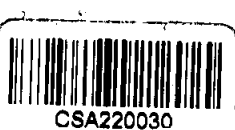


Industria y Comercio
SUPERINTENDENCIA



Delegatura de Propiedad Industrial
División de Nuevas Creaciones

PCT

SOLICITUD
PATENTE DE INVENCION

SUPERINTENDENCIA DE
INVEN

08-89267

21. EXPEDIENTE No.

34. TÍTULO

NOVEDOSAS 11~~3~~-HIDROXIANDROSTA-4-EN-3-ONAS

1. CLASIFICACIÓN INTERNACIONAL

1. SOLICITANTE

SUN PHARMACEUTICAL INDUSTRIES LIMITED

DOMICILIO

Acme Plaza, Andherikurla Road, Andheri (east), Mumbai 400 059 (IN)

APODERADO

JOSE LUIS REYES VILLAMIZAR

BOGOTÁ, D. C.,

**FORMULARIO UNICO DE SOLICITUD DE PATENTE
PCT
ENTRADA EN FASE NACIONAL****SOLICITUD DE: PATENTE EN COLOMBIA**

①

☒ Patente de Invención.☐ Patente de Modelo de Utilidad.☐ Capítulo I.☒ Capítulo II.

②

SOLICITANTE (71)Nombre: **SUN PHARMACEUTICAL
INDUSTRIES LIMITED**Dirección: **Acme Plaza, Andherikurla Road,
Andheri (east), Mumbai 400 059 (IN)**Nacionalidad o Domicilio: **India**Lugar de Constitución: **Mumbai - India**

Teléfono:

E-mail:

IDENTIFICACIÓNC.C. ☐ NIT ☐C.E. ☐ Otro ☐

Cual

Número

③

**REPRESENTANTE
O APODERADO (74)**Nombre: **JOSE LUIS REYES VILLAMIZAR**Dirección: **Cr. 17 No. 88-23 Of. 205**Teléfono: **655.77.95** Fax: **621.25.42**E-mail: **info@reyes-abogados.com****IDENTIFICACIÓN**C.C. ☒ NIT ☐C.E. ☐ Otro ☐

Cual

Número **79.152.473** TPA **44655**

④

INVENTOR (ES) (72)Nombre: **PATEL, Jiten Ranchhodhbhai; PATEL, Gopalkumar Chimanlal; SHETH,
Gaurav Sanjivkumar; SHAH, Samir Rameshchandra; MANDHANE, Sanjay Nandlal;
CHITTURI, Trinadha Rao; THENNATI, Rajamannar.**Dirección: **Sun Pharma Advanced Research Centre, Nima Compound, Near Pratham
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⑤

PCT (86)Solicitud Internacional No. **PCT/IN2007/000039**Fecha **29 de enero de 2007**Publicación Internacional No. **WO 2007/099548 A2**Fecha **07 de septiembre de 2007**

⑥

Título (54)**NOVEDOSAS 11 β -HIDROXIANDROSTA-4-EN-3-ONAS**

⑦

Clasificación Internacional (51)**C07D 3/00**

⑧

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Nombre de la exposición

Lugar de Celebración

Fecha

10

Anexos

☒ Comprobante de pago de la tasa de presentación de la solicitud

☐ Comprobante de pago de la tasa por concepto de excedente de palabras en la publicación (más de 150)

☒ Comprobante de pago de la tasa por concepto reivindicación de prioridad

☐ Poderes, si fuere el caso

☐ Certificado de existencia y representación legal cuando el solicitante sea persona jurídica

☐ Artes finales 12 x 12 cm, 2 ejemplares

☒ Copia de la primera solicitud si se reivindica prioridad

☒ Traducción simple de la primera solicitud, si se reivindica prioridad

☐ Certificado de registro en el caso del artículo 6º quinquies del Convenio de París

☐ Autorizaciones requeridas según los artículos 135 y 136 de la Decisión 486

☐ Reglamento de uso, si es el caso (marcas de certificación, colectivas y denominaciones de origen)

☐ Designación de zona geográfica, si es el caso (denominaciones de origen)

☐ Reseña de calidades, reputación y características de los productos, (denominaciones de origen)

☐ Designacion de zona geográfica, si es el caso (denominaciones de origen)

☐ Copia de estatutos del solicitante, si es el caso (marcas colectivas, de certificación, denominaciones de origen)

☐ Lista de integrantes, si es el caso (marcas colectivas o de certificación)

11

REPRODUCCIÓN DEL SIGNO A REGISTRAR

12

NOMBRE:

JOSE LUIS REYES VILLAMIZAR

FIRMA:

C.C.79.152.473 T.P.44655

(12) SOLICITUD INTERNACIONAL PUBLICADA SEGÚN EL TRATADO DE COOPERACIÓN INTERNACIONAL
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Rajamannar; Sun Pharma Advanced Research
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BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM,
DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT,
HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP,
KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD,
MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ,
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(71) Solicitante (para todos los países destinatarios con
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(84) Países designados (a menos que se indique lo
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SZ, TZ, UG, ZM, ZW), Eurasiática (AM, AZ, BY, KG,
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(72) Inventores, e

(75) Inventores/Solicitantes (para US únicamente):
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Gopalkumar Chimanlal**; Sun Pharma Advanced
Research Centre, Nima Compound, Near Pratham
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Gaurav Sanjivkumar**; Sun Pharma Advanced Research
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Sanjay Nandlal**; Sun Pharma Advanced Research
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Trinadha Rao**; Sun Pharma Advanced Research
Centre, Nima Compound, Near Pratham Enclave,
Tandelja Road, Baroda 390 020 (IN). **THENNATI,**

Declaraciones bajo la Regla 4.17:

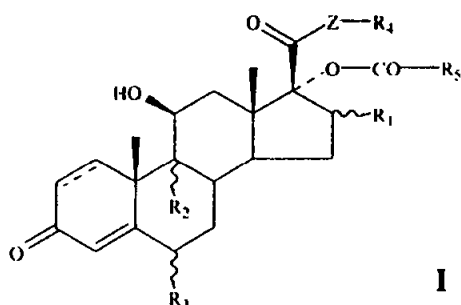
- de la condición de inventor (Regla 4.17(ii))
- en lo que respecta al derecho del solicitante de solicitar
y de que se le otorgue una patente, (Regla 4.17(ii))
- de la condición de inventor (Regla 4.17(iv))

Publicado:

- con informe internacional de búsqueda y para volverse
a publicar en el caso de recibo.

Para códigos de dos letras y otras abreviaturas, remitase a
las "Notas Guía sobre Códigos y Abreviaturas" que aparece
al comienzo de cada edición regular del Boletín Oficial PCT.

(54) Título: NOVEDOSAS 11 β -HIDROXIANDROSTA-4-EN-3-ONAS

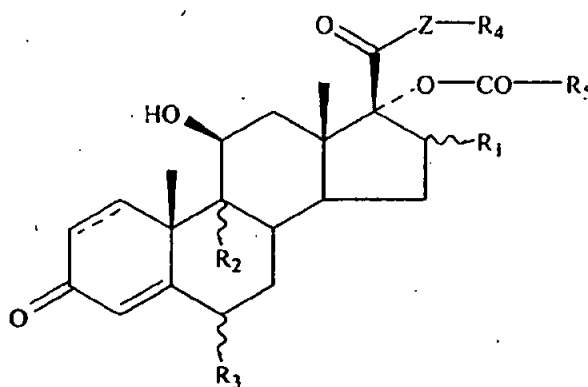


(57) Extracto: 11 β -hidroxiandrosta-4-en-3-ona, compuesto de
fórmula (I), y su sal fisiológicamente aceptable; en donde R₄
representa una fracción seleccionada de un grupo conformado
por (A), (B) y (C), siempre que, si R₄ representa una fracción
(C), Z es S.

WO 2007/099548 A2

NOVEDOSAS 11 β -HIDROXIANDROSTA-4-EN-3-ONAS

La presente invención se refiere a análogos anti-inflamatorios y antialérgicos novedosos de las 11 β -hidroxiandrosta-4-en-3-onas, representados como fórmula I y su sal fisiológicamente aceptable, que tienen efectos sistémicos insignificantes o no dignos de mención con múltiplos de una dosis eficaz.

**Fórmula I****ANTECEDENTES DE LA INVENCION**

Corticoesteroides (o glucocorticoides) con propiedades anti-inflamatorias se usan ampliamente para el tratamiento de enfermedades o trastornos inflamatorios de la piel, vías respiratorias, ojos, tracto digestivo, articulaciones, SNC, etc, y varios trastornos autoinmunitarios. Algunos de los trastornos inflamatorios de la piel, en los que se prescribe el tratamiento con glucocorticoides son eczema, psoriasis, dermatitis alérgica, picazón, reacciones de hipersensibilidad, etc. Las afecciones inflamatorias o alérgicas de las vías respiratorias para las cuales se emplean glucocorticoides incluyen trastornos de la nariz, garganta o pulmones tales como rinitis (incluida fiebre del heno), pólipos nasales, asma (incluida reacción asmática inducida por alérgenos), enfermedad pulmonar obstructiva crónica, enfermedad pulmonar intersticial, fibrosis, etc. La administración de glucocorticoides se emplea igualmente para síndrome de intestino irritable tales como colitis ulcerosa y enfermedad de Crohn; y

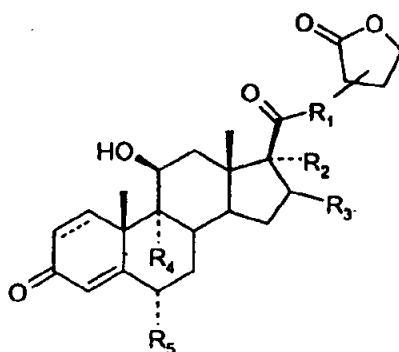
trastornos inflamatorios de las articulaciones tales como artritis reumatoide, que son enfermedades autoinmunitarias. Sin embargo, la administración de Corticoesteroides en general, además del efecto farmacológico deseado, puede ocasionar efectos secundarios adversos o indeseados en sitios distantes del tejido diana, los llamados efectos sistémicos. Algunos de los efectos sistémicos indeseados encontrados incluyen inmunosupresión ampliada, recambio óseo incrementado, crecimiento deficiente, adelgazamiento de la piel, diabetes, obesidad, retención de agua, trastornos relacionados con progesterona y estrógenos. En consecuencia, es deseable tener glucocorticoides que posean una potente actividad anti-inflamatoria en el tejido diana, con actividad sistémica mínima o, preferiblemente, ninguna con dosis terapéuticas cuando se emplean para tratamiento crónicos.

Glucocorticoides clásicos se describen en —

- **Patente de los Estados Unidos No. 4335121** (la patente '121; Referencia de la India no disponible) ----
(*S*)-fluorometil 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-17 α -propioniloxi-3-oxoandrosta-1,4-dien-17 β -carbotioato
(Fluticasona)
- **Patente de los Estados Unidos No. 3007923** (la patente '923; Referencia de la India no disponible) ----
16 α -metil-9 α -fluoro-1,4-pregnadien-11 β ,17 α ,21-triol-3,20-diona
(Dexametasona)
- **Patente de los Estados Unidos No 3929768** (la patente '768; Referencia de la India no disponible) ejemplifica (11 β ,16 α)-16,17-[Butilidenbis(oxi)]-11,21-dihidroxipregna-1,4-dien-3,20-diona (Budesonida)
- **Patente de los Estados Unidos No. 4472393** (la patente '393; Referencia de la India no disponible) ejemplifica (11 β ,16 α)-9,21-Dicloro-17-[(2-furanilcarbonil)oxi]-11-hidroxi-16-metilpregna-1,4-dien-3,20-diona (Furoato de mometasona)

Los medicamentos mencionados anteriormente son potentes glucocorticoides que ya se encuentran en uso clínico. Sin embargo, con múltiples elevados de dosis eficaz, estos medicamentos tienen el potencial de causar efectos secundarios sistémicos.

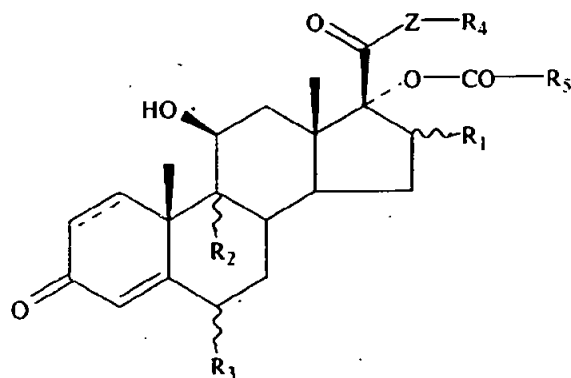
Publicación PCT WO 99/01467 describe compuestos esteroideos terapéuticamente activos o sales o solvatos con un grupo lactona conectado al anillo ciclopentano del núcleo esteroide (como se indica a continuación). Se ha descrito que estos compuestos tienen un potencial reducido de actividad sistémica, debido a la inestabilidad relativa del sistema lactona en el plasma. Los compuestos de la presente invención no poseen un grupo lactona conectado al anillo ciclopentano.



Nuestro interés en desarrollar compuestos que actúen en el sitio específico de inflamación con efectos secundarios insignificantes o no dignos de mención no ha llevado al descubrimiento de compuestos seguros de 11 β -hidroxiandrosta-4-en-3-ona, novedosos, descritos en esta invención. Estos compuestos poseen una actividad anti-inflamatoria útil teniendo al mismo tiempo efectos sistémicos insignificantes o no dignos de mención con múltiples de una dosis eficaz.

DESCRIPCIÓN DE LA INVENCION

La presente invención provee 11 β -hidroxiandrosta-4-en-3-ona, compuesto de fórmula I, y su sal fisiológicamente aceptable,

**Fórmula I**

----- representa un enlace único o doble y

~~~~~ representa una configuración  $\alpha$  o  $\beta$ .

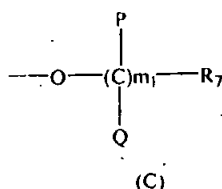
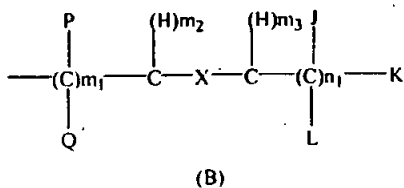
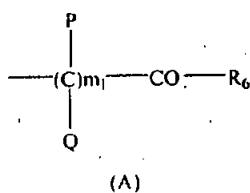
en donde

Z representa O ó S;

$R_1$  representa hidrógeno o metilo, el cual puede estar en una configuración  $\alpha$  o  $\beta$ , o metileno;  $R_2$  y  $R_3$  son los mismos o diferentes y cada uno independientemente representa hidrógeno, halógeno o un grupo metilo;

$R_5$  representa un grupo seleccionado de (C<sub>1</sub>-C<sub>10</sub>)-alquilo, (C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, -O-(C<sub>1</sub>-C<sub>10</sub>)-alquilo, arilo o anillo heterocíclico en donde el anillo o sistema de anillo es no sustituido o sustituido por uno o más halógeno, -OH, (C<sub>1</sub>-C<sub>3</sub>)-alquilo, -O-(C<sub>1</sub>-C<sub>3</sub>)-alquilo, (C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo; en donde los grupos alquilo o cicloalquilo pueden contener opcionalmente una o más insaturaciones y/o pueden tener uno o más heteroátomos incorporados en ellas y, opcionalmente, en cada caso, uno o más átomos de hidrógeno reemplazados por halógeno, -OH, (C<sub>1</sub>-C<sub>3</sub>)-alquilo, -O-(C<sub>1</sub>-C<sub>3</sub>)-alquilo, (C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo; y

$R_4$  representa una fracción seleccionada de un grupo conformado por (A), (B) y (C), siempre que cuando  $R_4$  representa una fracción (C), Z es S:



en donde

$m_1$  es 1, 2 ó 3;

$m_2$  es 0 ó 1;

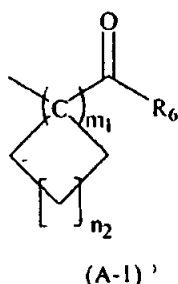
$m_3$  es 0 ó 1;

$n_1$  es 0, 1 ó 2;

$R_6$  representa un grupo seleccionado de  $(C_1-C_8)$ -alquilo,  $(C_3-C_{13})$ -cicloalquilo, arilo y un radical heterocíclico, donde el anillo o sistema de anillo es no sustituido o sustituido por uno o más radicales seleccionados de  $(C_1-C_8)$ -alquilo,  $(C_3-C_{13})$ -cicloalquilo, halógeno,  $O-(C_1-C_8)$ -alquilo,  $O-(C_3-C_{13})$ -cicloalquilo,  $OCO-(C_1-C_3)$ -alquilo,  $S(O)_{0-2}(C_1-C_8)$ -alquilo,  $COO-(C_1-C_8)$ -alquilo,  $-OCO-O-(C_1-C_3)$ -alquilo,  $-OCO-CO-O-(C_1-C_3)$ -alquilo,  $CONH_2$ ,  $CONH-(C_1-C_8)$ -alquilo,  $CON-[(C_1-C_8)\text{-alquil}]_2$ ,  $-NHCO-(C_1-C_8)$ -alquilo,  $N-(C_1-C_8)$ -alquil-CO- $(C_1-C_8)$ -alquilo,  $-NHCO-O-(C_1-C_8)$ -alquilo,  $-N-(C_1-C_8)$ -alquil-CO-O- $(C_1-C_8)$ -alquilo,  $-NHCONH-(C_1-C_8)$ -alquilo,  $-N-(C_1-C_8)$ -alquil-CONH- $(C_1-C_8)$ -alquilo,  $-NHCONH-SO_2-(C_1-C_8)$ -alquilo,  $-N-(C_1-C_8)$ -alquil-CONH- $SO_2-(C_1-C_8)$ -alquilo,  $-NO_2$ ,  $-CN$ ; en donde los grupos alquilo o cicloalquilo pueden contener opcionalmente una o más insaturaciones y/o pueden tener uno o más heteroátomos incorporados en ellas y, opcionalmente, en cada caso, uno o más átomos de hidrógeno reemplazados por halógeno,  $-OH$ ,  $(C_1-C_3)$ -alquilo,  $-OCO-(C_1-C_3)$ -alquilo o  $(C_3-C_{13})$ -cicloalquilo;

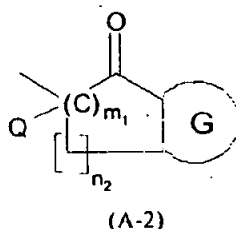
siempre que cuando  $R_4$  representa una fracción (A) en donde  $R_6$  representa  $(C_3-C_{13})$ -cicloalquilo que contiene opcionalmente uno o más heteroátomos incorporados en ellas, el heteroátomo no sea nitrógeno;

P y Q se seleccionan independientemente de hidrógeno y C<sub>1</sub> a C<sub>3</sub> alquilo;  
o P y Q pueden unirse conjuntamente con el átomo de carbono al cual se  
enlazan para formar (C<sub>3</sub>-C<sub>8</sub>)-cicloalquilo, como se representa por la fracción  
(A-1):



en donde m<sub>1</sub> es 1 y n<sub>2</sub> es 0, 1, 2, 3, 4 ó 5 y R<sub>6</sub> es un arilo como se define  
anteriormente;

o P y R<sub>6</sub> pueden unirse conjuntamente para formar un sistema cíclico, como  
se representa por la fracción (A-2):



en donde m<sub>1</sub> es 1 y n<sub>2</sub> es 0, 1, 2, 3 ó 4 y anillo G es un arilo como se define  
anteriormente;

X representa un enlace doble o un enlace triple; y

J, K y L se seleccionan independientemente de un grupo conformado por  
hidrógeno, halógeno, (C<sub>1</sub>-C<sub>10</sub>)-alquilo, (C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, -OH, -O-(C<sub>1</sub>-  
C<sub>10</sub>)-alquilo, -O-(C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, -OCO-(C<sub>1</sub>-C<sub>10</sub>)-alquilo, -OCO-(C<sub>3</sub>-  
C<sub>13</sub>)-cicloalquilo, -OCO-CO-O-(C<sub>1</sub>-C<sub>10</sub>)-alquilo, -OCO-CO-O-(C<sub>3</sub>-C<sub>13</sub>)-  
cicloalquilo, -OCO-O-(C<sub>1</sub>-C<sub>10</sub>)-alquilo, -OCO-O-(C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, -  
OCO-NH-(C<sub>1</sub>-C<sub>10</sub>)-alquilo, -OCO-NH-(C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, -OCO-N-[(C<sub>1</sub>-  
C<sub>10</sub>)-alquil]<sub>2</sub>, -OCO-N-[(C<sub>3</sub>-C<sub>13</sub>)-cicloalquil]<sub>2</sub>, -OCO-NHSO<sub>2</sub>-(C<sub>1</sub>-C<sub>10</sub>)-  
alquilo, -OCO-NHSO<sub>2</sub>-(C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, -NH<sub>2</sub>, -NH-(C<sub>1</sub>-C<sub>8</sub>)-alquilo, -  
N-[(C<sub>1</sub>-C<sub>8</sub>)-alquil]<sub>2</sub>, -NO<sub>2</sub> y -CN;

en donde los grupos alquilo o cicloalquilo pueden contener opcionalmente  
una o más insaturaciones y/o pueden tener uno o más heteroátomos

incorporados en ellas y, opcionalmente, en cada caso, uno o más átomos de hidrógeno reemplazados por halógeno, -OH, (C<sub>1</sub>-C<sub>3</sub>)-alquilo, -O-(C<sub>1</sub>-C<sub>3</sub>)-alquilo, -OCO-(C<sub>1</sub>-C<sub>3</sub>)-alquilo, -COOH, -COO-(C<sub>1</sub>-C<sub>5</sub>)-alquilo, -COO-(C<sub>1</sub>-C<sub>5</sub>)-haloalquilo, -NHCO-(C<sub>1</sub>-C<sub>8</sub>)-alquilo, -ONO<sub>2</sub>, -NH-(C<sub>1</sub>-C<sub>8</sub>)-alquilo, -N-[(C<sub>1</sub>-C<sub>8</sub>)-alquil]<sub>2</sub>, -NO<sub>2</sub>, -CN, (C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, arilo o un radical heterocíclico;

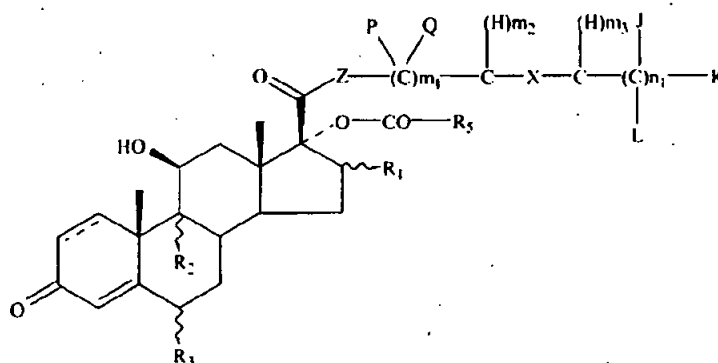
o J y K pueden unirse conjuntamente con el átomo de carbono al cual se enlazan para representar un grupo (C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo o -CO- y L es como se define anteriormente;

o J, K y L están ausentes cuando n<sub>1</sub> es 0;

R<sub>7</sub> representa un grupo seleccionado de hidrógeno, halógeno, arilo y CO-arilo, en donde el anillo o sistema de anillo es no sustituido o sustituido como se define anteriormente;

Preferiblemente,

11β-hidroxiandrost-4-en-3-ona, compuesto de fórmula I-B, y su sal fisiológicamente aceptable:



**Fórmula I-B**

en donde

Z representa O ó S;

R<sub>1</sub> representa hidrógeno o metilo, el cual puede estar en una configuración α o β, o metileno;

R<sub>2</sub> y R<sub>3</sub> son los mismos o diferentes y cada uno independientemente representa hidrógeno, halógeno o un grupo metilo;

R<sub>5</sub> representa un grupo seleccionado de (C<sub>1</sub>-C<sub>10</sub>)-alquilo, (C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo,

-O-(C<sub>1</sub>-C<sub>10</sub>)-alquilo, arilo o anillo heterocíclico en donde el anillo o sistema de anillo es no sustituido o sustituido por uno o más halógeno, -OH, (C<sub>1</sub>-C<sub>3</sub>)-alquilo, -O-(C<sub>1</sub>-C<sub>3</sub>)-alquilo, (C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo; en donde los grupos alquilo o cicloalquilo pueden contener opcionalmente una o más insaturaciones y/o pueden tener uno o más heteroátomos incorporados en ellas y, opcionalmente, en cada caso, uno o más átomos de hidrógeno reemplazados por halógeno, -OH, (C<sub>1</sub>-C<sub>3</sub>)-alquilo, -O-(C<sub>1</sub>-C<sub>3</sub>)-alquilo, (C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo; y

m<sub>1</sub> es 1;

m<sub>2</sub> es 0 ó 1;

m<sub>3</sub> es 0 ó 1;

n<sub>1</sub> es 0, 1 ó 2;

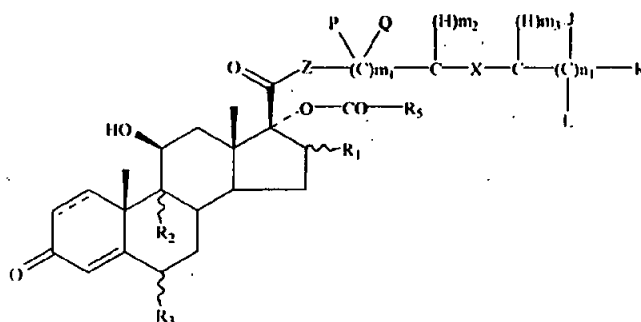
P y Q son hidrógeno;

X representa un enlace doble o un enlace triple; y

J, K y L se seleccionan independientemente de un grupo conformado por hidrógeno, halógeno, (C<sub>1</sub>-C<sub>10</sub>)-alquilo, (C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, -OH, -O-(C<sub>1</sub>-C<sub>10</sub>)-alquilo, -O-(C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, -OCO-(C<sub>1</sub>-C<sub>10</sub>)-alquilo, -OCO-(C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, -OCO-CO-O-(C<sub>1</sub>-C<sub>10</sub>)-alquilo, -OCO-CO-O-(C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, -OCO-O-(C<sub>1</sub>-C<sub>10</sub>)-alquilo, -OCO-O-(C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, -OCO-NH-(C<sub>1</sub>-C<sub>10</sub>)-alquilo, -OCO-NH-(C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, -OCO-N-[(C<sub>1</sub>-C<sub>10</sub>)-alquil]<sub>2</sub>, -OCO-N-[(C<sub>3</sub>-C<sub>13</sub>)-cicloalquil]<sub>2</sub>, -OCO-NHSO<sub>2</sub>-, (C<sub>1</sub>-C<sub>10</sub>)-alquilo, -OCO-NHSO<sub>2</sub>-(C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, -NH<sub>2</sub>, -NH-(C<sub>1</sub>-C<sub>8</sub>)-alquilo, -N-[(C<sub>1</sub>-C<sub>8</sub>)-alquil]<sub>2</sub>, -NO<sub>2</sub> y -CN.

Muy preferiblemente,

11β-hidroxiandrost-4-en-3-ona, compuesto de fórmula I-B, y su sal fisiológicamente aceptable:

**Formula I-B**

en donde

Z representa S;

R<sub>1</sub> representa hidrógeno o metilo, el cual puede estar en una configuración  $\alpha$  o  $\beta$ , o metileno;

R<sub>2</sub> y R<sub>3</sub> son los mismos o diferentes y cada uno independientemente representa hidrógeno, halógeno o un grupo metilo;

R<sub>5</sub> representa un grupo seleccionado de (C<sub>1</sub>-C<sub>10</sub>)-alquilo, (C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo,

-O-(C<sub>1</sub>-C<sub>10</sub>)-alquilo, arilo o anillo heterocíclico en donde el anillo o sistema de anillo es no sustituido o sustituido por uno o más halógeno, -OH, (C<sub>1</sub>-C<sub>3</sub>)-alquilo, -O-(C<sub>1</sub>-C<sub>3</sub>)-alquilo, (C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo; en donde los grupos alquilo o cicloalquilo pueden contener opcionalmente una o más insaturaciones y/o pueden tener uno o más heteroátomos incorporados en ellas y, opcionalmente, en cada caso, uno o más átomos de hidrógeno reemplazados por halógeno, -OH, (C<sub>1</sub>-C<sub>3</sub>)-alquilo, -O-(C<sub>1</sub>-C<sub>3</sub>)-alquilo, (C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo; y

m<sub>1</sub> es 1;

m<sub>2</sub> es 0;

m<sub>3</sub> es 0;

n<sub>1</sub> es 0, 1 ó 2;

P y Q son hidrógeno;

X representa un enlace triple; y

J, K y L se seleccionan independientemente de un grupo conformado por hidrógeno, halógeno, (C<sub>1</sub>-C<sub>10</sub>)-alquilo, (C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, -OH, -O-(C<sub>1</sub>-C<sub>10</sub>)-alquilo, -O-(C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, -OCO-(C<sub>1</sub>-C<sub>10</sub>)-alquilo, -OCO-(C<sub>3</sub>-

C<sub>13</sub>)-cicloalquilo, -OCO-CO-O-(C<sub>1</sub>-C<sub>10</sub>)-alquilo, -OCO-CO-O-(C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, -OCO-O-(C<sub>1</sub>-C<sub>10</sub>)-alquilo, -OCO-O-(C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, -OCO-NH-(C<sub>1</sub>-C<sub>10</sub>)-alquilo, -OCO-NH-(C<sub>1</sub>-C<sub>13</sub>)-cicloalquilo, -OCO-N-[(C<sub>1</sub>-C<sub>10</sub>)-alquil]<sub>2</sub>, -OCO-N-[(C<sub>3</sub>-C<sub>13</sub>)-cicloalquil]<sub>2</sub>, -OCO-NHSO<sub>2</sub>-(C<sub>1</sub>-C<sub>10</sub>)-alquilo, -OCO-NHSO<sub>2</sub>-(C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, -NH<sub>2</sub>, -NH-(C<sub>1</sub>-C<sub>8</sub>)-alquilo, -N-[(C<sub>1</sub>-C<sub>8</sub>)-alquil]<sub>2</sub>, -NO<sub>2</sub> y -CN.

## DESCRIPCIÓN DETALLADA DE LA INVENCION

La presente invención se refiere a una 11 $\beta$ -hidroxiandrosta-4-en-3-ona segura, novedosa, compuesto de fórmula 1, y su sal fisiológicamente aceptable.

Compuesto de fórmula 1 puede estar en la forma de diastereómeros y sus mezclas. Tal como se emplea en esta solicitud, cualquier forma estereoisomérica incluye diastereómeros y sus mezclas.

Referencia al compuesto de fórmula I incluye en lo sucesivo un compuesto de fórmula 1 y su sal fisiológicamente aceptable.

Con respecto a los diferentes grupos abarcados por los términos genéricos empleados aquí y a lo largo de esta especificación, se aplican las siguientes definiciones y explicaciones:

Tal como se emplea en esta solicitud 'alquilo' puede ser de cadena recta o ramificada y puede contener opcionalmente una o más insaturaciones y/o puede tener uno o más heteroátomos incorporados en ellas y, opcionalmente, en cada caso, tener uno o más átomos de hidrógeno reemplazados por -F, -Cl, -Br, -I, -OH, -OCO-(C<sub>1</sub>-C<sub>3</sub>)-alquilo, (C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, arilo o un radical heterocíclico.

Tal como se emplea en esta solicitud 'alquilo' incluidas una o más insaturaciones' tiene que entenderse como significando 'alquenilo' y/o 'alquinilo'. Grupos alquilo ejemplares incluyen metilo, etilo, *n*-propilo, *i*-propilo, *n*-butilo, *t*-butilo, *n*-pentilo, 3-pentilo, 2-octilo y similares. Grupos alquenilo ejemplares incluyen etenilo, propenilo, 1-butenilo, (*Z*)-2-butenilo, (*E*)-3-metilbut-2-enilo, (*E*)-2,4-pentadienilo, (*Z*)-3-heptenilo y similares. Grupos alquinilo ejemplares incluyen etinilo, propinilo, 1-butinilo, 2-butinilo, 4-metil-2-pentinilo, 2,4-hexadiinilo y similares.

Tal como se emplea en esta solicitud, 'cicloalquilo' tiene que entenderse como significando sistemas de anillo monocíclicos, bicíclicos, tricíclicos y policíclicos tales como norbornilo, adamantilo y similares. El término 'cicloalquilo', tal como se emplea en esta solicitud, puede contener opcionalmente una o más insaturaciones y/o puede tener uno o más heteroátomos incorporados en ellas -F, -Cl, -Br, -I, -OH, -OCO-(C<sub>1</sub>-C<sub>3</sub>)-alquilo, (C<sub>1</sub>-C<sub>13</sub>)-cicloalquilo, arilo o un radical heterocíclico.

Tal como se emplea en esta solicitud, 'grupo halógeno' o 'halo' se refiere a flúor, cloro, bromo o yodo.

Tal como se emplea en esta solicitud, arilo tiene que entenderse como significando sistemas de anillo tales como fenilo, naftilo, antracenilo, fenantrilo, preferiblemente arilo es fenilo.

Tal como se emplea en esta solicitud, heterociclo o anillo heterocíclico tiene que entenderse como significando sistemas de anillo que, además de carbono, contengan asimismo heteroátomos, tales como, por ejemplo, nitrógeno, oxígeno o azufre. Esta definición incluye además sistemas de anillo en los cuales el heterociclo o radical heterocíclico se fusiona con anillos benceno. Ejemplos de heterociclos o anillo heterocíclicos son: heteroarilos, tales como

15

benzimidazolilo,  
1-[(C<sub>1</sub>-C<sub>6</sub>)-alquil]benzimidazolilo,  
imidazolilo,  
2- ó 3-tienilo,  
2- ó 3-furilo,  
benzoxazolilo,  
benzotiazolilo,  
2-, 3- ó 4-piridilo,  
pirimidinilo,  
4-, 5- ó 6-piridazin-2*H*-il-3-ona,  
4-, 5- ó 6-piridazin-2-(C<sub>1</sub>-C<sub>8</sub>)-alquil-2*H*-il-3-ona,  
2-bencil-4-, -5- ó -6-piridazin-2*H*-il-3-ona,  
3- ó 4-piridazinilo,  
2-, 3-, 4- ó 8-quinolinilo,  
1-, 3- ó 4-isoquinolinilo,  
1-ftalazinilo,  
3- ó 4-cinnolinilo,  
2- ó 4-quinazolinilo,  
2-pirazinilo,  
2-quinoxalinilo,  
2-, 4- ó 5-oxazolilo,  
3-, 4- ó 5-isoxazolilo,  
2-, 4- ó 5-tiazolilo,  
3-, 4- ó 5-isotiazolilo,  
1-[(C<sub>1</sub>-C<sub>6</sub>)-alquil]-2-, -4- ó -5-imidazolilo,  
3-, 4- ó 5-pirazolilo,  
1-[(C<sub>1</sub>-C<sub>6</sub>)-alquil]-3-, -4- ó -5-pirazolilo,  
1- ó 4-[1,2,4]-triazolilo,  
4- ó 5-[1,2,3]-triazolilo,  
1-[(C<sub>1</sub>-C<sub>6</sub>)-alquil]-4- ó -5-[1,2,3]triazolilo,  
3-, 4- ó 7-indolilo,  
*N*-[(C<sub>1</sub>-C<sub>6</sub>)-alquil]-3-, -4- ó -7-indolilo,

2-[(C<sub>1</sub>-C<sub>6</sub>)-alquil]-3(2*H*)-indazolilo,  
1-[(C<sub>1</sub>-C<sub>6</sub>)-alquil]-3(1*H*)-indazolilo,  
5-tetrazolilo,  
1-[(C<sub>1</sub>-C<sub>6</sub>)-alquil]-1*H*-tetrazolilo,  
2-[(C<sub>1</sub>-C<sub>6</sub>)-alquil]-2*H*-tetrazolilo.

En una incorporación los compuestos preferidos de fórmula I se seleccionan del compuesto en donde m<sub>1</sub> es 1

En una incorporación los compuestos preferidos de fórmula I se seleccionan del compuesto en donde m<sub>1</sub> es 1 y P y Q son hidrógeno.

En una incorporación los compuestos de fórmula I se seleccionan de los compuestos en donde R representa una fracción (A).

En una incorporación los compuestos de fórmula I se seleccionan de los compuestos en donde R<sub>4</sub> representa una fracción (B).

En una incorporación los compuestos de fórmula I se seleccionan de los compuestos en donde R<sub>4</sub> representa una fracción (C).

En una incorporación los compuestos de fórmula I se seleccionan de los compuestos en donde m<sub>1</sub> es 1; P y Q son ambos hidrógeno y R<sub>4</sub> representa una fracción (A).

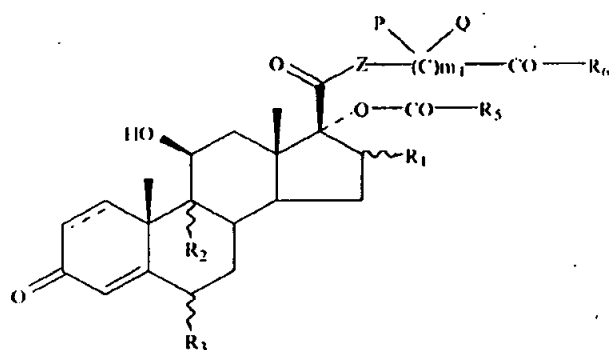
En una incorporación los compuestos de fórmula I se seleccionan de los compuestos en donde m<sub>1</sub> es 1; P y Q son ambos hidrógeno y R<sub>4</sub> representa una fracción (B).

En una incorporación los compuestos de fórmula I se seleccionan de los compuestos en donde m<sub>1</sub> es 1; P y Q son ambos hidrógeno y R<sub>4</sub> representa una fracción (C).

En una incorporación los compuestos de fórmula I se seleccionan de los compuestos en donde  $R_6$  se selecciona de un grupo conformado por  $(C_1-C_8)$ -alquilo, arilo y un radical heterocíclico en donde el anillo o sistema de anillo es no sustituido o sustituido como se define anteriormente.

En una incorporación los compuestos de fórmula I se seleccionan de los compuestos en donde  $R_5$  representa un grupo seleccionado de  $R_6$ , en donde  $R_6$  se selecciona de un grupo conformado por  $(C_1-C_8)$ -alquilo y un radical heterocíclico en donde el anillo o sistema de anillo es no sustituido o sustituido como se define anteriormente.

En una incorporación la presente invención provee 11 $\beta$ -hidroxiandrosta-4-en-3-ona, un compuesto de fórmula I-A y su sal fisiológicamente aceptable:



**Fórmula I-A**

— represents a single or double bond and

~~~~~ represents an  $\alpha$  or  $\beta$  configuration.

en donde

Z representa O, S;

R_1 representa hidrógeno o metilo, el cual puede estar en una configuración α o β o ser metileno;

R_2 y R_3 son los mismos o diferentes y cada uno independientemente representa hidrógeno, halógeno o un grupo metilo;

m_1 es 1, 2 ó 3;

R_6 representa un grupo seleccionado de (C_1-C_8) -alquilo, (C_3-C_{13}) -cicloalquilo, arilo y un radical heterocíclico, donde el anillo o sistema de

anillo es no sustituido o sustituido por uno o más radicales seleccionados de:

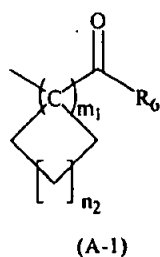
C₁-C₈-alquilo, (C₃-C₁₃)-cicloalquilo, halógeno, O-(C₁-C₈)-alquilo, O-(C₃-C₁₃)-cicloalquilo, OCO-(C₁-C₃)-alquilo, S(O)₀₋₂(C₁-C₈)-alquilo, COO-(C₁-C₈)-alquilo, -OCO-O-(C₁-C₃)-alquilo, -OCO-CO-O-(C₁-C₃)-alquilo, CONH₂, CONH-(C₁-C₈)-alquilo, CON-[(C₁-C₈)-alquil]₂, -NHCO-(C₁-C₈)-alquilo, N-(C₁-C₈)-alquil-CO-(C₁-C₈)-alquilo, -NHCO-O-(C₁-C₈)-alquilo, -N-(C₁-C₈)-alquil-CO-O-(C₁-C₈)-alquilo, -NHCONH-(C₁-C₈)-alquilo, -N-(C₁-C₈)-alquil-CONH-(C₁-C₈)-alquilo, -NHCONH-SO₂-(C₁-C₈)-alquilo, -N-(C₁-C₈)-alquil-CONH-SO₂-(C₁-C₈)-alquilo, -NO₂, -CN;

en donde los grupos alquilo o cicloalquilo pueden contener opcionalmente una o más insaturaciones y/o pueden tener uno o más heteroátomos incorporados en ellas y, opcionalmente, en cada caso, uno o más átomos de hidrógeno reemplazados por -F, -Cl, -Br, -I, -OH, -OCO-(C₁-C₃)-alquilo, (C₁-C₁₃)-cicloalquilo, arilo o un radical heterocíclico; siempre que cuando R₄ representa una fracción A en donde

R₆ representa (C₃-C₁₃)-cicloalquilo que contiene opcionalmente uno o más heteroátomos incorporados en ellas, el heteroátomo no sea nitrógeno;

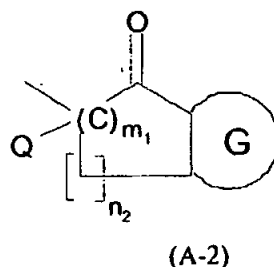
P y Q se seleccionan independientemente de hidrógeno, halógeno y C₁ a C₃-alquilo;

o P y Q pueden unirse conjuntamente con el átomo de carbono al cual se enlazan para formar (C₃-C₈)-cicloalquilo, como se representa por la fracción (A-1):



en donde m₁ es 1 y n₂ es 0, 1, 2, 3, 4 ó 5;

o P y R₆ pueden unirse conjuntamente para formar un sistema cíclico, como se representa por la fracción (A-2):



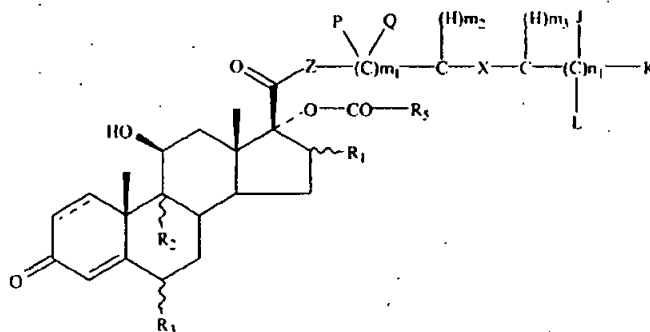
en donde m_1 es 1 y n_2 es 0, 1, 2, 3 ó 4 y anillo G está opcionalmente presente, en donde G representa un (C₃-C₈)-cicloalquilo, arilo o un radical heterocíclico como se define anteriormente;

R_5 representa un grupo seleccionado de R_6 , -O- R_6 ó -N(R_8) R_6 , en donde R_6 es como se define anteriormente y R_8 representa hidrógeno, (C₁-C₆)-alquilo o (C₃-C₆)-cicloalquilo.

En una incorporación los compuestos de fórmula I-A se seleccionan de los compuestos en donde m_1 es 1; P y Q son ambos hidrógeno; R_6 se selecciona del grupo conformado por (C₁-C₈)-alquilo, arilo y un radical heterocíclico; o en donde m_1 es 1; P y Q son ambos hidrógeno; R_6 es arilo en donde el anillo o sistema de anillo es no sustituido o sustituido como se define anteriormente; o

en donde R_6 es fenilo en donde el anillo o sistema de anillo es no sustituido o sustituido como se define anteriormente.

En una incorporación la presente invención provee 11 β -hidroxiandrosta-4-en-3-ona, un compuesto de fórmula 1-B y su sal fisiológicamente aceptable:



Fórmula I-B

----- representa un enlace único o doble y

~~~~~ representa una configuración  $\alpha$  o  $\beta$

en donde

Z representa O, S;

R<sub>1</sub> representa hidrógeno o metilo, el cual puede estar en una configuración  $\alpha$  o  $\beta$ , o ser metileno;

R<sub>2</sub> y R<sub>3</sub> son los mismos o diferentes y cada uno independientemente representa hidrógeno, halógeno o un grupo metilo;

m<sub>1</sub> es 1, 2 ó 3;

m<sub>2</sub> es 0 ó 1;

m<sub>3</sub> es 0 ó 1;

n<sub>1</sub> es 0, 1 ó 2;

P y Q se seleccionan independientemente de hidrógeno, halógeno y C<sub>1</sub> a C<sub>3</sub> alquilo;

X representa un enlace doble o un enlace triple; y

J, K y L se seleccionan independientemente de un grupo conformado por hidrógeno, halógeno, (C<sub>1</sub>-C<sub>10</sub>)-alquilo, (C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, -OH, -O-(C<sub>1</sub>-C<sub>10</sub>)-alquilo, -O-(C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, -OCO-(C<sub>1</sub>-C<sub>10</sub>)-alquilo, -OCO-(C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, -OCO-CO-O-(C<sub>1</sub>-C<sub>10</sub>)-alquilo, -OCO-CO-O-(C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, -OCO-O-(C<sub>1</sub>-C<sub>10</sub>)-alquilo, -OCO-O-(C<sub>1</sub>-C<sub>10</sub>)-cicloalquilo, -OCO-NH-(C<sub>1</sub>-C<sub>10</sub>)-alquilo, -OCO-NH-(C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, -OCO-N-[(C<sub>1</sub>-C<sub>10</sub>)-alquil]<sub>2</sub>, -OCO-N-[(C<sub>3</sub>-C<sub>13</sub>)-cicloalquil]<sub>2</sub>, -OCO-NHSO<sub>2</sub>-(C<sub>1</sub>-C<sub>10</sub>)-alquilo,

-OCO-NHSO<sub>2</sub>-(C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, -CO-[(C<sub>3</sub>-C<sub>10</sub>)N-ciclo], -OCO-[(C<sub>3</sub>-C<sub>10</sub>)N-ciclo], -NH<sub>2</sub>, -NH-(C<sub>1</sub>-C<sub>8</sub>)-alquilo, -N-[(C<sub>1</sub>-C<sub>8</sub>)-alquil]<sub>2</sub>, -NO<sub>2</sub>, -CN, arilo y un radical heterocíclico como se define anteriormente;

o J y K pueden unirse conjuntamente con el átomo de carbono al cual se enlazan para representar un grupo (C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo o -CO- y L es como se define anteriormente;

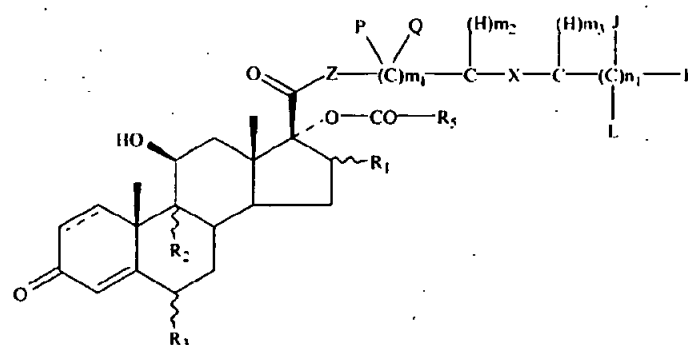
R<sub>5</sub> representa un grupo seleccionado de R<sub>6</sub>, -O-R<sub>6</sub> ó -N(R<sub>8</sub>)R<sub>6</sub>, en donde R<sub>6</sub> es como se define anteriormente, y

R<sub>8</sub> representa hidrógeno, (C<sub>1</sub>-C<sub>6</sub>)-alquilo o (C<sub>3</sub>-C<sub>6</sub>)-cicloalquilo;

En una incorporación los compuestos de fórmula I-B se seleccionan de los compuestos en donde,  $m_1$  es 1; P y Q son ambos hidrógeno; X representa un enlace doble o un enlace triple;  $m_2$  es 0;  $m_3$  es 0;  $n_1$  es 1 y J, K y L se seleccionan independientemente de hidrógeno, halógeno, -OH, -OCO-(C<sub>1</sub>-C<sub>10</sub>)-alquilo y -OCO-O-(C<sub>1</sub>-C<sub>10</sub>)-alquilo.

Preferiblemente,

11 $\beta$ -hidroxiandrosta-4-en-3-ona, compuesto de fórmula I-B, y su sal fisiológicamente aceptable:



**Fórmula I-B**

en donde

Z representa O ó S;

$R_1$  representa hidrógeno o metilo, el cual puede estar en una configuración  $\alpha$  o  $\beta$ , o metileno;

$R_2$  y  $R_3$  son los mismos o diferentes y cada uno independientemente representa hidrógeno, halógeno o un grupo metilo;

$R_5$  representa un grupo seleccionado de (C<sub>1</sub>-C<sub>10</sub>)-alquilo, (C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, -O-(C<sub>1</sub>-C<sub>10</sub>)-alquilo, arilo o anillo heterocíclico en donde el anillo o sistema de anillo es no sustituido o sustituido por uno o más halógeno, -OH, (C<sub>1</sub>-C<sub>3</sub>)-alquilo, -O-(C<sub>1</sub>-C<sub>3</sub>)-alquilo, (C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo; en donde los grupos alquilo o cicloalquilo pueden contener opcionalmente una o más insaturaciones y/o pueden tener uno o más heteroátomos incorporados en ellas y, opcionalmente, en cada caso, uno o más átomos de hidrógeno reemplazados por halógeno, -OH, (C<sub>1</sub>-C<sub>3</sub>)-alquilo, -O-(C<sub>1</sub>-C<sub>3</sub>)-alquilo, (C<sub>1</sub>-C<sub>13</sub>)-cicloalquilo; y

$m_1$  es 1;

$m_2$  es 0 ó 1;

$m_3$  es 0 ó 1;

$n_1$  es 0, 1 ó 2;

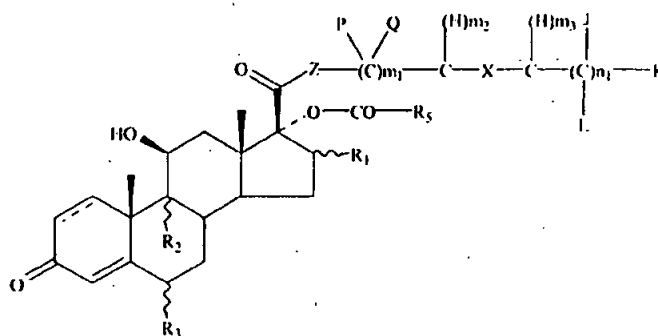
P y Q son hidrógeno;

X representa un enlace doble o un enlace triple; y

J, K y L se seleccionan independientemente de un grupo conformado por hidrógeno, halógeno, (C<sub>1</sub>-C<sub>10</sub>)-alquilo, (C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, -OH, -O-(C<sub>1</sub>-C<sub>10</sub>)-alquilo, -O-(C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, -OCO-(C<sub>1</sub>-C<sub>10</sub>)-alquilo, -OCO-(C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, -OCO-CO-O-(C<sub>1</sub>-C<sub>10</sub>)-alquilo, -OCO-CO-O-(C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, -OCO-O-(C<sub>1</sub>-C<sub>10</sub>)-alquilo, -OCO-O-(C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, -OCO-NH-(C<sub>1</sub>-C<sub>10</sub>)-alquilo, -OCO-NH-(C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, -OCO-N-[(C<sub>1</sub>-C<sub>10</sub>)-alquil]<sub>2</sub>, -OCO-N-[(C<sub>3</sub>-C<sub>13</sub>)-cicloalquil]-OCO-NHSO<sub>2</sub>-(C<sub>1</sub>-C<sub>10</sub>)-alquilo, -OCO-NHSO<sub>2</sub>-(C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, -NH<sub>2</sub>, -NH-(C<sub>1</sub>-C<sub>8</sub>)-alquil-N-[(C<sub>1</sub>-C<sub>8</sub>)-alquil]<sub>2</sub>, -NO<sub>2</sub> y -CN.

Muy preferiblemente,

11 $\beta$ -hidroxiandrosta-4-en-3-ona, compuesto de fórmula I-B, y su sal fisiológicamente aceptable:



**Fórmula I-B**

en donde

Z representa S;

R<sub>1</sub> representa hidrógeno o metilo, el cual puede estar en una configuración  $\alpha$  o  $\beta$ , o ser metileno;

$R_2$  y  $R_3$  son los mismos o diferentes y cada uno independientemente representa hidrógeno, halógeno o un grupo metilo;

$R_5$  representa un grupo seleccionado de  $(C_1-C_{10})$ -alquilo,  $(C_3-C_{13})$ -cicloalquilo,  $-O-(C_1-C_{10})$ -alquilo, arilo o anillo heterocíclico en donde el anillo o sistema de anillo es no sustituido o sustituido por uno o más halógeno,  $-OH$ ,  $(C_1-C_3)$ -alquilo,  $-O-(C_1-C_3)$ -alquilo,  $(C_3-C_{13})$ -cicloalquilo; en donde los grupos alquilo o cicloalquilo pueden contener opcionalmente una o más insaturaciones y/o pueden tener uno o más heteroátomos incorporados en ellas y, opcionalmente, en cada caso, uno o más átomos de hidrógeno reemplazados por halógeno,  $-OH$ ,  $(C_1-C_3)$ -alquilo,  $-O-(C_1-C_3)$ -alquilo,  $(C_3-C_{13})$ -cicloalquilo; y

$m_1$  es 1;

$m_2$  es 0;

$m_3$  es 0;

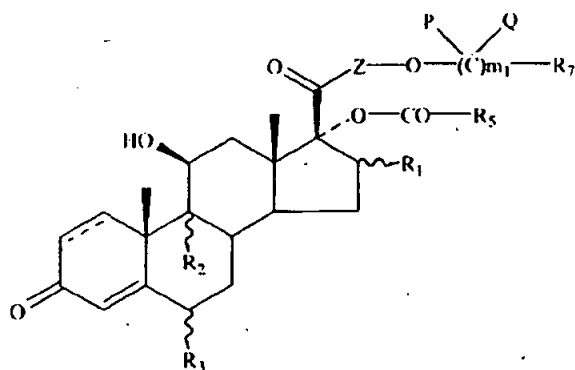
$n_1$  es 0, 1 ó 2;

P y Q son hidrógeno;

X representa un enlace triple; y

J, K y L se seleccionan independientemente de un grupo conformado por hidrógeno, halógeno,  $(C_1-C_{10})$ -alquilo,  $(C_3-C_{13})$ -cicloalquilo,  $-OH$ ,  $-O-(C_1-C_{10})$ -alquilo,  $-O-(C_3-C_{13})$ -cicloalquilo,  $-OCO-(C_1-C_{10})$ -alquilo,  $-OCO-(C_3-C_{13})$ -cicloalquilo,  $-OCO-CO-O-(C_1-C_{10})$ -alquilo,  $-OCO-CO-O-(C_1-C_{10})$ -cicloalquilo,  $-OCO-O-(C_1-C_{10})$ -alquilo,  $-OCO-O-(C_3-C_{13})$ -cicloalquilo,  $-OCO-NH-(C_1-C_{10})$ -alquilo,  $-OCO-NH-(C_3-C_{13})$ -cicloalquilo,  $-OCO-N-[(C_1-C_{10})-alquil]_2$ ,  $-OCO-N-[(C_3-C_{13})-cicloalquil]_2$ ,  $-OCO-NHSO_2-(C_1-C_{10})$ -alquilo,  $-OCO-NHSO_2-(C_3-C_{13})$ -cicloalquilo,  $-NH_2$ ,  $-NH-(C_1-C_8)$ -alquilo,  $N-[(C_1-C_8)-alquil]_2$ ,  $-NO_2$  y  $-CN$ .

En una incorporación la presente invención provee 11 $\beta$ -hidroxiandrosta-4-en-3-ona, un compuesto de fórmula I-C y su sal fisiológicamente aceptable:

**Fórmula I-C**

— representa un enlace único o doble y

~~~~~ representa una configuración  $\alpha$  o  $\beta$ .

en donde

Z representa S;

R_1 representa hidrógeno o metilo, el cual puede estar en una configuración α o β , o ser metileno, R_2 y R_3 son los mismos o diferentes y cada uno independientemente representa hidrógeno, halógeno o un grupo metilo;

m_1 es 1, 2 ó 3;

P y Q se seleccionan independientemente de hidrógeno, halógeno y C_1 a C_3 -alquilo, R_7 representa un grupo seleccionado de halógeno, CO-arilo y R_6 , en donde el anillo arilo de CO-arilo es no sustituido o sustituido por uno o más radicales como se define anteriormente para el anillo o sistema de anillo;

R_6 representa un grupo seleccionado de (C_1-C_8) -alquilo, (C_3-C_{13}) -cicloalquilo, arilo y un radical heterocíclico, donde el anillo o sistema de anillo es no sustituido o sustituido por uno o más radicales seleccionados de (C_1-C_8) -alquilo, (C_3-C_{13}) -cicloalquilo, halógeno O- (C_1-C_8) -alquilo, O- (C_3-C_{13}) -cicloalquilo, OCO- (C_1-C_3) -alquilo, S(O)₀₋₂ (C_1-C_8) -alquilo, COO- (C_1-C_8) -alquilo, -OCO-O- (C_1-C_3) -alquilo, -OCO-CO-O- (C_1-C_3) -alquilo, CONH₂, CONH- (C_1-C_8) -alquilo, CON-[(C_1-C_8)-alquil]₂, -NHCO- (C_1-C_8) -alquilo, N- (C_1-C_8) -alquil-CO- (C_1-C_8) -alquilo, -NHCO-O- (C_1-C_8) -alquilo, -N- (C_1-C_8) -alquil-CO-O- (C_1-C_8) -alquilo, -NHCONH- (C_1-C_8) -alquilo, -N-

(C₁-C₈)-alquil-CONH-(C₁-C₈)-alquilo, -NHCONH-SO₂-(C₁-C₈)-alquilo, -N-(C₁-C₈)-alquil-CONH-SO₂-(C₁-C₈)-alquilo, -NO₂, -CN;

en donde los grupos alquilo o cicloalquilo pueden contener opcionalmente una o más insaturaciones y/o pueden tener uno o más heteroátomos incorporados en ellas y, opcionalmente, en cada caso, uno o más átomos de hidrógeno reemplazados por -F, -Cl, -Br, -I, -OH, -OCO-(C₁-C₃)-alquilo, (C₃-C₁₃)-cicloalquilo, arilo o un radical heterocíclico;

R₅ representa un grupo seleccionado de R₆, -O-R₆ ó -N(R₈)R₆, en donde R₆ y R₈ son como se define anteriormente.

En una incorporación los compuestos de fórmula I-C se seleccionan de los compuestos en donde m₁ es 1; P y Q son ambos hidrógeno y R₇ representa R₆, en donde, R₆ se selecciona del grupo conformado por (C₁-C₈)-alquilo o arilo en donde el anillo o sistema de anillo es no sustituido o sustituido como se define anteriormente.

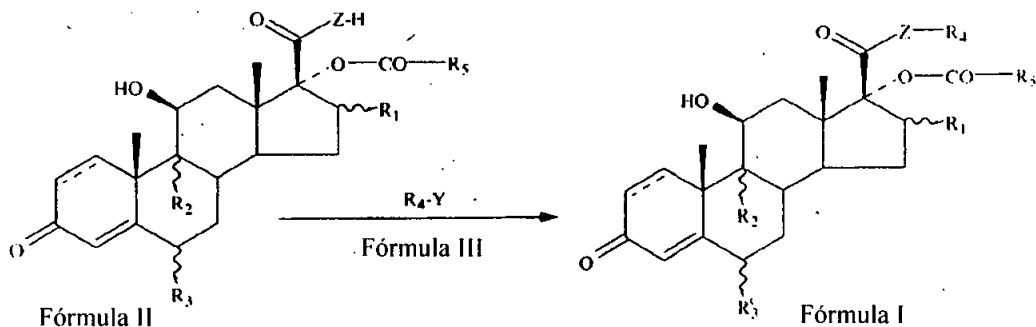
Sales fisiológicamente aceptables son particularmente apropiadas para aplicaciones médicas, debido a su mayor solubilidad en agua, comparadas con los compuestos de partida o básicos. Sales de adición de ácido fisiológicamente aceptables de los compuestos de la invención pueden ser sales de ácidos inorgánicos tales como ácido clorhídrico, ácido bromhídrico, ácido fosfórico, y similares, o de ácidos orgánicos tales como, por ejemplo, ácido acético, ácido benceno sulfónico, ácido benzoico, ácido cítrico y similares. Ejemplos de sales básicas fisiológicamente aceptables apropiadas son sales de amonio, sales de metal alcalino tales como sales de sodio y sales de potasio y sales de metal alcalinotérreo tales como sales de magnesio y sales de calcio.

Los compuestos de fórmula I son útiles en medicina humana o veterinaria, en particular como agentes anti-inflamatorios o antialérgicos.

Los compuestos de fórmula I tienen efectos anti-inflamatorios o antialérgicos potencialmente benéficos, que se demuestran, por ejemplo, por su capacidad de unirse al receptor glucocorticoide *in vitro*; e inhiben el edema en la oreja del ratón inducido por aceite de croto, granuloma inducido por torunda de algodón, edema pulmonar inducido por sephadex en modelos *in vivo*, sin causar efectos secundarios sistémicos como involución del timo, deposición incrementada de glucógeno en el hígado, o cambio apreciable en el peso corporal.

Todas las referencias al compuesto(s) de la fórmula I en esta solicitud aluden a un compuesto/compuestos de la fórmula (1) y a una sal del mismo.

La presente invención provee un proceso para la preparación de los compuestos de la fórmula I, que comprende hacer reaccionar el compuesto de fórmula II con R_4 -i, un compuesto de fórmula III (Esquema-I):



Esquema-I

----- representa un enlace único o doble y

~~~~~ representa una configuración  $\alpha$  o  $\beta$

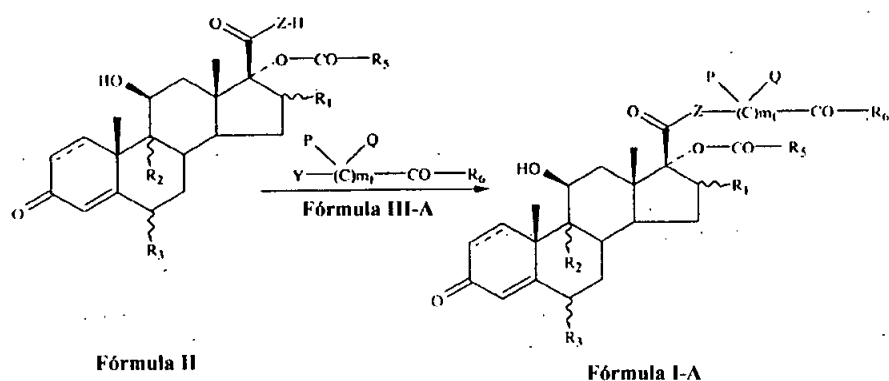
en donde Z representa O ó S;

$R_1$ ,  $R_2$ ,  $R_3$ ,  $R_4$  y  $R_5$  son como se define anteriormente; Y representa un grupo saliente;

En el compuesto de fórmula III, Y representa un grupo saliente apropiado. Un grupo saliente apropiado es cualquier grupo que, luego de la reacción de

un compuesto de fórmula II con el compuesto de fórmula III, facilita la formación de un compuesto de fórmula I. Por ejemplo, Y puede ser un grupo halógeno, alquilsulfonato o arilsulfonato, como un grupo metanosulfonato, *p*-toluenosulfonato o trifluorometanosulfonato.

En una incorporación la presente invención provee igualmente un compuesto de fórmula I-A y un proceso para la preparación de un compuesto de fórmula IA, que comprende hacer reaccionar un compuesto de ácido carboxílico de fórmula II-A (un compuesto de fórmula II, en donde Z es O) o un compuesto de ácido carbotioico de fórmula II-B (un compuesto de fórmula II, en donde Z es S) con un compuesto de fórmula III-A (Esquema-II):



**Esquema-II**

----- representa un enlace único o doble y

~~~~~ representa una configuración  $\alpha$  o  $\beta$

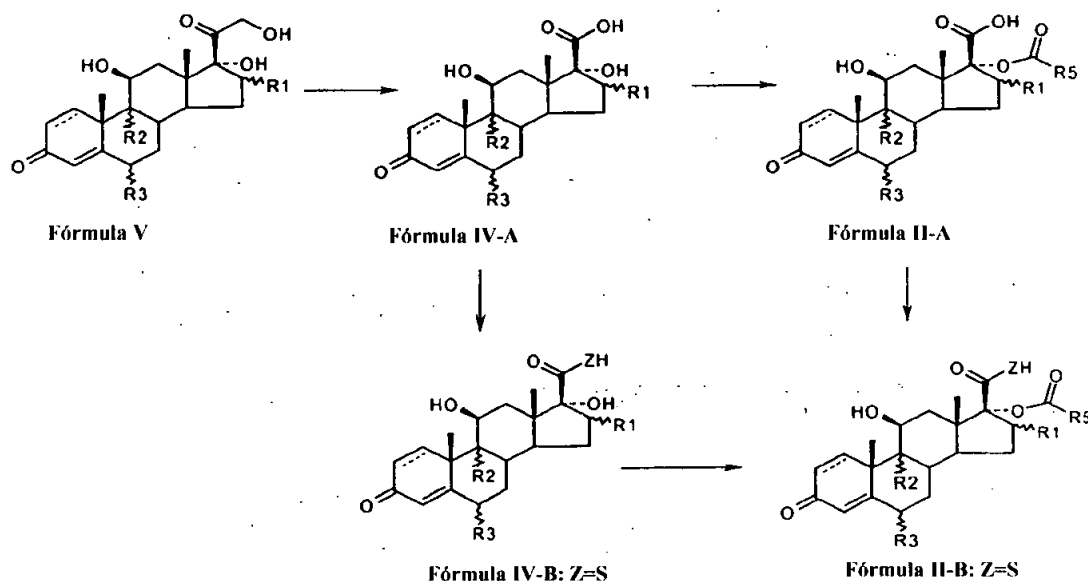
en donde Z representa O, S;

R_1 , R_2 , R_3 , R_5 , R_6 , Y, P, Q y m_1 son como se define anteriormente.

Las reacciones representadas por los Esquemas I o II pueden llevarse ventajosamente a cabo en un disolvente polar orgánico inerte apropiado o sistema disolvente, por ejemplo, acetona, acetonitrilo, *N,N*-dimetilformamida, *N,N*-dimetilacetamida, sulfóxido de dimetilo y similares o una mezcla de los mismos en la presencia de una base adecuada, por ejemplo, carbonatos de metal alcalino o alcalinotérreo como carbonato de potasio, carbonato de sodio, bicarbonato de sodio y similares.

Los compuestos de partida de fórmula formula II o bien son conocidos en el arte o bien pueden prepararse por los siguientes métodos conocidos, por ejemplo, Gordon J. Phillips et al., J. Med. Chem., 37, 3717-3729 (1994); Patente de los Estados Unidos No. 4335121; publicación PCT No. WO 04/001369 o WO 04/039827, incorporadas en esta solicitud por referencia.

Esquema-III representa una secuencia de reacción según la cual puede prepararse el compuesto de fórmula II.



Esquema-III

Preferiblemente, los compuestos de fórmula II-A (compuesto de fórmula II, en donde Z es O) pueden prepararse tratando un compuesto de fórmula IV-A con compuestos de fórmula $R_5\text{COOH}$ o un derivado activo de los mismos tal como un éster, anhídrido o haluro activado de los mismos, especialmente haluro ácido, por ejemplo, un cloruro ácido, en la presencia de una base orgánica como trietilamina o una base inorgánica como carbonato de potasio. Para obtener compuestos de fórmula II-A, en donde R_5 representa -O- R_6 ó -N(R_8) R_6 , el compuesto de fórmula IV-A se hace reaccionar con el correspondiente $R_6\text{-O-CO-i'}$ ó $R_6(R_8)\text{N-CO-i'}$ donde Y' representa un grupo saliente tal como un haluro, 4-nitrofenolato, etc, en la presencia de una base orgánica como trietilamina o una base inorgánica como carbonato de

potasio. Para obtener compuestos de fórmula II-A, donde R_5 representa $-N(R_8)R_6$, y R_8 es hidrógeno, el compuesto de fórmula IV-A puede hacerse reaccionar con el correspondiente isocianato $OCN-R_6$. Los compuestos de fórmula IV-A pueden prepararse por oxidación de compuestos de fórmula V en la presencia de un agente oxidante químico como ácido peryódico o peryodato de sodio.

Preferiblemente, los compuestos de fórmula II-B (compuesto de fórmula II, en donde Z es S) pueden prepararse del compuesto de fórmula II-A por reacción inicial con cloruro de *N,N*-dimetiltiocarbamoilo, seguido por aminólisis del anhídrido mezclado reordenado resultante con dietilamina, o metanólisis y carbonato de potasio, o reacción con hidrosulfuro de sodio en un disolvente apropiado, por ejemplo, *N,N*-dimetilformamida.

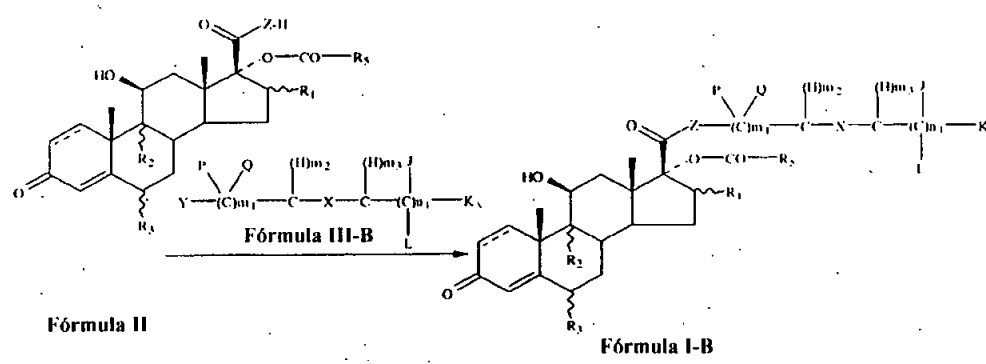
Los compuestos de fórmula II-B, donde Z es S pueden prepararse igualmente tratando un compuesto de fórmula IV-B con compuestos de fórmula R_5COOH o un derivado activo de los mismos, tal como un éster, anhídrido o haluro activado de los mismos, especialmente un haluro ácido, por ejemplo, un cloruro ácido, en la presencia de una base orgánica como trietilamina o una base inorgánica como carbonato de potasio. En compuestos de fórmula II-B en donde R_5 representa $-O-R_6$, ó $-N(R_8)R_6$, el compuesto de fórmula IV-B se hace reaccionar con el correspondiente $R_6-O-CO-i'$ ó $R_6(R_8)N-CO-i'$ donde Y' representa un grupo saliente tal como un haluro, 4-nitrofenolato, etc, en la presencia de una base orgánica como trietilamina o una base inorgánica como carbonato de potasio.

Los compuestos de fórmula IV-B, donde Z es S pueden prepararse del compuesto de fórmula IV-A por activación de carbonilo con 1,1'-carbonildiimidazol y reacción con sulfuro de hidrógeno o hidrosulfuro de sodio en un disolvente apropiado, por ejemplo, *N,N*-dimetilformamida.

Los compuestos de fórmula II pueden usarse convenientemente como sus sales de adición de ácido, preferiblemente en forma cristalina. Pueden emplearse cualesquiera sales de adición de ácido, por ejemplo, sal de sodio o de potasio.

Los compuestos de fórmula III-A son conocidos o pueden prepararse por métodos conocidos en el arte.

En una incorporación la presente invención provee un compuesto de fórmula I-B y un proceso para su preparación, que comprende hacer reaccionar un compuesto de ácido carboxílico de fórmula II-A (un compuesto de fórmula II, en donde Z es O) o un compuesto de ácido carbotioico de fórmula II-B (un compuesto de fórmula II, en donde Z es S) con un compuesto de fórmula III-B (Esquema-IV):



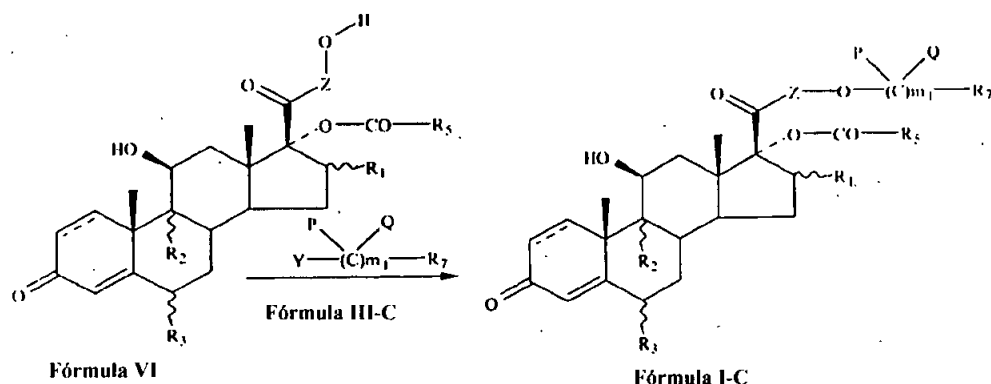
Esquema-IV

----- representa un enlace único o doble y
~~~~~ representa una configuración  $\alpha$  o  $\beta$   
en donde Z representa O ó S;  
 $R_1, R_2, R_3, R_5, Y, P, Q, J, K, L, m_1$  y  $n_1$  son como se define anteriormente, X representa un enlace doble o un enlace triple,  $m_2$  es 0 ó 1 y  $m_3$  es 0 ó 1;

El compuesto de fórmula I-B puede prepararse por alquilación del compuesto de fórmula II con el compuesto de fórmula III-B, que se lleva ventajosamente a cabo en un disolvente polar orgánico inerte o sistema

disolvente, por ejemplo, acetona, acetonitrilo, *N,N*-dimetilformamida, *N,N*-dimetilacetamida, sulfóxido de dimetilo y similares en la presencia de una base adecuada, por ejemplo, carbonatos de metal alcalino o alcalinotérreo como carbonato de potasio, carbonato de sodio, bicarbonato de sodio y similares. Los compuestos de fórmula III-B son conocidos o pueden prepararse por métodos conocidos en el arte.

En una incorporación preferida, la presente invención provee un compuesto de fórmula I-C y un proceso para su preparación, que comprende hacer reaccionar un compuesto de fórmula VI con un compuesto de fórmula III-C (Esquema-V):



### Esquema-V

— representa un enlace único o doble y

~~~~~ representa una configuración  $\alpha$  o  $\beta$

en donde Z representa S;

R_1 , R_2 , R_3 , R_5 , R_7 , Y, P, Q y m_1 son como se define anteriormente;

El compuesto de fórmula I-C puede prepararse por alquilación del compuesto de fórmula VI con el compuesto de fórmula III-C, que se lleva ventajosamente a cabo en un disolvente polar orgánico inerte o sistema disolvente, por ejemplo, acetona, acetonitrilo, *N,N*-dimetilformamida, *N,N*-dimetilacetamida, sulfóxido de dimetilo y similares en la presencia de una

base adecuada, por ejemplo, carbonatos de metal alcalino o alcalinotérreo como carbonato de potasio, carbonato de sodio, bicarbonato de sodio y similares. Los compuestos de fórmula III-C son conocidos o pueden prepararse por métodos conocidos en el arte.

El compuesto de fórmula VI puede prepararse por oxidación del compuesto de fórmula II-B con un agente oxidante, por ejemplo, peróxido de hidrógeno, peróxido de hidrógeno-urea, ácido peracético, ácido *m*-cloroperbenzoico, peryodato de sodio y similares en un disolvente polar orgánico tal como metanol, etanol, 2-propanol, ácido acético y similares.

El compuesto de fórmula I y su sal fisiológicamente aceptable pueden emplearse igualmente como intermedios para la preparación de derivados de los mismos, por ejemplo, el grupo -OH puede convertirse en el grupo halo o acetilarse, sulfonarse, etc.

La presente invención se refiere asimismo a las formas farmacéuticas para aplicación local, las cuales dependen del tipo exacto de la formulación que se va a preparar, pero generalmente pueden estar en el rango de 0.001 a 10% en peso. Por lo general, sin embargo, para la mayoría de los tipos de preparaciones, ventajosamente la proporción utilizada estará en el rango de 0.005 a 1% y, preferiblemente, 0.01 a 0.5%. No obstante, en polvos para inhalación o insuflación la proporción empleada puede estar en el rango de 0.1 a 5%. La dosis diaria puede variar y sería dependiente de la enfermedad que se está tratando, y la duración del tratamiento deseada.

En una incorporación, la cantidad de un compuesto de acuerdo con la fórmula I, usada para lograr el efecto biológico deseado, depende de un número de factores, por ejemplo el compuesto específico seleccionado, el uso previsto, el tipo de administración y el estado clínico del paciente. En general, la dosis diaria está en el rango de 0.01mg a 500mg (típicamente desde 0.1 mg a 10mg). Formulaciones farmacéuticas administrables

oralmente tales como, por ejemplo, tabletas o cápsulas pueden contener, por ejemplo, desde 0.1 mg a 500mg, típicamente desde 1mg a 100mg.

En el caso de sales fisiológicamente aceptables, las masas ya mencionadas se refieren a la masa del compuesto libre en la cual se basa la sal de adición. Los compuestos usados para la profilaxis o terapia pueden ser los compuestos de acuerdo con la fórmula I en sí mismos, o, en una incorporación, pueden estar presentes en la forma de una composición farmacéutica junto con una sustancia portadora aceptable. En una incorporación, la sustancia portadora tiene que ser naturalmente aceptable, en el sentido de que sea compatible con los demás ingredientes de la citada composición y no sea nociva para la salud del paciente. La sustancia portadora puede ser un sólido o un líquido, o ambos, y se formula preferiblemente con el compuesto como una dosis individual, por ejemplo como una tableta que puede contener desde 0.05% a 95% en peso del compuesto activo. Las composiciones farmacéuticas de la invención pueden prepararse de acuerdo con cualquiera de los métodos farmacéuticos conocidos, los cuales comprenden esencialmente mezclar los ingredientes con sustancias portadoras y/o excipientes farmacológicamente aceptables.

Otro aspecto de la presente invención se refiere a la formulación de compuestos de fórmula I en una forma apropiada para administración a un sujeto.

Composiciones farmacéuticas de la invención son aquellas que son apropiadas para administración oral, rectal, tópica, peroral (por ejemplo, sublingual) y parenteral (por ejemplo, subcutánea, intradérmica o intra-articular), aunque la manera más apropiada de administración depende en cada caso individual de la naturaleza y gravedad de la enfermedad a tratarse y de la naturaleza del compuesto de acuerdo con la fórmula I, empleado en cada caso. Asimismo formulaciones recubiertas con azúcar y formulaciones de liberación retardada, recubiertas con azúcar, se incluyen dentro del

ámbito de la invención. En una incorporación, se da preferencia a formulaciones resistentes a los ácidos y gastrorresistentes. Cubiertas gastrorresistentes apropiadas incluyen ftalato de acetato de celulosa, ftalato de acetato de polivinilo, ftalato de hidroxipropilmetilcelulosa y polímeros aniónicos de ácido metacrílico y metacrilato de metilo.

Compuestos farmacéuticos apropiados para administración oral pueden estar presentes en unidades separadas como, por ejemplo, cápsulas, sobre cápsulas amiláceas, pastillas para chupar o tabletas, que en cada caso contienen una cantidad particular del compuesto de acuerdo con fórmula I; como polvos o gránulos; como solución o suspensión en un líquido acuoso o no acuoso; o como una emulsión aceite en agua, o agua en aceite. Estas composiciones pueden prepararse de acuerdo con cualquier método farmacéutico apropiado, que incluye un paso en el cual se contactan el compuesto activo y la sustancia portadora (que puede comprender uno o más componentes adicionales). En general, las composiciones se preparan mezclando de manera uniforme y homogénea el compuesto activo con una sustancia portadora líquida y/o sólida finamente dispersada, luego de lo cual el producto se moldea, si es necesario. Por consiguiente una tableta, por ejemplo, puede prepararse prensando o moldeando un polvo o gránulos del compuesto, donde sea apropiado, con uno o más componentes adicionales. Tabletas prensadas pueden prepararse tableteando el compuesto en forma de deslizamiento libre, por ejemplo un polvo o gránulos, mezclados, donde sea apropiado, con un aglutinante, lubricante, diluyente inerte y/o uno o más agentes tensioactivos/dispersantes en una máquina adecuada. Tabletas moldeadas pueden prepararse moldeando el compuesto pulverulento, humedecido con un diluyente líquido inerte, en una máquina apropiada.

Composiciones farmacéuticas que son apropiadas para administración peroral (sublingual) incluyen pastillas para chupar, las cuales contienen un compuesto de acuerdo con fórmula I con un agente saborizante, usualmente sacarosa y goma arábica o tragacanto, y pastillas que contienen el

compuesto en una base inerte tal como gelatina y glicerol o sacarosa y goma arábica.

Composiciones farmacéuticas apropiadas para administración parenteral, por ejemplo, comprenden preparaciones estériles de un compuesto de acuerdo con fórmula I. Estas preparaciones pueden administrarse intradérmicamente, aunque pueden administrarse igualmente subcutánea, intramuscular o intra-articularmente como una inyección. Estas preparaciones pueden elaborarse mezclando el compuesto con agua y haciendo estéril la solución obtenida. Composiciones inyectables de la invención contienen generalmente desde 0.01 a 5% en peso del compuesto activo.

Composiciones farmacéuticas apropiadas para administración rectal están presentes como supositorios de dosis individual. Éstas pueden prepararse mezclando un compuesto de acuerdo con fórmula I con una o más soluciones portadoras sólidas convencionales, por ejemplo manteca de cacao, y moldear la mezcla resultante.

Composiciones farmacéuticas apropiadas para aplicación tópica a la piel pueden estar presentes como ungüento, crema, loción, pasta, atomizador, aerosol o aceite. Las sustancias portadoras que pueden usarse incluyen, por ejemplo, vaselina, lanolina, polietilen glicoles, alcoholes y combinaciones de dos o más de estas sustancias. En una incorporación, el compuesto activo está presente en un rango de concentración que varía desde 0.1 a 15%, por ejemplo desde 0.5 a 2%, en peso de la composición.

Es también posible la administración transdérmica. Composiciones farmacéuticas apropiadas para administración transdérmica pueden estar presentes como parches individuales, que son apropiados para contacto estrecho a largo plazo con la epidermis del paciente. Tales parches contienen convenientemente el compuesto activo en una solución acuosa

opcionalmente amortiguada, disuelta y/o dispersada en un adhesivo o dispersada en un polímero. Una concentración apropiada de un compuesto activo va desde aprox. 0.1 % a 35%, preferiblemente aprox. 1 a 15%. Una posibilidad particular es la liberación del compuesto activo por electrotransferencia o ionoforesis, como se describe, por ejemplo, en *Pharmaceutical Research*, 2(6): 318 (1986).

En una incorporación preferida, los compuestos de fórmula I se adaptan para administración local. Administración local, tal como se emplea en esta solicitud, incluye administración mediante insuflación e inhalación. Los diferentes tipos de formas farmacéuticas útiles para administración local incluyen ungüentos, lociones, cremas, geles, espumas, preparaciones para aplicación transdérmica mediante parches, polvos, atomizadores, aerosoles, cápsulas o cartuchos para uso en un inhalador o insuflador o gotas (por ejemplo, colirios o gotas nasales), soluciones/suspensiones para nebulización, supositorios, dispositivos intrauterinos, enemas de retención y tabletas o píldoras masticables o para chupar o preparaciones en microencapsulación.

Ungüentos, cremas y geles, por ejemplo, pueden formularse con una base aceitosa o acuosa con la adición de agentes espesantes y/o gelificantes apropiados y/o disolventes. Por lo tanto, tales bases pueden incluir, por ejemplo, agua y/o aceite, tal como parafina líquida o un aceite vegetal tal como aceite de maní o aceite de ricino, o un disolvente tal como polietilen glicol. Agentes espesantes y agentes gelificantes que pueden usarse de acuerdo con la naturaleza de la base incluyen parafina blanda, estearato de aluminio, alcohol cetoestearílico, polietilen glicoles, lanolina, cera de abejas, carboxipolimetileno y derivados de celulosa, y/o gliceril monosterato y agentes emulsionantes no iónicos.

Polvos para aplicación externas pueden formarse con ayuda de cualquier base en polvo apropiada, por ejemplo, talco, lactosa o almidón. Pueden

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formularse gotas con una base acuosa o no acuosa que contenga igualmente agentes, agentes solubilizantes, agentes de suspensión o preservantes.

Composiciones atomizables pueden formularse por ejemplo como solución acuosa o suspensiones o como aerosoles aplicados de envases presurizados, tales como un inhalador con dosis medidas, con el uso de un propelente licuado apropiado. Composiciones en aerosol adecuadas para inhalación puede ser o bien una suspensión o una solución y, generalmente, contienen un compuesto de fórmula I y un propelente apropiado tal como un fluorocarbono o clorofluorocarbono con contenido de hidrógeno o sus mezclas, particularmente hidrofluoroalcanos, especialmente 1,1,1,2-tetrafluoroetano, 1,1,1,2,3,3,3-heptafluoro-*n*-propano o sus mezclas. La composición en aerosol puede contener opcionalmente excipientes de formulación adicionales bien conocidos en el arte tales como tensioactivos, por ejemplo ácido oleico o lecitina y co-disolventes, por ejemplo etanol.

Ventajosamente, las formulaciones de la invención pueden amortiguarse mediante la adición de agentes amortiguadores apropiados.

Cápsulas y cartuchos para uso en un inhalador o insuflador, por ejemplo de gelatina, pueden formularse conteniendo una mezcla de polvo o, para inhalación de un compuesto de la invención, conteniendo una base de polvo apropiada tal como lactosa o almidón. Cada cápsula o cartucho puede contener por lo general entre 20µg-1.000µg del compuesto de fórmula I. Alternativamente, el compuesto de la invención puede presentarse sin excipientes tales como lactosa.

La proporción del compuesto activo de fórmula I en las composiciones locales de acuerdo con la invención depende del tipo exacto de formulación a prepararse, pero estará generalmente en el rango de desde 0.001 a 10% en peso. Por lo general, sin embargo, para la mayoría de los tipos de preparaciones, ventajosamente la proporción usada estará en el rango de

desde 0.005 a 1% y, preferiblemente, 0.01 a 0.5%. No obstante, en polvos para inhalación o insuflación, la proporción utilizada estará en el rango de desde 0.1 a 5%.

Las formulaciones en aerosol se disponen preferiblemente de tal manera que cada dosis medida o "emisión" de aerosol contenga 20µg-2.000µg, preferiblemente alrededor de 20µg-500µg de un compuesto de fórmula I. La administración puede ser una vez al día o varias veces al día, por ejemplo 2, 3, 4 u 8 veces, aplicando por ejemplo 1, 2 ó 3 dosis cada vez. La dosis diaria total con un aerosol estará en el rango de de 100µg-1.000µg preferiblemente, 200µg-2.000µg. La dosis diaria total y la dosis medida entregada por cápsulas y cartuchos en un inhalador o insuflador será generalmente el doble de las aplicadas con formulaciones en aerosol.

La preparación tópica puede administrarse mediante una o más aplicaciones al día al área afectada; ventajosamente puede utilizarse un apósito oclusivo. Una aplicación continua o prolongada puede lograrse mediante un sistema reservorio adhesivo.

Una composición farmacéutica puede ser una solución o suspensión que contenga una concentración terapéuticamente efectiva del compuesto de fórmula I, con o sin otros bioactivos en concentraciones farmacéuticamente efectivas. La composición puede constar adicionalmente de varios excipientes farmacéuticamente aceptables tales como agentes quelantes, modificadores de pH, soluciones amortiguadoras, mejoradores de viscosidad, agentes de isotonicidad, solubilizantes, preservantes, antioxidantes y similares.

Un compuesto de fórmula I puede formularse en la forma de sistemas de administración de medicamentos tales como soluciones formadoras de gel.

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Para administración interna los compuestos de acuerdo con la invención pueden, por ejemplo, formularse de manera convencional para administración oral, parenteral o rectal. La formulación para administración oral incluye jarabes, elixires, polvos, gránulos, tabletas y cápsulas que típicamente contienen excipientes convencionales tales como agentes aglutinantes, agentes de relleno, lubricantes, desagregantes, agentes humectantes, agentes de suspensión, agentes emulsionantes, preservantes, sales amortiguadoras, agentes saborizantes, colores y/o edulcorantes, según sea apropiado. No obstante se prefieren formas farmacéuticas unitarias, como se describe más adelante.

Formulaciones de liberación lenta o gastrorresistentes pueden ser ventajosas, particularmente para síndrome de intestino irritable.

Formas preferidas de preparación para administración interna son presentaciones farmacéuticas unitarias, es decir, tabletas y cápsulas. Tales presentaciones farmacéuticas unitarias contienen desde 0.01mg a 20mg, preferiblemente desde 2.5mg a 10mg de los compuestos de la invención.

La presente invención provee una composición farmacéutica que comprende 11β -hidroxiandrosta-4-en-3-ona, un compuesto de fórmula I y su sal fisiológicamente aceptable.

La presente invención en una incorporación provee una composición farmacéutica que comprende 11β -hidroxiandrosta-4-en-3-ona, un compuesto de fórmula I-A, y su sal fisiológicamente aceptable.

La presente invención en una incorporación provee una composición farmacéutica que comprende 11β -hidroxiandrosta-4-en-3-ona, un compuesto de fórmula I-B, y su sal fisiológicamente aceptable.

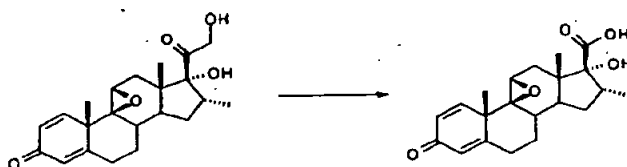
La presente invención en una incorporación provee una composición farmacéutica que comprende 11β -hidroxiandrosta-4-en-3-ona, un compuesto de fórmula I-C, y su sal fisiológicamente aceptable.

La invención se ilustra pero no se limita por la descripción en los siguientes ejemplos.

EJEMPLOS

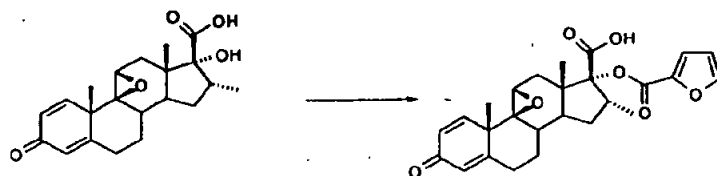
Ejemplo 1

Ácido 9, 11-epoxi-17 α -hidroxi-16 α -metil-3-oxandrosta-1,4-dien-17 β -carboxílico



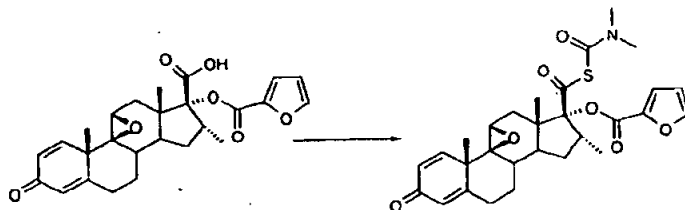
Una solución de ácido peryódico (4.59g, 0.0201mol) en agua (25ml) (preparada calentando a 50-55°C y enfriando luego a 30-35°C) se agregó gota a gota a una suspensión agitada de 17 α ,21-dihidroxi-9,11-epoxi-16 α -metilpregna-1,4-dien-3,20-diona (5.0g, 0.0134mol) en tetrahidrofurano (25ml) a 0-5°. La mezcla de reacción se agitó a 0-5°C durante 2 horas, se agregó agua a la mezcla de reacción a 0-5°C. El producto precipitado se filtró, se lavó con agua y se secó para producir el compuesto del título como sólido blanco (4.75g, 98.7%).

^1H NMR (400 MHz en CDCl_3), δ : 0.92(d, $J=6.99\text{Hz}$, 3H), 1.04(s, 3H), 1.29-1.36(m, 1H), 1.44(s, 3H), 1.41-1.82(m, 4H), 2.12-2.94(m, 6H), 3.19(s, 1H), 3.55-3.65(m, 1H), 6.11(s, 1H), 6.14(dd, $J_1=10.09\text{Hz}$, $J_2=1.68\text{Hz}$, 1H), 6.60(d, $J=10.06\text{Hz}$, 1H).

Ejemplo 2**Ácido 9,11-epoxi-17 α -[(2-furanilcarbonil)oxi]16 α -metil-3-oxoandrosta-1,4-dien-17 β -carboxílico**

A una suspensión de ácido 9,11-epoxi-17 α -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carboxílico (4.5g, 0.012mol) en acetona (25ml) a 10-15°C se agregó secuencialmente trietilamina (5.3ml, 0.038mol) y cloruro de 2-furoilo (4.96g, 0.038mol). Luego de agitar durante 4 horas a 25-30°C, se agregó gota a gota dietilamina (2.63ml, 0.025mol) a 10-15°C y luego se agitó a temperatura ambiente durante 1 hora. Posteriormente la mezcla de reacción se acidificó a pH 1.0-1.5 a 0-5°C, el producto precipitado se filtró, se lavó con agua y se secó para producir el compuesto del título como sólido blanco (5.96g, 99%).

¹H NMR (400 MHz en CDCl₃+DMSO-d₆), δ : 0.98(d, J =7.09Hz, 3H), 1.07(s, 3H), 1.25-1.48(m, 2H), 1.46(s, 3H), 1.66-1.81(m, 3H), 2.02-2.74(m, 6H), 3.26(s, 1H), 3.26-3.32 (m, 1H), 6.19(s, 1H), 6.22(dd, J_1 =10.13Hz, J_2 =1.76Hz, 1H), 6.53(dd, J_1 =3.44Hz, J_2 =1.61 Hz, 1H), 6.64(d, J =10.04Hz, 1H), 7.15 (d, J =3.37Hz, 1H), 7.62(d, J =0.81Hz, 1H).

Ejemplo 3**17 β -[(*N,N*-Dimetilcarbamoil)tio]carbonil-9,11-epoxi-17 α -[(2-furanilcarbonil)oxi]-16 α -metil-3-oxoandrosta-1,4-dieno**

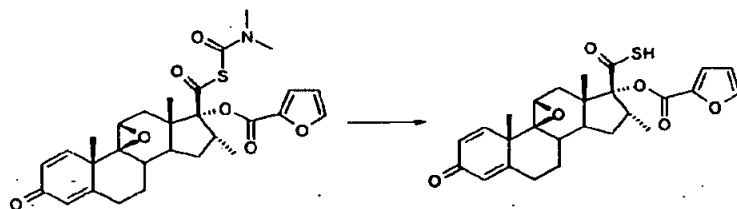
Una solución de ácido 9,11-epoxi-17 α -[(2-furanilcarbonil)oxi]16 α -metil-3-oxoandrosta-1,4-dien-17 β -carboxílico (7.0g, 0.0129mol) y cloruro de *N,N*-dimetiltiocarbamoilo (2.74g, 0.0259mol) en tetrahidrofurano (35ml) se

enfrió a 10 a 15°C y se trató con trietilamina (2.86g, 0.0283mol) y yoduro de tetrabutilamonio (0.5g). La mezcla de reacción se calentó entonces a temperatura ambiente, se agitó durante 4 horas y luego se agregó *N,N*-dimetilacetamida (21 ml) seguida por agua (140ml). La mezcla resultante se enfrió a 0°C, el producto se filtró, se lavó con agua y se secó para producir el compuesto del título como un sólido amarillo pálido. (6.6g, 79.1%)

¹H NMR (400 MHz en CDCl₃+DMSO-d₆), δ : 1.01(d, J =7.11Hz, 3H), 1.15(s, 3H), 1.41-1.49(m, 2H), 1.46(s, 3H), 1.72-1.87(m, 3H), 2.19-2.73(m, 6H), 3.06(s, 3H), 3.16(s, 3H), 3.30(s, 1H), 3.30-3.32(m, 1H), 6.19(s, 1H), 6.22(dd, J_1 =3.51 Hz, J_2 =1.68Hz, 1H), 6.64(d, J =10.09Hz, 1H), 7.22(d, J =3.51 Hz), 7.67(d, J =0.90Hz, 1H).

Ejemplo 4

Ácido 9,11-epoxi-17 α -(2-furanilcarbonil)oxi]-17 α -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotioico



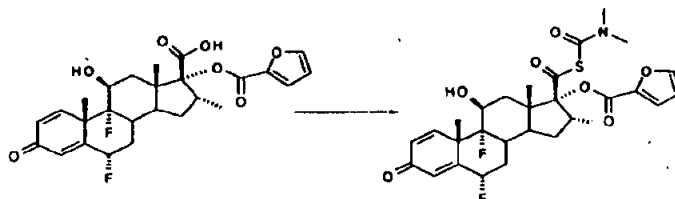
Una suspensión de 17 β -[(*N,N*-dimetilcarbamoil)tio]carbonil-9,11-epoxi-17 α -[(2-furanilcarbonil)oxi]-16 α -metil-3-oxoandrosta-1,4-dieno (5.0g, 0.0106 mol) y carbonato de potasio (2.94g, 0.0213mol) en metanol (25ml) se agitó a temperatura ambiente durante 5 horas bajo una cubierta de nitrógeno. Posteriormente, se agregó agua a la mezcla de reacción y la solución clara resultante se lavó con tolueno. La capa acuosa que contenía el producto se puso en carbón vegetal y luego se acidificó con 2N HCl hasta que el pH fue 1.5 a 2.0. El producto precipitado se filtró, se lavó con agua y se secó para producir el compuesto del título como un sólido blancuzco (3.6g, 83%).

¹H NMR (400 MHz en CDCl₃), δ : 1.01(d, J =7.11Hz, 3H), 1.12(s, 3H), 1.36-1.48(m, 2H), 1.46(s, 3H), 1.72-1.81(m, 3H), 2.18-2.69(m, 6H), 3.28-3.31(m, 1H), 3.31(s, 1H), 6.21(s, 1H), 6.25(dd, J_1 = 10.08Hz, J_2 =1.76Hz,

1H), 6.55(dd, $J_1=3.48\text{Hz}$, $J_2=1.61\text{Hz}$, 1H), 6.63(d, $J=10.06\text{Hz}$, 1H), 7.23(dd, 1H).

Ejemplo 5

17 β -[(*N,N*-Dimetilcarbamoil)tio]carbonil-6 α ,9 α -difluoro-17 α -[(2-furanil-carbonil)oxi]-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dieno

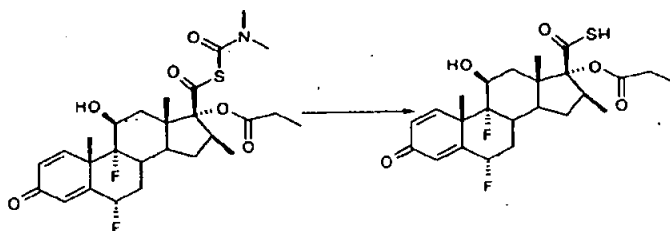


A una solución de ácido 6 α ,9 α -difluoro-17 α -[(2-furanilcarbonil)oxi]-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carboxílico (12.3g, 0.025mol) y cloruro de *N,N*-dimetiltiocarbamoilo (9.29g, 0.075mol) en tetrahidrofurano (60ml) se agregó trietilamina (10.48ml, 0.075mol) a 10-15°C y yoduro de tetrabutilamonio (0.92g) y la mezcla se agitó durante 4 horas a temperatura ambiente. Se agregaron dimetilacetamida (37ml) y agua (310ml) a la mezcla de reacción y se agitó durante 2 horas a 0°C. El sólido obtenido se filtró, se lavó con agua y se secó para producir el compuesto del título como un sólido blanco (14.3g, 99%).

^1H NMR (400 MHz en $\text{CDCl}_3+\text{DMSO}-d_6$), δ : 1.00(d, $J=7.10\text{Hz}$, 3H), 1.19(s, 3H), 1.30-1.36(m, 1H), 1.54(s, 3H), 1.63-2.00(m, 3H), 2.22-2.60(m, 4H), 3.03(s, 3H), 3.16(s, 3H), 3.31-3.36(m, 1H), 4.29(d, $J=8.91\text{Hz}$, 1H), 5.39(br-s, 1H), 5.43-5.59(m, 1H), 6.22(s, 1H), 6.27(dd, 1H), 7.26(d, $J=9.85\text{Hz}$, 1H), 7.80(d, $J=0.92\text{Hz}$, 1H).

Ejemplo 6

Ácido 6 α ,9 α -difluoro-11 β -hidroxi-16 β -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carbotioico

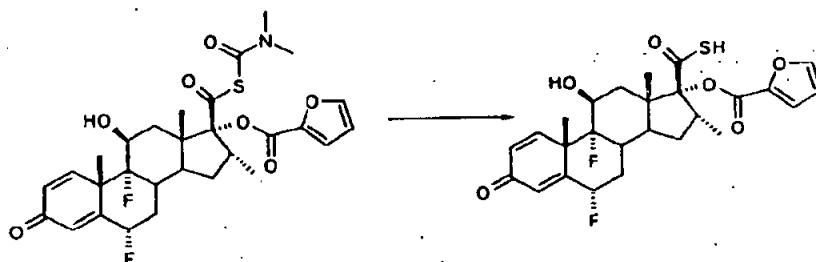


Una suspensión de 17β-[(*N,N*-dimetilcarbamoil)tio]carbonil-6α,9α-difluoro-11β-hidroxi-16β-metil-3-oxo-17α-propioniloxiandrosta-1,4-dieno (5.0g, 9.27 mmol) en 75ml dietilamina se calentó bajo reflujo durante 8 horas. La mezcla de reacción enfriada se virtió en agua helada acidificada con 2N HCl a pH 2 y se extrajo con acetato de etilo. El extracto de acetato de etilo se lavó con agua, se secó y se concentró *in vacuo*. El residuo obtenido se cristalizó de acetato de etilo para producir el compuesto del título como un sólido amarillo pálido (3.2g, 73.7%).

¹H NMR (400 MHz en CDCl₃), δ: 1.06(s, 3H), 1.16(t, *J*=7.52Hz, 3H), 1.20-1.25(m, 1H), 1.39(d, *J*=7.23Hz, 3H), 1.54(s, 3H), 1.67-2.05(m, 4H), 2.22-2.80(m, 4H), 2.39(q, *J*=7.69Hz, 2H), 4.45(br-d, *J*=7.69Hz, 1H), 5.30-5.50(m, 1H), 6.38(d, *J*=9.93Hz, 1H), 6.43(s, 1H), 7.15(dd, *J*=10.17Hz, 1H). En una manera análoga se preparó ácido 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16β-metil-3-oxoandrosta-1,4-dien-17β-carbotioico.

Ejemplo 7

Ácido 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotioico



Una suspensión de 17β-[(*N,N*-dimetilcarbamoil)tio]carbonil-6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dieno (14.2g, 0.024mol) y carbonato de potasio (6.78g, 0.0491mol) en metanol (70ml) se agitó a temperatura ambiente durante 6 horas bajo una

cubierta de nitrógeno. Posteriormente, se agregó agua a la mezcla de reacción y la solución clara resultante se lavó con tolueno. La capa acuosa que contenía el producto se puso en carbón vegetal y luego se acidificó con 2N HCl hasta que el pH fue 1.5 a 2.0. El producto precipitado se filtró, se lavó con agua y se secó para producir el compuesto del título como sólido blanco (11.8g, 94.8%).

¹H NMR (400 MHz en CDCl₃+DMSO-d₆), δ : 1.03(d, J =7.17Hz, 3H), 1.20(s, 3H), 1.31-1.37(m, 1H), 1.56(s, 3H), 1.73-2.03(m, 3H), 2.28-2.59(m, 4H), 3.37-3.42(m, 1H), 4.35-4.38(br-d, 1H), 4.89(d, J =1.22Hz, 1H), 5.34-5.51(m, 1H), 6.34(dd, J_1 =10.06Hz, J_2 =1.88Hz, 1H), 6.39(s, 1H), 6.53(dd, J_1 =3.45Hz, J_2 =1.73Hz, 1H), 7.14(dd, J_1 =3.28Hz, J_2 =0.49Hz, 1H), 7.25(dd, J_1 =10.12Hz, J_2 =1.30Hz, 1H), 7.63(dd, J_1 =1.73Hz, J_2 =0.63Hz, 1H).

Los siguientes ácidos 17 β -carbotioicos se prepararon por un método análogo a ejemplo 7:

Ácido 9 α -fluoro-17 α -[(2-furanilcarbonil)oxi]-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotioico.

Ácido 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-17 α -[(3-metil-2-furanil)carbonil]oxi]-3-oxoandrosta-1,4-dien-17 β -carbotioico.

Ácido 6 α ,9 α -difluoro-17 α -[(3-furanilcarbonil)oxi]-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotioico.

Ácido 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -[(2-tienilcarbonil)oxi]-androsta-1,4-dien-17 β -carbotioico.

Ácido 17 α -[(5-cloro-2-tioenil)carbonil]oxi]-6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotioico.

Ácido 17 α -ciclopropilcarboniloxi-6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotioico.

Ácido 17 α -ciclobutilcarboniloxi-6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotioico.

Ácido 17 α -ciclopentilcarboniloxi-6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotioico.

Ácido 17 α -ciclohexilcarboniloxi-6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotioico.

Ácido 17 α -ciclohexilmetilcarboniloxi-6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotioico.

Ácido 9 α -fluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carbotioico.

Ácido 9 α -fluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carbotioico.

Ácido 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carbotioico.

Ácido 6 α ,9 α -difluoro-11 β -hidroxi-16 β -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carbotioico.

Ácido 17 α -butiloxi-6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotioico.

Ácido 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -valeriloxiandrosta-1,4-dien-17 β -carbotioico.

Ácido 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-17 α -(2-metilpropionil)oxi-3-oxoandrosta-1,4-dien-17 β -carbotioico.

Ácido 17 α -dicloroacetoxi-6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotioico.

Ácido 6 α ,9 α -difluoro-11 β -hidroxi-17 α -(metoximetilcarbonil)oxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotioico.

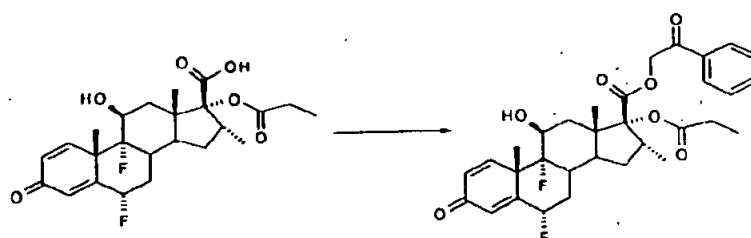
Ácido 6 α ,9 α -difluoro-17 α -(etoximetilcarbonil)oxi-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotioico.

Ácido 17 α -(etoxicarbonil)oxi-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotioico.

Ácido 6 α ,9 α -difluoro-17 α -(etoxicarbonil)oxi-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotioico.

Ejemplo 8 – Compuesto IA.44

2-Fenil-2-oxoetil 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carboxilato



2-Bromo-1-feniletanona (0.438g, 2.2mmol) y yoduro de sodio (50mg) se agregaron a una mezcla agitada de ácido 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxi-androsta-1,4-dien-17 β -carboxílico (1.0g, 2.20mmol) y carbonato de potasio anhidro (0.360g, 2.6mmol) en acetona (15ml). La mezcla se agitó bajo una cubierta de nitrógeno entre 25 a 30°C

48

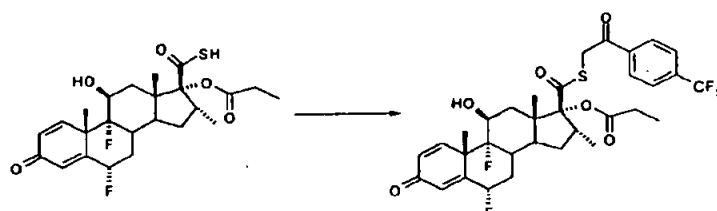
durante 8 horas, luego se virtió en agua y se extrajo con acetato de etilo. La capa orgánica se lavó dos veces con agua, se secó y se concentró *in vacuo*. El residuo se purificó por cromatografía de columna (40% acetato de etilo en hexanos) para producir el compuesto del título como un sólido blanco.

Los siguientes compuestos se prepararon en una manera similar a ejemplo 8 usando un ácido carboxílico apropiado de fórmula II y compuesto de fórmula III-A:

IA.1, IA.2, IA.4, IA.5, IA.7 a IA.10, IA.12, IA.15 a IA.19, IA.21, IA.23 a 25, IA.28 a 30, IA.32, IA.33, IA.36, IA.37, IA.42, IA.46, IA.48, IA.50, IA.52, IA.54, IA.57, IA.60, IA.62 a IA.67, IA.71, IA.72, IA.74, IA.76, IA.77, IA.80, IA.82, IA.84, IA.87, IA.91, IA.103, IA.115, IA.118, IA.121, IA.133.

Ejemplo 9- Compuesto IA.38

***S*-[2-Oxo-2-(4-trifluorometilfenil)etil] 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carbotioato**



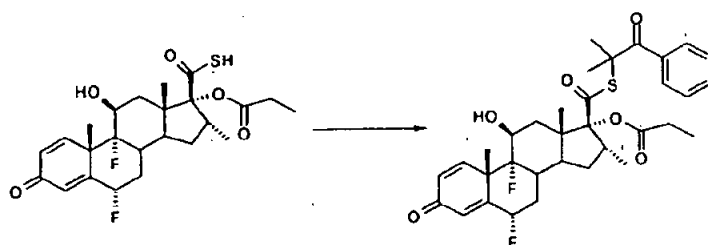
Una mezcla de 2-bromo-1-(4-trifluorometilfenil)etan-1-ona (0.569g, 2.13mmol), ácido 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carbotioico (1.0g, 2.13mmol) y carbonato de potasio anhidro (0.295g, 2.13mmol) en acetona (25ml) se agitó bajo una cubierta de nitrógeno entre 25 a 30°C durante 3 horas. La mezcla de reacción se vertió entonces en agua y se extrajo con acetato de etilo. La capa orgánica se lavó con agua, se secó y se concentró *in vacuo*. El residuo se purificó por cromatografía de columna (40% acetato de etilo en hexano) para producir el compuesto del título como un sólido blanco. Los siguientes compuestos se prepararon en una manera similar a ejemplo 9

usando un ácido tioico apropiado de fórmula II y compuesto de fórmula III-A:

IA.3, IA.6, IA.11, IA.13, IA.14, IA.20, IA.22, IA.26, IA.27, IA.31, IA.34, IA.35, IA.39, IA.40, IA.43, IA.45, IA.47, IA.49, IA.51, IA.53, IA.55, IA.56, IA.58, IA.59, IA.61, IA.63, IA.68 a IA.70, IA.73, IA.75, IA.78, IA.79, IA.81, IA.83, IA.85, IA.86, IA.88 a IA.90, IA.92 a IA.102, IA.104 a IA.108, IA.110 a IA.114, IA.116, IA.117, IA.119, IA.120, IA.122 a IA.124, IA.126 a IA.132, IA.134 a IA.186, IA.198.

Ejemplo 10 – Compuesto IA.59

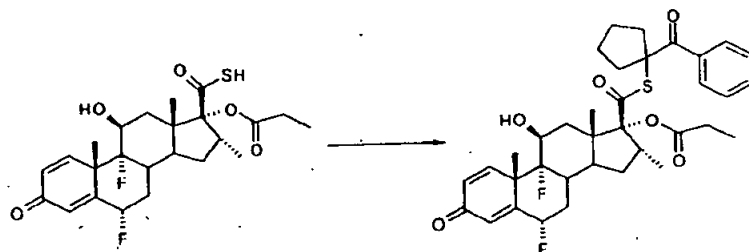
S-[1,1-Dimetil-2-oxo-2-feniletíl] 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carbotioato



2-Bromo-2-metil-1-fenil-propan-1-ona (0.483g, 2.13mmol) se agregó a una mezcla agitada de ácido 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-11 β -carbotioico (1.0g, 2.13mmol) y carbonato de potasio anhidro (0.295g, 2.13mmol) en acetona (20ml) y la mezcla se agitó bajo una cubierta de nitrógeno entre 25 a 30°C durante 3 horas. La mezcla de reacción se virtió entonces en agua y se extrajo con acetato de etilo. La capa orgánica se lavó con agua, se secó y se concentró *in vacuo*. El residuo se purificó por cromatografía de columna (40% acetato de etilo en hexano) para producir el compuesto del título como un sólido blanco.

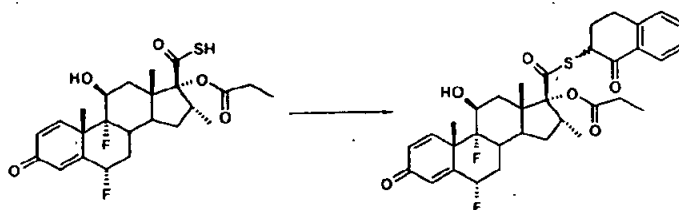
Los siguientes compuestos se prepararon en una manera similar a ejemplo 10 usando un ácido tioico apropiado de fórmula II y compuesto de fórmula III-A:

IA.109, IA.187 a IA.197.

Ejemplo 11- Compuesto IA-1.2**S-(1-Benzoilciclopentil) 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carbotioato**

(1-Bromociclopentil) fenil metanona (0.539g, 2.13mmol) se agregó a una mezcla agitada de ácido 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carbotioico (1.0g, 2.13mmol) y carbonato de potasio anhidro (0.295g, 2.13mmol) en acetona (25ml), y la mezcla se agitó bajo una cubierta de nitrógeno entre 25 a 30°C durante 3 horas. La mezcla de reacción se vertió entonces en agua y se extrajo con acetato de etilo. La capa orgánica se lavó con agua, se secó y se concentró *in vacuo*. El residuo se purificó en cromatografía de columna (35% acetato de etilo en hexano) para producir el compuesto del título como un sólido blanco.

El compuesto IA-1.1 se preparó en una manera similar a ejemplo 11.

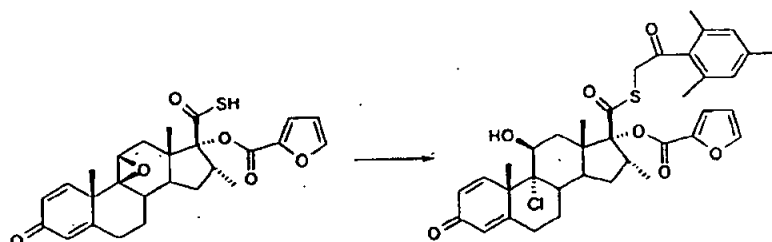
Ejemplo 12- Compuesto IA-2.1**S-(1-Oxo-1,2,3,4-tetrahidronaftalen-2-il) 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-17 α -propioniloxi-3-oxoandrosta-1,4-dien-17 β -carbotioato**

2-Bromo-1-tetralona (0.395g, 1.75mmol) se agregó a una mezcla agitada de ácido 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carbotioico (0.500g, 1.06mmol) y carbonato de potasio anhidro (0.161g, 1.17mmol) en acetona (10ml) y la

mezcla se agitó bajo una cubierta de nitrógeno entre 25 a 30°C durante 3 horas. La mezcla de reacción se vertió entonces en agua y se extrajo con acetato de etilo. La capa orgánica se lavó con agua, se secó y se concentró *in vacuo*. El residuo se purificó por cromatografía de columna (40% acetato de etilo en hexano) para producir el compuesto del título como un sólido blanco.

Ejemplo 13- Compuesto IA.41

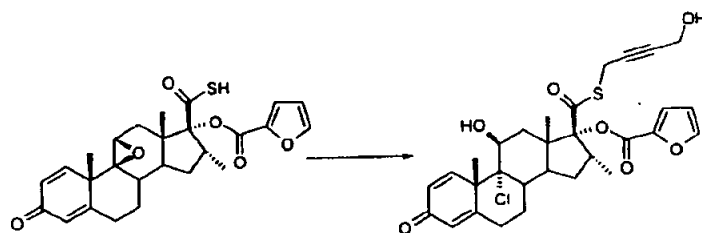
***S*-[2-Oxo-2-(2,4,6-Trimetilfenil)etil] 9 α -cloro-17 α -[(2-furanilcarbonil)oxi]-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotioato**



2-Bromo-1-(2,4,6-trimetilfenil)etanona (0.287g, 1.13mmol) se agregó a una mezcla agitada de ácido 9,11-epoxi-17 α -[(2-furanilcarbonil)oxi]-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotioico (0.600g, 1.28mmol) y carbonato de potasio anhidro (0.194g, 1.40mmol) en acetona (25ml) y la mezcla se agitó bajo una cubierta de nitrógeno entre 25 a 30°C durante 2.5 horas. La mezcla de reacción se vertió entonces en agua y se extrajo con acetato de etilo. La capa orgánica se lavó con agua, se secó y se concentró *in vacuo*. El sólido crudo se disolvió en ácido acético glacial (10ml) y se agregó ácido clorhídrico concentrado (1ml) a 10-15°C. La mezcla se agitó a 15-20°C durante 30 minutos, se vertió en agua helada (400ml), el producto se filtró, se lavó con agua y, finalmente, se secó en un horno de aire. El sólido crudo se purificó por cromatografía de columna (35% acetato de etilo en hexano) para producir el compuesto del título como un sólido blanco.

Ejemplo 14 - Compuesto IB.45

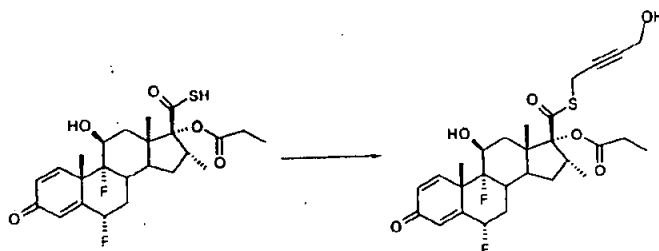
5-[4-Hidroxi-but-2-inil] 9 α -cloro-17 α -[(2-furanilcarbonil)oxi]-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotioato



Éster de ácido 4-(tetrahidropiran-2-iloxi)-but-2-inil tolueno-4-sulfónico (0.727g, 2.24mmol) se agregó a una mezcla agitada de ácido 9,11-epoxi-17 α -[(2-furanilcarbonil)oxi]-17 α -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotioico (1.0g, 2.13 mmol) y carbonato de potasio anhidro (0.300g, 2.34mmol) en acetona (20ml) y la mezcla se agitó bajo una cubierta de nitrógeno entre 25 a 30°C durante 4 horas. La mezcla de reacción se virtió entonces en agua y se extrajo con acetato de etilo. La capa orgánica se lavó con agua, se secó y se concentró *in vacuo*. El sólido crudo se disolvió en metanol (15ml) y se agregó ácido clorhídrico concentrado (4ml) a 10-15°C. La mezcla se agitó entre 25-30°C durante 30 minutos y luego se calentó a 60°C durante 4 horas. La mezcla se enfrió entonces y se virtió en agua helada. El sólido se filtró, se lavó con agua y se secó. El sólido crudo se purificó por cromatografía de columna (3% metanol en diclorometano) para producir el compuesto del título como un sólido blanco.

Ejemplo 15 - Compuesto IB.2

S-(4-Hidroxi-but-2-inil) 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carbotioato



4-Cloro-but-2-in-1-ol (0.169g, 1.62mmol) se agregó a una mezcla agitada de ácido 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carbotioico (0.800g, 1.54 mmol) y carbonato de potasio anhidro (0.234g, 1.70 mmol) en acetona (20ml) y la

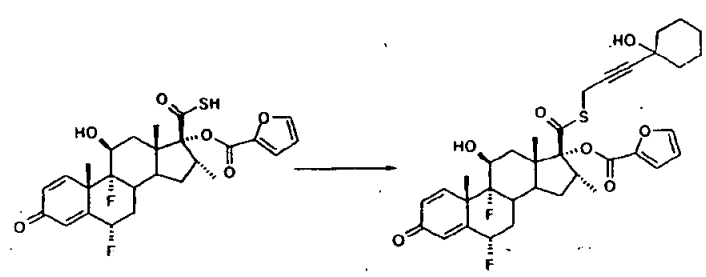
mezcla se agitó bajo una cubierta de nitrógeno entre 25 a 30°C durante 3 horas. La mezcla de reacción se virtió entonces en agua y se extrajo con acetato de etilo. La capa orgánica se lavó con agua, se secó y se concentró *in vacuo*. El residuo se purificó por cromatografía de columna (3% metanol en diclorometano) para producir el compuesto del título como un sólido blanco.

Los siguientes compuestos se prepararon en una manera similar a ejemplo 15 usando un ácido tioico apropiado de fórmula II y compuesto de fórmula III-B:

IB.1, IB.4, IB.5, IB.7 a IB.11, IB.20 a IB.24, IB.26 a IB.29, IB.38, IB.39, IB.61, IB.62, IB.132.

Ejemplo 16 - Compuesto IB.25

S-[3-(1-Hidroxiciclohexil)prop-2-inil] 6 α ,9 α -difluoro-17 α -[(2-furanilcarbonil)oxi]-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotioato

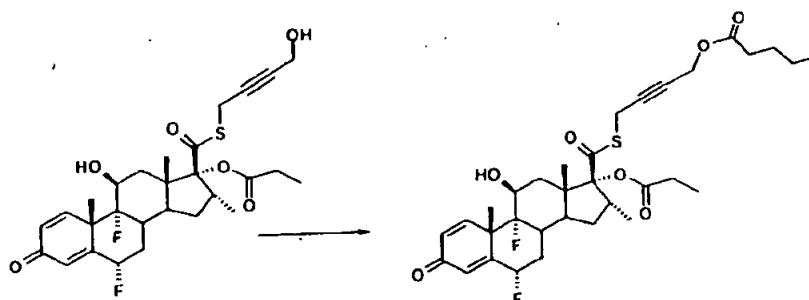


4-Metil-[3-(hidroxiciclohexil)prop-2-inil]bencenosulfonato (0.222g, 0.72mmol) se agregó a una mezcla agitada de ácido 6 α ,9 α -difluoro-17 α -[(2-furanilcarbonil)oxi]-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dieno 17 β -carbotioico (0.350g, 0.688mmol) y carbonato de potasio anhidro (0.104g, 0.756mmol) en acetona (20ml) y la mezcla se agitó bajo una cubierta de nitrógeno a 25 a 30°C durante 3 horas. La mezcla de reacción se virtió entonces en agua y se extrajo con acetato de etilo. La capa orgánica se lavó con agua, se secó y se concentró *in vacuo*. El residuo se purificó por cromatografía de columna (35% acetato de etilo en hexano) para producir el compuesto del título como un sólido blanco.

Compuesto IB.40 se preparó en una manera similar a ejemplo 16.

Ejemplo 17 - Compuesto IB.35

***S*-[4-*n*-Butilcarboniloxi-but-2-inil] 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carbotioato**



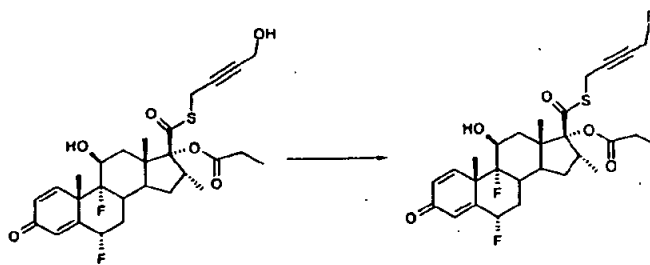
Cloruro de valerilo (0.337g, 2.79mmol) se agregó entre 10-15°C a una mezcla agitada de *S*-(4-hidroxi-but-2-inil)6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propionil-oxiandrosta-1,4-dien-17 β -carbotioato (0.5g, 0.93mmol) y trietilamina (0.282g, 2.79mmol) en acetona (20ml) y la mezcla se agitó bajo una cubierta de nitrógeno entre 25-30°C durante 8 horas. La mezcla de reacción se virtió entonces en agua y se extrajo con acetato de etilo. La capa orgánica se lavó con agua, se secó y se concentró *in vacuo*. El residuo se purificó por cromatografía de columna (35% acetato de etilo en hexano) para producir el compuesto del título como un sólido blanco.

Los siguientes compuestos se prepararon de una manera similar a ejemplo 17:

IB.31 a IB.37, IB.48 a IB.53, IB.55 a IB.60, IB.67 a IB.73, IB.75 a IB.86, IB.88, IB.92, IB.102, IB.104 a IB.122, IB.124, IB.133, IB.135, IB.148, IB.155, IB.157.

Ejemplo 18 - Compuesto IB.3

***S*-(4-Fluorobut-2-inil) 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propionil-oxiandrosta-1,4-dien-17 β -carbotioato**

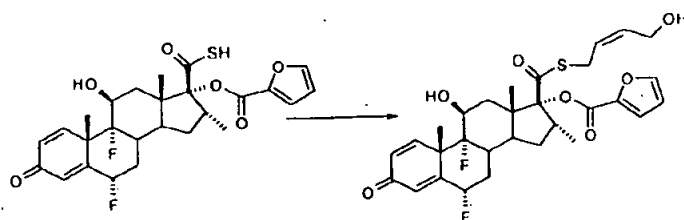


Trifluoruro de dietilaminoazufre (DAST) (0.151g, 0.93mmol) se agregó a una solución agitada de S-(4-hidroxi-but-2-enil) 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carbotioato (0.450g, 0.783mmol) en diclorometano seco (20ml) entre 25-30°C y la mezcla se agitó bajo una cubierta de nitrógeno entre 25-30°C durante 2 horas. La mezcla de reacción se lavó con solución de bicarbonato de sodio (25ml), agua, se secó y se concentró *in vacuo*. El residuo se purificó por cromatografía de columna (40% acetato de etilo en hexano) para producir el compuesto del título como un sólido blanco.

El compuesto IB.6 se preparó en una manera similar a ejemplo 18.

Ejemplo 19 - Compuesto IB.15

S-(4-Hidroxi-Z)-but-2-enil) 6 α ,9 α -difluoro-17 α -[(2-furanilcarbonil)oxi]-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotioato



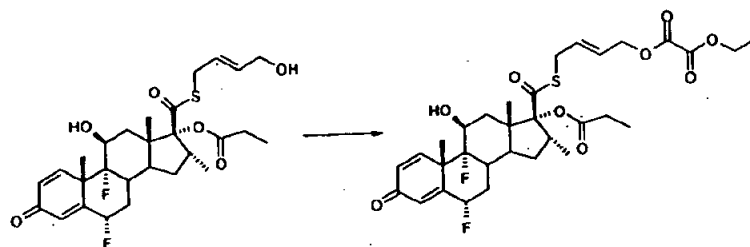
(Z)-4-Cloro-but-2-en-1-ol (0.691g, 6.48mmol) se agregó a una mezcla agitada de ácido 6 α ,9 α - difluoro-17 α -[(2-furanilcarbonil)oxi]-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotioico (3.0g, 5.87mmol) y carbonato de potasio anhidro (0.895g, 6.48 mmol) en acetona (60ml) y la mezcla se agitó bajo una cubierta de nitrógeno entre 25 a 30°C durante 3 horas. La mezcla de reacción se virtió entonces en agua y se extrajo con acetato de etilo. La capa orgánica se lavó con agua, se secó y se concentró

in vacuo. El residuo se purificó por cromatografía de columna (1% metanol en diclorometano) para producir el compuesto del título como un sólido blanco.

Los compuestos IB.16, IB.30 se prepararon en una manera similar a ejemplo 19. Los compuestos IB.13, IB.14, IB.17 se prepararon en una manera similar usando (*E*)-4-bromo-but-2-en-1-ol y un ácido tioico apropiado de fórmula II.

Ejemplo 20 - Compuesto IB.44

S-[4-(2-Etoxi-1,2-dioxoetil)oxi-(*E*)-but-2-enil] 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carbotioato

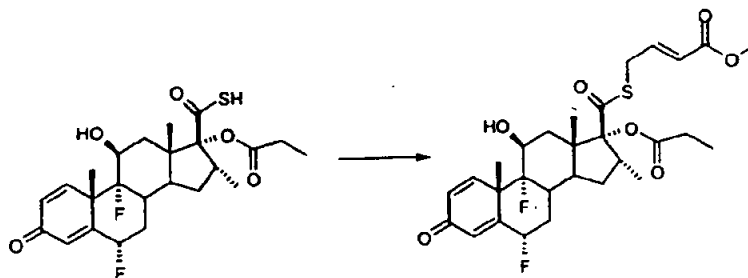


Cloruro de etil oxalilo (0.352g, 2.58mmol) se agregó entre 10-15°C a una mezcla agitada de *S*-(4- hidroxi-(*E*)-but-2-enil)-6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carbotioato (0.7g, 1.29mmol) y trietilamina (0.260g, 2.58mmol) en acetona (20ml) y la mezcla se agitó bajo una cubierta de nitrógeno entre 25-30°C durante 8 horas. La mezcla de reacción se virtió entonces en agua y se extrajo con acetato de etilo. La capa orgánica se lavó con agua, se secó y se concentró *in vacuo*. El residuo se purificó por cromatografía de columna (35% acetato de etilo en hexano) para producir el compuesto del título como un sólido blanco.

El compuesto IB.46 se preparó en una manera similar a ejemplo 20. Los compuestos IB.47 y IB.54 se prepararon de IB.15 y IB.4 respectivamente, en una manera similar a ejemplo 20.

Ejemplo 21- Compuesto IB.42

4-Metoxi-4-oxo-(E)-but-2-enil 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α - propioniloxiandrosta-1,4 dien-17 β -carbotioato

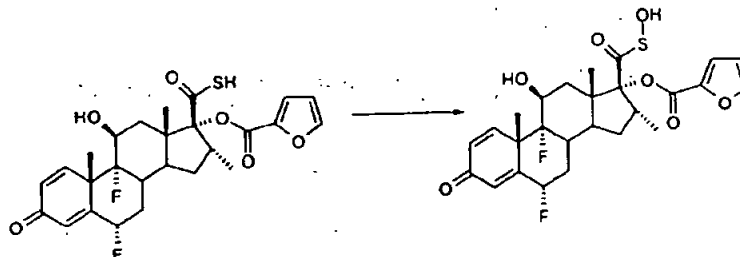


Metil 4-bromocrotonato (0.191g, 1.06mmol) se agregó entre 25-30°C a una mezcla agitada de ácido 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carbotioico (0.5g, 1.06mmol) y carbonato de potasio anhidro (0.146g, 1.06mmol) en *N,N*-dimetilformamida (10ml) y la mezcla se agitó bajo una cubierta de nitrógeno entre 25-30°C durante 1.5 horas. La mezcla de reacción se virtió entonces en agua y se extrajo con acetato de etilo. La capa orgánica se lavó con agua, se secó y se concentró *in vacuo*. El residuo se purificó por cromatografía de columna (40% acetato de etilo en hexano) para producir el compuesto del título como un sólido blanco.

Compuestos IB.41 y IB.43 se prepararon en una manera similar a ejemplo 21.

Ejemplo 22

Ácido 6 α ,9 α -difluoro-17 α -[(2-furanilcarbonyl)oxil]11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbonilsulfénico

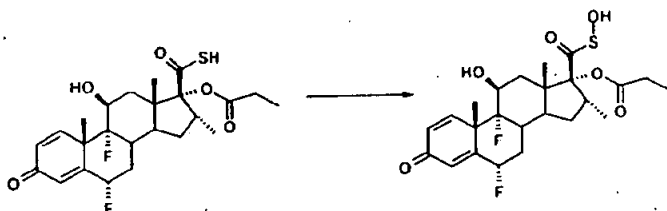


Una solución de peróxido de hidrógeno - urea (2.41g, 0.0256mol) en *N,N*-dimetilformamida se agregó entre 10 a 15°C a una solución clara de ácido 6 α ,9 α -difluoro-17 α -[(2-furanilcarbonil)oxi]-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotioico (13.0g, 0.0256mol) en *N,N*-dimetilformamida (40ml). La mezcla de reacción se agitó a 10-15°C durante 30 minutos, luego se vertió en agua helada. El sólido se filtró, se lavó con agua y se secó entre 50-60°C para producir el compuesto del título como sólido blanco (12.0g, 89.48%).

¹H NMR (400 MHz en CDCl₃+DMSO-d₆), δ : 1.06(d, J =7.09Hz, 3H), 1.19(s, 3H), 1.33-1.38(m, 1H), 1.55(s, 3H), 1.58-1.98(m, 4H), 2.26-2.52(m, 4H), 3.02-3.06(m, 1H), 4.32(br-d, J =8.76Hz, 1H), 5.14-5.19(br-s, 1H), 5.38-5.54(m, 1H), 6.29(s, 1H), 6.30(d, J =8.71Hz, 1H), 6.54(dd, J_1 =3.32Hz, J_2 =1.53Hz, 1H), 7.08(d, J =3.37Hz, 1H), 7.27(d, J =10.30Hz, 1H), 7.67(s, 1H).

Ejemplo 23

Ácido 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carbonilsulfénico



Peróxido de hidrógeno (30vol, 60ml) se agregó a una suspensión de ácido 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carbotioico (20.0g, 42.68mmol) en metanol (120ml) entre 10 a 15°C. La mezcla de reacción se agitó a temperatura ambiente durante 1 hora. Se neutralizó el exceso de peróxido con 10% de solución de metabisulfito de sodio, el producto se filtró, se lavó con agua y se secó para producir el compuesto del título como sólido blanco (19.9g, 96.22%).

¹H NMR (400 MHz en CDCl₃+DMSO-d₆), δ : 0.98(d, J =7.10Hz, 3H), 1.08(t, J =7.55Hz, 3H), 1.12(s, 3H), 1.25-1.33(m, 1H), 1.53(s, 3H), 1.58-1.93(m, 4H), 2.12-2.47(m, 4H), 2.33(q, J =7.57Hz, 2H), 2.95-2.99(m, 1H),

4.24-4.27(br-d, 1H), 5.15(br-s, 1H), 5.36-5.53(m, 1H), 6.26(s, 1H), 6.27(dd, $J_1=10.21\text{Hz}$, $J_2=1.68\text{Hz}$, 1H), 7.24(d, $J=9.73\text{Hz}$, 1H).

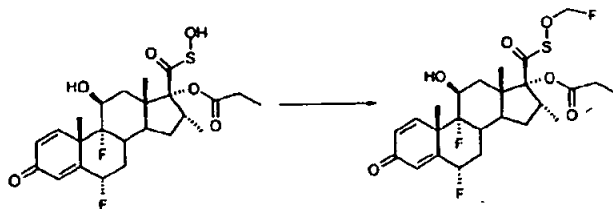
Los siguientes ácidos 17 β -carbonilsulfénicos se prepararon por un método análogo a ejemplo 23:

Ácido 9 α -fluoro-17 α -[(2-furanilcarbonil)oxi]-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbonilsulfénico.

Ácido 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-17 α -penatanoiloxi-3-oxoandrosta-1,4-dien-17 β -carbonilsulfénico.

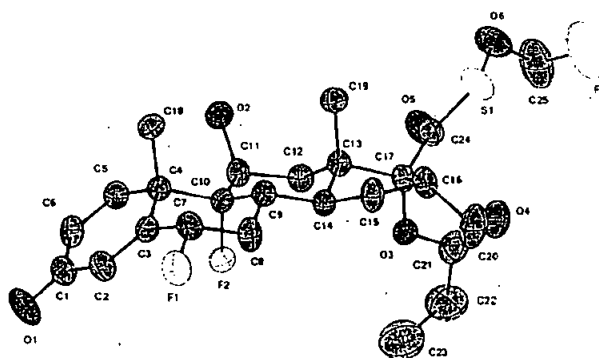
Ejemplo 24 - Compuesto IC.3

Éster fluorometílico de ácido 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-11 β -carbonilsulfénico



Bromofluorometano (1.5ml) se agregó a 0°C en una mezcla agitada de ácido 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-17 α -propioniloxi-3-oxoandrosta-1,4-dien-17 β -carbonilsulfénico (1.5g, 3.1mmol) y carbonato de potasio anhidro (0.427g, 3.1mmol) en acetona (50ml). La mezcla se agitó bajo una cubierta de nitrógeno entre 5 a 10°C durante 1 hora. La mezcla de reacción se vertió entonces en agua y se extrajo con acetato de etilo. La capa orgánica se lavó con agua, se secó y se concentró *in vacuo*. El residuo se purificó mediante HPLC preparativa para producir el compuesto del título como un sólido blanco.

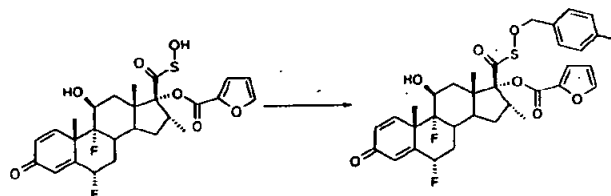
La estructura del compuesto IC.3 se confirmó mediante rayos X de cristal único como se muestra a continuación:



Los compuestos IC.4, IC.11 a IC.14 se prepararon en una manera similar a ejemplo 24 usando un ácido carbonilsulfénico apropiado de fórmula VI y compuesto de HI-C.

Ejemplo 25 - Compuesto IC.5

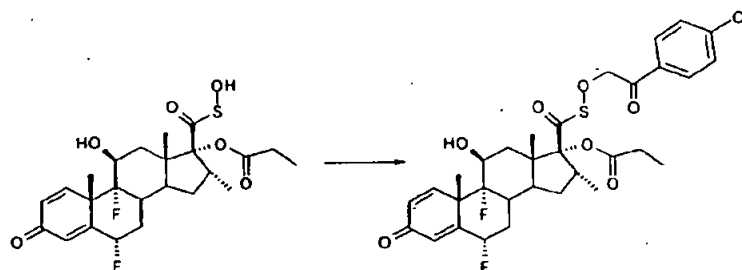
Éster (4-fluorofenil)metílico de ácido 6 α ,9 α -difluoro-17 α -[(2-furanilcarbonil)oxi]-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbonilsulfénico



Cloruro 4-fluorobencílico (0.277g, 1.91mmol) se agregó entre 25-30°C en una mezcla agitada de ácido 6 α ,9 α -difluoro-17 α -[(2-furanilcarbonil)oxi]-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbonilsulfénico (1.0g, 1.91mmol) y carbonato de potasio anhidro (0.344g, 2.49mmol) en *N,N*-dimetilformamida (15ml), y la mezcla se agitó bajo una cubierta de nitrógeno entre 25-30°C durante 2 horas. La mezcla de reacción se virtió entonces en agua y se extrajo con acetato de etilo. La capa orgánica se lavó con agua y se concentró *in vacuo*. El residuo se purificó por cristalización de acetona para producir el compuesto del título como un sólido blanco. Los compuestos IC.1, IC.2, IC.6 a IC.9, IC.15, IC.16, IC.18 a IC.23 se prepararon en una manera similar a ejemplo 25.

Ejemplo 26 - Compuesto IC.10

[2-(4-Clorofenil)-2-oxoetil]éster de ácido 6 α ,9 α -difluoro-17 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carbonilsulfénico

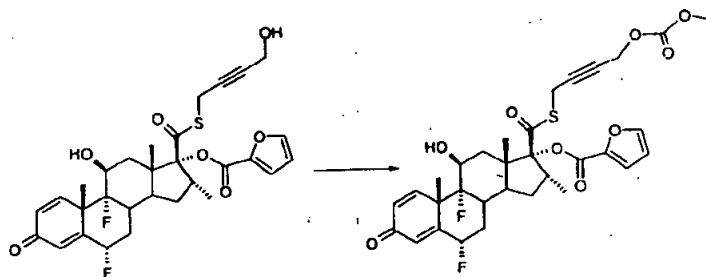


2-Bromo-1-(4-clorofenil)etanona (0.120g, 0.51mmol) se agregó entre 25-30°C a una mezcla agitada de ácido 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carbonilsulfénico (0.25g, 0.51mmol) y carbonato de potasio anhidro (0.070g, 0.51mmol) en acetona (20ml) y la mezcla se agitó bajo una cubierta de nitrógeno entre 25-30°C durante 2 horas. La mezcla de reacción se vertió entonces en agua y se extrajo con acetato de etilo. La capa orgánica se lavó con agua, se secó y se concentró *in vacuo*. El residuo se purificó por cromatografía de columna (35% acetato de etilo en hexano) para producir el compuesto del título como un sólido blanco.

Compuesto IC.17 se preparó en una manera similar a ejemplo 26.

Ejemplo 27 - Compuesto IB.63

S-(4-Metoxicarboniloxi-but-2-inil) 6 α ,9 α -difluoro-17 α -[(2-furanilcarbonil)-oxi]-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotioato

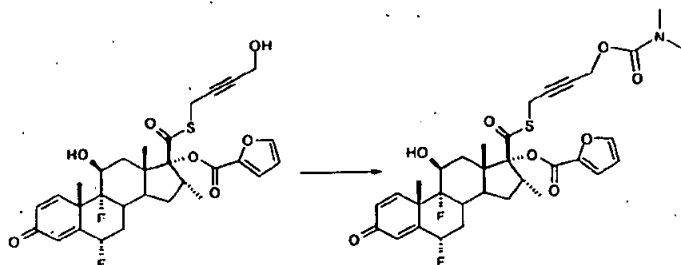


Metil cloroformiato (0.33g, 3.48mmol) se agregó entre 25-30°C a una mezcla agitada de *S*-[4-hidroxi-but-2-inil] 6 α ,9 α -difluoro-17 α -[(2-furanilcarbonil)oxi]-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotioato (1.0g, 1.74mmol) y trietilamina (0.70g, 6.96mmol) en diclorometano seco (30ml). La mezcla se agitó entre 25 a 30°C durante 6 horas, luego se lavó con agua y se concentró *in vacuo*. El residuo se purificó por cromatografía de columna (30% acetato de etilo en hexano) para producir el compuesto del título como un sólido blanco.

Los compuestos IB.12, IB.18, IB.19, IB.64 a IB.66, IB.89, IB.91, IB.123, IB.125 a IB.129, IB.131, IB.134, IB.137 a IB.147, IB.149, IB.150, IB.153, IB.154, IB 156 se prepararon en una manera similar a ejemplo 27.

Ejemplo 28 - Compuesto IB.103

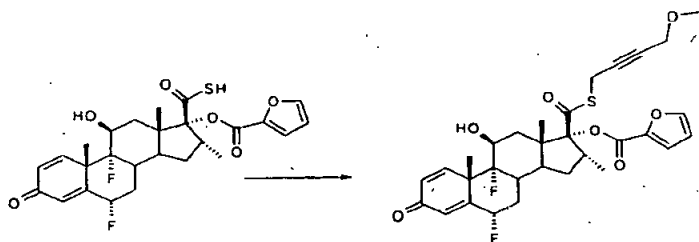
***S*-[4-(*N,N*-Dimetilaminocarboniloxi)-but-2-inil] 6 α ,9 α -difluoro-17 α -[(2-furanil-carbonil)oxi]-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotioato**



Cloruro de *N,N*-dimetilcarbamoilo (0.23g, 2.0mmol) se agregó entre 25-30°C a una mezcla agitada de *S*-(4-hidroxi-but-2-inil) 6 α ,9 α -difluoro-17 α -[(2-furanilcarbonil)oxi]-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotioato (1.0g, 1.74mmol) y trietilamina (0.70g, 6.96mmol) en diclorometano (30ml). La mezcla se agitó entre 25 a 30°C durante 4 horas, luego se lavó con agua y se concentró *in vacuo*. El residuo se purificó por cromatografía de columna (40% acetato de etilo en hexano) para producir el compuesto del título como un sólido blanco. Los compuestos IB.129 a IB.131 se prepararon en una manera similar a ejemplo 28.

Ejemplo 29 - Compuesto IB.158

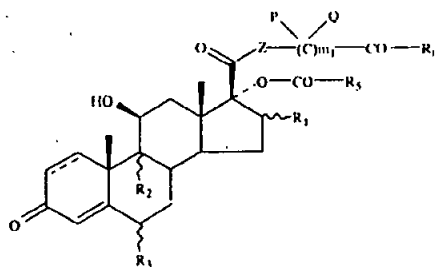
S-[4-Metoxibut-2-inil] 6 α ,9 α -difluoro-17 α -[(2-furanilcarbonil)oxil]-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotoiato.



1-Cloro-4-metoxibut-2-ino (0.086g, 0.72mmol) se agregó a una mezcla agitada de ácido 6 α ,9 α -difluoro-17 α -[(2-furanilcarbonil)oxil]-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-11 β -carbotoiico (0.350g, 0.688mmol) y carbonato de potasio anhidro (0.104g, 0.756mmol) en acetona (20ml). La mezcla se agitó bajo una cubierta de nitrógeno entre 25 a 30°C durante 3 horas, luego se virtió en agua y se extrajo con acetato de etilo. La capa orgánica se lavó con agua, se secó y se concentró *in vacuo*. El residuo se purificó por cromatografía de columna (35% acetato de etilo en hexano) para producir el compuesto del título como un sólido blanco.

Compuestos IB.159, IB.160 se prepararon en una manera similar a ejemplo 29.

Tabla 1- enumera los compuestos de fórmula I-A que se han sintetizado.



Fórmula I-A

Tabla-1

| No. | R ₁ | R ₂ | R ₃ | R ₄ | R ₅ | P | Q | m ₁ | Z | Nombre Químico |
|-------|---------------------------|----------------|----------------|-------------------|-----------------------------|---|---|----------------|---|---|
| IA.1 | H | H | H | Etoxi | 4-Cloro-fenilo | H | H | 1 | O | 2-(4-Clorofenil)-2-oxoetil 17 α -etoxicarboniloxi-11 β -hidroxi-3-oxoandrosta-1,4-dien-17 β -carboxilato |
| IA.2 | α -CH ₃ | F | F | Etilo | 4-Cloro-fenilo | H | H | 1 | O | 2-(4-Clorofenil)-2-oxoetil 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carboxilato |
| IA.3 | α -CH ₃ | F | F | Etilo | 4-Cloro-fenilo | H | H | 1 | S | S-[2-(4-Clorofenil)-2-oxoetil] 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carboxilato |
| IA.4 | H | H | H | Etoxi | 4-Fluoro-fenilo | H | H | 1 | O | 2-(4-Fluorofenil)-2-oxoetil 17 α -etoxicarboniloxi-11 β -hidroxi-3-oxoandrosta-1,4-dien-17 β -carboxilato |
| IA.5 | α -CH ₃ | F | F | Etilo | 4-Fluoro-fenilo | H | H | 1 | O | 2-(4-Fluorofenil)-2-oxoetil 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carboxilato |
| IA.6 | α -CH ₃ | F | F | Etilo | 4-Fluoro-fenilo | H | H | 1 | S | S-[2-(4-Fluorofenil)-2-oxoetil] 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carboxilato |
| IA.7 | H | H | H | Etoxi | 2,4-Difluoro-fenilo | H | H | 1 | O | 2-(2,4-Difluorofenil)-2-oxoetil 17 α -(etoxicarbonil)oxi-11 β -hidroxi-3-oxoandrosta-1,4-dien-17 β -carboxilato |
| IA.8 | H | H | H | Etoxi | 2,4-Dicloro-fenilo | H | H | 1 | O | 2-(2,4-Diclorofenil)-2-oxoetil 17 α -(etoxicarbonil)oxi-11 β -hidroxi-3-oxoandrosta-1,4-dien-17 β -carboxilato |
| IA.9 | α -CH ₃ | F | F | Etilo | 2,4-Difluoro-fenilo | H | H | 1 | O | 2-(2,4-Difluorofenil)-2-oxoetil 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carboxilato |
| IA.10 | α -CH ₃ | F | F | Etilo | 2,4-Dicloro-fenilo | H | H | 1 | O | 2-(2,4-Diclorofenil)-2-oxoetil 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carboxilato |
| IA.11 | α -CH ₃ | F | F | Etilo | 2,4-Difluoro-fenilo | H | H | 1 | S | S-[2-(2,4-Difluorofenil)-2-oxoetil] 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carboxilato |
| IA.12 | H | H | H | Etoxi | 3,4-Dicloro-fenilo | H | H | 1 | O | 2-(3,4-Diclorofenil)-2-oxoetil 17 α -etoxicarboniloxi-11 β -hidroxi-3-oxoandrosta-1,4-dien-17 β -carboxilato |
| IA.13 | α -CH ₃ | F | F | Etilo | 2,4-Dicloro-fenilo | H | H | 1 | S | S-[2-(2,4-Diclorofenil)-2-oxoetil] 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carboxilato |
| IA.14 | α -CH ₃ | F | F | Etilo | 3,4-Dicloro-fenilo | H | H | 1 | S | S-[2-(3,4-Diclorofenil)-2-oxoetil] 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carboxilato |
| IA.15 | α -CH ₃ | F | F | Etilo | 3,4-Dicloro-fenilo | H | H | 1 | O | 2-(3,4-Diclorofenil)-2-oxoetil 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carboxilato |
| IA.16 | H | H | H | Etoxi | 2-Tienilo | H | H | 1 | O | 2-Oxo-2-(tiofen-2-il)etil 17 α -(etoxicarbonil)oxi-11 β -hidroxi-3-oxoandrosta-1,4-dien-17 β -carboxilato |
| IA.17 | H | H | H | Etoxi | 5-Cloro-2-tienilo | H | H | 1 | O | 2-(5-Clorotiofen-2-il)-2-oxoetil 17 α -(etoxicarbonil)oxi-11 β -hidroxi-3-oxoandrosta-1,4-dien-17 β -carboxilato |
| IA.18 | α -CH ₃ | F | F | Etilo | 5-Cloro-2-tienilo | H | H | 1 | O | 2-(5-Clorotiofen-2-il)-2-oxoetil 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carboxilato |
| IA.19 | H | H | H | Etoxi | 5-Metil-2-furilo | H | H | 1 | O | 2-(5-Metilfuran-2-il)-2-oxoetil 17 α -(etoxicarbonil)oxi-11 β -hidroxi-3-oxoandrosta-1,4-dien-17 β -carboxilato |
| IA.20 | α -CH ₃ | F | F | Etilo | 5-Cloro-2-tienilo | H | H | 1 | S | S-[2-(5-Clorotiofen-2-il)-2-oxoetil] 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carboxilato |
| IA.21 | α -CH ₃ | F | F | Etilo | 5-Metil-2-furilo | H | H | 1 | O | 2-(5-Metilfuran-2-il)-2-oxoetil 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carboxilato |
| IA.22 | α -CH ₃ | F | F | Etilo | 5-Metil-2-furilo | H | H | 1 | S | S-[2-(5-Metilfuran-2-il)-2-oxoetil] 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carboxilato |
| IA.23 | H | H | H | Etoxi | 1-Butilo | H | H | 1 | O | 3,3-Dimetil-2-oxobutil 17 α -(etoxicarbonil) 11 β -hidroxi-3-oxoandrosta-1,4-dien-17 β -carboxilato |
| IA.24 | H | H | H | Etoxi | Metilo | H | H | 1 | O | 2-Oxopropil 17 α -(etoxicarbonil)oxi-11 β -hidroxi-3-oxoandrosta-1,4-dien-17 β -carboxilato |
| IA.25 | α -CH ₃ | F | F | Etilo | 1-Butilo | H | H | 1 | O | 3,3-Dimetil-2-oxobutil 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carboxilato |
| IA.26 | α -CH ₃ | F | F | Etilo | 1-Butilo | H | H | 1 | S | S-[3,3-Dimetil-2-oxobutil] 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carboxilato |
| IA.27 | α -CH ₃ | F | F | Etilo | Metilo | H | H | 1 | S | S-[2-Oxopropil] 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carboxilato |
| IA.28 | α -CH ₃ | F | F | Etilo | Metilo | H | H | 1 | O | 2-Oxopropil 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carboxilato |
| IA.29 | H | H | H | Etoxi | 4-Metoxi-fenilo | H | H | 1 | O | 2-(4-Metoxifenil)-2-oxoetil 17 α -(etoxicarbonil)oxi-11 β -hidroxi-3-oxoandrosta-1,4-dien-17 β -carboxilato |
| IA.30 | α -CH ₃ | F | F | Etilo | 4-Metoxi-fenilo | H | H | 1 | O | 2-(4-Metoxifenil)-2-oxoetil 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carboxilato |
| IA.31 | α -CH ₃ | F | F | Etilo | 4-Metoxi-fenilo | H | H | 1 | S | S-[2-(4-Metoxifenil)-2-oxoetil] 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carboxilato |
| IA.32 | H | H | H | Etoxi | 1-Adamantilo | H | H | 1 | O | 2-(Adamantan-1-il)-2-oxoetil 17 α -(etoxicarbonil)oxi-11 β -hidroxi-3-oxoandrosta-1,4-dien-17 β -carboxilato |
| IA.33 | α -CH ₃ | F | F | Etilo | 1-Adamantilo | H | H | 1 | O | 2-(Adamantan-1-il)-2-oxoetil 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carboxilato |
| IA.34 | α -CH ₃ | F | F | Etilo | 1-Adamantilo | H | H | 1 | S | S-[2-(Adamantan-1-il)-2-oxoetil] 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carboxilato |
| IA.35 | α -CH ₃ | F | F | Etilo | 4-Trifluoro metiloxifenilo | H | H | 1 | S | S-[2-Oxo-2-(4-trifluorometiloxifenil)etil] 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carboxilato |
| IA.36 | α -CH ₃ | F | F | Etilo | 4-Trifluoro metiloxi-fenilo | H | H | 1 | O | 2-Oxo-2-(4-trifluorometiloxifenil)etil 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carboxilato |
| IA.37 | H | H | H | Etoxi | 4-Trifluoro metiloxi-fenilo | H | H | 1 | O | 2-Oxo-2-(4-trifluorometiloxifenil)etil 17 α -(etoxicarbonil)oxi-11 β -hidroxi-3-oxoandrosta-1,4-dien-17 β -carboxilato |
| IA.38 | α -CH ₃ | F | F | Etilo | 4-Trifluoro metilfenilo | H | H | 1 | S | S-[2-Oxo-2-(4-trifluorometilfenil)etil] 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carboxilato |
| IA.39 | α -CH ₃ | F | F | 5-Cloro-2-tienilo | 4-Trifluoro metilfenilo | H | H | 1 | S | S-[2-Oxo-2-(4-trifluorometilfenil)etil] 17 α -[(5-cloro-2-tienil)carbonil]oxi-6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carboxilato |
| IA.40 | α -CH ₃ | F | F | 5-Cloro-2-tienilo | 2,4,6-Trimetil-fenilo | H | H | 1 | S | S-[2-Oxo-2-(2,4,6-trimetilfenil)etil] 17 α -[(5-cloro-2-tienil)carbonil]oxi-6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carboxilato |
| IA.41 | α -CH ₃ | Cl | H | 2-Furilo | 2,4,6-Trimetil-fenilo | H | H | 1 | S | S-[2-Oxo-2-(2,4,6-trimetilfenil)etil] 9 α -cloro-17 α -[(2-furanilcarbonil)oxi]-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carboxilato |

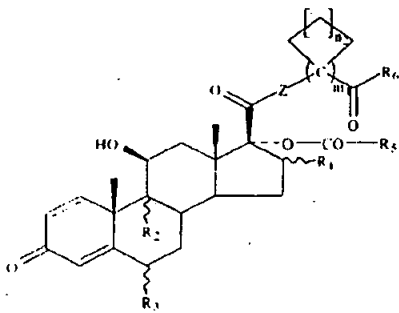
HOJA DE REEMPLAZO (REGLA 26)

HOJA DE REEMPLAZO (REGLA 26)

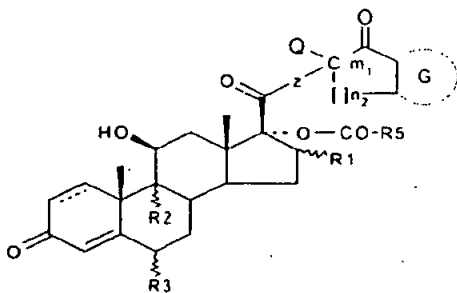
| No. | R ₁ | R ₂ | R ₃ | R ₄ | R ₅ | P | Q | m ₁ | Z | Nombre Químico |
|--------|-------------------|----------------|----------------|--------------------|--------------------------|---|---|----------------|---|--|
| IA.130 | CH ₃ | F | F | n-Butilo | 2,4-Difluoro-fenilo | H | H | 1 | S | hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoato. |
| IA.131 | α-CH ₃ | F | F | n-Butilo | 4-Fluoro-fenilo | H | H | 1 | S | S-[2-(2,4-Difluorofenil)-2-oxoetil] 17a-n-butylcarboniloxi-6a,9a-difluoro-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoato. |
| IA.132 | α-CH ₃ | F | F | Isopropilo | 4-Cloro-fenilo | H | H | 1 | S | S-[2-(4-Fluorofenil)-2-oxoetil] 17a-n-butylcarboniloxi-6a,9a-difluoro-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoato. |
| IA.133 | α-CH ₃ | F | F | Ciclo-butilo | 4-Fluoro-fenilo | H | H | 1 | O | S-[2-(4-Clorofenil)-2-oxoetil] 6a,9a-difluoro-11β-hidroxi-16a-metil-17a-(2-metilpropioniloxi)-3-oxoandrosta-1,4-dien-17β-carbotoato. |
| IA.134 | α-CH ₃ | F | F | Ciclo-pentilo | 4-Trifluoro-metilfenilo | H | H | 1 | S | S-[2-(4-Fluorofenil)-2-oxoetil] 17a-ciclobutylcarboniloxi-6a,9a-difluoro-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carboxilato. |
| IA.135 | α-CH ₃ | F | F | Ciclo-butilo | 4-Cloro-fenilo | H | H | 1 | S | S-[2-Oxo-2-(4-trifluorometilfenil)etil] 17a-ciclopentylcarboniloxi-6a,9a-difluoro-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoato. |
| IA.136 | α-CH ₃ | F | F | Ciclo-butilo | 4-Trifluoro-metilfenilo | H | H | 1 | S | S-[2-(4-Clorofenil)-2-oxoetil] 17a-ciclobutylcarboniloxi-6a,9a-difluoro-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoato. |
| IA.137 | α-CH ₃ | F | F | Ciclo-butilo | 2,4-Difluoro-fenilo | H | H | 1 | S | S-[2-Oxo-2-(4-trifluorometilfenil)etil] 17a-ciclobutylcarboniloxi-6a,9a-difluoro-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoato. |
| IA.138 | α-CH ₃ | F | F | Ciclo-butilo | 4-Metoxi-fenilo | H | H | 1 | S | S-[2-(4-Metoxifenil)-2-oxoetil] 17a-ciclobutylcarboniloxi-6a,9a-difluoro-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoato. |
| IA.139 | α-CH ₃ | F | H | 2-Furilo | 4-Trifluoro-metilfenilo | H | H | 1 | S | S-[2-(4-Clorofenil)-2-oxoetil] 17a-ciclobutylcarboniloxi-6a,9a-difluoro-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoato. |
| IA.140 | α-CH ₃ | F | H | 2-Furilo | 2,4-Difluoro-fenilo | H | H | 1 | S | S-[2-Oxo-2-(4-trifluorometilfenil)etil]-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoato. |
| IA.141 | α-CH ₃ | F | H | 2-Furilo | 4-Cloro-fenilo | H | H | 1 | S | S-[2-(2,4-Difluorofenil)-2-oxoetil] 9a-fluoro-17a-[(2-furanilcarbonil)oxi]-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoato. |
| IA.142 | α-CH ₃ | F | H | 2-Furilo | 4-Metoxi-fenilo | H | H | 1 | S | S-[2-(4-Clorofenil)-2-oxoetil] 9a-fluoro-17a-[(2-furanilcarbonil)oxi]-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoato. |
| IA.143 | α-CH ₃ | F | H | 2-Furilo | 4-Fluoro-fenilo | H | H | 1 | S | S-[2-(4-Metoxifenil)-2-oxoetil] 9a-fluoro-17a-[(2-furanilcarbonil)oxi]-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoato. |
| IA.144 | α-CH ₃ | F | F | Isopropilo | 2,4,6-Trimetil-fenilo | H | H | 1 | S | S-[2-(4-Fluorofenil)-2-oxoetil] 9a-fluoro-17a-[(2-furanilcarbonil)oxi]-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoato. |
| IA.145 | α-CH ₃ | F | F | Ciclo-hexilo | 2,4,6-Trimetil-fenilo | H | H | 1 | S | S-[2-Oxo-2-(2,4,6-trimetilfenil)etil] 6a,9a-difluoro-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoato. |
| IA.146 | α-CH ₃ | F | F | Ciclo-pentilo | 2,4,6-Trimetil-fenilo | H | H | 1 | S | S-[2-Oxo-2-(2,4,6-trimetilfenil)etil] 17a-ciclohexilcarboniloxi-6a,9a-difluoro-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoato. |
| IA.147 | α-CH ₃ | F | F | Ciclo-butilo | 2,4,6-Trimetil-fenilo | H | H | 1 | S | S-[2-Oxo-2-(2,4,6-trimetilfenil)etil] 17a-ciclopentylcarboniloxi-6a,9a-difluoro-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoato. |
| IA.148 | α-CH ₃ | F | F | Ciclo-hexil-metilo | 2,4,6-Trimetil-fenilo | H | H | 1 | S | S-[2-Oxo-2-(2,4,6-trimetilfenil)etil] 17a-ciclobutylcarboniloxi-6a,9a-difluoro-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoato. |
| IA.149 | α-CH ₃ | F | F | 2-Tienilo | 2,4,6-Trimetil-fenilo | H | H | 1 | S | S-[2-Oxo-2-(2,4,6-trimetilfenil)etil] 17a-ciclohexilmetilcarboniloxi-6a,9a-difluoro-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoato. |
| IA.150 | α-CH ₃ | F | F | Ciclo-hexil-metilo | 2,4-Difluoro-fenilo | H | H | 1 | S | S-[2-Oxo-2-(2,4,6-trimetilfenil)etil] 6a,9a-difluoro-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoato. |
| IA.151 | α-CH ₃ | F | F | Ciclo-hexil-metilo | 4-Cloro-fenilo | H | H | 1 | S | S-[2-(2,4-Difluorofenil)-2-oxoetil] 17a-ciclohexilmetilcarboniloxi-6a,9a-difluoro-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoato. |
| IA.152 | α-CH ₃ | F | F | Ciclo-hexil-metilo | 4-Trifluoro-metil-fenilo | H | H | 1 | S | S-[2-(4-Clorofenil)-2-oxoetil] 17a-ciclohexilmetilcarboniloxi-6a,9a-difluoro-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoato. |
| IA.153 | α-CH ₃ | F | F | Ciclo-hexil-metilo | 4-metoxi-fenilo | H | H | 1 | S | S-[2-Oxo-2-(4-trifluorometilfenil)etil] 17a-ciclohexilmetilcarboniloxi-6a,9a-difluoro-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoato. |
| IA.154 | α-CH ₃ | F | F | n-Butilo | 2,4,6-Trimetil-fenilo | H | H | 1 | S | S-[2-(4-Metoxifenil)-2-oxoetil] 17a-ciclohexilmetilcarboniloxi-6a,9a-difluoro-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoato. |
| IA.155 | α-CH ₃ | F | F | Etoxi | 2,4,6-Trimetil-fenilo | H | H | 1 | S | S-[2-Oxo-2-(2,4,6-trimetilfenil)etil] 17a-n-butylcarboniloxi-6a,9a-difluoro-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoato. |
| IA.156 | α-CH ₃ | F | F | 2-Furilo | 2,4,6-Trimetil-fenilo | H | H | 1 | S | S-[2-Oxo-2-(2,4,6-trimetilfenil)etil] 6a,9a-difluoro-17a-[(2-furanilcarbonil)oxi]-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoato. |
| IA.157 | α-CH ₃ | F | F | 2-Furilo | 4-Cloro-fenilo | H | H | 1 | S | S-[2-Oxo-2-(2,4,6-trimetilfenil)etil] 6a,9a-difluoro-17a-[(2-furanilcarbonil)oxi]-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoato. |
| IA.158 | β-CH ₃ | F | F | Etilo | 4-Cloro-fenilo | H | H | 1 | S | S-[2-(4-Fluorofenil)-2-oxoetil] 6a,9a-difluoro-11β-hidroxi-16a-metil-3-oxo-17a-propioniloxiandrosta-1,4-dien-17β-carbotoato. |
| IA.159 | α-CH ₃ | F | F | 2-Tienilo | 4-Trifluoro-metilfenilo | H | H | 1 | S | S-[2-(4-Clorofenil)-2-oxoetil] 6a,9a-difluoro-11β-hidroxi-16a-metil-3-oxo-17a-propioniloxiandrosta-1,4-dien-17β-carbotoato. |
| IA.160 | α-CH ₃ | F | F | Etilo | 3-Nitrofenilo | H | H | 1 | S | S-[2-Oxo-2-(4-trifluorometilfenil)etil] 6a,9a-difluoro-17a-[(2-tienilcarbonil)oxi]-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoato. |
| IA.161 | α-CH ₃ | F | F | Etilo | 3,4-Dimetil-fenilo | H | H | 1 | S | S-[2-(3-Nitrofenil)-2-oxoetil] 6a,9a-difluoro-11β-hidroxi-16a-metil-3-oxo-17a-propioniloxiandrosta-1,4-dien-17β-carbotoato. |
| IA.162 | β-CH ₃ | F | F | Etilo | 4-Trifluoro-metilfenilo | H | H | 1 | S | S-[2-(3,4-Dimetilfenil)-2-oxoetil] 6a,9a-difluoro-11β-hidroxi-16a-metil-3-oxo-17a-propioniloxiandrosta-1,4-dien-17β-carbotoato. |
| IA.163 | α-CH ₃ | F | F | n-Propilo | 4-Trifluoro-metilfenilo | H | H | 1 | S | S-[2-Oxo-2-(4-trifluorometilfenil)etil] 6a,9a-difluoro-11β-hidroxi-16a-metil-3-oxo-17a-n-propylcarboniloxiandrosta-1,4-dien-17β-carbotoato. |
| IA.164 | α-CH ₃ | F | F | n-Propilo | 4-Cloro-fenilo | H | H | 1 | S | S-[2-(4-Clorofenil)-2-oxoetil] 6a,9a-difluoro-11β-hidroxi-16a-metil-3-oxo-17a-n-propylcarboniloxiandrosta-1,4-dien-17β-carbotoato. |
| IA.165 | α-CH ₃ | F | F | n-Propilo | 2,4-Difluoro-fenilo | H | H | 1 | S | S-[2-(4-Clorofenil)-2-oxoetil] 6a,9a-difluoro-11β-hidroxi-16a-metil-3-oxo-17a-n-propylcarboniloxiandrosta-1,4-dien-17β-carbotoato. |
| IA.166 | α-CH ₃ | F | F | n-Propilo | 4-Fluoro-fenilo | H | H | 1 | S | S-[2-(4-Fluorofenil)-2-oxoetil] 6a,9a-difluoro-11β-hidroxi-16a-metil-3-oxo-17a-n-propylcarboniloxiandrosta-1,4-dien-17β-carbotoato. |
| IA.167 | α-CH ₃ | F | F | n-Propilo | 4-Metoxi-fenilo | H | H | 1 | S | S-[2-(4-Fluorofenil)-2-oxoetil] 6a,9a-difluoro-11β-hidroxi-16a-metil-3-oxo-17a-n-propylcarboniloxiandrosta-1,4-dien-17β-carbotoato. |
| IA.168 | α-CH ₃ | F | F | 2-Furilo | 3-Cloro-fenilo | H | H | 1 | S | S-[2-(4-Metoxifenil)-2-oxoetil] 6a,9a-difluoro-11β-hidroxi-16a-metil-3-oxo-17a-n-propylcarboniloxiandrosta-1,4-dien-17β-carbotoato. |
| IA.169 | β-CH ₃ | F | F | 2-Furilo | 4-Trifluoro-metilfenilo | H | H | 1 | S | S-[2-(3-Clorofenil)-2-oxoetil] 6a,9a-difluoro-17a-[(2-furanilcarbonil)oxi]-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoato. |

| No. | R ₁ | R ₂ | R ₃ | R ₄ | R ₅ | P | Q | m ₁ | Z | Nombre Químico |
|--------|---------------------------|----------------|----------------|-------------------|-------------------------|-----------------|-----------------|----------------|---|---|
| IA.170 | <i>α</i> -CH ₃ | F | F | 2-Furilo | 3,5-Dimetoxi-fenilo | H | H | I | S | S-[2-(3,5-Dimetoxifenil)-2-oxoetil] 6 <i>α</i> ,9 <i>α</i> -difluoro-17 <i>α</i> -[(2-furanilcarbonil)oxi]-11 <i>β</i> -hidroxi-16 <i>α</i> -metil-3-oxoandrosta-1,4-dien-17 <i>β</i> -carbotoiato. |
| IA.171 | <i>α</i> -CH ₃ | F | F | 2-Furilo | 4-Nitrofenilo | H | H | I | S | S-[2-(4-Nitrofenil)-2-oxoetil] 6 <i>α</i> ,9 <i>α</i> -difluoro-17 <i>α</i> -[(2-furanilcarbonil)oxi]-11 <i>β</i> -hidroxi-16 <i>α</i> -metil-3-oxoandrosta-1,4-dien-17 <i>β</i> -carbotoiato. |
| IA.172 | <i>α</i> -CH ₃ | F | F | Metoxi-metilo | 4-Trifluoro-metilfenilo | H | H | I | S | S-[2-Oxo-2-(4-trifluorometilfenil)etil] 6 <i>α</i> ,9 <i>α</i> -difluoro-11 <i>β</i> -hidroxi-17 <i>α</i> -(metoximetilcarbonil)oxi-16 <i>α</i> -metil-3-oxoandrosta-1,4-dien-17 <i>β</i> -carbotoiato. |
| IA.173 | <i>α</i> -CH ₃ | F | F | Metoxi-metilo | 2,4,6-Trimetil-fenilo | H | H | I | S | S-[2-Oxo-2-(2,4,6-trimetilfenil)etil] 6 <i>α</i> ,9 <i>α</i> -difluoro-11 <i>β</i> -hidroxi-17 <i>α</i> -(metoximetilcarbonil)oxi-16 <i>α</i> -metil-3-oxoandrosta-1,4-dien-17 <i>β</i> -carbotoiato. |
| IA.174 | <i>α</i> -CH ₃ | F | F | Etilo | 3-Cloro-4-fluorofenilo | H | H | I | S | S-[2-(3-Cloro-4-fluorofenil)-2-oxoetil] 6 <i>α</i> ,9 <i>α</i> -difluoro-11 <i>β</i> -hidroxi-16 <i>α</i> -metil-3-oxo-17 <i>α</i> -propioniloxiandrosta-1,4-dien-17 <i>β</i> -carbotoiato. |
| IA.175 | <i>β</i> -CH ₃ | F | F | 2-Furilo | 2,4,6-Trimetil-fenilo | H | H | I | S | S-[2-Oxo-2-(2,4,6-trimetilfenil)etil] 6 <i>α</i> ,9 <i>α</i> -difluoro-17 <i>α</i> -[(2-furanilcarbonil)oxi]-11 <i>β</i> -hidroxi-16 <i>β</i> -metil-3-oxoandrosta-1,4-dien-17 <i>β</i> -carbotoiato. |
| IA.176 | <i>α</i> -CH ₃ | F | F | Etoxi-metilo | 2,4,6-Trimetil-fenilo | H | H | I | S | S-[2-Oxo-2-(2,4,6-trimetilfenil)etil] 6 <i>α</i> ,9 <i>α</i> -difluoro-17 <i>α</i> -(etoximetilcarbonil)oxi-11 <i>β</i> -hidroxi-16 <i>α</i> -metil-3-oxoandrosta-1,4-dien-17 <i>β</i> -carbotoiato. |
| IA.177 | <i>α</i> -CH ₃ | F | F | Etoxi-metilo | 4-Trifluoro-metilfenilo | H | H | I | S | S-[2-Oxo-2-(4-trifluorometilfenil)etil] 6 <i>α</i> ,9 <i>α</i> -difluoro-17 <i>α</i> -(etoximetilcarbonil)oxi-11 <i>β</i> -hidroxi-16 <i>α</i> -metil-3-oxoandrosta-1,4-dien-17 <i>β</i> -carbotoiato. |
| IA.179 | <i>α</i> -CH ₃ | F | F | 2-Furilo | 2-Naftilo | H | H | I | S | S-[2-(Naftalen-2-il)-2-oxoetil] 6 <i>α</i> ,9 <i>α</i> -difluoro-17 <i>α</i> -[(2-furanilcarbonil)oxi]-11 <i>β</i> -hidroxi-16 <i>α</i> -metil-3-oxoandrosta-1,4-dien-17 <i>β</i> -carbotoiato. |
| IA.180 | <i>α</i> -CH ₃ | F | F | 2-Furilo | 1-Naftilo | H | H | I | S | S-[2-(Naftalen-1-il)-2-oxoetil] 6 <i>α</i> ,9 <i>α</i> -difluoro-17 <i>α</i> -[(2-furanilcarbonil)oxi]-11 <i>β</i> -hidroxi-16 <i>α</i> -metil-3-oxoandrosta-1,4-dien-17 <i>β</i> -carbotoiato. |
| IA.181 | <i>α</i> -CH ₃ | F | F | 3-Metil-2-furilo | 4-Trifluoro-metilfenilo | H | H | I | S | S-[2-Oxo-2-(4-trifluorometilfenil)etil] 6 <i>α</i> ,9 <i>α</i> -difluoro-11 <i>β</i> -hidroxi-17 <i>α</i> -[(3-metil-2-furanil)-carbonil]oxi-16 <i>α</i> -metil-3-oxoandrosta-1,4-dien-17 <i>β</i> -carbotoiato. |
| IA.182 | <i>α</i> -CH ₃ | F | F | 3-Metil-2-furilo | 2,4,6-Trimetil-fenilo | H | H | I | S | S-[2-Oxo-2-(2,4,6-trimetilfenil)etil] 6 <i>α</i> ,9 <i>α</i> -difluoro-11 <i>β</i> -hidroxi-17 <i>α</i> -[(3-metil-2-furanil)-carbonil]oxi-16 <i>α</i> -metil-3-oxoandrosta-1,4-dien-17 <i>β</i> -carbotoiato. |
| IA.183 | <i>α</i> -CH ₃ | F | F | 2-Furilo | 3-Nitro-4-metoxi-fenilo | H | H | I | S | S-[2-(3-Nitro-4-metoxifenil)-2-oxoetil] 6 <i>α</i> ,9 <i>α</i> -difluoro-17 <i>α</i> -[(2-furanilcarbonil)oxi]-11 <i>β</i> -hidroxi-16 <i>α</i> -metil-3-oxoandrosta-1,4-dien-17 <i>β</i> -carbotoiato. |
| IA.184 | <i>α</i> -CH ₃ | F | F | 2-Furilo | 3,4-Dimetil-fenilo | H | H | I | S | S-[2-(3,4-Dimetilfenil)-2-oxoetil] 6 <i>α</i> ,9 <i>α</i> -difluoro-17 <i>α</i> -[(2-furanilcarbonil)oxi]-11 <i>β</i> -hidroxi-16 <i>α</i> -metil-3-oxoandrosta-1,4-dien-17 <i>β</i> -carbotoiato. |
| IA.185 | <i>α</i> -CH ₃ | F | F | 3-Furilo | 4-Trifluoro-metilfenilo | H | H | I | S | S-[2-Oxo-2-(4-trifluorometilfenil)etil] 6 <i>α</i> ,9 <i>α</i> -difluoro-17 <i>α</i> -[(3-furanilcarbonil)oxi]-11 <i>β</i> -hidroxi-16 <i>α</i> -metil-3-oxoandrosta-1,4-dien-17 <i>β</i> -carbotoiato. |
| IA.186 | <i>α</i> -CH ₃ | F | F | 3-Furilo | 2,4,6-Trimetil-fenilo | H | H | I | S | S-[2-Oxo-2-(2,4,6-trimetilfenil)etil] 6 <i>α</i> ,9 <i>α</i> -difluoro-17 <i>α</i> -[(3-furanilcarbonil)oxi]-11 <i>β</i> -hidroxi-16 <i>α</i> -metil-3-oxoandrosta-1,4-dien-17 <i>β</i> -carbotoiato. |
| IA.187 | <i>α</i> -CH ₃ | F | F | Etilo | 4-Trifluoro-metilfenilo | CH ₃ | CH ₃ | I | S | S-[1,1-Dimetil-2-oxo-2-(4-trifluorometilfenil)-etil] 6 <i>α</i> ,9 <i>α</i> -difluoro-11 <i>β</i> -hidroxi-16 <i>α</i> -metil-3-oxo-17 <i>α</i> -propioniloxiandrosta-1,4-dien-17 <i>β</i> -carbotoiato. |
| IA.188 | <i>α</i> -CH ₃ | F | F | Etilo | 4-Fluoro-fenilo | CH ₃ | CH ₃ | I | S | S-[1,1-Dimetil-2-(4-fluorofenil)-2-oxoetil] 6 <i>α</i> ,9 <i>α</i> -difluoro-11 <i>β</i> -hidroxi-16 <i>α</i> -metil-3-oxo-17 <i>α</i> -propioniloxiandrosta-1,4-dien-17 <i>β</i> -carbotoiato. |
| IA.189 | <i>α</i> -CH ₃ | F | H | Etilo | Fenilo | CH ₃ | CH ₃ | I | S | S-[1,1-Dimetil-2-fenil-2-oxoetil] 9 <i>α</i> -fluoro-11 <i>β</i> -hidroxi-16 <i>α</i> -metil-3-oxo-17 <i>α</i> -propioniloxiandrosta-1,4-dien-17 <i>β</i> -carbotoiato. |
| IA.190 | <i>α</i> -CH ₃ | F | F | Ciclo-hexilo | Fenilo | CH ₃ | CH ₃ | I | S | S-[1,1-Dimetil-2-fenil-2-oxoetil] 17 <i>α</i> -ciclohexilcarboniloxi-6 <i>α</i> ,9 <i>α</i> -difluoro-11 <i>β</i> -hidroxi-16 <i>α</i> -metil-3-oxoandrosta-1,4-dien-17 <i>β</i> -carbotoiato. |
| IA.191 | <i>α</i> -CH ₃ | F | F | Ciclo-pentilo | Fenilo | CH ₃ | CH ₃ | I | S | S-[1,1-Dimetil-2-fenil-2-oxoetil] 17 <i>α</i> -ciclopentilcarboniloxi-6 <i>α</i> ,9 <i>α</i> -difluoro-11 <i>β</i> -hidroxi-16 <i>α</i> -metil-3-oxoandrosta-1,4-dien-17 <i>β</i> -carbotoiato. |
| IA.192 | <i>α</i> -CH ₃ | F | F | Isopropilo | Fenilo | CH ₃ | CH ₃ | I | S | S-[1,1-Dimetil-2-fenil-2-oxoetil] 6 <i>α</i> ,9 <i>α</i> -difluoro-11 <i>β</i> -hidroxi-16 <i>α</i> -metil-17 <i>α</i> -(2-propioniloxi)-3-oxoandrosta-1,4-dien-17 <i>β</i> -carbotoiato. |
| IA.193 | <i>α</i> -CH ₃ | F | F | Ciclo-butilo | Fenilo | CH ₃ | CH ₃ | I | S | S-[1,1-Dimetil-2-fenil-2-oxoetil] 17 <i>α</i> -ciclobutilcarboniloxi-6 <i>α</i> ,9 <i>α</i> -difluoro-11 <i>β</i> -hidroxi-16 <i>α</i> -metil-3-oxoandrosta-1,4-dien-17 <i>β</i> -carbotoiato. |
| IA.194 | <i>α</i> -CH ₃ | F | H | 2-Furilo | Fenilo | CH ₃ | CH ₃ | I | S | S-[1,1-Dimetil-2-fenil-2-oxoetil] 9 <i>α</i> -fluoro-17 <i>α</i> -[(2-furanilcarbonil)oxi]-11 <i>β</i> -hidroxi-16 <i>α</i> -metil-3-oxoandrosta-1,4-dien-17 <i>β</i> -carbotoiato. |
| IA.195 | <i>α</i> -CH ₃ | F | F | Ciclohe-xilmetilo | Fenilo | CH ₃ | CH ₃ | I | S | S-[1,1-Dimetil-2-fenil-2-oxoetil] 17 <i>α</i> -ciclohexilmetilcarboniloxi-6 <i>α</i> ,9 <i>α</i> -difluoro-11 <i>β</i> -hidroxi-16 <i>α</i> -metil-3-oxoandrosta-1,4-dien-17 <i>β</i> -carbotoiato. |
| IA.196 | <i>α</i> -CH ₃ | F | F | 2-Furilo | 4-Fluoro-fenilo | CH ₃ | CH ₃ | I | S | S-[1,1-Dimetil-2-(4-fluorofenil)-2-oxoetil] 6 <i>α</i> ,9 <i>α</i> -difluoro-17 <i>α</i> -[(2-furanilcarbonil)oxi]-11 <i>β</i> -hidroxi-16 <i>α</i> -metil-3-oxoandrosta-1,4-dien-17 <i>β</i> -carbotoiato. |
| IA.197 | <i>α</i> -CH ₃ | F | F | 2-Furilo | 4-Trifluoro-metilfenilo | CH ₃ | CH ₃ | I | S | S-[1,1-Dimetil-2-oxo-2-(4-trifluorometilfenil)etil] 6 <i>α</i> ,9 <i>α</i> -difluoro-17 <i>α</i> -[(2-furanilcarbonil)oxi]-11 <i>β</i> -hidroxi-16 <i>α</i> -metil-3-oxoandrosta-1,4-dien-17 <i>β</i> -carbotoiato. |
| IA.198 | <i>α</i> -CH ₃ | F | F | 5-Cloro-2-tienilo | 3,4-Dimetil-fenilo | H | H | I | S | S-[2-(3,4-Dimetilfenil)-2-oxoetil] 17 <i>α</i> -[(5-cloro-2-tienil)carbonil]oxi-6 <i>α</i> ,9 <i>α</i> -difluoro-11 <i>β</i> -hidroxi-16 <i>α</i> -metil-3-oxoandrosta-1,4-dien-17 <i>β</i> -carbotoiato. |

Tabla 2- Enumera los compuestos de fórmula I-A-1 y la Tabla-3 enumera los compuestos de fórmula I-A-2 que se han sintetizado



Fórmula I-A-1



Fórmula I-A-2

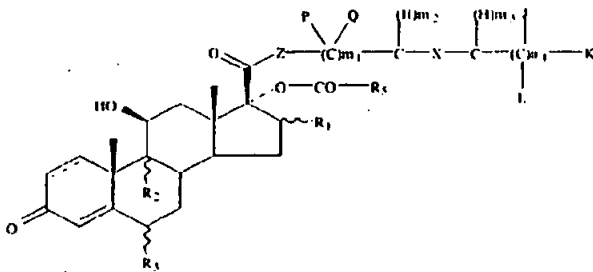
Tabla 2

| Serie No. | R ₁ | R ₂ | R ₃ | R ₅ | R ₆ | n ₂ | m ₁ | Z | Nombre Químico |
|-----------|---------------------------|----------------|----------------|----------------|----------------|----------------|----------------|---|--|
| IA.1.1 | α -CH ₃ | F | F | Etilo | 4-Fluorofenilo | 2 | 1 | | S-[1-(4-Fluorobenzil)ciclopentil] 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxi-androsta-1,4-dien-17 β -carbotoiato. |
| IA.1.2 | α -CH ₃ | F | F | Etilo | Fenilo | 2 | 1 | 5 | S-[1-Benzilciclopentil] 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carbotoiato. |

Tabla 3

| Serie No. | R ₁ | R ₂ | R ₃ | R ₅ | n ₂ | Q | G | m ₁ | Z | Nombre Químico |
|-----------|---------------------------|----------------|----------------|----------------|----------------|---|--------|----------------|---|---|
| IA.2.1 | α -CH ₃ | F | F | Etilo | 2 | H | Fenilo | 1 | S | S-(1-oxo-1,2,3,4-tetrahidronaftalen-2-il) 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carbotoiato. |

Tabla 4- Enumera los compuestos de fórmula I-B que se han sintetizado



Fórmula I-B

Tabla-4

| Serie No. | R ₁ | R ₂ | R ₃ | R ₅ | P | Q | J | K | Z | X | m ₁ | m ₂ | m ₃ | n ₁ | L | Nombre Químico |
|-----------|---------------------------|----------------|----------------|----------------|---|---|---|---|---|----------|----------------|----------------|----------------|----------------|----|--|
| IB.1 | α -CH ₃ | F | F | Etilo | H | H | H | H | O | $\equiv$ | 1 | 0 | 0 | 1 | OH | 4-Hidroxi-but-2-inil 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carboxilato. |
| IB.2 | α -CH ₃ | F | F | Etilo | H | H | H | H | S | $\equiv$ | 1 | 0 | 0 | 1 | OH | S-(4-Hidroxi-but-2-inil) 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carbotoiato. |
| IB.3 | α -CH ₃ | F | F | Etilo | H | H | H | H | S | $\equiv$ | 1 | 0 | 0 | 1 | F | S-(4-Fluoro-but-2-inil) 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carbotoiato. |
| IB.4 | α -CH ₃ | F | F | 2-Furilo | H | H | H | H | S | $\equiv$ | 1 | 0 | 0 | 1 | OH | S-(4-Hidroxi-but-2-inil) 6 α ,9 α -difluoro-17 α -(2-furanilcarbonyloxi)-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotoiato. |

| Serie No. | R ₁ | R ₂ | R ₃ | R ₄ | P | Q | J | K | Z | X | m ₁ | m ₂ | m ₃ | n ₁ | I. | Nombre Químico |
|-----------|---------------------------|----------------|----------------|--------------------|---|---|---------------------------------|----|---|-----------------|----------------|----------------|----------------|----------------|--|---|
| IB.5 | α -CH ₃ | F | H | Etilo | H | H | H | H | S | $\equiv$ | 1 | 0 | 0 | 1 | OH | S-(4-Hidroxi-but-2-inil) 9 α -fluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carbotoato. |
| IB.6 | α -CH ₃ | F | F | 2-Furilo | H | H | H | H | S | $\equiv$ | 1 | 0 | 0 | 1 | F | S-(4-Fluoro-but-2-inil) 6 α ,9 α -difluoro-17 α -[(2-furanilcarbonil)oxi]-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotoato. |
| IB.7 | α -CH ₃ | F | F | Iso-propilo | H | H | H | H | S | $\equiv$ | 1 | 0 | 0 | 1 | OH | S-(4-Hidroxi-but-2-inil) 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-17 α -(2-metil-propioniloxi)-3-oxoandrosta-1,4-dien-17 β -carbotoato. |
| IB.8 | α -CH ₃ | F | F | Ciclo-butilo | H | H | H | H | S | $\equiv$ | 1 | 0 | 0 | 1 | OH | S-(4-Hidroxi-but-2-inil) 17 α -ciclobutilcarboniloxi-6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotoato. |
| IB.9 | α -CH ₃ | F | H | 2-Furilo | H | H | H | H | S | $\equiv$ | 1 | 0 | 0 | 1 | OH | S-(4-Hidroxi-but-2-inil) 9 α -fluoro-17 α -[(2-furanilcarbonil)oxi]-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotoato. |
| IB.10 | α -CH ₃ | F | F | 2-Tienilo | H | H | H | H | S | $\equiv$ | 1 | 0 | 0 | 1 | OH | S-(4-Hidroxi-but-2-inil) 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -[(2-tienilcarbonil)oxi]-androsta-1,4-dien-17 β -carbotoato. |
| IB.11 | α -CH ₃ | F | F | Etilo | H | H | -- | -- | S | $\equiv$ | 1 | 0 | 1 | 0 | -- | S-(Prop-2-inil) 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carbotoato. |
| IB.12 | α -CH ₃ | F | F | 2-Furilo | H | H | H | H | S | $\equiv$ | 1 | 0 | 0 | 1 | 1,4-Dioxaspiro[4,5]decan-2-ilmetoxi-carboniloxi | S-[4-(1,4-Dioxaspiro[4,5]decan-2-ilmetoxi-carboniloxi)-but-2-inil] 6 α ,9 α -difluoro-17 α -[(2-furanilcarbonil)oxi]-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotoato. |
| IB.13 | α -CH ₃ | F | F | Etilo | H | H | H | H | S | $\equiv$
(E) | 1 | 1 | 1 | 1 | OH | S-[4-Hidroxi-(E)-but-2-enil] 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carbotoato. |
| IB.14 | α -CH ₃ | F | F | 2-Furilo | H | H | H | H | S | $\equiv$
(E) | 1 | 1 | 1 | 1 | OH | S-[4-Hidroxi-(E)-but-2-enil] 6 α ,9 α -difluoro-17 α -[(2-furanilcarbonil)oxi]-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotoato. |
| IB.15 | α -CH ₃ | F | F | 2-Furilo | H | H | H | H | S | $\equiv$
(Z) | 1 | 1 | 1 | 1 | OH | S-[4-Hidroxi-(Z)-but-2-enil] 6 α ,9 α -difluoro-17 α -[(2-furanilcarbonil)oxi]-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotoato. |
| IB.16 | α -CH ₃ | F | F | 2-Tienilo | H | H | H | H | S | $\equiv$
(Z) | 1 | 1 | 1 | 1 | OH | S-[4-Hidroxi-(Z)-but-2-enil] 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -[(2-tienilcarbonil)oxi]-androsta-1,4-dien-17 β -carbotoato. |
| IB.17 | α -CH ₃ | F | F | 2-Tienilo | H | H | H | H | S | $\equiv$
(E) | 1 | 1 | 1 | 1 | OH | S-[4-Hidroxi-(E)-but-2-enil] 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -[(2-tienilcarbonil)oxi]-androsta-1,4-dien-17 β -carbotoato. |
| IB.18 | α -CH ₃ | F | F | 2-Furilo | H | H | H | H | S | $\equiv$ | 1 | 0 | 0 | 1 | 1,4-Dioxaspiro[4,4]nonan-2-ilmetoxi-carboniloxi | S-[4-(1,4-Dioxaspiro[4,4]nonan-2-ilmetoxi-carboniloxi)-but-2-inil] 6 α ,9 α -difluoro-17 α -[(2-furanilcarbonil)oxi]-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotoato. |
| IB.19 | α -CH ₃ | F | F | 2-Furilo | H | H | H | H | S | $\equiv$ | 1 | 0 | 0 | 1 | OCO-
O(CH ₂) ₄ -
ONO ₂ | S-(4-(4-Nitroxibutiloxi-carboniloxi)-but-2-inil) 6 α ,9 α -difluoro-17 α -[(2-furanilcarbonil)oxi]-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotoato. |
| IB.20 | α -CH ₃ | F | F | 5-Cloro-2-tienilo | H | H | H | H | S | $\equiv$ | 1 | 0 | 0 | 1 | OH | S-[4-Hidroxi-but-2-inil] 17 α -[(5-cloro-2-tienil)carbonil]oxi] 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotoato. |
| IB.21 | α -CH ₃ | F | F | 2-Furilo | H | H | H | H | S | $\equiv$ | 1 | 0 | 0 | 1 | H | S-[But-2-inil] 6 α ,9 α -difluoro-17 α -[(2-furanilcarbonil)oxi]-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotoato. |
| IB.22 | α -CH ₃ | F | F | 3-Metil-2-furilo | H | H | H | H | S | $\equiv$ | 1 | 0 | 0 | 1 | OH | S-[4-Hidroxi-but-2-inil] 6 α ,9 α -difluoro-11 β -hidroxi-17 α -[(3-metil-2-furanil)-carbonil]oxi]-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotoato. |
| IB.23 | α -CH ₃ | F | F | Etoxi-metilo | H | H | H | H | S | $\equiv$ | 1 | 0 | 0 | 1 | OH | S-[4-Hidroxi-but-2-inil] 6 α ,9 α -difluoro-17 α -(etoximetilcarbonil)oxi]-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotoato. |
| IB.24 | α -CH ₃ | F | F | Metoxi-metilo | H | H | H | H | S | $\equiv$ | 1 | 0 | 0 | 1 | OH | S-[4-Hidroxi-but-2-inil] 6 α ,9 α -difluoro-11 β -hidroxi-17 α -(metoximetil-carbonil)oxi]-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotoato. |
| IB.25 | α -CH ₃ | F | F | 2-Furilo | H | H | (CH ₂) ₅ | | S | $\equiv$ | 1 | 0 | 0 | 1 | OH | S-[3-(1-Hidroxiciclohexil)prop-2-inil] 6 α ,9 α -difluoro-17 α -[(2-furanilcarbonil)-oxi]-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotoato. |
| IB.26 | α -CH ₃ | F | F | Ciclo-hexil-metilo | H | H | H | H | S | $\equiv$ | 1 | 0 | 0 | 1 | OH | S-[4-Hidroxi-but-2-inil] 17 α -ciclohexilmetilcarboniloxi-6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotoato. |
| IB.27 | α -CH ₃ | F | F | n-Butilo | H | H | H | H | S | $\equiv$ | 1 | 0 | 0 | 1 | OH | S-[4-Hidroxi-but-2-inil] 17 α -n-butilcarboniloxi-6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotoato. |
| IB.28 | α -CH ₃ | F | F | Etilo | H | H | -- | -- | O | $\equiv$ | 1 | 0 | 1 | 0 | -- | Prop-2-inil 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carbotoato. |
| IB.29 | α -CH ₃ | F | F | Ciclo-pentilo | H | H | H | H | S | $\equiv$ | 1 | 0 | 0 | 1 | OH | S-[4-Hidroxi-but-2-inil] 17 α -ciclopentilcarboniloxi-6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotoato. |
| IB.30 | α -CH ₃ | F | F | Etilo | H | H | H | H | S | $\equiv$
(Z) | 1 | 1 | 1 | 1 | OH | S-[4-Hidroxi-(Z)-but-2-enil] 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α - |

| Serie No. | R ₁ | R ₂ | R ₃ | R ₅ | P | Q | J | K | Z | X | m ₁ | m ₂ | m ₃ | n ₁ | L | Nombre Químico |
|-----------|---------------------------|----------------|----------------|----------------|---|---|-----------------|-----------------|--------------------------|--------------------------|----------------|----------------|----------------|----------------|--|---|
| IB.31 | α -CH ₃ | F | F | Etilo | H | H | H | H | S | $\equiv$ | 1 | 0 | 0 | 1 | OCOC ₂ H ₅ | propioniloxiandrosta-1,4-dien-17 β -carbotoiato
S-[4-Propioniloxi-but-2-inil] 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carbotoiato |
| IB.32 | α -CH ₃ | F | F | Etilo | H | H | H | H | S | $\equiv$ | 1 | 0 | 0 | 1 | OCOCH ₃ | S-[4-Acetoxi-but-2-inil] 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carbotoiato |
| IB.33 | α -CH ₃ | F | F | Etilo | H | H | H | H | S | $\equiv$ | 1 | 0 | 0 | 1 | OCO-
<i>n</i> -C ₃ H ₇ | S-[4- <i>n</i> -Propilcarboniloxi-but-2-inil] 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carbotoiato |
| IB.34 | α -CH ₃ | F | F | Etilo | H | H | H | H | S | $\equiv$ | 1 | 0 | 0 | 1 | OCO-
CH(CH ₃) ₂ | S-[4-(2-Metilpropioniloxi)-but-2-inil] 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carbotoiato |
| IB.35 | α -CH ₃ | F | F | Etilo | H | H | H | H | S | $\equiv$ | 1 | 0 | 0 | 1 | OCO-
<i>n</i> -C ₄ H ₉ | S-[4- <i>n</i> -Butilcarboniloxi-but-2-inil] 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carbotoiato |
| IB.36 | α -CH ₃ | F | F | Etilo | H | H | H | H | S | $\equiv$ | 1 | 0 | 0 | 1 | OCO-
ciclobutil | S-[4-Ciclobutilcarboniloxi-but-2-inil] 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carbotoiato |
| IB.37 | α -CH ₃ | F | F | Etilo | H | H | H | H | S | $\equiv$ | 1 | 0 | 0 | 1 | OCO-
<i>n</i> -C ₅ H ₁₁ | S-[4- <i>n</i> -Pentilcarboniloxi-but-2-inil] 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carbotoiato |
| IB.38 | β -CH ₃ | F | H | Etilo | H | H | H | H | S | $\equiv$ | 1 | 0 | 0 | 1 | OH | S-[4-Hidroxi-but-2-inil] 9 α -fluoro-11 β -hidroxi-16 β -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carbotoiato |
| IB.39 | β -CH ₃ | F | F | Etilo | H | H | H | H | S | $\equiv$ | 1 | 0 | 0 | 1 | OH | S-[4-Hidroxi-but-2-inil] 6 α ,9 α -difluoro-11 β -hidroxi-16 β -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carbotoiato |
| IB.40 | α -CH ₃ | F | F | 2-Furilo | H | H | CH ₃ | CH ₃ | S | $\equiv$ | 1 | 0 | 0 | 1 | OH | S-[4-Hidroxi-4-metil-pent-2-inil] 6 α ,9 α -difluoro-17 α -[(2-furanilcarbonil)-oxi]-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotoiato. |
| IB.41 | α -CH ₃ | F | F | Etilo | H | H | O | O | $\equiv$
(<i>E</i>) | $\equiv$ | 1 | 1 | 1 | 1 | OCH ₃ | 4-Metoxi-4-oxo-(<i>E</i>)-but-2-enil 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carboxilato |
| IB.42 | α -CH ₃ | F | F | Etilo | H | H | O | S | $\equiv$
(<i>E</i>) | $\equiv$ | 1 | 1 | 1 | 1 | OCH ₃ | S-[4-Metoxi-4-oxo-(<i>E</i>)-but-2-enil] 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carbotoiato |
| IB.43 | - | H | H | Etoxi | H | H | O | O | $\equiv$
(<i>E</i>) | $\equiv$ | 1 | 1 | 1 | 1 | OCH ₃ | 4-Metoxi-4-oxo-(<i>E</i>)-but-2-enil 17 α -(etoxicarbonil) oxi-11 β -hidroxi-3-oxoandrosta-1,4-dien-17 β -carboxilato. |
| IB.44 | α -CH ₃ | F | F | Etilo | H | H | H | H | S | $\equiv$
(<i>E</i>) | 1 | 1 | 1 | 1 | OCOCO-
OC ₂ H ₅ | S-[4-(2-Etoxi-1,2-dioxoetil)oxi-(<i>E</i>)-but-2-enil] 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carbotoiato |
| IB.45 | α -CH ₃ | Cl | H | 2-Furilo | H | H | H | H | S | $\equiv$ | 1 | 0 | 0 | 1 | OH | S-[4-Hidroxi-but-2-inil] 9 α -cloro 17 α -[(2-furanilcarbonil)oxi]-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotoiato |
| IB.46 | α -CH ₃ | F | F | 2-Furilo | H | H | H | H | S | $\equiv$
(<i>E</i>) | 1 | 1 | 1 | 1 | OCOCO-
OC ₂ H ₅ | S-[4-(2-Etoxi-1,2-dioxoetil)oxi-(<i>E</i>)-but-2-enil] 6 α ,9 α -difluoro-17 α -[(2-furanilcarbonil)oxi]-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotoiato. |
| IB.47 | α -CH ₃ | F | F | 2-Furilo | H | H | H | H | S | $\equiv$
(<i>Z</i>) | 1 | 1 | 1 | 1 | OCOCO-
OC ₂ H ₅ | S-[4-(2-Etoxi-1,2-dioxoetil)oxi-(<i>Z</i>)-but-2-enil] 6 α ,9 α -difluoro-17 α -[(2-furanilcarbonil)oxi]-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotoiato. |
| IB.48 | α -CH ₃ | F | F | 2-Furilo | H | H | H | H | S | $\equiv$ | 1 | 0 | 0 | 1 | (<i>S</i>)-(-)-2-Acetoxi-propionil-oxi | S-[4-(<i>s</i>)-(-)-2-Acetoxipropioniloxi] but-2-inil] 6 α ,9 α -difluoro-17 α -[(2-furanilcarbonil)oxi]-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotoiato. |
| IB.49 | α -CH ₃ | F | F | 2-Furilo | H | H | H | H | S | $\equiv$ | 1 | 0 | 0 | 1 | OCO-
<i>n</i> -C ₃ H ₇ | S-[4- <i>n</i> -Propilcarboniloxi-but-2-inil] 6 α ,9 α -difluoro-17 α -[(2-furanilcarbonil)-oxi]-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotoiato. |
| IB.50 | α -CH ₃ | F | F | 2-Furilo | H | H | H | H | S | $\equiv$ | 1 | 0 | 0 | 1 | OCO-
CH(CH ₃) ₂ | S-[4-(2-Metilpropioniloxi)-but-2-inil] 6 α ,9 α -difluoro-17 α -[(2-furanilcarbonil)-oxi]-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotoiato. |
| IB.51 | α -CH ₃ | F | F | 2-Furilo | H | H | H | H | S | $\equiv$ | 1 | 0 | 0 | 1 | OCO-
C(CH ₃) ₃ | S-[4-(2,2-Dimetilpropioniloxi)-but-2-inil] 6 α ,9 α -difluoro-17 α -[(2-furanilcarbonil)oxi]-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotoiato. |
| IB.52 | α -CH ₃ | F | F | Etilo | H | H | H | H | S | $\equiv$ | 1 | 0 | 0 | 1 | OCO-
C(CH ₃) ₃ | S-[4-(2,2-Dimetilpropioniloxi)-but-2-inil] 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -propioniloxiandrosta-1,4-dien-17 β -carbotoiato |
| IB.53 | α -CH ₃ | F | F | 2-Furilo | H | H | H | H | S | $\equiv$
(<i>Z</i>) | 1 | 1 | 1 | 1 | OCO-
<i>n</i> -C ₃ H ₇ | S-[4- <i>n</i> -Propilcarboniloxi-(<i>Z</i>)-but-2-enil] 6 α ,9 α -difluoro-17 α -[(2-furanilcarbonil)oxi]-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotoiato. |
| IB.54 | α -CH ₃ | F | F | 2-Furilo | H | H | H | H | S | $\equiv$ | 1 | 0 | 0 | 1 | OCOCO-
OC ₂ H ₅ | S-[4-(2-Etoxi-1,2-dioxoetil)oxi-but-2-inil] 6 α ,9 α -difluoro-17 α -[(2-furanilcarbonil)oxi]-11 β -hidroxi-16 α -metil-3-oxoandrosta-1,4-dien-17 β -carbotoiato. |
| IB.55 | α -CH ₃ | F | F | 2-Tienilo | H | H | H | H | S | $\equiv$ | 1 | 0 | 0 | 1 | OCO-
<i>n</i> -C ₃ H ₇ | S-[4- <i>n</i> -Propilcarboniloxi-but-2-inil] 6 α ,9 α -difluoro-11 β -hidroxi-16 α -metil-3-oxo-17 α -[(2-tienilcarbonil)oxi]-androsta-1,4-dien-17 β -carbotoiato. |
| IB.56 | α -CH ₃ | F | F | 5-Cl-2-Tienil | H | H | H | H | S | $\equiv$ | 1 | 0 | 0 | 1 | OCO-
<i>n</i> -C ₃ H ₇ | S-[4- <i>n</i> -Propilcarboniloxi-but-2-inil] 17 α -[(5-cloro-2-tienil)carbonil]-oxi]-6 α ,9 α -difluoro- |

| Serie No. | R ₁ | R ₂ | R ₃ | R ₄ | P | Q | J | K | Z | X | m ₁ | m ₂ | m ₃ | n ₁ | L | Nombre Químico |
|-----------|-------------------|----------------|----------------|----------------|---|---|---|---|---|----------|----------------|----------------|----------------|----------------|--|--|
| | | | | | | | | | | | | | | | | 11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.57 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCO-ciclopropil | S-[(4-Ciclopropilcarboniloxi)-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)-oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.58 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCO-ciclobutil | S-[(4-Ciclobutilcarboniloxi)-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)-oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.59 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCO-ciclopentil | S-[(4-Ciclopentilcarboniloxi)-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)-oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.60 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | =
(E) | 1 | 1 | 1 | 1 | OCO-n-C ₄ H ₉ | S-[4- <i>n</i> -Propilcarboniloxi-(E)-but-2-enil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)-oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.61 | α-CH ₃ | F | F | 4-Cl-fenilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OH | S-[4-Hidroxi-but-2-inil] 17α-(4-clorofenil) carboniloxi-6α,9α-difluoro-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.62 | α-CH ₃ | F | F | 3-Cl-fenilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OH | S-[4-Hidroxi-but-2-inil] 17α-(3-clorofenil) carboniloxi-6α,9α-difluoro-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.63 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCO-OCH ₃ | S-[(4-Metoxicarboniloxi)-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)-oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.64 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCO-OC ₂ H ₅ | S-[(4-Etoxicarboniloxi)-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)-oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.65 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCO-OC(CH ₃) ₃ | S-[4-(2,2-Dimetiletiloxicarboniloxi)-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)-oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.66 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCO-OCH ₂ CH(CH ₃) ₂ | S-[4-(2-Metilpropiloxicarboniloxi)-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)-oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.67 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCO-(CH ₂) ₂ CH ₂ Cl | S-[4-(3-Clorofenilcarboniloxi)-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)-oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.68 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | =
(Z) | 1 | 1 | 1 | 1 | OCO-C(CH ₃) ₃ | S-[4-(2,2-Dimetilpropioniloxi)-(Z)-but-2-enil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)-oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.69 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | =
(E) | 1 | 1 | 1 | 1 | OCO-C(CH ₃) ₃ | S-[4-(2,2-Dimetilpropioniloxi)-(E)-but-2-enil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)-oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.70 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCOCHCl ₂ | S-[4-Dicloroacetoxi-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)-oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.71 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | 2-metil propil-etil-carboniloxi | S-[4-(2-Metilpropilcarboniloxi)-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)-oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.72 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCOCH ₂ -C(CH ₃) ₃ | S-[4-(3,3-Dimetilpropilcarboniloxi)-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil) oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.73 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCO-CH ₂ CH ₃ | S-[4-Propioniloxi-but-2-inil] 6α,9α-difluoro-11β-hidroxi-17α-[(2-furanilcarbonil)-oxi]-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.74 | α-CH ₃ | F | F | Ciclo-butilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCO-COOCH ₂ CH ₃ | S-[4-(2-Etoxi-1,2-dioxoetil)oxi-but-2-inil] 17α-ciclobutilcarboniloxi-6α,9α-difluoro-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.75 | α-CH ₃ | F | F | Ciclo-butilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCO-CH(CH ₃) ₂ | S-[4-(2-Metilpropioniloxi)-but-2-inil] 17α-ciclobutilcarboniloxi-6α,9α-difluoro-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.76 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | Adamantil-carboniloxi | S-[4-(Adamantilcarboniloxi)-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.77 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCOCH ₂ -CF ₃ | S-[4-(3,3,3-Trifluoropropioniloxi)-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.78 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCOCH ₂ -OCH ₃ | S-[4-(Metoxiacetiloxi)-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.79 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCOCH ₂ -OCH ₂ CH ₃ | S-[4-(Etoxiacetiloxi)-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.80 | α- | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCOCH ₂ - | S-[4-(4-Hidroxibutil-1,4-dien)-oxi-but-2-inil] |

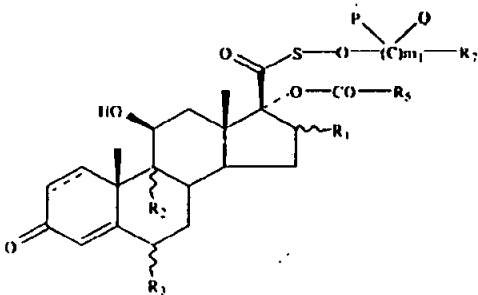
| Serie No. | R ₁ | R ₂ | R ₃ | R ₄ | P | Q | J | K | Z | X | m ₁ | m ₂ | m ₃ | n ₁ | L | Nombre Químico |
|-----------|-------------------|----------------|----------------|-------------------|---|---|---|---|---|-------|----------------|----------------|----------------|----------------|---|--|
| | CH ₃ | | | | | | | | | | | | | | CH ₂ COOH | 6α,9α-difluoro-11β-hidroxi-16α-metil-17α-[(2-furanilcarbonil)oxi]-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.81 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCOCH ₃ | S-[4-Acetoxi-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.82 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | = (E) | 1 | 1 | 1 | 1 | OCO-CH(CH ₃) ₂ | S-[4-(2-Metilpropioniloxi)-(E)-but-2-enil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.83 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | = (Z) | 1 | 1 | 1 | 1 | OCO-CH(CH ₃) ₂ | S-[4-(2-Metilpropioniloxi)-(Z)-but-2-enil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.84 | α-CH ₃ | F | F | Ciclo-butilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCO-C(CH ₃) ₃ | S-[4-(2,2-Dimetilpropioniloxi)-but-2-inil] 17α-ciclobutilcarboniloxi-6α,9α-difluoro-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.85 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | 2,2-Dimetil-butylcarbonyloxi | S-[4-(2,2-Dimetilbutylcarboniloxi)-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.86 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | (1S)-Canfanil-carboniloxi | S-[4-(1S)-Canfanilcarboniloxi-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.87 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OC(=O)NH-C(CH ₃) ₃ | S-[4-(1,1-Dimetiletilcarbamoiloxi)-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.88 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCO(CH ₂) ₂ -COOC ₂ H ₅ | S-[4-(4-Etoxibutil-1,4-dion)oxi-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.89 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | Metil-carboniloxi | S-[4-Metilcarboniloxi-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.90 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCOCH ₂ NH-COCH ₃ | S-[4-Acetamidacetoxi-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.91 | α-CH ₃ | F | F | 5-Cloro-2-tienilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCOCH ₂ -CH(CH ₃) ₂ | S-[4-(2-Metilpropiloxycarboniloxi)-but-2-inil] 17α-[(5-cloro-2-tienil)carbonil]oxi-6α,9α-difluoro-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.92 | α-CH ₃ | F | F | 5-Cloro-2-tienilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCO-CH(CH ₃) ₂ | S-[4-(2-Metilpropioniloxi)-but-2-inil] 17α-[(5-cloro-2-tienil)carbonil]oxi-6α,9α-difluoro-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.93 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCOCH=CH-COOC ₂ H ₅ | S-[4-(4-Etiloxi)-(Z)-but-2-en-1,4-dion)oxi-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.94 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCO(CH ₂) ₂ -COOCH ₃ | S-[4-(4-Metoxibutil-1,4-dion)oxi-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.95 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCO(CH ₂) ₂ -COOCH-(CH ₃) ₂ | S-[4-(4-Isopropiloxibutil-1,4-dion)oxi-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.96 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCO(CH ₂) ₂ -COOCH ₂ CH-(CH ₃) ₂ | S-[4-(4-Isobutiloxibutil-1,4-dion)oxi-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.97 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCO(CH ₂) ₂ -COO(CH ₂) ₂ -CH ₃ | S-[4-(4-n-Butiloxibutil-1,4-dion)oxi-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.98 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | 3-Cloro-2,2-dimetil-propioniloxi | S-[4-(3-Cloro-2,2-dimetilpropioniloxi)-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.99 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCOCH=CH-COOC ₂ H ₅ -CH(CH ₃) ₂ | S-[4-(4-Isobutiloxi)-(Z)-but-2-en-1,4-dion)oxi-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.100 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCOCH=CH-COOC ₂ H ₅ | S-[4-(4-Metoxi)-(E)-but-2-en-1,4-dion)oxi-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.101 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCO-CH ₂ CH(CH ₃) ₂ | S-[4-(3-Metil-1-oxobutiloxi)-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.102 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCO-CH(C ₂ H ₅) ₂ | S-[4-(2-Etil-1-oxobutiloxi)-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.103 | α- | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCON(CH ₃) ₂ | S-[4-(N,N-Dimetilaminocarbonil-oxi)-but-2- |

| Serie No. | R ₁ | R ₂ | R ₃ | R ₅ | P | Q | J | K | Z | X | m ₁ | m ₂ | m ₃ | n ₁ | I. | Nombre Químico |
|-----------|-------------------|----------------|----------------|----------------|---|---|---|---|---|---|----------------|----------------|----------------|----------------|---|---|
| | CH ₃ | | | | | | | | | | | | | | | inil] 6a,9a-difluoro-17a-[(2-furanilcarbonil) oxi]-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.104 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCO-CCl(CH ₃) ₂ | S-[4-(2-Cloro-2-metilpropionil-oxi)-but-2-inil] 6a,9a-difluoro-17a-[(2-furanilcarbonil) oxi]-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.105 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCO(CH ₂) ₂ -CH(CH ₃) ₂ | S-[4-(4-Metil-1-oxopentiloxi)-but-2-inil] 6a,9a-difluoro-17a-[(2-furanilcarbonil) oxi]-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.106 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCO(CH ₂) ₂ -COOCH ₃ F | S-[4-(4-Fluorometoxi-1,4-dioxo-butil)oxi]-but-2-inil] 6a,9a-difluoro-17a-[(2-furanilcarbonil) oxi]-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.107 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCOCH=CH-COOCH ₂ F | S-[4-(4-Fluorometiloxi-1,4-dioxo-(Z)-but-2-en)oxi]-but-2-inil] 6a,9a-difluoro-17a-[(2-furanilcarbonil) oxi]-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.108 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCOCH ₂ -COOCH ₃ | S-[4-(3-Metoxipropil-1,3-dion)oxi]-but-2-inil] 6a,9a-difluoro-17a-[(2-furanilcarbonil) oxi]-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.109 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCOC(CH ₃) ₂ -COOCH ₂ | S-[4-(3-Metoxi-2,2-dimetilpropil-1,3-dion)oxi]-but-2-inil] 6a,9a-difluoro-17a-[(2-furanilcarbonil) oxi]-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.110 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCOC(OH)-(CH ₃) ₂ | S-[4-(2-Hidroxi-2-metilpropioniloxi)-but-2-inil] 6a,9a-difluoro-17a-[(2-furanilcarbonil) oxi]-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.111 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCOCF(CH ₃) ₂ | S-[4-(2-Fluoro-2-metilpropioniloxi)-but-2-inil] 6a,9a-difluoro-17a-[(2-furanilcarbonil) oxi]-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.112 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCOCH=CH-COOCH ₃ | S-[4-(4-Metoxi-(Z)-but-2-en-1,4-dion)oxi]-but-2-inil] 6a,9a-difluoro-17a-[(2-furanilcarbonil) oxi]-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.113 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCOCH=CH-COOC ₂ H ₅ | S-[4-(4-Etoxi-(E)-but-2-en-1,4-dion)oxi]-but-2-inil] 6a,9a-difluoro-17a-[(2-furanilcarbonil) oxi]-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.114 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCOCH=CH-COOCH ₂ -CH(CH ₃) ₂ | S-[4-(4-Isobutiloxi-1,4-dioxo-(E)-but-2-en)oxi]-but-2-inil] 6a,9a-difluoro-17a-[(2-furanilcarbonil) oxi]-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.115 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCOC(CH ₃)=CH-COO(CH ₂) ₃ -CH ₃ | S-[4-(4-n-butiloxi-1,4-dioxo-(E)-but-2-en)oxi]-but-2-inil] 6a,9a-difluoro-17a-[(2-furanilcarbonil) oxi]-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.116 | α-CH ₃ | Cl | H | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCOC(CH ₃)=CH-(CH ₃) ₂ | S-[4-(2-Metilpropioniloxi)-but-2-inil] 9a-cloro-17a-[(2-furanilcarbonil) oxi]-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.117 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | 2-(S)-Metil-butiriloxi | S-[4-(2-(S)-Metilbutiriloxi)-but-2-inil] 6a,9a-difluoro-17a-[(2-furanilcarbonil) oxi]-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.118 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCO-(2-Furil) | S-[4-((Furan-2-il)carboniloxi)-but-2-inil] 6a,9a-difluoro-17a-[(2-furanilcarbonil) oxi]-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.119 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCOCH=CH-COOCH-(CH ₃) ₂ | S-[4-(4-Isopropiloxi-1,4-dioxo-(E)-but-2-en)oxi]-but-2-inil] 6a,9a-difluoro-17a-[(2-furanilcarbonil) oxi]-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.120 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | 3-Hidroxi-2,2-dimetil-Propionil-oxi | S-[4-(3-Hidroxi-2,2-dimetil-propionil-oxi)-but-2-inil] 6a,9a-difluoro-17a-[(2-furanilcarbonil) oxi]-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.121 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCO-CH=CH ₂ | S-[4-(4-Acridiloxi)-but-2-inil] 6a,9a-difluoro-17a-[(2-furanilcarbonil) oxi]-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.122 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCOC(OH)-(C ₂ H ₅) ₂ | S-[4-(1-Etil-1-hidroxiipropilcarbonil-oxi)-but-2-inil] 6a,9a-difluoro-17a-[(2-furanilcarbonil) oxi]-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.123 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCOCH ₂ -ciclopropil | S-[4-(Ciclopropilmetiloxi-carbonil-oxi)-but-2-inil] 6a,9a-difluoro-17a-[(2-furanilcarbonil) oxi]-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.124 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCOC=C-COOCH ₃ | S-[4-(4-Metoxibut-2-in-1,4-dion)oxi]-but-2-inil] 6a,9a-difluoro-17a-[(2-furanilcarbonil) oxi]-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.125 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCOO-ciclopentil | S-[4-(Ciclopentilmetiloxi-carbonil-oxi)-but-2-inil] 6a,9a-difluoro-17a-[(2-furanilcarbonil) oxi]-11β-hidroxi-16a-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.126 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCOO-CH ₂ -ciclopentil | S-[4-(Ciclopentilmetiloxi-carbonil-oxi)-but-2-inil] 6a,9a-difluoro-17a-[(2-furanilcarbonil) |

| Serie No. | R ₁ | R ₂ | R ₃ | R ₅ | P | Q | J | K | Z | X | m ₁ | m ₂ | m ₃ | n ₁ | L | Nombre Químico |
|-----------|-------------------|----------------|----------------|----------------|---|---|---|---|---|---|----------------|----------------|----------------|----------------|--|--|
| | | | | | | | | | | | | | | | | oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.127 | α-CH ₃ | Cl | H | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCOO-CH ₂ -CH(CH ₃) ₂ | S-[4-(2-Metilpropiloxycarboniloxi)-but-2-inil] 9α-cloro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16β-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.128 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | 2,2-Dimetil-1,3-dioxolan-4-il-metoxi-etil-carboniloxi | S-[4-(2,2-Dimetil-1,3-dioxolan-4-il-metoxycarboniloxi)-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.129 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCOC(C ₂ H ₅) ₂ | S-[4-(N,N-Dietilaminocarboniloxi)-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.130 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | Piperidin-1-il-etil-carboniloxi | S-[4-(Piperidin-1-ilcarboniloxi)-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.131 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | 4-Metil-piperazin-1-il-etil-carboniloxi | S-[4-(4-Metil-piperazin-1-il-carbonil-oxi)-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.132 | β-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OH | S-(4-Hidroxi-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16β-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.133 | β-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCOCH-(CH ₃) ₂ | S-[4-(2-Metilpropioniloxi)-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16β-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.134 | β-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCOOCH ₂ -CH(CH ₃) ₂ | S-[4-(2-Metilpropiloxycarboniloxi)-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16β-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.135 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCOCCL ₂ -CH ₃ | S-[4-(2,2-Dicloropropioniloxi)-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.136 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | N(C ₂ H ₅) ₂ | S-[4-(N,N-Dietilamino)-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.137 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCOOCH-(CH ₃) ₂ | S-[4-(Isopropiloxycarboniloxi)-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.138 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCOOCH ₂ -CH=C(CH ₃) ₂ | S-[4-(3-Metilbut-2-enoxycarbonil-oxi)-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.139 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCOO-(CH ₂) ₃ -CH ₃ | S-[4-(n-Hexiloxycarboniloxi)-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.140 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCOOCH ₂ -ciclohexil | S-[4-(Ciclohexilmetiloxycarbonil-oxi)-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.141 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCOO-ciclohexil | S-[4-(Ciclohexiloxycarboniloxi)-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.142 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCOO-(CH ₂) ₈ -CH ₃ | S-[4-(n-Nonaniloxycarboniloxi)-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.143 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCOOCH ₂ -C(CH ₃) ₃ | S-[4-(2,2-Dimetilpropiloxycarbonil-oxi)-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.144 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCOOCH ₂ -Ciclobutil | S-[4-(Ciclobutilmetiloxycarboniloxi)-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.145 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCOOCH ₂ -(furan-2-il) | S-[4-(2-Metilfuraniloxycarboniloxi)-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.146 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCOO-(CH ₂) ₃ -CH ₃ | S-[4-(n-Butiloxycarboniloxi)-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.147 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCOO-(CH ₂) ₅ -CH ₃ | S-[4-(n-Pentiloxycarboniloxi)-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |
| IB.148 | α-CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | 2,2-Dimetil-3-fluoro-propioniloxi | S-[4-(2,2-Dimetil-3-fluoro-propioniloxi)-but-2-inil] 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbotoiato. |

| Serie No. | R ₁ | R ₂ | R ₃ | R ₄ | P | Q | J | K | Z | X | m ₁ | m ₂ | m ₃ | n ₁ | I. | Nombre Químico |
|-----------|---------------------------|----------------|----------------|----------------|---|---|---|---|---|---|----------------|----------------|----------------|----------------|--|--|
| IB.149 | <i>α</i> -CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | (S)-2,2-Dimetil-1,3-dioxolan-4-il-metoxicarboniloxi-but-2-inil | S-[4-((S)-2,2-Dimetil-1,3-dioxolan-4-il-metoxicarboniloxi)-but-2-inil] 6 <i>α</i> ,9 <i>α</i> -difluoro-17 <i>α</i> -[(2-furanilcarbonil)oxi]-carboniloxi-11 <i>β</i> -hidroxi-16 <i>α</i> -metil-3-oxoandrosta-1,4-dien-17 <i>β</i> -carbotoiato. |
| IB.150 | <i>α</i> -CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | (R)-2,2-Dimetil-1,3-dioxolan-4-il-metoxicarboniloxi-but-2-inil | S-[4-((R)-2,2-Dimetil-1,3-dioxolan-4-il-metoxicarboniloxi)-but-2-inil] 6 <i>α</i> ,9 <i>α</i> -difluoro-17 <i>α</i> -[(2-furanilcarbonil)oxi]-11 <i>β</i> -hidroxi-16 <i>α</i> -metil-3-oxoandrosta-1,4-dien-17 <i>β</i> -carbotoiato. |
| IB.151 | <i>α</i> -CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | (Morfolin-4-il)-etil-carboniloxi | S-[4-(Morfolin-4-il)carboniloxi-but-2-inil] 6 <i>α</i> ,9 <i>α</i> -difluoro-17 <i>α</i> -[(2-furanilcarbonil)oxi]-11 <i>β</i> -hidroxi-16 <i>α</i> -metil-3-oxoandrosta-1,4-dien-17 <i>β</i> -carbotoiato. |
| IB.152 | <i>α</i> -CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | 2,2-Dimetil-1,3-dioxolan-4-ilmetil-carbamooxi | S-[4-(2,2-Dimetil-1,3-dioxolan-4-il-metilcarbamooxi)-but-2-inil] 6 <i>α</i> ,9 <i>α</i> -difluoro-17 <i>α</i> -[(2-furanilcarbonil)oxi]-11 <i>β</i> -hidroxi-16 <i>α</i> -metil-3-oxoandrosta-1,4-dien-17 <i>β</i> -carbotoiato. |
| IB.153 | <i>α</i> -CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCOO(CH ₂) ₂ -ciclopentil | S-[4-(2-Ciclopentiletoxicarboniloxi)-but-2-inil] 6 <i>α</i> ,9 <i>α</i> -difluoro-17 <i>α</i> -[(2-furanilcarbonil)oxi]-11 <i>β</i> -hidroxi-16 <i>α</i> -metil-3-oxoandrosta-1,4-dien-17 <i>β</i> -carbotoiato. |
| IB.154 | <i>α</i> -CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCOO-(CH ₂) ₂ -CH(CH ₃) ₂ | S-[4-(Isoamiloxicarboniloxi)-but-2-inil] 6 <i>α</i> ,9 <i>α</i> -difluoro-17 <i>α</i> -[(2-furanilcarbonil)oxi]-11 <i>β</i> -hidroxi-16 <i>α</i> -metil-3-oxoandrosta-1,4-dien-17 <i>β</i> -carbotoiato. |
| IB.155 | <i>α</i> -CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCO(CH ₂) ₃ -ONO ₂ | S-[4-(3-Nitroxipropilcarboniloxi)-but-2-inil] 6 <i>α</i> ,9 <i>α</i> -difluoro-17 <i>α</i> -[(2-furanilcarbonil)oxi]-11 <i>β</i> -hidroxi-16 <i>α</i> -metil-3-oxoandrosta-1,4-dien-17 <i>β</i> -carbotoiato. |
| IB.156 | <i>α</i> -CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | 2,2,7,7-Tetrametil tetrahidro-bis[1,3]dioxolo[4,5-b;4',5'-d]piran-5-il metoxi-etil-carboniloxi | S-[4-(2,2,7,7-Tetrametiltetrahidro-bis[1,3]dioxolo[4,5-b;4',5'-d]piran-5-il metoxicarboniloxi)-but-2-inil] 6 <i>α</i> ,9 <i>α</i> -difluoro-17 <i>α</i> -[(2-furanilcarbonil)oxi]-11 <i>β</i> -hidroxi-16 <i>α</i> -metil-3-oxoandrosta-1,4-dien-17 <i>β</i> -carbotoiato. |
| IB.157 | <i>α</i> -CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCO(CH ₂) ₄ -ONO ₂ | S-[4-(4-Nitroxibutilcarboniloxi)-but-2-inil] 6 <i>α</i> ,9 <i>α</i> -difluoro-17 <i>α</i> -[(2-furanilcarbonil)oxi]-11 <i>β</i> -hidroxi-16 <i>α</i> -metil-3-oxoandrosta-1,4-dien-17 <i>β</i> -carbotoiato. |
| IB.158 | <i>α</i> -CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCH ₃ | S-(4-Metoxi-but-2-inil) 6 <i>α</i> ,9 <i>α</i> -difluoro-17 <i>α</i> -[(2-furanilcarbonil)oxi]-11 <i>β</i> -hidroxi-16 <i>α</i> -metil-3-oxoandrosta-1,4-dien-17 <i>β</i> -carbotoiato. |
| IB.159 | <i>α</i> -CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCH ₂ CH ₃ | S-(4-Etoxi-but-2-inil) 6 <i>α</i> ,9 <i>α</i> -difluoro-17 <i>α</i> -[(2-furanilcarbonil)oxi]-11 <i>β</i> -hidroxi-16 <i>α</i> -metil-3-oxoandrosta-1,4-dien-17 <i>β</i> -carbotoiato. |
| IB.160 | <i>α</i> -CH ₃ | F | F | 2-Furilo | H | H | H | H | S | ≡ | 1 | 0 | 0 | 1 | OCH ₂ CH-(CH ₃) ₂ | S-[4-Isobutoxi-but-2-inil] 6 <i>α</i> ,9 <i>α</i> -difluoro-17 <i>α</i> -[(2-furanilcarbonil)oxi]-11 <i>β</i> -hidroxi-16 <i>α</i> -metil-3-oxoandrosta-1,4-dien-17 <i>β</i> -carbotoiato. |

Tabla 5- Enumera los compuestos de fórmula I-C que se han sintetizado



Fórmula I-C

Tabla 5

| Serie No. | R ₁ | R ₂ | R ₃ | R ₄ | m ₁ | R ₇ | P | Q | Nombre Químico |
|-----------|---------------------------|----------------|----------------|----------------|----------------|--------------------|---|---|---|
| IC.1 | <i>α</i> -CH ₃ | F | F | Etilo | 1 | 4-Fluoro-fenilo | H | H | (4-Fluorofenil)metil éster de ácido 6 <i>α</i> ,9 <i>α</i> -difluoro-11 <i>β</i> -hidroxi-16 <i>α</i> -metil-3-oxo-17 <i>α</i> -propioniloxiandrosta-1,4-dien-17 <i>β</i> -carbonilsulfónico. |
| IC.2 | <i>α</i> - | F | F | Etilo | 1 | 3,4-Dicloro-fenilo | H | H | (3,4-Diclorofenil)metil éster de ácido 6 <i>α</i> ,9 <i>α</i> -difluoro-11 <i>β</i> -hidroxi-16 <i>α</i> -metil-3-oxo-17 <i>α</i> - |

| Serie No. | R ₁ | R ₂ | R ₃ | R ₄ | m ₁ | R ₇ | P | Q | Nombre Químico |
|-----------|-------------------|----------------|----------------|---------------------------------|----------------|--------------------------------|---|---|---|
| | CH ₃ | | | | | | | | propioniloxiandrosta-1,4-dien-17β-carbonilsulfénico. |
| IC.3 | α-CH ₃ | F | F | Étilo | 1 | F | H | H | Fluorometil éster de ácido 6α,9α-difluoro-11β-hidroxi-16α-metil-3-oxo-17α-propioniloxiandrosta-1,4-dien-17β-carbonilsulfénico. |
| IC.4 | α-CH ₃ | F | F | 2-Furilo | 1 | F | H | H | Fluorometil éster de ácido 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbonilsulfénico. |
| IC.5 | α-CH ₃ | F | F | 2-Furilo | 1 | 4-Fluoro-fenilo | H | H | (4-Fluorofenil)metil éster de ácido 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbonilsulfénico. |
| IC.6 | α-CH ₃ | F | F | 2-Furilo | 1 | 4-Trifluoro-metilfenilo | H | H | (4-Trifluorometilfenil)metil éster de ácido 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbonilsulfénico. |
| IC.7 | α-CH ₃ | F | F | 2-Furilo | 1 | 4-Cloro-fenilo | H | H | (4-Clorofenil)metil éster de ácido 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbonilsulfénico. |
| IC.8 | α-CH ₃ | F | F | Étilo | 1 | 4-Trifluoro-metilfenilo | H | H | (4-Trifluorometilfenil)metil éster de ácido 6α,9α-difluoro-11β-hidroxi-16α-metil-3-oxo-17α-propioniloxiandrosta-1,4-dien-17β-carbonilsulfénico. |
| IC.9 | α-CH ₃ | F | H | 2-Furilo | 1 | 4-Fluoro-fenilo | H | H | (4-Fluorofenil)metil éster de ácido 9α-fluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbonilsulfénico. |
| IC.10 | α-CH ₃ | F | F | Étilo | 1 | 4-Clorofenil-carbonilo | H | H | [2-(4-Clorofenil)-2-oxoetil] éster de ácido 6α,9α-difluoro-11β-hidroxi-16α-metil-3-oxo-17α-propioniloxiandrosta-1,4-dien-17β-carbonilsulfénico. |
| IC.11 | α-CH ₃ | F | H | 2-Furilo | 1 | F | H | H | Fluorometil éster de ácido 9α-fluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbonilsulfénico. |
| IC.12 | α-CH ₃ | F | F | n-C ₄ H ₉ | 1 | F | H | H | Fluorometil éster de ácido 17α-n-butilcarboniloxi-6α,9α-difluoro-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbonilsulfénico. |
| IC.13 | α-CH ₃ | F | F | Étilo | 1 | H | H | H | Éster metílico de ácido 6α,9α-difluoro-11β-hidroxi-16α-metil-3-oxo-17α-propioniloxiandrosta-1,4-dien-17β-carbonilsulfénico. |
| IC.14 | α-CH ₃ | F | F | 2-Furilo | 1 | H | H | H | Éster metílico de ácido 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbonilsulfénico. |
| IC.15 | α-CH ₃ | F | F | Étilo | 1 | Fenilo | H | H | Éster fenilmetílico de ácido 6α,9α-difluoro-11β-hidroxi-16α-metil-3-oxo-17α-propioniloxiandrosta-1,4-dien-17β-carbonilsulfénico. |
| IC.16 | α-CH ₃ | F | F | 2-Furilo | 1 | Fenilo | H | H | Éster fenilmetílico de ácido 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbonilsulfénico. |
| IC.17 | α-CH ₃ | F | F | Étilo | 1 | 2,4,6-Tri-metilfenil-carbonilo | H | H | [2-(2,4,6-Trimetilfenil)-2-oxoetil] éster de ácido 6α,9α-difluoro-11β-hidroxi-16α-metil-3-oxo-17α-propioniloxiandrosta-1,4-dien-17β-carbonilsulfénico. |
| IC.18 | α-CH ₃ | F | F | Étilo | 1 | 4-Cloro-fenilo | H | H | (4-Clorofenil)metil éster de ácido 6α,9α-difluoro-11β-hidroxi-16α-metil-3-oxo-17α-propioniloxiandrosta-1,4-dien-17β-carbonilsulfénico. |
| IC.19 | α-CH ₃ | F | F | 2-Furilo | 1 | 3,4-Dicloro-fenilo | H | H | (3,4-Diclorofenil)metil éster de ácido 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbonilsulfénico. |
| IC.20 | α-CH ₃ | F | F | 2-Furilo | 1 | 2,4-Dicloro-fenilo | H | H | (2,4-Diclorofenil)metil éster de ácido 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbonilsulfénico. |
| IC.21 | α-CH ₃ | F | F | 2-Furilo | 1 | 3-Cloro-fenilo | H | H | (3-Clorofenil)metil éster de ácido 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbonilsulfénico. |
| IC.22 | α-CH ₃ | F | F | 2-Furilo | 1 | 2,4,6-Trifluoro-fenilo | H | H | (2,4,6-Trifluorofenil)metil éster de ácido 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbonilsulfénico. |
| IC.23 | α-CH ₃ | F | F | 2-Furilo | 1 | 3-(Trifluoro-metil)fenilo | H | H | (3-Trifluorometilfenil)metil éster de ácido 6α,9α-difluoro-17α-[(2-furanilcarbonil)oxi]-11β-hidroxi-16α-metil-3-oxoandrosta-1,4-dien-17β-carbonilsulfénico. |

Tabla-6: Datos de espectro de los compuestos sintetizados

| Com-puesto No. | ¹ H-NMR (δ ppm). MASA (EI / ES+, m/z) |
|----------------|---|
| IA.1 | 1.19 (s, 3H), 1.29 (t, 3H, J=7.1Hz), 1.45 (s, 3H), 1.5-1.54 (m, 1H), 1.66-1.73 (m, 3H), 1.81-1.84 (m, 1H), 1.95-2.24 (m, 6H), 2.32-2.36 (m, 1H), 2.56-2.62 (m, 1H), 2.9-3.0 (m, 1H), 4.1-4.2 (q, 2H, J=7.1), 4.51 (br, d, 1H, J=2.51Hz), 5.07 (d, 1H, J=16.4Hz), 5.62 (d, 1H, J=16.4Hz), 6.17 (s, 1H), 6.27 (dd, 1H, J ₁ =10.1Hz, J ₂ =1.8Hz), 7.27 (d, 1H, J=10.4Hz), 7.47 (d, 2H, J=6.9Hz), 7.84 (d, 2H, J=6.9Hz). MASA (ES+): 592.9 (M+Na) ⁺ . |
| IA.2 | 0.96 (d, 3H, J=7.16Hz), 1.11-1.15 (m, 3H), 1.24 (s, 3H), 1.55 (s, 3H), 1.67 (s, 2H), 1.71-1.89 (m, 3H), 2.25-2.40 (m, 6H), 3.3-3.4 (m, 1H), 4.42 (br, 1H), 4.95 (d, 1H, J=16.6Hz), 5.69 (d, 1H, J=16.6Hz), 5.3-5.37 & 5.43-5.49 (m, 1H), 6.38 (dd, 1H, J ₁ =10.14Hz, J ₂ =1.8Hz), 6.45 (s, 1H), 7.16 (dd, 1H, J ₁ =10.1Hz, J ₂ =1.8Hz), 7.49 (d, 2H, J=8.8Hz), 7.56 (d, 2H, J=8.6Hz). MASA (ES+): 627.0 (M+Na) ⁺ . |
| IA.3 | 0.99 (d, 3H, J=7.14Hz), 1.11-1.14 (m, 6H), 1.53 (s, 3H), 1.62 (s, 2H), 1.7-1.91 (m, 4H), 2.21-2.29 (m, 2H), 2.34-2.38 (m, 4H), 3.35-3.42 (m, 1H), 4.3 (d, 1H, J=16.5Hz), 4.41 (br, 1H), 4.48 (d, 1H, J=16.5Hz), 5.30-5.35 & 5.42-5.47 (m, 1H), 6.38 (dd, 1H, J ₁ =10.15Hz, J ₂ =1.75Hz), 6.43 (s, 1H), 7.12 (d, 1H, J=10.15Hz), 7.47 (d, 2H, J=8.5Hz), 7.9 (d, 2H, J=8.5Hz). MASA (ES+): 643.1 (M+Na) ⁺ . |
| IA.4 | 1.16 (d, 1H, J=3.30Hz), 1.20 (s, 3H), 1.29 (t, 3H, J=7.10Hz), 1.48 (s, 3H), 1.54 (m, 2H), 1.70 (m, 1H), 1.83 (m, 2H), 1.96-2.22 (m, 5H), 2.34 (m, 1H), 2.59 (m, 1H), 2.95 (m, 1H), 4.16 (q, 2H, J=7.00Hz), 4.52 (br, 1H), 5.08 (d, 1H, J=16.32Hz), 5.63 (d, 1H, J=16.32Hz), 6.02 (s, 1H), 6.27 (dd, 1H, J ₁ =10.59Hz, J ₂ =1.67Hz), 7.17 (dd, 2H, J ₁ =J ₂ =8.55Hz), 7.28 (d, 1H, J=10.19Hz), 7.94 (dd, 2H, J ₁ =8.76, J ₂ =5.31). MASA (EI): 554 |
| IA.5 | 0.96 (s, 3H), 1.13 (t, 3H, J=7.55Hz), 1.24 (s, 3H), 1.30 (m, 1H), 1.55 (s, 3H), 1.82 (m, 2H), 2.05 (m, 2H), 2.20 (br, 1H), 2.25-2.50 (m, 6H), 3.35 (m, 1H), 4.41 (d, 1H, J=8.52Hz), 5.00 (d, 1H, J=16.53), 5.33 & 5.46 (m, 1H), 5.69 (d, 1H, J=16.53Hz), 6.38 (1H, dd, J ₁ =10.15Hz, J ₂ =1.64Hz), 6.44 (s, 1H), 7.18 (dd, 2H, J ₁ =J ₂ =8.50Hz), 7.95 (dd, 2H, J ₁ =8.70Hz, J ₂ =5.30Hz). MASA (ES+): 611.1 (M+Na) ⁺ . |
| IA.6 | 0.99 (d, 3H, J=7.15Hz), 1.13 (m, 6H), 1.25 (s, 1H), 1.33 (m, 1H), 1.53 (s, 3H), 1.86 (m, 3H), 2.26 (m, 2H), 2.39 (m, 4H), 3.39 (m, 1H), 4.32 (d, 1H, J=16.48Hz), 4.41 (d, 1H, J=8.92Hz), 4.48 (d, 1H, J=16.49Hz), 5.32 & 5.44 (m, 1H), 6.38 (dd, 1H, J ₁ =10.15Hz, J ₂ =1.69Hz), 6.44 (s, 1H), 7.12 (dd, 1H, J ₁ =10.19Hz, J ₂ =0.95Hz), 7.17 (dd, 2H, J ₁ =J ₂ =8.50Hz), 8.05 (dd, 2H, J ₁ =10.26Hz, J ₂ =5.35Hz). MASA (ES+): 627.1 (M+Na) ⁺ . |
| IA.7 | 1.18 (dd, 2H, J ₁ =11.44Hz, J ₂ =3.21Hz), 1.21 (s, 3H), 1.29 (t, 3H, J=7.11Hz), 1.48 (s, 3H), 1.52 (m, 1H), 1.66-1.84 (m, 2H), 1.95-2.22 (m, 6H), 2.32-2.36 (m, 1H), 2.91-2.98 (m, 1H), 4.16 (q, 2H, J=7.14Hz), 4.52 (s, 1H), 5.00 (dd, 1H, J ₁ =17.35Hz, J ₂ =1Hz 3.61), 5.48 (dd, 1H, J ₁ =17.35Hz, J ₂ =3.61Hz), 6.02 (s, 1H), 6.22 (dd, 1H, J ₁ =10.09Hz, J ₂ =1.73Hz), 6.92 (t, 1H, J=6.67Hz), 7.00 (1H, t, |

| Com-
puesto
No. | 1H-NMR (δ ppm). MASA (EI / ES+, m/z) |
|-----------------------|--|
| | J=6.67Hz), 7.29 (1H, d, J=10.15Hz), 8.01 (dd, 1H, J ₁ =8.25Hz, J ₂ =6.75Hz). MASA (ES+): 595.1 (M+Na) ⁺ |
| IA.8 | 1.13 (s, 3H), 1.16 (dd, 2H, J ₁ =11.37Hz, J ₂ =3.2Hz), 1.28 (t, 3H, J=7.13Hz), 1.47 (s, 3H), 1.50-1.52 (m, 1H), 1.64-1.68 (m, 1H), 1.80-1.83 (m, 1H), 1.91-2.20 (m, 6H), 2.33 (dd, 1H, J ₁ =13.36Hz, J ₂ =2.80Hz), 2.53-2.61 (m, 1H), 2.88-2.95 (m, 1H), 4.14 (q, 2H, J=7.12Hz), 4.51 (s, 1H), 5.00 (d, 1H, J=16.75Hz), 5.41 (d, 1H, J=16.75Hz), 6.02 (s, 1H), 6.26 (dd, 1H, J ₁ =10.01, J ₂ =1.78Hz), 7.27 (d, 1H, J=10.09Hz), 7.36 (dd, 1H, J ₁ =8.38Hz, J ₂ =1.93Hz), 7.47 (d, 1H, J=1.89Hz), 7.62 (d, 1H, J=8.37Hz). MASA (ES+): 627.0 (M+Na) ⁺ . |
| IA.9 | 0.96 (d, 3H, J=7.14Hz), 1.14 (t, 3H, J=7.57Hz), 1.26 (s, 3H), 1.29-1.34 (m, 3H), 1.56 (s, 3H), 1.71-1.88 (m, 4H), 2.02-2.05 (m, 1H), 2.25-2.50 (m, 6H), 3.33-3.38 (m, 1H), 4.42 (d, 1H, J=8.87Hz), 4.92 (dd, 1H, J ₁ =17.59Hz, J ₂ =3.07Hz), 5.35 & 5.46 (m, 1H), 5.56 (dd, 1H, J ₁ =17.59Hz, J ₂ =3.07Hz), 6.38 (dd, 1H, J ₁ =10.14Hz, J ₂ =1.70Hz), 6.44 (s, 1H), 6.90-7.04 (m, 1H), 7.15 (d, 1H, J=10.12Hz), 8.00 (dd, 1H, J ₁ =15.04Hz, J ₂ =8.43Hz). MASA (ES+): 629.0 (M+Na) ⁺ . |
| IA.10 | 0.94 (d, 3H, J=6.91Hz), 1.12 (t, 3H, J=7.51Hz), 1.18 (s, 3H), 1.24-1.32 (m, 2H), 1.55 (s, 3H), 1.71-1.96 (m, 4H), 2.27-2.48 (m, 5H), 3.32 (s, 1H), 4.40 (d, 1H, J=7.18Hz), 4.90 (d, 1H, J=16.85Hz); 5.33 (m, 0.5H), 5.46 (d, 1.5H, J=16.87Hz), 6.38 (d, 1H, J=10.07Hz), 6.44 (s, 1H), 7.15 (d, 1H, J=9.95Hz), 7.37 (d, 1H, J=8.30Hz), 7.49 (s, 1H), 7.64 (d, 1H, J=8.33). MASA (ES+): 661.0 (M+Na) ⁺ . |
| IA.11 | 0.98 (d, 3H, J=7.13Hz), 1.10-1.13 (m, 6H), 1.26-1.35 (m, 2H), 1.54 (s, 3H), 1.72-2.01 (m, 4H), 2.23-2.46 (m, 5H), 3.37 (m, 1H), 4.92 (dd, 1H, J ₁ =17.43Hz, J ₂ =2.69Hz), 4.43 (dd, 2H, J ₁ =17.44Hz, J ₂ =2.76Hz), 5.33 & 5.45 (m, 1H), 6.37 (dd, 1H, J ₁ =10.13Hz, J ₂ =1.73Hz), 6.43 (s, 1H), 6.89-7.01 (m, 2H), 7.16 (dd, 1H, J ₁ =10.14Hz, J ₂ =1.05Hz), 7.94 (dd, 1H, J ₁ =15.09Hz, J ₂ =8.50Hz). M ASS (ES+): 645.0 (M + Na) ⁺ . |
| IA.12 | 1.15 (d, 1H, J=3.26Hz), 1.17 (s, 4H), 1.29 (t, 3H, J=7.13Hz), 1.48 (s, 3H), 1.51-1.54 (m, 1H), 1.66-1.73 (m, 2H), 1.81-1.84 (m, 1H), 1.95-2.22 (m, 5H), 2.34 (dd, 1H, J ₁ =13.41Hz, J ₂ =2.71Hz), 2.56-2.62 (m, 1H), 2.90-2.97 (m, 1H), 4.15 (q, 2H, J=7.15Hz), 4.52 (s, 1H), 5.06 (d, 1H, J=16.43Hz), 5.56 (d, 1H, J=16.43Hz), 6.02 (s, 1H), 6.27 (dd, 1H, J ₁ =10.08Hz, J ₂ =1.70Hz), 7.29 (d, 1H, J=10.08Hz), 7.59 (d, 1H, J=8.34Hz), 7.73 (dd, 1H, J ₁ =8.35Hz, J ₂ =1.92Hz), 7.99 (d, 1H, J=1.88Hz). MASA (ES+): 627.0 (M+Na) ⁺ . |
| IA.13 | 0.97 (d, 3H, J=7.16Hz), 1.05 (s, 3H), 1.12 (t, 3H, J=7.58Hz), 1.28-1.35 (m, 2H), 1.53 (s, 3H), 1.72-1.94 (m, 3H), 2.24-2.42 (m, 6H), 3.35 (m, 1H), 4.21 (d, 1H, J=16.84Hz), 4.34 (d, 1H, J=6.84Hz), 5.32 & 5.44 (m, 1H), 6.38 (dd, 1H, J ₁ =10.14Hz, J ₂ =1.78Hz), 6.43 (s, 1H), 7.11 (dd, 1H, J ₁ =10.12Hz, J ₂ =1.22Hz), 7.35 (dd, 1H, J ₁ =8.34Hz, J ₂ =1.92Hz), 7.46 (d, 1H, J=8.33Hz). MASA (ES+): 677.0 (M+Na) ⁺ . |
| IA.14 | 0.99 (3H, d, J=7.10Hz), 1.10 (s, 3H), 1.12 (t, 3H, J=7.57Hz), 1.33 (m, 1H), 1.53 (s, 3H), 1.73-1.97 (m, 5H), 2.20-2.46 (m, 5H), 3.37 (m, 1H), 4.28 (d, 2H, J=16.38Hz), 4.41 (d, 2H, J=15.93Hz), 5.32 & 5.44 (m, 1H), 6.36 (d, 1H, J=10.14Hz), 6.43 (s, 1H), 7.13 (d, 1H, J=10.14Hz), 7.58 (d, 1H, J=8.35Hz), 7.83 (dd, 1H, J ₁ =8.23Hz, J ₂ =1.66Hz), 8.08 (d, 1H, J=1.71Hz). MASA (ES+): 677.0 (M+Na) ⁺ . |
| IA.15 | 0.96 (d, 3H, J=7.10Hz), 1.13 (t, 3H, J=7.56Hz), 1.22 (s, 3H), 1.26-1.33 (m, 2H), 1.55 (s, 3H), 1.71-1.90 (m, 3H), 2.00 (d, 1H, J=14.88Hz), 2.27-2.50 (m, 5H), 3.34 (m, 1H), 4.41 (d, 1H, J=8.73Hz), 4.96 (d, 1H, J=16.66Hz), 5.33 & 5.45 (m, 1H), 5.64 (d, 1H, J=16.59Hz), 6.38 (d, 1H, J=10.14Hz), 6.44 (s, 1H), 7.14 (d, 1H, J=10.14Hz), 7.59 (d, 1H, J=8.35Hz), 8.01 (s, 1H). |
| IA.16 | 1.15 (m, 2H), 1.19 (s, 3H), 1.29 (t, 3H, J=7.13Hz), 1.61 (s, 3H), 1.66-1.84 (m, 2H), 1.95-2.22 (m, 6H), 2.32-2.36 (m, 1H), 2.55-2.63 (m, 2H), 2.92-2.98 (m, 1H), 4.15 (q, 2H, J=7.04Hz), 4.51 (br, 1H), 5.00 (d, 1H, J=16.00Hz), 5.58 (d, 1H, J=16.00Hz), 6.02 (s, 1H), 6.27 (dd, 1H, J ₁ =10.09Hz, J ₂ =1.74Hz), 7.18 (t, 1H, J=3.94Hz), 7.29 (s, 1H), 7.72 (d, 1H, J=4.92Hz), 7.75 (d, 1H, J=3.82Hz). MASA (ES+): 565.1 (M+Na) ⁺ . |
| IA.17 | 1.16 (s, 3H), 1.19 (m, 2H), 1.28 (t, 3H, J=7.13Hz), 1.45 (m, 2H), 1.47 (s, 3H), 1.67-2.38 (m, 6H), 2.51-2.67 (m, 1H), 2.88-3.00 (m, 1H), 4.14 (q, 2H, J ₁ =14.24Hz, J ₂ =7.11Hz), 4.51 (br, 1H), 4.94 (d, 1H, J=15.95Hz), 5.49 (d, 1H, J=15.98Hz), 6.02 (s, 1H), 6.27 (dd, 1H, J ₁ =10.07Hz, J ₂ =1.72Hz), 7.00 (d, 1H, J=4.08Hz), 7.27 (d, 1H, J=9.96Hz), 7.54 (d, 1H, J=4.09Hz). MASA (ES+): 599.0 (M+Na). |
| IA.18 | 0.95 (d, 3H, J=7.14Hz), 1.13 (t, 3H, J=7.56Hz), 1.20 (s, 3H), 1.26-1.36 (m, 1H), 1.54 (s, 3H), 1.77-2.04 (m, 4H), 2.25-2.43 (m, 6H), 3.30-3.37 (m, 1H), 4.40 (d, 1H, J=9.64Hz), 4.85 (d, 1H, J=16.19Hz), 5.28 & 5.51 (m, 1H), 5.56 (d, 1H, J=16.17Hz), 6.35-6.44 (m, 2H), 7.00 (d, 1H, J=4.09Hz), 7.14 (d, 1H, J=10.02Hz), 7.54 (d, 1H, J=4.08Hz). MASA (ES+): 633.0 (M+Na) ⁺ . |
| IA.19 | 1.17 (m, 2H), 1.18 (s, 3H), 1.28 (t, 3H, J=7.11Hz), 1.47 (s, 5H), 1.70-2.38 (m, 8H), 2.41 (s, 3H), 2.51-2.66 (m, 1H), 2.88-3.01 (m, 1H), 4.15 (q, 2H, J ₁ =14.21Hz, J ₂ =7.09Hz), 4.49 (br, 1H), 4.89 (d, 1H, J=16.20Hz), 5.49 (d, 1H, J=16.21Hz), 6.02 (s, 1H), 6.21 (d, 1H, J=3.51Hz), 6.27 (dd, 1H, J ₁ =10.11Hz, J ₂ =1.72Hz), 7.19 (d, 1H, J=3.46Hz), 7.28 (d, 1H, J=9.26Hz). MASA (EI): 540 |
| IA.20 | 0.99 (d, 3H, J=7.35Hz), 1.10-1.16 (m, 6H), 1.21-1.38 (m, 1H), 1.53 (s, 3H), 1.69-2.02 (m, 4H), 2.16-2.49 (m, 6H), 3.34-3.46 (m, 1H), 4.17 (d, 1H, J=16.03Hz), 4.35 (d, 1H, J=16.01Hz), 4.43 (br, 1H), 5.28 & 5.51 (m, 1H), 6.37 (d, 1H, J=10.33Hz), 6.99 (d, 1H, J=4.03Hz), 7.16 (d, 1H, J=10.03Hz), 7.65 (d, 1H, J=4.04Hz). MASA (ES+): 649.0 (M+Na) ⁺ . |
| IA.21 | 0.95 (d, 3H, J=7.13Hz), 1.13 (t, 3H, J=7.56Hz), 1.22 (s, 3H), 1.54 (s, 3H), 1.70-1.88 (m, 2H), 2.03-2.08 (m, 1H), 2.25-2.51 (m, 8H), 2.40 (s, 3H), 3.30-3.38 (m, 1H), 4.39 (d, 1H, J=8.28Hz), 4.80 (d, 1H, J=16.31Hz), 5.28 & 5.50 (m, 1H), 5.52 (d, 1H, J=16.33Hz), 6.21 (d, 1H, J=2.99Hz), 6.37 (dd, 1H, J ₁ =10.12Hz, J ₂ =1.77Hz), 6.43 (s, 1H), 7.15-7.20 (m, 2H). MASA (EI): 574. |
| IA.22 | 0.98 (d, 3H, J=7.13Hz), 1.09-1.16 (m, 6H), 1.22-1.37 (m, 1H), 1.53 (s, 3H), 1.69-2.56 (m, 10H), 2.41 (s, 3H), 3.36-3.43 (m, 1H), 4.12 (d, 1H, J=16.31Hz), 4.33 (d, 1H, J=16.33Hz), 4.43 (br, 1H), 5.28 & 5.52 (m, 1H), 6.21 (d, 1H, J=3.12Hz), 6.34-6.43 (m, 2H), 7.18 (dd, 1H, J ₁ =10.04Hz, J ₂ =1.03Hz), 7.27 (d, 1H, J=3.60Hz). MASA (ES+): 613.1 (M+Na) ⁺ . |
| IA.23 | 1.17 (s, 3H), 1.20 (s, 1H), 1.21 (s, 9H), 1.28 (t, 3H, J=7.12Hz), 1.43 (s, 1H), 1.47 (s, 3H), 1.63-2.97 (m, 12H), 4.14 (q, 2H, J ₁ =14.26Hz, J ₂ =7.12Hz), 4.49 (br, 1H), 4.63 (d, 1H, J=16.68Hz), 5.23 (d, 1H, J=16.69Hz), 6.01 (s, 1H), 6.27 (dd, 1H, J ₁ =10.10Hz, J ₂ =1.84Hz), 7.27 (d, 1H, J=9.73Hz). MASA (EI): 516. |
| IA.24 | 1.13 (s, 3H), 1.18-1.25 (m, 3H), 1.28 (t, 3H, J=7.12Hz), 1.47 (s, 3H), 1.55-2.16 (m, 8H), 2.18 (s, 3H), 2.36-2.96 (m, 3H), 4.14 (q, 2H, J=7.13Hz), 4.50 (d, 1H, J=16.83Hz), 4.51 (m, 1H), 4.92 (d, 1H, J=16.84Hz), 6.02 (s, 1H), 6.26 (dd, 1H, J ₁ =10.09Hz, J ₂ =1.82Hz), 7.28 (d, 1H, J=10.10Hz). MASA (EI): 474 |
| IA.25 | 0.94 (d, 3H, J=7.17Hz), 1.12 (t, 3H, J=7.56Hz), 1.21 (s, 12H), 1.26-1.39 (m, 1H), 1.54 (s, 3H), 1.77-2.41 (m, 10H), 3.28-3.35 (m, 1H), 4.38 (br, 1H), 4.54 (d, 1H, J=16.98Hz), 5.28 & 5.52 (m, 1H), 5.29 (d, 1H, J=16.91Hz), 6.38 (dd, 1H, J ₁ =10.10Hz, J ₂ =1.73Hz), 6.43 (s, 1H), 7.17 (dd, 1H, J ₁ =10.05Hz, J ₂ =1.10Hz). MASA (ES+): 573.2 (M+Na) ⁺ . |
| IA.26 | 0.98 (d, 3H, J=7.12Hz), 1.12 (s, 3H), 1.12 (t, 3H, J=7.54Hz), 1.24 (s, 9H), 1.23-1.34 (m, 1H), 1.54 (s, 3H), 1.75-2.50 (m, 10H), 3.34-3.42 (m, 1H), 3.89 (d, 1H, J=17.40Hz), 4.14 (d, 1H, J=17.38Hz), 4.38-4.42 (br, 1H), 5.28 & 5.52 (m, 1H), 6.37 (dd, 1H, J ₁ =10.20Hz, J ₂ =1.64Hz), 6.43 (s, 1H), 7.17 (d, 1H, J=9.96Hz). MASA (ES+): 589.1 (M+Na) ⁺ . |
| IA.27 | 0.99 (d, 3H, J=7.13Hz), 1.10 (s, 3H), 1.12 (t, 3H, J=7.55Hz), 1.20-1.39 (m, 2H), 1.53 (s, 3H), 1.69-1.97 (m, 4H), 2.22-2.42 (m, 8H), 3.33-3.40 (m, 1H), 3.72 (d, 1H, J=16.52Hz), 3.83 (d, 1H, J=16.51Hz), 4.40 (br, 1H), 5.28 & 5.50 (m, 1H), 6.38 (dd, 1H, J ₁ =10.08Hz, J ₂ =1.28Hz), 6.43 (s, 1H), 7.13 (dd, 1H, J ₁ =10.08Hz, J ₂ =1.37Hz). MASA (ES+): 547.1 (M+Na) ⁺ . |
| IA.28 | 0.94 (d, 3H, J=7.12Hz), 1.12 (t, 3H, J=7.58Hz), 1.17 (s, 3H), 1.24-1.35 (m, 1H), 1.55 (s, 3H), 1.70-1.95 (m, 3H), 2.18 (s, 3H), 2.24-2.42 (m, 7H), 3.30 (m, 1H), 4.39 (br, 1H), 4.43 (d, 1H, J=17.04Hz), 4.96 (d, 1H, J=17.04Hz), 5.28 & 5.52 (m, 1H), 6.37 (dd, 1H, J ₁ =10.10Hz, J ₂ =1.79Hz), 6.42 (s, 1H), 7.17 (dd, 1H, J ₁ =10.07Hz, J ₂ =1.11Hz). MASA (ES+): 531.1 (M+Na) ⁺ . |
| IA.29 | 1.15 (d, J=3.31Hz, 3H), 1.21 (s, 3H), 1.29 (t, J=7.08, 3H), 1.48 (s, 3H), 1.71-2.38 (m, 6H), 2.58 (m, 1H), 2.97 (m, 1H), 3.89 (s, 3H), 4.16 (q, J=7.07Hz, 2H), 4.51 (d, 1H), 5.05 (d, J=16.2Hz, 1H), 5.60 (d, J=16.2Hz, 1H), 6.02 (s, 1H), 6.27 (dd, J ₁ =10.11Hz, J ₂ =1.83Hz, 1H), 6.96 (d, J=8.9Hz, 2H), 7.28 (d, J=10.3Hz, 1H), 7.88 (d, J=8.9Hz, 2H). |
| IA.30 | 0.96 (d, J=7.11Hz 3H), 1.13 (t, J=7.5Hz 3H), 1.25 (s, 3H), 1.55 (s, 3H), 1.70-1.88 (m, 2H), 2.08 (d, J=15.9Hz, 1H), 2.26-2.46 (m, 7H), 2.56 (m, 1H), 3.34 (m, 1H), 3.38 (s, 3H), 4.40 (d, J=8.63Hz, 1H), 4.97 (d, J=16.41Hz, 1H), 5.42 (m, 1H), 5.70 (d, J=16.42, 1Hz, |

| Com-
puesto
No. | ¹ H-NMR (δ ppm). MASA (EI / ES+, m/z) |
|-----------------------|---|
| | 1H, 6.37 (dd, $J_1=10.1\text{Hz}$, $J_2=1.76\text{Hz}$, 1H), 6.43 (s, 1H), 6.95 (d, $J=10.9\text{Hz}$, 2H), 7.175 (dd, $J_1=10.1\text{Hz}$, $J_2=1.03\text{Hz}$, 1H), 7.88 (d, $J=8.89\text{Hz}$, 1H). MASA (ES+): 623.1 (M+Na) ⁺ . |
| IA.31 | 0.98 (d, $J=6.2\text{Hz}$, 3H), 1.11 (s, 3H), 1.13 (t, $J=7.3\text{Hz}$, 3H), 1.22-1.37 (m, 2H), 1.53 (s, 3H), 1.69-2.27 (m, 3H), 2.37 (q, $J=7.52\text{Hz}$, 2H), 2.15-2.35 (m, 4H), 3.40 (m, 1H), 3.88 (s, 3H), 4.30 (d, $J=16.5\text{Hz}$, 1H), 4.39 (bd, 1H), 4.52 (d, $J=16.5\text{Hz}$, 1H), 5.25-5.60 (m, 1H), 6.38 (dd, $J_1=10.10\text{Hz}$, $J_2=1.7\text{Hz}$, 1H), 6.42 (s, 1H), 6.95 (d, $J=8.8\text{Hz}$, 2H), 7.16 (d, $J=10\text{Hz}$, 1H), 7.98 (d, $J=8.89\text{Hz}$, 2H). MASA (ES+): 639.1 (M+Na) ⁺ . |
| IA.32 | 1.16 (s, 6H), 1.26 (t, $J=7.07\text{Hz}$, 3H), 1.47 (s, 3H), 1.54-2.36 (m, 24H), 2.57 (m, 1H), 2.90 (t, $J=11.31\text{Hz}$, 1H), 4.13 (q, $J=7.14\text{Hz}$, 2H), 4.49 (d, $J=1.39\text{Hz}$, 1H), 4.60 (d, $J=16.61\text{Hz}$, 1H), 5.21 (d, $J=16.70\text{Hz}$, 1H), 6.01 (s, 1H), 6.26 (dd, $J_1=1.64\text{Hz}$, $J_2=10.82\text{Hz}$, 1H), 7.27 (d, $J=3.22\text{Hz}$, 1H). MASA (ES+): 617.2 (M+Na) ⁺ . |
| IA.33 | 0.935 (d, $J=7.11\text{Hz}$, 3H), 1.11 (t, $J=7.66\text{Hz}$, 3H), 1.20-1.34 (m, 3H), 1.54 (s, 3H), 1.66-1.94 (m, 14H), 2.05 (d, $J=4.87\text{Hz}$, 6H), 2.18-2.51 (m, 6H), 3.30 (m, 1H), 4.38 (d, $J=8.13\text{Hz}$, 1H), 4.51 (d, $J=16.91\text{Hz}$, 1H), 5.25 (d, $J=17.23\text{Hz}$, 1H), 5.40-5.60 (m, 1H), 6.37 (dd, $J_1=1.73\text{Hz}$, $J_2=10.09\text{Hz}$, 1H), 6.42 (s, 1H), 7.15 (d, $J=9.011\text{Hz}$, 1H). MASA (ES+): 651.2 (M+Na) ⁺ . |
| IA.34 | 0.97 (d, $J=7.14\text{Hz}$, 3H), 1.12 (t, $J=7.57\text{Hz}$, 6H), 1.22-1.36 (m, 2H), 1.52 (s, 3H), 1.71 (s, 6H), 1.82-1.91 (m, 9H), 2.06 (s, 3H), 2.21-2.26 (m, 4H), 2.35 (q, $J=7.15\text{Hz}$, 2H), 3.39 (m, 1H), 3.84 (d, $J=17.48\text{Hz}$, 1H), 4.11 (d, $J=17.49\text{Hz}$, 1H), 4.40 (d, $J=7.69\text{Hz}$, 1H), 5.40-5.60 (m, 1H), 6.35 (d, $J=1.81\text{Hz}$, 1H), 6.41 (d, $J=6.48\text{Hz}$, 1H), 7.16 (dd, $J_1=1.21\text{Hz}$, $J_2=10.06\text{Hz}$, 1H). MASA (ES+): 667.1 (M+Na) ⁺ . |
| IA.35 | 0.99 (d, $J=7.06\text{Hz}$, 3H), 1.12 (t, $J=7.44\text{Hz}$, 6H), 1.22-1.38 (m, 2H), 1.53 (s, 3H), 1.69-2.02 (m, 3H), 2.16-2.38 (m, 6H), 3.38 (m, 1H), 4.30 (d, $J=16.50\text{Hz}$, 1H), 4.39 (s, 1H), 4.48 (d, $J=16.51\text{Hz}$, 1H), 5.20-5.50 (m, 1H), 6.345 (d, $J=1.69\text{Hz}$, 1H), 6.41 (d, $J=4.53\text{Hz}$, 1H), 7.16 (d, $J=10.03\text{Hz}$, 1H), 7.31 (d, $J=8.31\text{Hz}$, 2H), 8.06 (d, $J=8.87\text{Hz}$, 2H). MASA (ES+): 693.1 (M+Na) ⁺ . |
| IA.36 | 0.96 (d, $J=7.02\text{Hz}$, 3H), 1.12 (t, $J=7.50\text{Hz}$, 3H), 1.24-1.36 (m, 4H), 1.55 (s, 3H), 1.64-2.07 (m, 3H), 2.26-2.58 (m, 6H), 3.31-3.38 (m, 1H), 4.41 (d, $J=8.22\text{Hz}$, 1H), 5.03 (d, $J=16.58\text{Hz}$, 1H), 5.40 (m, 1H), 5.65 (d, $J=16.59\text{Hz}$, 1H), 6.35 (d, $J=1.62\text{Hz}$, 1H), 6.42 (d, $J=5.32\text{Hz}$, 1H), 7.17 (d, $J=9.99\text{Hz}$, 1H), 7.32 (d, $J=8.23\text{Hz}$, 2H), 7.97 (d, $J=8.76\text{Hz}$, 2H). MASA (ES+): 677.0 (M+Na) ⁺ . |
| IA.37 | 0.88-1.32 (m, 10H), 1.48 (s, 3H), 1.53-2.37 (m, 7H), 2.51-3.01 (m, 2H), 4.15 (q, $J=7.13\text{Hz}$, 2H), 4.52 (d, $J=2.46\text{Hz}$, 1H), 5.08 (d, $J=16.41\text{Hz}$, 1H), 5.64 (d, $J=16.41\text{Hz}$, 1H), 6.02 (s, 1H), 6.28 (dd, $J_1=1.78\text{Hz}$, $J_2=10.07\text{Hz}$, 1H), 7.26 (s, 1H), 7.33 (d, $J=8.60\text{Hz}$, 2H), 7.97 (d, $J=8.84\text{Hz}$, 2H). MASA (ES+): 643.1 (M+Na) ⁺ . |
| IA.38 | 1.00 (d, $J=7.18\text{Hz}$, 3H), 1.05-1.50 (m, 8H), 1.53 (s, 3H), 1.69-2.42 (m, 9H), 3.38 (m, 1H), 4.32 (d, $J=16.14\text{Hz}$, 1H), 4.40 (s, 1H), 4.50 (d, $J=16.10\text{Hz}$, 1H), 5.30 (m, 1H), 6.38 (dd, $J_1=1.67\text{Hz}$, $J_2=10.12\text{Hz}$, 1H), 6.43 (s, 1H), 7.12 (d, $J=10.05\text{Hz}$, 1H), 7.76 (d, $J=8.21\text{Hz}$, 2H), 8.12 (d, $J=8.08\text{Hz}$, 2H). MASA (ES+): 677.1 (M+Na) ⁺ . |
| IA.39 | 1.06 (d, $J=7.12\text{Hz}$, 3H), 1.17 (s, 3H), 1.36-1.41 (m, 1H), 1.55 (s, 3H), 1.72-2.01 (m, 4H), 2.28-2.49 (m, 4H), 3.43-3.48 (m, 1H), 4.38 (d, $J=16.56\text{Hz}$, 1H), 4.47 (d, $J=10.79\text{Hz}$, 1H), 4.52 (d, $J=16.65\text{Hz}$, 1H), 5.32-5.49 (m, 1H), 6.41 (d, $J_1=10.13\text{Hz}$, $J_2=1.79\text{Hz}$, 1H), 6.46 (s, 1H), 6.93 (d, $J=4.181\text{Hz}$, 1H), 7.14 (d, $J_1=10.19\text{Hz}$, $J_2=1.16\text{Hz}$, 1H), 7.52 (d, $J=4.00\text{Hz}$, 1H), 7.77 (d, $J=8.24\text{Hz}$, 2H), 8.12 (d, $J=8.13\text{Hz}$, 2H). MASA (ES+): 743.5 |
| IA.40 | 1.05 (d, $J=7.15\text{Hz}$, 3H), 1.11 (s, 3H), 1.34-1.40 (m, 1H), 1.54 (s, 3H), 1.77-2.01 (m, 4H), 2.25 (s, 6H), 2.28 (s, 3H), 2.28-2.50 (m, 4H), 3.45-3.50 (m, 1H), 4.09 (d, $J=17.76\text{Hz}$, 1H), 4.29 (d, $J=17.83\text{Hz}$, 1H), 4.43 (d, $J=8.40\text{Hz}$, 1H), 5.32-5.48 (m, 1H), 6.40 (dd, $J_1=10.15\text{Hz}$, $J_2=1.79\text{Hz}$, 1H), 6.46 (s, 1H), 6.85 (s, 2H), 6.93 (d, $J=4.09\text{Hz}$, 1H), 7.14 (dd, $J_1=10.11\text{Hz}$, $J_2=1.00\text{Hz}$, 1H), 7.52 (d, $J=4.07\text{Hz}$, 1H). MASA (ES+): 717.5 |
| IA.41 | 1.06 (d, $J=7.16\text{Hz}$, 3H), 1.10 (s, 3H), 1.29-1.35 (m, 1H), 1.67 (s, 3H), 1.77-1.92 (m, 4H), 2.25 (s, 6H), 2.28 (s, 3H), 2.42-2.87 (m, 5H), 3.45-3.48 (m, 1H), 4.07 (d, $J=17.54\text{Hz}$, 1H), 4.31 (d, $J=17.68\text{Hz}$, 1H), 4.59 (s, 1H), 6.11 (s, 1H), 6.36 (dd, $J_1=10.09\text{Hz}$, $J_2=1.74\text{Hz}$, 1H), 6.49 (dd, $J_1=3.45\text{Hz}$, $J_2=1.67\text{Hz}$, 1H), 6.85 (s, 2H), 7.17 (d, $J=3.45\text{Hz}$, 1H), 7.20 (d, $J=10.13\text{Hz}$, 1H), 7.58 (d, $J=0.8\text{Hz}$, 1H). MASA (ES+): 687.5 (M+Na) ⁺ . |
| IA.42 | 0.96 (d, $J=7.10\text{Hz}$, 3H), 1.13 (t, $J=7.35\text{Hz}$, 2H), 1.22-1.34 (m, 4H), 1.55 (s, 3H), 1.64-2.04 (m, 7H), 2.17-2.51 (m, 4H), 3.10 (s, 3H), 3.34 (m, 1H), 4.41 (d, $J=8.44\text{Hz}$, 1H), 5.02 (d, $J=16.63\text{Hz}$, 1H), 5.44 (m, 1H), 5.70 (d, $J=16.73\text{Hz}$, 1H), 6.38 (d, $J=10.14\text{Hz}$, 1H), 6.44 (s, 1H), 7.14 (d, $J=10.14\text{Hz}$, 1H), 8.09 (s, 4H). MASA (ES+): 671.0 (M+Na) ⁺ . |
| IA.43 | 0.99 (d, $J=7.11\text{Hz}$, 3H), 1.12 (t, $J=7.54\text{Hz}$, 3H), 1.24-1.52 (m, 4H), 1.72-1.90 (m, 8H), 2.23-2.43 (m, 6H), 3.10 (s, 3H), 3.35 (m, 1H), 4.36 (d, $J=16.36\text{Hz}$, 1H), 4.40 (d, 1H), 4.43 (d, $J=16.19\text{Hz}$, 1H), 5.40 (m, 1H), 6.37 (d, $J=10.14\text{Hz}$, 1H), 6.43 (s, 1H), 7.11 (d, $J=10.09\text{Hz}$, 1H), 8.04 (d, $J=8.32\text{Hz}$, 2H), 8.17 (d, $J=8.33\text{Hz}$, 2H). MASA (ES+): 687.0 (M+Na) ⁺ . |
| IA.44 | 0.96 (d, $J=7.14\text{Hz}$, 3H), 1.13 (t, $J=7.56\text{Hz}$, 3H), 1.24-1.33 (m, 3H), 1.70-2.08 (m, 8H), 2.25-2.42 (m, 6H), 3.36 (m, 1H), 4.41 (d, $J=8.98\text{Hz}$, 1H), 5.02 (d, $J=16.63\text{Hz}$, 1H), 5.40 (m, 1H), 5.75 (d, $J=16.64\text{Hz}$, 1H), 6.38 (dd, $J_1=1.52\text{Hz}$, $J_2=10.13\text{Hz}$, 1H), 6.44 (s, 1H), 7.12 (d, $J=10.09\text{Hz}$, 1H), 7.50 (t, $J=7.73\text{Hz}$, 2H), 7.63 (t, $J=7.38\text{Hz}$, 1H), 7.91 (d, $J=7.47\text{Hz}$, 2H). MASA (ES+): 593.1 (M+Na) ⁺ . |
| IA.45 | 1.00 (d, $J=7.12\text{Hz}$, 3H), 1.13 (t, $J=7.67\text{Hz}$, 6H), 1.14-1.35 (m, 3H), 1.67-2.00 (m, 6H), 2.23-2.44 (m, 5H), 3.40 (m, 1H), 4.35 (d, $J=16.72\text{Hz}$, 1H), 4.40 (d, $J=9.27\text{Hz}$, 1H), 4.53 (d, $J=16.82\text{Hz}$, 1H), 5.40 (m, 1H), 6.38 (dd, $J_1=1.22\text{Hz}$, $J_2=10.10\text{Hz}$, 1H), 6.43 (s, 1H), 7.12 (d, $J=10.05\text{Hz}$, 1H), 7.49 (t, $J=7.71\text{Hz}$, 2H), 7.61 (t, $J=7.43\text{Hz}$, 1H), 8.01 (d, $J=1\text{Hz}$, 2H). MASA (ES+): 609.1 (M+Na) ⁺ . |
| IA.46 | 0.96 (d, $J=7.11\text{Hz}$, 3H), 1.13 (t, $J=7.55\text{Hz}$, 3H), 1.24 (s, 3H), 1.27-2.09 (m, 8H), 2.24-2.40 (m, 6H), 2.43 (s, 3H), 3.36 (m, 1H), 4.41 (d, $J=8.93\text{Hz}$, 1H), 5.00 (d, $J=16.55\text{Hz}$, 1H), 5.40 (m, 1H), 5.73 (d, $J=16.56\text{Hz}$, 1H), 6.37 (dd, $J_1=10.18\text{Hz}$, $J_2=1.37\text{Hz}$, 1H), 6.44 (s, 1H), 7.15 (d, $J=10.15\text{Hz}$, 1H), 7.29 (d, $J=8.01\text{Hz}$, 2H), 7.80 (d, $J=8.08\text{Hz}$, 2H). MASA (ES+): 607.1 (M+Na) ⁺ . |
| IA.47 | 0.99 (d, $J=7.15\text{Hz}$, 3H), 1.12 (t, $J=7.49\text{Hz}$, 6H), 1.29-2.00 (m, 8H), 2.20-2.42 (m, 6H), 2.42 (s, 3H), 3.40 (m, 1H), 4.34 (d, $J=16.63\text{Hz}$, 1H), 4.40 (d, $J=8.60\text{Hz}$, 1H), 4.52 (d, $J=16.61\text{Hz}$, 1H), 5.40 (m, 1H), 6.37 (dd, $J_1=10.17\text{Hz}$, $J_2=1\text{Hz}$, 1H), 6.43 (s, 1H), 7.13 (d, $J=10.15\text{Hz}$, 1H), 7.28 (d, $J=8.05\text{Hz}$, 2H), 7.90 (d, $J=8.17\text{Hz}$, 2H). MASA (ES+): 623.1 (M+Na) ⁺ . |
| IA.48 | 0.93 (d, $J=7.14\text{Hz}$, 3H), 1.11 (t, $J=7.56\text{Hz}$, 3H), 1.15 (s, 3H), 1.25-1.84 (m, 8H), 2.21-2.38 (m, 6H), 3.32 (m, 1H), 4.34 (d, $J=8.93\text{Hz}$, 1H), 4.81 (d, $J=17.90\text{Hz}$, 1H), 5.40 (m, 1H), 5.41 (d, $J=17.68\text{Hz}$, 1H), 6.38 (dd, $J_1=10.17\text{Hz}$, $J_2=1.49\text{Hz}$, 1H), 6.43 (s, 1H), 7.11 (d, $J=10.07\text{Hz}$, 1H), 7.36 (d, $J=2.95\text{Hz}$, 3H). MASA (ES+): 661.0 (M+Na) ⁺ . |
| IA.49 | 0.98 (d, $J=7.13\text{Hz}$, 3H), 1.07 (s, 3H), 1.12 (t, $J=7.554\text{Hz}$, 3H), 1.25-2.01 (m, 8H), 2.23-2.43 (m, 6H), 3.40 (m, 1H), 4.25 (d, $J=17.50\text{Hz}$, 1H), 4.42 (d, $J=8.45\text{Hz}$, 1H), 4.45 (d, $J=17.57\text{Hz}$, 1H), 5.40 (m, 1H), 6.39 (d, $J=10.15\text{Hz}$, 1H), 6.43 (s, 1H), 7.13 (d, $J=10.11\text{Hz}$, 1H), 7.26-7.36 (m, 3H). MASA (ES+): 677.0 (M+Na) ⁺ . |
| IA.50 | 0.93 (d, $J=7.14\text{Hz}$, 3H), 1.08 (s, 3H), 1.12 (t, $J=7.53\text{Hz}$, 3H), 1.26-1.86 (m, 8H), 2.24-2.38 (m, 6H), 3.29 (m, 1H), 4.39 (d, $J=8.69\text{Hz}$, 1H), 4.85 (d, $J=19.97\text{Hz}$, 1H), 5.36 (d, $J=17.05\text{Mz}$, 1H), 5.40 (m, 1H), 6.38 (dd, $J_1=10.10\text{Hz}$, $J_2=1.50\text{Hz}$, 1H), 6.43 (s, 1H), 7.15 (d, $J=10.11\text{Hz}$, 1H), 7.33 (t, $J=7.90\text{Hz}$, 1H), 7.47 (dd, $J_1=7.60\text{Hz}$, $J_2=1.21\text{Hz}$, 1H), 7.62 (dd, $J_1=73871\text{Hz}$, $J_2=1.11\text{Hz}$, 1H). MASA (ES+): 661.0 (M+Na) ⁺ . |
| IA.51 | 0.97 (d, $J=7.13\text{Hz}$, 3H), 1.01 (s, 3H), 1.12 (t, $J=7.55\text{Hz}$, 3H), 1.29-1.95 (m, 8H), 2.24-2.40 (m, 6H), 3.35 (m, 1H), 4.17 (d, $J=16.89\text{Hz}$, 1H), 4.32 (d, $J=16.88\text{Hz}$, 1H), 4.41 (d, $J=8.19\text{Hz}$, 1H), 5.40 (m, 1H), 6.38 (dd, $J_1=10.04\text{Hz}$, $J_2=1.50\text{Hz}$, 1H), 6.43 (s, 1H), 7.13 (d, $J=10.14\text{Hz}$, 1H), 7.31 (d, $J=7.89\text{Hz}$, 1H), 7.53 (dd, $J_1=7.62\text{Hz}$, $J_2=1.15\text{Hz}$, 1H), 7.58 (dd, $J_1=8.01\text{Hz}$, $J_2=1.19\text{Hz}$, 1H). MASA (ES+): 677.0 (M+Na) ⁺ . |
| IA.52 | 0.94 (d, $J=7.16\text{Hz}$, 3H), 1.12 (t, $J=7.55\text{Hz}$, 3H), 1.19 (s, 3H), 1.25-1.97 (m, 8H), 2.17-2.41 (m, 6H), 3.34 (m, 1H), 4.39 (d, $J=8.73\text{Hz}$, 1H), 4.81 (d, $J=17.22\text{Hz}$, 1H), 5.38 (m, 1H), 5.42 (d, $J=17.55\text{Hz}$, 1H), 6.38 (dd, $J_1=10.13\text{Hz}$, $J_2=1.37\text{Hz}$, 1H), 6.43 (s, 1H), 7.02 (d, $J=8.53\text{Hz}$, 2H), 7.15 (d, $J=10.17\text{Hz}$, 1H), 7.47-7.51 (m, 1H). MASA (ES+): 629.1 (M+Na) ⁺ . |
| IA.53 | 0.97 (d, $J=7.13\text{Hz}$, 3H), 1.07 (s, 3H), 1.10 (t, $J=7.54\text{Hz}$, 3H), 1.16-1.95 (m, 8H), 2.22-2.44 (m, 6H), 3.36 (m, 1H), 4.17 (d, $J=16.90\text{Hz}$, 1H), 4.29 (d, $J=16.88\text{Hz}$, 1H), 4.40 (d, $J=8.72\text{Hz}$, 1H), 5.40 (m, 1H), 6.37 (dd, $J_1=10.16\text{Hz}$, $J_2=1.46\text{Hz}$, 1H), 6.43 (s, 1H), 7.13 (d, $J=10.11\text{Hz}$, 1H), 7.33 (t, $J=7.90\text{Hz}$, 1H), 7.47 (dd, $J_1=7.60\text{Hz}$, $J_2=1.21\text{Hz}$, 1H), 7.62 (dd, $J_1=73871\text{Hz}$, $J_2=1.11\text{Hz}$, 1H). MASA (ES+): 661.0 (M+Na) ⁺ . |

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No. | ¹ H-NMR (δ ppm). MASA (EI / ES+, m/z) |
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| | 1H), 6.98 (t, J=8.34Hz, 2H), 7.13 (d, J=9.90Hz, 1H), 7.44 (d, J=7.62Hz, 1H). MASA (ES+): 645.0 (M+Na) ⁺ . |
| IA.54 | 0.96 (d, J=7.13Hz, 3H), 1.13 (t, J=7.55Hz, 3H), 1.24 (s, 3H), 1.25-1.99 (m, 8H), 2.17-2.43 (m, 6H), 3.35 (m, 1H), 4.42 (d, J=8.41Hz, 1H), 4.95 (dd, J ₁ =17.53Hz, J ₂ =2.75Hz, 1H), 5.40 (m, 1H), 5.57 (dd, J ₁ =17.55Hz, J ₂ =2.80Hz, 1H), 6.38 (d, J ₁ =10.10Hz, J ₂ =1.06Hz, 1H), (6.44 (s, 1H), 7.15 (d, J=10.15Hz, 1H), 7.22 (d, J ₁ =10.05Hz, J ₂ =5.61Hz, 1H), 7.43 (d, J ₁ =16.25Hz, J ₂ =8.85Hz, 1H), 7.69 (t, J=7.42Hz, 1H). MASA (ES+): 629.1 (M+Na) ⁺ . |
| IA.55 | 0.98 (d, J=7.08Hz, 3H), 1.10-1.14 (m, 6H), 1.24-1.99 (m, 8H), 2.23-2.43 (m, 6H), 3.36 (m, 1H), 4.20 (dd, J ₁ =17.37Hz, J ₂ =1.85Hz, 1H), 4.43 (dd, J ₁ =17.25Hz, J ₂ =2.03Hz, 2H), 5.40 (m, 1H), 6.38 (d, J=10.14Hz, 1H), 6.43 (s, 1H), 7.13 (d, J=10.11Hz, 1H), 7.21 (dd, J ₁ =12.35Hz, J ₂ =7.03Hz, 1H), 7.40 (d, J=8.21Hz, 1H), 7.63 (t, J=6.40Hz, 1H). MASA (ES+): 645.1 (M+Na) ⁺ . |
| IA.56 | 1.06 (d, J=7.11Hz, 3H), 1.17 (s, 3H), 1.35-1.41 (m, 1H), 1.54 (s, 3H), 1.77-2.03 (m, 4H), 2.28-2.40 (m, 4H), 3.43-3.49 (m, 1H), 4.34 (d, 1H, J=16.58Hz), 4.47 (d, J=6.32Hz, 1H), 4.50 (d, J=16.57Hz, 1H), 5.32-5.49 (m, 1H), 6.40 (dd, J ₁ =10.19Hz, J ₂ =1.84Hz, 1H), 6.46 (s, 1H), 6.93 (d, J=3.95Hz, 1H), 7.14 (dd, J ₁ =10.12Hz, J ₂ =1.10Hz, 1H), 7.47 (d, J=8.60Hz, 2H), 7.52 (d, J=406Hz, 1H), 7.95 (d, J=8.60Hz, 2H). MASA (ES+): 731.5 (M+Na) ⁺ . |
| IA.57 | 0.93 (d, J=7.11Hz, 3H), 1.07 (s, 3H), 1.11 (t, J=7.54Hz, 3H), 1.25-1.82 (m, 8H), 2.25 (s, 9H), 2.22-2.37 (m, 6H), 3.31 (m, 1H), 4.27 (d, J=8.71Hz, 1H), 4.55 (d, J=17.82Hz, 1H), 5.33 (d, J=17.85Hz, 1H), 5.40 (m, 1H), 6.38 (d, J ₁ =10.14Hz, J ₂ =1.44Hz, 1H), 6.43 (s, 1H), 6.87 (s, 2H), 7.11 (d, J=9.94Hz, 1H). MASA (ES-): 611.3 (M-H) ⁺ . |
| IA.58 | 0.98 (d, J=7.07Hz, 3H), 1.03 (s, 3H), 1.12 (t, J=7.53Hz, 3H), 1.25-1.95 (m, 8H), 2.25 (s, 9H), 2.22-2.41 (m, 6H), 3.40 (m, 1H), 4.05 (d, J=17.72Hz, 1H), 4.28 (d, J=17.74Hz, 1H), 4.38 (d, J=8.06Hz, 1H), 5.41 (m, 1H), 6.38 (d, J=10.17Hz, 1H), 6.43 (s, 1H), 6.85 (s, 2H), 7.12 (d, J=10.13Hz, 1H). MASA (ES+): 651.1 (M+Na) ⁺ . |
| IA.59 | 0.44 (s, 3H), 0.95 (d, J=7.02Hz, 3H), 1.08 (t, J=7.53Hz, 3H), 1.22-1.75 (m, 15H), 2.17-2.32 (m, 6H), 3.15 (m, 1H), 4.20 (d, J=6.81Hz, 1H), 5.40 (m, 1H), 6.35 (dd, J ₁ =10.11Hz, J ₂ =1.43Hz, 1H), 6.40 (s, 1H), 7.05 (d, J=9.98Hz, 1H), 7.36 (t, J=7.70Hz, 2H), 7.46 (t, J=7.20Hz, 1H), 7.95 (d, J=7.43Hz, 2H). MASA (ES+): 637.1 (M+Na) ⁺ . |
| IA.60 | 0.96 (d, J=7.10Hz, 3H), 1.13 (t, J=7.56Hz, 3H), 1.23-2.06 (m, 11H), 2.17-2.49 (m, 6H), 3.35 (m, 1H), 4.40 (d, J=8.55Hz, 1H), 4.93 (d, J=16.21Hz, 1H), 5.39 (m, 1H), 5.64 (d, J=16.21Hz, 1H), 6.38 (d, J ₁ =10.18Hz, J ₂ =1.30Hz, 1H), 6.43 (s, 1H), 7.15 (d, J=10.22Hz, 1H), 7.18 (t, J=4.56Hz, 1H), 7.73 (d, J=4.96Hz, 1H), 7.75 (d, J=3.66Hz, 1H). MASA (ES+): 599.2 (M+Na) ⁺ . |
| IA.61 | 0.99 (d, J=7.11Hz, 3H), 1.11-1.14 (m, 6H), 1.25-1.96 (m, 8H), 2.17-2.41 (m, 6H), 3.39 (m, 1H), 4.27 (d, J=16.28Hz, 1H), 4.41 (d, J=13.26Hz, 1H), 4.44 (d, J=16.48Hz, 1H), 5.42 (m, 1H), 6.38 (dd, J ₁ =10.16Hz, J ₂ =1.46Hz, 1H), 6.43 (s, 1H), 7.13 (d, J=9.66Hz, 1H), 7.17 (t, J=4.16Hz, 1H), 7.71 (d, J=4.90Hz, 1H), 7.86 (d, J=3.51Hz, 1H). MASA (ES+): 615.2 (M+Na) ⁺ . |
| IA.62 | 0.96 (d, J=7.11Hz, 3H), 1.13 (t, J=7.54Hz, 3H), 1.23 (s, 3H), 1.25-2.03 (m, 8H), 2.24-2.42 (m, 6H), 3.34 (m, 1H), 4.40-4.42 (m, 1H), 4.97 (d, J=16.57Hz, 1H), 5.40 (m, 1H), 5.64 (d, J=16.56Hz, 1H), 6.37 (d, J=10.15Hz, 1H), 6.44 (s, 1H), 7.14 (d, J=10.11Hz, 1H), 7.33-7.26 (m, 1H), 7.68-7.79 (m, 2H). MASA (ES+): 629.2 (M+Na) ⁺ . |
| IA.63 | 0.99 (d, J=7.09Hz, 3H), 1.11 (t, J=7.80Hz, 6H), 1.25-1.03 (m, 8H), 2.17-2.44 (m, 6H), 3.36 (m, 1H), 4.18-4.38 (m, 3H), 4.40 (d, J=16.10Hz, 1H), 5.38 (m, 1H), 6.33 (d, J=10.07Hz, 1H), 6.39 (s, 1H), 7.20 (d, J=10.05Hz, 1H), 7.28-7.32 (m, 1H), 7.79-7.85 (m, 1H). MASA (ES+): 645.1 (M+Na) ⁺ . |
| IA.64 | 0.95 (d, J=7.13Hz, 3H), 1.13 (t, J=7.56Hz, 3H), 1.22 (s, 3H), 1.25-2.05 (m, 8H), 2.24-2.49 (m, 6H), 3.32-3.37 (m, 1H), 4.40 (d, J=8.68Hz, 1H), 4.86 (d, J=16.63Hz, 1H), 5.32-5.48 (m, 1H), 5.58 (d, J=16.63Hz, 1H), 6.38 (d, J ₁ =10.13Hz, J ₂ =1.29Hz, 1H), 6.43 (s, 1H), 6.60 (d, J ₁ =3.19Hz, J ₂ =1.29Hz, 1H), 7.14 (d, J=10.16Hz, 1H), 7.27 (d, J=3.65Hz, 1H), 7.63 (s, 1H). MASA (ES+): 583.2 (M+Na) ⁺ . |
| IA.65 | 1.03 (d, J=7.10Hz, 3H), 1.25-1.95 (m, 10H), 2.07 (d, J=14.85Hz, 1H), 2.28-2.51 (m, 4H), 3.41-3.44 (m, 1H), 4.44 (d, J=8.26Hz, 1H), 5.02 (d, J=16.48Hz, 1H), 5.32-5.49 (m, 1H), 5.73 (d, J=16.48Hz, 1H), 5.97 (s, 1H), 6.38 (d, J=10.19Hz, 1H), 6.44 (s, 1H), 7.13-7.21 (m, 3H), 7.95 (d, J ₁ =8.18Hz, J ₂ =5.45Hz, 2H). MASA (ES-): 641.2 (M-H) ⁺ . |
| IA.66 | 1.03 (d, J=7.12Hz, 3H), 1.25-2.07 (m, 11H), 2.28-2.52 (m, 4H), 3.41-3.44 (m, 1H), 4.44 (d, J=8.40Hz, 1H), 4.93 (d, J ₁ =17.51Hz, J ₂ =3.47Hz, 1H), 5.32-5.49 (m, 1H), 5.67 (d, J ₁ =17.49Hz, J ₂ =3.40Hz, 1H), 5.96 (s, 1H), 6.38 (d, J ₁ =10.16Hz, J ₂ =1.38Hz, 1H), 6.44 (s, 1H), 6.91-6.97 (m, 1H), 7.01-7.05 (m, 1H), 7.15 (d, J=10.12Hz, 1H), 8.01 (d, J ₁ =14.98Hz, J ₂ =8.29Hz, 1H). MASA (ES+): 683.1 (M+Na) ⁺ . |
| IA.67 | 0.97 (d, J=7.10Hz, 3H), 1.14 (t, J=7.53Hz, 3H), 1.24-2.05 (m, 8H), 2.27-2.44 (m, 6H), 3.32-3.36 (m, 1H), 4.40 (d, J=9.07Hz, 1H), 5.00 (d, J=16.85Hz, 1H), 5.20-5.60 (m, 1H), 5.72 (d, J=16.81Hz, 1H), 6.38 (d, J ₁ =10.11Hz, J ₂ =1.74Hz, 1H), 6.44 (s, 1H), 7.15 (d, J=10.06Hz, 1H), 7.31-7.39 (m, 1H), 7.49-7.59 (m, 3H), 7.74 (d, J=7.85Hz, 1H). MASA (ES+): 633.2 (M+Na) ⁺ . |
| IA.68 | 0.99 (d, J=7.11Hz, 3H), 1.13 (d, J=7.32Hz, 6H), 1.25-1.99 (m, 8H), 2.23-2.45 (m, 6H), 3.38 (m, 1H), 4.19 (d, J=16.55Hz, 1H), 4.36 (d, J=16.90Hz, 1H), 4.40 (d, J=13.09Hz, 1H), 5.39 (m, 1H), 6.38 (dd, J ₁ =10.15Hz, J ₂ =1.46Hz, 1H), 6.43 (s, 1H), 7.13 (d, J=10.16Hz, 1H), 7.33 (d, J=3.51Hz, 1H), 7.64 (s, 1H). MASA (ES+): 599.1 (M+Na) ⁺ . |
| IA.69 | 0.99 (d, J=7.07Hz, 3H), 1.13 (t, J=7.22Hz, 6H), 1.25-1.93 (m, 8H), 2.00-2.48 (m, 6H), 3.35-3.42 (m, 1H), 4.27-4.52 (m, 3H), 5.25-5.52 (m, 1H), 6.34-6.40 (m, 1H), 6.43 (s, 1H), 7.13 (d, J=9.96Hz, 1H), 7.33 (t, J=6.94Hz, 1H), 7.47-7.76 (m, 4H). MASA (ES+): 649.1 (M+Na) ⁺ . |
| IA.70 | 0.95 (d, J=7.18Hz, 3H), 1.09-1.16 (m, 6H), 1.25-1.30 (m, 2H), 1.34 (s, 9H), 1.42-1.905 (m, 6H), 2.17-2.43 (m, 6H), 3.37-3.44 (m, 1H), 4.28-4.49 (m, 2H), 4.53 (d, J=16.72Hz, 1H), 5.20-5.60 (m, 1H), 6.37 (dd, J ₁ =10.12Hz, J ₂ =1.73Hz, 1H), 6.43 (s, 1H), 7.13 (d, J=10.19Hz, 1H), 7.50 (d, J=8.52Hz, 2H), 7.95 (d, J=8.52Hz, 2H). MASA (ES+): 665.2 (M+Na) ⁺ . |
| IA.71 | 0.96 (d, J=7.11Hz, 3H), 1.14 (t, J=7.52Hz, 3H), 1.24-1.36 (m, 5H), 1.55-2.07 (m, 6H), 2.20-2.46 (m, 6H), 3.32-3.39 (m, 1H), 4.02 (s, 3H), 4.40 (d, J=9.33Hz, 1H), 5.02 (d, J=16.95Hz, 1H), 5.20-5.60 (m, 1H), 5.74 (d, J=16.94Hz, 1H), 6.37 (d, J ₁ =10.13Hz, J ₂ =1.73Hz, 1H), 6.44 (s, 1H), 6.97 (d, J ₁ =6.86Hz, J ₂ =1.97Hz, 1H), 7.13-7.28 (m, 3H), 7.56 (s, 1H). MASA (ES+): 663.2 (M+Na) ⁺ . |
| IA.72 | 0.96 (d, J=7.11Hz, 3H), 1.14 (t, J=7.52Hz, 3H), 1.24-1.30 (m, 6H), 1.34 (s, 8H), 1.42-1.92 (m, 6H), 2.11-2.54 (m, 6H), 3.30-3.41 (m, 1H), 4.41 (d, J=9.37Hz, 1H), 5.00 (d, J=16.55Hz, 1H), 5.26-5.53 (m, 1H), 5.74 (d, J=16.56Hz, 1H), 6.38 (d, J ₁ =10.12Hz, J ₂ =1.67Hz, 1H), 6.44 (s, 1H), 7.15 (d, J=10.03Hz, 1H), 7.50 (d, J=8.48Hz, 2H), 7.85 (d, J=8.47Hz, 2H). MASA (ES+): 649.2 (M+Na) ⁺ . |
| IA.73 | 1.00 (d, J=7.18Hz, 3H), 1.05-1.50 (m, 8H), 1.53 (s, 3H), 1.69-2.42 (m, 9H), 3.38 (m, 1H), 4.32 (d, J=16.14Hz, 1H), 4.40 (s, 1H), 4.50 (d, J=16.10Hz, 1H), 5.30 (m, 1H), 6.38 (dd, J ₁ =1.67Hz, J ₂ =10.12Hz, 1H), 6.43 (s, 1H), 7.12 (d, J=10.05Hz, 1H), 7.76 (d, J=8.21Hz, 2H), 8.12 (d, J=8.08Hz, 2H). MASA (ES+): 679.1 (M+Na) ⁺ . |
| IA.74 | 0.96 (d, J=7.10Hz, 3H), 1.13 (t, J=7.54Hz, 3H), 1.25-1.99 (m, 8H), 2.11-2.43 (m, 6H), 3.30-3.50 (m, 1H), 3.88 (s, 3H), 4.40 (d, J=9.28Hz, 1H), 4.85 (d, J ₁ =17.50Hz, J ₂ =3.72Hz, 1H), 5.20-5.60 (m, 1H), 5.60 (d, J ₁ =17.50Hz, J ₂ =3.65Hz, 1H), 6.37 (d, J ₁ =10.11Hz, J ₂ =1.74Hz, 1H), 6.44 (s, 1H), 6.65 (d, J ₁ =13.13Hz, J ₂ =2.25Hz, 1H), 6.79 (d, J ₁ =8.90Hz, J ₂ =2.35Hz, 1H), 7.15 (d, J ₁ =10.14Hz, J ₂ =1.04Hz, 1H), 7.91 (t, J=8.54Hz, 1H). MASA (ES+): 641.2 (M+Na) ⁺ . |
| IA.75 | 0.99 (d, J=7.17Hz, 3H), 1.09-1.16 (m, 6H), 1.25-1.97 (m, 8H), 2.05-2.44 (m, 6H), 3.30-3.50 (m, 1H), 3.87 (s, 3H), 4.25-4.54 (m, 3H), 5.20-5.60 (m, 1H), 6.38 (dd, J ₁ =10.09Hz, J ₂ =1.73Hz, 1H), 6.43 (s, 1H), 6.65 (dd, J ₁ =13.18Hz, J ₂ =2.35Hz, 1H), 6.77 (dd, J ₁ =8.40Hz, J ₂ =2.38Hz, 1H), 7.14 (d, J=9.05Hz, 1H), 7.89 (t, J=8.67Hz, 1H). MASA (ES+): 657.1 (M+Na) ⁺ . |
| IA.76 | 0.96 (d, J=7.15Hz, 3H), 1.15 (t, J=7.60Hz, 3H), 1.25-1.94 (m, 8H), 2.04-2.43 (m, 6H), 3.33-3.41 (m, 1H), 3.95 (s, 3H), 4.41 (d, J=8.47Hz, 1H), 4.97 (d, J=17.66Hz, 1H), 5.20-5.60 (m, 1H), 5.65 (d, J=17.71Hz, 1H), 6.34-6.44 (m, 2H), 6.98-7.08 (m, 2H), 7.15 (d, J=10.01Hz, 1H), 7.52 (t, J=6.82Hz, 1H), 7.89 (dd, J ₁ =7.79Hz, J ₂ =1.66Hz, 1H). MASA (ES+): 623.2 (M+Na) ⁺ . |
| IA.77 | 0.96 (d, J=7.13Hz, 3H), 1.09 (t, J=7.55Hz, 3H), 1.24-2.43 (m, 17H), 3.31-3.40 (m, 1H), 3.87 (s, 3H), 3.92 (s, 3H), 4.41 (d, J=9.87Hz, 1H), 4.88 (d, J=17.64Hz, 1H), 5.20-5.68 (m, 2H), 6.34-6.59 (m, 4H), 7.17 (d, J ₁ =10.11Hz, J ₂ =0.97Hz, 1H), 7.92 (d, J=8.80Hz, 1H). |

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No. | ¹ H-NMR (δ ppm). MASA (EI / ES+, m/z) |
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| | MASA (ES+): 635.2 (M+Na)⁺. |
| IA.78 | 0.98 (d, J=7.16Hz, 3H), 1.09-1.16 (m, 6H), 1.25-1.88 (m, 8H), 2.05-2.41 (m, 6H), 3.36-3.45 (m, 1H), 3.86 (s, 3H), 3.93 (s, 3H), 4.30-4.61 (m, 3H), 5.20-5.60 (m, 1H), 6.34-6.57 (m, 4H), 7.15 (dd, J ₁ =10.05Hz, J ₂ =1.00Hz, 1H), 7.85 (d, J=8.73Hz, 1H). MASA (ES+): 669.1 (M+Na)⁺. |
| IA.79 | 0.97 (d, J=7.16Hz, 3H), 1.09-1.25 (m, 6H), 1.29-1.96 (m, 8H), 2.03-2.41 (m, 6H), 3.36-3.43 (m, 1H), 3.95 (s, 3H), 4.31-4.60 (m, 3H), 5.20-5.6 (m, 1H), 6.35-6.45 (m, 2H), 6.97-7.05 (m, 2H), 7.14 (d, J=9.89Hz, 1H), 7.46-7.55 (m, 1H), 7.77 (dd, J ₁ =7.11Hz, J ₂ =1.58Hz, 1H). MASA (ES+): 639.1 (M+Na)⁺. |
| IA.80 | 0.95 (d, J=7.16Hz, 3H), 1.08-1.18 (m, 6H), 1.22-1.93 (m, 8H), 2.19-2.41 (m, 6H), 3.28-3.37 (m, 1H), 4.39 (d, J=8.09Hz, 1H), 4.73 (d, J=17.18Hz, 1H), 5.22-5.53 (m, 2H), 6.38 (d, J ₁ =10.09Hz, J ₂ =1.78Hz, 1H), 6.43 (s, 1H), 7.14 (d, J ₁ =10.07Hz, J ₂ =1.16Hz, 1H), 7.63-7.88 (m, 4H). MASA (ES+): 661.1 (M+Na)⁺. |
| IA.81 | 0.99 (d, J=7.15Hz, 3H), 1.09-1.17 (m, 6H), 1.25-2.02 (m, 8H), 2.17-2.44 (m, 6H), 3.34-3.41 (m, 1H), 4.11 (d, J=17.43Hz, 1H), 4.30 (d, J=17.42Hz, 1H), 4.41 (d, J=9.75Hz, 1H), 5.20-5.60 (m, 1H), 6.38 (dd, J ₁ =10.11Hz, J ₂ =1.74Hz, 1H), 6.43 (s, 1H), 7.13 (dd, J ₁ =10.13Hz, J ₂ =1.07Hz, 1H), 7.60-7.88 (m, 4H). MASA (ES+): 677.1 (M+Na)⁺. |
| IA.82 | 1.03 (d, J=7.07Hz, 3H), 1.25-1.79 (m, 7H), 1.79-2.55 (m, 8H), 3.41-3.45 (m, 1H), 4.45 (d, J=8.28Hz, 1H), 4.98 (d, J=16.58Hz, 1H), 5.34-5.50 (m, 1H), 5.79 (d, J=16.48Hz, 1H), 6.40 (d, J ₁ =10.16Hz, J ₂ =1.38Hz, 1H), 6.46 (s, 1H), 6.51 (s, 1H), 7.14-7.19 (m, 4H), 7.60 (s, 1H), 7.93 (d, J ₁ =8.55Hz, J ₂ =5.35Hz, 2H). MASA (ES+): 649.1 (M+Na)⁺. |
| IA.83 | 1.07 (d, J=6.86Hz, 3H), 1.17 (s, 3H), 1.38-1.92 (m, 6H), 1.95-2.54 (m, 6H), 3.47 (m, 1H), 4.31 (d, J=16.60Hz, 1H), 4.45-4.67 (m, 2H), 5.32-5.49 (m, 1H), 6.39-6.51 (m, 3H), 7.14-7.19 (m, 4H), 7.59 (s, 1H), 8.05 (dd, J ₁ =8.14Hz, J ₂ =5.42Hz, 2H). MASA (ES+): 665.1 (M+Na)⁺. |
| IA.84 | 1.03 (d, J=7.08Hz, 3H), 1.25-1.66 (m, 7H), 1.76-2.56 (m, 8H), 3.41-3.45 (m, 1H), 4.45 (d, J=8.26Hz, 1H), 4.90 (d, J ₁ =17.59Hz, J ₂ =3.07Hz, 1H), 5.34-5.51 (m, 1H), 5.65 (d, J ₁ =17.61Hz, J ₂ =3.17Hz, 1H), 6.41 (d, J ₁ =10.05Hz, J ₂ =1.50Hz, 1H), 6.46 (s, 1H), 6.51 (d, J ₁ =3.20Hz, J ₂ =1.52Hz, 1H), 6.90-7.04 (m, 2H), 7.13-7.19 (m, 2H), 7.59 (s, 1H), 7.99 (d, J ₁ =15.08Hz, J ₂ =8.28Hz, 1H). MASA (ES+): 683.1 (M+Na)⁺. |
| IA.85 | 1.06 (d, J=7.02Hz, 3H), 1.19 (s, 3H), 1.36-1.66 (m, 6H), 1.71-2.55 (m, 6H), 3.44-3.48 (m, 1H), 4.31 (d, J=17.67Hz, 1H), 4.46-4.50 (m, 2H), 5.33-5.66 (m, 1H), 6.41 (dd, J ₁ =10.18Hz, J ₂ =0.81Hz, 1H), 6.45 (s, 1H), 6.50 (d, J=1.54Hz, 1H), 6.89-7.01 (m, 2H), 7.12-7.17 (m, 2H), 7.59 (s, 1H), 7.95 (dd, J ₁ =15.16Hz, J ₂ =8.35Hz, 1H). MASA (ES+): 683.1 (M+Na)⁺. |
| IA.86 | 0.96 (d, J=7.14Hz, 3H), 1.11 (s, 3H), 1.12 (t, J=7.53Hz, 3H), 1.24-1.34 (m, 1H), 1.54 (s, 3H), 1.59-1.64 (m, 1H), 1.75-1.98 (m, 4H), 2.13-2.61 (m, 7H), 3.37 (m, 1H), 4.36 (d, J=11.18, 1H), 4.42 (d, J=87.1H), 4.49 (d, J=16.46, 1H), 6.34 (s, 1H), 6.34 (d, J ₁ =10.12Hz, J ₂ =1.79Hz, 1H), 7.11-7.23 (m, 3H), 8.01 (m, 2H). MASA (ES+): 609.1 (M+Na)⁺. |
| IA.87 | 0.94 (d, J=7.09Hz, 3H), 1.12 (t, J=7.54Hz, 3H), 1.24 (s, 3H), 1.27-1.31 (m, 1H), 1.57 (s, 3H), 1.59-1.62 (m, 1H), 1.81-1.87 (m, 2H), 1.97-2.03 (m, 2H), 2.15-2.23 (m, 1H), 2.34-2.46 (m, 6H), 2.60-2.66 (m, 1H), 3.30-3.36 (m, 1H), 4.41 (d, J=8.85Hz, 1H), 4.98 (d, J=16.51Hz, 1H), 5.69 (d, J=16.54Hz, 1H), 6.13 (s, 1H), 6.34 (d, J ₁ =9.98Hz, J ₂ =1.40Hz, 1H), 7.17 (t, J=8.50Hz, 2H), 7.23 (d, J=10.14Hz, 1H), 7.95 (dd, J ₁ =8.58Hz, J ₂ =5.36Hz, 2H). MASA (ES+): 593.2 (M+Na)⁺. |
| IA.88 | 0.98 (d, J=6.7Hz, 3H), 1.09 (m, 6H), 1.31-1.35 (m, 2H), 1.54 (s, 3H), 1.71-1.84 (m, 1H), 1.87-2.00 (m, 2H), 2.20-2.33 (m, 6H), 2.88 (s, 1H), 3.36 (m, 1H), 4.39 (d, 1H, J=31.8Hz), 4.47 (d, 1H, J=31.7Hz), 5.31-5.48 (m, 1H), 6.36 (d, 1H, J=10.1Hz), 6.41 (s, 1H), 7.21 (d, 1H, J=10.01-8.10 (s, 1H), 8.44 (s, 2H). MASA (ES+): 745.1 (M+Na)⁺. |
| IA.89 | 0.99 (d, J=6.91Hz, 3H), 1.10 (m, 5H), 1.32 (m, 1H), 1.54 (s, 3H), 1.80 (m, 2H), 2.20-2.48 (m, 7H), 3.21 (m, 1H), 3.38 (m, 1H), 4.36-4.47 (m, 3H), 5.32-5.48 (m, 1H), 6.36 (d, 1H, J=10.0Hz), 6.41 (s, 1H), 7.22 (d, 1H, J=10.0Hz), 7.65 (t, 1H, J=7.7Hz), 7.85 (d, 1H, J=7.6Hz), 8.19 (d, 1H, J=7.8Hz), 8.24 (s, 1H). MASA (ES+): 677.1 (M+Na)⁺. |
| IA.90 | 0.90 (d, J=6.41Hz, 6H), 0.99 (d, 3H, J=6.7Hz), 1.12 (s, 3H), 1.30-1.34 (m, 1H), 1.52 (s, 3H), 1.72-1.89 (m, 3H), 1.91-2.19 (m, 4H), 2.25-2.47 (m, 7H), 2.53 (m, 3H), 3.40 (m, 1H), 4.36 (d, 1H, J=17.0Hz), 4.51 (d, 1H, J=16.5Hz), 5.30-5.50 (m, 1H), 6.37 (d, 1H, J=10.0Hz), 6.43 (s, 1H), 7.17 (d, 1H, J=10.0Hz), 7.25 (d, 2H, J=7.8Hz), 7.91 (d, 2H, J=7.8Hz). MASA (ES+): 665.2 (M+Na)⁺. |
| IA.91 | 1.11 (t, J=7.57Hz, 3H), 1.18 (s, 3H), 1.23-1.25 (m, 1H), 1.43 (d, J=7.34Hz, 3H), 1.58 (s, 3H), 1.61-1.64 (m, 1H), 1.91-2.07 (m, 4H), 2.13-2.22 (m, 2H), 2.29-2.55 (m, 7H), 2.61-2.66 (m, 1H), 4.43 (d, J=8.38Hz, 1H), 4.88 (d, J=16.49Hz, 1H), 5.68 (d, J=16.4Hz, 1H), 6.14 (s, 1H), 6.35 (d, J ₁ =10.12Hz, J ₂ =1.44Hz, 1H), 7.17 (t, J=8.52Hz, 2H), 7.25 (d, J=9.93Hz, 1H), 7.92 (dd, J=8.67Hz, J ₂ =5.31Hz, 2H). MASA (ES+): 593.2 (M+Na)⁺. |
| IA.92 | 0.99 (d, 3H, J=6.95Hz), 1.06-1.14 (m, 6H), 1.26 (t, 3H, J=7.52), 1.30-1.34 (m, 1H), 1.52 (s, 3H), 1.72-1.96 (m, 4H), 2.0-2.28 (m, 2H), 2.34-2.44 (m, 4H), 2.72 (q, 2H, J ₁ =15.05Hz, J ₂ =7.51Hz, 3.39-3.42 (m, 1H), 4.33-4.41 (m, 2H), 4.52 (1H, d, J=16.60Hz), 5.25-5.50 (m, 1H), 6.37 (1H, d, J=10.09Hz), 6.43 (s, 1H), 7.13 (d, 1H, J=10.07Hz), 7.31 (d, 2H, J=7.92Hz), 7.93 (d, 2H, J=8.00Hz). MASA (ES+): 637.1 (M+Na)⁺. |
| IA.93 | 0.99 (d, J=7.0Hz, 3H), 1.11-1.50 (m, 5H), 1.26-1.48 (m, 7H), 1.52 (s, 3H), 1.67 (s, 3H), 1.70-1.80 (m, 2H), 1.87-2.00 (m, 6H), 2.20-2.45 (m, 3H), 2.57 (m, 1H), 3.38-3.42 (m, 1H), 4.32 (d, 1H, J=16.7Hz), 4.40 (d, 1H, J=8.01Hz), 4.54 (d, 1H, J=16.7Hz), 5.30-5.47 (m, 1H), 6.38 (dd, 1H, J ₁ =10.01Hz, J ₂ =1.09Hz), 6.43 (s, 1H), 7.13 (d, 1H, J=5.05Hz), 7.32 (d, 2H, J=8.13Hz), 7.94 (d, 2H, J=8.12Hz). MASA (ES+): 691.2 (M+Na)⁺. |
| IA.94 | 0.99 (s, 3H), 1.14 (t, J=7.53Hz, 3H), 1.22-1.29 (m, 1H), 1.36 (d, J=7.31Hz, 3H), 1.56 (s, 3H), 1.63-2.11 (m, 6H), 2.25-2.65 (m, 7H), 4.01 (d, J ₁ =17.65Hz, J ₂ =3.11Hz, 1H), 4.47 (d, J ₁ =17.62Hz, J ₂ =3.11Hz, 1H), 4.49 (d, J=7.05Hz, 1H), 6.13 (s, 1H), 6.34 (d, J ₁ =10.11Hz, J ₂ =1.81Hz, 1H), 6.86-7.04 (m, 2H), 7.22 (d, J=10.18Hz, 1H), 7.87-7.98 (m, 1H). MASA (ES+): 627.1 (M+Na)⁺. |
| IA.95 | 0.99 (d, J=7.08Hz, 6H), 1.11-1.15 (m, 5H), 1.27 (d, 6H, J=6.8Hz), 1.52 (s, 3H), 1.67 (s, 3H), 1.72-1.89 (m, 3H), 1.99 (d, 1H, J=14.47Hz, 2.37 (q, 2H), 2.96-2.99 (m, 1H), 3.39-3.42 (m, 1H), 4.32 (d, 1H, J=16.63Hz), 4.40 (d, 1H, J=8.64Hz), 4.54 (d, 1H, J=16.7Hz), 5.30-5.47 (m, 1H), 6.37 (d, 1H, J=10.0Hz), 6.43 (s, 1H), 7.14 (d, 1H, J=10.0Hz), 7.34 (d, 2H, J=8.17Hz), 7.94 (d, 2H, J=8.1Hz). MASA (ES+): 651.1 (M+Na)⁺. |
| IA.96 | 0.83-0.95 (m, 1H), 0.99 (d, 3H, J=7.0Hz), 1.11 (d, 3H, J=4.13Hz), 1.26-1.34 (m, 2H), 1.65-1.69 (m, 2H), 1.72-2.08 (m, 11H), 2.14-2.32 (m, 2H), 2.36 (q, 2H, J ₁ =15.04, J ₂ =7.58), 3.39-3.42 (m, 1H), 4.32 (d, 1H, J=16.43Hz), 4.40 (1H, d, J=8.26Hz), 4.49 (d, 1H, J=16.4Hz), 5.30-5.46 (m, 1H), 6.37 (d, 1H, J=9.92Hz), 6.43 (s, 1H), 6.90 (d, 2H, J=8.71Hz), 7.13 (d, 1H, J=10.04Hz), 7.95 (d, 2H, J=8.71Hz). MASA (ES+): 693.1 (M+Na)⁺. |
| IA.97 | 0.94 (d, J=7.11Hz, 3H), 1.04 (s, 3H), 1.11 (t, J=7.55Hz, 3H), 1.21-1.44 (m, 1H), 1.54 (s, 3H), 1.75-2.04 (m, 4H), 2.12-2.41 (m, 7H), 3.1 (s, 3H), 3.29-3.33 (m, 1H), 4.34 (d, J=16.23, 1H), 4.44 (d, J=16.35, 1H), 6.12 (s, 1H), 6.34 (d, J ₁ =10.12Hz, J ₂ =1.77Hz, 1H), 7.19 (d, J=10.15Hz, 1H), 8.06 (d, J=8.59Hz, 2H), 8.18 (d, J=8.62Hz, 2H). MASA (ES+): 669.1 (M+Na)⁺. |
| IA.98 | 0.97 (d, J=7.14Hz, 3H), 1.11 (t, J=7.54Hz, 3H), 1.13 (s, 3H), 1.21-1.45 (m, 1H), 1.55 (s, 3H), 1.60-2.07 (m, 5H), 2.17-2.68 (m, 7H), 3.31-3.41 (m, 1H), 4.22 (dd, J ₁ =17.96Hz, J ₂ =3.50Hz, 1H), 4.40-4.42 (d, 1H), 4.43 (dd, J ₁ =17.47Hz, J ₂ =2.98Hz, 1H), 6.13 (s, 1H), 6.35 (d, J ₁ =10.13Hz, J ₂ =1.83Hz, 1H), 6.86-7.03 (m, 2H), 7.21 (d, J=10.16Hz, 1H), 7.89-8.01 (m, 1H). MASA (ES+): 627.1 (M+Na)⁺. |
| IA.99 | 0.94 (s, 3H), 1.12 (t, J=7.54Hz, 3H), 1.20-1.29 (m, 1H), 1.37 (d, J=7.28Hz, 3H), 1.55 (s, 3H), 1.60-1.95 (m, 6H), 2.25-2.46 (m, 7H), 3.1 (s, 3H), 4.00 (d, J=16.59Hz, 1H), 4.42 (d, J=9.05Hz, 1H), 4.53 (d, J=16.61Hz, 1H), 6.12 (s, 1H), 6.35 (d, J ₁ =10.12Hz, J ₂ =1.75Hz, 1H), 7.19 (d, J=10.15Hz, 1H), 8.07 (d, J=6.69Hz, 2H), 8.13 (d, J=8.73Hz, 2H). MASA (ES+): 669.0 (M+Na)⁺. |
| IA.100 | 0.98 (d, J=7.10Hz, 3H), 1.11 (s, 3H), 1.11 (t, J=7.46Hz, 3H), 1.27-1.33 (m, 1H), 1.54 (s, 3H), 1.57-1.65 (m, 4H), 2.14-2.41 (m, 7H), 2.61-2.63 (m, 1H), 3.35-3.37 (m, 1H), 4.30 (d, 1H, J=16.48Hz), 4.40 (d, 1H, J=8.83Hz), 4.47 (d, 1H, J=16.47Hz), 6.13 (s, 1H), 6.34 (d, J ₁ =10.13Hz, J ₂ =1.45Hz, 1H), 7.20 (d, J=10.15Hz, 1H), 7.47 (d, J=8.51Hz, 2H), 7.95 (d, J=8.51Hz, 2H). MASA (ES+): 625.1 |

| Com-
puesto
No. | 1H-NMR (δ ppm). MASA (EI / ES+, m/z) |
|-----------------------|--|
| | (M+Na) ⁺ |
| IA.101 | 0.97 (s, 3H), 1.14 (t, $J=7.50$ Hz, 3H), 1.18-1.27 (m, 1H), 1.38 (d, $J=7.26$ Hz, 3H), 1.56 (s, 3H), 1.60-1.64 (m, 1H), 1.89-2.29 (m, m, 6H), 2.35-2.47 (m, 5H), 2.59-2.64 (m, 1H), 3.97 (d, $J=16.8$ Hz, 1H), 4.45 (d, $J=8.17$ Hz, 1H), 4.55 (d, $J=16.82$ Hz, 1H), 6.13 (s, 1H), 6.35 (d, $J=10.18$ Hz, 1H), 7.22 (d, $J=10.13$ Hz, 1H), 7.47 (d, $J=8.37$ Hz, 2H), 7.92 (d, $J=8.38$ Hz, 2H). MASA (ES+): 625.1 (M+Na) ⁺ |
| IA.102 | 1.05-1.15 (m, 6H), 1.22-1.52 (m, 9H), 1.76-2.47 (m, 8H), 3.34-3.41 (m, 1H), 4.07-4.16 (m, 2H), 4.16-4.56 (m, 3H), 5.23-5.48 (m, 1H), 6.36 (d, $J=11.36$ Hz, 1H), 6.42 (s, 1H), 7.11 (d, $J=9.95$ Hz, 1H), 7.76 (d, $J=8.11$ Hz, 2H), 8.11 (d, $J=8.12$ Hz, 2H). MASA (ES+): 693.5 (M+Na) ⁺ |
| IA.103 | 0.87 (m, 4H), 0.96 (d, $J=6.88$ Hz, 3H), 1.24 (s, 3H), 1.29-1.35 (m, 1H), 1.55 (s, 3H), 1.61-1.66 (m, 1H), 1.81-2.09 (m, 2H), 2.28-2.50 (m, 6H), 3.31-3.36 (m, 1H), 4.42 (d, $J=8.86$ Hz, 1H), 4.97 (d, $J=16.53$ Hz, 1H), 5.32-5.48 (m, 1H), 5.69 (d, $J=16.53$ Hz, 1H), 6.38 (d, $J_1=10.17$ Hz, $J_2=1.46$ Hz, 1H), 6.44 (s, 1H), 7.16 (d, $J=8.50$ Hz, 2H), 7.23 (t, $J=8.64$ Hz, 3H), 7.94 (dd, $J_1=8.60$ Hz, $J_2=5.35$ Hz, 2H). MASA (ES+): 623.0 (M+Na) ⁺ |
| IA.104 | 0.86-0.96 (m, 4H), 0.98 (d, $J=7.35$ Hz, 3H), 1.12 (s, 3H), 1.31-1.36 (m, 1H), 1.53 (s, 3H), 1.60-1.65 (m, 1H), 1.70-2.03 (m, 5H), 2.22-2.29 (m, 2H), 2.39-2.45 (m, 2H), 3.35-3.39 (m, 1H), 4.26 (d, $J=17.62$ Hz, 1H), 4.42 (d, $J=8.24$ Hz, 1H), 4.43 (d, $J=17.30$ Hz, 1H), 5.31-5.47 (m, 1H), 6.38 (d, $J_1=10.11$ Hz, $J_2=1.09$ Hz, 1H), 6.43 (s, 1H), 6.89-6.94 (m, 1H), 6.96-7.01 (m, 1H), 7.14 (d, $J=10.14$ Hz, 1H), 7.95 (dd, $J_1=15.13$ Hz, $J_2=8.38$ Hz, 1H). MASA (ES+): 657.5 (M+Na) ⁺ |
| IA.105 | 1.07 (d, $J=7.14$ Hz, 3H), 1.10 (s, 3H), 1.27 (t, $J=7.60$ Hz, 3H), 1.32-1.97 (m, 8H), 2.23-2.44 (m, 4H), 3.36-3.42 (m, 1H), 4.09-4.14 (m, 2H), 4.30 (d, $J=16.57$ Hz, 1H), 4.40 (d, $J=8.43$ Hz, 1H), 4.51 (d, $J=16.58$ Hz, 1H), 5.20-5.60 (m, 1H), 6.36 (dd, $J_1=10.15$ Hz, $J_2=1.20$ Hz, 1H), 6.42 (s, 1H), 7.12 (d, $J=10.14$ Hz, 1H), 7.47 (d, $J=8.52$ Hz, 2H), 7.95 (d, $J=8.54$ Hz, 2H). MASA (ES+): 659.4 (M+Na) ⁺ |
| IA.106 | 0.87-0.97 (m, 4H), 0.99 (d, $J=7.12$ Hz, 3H), 1.00 (s, 3H), 1.31-1.36 (m, 1H), 1.53 (s, 3H), 1.62-1.66 (m, 1H), 1.77-2.01 (m, 3H), 2.25-2.42 (m, 4H), 3.36-3.39 (m, 1H), 4.28 (d, $J=16.54$ Hz, 1H), 4.42 (d, $J=14.05$ Hz, 1H), 4.46 (d, $J=16.73$ Hz, 1H), 5.30-5.48 (m, 1H), 6.38 (d, $J_1=9.63$ Hz, $J_2=1.85$ Hz, 1H), 6.43 (s, 1H), 7.14 (d, $J=10.10$ Hz, 1H), 7.46 (d, $J=8.51$ Hz, 2H), 7.94 (d, $J=8.53$ Hz, 2H). MASA (ES+): 655.2 (M+Na) ⁺ |
| IA.107 | 0.98 (s, 3H), 1.14 (t, $J=7.56$ Hz, 3H), 1.20-1.27 (m, 1H), 1.38 (d, $J=7.23$ Hz, 3H), 1.56 (s, 3H), 1.60-1.65 (m, 1H), 1.91-1.98 (m, 3H), 2.04-2.30 (m, 2H), 2.36-2.66 (m, 7H), 3.88 (s, 3H), 3.97 (d, 1H, $J=16.74$ Hz), 4.44 (d, 1H, $J=8.41$ Hz), 4.58 (d, 1H, $J=16.74$ Hz), 6.13 (s, 1H), 6.35 (d, $J=10.07$ Hz, 1H), 6.95 (d, $J=8.74$ Hz, 2H), 7.24 (d, $J=10.33$ Hz, 1H), 7.97 (d, $J=8.74$ Hz, 2H). MASA (ES+): 621.3 (M+Na) ⁺ |
| IA.108 | 0.98 (d, $J=7.15$ Hz, 3H), 1.11 (s, 3H), 1.11 (t, $J=7.56$ Hz, 3H), 1.27-1.33 (m, 1H), 1.54 (s, 3H), 1.57-1.94 (m, 5H), 2.13-2.17 (m, 1H), 2.32-2.41 (m, 5H), 2.62-2.63 (m, 1H), 3.33-3.38 (m, 1H), 4.33 (d, 1H, $J=16.52$ Hz), 4.41 (d, 1H, $J=9.09$ Hz), 4.49 (d, 1H, $J=16.49$ Hz), 6.13 (s, 1H), 6.34 (d, $J_1=10.12$ Hz, $J_2=1.81$ Hz, 1H), 7.21 (d, $J=10.12$ Hz, 1H), 7.76 (d, $J=8.25$ Hz, 2H), 8.12 (d, $J=8.14$ Hz, 2H). MASA (ES+): 659.3 (M+Na) ⁺ |
| IA.109 | 0.53 (s, 3H), 0.93 (d, $J=6.88$ Hz, 3H), 1.07 (t, $J=7.52$ Hz, 3H), 1.12-1.90 (m, 14H), 2.07-2.42 (m, 6H), 3.14-3.17 (m, 1H), 3.84 (s, 3H), 4.28 (d, $J=7.12$ Hz, 1H), 5.25-5.42 (m, 1H), 6.34 (dd, $J_1=10.14$ Hz, $J_2=1.19$ Hz, 1H), 6.40 (s, 1H), 6.87 (d, $J=8.84$ Hz, 2H), 7.03 (d, $J=10.07$ Hz, 1H), 8.02 (d, $J=8.80$ Hz, 2H). MASA (ES+): 667.3 (M+Na) ⁺ |
| IA.110 | 1.07 (d, $J=7.20$ Hz, 3H), 1.11 (s, 3H), 1.27 (t, $J=7.12$ Hz, 3H), 1.33-1.39 (m, 1H), 1.52 (s, 3H), 1.74-1.98 (m, 6H), 2.33-2.45 (m, 4H), 3.36-3.42 (m, 1H), 4.08-4.14 (m, 2H), 4.31 (d, $J=16.55$ Hz, 1H), 4.41 (d, $J=8.80$ Hz, 1H), 4.52 (d, $J=16.55$ Hz, 1H), 5.29-5.46 (m, 1H), 6.37 (dd, $J_1=10.15$ Hz, $J_2=1.75$ Hz, 1H), 6.42 (s, 1H), 7.13 (dd, $J_1=10.15$ Hz, $J_2=1.05$ Hz, 1H), 7.17-7.19 (m, 2H), 8.03-8.07 (m, 2H). MASA (ES+): 643.2 (M+Na) ⁺ |
| IA.111 | 0.97 (s, 3H), 1.13 (t, $J=7.55$ Hz, 3H), 1.15-1.29 (m, 1H), 1.38 (d, $J=7.33$ Hz, 3H), 1.56 (s, 3H), 1.58-1.66 (m, 1H), 1.88-2.14 (m, 5H), 2.17-2.30 (m, 1H), 2.35-2.64 (m, 5H), 4.01 (d, $J=16.84$ Hz, 1H), 4.45 (d, $J=8.23$ Hz, 1H), 4.57 (d, $J=16.84$ Hz, 1H), 6.13 (s, 1H), 6.35 (d, $J_1=10.12$ Hz, $J_2=1.77$ Hz, 1H), 7.22 (d, $J=10.13$ Hz, 1H), 7.77 (d, $J=8.24$ Hz, 2H), 8.09 (d, $J=8.14$ Hz, 2H). MASA (ES+): 659.2 (M+Na) ⁺ |
| IA.112 | 0.97 (d, $J=7.05$ Hz, 3H), 1.10 (s, 3H), 1.12-1.48 (m, 7H), 1.53 (s, 3H), 1.71-2.01 (m, 8H), 2.20-2.43 (m, 5H), 3.36-3.39 (m, 1H), 4.30 (d, $J=16.59$ Hz, 1H), 4.43 (d, $J=8.27$ Hz, 1H), 4.51 (d, $J=16.56$ Hz, 1H), 5.31-5.47 (m, 1H), 6.38 (d, $J_1=10.12$ Hz, $J_2=1.33$ Hz, 1H), 6.44 (s, 1H), 7.16 (d, $J=10.07$ Hz, 1H), 7.76 (d, $J=8.15$ Hz, 1H), 8.11 (d, $J=8.08$ Hz, 2H). MASA (ES+): 731.2 (M+Na) ⁺ |
| IA.113 | 0.97 (d, $J=7.06$ Hz, 3H), 1.10 (s, 3H), 1.15-1.45 (m, 6H), 1.53 (s, 3H), 1.58-1.66 (m, 1H), 1.72-2.0 (m, 8H), 2.20-2.44 (m, 5H), 3.36-3.40 (m, 1H), 4.28 (d, $J=16.54$ Hz, 1H), 4.43 (d, $J=8.81$ Hz, 1H), 4.48 (d, $J=16.56$ Hz, 1H), 5.31-5.47 (m, 1H), 6.38 (d, $J_1=10.15$ Hz, $J_2=1.46$ Hz, 1H), 6.44 (s, 1H), 7.14 (d, $J=10.06$ Hz, 1H), 7.46 (d, $J=8.53$ Hz, 2H), 7.94 (d, $J=8.54$ Hz, 2H). MASA (ES+): 697.2 (M+Na) ⁺ |
| IA.114 | 0.96 (d, $J=7.05$ Hz, 3H), 1.12 (s, 3H), 1.17-1.48 (m, 6H), 1.53 (s, 3H), 1.58-1.65 (m, 1H), 1.71-2.06 (m, 8H), 2.20-2.43 (m, 5H), 3.36-3.39 (m, 1H), 4.27 (d, $J=17.51$ Hz, 1H), 4.24-4.45 (m, 2H), 5.31-5.47 (m, 1H), 6.38 (d, $J_1=10.12$ Hz, $J_2=1.43$ Hz, 1H), 6.44 (s, 1H), 6.89-7.01 (m, 2H), 7.14 (d, $J=10.11$ Hz, 1H), 7.94 (dd, $J_1=15.11$ Hz, $J_2=8.41$ Hz, 1H). MASA (ES+): 699.2 (M+Na) ⁺ |
| IA.115 | 0.94 (d, $J=7.07$ Hz, 3H), 1.24 (s, 3H), 1.28-1.46 (m, 5H), 1.55 (s, 3H), 1.61-2.06 (m, 10H), 2.24-2.50 (m, 5H), 3.32-3.37 (m, 1H), 4.42 (d, $J=8.32$ Hz, 1H), 4.96 (d, $J=16.52$ Hz, 1H), 5.32-5.48 (m, 1H), 5.68 (d, $J=16.53$ Hz, 1H), 6.38 (d, $J_1=10.12$ Hz, $J_2=1.30$ Hz, 1H), 6.44 (s, 1H), 7.17 (d, $J=9.91$ Hz, 1H), 7.16-7.19 (m, 2H), 7.94 (dd, $J_1=8.62$ Hz, $J_2=5.31$ Hz, 2H). MASS (ES+): 665.5 (M+Na) ⁺ |
| IA.116 | 0.96 (d, $J=7.14$ Hz, 3H), 1.10 (s, 3H), 1.14-1.43 (m, 6H), 1.53 (s, 3H), 1.62-2.06 (m, 10H), 2.23-2.45 (m, 4H), 3.38-3.42 (m, 1H), 3.88 (s, 3H), 4.27 (d, $J=16.51$ Hz, 1H), 4.42 (d, $J=8.73$ Hz, 1H), 4.53 (d, $J=16.53$ Hz, 1H), 5.31-5.47 (m, 1H), 6.38 (d, $J_1=10.11$ Hz, $J_2=1.66$ Hz, 1H), 6.44 (s, 1H), 6.95 (d, $J=8.90$ Hz, 2H), 7.15 (d, $J=10.10$ Hz, 1H), 7.99 (d, $J_1=8.89$ Hz, 2H). MASA (ES+): 693.2 (M+Na) ⁺ |
| IA.117 | 0.98 (d, $J=7.03$ Hz, 3H), 1.10 (s, 3H), 1.24-1.34 (m, 1H), 1.53 (s, 3H), 1.55-1.68 (m, 2H), 1.73-2.04 (m, 9H), 2.20-2.41 (m, 4H), 2.74-2.78 (m, 1H), 3.36-3.40 (m, 1H), 4.27 (d, $J=16.55$ Hz, 1H), 4.41 (d, $J=7.75$ Hz, 1H), 4.49 (d, $J=16.55$ Hz, 1H), 5.30-5.47 (s, 1H), 6.37 (d, $J_1=10.15$ Hz, 1H), 6.43 (s, 1H), 7.13 (d, $J=10.12$ Hz, 1H), 7.47 (d, $J=8.36$ Hz, 1H), 7.95 (d, $J=8.36$ Hz, 2H). MASA (ES+): 661.2 |
| IA.118 | 0.96 (d, $J=7.08$ Hz, 3H), 1.24 (s, 3H), 1.24-1.33 (m, 1H), 1.55 (s, 3H), 1.56-1.92 (m, 9H), 2.022.50 (m, 5H), 2.73-2.81 (m, 1H), 3.32-3.36 (m, 1H), 4.42 (d, $J=7.77$ Hz, 1H), 4.97 (d, $J=16.51$ Hz, 1H), 5.32-5.48 (m, 1H), 5.68 (d, $J=16.56$ Hz, 1H), 6.38 (d, $J_1=10.08$ Hz, $J_2=1.22$ Hz, 1H), 6.44 (s, 1H), 7.14-7.19 (m, 3H), 7.93-7.96 (m, 2H). MASA (ES+): 629.3 |
| IA.119 | 0.98 (d, $J=6.93$ Hz, 3H), 1.10 (s, 3H), 1.16 (t, $J=6.88$ Hz, 6H), 1.31-1.35 (m, 1H), 1.53 (s, 3H), 1.58-2.01 (m, 4H), 2.21-2.62 (m, 5H), 3.36-3.38 (m, 1H), 4.31 (d, 1H, $J=16.58$ Hz), 4.42 (d, $J=7.40$ Hz, 1H), 4.51 (d, $J=16.58$ Hz, 1H), 5.30-5.47 (m, 1H), 6.38 (d, $J_1=10.15$ Hz, 1H), 6.43 (s, 1H), 7.13 (d, $J=10.11$ Hz, 1H), 7.76 (d, $J=7.98$ Hz, 2H), 8.11 (d, $J=7.91$ Hz, 2H). MASA (ES+): 669.2 |
| IA.120 | 0.98 (d, $J=7.12$ Hz, 3H), 1.12 (s, 3H), 1.29-1.35 (m, 1H), 1.53 (s, 3H), 1.56-1.66 (m, 5H), 1.70-2.00 (m, 7H), 2.20-2.40 (m, 4H), 2.73-2.77 (m, 1H), 3.35-3.40 (m, 1H), 4.26 (d, $J_1=17.47$ Hz, $J_2=2.37$ Hz, 1H), 4.42 (d, $J=5.81$ Hz, 1H), 4.54 (d, $J_1=17.35$ Hz, $J_2=2.61$ Hz, 1H), 5.31-5.47 (m, 1H), 6.38 (d, $J_1=10.14$ Hz, $J_2=1.38$ Hz, 1H), 6.43 (s, 1H), 6.89-7.01 (m, 1H), 7.13 (d, $J=10.09$ Hz, 1H), 7.94 (dd, $J_1=15.10$ Hz, $J_2=8.46$ Hz, 2H). MASA (ES+): 663.3 |
| IA.121 | 0.95 (d, $J=7.14$ Hz, 3H), 1.16 (d, $J=7.00$ Hz, 6H), 1.22 (s, 3H), 1.28-1.34 (m, 1H), 1.55 (s, 3H), 1.74-2.18 (m, 4H), 2.28-2.57 (m, 4H), 2.58-2.62 (m, 1H), 2.30-2.38 (m, 1H), 3.30-3.38 (m, 1H), 4.42 (d, $J=8.92$ Hz, 1H), 4.97 (d, $J=16.51$ Hz, 1H), 5.32-5.49 (m, 1H), 5.69 (d, $J=16.53$ Hz, 1H), 6.38 (d, $J_1=10.13$ Hz, $J_2=1.75$ Hz, 1H), 6.44 (s, 1H), 7.14-7.20 (m, 3H), 7.93-7.97 (m, 2H). MASA (ES+): 603.3 |
| IA.122 | 0.98 (d, $J=7.14$ Hz, 3H), 1.11 (s, 3H), 1.16 (d, $J=2.98$ Hz, 3H), 1.17 (d, $J=3.00$ Hz, 3H), 1.31-1.34 (m, 1H), 1.53 (s, 3H), 1.71-2.03 (m, 3H), 2.24-2.42 (m, 4H), 2.57-2.61 (m, 1H), 3.40-3.43 (m, 1H), 3.88 (s, 3H), 4.28 (d, $J=16.49$ Hz, 1H), 4.42 (d, $J=8.74$ Hz, 1H), 4.54 (d, $J=16.50$ Hz, 1H), 5.30-5.47 (m, 1H), 6.37 (d, $J_1=10.13$ Hz, $J_2=1.77$ Hz, 1H), 6.43 (s, 1H), 6.95 (d, $J=8.89$ Hz, 2H), 7.14 (dd, |

| Com-
puesto
No. | III-NMR (δ ppm). MASA (EI / ES+, m/z) |
|-----------------------|--|
| | $J_1=10.18\text{Hz}$, $J_2=1.12\text{Hz}$, 2H), 7.99 (d, $J=8.87\text{Hz}$, 2H). MASA (ES+): 653.3 |
| IA.123 | 0.97 (d, $J=7.14\text{Hz}$, 3H), 1.13 (s, 3H), 1.16 (d.d, $J_1=6.99\text{Hz}$, $J_2=3.08\text{Hz}$, 6H), 1.29-1.33 (m, 3H), 1.53 (s, 3H), 1.73-2.02 (m, 4H), 2.23-2.47 (m, 4H), 2.55-2.62 (m, 1H), 3.36-3.41 (m, 1H), 4.28 (d.d, $J_1=17.54\text{Hz}$, $J_2=2.63\text{Hz}$, 1H), 4.42 (d, 1H), 4.44 (d.d, $J_1=17.54\text{Hz}$, $J_2=2.90\text{Hz}$, 1H), 5.31-5.48 (m, 1H), 6.38 (d.d, $J_1=10.13\text{Hz}$, $J_2=1.79\text{Hz}$, 1H), 6.44 (s, 1H), 6.89-7.01 (m, 2H), 7.13 (d.d, $J_1=10.10\text{Hz}$, $J_2=1.16\text{Hz}$, 1H), 7.92-7.98 (m, 1H). MASA (ES+): 637.3 |
| IA.124 | 1.07 (d, $J=7.13\text{Hz}$, 3H), 1.17 (s, 3H), 1.33-1.41 (m, 1H), 1.55 (s, 3H), 1.73-2.04 (m, 3H), 2.28-2.54 (m, 5H), 3.43-3.48 (m, 1H), 4.35 (d, $J=16.65\text{Hz}$, 1H), 4.46 (d, $J=8.34\text{Hz}$, 1H), 4.54 (d, $J=16.65\text{Hz}$, 1H), 5.33-5.49 (m, 1H), 6.41 (dd, $J_1=10.12\text{Hz}$, $J_2=1.69\text{Hz}$, 1H), 6.42 (s, 1H), 6.51 (dd, $J_1=3.46\text{Hz}$, $J_2=1.69\text{Hz}$, 1H), 7.09-7.21 (m, 2H), 7.59 (d, $J=0.72\text{Hz}$, 1H), 7.77 (d, $J=8.25\text{Hz}$, 2H), 8.72 (d, $J=8.18\text{Hz}$, 2H). MASA (ES+): 693.3 |
| IA.125 | 0.59 (s, 3H), 0.93 (d, $J=6.99\text{Hz}$, 3H), 1.07 (t, $J=7.54\text{Hz}$, 3H), 1.21-1.88 (m, 14H), 2.09-2.36 (m, 6H), 3.13-3.17 (m, 1H), 4.31 (d, $J=7.52\text{Hz}$, 1H), 5.27-5.42 (m, 1H), 6.35 (dd, $J_1=10.08\text{Hz}$, $J_2=1.16\text{Hz}$, 1H), 6.41 (s, 1H), 7.07 (d, $J=10.11\text{Hz}$, 1H), 7.36 (d, $J=8.47\text{Hz}$, 2H), 7.29 (d, $J=8.49\text{Hz}$, 2H). MASA (ES+): 649.2 |
| IA.126 | 1.07 (d, $J=7.12\text{Hz}$, 3H), 1.11 (s, 3H), 1.16-1.87 (m, 11H), 1.90-2.09 (m, 2H), 2.13-2.44 (m, 4H), 3.38-3.42 (m, 1H), 4.06-4.19 (m, 2H), 4.31 (d, $J=16.58\text{Hz}$, 1H), 4.40 (d, $J=8.68\text{Hz}$, 1H), 4.55 (d, $J=16.55\text{Hz}$, 1H), 5.29-5.47 (m, 1H), 6.37 (dd, $J_1=10.17\text{Hz}$, $J_2=1.45\text{Hz}$, 1H), 6.42 (s, 1H), 6.96 (d, $J=8.81\text{Hz}$, 2H), 7.13 (d, $J=10.19\text{Hz}$, 1H), 8.00 (d, $J=8.83\text{Hz}$, 2H). MASA (ES+): 633 |
| IA.127 | 1.07 (d, $J=7.06\text{Hz}$, 3H), 1.17 (s, 3H), 1.23-2.10 (m, 8H), 2.17-2.53 (m, 4H), 3.46-3.50 (m, 1H), 3.88 (s, 3H), 4.31 (d, $J=16.63\text{Hz}$, 1H), 4.45 (d, $J=8.39\text{Hz}$, 1H), 4.57 (d, $J=16.60\text{Hz}$, 1H), 5.32-5.49 (m, 1H), 6.40 (dd, $J_1=10.14\text{Hz}$, $J_2=1.36\text{Hz}$, 1H), 6.45 (s, 1H), 6.50 (dd, $J_1=3.1\text{Hz}$, $J_2=1.47\text{Hz}$, 1H), 6.96 (d, $J=8.82\text{Hz}$, 2H), 7.13-7.21 (m, 2H), 7.59 (s, 1H), 8.00 (d, $J=8.80\text{Hz}$, 2H). MASA (ES+): 655.2 |
| IA.128 | 0.88 (t, $J=1\text{Hz}$, 3H), 0.99 (d, $J=1\text{Hz}$, 3H), 1.11 (s, 3H), 1.22-1.32 (m, 4H), 1.53-1.97 (m, 8H), 2.20-2.46 (m, 6H), 3.36-3.40 (m, 1H), 4.33 (d, $J=1\text{Hz}$, 1H), 4.41 (d, $J=1\text{Hz}$, 1H), 4.49 (d, $J=1\text{Hz}$, 1H), 5.30-5.47 (m, 1H), 6.38 (dd, $J_1=1\text{Hz}$, $J_2=1\text{Hz}$, 1H), 6.43 (s, 1H), 7.13 (dd, $J_1=1\text{Hz}$, $J_2=1\text{Hz}$, 1H), 7.76 (d, $J=1\text{Hz}$, 2H), 8.12 (d, $J=1\text{Hz}$, 2H). MASA (ES+): 683.2 |
| IA.129 | 0.88 (t, $J=7.32\text{Hz}$, 3H), 0.99 (d, $J=7.10\text{Hz}$, 3H), 1.11 (s, 3H), 1.19-1.32 (m, 4H), 1.48-1.97 (m, 8H), 2.20-2.48 (m, 6H), 3.36-3.40 (m, 1H), 4.30 (d, $J=16.53\text{Hz}$, 1H), 4.41 (d, $J=7.86\text{Hz}$, 1H), 4.47 (d, $J=16.56\text{Hz}$, 1H), 5.30-5.47 (m, 1H), 6.38 (dd, $J_1=10.12\text{Hz}$, $J_2=1.53\text{Hz}$, 1H), 6.43 (s, 1H), 7.13 (d, $J=10.02\text{Hz}$, 1H), 7.47 (d, $J=8.48\text{Hz}$, 2H), 7.95 (d, $J=8.48\text{Hz}$, 2H). MASA (ES+): 649.3 |
| IA.130 | 0.88 (t, $J=7.32\text{Hz}$, 3H), 0.98 (d, $J=7.11\text{Hz}$, 3H), 1.13 (s, 3H), 1.18-1.42 (m, 4H), 1.45-1.99 (m, 8H), 2.20-2.46 (m, 6H), 3.36-3.39 (m, 1H), 4.30 (d, $J=17.38\text{Hz}$, 1H), 4.41-4.46 (m, 2H), 5.30-5.47 (m, 1H), 6.38 (dd, $J_1=10.13\text{Hz}$, $J_2=1.55\text{Hz}$, 1H), 6.43 (s, 1H), 6.89-6.95 (m, 1H), 6.97-7.01 (m, 1H), 7.13 (d, $J=9.99\text{Hz}$, 1H), 7.92-7.98 (m, 1H). MASA (ES+): 651.4 |
| IA.131 | 0.88 (t, $J=7.35\text{Hz}$, 3H), 0.99 (d, $J=7.12\text{Hz}$, 3H), 1.11 (s, 3H), 1.21-1.38 (m, 3H), 1.45-1.99 (m, 9H), 2.20-2.46 (m, 6H), 3.36-3.40 (m, 1H), 4.31 (d, $J=16.51\text{Hz}$, 1H), 4.41 (d, $J=7.65\text{Hz}$, 1H), 4.49 (d, $J=16.50\text{Hz}$, 1H), 5.30-5.47 (m, 1H), 6.38 (dd, $J_1=10.12\text{Hz}$, $J_2=1.69\text{Hz}$, 1H), 6.43 (s, 1H), 7.12-7.18 (m, 3H), 8.03-8.06 (m, 2H). MASA (ES+): 633.4 |
| IA.132 | 0.98 (d, $J=7.04\text{Hz}$, 3H), 1.11 (s, 3H), 1.16 (d, $J=5.61\text{Hz}$, 6H), 1.30-1.35 (m, 1H), 1.53 (s, 3H), 1.73-2.01 (m, 4H), 2.21-2.60 (m, 5H), 3.37-3.40 (m, 1H), 4.28 (d, $J=16.48\text{Hz}$, 1H), 4.42 (d, $J=7.47\text{Hz}$, 1H), 4.48 (d, $J=16.59\text{Hz}$, 1H), 5.30-5.47 (m, 1H), 6.38 (d, $J=10.17\text{Hz}$, 1H), 6.43 (s, 1H), 7.13 (d, $J=10.11\text{Hz}$, 1H), 7.473 (d, $J=8.33\text{Hz}$, 2H), 7.95 (d, $J=8.39\text{Hz}$, 2H). MASA (ES+): 635.2 |
| IA.133 | 0.96 (d, $J=7.13\text{Hz}$, 3H), 1.24 (s, 3H), 1.27-1.33 (m, 1H), 1.55 (s, 3H), 1.75-2.06 (m, 6H), 2.19-2.38 (m, 8H), 3.13-3.19 (m, 1H), 3.33-3.37 (m, 1H), 4.41 (d, $J=9.04\text{Hz}$, 1H), 5.00 (d, $J=16.54\text{Hz}$, 1H), 5.31-5.48 (m, 1H), 5.71 (d, $J=16.57\text{Hz}$, 1H), 6.38 (dd, $J_1=10.15\text{Hz}$, $J_2=1.70\text{Hz}$, 1H), 6.44 (s, 1H), 7.15 (dd, $J_1=9.99\text{Hz}$, $J_2=1.10\text{Hz}$, 1H), 7.18 (t, $J=8.54\text{Hz}$, 2H), 7.94-7.97 (m, 2H). MASS (ES+): 615.1 |
| IA.134 | 0.98 (d, $J=7.16\text{Hz}$, 3H), 1.10 (s, 3H), 1.30-1.36 (m, 1H), 1.53 (s, 3H), 1.53-1.98 (m, 12H), 2.23-2.42 (m, 4H), 2.72-2.80 (m, 1H), 3.36-3.40 (m, 1H), 4.33 (d, $J=16.54\text{Hz}$, 1H), 4.42 (d, $J=8.83\text{Hz}$, 1H), 4.49 (d, $J=16.53\text{Hz}$, 1H), 5.30-5.47 (m, 1H), 6.38 (dd, $J_1=10.14\text{Hz}$, $J_2=1.80\text{Hz}$, 1H), 6.43 (s, 1H), 7.12 (dd, $J_1=10.19\text{Hz}$, $J_2=1.24\text{Hz}$, 1H), 7.76 (d, $J=8.27\text{Hz}$, 2H), 8.11 (d, $J=8.14\text{Hz}$, 2H). MASA (ES+): 695.3 |
| IA.135 | 0.99 (d, $J=7.13\text{Hz}$, 3H), 1.11 (s, 3H), 1.25-1.32 (m, 1H), 1.52 (s, 3H), 1.72-2.04 (m, 6H), 2.18-2.40 (m, 8H), 3.14-3.16 (m, 1H), 4.31 (d, $J=16.5\text{Hz}$, 1H), 4.40 (d, $J=8.48\text{Hz}$, 1H), 4.48 (d, $J=16.52\text{Hz}$, 1H), 6.37 (dd, $J_1=10.12\text{Hz}$, $J_2=1.72\text{Hz}$, 1H), 6.43 (s, 1H), 7.12 (dd, $J_1=10.12\text{Hz}$, $J_2=0.8\text{Hz}$, 1H), 7.47 (d, $J=8.57\text{Hz}$, 2H), 7.95 (d, $J=8.59\text{Hz}$, 2H). MASA (ES+): 647.2 |
| IA.136 | 0.99 (d, $J=7.12\text{Hz}$, 3H), 1.10 (s, 3H), 1.29-1.35 (m, 1H), 1.53 (s, 3H), 1.76-1.99 (m, 6H), 2.17-2.45 (m, 8H), 3.12-3.21 (m, 1H), 3.35-3.41 (m, 1H), 4.33 (d, 1H, $J=16.59\text{Hz}$), 4.41 (d, $J=8.63\text{Hz}$, 1H), 4.51 (d, 1H, $J=16.56\text{Hz}$), 5.30-5.47 (m, 1H), 6.37 (dd, $J_1=10.16\text{Hz}$, $J_2=1.61\text{Hz}$, 1H), 6.43 (s, 1H), 7.13 (dd, $J_1=10.18\text{Hz}$, $J_2=0.73\text{Hz}$, 1H), 7.77 (d, $J=8.24\text{Hz}$, 2H), 8.12 (d, $J=8.14\text{Hz}$, 2H). MASA (ES+): 681.2 |
| IA.137 | 0.98 (d, $J=7.13\text{Hz}$, 3H), 1.12 (s, 3H), 1.29-1.35 (m, 1H), 1.53 (s, 3H), 1.70-2.00 (m, 5H), 2.16-2.45 (m, 7H), 3.13-3.18 (m, 1H), 3.36-3.43 (m, 1H), 4.29 (dd, $J_1=17.52\text{Hz}$, $J_2=2.62\text{Hz}$, 1H), 4.41 (d, $J=9.87\text{Hz}$, 1H), 4.45 (dd, $J_1=17.67\text{Hz}$, $J_2=2.71\text{Hz}$, 1H), 5.31-5.47 (m, 1H), 6.38 (dd, $J_1=10.12\text{Hz}$, $J_2=1.71\text{Hz}$, 1H), 6.43 (s, 1H), 6.89-7.02 (m, 2H), 7.14 (d, $J=10.13\text{Hz}$, 1H), 7.92-7.98 (m, 1H). MASA (ES+): 649.3 |
| IA.138 | 0.96 (d, $J=7.16\text{Hz}$, 3H), 1.11 (s, 3H), 1.29-1.34 (m, 1H), 1.52 (s, 3H), 1.84-2.04 (m, 6H), 2.17-2.39 (m, 8H), 3.14-3.19 (m, 1H), 3.38-3.43 (m, 1H), 3.88 (s, 3H), 4.30 (d, $J=16.51\text{Hz}$, 1H), 4.40 (d, $J=8.92\text{Hz}$, 1H), 4.53 (d, $J=16.51\text{Hz}$, 1H), 5.30-5.47 (m, 1H), 6.37 (dd, $J_1=10.13\text{Hz}$, $J_2=1.74\text{Hz}$, 1H), 6.43 (s, 1H), 6.96 (d, $J=8.85\text{Hz}$, 2H), 7.14 (d, $J=10.11\text{Hz}$, 1H), 7.99 (d, $J=8.85\text{Hz}$, 2H). MASA (ES+): 643.3 |
| IA.139 | 1.06 (d, $J=7.12\text{Hz}$, 3H), 1.17 (s, 3H), 1.33-1.38 (m, 1H), 1.56 (s, 3H), 1.60-1.99 (m, 5H), 2.29-2.65 (m, 4H), 3.41-3.46 (m, 1H), 4.35 (d, 1H, $J=16.58\text{Hz}$), 4.46 (d, 1H, $J=8.88\text{Hz}$), 4.53 (d, 1H, $J=16.55\text{Hz}$), 6.15 (s, 1H), 6.37 (dd, $J_1=10.13\text{Hz}$, $J_2=1.68\text{Hz}$, 1H), 6.49 (dd, $J_1=3.42\text{Hz}$, $J_2=1.65\text{Hz}$, 1H), 7.12 (d, $J=3.47\text{Hz}$, 1H), 7.22 (d, $J=10.12\text{Hz}$, 1H), 7.58 (d, $J=1.48\text{Hz}$, 1H), 7.76 (d, $J=8.35\text{Hz}$, 2H), 8.12 (d, $J=8.26\text{Hz}$, 2H). MASA (ES+): 675.3 |
| IA.140 | 1.05 (d, $J=7.1\text{Hz}$, 3H), 1.19 (s, 3H), 1.32-1.37 (m, 1H), 1.57 (s, 3H), 1.60-2.02 (m, 5H), 2.29-2.67 (m, 5H), 3.42-3.47 (m, 1H), 4.31 (dd, $J_1=17.52\text{Hz}$, $J_2=2.24\text{Hz}$, 1H), 4.46 (d, $J=8.89\text{Hz}$, 1H), 4.47 (dd, 1H), 6.15 (s, 1H), 6.37 (dd, $J_1=10.11\text{Hz}$, $J_2=1.09\text{Hz}$, 1H), 6.48 (dd, $J_1=3.04\text{Hz}$, $J_2=1.33\text{Hz}$, 1H), 6.88-7.01 (m, 2H), 7.12 (d, $J=3.45\text{Hz}$, 1H), 7.23 (d, $J=10.12\text{Hz}$, 1H), 7.58 (d), 7.95 (dd, $J_1=15.1\text{Hz}$, $J_2=8.46\text{Hz}$, 1H). MASA (ES+): 643.2 |
| IA.141 | 1.05 (d, $J=7.09\text{Hz}$, 3H), 1.17 (s, 3H), 1.25-1.38 (m, 1H), 1.56 (s, 3H), 1.60-2.00 (m, 5H), 2.29-2.65 (m, 4H), 3.43-3.45 (m, 1H), 4.32 (d, 1H, $J=16.52\text{Hz}$), 4.45 (d, 1H, $J=9.02\text{Hz}$), 4.50 (d, 1H, $J=16.61\text{Hz}$), 6.15 (s, 1H), 6.37 (dd, $J_1=10.07\text{Hz}$, $J_2=0.81\text{Hz}$, 1H), 6.49 (d, $J=3.33\text{Hz}$, 1H), 7.12 (d, $J=3.43\text{Hz}$, 1H), 7.22 (d, $J=10.12\text{Hz}$, 1H), 7.47 (d, $J=8.40\text{Hz}$, 2H), 7.58 (s, 1H), 7.95 (d, $J=8.45\text{Hz}$, 2H). MASA (ES+): 641.3 |
| IA.142 | 1.06 (d, $J=7.12\text{Hz}$, 3H), 1.18 (s, 3H), 1.31-1.37 (m, 1H), 1.56 (s, 3H), 1.60-2.04 (m, 4H), 2.29-2.65 (m, 5H), 3.44-3.48 (m, 1H), 3.88 (s, 3H), 4.33 (d, $J=16.64\text{Hz}$, 1H), 4.45 (d, $J=8.94\text{Hz}$, 1H), 4.54 (d, $J=16.50\text{Hz}$, 1H), 6.15 (s, 1H), 6.36 (dd, $J_1=10.11\text{Hz}$, $J_2=1.73\text{Hz}$, 1H), 6.49 (dd, $J_1=3.46\text{Hz}$, $J_2=1.70\text{Hz}$, 1H), 6.95 (d, $J=8.89\text{Hz}$, 2H), 7.12 (d, $J=13.39\text{Hz}$, 1H), 7.23 (d, $J=10.15\text{Hz}$, 1H), 7.58 (s, 1H), 7.99 (d, $J_1=8.66\text{Hz}$, 2H). MASA (ES+): 637.4 |
| IA.143 | 1.05 (d, $J=7.12\text{Hz}$, 3H), 1.18 (s, 3H), 1.25-1.35 (m, 1H), 1.57 (s, 3H), 1.63-1.99 (m, 5H), 2.03-2.64 (m, 5H), 3.45 (m, 1H), 4.32 (d, $J=16.52$, 1H), 4.45 (d, $J=9.01$, 1H), 4.53 (d, $J=16.54$, 1H), 6.15 (s, 1H), 6.37 (dd, $J_1=10.11\text{Hz}$, $J_2=1.75\text{Hz}$, 1H), 6.49 (dd, $J_1=3.47\text{Hz}$, $J_2=1.71\text{Hz}$, 1H), 7.13-7.25 (m, 4H), 7.58 (d, $J=0.81\text{Hz}$, 1H), 8.03-8.07 (m, 2H). MASA (ES+): 647.2 M+Na ⁺ |
| IA.144 | 0.96 (d, $J=7.17\text{Hz}$, 3H), 1.04 (s, 3H), 1.15 (d, $J=3.84\text{Hz}$, 3H), 1.17 (d, $J=3.86\text{Hz}$, 3H), 1.28-1.34 (m, 1H), 1.52 (s, 3H), 1.76-1.89 (m, 4H), 2.25 (s, 6H), 2.28 (s, 3H), 2.22-2.41 (m, 4H), 2.55-2.62 (m, 1H), 3.38-3.43 (m, 1H), 4.03 (d, $J=17.76\text{Hz}$, 1H), 4.30 (d, $J=17.79\text{Hz}$, 1H), 4.37 (d, $J=8.81\text{Hz}$, 1H), 5.30-5.47 (m, 1H), 6.37 (dd, $J_1=10.14\text{Hz}$, $J_2=1.86\text{Hz}$, 1H), 6.43 (s, 1H), 6.85 (s, 2H), 7.12 |

| Com-
puesto
No. | III-NMR (δ ppm). MASA (EI / ES+, m/z) |
|-----------------------|--|
| | (dd, $J_1=10.13$ Hz, $J_2=1.29$ Hz, 1H). MASA (ES+): 643.5 |
| IA.145 | 0.95 (d, $J=7.15$ Hz, 3H), 1.02 (s, 3H), 1.20-1.42 (m, 8H), 1.52 (s, 3H), 1.72-1.89 (m, 6H), 2.25 (s, 6H), 2.28 (s, 3H), 2.25-2.41 (m, 5H), 3.37-3.43 (m, 1H), 4.02 (d, $J=17.62$ Hz, 1H), 4.30 (d, $J=17.83$ Hz, 1H), 4.38 (d, $J=8.83$ Hz, 1H), 5.30-5.47 (m, 1H), 6.38 (dd, $J_1=10.14$ Hz, $J_2=1.86$ Hz, 1H), 6.44 (s, 1H), 6.85 (s, 2H), 7.13 (dd, $J_1=10.14$ Hz, $J_2=1.39$ Hz, 1H). MASA (ES+): 705.3 (M+Na) ⁺ |
| IA.146 | 0.96 (d, $J=7.16$ Hz, 3H), 1.03 (s, 3H), 1.25-1.34 (m, 1H), 1.52 (s, 3H), 1.54-1.69 (m, 4H), 1.76-1.89 (m, 7H), 2.25 (s, 6H), 2.28 (s, 3H), 2.27-2.80 (m, 1H), 3.37-3.43 (m, 1H), 4.03 (d, $J=17.77$ Hz, 1H), 4.30 (d, $J=17.77$ Hz, 1H), 4.37 (d, $J=8.7$ Hz, 1H), 5.30-5.47 (m, 1H), 6.37 (dd, $J_1=10.14$ Hz, $J_2=1.82$ Hz, 1H), 6.43 (s, 1H), 6.85 (s, 2H), 7.12 (dd, $J_1=10.14$ Hz, $J_2=1.12$ Hz, 1H). MASA (ES+): 669.4 |
| IA.147 | 0.97 (d, $J=7.17$ Hz, 3H), 1.02 (s, 3H), 1.28-1.34 (m, 1H), 1.52 (s, 3H), 1.72-1.97 (m, 6H), 2.18-2.23 (m, 5H), 2.26 (s, 6H), 2.28 (s, 3H), 2.30-2.43 (m, 2H), 3.12-3.20 (m, 1H), 3.38-3.43 (m, 1H), 4.06 (d, $J=17.72$ Hz, 1H), 4.29 (d, $J=17.72$ Hz, 1H), 4.37 (d, $J=8.92$ Hz, 1H), 5.30-5.47 (m, 1H), 6.38 (dd, $J_1=10.15$ Hz, $J_2=1.87$ Hz, 1H), 6.43 (s, 1H), 6.85 (s, 2H), 7.11 (dd, $J_1=10.13$ Hz, $J_2=1.27$ Hz, 1H). MASA (ES+): 655.4 |
| IA.148 | 0.91-0.94 (m, 2H), 0.98 (d, $J=7.11$ Hz, 3H), 1.03 (s, 3H), 1.09-1.26 (m, 5H), 1.52- (s, 3H), 1.65-1.75 (m, 8H), 1.83-1.93 (m, 2H), 2.17-2.22 (m, 3H), 2.25 (s, 6H), 2.28 (s, 3H), 2.34-2.38 (m, 1H), 3.37-3.41 (m, 1H), 4.06 (d, $J=17.78$ Hz, 1H), 4.27 (d, $J=17.79$ Hz, 1H), 4.27 (d, $J=9.08$ Hz, 1H), 5.30-5.46 (m, 1H), 6.38 (d, $J_1=10.14$ Hz, $J_2=1.85$ Hz, 1H), 6.43 (s, 1H), 6.85 (s, 2H), 7.12 (d, $J_1=10.12$ Hz, $J_2=1.20$ Hz, 1H). MASA (ES+): 719.4 (M+Na) ⁺ |
| IA.149 | 1.07 (d, $J=7.13$ Hz, 3H), 1.20 (s, 3H), 1.35-1.40 (m, 1H), 1.56 (s, 3H), 1.72-1.98 (m, 3H), 2.25 (s, 6H), 2.28 (s, 3H), 2.32-2.44 (m, 4H), 3.44-3.49 (m, 1H), 4.13 (d, $J=17.69$ Hz, 1H), 4.23 (d, $J=17.69$ Hz, 1H), 4.40 (d, $J=8.86$ Hz, 1H), 4.53-4.55 (m, 1H), 5.34-5.51 (m, 1H), 6.36 (dd, $J_1=10.10$ Hz, $J_2=1.79$ Hz, 1H), 6.41 (s, 1H), 6.86 (s, 2H), 7.10 (dd, $J_1=4.94$ Hz, $J_2=3.81$ Hz, 1H), 7.25 (dd, $J_1=10.12$ Hz, $J_2=1.05$ Hz, 1H), 7.58 (dd, $J_1=4.98$ Hz, $J_2=1.15$ Hz, 1H), 7.73 (dd, $J_1=3.65$ Hz, $J_2=1.16$ Hz, 1H). MASA (ES+): 683.9 |
| IA.150 | 0.88-0.94 (m, 2H), 0.99 (d, $J=7.10$ Hz, 3H), 1.13 (s, 3H), 1.17-1.35 (m, 4H), 1.53 (s, 3H), 1.64-1.98 (m, 10H), 2.17-2.46 (m, 6H), 3.35-3.39 (m, 1H), 4.30 (d, $J_1=15.16$ Hz, $J_2=2.50$ Hz, 1H), 4.40 (d, 1H), 4.42 (d, $J_1=17.58$ Hz, $J_2=2.47$ Hz, 1H), 5.31-5.45 (m, 1H), 6.38 (d, $J_1=10.13$ Hz, $J_2=1.65$ Hz, 1H), 6.43 (s, 1H), 6.89-7.01 (m, 2H), 7.13 (d, $J_1=10.11$ Hz, $J_2=1.11$ Hz, 1H), 7.92-7.98 (m, 1H). MASA (ES+): 691.5 |
| IA.151 | 0.91-0.97 (m, 2H), 0.99 (d, $J=7.15$ Hz, 3H), 1.11 (s, 3H), 1.13-1.35 (m, 4H), 1.52 (s, 3H), 1.61-1.95 (m, 9H), 2.19-2.40 (m, 6H), 3.35-3.40 (m, 1H), 4.33 (d, $J=16.4$ Hz, 1H), 4.41 (d, $J=12.88$ Hz, 1H), 4.45 (d, $J=16.53$ Hz, 1H), 5.30-5.47 (m, 1H), 6.38 (d, $J_1=10.12$ Hz, $J_2=1.80$ Hz, 1H), 6.43 (s, 1H), 7.13 (d, $J_1=10.14$ Hz, $J_2=1.27$ Hz, 1H), 7.46 (d, $J=8.55$ Hz, 2H), 7.94 (d, $J=8.61$ Hz, 2H). MASA (ES+): 711.3 (M+Na) ⁺ |
| IA.152 | 0.91-0.97 (m, 2H), 1.00 (d, $J=7.13$ Hz, 3H), 1.11 (s, 3H), 1.13-1.36 (m, 4H), 1.53 (s, 3H), 1.61-1.91 (m, 10H), 2.20-2.45 (m, 6H), 3.34-3.40 (m, 1H), 4.35 (d, $J=16.56$ Hz, 1H), 4.41 (d, $J=8.94$ Hz, 1H), 4.48 (d, $J=16.54$ Hz, 1H), 5.30-5.47 (m, 1H), 6.38 (d, $J_1=10.15$ Hz, $J_2=1.87$ Hz, 1H), 6.43 (s, 1H), 7.12 (d, $J_1=10.13$ Hz, $J_2=1.26$ Hz, 1H), 7.76 (d, $J=8.28$ Hz, 2H), 8.11 (d, $J=8.16$ Hz, 2H). MASA (ES+): 723.1 |
| IA.153 | 0.91-0.97 (m, 2H), 1.00 (d, $J=7.11$ Hz, 3H), 1.12 (s, 3H), 1.09-1.36 (m, 4H), 1.52 (s, 3H), 1.61-1.87 (m, 10H), 2.20-2.39 (m, 6H), 3.37-3.42 (m, 1H), 3.88 (s, 3H), 4.34 (d, $J=16.49$ Hz, 1H), 4.40 (d, $J=9.19$ Hz, 1H), 4.48 (d, $J=16.43$ Hz, 1H), 5.30-5.47 (m, 1H), 6.37 (d, $J_1=10.14$ Hz, $J_2=1.76$ Hz, 1H), 6.43 (s, 1H), 6.95 (d, $J=8.87$ Hz, 2H), 7.13 (d, $J_1=10.13$ Hz, $J_2=1.02$ Hz, 1H), 7.99 (d, $J=8.89$ Hz, 2H). MASA (ES+): 707.3 (M+Na) ⁺ |
| IA.154 | 0.89 (t, $J=7.34$ Hz, 3H), 0.97 (d, $J=7.10$ Hz, 3H), 1.03 (s, 3H), 1.25-1.96 (m, 8H), 2.09-2.40 (m, 15H), 3.38-3.42 (m, 1H), 4.05 (d, $J=17.80$ Hz, 1H), 4.29 (d, $J=17.72$ Hz, 1H), 4.39 (d, $J=7.99$ Hz, 1H), 5.30-5.47 (m, 1H), 6.39 (dd, $J_1=10.10$ Hz, $J_2=1.65$ Hz, 1H), 6.43 (s, 1H), 6.85 (s, 2H), 7.13 (d, $J=10.07$ Hz, 1H). MASA (ES+): 657.3 |
| IA.155 | 1.03 (s, 3H), 1.06 (d, $J=7.19$ Hz, 3H), 1.26 (t, $J=7.09$ Hz, 3H), 1.32-1.94 (m, 10H), 2.22-2.44 (m, 12H), 3.37-3.42 (m, 1H), 4.04-4.18 (m, 3H), 4.30 (d, $J=17.74$ Hz, 1H), 4.36-4.38 (m, 1H), 5.30-5.45 (m, 1H), 6.37 (dd, $J_1=10.14$ Hz, $J_2=1.67$ Hz, 1H), 6.42 (s, 1H), 6.86 (s, 2H), 7.12 (d, $J=10.21$ Hz, 1H). MASA (ES+): 645.1 |
| IA.156 | 1.06 (d, $J=7.19$ Hz, 3H), 1.11 (s, 3H), 1.25-1.97 (m, 8H), 2.25 (s, 6H), 2.28 (s, 3H), 2.30-2.53 (m, 3H), 3.46-3.51 (m, 1H), 4.07 (d, $J=17.84$ Hz, 1H), 4.31 (d, $J=17.82$ Hz, 1H), 5.34-5.46 (m, 1H), 6.41 (dd, $J_1=10.14$ Hz, $J_2=1.87$ Hz, 1H), 6.51 (dd, $J_1=3.50$ Hz, $J_2=1.73$ Hz, 1H), 6.81 (s, 2H), 7.12-7.16 (m, 2H), 7.59 (d, $J=1.01$ Hz, 1H). MASA (ES+): 667.3 |
| IA.157 | 1.07 (d, $J=7.10$ Hz, 3H), 1.17 (s, 3H), 1.21-2.03 (m, 8H), 2.17-2.55 (m, 4H), 3.45-3.48 (m, 1H), 4.32 (d, $J=16.56$ Hz, 1H), 4.46 (d, $J=8.46$ Hz, 1H), 4.51 (d, $J=15.90$ Hz, 1H), 5.7-5.49 (m, 1H), 6.40 (dd, $J_1=10.14$ Hz, $J_2=1.70$ Hz, 1H), 6.45 (s, 1H), 6.51 (dd, $J_1=3.44$ Hz, $J_2=1.67$ Hz, 1H), 7.13-7.16 (m, 2H), 7.47 (d, $J=8.56$ Hz, 2H), 7.59 (s, 1H), 7.96 (d, $J=8.59$ Hz, 2H). MASA (ES+): 659.5 |
| IA.158 | 0.97 (s, 3H), 1.14 (t, $J=7.54$ Hz, 3H), 1.19-1.25 (m, 1H), 1.38 (d, $J=7.35$ Hz, 3H), 1.54 (s, 3H), 1.92-2.14 (m, 4H), 2.26-2.48 (m, 5H), 3.97 (d, $J=16.90$ Hz, 1H), 4.45 (d, $J=8.33$ Hz, 1H), 4.56 (d, $J=16.89$ Hz, 1H), 5.31-5.48 (m, 1H), 6.38 (dd, $J_1=10.14$ Hz, $J_2=1.85$ Hz, 1H), 6.44 (s, 1H), 7.14 (dd, $J_1=10.12$ Hz, $J_2=1.22$ Hz, 1H), 7.47 (d, $J=8.60$ Hz, 2H), 7.93 (d, $J=8.59$ Hz, 2H). MASA (ES+): 643.3 (M+Na) ⁺ |
| IA.159 | 1.08 (d, $J=7.14$ Hz, 3H), 1.17 (s, 3H), 1.37-1.42 (m, 1H), 1.55 (s, 3H), 1.78-1.94 (m, 4H), 2.00-2.57 (m, 4H), 3.44-3.49 (m, 1H), 4.37 (d, $J=16.62$ Hz, 1H), 4.47 (d, $J=6.55$ Hz, 1H), 4.53 (d, $J=16.57$ Hz, 1H), 5.33-5.55 (m, 1H), 6.40 (d, $J_1=10.15$ Hz, $J_2=1.80$ Hz, 1H), 6.46 (s, 1H), 7.11 (dd, $J_1=4.95$ Hz, $J_2=3.87$ Hz, 1H), 7.15 (d, $J=10.14$ Hz, 1H), 7.58 (dd, $J_1=5.02$ Hz, $J_2=1.10$ Hz, 1H), 7.74 (d, $J_1=3.85$ Hz, $J_2=1.12$ Hz, 1H), 7.76 (d, $J=8.39$ Hz, 2H), 8.10 (d, $J=8.23$ Hz, 2H). MASA (ES+): 709.3 |
| IA.160 | 0.99 (d, $J=7.10$ Hz, 3H), 1.09 (s, 3H), 1.11 (t, $J=7.59$ Hz, 3H), 1.31-1.36 (m, 1H), 1.53 (s, 3H), 1.72-1.97 (m, 4H), 2.23-2.44 (m, 6H), 3.32-3.37 (m, 1H), 4.38-4.48 (m, 3H), 5.30-5.47 (m, 1H), 6.38 (d, $J_1=10.14$ Hz, $J_2=1.5$ Hz, 1H), 6.43 (s, 1H), 7.13 (d, $J=10.08$ Hz, 1H), 7.72 (t, $J=7.99$ Hz, 1H), 8.34 (d, $J=7.78$ Hz, 1H), 8.46 (d, $J_1=8.17$ Hz, $J_2=1.14$ Hz, 1H), 8.82 (s, 1H). MASA (ES+): 654.3 (M+Na) ⁺ |
| IA.161 | 0.99 (d, $J=7.16$ Hz, 3H), 1.12 (t, $J=7.58$ Hz, 3H), 1.13 (s, 3H), 1.31-1.35 (m, 1H), 1.52 (s, 3H), 1.76-2.01 (m, 3H), 2.23-2.45 (m, 6H), 2.32 (s, 3H), 2.33 (s, 3H), 3.38-3.43 (m, 1H), 4.34 (d, $J=16.65$ Hz, 1H), 4.39-4.41 (m, 1H), 4.52 (d, $J=16.66$ Hz, 1H), 5.30-5.47 (m, 1H), 6.37 (dd, $J_1=10.14$ Hz, $J_2=1.81$ Hz, 1H), 6.43 (s, 1H), 7.13 (dd, $J_1=10.13$ Hz, $J_2=1.23$ Hz, 1H), 7.24 (d, $J=7.86$ Hz, 1H), 7.74 (dd, $J_1=8.51$ Hz, $J_2=1.38$ Hz, 1H), 7.77 (s, 1H). MASA (ES+): 615.4 |
| IA.162 | 0.97 (s, 3H), 1.14 (t, $J=7.51$ Hz, 3H), 1.21-1.27 (m, 1H), 1.38 (d, $J=7.37$ Hz, 3H), 1.54 (s, 3H), 1.73-2.12 (m, 5H), 2.26-2.50 (m, 6H), 4.01 (d, 1H, $J=16.98$ Hz), 4.46 (d, $J=8.09$ Hz, 1H), 4.58 (d, $J=16.98$ Hz, 1H), 5.31-5.48 (m, 1H), 6.38 (dd, $J_1=10.11$ Hz, $J_2=1.78$ Hz, 1H), 6.44 (s, 1H), 7.13 (dd, $J_1=10.17$ Hz, $J_2=1.27$ Hz, 1H), 7.77 (d, $J=8.35$ Hz, 2H), 8.09 (d, $J=8.05$ Hz, 2H). MASA (ES+): 655.4 |
| IA.163 | 0.93 (t, $J=7.36$ Hz, 3H), 1.00 (d, $J=7.20$ Hz, 3H), 1.11 (s, 3H), 1.25-1.97 (m, 10H), 2.20-2.41 (m, 6H), 3.35-3.39 (m, 1H), 4.33 (d, $J=16.58$ Hz, 1H), 4.41 (d, $J=8.84$ Hz, 1H), 4.50 (d, $J=16.57$ Hz, 1H), 5.30-5.47 (m, 1H), 6.38 (dd, $J_1=10.14$ Hz, $J_2=1.81$ Hz, 1H), 6.43 (s, 1H), 7.12 (dd, $J_1=10.12$ Hz, $J_2=1.17$ Hz, 1H), 7.76 (d, $J=8.29$ Hz, 2H), 8.12 (d, $J=8.12$ Hz, 2H). MASA (ES+): 669.3 |
| IA.164 | 0.94 (t, $J=7.40$ Hz, 3H), 0.99 (d, $J=7.15$ Hz, 3H), 1.11 (s, 3H), 1.24-1.98 (m, 10H), 2.22-2.41 (m, 6H), 3.36-3.40 (m, 1H), 4.29 (d, $J=16.51$ Hz, 1H), 4.41 (d, $J=8.74$ Hz, 1H), 4.47 (d, $J=16.54$ Hz, 1H), 5.30-5.47 (m, 1H), 6.37 (dd, $J_1=10.12$ Hz, $J_2=1.75$ Hz, 1H), 6.43 (s, 1H), 7.13 (dd, $J_1=10.12$ Hz, $J_2=1.14$ Hz, 1H), 7.46-7.48 (m, 2H), 7.95 (d, $J=8.61$ Hz, 2H). MASA (ES+): 635.3 |
| IA.165 | 0.94 (t, $J=7.39$ Hz, 3H), 0.99 (d, $J=7.16$ Hz, 3H), 1.13 (s, 3H), 1.22-2.01 (m, 10H), 2.20-2.45 (m, 6H), 3.36-3.40 (m, 1H), 4.30 (d, $J=16.52$ Hz, 1H), 4.28 (dd, $J_1=17.53$ Hz, $J_2=2.68$ Hz), 4.42-4.47 (m, 2H), 5.30-5.47 (m, 1H), 6.38 (dd, $J_1=10.14$ Hz, $J_2=1.76$ Hz, 1H), 6.43 (s, 1H), 6.89-7.01 (m, 2H), 7.12-7.15 (m, 1H), 7.92-7.98 (m, 1H). MASA (ES+): 637.3 |
| IA.166 | 0.94 (t, $J=7.36$ Hz, 3H), 0.99 (d, $J=7.16$ Hz, 3H), 1.11 (s, 3H), 1.24-1.99 (m, 10H), 2.20-2.41 (m, 6H), 3.37-3.41 (m, 1H), 4.30 (d, $J=16.52$ Hz, 1H), 4.41 (d, $J=8.86$ Hz, 1H), 4.49 (d, $J=16.51$ Hz, 1H), 5.30-5.47 (m, 1H), 6.38 (dd, $J_1=10.14$ Hz, $J_2=1.74$ Hz, 1H), 6.43 (s, 1H), 7.12-7.18 (m, 3H), 8.03-8.06 (m, 2H). MASA (ES+): 619.4 |

| Com-
puesto
No. | ¹ H-NMR (δ ppm). MASA (EI / ES+, <i>m/z</i>) |
|-----------------------|--|
| IA.167 | 0.94 (t, <i>J</i> =7.40Hz, 3H), 0.99 (d, <i>J</i> =7.15Hz, 3H), 1.20 (s, 3H), 1.17-1.87 (m, 10H), 2.20-2.45 (m, 6H), 3.38-3.43 (m, 1H), 3.88 (s, 3H), 4.30 (d, <i>J</i> =16.44Hz, 1H), 4.41 (d, <i>J</i> =9.06Hz, 1H), 4.52 (d, <i>J</i> =16.51Hz, 1H), 5.30-5.47 (m, 1H), 6.38 (dd, <i>J</i> ₁ =10.15Hz, <i>J</i> ₂ =1.85Hz, 1H), 6.43 (s, 1H), 6.94-6.97 (m, 2H), 7.13 (dd, <i>J</i> ₁ =10.12Hz, <i>J</i> ₂ =1.21Hz, 1H), 7.98-8.00 (m, 2H). MASA (ES+): 631.3 |
| IA.168 | 1.07 (d, <i>J</i> =7.15Hz, 3H), 1.16 (s, 3H), 1.35-1.41 (m, 1H), 1.55 (s, 3H), 1.74-2.03 (m, 4H), 2.28-2.55 (m, 1H), 3.43-3.48 (m, 1H), 4.33 (d, <i>J</i> =16.67Hz, 1H), 4.46 (d, <i>J</i> =H, 14Hz, 1H), 4.49 (d, <i>J</i> =16.89Hz, 1H), 5.32-5.49 (m, 1H), 6.40 (dd, <i>J</i> ₁ =10.14Hz, <i>J</i> ₂ =1.69Hz, 1H), 6.45 (s, 1H), 6.50 (dd, <i>J</i> ₁ =3.47Hz, <i>J</i> ₂ =1.69Hz, 1H), 7.13 (d, <i>J</i> =2.81Hz, 1H), 7.14 (dd, <i>J</i> ₁ =9.98Hz, <i>J</i> ₂ =1.20Hz, 1H), 7.45 (t, <i>J</i> =7.89Hz, 1H), 7.57 (dd, <i>J</i> ₁ =1.86Hz, <i>J</i> ₂ =0.89Hz, 1H), 7.59 (m, 1H), 7.88-7.91 (m, 1H), 7.98 (t, <i>J</i> =1.75Hz, 1H). MASA (ES+): 681.3 (M+Na) ⁺ |
| IA.169 | 1.03 (s, 3H), 1.13-1.36 (m, 1H), 1.43 (d, <i>J</i> =7.23Hz, 3H), 1.56 (s, 3H), 1.77-2.23 (m, 5H), 2.31-2.67 (m, 4H), 3.97 (d, 1H, <i>J</i> =17.00Hz), 4.53 (d, <i>J</i> =7.381Hz, 1H), 4.62 (d, <i>J</i> =17.03Hz, 1H), 5.24-5.57 (m, 1H), 6.41 (d, <i>J</i> =10.09Hz, 1H), 6.44 (s, 1H), 6.53 (dd, <i>J</i> ₁ =3.24Hz, <i>J</i> ₂ =1.49Hz, 1H), 7.17 (d, <i>J</i> =9.71Hz, 1H), 7.20 (d, <i>J</i> =3.03Hz, 1H), 7.62 (s, 1H), 7.76 (d, <i>J</i> =8.15Hz, 2H), 8.09 (d, <i>J</i> =8.09Hz, 2H). MASA (ES+): 093.2 |
| IA.170 | 1.07 (d, <i>J</i> =7.13Hz, 3H), 1.17 (s, 3H), 1.35-1.41 (m, 1H), 1.54 (s, 3H), 1.76-2.04 (m, 4H), 2.28-2.54 (m, 4H), 3.45-3.50 (m, 1H), 3.83 (s, 3H), 4.36 (d, 1H, <i>J</i> =10.61Hz), 4.45 (d, <i>J</i> =8.19Hz, 1H), 4.51 (d, <i>J</i> =16.68Hz, 1H), 5.32-5.49 (m, 1H), 6.39 (dd, <i>J</i> ₁ =10.15Hz, <i>J</i> ₂ =1.84Hz, 1H), 0.45 (s, 1H), 6.50 (dd, <i>J</i> ₁ =3.50Hz, <i>J</i> ₂ =1.70Hz, 1H), 6.68 (t, <i>J</i> =2.27Hz, 1H), 7.13-7.17 (m, 4H), 7.59 (m, 1H). MASA (ES+): 685.2 |
| IA.171 | 1.07 (d, <i>J</i> =7.12Hz, 3H), 1.17 (s, 3H), 1.34-1.42 (m, 1H), 1.55 (s, 3H), 1.73-1.99 (m, 4H), 2.28-2.55 (m, 4H), 3.41-3.47 (m, 1H), 4.35 (d, 1H, <i>J</i> =16.49Hz), 4.46 (d, <i>J</i> =8.61Hz, 1H), 4.52 (d, <i>J</i> =16.49Hz, 1H), 5.33-5.49 (m, 1H), 6.40 (dd, <i>J</i> ₁ =10.12Hz, <i>J</i> ₂ =1.73Hz, 1H), 6.45 (s, 1H), 6.51 (dd, <i>J</i> ₁ =3.47Hz, <i>J</i> ₂ =1.71Hz, 1H), 7.13 (d, <i>J</i> =3.46Hz, 1H), 7.14 (d, <i>J</i> =10.8Hz, 1H), 7.59-7.60 (m, 1H), 8.17 (d, <i>J</i> =8.8Hz, 2H), 8.34 (d, <i>J</i> =8.72Hz, 2H). MASA (ES+): 692.3 (M+Na) ⁺ |
| IA.172 | 1.03 (d, <i>J</i> =7.16Hz, 3H), 1.13 (s, 3H), 1.33-1.38 (m, 1H), 1.52 (s, 3H), 1.66-1.96 (m, 4H), 2.18-2.38 (m, 4H), 3.36-3.43 (m, 1H), 3.41 (s, 3H), 4.05 (s, 2H), 4.35 (d, 1H, <i>J</i> =16.67Hz), 4.40 (d, <i>J</i> =9.01Hz, 1H), 4.49 (d, <i>J</i> =16.66Hz, 1H), 5.30-5.47 (m, 1H), (6.37 (dd, <i>J</i> ₁ =10.12Hz, <i>J</i> ₂ =1.73Hz, 1H), 6.43 (s, 1H), 7.11 (dd, <i>J</i> ₁ =10.11Hz, <i>J</i> ₂ =1.01Hz, 1H), 7.77 (d, <i>J</i> =8.33Hz, 2H), 8.11 (d, <i>J</i> =8.18Hz, 2H). MASA (ES+): 693.3 (M+Na) ⁺ |
| IA.173 | 1.01 (d, <i>J</i> =7.14Hz, 3H), 1.07 (s, 3H), 1.31-1.35 (m, 1H), 1.52 (s, 3H), 1.75-1.95 (m, 4H), 2.19-2.35 (m, 4H), 2.25 (s, 6H), 2.28 (s, 3H), 3.41 (s, 3H), 3.41-3.49 (m, 1H), 4.05 (s, 3H), 4.07 (d, <i>J</i> =13.34Hz, 1H), 4.27 (d, <i>J</i> =17.85Hz, 1H), 4.37 (d, <i>J</i> =8.04Hz, 1H), 5.30-5.46 (m, 1H), 6.37 (dd, <i>J</i> ₁ =10.13Hz, <i>J</i> ₂ =1.65Hz, 1H), 6.43 (s, 1H), 6.86 (s, 2H), 7.12 (d, <i>J</i> ₁ =10.09Hz, 1H). MASA (ES+): 667.2 (M+Na) ⁺ |
| IA.174 | 0.99 (d, <i>J</i> =7.00Hz, 3H), 1.10-1.14 (m, 6H), 1.22-1.97 (m, 8H), 2.20-2.45 (m, 6H), 3.35-3.39 (m, 1H), 4.27 (d, <i>J</i> =16.36Hz, 1H), 4.40-4.45 (m, 2H), 5.30-5.47 (m, 1H), 6.37 (dd, <i>J</i> ₁ =10.14Hz, <i>J</i> ₂ =1.74Hz, 1H), 6.43 (s, 1H), 7.13 (dd, <i>J</i> ₁ =10.15Hz, <i>J</i> ₂ =0.90Hz, 1H), 7.24-7.28 (m, 1H), 7.91-7.95 (m, 1H), 8.08-8.10 (m, 1H). MASA (ES+): 639.4 |
| IA.175 | 0.91 (s, 3H), 1.25-1.27 (m, 1H), 1.44 (d, <i>J</i> =7.23Hz, 3H), 1.55 (s, 3H), 1.74-2.17 (m, 4H), 2.23 (s, 6H), 2.28 (s, 3H), 2.31-2.58 (m, 4H), 3.69 (d, <i>J</i> =17.64Hz, 1H), 4.43 (d, <i>J</i> =17.63Hz, 1H), 4.46 (d, <i>J</i> =11.28Hz, 1H), 5.32-5.48 (m, 1H), 6.40 (dd, <i>J</i> ₁ =10.11Hz, <i>J</i> ₂ =1.68Hz, 1H), 6.44 (s, 1H), 6.52 (dd, <i>J</i> ₁ =3.63Hz, <i>J</i> ₂ =1.51Hz, 1H), 6.85 (s, 2H), 7.16 (dd, <i>J</i> ₁ =10.15Hz, <i>J</i> ₂ =0.99Hz, 1H), 7.19 (d, <i>J</i> =3.31Hz, 1H), 7.61 (d, <i>J</i> =0.79Hz, 1H). MASA (ES+): 667.1 |
| IA.176 | 1.01 (d, <i>J</i> =7.14Hz, 3H), 1.06 (s, 3H), 1.21 (d, <i>J</i> =7.00Hz, 3H), 1.32-1.36 (m, 1H), 1.52 (s, 3H), 1.75-1.94 (m, 4H), 2.25 (s, 6H), 2.28 (s, 3H), 2.20-2.36 (m, 4H), 3.35-3.45 (m, 1H), 3.54 (q, <i>J</i> =7.02Hz, 2H), 4.06 (d, <i>J</i> =17.75Hz, 1H), 4.09 (s, 2H), 4.26 (d, <i>J</i> =17.82Hz, 1H), 4.36 (d, <i>J</i> =8.94Hz, 1H), 5.29-5.47 (m, 1H), 6.37 (dd, <i>J</i> ₁ =10.14Hz, <i>J</i> ₂ =1.78Hz, 1H), 6.43 (s, 1H), 6.86 (s, 2H), 7.10 (dd, <i>J</i> ₁ =10.11Hz, <i>J</i> ₂ =0.82Hz, 1H). MASA (ES+): 659.1 |
| IA.177 | 1.03 (d, <i>J</i> =7.13Hz, 3H), 1.13 (s, 3H), 1.21 (t, <i>J</i> =7.00Hz, 3H), 1.32-1.37 (m, 1H), 1.52 (s, 3H), 1.68-1.95 (m, 4H), 2.20-2.45 (m, 4H), 3.38-3.43 (m, 1H), 3.54 (qd, <i>J</i> ₁ =6.98Hz, <i>J</i> ₂ =1.49Hz, 2H), 4.09 (s, 2H), 4.25 (d, <i>J</i> =16.66Hz, 1H), 4.40 (d, <i>J</i> =10.48Hz, 1H), 4.49 (d, <i>J</i> =16.63Hz, 1H), 5.30-5.46 (m, 1H), 6.37 (dd, <i>J</i> ₁ =10.15Hz, <i>J</i> ₂ =1.72Hz, 1H), 6.43 (s, 1H), 7.11 (dd, <i>J</i> ₁ =10.11Hz, <i>J</i> ₂ =0.73Hz, 1H), 7.77 (d, <i>J</i> =8.28Hz, 2H), 8.11 (d, <i>J</i> =8.15Hz, 2H). MASA (ES+): 685.1 |
| IA.178 | 1.07 (d, <i>J</i> =7.12Hz, 3H), 1.19 (s, 3H), 1.31-1.40 (m, 1H), 1.55 (s, 3H), 1.77-2.06 (m, 4H), 2.21-2.54 (m, 4H), 2.37 (s, 6H), 3.46-3.50 (m, 1H), 4.35 (d, <i>J</i> =10.85Hz, 1H), 4.45 (d, <i>J</i> =8.61Hz, 1H), 4.56 (d, <i>J</i> =16.77Hz, 1H), 5.32-5.49 (m, 1H), 6.39 (dd, <i>J</i> ₁ =10.15Hz, <i>J</i> ₂ =1.7Hz, 1H), 6.45 (s, 1H), 6.50 (dd, <i>J</i> ₁ =3.43Hz, <i>J</i> ₂ =1.68Hz, 1H), 7.13 (s, 1H), 7.14 (s, 1H), 7.16 (dd, <i>J</i> ₁ =11.79Hz, <i>J</i> ₂ =0.67Hz, 1H), 7.24 (s, 1H), 7.59 (s, 1H), 7.61 (s, 1H). MASA (ES+): 653.1 |
| IA.179 | 1.08 (d, <i>J</i> =7.11Hz, 3H), 1.16 (s, 3H), 1.33-1.41 (s, 1H), 1.53 (s, 3H), 1.71-2.04 (m, 4H), 2.28-2.51 (m, 4H), 3.46-3.51 (m, 1H), 4.44 (d, <i>J</i> =8.45Hz, 1H), 4.53 (d, <i>J</i> =16.43Hz, 1H), 4.69 (d, <i>J</i> =16.48Hz, 1H), 5.31-5.48 (m, 1H), 6.39 (dd, <i>J</i> ₁ =10.15Hz, <i>J</i> ₂ =1.84Hz, 1H), 6.45 (s, 1H), 6.50 (dd, <i>J</i> ₁ =3.48Hz, <i>J</i> ₂ =1.69Hz, 1H), 7.13 (s, 1H), 7.14 (dd, <i>J</i> ₁ =8.47Hz, <i>J</i> ₂ =1.99Hz, 1H), 7.56-7.65 (m, 3H), 7.87-8.04 (m, 4H), 8.58 (s, 1H). MASA (ES+): 675.1 |
| IA.180 | 0.98 (s, 3H), 1.06 (d, <i>J</i> =7.15Hz, 3H), 1.33-1.39 (m, 1H), 1.51 (s, 3H), 1.71-1.93 (m, 4H), 2.35-2.49 (m, 4H), 3.42-3.47 (m, 1H), 4.37 (d, <i>J</i> =13.12Hz, 1H), 4.39 (d, <i>J</i> =4.87Hz, 1H), 4.59 (d, <i>J</i> =16.48Hz, 1H), 5.30-5.47 (m, 1H), 6.37 (dd, <i>J</i> ₁ =10.12Hz, <i>J</i> ₂ =1.80Hz, 1H), 6.44 (s, 1H), 6.50 (dd, <i>J</i> ₁ =3.14Hz, <i>J</i> ₂ =1.36Hz, 1H), 7.11 (dd, <i>J</i> ₁ =6.33Hz, <i>J</i> ₂ =1.21Hz, 1H), 7.13 (s, 1H), 7.52-7.61 (m, 4H), 7.89 (dd, <i>J</i> ₁ =8.54Hz, <i>J</i> ₂ =1.43Hz, 1H), 8.02 (d, <i>J</i> =8.22Hz, 1H), 8.07 (dd, <i>J</i> ₁ =7.22Hz, <i>J</i> ₂ =0.94Hz, 1H), 8.49 (d, <i>J</i> =8.42Hz, 1H). MASA (ES+): 674.9 |
| IA.181 | 1.06 (d, <i>J</i> =7.10Hz, 3H), 1.16 (s, 3H), 1.34-1.42 (m, 1H), 1.54 (s, 3H), 1.65-2.02 (m, 4H), 2.29 (s, 3H), 2.24-2.61 (m, 4H), 3.44-3.49 (m, 1H), 4.37 (d, 1H, <i>J</i> =16.53Hz), 4.44 (d, <i>J</i> =8.48Hz, 1H), 4.53 (d, <i>J</i> =16.51Hz, 1H), 5.31-5.48 (m, 1H), 6.34 (d, <i>J</i> =1.44Hz, 1H), 6.38 (dd, <i>J</i> ₁ =12.12Hz, <i>J</i> ₂ =1.75Hz, 1H), 6.44 (s, 1H), 7.13 (dd, <i>J</i> ₁ =10.11Hz, <i>J</i> ₂ =1.05Hz, 1H), 7.44 (d, <i>J</i> =1.43Hz, 1H), 7.76 (d, <i>J</i> =8.26Hz, 2H), 8.12 (d, <i>J</i> =8.13Hz, 2H). MASA (ES+): 707.2 |
| IA.182 | 1.05 (d, <i>J</i> =7.13Hz, 3H), 1.09 (s, 3H), 1.36-1.43 (m, 1H), 1.54 (s, 3H), 1.75-2.00 (m, 4H), 2.26 (s, 6H), 2.28 (s, 3H), 2.30 (s, 3H), 2.41-2.60 (m, 4H), 3.47-3.50 (m, 1H), 4.09 (d, <i>J</i> =17.81Hz, 1H), 4.32 (d, <i>J</i> =17.76Hz, 1H), 4.41 (d, <i>J</i> =8.28Hz, 1H), 5.32-5.48 (m, 1H), 6.34 (d, <i>J</i> =1.21Hz, 1H), 6.38 (dd, <i>J</i> ₁ =10.16Hz, <i>J</i> ₂ =1.66Hz, 1H), 6.44 (s, 1H), 6.85 (s, 2H), 7.14 (d, <i>J</i> =10.11Hz), 7.43 (d, <i>J</i> =1.18Hz, 1H). MASA (ES+): 681.1 |
| IA.183 | 1.07 (d, <i>J</i> =7.10Hz, 3H), 1.12 (s, 3H), 1.32-1.42 (m, 1H), 1.54 (s, 3H), 1.73-2.00 (m, 4H), 2.27-2.53 (m, 4H), 3.40-3.44 (m, 1H), 4.05 (s, 3H), 4.39 (s, 2H), 4.46 (d, <i>J</i> =8.45Hz, 1H), 5.32-5.48 (m, 1H), 6.40 (dd, <i>J</i> ₁ =10.12Hz, <i>J</i> ₂ =1.68Hz, 1H), 6.45 (s, 1H), 6.50 (dd, <i>J</i> ₁ =3.44Hz, <i>J</i> ₂ =1.68Hz, 1H), 7.13 (s, 1H), 7.15 (dd, <i>J</i> ₁ =11.15Hz, <i>J</i> ₂ =0.94Hz, 1H), 7.19 (d, <i>J</i> =8.88Hz, 1H), 7.59 (d, <i>J</i> =0.69Hz, 1H), 8.22 (dd, <i>J</i> ₁ =8.81Hz, <i>J</i> ₂ =2.16Hz, 1H), 8.49 (d, <i>J</i> =2.15Hz, 1H). MASA (ES+): 700.1 |
| IA.184 | 1.07 (d, <i>J</i> =7.16Hz, 3H), 1.18 (s, 3H), 1.32-1.40 (m, 1H), 1.55 (s, 3H), 1.73-2.08 (m, 4H), 2.25-2.43 (m, 4H), 2.32 (s, 3H), 2.32 (s, 3H), 3.46-3.51 (m, 1H), 4.34 (d, <i>J</i> =16.73Hz, 1H), 4.45 (d, <i>J</i> =8.08Hz, 1H), 4.57 (d, <i>J</i> =16.76Hz, 1H), 5.32-5.49 (m, 1H), 6.39 (dd, <i>J</i> ₁ =10.14Hz, <i>J</i> ₂ =1.82Hz, 1H), 6.45 (s, 1H), 6.50 (dd, <i>J</i> ₁ =3.53Hz, <i>J</i> ₂ =1.74Hz, 1H), 7.13 (dd, <i>J</i> ₁ =3.63Hz, <i>J</i> ₂ =0.62Hz, 1H), 7.16 (dd, <i>J</i> ₁ =10.14Hz, <i>J</i> ₂ =1.18Hz, 1H), 7.24 (d, <i>J</i> =7.87Hz, 1H), 7.59 (m, 4H), 7.74 (dd, <i>J</i> ₁ =8.69Hz, <i>J</i> ₂ =1.66Hz, 1H), 7.77 (s, 1H). MASA (ES+): 653.5 (M+H) ⁺ |
| IA.185 | 1.05 (d, <i>J</i> =7.17Hz, 3H), 1.16 (s, 3H), 1.14-1.40 (m, 1H), 1.54 (s, 3H), 1.72-2.03 (m, 4H), 2.29-2.48 (m, 4H), 3.42-3.47 (m, 1H), 4.35 (d, 1H, <i>J</i> =16.60Hz), 4.46 (d, <i>J</i> =8.55Hz, 1H), 4.53 (d, <i>J</i> =16.65Hz, 1H), 5.32-5.49 (m, 1H), 6.39 (dd, <i>J</i> ₁ =10.14Hz, <i>J</i> ₂ =1.84Hz, 1H), 6.45 (s, 1H), 6.65 (d, <i>J</i> =1.52Hz, 1H), 7.13 (dd, <i>J</i> ₁ =10.12Hz, <i>J</i> ₂ =1.21Hz, 1H), 7.42 (t, <i>J</i> =1.70Hz, 1H), 7.76 (d, <i>J</i> =8.27Hz, 2H), 7.97 (d, <i>J</i> =0.75Hz, 1H), 8.12 (d, <i>J</i> =8.08Hz, 2H). MASA (ES+): 693.2 (M+H) ⁺ |
| IA.186 | 1.04 (d, <i>J</i> =7.12Hz, 3H), 1.10 (s, 3H), 1.33-1.38 (m, 1H), 1.54 (s, 3H), 1.75-2.04 (m, 4H), 2.25 (s, 6H), 2.28 (s, 3H), 2.17-2.46 (m, |

| Com-
puesto
No. | ¹ H-NMR (δ ppm). MASA (EI / ES+, <i>m/z</i>) |
|-----------------------|---|
| | 4.11), 3.46-3.49 (m, 1H), 4.09 (d, <i>J</i> =17.58Hz, 1H), 4.30 (d, <i>J</i> =17.79Hz, 1H), 4.42 (d, <i>J</i> =7.85Hz, 1H), 5.32-5.48 (m, 1H), 6.40 (dd, <i>J</i> ₁ =10.12Hz, <i>J</i> ₂ =1.70Hz, 1H), 6.45 (s, 1H), 6.65 (d, <i>J</i> =1.50Hz, 1H), 6.85 (s, 2H), 7.13 (dd, <i>J</i> ₁ =10.09Hz, <i>J</i> ₂ =0.79Hz, 1H), 7.42 (t, <i>J</i> =1.40Hz, 1H), 7.97 (s, 1H). MASA (ES+): 667.1 (M+H) ⁺ |
| IA.187 | 0.44 (s, 3H), 0.95 (d, <i>J</i> =7.02Hz, 3H), 1.08 (t, <i>J</i> =7.53Hz, 3H), 1.22-1.75 (m, 15H), 2.17-2.32 (m, 6H), 3.15 (m, 1H), 4.29 (d, <i>J</i> =6.81Hz, 1H), 5.40 (m, 1H), 6.35 (dd, <i>J</i> ₁ =10.11Hz, <i>J</i> ₂ =1.43Hz, 1H), 6.40 (s, 1H), 7.05 (d, <i>J</i> =9.98Hz, 1H), 7.36 (t, <i>J</i> =7.70Hz, 2H), 7.46 (t, <i>J</i> =7.20Hz, 1H), 7.95 (d, <i>J</i> =7.43Hz, 2H). MASA (ES+): 705.4 (M+Na) ⁺ |
| IA.188 | 0.60 (s, 3H), 0.93 (d, <i>J</i> =7.04Hz, 3H), 1.06 (t, <i>J</i> =7.54Hz, 3H), 1.10-1.89 (m, 14H), 2.09-2.36 (m, 6H), 3.14-3.17 (m, 1H), 4.30 (d, <i>J</i> =7.66Hz, 1H), 5.26-5.43 (m, 1H), 6.34 (dd, <i>J</i> ₁ =10.14Hz, <i>J</i> ₂ =1.67Hz, 1H), 6.41 (s, 1H), 7.06 (m, 3H), 8.02-8.05 (m, 2H). MASA (ES+): (655.5 (M+Na)) ⁺ |
| IA.189 | 0.42 (s, 3H), 0.93 (d, <i>J</i> =7.1Hz, 3H), 1.08 (t, <i>J</i> =7.57Hz, 3H), 1.20-1.25 (m, 1H), 1.49 (s, 3H), 1.51-1.79 (m, 4H), 1.75 (s, 6H), 1.80-2.37 (m, 7H), 3.31 (m, 1H), 4.28 (d, <i>J</i> =8.59Hz, 1H), 6.10 (s, 1H), 6.31 (d, <i>J</i> ₁ =10.12Hz, <i>J</i> ₂ =1.80Hz, 1H), 7.13 (d, <i>J</i> =10.14Hz, 1H), 7.38 (t, <i>J</i> =7.53Hz, 2H), 7.45-7.47 (m, 1H), 7.95-7.97 (m, 1H). MASA (ES+): 619.6 (M+Na) ⁺ |
| IA.190 | 0.44 (s, 3H), 0.82-1.15 (m, 2H), 0.92 (d, <i>J</i> =6.92Hz, 3H), 1.21-1.42 (m, 8H), 1.48 (s, 3H), 1.52-1.84 (m, 6H), 1.71 (s, 6H), 2.10-2.29 (m, 5H), 3.14-3.17 (m, 1H), 4.40 (d, <i>J</i> =7.44Hz, 1H), 5.24-5.44 (m, 1H), 6.35 (d, <i>J</i> =9.7Hz, 1H), 6.41 (s, 1H), 7.07 (d, <i>J</i> =10.11Hz, 1H), 7.37 (t, <i>J</i> =7.54Hz, 2H), 7.46 (t, <i>J</i> =7.28Hz, 1H), 7.95 (d, <i>J</i> =7.61Hz, 2H). MASA (ES+): 691.6 (M+Na) ⁺ |
| IA.191 | 0.44 (s, 3H), 0.93 (d, <i>J</i> =7.07Hz, 3H), 1.23-1.25 (m, 1H), 1.47 (s, 3H), 1.52-1.83 (m, 12H), 1.74 (s, 6H), 2.19-2.25 (m, 4H), 2.67-2.71 (m, 1H), 3.13-3.17 (m, 1H), 4.30 (d, <i>J</i> =7.27Hz, 1H), 5.25-5.42 (m, 1H), 6.34 (d, <i>J</i> ₁ =10.19Hz, <i>J</i> ₂ =1.75Hz, 1H), 6.41 (s, 1H), 7.06 (d, <i>J</i> =10.22Hz, 1H), 7.37 (t, <i>J</i> =7.57Hz, 2H), 7.46 (t, 1H, <i>J</i> =7.34Hz), 7.95 (d, 2H, <i>J</i> =7.22Hz). MASA (ES+): 655.2 |
| IA.192 | 0.45 (s, 3H), 0.93 (d, <i>J</i> =7.14Hz, 3H), 1.11 (d, <i>J</i> =6.96Hz, 3H), 1.21-1.26 (m, 1H), 1.48 (s, 3H), 1.55-1.75 (m, 4H), 1.75 (d, <i>J</i> =1.51Hz, 6H), 2.10-2.27 (m, 4H), 2.47-2.52 (m, 1H), 3.13-3.18 (m, 1H), 4.30 (d, <i>J</i> =7.45Hz, 1H), 5.25-5.42 (m, 1H), 6.34 (d, <i>J</i> ₁ =10.13Hz, <i>J</i> ₂ =1.77Hz, 1H), 6.41 (s, 1H), 7.06 (dd, <i>J</i> ₁ =10.13Hz, <i>J</i> ₂ =1.06Hz, 1H), 7.37 (t, <i>J</i> =7.59Hz, 2H), 7.47 (t, <i>J</i> =7.59Hz, 2H), 7.47 (t, <i>J</i> =7.35Hz, 1H), 7.95 (d, <i>J</i> =7.28Hz, 2H). MASA (ES+): 629.2. |
| IA.193 | 0.45 (s, 3H), 0.94 (d, <i>J</i> =7.06Hz, 3H), 1.16-1.26 (m, 2H), 1.47 (s, 3H), 1.55-1.96 (m, 5H), 1.7 (T'wos, 6H), 2.09-2.29 (m, 8H), 3.06-3.17 (m, 2H), 4.28 (d, <i>J</i> =7.88Hz, 1H), 5.25-5.43 (m, 1H), 6.33 (dd, <i>J</i> ₁ =10.13Hz, <i>J</i> ₂ =1.66Hz, 1H), 6.40 (s, 1H), 7.05 (d, <i>J</i> =10.13Hz, 1H), 7.38 (t, <i>J</i> =7.58Hz, 2H), 7.47 (t, <i>J</i> =7.83Hz, 1H), 7.96 (d, <i>J</i> =8.66Hz, 2H). MASA (ES+): 641.5 |
| IA.194 | 0.5 (s, 3H), 1.0 (d, <i>J</i> =6.97Hz, 3H), 1.22-1.28 (m, 1H), 1.51 (s, 3H), 1.41-1.74 (m, 5H), 1.77 (s, 3H), 1.78 (s, 3H), 2.15-2.60 (m, 5H), 3.19-3.33 (m, 1H), 4.33 (d, <i>J</i> =8.07Hz, 1H), 6.12 (s, 1H), 6.35 (d, <i>J</i> =10.10Hz, 1H), 6.46 (d, <i>J</i> =3.25Hz, 1H), 7.04 (d, <i>J</i> =3.27Hz, 1H), 7.16 (d, <i>J</i> =1.10Hz, 1H), 7.38 (t, <i>J</i> =7.57Hz, 2H), 7.47 (t, <i>J</i> =7.30Hz, 1H), 7.56 (s, 1H), 7.95 (d, <i>J</i> =7.71Hz, 2H). MASA (ES+): 635.4 |
| IA.195 | 0.44 (s, 3H), 0.88-0.91 (m, 2H), 0.94 (d, <i>J</i> =7.11Hz, 3H), 1.09-1.36 (m, 5H), 1.47 (s, 3H), 1.52-1.73 (m, 8H), 1.74 (s, 6H), 2.12-2.22 (m, 6H), 3.13-3.16 (m, 1H), 5.29 (d, <i>J</i> =8.09Hz, 1H), 5.25-5.42 (m, 1H), 6.35 (dd, <i>J</i> ₁ =10.12Hz, <i>J</i> ₂ =1.79Hz, 1H), 6.40 (s, 3H), 7.06 (dd, <i>J</i> ₁ =10.14Hz, <i>J</i> ₂ =1.36Hz, 1H), 7.37 (t, <i>J</i> =7.54Hz, 2H), 7.44-7.47 (m, 1H), 7.95 (dd, <i>J</i> ₁ =8.31Hz, <i>J</i> ₂ =1.23Hz, 2H). MASA (ES+): 683.4. |
| IA.196 | 0.66 (s, 3H), 1.02 (d, <i>J</i> =7.03Hz, 3H), 1.10-1.43 (m, 2H), 1.50 (s, 3H), 1.54-1.82 (m, 9H), 2.22-2.41 (m, 4H), 3.22-3.25 (m, 1H), 4.34 (d, <i>J</i> =6.85Hz, 1H), 5.28-5.45 (m, 1H), 6.38 (dd, <i>J</i> ₁ =10.17Hz, <i>J</i> ₂ =1.68Hz, 1H), 6.43 (s, 1H), 6.47 (dd, <i>J</i> ₁ =3.39Hz, <i>J</i> ₂ =1.86Hz, 1H), 7.03-7.09 (m, 4H), 7.56 (s, 1H), 8.01-8.01 (m, 2H). MASA (ES+): 671.3 |
| IA.197 | 0.58 (s, 3H), 1.02 (d, <i>J</i> =7.09Hz, 3H), 1.08-1.37 (m, 3H), 1.50 (s, 3H), 1.61-1.80 (m, 8H), 2.22-2.38 (m, 4H), 3.20-3.25 (m, 1H), 4.34-4.36 (m, 1H), 5.28-5.48 (m, 1H), 6.39 (dd, <i>J</i> ₁ =10.12Hz, <i>J</i> ₂ =1.77Hz, 1H), 6.43 (s, 1H), 6.48 (dd, <i>J</i> ₁ =3.47Hz, <i>J</i> ₂ =1.71Hz, 1H), 7.05 (d, <i>J</i> =3.34Hz, 1H), 7.09 (dd, <i>J</i> ₁ =10.12Hz, <i>J</i> ₂ =1.07Hz, 1H), 7.57 (t, <i>J</i> =0.85Hz, 1H), 7.65 (d, <i>J</i> =8.33Hz, 2H), 8.01 (d, <i>J</i> =8.21Hz, 2H). MASA (ES+): 721.2 |
| IA.198 | 1.05 (d, <i>J</i> =7.15Hz, 3H), 1.17 (s, 3H), 1.34-1.39 (m, 1H), 1.55 (s, 3H), 1.74-1.92 (m, 4H), 2.09-2.50 (m, 4H), 2.32 (s, 3H), 2.33 (s, 3H), 3.45-3.49 (m, 1H), 4.32 (d, <i>J</i> =16.76Hz, 1H), 4.46 (d, <i>J</i> =8.58Hz, 1H), 4.59 (d, <i>J</i> =16.79Hz, 1H), 5.32-5.49 (m, 1H), 6.40 (dd, <i>J</i> ₁ =10.12Hz, <i>J</i> ₂ =1.65Hz, 1H), 6.46 (s, 1H), 6.93 (d, <i>J</i> =4.02Hz, 1H), 7.17 (d, <i>J</i> =10.13Hz, 1H), 7.24 (d, <i>J</i> =7.93Hz, 1H), 7.53 (dd, <i>J</i> =3.95Hz, 1H), 7.75 (d, <i>J</i> =7.93Hz, 1H), 7.78 (s, 1H). MASA (ES+): 703.7 |
| IA-1.1 | 0.33 (s, 3H), 0.92 (d, <i>J</i> =7.14Hz, 3H), 1.07 (t, <i>J</i> =7.55Hz, 3H), 1.17-1.88 (m, 12H), 2.08-2.30 (m, 8H), 2.66-2.63 (m, 2H), 3.10-3.13 (m, 1H), 4.28-4.30 (m, 1H), 5.25-5.41 (m, 1H), 6.36 (dd, <i>J</i> ₁ =10.13Hz, <i>J</i> ₂ =1.77Hz, 1H), 6.40 (s, 1H), 7.03-7.07 (m, 3H), 7.94-7.97 (m, 2H). MASA (ES+): 660.5 |
| IA-1.2 | 0.15 (s, 3H), 0.91 (d, <i>J</i> =7.10Hz, 3H), 1.08 (t, <i>J</i> =7.68Hz, 3H), 1.17-1.88 (m, 12H), 2.04-2.31 (m, 8H), 2.63-2.67 (m, 2H), 3.05-3.15 (m, 1H), 4.26 (d, <i>J</i> =7.89Hz, 1H), 5.23-5.39 (m, 1H), 6.35 (dd, <i>J</i> ₁ =10.11Hz, <i>J</i> ₂ =1.47Hz, 1H), 6.39 (s, 1H), 7.05 (d, <i>J</i> =10.11Hz, 2H), 7.36-7.39 (m, 2H), 7.45-7.49 (m, 2H), 7.90 (d, <i>J</i> =7.49Hz, 2H). MASA (ES+): 663.0 (M+Na) ⁺ |
| IB.1 | 0.94 (d, <i>J</i> =7.16Hz, 3H), 1.10 (s, 3H), 1.12 (t, <i>J</i> =7.53Hz, 3H), 1.23-1.35 (m, 1H), 1.53 (s, 3H), 1.69-1.85 (m, 3H), 2.17-2.49 (m, 7H), 3.29-3.36 (m, 1H), 4.30-4.40 (m, 3H), 4.55 (d, <i>J</i> =15.48, 1H), 5.04 (d, <i>J</i> =15.46, 1H), 5.27-5.52 (m, 1H), 6.37 (d, <i>J</i> ₁ =10.11Hz, <i>J</i> ₂ =1.69Hz, 1H), 6.43 (s, 1H), 7.13 (d, <i>J</i> =10.10Hz, 1H). MASA (ES+): 543.5 (M+Na) ⁺ |
| IB.2 | 0.97 (d, <i>J</i> =6.99Hz, 3H), 1.11 (s, 3H), 1.12 (t, <i>J</i> =7.33Hz, 3H), 1.29-1.33 (m, 1H), 1.53 (s, 3H), 1.70-1.98 (m, 3H), 2.17-2.54 (m, 7H), 3.33-3.34 (m, 1H), 3.67 (d, <i>J</i> =14.69, 1H), 3.74 (d, <i>J</i> =16.44, 1H), 4.19 (s, 2H), 4.32 (d, <i>J</i> =7.28, 1H), 4.59 (s, 1H), 5.31-5.48 (m, 1H), 6.33 (d, <i>J</i> =10.16Hz, 1H), 6.37 (s, 1H), 7.22 (d, <i>J</i> =10.02Hz, 1H). MASA (ES+): 559.5 (M+Na) ⁺ |
| IB.3 | 0.99 (d, <i>J</i> =7.10Hz, 3H), 1.10 (s, 3H), 1.12 (t, <i>J</i> =7.59Hz, 3H), 1.31-1.36 (m, 1H), 1.52 (s, 3H), 1.70-1.91 (m, 4H), 2.19-2.45 (m, 6H), 3.33-3.37 (m, 1H), 3.72-3.78 (m, 2H), 4.41 (d, <i>J</i> =6.54, 1H), 4.94 (d, <i>J</i> =47.47Hz, 2H), 5.30-5.47 (m, 1H), 6.38 (d, <i>J</i> =10.13Hz, 1H), 6.43 (s, 1H), 7.12 (d, <i>J</i> =10.13Hz, 1H). MASA (ES+): 561.2 (M+Na) ⁺ |
| IB.4 | 1.02 (d, <i>J</i> =7.08Hz, 3H), 1.13 (s, 3H), 1.32-1.37 (m, 1H), 1.55 (s, 3H), 1.66-2.02 (m, 4H), 2.07-2.32 (m, 4H), 3.38-3.41 (m, 1H), 3.70 (d, <i>J</i> =16.32, 1H), 3.78 (d, <i>J</i> =16.35Hz, 1H), 1.12-4.15 (m, 2H), 4.33 (d, <i>J</i> =6.37, 1H), 4.88 (t, <i>J</i> =5.92, 1H), 5.14 (m, 1H), 5.36-5.53 (m, 1H), 6.29-6.32 (m, 2H), 6.54 (dd, <i>J</i> ₁ =3.47Hz, <i>J</i> ₂ =1.72Hz, 1H), 7.11 (d, <i>J</i> =3.46, 1H), 7.25 (d, <i>J</i> =10.45Hz, 1H), 7.66 (m, 1H). MASA (ES+): 597.5 (M+Na) ⁺ |
| IB.5 | 0.98 (d, <i>J</i> =7.03Hz, 3H), 1.11 (s, 3H), 1.12 (t, <i>J</i> =7.72Hz, 3H), 1.27-1.33 (m, 1H), 1.54 (s, 3H), 1.78-1.88 (m, 5H), 2.04-2.31 (m, 2H), 2.33-2.63 (m, 6H), 3.31-3.34 (m, 1H), 3.66 (d, <i>J</i> =16.48, 1H), 3.74 (d, <i>J</i> =16.56, 1H), 4.24 (s, 2H), 4.40 (d, <i>J</i> =8.44, 1H), 6.13 (s, 1H), 6.35 (d, <i>J</i> =10.06Hz, 1H), 7.20 (d, <i>J</i> =10.07Hz, 1H). MASA (ES+): 541.6 (M+Na) ⁺ |
| IB.6 | 1.07 (d, <i>J</i> =7.08Hz, 3H), 1.15 (s, 3H), 1.32-1.41 (m, 1H), 1.54 (s, 3H), 1.58-1.95 (m, 5H), 2.29-2.53 (m, 3H), 3.41-3.45 (m, 1H), 3.75 (dd, <i>J</i> ₁ =15.74Hz, <i>J</i> ₂ =5.95Hz, 1H), 3.83 (dd, <i>J</i> ₁ =16.61Hz, <i>J</i> ₂ =6.93Hz, 1H), 4.46 (d, <i>J</i> =8.11Hz, 1H), 4.94 (d, <i>J</i> =47.47Hz, 2H), 5.32-5.49 (m, 1H), 6.40 (dd, <i>J</i> ₁ =10.11Hz, <i>J</i> ₂ =1.43Hz, 1H), 6.45 (s, 1H), 6.50 (dd, <i>J</i> ₁ =3.14Hz, <i>J</i> ₂ =1.5Hz, 1H), 7.12 (s, 1H), 7.14 (d, <i>J</i> =10.36Hz, 1H), 7.59 (s, 1H). MASA (ES+): 599.5 (M+Na) ⁺ |
| IB.7 | 0.95 (d, <i>J</i> =7.14Hz, 3H), 1.10 (s, 3H), 1.14 (d, <i>J</i> =4.89Hz, 3H), 1.16 (d, <i>J</i> =4.92Hz, 3H), 1.23-1.33 (m, 1H), 1.53 (s, 3H), 1.68-2.00 (m, 3H), 2.16-2.29 (m, 2H), 2.54-2.62 (m, 2H), 3.32-3.36 (m, 1H), 3.64-3.78 (m, 2H), 4.15-4.17 (m, 2H), 4.30-4.33 (m, 1H), 4.72 (t, <i>J</i> =5.89, 1H), 4.99 (t, <i>J</i> =2.77, 1H), 5.34-5.50 (m, 1H), 6.31 (d, <i>J</i> ₁ =12.18Hz, <i>J</i> ₂ =1.97Hz, 1H), 6.32 (s, 1H), 7.24 (d, <i>J</i> =10.03Hz, 1H). MASA (ES+): 551.2 |
| IB.8 | 0.99 (d, <i>J</i> =7.31Hz, 3H), 1.11 (s, 3H), 1.27-1.35 (m, 1H), 1.52 (s, 3H), 1.72-1.99 (m, 7H), 2.04-2.37 (m, 8H), 3.14-3.18 (m, 1H), 3.33-3.36 (m, 1H), 3.65-3.77 (m, 2H), 4.24 (d, <i>J</i> =2.11, 2H), 4.39 (d, <i>J</i> =8.66, 1H), 5.28-5.48 (m, 1H), 6.37 (dd, <i>J</i> ₁ =10.12Hz, <i>J</i> ₂ =1.60Hz, 1H), 6.43 (s, 1H), 7.12 (d, <i>J</i> =10.18Hz, 1H). MASA (ES+): 564.3 |
| IB.9 | 1.02 (d, <i>J</i> =7.10Hz, 3H), 1.16 (s, 3H), 1.13-1.36 (m, 1H), 1.57 (s, 3H), 1.60-2.00 (m, 4H), 2.24-2.66 (m, 6H), 3.38-3.42 (m, 1H), 3.70 (d, <i>J</i> =16.38, 1H), 3.78 (d, <i>J</i> =16.39, 1H), 4.15-4.17 (m, 2H), 4.34-4.37 (m, 1H), 4.73 (t, <i>J</i> =5.85, 1H), 4.78 (s, 1H), 6.09 (s, 1H), 6.29 |

| Com-
puesto
No. | ¹ H-NMR (δ ppm). MASA (EI / ES+, m/z) |
|-----------------------|--|
| | (dd, $J_1=10.10$ Hz, $J_2=1.45$ Hz, 1H), 6.52 (dd, $J_1=3.33$ Hz, $J_2=1.60$ Hz, 1H), 7.11 (d, $J=3.43$ Hz, 1H), 7.32 (d, $J=10.12$ Hz, 1H), 7.63 (s, 1H). MASA (ES+): 557.3 |
| IB.10 | 1.03 (d, $J=6.98$ Hz, 3H), 1.13 (s, 3H), 1.33-1.37 (m, 1H), 1.55 (s, 3H), 1.62-1.98 (m, 3H), 2.24-2.54 (m, 4H), 3.3 (m, 1H), 3.71 (d, $J=16.40$, 1H), 3.79 (d, $J=16.39$ Hz, 1H), 4.08 (d, $J=7.17$ Hz, 1H), 4.12 (d, $J=5.83$ Hz, 2H), 4.99 (t, $J=5.92$, 1H), 5.27 (s, 1H), 5.40-5.56 (m, 1H), 6.28 (s, 1H), 6.29 (d, $J=13.05$ Hz, 1H), 7.14 (t, $J=4.33$ Hz, 1H), 7.27 (d, $J=10.03$, 1H), 7.71 (m, 2H). MASA (ES+): 591.4 |
| IB.11 | 0.99 (d, $J=7.15$ Hz, 3H), 1.09 (s, 3H), 1.12 (t, $J=7.66$ Hz, 3H), 1.30-1.36 (m, 1H), 1.52 (s, 3H), 1.64-1.90 (m, 4H), 2.18-2.44 (m, 7H), 3.34-3.38 (m, 1H), 3.65 (dd, $J_1=16.57$ Hz, $J_2=2.60$ Hz, 1H), 3.71 (dd, $J_1=16.58$ Hz, $J_2=2.58$ Hz, 1H), 4.41 (d, $J=7.42$, 1H), 5.30-5.47 (m, 1H), 6.37 (dd, $J_1=10.14$ Hz, $J_2=1.54$ Hz, 1H), 6.43 (s, 1H), 7.12 (d, $J=10.05$ Hz, 1H). MASA (ES+): 507.3 |
| IB.12 | 1.06 (d, $J=7.11$ Hz, 3H), 1.18 (s, 3H), 1.35-1.61 (m, 1H), 1.55 (s, 3H), 1.80-1.97 (m, 3H), 2.39-2.60 (m, 5H), 3.43-3.46 (m, 1H), 3.70-3.82 (m, 3H), 4.06-4.33 (m, 4H), 4.45 (d, $J=7.47$ Hz, 1H), 4.69-4.71 (m, 2H), 5.32-5.49 (m, 1H), 6.39 (d, $J=10.13$ Hz, 1H), 6.45 (s, 1H), 6.50 (d, $J_1=3.26$ Hz, $J_2=1.48$ Hz, 1H), 7.13 (d, $J=3.42$ Hz, 1H), 7.16 (d, $J=10.32$ Hz, 1H), 7.59 (s, 1H). MASA (ES+): 773.2 |
| IB.13 | 0.70 (d, $J=7.16$ Hz, 3H), 1.07 (s, 3H), 1.11 (t, $J=7.53$ Hz, 3H), 1.25-1.35 (m, 1H), 1.53 (s, 3H), 1.70-2.03 (m, 3H), 2.18-2.60 (m, 7H), 3.34-3.37 (m, 1H), 3.56-3.60 (m, 2H), 4.04 (d, $J=3.79$ Hz, 2H), 4.28 (d, $J=9.37$ Hz, 1H), 4.93 (s, 1H), 5.32-5.51 (m, 1H), 5.63-5.81 (m, 1H), 5.80-5.88 (m, 1H), 6.30 (dd, $J_1=10.12$ Hz, $J_2=1.88$ Hz, 1H), 6.33 (s, 1H), 7.24 (d, $J=9.87$ Hz, 1H). MASA (ES+): 539.2 |
| IB.14 | 1.04 (d, $J=7.10$ Hz, 3H), 1.12 (s, 3H), 1.12-1.37 (m, 1H), 1.55 (s, 3H), 1.70-1.95 (m, 4H), 2.29-2.59 (m, 4H), 3.40-3.44 (m, 1H), 3.55-3.68 (m, 2H), 4.02 (d, $J=4.19$ Hz, 1H), 4.23 (br-s, 1H), 4.33 (br-d, $J=10.86$ Hz, 1H), 5.07-5.09 (m, 1H), 5.36-5.53 (m, 1H), 5.65-5.71 (m, 1H), 5.81-5.87 (m, 1H), 6.31 (dd, $J_1=10.68$ Hz, $J_2=1.76$ Hz, 1H), 6.33 (s, 1H), 6.53 (dd, $J_1=3.46$ Hz, $J_2=1.75$ Hz, 1H), 7.10 (d, $J=3.47$ Hz, 1H), 7.26 (d, $J=10.00$ Hz, 1H), 7.64 (d, $J=1.37$ Hz, 1H). MASA (ES+): 599.3 (M+Na) ⁺ |
| IB.15 | 1.02 (d, $J=7.10$ Hz, 3H), 1.10 (s, 3H), 1.31-1.38 (m, 1H), 1.54 (s, 3H), 1.65-1.96 (m, 3H), 2.26-2.53 (m, 4H), 3.38-3.41 (m, 1H), 3.64 (d, $J=7.8$ Hz, 2H), 4.16 (d, $J=5.94$ Hz, 2H), 4.29 (b.d, 1H), 4.48 (bs, 1H), 5.27 (m, 1H), 5.40-5.57 (m, 2H), 5.62-5.69 (m, 1H), 6.26 (s, 1H), 6.28 (dd, $J_1=10.12$ Hz, $J_2=1.79$ Hz, 1H), 6.56 (dd, $J_1=3.47$ Hz, $J_2=1.72$ Hz, 1H), 7.10 (d, $J=3.48$ Hz, 1H), 7.26 (d, $J=10.10$ Hz, 1H), 7.72 (d, $J=1.51$ Hz, 1H). MASA (ES+): 599.3 (M+Na) ⁺ |
| IB.16 | 1.03 (d, $J=7.09$ Hz, 3H), 1.11 (s, 3H), 1.31-1.37 (m, 1H), 1.55 (s, 3H), 1.65-2.01 (m, 4H), 2.28-2.58 (m, 4H), 3.36-3.41 (m, 1H), 3.64 (d, $J=7.76$ Hz, 2H), 4.16 (m, 2H), 3.31 (d, $J=6.77$ Hz, 1H), 4.49 (t, $J=5.37$ Hz, 1H), 5.28 (m, 1H), 5.41-5.57 (m, 2H), 5.64-5.69 (m, 1H), 6.26 (s, 1H), 6.29 (dd, $J_1=10.11$ Hz, $J_2=1.82$ Hz, 1H), 7.14 (t, $J=4.36$ Hz, 1H), 7.27 (dd, $J_1=10.11$ Hz, $J_2=0.74$ Hz, 1H), 7.70-7.71 (m, 2H). MASA (ES+): 615.0 (M+Na) |
| IB.17 | 1.04 (d, $J=7.11$ Hz, 3H), 1.12 (s, 3H), 1.32-1.38 (m, 1H), 1.55 (s, 3H), 1.60-1.99 (m, 4H), 2.29-2.59 (m, 4H), 3.39-3.43 (m, 1H), 3.56-3.67 (m, 2H), 4.00 (d, $J=5.11$ Hz, 1H), 4.22 (dd, $J_1=4.85$ Hz, $J_2=0.81$ Hz, 1H), 4.32 (d, $J=6.73$ Hz, 1H), 4.43 (t, $J=5.49$ Hz, 1H), 5.21-5.22 (m, 1H), 5.39-5.56 (m, 1H), 5.63-5.70 (m, 1H), 5.83 (d, t, $J_1=15.27$ Hz, $J_2=5.03$ Hz, 1H), 6.29 (s, 1H), 6.30 (dd, $J_1=10.58$ Hz, $J_2=1.77$ Hz, 1H), 7.13 (dd, $J_1=4.87$ Hz, $J_2=3.87$ Hz, 1H), 7.27 (d, $J=9.68$ Hz, 1H), 7.67 (dd, $J_1=4.97$ Hz, $J_2=0.99$ Hz, 1H), 7.70 (dd, $J_1=3.70$ Hz, $J_2=1.05$ Hz, 1H). MASA (ES+): 592.7 |
| IB.18 | 1.06 (d, $J=7.11$ Hz, 3H), 1.18 (s, 3H), 1.35-1.41 (m, 1H), 1.55 (s, 3H), 1.67-1.97 (m, 4H), 2.28-2.56 (m, 5H), 3.44 (m, 1H), 3.66-3.81 (m, 3H), 3.99-4.31 (m, 4H), 4.45 (d, $J=7.88$ Hz, 1H), 4.65-4.75 (m, 2H), 5.32-5.49 (m, 1H), 6.39 (dd, $J_1=10.15$ Hz, $J_2=1.29$ Hz, 1H), 6.45 (s, 1H), 6.50 (dd, $J_1=3.34$ Hz, $J_2=1.69$ Hz, 1H), 7.13 (d, $J=3.45$ Hz, 1H), 7.16 (d, $J=10.13$ Hz, 1H), 7.59 (d, $J=0.66$ Hz, 1H). MASA (ES+): 759.1 |
| IB.19 | 1.06 (d, $J=7.05$ Hz, 3H), 1.18 (s, 3H), 1.36-1.41 (m, 1H), 1.54 (s, 3H), 1.74-1.97 (m, 7H), 2.29-2.50 (m, 5H), 3.42-3.45 (m, 1H), 3.72-3.74 (m, 2H), 4.20 (t, $J=5.74$ Hz, 2H), 4.44-4.47 (m, 1H), 4.48 (t, $J=5.90$ Hz, 2H), 4.65-4.74 (m, 2H), 5.33-5.50 (m, 1H), 6.40 (dd, $J_1=10.14$ Hz, $J_2=1.52$ Hz, 1H), 6.45 (s, 1H), 6.50 (dd, $J_1=3.22$ Hz, $J_2=1.48$ Hz, 1H), 7.13-7.16 (m, 2H), 7.59 (s, 1H). MASA (ES+): 736.1 |
| IB.20 | 1.03 (d, $J=7.10$ Hz, 3H), 1.15 (s, 3H), 1.33-1.39 (m, 1H), 1.55 (s, 3H), 1.60-2.00 (m, 4H), 2.25-2.60 (m, 4H), 3.30-3.42 (m, 1H), 3.71 (d, $J=16.35$ Hz, 1H), 3.78 (d, t, $J_1=16.38$ Hz, $J_2=1.86$ Hz, 1H), 4.15-4.17 (m, 2H), 4.36 (d, $J=9.1$ Hz, 1H), 4.71 (t, $J=5.90$, 1H), 5.03 (d, $J=2.42$ Hz, 1H), 5.16-5.52 (m, 1H), 6.34 (dd, $J_1=10.97$ Hz, $J_2=1.70$ Hz, 1H), 6.36 (s, 1H), 6.97 (d, $J=13.05$ Hz, 1H), 7.26 (d, $J=10.17$ Hz, 1H), 7.52 (s, 1H). MASA (ES+): 647.0 (M+Na) ⁺ |
| IB.21 | 1.06 (d, $J=7.13$ Hz, 3H), 1.14 (s, 3H), 1.35-1.40 (m, 1H), 1.54 (s, 3H), 1.79 (t, $J=2.34$ Hz, 3H), 1.73-1.96 (m, 4H), 2.28-2.54 (m, 4H), 3.41-3.46 (m, 1H), 3.66 (dd, $J_1=16.08$ Hz, $J_2=2.46$ Hz, 1H), 3.73 (dd, $J_1=16.12$ Hz, $J_2=2.45$ Hz, 1H), 4.45 (d, $J=8.43$ Hz, 1H), 5.32-5.48 (m, 1H), 6.40 (d, $J=10.71$ Hz, 1H), 6.45 (s, 1H), 6.50 (dd, $J_1=3.21$ Hz, $J_2=1.11$ Hz, 1H), 7.11 (d, $J=3.39$, 1H), 7.13 (d, $J=9.96$ Hz, 1H), 7.58 (m, 1H). MASA (ES+): 559.5 |
| IB.22 | 1.06 (d, $J=7.10$ Hz, 3H), 1.17 (s, 3H), 1.36-1.43 (m, 1H), 1.53 (s, 3H), 1.56-1.96 (m, 4H), 2.30 (s, 3H), 2.38-2.58 (m, 4H), 3.41-3.45 (m, 1H), 3.70 (d, $J=16.56$, 1H), 3.79 (d, $J=16.56$ Hz, 1H), 4.22 (d, $J=14.06$, 1H), 4.27 (d, $J=15.99$ Hz, 1H), 4.42 (d, $J=8.53$, 1H), 5.31-5.48 (m, 1H), 6.34 (d, $J=0.96$, 1H), 6.38 (dd, $J_1=10.16$ Hz, $J_2=1.43$ Hz, 1H), 6.44 (s, 1H), 7.14 (d, $J=10.2$, 1H), 7.44 (s, 1H). MASA (ES+): 589.3 |
| IB.23 | 1.03 (d, $J=7.10$ Hz, 3H), 1.12 (s, 3H), 1.21 (t, $J=6.99$ Hz, 3H), 1.32-1.37 (m, 1H), 1.52 (s, 3H), 1.66-1.92 (m, 4H), 2.17-2.45 (m, 5H), 3.35-3.38 (m, 1H), 3.54 (q, $J=6.98$ Hz, 2H), 3.69 (d, $J=14.78$ Hz, 1H), 3.73 (d, $J=14.72$ Hz, 1H), 4.09 (s, 2H), 4.19-4.28 (m, 2H), 4.39 (d, $J=8.39$ Hz, 1H), 5.30-5.46 (m, 1H), 6.37 (dd, $J_1=10.13$ Hz, $J_2=1.65$ Hz, 1H), 6.43 (s, 1H), 7.13 (dd, $J_1=10.07$ Hz, $J_2=0.65$ Hz, 1H). MASA (ES+): 567.1 |
| IB.24 | 1.03 (d, $J=7.11$ Hz, 3H), 1.12 (s, 3H), 1.32-1.38 (m, 1H), 1.52 (s, 3H), 1.68-1.93 (m, 5H), 2.16-2.32 (m, 4H), 3.35-3.39 (m, 1H), 3.41 (s, 3H), 3.71-3.73 (m, 2H), 4.05 (s, 2H), 4.23 (t, $J=2.22$, 1H), 4.25 (t, $J=2.23$, 1H), 4.39 (d, $J=8.92$, 1H), 5.30-5.47 (m, 1H), 6.37 (dd, $J_1=10.17$ Hz, $J_2=1.78$ Hz, 1H), 6.43 (s, 1H), 7.14 (d, $J=10.13$ Hz, 1H). MASA (ES+): 553.2 |
| IB.25 | 1.07 (d, $J=7.15$ Hz, 3H), 1.18 (s, 3H), 1.28-1.42 (m, 1H), 1.46-1.67 (m, 10H), 1.54 (s, 3H), 1.74-2.02 (m, 9H), 2.28-2.50 (m, 1H), 3.40-3.46 (m, 1H), 3.70 (d, $J=16.45$ Hz, 1H), 3.78 (d, $J=16.43$ Hz, 1H), 4.44 (d, $J=8.82$ Hz, 1H), 5.32-5.49 (m, 1H), 6.39 (dd, $J_1=10.13$ Hz, $J_2=1.66$ Hz, 1H), 6.45 (s, 1H), 6.49 (dd, $J_1=3.42$ Hz, $J_2=1.66$ Hz, 1H), 7.12 (d, $J=3.71$ Hz, 1H), 7.14 (d, $J=12.28$ Hz, 1H), 7.59 (s, 1H). MASA (ES+): 643.3 |
| IB.26 | 0.89-0.94 (m, 2H), 1.0 (d, $J=7.14$ Hz, 3H), 1.12 (s, 3H), 1.08-1.36 (m, 4H), 1.52 (s, 3H), 1.61-1.91 (m, 10H), 2.16-2.44 (m, 7H), 3.31-3.35 (m, 1H), 3.65-3.76 (m, 2H), 4.19-4.28 (m, 2H), 4.40 (d, $J=8.88$, 1H), 5.30-5.47 (m, 1H), 6.38 (dd, $J_1=10.12$ Hz, $J_2=1.78$ Hz, 1H), 6.43 (s, 1H), 7.14 (dd, $J_1=10.12$ Hz, $J_2=1.31$ Hz, 1H). MASA (ES+): 605.5 |
| IB.27 | 0.89 (t, $J=7.32$ Hz, 3H), 0.99 (d, $J=7.11$ Hz, 3H), 1.11 (s, 3H), 1.34 (q, $J=7.53$ Hz, 2H), 1.52 (s, 3H), 1.55-1.59 (m, 2H), 1.73-2.04 (m, 4H), 2.22-2.37 (m, 7H), 3.34 (m, 1H), 3.69-3.73 (m, 2H), 4.24 (d, $J=1.36$ Hz, 2H), 4.40 (d, $J=8.57$, 1H), 5.30-5.48 (m, 1H), 6.38 (dd, $J_1=10.13$ Hz, $J_2=1.70$ Hz, 1H), 6.43 (s, 1H), 7.13 (d, $J=10.12$ Hz, 1H). MASA (ES+): 565.3 |
| IB.28 | 0.94 (d, $J=7.17$ Hz, 3H), 1.08 (s, 3H), 1.12 (t, $J=7.58$ Hz, 3H), 1.27-1.32 (m, 1H), 1.53 (s, 3H), 1.64-1.83 (m, 4H), 2.22-2.48 (m, 7H), 3.30-3.34 (m, 1H), 4.40 (d, $J=7.59$, 1H), 4.60 (dd, $J_1=15.58$ Hz, $J_2=1.63$ Hz, 1H), 4.84 (dd, $J_1=15.60$ Hz, $J_2=2.18$ Hz, 1H), 5.30-5.47 (m, 1H), 6.37 (dd, $J_1=10.17$ Hz, $J_2=1.46$ Hz, 1H), 6.43 (s, 1H), 7.12 (d, $J=10.10$ Hz, 1H). MASA (ES+): 491.2 |
| IB.29 | 0.99 (d, $J=7.12$ Hz, 3H), 1.12 (s, 3H), 1.31-1.36 (m, 1H), 1.52 (s, 3H), 1.54-1.70 (m, 5H), 1.73-1.92 (m, 6H), 2.18-2.38 (m, 6H), 2.72-2.80 (m, 1H), 3.32-3.37 (m, 1H), 3.64-3.76 (m, 2H), 4.24 (s, 2H), 4.41 (d, $J=8.75$, 1H), 5.31-5.47 (m, 1H), 6.38 (d, d, $J_1=10.16$ Hz, $J_2=1.64$ Hz, 1H), 6.44 (s, 1H), 7.14 (d, $J=10.17$ Hz, 1H). MASA (ES+): 577.2 |
| IB.30 | 0.99 (d, $J=7.13$ Hz, 3H), 1.06 (s, 3H), 1.11 (t, $J=7.59$ Hz, 3H), 1.30-1.35 (m, 1H), 1.52 (s, 3H), 1.72-2.04 (m, 4H), 2.17-2.43 (m, 7H), 3.31-3.36 (m, 1H), 3.57 (dd, $J_1=13.64$ Hz, $J_2=7.49$ Hz, 1H), 3.73 (dd, $J_1=13.86$ Hz, $J_2=8.50$ Hz, 1H), 4.21 (dd, $J_1=12.64$ Hz, $J_2=0.89$ Hz, 1H), 4.33 (dd, $J_1=12.89$ Hz, $J_2=8.13$ Hz, 1H), 4.37 (d, $J=10.81$ Hz, 1H), 5.30-5.46 (m, 1H), 5.52-5.59 (m, 1H), 5.73-5.79 (m, 1H), 6.37 |

| Com-
puesto
No. | ¹ H-NMR (δ ppm). MASA (EI / ES+, <i>m/z</i>) |
|-----------------------|--|
| | (dd, $J_1=10.14$ Hz, $J_2=1.74$ Hz, 1H), 6.43 (s, 1H), 7.22 (dd, $J_1=10.10$ Hz, $J_2=1.03$ Hz, 1H). MASA (ES+): 539.3 |
| IB.31 | 0.98 (d, $J=7.11$ Hz, 3H), 1.10-1.17 (m, 6H), 1.15 (s, 3H), 1.30-1.36 (m, 1H), 1.54 (s, 3H), 1.73-1.90 (m, 3H), 2.20-2.44 (m, 8H), 3.03 (d, $J=2.56$ Hz, 1H), 3.34-3.38 (m, 1H), 3.68 (dd, 2H), 4.40 (d, $J=8.47$, 1H), 4.55 (d, $J=15.4$ Hz, 1H), 7.72 (d, $J=15.4$ Hz, 1H), 5.31-5.49 (m, 1H), 6.36 (dd, $J_1=10.11$ Hz, $J_2=1.16$ Hz, 1H), 6.43 (s, 1H), 7.16 (d, $J=10.11$ Hz, 1H). MASA (ES+): 615.5 (M+Na) ⁺ . |
| IB.32 | 0.98 (d, $J=7.11$ Hz, 3H), 1.12 (t, $J=7.49$ Hz, 3H), 1.13 (s, 3H), 1.20-1.36 (m, 1H), 1.54 (s, 3H), 1.70-1.93 (m, 3H), 2.10 (s, 3H), 2.19-2.42 (m, 6H), 2.88 (s, 1H), 3.34-3.37 (m, 1H), 3.64 (d, $J=16.77$, 1H), 3.72 (d, $J=16.82$, 1H), 4.41-1.12 (d, $J=8.07$ Hz, 1H), 4.56 (d, $J=15.4$ Hz, 1H), 4.69-1.12 (d, $J=15.4$ Hz, 1H), 5.30-5.47 (m, 1H), 6.38 (dd, $J_1=10.12$ Hz, $J_2=1.50$ Hz, 1H), 6.43 (s, 1H), 7.17 (d, $J=10.15$ Hz, 1H). MASA (ES+): 601.0 (M+Na) ⁺ . |
| IB.33 | 0.97 (t, $J=7.47$ Hz, 3H), 0.98 (d, $J=7.44$ Hz, 3H), 1.12 (t, $J=7.64$ Hz, 3H), 1.15 (s, 3H), 1.30-1.36 (m, 1H), 1.54 (s, 3H), 1.66 (q, $J=7.42$ Hz, 2H), 1.70-1.94 (m, 4H), 2.19-2.46 (m, 8H), 3.01 (d, $J=2.63$ Hz, 1H), 3.33-3.38 (m, 1H), 3.64 (d, $J=16.88$ Hz, 1H), 3.72 (d, $J=16.75$ Hz, 1H), 4.40 (d, $J=8.68$ Hz, 1H), 4.53 (t, d, $J_1=15.38$ Hz, $J_2=1.70$ Hz, 1H), 4.72 (dd, $J_1=15.39$ Hz, $J_2=1.62$ Hz, 1H), 5.31-5.48 (m, 1H), 6.37 (dd, $J_1=10.12$ Hz, $J_2=1.77$ Hz, 1H), 6.43 (s, 1H), 7.16 (dd, $J_1=10.15$ Hz, $J_2=1.26$ Hz, 1H). MASA (ES+): 607.5 |
| IB.34 | 0.98 (d, $J=7.15$ Hz, 3H), 1.12 (t, $J=7.59$ Hz, 3H), 1.16 (s, 3H), 1.18 (d, $J=7.00$ Hz, 3H), 1.19 (d, $J=6.96$ Hz, 3H), 1.30-1.36 (m, 1H), 1.54 (s, 3H), 1.70-1.94 (m, 4H), 2.19-2.48 (m, 4H), 2.36 (q, $J=7.55$ Hz, 2H), 2.56-2.63 (m, 1H), 3.11 (d, $J=3.05$ Hz, 1H), 3.33-3.37 (m, 1H), 3.65 (d, $J=16.93$ Hz, 1H), 3.71 (d, $J=17.26$ Hz, 1H), 4.40 (d, $J=8.83$ Hz, 1H), 4.53 (t, d, $J_1=15.38$ Hz, $J_2=1.72$ Hz, 1H), 4.73 (dd, $J_1=15.36$ Hz, $J_2=1.61$ Hz, 1H), 5.31-5.48 (m, 1H), 6.37 (dd, $J_1=10.12$ Hz, $J_2=1.79$ Hz, 1H), 6.43 (s, 1H), 7.16 (dd, $J_1=10.12$ Hz, $J_2=1.17$ Hz, 1H). MASA (ES+): 607.7 |
| IB.35 | 0.93 (t, $J=7.31$ Hz, 3H), 0.98 (d, $J=7.15$ Hz, 3H), 1.12 (t, $J=7.71$ Hz, 3H), 1.15 (s, 3H), 1.25-1.41 (m, 3H), 1.54 (s, 3H), 1.55-1.94 (m, 6H), 2.19-2.46 (m, 8H), 3.03 (d, $J=2.91$ Hz, 1H), 3.33-3.38 (m, 1H), 3.64 (d, $J=16.76$ Hz, 1H), 3.72 (d, $J=16.71$ Hz, 1H), 4.40 (d, $J=8.90$ Hz, 1H), 4.53 (t, d, $J_1=15.40$ Hz, $J_2=1.75$ Hz, 1H), 4.71 (dd, $J_1=15.41$ Hz, $J_2=1.43$ Hz, 1H), 5.31-5.48 (m, 1H), 6.37 (dd, $J_1=10.13$ Hz, $J_2=1.78$ Hz, 1H), 6.43 (s, 1H), 7.16 (dd, $J_1=10.11$ Hz, $J_2=1.19$ Hz, 1H). MASA (ES+): 621.5 |
| IB.36 | 0.98 (d, $J=7.18$ Hz, 3H), 1.12 (t, $J=7.59$ Hz, 3H), 1.15 (s, 3H), 1.25-1.36 (m, 1H), 1.55 (s, 3H), 1.73-2.04 (m, 6H), 2.20-2.47 (m, 10H), 3.16-3.20 (m, 2H), 3.34-3.37 (m, 1H), 3.68 (Two d, 2H), 4.41 (d, $J=8.64$ Hz, 1H), 4.54 (t, d, $J_1=15.38$ Hz, $J_2=1.74$ Hz, 1H), 4.72 (t, d, $J_1=15.37$ Hz, $J_2=1.66$ Hz, 1H), 5.33-5.45 (m, 1H), 6.37 (dd, $J_1=10.16$ Hz, $J_2=1.81$ Hz, 1H), 6.43 (s, 1H), 7.16 (dd, $J_1=10.10$ Hz, $J_2=1.26$ Hz, 1H). MASA (ES+): 619.7 |
| IB.37 | 0.91 (t, $J=6.86$ Hz, 3H), 0.98 (d, $J=7.15$ Hz, 3H), 1.12 (t, $J=7.59$ Hz, 3H), 1.15 (s, 3H), 1.25-1.36 (m, 3H), 1.54 (s, 3H), 1.61-1.94 (m, 6H), 2.19-2.38 (m, 8H), 3.05 (d, $J=3.03$ Hz, 1H), 3.34-3.38 (m, 1H), 3.64 (d, $J=16.70$ Hz, 1H), 3.72 (d, $J=16.93$ Hz, 1H), 4.40 (d, $J=8.58$ Hz, 1H), 4.52 (d, $J=15.37$ Hz, 1H), 4.72 (d, $J=15.39$ Hz, 1H), 5.31-5.47 (m, 1H), 6.37 (dd, $J_1=10.14$ Hz, $J_2=1.75$ Hz, 1H), 6.43 (s, 1H), 7.16 (dd, $J_1=10.63$ Hz, $J_2=1.04$ Hz, 1H). MASA (ES+): 634.8 |
| IB.38 | 1.07 (s, 3H), 1.14 (t, $J=7.53$ Hz, 3H), 1.21-1.28 (m, 1H), 1.42 (d, $J=7.27$ Hz, 3H), 1.55 (s, 3H), 1.60-1.65 (m, 1H), 1.90-2.00 (m, 5H), 2.26-2.42 (m, 7H), 2.61-2.71 (m, 1H), 3.36 (d, $J=16.65$, 1H), 3.80 (d, $J=16.65$, 1H), 4.26 (m, 2H), 4.40 (d, $J=8.38$, 1H), 6.14 (s, 1H), 6.35 (dd, $J_1=10.06$ Hz, $J_2=1.39$ Hz, 1H), 7.24 (d, $J=10.23$ Hz, 1H). MASA (ES+): 541.6 (M+Na) ⁺ . |
| IB.39 | 1.06 (s, 3H), 1.15 (t, $J=7.54$ Hz, 3H), 1.21-1.29 (m, 1H), 1.43 (d, $J=7.35$ Hz, 3H), 1.53 (s, 3H), 1.70-2.06 (m, 6H), 2.27-2.41 (m, 6H), 3.35 (d, d, $J_1=16.67$, $J_2=2.34$ Hz, 1H), 3.81 (d, t, $J_1=16.67$, $J_2=2.08$, 1H), 4.25-4.28 (m, 2H), 4.40 (d, $J=8.32$ Hz, 1H), 5.31-5.48 (m, 1H), 6.37 (dd, $J_1=10.12$ Hz, $J_2=1.77$ Hz, 1H), 6.44 (s, 1H), 7.16 (dd, $J_1=10.12$ Hz, $J_2=1.16$ Hz, 1H). MASA (ES+): 559.2 (M+Na) ⁺ . |
| IB.40 | 1.04 (d, $J=7.13$ Hz, 3H), 1.16 (s, 3H), 1.25-1.39 (m, 2H), 1.43 (s, 3H), 1.44 (s, 3H), 1.55 (s, 3H), 1.72-1.94 (m, 3H), 2.28-2.51 (m, 4H), 3.39-3.44 (m, 1H), 3.67 (d, $J=16.29$ Hz, 1H), 3.75 (d, $J=16.24$ Hz, 1H), 4.60 (s, 1H), 4.98-4.99 (m, 1H), 5.37-5.50 (m, 1H), 6.32-6.35 (m, 2H), 6.53 (dd, $J_1=3.41$ Hz, $J_2=1.65$ Hz, 1H), 7.12 (d, $J=3.48$ Hz, 1H), 7.26 (d, $J=10.03$ Hz, 1H), 7.64 (s, 1H). MASA (ES+): 625.0 (M+Na) ⁺ . |
| IB.41 | 0.96 (d, 3H, $J=7.16$ Hz), 1.06 (s, 3H), 1.12 (t, 3H, $J=7.57$ Hz), 1.26-1.34 (m, 1H), 1.53 (s, 3H), 1.71-1.91 (m, 3H), 2.24-2.39 (m, 6H), 3.30-3.35 (m, 1H), 3.76 (s, 3H), 4.41 (m, 1H), 4.71 (1H, ddd, $J_1=15.93$ Hz, $J_2=4.75$ Hz, $J_3=1.81$ Hz), 4.84 (ddd, 1H, $J_1=16.00$ Hz, $J_2=4.75$ Hz, $J_3=1.82$ Hz), 5.34 & 5.46 (m, 1H), 6.03 (d, 1H, $J=15.77$ Hz), 6.37 (dd, 1H, $J_1=10.15$ Hz, $J_2=1.78$ Hz), 6.44 (s, 1H), 6.93-6.97 (m, 1H), 7.12 (dd, $J_1=10.13$ Hz, $J_2=1.18$ Hz). MASA (ES+): 573.1 (M+Na) ⁺ . |
| IB.42 | 1.00 (d, 3H, $J=7.15$ Hz), 1.06 (s, 3H), 1.12 (t, 3H, $J=7.56$ Hz), 1.30-1.35 (m, 1H), 1.52 (s, 3H), 1.73-1.87 (m, 4H), 2.22-2.40 (m, 6H), 3.34-3.36 (m, 1H), 3.71 (d, 2H, $J=7.09$ Hz), 3.74 (s, 3H), 4.40 (d, 1H, $J=8.85$ Hz), 5.32 & 5.44 (m, 1H), 6.02 (d, 1H, $J=15.46$ Hz), 6.38 (dd, 1H, $J_1=10.15$ Hz, $J_2=1.79$ Hz), 6.43 (s, 1H), 6.85-6.89 (m, 1H), 7.12 (dd, 1H, $J_1=10.15$ Hz, $J_2=1.18$ Hz). MASA (ES+): 589.1 (M+Na) ⁺ . |
| IB.43 | 1.03 (s, 3H), 1.15-1.23 (m, 3H), 1.27 (t, 3H, $J=7.12$ Hz), 1.45 (s, 3H), 1.47-1.55 (m, 1H), 1.63-1.70 (m, 2H), 1.80-1.87 (m, 1H), 1.93-2.00 (m, 1H), 2.09-2.16 (m, 3H), 2.32-2.36 (m, 1H), 2.53-2.61 (m, 1H), 2.91-2.98 (m, 1H), 3.76 (s, 3H), 4.13 (d de q, 2H, $J_1=14.22$ Hz, $J_2=7.10$ Hz, $J_3=2.13$ Hz), 4.51 (s, 1H), 4.79 (d, 1H, $J=1.62$ Hz), 4.80 (d, 1H, $J=1.62$ Hz), 6.02 (s, 1H), 6.06 (d, 1H, $J=15.77$ Hz), 6.27 (dd, 1H, $J_1=10.09$ Hz, $J_2=1.75$ Hz), 6.94 (d de t, 1H, $J_1=15.76$ Hz, $J_2=4.71$ Hz), 7.23 (d, 1H, $J=10.11$ Hz). MASA (EI): 516 |
| IB.44 | 0.99 (d, $J=7.13$ Hz, 3H), 1.09 (s, 3H), 1.11 (t, $J=7.38$ Hz, 3H), 1.29-1.35 (m, 1H), 1.39 (t, $J=7.18$ Hz, 3H), 1.53 (s, 3H), 1.72-1.89 (m, 3H), 2.20-2.50 (m, 6H), 3.32-3.37 (m, 1H), 3.52 (d, $J=13.42$ Hz, 1H), 3.62 (dd, $J_1=15.97$ Hz, $J_2=4.53$ Hz, 1H), 4.37 (q, $J=7.15$ Hz, 2H), 4.38-4.40 (m, 1H), 4.70-4.82 (m, 1H), 5.30-5.47 (m, 1H), 5.82-5.83 (m, 2H), 6.37 (dd, $J_1=10.13$ Hz, $J_2=1.77$ Hz, 1H), 6.43 (s, 1H), 7.15 (dd, $J_1=10.12$ Hz, $J_2=1.18$ Hz, 1H). |
| IB.45 | 1.04 (d, $J=7.06$ Hz, 3H), 1.16 (s, 3H), 1.29-1.34 (m, 1H), 1.68 (s, 3H), 1.71-1.97 (m, 4H), 2.37-2.70 (m, 5H), 3.38-3.41 (m, 1H), 3.70 (d, $J=16.35$, 1H), 3.79 (d, $J=16.32$ Hz, 1H), 4.15-4.16 (m, 2H), 4.53 (d, $J=2.4$ Hz, 1H), 4.74 (t, $J=5.94$, 1H), 5.03 (d, $J=3.67$ Hz, 1H), 6.05 (s, 1H), 6.28 (dd, $J_1=10.07$ Hz, $J_2=1.27$ Hz, 1H), 6.53 (dd, $J_1=3.15$ Hz, $J_2=1.47$ Hz, 1H), 7.18 (d, $J=3.35$, 1H), 7.31 (d, $J=10.11$ Hz, 1H), 7.63 (br-s, 1H). MASA (ES+): 595.4 (M+Na) ⁺ . |
| IB.46 | 1.07 (d, $J=7.16$ Hz, 3H), 1.15 (s, 3H), 1.35-1.38 (m, 1H), 1.39 (t, $J=7.14$ Hz, 3H), 1.56 (s, 3H), 1.76-1.97 (m, 3H), 2.28-2.50 (m, 5H), 3.40-3.44 (m, 1H), 3.55 (dd, $J_1=14.06$ Hz, $J_2=2.91$ Hz, 1H), 3.65 (dd, $J_1=15.79$ Hz, $J_2=4.86$ Hz, 1H), 4.36 (q, $J=7.17$ Hz, 2H), 4.43 (d, $J=8.99$ Hz, 1H), 4.95-5.05 (m, 2H), 5.31-5.50 (m, 1H), 5.67-5.71 (m, 1H), 5.77-5.81 (m, 1H), 6.39 (dd, $J_1=10.13$ Hz, $J_2=1.82$ Hz, 1H), 6.45 (s, 1H), 6.48 (dd, $J_1=3.49$ Hz, $J_2=1.73$ Hz, 1H), 7.11 (dd, $J_1=3.49$ Hz, $J_2=0.64$ Hz, 1H), 7.18 (dd, $J_1=10.11$ Hz, $J_2=1.20$ Hz, 1H), 7.57 (dd, $J_1=1.6$ Hz, $J_2=0.70$ Hz, 1H). |
| IB.47 | 1.06 (d, $J=7.13$ Hz, 3H), 1.12 (s, 3H), 1.34-1.38 (m, 1H), 1.38 (t, $J=7.16$ Hz, 3H), 1.55 (s, 3H), 1.77-1.98 (m, 3H), 2.25-2.48 (m, 5H), 3.42-3.45 (m, 1H), 3.63 (dd, $J_1=13.76$ Hz, $J_2=7.57$ Hz, 1H), 3.76 (dd, $J_1=13.79$ Hz, $J_2=8.48$ Hz, 1H), 4.36 (q, $J=7.17$ Hz, 2H), 4.43 (d, $J=8.99$ Hz, 1H), 4.95-5.05 (m, 2H), 5.31-5.50 (m, 1H), 5.67-5.71 (m, 1H), 5.77-5.81 (m, 1H), 6.39 (dd, $J_1=10.14$ Hz, $J_2=1.55$ Hz, 1H), 6.45 (s, 1H), 6.49 (dd, $J_1=3.32$ Hz, $J_2=1.55$ Hz, 1H), 7.11 (dd, $J=3.48$ Hz, 1H), 7.16 (d, $J=10.14$ Hz, 1H), 7.58 (s, 1H). |
| IB.48 | 1.05 (d, $J=7.15$ Hz, 3H), 1.17 (s, 3H), 1.37-1.40 (m, 1H), 1.49 (d, $J=7.07$ Hz, 3H), 1.55 (s, 3H), 1.77-1.99 (m, 4H), 2.13 (s, 3H), 2.17-2.48 (m, 4H), 3.42-3.46 (m, 1H), 3.67 (d, $J=16.90$, 1H), 3.77 (d, $J=16.82$ Hz, 1H), 4.44 (d, $J=8.50$ Hz, 1H), 4.64 (t, d, $J_1=15.4$ Hz, $J_2=1.87$ Hz, 1H), 4.78 (t, d, $J_1=15.41$ Hz, $J_2=1.86$ Hz, 1H), 5.09 (q, $J=6.37$ Hz, 1H), 5.32-5.51 (m, 1H), 6.39 (dd, $J_1=10.12$ Hz, $J_2=1.78$ Hz, 1H), 6.45 (s, 1H), 6.50 (dd, $J_1=3.49$ Hz, $J_2=1.73$ Hz, 1H), 7.12 (dd, $J_1=3.47$ Hz, $J_2=0.49$ Hz, 1H), 7.16 (dd, $J_1=10.14$ Hz, $J_2=1.31$ Hz, 1H), 7.59 (d, $J=0.75$ Hz, 1H). MASA (ES+): 689.0 |
| IB.49 | 0.97 (t, $J=7.47$ Hz, 3H), 0.98 (d, $J=7.44$ Hz, 3H), 1.12 (t, $J=7.64$ Hz, 3H), 1.15 (s, 3H), 1.30-1.36 (m, 1H), 1.54 (s, 3H), 1.66 (q, $J=7.42$ Hz, 2H), 1.70-1.94 (m, 4H), 2.19-2.46 (m, 8H), 3.01 (d, $J=2.63$ Hz, 1H), 3.33-3.38 (m, 1H), 3.64 (d, $J=16.88$ Hz, 1H), 3.72 (d, $J=16.75$ Hz, 1H), 4.40 (d, $J=8.68$ Hz, 1H), 4.53 (t, d, $J_1=15.38$ Hz, $J_2=1.70$ Hz, 1H), 4.72 (dd, $J_1=15.39$ Hz, $J_2=1.62$ Hz, 1H), 5.31-5.48 (m, 1H), 6.37 (dd, $J_1=10.12$ Hz, $J_2=1.77$ Hz, 1H), 6.43 (s, 1H), 7.16 (dd, $J_1=10.15$ Hz, $J_2=1.26$ Hz, 1H). MASA (ES+): 607.5 |

| Com-puesto No. | III-NMR (δ ppm). MASA (EI / ES+, m/z) |
|----------------|---|
| IB.50 | 1.06 (d, $J=7.16$ Hz, 3H), 1.17 (d, $J=2.39$ Hz, 3H), 1.18 (d, $J=2.37$ Hz, 3H), 1.21 (s, 3H), 1.35-1.41 (m, 1H), 1.56 (s, 3H), 1.77-2.00 (m, 3H), 2.29-2.62 (m, 5H), 3.21 (d, $J=2.62$ Hz, 1H), 3.42-3.49 (m, 1H), 3.67 (d, $J=16.86$ Hz, 1H), 3.75 (d, $J=16.81$ Hz, 1H), 4.45 (d, $J=8.59$ Hz, 1H), 4.52 (d, $J=15.45$ Hz, 1H), 4.74 (d, $J=15.33$ Hz, 1H), 5.33-5.50 (m, 1H), 6.40 (dd, $J_1=10.05$ Hz, $J_2=1.65$ Hz, 1H), 6.45 (s, 1H), 6.50 (dd, $J_1=3.50$ Hz, $J_2=1.69$ Hz, 1H), 7.13 (dd, $J_1=3.56$ Hz, $J_2=0.57$ Hz, 1H), 7.19 (dd, $J_1=0.75$ Hz, $J_2=0.22$ Hz, 1H), 7.58 (s, 1H). MASA (ES+): 667.0 (M+Na) ⁺ |
| IB.51 | 1.06 (d, $J=7.16$ Hz, 3H), 1.21 (s, 9H), 1.22 (s, 3H), 1.35-1.41 (m, 1H), 1.56 (s, 3H), 1.77-2.00 (m, 1H), 2.29-2.53 (m, 1H), 3.27 (d, $J=3.09$ Hz, 1H), 3.42-3.47 (m, 1H), 3.67 (d, $J=16.88$ Hz, 1H), 3.74 (d, $J=16.89$ Hz, 1H), 4.45 (d, $J=8.56$ Hz, 1H), 4.50 (d, $J=15.35$ Hz, 1H), 4.75 (d, $J=15.40$ Hz, 1H), 5.33-5.40 (m, 1H), 6.40 (dd, $J_1=10.19$ Hz, $J_2=1.84$ Hz, 1H), 6.45 (s, 1H), 6.50 (dd, $J_1=3.51$ Hz, $J_2=1.68$ Hz, 1H), 7.14 (d, $J=3.43$ Hz, 1H), 7.17 (dd, $J_1=15.12$ Hz, $J_2=0.99$ Hz, 1H), 7.58 (d, $J=0.98$ Hz, 1H). MASA (ES+): 680.9 (M+Na) ⁺ |
| IB.52 | 0.98 (d, $J=7.14$ Hz, 3H), 1.12 (t, $J=7.56$ Hz, 3H), 1.17 (s, 3H), 1.22 (s, 9H), 1.30-1.36 (m, 1H), 1.54 (s, 3H), 1.73-1.95 (m, 3H), 2.21-2.40 (m, 6H), 3.20 (d, $J=3.29$ Hz, 1H), 3.34-3.38 (m, 1H), 3.68 (br-s, 2H), 4.40 (d, $J=8.77$ Hz, 1H), 4.50 (d, $J=14.59$ Hz, 1H), 4.74 (d, $J=15.33$ Hz, 1H), 5.30-5.50 (m, 1H), 6.37 (dd, $J_1=10.12$ Hz, $J_2=1.77$ Hz, 1H), 6.43 (s, 1H), 7.15 (dd, $J_1=10.09$ Hz, $J_2=1.04$ Hz, 1H). MASA (ES+): 643.0 (M+Na) ⁺ |
| IB.53 | 0.94 (d, $J=7.45$ Hz, 3H), 1.06 (d, $J=7.18$ Hz, 3H), 1.12 (s, 3H), 1.34-1.40 (m, 1H), 1.55 (s, 3H), 1.66 (t, $J=7.41$ Hz, 2H), 1.77-2.05 (m, 3H), 2.30 (t, $J=7.45$ Hz, 2H), 2.35-2.48 (m, 4H), 3.43-3.47 (m, 1H), 3.66 (d, $J=7.79$ Hz, 1H), 3.43 (d, $J=9.05$ Hz, 1H), 4.76-4.79 (m, 2H), 5.59-5.72 (m, 1H), 6.39 (dd, $J_1=10.17$ Hz, $J_2=1.80$ Hz, 1H), 6.45 (s, 1H), 6.49 (dd, $J_1=3.48$ Hz, $J_2=1.81$ Hz, 1H), 7.12 (d, $J=3.42$ Hz, 1H), 7.17 (dd, $J_1=10.08$ Hz, $J_2=1.02$ Hz, 1H), 7.58 (d, $J=0.93$ Hz, 1H). MASA (ES+): 669.0 (M+Na) ⁺ |
| IB.54 | 1.06 (d, 3H, $J=7.14$ Hz), 1.21 (s, 3H), 1.38-1.41 (m, 1H), 1.39 (t, 3H, $J=7.15$ Hz), 1.56 (s, 3H), 1.77-1.96 (m, 3H), 2.28-2.64 (m, 5H), 3.37-3.45 (m, 1H), 3.72 (br-s, 2H), 4.38 (q, $J=7.12$ Hz, 2H), 4.46 (d, $J=8.96$ Hz, 1H), 4.79 (d, $J=15.27$ Hz, 1H), 4.89 (d, $J=15.31$ Hz, 1H), 5.32-5.51 (m, 1H), 6.40 (dd, $J_1=10.14$ Hz, $J_2=1.77$ Hz, 1H), 6.45 (s, 1H), 6.50 (dd, $J_1=3.47$ Hz, $J_2=1.69$ Hz, 1H), 7.12 (d, $J=3.25$ Hz, 1H), 7.19 (dd, $J_1=10.11$ Hz, $J_2=0.85$ Hz, 1H), 7.58 (d, $J=0.72$ Hz, 1H). |
| IB.55 | 0.96 (t, $J=7.42$ Hz, 3H), 1.07 (d, $J=7.18$ Hz, 3H), 1.21 (s, 3H), 1.36-1.42 (m, 1H), 1.56 (s, 3H), 1.65 (q, $J=7.43$ Hz, 2H), 1.70-2.02 (m, 3H), 2.29-2.53 (m, 6H), 3.09 (d, $J=2.87$ Hz, 1H), 3.43-3.47 (m, 1H), 3.67 (d, $J=16.68$ Hz, 1H), 3.77 (d, $J=16.66$ Hz, 1H), 4.46 (d, $J=8.60$ Hz, 1H), 4.53 (d, $J=18.41$ Hz, 1H), 4.73 (d, $J=15.35$ Hz, 1H), 5.33-5.50 (m, 1H), 6.40 (dd, $J_1=10.17$ Hz, $J_2=1.81$ Hz, 1H), 6.46 (s, 1H), 7.10 (dd, $J_1=4.83$ Hz, $J_2=3.94$ Hz, 1H), 7.19 (dd, $J_1=10.10$ Hz, $J_2=1.02$ Hz, 1H), 7.57 (dd, $J_1=5.01$ Hz, $J_2=1.05$ Hz, 1H), 7.75 (dd, $J_1=3.71$ Hz, $J_2=1.03$ Hz, 1H). MASA (ES+): 682.9 (M+Na) ⁺ |
| IB.56 | 0.92 (t, $J=7.40$ Hz, 3H), 1.05 (d, $J=7.16$ Hz, 3H), 1.21 (s, 3H), 1.37-1.40 (m, 1H), 1.56 (s, 3H), 1.66 (q, $J=7.42$ Hz, 2H), 1.78-2.0 (m, 3H), 2.28-2.41 (m, 6H), 3.11 (d, $J=3.03$ Hz, 1H), 3.38-3.45 (m, 1H), 3.71 (d, $J=11.09$ Hz, 1H), 4.46 (d, $J=8.70$ Hz, 1H), 4.52 (d, $J=15.37$ Hz, 1H), 4.74 (d, $J=15.34$ Hz, 1H), 6.42 (dd, $J_1=10.18$ Hz, $J_2=1.82$ Hz, 1H), 6.46 (s, 1H), 6.94 (d, $J=4.09$ Hz, 1H), 7.19 (dd, $J_1=10.09$ Hz, $J_2=1.06$ Hz, 1H), 7.54 (d, $J=4.07$ Hz, 1H). MASA (ES+): 716.9 (M+Na) ⁺ |
| IB.57 | 0.92-1.03 (m, 4H), 1.05 (d, $J=7.26$ Hz, 3H), 1.19 (s, 3H), 1.35-1.40 (m, 1H), 1.56 (s, 3H), 1.61-1.98 (m, 4H), 2.28-2.51 (m, 4H), 3.06 (d, $J=2.41$ Hz, 1H), 3.43-3.46 (m, 1H), 3.66 (d, $J=16.84$ Hz, 1H), 3.77 (d, $J=16.84$ Hz, 1H), 4.44 (d, $J=8.44$ Hz, 1H), 4.55 (d, $J=16.23$ Hz, 1H), 4.70 (d, $J=14.68$ Hz, 1H), 5.33-5.50 (m, 1H), 6.40 (dd, $J_1=10.15$ Hz, $J_2=1.79$ Hz, 1H), 6.45 (s, 1H), 6.50 (dd, $J_1=3.47$ Hz, $J_2=1.65$ Hz, 1H), 7.13 (d, $J=3.31$ Hz, 1H), 7.18 (dd, $J_1=10.10$ Hz, $J_2=1.04$ Hz, 1H), 7.59 (d, $J=0.83$ Hz, 1H). MASA (ES+): 693.0 (M+Na) ⁺ |
| IB.58 | 1.06 (d, $J=7.14$ Hz, 3H), 1.21 (s, 3H), 1.35-1.41 (m, 1H), 1.57 (s, 3H), 1.77-2.04 (m, 5H), 2.21-2.53 (m, 8H), 3.15-3.21 (m, 2H), 3.42-3.47 (m, 1H), 3.67 (d, $J=16.81$ Hz, 1H), 3.75 (d, $J=17.06$ Hz, 1H), 4.45 (d, $J=8.61$ Hz, 1H), 4.43 (d, $J=15.33$ Hz, 1H), 4.73 (d, $J=15.39$ Hz, 1H), 5.33-5.50 (m, 1H), 6.40 (dd, $J_1=10.14$ Hz, $J_2=1.82$ Hz, 1H), 6.45 (s, 1H), 6.50 (dd, $J_1=3.47$ Hz, $J_2=1.60$ Hz, 1H), 7.13 (d, $J=3.26$ Hz, 1H), 7.18 (dd, $J_1=10.18$ Hz, $J_2=1.26$ Hz, 1H), 7.58 (d, $J=1.71$ Hz, 1H). MASA (ES+): 678.9 (M+Na) ⁺ |
| IB.59 | 1.06 (d, $J=7.16$ Hz, 3H), 1.21 (s, 3H), 1.35-1.41 (m, 1H), 1.56 (s, 3H), 1.62-1.9 (m, 1H), 2.28-2.51 (m, 4H), 2.73-2.81 (m, 1H), 3.37 (d, $J=2.84$ Hz, 1H), 3.42-3.49 (m, 1H), 3.66 (d, $J=16.87$ Hz, 1H), 3.75 (d, $J=16.86$ Hz, 1H), 4.44 (d, $J=8.46$ Hz, 1H), 4.51 (d, $J=15.31$ Hz, 1H), 4.74 (d, $J=15.33$ Hz, 1H), 5.33-5.50 (m, 1H), 6.40 (dd, $J_1=10.18$ Hz, $J_2=1.82$ Hz, 1H), 6.45 (s, 1H), 6.50 (dd, $J_1=3.48$ Hz, $J_2=1.79$ Hz, 1H), 7.13 (d, $J=3.41$ Hz, 1H), 7.17 (dd, $J_1=10.08$ Hz, $J_2=1.08$ Hz, 1H), 7.59 (d, $J=1.89$ Hz, 1H). MASA (ES+): 693.0 (M+Na) ⁺ |
| IB.60 | 0.95 (t, $J=7.38$ Hz, 3H), 1.06 (d, $J=7.18$ Hz, 3H), 1.12 (s, 3H), 1.34-1.40 (m, 1H), 1.55 (s, 3H), 1.64 (q, $J=7.44$ Hz, 2H), 1.74-1.94 (m, 3H), 2.30 (t, $J=7.46$ Hz, 2H), 2.36-2.50 (m, 4H), 2.72 (s, 1H), 3.42-3.47 (m, 1H), 3.53 (dd, $J_1=14.08$ Hz, $J_2=6.92$ Hz, 1H), 3.67 (dd, $J_1=14.01$ Hz, $J_2=5.33$ Hz, 1H), 4.42 (d, $J=8.53$ Hz, 1H), 4.50 (dd, $J_1=13.23$ Hz, $J_2=4.74$ Hz, 1H), 4.62 (dd, $J_1=13.20$ Hz, $J_2=5.70$ Hz, 1H), 5.32-5.49 (m, 1H), 5.67-5.81 (m, 2H), 6.39 (dd, $J_1=10.19$ Hz, $J_2=1.80$ Hz, 1H), 6.45 (s, 1H), 6.49 (dd, $J_1=3.49$ Hz, $J_2=1.56$ Hz, 1H), 7.12 (d, $J=3.42$ Hz, 1H), 7.16 (dd, $J_1=10.15$ Hz, $J_2=1.02$ Hz, 1H), 7.58 (d, $J=0.79$ Hz, 1H). MASA (ES+): 669.0 (M+Na) ⁺ |
| IB.61 | 1.03 (d, $J=7.12$ Hz, 3H), 1.19 (s, 3H), 1.25-1.42 (m, 2H), 1.55 (s, 3H), 1.65-1.96 (m, 3H), 2.21-2.46 (m, 4H), 3.45 (m, 1H), 3.71 (d, $J=16.51$ Hz, 1H), 3.79 (d, $J=16.46$ Hz, 1H), 4.20-4.30 (m, 2H), 4.46 (d, $J=8.42$ Hz, 1H), 5.30-5.50 (m, 1H), 6.42 (dd, $J_1=10.05$ Hz, $J_2=1.80$ Hz, 1H), 6.47 (s, 1H), 7.15 (dd, $J_1=10.15$ Hz, $J_2=1.21$ Hz, 1H), 7.43 (d, $J=8.59$ Hz, 2H), 7.86 (d, $J=8.55$ Hz, 2H). MASA (ES+): 640.9 (M+Na) ⁺ |
| IB.62 | 1.03 (d, $J=7.05$ Hz, 3H), 1.20 (s, 3H), 1.22-1.93 (m, 8H), 2.29-2.51 (m, 4H), 3.44-3.50 (m, 1H), 3.71 (d, $J=16.42$ Hz, 1H), 3.80 (d, $J=16.52$ Hz, 1H), 4.26-4.32 (m, 2H), 4.46 (d, $J=8.81$ Hz, 1H), 5.33-5.50 (m, 1H), 6.40-6.42 (m, 1H), 6.46 (s, 1H), 7.16 (dd, $J_1=10.15$ Hz, 1H), 7.39 (d, $J=7.91$ Hz, 1H), 7.55 (d, $J=7.56$ Hz, 1H), 7.79 (d, $J=7.76$ Hz, 1H), 7.91 (s, 1H). MASA (ES+): 640.9 (M+Na) ⁺ |
| IB.63 | 1.06 (d, $J=7.14$ Hz, 3H), 1.19 (s, 3H), 1.36-1.41 (m, 1H), 1.55 (s, 3H), 1.74-1.99 (m, 3H), 2.17-2.51 (m, 5H), 3.42-3.46 (m, 1H), 3.69 (d, $J=16.73$ Hz, 1H), 3.76 (d, $J=16.91$ Hz, 1H), 3.81 (s, 3H), 4.45 (d, $J=8.63$ Hz, 1H), 4.66 (td, $J_1=15.52$ Hz, $J_2=1.70$ Hz, 1H), 4.73 (td, $J_1=15.49$ Hz, $J_2=1.71$ Hz, 1H), 5.33-5.49 (m, 1H), 6.40 (dd, $J_1=10.12$ Hz, $J_2=1.72$ Hz, 1H), 6.45 (s, 1H), 6.50 (dd, $J_1=3.48$ Hz, $J_2=1.68$ Hz, 1H), 7.14 (d, $J=3.43$ Hz, 1H), 7.16 (dd, $J_1=10.09$ Hz, $J_2=0.99$ Hz, 1H), 7.59 (d, $J=0.92$ Hz, 1H). MASA (ES+): 654.9 (M+Na) ⁺ |
| IB.64 | 1.06 (d, $J=7.16$ Hz, 3H), 1.19 (s, 3H), 1.33 (t, $J=7.05$ Hz, 3H), 1.36-1.41 (m, 1H), 1.55 (s, 3H), 1.74-1.99 (m, 3H), 2.28-2.50 (m, 4H), 2.56 (d, $J=1.85$ Hz, 1H), 3.42-3.47 (m, 1H), 3.69 (d, $J=16.88$ Hz, 1H), 3.76 (d, $J=16.88$ Hz, 1H), 4.22 (q, $J=7.13$ Hz, 2H), 4.44 (d, $J=8.65$ Hz, 1H), 4.65 (d, $J=15.49$ Hz, 1H), 4.72 (d, $J=15.41$ Hz, 1H), 5.33-5.49 (m, 1H), 6.40 (dd, $J_1=10.13$ Hz, $J_2=1.63$ Hz, 1H), 6.45 (s, 1H), 6.51 (dd, $J_1=3.44$ Hz, $J_2=1.69$ Hz, 1H), 7.14 (d, $J=3.50$ Hz, 1H), 7.16 (d, $J=10.20$ Hz, 1H), 7.59 (d, $J=0.87$ Hz, 1H). MASA (ES+): 669.1 (M+Na) ⁺ |
| IB.65 | 1.06 (d, $J=7.19$ Hz, 3H), 1.20 (s, 3H), 1.34-1.43 (m, 1H), 1.50 (s, 9H), 1.55 (s, 3H), 1.62-1.99 (m, 3H), 2.28-2.54 (m, 5H), 3.43-3.48 (m, 1H), 3.68 (d, $J=16.70$ Hz, 1H), 3.77 (d, $J=16.65$ Hz, 1H), 4.44 (d, $J=8.51$ Hz, 1H), 4.57-4.68 (m, 2H), 5.33-5.49 (m, 1H), 6.40 (dd, $J_1=10.06$ Hz, $J_2=1.79$ Hz, 1H), 6.45 (s, 1H), 6.50 (dd, $J_1=3.48$ Hz, $J_2=1.78$ Hz, 1H), 7.11-7.14 (m, 2H), 7.59 (d, $J=1.00$ Hz, 1H). MASA (ES+): 697.0 (M+Na) ⁺ |
| IB.66 | 0.96 (d, $J=6.74$ Hz, 6H), 1.06 (d, $J=7.13$ Hz, 3H), 1.19 (s, 3H), 1.35-1.41 (m, 1H), 1.55 (s, 3H), 1.74-2.00 (m, 4H), 2.28-2.52 (m, 5H), 3.43-3.46 (m, 1H), 3.69 (d, $J=16.80$ Hz, 1H), 3.77 (d, $J=16.79$ Hz, 1H), 3.93 (d, $J=6.72$ Hz, 2H), 4.44 (d, $J=8.62$ Hz, 1H), 4.66 (d, $J=15.49$ Hz, 1H), 4.71 (d, $J=15.48$ Hz, 1H), 5.33-5.49 (m, 1H), 6.40 (dd, $J_1=10.18$ Hz, $J_2=1.48$ Hz, 1H), 6.45 (s, 1H), 6.50 (dd, $J_1=3.36$ Hz, $J_2=1.59$ Hz, 1H), 7.13-7.16 (m, 2H), 7.59 (s, 1H). MASA (ES+): 697.0 (M+Na) ⁺ |
| IB.67 | 1.06 (d, $J=7.14$ Hz, 3H), 1.19 (s, 3H), 1.35-1.41 (m, 1H), 1.55 (s, 3H), 1.77-2.14 (m, 5H), 2.28-2.72 (m, 5H), 2.55 (t, $J=7.26$ Hz, 2H), 3.42-3.47 (m, 1H), 3.59 (t, $J=6.37$ Hz, 2H), 3.64 (d, $J=16.76$ Hz, 1H), 3.76 (d, $J=16.58$ Hz, 1H), 4.46 (d, $J=8.65$ Hz, 1H), 4.58 (d, |

| Com-
puesto
No. | 1H-NMR (δ ppm). MASA (EI / ES+, m/z) |
|-----------------------|---|
| | J=15.39Hz, 1H), 4.73 (d, J=15.40Hz, 1H), 5.33-5.49 (m, 1H), 6.40 (dd, J ₁ =10.14Hz, J ₂ =1.64Hz, 1H), 6.45 (s, 1H), 6.50 (dd, J ₁ =3.4Hz, J ₂ =1.57Hz, 1H), 7.13 (d, J=3.45Hz, 1H), 7.18 (d, J=9.98Hz, 1H), 7.59 (d, J=0.75Hz, 1H). MASA (ES+): 679.0 |
| IB.68 | 1.05 (d, J=7.14Hz, 3H), 1.12 (s, 3H), 1.19 (s, 9H), 1.34-1.40 (m, 1H), 1.55 (s, 3H), 1.71-2.06 (m, 3H), 2.27-2.52 (m, 4H), 3.42-3.47 (m, 1H), 3.63 (d, J=11.76Hz, 1H), 3.68 (d, J=11.84Hz, 1H), 4.43 (d, J=9.20Hz, 1H), 4.74 (dd, J ₁ =13.06Hz, J ₂ =6.26Hz, 1H), 4.79 (dd, J ₁ =13.58Hz, J ₂ =6.06Hz, 1H), 5.32-5.49 (m, 1H), 5.55-5.74 (m, 1H), 6.39 (dd, J ₁ =10.19Hz, J ₂ =1.41Hz, 1H), 6.45 (s, 2H), 6.49 (dd, J ₁ =3.34Hz, J ₂ =1.53Hz, 1H), 7.12 (d, J=3.45Hz, 1H), 7.15 (d, J=10.17Hz, 1H), 7.58 (s, 1H). MASA (ES+): 683.0 (M+Na) ⁺ |
| IB.69 | 1.06 (d, J=7.15Hz, 3H), 1.13 (s, 3H), 1.20 (s, 9H), 1.34-1.42 (m, 1H), 1.55 (s, 3H), 1.71-1.95 (m, 3H), 2.17-2.53 (m, 4H), 2.81 (s, 1H), 3.42-3.49 (m, 1H), 3.54 (dd, J ₁ =14.17Hz, J ₂ =7.36Hz, 1H), 3.67 (dd, J ₁ =14.01Hz, J ₂ =5.52Hz, 1H), 4.42 (d, J=8.46Hz, 1H), 4.50 (dd, J ₁ =13.61Hz, J ₂ =4.34Hz, 1H), 4.62 (dd, J ₁ =13.51Hz, J ₂ =5.59Hz, 1H), 5.32-5.49 (m, 1H), 5.64-5.80 (m, 2H), 6.39 (dd, J ₁ =10.18Hz, J ₂ =1.77Hz, 1H), 6.45 (s, 1H), 6.49 (dd, J ₁ =3.43Hz, J ₂ =1.80Hz, 1H), 7.12 (d, J=3.31Hz, 1H), 7.15 (dd, J ₁ =10.24Hz, J ₂ =0.78Hz, 1H), 7.58 (d, J=0.85Hz, 1H). MASA (ES+): 683.1 (M+Na) ⁺ |
| IB.70 | 1.06 (d, 3H, J=7.16Hz), 1.19 (s, 3H), 1.36-1.42 (m, 1H), 1.56 (s, 3H), 1.77-1.96 (m, 3H), 2.29-2.52 (m, 5H), 3.41-3.45 (m, 1H), 3.70 (d, 1H, J=16.78Hz), 3.77 (d, J=16.93Hz, 1H), 4.46 (d, J=8.62Hz, 1H), 4.77 (d, J=15.30Hz, 1H), 4.89 (d, J=15.31Hz, 1H), 5.33-5.50 (m, 1H), 5.99 (s, 1H), 6.40 (dd, J ₁ =10.16Hz, J ₂ =1.75Hz, 1H), 6.45 (s, 1H), 6.50 (dd, J ₁ =3.47Hz, J ₂ =1.67Hz, 1H), 7.12 (d, J=3.41Hz, 1H), 7.17 (d, J=10.19Hz, 1H), 7.59 (s, 1H). MASA (ES+): 597.2 [(M+Na) ⁺ de IB.4] |
| IB.71 | 0.92 (q, J=4.52Hz, 3H), 1.06 (d, J=7.11Hz, 3H), 1.15 (dd, 3H), 1.22 (s, 3H), 1.22 (s, 3H), 1.35-1.41 (m, 1H), 1.56 (s, 3H), 1.46-2.00 (m, 5H), 2.29-2.53 (m, 5H), 3.22-3.26 (dd, 1H), 3.40-3.50 (m, 1H), 3.66 (d, J=16.58Hz, 1H), 3.75 (d, J=16.83Hz, 1H), 4.45 (d, J=8.39Hz, 1H), 4.48-4.53 (m, 1H), 5.33-5.50 (m, 1H), 6.40 (dd, J ₁ =10.15Hz, J ₂ =1.71Hz, 1H), 6.45 (s, 1H), 6.50 (dd, J ₁ =3.39Hz, J ₂ =1.67Hz, 1H), 7.13 (d, J=3.49Hz, 1H), 7.19 (d, J=10.13Hz, 1H), 7.58 (s, 1H). MASA (ES+): 659.3 |
| IB.72 | 1.03 (s, 9H), 1.05 (d, J=7.35Hz, 3H), 1.20 (s, 3H), 1.35-1.40 (m, 1H), 1.56 (s, 3H), 1.72-2.03 (m, 3H), 2.20 (d, J=13.11Hz, 1H), 2.24 (d, J=13.16Hz, 1H), 2.29-2.54 (m, 4H), 3.07 (s, 1H), 3.44-3.48 (m, 1H), 3.63 (d, J=16.81Hz, 1H), 3.78 (d, J=16.84Hz, 1H), 4.44 (d, J=8.47Hz, 1H), 4.50 (d, J=15.41Hz, 1H), 4.73 (d, J=15.35Hz, 1H), 5.33-5.50 (m, 1H), 6.40 (dd, J ₁ =10.17Hz, J ₂ =1.78Hz, 1H), 6.45 (s, 1H), 6.50 (dd, J ₁ =3.45Hz, J ₂ =1.78Hz, 1H), 7.14 (d, J=3.37Hz, 1H), 7.18 (dd, J ₁ =9.63Hz, J ₂ =1.07Hz, 1H), 7.59 (s, 1H). MASA (ES+): 673.3 |
| IB.73 | 1.06 (d, J=7.17Hz, 3H), 1.15 (t, J=7.57Hz, 3H), 1.20 (s, 3H), 1.35-1.41 (m, 1H), 1.56 (s, 3H), 1.74-2.00 (m, 3H), 2.28-2.52 (m, 6H), 3.10 (d, J=2.84Hz, 1H), 3.42-3.46 (m, 1H), 3.66 (d, J=16.80Hz, 1H), 3.75 (d, J=16.82Hz, 1H), 4.45 (d, J=8.54Hz, 1H), 4.54 (d, J=15.48Hz, 1H), 4.73 (d, J=15.38Hz, 1H), 5.33-5.40 (m, 1H), 6.40 (dd, J ₁ =10.11Hz, J ₂ =1.76Hz, 1H), 6.45 (s, 1H), 6.50 (dd, J ₁ =3.49Hz, J ₂ =1.65Hz, 1H), 7.13 (d, J=3.35Hz, 1H), 7.18 (dd, J ₁ =10.06Hz, J ₂ =1.04Hz, 1H), 7.59 (d, J=0.80Hz, 1H). MASA (ES+): 631.3 |
| IB.74 | 0.98 (d, J=7.10Hz, 3H), 1.16 (s, 3H), 1.30-1.36 (m, 1H), 1.40 (t, J=7.12Hz, 3H), 1.54 (s, 3H), 1.73-1.99 (m, 5H), 2.10-2.47 (m, 8H), 2.61 (m, 1H), 3.11-3.19 (m, 1H), 3.31-3.35 (m, 1H), 3.67 (d, J=16.90Hz, 1H), 3.73 (d, J=16.78Hz, 1H), 4.36-4.41 (m, 3H), 4.79 (d, J=15.23Hz, 1H), 4.88 (d, J=15.28Hz, 1H), 5.31-5.48 (m, 1H), 6.38 (d, J ₁ =10.17Hz, 1H), 6.43 (s, 1H), 7.17 (d, J=10.05Hz, 1H). MASA (ES+): 585.22 [(M+Na) ⁺ de IB.08] |
| IB.75 | 0.98 (d, J=7.18Hz, 3H), 1.16 (s, 3H), 1.18 (d, J=3.67Hz, 3H), 1.20 (d, J=3.71Hz, 1H), 1.29-1.35 (m, 1H), 1.54 (s, 3H), 1.70-1.99 (m, 5H), 2.16-2.61 (m, 9H), 3.12 (d, J=3.61Hz, 1H), 3.12-3.20 (m, 1H), 3.33-3.38 (m, 1H), 3.65 (d, J=16.64Hz, 1H), 3.72 (d, J=16.26Hz, 1H), 4.40 (d, J=8.93, 1H), 4.52 (d, J=15.32, 1H), 4.73 (d, J=15.33Hz, 1H), 5.31-5.48 (m, 1H), 6.37 (dd, J ₁ =10.09Hz, J ₂ =1.77Hz, 1H), 6.43 (s, 1H), 7.16 (d, J ₁ =10.10Hz, J ₂ =1.10Hz, 1H). MASA (ES+): 633.25 |
| IB.76 | 1.06 (d, J=7.17Hz, 3H), 1.22 (s, 3H), 1.35-1.41 (m, 1H), 1.57 (s, 3H), 1.67-2.03 (m, 1H), 2.29-2.53 (m, 4H), 3.31 (d, J=3.06Hz, 1H), 3.45 (m, 1H), 3.67 (d, J=16.78Hz, 1H), 3.73 (d, J=17.10Hz, 1H), 4.45 (d, J=7.42Hz, 1H), 4.48 (d, J=15.41Hz, 1H), 4.73 (d, J=15.40Hz, 1H), 5.33-5.40 (m, 1H), 6.40 (dd, J ₁ =10.07Hz, J ₂ =1.79Hz, 1H), 6.45 (s, 1H), 6.50 (dd, J ₁ =3.47Hz, J ₂ =1.81Hz, 1H), 7.14 (d, J=3.28Hz, 1H), 7.18 (dd, J ₁ =10.07Hz, J ₂ =1.07Hz, 1H), 7.58 (d, J=0.97Hz, 1H). MASA (ES+): 737.4 |
| IB.77 | 1.06 (d, J=7.12Hz, 3H), 1.19 (s, 3H), 1.25-1.43 (m, 2H), 1.55 (s, 3H), 1.74-1.97 (m, 3H), 2.28-2.50 (m, 4H), 3.24 (q, J=10.07Hz, 2H), 3.42-3.45 (m, 1H), 3.68 (d, J=16.80Hz, 1H), 3.76 (d, J=16.82Hz, 1H), 4.45 (d, J=8.56Hz, 1H), 4.65 (d, J=15.34Hz, 1H), 4.83 (d, J=15.37Hz, 1H), 5.33-5.49 (m, 1H), 6.41 (dd, J ₁ =10.14Hz, J ₂ =1.72Hz, 1H), 6.41 (s, 1H), 6.51 (dd, J ₁ =3.42Hz, J ₂ =1.62Hz, 1H), 7.13 (d, J=3.42Hz, 1H), 7.16 (d, J=10.14Hz, 1H), 7.59 (s, 1H). MASA (ES+): 707.13 (M + Na) ⁺⁺ |
| IB.78 | 1.06 (d, J=7.14Hz, 3H), 1.23 (s, 3H), 1.35-1.41 (m, 1H), 1.57 (s, 3H), 1.77-1.99 (m, 3H), 2.28-2.53 (m, 4H), 3.11 (s, 1H), 3.39-3.45 (m, 1H), 3.45 (s, 3H), 3.67 (d, J=17.19Hz, 1H), 3.73 (d, J=16.96Hz, 1H), 4.03 (d, J=16.48Hz, 1H), 4.10 (d, J=16.55Hz, 1H), 4.43 (d, J=8.74Hz, 1H), 4.58 (d, J=15.30Hz, 1H), 4.58 (d, J=15.33Hz, 1H), 5.33-5.50 (m, 1H), 6.39 (dd, J ₁ =10.14Hz, J ₂ =1.71Hz, 1H), 6.45 (s, 1H), 6.50 (dd, J ₁ =3.41Hz, J ₂ =1.76Hz, 1H), 7.12 (d, J=3.55Hz, 1H), 7.17 (dd, J ₁ =10.19Hz, J ₂ =0.74Hz, 1H), 7.58 (d, J=0.71Hz, 1H). MASA (ES+): 647.24 |
| IB.79 | 1.06 (d, J=7.16Hz, 3H), 1.23 (s, 3H), 1.27 (t, J=7.04Hz, 3H), 1.35-1.41 (m, 1H), 1.56 (s, 3H), 1.73-1.99 (m, 3H), 2.28-2.53 (m, 4H), 3.17 (s, 1H), 3.39-3.42 (m, 1H), 3.57 (dd, J ₁ =7.03Hz, J ₂ =2.38Hz, 1H), 3.60 (dd, J ₁ =4.44Hz, J ₂ =2.44Hz, 1H), 3.65 (d, J=16.18Hz, 1H), 3.73 (d, J=16.94Hz, 1H), 4.07 (d, J=16.64Hz, 1H), 4.14 (d, J=16.63Hz, 1H), 4.43 (d, J=8.74Hz, 1H), 4.56 (d, J=15.41Hz, 1H), 4.85 (d, J=15.30Hz, 1H), 5.33-5.50 (m, 1H), 6.38 (dd, J ₁ =10.11Hz, J ₂ =1.72Hz, 1H), 6.45 (s, 1H), 6.50 (dd, J ₁ =3.49Hz, J ₂ =1.65Hz, 1H), 7.12 (d, J=3.37Hz, 1H), 7.17 (d, J=10.17Hz, 1H), 7.58 (d, J=1.57Hz, 1H). MASA (ES+): 661.22 |
| IB.80 | 1.05 (d, J=7.10Hz, 3H), 1.18 (s, 3H), 1.25-1.42 (m, 2H), 1.55 (s, 3H), 1.71-2.00 (m, 3H), 2.17-2.51 (m, 4H), 2.62-2.68 (m, 4H), 3.43-3.49 (m, 1H), 3.68 (d, J=16.72Hz, 1H), 3.75 (d, J=16.78Hz, 1H), 4.45 (d, J=8.41Hz, 1H), 4.58 (d, J=15.45Hz, 1H), 4.74 (d, J=15.45Hz, 1H), 5.33-5.49 (m, 1H), 6.42 (dd, J ₁ =10.09Hz, J ₂ =1.58Hz, 1H), 6.45 (s, 1H), 6.51 (dd, J ₁ =3.41Hz, J ₂ =1.69Hz, 1H), 7.14 (d, J=3.41Hz, 1H), 7.22 (d, J=10.04Hz, 1H), 7.59 (s, 1H). MASA (ES+): 697.16 (M+Na) ⁺ |
| IB.81 | 1.06 (d, 3H, J=7.17Hz), 1.18 (s, 3H), 1.35-1.41 (m, 1H), 1.56 (s, 3H), 1.77-1.99 (m, 3H), 2.09 (s, 3H), 2.28-2.51 (m, 4H), 2.91 (d, 1H, J=2.60Hz), 3.42-3.47 (m, 1H), 3.66 (d, 1H, J=16.74Hz), 3.76 (d, J=16.78Hz, 1H), 4.46 (d, J=8.63Hz, 1H), 4.56 (d, 1H, J=15.46Hz, J ₂ =1.78Hz, 1H), 4.70 (d, J ₁ =15.39Hz, J ₂ =1.65Hz, 1H), 5.32-5.50 (m, 1H), 6.39 (dd, J ₁ =10.07Hz, J ₂ =1.79Hz, 1H), 6.45 (s, 1H), 6.50 (dd, J ₁ =3.53Hz, J ₂ =1.68Hz, 1H), 7.14 (d, J=3.37Hz, 1H), 7.20 (dd, J ₁ =10.18Hz, J ₂ =1.23Hz, 1H), 7.59 (d, J=0.86Hz, 1H). MASA (ES+): 617.1 |
| IB.82 | 1.06 (d, J=7.18Hz, 3H), 1.13 (s, 3H), 1.16 (d, J=1.26Hz, 3H), 1.18 (d, J=1.30Hz, 3H), 1.34-1.43 (m, 1H), 1.55 (s, 3H), 1.77-1.95 (m, 3H), 2.28-2.53 (m, 4H), 2.53-2.80 (m, 1H), 2.81 (m, 1H), 3.43-3.48 (m, 1H), 3.54 (dd, J ₁ =14.12Hz, J ₂ =7.29Hz, 1H), 3.66 (dd, J ₁ =14.07Hz, J ₂ =5.45Hz, 1H), 4.43 (d, J=8.57Hz, 1H), 4.50 (dd, J ₁ =13.32Hz, J ₂ =4.52Hz, 1H), 4.62 (dd, J ₁ =13.25Hz, J ₂ =5.69Hz, 1H), 5.32-5.49 (m, 1H), 5.65-5.80 (m, 2H), 6.39 (dd, J ₁ =10.15Hz, J ₂ =1.79Hz, 1H), 6.45 (s, 1H), 6.50 (dd, J ₁ =3.46Hz, J ₂ =1.64Hz, 1H), 7.11 (d, J=3.43Hz, 1H), 7.16 (dd, J ₁ =10.03Hz, J ₂ =0.93Hz, 1H), 7.58 (d, J=0.86Hz, 1H). MASA (ES+): 647.1 |
| IB.83 | 1.06 (d, J=7.17Hz, 3H), 1.12 (s, 3H), 1.16 (d, J=6.98Hz, 6H), 1.34-1.40 (m, 1H), 1.55 (s, 3H), 1.77-2.06 (m, 3H), 2.28-2.59 (m, 5H), 3.42-3.47 (m, 1H), 3.66 (d, J=7.82Hz, 2H), 4.44 (d, J=9.08Hz, 1H), 4.75-4.79 (m, 2H), 5.34-5.47 (m, 1H), 5.58-5.72 (m, 2H), 6.39 (dd, J ₁ =10.16Hz, J ₂ =1.79Hz, 1H), 6.45 (s, 1H), 6.49 (dd, J ₁ =3.41Hz, J ₂ =1.82Hz, 1H), 7.12 (d, J=3.19Hz, 1H), 7.16 (dd, J ₁ =10.08Hz, J ₂ =1.06Hz, 1H), 7.58 (br-s, 1H). MASA (ES+): 647.1 |
| IB.84 | 0.98 (d, J=7.15Hz, 3H), 1.17 (s, 3H), 1.22 (s, 9H), 1.27-1.38 (m, 1H), 1.54 (s, 3H), 1.70-1.99 (m, 5H), 2.17-2.50 (m, 8H), 3.12-3.18 (m, 1H), 3.21 (d, J=3.24Hz, 1H), 3.35-3.38 (m, 1H), 3.65 (d, J=16.86Hz, 1H), 3.65 (d, J=16.86Hz, 1H), 3.72 (d, J=17.02Hz, 1H), 4.39 (d, J=8.61Hz, 1H), 4.51 (d, J=15.31Hz, 1H), 4.73 (d, J=15.33Hz, 1H), 5.31-5.48 (m, 1H), 6.37 (dd, J ₁ =10.11Hz, J ₂ =1.61Hz, 1H), 6.43 (s, 1H), 7.15 (d, J=10.16Hz, 1H). MASA (ES+): 647.1 |
| IB.85 | 0.80 (t, J=7.46Hz, 3H), 1.05 (d, J=7.15Hz, 3H), 1.17 (s, 6H), 1.23 (s, 3H), 1.35-1.41 (m, 1H), 1.56 (s, 3H), 1.73-2.01 (m, 3H), 2.29- |

| Com-
puesto
No. | 1H-NMR (δ ppm). MASA (EI / ES+, m/z) |
|-----------------------|--|
| | 2.56 (m, 4H), 3.36 (br-s, 1H), 3.43-3.49 (m, 1H), 4.40 (d, 1H), 4.48 (d, $J=15.37$ Hz, 1H), 4.76 (d, $J=15.31$ Hz, 1H), 5.34-5.50 (m, 1H), 6.40 (dd, $J_1=10.17$ Hz, $J_2=1.72$ Hz, 1H), 6.45 (s, 1H), 6.50 (dd, $J_1=3.44$ Hz, $J_2=1.67$ Hz, 1H), 7.13 (d, $J=3.37$ Hz, 1H), 7.17 (dd, $J_1=10.07$ Hz, $J_2=0.60$ Hz, 1H), 7.58 (s, 1H). MASA (ES+): 673.26 |
| IB.86 | 0.96 (s, 3H), 1.06 (d, $J=5.33$ Hz, 3H), 1.07 (s, 3H), 1.13 (s, 3H), 1.25 (s, 3H), 1.35-1.41 (m, 1H), 1.56 (s, 3H), 1.69-2.13 (m, 6H), 2.28-2.57 (m, 5H), 3.10 (s, 1H), 3.39-3.42 (m, 1H), 3.66 (d, $J=16.62$ Hz, 1H), 3.73 (d, $J=17.10$ Hz, 1H), 4.53 (d, $J=8.29$ Hz, 1H), 4.64 (d, $J=15.20$ Hz, 1H), 4.92 (d, $J=15.23$ Hz, 1H), 5.33-5.50 (m, 1H), 6.41 (dd, $J_1=10.07$ Hz, $J_2=1.78$ Hz, 1H), 6.44 (s, 1H), 6.49 (dd, $J_1=3.51$ Hz, $J_2=1.70$ Hz, 1H), 7.12 (d, $J=3.41$ Hz, 1H), 7.29 (dd, $J_1=10.04$ Hz, $J_2=0.99$ Hz, 1H), 7.58 (d, $J=0.95$ Hz, 1H). MASA (ES+): 777.18 (M+Na) ⁺ |
| IB.87 | 1.06 (d, $J=7.17$ Hz, 3H), 1.18 (s, 3H), 1.33 (s, 9H), 1.33-1.38 (m, 1H), 1.56 (s, 3H), 1.77-2.08 (m, 3H), 2.29-2.53 (m, 4H), 3.47 (m, 1H), 3.61 (d, $J=16.75$ Hz, 1H), 3.80 (d, $J=16.80$ Hz, 1H), 4.38 (d, $J=16.03$ Hz, 1H), 4.44 (d, $J=8.47$ Hz, 1H), 4.72 (d, $J=15.70$ Hz, 1H), 4.78 (s, 1H), 5.33-5.49 (m, 1H), 6.39 (dd, $J_1=10.09$ Hz, $J_2=1.72$ Hz, 1H), 6.45 (s, 1H), 6.50 (dd, $J_1=3.45$ Hz, $J_2=1.62$ Hz, 1H), 7.14 (m, 2H), 7.59 (d, $J=0.74$ Hz, 1H). MASA (ES+): 696.20 (M+Na) ⁺ |
| IB.88 | 1.06 (d, $J=7.17$ Hz, 3H), 1.18 (s, 3H), 1.35-1.41 (m, 2H), 1.55 (s, 3H), 1.77-1.96 (m, 3H), 2.17-2.47 (m, 4H), 3.42-3.46 (m, 1H), 3.66 (d, $J=16.77$ Hz, 1H), 3.76 (d, $J=16.80$ Hz, 1H), 4.15 (q, $J=7.15$ Hz, 2H), 4.45 (d, $J=8.67$ Hz, 1H), 4.59 (d, $J=15.47$ Hz, 1H), 4.73 (d, $J=15.36$ Hz, 1H), 5.32-5.49 (m, 1H), 6.40 (dd, $J_1=10.09$ Hz, $J_2=1.75$ Hz, 1H), 6.41 (s, 1H), 6.51 (dd, $J_1=3.46$ Hz, $J_2=1.81$ Hz, 1H), 7.13 (d, $J=3.36$ Hz, 1H), 7.20 (dd, $J_1=10.14$ Hz, $J_2=1.08$ Hz, 1H), 7.59 (s, 1H). MASA (ES+): 725.18 (M+Na) ⁺ |
| IB.89 | 0.78 (d, $J=6.98$ Hz, 3H), 0.88 (d, $J=7.03$ Hz, 3H), (d, $J=6.41$ Hz, 3H), 1.02-1.10 (m, 5H), 1.20 (s, 3H), 1.30-1.49 (m, 3H), 1.55 (s, 3H), 1.69-2.00 (m, 7H), 2.28-2.51 (m, 4H), 2.59 (s, 1H), 3.42-3.46 (m, 1H), 3.69 (d, $J=16.56$ Hz, 1H), 3.76 (d, $J=16.91$ Hz, 1H), 4.42 (d, $J=8.58$ Hz, 1H), 4.59 (td, $J_1=10.91$ Hz, $J_2=4.39$ Hz, 1H), 4.62 (d, $J=15.52$ Hz, 1H), 4.72 (d, $J=15.41$ Hz, 1H), 5.32-5.49 (m, 1H), 6.40 (dd, $J_1=10.18$ Hz, $J_2=1.81$ Hz, 1H), 6.45 (s, 1H), 6.50 (dd, $J_1=3.47$ Hz, $J_2=1.78$ Hz, 1H), 7.12-7.14 (m, 2H), 7.59 (s, 1H). MASA (ES+): 779.32 (M+Na) ⁺ |
| IB.90 | 1.06 (d, $J=7.14$ Hz, 3H), 1.17 (s, 3H), 1.34-1.40 (m, 1H), 1.55 (s, 3H), 1.76-1.97 (m, 3H), 2.06 (s, 3H), 2.28-2.54 (m, 4H), 3.41-3.41 (m, 1H), 3.67-3.75 (m, 2H), 4.00 (dd, $J_1=18.22$ Hz, $J_2=5.46$ Hz, 1H), 4.09 (dd, $J_1=18.22$ Hz, $J_2=5.84$ Hz, 1H), 4.41 (d, $J=5.81$ Hz, 1H), 4.71 (s, 2H), 5.32-5.49 (m, 1H), 6.11 (s, 1H), 6.39 (dd, $J_1=10.16$ Hz, $J_2=1.79$ Hz, 1H), 6.45 (s, 1H), 6.50 (dd, $J_1=3.45$ Hz, $J_2=1.77$ Hz, 1H), 7.12 (d, $J=3.51$ Hz, 1H), 7.19 (dd, $J_1=10.09$ Hz, $J_2=0.96$ Hz, 1H), 7.58 (d, $J=0.90$ Hz, 1H). MASA (ES+): 696.13 (M+Na) ⁺ |
| IB.91 | 0.96 (d, $J=6.72$ Hz, 3H), 1.05 (d, $J=7.15$ Hz, 3H), 1.19 (s, 3H), 1.35-1.41 (m, 1H), 1.55 (s, 3H), 1.78-2.02 (m, 4H), 2.30-2.63 (m, 5H), 3.41-3.45 (m, 1H), 3.70 (d, $J=16.81$ Hz, 1H), 3.76 (d, $J=16.76$ Hz, 1H), 3.93 (d, $J=6.80$ Hz, 2H), 4.44-4.46 (m, 1H), 4.66 (d, $J=15.53$ Hz, 1H), 4.71 (d, $J=15.50$ Hz, 1H), 5.33-5.49 (m, 1H), 6.40 (dd, $J_1=10.13$ Hz, $J_2=1.67$ Hz, 1H), 6.46 (s, 1H), 6.94 (d, $J=4.00$ Hz, 1H), 7.15 (d, $J=10.22$ Hz, 1H), 7.53 (d, $J=4.01$ Hz, 1H). MASA (ES+): 747.0 (M+Na) ⁺ |
| IB.92 | 1.05 (d, $J=7.14$ Hz, 3H), 1.18 (d, $J=6.98$ Hz, 3H), 1.19 (d, $J=7.13$ Hz, 3H), 1.22 (s, 3H), 1.35-1.41 (m, 1H), 1.56 (s, 3H), 1.78-2.00 (m, 3H), 2.28-2.63 (m, 5H), 3.23 (d, $J=3.19$ Hz, 1H), 3.40-3.45 (m, 1H), 3.67-3.75 (m, 2H), 3.45-3.47 (m, 1H), 3.49-3.77 (m, 2H), 5.33-5.50 (m, 1H), 6.41 (dd, $J_1=10.15$ Hz, $J_2=1.79$ Hz, 1H), 6.46 (s, 1H), 6.93 (d, $J=4.0$ Hz, 1H), 7.18 (dd, $J_1=10.14$ Hz, $J_2=1.08$ Hz, 1H), 7.53 (d, $J=4.08$ Hz, 1H). MASA (ES+): 717.12 (M+Na) ⁺ |
| IB.93 | 1.06 (d, $J=7.16$ Hz, 3H), 1.17 (s, 3H), 1.33 (t, $J=7.12$ Hz, 3H), 1.36-1.40 (m, 1H), 1.55 (s, 3H), 1.71-1.97 (m, 3H), 2.28-2.48 (m, 4H), 2.71 (s, 1H), 3.42-3.48 (m, 1H), 3.68 (d, $J=16.79$ Hz, 1H), 3.77 (d, $J=16.60$ Hz, 1H), 4.25-4.30 (m, 2H), 4.44 (m, 1H), 4.68 (d, $J=15.47$ Hz, 1H), 4.81 (d, $J=15.45$ Hz, 1H), 5.32-5.49 (m, 1H), 6.21 (d, $J=12.01$ Hz, 1H), 6.32 (d, $J=1.98$ Hz, 1H), 6.40 (dd, $J_1=10.10$ Hz, $J_2=1.75$ Hz, 1H), 6.45 (s, 1H), 6.50 (dd, $J_1=3.47$ Hz, $J_2=1.75$ Hz, 1H), 7.13 (d, $J=3.42$ Hz, 1H), 7.19 (dd, $J_1=10.25$ Hz, $J_2=0.81$ Hz, 1H), 7.59 (d, $J=0.88$ Hz, 1H). MASA (ES+): 723.22 (M+Na) ⁺ |
| IB.94 | 1.06 (d, $J=7.17$ Hz, 3H), 1.18 (s, 3H), 1.35-1.41 (m, 1H), 1.56 (s, 3H), 1.74-1.99 (m, 3H), 2.28-2.47 (m, 4H), 2.63-2.69 (m, 4H), 2.93 (s, 1H), 3.43-3.47 (m, 1H), 3.66 (d, $J=16.86$ Hz, 1H), 3.70 (s, 3H), 3.76 (d, $J=17.21$ Hz, 1H), 4.45 (d, $J=8.60$ Hz, 1H), 4.59 (d, $J=15.38$ Hz, 1H), 4.68 (d, $J=15.45$ Hz, 1H), 5.33-5.50 (m, 1H), 6.41 (dd, $J_1=10.15$ Hz, $J_2=1.76$ Hz, 1H), 6.46 (s, 1H), 6.51 (dd, $J_1=3.45$ Hz, $J_2=1.64$ Hz, 1H), 7.13 (d, $J=3.43$ Hz, 1H), 7.19 (d, $J=9.97$ Hz, 1H), 7.59 (d, $J=0.73$ Hz, 1H). MASA (ES+): 711.19 (M+Na) ⁺ |
| IB.95 | 1.06 (d, $J=7.07$ Hz, 3H), 1.18 (s, 3H), 1.23 (d, $J=6.20$ Hz, 3H), 1.246 (d, $J=6.25$ Hz, 3H), 1.35-1.41 (m, 1H), 1.56 (s, 3H), 1.74-2.00 (m, 3H), 2.28-2.51 (m, 4H), 2.58-2.67 (m, 4H), 3.00 (s, 1H), 3.43-3.47 (m, 1H), 3.65 (d, $J=16.97$ Hz, 1H), 3.76 (d, $J=17.57$ Hz, 1H), 4.46 (d, $J=8.05$ Hz, 1H), 4.59 (d, $J=15.43$ Hz, 1H), 4.72 (d, $J=15.40$ Hz, 1H), 4.96-5.06 (m, 1H), 5.33-5.49 (m, 1H), 6.41 (dd, $J_1=10.20$ Hz, $J_2=1.24$ Hz, 1H), 6.46 (s, 1H), 6.51 (dd, $J_1=3.13$ Hz, $J_2=1.24$ Hz, 1H), 7.13 (d, $J=3.33$ Hz, 1H), 7.19 (d, $J=10.11$ Hz, 1H), 7.59 (s, 1H). MASA (ES+): 739.31 (M+Na) ⁺ |
| IB.96 | 0.92 (d, $J=6.64$ Hz, 6H), 1.06 (d, $J=6.64$ Hz, 3H), 1.18 (s, 3H), 1.36-1.41 (m, 1H), 1.56 (s, 3H), 1.74-2.06 (m, 4H), 2.29-2.51 (m, 4H), 2.66-2.69 (m, 4H), 2.99 (s, 1H), 3.43-3.45 (m, 1H), 3.66 (d, $J=16.76$ Hz, 1H), 3.77 (d, $J=16.64$ Hz, 1H), 3.88 (d, $J=6.57$ Hz, 2H), 4.46 (d, $J=6.66$ Hz, 1H), 4.59 (d, $J=15.40$ Hz, 1H), 4.73 (d, $J=15.33$ Hz, 1H), 5.33-5.49 (m, 1H), 6.41 (d, $J_1=10.11$ Hz, 1H), 6.45 (s, 1H), 6.50 (dd, $J_1=2.62$ Hz, $J_2=1.21$ Hz, 1H), 7.13 (d, $J=3.43$ Hz, 1H), 7.19 (d, $J=10.11$ Hz, 1H), 7.59 (s, 1H). MASA (ES+): 753.35 (M+Na) ⁺ |
| IB.97 | 0.92 (t, $J=7.32$ Hz, 3H), 1.05 (d, $J=7.15$ Hz, 3H), 1.18 (s, 3H), 1.20-1.38 (m, 5H), 1.40-1.62 (m, 4H), 1.77-2.00 (m, 3H), 2.25-2.50 (m, 4H), 2.61-2.69 (m, 4H), 2.97 (s, 1H), 3.42-3.47 (m, 1H), 3.65 (d, $J=16.71$ Hz, 1H), 3.76 (d, $J=16.87$ Hz, 1H), 4.10 (t, $J=6.71$ Hz, 2H), 4.45 (d, $J=8.59$ Hz, 1H), 4.59 (d, $J=15.45$ Hz, 1H), 4.72 (d, $J=15.43$ Hz, 1H), 5.32-5.49 (m, 1H), 6.39 (dd, $J_1=10.16$ Hz, $J_2=1.78$ Hz, 1H), 6.46 (s, 1H), 6.50 (dd, $J_1=3.74$ Hz, $J_2=1.47$ Hz, 1H), 7.13 (d, $J=3.44$ Hz, 1H), 7.19 (dd, $J_1=10.10$ Hz, $J_2=0.91$ Hz, 1H), 7.59 (d, $J=1.08$ Hz, 1H). MASA (ES+): 753.18 (M+Na) ⁺ |
| IB.98 | 1.06 (d, $J=7.12$ Hz, 3H), 1.21 (s, 3H), 1.31 (s, 6H), 1.35-1.41 (m, 1H), 1.56 (s, 3H), 1.77-2.01 (m, 3H), 2.29-2.53 (m, 4H), 2.91 (d, $J=2.26$ Hz, 1H), 3.43-3.47 (m, 1H), 3.58-3.64 (m, 2H), 3.66 (d, $J=17.24$ Hz, 1H), 3.76 (d, $J=16.76$ Hz, 1H), 4.45-4.47 (m, 1H), 4.57 (d, $J=15.36$ Hz, 1H), 4.78 (d, $J=15.36$ Hz, 1H), 5.34-5.50 (m, 1H), 6.40 (dd, $J_1=10.15$ Hz, $J_2=1.46$ Hz, 1H), 6.45 (s, 1H), 6.50 (dd, $J_1=3.28$ Hz, $J_2=1.48$ Hz, 1H), 7.14 (d, $J=3.49$ Hz, 1H), 7.18 (dd, $J_1=10.12$ Hz, 1H), 7.59 (s, 1H). MASA (ES+): 715.02 (M+Na) ⁺ |
| IB.99 | 0.94 (d, $J=6.70$ Hz, 6H), 1.06 (d, $J=7.12$ Hz, 3H), 1.17 (s, 3H), 1.25-1.40 (m, 1H), 1.55 (s, 3H), 1.73-1.99 (m, 4H), 2.28-2.46 (m, 4H), 2.73 (s, 1H), 3.43-3.47 (m, 1H), 3.67 (d, $J=16.91$ Hz, 1H), 3.78 (d, $J=17.01$ Hz, 1H), 3.99 (d, $J=6.69$ Hz, 2H), 4.44 (d, $J=8.42$ Hz, 1H), 4.67 (d, $J=15.51$ Hz, 1H), 4.81 (d, $J=15.46$ Hz, 1H), 5.32-5.49 (m, 1H), 6.22 (d, $J=12.05$ Hz, 1H), 6.34 (d, $J=12.03$ Hz, 1H), 6.39 (dd, $J_1=10.13$ Hz, $J_2=1.65$ Hz, 1H), 6.45 (s, 1H), 6.50 (dd, $J_1=3.57$ Hz, $J_2=1.85$ Hz, 1H), 7.13 (d, $J=3.44$ Hz, 1H), 7.19 (d, $J=10.20$ Hz, 1H), 7.59 (d, $J=0.67$ Hz, 1H). MASA (ES+): 751.16 (M+Na) ⁺ |
| IB.100 | 1.06 (d, $J=7.15$ Hz, 3H), 1.16 (s, 3H), 1.25-1.41 (m, 1H), 1.56 (s, 3H), 1.77-1.96 (m, 3H), 2.28-2.49 (m, 4H), 2.71 (s, 1H), 3.41-3.45 (m, 1H), 3.67 (d, $J=16.72$ Hz, 1H), 3.77 (d, $J=16.87$ Hz, 1H), 3.82 (s, 3H), 4.46 (m, 1H), 4.74 (d, $J=15.44$ Hz, 1H), 4.80 (d, $J=15.44$ Hz, 1H), 5.32-5.49 (m, 1H), 6.42 (dd, $J_1=10.16$ Hz, $J_2=1.79$ Hz, 1H), 6.46 (s, 1H), 6.50 (dd, $J_1=3.45$ Hz, $J_2=1.76$ Hz, 1H), 6.86 (d, $J=15.85$ Hz, 1H), 6.90 (d, $J=15.82$ Hz, 1H), 7.13 (d, $J=3.51$ Hz, 1H), 7.20 (dd, $J_1=10.00$ Hz, $J_2=1.00$ Hz, 1H), 7.59 (d, $J=0.73$ Hz, 1H). MASA (ES+): 709.11 (M+Na) ⁺ |
| IB.101 | 0.96 (d, $J=6.59$ Hz, 6H), 1.05 (d, $J=7.11$ Hz, 3H), 1.20 (s, 3H), 1.35-1.41 (m, 1H), 1.56 (s, 3H), 1.77-2.01 (m, 3H), 2.052.12 (m, 1H), 2.21-2.52 (m, 6H), 3.07 (d, $J=2.84$ Hz, 1H), 3.43-3.47 (m, 1H), 3.65 (d, $J=16.86$ Hz, 1H), 3.77 (d, $J=16.79$ Hz, 1H), 4.45 (d, $J=8.63$ Hz, 1H), 4.52 (d, $J=15.42$ Hz, 1H), 4.73 (d, $J=15.34$ Hz, 1H), 5.33-5.48 (m, 1H), 6.40 (dd, $J_1=10.12$ Hz, $J_2=1.71$ Hz, 1H), 6.45 (s, 1H), 6.50 (dd, $J_1=3.43$ Hz, $J_2=1.61$ Hz, 1H), 7.13 (d, $J=3.43$ Hz, 1H), 7.19 (dd, $J_1=10.19$ Hz, 1H), 7.58 (d, $J=0.85$ Hz, 1H). MASA (ES+): 681.0 (M+Na) ⁺ |
| IB.102 | 0.90 (q, $J=7.40$ Hz, 3H), 1.05 (d, $J=7.14$ Hz, 3H), 1.23 (s, 3H), 1.35-1.41 (m, 1H), 1.50-1.65 (m, 4H), 1.57 (s, 3H), 1.77-2.01 (m, 3H), 2.21-2.55 (m, 5H), 3.31 (d, $J=2.47$ Hz, 1H), 3.44-3.47 (m, 1H), 3.64 (d, $J=16.73$ Hz, 1H), 3.76 (d, $J=16.70$ Hz, 1H), 4.43-4.46 (m, |

| Com-
puesto
No. | ¹ H-NMR (δ ppm). MASA (EI / ES+, m/z) |
|-----------------------|---|
| | 1H), 4.49 (d, $J=15.39$ Hz, 1H), 4.78 (d, $J=15.38$ Hz, 1H), 5.34-5.50 (m, 1H), 6.40 (dd, $J_1=10.08$ Hz, $J_2=1.62$ Hz, 1H), 6.45 (s, 1H), 6.50 (dd, $J_1=3.37$ Hz, $J_2=1.57$ Hz, 1H), 7.13 (d, $J=3.45$ Hz, 1H), 7.19 (dd, $J_1=10.16$ Hz, 1H), 7.59 (s, 1H). MASA (ES+): 695.0 (M+Na) ⁺ |
| IB.103 | 1.05 (d, $J=7.18$ Hz, 3H), 1.23 (s, 3H), 1.34-1.40 (m, 1H), 1.56 (s, 3H), 1.77-2.08 (m, 3H), 2.17-2.53 (m, 4H), 2.92 (s, 6H), 3.44-3.48 (m, 1H), 3.64 (d, $J=16.62$ Hz, 1H), 3.76 (d, $J=16.16$ Hz, 1H), 4.01 (d, $J=3.45$ Hz, 1H), 4.41-4.43 (m, 1H), 4.49 (d, $J=15.61$ Hz, 1H), 4.76 (d, $J=15.59$ Hz, 1H), 5.33-5.50 (m, 1H), 6.39 (dd, $J_1=10.11$ Hz, $J_2=1.75$ Hz, 1H), 6.45 (s, 1H), 6.50 (dd, $J_1=3.47$ Hz, $J_2=1.74$ Hz, 1H), 7.14 (d, $J=3.40$ Hz, 1H), 7.18 (dd, $J_1=10.16$ Hz, $J_2=0.91$ Hz, 1H), 7.59 (s, 1H). MASA (ES+): 668.0 (M+Na) ⁺ |
| IB.104 | 1.06 (d, $J=7.12$ Hz, 3H), 1.21 (s, 3H), 1.35-1.41 (m, 1H), 1.56 (s, 3H), 1.79 (s, 3H), 1.80 (s, 3H), 1.80-1.98 (m, 3H), 2.28-2.52 (m, 4H), 2.70 (d, $J=2.16$ Hz, 1H), 3.42-3.46 (m, 1H), 3.67-3.77 (m, 2H), 3.44-3.46 (m, 1H), 4.62-4.85 (m, 2H), 5.33-5.49 (m, 1H), 6.39 (dd, $J_1=10.15$ Hz, $J_2=1.70$ Hz, 1H), 6.45 (s, 1H), 6.50 (dd, $J_1=3.44$ Hz, $J_2=1.71$ Hz, 1H), 7.12 (dd, $J=3.42$ Hz, 1H), 7.16 (dd, $J_1=10.07$ Hz, $J_2=0.93$ Hz, 1H), 7.58 (s, 1H). MASA (ES+): 679.0 |
| IB.105 | 0.90 (d, $J=6.31$ Hz, 3H), 0.91 (d, $J=6.24$ Hz, 3H), 1.06 (d, $J=7.14$ Hz, 3H), 1.20 (s, 3H), 1.35-1.41 (m, 1H), 1.47-1.59 (m, 3H), 1.56 (s, 3H), 1.77-2.00 (m, 3H), 2.29-2.52 (m, 4H), 2.35 (t, $J=7.72$ Hz, 2H), 3.10 (d, $J=2.65$ Hz, 1H), 3.43-3.46 (m, 1H), 3.65 (d, $J=16.80$ Hz, 1H), 3.77 (d, $J=16.81$ Hz, 1H), 4.44-4.46 (m, 1H), 4.53 (d, $J=15.38$ Hz, 1H), 4.71 (d, $J=15.33$ Hz, 1H), 5.33-5.50 (m, 1H), 6.39 (dd, $J_1=19.16$ Hz, $J_2=1.74$ Hz, 1H), 6.45 (s, 1H), 6.50 (dd, $J_1=3.43$ Hz, $J_2=1.77$ Hz, 1H), 7.13 (d, $J=3.60$ Hz, 1H), 7.18 (dd, $J_1=10.22$ Hz, $J_2=0.72$ Hz, 1H), 7.59 (s, 1H). MASA (ES+): 073.0 |
| IB.106 | 1.06 (d, $J=7.18$ Hz, 3H), 1.17 (s, 3H), 1.35-1.41 (m, 1H), 1.55 (s, 3H), 1.74-1.97 (m, 3H), 2.28-2.48 (m, 4H), 2.65 (s, 1H), 2.69-2.77 (m, 4H), 3.43-3.47 (m, 1H), 3.67 (d, $J=16.80$ Hz, 1H), 3.76 (d, $J=16.76$ Hz, 1H), 4.45 (d, $J=8.68$ Hz, 1H), 4.61 (d, $J=15.48$ Hz, 1H), 4.74 (d, $J=15.38$ Hz, 1H), 5.32-5.49 (m, 1H), 5.71 (d, $J=50.60$ Hz, 2H), 6.41 (dd, $J_1=10.18$ Hz, $J_2=1.81$ Hz, 1H), 6.45 (s, 1H), 6.51 (dd, $J_1=3.49$ Hz, $J_2=1.64$ Hz, 1H), 7.13 (d, $J=3.29$ Hz, 1H), 7.18 (dd, $J_1=10.16$ Hz, $J_2=0.91$ Hz, 1H), 7.59 (d, $J=0.79$ Hz, 1H). MASA (ES+): 729.28 (M + Na) ⁺ |
| IB.107 | 1.06 (d, $J=7.17$ Hz, 3H), 1.17 (s, 3H), 1.25-1.41 (m, 1H), 1.54 (s, 3H), 1.77-1.98 (m, 3H), 2.28-2.49 (m, 5H), 3.42-3.47 (m, 1H), 3.69 (d, $J=16.78$ Hz, 1H), 3.78 (d, $J=16.84$ Hz, 1H), 4.44 (d, $J=8.74$ Hz, 1H), 4.66 (d, $J=17.09$ Hz, 1H), 4.84 (d, $J=17.31$ Hz, 1H), 5.32-5.49 (m, 1H), 5.78 (dd, $J_1=50.72$ Hz, $J_2=1.89$ Hz, 1H), 5.82 (dd, $J_1=50.31$ Hz, $J_2=1.91$ Hz, 1H), 6.34 (d, $J=12.00$ Hz, 1H), 6.38 (d, $J=12.14$ Hz, 1H), 6.39 (dd, $J_1=3.46$ Hz, $J_2=1.60$ Hz, 1H), 6.45 (s, 1H), 6.51 (dd, $J_1=3.46$ Hz, $J_2=1.60$ Hz, 1H), 7.13 (d, $J=3.42$ Hz, 1H), 7.17 (d, $J=10.16$ Hz, 1H), 7.59 (d, $J=0.84$ Hz, 1H). MASA (ES+): 727.26 (M+Na) ⁺ |
| IB.108 | 1.06 (d, $J=7.15$ Hz, 3H), 1.19 (s, 3H), 1.25-1.41 (m, 1H), 1.55 (s, 3H), 1.74-1.97 (m, 3H), 2.29-2.50 (m, 4H), 2.81 (s, 1H), 3.43 (m, 3H), 3.68 (d, $J=17.09$ Hz, 1H), 3.75 (d, $J=16.15$ Hz, 1H), 3.77 (s, 3H), 4.46 (d, $J=8.71$ Hz, 1H), 4.62 (d, $J=15.45$ Hz, 1H), 4.80 (d, $J=15.32$ Hz, 1H), 5.33-5.50 (m, 1H), 6.41 (dd, $J_1=10.09$ Hz, $J_2=1.69$ Hz, 1H), 6.45 (s, 1H), 6.51 (dd, $J_1=3.43$ Hz, $J_2=1.69$ Hz, 1H), 7.13 (d, $J=3.39$ Hz, 1H), 7.18 (d, $J=10.15$ Hz, 1H), 7.59 (d, $J=0.88$ Hz, 1H). MASA (ES+): 697.29 (M+Na) ⁺ |
| IB.109 | 1.06 (d, $J=7.15$ Hz, 3H), 1.21 (s, 3H), 1.37-1.41 (m, 1H), 1.44 (s, 3H), 1.45 (s, 3H), 1.56 (s, 3H), 1.77-1.97 (m, 3H), 2.29-2.52 (m, 4H), 3.05 (d, $J=2.12$ Hz, 1H), 3.42-3.47 (m, 3H), 2.71-3.75 (m, 5H), 4.46 (d, $J=8.69$ Hz, 1H), 4.62 (d, $J=15.42$ Hz, 1H), 4.74 (d, $J=15.43$ Hz, 1H), 5.33-5.50 (m, 1H), 6.41 (dd, $J_1=10.15$ Hz, $J_2=1.76$ Hz, 1H), 6.45 (s, 1H), 6.50 (dd, $J_1=3.48$ Hz, $J_2=1.64$ Hz, 1H), 7.13 (d, $J=3.41$ Hz, 1H), 7.18 (dd, $J_1=10.12$ Hz, $J_2=0.95$ Hz, 1H), 7.59 (d, $J=0.88$ Hz, 1H). MASA (ES+): 725.30 (M+Na) ⁺ |
| IB.110 | 1.06 (d, $J=7.15$ Hz, 3H), 1.18 (s, 1H), 1.35-1.42 (m, 1H), 1.15 (s, 3H), 1.47 (s, 3H), 1.55 (s, 3H), 1.59-1.98 (m, 3H), 2.17-2.51 (m, 4H), 3.88 (m, 1H), 2.97 (s, 1H), 3.39-3.45 (m, 1H), 3.72 (s, 2H), 4.43-4.45 (m, 1H), 4.64-4.81 (m, 2H), 5.33-5.49 (m, 1H), 6.39 (dd, $J_1=10.16$ Hz, $J_2=1.75$ Hz, 1H), 6.45 (s, 1H), 6.50 (dd, $J_1=3.45$ Hz, $J_2=1.76$ Hz, 1H), 7.13 (d, $J=3.44$ Hz, 1H), 7.17 (dd, $J_1=10.12$ Hz, $J_2=0.76$ Hz, 1H), 7.58 (d, $J=0.90$ Hz, 1H). MASA (ES+): 683.10 (M+Na) ⁺ |
| IB.111 | 1.06 (d, $J=7.13$ Hz, 3H), 1.23 (s, 3H), 1.36-1.41 (m, 1H), 1.56 (d, $J=21.29$ Hz, 3H), 1.62 (d, $J=21.37$ Hz, 3H), 1.77-1.99 (m, 3H), 2.28-2.53 (m, 4H), 2.95 (s, 1H), 3.39-3.43 (m, 1H), 3.67 (d, $J=16.95$ Hz, 1H), 3.74 (d, $J=16.49$ Hz, 1H), 4.44 (d, $J=8.03$ Hz, 1H), 4.60 (d, $J=15.23$ Hz, 1H), 4.86 (d, $J=15.34$ Hz, 1H), 5.33-5.50 (m, 1H), 6.39 (dd, $J_1=10.11$ Hz, $J_2=1.63$ Hz, 1H), 6.45 (s, 1H), 6.50 (dd, $J_1=3.35$ Hz, $J_2=1.50$ Hz, 1H), 7.12 (d, $J=3.42$ Hz, 1H), 7.19 (d, $J=10.13$ Hz, 1H), 7.58 (s, 1H). MASA (ES+): 685.10 (M+Na) ⁺ |
| IB.112 | 1.06 (d, $J=7.15$ Hz, 3H), 1.17 (s, 3H), 1.35-1.40 (m, 1H), 1.55 (s, 3H), 1.76-1.97 (m, 3H), 2.28-2.47 (m, 4H), 2.71 (s, 1H), 3.42-3.47 (m, 1H), 3.69 (d, $J=16.76$ Hz, 1H), 3.78 (d, $J=16.97$ Hz, 1H), 3.82 (s, 3H), 4.44 (d, $J=8.22$ Hz, 1H), 4.69 (d, $J=15.50$ Hz, 1H), 4.82 (d, $J=15.54$ Hz, 1H), 5.30-5.60 (m, 1H), 6.23 (d, $J=11.91$ Hz, 1H), 6.33 (d, $J=12.06$ Hz, 1H), 6.40 (dd, $J_1=10.14$ Hz, $J_2=1.58$ Hz, 1H), 6.45 (s, 1H), 6.50 (dd, $J_1=3.31$ Hz, $J_2=1.51$ Hz, 1H), 7.13 (d, $J=3.47$ Hz, 1H), 7.19 (d, $J=10.14$ Hz, 1H), 7.59 (s, 1H). MASA (ES+): 687.73 |
| IB.113 | 1.06 (d, $J=7.12$ Hz, 3H), 1.16 (s, 3H), 1.32 (t, 3H), 1.35-1.42 (m, 2H), 1.56 (s, 3H), 1.72-1.97 (m, 3H), 2.28-2.48 (m, 4H), 2.86 (s, 1H), 3.42-3.45 (m, 1H), 3.68 (d, $J=16.77$ Hz, 1H), 3.77 (d, $J=16.62$ Hz, 1H), 4.26 (q, $J=7.07$ Hz, 2H), 4.46 (d, $J=8.36$ Hz, 1H), 4.75 (d, $J=15.39$ Hz, 1H), 4.80 (d, $J=15.39$ Hz, 1H), 5.30-5.49 (m, 1H), 6.41 (dd, $J_1=10.14$ Hz, $J_2=1.76$ Hz, 1H), 6.46 (s, 1H), 6.50 (dd, $J_1=3.45$ Hz, $J_2=1.76$ Hz, 1H), 6.85 (d, $J=15.75$ Hz, 1H), 6.90 (d, $J=15.90$ Hz, 1H), 7.13 (d, $J=3.74$ Hz, 1H), 7.20 (dd, $J_1=10.19$ Hz, $J_2=0.84$ Hz, 1H), 7.59 (d, $J=0.87$ Hz, 1H). MASA (ES+): 701.0 |
| IB.114 | 0.96 (d, $J=6.72$ Hz, 6H), 1.06 (d, $J=7.13$ Hz, 3H), 1.17 (s, 3H), 1.25-1.41 (m, 1H), 1.56 (s, 3H), 1.74-2.00 (m, 4H), 2.28-2.49 (m, 4H), 2.86 (s, 1H), 3.42-3.45 (m, 1H), 3.68 (d, $J=16.76$ Hz, 1H), 3.78 (d, $J=16.83$ Hz, 1H), 4.00 (d, $J=6.70$ Hz, 2H), 4.46 (d, $J=8.56$ Hz, 1H), 4.75 (d, $J=15.47$ Hz, 1H), 4.80 (d, $J=15.38$ Hz, 1H), 5.30-5.49 (m, 1H), 6.41 (dd, $J_1=10.15$ Hz, $J_2=1.80$ Hz, 1H), 6.46 (s, 1H), 6.50 (dd, $J_1=3.50$ Hz, $J_2=1.73$ Hz, 1H), 6.85 (d, $J=15.79$ Hz, 1H), 6.92 (d, $J=15.93$ Hz, 1H), 7.13 (d, $J=3.32$ Hz, 1H), 7.20 (dd, $J_1=10.12$ Hz, $J_2=0.96$ Hz, 1H), 7.59 (d, $J=0.90$ Hz, 1H). MASA (ES+): 729.1 |
| IB.115 | 0.95 (t, $J=7.37$ Hz, 6H), 1.06 (d, $J=7.10$ Hz, 3H), 1.17 (s, 3H), 1.36-1.45 (m, 3H), 1.56 (s, 3H), 1.67-1.97 (m, 7H), 2.28-2.51 (m, 4H), 2.82 (s, 1H), 3.42-3.45 (m, 1H), 3.72 (d, $J=16.78$ Hz, 1H), 3.77 (d, $J=16.74$ Hz, 1H), 4.22 (t, $J=6.67$ Hz, 2H), 4.47 (d, $J=8.32$ Hz, 1H), 4.75 (d, $J=15.54$ Hz, 1H), 4.79 (d, $J=15.52$ Hz, 1H), 5.33-5.49 (m, 1H), 6.41 (dd, $J_1=10.13$ Hz, $J_2=1.63$ Hz, 1H), 6.46 (s, 1H), 6.50 (dd, $J_1=3.33$ Hz, $J_2=1.52$ Hz, 1H), 6.84 (d, $J=15.81$ Hz, 1H), 6.90 (d, $J=15.77$ Hz, 1H), 7.13 (d, $J=3.40$ Hz, 1H), 7.20 (d, $J=10.18$ Hz, 1H), 7.59 (s, 1H). MASA (ES+): 729.1 |
| IB.116 | 1.06 (d, $J=7.16$ Hz, 3H), 1.18 (d, $J=7.07$ Hz, 3H), 1.19 (d, $J=6.98$ Hz, 3H), 1.23 (s, 3H), 1.31-1.36 (m, 1H), 1.62 (s, 3H), 1.75-2.04 (m, 4H), 2.17-2.82 (m, 6H), 3.19 (s, 1H), 3.41-3.45 (m, 1H), 3.65-3.75 (m, 1H), 4.53 (d, $J=15.43$ Hz, 1H), 4.63 (s, 1H), 4.73 (d, $J=15.42$ Hz, 1H), 6.11 (s, 1H), 6.38 (dd, $J_1=10.04$ Hz, $J_2=1.72$ Hz, 1H), 6.49 (dd, $J_1=3.43$ Hz, $J_2=1.62$ Hz, 1H), 7.18 (d, $J=3.35$ Hz, 1H), 7.24 (d, $J=10.57$ Hz, 1H), 7.58 (d, $J=0.75$ Hz, 1H). MASA (ES+): 665.1 (M+Na) ⁺ |
| IB.117 | 0.91 (t, $J=7.48$ Hz, 3H), 1.05 (d, $J=7.13$ Hz, 3H), 1.15 (d, 3H, $J=7.02$ Hz), 1.22 (s, 3H), 1.38-2.00 (m, 6H), 1.56 (s, 3H), 2.28-2.46 (m, 5H), 3.19 (d, 1H, $J=3.09$ Hz), 3.45 (m, 3H), 3.68-3.73 (m, 2H), 4.44-4.46 (m, 1H), 4.51 (d, $J=15.29$ Hz, 1H), 4.75 (d, $J=15.38$ Hz, 1H), 5.33-5.52 (m, 1H), 6.40 (dd, $J_1=10.18$ Hz, $J_2=1.78$ Hz, 1H), 6.45 (s, 1H), 6.50 (dd, $J_1=3.46$ Hz, $J_2=1.61$ Hz, 1H), 7.13 (d, $J=3.32$ Hz, 1H), 7.18 (d, $J_1=10.03$ Hz, $J_2=0.94$ Hz, 1H), 7.58 (d, $J=0.89$ Hz, 1H). MASA (ES+): 659.1 |
| IB.118 | 1.05 (d, $J=7.15$ Hz, 3H), 1.20 (s, 3H), 1.35-1.40 (m, 1H), 1.59 (s, 3H), 1.77-2.00 (m, 3H), 2.28-2.52 (m, 4H), 3.12 (d, $J=2.71$ Hz, 1H), 3.41-3.45 (m, 1H), 3.68 (d, $J=16.77$ Hz, 1H), 3.75 (d, $J=16.87$ Hz, 1H), 4.48-4.50 (m, 1H), 4.75-4.96 (m, 2H), 5.33-5.50 (m, 1H), 6.41 (dd, $J_1=10.08$ Hz, $J_2=1.70$ Hz, 1H), 6.46 (s, 1H), 6.49 (dd, $J_1=3.44$ Hz, $J_2=1.76$ Hz, 1H), 6.55 (dd, $J_1=3.51$ Hz, $J_2=1.65$ Hz, 1H), 7.11 (d, $J=3.34$ Hz, 1H), 7.22-7.25 (m, 2H), 7.57 (d, $J=0.83$ Hz, 1H), 7.61 (d, $J=0.85$ Hz, 1H). MASA (ES+): 669.1 |
| IB.119 | 1.06 (d, $J=7.12$ Hz, 3H), 1.17 (s, 3H), 1.30 (d, $J=6.20$ Hz, 6H), 1.36-1.41 (m, 1H), 1.56 (s, 3H), 1.72-1.97 (m, 3H), 2.28-2.50 (m, 4H), 2.82 (s, 1H), 3.42-3.45 (m, 1H), 3.67 (d, $J=16.71$ Hz, 1H), 3.76 (d, $J=16.51$ Hz, 1H), 4.46 (d, $J=8.56$ Hz, 1H), 4.74 (d, $J=15.47$ Hz, 1H), 4.79 (d, $J=15.41$ Hz, 1H), 5.08-5.13 (m, 1H), 5.33-5.49 (m, 1H), 6.41 (dd, $J_1=10.16$ Hz, $J_2=1.58$ Hz, 1H), 6.46 (s, 1H), 6.50 (dd, $J_1=3.36$ Hz, $J_2=1.62$ Hz, 1H), 6.83 (d, $J=15.87$ Hz, 1H), 6.88 (d, $J=15.76$ Hz, 1H), 7.13 (d, $J=3.39$ Hz, 1H), 7.20 (d, $J=10.29$ Hz, 1H), 7.58 (s, 1H). MASA (ES+): 715.1 |
| IB.120 | 1.03 (d, 3H, $J=7.05$ Hz), 1.15 (s, 3H), 1.16 (s, 6H), 1.33-1.39 (m, 1H), 1.55 (s, 1H), 1.67-2.00 (m, 3H), 2.29-2.59 (m, 4H), 3.39-3.49 |

| Com-
puesto
No. | ¹ H-NMR (δ ppm). MASA (EI / ES+, <i>m/z</i>) |
|-----------------------|--|
| | (m, 1H), 3.51 (d, 1H, $J=4.8$ Hz), 3.54 (d, 1H, $J=11.65$ Hz), 3.71 (d, 1H, $J=16.53$ Hz), 3.77 (d, 1H, $J=16.53$ Hz), 4.73 (t, 1H, $J=5.86$ Hz), 4.33-4.35 (m, 1H), 4.64 (d, 1H, $J=15.64$ Hz), 4.68 (d, 1H, $J=15.66$ Hz), 5.07 (s, 1H), 5.37-5.53 (m, 1H), 6.31-6.33 (m, 1H), 6.33 (s, 1H), 6.54 (dd, 1H, $J_1=3.41$ Hz, $J_2=1.58$ Hz), 7.12 (d, 1H, $J=3.37$ Hz), 7.26 (d, 1H, $J=10.30$ Hz), 7.66 (s, 1H). MASA (ES+): 697.07 (M+Na) ⁺ |
| IB.121 | 1.05 (d, 3H, $J=7.11$ Hz), 1.18 (s, 3H), 1.35-1.40 (m, 1H), 1.56 (s, 1H), 1.73-2.00 (m, 3H), 2.28-2.55 (m, 4H), 3.01 (d, 1H, $J=2.36$ Hz), 3.42-3.46 (m, 1H), 3.66 (d, 1H, $J=16.75$ Hz), 3.77 (d, 1H, $J=16.77$ Hz), 4.46 (d, 1H, $J=8.20$ Hz), 4.67 (d, 1H, $J=15.43$ Hz), 4.78 (d, 1H, $J=15.43$ Hz), 5.33-5.49 (m, 1H), 5.92 (d, 1H, $J=10.35$ Hz), 6.12 (dd, 1H, $J_1=17.32$ Hz, $J_2=10.52$ Hz), 6.39-6.46 (m, 1H), 6.43 (d, 1H, $J=13.3$ Hz), 6.50 (dd, 1H, $J_1=3.27$ Hz, $J_2=1.52$ Hz), 7.12 (d, 1H, $J=3.39$ Hz), 7.19 (d, 1H, $J=10.12$ Hz), 7.58 (s, 1H). MASA (ES+): 629.05 |
| IB.122 | 0.86 (t, $J=6.57$ Hz, 6H), 1.06 (d, $J=7.13$ Hz, 3H), 1.16 (s, 3H), 1.27-1.41 (m, 1H), 1.55 (s, 3H), 1.61-1.98 (m, 8H), 2.29-2.51 (m, 4H), 3.38-3.42 (m, 1H), 3.64-3.79 (m, 3H), 4.36 (d, $J=6.47$ Hz, 1H), 4.68-4.82 (m, 3H), 5.35-5.51 (m, 1H), 6.35 (dd, $J_1=10.15$ Hz, $J_2=1.67$ Hz, 1H), 6.38 (s, 1H), 6.52 (dd, $J_1=3.40$ Hz, $J_2=1.68$ Hz, 1H), 7.12 (d, $J=3.46$ Hz, 1H), 7.27 (d, $J=9.97$ Hz, 1H), 7.62 (s, 1H). MASA (ES+): 689.1 |
| IB.123 | 0.30-0.34 (m, 2H), 0.60-0.64 (m, 2H), 1.06 (d, $J=7.15$ Hz, 3H), 1.19 (s, 3H), 1.36-1.41 (m, 1H), 1.55 (s, 3H), 1.64-1.99 (m, 4H), 2.29-2.51 (m, 4H), 2.61 (s, 1H), 3.42-3.47 (m, 1H), 3.69 (d, $J=16.73$ Hz, 1H), 3.77 (d, $J=16.72$ Hz, 1H), 3.99 (d, $J=7.39$ Hz, 2H), 4.44 (d, $J=8.47$ Hz, 1H), 4.65-4.74 (m, 2H), 5.33-5.49 (m, 1H), 6.41 (dd, $J_1=10.13$ Hz, $J_2=1.66$ Hz, 1H), 6.46 (s, 1H), 6.51 (dd, $J_1=3.43$ Hz, $J_2=1.68$ Hz, 1H), 7.13-7.17 (m, 2H), 7.59 (s, 1H). MASA (ES+): 673.0 |
| IB.124 | 1.05 (d, $J=7.07$ Hz, 3H), 1.15 (s, 3H), 1.29-1.41 (m, 1H), 1.54 (s, 3H), 1.72-2.00 (m, 3H), 2.28-2.50 (m, 4H), 2.76 (s, 3H), 3.39-3.43 (m, 1H), 3.73 (d, $J=16.53$ Hz, 1H), 3.79 (d, $J=16.54$ Hz, 1H), 4.16 (m, 2H), 4.36 (d, $J=6.03$ Hz, 1H), 4.93 (s, 1H), 5.35-5.51 (m, 1H), 6.35 (d, $J=10.19$ Hz, 1H), 6.37 (s, 1H), 6.52 (dd, $J_1=3.09$ Hz, $J_2=1.32$ Hz, 1H), 7.12 (d, $J=3.40$ Hz, 1H), 7.27 (d, $J=10.15$ Hz, 1H), 7.62 (s, 1H). MASA (ES+): 707.1 (M+Na) ⁺ |
| IB.125 | 1.06 (d, $J=7.13$ Hz, 3H), 1.20-1.42 (m, 8H), 1.55 (s, 3H), 1.71-2.00 (m, 7H), 2.28-2.49 (m, 4H), 2.66 (s, 1H), 3.43-3.47 (m, 1H), 3.69 (d, $J=17.44$ Hz, 1H), 3.76 (d, $J=16.97$ Hz, 1H), 4.44 (d, $J=8.32$ Hz, 1H), 4.63 (d, $J=15.47$ Hz, 1H), 4.70 (d, $J=15.45$ Hz, 1H), 5.05-5.09 (m, 1H), 5.33-5.49 (m, 1H), 6.40 (dd, $J_1=10.14$ Hz, $J_2=1.48$ Hz, 1H), 6.46 (s, 1H), 6.51 (dd, $J_1=3.32$ Hz, $J_2=1.53$ Hz, 1H), 7.13-7.16 (m, 2H), 7.59 (s, 1H). MASA (ES+): 687.1 |
| IB.126 | 1.06 (d, $J=7.07$ Hz, 3H), 1.20-1.99 (m, 15H), 2.20-2.49 (m, 5H), 2.60 (s, 1H), 3.44 (m, 1H), 3.69 (d, $J=16.73$ Hz, 1H), 3.77 (d, $J=16.67$ Hz, 1H), 4.04 (d, $J=7.15$ Hz, 2H), 4.44 (d, $J=7.91$ Hz, 1H), 4.64-4.73 (m, 2H), 5.33-5.49 (m, 1H), 6.40 (d, $J=10.02$ Hz, 1H), 6.46 (s, 1H), 6.50 (m, 1H), 7.13-7.17 (m, 2H), 7.59 (s, 1H). MASA (ES+): 701.1 |
| IB.127 | 1.06 (d, $J=7.16$ Hz, 3H), 1.17 (d, $J=2.39$ Hz, 3H), 1.18 (d, $J=2.37$ Hz, 3H), 1.21 (s, 3H), 1.35-1.41 (m, 1H), 1.56 (s, 3H), 1.77-2.00 (m, 3H), 2.29-2.62 (m, 5H), 3.21 (d, $J=2.62$ Hz, 1H), 3.42-3.49 (m, 1H), 3.67 (d, $J=16.86$ Hz, 1H), 3.75 (d, $J=16.81$ Hz, 1H), 4.45 (d, $J=8.59$ Hz, 1H), 4.52 (d, $J=15.45$ Hz, 1H), 4.74 (d, $J=15.33$ Hz, 1H), 5.33-5.50 (m, 1H), 6.40 (dd, $J_1=10.05$ Hz, $J_2=1.65$ Hz, 1H), 6.45 (s, 1H), 6.50 (dd, $J_1=3.50$ Hz, $J_2=1.69$ Hz, 1H), 7.13 (dd, $J_1=3.56$ Hz, $J_2=0.57$ Hz, 1H), 7.19 (dd, $J_1=0.75$ Hz, $J_2=0.22$ Hz, 1H), 7.58 (s, 1H). MASA (ES+): 673.1 |
| IB.128 | 1.06 (d, $J=7.12$ Hz, 3H), 1.18 (s, 3H), 1.35 (s, 3H), 1.38-1.41 (m, 1H), 1.43 (s, 3H), 1.55 (s, 3H), 1.80-1.97 (m, 3H), 2.40-2.64 (m, 5H), 3.39-3.50 (m, 1H), 3.71-3.83 (m, 3H), 4.07-4.33 (m, 4H), 4.44 (d, $J=8.59$ Hz, 1H), 4.69-4.72 (m, 2H), 5.31-5.51 (m, 1H), 6.40 (dd, $J_1=10.17$ Hz, $J_2=1.73$ Hz, 1H), 6.45 (s, 1H), 6.50 (dd, $J_1=3.47$ Hz, $J_2=1.64$ Hz, 1H), 7.13 (d, $J=3.43$ Hz, 1H), 7.16 (d, $J=10.04$ Hz, 1H), 7.59 (s, 1H). MASA (ES+): 733.0 |
| IB.129 | 1.05 (d, $J=7.13$ Hz, 3H), 1.12-1.14 (m, 6H), 1.24 (s, 3H), 1.35-1.39 (m, 1H), 1.56 (s, 3H), 1.80-2.11 (m, 3H), 2.30-2.42 (m, 4H), 3.19-3.35 (m, 4H), 3.43-3.52 (m, 1H), 3.60-3.82 (m, 2H), 4.12 (d, $J=3.12$ Hz, 1H), 4.42 (d, $J=8.25$ Hz, 1H), 4.48 (d, $J=15.61$ Hz, 1H), 4.76 (d, $J=15.96$ Hz, 1H), 5.32-5.52 (m, 1H), 6.39 (dd, $J_1=10.12$ Hz, $J_2=1.75$ Hz, 1H), 6.45 (s, 1H), 6.50 (dd, $J_1=3.47$ Hz, $J_2=1.67$ Hz, 1H), 7.14 (d, $J=3.39$ Hz, 1H), 7.16 (dd, $J_1=10.13$ Hz, $J_2=0.97$ Hz, 1H), 7.58 (d, $J=0.78$ Hz, 1H). MASA (ES+): 674.1 |
| IB.130 | 1.05 (d, $J=7.17$ Hz, 3H), 1.22 (s, 3H), 1.34-1.40 (m, 1H), 1.56 (s, 3H), 1.56-1.60 (m, 6H), 1.77-2.07 (m, 3H), 2.28-2.42 (m, 4H), 3.40-3.49 (m, 5H), 3.62-3.82 (m, 2H), 3.86 (d, $J=3.25$ Hz, 1H), 3.42 (d, $J=8.41$ Hz, 1H), 4.52 (d, $J=15.61$ Hz, 1H), 4.74 (d, $J=15.58$ Hz, 1H), 5.32-5.51 (m, 1H), 6.39 (dd, $J_1=10.11$ Hz, $J_2=1.68$ Hz, 1H), 6.45 (s, 1H), 6.50 (dd, $J_1=3.41$ Hz, $J_2=1.58$ Hz, 1H), 7.13 (d, $J=3.41$ Hz, 1H), 7.18 (d, $J=10.00$ Hz, 1H), 7.59 (d, $J=0.74$ Hz, 1H). MASA (ES+): 686.1 |
| IB.131 | 1.05 (d, $J=7.11$ Hz, 3H), 1.20 (s, 3H), 1.34-1.40 (m, 1H), 1.55 (s, 3H), 1.77-2.04 (m, 3H), 2.30 (s, 3H), 2.39-2.53 (m, 8H), 3.48 (m, 5H), 3.64 (d, $J=15.98$ Hz, 1H), 3.66 (s, 1H), 3.77 (d, $J=17.39$ Hz, 1H), 4.42 (d, $J=8.06$ Hz, 1H), 4.57 (d, $J=15.59$ Hz, 1H), 4.73 (d, $J=15.61$ Hz, 1H), 5.32-5.49 (m, 1H), 6.39 (dd, $J_1=10.15$ Hz, $J_2=1.22$ Hz, 1H), 6.45 (s, 1H), 6.50 (dd, $J_1=3.11$ Hz, $J_2=1.26$ Hz, 1H), 7.14 (d, $J=3.49$ Hz, 1H), 7.17 (d, $J=10.13$ Hz, 1H), 7.59 (s, 1H). MASA (ES+): 701.1 |
| IB.132 | 1.12 (s, 3H), 1.29-1.34 (m, 1H), 1.48 (d, $J=7.34$ Hz, 3H), 1.55 (s, 3H), 1.74-2.16 (m, 4H), 2.33-2.81 (m, 4H), 3.35 (t, d, $J_1=16.65$ Hz, $J_2=2.31$ Hz, 1H), 3.82 (t, d, $J_1=16.66$ Hz, $J_2=1.98$ Hz, 1H), 4.26 (m, 2H), 4.46 (d, $J=8.42$ Hz, 1H), 5.32-5.49 (m, 1H), 6.39 (dd, $J_1=10.13$ Hz, $J_2=1.75$ Hz, 1H), 6.44 (s, 1H), 6.51 (dd, $J_1=3.50$ Hz, $J_2=1.65$ Hz, 1H), 7.17-7.19 (m, 1H), 7.61 (s, 1H). MASA (ES+): 575.1 |
| IB.133 | 1.14 (s, 3H), 1.19 (d, $J=6.97$ Hz, 3H), 1.25-1.32 (m, 1H), 1.48 (d, $J=7.33$ Hz, 3H), 1.58 (s, 3H), 1.75-2.15 (m, 4H), 2.33-2.62 (m, 5H), 3.20 (dd, $J_1=17.13$ Hz, $J_2=0.74$ Hz, 1H), 3.84-3.90 (m, 2H), 4.40 (m, 2H), 4.72 (dd, $J_1=15.25$ Hz, $J_2=1.33$ Hz, 1H), 5.33-5.51 (m, 1H), 6.40 (dd, $J_1=10.13$ Hz, $J_2=1.69$ Hz, 1H), 6.44 (s, 1H), 6.51 (dd, $J_1=3.43$ Hz, $J_2=1.57$ Hz, 1H), 7.18-7.20 (m, 2H), 7.61 (d, $J=0.73$ Hz, 1H). MASA (ES+): 645.0 |
| IB.134 | 1.06 (d, $J=7.16$ Hz, 3H), 1.17 (d, $J=2.39$ Hz, 3H), 1.18 (d, $J=2.37$ Hz, 3H), 1.21 (s, 3H), 1.35-1.41 (m, 1H), 1.56 (s, 3H), 1.77-2.00 (m, 3H), 2.29-2.62 (m, 5H), 3.21 (d, $J=2.62$ Hz, 1H), 3.42-3.49 (m, 1H), 3.67 (d, $J=16.86$ Hz, 1H), 3.75 (d, $J=16.81$ Hz, 1H), 4.45 (d, $J=8.59$ Hz, 1H), 4.52 (d, $J=15.45$ Hz, 1H), 4.74 (d, $J=15.33$ Hz, 1H), 5.33-5.50 (m, 1H), 6.40 (dd, $J_1=10.05$ Hz, $J_2=1.65$ Hz, 1H), 6.45 (s, 1H), 6.50 (dd, $J_1=3.50$ Hz, $J_2=1.69$ Hz, 1H), 7.13 (dd, $J_1=3.56$ Hz, $J_2=0.57$ Hz, 1H), 7.19 (dd, $J_1=0.75$ Hz, $J_2=0.22$ Hz, 1H), 7.58 (s, 1H). MASA (ES+): 675.0 |
| IB.135 | 1.06 (d, $J=7.12$ Hz, 3H), 1.19 (s, 3H), 1.36-1.41 (m, 1H), 1.55 (s, 3H), 1.77-1.97 (m, 3H), 2.32 (s, 3H), 2.29-2.49 (m, 5H), 3.41-3.58 (m, 1H), 3.73-3.75 (m, 2H), 4.45 (d, $J=8.67$ Hz, 1H), 4.77 (d, $J=15.28$ Hz, 1H), 4.98 (d, $J=15.27$ Hz, 1H), 5.31-5.50 (m, 1H), 6.40 (dd, $J_1=10.15$ Hz, $J_2=1.65$ Hz, 1H), 6.45 (s, 1H), 6.50 (dd, $J_1=3.39$ Hz, $J_2=1.64$ Hz, 1H), 7.12 (d, $J=3.45$ Hz, 1H), 7.15 (dd, $J=9.90$ Hz, 1H), 7.59 (s, 1H). MASA (ES+): 699.0 |
| IB.136 | 1.05 (t, $J=7.09$ Hz, 6H), 1.05 (d, $J=6.67$ Hz, 3H), 1.34-1.40 (m, 1H), 1.55 (s, 3H), 1.76-2.02 (m, 3H), 2.28-2.62 (m, 4H), 2.56 (q, $J=7.22$ Hz, 2H), 3.26-3.39 (m, 3H), 3.44-3.47 (m, 1H), 3.63 (d, $J=16.46$ Hz, 1H), 3.85 (d, $J=16.45$ Hz, 1H), 4.42 (d, $J=8.63$ Hz, 1H), 5.30-5.81 (m, 1H), 6.39 (dd, $J_1=10.17$ Hz, $J_2=1.45$ Hz, 1H), 6.45 (s, 1H), 6.50 (dd, $J_1=3.30$ Hz, $J_2=1.61$ Hz, 1H), 7.14 (d, $J=3.21$ Hz, 1H), 7.15 (d, $J=9.85$ Hz, 1H), 7.59 (s, 1H). MASA (ES+): 630.1 |
| IB.137 | 1.06 (d, $J=7.13$ Hz, 3H), 1.20 (s, 3H), 1.32 (d, $J=6.25$ Hz, 3H), 1.32 (d, $J=6.13$ Hz, 3H), 1.35-1.39 (m, 1H), 1.55 (s, 3H), 1.71-1.99 (m, 3H), 2.28-2.49 (m, 4H), 2.53 (s, 1H), 3.42-3.46 (m, 1H), 3.69 (d, $J=16.80$ Hz, 1H), 3.76 (d, $J=16.64$ Hz, 1H), 4.44 (d, $J=8.28$ Hz, 1H), 4.64 (d, $J=15.56$ Hz, 1H), 4.70 (d, $J=15.45$ Hz, 1H), 4.82-4.90 (m, 1H), 5.33-5.49 (m, 1H), 6.41 (dd, $J_1=10.17$ Hz, $J_2=1.38$ Hz, 1H), 6.46 (s, 1H), 6.50 (dd, $J_1=3.26$ Hz, $J_2=1.44$ Hz, 1H), 7.13-7.16 (m, 2H), 7.59 (s, 1H). MASA (ES+): 661.1 |
| IB.138 | 1.06 (d, $J=7.13$ Hz, 3H), 1.20 (s, 3H), 1.35-1.41 (m, 1H), 1.55 (s, 3H), 1.72 (s, 1H), 1.76 (s, 3H), 1.74-1.98 (m, 3H), 2.28-2.53 (m, 5H), 3.42-3.46 (m, 1H), 3.69 (d, $J=16.85$ Hz, 1H), 3.76 (d, $J=16.94$ Hz, 1H), 4.43 (d, $J=8.85$ Hz, 1H), 4.64-4.68 (m, 3H), 5.33-5.49 (m, 1H), 6.39 (dd, $J_1=10.11$ Hz, $J_2=1.71$ Hz, 1H), 6.46 (s, 1H), 6.50 (dd, $J_1=3.45$ Hz, $J_2=1.71$ Hz, 1H), 7.13-7.16 (m, 2H), 7.59 (d, $J=0.83$ Hz, 1H). MASA (ES+): 687.1 |

| Com-puesto No. | ¹ H-NMR (δ ppm). MASA (EI / ES+, <i>m/z</i>) |
|----------------|--|
| IB.139 | 0.87 (t, <i>J</i> =6.15Hz, 3H), 1.06 (d, <i>J</i> =7.15Hz, 3H), 1.19 (s, 3H), 1.28-1.40 (m, 1H), 1.55 (s, 3H), 1.64-1.99 (m, 5H), 2.28-2.59 (m, 5H), 3.43-3.46 (m, 1H), 3.69 (d, <i>J</i> =16.84Hz, 1H), 3.76 (d, <i>J</i> =16.70Hz, 1H), 4.14 (t, <i>J</i> =6.75Hz, 1H), 4.44 (d, <i>J</i> =8.29Hz, 1H), 4.65 (d, <i>J</i> =15.47Hz, 1H), 4.65 (d, <i>J</i> =15.48Hz, 1H), 5.32-5.49 (m, 1H), 6.40 (dd, <i>J</i> ₁ =10.13Hz, <i>J</i> ₂ =1.66Hz, 1H), 6.46 (s, 1H), 6.50 (dd, <i>J</i> ₁ =3.42Hz, <i>J</i> ₂ =1.70Hz, 1H), 7.13-7.16 (m, 2H), 7.59 (s, 1H). MASA (ES+): 703.1 |
| IB.140 | 0.94-1.02 (m, 2H), 1.06 (d, <i>J</i> =7.14Hz, 3H), 1.19 (s, 3H), 1.23-1.41 (m, 3H), 1.55 (s, 3H), 1.66-1.99 (m, 9H), 2.29-2.49 (m, 4H), 2.58 (d, <i>J</i> =2.05Hz, 1H), 3.43-3.46 (m, 1H), 3.68 (d, <i>J</i> =16.65Hz, 1H), 3.77 (d, <i>J</i> =16.93Hz, 1H), 3.97 (d, <i>J</i> =6.45Hz, 2H), 4.44 (d, <i>J</i> =8.23Hz, 1H), 4.65 (d, <i>J</i> =15.56Hz, 1H), 4.71 (d, <i>J</i> =15.48Hz, 1H), 5.33-5.49 (m, 1H), 6.40 (dd, <i>J</i> ₁ =10.16Hz, <i>J</i> ₂ =1.50Hz, 1H), 6.46 (s, 1H), 6.51 (dd, <i>J</i> ₁ =3.33Hz, <i>J</i> ₂ =1.61Hz, 1H), 7.13-7.16 (m, 2H), 7.59 (s, 1H). MASA (ES+): 715.2 |
| IB.141 | 1.06 (d, <i>J</i> =7.13Hz, 3H), 1.20 (s, 3H), 1.25-1.52 (m, 7H), 1.55 (s, 3H), 1.73-1.99 (m, 7H), 2.29-2.53 (m, 4H), 2.63 (s, 1H), 3.43-3.47 (m, 1H), 3.68 (d, <i>J</i> =16.79Hz, 1H), 3.77 (d, <i>J</i> =16.71Hz, 1H), 4.44 (d, <i>J</i> =8.52Hz, 1H), 4.56-4.62 (m, 1H), 4.64 (d, <i>J</i> =15.48Hz, 1H), 4.70 (d, <i>J</i> =15.53Hz, 1H), 5.33-5.50 (m, 1H), 6.40 (dd, <i>J</i> ₁ =10.11Hz, <i>J</i> ₂ =1.71Hz, 1H), 6.46 (s, 1H), 6.50 (dd, <i>J</i> ₁ =3.45Hz, <i>J</i> ₂ =1.58Hz, 1H), 7.13-7.16 (m, 2H), 7.59 (d, <i>J</i> =0.9Hz, 1H). MASA (ES+): 701.1 |
| IB.142 | 0.88 (m, 9H), 0.94-1.25 (m, 14H), 1.38-1.41 (m, 1H), 1.49-1.72 (m, 6H), 1.78-1.99 (m, 3H), 2.28-2.55 (m, 5H), 3.43-3.46 (m, 1H), 3.68 (d, <i>J</i> =17.42Hz, 1H), 3.76 (d, <i>J</i> =16.72Hz, 1H), 4.17 (m, 2H), 4.44 (d, <i>J</i> =7.54Hz, 1H), 4.64 (d, <i>J</i> =15.74Hz, 1H), 4.76 (d, <i>J</i> =15.62Hz, 1H), 5.33-5.49 (m, 1H), 6.40 (d, <i>J</i> =10.10Hz, 1H), 6.46 (s, 1H), 6.50 (m, 1H), 7.13-7.16 (m, 2H), 7.59 (m, 1H). MASA (ES+): 745.1 |
| IB.143 | 0.96 (s, 9H), 1.06 (d, <i>J</i> =7.05Hz, 3H), 1.19 (s, 3H), 1.25-1.40 (m, 7H), 1.55 (s, 3H), 1.74-1.99 (m, 3H), 2.30-2.56 (m, 5H), 3.44 (m, 1H), 3.68 (d, <i>J</i> =16.89Hz, 1H), 3.79 (d, <i>J</i> =17.24Hz, 1H), 3.85 (s, 2H), 4.45 (d, <i>J</i> =7.73Hz, 1H), 4.67 (d, <i>J</i> =15.98Hz, 1H), 4.71 (d, <i>J</i> =15.98Hz, 1H), 5.33-5.49 (m, 1H), 6.40 (d, <i>J</i> =10.09Hz, 1H), 6.46 (s, 1H), 6.50-6.51 (m, 1H), 7.13-7.16 (m, 2H), 7.59 (s, 1H). MASA (ES+): 689.1 |
| IB.144 | 1.06 (d, <i>J</i> =7.16Hz, 3H), 1.19 (s, 3H), 1.25-1.39 (m, 1H), 1.55 (s, 3H), 1.76-2.10 (m, 9H), 2.28-2.67 (m, 6H), 3.43-3.47 (m, 1H), 3.67-3.79 (m, 2H), 4.12 (d, <i>J</i> =8.32Hz, 1H), 4.65-4.75 (m, 2H), 5.33-5.50 (m, 1H), 6.40 (dd, <i>J</i> ₁ =10.11Hz, <i>J</i> ₂ =1.64Hz, 1H), 6.46 (s, 1H), 6.51 (dd, <i>J</i> ₁ =3.45Hz, <i>J</i> ₂ =1.60Hz, 1H), 7.13-7.17 (m, 2H), 7.59 (m, 1H). MASA (ES+): 687.1 |
| IB.145 | 1.06 (d, <i>J</i> =7.07Hz, 3H), 1.19 (s, 3H), 1.36-1.41 (m, 1H), 1.54 (s, 3H), 1.70-1.94 (m, 3H), 2.17-2.49 (m, 5H), 3.44 (m, 1H), 3.68 (d, <i>J</i> =16.70Hz, 1H), 3.76 (d, <i>J</i> =16.66Hz, 1H), 4.42 (d, <i>J</i> =7.94Hz, 1H), 4.70 (s, 2H), 5.13 (s, 2H), 5.32-5.49 (m, 1H), 6.38-6.50 (m, 5H), 7.12-7.14 (m, 2H), 7.43 (s, 1H), 7.59 (s, 1H). MASA (ES+): 699.1 |
| IB.146 | 0.94 (t, <i>J</i> =7.29Hz, 3H), 1.06 (d, <i>J</i> =7.15Hz, 3H), 1.19 (s, 3H), 1.25-1.43 (m, 3H), 1.55 (s, 3H), 1.61-1.99 (m, 5H), 2.28-2.49 (m, 4H), 2.59 (s, 1H), 3.44-3.47 (m, 1H), 3.68-3.79 (m, 2H), 4.15 (t, <i>J</i> =6.69Hz, 1H), 4.44 (d, <i>J</i> =8.63Hz, 1H), 4.65 (d, <i>J</i> =15.51Hz, 1H), 4.71 (d, <i>J</i> =15.47Hz, 1H), 5.33-5.49 (m, 1H), 6.40 (dd, <i>J</i> ₁ =10.14Hz, <i>J</i> ₂ =1.59Hz, 1H), 6.46 (s, 1H), 6.50 (dd, <i>J</i> ₁ =3.39Hz, <i>J</i> ₂ =1.60Hz, 1H), 7.13-7.17 (m, 2H), 7.59 (s, 1H). MASA (ES+): 675.1 |
| IB.147 | 0.90 (t, <i>J</i> =6.86Hz, 3H), 1.06 (d, <i>J</i> =7.11Hz, 3H), 1.19 (s, 3H), 1.33-1.43 (m, 5H), 1.55 (s, 3H), 1.65-1.99 (m, 5H), 2.28-2.53 (m, 4H), 2.60 (s, 1H), 3.42-3.47 (m, 1H), 3.69 (d, <i>J</i> =16.86Hz, 1H), 3.76 (d, <i>J</i> =16.62Hz, 1H), 4.15 (t, <i>J</i> =6.78Hz, 2H), 4.44 (d, <i>J</i> =8.38Hz, 1H), 4.66 (d, <i>J</i> =15.54Hz, 1H), 4.71 (d, <i>J</i> =15.39Hz, 1H), 5.33-5.49 (m, 1H), 6.40 (dd, <i>J</i> ₁ =10.08Hz, <i>J</i> ₂ =1.55Hz, 1H), 6.46 (s, 1H), 6.50 (dd, <i>J</i> ₁ =3.36Hz, <i>J</i> ₂ =1.74Hz, 1H), 7.13-7.17 (m, 2H), 7.59 (s, 1H). MASA (ES+): 689.2 |
| IB.148 | 1.06 (d, <i>J</i> =7.17Hz, 3H), 1.20 (s, 3H), 1.24-1.25 (m, 6H), 1.35-1.41 (m, 1H), 1.56 (s, 3H), 1.77-1.98 (m, 3H), 2.28-2.52 (m, 4H), 2.82 (s, 1H), 3.42-3.46 (m, 1H), 3.67 (d, <i>J</i> =16.93Hz, 1H), 3.75 (d, <i>J</i> =16.87Hz, 1H), 4.33 (dd, <i>J</i> ₁ =13.35Hz, <i>J</i> ₂ =8.87Hz, 1H), 4.45 (dd, <i>J</i> ₁ =13.22Hz, <i>J</i> ₂ =8.77Hz, 1H), 4.42-4.48 (m, 1H), 4.58 (d, <i>J</i> =15.35Hz, 1H), 4.78 (d, <i>J</i> =15.36Hz, 1H), 5.31-5.49 (m, 1H), 6.40 (dd, <i>J</i> ₁ =10.12Hz, <i>J</i> ₂ =1.68Hz, 1H), 6.45 (s, 1H), 6.50 (dd, <i>J</i> ₁ =3.43Hz, <i>J</i> ₂ =1.64Hz, 1H), 7.12 (d, <i>J</i> =3.44Hz, 1H), 7.17 (dd, <i>J</i> =10.21Hz, 1H), 7.58 (d, <i>J</i> =0.71Hz, 1H). MASA (ES+): 677.1 |
| IB.149 | 1.06 (d, <i>J</i> =7.10Hz, 3H), 1.18 (s, 3H), 1.36 (s, 3H), 1.38-1.43 (m, 1H), 1.43 (s, 3H), 1.55 (s, 3H), 1.77-1.98 (m, 3H), 2.28-2.55 (m, 5H), 3.43-3.46 (m, 1H), 3.66-3.83 (m, 3H), 4.07-4.36 (m, 4H), 4.44 (d, <i>J</i> =7.86Hz, 1H), 4.67 (d, <i>J</i> =15.48Hz, 1H), 4.73 (d, <i>J</i> =15.48Hz, 1H), 5.32-5.49 (m, 1H), 6.39 (d, <i>J</i> =10.08Hz, 1H), 6.45 (s, 1H), 6.50 (d, <i>J</i> =1.59Hz, 1H), 7.13 (d, <i>J</i> =3.39Hz, 1H), 7.15 (d, <i>J</i> =10.24Hz, 1H), 7.59 (s, 1H). MASA (ES+): 733.1 |
| IB.150 | 1.06 (d, <i>J</i> =7.08Hz, 3H), 1.18 (s, 3H), 1.35 (s, 3H), 1.38-1.43 (m, 1H), 1.43 (s, 3H), 1.55 (s, 3H), 1.77-1.97 (m, 3H), 2.28-2.49 (m, 5H), 3.42-3.46 (m, 1H), 3.69 (d, <i>J</i> =16.77Hz, 1H), 3.77 (d, <i>J</i> =15.45Hz, 1H), 3.80 (d, <i>J</i> =5.40Hz, 1H), 3.82 (d, <i>J</i> =5.56Hz, 1H), 4.08 (d, <i>J</i> =6.42Hz, 1H), 4.10 (d, <i>J</i> =6.85Hz, 1H), 4.18 (d, <i>J</i> =5.35Hz, 2H), 4.32 (m, 1H), 4.45 (d, <i>J</i> =7.55Hz, 2H), 4.70 (m, 1H), 5.31-5.51 (m, 1H), 6.39 (d, <i>J</i> =10.13Hz, 1H), 6.45 (s, 1H), 6.50 (dd, <i>J</i> ₁ =3.47Hz, <i>J</i> ₂ =1.52Hz, 1H), 7.12 (d, <i>J</i> =3.44Hz, 1H), 7.14 (d, <i>J</i> =10.15Hz, 1H), 7.59 (s, 1H). MASA (ES+): 733.1 |
| IB.151 | 1.05 (d, <i>J</i> =7.11Hz, 3H), 1.20 (s, 3H), 1.35-1.40 (m, 1H), 1.54 (s, 3H), 1.77-2.03 (m, 3H), 2.28-2.52 (m, 4H), 3.39 (d, <i>J</i> =72.79Hz, 1H), 3.39-3.46 (m, 5H), 3.67-3.80 (m, 6H), 4.42 (d, <i>J</i> =8.10Hz, 1H), 4.59 (d, <i>J</i> =15.59Hz, 1H), 4.74 (d, <i>J</i> =15.59Hz, 1H), 5.32-5.49 (m, 1H), 6.39 (dd, <i>J</i> ₁ =10.16Hz, <i>J</i> ₂ =1.48Hz, 1H), 6.45 (s, 1H), 6.50 (dd, <i>J</i> ₁ =3.26Hz, <i>J</i> ₂ =1.59Hz, 1H), 7.14 (d, <i>J</i> =2.57Hz, 1H), 7.16 (d, <i>J</i> =10.25Hz, 1H), 7.59 (s, 1H). MASA (ES+): 688.1 |
| IB.152 | 1.05 (d, <i>J</i> =7.10Hz, 3H), 1.20 (s, 3H), 1.34 (s, 3H), 1.34-1.40 (m, 1H), 1.43 (s, 3H), 1.55 (s, 3H), 1.77-2.03 (m, 3H), 2.28-2.53 (m, 4H), 3.23-3.30 (m, 1H), 3.37-3.45 (m, 3H), 3.63-3.79 (m, 3H), 4.02-4.24 (m, 2H), 4.43 (d, <i>J</i> =7.99Hz, 1H), 4.53 (d, <i>J</i> =15.80Hz, 1H), 4.70 (d, <i>J</i> =15.61Hz, 1H), 5.15 (s, 1H), 5.33-5.49 (m, 1H), 6.39 (dd, <i>J</i> ₁ =10.16Hz, <i>J</i> ₂ =1.42Hz, 1H), 6.45 (s, 1H), 6.50 (d, <i>J</i> ₁ =3.31Hz, <i>J</i> ₂ =1.54Hz, 1H), 7.14 (d, <i>J</i> =3.39Hz, 1H), 7.18 (d, <i>J</i> =9.90Hz, 1H), 7.59 (s, 1H). MASA (ES+): 732.1 |
| IB.153 | 1.06 (d, <i>J</i> =7.12Hz, 3H), 1.09 (m, 2H), 1.20 (s, 3H), 1.36-1.41 (m, 1H), 1.51-1.99 (m, 15H), 2.29-2.49 (m, 4H), 2.64 (d, <i>J</i> =1.80Hz, 1H), 3.43-3.47 (m, 1H), 3.69 (d, <i>J</i> =16.81Hz, 1H), 3.76 (d, <i>J</i> =16.88Hz, 1H), 4.17 (t, <i>J</i> =6.97Hz, 2H), 4.44 (d, <i>J</i> =8.65Hz, 1H), 4.65 (d, <i>J</i> =15.48Hz, 1H), 4.71 (d, <i>J</i> =15.44Hz, 1H), 5.33-5.49 (m, 1H), 6.40 (dd, <i>J</i> ₁ =10.13Hz, <i>J</i> ₂ =1.56Hz, 1H), 6.46 (s, 1H), 6.51 (dd, <i>J</i> ₁ =3.37Hz, <i>J</i> ₂ =1.53Hz, 1H), 7.13-7.17 (m, 2H), 7.59 (d, <i>J</i> =0.70Hz, 1H). MASA (ES+): 715.1 |
| IB.154 | 0.93 (d, <i>J</i> =6.53Hz, 6H), 1.06 (d, <i>J</i> =7.11Hz, 3H), 1.20 (m, 2H), 1.35-1.41 (m, 1H), 1.55 (s, 3H), 1.57-1.66 (m, 2H), 1.66-1.99 (m, 4H), 2.29-2.49 (m, 4H), 2.57 (s, 1H), 3.43-3.46 (m, 1H), 3.69 (d, <i>J</i> =16.54Hz, 1H), 3.77 (d, <i>J</i> =16.68Hz, 1H), 4.19 (t, <i>J</i> =6.87Hz, 2H), 4.44 (d, <i>J</i> =8.08Hz, 1H), 4.65 (d, <i>J</i> =15.53Hz, 1H), 4.71 (d, <i>J</i> =15.51Hz, 1H), 5.33-5.49 (m, 1H), 6.40 (d, <i>J</i> =10.11Hz, 1H), 6.46 (s, 1H), 6.50 (dd, <i>J</i> ₁ =3.10Hz, <i>J</i> ₂ =1.63Hz, 1H), 7.13-7.17 (m, 2H), 7.59 (s, 1H). MASA (ES+): 689.1 |
| IB.155 | 1.06 (d, <i>J</i> =7.08Hz, 3H), 1.17 (s, 3H), 1.36-1.40 (m, 1H), 1.55 (s, 3H), 1.74-2.11 (m, 5H), 2.29-2.63 (m, 6H), 3.44 (m, 1H), 3.67 (d, <i>J</i> =16.71Hz, 1H), 3.76 (d, <i>J</i> =16.62Hz, 1H), 4.45 (d, <i>J</i> =8.31Hz, 1H), 4.51 (t, <i>J</i> =6.24Hz, 2H), 4.61 (d, <i>J</i> =15.49Hz, 1H), 4.73 (d, <i>J</i> =15.42Hz, 1H), 4.40 (d, <i>J</i> =11.18Hz, 1H), 5.33-5.50 (m, 1H), 6.40 (d, <i>J</i> =11.18Hz, 1H), 6.45 (s, 1H), 6.50 (m, 1H), 7.13 (d, <i>J</i> =3.30Hz, 1H), 7.17 (d, <i>J</i> =10.24Hz, 1H), 7.59 (s, 1H). MASA (ES+): 706.1 |
| IB.156 | 1.05 (d, <i>J</i> =7.06Hz, 3H), 1.19 (s, 3H), 1.31 (s, 3H), 1.33 (s, 3H), 1.37-1.41 (m, 1H), 1.44 (s, 3H), 1.50 (s, 3H), 1.55 (s, 3H), 1.77-2.00 (m, 3H), 2.28-2.50 (m, 4H), 2.68 (s, 1H), 3.45 (m, 1H), 3.66 (d, <i>J</i> =13.96Hz, 1H), 3.77 (d, <i>J</i> =16.58Hz, 1H), 4.05 (t, <i>J</i> =5.83Hz, 1H), 4.24-4.34 (m, 4H), 4.46 (d, <i>J</i> =7.50Hz, 1H), 4.62 (dd, <i>J</i> ₁ =7.80Hz, <i>J</i> ₂ =2.15Hz, 1H), 4.69 (s, 2H), 5.33-5.49 (m, 1H), 5.52 (d, <i>J</i> =4.93Hz, 1H), 6.38 (d, <i>J</i> =10.13Hz, 1H), 6.45 (s, 1H), 6.50 (dd, <i>J</i> ₁ =3.19Hz, <i>J</i> ₂ =1.47Hz, 1H), 7.13 (d, <i>J</i> =3.18Hz, 1H), 7.18 (d, <i>J</i> =10.10Hz, 1H), 7.59 (s, 1H). MASA (ES+): 861.1 |
| IB.157 | 1.06 (d, <i>J</i> =7.08Hz, 3H), 1.17 (s, 3H), 1.36-1.40 (m, 1H), 1.55 (s, 3H), 1.74-2.11 (m, 5H), 2.29-2.63 (m, 6H), 3.44 (m, 1H), 3.67 (d, <i>J</i> =16.71Hz, 1H), 3.76 (d, <i>J</i> =16.62Hz, 1H), 4.45 (d, <i>J</i> =8.31Hz, 1H), 4.51 (t, <i>J</i> =6.24Hz, 2H), 4.61 (d, <i>J</i> =15.49Hz, 1H), 4.73 (d, <i>J</i> =15.42Hz, 1H), 4.40 (d, <i>J</i> =11.18Hz, 1H), 5.33-5.50 (m, 1H), 6.40 (d, <i>J</i> =11.18Hz, 1H), 6.45 (s, 1H), 6.50 (m, 1H), 7.13 (d, <i>J</i> =3.30Hz, 1H), 7.17 (d, <i>J</i> =10.24Hz, 1H), 7.59 (s, 1H). MASA (ES+): 720.1 |
| IB.158 | 1.06 (d, <i>J</i> =7.14Hz, 3H), 1.16 (s, 3H), 1.35-1.41 (m, 1H), 1.55 (s, 3H), 1.77-1.97 (m, 3H), 2.12-2.51 (m, 5H), 3.36 (s, 3H), 3.43-3.47 |

| Com-
puesto
No. | ¹ H-NMR (δ ppm). MASA (EI / ES+, m/z) |
|-----------------------|---|
| | (m, 1H), 3.71 (d, J=16.48Hz, 1H), 3.83 (d, J=16.48Hz, 1H), 4.05 (d, J=15.61Hz, 1H), 4.10 (d, J=15.58Hz, 1H), 4.44 (d, J=8.60Hz, 1H), 5.34-5.47 (m, 1H), 6.41 (dd, J ₁ =10.16Hz, J ₂ =1.69Hz, 1H), 6.46 (s, 1H), 6.51 (dd, J ₁ =3.44Hz, J ₂ =1.75Hz, 1H), 7.13 (d, J=3.40Hz, 1H), 7.15 (d, J=10.20Hz, 1H), 7.59 (d, J=0.86Hz, 1H). MASA (ES+): 589.1 |
| IB.159 | 1.06 (d, J=7.16Hz, 3H), 1.16 (s, 3H), 1.22 (t, J=7.01Hz, 3H), 1.36-1.41 (m, 1H), 1.54 (s, 3H), 1.71-2.00 (m, 3H), 2.28-2.51 (m, 4H), 3.42-3.46 (m, 1H), 3.46-3.59 (m, 2H), 3.70 (d, J=16.51Hz, 1H), 3.83 (d, J=16.49Hz, 1H), 4.07-4.17 (m, 2H), 4.44 (d, J=8.80Hz, 1H), 5.32-5.49 (m, 1H), 6.41 (dd, J ₁ =10.12Hz, J ₂ =1.68Hz, 1H), 6.46 (s, 1H), 6.51 (dd, J ₁ =3.43Hz, J ₂ =1.63Hz, 1H), 7.13-7.16 (m, 2H), 7.59 (s, 1H). MASA (ES+): 603.1 |
| IB.160 | 0.91 (d, J=6.70Hz, 6H), 1.06 (d, J=7.07Hz, 3H), 1.15 (s, 3H), 1.25-1.41 (m, 1H), 1.54 (s, 3H), 1.67-1.97 (m, 5H), 2.28-2.53 (m, 4H), 3.22-3.28 (m, 2H), 3.42-3.46 (m, 1H), 3.71 (d, J=16.42Hz, 1H), 3.84 (d, J=16.45Hz, 1H), 4.06-4.16 (m, 2H), 4.44 (d, J=7.72Hz, 1H), 5.32-5.49 (m, 1H), 6.39-6.41 (m, 1H), 6.46 (s, 1H), 6.51 (dd, J ₁ =3.19Hz, J ₂ =1.44Hz, 1H), 7.12-7.15 (m, 2H), 7.59 (s, 1H). MASA (ES+): 631.1 |
| IC.1 | 1.03 (d, J=7.07Hz, 3H), 1.13 (d, J=7.68Hz, 3H), 1.15 (s, 3H), 1.20-1.89 (m, 8H), 2.15-2.44 (m, 6H), 2.85-2.88 (m, 1H), 4.30-4.33 (m, 1H), 4.82 (s, 2H), 5.30-5.47 (m, 1H), 6.34 (dd, J ₁ =10.13Hz, J ₂ =1.17Hz, 2H), 6.38 (s, 1H), 7.05 (dd, J=8.67Hz, 2H), 7.21 (d, J=10.17Hz, 1H), 7.43-7.47 (m, 2H). MASA (ES+): 615.5 (M+Na) ⁺ |
| IC.2 | 1.03 (d, J=7.01Hz, 3H), 1.11-1.14 (m, 6H), 1.32-1.89 (m, 8H), 2.20-2.44 (m, 6H), 2.80-2.84 (m, 1H), 4.40 (d, J=8.11Hz, 1H), 4.78 (d, J=11.17Hz, 1H), 4.4.81 (d, J=11.19Hz, 1H), 5.32-5.49 (m, 1H), 6.37 (d, J=10.14Hz, 1H), 7.10 (d, J=10.15Hz, 1H), 7.29 (d, J=8.19Hz, 1H), 7.44 (d, J=8.19Hz, 1H), 7.57 (s, 1H). MASA (ES+): 665.4 (M+Na) ⁺ |
| IC.3 | 1.03 (d, J=7.09Hz, 3H), 1.12 (t, J=7.50Hz, 3H), 1.16 (s, 3H), 1.16-1.95 (m, 8H), 2.20-2.40 (m, 6H), 2.78-2.84 (m, 1H), 4.41 (d, J=8.70Hz, 1H), 5.28-5.48 (m, 1H), 5.39 (d, J=50.31Hz, J ₂ =2.66Hz, 1H), 5.51 (d, J=49.30Hz, J ₂ =2.61Hz, 1H), 6.37 (dd, J ₁ =10.15Hz, J ₂ =1.74Hz, 1H), 6.43 (s, 1H), 7.10 (dd, J ₁ =10.12Hz, J ₂ =1.11Hz, 1H). MASA (ES+): 517.2 |
| IC.4 | 1.11 (d, J=7.09Hz, 3H), 1.21 (s, 3H), 1.24-1.97 (m, 8H), 2.28-2.50 (m, 4H), 2.86-2.90 (m, 1H), 4.45-4.47 (m, 1H), 5.30-5.52 (m, 1H), 5.41 (d, J=53.67Hz, J ₂ =2.34Hz, 1H), 5.56 (d, J=52.24Hz, J ₂ =2.33Hz, 1H), 6.39 (d, J=10.13Hz, J ₂ =1.77Hz, 1H), 6.45 (s, 1H), 6.51 (d, J=3.50Hz, J ₂ =1.72Hz, 1H), 7.12-7.15 (m, 2H), 7.60 (d, J=0.88Hz, 1H). MASA (ES+): 555.2 |
| IC.5 | 1.10 (d, J=7.17Hz, 3H), 1.21 (s, 1H), 1.25-1.38 (m, 2H), 1.55 (s, 1H), 1.85-1.99 (m, 3H), 2.16-2.59 (m, 4H), 2.88-2.93 (m, 1H), 4.83 (d, J=10.67Hz, 1H), 4.83 (d, J=10.69Hz, 1H), 5.03-5.09 (m, 1H), 6.31-6.35 (m, 2H), 6.54 (dd, J ₁ =3.47Hz, J ₂ =1.71Hz, 1H), 7.03-7.07 (m, 2H), 7.26 (d, J=10.03Hz, 1H), 7.45-7.49 (m, 2H), 7.65 (d, J=0.82Hz, 1H). MASA (ES+): 631.2 |
| IC.6 | 1.12 (d, J=7.07Hz, 3H), 1.21 (s, 3H), 1.26-1.48 (m, 1H), 1.53 (s, 3H), 1.59-1.96 (m, 4H), 2.28-2.52 (m, 4H), 2.82-2.86-2.89 (m, 1H), 4.44-4.46 (m, 1H), 4.93 (d, J=11.263Hz, 1H), 5.03 (d, J=11.24Hz, 1H), 5.32-5.48 (m, 1H), 6.39 (dd, J ₁ =10.11Hz, J ₂ =1.68Hz, 1H), 6.45 (s, 1H), 6.52 (dd, J ₁ =3.41Hz, J ₂ =1.70Hz, 1H), 7.11 (d, J=5.71Hz, 1H), 7.13 (s, 1H), 7.58-7.64 (m, 4H). MASA (ES+): 681.3 |
| IC.7 | 1.09 (d, J=6.89Hz, 3H), 1.20 (s, 3H), 1.25-1.50 (m, 1H), 1.55 (s, 3H), 1.60-2.03 (m, 4H), 2.16-2.52 (m, 4H), 2.92-3.13 (m, 1H), 4.32 (m, 1H), 4.83 (d, J=10.85Hz, 1H), 4.87 (d, J=10.88Hz, 1H), 5.13-5.51 (m, 1H), 6.30-6.33 (m, 2H), 6.55 (s, 1H), 7.13 (s, 1H), 7.26 (d, J=10.22Hz, 1H), 7.33-7.58 (m, 4H), 7.58-7.77 (m, 1H). MASA (ES+): 647.2 |
| IC.8 | 0.99 (d, J=7.09Hz, 3H), 1.09 (t, J=7.52Hz, 3H), 1.12 (s, 3H), 1.22-1.88 (m, 8H), 2.13-2.55 (m, 6H), 2.82-2.86 (m, 1H), 4.25-4.27 (m, 1H), 4.89 (s, 2H), 4.96-4.98 (m, 1H), 5.30-5.50 (m, 1H), 6.26-6.29 (m, 2H), 7.21 (dd, J ₁ =10.03Hz, J ₂ =1.05Hz, 1H), 7.56 (d, J=8.26Hz, 2H), 7.61 (d, J=8.30Hz, 2H). MASA (ES+): 643.0 |
| IC.9 | 1.05 (d, J=7.09Hz, 3H), 1.18 (s, 1H), 1.20-1.87 (m, 8H), 2.19-2.56 (m, 4H), 2.58-2.70 (m, 1H), 2.86-2.90 (m, 1H), 4.30-4.32 (m, 1H), 4.80 (d, J=10.70Hz, 1H), 4.85 (d, J=10.70Hz, 1H), 4.92-4.94 (m, 1H), 6.05 (m, 1H), 6.25 (dd, J ₁ =10.13Hz, J ₂ =1.77Hz, 1H), 6.51 (dd, J ₁ =3.45Hz, J ₂ =1.70Hz, 1H), 7.00-7.02 (m, 2H), 7.29 (d, J=10.11Hz, 1H), 7.43-7.46 (m, 2H), 7.63 (d, J=0.85Hz, 1H). MASA (ES+): 613.0 |
| IC.10 | 1.00 (d, J=7.06Hz, 3H), 1.07 (t, J=7.54Hz, 3H), 1.15 (s, 3H), 1.25-1.92 (m, 8H), 2.16-2.44 (m, 6H), 2.81-2.84 (m, 1H), 4.41 (d, J=8.51Hz, 1H), 5.10 (d, J=16.55Hz, 1H), 5.21 (d, J=16.64Hz, 1H), 5.30-5.46 (m, 1H), 6.38 (dd, J ₁ =10.13Hz, J ₂ =1.69Hz, 1H), 7.14 (d, J=10.13Hz, 1H), 7.46 (d, J=8.54Hz, 2H), 7.85 (d, J=8.58Hz, 2H). MASA (ES+): 637.1 |
| IC.11 | 1.10 (d, J=7.08Hz, 3H), 1.22 (s, 3H), 1.25-1.94 (m, 8H), 2.27-2.65 (m, 5H), 2.80-2.92 (m, 1H), 4.45-4.56 (m, 1H), 5.41 (dd, J ₁ =52.28Hz, J ₂ =2.31Hz, 1H), 5.56 (dd, J ₁ =53.72Hz, J ₂ =2.34Hz, 1H), 6.15 (s, 1H), 6.37 (dd, J ₁ =10.13Hz, J ₂ =1.82Hz, 1H), 6.50 (dd, J ₁ =3.48Hz, J ₂ =1.70Hz, 1H), 7.12 (d, J=3.40Hz, 1H), 7.21 (d, J=10.12Hz, 1H), 7.59 (d, J=0.86Hz, 1H). MASA (ES+): 537.1 |
| IC.12 | 0.89 (t, J=7.33Hz, 3H), 1.03 (d, J=7.07Hz, 3H), 1.16 (s, 3H), 1.25-1.91 (m, 12H), 2.17-2.44 (m, 6H), 2.80-2.84 (m, 1H), 4.1-4.33 (m, 1H), 5.30-5.58 (m, 3H), 6.38 (dd, J ₁ =10.13Hz, J ₂ =1.69Hz, 1H), 6.43 (s, 1H), 7.11 (dd, J ₁ =10.12Hz, J ₂ =0.98 Hz, 1H). MASA (ES+): 537.1 |
| IC.13 | 1.02 (d, J=7.08Hz, 3H), 1.12 (t, J=7.70Hz, 3H), 1.15 (s, 3H), 1.32-1.37 (m, 1H), 1.52 (s, 3H), 1.68-1.92 (m, 4H), 2.22-2.39 (m, 4H), 2.76-2.81 (m, 1H), 3.84 (s, 3H), 4.40-4.42 (m, 1H), 5.29-5.47 (m, 1H), 6.38 (dd, J ₁ =10.12Hz, J ₂ =1.79Hz, 1H), 6.43 (s, 1H), 7.12 (dd, J ₁ =10.14Hz, J ₂ =1.32Hz, 1H). MASA (ES+): 499.0 |
| IC.14 | 1.08 (d, J=7.08Hz, 3H), 1.20 (s, 3H), 1.29-1.40 (m, 1H), 1.55 (s, 3H), 1.59-2.00 (m, 4H), 2.27-2.51 (m, 4H), 2.88-2.92 (m, 1H), 3.85 (s, 3H), 4.33-4.35 (m, 1H), 4.95-4.97 (m, 1H), 5.34-5.51 (m, 3H), 6.33 (dd, J ₁ =10.10Hz, J ₂ =1.85Hz, 1H), 6.36 (s, 1H), 6.52 (dd, J ₁ =3.49Hz, J ₂ =1.72Hz, 1H), 7.11 (dd, J ₁ =3.48Hz, J ₂ =0.53Hz, 1H), 7.26 (dd, J ₁ =10.05Hz, J ₂ =0.96Hz, 1H), 7.62-7.63 (m, 1H). MASA (ES+): 537.0 |
| IC.15 | 1.04 (d, J=7.09Hz, 3H), 1.11-1.15 (m, 6H), 1.34-1.85 (m, 8H), 2.20-2.39 (m, 6H), 2.80-2.90 (m, 1H), 4.38 (d, J=8.66Hz, 1H), 4.86 (d, J=10.78Hz, 1H), 4.92 (d, J=10.77Hz, 1H), 5.27-5.49 (m, 1H), 6.36 (dd, J ₁ =10.14Hz, J ₂ =1.80Hz, 1H), 6.43 (s, 1H), 7.09 (dd, J ₁ =10.13Hz, J ₂ =1.20Hz, 1H), 7.35-7.45 (m, 5H). MASA (ES+): 575.0 |
| IC.16 | 1.08 (d, J=7.08Hz, 3H), 1.20 (s, 3H), 1.22-1.97 (m, 8H), 2.26-2.54 (m, 4H), 2.91-2.95 (m, 1H), 4.31 (d, J=6.59Hz, 1H), 4.85 (d, J=10.66Hz, 1H), 4.88 (d, J=10.66Hz, 1H), 5.24-5.56 (m, 1H), 6.28-6.31 (m, 2H), 6.56 (dd, J ₁ =3.39Hz, J ₂ =1.64Hz, 1H), 7.31 (d, J=3.45Hz, 1H), 7.18-7.46 (m, 6H), 7.72 (s, 1H). MASA (ES+): 613.0 |
| IC.17 | 6.99 (d, J=7.07Hz, 3H), 1.99 (t, J=7.51Hz, 3H), 1.14 (s, 3H), 1.19-1.96 (m, 8H), 2.09-2.47 (m, 12H), 2.77-2.81 (m, 1H), 4.40 (d, J=6.30Hz, 1H), 4.74 (d, J=18.25Hz, 1H), 4.82 (d, J=18.27Hz, 1H), 5.30-5.46 (m, 1H), 6.38 (dd, J ₁ =10.15Hz, J ₂ =1.79Hz, 1H), 6.43 (s, 1H), 6.84 (s, 2H), 7.12 (d, J=9.89Hz, 1H). MASA (ES+): 645.3 |
| IC.18 | 1.03 (d, J=7.09Hz, 3H), 1.14 (s, 3H), 1.13 (t, J=7.54Hz, 3H), 1.25-1.89 (m, 8H), 2.17-2.40 (m, 6H), 2.81-2.83 (m, 1H), 4.38-4.41 (m, 1H), 4.81 (d, J=10.91Hz, 1H), 4.88 (d, J=10.91Hz, 1H), 5.25-5.50 (m, 1H), 6.35 (d, J=10.13Hz, J ₂ =1.65Hz), 6.43 (s, 1H), 7.10 (d, J=10.10Hz, J ₂ =0.67Hz, 1H), 7.34 (d, J=8.40Hz, 2H), 7.40 (d, J=8.39Hz, 2H). MASA (ES+): 609.0 |
| IC.19 | 1.10 (d, J=7.04Hz, 3H), 1.21 (s, 3H), 1.30-1.96 (m, 8H), 2.29-2.54 (m, 4H), 2.90-2.93 (m, 1H), 4.33-4.36 (m, 1H), 4.82 (d, J=11.11Hz, 1H), 4.87 (d, J=11.10Hz, 1H), 4.95-4.98 (m, 1H), 5.36-5.51 (m, 1H), 6.33 (dd, J ₁ =10.13Hz, J ₂ =1.75Hz, 1H), 7.14 (d, J=3.45Hz, 1H), 7.25 (d, J=10.09Hz, 1H), 7.32 (dd, J ₁ =8.22Hz, J ₂ =1.89Hz, 1H), 7.44-7.46 (m, 1H), 7.64 (s, 1H). MASA (ES+): 680.9 |
| IC.20 | 1.09 (d, J=7.00Hz, 3H), 1.20 (s, 3H), 1.30-2.02 (m, 8H), 2.26-2.53 (m, 4H), 2.91-2.95 (m, 1H), 4.32 (d, J=6.99Hz, 1H), 4.97 (d, J=11.64Hz, 1H), 5.03 (d, J=11.59Hz, 1H), 5.37-5.54 (m, 1H), 6.31-6.32 (m, 2H), 6.56 (dd, J ₁ =3.28Hz, J ₂ =1.56Hz, 1H), 7.13 (d, J=3.41Hz, 1H), 7.18-7.31 (m, 2H), 7.42 (d, J=1.43Hz, 1H), 7.58 (d, J=8.25Hz, 1H), 7.70 (s, 1H). MASA (ES+): 681.5 |
| IC.21 | 1.11 (d, J=6.97Hz, 3H), 1.22 (s, 3H), 1.25-1.96 (m, 8H), 2.28-2.58 (m, 4H), 2.90-3.95 (m, 1H), 4.36 (m, 1H), 4.83-4.88 (m, 3H), 5.30-5.55 (m, 1H), 6.34 (d, J=10.10Hz, J ₂ =1.68Hz, 1H), 6.38 (m, 1H), 6.53 (d, J=3.39Hz, J ₂ =1.65Hz, 1H), 7.13 (d, J=3.43Hz, 1H), 7.124-7.42 (m, 4H), 7.50 (s, 1H), 7.63 (s, 1H). MASA (ES+): 647.7 |
| IC.22 | 1.09 (d, J=7.04Hz, 3H), 1.20 (s, 3H), 1.25-1.97 (m, 8H), 2.03-2.57 (m, 4H), 2.89-2.93 (m, 1H), 4.33 (d, J=6.78Hz, 1H), 4.95 (d, J=10.92Hz, 1H), 5.05 (d, J=10.89Hz, 1H), 5.12 (m, 1H), 5.30-5.30 (m, 1H), 6.30-6.33 (m, 2H), 6.54 (dd, J ₁ =3.39Hz, J ₂ =1.63Hz, 1H), 7.13 (d, J=3.43Hz, 1H), 7.124-7.42 (m, 4H), 7.50 (s, 1H), 7.63 (s, 1H). MASA (ES+): 647.7 |

| Com-puesto No. | ¹ H-NMR (δ ppm). MASA (EI / ES+, m/z) |
|----------------|--|
| | 1H), 6.74-6.78 (m, 2H), 7.11 (d, J=3.36Hz, 1H), 7.26 (d, J=10.07Hz, 1H), 7.66 (s, 1H). MASA (ES+): 667.0 |
| IC.23 | 1.10 (d, J=7.05Hz, 3H), 1.22 (s, 3H), 1.36-1.42 (m, 1H), 1.55 (s, 3H), 1.72-2.00 (m, 4H), 2.29-2.52 (m, 4H), 2.87-2.92 (m, 1H), 4.32-4.35 (m, 1H), 4.93 (d, J=11.04Hz, 1H), 4.97 (d, J=11.07Hz, 1H), 5.05-5.06 (m, 1H), 5.30-5.52 (m, 1H), 6.33 (dd, J ₁ =10.09Hz, J ₂ =1.88Hz, 1H), 6.35 (s, 1H), 6.54 (dd, J ₁ =3.49Hz, J ₂ =1.72Hz, 1H), 7.13 (d, J=3.39Hz, 1H), 7.26 (dd, J ₁ =10.07Hz, J ₂ =1.01Hz, 1H), 7.51-7.69 (m, 4H), 7.74 (s, 1H). MASA (ES+): 681.5 |

Ejemplo 30: Actividad Farmacológica:

(a) Análisis de Unión de Receptor Esteroide:

Los análisis de unión de receptor esteroide se llevaron a cabo por MDS Pharma Services en su laboratorio de farmacología de Taipei (Taiwán).

(i) Análisis de Unión de Receptor Glucocorticoide

Se evaluó la actividad de los compuestos de prueba sobre el receptor glucocorticoide usando análisis de radioligando. Células HeLa humanas transfectadas con receptores glucocorticoides se incubaron con [³H]dexametasona a 25 °C durante 2 horas en medio de incubación RPMI-1640, 10nM HEPES, pH 7.2, en la ausencia o presencia de compuestos de prueba con una concentración de 3nM y/o 10nM. Se retiró la [³H]dexametasona libre del medio mediante centrifugación y se determinó la concentración del ligando unido a receptor en el sobrenadante mediante contador de centelleo líquido.

La Dexametasona como compuesto de referencia se probó concurrentemente como parte integral de cada análisis para garantizar la validez de los resultados obtenidos. La inhibición % se evaluó usando una sola concentración del compuesto de prueba y el ligando radiomarcado correspondiente. Los resultados se presentan como la inhibición porcentual de la unión específica. Los valores son el promedio de determinaciones duplicadas de cada concentración.

Tabla 7: Tamizaje de Unión de Receptor Glucocoticoide (*in vitro*)

| Compuesto No. | Inhibición % de la Unión
de Receptor
Glucocorticoide |
|------------------------------|--|
| IA.143 | 58 ^b |
| IA.161 | 55 ^b |
| IA.157 | 56 ^b |
| IA.159 | 36 ^b |
| IA.168 | 40 ^a |
| IB.2 | 55 ^a |
| IB.4 | 88 ^b |
| IB.6 | 92 ^b |
| IB.7 | 82 ^b |
| IB.8 | 93 ^b |
| IB.10 | 82 ^b |
| IB.13 | 79 ^b |
| IB.14 | 85 ^b |
| IB.15 | 83 ^b |
| IB.50 | 74 ^b |
| IB.51 | 67 ^b |
| IB.54 | 82 ^b |
| IB.66 | 72 ^b |
| IB.67 | 77 ^b |
| IB.70 | 43 ^a |
| IB.73 | 45 ^a |
| IB.88 | 46 ^a |
| IB.100 | 45 ^a |
| IB.101 | 45 ^a |
| IB.103 | 78 ^b |
| IB.104 | 72 ^b |
| IB.105 | 42 ^a |
| IC.3 | 72 ^c |
| IC.4 | 73 ^b |
| IC.5 | 75 ^c |
| IC.7 | 41 ^b |
| Propionato de
Fluticasona | 88 ^b |
| Budesonida | 85 ^b |

^a % Inhibición con 3nM: ^b %Inhibición con 10nM: ^c % Inhibición con 100nM.

(b) Edema en la oreja del ratón inducido por aceite de croto

Ratones (machos, CD-1) se asignaron en diferentes grupos. Compuestos de prueba se disolvieron en solución de piridina-agua-acetona (4:2:14). De

aplicaron 10µl de compuesto o solución vehículo a la oreja izquierda de cada ratón. A la oreja derecha de cada ratón se aplicaron simultáneamente 10µl de solución piridina-agua- (4:2:14). Luego de 2 horas de la aplicación de compuesto o vehículo, se aplicaron 10µl de solución de aceite de croto a la oreja izquierda de todos los animales. Después de 6 horas de tratamiento con aceite de croto los animales se sacrificaron; se extirparon las orejas y se pesaron por separado.

Tabla 8: Tamizaje del Edema en la Oreja del Ratón inducido por Aceite de Croto

| Compuesto No. | Inhibición % Media |
|---------------------------|--------------------|
| IA.3 | 45.31 ^a |
| IA.56 | 34.59 ^a |
| IA.184 | 49.06 ^a |
| IA.185 | 49.06 ^a |
| IB.20 | 61.49 ^a |
| IB.33 | 76.16 ^a |
| IB.34 | 64.39 ^a |
| IB.35 | 60.18 ^a |
| IB.37 | 57.12 ^a |
| IB.44 | 75.19 ^a |
| IB.46 | 75.97 ^a |
| IB.49 | 71.82 ^a |
| IB.52 | 78.12 ^a |
| IB.53 | 71.19 ^a |
| IB.55 | 74.78 ^a |
| IB.57 | 74.43 ^a |
| IB.64 | 72.75 ^a |
| IB.73 | 76.24 ^a |
| IB.77 | 71.71 ^a |
| IB.81 | 77.75 ^a |
| IB.98 | 73.71 ^b |
| IB.102 | 73.63 ^b |
| IB.112 | 66.94 ^b |
| IB.138 | 72.48 ^b |
| IB.150 | 77.76 ^b |
| IB.159 | 66.02 ^b |
| IC.13 | 41.79 ^a |
| IC.14 | 61.46 ^a |
| Propionato de Fluticasona | 81.09 ^a |
| Dexametasona | 50.05 ^a |

^a Inhibición con 1.6µg: ^b Inhibición con 0.5µg

(c) Granuloma inducido por Torunda de Algodón

Ratas SD se utilizaron para evaluar la actividad anti-inflamatoria del compuesto de prueba empleando el método de granuloma inducido por torunda de algodón. Se prepararon torundas de algodón esterilizadas que pesaban 20mg. Se disolvieron los compuestos de prueba en acetona con el fin de obtener la cantidad requerida para cada torunda de algodón en 500µl. Diferentes torundas se impregnaron con 500µl de acetona para contener la cantidad requerida de compuesto de prueba y se pusieron a secar. Torundas de control de vehículo se impregnaron con 500µl de acetona. Las ratas se distribuyeron en diferentes grupos. Dos torundas de algodón se implantaron quirúrgicamente en la región escapular de cada rata. El día sexto de tal implante, se extrajeron las torundas junto con el granuloma. También se separó la glándula timo de cada animal y se pesó. Las torundas con granuloma se secaron durante 20 horas a 60°C y se pesaron. Se calcularon los pesos medios del granuloma seco y el timo, el aumento de peso corporal/100g de pesos corporales.

Tabla 9: Prueba de Granuloma inducido por Torunda de Algodón

| Compuesto No. | Dosis (mcg) | Inhibición % Media de Granuloma | Peso del Timo * (% Disminución) |
|---------------|-------------|---------------------------------|---------------------------------|
| IA.3 | 1000 | 74.76 | -11.72 |
| IA.6 | 1000 | 61.25 | -6.95 |
| IA.11 | 1000 | 61.36 | -4.72 |
| IA.13 | 1000 | 62.52 | 6.46 |
| IA.14 | 1000 | 70.74 | -13.26 |
| IA.20 | 1000 | 67.57 | 0.73 |
| IA.27 | 10 | 31.28 | 8.71 |
| | 1000 | 69.84 | 11.74 |
| IA.28 | 1000 | 73.73 | 13.5 |
| IA.35 | 1000 | 67.16 | -11.43 |
| IA.36 | 1000 | 70.74 | -13.26 |
| IA.38 | 10 | 67.17 | -1.28 |
| IA.42 | 1000 | 65.63 | -1.33 |
| IA.43 | 10 | 27.72 | -0.55 |
| | 1000 | 72.03 | 1.47 |
| IA.44 | 1000 | 71.79 | 4.58 |
| IA.45 | 1000 | 80.06 | -4.46 |
| IA.58 | 10 | 59.00 | 6.00 |

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| Compuesto No. | Dosis (mcg) | Inhibición % Media de Granuloma | Peso del Timo * (% Disminución) |
|---------------------------|-------------|---------------------------------|---------------------------------|
| IA.59 | 1000 | 76.86 | -2.51 |
| IA.122 | 3 | 37.29 | 2.25 |
| IA.136 | 10 | 37.74 | 4.44 |
| | 1000 | 67.79 | 2.14 |
| IA.137 | 1000 | 65.58 | 1.59 |
| IA.138 | 1000 | 66.16 | 15.45 |
| IA.140 | 1000 | 62.54 | -36.16 |
| IA.141 | 1000 | 63.1 | -18.26 |
| IA.142 | 10 | 45.36 | -8.43 |
| IA.197 | 1000 | 79.04 | -8.89 |
| IB.5 | 10 | 39.79 | -0.39 |
| IB.7 | 1000 | 78.82 | 14.89 |
| IB.16 | 3 | 68.92 | -11.06 |
| | 1000 | 77.36 | -11.65 |
| IB.163 | 3 | 45.8 | -5.44 |
| | 10 | 76.13 | 13.77 |
| IC.6 | 1000 | 84.96 | 10.96 |
| IC.8 | 3 | 45.15 | 3.38 |
| IC.9 | 3 | 34.3 | 2.51 |
| Propionato de Fluticasona | 1000 | 75.03 | 82.36 |
| Dexametasona | 1000 | 44.73 | 68.66 |

** En todos los compuestos (distintos de los compuestos de referencia) el peso del timo y el aumento en peso corporal fueron estadísticamente no significativos comparados con el control vehículo*

(d) Edema Pulmonar Inducido por Sephadex en la Rata SD

Se preparó Sephadex G-200 en solución salina estéril (10mg/ml) y se dejó esponjar durante un mínimo de 3 días a temperatura ambiente. Se prepararon compuestos de prueba como suspensiones moliendo y sonicando el sólido en solución salina enfriada. Todos los compuestos se administraron intratraquealmente a 24 horas y 2 horas antes de la administración intratraqueal de Sephadex (5 mg/kg) bajo anestesia ligera con éter. A los animales de control vehículo se administró vehículo en lugar de Sepahdex. 24 horas después de la instilación de Sephadex, se extirparon el pulmón y el timo de animales individuales y se pesaron. El peso húmedo del pulmón y el timo se corrigió por 100g del peso corporal inicial. Se calcularon el aumento porcentual en el peso del pulmón causado por

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Sephadex y sus inhibiciones por los compuestos. Se calcularon igualmente las inhibiciones porcentuales del timo comparadas con el grupo de control con vehículo.

Tabla 10: Edema Pulmonar Inducido por Sephadex en la Rata SD

| Compuesto No. | Dosis (meg/kg) | Inhibición % Media* | |
|---------------|----------------|---------------------|-------|
| | | Edema Pulmonar | Timo |
| IA.168 | 3000 | 95.3 | 9.2 |
| IB. 15 | 1000 | 70.3 | 4.5 |
| IB.15 | 3000 | 71.1 | 6.4 |
| IB.51 | 3000 | 120.5 | 29.8 |
| IB.54 | 3000 | 110.4 | 29.7 |
| IB.64 | 1000 | 86.4 | 2.0 |
| IB.64 | 3000 | 104.6 | 20.0 |
| IB.67 | 3000 | 121.8 | 33.4 |
| IB.79 | 3000 | 99.3 | 15.2 |
| IB.94 | 3000 | 99.7 | 8.1 |
| IB.100 | 3000 | 120.8 | 36.0 |
| IB.101 | 3000 | 114.8 | 8.9 |
| IB.150 | 3000 | 106.2 | 18.0 |
| Budesonida | 3000 | 119.38 | 67.08 |

** En todos los compuestos (distintos de los compuestos de referencia) el aumento de peso corporal fue estadísticamente no significativo comparado con el control con vehículo*

Tabla 10a: Índice Terapéutico para Compuestos en el Modelo de Edema Pulmonar Inducido por Sephadex en Rata SD

| Compuesto No. | ED50 Edema Pulmonar (mg/kg, i.t.) | ED ₅₀ Timo (mg/kg, i.t.) | Índice Terapéutico ED ₅₀ Involución del Timo / ED ₅₀ Edema Pulmonar |
|---------------------------|-----------------------------------|-------------------------------------|---|
| IB.51 | 0.641 | 13.31 | 20.76 |
| IB.67 | 0.232 | 8.84 | 38.10 |
| IB.70 | 0.323 | 7.67 | 23.75 |
| IB.88 | 0.300 | 4.09 | 13.63 |
| Budesonida | 0.101 | 0.68 | 6.73 |
| Propionato de Fluticasona | 0.086 | 0.36 | 4.18 |

(e) Deposición de Glucógeno Hepático en Ratas

A ratas macho Sprague Dawley, que pesaban 190-220g se les extirparon las glándulas suprarrenales bilateralmente y se mantuvieron en solución salina al 0.9% de principio a fin del experimento. Los días 5 y 6 de la adrenalectomía, los animales se repartieron en diferentes grupos, compuestos preparados en solución salina fría (sonicada durante 30 minutos) se instilaron intratraquealmente en 2 dosis @ 3mg/kg, con intervalos de 24 horas. 15 horas después del último tratamiento, los animales se sacrificaron y se extirparon los hígados y se pesaron. Se determinó el contenido de glucógeno de los hígados por el método de antrona. Concretamente, una cantidad pesada de tejido hepático se homogeneizó con 5% de ácido tricloroacético, el sobrenadante se mezcló con etanol y se mantuvo de un día para otro para precipitación. El glucógeno así extraído se calculó como glucosa generada luego de la hidrólisis ácida por la adición del reactivo antrona a 620nm. El contenido de glucógeno se expresó como mg/100g hígado.

Tabla 11: Deposición de Glucógeno Hepático en Ratas

| Compuesto No. | Dosis (mg/kg) | Contenido de Glucógeno (mg/100g hígado) | Inhibición % de Timo |
|---------------------------|---------------|---|----------------------|
| IA.3 | 3 | -13.6 | -2.42 |
| IB.4 | 3 | -5.77 | -9.68 |
| IB.50 | 3 | 6.67 | 5.48 |
| IC.3 | 3 | -11.34 | -2.43 |
| Propionato de Fluticasona | 3 | 1514.65 | 70.17 |
| Furoato de Mometasona | 3 | 1117.32 | 43.51 |
| Budesonida | 3 | 552.77 | 65.02 |

(f) Evaluación de la Actividad Sistémica por Vía de Administración i.v.

Para evaluar los efectos secundarios sistémicos con la administración i.v., se llevó a cabo el análisis de granuloma inducido por torunda de algodón (blanco torunda de algodón) en ratas macho SD. Torundas de algodón esterilizadas que pesaban 20mg se implantaron quirúrgicamente en la región escapular en ambos lados. A partir del día siguiente del implante, los

compuestos disueltos en Pharmasolve (Pharmasolve 66.67% en solución salina) o vehículo se administraron intravenosamente a 1.6mg/kg dosis durante 3 días consecutivos. El día 5 del implante se extirparon las torundas junto con el granuloma. Se extrajo igualmente la glándula timo de cada animal y se pesó. Las torundas con granuloma se secaron durante 20 horas a 60°C y se pesaron. Los pesos medios del granuloma seco y el timo y el aumento de peso corporal /100g de pesos corporales se compararon con los grupos de control con vehículo.

Los compuestos de fórmula I de la presente invención no indujeron una supresión significativa del timo y aumento del peso corporal por administración i.v. Además, no hubo inhibición significativa del granuloma inducido por torunda de algodón por la vía i.v. de administración, indicando así claramente falta de actividad sistémica y, en consecuencia, un perfil excelente de seguridad sistémica para los compuestos de fórmula I.

Tabla 12: Actividad por Vías i.v. de Administración

| Compuesto No. | Dosis mcg (durante 3 días), i.v. | Inhibición Media de Granuloma (%) | Disminución del Peso Medio del Timo (%)* |
|---------------------------|----------------------------------|-----------------------------------|--|
| IA.3 | 1600 | 3.98 | 6.37 |
| IA.11 | 1600 | 16.65 | -17.88 |
| IA.89 | 1600 | 15.90 | 6.54 |
| IC.3 | 1600 | 12.09 | -10.38 |
| IC.5 | 1600 | -22.20 | 1.67 |
| IA.143 | 1600 | -3.01 | 5.51 |
| Propionato de Fluticasona | 1600 | 55.62 | 75.71 |

* El aumento de peso corporal en todos los compuestos no fue estadísticamente significativo comparado con el control con vehículo

Conclusión

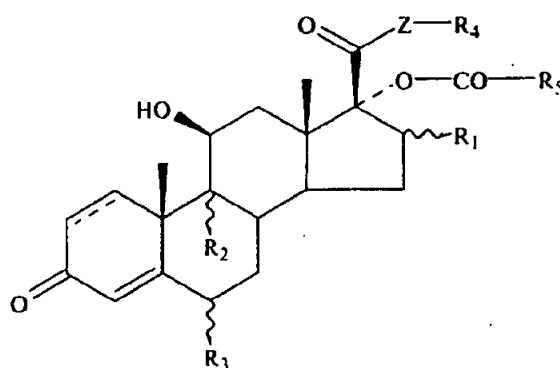
Los compuestos de fórmula I de la presente invención tienen una potente unión al receptor glucocorticoide *in vitro*. En los modelos *in vivo*, que incluyen tamizajes de edema en oreja de ratón inducido por aceite de croto, granuloma inducido por torunda de algodón y edema de pulmón inducido

por Sephadex, los compuestos de la presente invención exhiben una actividad anti-inflamatoria significativa. En el granuloma inducido por torunda de algodón, la involución del timo y el aumento del peso corporal debidas a los compuestos o bien estuvieron ausentes o bien fueron insignificantes incluso con niveles de dosis tal altas como 100-1.000mcg por torunda. Un comportamiento similar se observó nuevamente en el caso de los modelos de edema pulmonar inducido por Sephadex, incluso cuando los compuestos se administraron con dosis muy elevadas, demostrando claramente que estos compuestos no causan efectos sistémicos adversos luego de la administración. La ausencia o no significación de los efectos secundarios sistémicos se confirmó además por la medición de la deposición de glucógeno hepático en ratas luego de la administración intratraqueal, y por la medición de la supresión del aumento del timo y peso corporal luego de la administración i.v.

En consecuencia, los compuestos de fórmula I descritos en la presente invención son potentes glucocorticoides anti-inflamatorios que poseen actividad sistémica insignificante o no digna de mención incluso con dosis significativamente más elevadas que las dosis terapéuticas. Debido a los efectos sistémicos no significativos, los compuestos de la presente invención tienen un índice terapéutico elevado para actividad anti-inflamatoria vs efectos secundarios sistémicos, una propiedad que es altamente deseable para terapias que emplean glucocorticoides.

REIVINDICAMOS:

1. 11β -hidroxiandrosta-4-en-3-ona, compuesto de fórmula I, y su sal fisiológicamente aceptable:

**Formula I**

— represents a single or double bond and

~~~~~ represents a configuration  $\alpha$  or  $\beta$

in where

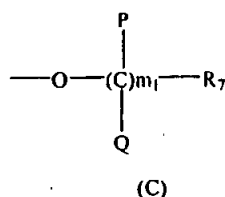
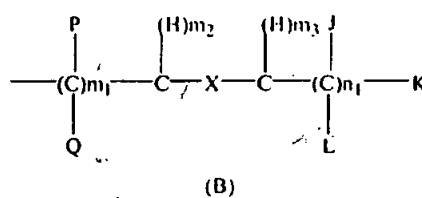
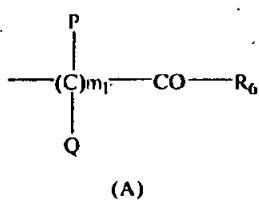
Z represents O or S;

$R_1$  represents hydrogen or methyl, which can be in a configuration  $\alpha$  or  $\beta$ , or be methylene;

$R_2$  and  $R_3$  are the same or different and each one independently represents hydrogen, halogen or a methyl group;

$R_5$  represents a group selected from  $(C_1-C_{10})$ -alkyl,  $(C_3-C_{13})$ -cycloalkyl,  $-O-(C_1-C_{10})$ -alkyl, aryl or heterocyclic ring in where the ring or ring system is not substituted or substituted by one or more halogen,  $-OH$ ,  $(C_1-C_3)$ -alkyl,  $-O-(C_1-C_3)$ -alkyl,  $(C_3-C_{13})$ -cycloalkyl; in where the alkyl or cycloalkyl groups can optionally contain one or more unsaturations and/or can have one or more heteroatoms incorporated in them and, optionally, in each case, one or more hydrogen atoms replaced by halogen,  $-OH$ ,  $(C_1-C_3)$ -alkyl,  $-O-(C_1-C_3)$ -alkyl,  $(C_3-C_{13})$ -cycloalkyl; and

$R_4$  representa una fracción seleccionada de un grupo conformado por (A), (B) y (C), siempre que cuando  $R_4$  representa la fracción (C), Z es S:



en donde

$m_1$  es 1, 2 ó 3;

$m_2$  es 0 ó 1;

$m_3$  es 0 ó 1;

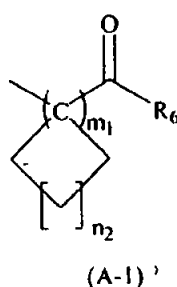
$n_1$  es 0, 1 ó 2;

$R_6$  representa un grupo seleccionado de  $(\text{C}_1\text{-C}_8)$ -alquilo,  $(\text{C}_3\text{-C}_{13})$ -cicloalquilo, arilo y un radical heterocíclico, donde el anillo o sistema de anillo es no sustituido o sustituido por uno o más radicales seleccionados de  $(\text{C}_1\text{-C}_8)$ -alquilo,  $(\text{C}_3\text{-C}_{13})$ -cicloalquilo, halógeno O- $(\text{C}_1\text{-C}_8)$ -alquilo, O- $(\text{C}_3\text{-C}_{13})$ -cicloalquilo, OCO- $(\text{C}_1\text{-C}_3)$ -alquilo, S(O)<sub>0-2</sub> $(\text{C}_1\text{-C}_8)$ -alquilo, COO- $(\text{C}_1\text{-C}_8)$ -alquilo, -OCO-O- $(\text{C}_1\text{-C}_3)$ -alquilo, -OCO-CO-O- $(\text{C}_1\text{-C}_3)$ -alquilo, CONH<sub>2</sub>, CONH- $(\text{C}_1\text{-C}_8)$ -alquilo, CON- $[(\text{C}_1\text{-C}_8)\text{-alquil}]_2$ , -NHCO- $(\text{C}_1\text{-C}_8)$ -alquilo, N- $(\text{C}_1\text{-C}_8)$ -alquil-CO- $(\text{C}_1\text{-C}_8)$ -alquilo, -NHCO-O- $(\text{C}_1\text{-C}_8)$ -alquilo, -N- $(\text{C}_1\text{-C}_8)$ -alquil-CO-O- $(\text{C}_1\text{-C}_8)$ -alquilo, -NHCONH- $(\text{C}_1\text{-C}_8)$ -alquilo, -N- $(\text{C}_1\text{-C}_8)$ -alquil-CONH- $(\text{C}_1\text{-C}_8)$ -alquilo, -NHCONH-SO<sub>2</sub>- $(\text{C}_1\text{-C}_8)$ -alquilo, -N- $(\text{C}_1\text{-C}_8)$ -alquil-CONH-SO<sub>2</sub>- $(\text{C}_1\text{-C}_8)$ -alquilo, -NO<sub>2</sub>, -CN; en donde los grupos alquilo o cicloalquilo pueden contener opcionalmente una o más insaturaciones y/o pueden tener uno o más heteroátomos incorporados en ellas y, opcionalmente, en cada caso, uno o más átomos de hidrógeno reemplazados por halógeno, -OH,  $(\text{C}_1\text{-C}_3)$ -alquilo, -OCO- $(\text{C}_1\text{-C}_3)$ -alquilo o  $(\text{C}_3\text{-C}_{13})$ -cicloalquilo;

siempre que cuando  $R_4$  representa una fracción A en donde  $R_6$  representa  $(C_3-C_{13})$ -cicloalquilo que contiene opcionalmente uno o más heteroátomos incorporados en ellas, el heteroátomo no sea nitrógeno;

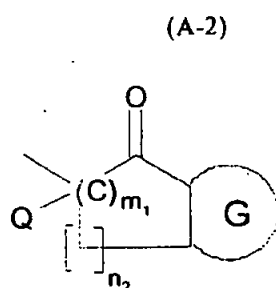
P y Q se seleccionan independientemente de hidrógeno y  $C_1$  a  $C_3$  alquilo;

o P y Q pueden unirse conjuntamente con el átomo de carbono al cual se enlazan para formar  $(C_3-C_8)$ -cicloalquilo, como se representa por la fracción (A-1):



en donde  $m_1$  es 1 y  $n_2$  es 0, 1, 2, 3, 4 ó 5 y  $R_6$  es un arilo, como se define anteriormente;

o P y  $R_6$  pueden unirse conjuntamente para formar un sistema cíclico, como se representa por la fracción (A-2):



en donde  $m_1$  es 1 y  $n_2$  es 0, 1, 2, 3 ó 4 y anillo G es un arilo como se define anteriormente;

X representa un enlace doble o un enlace triple; y

J, K y L se seleccionan independientemente de un grupo conformado por hidrógeno, halógeno,  $(C_1-C_{10})$ -alquilo,  $(C_3-C_{13})$ -cicloalquilo, -OH, -O- $(C_1-C_{10})$ -alquilo, -O- $(C_3-C_{13})$ -cicloalquilo, -OCO- $(C_1-C_{10})$ -alquilo, -OCO- $(C_3-C_{13})$ -cicloalquilo, -OCO-CO-O- $(C_1-C_{10})$ -alquilo, -OCO-CO-O- $(C_3-C_{13})$ -cicloalquilo, -OCO-O- $(C_1-C_{10})$ -alquilo, -OCO-O- $(C_3-C_{13})$ -cicloalquilo, -OCO-NH- $(C_1-C_{10})$ -alquilo, -OCO-NH- $(C_3-C_{13})$ -cicloalquilo, -OCO-N- $[(C_1-C_{10})$ -alquil]<sub>2</sub>, -OCO-N- $[(C_3-C_{13})$ -cicloalquil]<sub>2</sub>, -OCO-NHSO<sub>2</sub>- $(C_1-C_{10})$ -

alquilo, -OCO-NHSO<sub>2</sub>-(C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, -NH<sub>2</sub>, -NH-(C<sub>1</sub>-C<sub>8</sub>)-alquilo, -N-[(C<sub>1</sub>-C<sub>8</sub>)-alquil]<sub>2</sub>, -NO<sub>2</sub> y -CN;

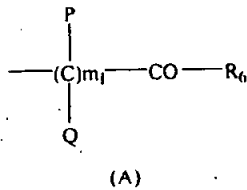
en donde los grupos alquilo o cicloalquilo pueden contener opcionalmente una o más insaturaciones y/o pueden tener uno o más heteroátomos incorporados en ellas y, opcionalmente, en cada caso, uno o más átomos de hidrógeno reemplazados por halógeno, -OH, (C<sub>1</sub>-C<sub>3</sub>)-alquilo, -O-(C<sub>1</sub>-C<sub>3</sub>)-alquilo, -OCO-(C<sub>1</sub>-C<sub>3</sub>)-alquilo, -COOH, -COO-(C<sub>1</sub>-C<sub>5</sub>)-alquilo, -COO-(C<sub>1</sub>-C<sub>5</sub>)-haloalquilo, -NHCO-(C<sub>1</sub>-C<sub>8</sub>)-alquilo, -ONO<sub>2</sub>, -NH-(C<sub>1</sub>-C<sub>8</sub>)-alquilo, -N-[(C<sub>1</sub>-C<sub>8</sub>)-alquil]<sub>2</sub>, -NO<sub>2</sub>, -CN, (C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, arilo o un radical heterocíclico;

o J y K pueden unirse conjuntamente con el átomo de carbono al cual se enlazan para representar un grupo (C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo o -CO- y L es como se define anteriormente;

o J, K y L están ausentes cuando n<sub>1</sub> es 0;

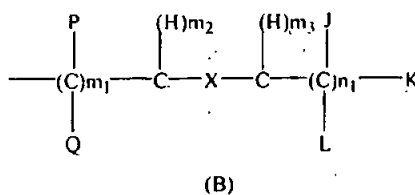
R<sub>7</sub> representa un grupo seleccionado de hidrógeno, halógeno, arilo y CO-arilo, en donde el anillo o sistema de anillo es no sustituido o sustituido como se define anteriormente.

2. 11β-hidroxiandrosta-4-en-3-ona, compuesto de fórmula I, y su sal fisiológicamente aceptable, como se reivindica en la reivindicación 1, en donde R<sub>4</sub> representa una fracción (A).



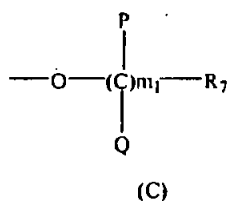
en donde m<sub>1</sub>, P, Q y R<sub>6</sub> son como se define en la reivindicación 1.

3. 11β-hidroxiandrosta-4-en-3-ona, compuesto de fórmula I, y su sal fisiológicamente aceptable, como se reivindica en la reivindicación 1, en donde R<sub>4</sub> representa una fracción (B).



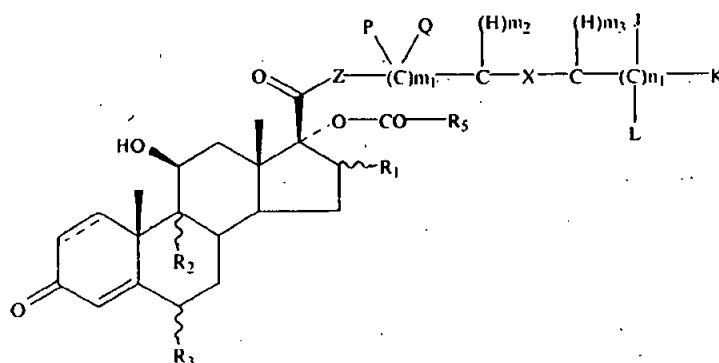
en donde  $m_1$ ,  $m_2$ ,  $m_3$ ,  $n_1$ , P, Q, J, K, L y X son como se define en la reivindicación 1.

4.  $11\beta$ -hidroxiandrosta-4-en-3-ona, compuesto de fórmula I, y su sal fisiológicamente aceptable, como se reivindica en la reivindicación 1, en donde  $R_4$  representa una fracción (C).



en donde  $m_1$ , P, Q y  $R_7$  son como se define en la reivindicación 1.

5.  $11\beta$ -hidroxiandrosta-4-en-3-ona, compuesto de fórmula I-B, y su sal fisiológicamente aceptable:



**Fórmula I-B**

en donde

Z representa O ó S;

$R_1$  representa hidrógeno o metilo, el cual puede estar en una configuración  $\alpha$  o  $\beta$ , o ser metileno;

$R_2$  y  $R_3$  son los mismos o diferentes y cada uno independientemente representa hidrógeno, halógeno o un grupo metilo;

R<sub>5</sub> representa un grupo seleccionado de (C<sub>1</sub>-C<sub>10</sub>)-alquilo, (C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, -O-(C<sub>1</sub>-C<sub>10</sub>)-alquilo, arilo o anillo heterocíclico en donde el anillo o sistema de anillo es no sustituido o sustituido por uno o más halógeno, -OH, (C<sub>1</sub>-C<sub>3</sub>)-alquilo, -O-(C<sub>1</sub>-C<sub>3</sub>)-alquilo, (C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo; en donde los grupos alquilo o cicloalquilo pueden contener opcionalmente una o más insaturaciones y/o pueden tener uno o más heteroátomos incorporados en ellas y, opcionalmente, en cada caso, uno o más átomos de hidrógeno reemplazados por halógeno, -OH, (C<sub>1</sub>-C<sub>3</sub>)-alquilo, -O-(C<sub>1</sub>-C<sub>3</sub>)-alquilo, (C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo; y

m<sub>1</sub> es 1;

m<sub>2</sub> es 0 ó 1;

m<sub>3</sub> es 0 ó 1;

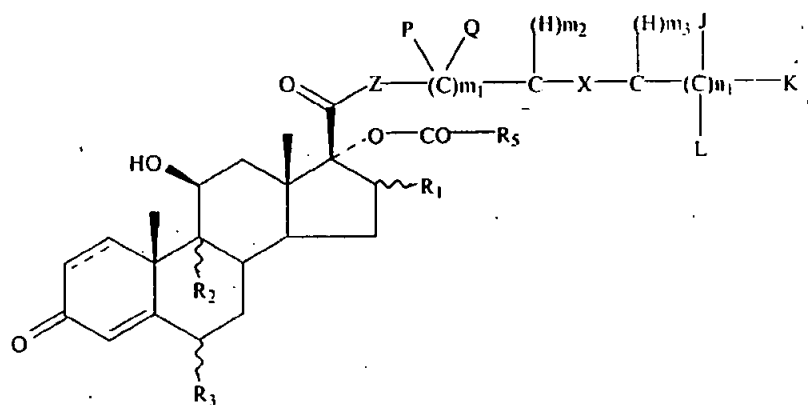
n<sub>1</sub> es 0, 1 ó 2;

P y Q son hidrógeno;

X representa un enlace doble o un enlace triple; y

J, K y L se seleccionan independientemente de un grupo conformado por hidrógeno, halógeno, (C<sub>1</sub>-C<sub>10</sub>)-alquilo, (C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, -OH, -O-(C<sub>1</sub>-C<sub>10</sub>)-alquilo, -O-(C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, -OCO-(C<sub>1</sub>-C<sub>10</sub>)-alquilo, -OCO-(C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, -OCO-CO-O-(C<sub>1</sub>-C<sub>10</sub>)-alquilo, -OCO-CO-O-(C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, -OCO-O-(C<sub>1</sub>-C<sub>10</sub>)-alquilo, -OCO-O-(C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, -OCO-NH-(C<sub>1</sub>-C<sub>10</sub>)-alquilo, -OCO-NH-(C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, -OCO-N-[(C<sub>1</sub>-C<sub>10</sub>)-alquil]<sub>2</sub>, -OCO-N-[(C<sub>3</sub>-C<sub>13</sub>)-cicloalquil]<sub>2</sub>, -OCO-NHSO<sub>2</sub>-, (C<sub>1</sub>-C<sub>10</sub>)-alquilo, -OCO-NHSO<sub>2</sub>-(C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, -NH<sub>2</sub>, -NH-(C<sub>1</sub>-C<sub>8</sub>)-alquilo, -N-[(C<sub>1</sub>-C<sub>8</sub>)-alquil]<sub>2</sub>, -NO<sub>2</sub> y -CN.

6. 11β-hidroxiandrosta-4-en-3-ona, compuesto de fórmula I-B, y su sal fisiológicamente aceptable:

**Formula I-B**

en donde

Z representa S;

R<sub>1</sub> representa hidrógeno o metilo, el cual puede estar en una configuración  $\alpha$  o  $\beta$ , o ser metileno;

R<sub>2</sub> y R<sub>3</sub> son los mismos o diferentes y cada uno independientemente representa hidrógeno, halógeno o un grupo metilo;

R<sub>5</sub> representa un grupo seleccionado de (C<sub>1</sub>-C<sub>10</sub>)-alquilo, (C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo,

-O-(C<sub>1</sub>-C<sub>10</sub>)-alquilo, arilo o anillo heterocíclico en donde el anillo o sistema de anillo es no sustituido o sustituido por uno o más halógeno, -OH, (C<sub>1</sub>-C<sub>3</sub>)-alquilo, -O-(C<sub>1</sub>-C<sub>3</sub>)-alquilo, (C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo; en donde los grupos alquilo o cicloalquilo pueden contener opcionalmente una o más insaturaciones y/o pueden tener uno o más heteroátomos incorporados en ellas y, opcionalmente en cada caso, tienen uno o más átomos de hidrógeno reemplazados por halógeno -OH, (C<sub>1</sub>-C<sub>3</sub>)-alquilo, -O-(C<sub>1</sub>-C<sub>3</sub>)-alquilo, (C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo; y

m<sub>1</sub> es 1;

m<sub>2</sub> es 0;

m<sub>3</sub> es 0;

n<sub>1</sub> es 0, 1 ó 2;

P y Q son hidrógeno;

X representa un enlace triple, y

J, K y L se seleccionan independientemente de un grupo conformado por hidrógeno, halógeno, (C<sub>1</sub>-C<sub>10</sub>)-alquilo, (C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, -OH, -O-(C<sub>1</sub>-

C<sub>10</sub>)-alquilo, -O-(C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, -OCO-(C<sub>1</sub>-C<sub>10</sub>)-alquilo, -OCO-(C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, -OCO-CO-O-(C<sub>1</sub>-C<sub>10</sub>)-alquilo, -OCO-CO-O-(C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, -OCO-O-(C<sub>1</sub>-C<sub>10</sub>)-alquilo, -OCO-O-(C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, -OCO-NH-(C<sub>1</sub>-C<sub>10</sub>)-alquilo, -OCO-NH-(C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, -OCO-N-[(C<sub>1</sub>-C<sub>10</sub>)-alquil]<sub>2</sub>, -OCO-N-[(C<sub>3</sub>-C<sub>13</sub>)-cicloalquil]<sub>2</sub>, -OCO-NHSO<sub>2</sub>-(C<sub>1</sub>-C<sub>10</sub>)-alquilo, -OCO-NHSO<sub>2</sub>-(C<sub>3</sub>-C<sub>13</sub>)-cicloalquilo, -NH<sub>2</sub>, -NH-(C<sub>1</sub>-C<sub>8</sub>)-alquilo, -N-[(C<sub>1</sub>-C<sub>8</sub>)-alquil]<sub>2</sub>, -NO<sub>2</sub> y -CN.

7. 1 $\beta$ -Hidroxiandrosta-4-en-3-ona como se reivindica en la reivindicación 1 seleccionada del grupo conformado por

*S*-[2-(4-Clorofenil)-2-oxoetil] 6 $\alpha$ ,9 $\alpha$ -difluoro-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxo-17 $\alpha$ -propioniloxiandrosta-1,4-dien-17 $\beta$ -carbotioato,

2-(4-Fluorofenil)-2-oxoetil 6 $\alpha$ ,9 $\alpha$ -difluoro-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxo-17 $\alpha$ -propioniloxiandrosta-1,4-dien-17 $\beta$ -carboxilato,

*S*-[2-(4-Fluorofenil)-2-oxoetil] 6 $\alpha$ ,9 $\alpha$ -difluoro-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxo-17 $\alpha$ -propioniloxiandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[2-(2,4-Difluorofenil)-2-oxoetil] 6 $\alpha$ ,9 $\alpha$ -difluoro-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxo-17 $\alpha$ -propioniloxiandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[2-(2,4-Diclorofenil)-2-oxoetil] 6 $\alpha$ ,9 $\alpha$ -difluoro-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxo-17 $\alpha$ -propioniloxiandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[2-(3,4-Diclorofenil)-2-oxoetil] 6 $\alpha$ ,9 $\alpha$ -difluoro-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxo-17 $\alpha$ -propioniloxiandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[2-(5-Clorotiofen-2-il)-2-oxoetil] 6 $\alpha$ ,9 $\alpha$ -difluoro-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxo-17 $\alpha$ -propioniloxiandrosta-1,4-dien-17 $\beta$ -carboxilato,

*S*-[2-Oxopropil]6 $\alpha$ ,9 $\alpha$ -difluoro-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxo-17 $\alpha$ -propioniloxiandrosta-1,4-dien-17 $\beta$ -carbotioato,

2-Oxopropil 6 $\alpha$ ,9 $\alpha$ -difluoro-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxo-17 $\alpha$ -propioniloxiandrosta-1,4-dien-17 $\beta$ -carboxilato,

*S*-[2-(4-Metoxifenil)-2-oxoetil] 6 $\alpha$ ,9 $\alpha$ -difluoro-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxo-17 $\alpha$ -propioniloxiandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[2-Oxo-2-(4-trifluorometiloxifenil)etil] 6 $\alpha$ ,9 $\alpha$ -difluoro-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxo-17 $\alpha$ -propioniloxiandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[2-Oxo-2-(4-trifluorometilfenil)etil] 6 $\alpha$ ,9 $\alpha$ -difluoro-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxo-17 $\alpha$ -propioniloxiandrosta-1,4-dien-17 $\beta$ -carbotioato,

2-(4-Metanosulfonilfenil)-2-oxoetil 6 $\alpha$ ,9 $\alpha$ -difluoro-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxo-17 $\alpha$ -propioniloxiandrosta-1,4-dien-17 $\beta$ -carboxilato,

*S*-[2-(4-Metanosulfonilfenil)-2-oxoetil] 6 $\alpha$ ,9 $\alpha$ -difluoro-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxo-17 $\alpha$ -propioniloxiandrosta-1,4-dien-17 $\beta$ -carbotioato,

2-Oxo-2-feniletil 6 $\alpha$ ,9 $\alpha$ -difluoro-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxo-17 $\alpha$ -propioniloxiandrosta-1,4-dien-17 $\beta$ -carboxilato,

*S*-[2-Oxo-2-feniletil] 6 $\alpha$ ,9 $\alpha$ -difluoro-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxo-17 $\alpha$ -propioniloxiandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[2-Oxo-2-(2,4,6-trimetilfenil)etil] 6 $\alpha$ ,9 $\alpha$ -difluoro-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxo-17 $\alpha$ -propioniloxiandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[1,1-Dimetil-2-oxo-2-feniletil] 6 $\alpha$ ,9 $\alpha$ -difluoro-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxo-17 $\alpha$ -propioniloxiandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[2-(4-Metoxifenil)-2-oxoetil] 6 $\alpha$ ,9 $\alpha$ -difluoro-11 $\beta$ -hidroxi-16 $\alpha$ -metil-17 $\alpha$ -(2-metilpropioniloxi)-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[2-Oxo-2-(4-trifluorometilfenil)etil] 17 $\alpha$ -ciclobutilcarboniloxi-6 $\alpha$ ,9 $\alpha$ -difluoro-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[2-(2,4-Difluorofenil)-2-oxoetil] 17 $\alpha$ -ciclobutilcarboniloxi-6 $\alpha$ -9 $\alpha$ -difluoro-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[2-(4-Metoxifenil)-2-oxoetil] 17 $\alpha$ -ciclobutilcarboniloxi-6 $\alpha$ ,9 $\alpha$ -difluoro-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[2-(2,4-Difluorofenil)-2-oxoetil] 9 $\alpha$ -fluoro-17 $\alpha$ -[(2-furanilcarbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[2-(4-Clorofenil)-2-oxoetil] 9 $\alpha$ -fluoro-17 $\alpha$ -[(2-furanilcarbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[2-(4-Metoxifenil)-2-oxoetil] 9 $\alpha$ -fluoro-17 $\alpha$ -[(2-furanilcarbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[2-(4-Fluorofenil)-2-oxoetil] 9 $\alpha$ -fluoro-17 $\alpha$ -[(2-furanilcarbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[2-(4-Clorofenil)-2-oxoetil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanilcarbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[2-Oxo-2-(4-trifluorometilfenil)etil] 6 $\alpha$ ,9 $\alpha$ -difluoro-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxo-17 $\alpha$ -[(2-tienilcarbonil)oxi]androsta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[2-(3,4-Dimetilfenil)-2-oxoetil] 6 $\alpha$ ,9 $\alpha$ -difluoro-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxo-17 $\alpha$ -propioniloxiandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[2-(3-Clorofenil)-2-oxoetil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanilcarbonil) oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[2-Oxo-2-(4-trifluorometilfenil)etil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanilcarbonil)oxi]-11 $\beta$ -hidroxi-16 $\beta$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato.

*S*-(4-Hidroxi-but-2-inil) 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanilcarbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[4-*n*-Propilcarboniloxi-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxo-17 $\alpha$ -propioniloxiandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[4-(2-Etoxi-1,2-dioxoetil-(*E*)-but-2-enil] 6 $\alpha$ ,9 $\alpha$ -difluoro-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxo-17 $\alpha$ -propioniloxiandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[4-(2-Etoxi-1,2-dioxoetil)oxi-(*E*)-but-2-enil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanil-carbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[4-*n*-Propilcarboniloxi-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanilcarbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[4-(2-Metilpropioniloxi)-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanilcarbonil) oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[4-(2,2-Dimetilpropioniloxi)-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanil-carbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[4-(2,2-Dimetilpropioniloxi)-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxo-17 $\alpha$ -propioniloxiandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[4-*n*-Propilcarboniloxi-(*Z*)-but-2-enil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanilcarbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[4-(2-Etoxi-1,2-dioxoetil)oxi-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanil-carbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato.

*S*-[4-*n*-Propilcarboniloxi-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxo-17 $\alpha$ -[(2-tienilcarbonil)oxi]androsta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[(4-Ciclopropilcarboniloxi)-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanilcarbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[(4-Ciclobutilcarboniloxi)-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanilcarbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[(4-Ciclopentilcarboniloxi)-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanilcarbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

S-[4-*n*-Propilcarboniloxi-(*E*)-but-2-enil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanilcarbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

S-[(4-Metoxicarboniloxi)-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanilcarbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

S-[(4-Etoxicarboniloxi)-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanilcarbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

S-[4-(2,2-Dimetiletiloxicarboniloxi)-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanil-carbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

S-[4-(2-Metilpropiloxicarboniloxi)-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanil-carbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

S-[4-(3-Cloropropilcarboniloxi)-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanilcarbonil)-oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

S-[4-Dicloroacetoxi-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanilcarbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

S-[4-(2-Metilpropilcarboniloxi)-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanilcarbonil)-oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[4-(3,3-Dimetilpropilcarboniloxi)-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanil-carbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-(4-Propioniloxi-but-2-inil) 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanilcarbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[4-(3,3,3-Trifluoropropioniloxi)-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanilcarbonil)-oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[4-(Metoxiacetiloxi)-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanilcarbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[4-(Etoxiacetiloxi)-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanilcarbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-(4-Acetoxi-but-2-inil) 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanilcarbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[4-(2,2-Dimetilbutilcarboniloxi)-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanilcarbonil)-oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[4-((1*S*)-Canfanilcarboniloxi)-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanilcarbonil)-oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[4-(4-Etoxibutil-1,4-diona)oxi-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanilcarbonil)-oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[4-(4-Etiloxi-(*Z*)but-2-en-1,4-diona)oxi-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanil-carbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[4-(4-Metoxibutil-1,4-diona)oxi-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanilcarbonil)-oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[4-(4-Isopropiloxibutil-1,4-diona)oxi-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-11 $\beta$ -hidroxi-16 $\alpha$ -metil-17 $\alpha$ -[(2-furanilcarbonil)oxi]-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[4-(4-Isobutiloxibutil-1,4-diona)oxi-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanil-carbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[4-(4-*n*-Butiloxibutil-1,4-diona)oxi-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanil-carbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[4-(3-Cloro-2,2-dimetilpropioniloxi)-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanil-carbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[4-(4-Metoxi-(*E*)-but-2-en-1,4-diona)-oxi-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanil-carbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[4-(3-Metil-1-oxobutiloxi)-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanilcarbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[4-(2-Etil-1-oxobutiloxi)-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanilcarbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[4-(*N,N*-Dimetilaminocarboniloxi)-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanil-carbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[4-(2-Cloro-2-metilpropioniloxi)-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanil-carbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[4-(4-Metil-1-oxopentiloxi)-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanilcarbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[4-(2-Hidroxi-2-metilpropioniloxi)-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanil-carbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[4-(2-Fluoro-2-metilpropioniloxi)-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanil-carbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[4-(4-Metoxi-(*Z*)-but-2-en-1,4-diona)oxi-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanil-carbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[4-(4-Etoxi-(*E*)-but-2-en-1,4-diona)oxi-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanil-carbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[4-(4-Isobutiloxi-(*E*)-but-2-en-1,4-diona)oxi-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanilcarbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[4-Acridoiloxi-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanilcarbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[4-(Ciclopentilmetiloxicarboniloxi)-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanil-carbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[4-(3-Metilbut-2-enoxicarboniloxi)-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanil-carbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[4-(*n*-Pentiloxicarboniloxi)-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanilcarbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[4-(2,2-Dimetil-3-fluoropropioniloxi)-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanil-carbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[4-((*S*)-2,2-Dimetil-1,3-dioxolan-4-il-metoxicarboniloxi)-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanilcarbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-[4-(*R*)-2,2-Dimetil-1,3-dioxolan-4-il-metoxicarboniloxi)-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanilcarbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-11 $\beta$ -carbotioato,

*S*-[4-(Isoamiloxicarboniloxy)-but-2-inil] 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanilcarbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

*S*-(4-Etoxi-but-2-inil) 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanilcarbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbotioato,

Éster fluorometílico de ácido 6 $\alpha$ ,9 $\alpha$ -difluoro-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxo-17 $\alpha$ -propioniloxiandrosta-1,4-dien-17 $\beta$ -carbonilsulfénico,

Éster fluorometílico de ácido 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanilcarbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbonilsulfénico,

Éster (4-fluorofenil)metílico de ácido 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanilcarbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbonilsulfénico,

Éster (4-trifluorometilfenil)metílico de ácido 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanilcarbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbonilsulfénico,

Éster (4-clorofenil)metílico de ácido 6 $\alpha$ ,9 $\alpha$ -difluoro-17 $\alpha$ -[(2-furanilcarbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbonilsulfénico,

Éster (4-trifluorometilfenil)metílico de ácido 6 $\alpha$ ,9 $\alpha$ -difluoro-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxo-17 $\alpha$ -propioniloxiandrosta-1,4-dien-17 $\beta$ -carbonilsulfénico,

Éster (4-fluorofenil)metílico de ácido 9 $\alpha$ -fluoro-17 $\alpha$ -[(2-furanilcarbonil)oxi]-11 $\beta$ -hidroxi-16 $\alpha$ -metil-3-oxoandrosta-1,4-dien-17 $\beta$ -carbonilsulfénico,

Éster metílico de ácido  $6\alpha,9\alpha$ -difluoro- $11\beta$ -hidroxi- $16\alpha$ -metil-3-oxo- $17\alpha$ -propioniloxiandrosta- $1,4$ -dien- $17\beta$ -carbonilsulfénico,

Éster metílico de ácido  $6\alpha,9\alpha$ -difluoro- $17\alpha$ -[(2-furanilcarbonil)oxi]- $11\beta$ -hidroxi- $16\alpha$ -metil-3-oxoandrosta- $1,4$ -dien- $17\beta$ -carbonilsulfénico,

*S*-[4-(4-Metil-1-oxopentiloxi)-but-2-inil]  $6\alpha,9\alpha$ -difluoro- $17\alpha$ -[(2-furanilcarbonil)-oxi]- $11\beta$ -hidroxi- $16\alpha$ -metil-3-oxoandrosta- $1,4$ -dien- $17\beta$ -carbotioato.

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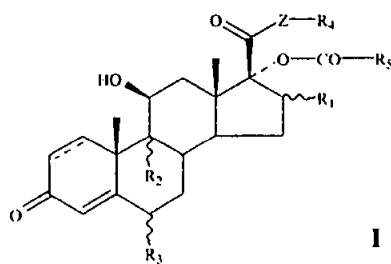
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(54) Title: NOVEL 11 BETA - HYDROXYANDROSTA-4-ENE-3-ONES

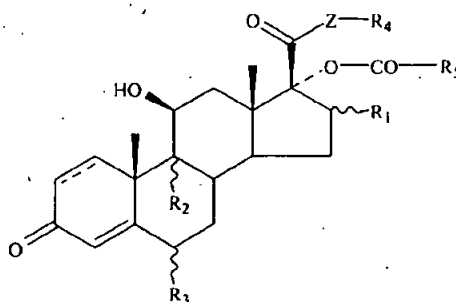


(57) Abstract: 11  $\beta$ -hydroxyandrosta-4-ene-3-one, compound of  
formula (I), and physiologically acceptable salt thereof; wherein  
 $R_4$  represents moiety selected from a group consisting of (A), (B)  
and (C), with a proviso that when  $R_4$  represents moiety (C), Z is S.

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NOVEL 11 $\beta$ -HYDROXYANDROSTA-4-ENE-3-ONES

- 5 The present invention relates to novel anti-inflammatory and antiallergic analogues of the 11 $\beta$ -hydroxyandrosta-4-ene-3-ones, represented as formula I and physiologically acceptable salt thereof, having insignificant or no noteworthy systemic effects at multiples of efficacious dose.



Formula I

## BACKGROUND OF THE INVENTION

- Corticosteroids (or glucocorticoids) having anti-inflammatory properties are widely used for the treatment of inflammatory conditions or disorders of skin, airways, eye, GI tract, joints, CNS etc, and several autoimmune disorders. Some of the inflammatory skin disorders where treatment with glucocorticoids is prescribed are eczema, psoriasis, allergic dermatitis, pruritis, hypersensitivity reactions etc. Inflammatory or allergic conditions of the airways for which glucocorticoids are used include disorders of nose, throat or lungs such as rhinitis (including hay fever), nasal polyps, asthma (including allergen-induced asthmatic reaction), chronic obstructive pulmonary disease, interstitial lung disease, fibrosis, etc. Glucocorticoid administration is also used for inflammatory bowel disorders such as ulcerative colitis and Crohn's diseases; and inflammatory joint disorders such as rheumatoid arthritis which are autoimmune diseases. However, administration of corticosteroids in general may cause, in addition to the desired pharmacological effect, undesirable or adverse side effects at sites distant from the target tissue, the so-called systemic effects. Some of the undesired systemic effects encountered include

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widespread immunosuppression, increased bone turnover, impaired growth, skin thinning, diabetes, obesity, water retention, progesterone and estrogen related disorders. It is therefore desirable to have glucocorticoids which possess potent anti-inflammatory activity at the target tissue, with minimal or preferably no systemic activity at therapeutic doses when used for chronic treatment.

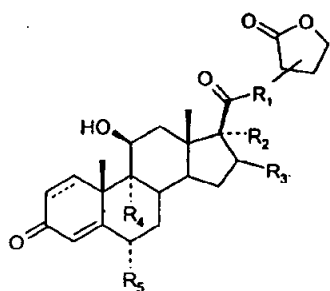
Classical glucocorticoids are described in —

- United States patent No. 4335121 (the '121 patent; Indian reference not available) ---  
(S)-fluoromethyl 6 $\alpha$ ,9 $\alpha$ -difluoro-11 $\beta$ -hydroxy-16 $\alpha$ -methyl-17 $\alpha$ -propionyloxy-3-oxoandrosta-1,4-diene-17 $\beta$ -carbothioate (Fluticasone)
- United states patent No. 3007923 (the '923 patent; Indian reference not available) ---  
16 $\alpha$ -methyl-9 $\alpha$ -fluoro-1,4-pregnadiene-11 $\beta$ ,17 $\alpha$ ,21-triol-3,20-dione (Dexamethasone)
- United states patent No 3929768 (the '768 patent; Indian reference not available)  
exemplifies (11 $\beta$ ,16 $\alpha$ )-16,17-[Butylidenebis(oxy)]-11,21-dihydroxypregna-1,4-diene-3,20-dione (Budesonide)
- United states patent No 4472393 (the '393 patent; Indian reference not available)  
exemplifies (11 $\beta$ ,16 $\alpha$ )-9,21-Dichloro-17-[(2-furanylcarbonyl)oxy]-11-hydroxy-16-methylpregna-1,4-diene-3,20-dione (Mometasone furoate)

The above mentioned drugs are potent glucocorticoids which are already in clinical use. However, at high multiples of efficacy dose these drugs have the potential to cause systemic side effects.

PCT publication WO 99/01467 describes therapeutically active steroidal compounds or salts or solvates having lactone group connected to the cyclopentane ring of the steroid nucleus (as given below). These compounds have been described to have reduced potential for systemic activity due to the relative instability of the lactone system in plasma. The compounds of the present invention do not possess a lactone group connected to the cyclopentane ring.

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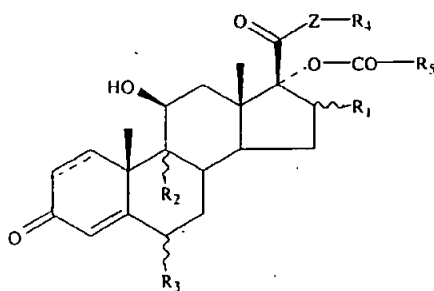


Our interest to develop compounds which act at the specific site of inflammation with insignificant or no noteworthy side effects has led us to the discovery of novel, safe 11 $\beta$ -hydroxyandrost-4-ene-3-one compounds described in this invention. These compounds possess useful anti-inflammatory activity whilst having insignificant or no noteworthy systemic effects at multiples of efficacious dose.

### DESCRIPTION OF THE INVENTION

10

The present invention provides 11 $\beta$ -hydroxyandrost-4-ene-3-one, compound of formula I, and physiologically acceptable salt thereof,



Formula I

15

— represents a single or double bond and

~~~~~ represents  $\alpha$  or  $\beta$ -configuration.

wherein

Z represents O or S;

R₁ represents hydrogen or methyl which may be either in α or β -configuration, or methylene;

R₂ and R₃ are the same or different and each independently represents hydrogen, halogen or a methyl group;

R₅ represents a group selected from (C₁-C₁₀)-alkyl, (C₃-C₁₃)-cycloalkyl,

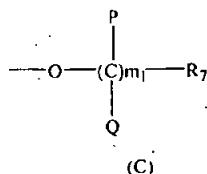
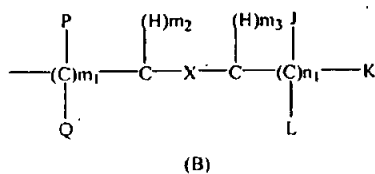
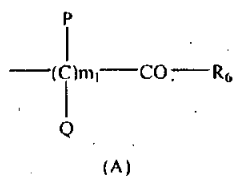
-O-(C₁-C₁₀)-alkyl, aryl or heterocyclic ring wherein the ring or ring system is unsubstituted or substituted by one or more halogen, -OH, (C₁-C₃)-alkyl, -O-(C₁-C₃)-alkyl, (C₃-C₁₃)-cycloalkyl;

wherein the alkyl or cycloalkyl groups can optionally contain one or more unsaturations and/or

can have one or more hetero atom incorporated therein and optionally in each case have one or more hydrogen atoms replaced by halogen, -OH, (C₁-C₃)-alkyl, -O-(C₁-C₃)-alkyl, (C₃-C₁₃)-cycloalkyl; and

R₄ represents moiety selected from a group consisting of (A), (B) and (C), with a proviso that

when R₄ represents moiety (C), Z is S:



wherein

m₁ is 1, 2 or 3;

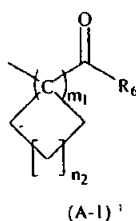
m₂ is 0 or 1;

m₃ is 0 or 1;

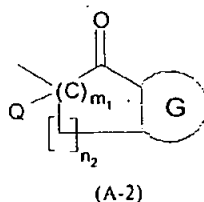
n₁ is 0, 1 or 2;

R₆ represents a group selected from (C₁-C₈)-alkyl, (C₃-C₁₃)-cycloalkyl, aryl and a heterocyclic radical, where the ring or ring system is unsubstituted or substituted by one or more substituents

- selected from (C₁-C₈)-alkyl, (C₃-C₁₃)-cycloalkyl, halogen, O-(C₁-C₈)-alkyl, O-(C₃-C₁₃)-cycloalkyl, OCO-(C₁-C₃)-alkyl, S(O)₀₋₂(C₁-C₈)-alkyl, COO-(C₁-C₈)-alkyl, -OCO-O-(C₁-C₃)-alkyl, -OCO-CO-O-(C₁-C₃)-alkyl, CONH₂, CONH-(C₁-C₈)-alkyl, CON-[(C₁-C₈)-alkyl]₂, -NHCO-(C₁-C₈)-alkyl, N-(C₁-C₈)-alkyl-CO-(C₁-C₈)-alkyl, -NHCO-O-(C₁-C₈)-alkyl, -N-(C₁-C₈)-alkyl-CO-O-(C₁-C₈)-alkyl, -NHCONH-(C₁-C₈)-alkyl, -N-(C₁-C₈)-alkyl-CONH-(C₁-C₈)-alkyl, -NHCONH-SO₂-(C₁-C₈)-alkyl, -N-(C₁-C₈)-alkyl-CONH-SO₂-(C₁-C₈)-alkyl, -NO₂, -CN; wherein the alkyl or cycloalkyl groups can optionally contain one or more unsaturations and/or can have one or more hetero atom incorporated therein and optionally, in each case have one or more hydrogen atoms replaced by halogen, -OH, (C₁-C₃)-alkyl, -OCO-(C₁-C₃)-alkyl or (C₃-C₁₃)-cycloalkyl; with a proviso that when R₄ represents moiety (A) wherein R₆ represents (C₃-C₁₃)-cycloalkyl optionally containing one or more hetero atom incorporated therein, the hetero atom is not nitrogen; P and Q are independently selected from hydrogen and C₁ to C₃ alkyl; or P and Q can be joined together with the carbon atom to which they are attached to form (C₃-C₈)-cycloalkyl as represented by moiety (A-1):



- wherein m₁ is 1 and n₂ is 0, 1, 2, 3, 4 or 5 and R₆ is an aryl as defined above; or P and R₆ can be joined together to form a cyclic system as represented by moiety (A-2):



wherein m₁ is 1 and n₂ is 0, 1, 2, 3 or 4 and ring G is an aryl as defined above;

X represents either a double bond or a triple bond; and

J, K and L are independently selected from a group consisting of hydrogen, halogen,

(C₁-C₁₀)-alkyl, (C₃-C₁₃)-cycloalkyl, -OH, -O-(C₁-C₁₀)-alkyl, -O-(C₃-C₁₃)-cycloalkyl,

-OCO-(C₁-C₁₀)-alkyl, -OCO-(C₃-C₁₃)-cycloalkyl, -OCO-CO-O-(C₁-C₁₀)-alkyl,

5 -OCO-CO-O-(C₃-C₁₃)-cycloalkyl, -OCO-O-(C₁-C₁₀)-alkyl, -OCO-O-(C₃-C₁₃)-cycloalkyl,

-OCO-NH-(C₁-C₁₀)-alkyl, -OCO-NH-(C₃-C₁₃)-cycloalkyl, -OCO-N-[(C₁-C₁₀)-alkyl]₂,

-OCO-N-[(C₃-C₁₃)-cycloalkyl]₂, -OCO-NHSO₂-(C₁-C₁₀)-alkyl, -OCO-NHSO₂-(C₃-C₁₃)-

cycloalkyl, -NH₂, -NH-(C₁-C₈)-alkyl, -N-[(C₁-C₈)-alkyl]₂, -NO₂ and -CN;

wherein the alkyl or cycloalkyl groups can optionally contain one or more unsaturations and/or

10 can have one or more hetero atom incorporated therein and optionally, in each case have one or more hydrogen atoms replaced by halogen, -OH, (C₁-C₃)-alkyl,

-O-(C₁-C₃)-alkyl, -OCO-(C₁-C₃)-alkyl, -COOH, -COO-(C₁-C₃)-alkyl,

-COO-(C₁-C₅)-haloalkyl, -NHCO-(C₁-C₈)-alkyl, -ONO₂, -NH-(C₁-C₈)-alkyl, -N-[(C₁-C₈)-alkyl]₂,

-NO₂, -CN, (C₃-C₁₃)-cycloalkyl, aryl or heterocyclic radical;

15 or J and K can be joined together with the carbon atom to which they are attached to represent a (C₃-C₁₃)-cycloalkyl or -CO- group and L is as defined above;

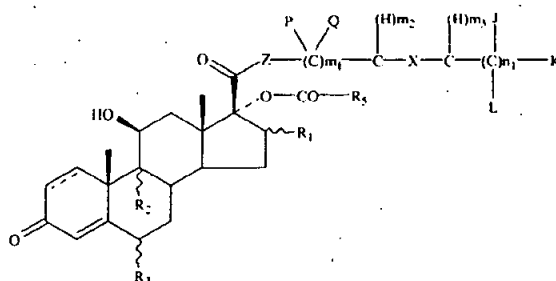
or J, K and L are absent when n₁ is 0;

R₇ represents a group selected from hydrogen, halogen, aryl and CO-aryl, wherein the ring or ring system is unsubstituted or substituted as defined above;

20

Preferably,

11β-hydroxyandrost-4-ene-3-one, compound of formula I-B, and physiologically acceptable salt thereof:



25

Formula I-B

wherein

Z represents O or S;

R₁ represents hydrogen or methyl which may be either in α or β -configuration, or methylene;

R₂ and R₃ are the same or different and each independently represents hydrogen, halogen or a methyl group;

R₅ represents a group selected from (C₁-C₁₀)-alkyl, (C₃-C₁₃)-cycloalkyl, -O-(C₁-C₁₀)-alkyl, aryl or heterocyclic ring wherein the ring or ring system is unsubstituted or substituted by one or more halogen, -OH, (C₁-C₃)-alkyl, -O-(C₁-C₃)-alkyl, (C₃-C₁₃)-cycloalkyl; wherein the alkyl or cycloalkyl groups can optionally contain one or more unsaturations and/or can have one or more hetero atom incorporated therein and optionally in each case have one or more hydrogen atoms replaced by halogen, -OH, (C₁-C₃)-alkyl, -O-(C₁-C₃)-alkyl, (C₃-C₁₃)-cycloalkyl; and

m₁ is 1;

m₂ is 0 or 1;

m₃ is 0 or 1;

n₁ is 0, 1 or 2;

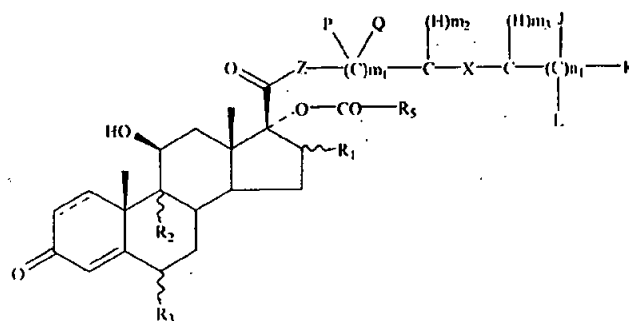
P and Q are hydrogen;

X represents either a double bond or a triple bond; and

J, K and L are independently selected from a group consisting of hydrogen, halogen, (C₁-C₁₀)-alkyl, (C₃-C₁₃)-cycloalkyl, -OH, -O-(C₁-C₁₀)-alkyl, -O-(C₃-C₁₃)-cycloalkyl, -OCO-(C₁-C₁₀)-alkyl, -OCO-(C₃-C₁₃)-cycloalkyl, -OCO-CO-O-(C₁-C₁₀)-alkyl, -OCO-CO-O-(C₃-C₁₃)-cycloalkyl, -OCO-O-(C₁-C₁₀)-alkyl, -OCO-O-(C₃-C₁₃)-cycloalkyl, -OCO-NH-(C₁-C₁₀)-alkyl, -OCO-NH-(C₃-C₁₃)-cycloalkyl, -OCO-N-[(C₁-C₁₀)-alkyl]₂, -OCO-N-[(C₃-C₁₃)-cycloalkyl]₂, -OCO-NHSO₂-(C₁-C₁₀)-alkyl, -OCO-NHSO₂-(C₃-C₁₃)-cycloalkyl, -NH₂, -NH-(C₁-C₈)-alkyl, -N-[(C₁-C₈)-alkyl]₃, -NO₂ and -CN.

Most preferably,

11 β -hydroxyandrost-4-ene-3-one, compound of formula I-B, and physiologically acceptable salt thereof:



Formula I-B

wherein

Z represents S;

5 R_1 represents hydrogen or methyl which may be either in α or β -configuration, or methylene;

R_2 and R_3 are the same or different and each independently represents hydrogen, halogen or a methyl group;

R_5 represents a group selected from (C_1-C_{10}) -alkyl, (C_3-C_{13}) -cycloalkyl,

10 -O- (C_1-C_{10}) -alkyl, aryl or heterocyclic ring wherein the ring or ring system is unsubstituted or substituted by one or more halogen, -OH, (C_1-C_3) -alkyl, -O- (C_1-C_3) -alkyl, (C_3-C_{13}) -cycloalkyl; wherein the alkyl or cycloalkyl groups can optionally contain one or more unsaturations and/or can have one or more hetero atom incorporated therein and optionally in each case have one or more hydrogen atoms replaced by halogen, -OH, (C_1-C_3) -alkyl, -O- (C_1-C_3) -alkyl, (C_3-C_{13}) -cycloalkyl; and

15 m_1 is 1;

m_2 is 0;

m_3 is 0;

n_1 is 0, 1 or 2;

P and Q are hydrogen;

20 X represents a triple bond; and

J, K and L are independently selected from a group consisting of hydrogen, halogen, (C_1-C_{10}) -alkyl, (C_3-C_{13}) -cycloalkyl, -OH, -O- (C_1-C_{10}) -alkyl, -O- (C_3-C_{13}) -cycloalkyl, -OCO- (C_1-C_{10}) -alkyl, -OCO- (C_3-C_{13}) -cycloalkyl, -OCO-CO-O- (C_1-C_{10}) -alkyl, -OCO-CO-O- (C_3-C_{13}) -cycloalkyl, -OCO-O- (C_1-C_{10}) -alkyl, -OCO-O- (C_3-C_{13}) -cycloalkyl, -OCO-NH- (C_1-C_{10}) -alkyl, -OCO-NH-

(C₃-C₁₃)-cycloalkyl, -OCO-N-[(C₁-C₁₀)-alkyl]₂, -OCO-N-[(C₃-C₁₃)-cycloalkyl]₂, -OCO-NHSO₂-(C₁-C₁₀)-alkyl, -OCO-NHSO₂-(C₃-C₁₃)-cycloalkyl, -NH₂, -NH-(C₁-C₈)-alkyl, -N-[(C₁-C₈)-alkyl]₂, -NO₂ and -CN.

5 DETAILED DESCRIPTION OF THE INVENTION

The present invention relates to novel, safe 11 β -hydroxyandrost-4-ene-3-one, compound of formula I, and physiologically acceptable salt thereof.

- 10 Compound of formula I, may be in the form of diastereomers and mixtures thereof. As used herein, any stereoisomeric form includes diastereomers and mixtures thereof.

Reference to compound of formula I hereinafter includes a compound of formula I and physiologically acceptable salt thereof.

15

With respect to the various groups encompassed by the generic terms used here and throughout this specification, the following definitions and explanations are applicable:

- 20 As used herein 'alkyl' can be straight-chain or branched and can optionally contain one or more unsaturations and/or can have one or more hetero atom incorporated therein and optionally, in each case have one or more hydrogen atoms replaced by -F, -Cl, -Br, -I,

-OH, -OCO-(C₁-C₃)-alkyl, (C₃-C₁₃)-cycloalkyl, aryl or heterocyclic radical.

- 25 As used herein 'alkyl including one or more unsaturations' is to be understood as meaning 'alkenyl' and/or 'alkynyl'. Exemplary alkyl groups include methyl, ethyl, *n*-propyl, *i*-propyl, *n*-butyl, *t*-butyl, *n*-pentyl, 3-pentyl, 2-octyl and the like. Exemplary alkenyl groups include ethenyl, propenyl, 1-butenyl, (*Z*)-2-butenyl, (*E*)-3-methylbut-2-enyl,

(*E*)-2,4-pentadienyl, (*Z*)-3-heptenyl and the like. Exemplary alkynyl groups include ethynyl, propynyl, 1-butylnyl, 2-butylnyl, 4-methyl-2-pentylnyl, 2,4-hexadiynyl and the like.

- 30 As used herein 'cycloalkyl' is to be understood as meaning monocyclic, bicyclic, tricyclic and polycyclic ring systems such as norbornyl, adamantyl and the like. The term 'cycloalkyl' as used herein can optionally contain one or more unsaturations and/or can have one or more hetero atom

incorporated therein -F, -Cl, -Br, -I, -OH, -OCO-(C₁-C₃)-alkyl, (C₃-C₁₁)-cycloalkyl, aryl or heterocyclic radical.

As used herein 'halogen' or 'halo group' refers to fluorine, chlorine, bromine or iodine.

5

As used herein aryl is to be understood as meaning ring systems such as phenyl, naphthyl, anthracenyl, phenanthryl, preferably aryl is phenyl.

As used herein heterocycle or heterocyclic ring is to be understood as meaning ring systems which, in addition to carbon, also contain hetero atoms, such as, for example, nitrogen, oxygen or sulfur. This definition furthermore includes ring systems in which the heterocycle or heterocyclic radical is fused with benzene rings. Examples of heterocycles or heterocyclic rings are:

heteroaryls, such as

- 15 benzimidazolyl,
1-[(C₁-C₆)-alkyl]benzimidazolyl,
imidazolyl,
2- or 3-thienyl,
2- or 3-furyl,
20 benzoxazolyl,
benzothiazolyl,
2-, 3- or 4-pyridyl,
pyrimidinyl,
4-, 5- or 6-pyridazin-2*H*-yl-3-one,
25 4-, 5- or 6-pyridazin-2-(C₁-C₈)-alkyl-2*H*-yl-3-one,
2-benzyl-4-, -5- or -6-pyridazin-2*H*-yl-3-one,
3- or 4-pyridazinyl,
2-, 3-, 4- or 8-quinolinyl,
1-, 3- or 4-isoquinolinyl,
30 1-phthalazinyl,
3- or 4-cinnolinyl,

- 2- or 4-quinazoliny,
2-pyraziny,
2-quinoxaliny,
2-, 4- or 5-oxazolyl,
5 3-, 4- or 5-isoxazolyl,
2-, 4- or 5-thiazolyl,
3-, 4- or 5-isothiazolyl,
1-[(C₁-C₆)-alkyl]-2-, -4- or -5-imidazolyl,
3-, 4- or 5-pyrazolyl,
10 1-[(C₁-C₆)-alkyl]-3-, -4- or -5-pyrazolyl,
1- or 4-[1,2,4]-triazolyl,
4- or 5-[1,2,3]-triazolyl,
1-[(C₁-C₆)-alkyl]-4- or -5-[1,2,3]triazolyl,
3-, 4- or 7-indolyl,
15 *N*-[(C₁-C₆)-alkyl]-3-, -4- or -7-indolyl
2-[(C₁-C₆)-alkyl]-3(2*H*)-indazolyl,
1-[(C₁-C₆)-alkyl]-3(1*H*)-indazolyl,
5-tetrazolyl,
1-[(C₁-C₆)-alkyl]-1*H*-tetrazolyl,
20 2-[(C₁-C₆)-alkyl]-2*H*-tetrazolyl.

In one embodiment the preferred compounds of formula I are selected from the compounds wherein m₁ is 1

- 25 In one embodiment the preferred compounds of formula I are selected from the compounds wherein m₁ is 1 and P and Q are hydrogen.

In one embodiment the compounds of formula I are selected from the compounds wherein R₁ represents moiety (A).

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In one embodiment the compounds of formula I are selected from the compounds wherein R₄ represents moiety (B).

In one embodiment the compounds of formula I are selected from the compounds wherein R₄ represents moiety (C).

In one embodiment the compounds of formula I are selected from the compounds wherein m₁ is 1; P and Q are both hydrogen and R₄ represents moiety (A).

10 In one embodiment the compounds of formula I are selected from the compounds wherein m₁ is 1; P and Q are both hydrogen and R₄ represents moiety (B).

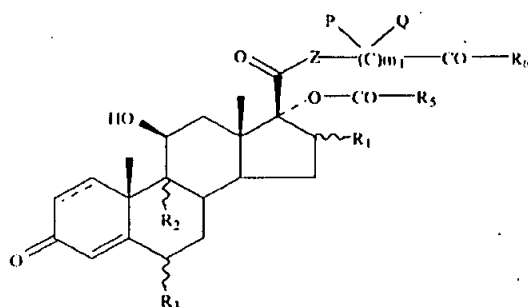
In one embodiment the compounds of formula I are selected from the compounds wherein m₁ is 1; P and Q are both hydrogen and R₄ represents moiety (C).

15

In one embodiment the compounds of formula I are selected from the compounds wherein R₆ is selected from a group consisting of (C₁-C₈)-alkyl, aryl and a heterocyclic radical wherein the ring or ring system is unsubstituted or substituted as defined above.

20 In one embodiment the compounds of formula I are selected from the compounds wherein R₅ represents a group selected from R₆, wherein R₆ is selected from a group consisting of (C₁-C₈)-alkyl and a heterocyclic radical wherein the ring or ring system is unsubstituted or substituted as defined above.

25 In one embodiment the present invention provides 11 β -hydroxyandrosta-4-ene-3-one, a compound of formula I-A and physiologically acceptable salt, thereof.



Formula I-A

5

----- represents a single or double bond and

~~~~~ represents  $\alpha$  or  $\beta$ -configuration.

wherein

Z represents O, S;

10  $R_1$  represents hydrogen or methyl which may be either in  $\alpha$  or  $\beta$ -configuration, or methylene;

$R_2$  and  $R_3$  are the same or different and each independently represents hydrogen, halogen or a methyl group;

$m_1$  is 1, 2 or 3;

15  $R_6$  represents a group selected from (C<sub>1</sub>-C<sub>8</sub>)-alkyl, (C<sub>3</sub>-C<sub>13</sub>)-cycloalkyl, aryl and a heterocyclic radical, where the ring or ring system is unsubstituted or substituted by one or more substituents selected from.

(C<sub>1</sub>-C<sub>8</sub>)-alkyl, (C<sub>3</sub>-C<sub>13</sub>)-cycloalkyl, halogen, O-(C<sub>1</sub>-C<sub>8</sub>)-alkyl, O-(C<sub>3</sub>-C<sub>13</sub>)-cycloalkyl, OCO-(C<sub>1</sub>-C<sub>3</sub>)-alkyl, S(O)<sub>0-2</sub>(C<sub>1</sub>-C<sub>8</sub>)-alkyl, COO-(C<sub>1</sub>-C<sub>8</sub>)-alkyl, -OCO-O-(C<sub>1</sub>-C<sub>3</sub>)-alkyl,

-OCO-CO-O-(C<sub>1</sub>-C<sub>3</sub>)-alkyl, CONH<sub>2</sub>, CONH-(C<sub>1</sub>-C<sub>8</sub>)-alkyl, CON-[(C<sub>1</sub>-C<sub>8</sub>)-alkyl]<sub>2</sub>,

20 -NHCO-(C<sub>1</sub>-C<sub>8</sub>)-alkyl, N-(C<sub>1</sub>-C<sub>8</sub>)-alkyl-CO-(C<sub>1</sub>-C<sub>8</sub>)-alkyl, -NHCO-O-(C<sub>1</sub>-C<sub>8</sub>)-alkyl,

-N-(C<sub>1</sub>-C<sub>8</sub>)-alkyl-CO-O-(C<sub>1</sub>-C<sub>8</sub>)-alkyl, -NHCONH-(C<sub>1</sub>-C<sub>8</sub>)-alkyl,

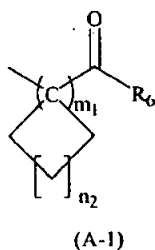
-N-(C<sub>1</sub>-C<sub>8</sub>)-alkyl-CONH-(C<sub>1</sub>-C<sub>8</sub>)-alkyl, -NHCONH-SO<sub>2</sub>-(C<sub>1</sub>-C<sub>8</sub>)-alkyl,

-N-(C<sub>1</sub>-C<sub>8</sub>)-alkyl-CONH-SO<sub>2</sub>-(C<sub>1</sub>-C<sub>8</sub>)-alkyl, -NO<sub>2</sub>, -CN;

wherein the alkyl or cycloalkyl groups can optionally contain one or more unsaturations and/or

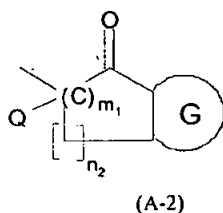
25 can have one or more hetero atom incorporated therein and optionally, in each case have one or

- more hydrogen atoms replaced by -F, -Cl, -Br, -I, -OH, -OCO-(C<sub>1</sub>-C<sub>3</sub>)-alkyl, (C<sub>3</sub>-C<sub>13</sub>)-cycloalkyl, aryl or heterocyclic radical; with a proviso that when R<sub>4</sub> represents moiety A wherein R<sub>6</sub> represents (C<sub>3</sub>-C<sub>13</sub>)-cycloalkyl optionally containing one or more hetero atom incorporated therein, the hetero atom is not nitrogen;
- 5 P and Q are independently selected from hydrogen, halogen and C<sub>1</sub> to C<sub>3</sub> alkyl; or P and Q can be joined together with the carbon atom to which they are attached to form (C<sub>3</sub>-C<sub>8</sub>)-cycloalkyl as represented by moiety (A-1):



wherein m<sub>1</sub> is 1 and n<sub>2</sub> is 0, 1, 2, 3, 4 or 5;

- 10 or P and Q can be joined together to form a cyclic system as represented by moiety (A-2):



wherein m<sub>1</sub> is 1 and n<sub>2</sub> is 0, 1, 2, 3 or 4 and ring G is optionally present, wherein G represents a (C<sub>3</sub>-C<sub>8</sub>)-cycloalkyl, aryl or a heterocyclic radical as defined above;

- 15 R<sub>5</sub> represents a group selected from R<sub>6</sub>, -O-R<sub>6</sub> or -N(R<sub>8</sub>)R<sub>6</sub>, wherein R<sub>6</sub> is as defined above and R<sub>8</sub> represents hydrogen, (C<sub>1</sub>-C<sub>6</sub>)-alkyl or (C<sub>3</sub>-C<sub>6</sub>)-cycloalkyl;

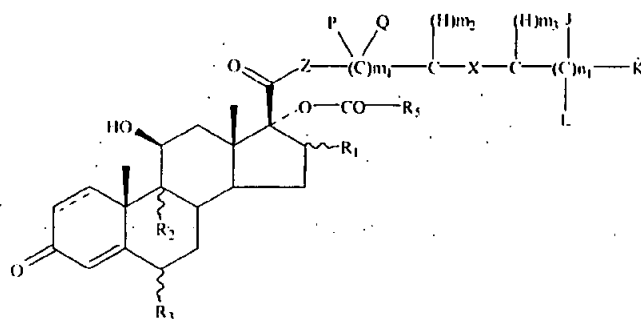
- In one embodiment the compounds of formula I-A are selected from the compounds wherein
- 20 m<sub>1</sub> is 1; P and Q are both hydrogen; R<sub>6</sub> is selected from group consisting of (C<sub>1</sub>-C<sub>8</sub>)-alkyl, aryl and a heterocyclic radical; or

wherein  $m_1$  is 1; P and Q are both hydrogen;  $R_6$  is aryl wherein the ring or ring system is unsubstituted or substituted as defined above; or

wherein  $R_6$  is phenyl wherein the ring or ring system is unsubstituted or substituted as defined above.

5

In one embodiment the present invention provides 11 $\beta$ -hydroxyandrosta-4-ene-3-one, a compound of formula I-B and physiologically acceptable salt thereof:



10

**Formula I-B**

— represents a single bond or double bond and

~~~~~ represents  $\alpha$  or  $\beta$ -configuration.

wherein

15 Z represents O, S;

R_1 represents hydrogen or methyl which may be either in α or β -configuration, or methylene;

R_2 and R_3 are the same or different and each independently represents hydrogen, halogen or a methyl group;

m_1 is 1, 2 or 3;

20 m_2 is 0 or 1;

m_3 is 0 or 1;

n_1 is 0, 1 or 2;

P and Q are independently selected from hydrogen, halogen and C_1 to C_3 alkyl;

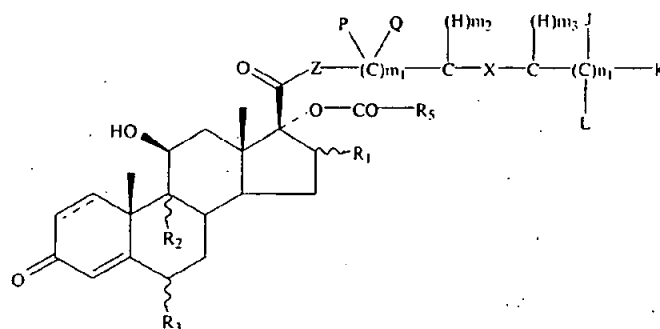
X represents either a double bond or a triple bond; and

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- J, K and L are independently selected from a group consisting of hydrogen, halogen, (C₁-C₁₀)-alkyl, (C₃-C₁₃)-cycloalkyl, -OH, -O-(C₁-C₁₀)-alkyl, -O-(C₃-C₁₃)-cycloalkyl, -OCO-(C₁-C₁₀)-alkyl, -OCO-(C₃-C₁₃)-cycloalkyl, -OCO-CO-O-(C₁-C₁₀)-alkyl, -OCO-CO-O-(C₃-C₁₃)-cycloalkyl, -OCO-O-(C₁-C₁₀)-alkyl, -OCO-O-(C₃-C₁₃)-cycloalkyl, -OCO-NH-(C₁-C₁₀)-alkyl, -OCO-NH-(C₃-C₁₃)-cycloalkyl, -OCO-N-[(C₁-C₁₀)-alkyl]₂, -OCO-N-[(C₃-C₁₃)-cycloalkyl]₂, -OCO-NHSO₂-(C₁-C₁₀)-alkyl, -OCO-NHSO₂-(C₃-C₁₃)-cycloalkyl, -CO-[(C₃-C₁₀)N-cyclo], -OCO-[(C₃-C₁₀)N-cyclo], -NH₂, -NH-(C₁-C₈)-alkyl, -N-[(C₁-C₈)-alkyl]₂, -NO₂, -CN, aryl and a heterocyclic radical as defined above;
- or J and K can be joined together with the carbon atom to which they are attached to represent a (C₃-C₁₃)-cycloalkyl or -CO- group and L is as defined above;
- R₅ represents a group selected from R₆, -O-R₆ or -N(R₈)R₆, wherein R₆ is as defined above and R₈ represents hydrogen, (C₁-C₆)-alkyl or (C₃-C₆)-cycloalkyl;
- In one embodiment the compounds of formula I-B are selected from the compounds wherein, m₁ is 1; P and Q are both hydrogen; X represents either a double bond or a triple bond; m₂ is 0; m₃ is 0; n₁ is 1 and J, K and L are independently selected from hydrogen, halogen, -OH, -OCO-(C₁-C₁₀)-alkyl and -OCO-O-(C₁-C₁₀)-alkyl.

Preferably,

- 11β-hydroxyandrost-4-ene-3-one, compound of formula I-B, and physiologically acceptable salt thereof:



Formula I-B

wherein

Z represents O or S;

R₁ represents hydrogen or methyl which may be either in α or β -configuration, or methylene;

R₂ and R₃ are the same or different and each independently represents hydrogen, halogen or a methyl group;

R₅ represents a group selected from (C₁-C₁₀)-alkyl, (C₃-C₁₃)-cycloalkyl,

-O-(C₁-C₁₀)-alkyl, aryl or heterocyclic ring wherein the ring or ring system is unsubstituted or substituted by one or more halogen, -OH, (C₁-C₃)-alkyl, -O-(C₁-C₃)-alkyl, (C₃-C₁₃)-cycloalkyl; wherein the alkyl or cycloalkyl groups can optionally contain one or more

unsaturations and/or can have one or more hetero atom incorporated therein and optionally in each case have one or more hydrogen atoms replaced by halogen, -OH, (C₁-C₃)-alkyl, -O-(C₁-C₃)-alkyl, (C₃-C₁₃)-cycloalkyl; and

m₁ is 1;

m₂ is 0 or 1;

m₃ is 0 or 1;

n₁ is 0, 1 or 2;

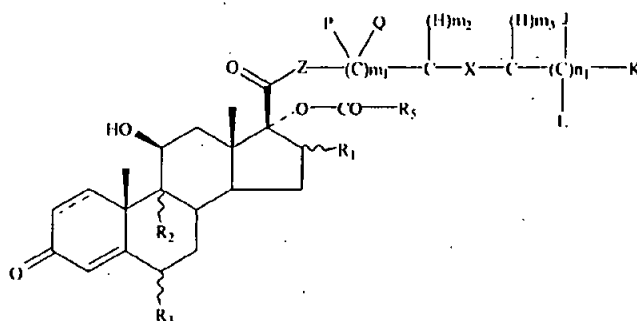
P and Q are hydrogen;

X represents either a double bond or a triple bond; and

J, K and L are independently selected from a group consisting of hydrogen, halogen, (C₁-C₁₀)-alkyl, (C₃-C₁₃)-cycloalkyl, -OH, -O-(C₁-C₁₀)-alkyl, -O-(C₃-C₁₃)-cycloalkyl, -OCO-(C₁-C₁₀)-alkyl, -OCO-(C₃-C₁₃)-cycloalkyl, -OCO-CO-O-(C₁-C₁₀)-alkyl, -OCO-CO-O-(C₃-C₁₃)-cycloalkyl, -OCO-O-(C₁-C₁₀)-alkyl, -OCO-O-(C₃-C₁₃)-cycloalkyl, -OCO-NH-(C₁-C₁₀)-alkyl, -OCO-NH-(C₃-C₁₃)-cycloalkyl, -OCO-N-[(C₁-C₁₀)-alkyl]₂, -OCO-N-[(C₃-C₁₃)-cycloalkyl]₂, -OCO-NHSO₂-(C₁-C₁₀)-alkyl, -OCO-NHSO₂-(C₃-C₁₃)-cycloalkyl, -NH₂, -NH-(C₁-C₈)-alkyl, N-[(C₁-C₈)-alkyl]₂, -NO₂ and -CN.

Most preferably,

11 β -hydroxyandrosta-4-ene-3-one, compound of formula I-B, and physiologically acceptable salt thereof.



Formula I-B

wherein

Z represents S;

5 R_1 represents hydrogen or methyl which may be either in α or β -configuration, or methylene;
 R_2 and R_3 are the same or different and each independently represents hydrogen, halogen or a methyl group;

R_5 represents a group selected from (C_1-C_{10}) -alkyl, (C_3-C_{13}) -cycloalkyl,

10 $-O-(C_1-C_{10})$ -alkyl, aryl or heterocyclic ring wherein the ring or ring system is unsubstituted or substituted by one or more halogen, $-OH$, (C_1-C_3) -alkyl, $-O-(C_1-C_3)$ -alkyl, (C_3-C_{13}) -cycloalkyl; wherein the alkyl or cycloalkyl groups can optionally contain one or more unsaturations and/or can have one or more hetero atom incorporated therein and optionally in each case have one or more hydrogen atoms replaced by halogen, $-OH$, (C_1-C_3) -alkyl, $-O-(C_1-C_3)$ -alkyl, (C_3-C_{13}) -cycloalkyl; and

15 m_1 is 1;

m_2 is 0;

m_3 is 0;

n_1 is 0, 1 or 2;

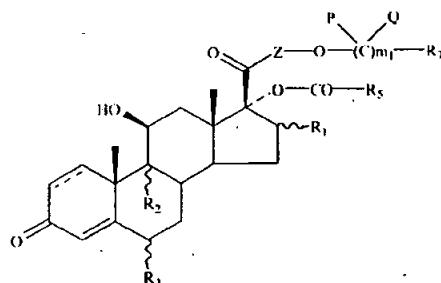
P and Q are hydrogen;

20 X represents a triple bond; and

J, K and L are independently selected from a group consisting of hydrogen, halogen, (C_1-C_{10}) -alkyl, (C_3-C_{13}) -cycloalkyl, $-OH$, $-O-(C_1-C_{10})$ -alkyl, $-O-(C_3-C_{13})$ -cycloalkyl, $-OCO-(C_1-C_{10})$ -alkyl, $-OCO-(C_3-C_{13})$ -cycloalkyl, $-OCO-CO-O-(C_1-C_{10})$ -alkyl, $-OCO-CO-O-(C_3-C_{13})$ -cycloalkyl, $-OCO-O-(C_1-C_{10})$ -alkyl, $-OCO-O-(C_3-C_{13})$ -cycloalkyl, $-OCO-NH-(C_1-C_{10})$ -alkyl.

-OCO-NH-(C₃-C₁₃)-cycloalkyl, -OCO-N-[(C₁-C₁₀)-alkyl]₂, -OCO-N-[(C₃-C₁₃)-cycloalkyl]₂, -OCO-NHSO₂-(C₁-C₁₀)-alkyl, -OCO-NHSO₂-(C₃-C₁₃)-cycloalkyl, -NH₂, -NH-(C₁-C₈)-alkyl, -N-[(C₁-C₈)-alkyl]₂, -NO₂ and -CN.

- 5 In one embodiment the present invention provides 11 β -hydroxyandrosta-4-ene-3-one, a compound of formula I-C and physiologically acceptable salt thereof:



Formula I-C

10

— represents a single or double bond and

~~~~~ represents  $\alpha$  or  $\beta$ -configuration.

wherein

Z represents S;

- 15 R<sub>1</sub> represents hydrogen or methyl which may be either in  $\alpha$  or  $\beta$ -configuration, or methylene;  
R<sub>2</sub> and R<sub>3</sub> are the same or different and each independently represents hydrogen, halogen or a methyl group;  
m<sub>1</sub> is 1, 2 or 3;  
P and Q are independently selected from hydrogen, halogen and C<sub>1</sub>-to-C<sub>3</sub> alkyl;  
20 R<sub>7</sub> represents a group selected from halogen, CO-aryl and R<sub>6</sub>, wherein the aryl ring of CO-aryl is unsubstituted or substituted by one or more substituents as defined above for the ring or ring system;  
R<sub>6</sub> represents a group selected from (C<sub>1</sub>-C<sub>8</sub>)-alkyl, (C<sub>3</sub>-C<sub>13</sub>)-cycloalkyl, aryl and a heterocyclic radical, where the ring or ring system is unsubstituted or substituted by one or more substituents  
25 selected from

(C<sub>1</sub>-C<sub>8</sub>)-alkyl, (C<sub>3</sub>-C<sub>13</sub>)-cycloalkyl, halogen, O-(C<sub>1</sub>-C<sub>8</sub>)-alkyl, O-(C<sub>3</sub>-C<sub>13</sub>)-cycloalkyl, OCO-(C<sub>1</sub>-C<sub>3</sub>)-alkyl, S(O)<sub>0-2</sub>(C<sub>1</sub>-C<sub>8</sub>)-alkyl, COO-(C<sub>1</sub>-C<sub>8</sub>)-alkyl, -OCO-O-(C<sub>1</sub>-C<sub>3</sub>)-alkyl, -OCO-CO-O-(C<sub>1</sub>-C<sub>3</sub>)-alkyl, CONH<sub>2</sub>, CONH-(C<sub>1</sub>-C<sub>8</sub>)-alkyl, CON-[(C<sub>1</sub>-C<sub>8</sub>)-alkyl]<sub>2</sub>, -NHCO-(C<sub>1</sub>-C<sub>8</sub>)-alkyl, N-(C<sub>1</sub>-C<sub>8</sub>)-alkyl-CO-(C<sub>1</sub>-C<sub>8</sub>)-alkyl, -NHCO-O-(C<sub>1</sub>-C<sub>8</sub>)-alkyl, 5 -N-(C<sub>1</sub>-C<sub>8</sub>)-alkyl-CO-O-(C<sub>1</sub>-C<sub>8</sub>)-alkyl, -NHCONH-(C<sub>1</sub>-C<sub>8</sub>)-alkyl, -N-(C<sub>1</sub>-C<sub>8</sub>)-alkyl-CONH-(C<sub>1</sub>-C<sub>8</sub>)-alkyl, -NHCONH-SO<sub>2</sub>-(C<sub>1</sub>-C<sub>8</sub>)-alkyl, -N-(C<sub>1</sub>-C<sub>8</sub>)-alkyl-CONH-SO<sub>2</sub>-(C<sub>1</sub>-C<sub>8</sub>)-alkyl, -NO<sub>2</sub>, -CN;

wherein the alkyl or cycloalkyl groups can optionally contain one or more unsaturations and/or can have one or more hetero atom incorporated therein and optionally, in each case have one or more hydrogen atoms replaced by -F, -Cl, -Br, -I, -OH, -OCO-(C<sub>1</sub>-C<sub>3</sub>)-alkyl, (C<sub>3</sub>-C<sub>13</sub>)-cycloalkyl, aryl or heterocyclic radical;

R<sub>5</sub> represents a group selected from R<sub>6</sub>, -O-R<sub>6</sub> or -N(R<sub>8</sub>)R<sub>6</sub>, wherein R<sub>6</sub> and R<sub>8</sub> are as defined above.

In one embodiment the compounds of formula I-C are selected from the compounds wherein m<sub>1</sub> is 1; P and Q are both hydrogen and R<sub>7</sub> represents R<sub>6</sub>, wherein, R<sub>6</sub> is selected from group consisting of (C<sub>1</sub>-C<sub>8</sub>)-alkyl or aryl wherein the ring or ring system is unsubstituted or substituted as defined above.

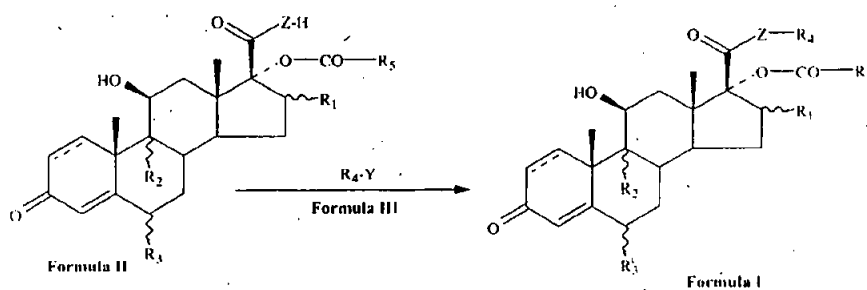
Physiologically acceptable salts are particularly suitable for medical applications, due to their greater solubility in water compared with the starting or base compounds. Suitable physiologically acceptable acid addition salts of the compounds of the invention may be salts of inorganic acids such as hydrochloric acid, hydrobromic acid, phosphoric acid, and the like or of organic acids such as, for example, acetic acid, benzenesulfonic acid, benzoic acid, citric acid and the like. Examples of suitable physiologically acceptable basic salts are ammonium salts, alkali metal salts such as sodium salts and potassium salts and alkaline earth metal salts such as magnesium salts and calcium salts.

The compounds of formula I are useful in human or veterinary medicine, in particular as anti-inflammatory and antiallergic agents.

The compounds of formula I have potentially beneficial anti-inflammatory or antiallergic effects, which are demonstrated by, for example, their ability to bind to the glucocorticoid receptor *in vitro*; and inhibit croton oil induced ear edema, cotton pellet induced granuloma, sephadex induced lung edema *in vivo* models, without causing systemic side effects like involution of thymus, enhanced deposition of glycogen in the liver, or appreciable change in body weight.

All references to compound(s) of the formula I herein refer to a compound/compounds of the formula (I) and to salt thereof.

- 10 The present invention provides process for preparation of the compounds of the formula I, comprising reacting the compound of formula II, with  $R_4$ -Y, a compound of formula III (Scheme-I):



----- represents a single or double bond and

~~~~~ represents  $\alpha$  or  $\beta$ -configuration.

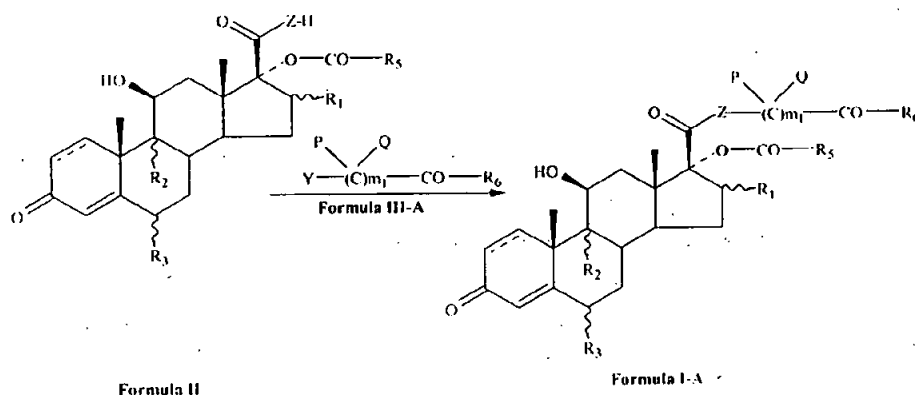
wherein Z represents O or S;

- 20 R_1 , R_2 , R_3 , R_4 and R_5 are as defined above; Y represents a leaving group;

In the compound of formula III, Y represents a suitable leaving group. A suitable leaving group is any group which upon reaction of a compound of formula II with the compound of formula III, facilitates formation of a compound of formula I. For example, Y may be halogen, alkylsulfonate

or arylsulfonate group, like methanesulfonate, *p*-toluenesulfonate or trifluoromethanesulfonate group.

- In one embodiment the present invention also provides a compound of formula I-A and a process for preparation of compound of formula IA comprising reacting a carboxylic acid compound of formula II-A (a compound of formula II, wherein Z is O) or a carbothioic acid compound of formula II-B (a compound of formula II, wherein Z is S) with a compound of formula III-A (Scheme-II):



Scheme-II

----- represents a single or double bond and

~~~~~ represents  $\alpha$  or  $\beta$ -configuration.

wherein Z represents O, S;

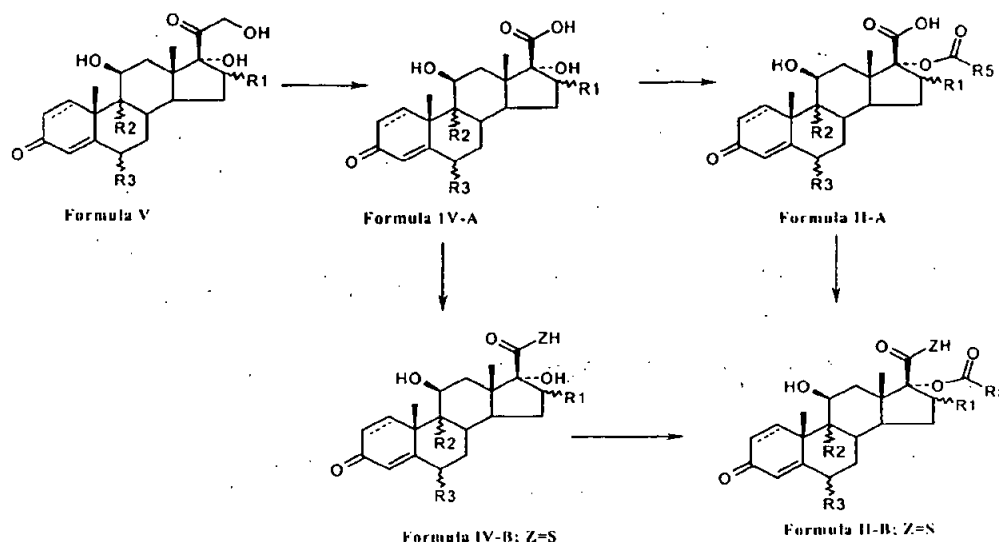
$R_1$ ,  $R_2$ ,  $R_3$ ,  $R_5$ ,  $R_6$ , Y, P, Q and  $m_1$  are as defined above;

- The reactions represented by Schemes I or II can be advantageously carried out in a suitable inert organic polar solvent or solvent system, for example, acetone, acetonitrile, *N,N*-dimethylformamide, *N,N*-dimethylacetamide, dimethyl sulfoxide and the like or mixture thereof, in presence of a suitable base, for example, alkali or alkaline earth metal carbonates like potassium carbonate, sodium carbonate, sodium bicarbonate and the like.

The starting compounds of formula II are either known in the art or can be prepared by following known methods, for example, Gordon J. Phillips et al., *J. Med. Chem.*, **37**, 3717-3729 (1994);

United States Patent No. 4335121; PCT publication No. WO 04/001369 or WO 04/039827, incorporated herein by reference.

Scheme-III represents a reaction sequence following which compound of formula II can be prepared.



Scheme-III

- 10 Preferably, the compounds of formula II-A ( compound of formula II, wherein Z is O) may be prepared by treating a compound of formula IV-A with compounds of formula  $R_5\text{COOH}$  or an active derivative thereof such as an activated ester, anhydride or halide thereof, especially an acid halide, for example, an acid chloride, in the presence of an organic base like triethylamine or an inorganic base like potassium carbonate. To obtain compounds of formula II-A, wherein  $R_5$
- 15 represents  $-\text{O}-R_6$  or  $-\text{N}(\text{R}_8)\text{R}_6$ , the compound of formula IV-A is reacted with corresponding  $\text{R}_6-\text{O}-\text{CO}-\text{Y}'$  or  $\text{R}_6(\text{R}_8)\text{N}-\text{CO}-\text{Y}'$  where  $\text{Y}'$  represents a leaving group such as a halide, 4-nitrophenolate etc, in the presence of an organic base like triethylamine or an inorganic base like potassium carbonate. To obtain compounds of formula II-A, where  $R_5$  represents  $-\text{N}(\text{R}_8)\text{R}_6$ , and  $\text{R}_8$  is hydrogen, the compound of formula IV-A can be reacted with the corresponding
- 20 isocyanate  $\text{OCN}-\text{R}_6$ . The compounds of formula IV-A may be prepared by oxidation of

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compounds of formula V in presence of of a chemical oxidizing agent like periodic acid or sodium periodate.

- 5 Preferably, the compounds of formula II-B ( compound of formula II, wherein Z is S) may be prepared from compound formula II-A by initial reaction with *N,N*-dimethylthiocarbamoyl chloride, followed by aminolysis of the resulting rearranged mixed anhydride with diethylamine, or methanolysis by methanol and potassium carbonate, or reaction with sodium hydrosulfide in a suitable solvent, for example, *N,N*-dimethylformamide.

10

- The compounds of formula II-B, where Z is S may also be prepared by treating a compound of formula IV-B with compounds of formula  $R_5\text{COOH}$  or an active derivative thereof such as an activated ester, anhydride or halide thereof, especially an acid halide, for example, an acid chloride, in the presence of an organic base like triethylamine or an inorganic abse like potassium carbonate. In compounds of formula II-B wherein  $R_5$  represents  $-\text{O}-R_6$  or  $-\text{N}(\text{R}_8)\text{R}_6$ ,  
15 the compound of formula IV-B is reacted with corresponding  $\text{R}_6-\text{O}-\text{CO}-\text{Y}'$  or  $\text{R}_6(\text{R}_8)\text{N}-\text{CO}-\text{Y}'$  where  $\text{Y}'$  represents a leaving group such as a halide, 4-nitrophenolate etc, in the in the presence of an organic base like triethylamine or an inorganic base like potassium carbonate.

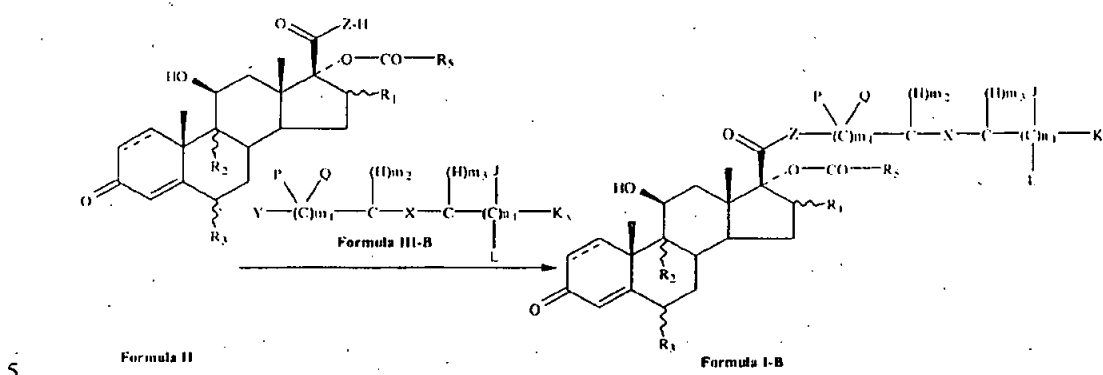
- 20 The compounds of formula IV-B, where Z is S may be prepared from compound formula IV-A by carbonyl activation with 1,1'-carbonyldiimidazole and reaction with hydrogen sulfide or sodium hydrosulfide in a suitable solvent, for example, *N,N*-dimethylformamide.

- The compounds of formula II may be conveniently used as acid addition salts thereof, preferably  
25 in crystalline form. Any suitable base addition salts can be used, for example, sodium or potassium salt.

The compound of formula III-A are known or may be prepared by methods known in the art.

- 30 In one embodiment the present invention provides a compound of formula I-B and a process for preparation thereof comprising reacting a carboxylic acid compound of formula II-A (a

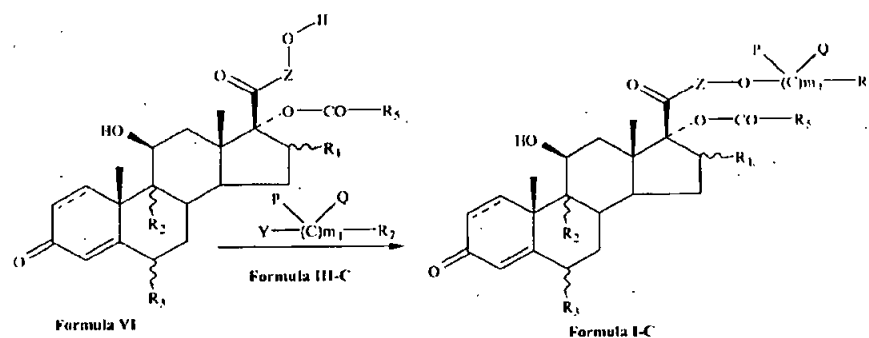
compound of formula II, wherein Z is O) or carbothioic acid compound of formula II-B (a compound of formula II, wherein Z is S) with a compound of formula III-B (Scheme-IV):



Scheme-IV

- represents a single or double bond and
- 10    ~~~~~ represents  $\alpha$  or  $\beta$ -configuration.
- wherein Z represents O or S;
- R<sub>1</sub>, R<sub>2</sub>, R<sub>3</sub>, R<sub>5</sub>, Y, P, Q, J, K, L, m<sub>1</sub> and n<sub>1</sub> are as defined above, X represents either a double bond or a triple bond, m<sub>2</sub> is 0 or 1 and m<sub>3</sub> is 0 or 1;
- 15    The compound of formula I-B can be prepared by alkylation of compound of formula II with compound of formula III-B, advantageously carried out in an inert organic polar solvent, for example, acetone, acetonitrile, *N,N*-dimethylformamide, *N,N*-dimethylacetamide, dimethyl sulfoxide and the like in presence of a suitable base, for example, alkali or alkaline earth metal carbonates like potassium carbonate, sodium carbonate, sodium bicarbonate and the like. The
- 20    compound of formula III-B are known or can be prepared by methods known in the art.

In one preferred embodiment, the present invention provides a compound of formula I-C and a process for preparation thereof comprising reacting a compound of formula VI with a compound of formula III-C (Scheme-V):



5

Scheme-V

==== represents a single or double bond and

~~~~~ represents  $\alpha$  or  $\beta$ -configuration.

wherein Z represents S;

10 $R_1, R_2, R_3, R_5, R_7, Y, P, Q$ and m_1 are as defined above;

The compound of formula I-C can be prepared by the alkylation of compound of formula VI with compound of formula III-C, advantageously carried out in an inert organic polar solvent, for example, acetone, acetonitrile, *N,N*-dimethylformamide, *N,N*-dimethylacetamide, dimethyl sulfoxide and the like in presence of a suitable base, for example, alkali or alkaline earth metal carbonates like potassium carbonate, sodium carbonate, sodium bicarbonate and the like. The compound of formula III-C are known or can be prepared by methods known in the art.

20 The compound of formula VI may be prepared by oxidation of compound of formula II-B with oxidizing agent, for example, hydrogen peroxide, urea-hydrogen peroxide, peracetic acid, *m*-chloroperbenzoic acid, sodium periodate and the like in a polar organic solvent such as methanol, ethanol, 2-propanol, acetic acid and the like.

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The compound of formula I and physiologically acceptable salt thereof can also be used as intermediates for preparation of derivatives thereof, for example, the -OH group can be converted to halo group or acetylated, sulfonated etc.

- 5 The present invention also relates to the dosage forms for local application depends on the precise type of formulation to be prepared but generally may be within the range of 0.001 to 10% by weight. Generally, however for most types of preparations advantageously the proportion used will be within the range of 0.005 to 1% and preferably 0.01 to 0.5%. However, in powders for inhalation or insufflation the proportion used may be within the range of 0.1 to 5%. The daily
10 dose may vary and would be dependent on the condition being treated, and the duration of treatment desired.

- In one embodiment, the amount of a compound according to formula I used to attain the desired biological effect depends on a number of factors, for example the specific compound selected,
15 the intended use, the type of administration and the clinical state of the patient. In general, the daily dose is in the range of 0.01mg to 500mg (typically from 0.1mg to 10mg). Orally administrable individual dose formulations such as, for example, tablets or capsules can contain, for example, from 0.1mg to 500mg, typically from 1mg to 100mg.

- 20 In the case of physiologically acceptable salts, the above mentioned masses relate to the mass of the free compound on which the addition salt is based. The compounds used for the prophylaxis or therapy may be the compounds according to formula I themselves, or, in one embodiment, they are present in the form of a pharmaceutical composition together with an acceptable carrier. In one embodiment, the carrier must be naturally acceptable, in the sense that it is compatible
25 with the other ingredients of said composition and is not harmful to the patient's health. The carrier may be a solid or a liquid or both and is preferably formulated with the compound as an individual dose, for example as a tablet that may contain from 0.05% to 95% by weight of the active compound. The pharmaceutical compositions of the invention may be prepared according to any of the known pharmaceutical methods which essentially comprise mixing the ingredients
30 with pharmacologically acceptable carriers and/or excipients.

Another aspect of the present invention relates to formulation of compounds of formula I in a suitable form for administration to a subject.

Pharmaceutical compositions of the invention are those which are suitable for oral, rectal, topical, peroral (e.g. sublingual) and parenteral (e.g. subcutaneous, intradermal or intraarticular) administration, although the most suitable manner of administration depends in each individual case on the nature and severity of the condition to be treated and on the nature of the compound according to formula I used in each case. Sugar-coated formulations and sugar-coated delayed-release formulations, too, are included within the scope of the invention. In one embodiment, preference is given to acid-resistant and enteric formulations. Suitable enteric coatings include cellulose acetate phthalate, polyvinyl acetate phthalate, hydroxypropylmethylcellulose phthalate and anionic polymers of methacrylic acid and methyl methacrylate.

Suitable pharmaceutical compounds for oral administration may be present in separate units as, for example, capsules, cachets, lozenges or tablets, which in each case contain a particular amount of the compound according to formula I; as powders or granules; as solution or suspension in an aqueous or non-aqueous liquid; or as an oil-in-water or water-in-oil emulsion. These compositions can be prepared according to any suitable pharmaceutical method which includes a step in which the active compound and the carrier (which may comprise one or more additional components) are contacted. In general, the compositions are prepared by uniform and homogeneous mixing of the active compound with a liquid and/or finely dispersed solid carrier, after which the product is shaped, if necessary. Thus a tablet, for example, may be prepared by pressing or shaping a powder or granules of the compound, where appropriate with one or more additional components. Pressed tablets can be prepared by tableting the compound in free-flowing form, for example a powder or granules, mixed, where appropriate, with a binder, lubricant, inert diluent and/or one or more surface active/dispersing agents in a suitable machine. Shaped tablets can be prepared by shaping the pulverulent compound, moistened with an inert liquid diluent, in a suitable machine.

Pharmaceutical compositions which are suitable for peroral (sublingual) administration include lozenges which contain a compound according to formula I with a flavoring agent, usually

sucrose and gum arabic or tragacanth, and pastilles which comprise the compound in an inert base such as gelatin and glycerol or sucrose and gum arabic.

5 Suitable pharmaceutical compositions for parenteral administration may, for example, comprise sterile preparations of a compound according to formula I. These preparations may be administered intradermally, although they may also be administered subcutaneously, intramuscularly or intraarticularly as an injection. These preparations may be prepared by mixing the compound with water and rendering the obtained solution sterile. Injectable compositions of the invention generally contain from 0.01 to 5% by weight of the active compound.

10

Suitable pharmaceutical compositions for rectal administration are present as individual dose suppositories. These may be prepared by mixing a compound according to formula I with one or more conventional solid carriers, for example cocoa butter, and shaping the resulting mixture.

15 Suitable pharmaceutical compositions for topical application to the skin may be present as ointment, cream, lotion, paste, spray, aerosol or oil. The carriers which may be used include, for example, petroleum jelly, lanolin, polyethylene glycols, alcohols and combinations of two or more of these substances. In one embodiment, the active compound is present at a concentration ranging from 0.1 to 15%, for example from 0.5 to 2%, by weight of the composition.

20

Transdermal administration is also possible. Suitable pharmaceutical compositions for transdermal administration may be present as individual patches, which are suitable for long-term close contact with the epidermis of the patient. Such patches suitably contain the active compound in an optionally buffered aqueous solution, dissolved and/or dispersed in an adhesive or dispersed in a polymer. A suitable active compound concentration is from approx. 0.1% to 25 35%, preferably approx. 1 to 15%. A particular possibility is the release of the active compound by electro-transport or ionophoresis, as described, for example, in Pharmaceutical Research, 2(6): 318 (1986).

30 In one preferred embodiment the compounds of formula I are adapted for local administration. Local administration as used herein includes administration by insufflations and inhalation. The

various types of dosage forms useful for local administration include ointments, lotions, creams, gels, foams, preparations for transdermal delivery by patches, powders, sprays, aerosols, capsules or cartridges for use in inhaler or insufflator or drops (for example, eye or nose drops), solution/suspensions for nebulisation, suppositories, pessaries, retention enemas and chewable or
5 suckable tablets or pellets or microencapsulation preparations.

Ointments, creams and gels, may for example, be formulated with an aqueous or oily base with the addition of suitable thickening and/or gelling agent and/or solvents. Such bases may thus, for example, include water and/or oil such as liquid paraffin or a vegetable oil such as arachis oil or
10 castor oil, or a solvent such as polyethylene glycol. Thickening agents and gelling agents which may be used according to the nature of the base include soft paraffin, aluminum stearate, cetostearyl alcohol, polyethylene glycols, woolfat, beeswax, carboxypolymethylene and cellulose derivatives, and/or glyceryl monostearate and non-ionic emulsifying agents.

15 Powders for external application may be formed with the aid of any suitable powder base, for example, talc, lactose or starch. Drops may be formulated with an aqueous or non aqueous base also comprising agents, solubilizing agents, suspending agents or preservatives.

Spray compositions may for example be formulated as aqueous solution or suspensions or as
20 aerosols delivered from pressurized packs, such as a metered dose inhaler, with the use of a suitable liquefied propellant. Aerosol compositions suitable for inhalation can be either a suspension or a solution and generally contain a compound of formula I and suitable propellant such as a fluorocarbon or hydrogen containing chlorofluorocarbon or mixtures thereof, particularly hydrofluoroalkanes, especially 1,1,1,2-tetrafluoroethane, 1,1,1,2,3,3,3-heptafluoro-*n*-
25 propane or a mixture thereof. The aerosol composition may optionally contain additional formulation excipients well known in the art such as surfactants e.g. oleic acid or lecithin and co solvents e.g. ethanol.

Advantageously, the formulations of the invention may be buffered by the addition of suitable
30 buffering agents.

Capsules and cartridges for use in an inhaler or insufflator, for example gelatine, may be formulated containing a powder mix or for inhalation of a compound of the invention suitable powder base such as lactose or starch. Each capsule or cartridge may generally contain between 20µg-1000µg of the compound of formula I. Alternatively, the compound of the invention may be presented without excipients such as lactose.

The proportion of the active compound of formula I in the local compositions according to the invention depends on the precise type of formulation to be prepared but will generally be within the range of from 0.001 to 10% by weight. Generally, however for most types of preparations advantageously the proportion used will be within the range of from 0.005 to 1% and preferably 0.01 to 0.5%. However, in powders for inhalation or insufflation the proportion used will be within the range of from 0.1 to 5%.

Aerosol formulations are preferably arranged so that each metered dose or "puff" of aerosol contains 20µg-2000µg, preferably about 20µg-500µg of a compound of formula I. Administration may be once daily or several times daily, for example 2, 3, 4 or 8 times, giving for example 1, 2 or 3 doses each time. The overall daily dose with an aerosol will be within the range 100µg-1000µg preferably, 200µg-2000µg. The overall daily dose and the metered dose delivered by capsules and cartridges in an inhaler or insufflator will generally be double those with aerosol formulations.

Topical preparation may be administered by one or more applications per day to the affected area, occlusive dressing may advantageously be used. A continuous or prolonged delivery may be achieved by an adhesive reservoir system.

A pharmaceutical composition may be a solution or suspension comprising a therapeutically effective concentration of compound of formula I, with or without other bioactives in pharmaceutically effective concentrations. The composition may additionally comprise of various pharmaceutically acceptable excipients such as chelating agents, pH modifiers, buffers, viscosity enhancers, isotonicity agents, solubilizers, preservatives, antioxidants and the like.

A compound of formula I may be formulated in the form of drug delivery systems such as gel forming solutions.

For internal administration the compounds according to the invention may, for example, be formulated in conventional manner for oral, parenteral or rectal administration. Formulation for oral administration include syrups, elixirs, powders, granules, tablets and capsules which typically contain conventional excipients such as binding agents, fillers, lubricants, disintegrants, wetting agents, suspending agents, emulsifying agents, preservatives, buffer salts, flavoring, coloring and/or sweetening agents as appropriate. Dosage unit forms are, however, preferred as described below.

Slow release or enteric coated formulations may be advantageous, particularly for inflammatory bowel disorders.

Preferred forms of preparation for internal administration are dosage unit forms i.e. tablets and capsules. Such dosage unit forms contain from 0.01mg to 20mg preferably from 2.5mg to 10mg of the compounds of the invention.

The present invention provides a pharmaceutical composition comprising 11 β -hydroxyandrost-4-ene-3-one, a compound of formula I and physiologically acceptable salt thereof.

The present invention in one embodiment provides a pharmaceutical composition comprising 11 β -hydroxyandrost-4-ene-3-one; a compound of formula I-A, and physiologically acceptable salt thereof.

The present invention in one embodiment provides a pharmaceutical composition comprising 11 β -hydroxy androst-4-ene-3-one, a compound of formula I-B, physiologically acceptable salt thereof.

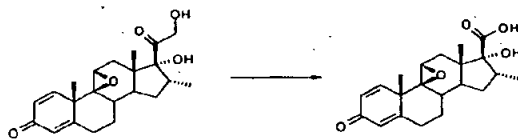
The present invention in one embodiment provides a pharmaceutical composition comprising 11 β -hydroxyandrost-4-ene-3-one, a compound of formula I-C, and physiologically acceptable salt thereof.

5 The invention is illustrated but not restricted by the description in the following examples.

EXAMPLES

10 Example 1

9,11-Epoxy-17 α -hydroxy-16 α -methyl-3-oxandrosta-1,4-diene-17 β -carboxylic acid

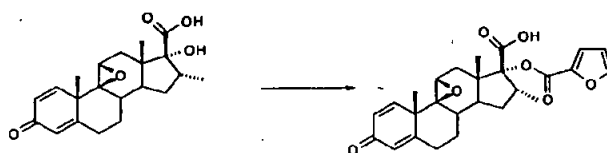


A solution of periodic acid (4.59g, 0.0201mol) in water (25ml) (prepared by heating to 50-55°C and then cooling to 30-35°C) was added dropwise to a stirred suspension of 17 α ,21-dihydroxy-9,11-epoxy-16 α -methylpregna-1,4-diene-3,20-dione (5.0g, 0.0134mol) in tetrahydrofuran (25ml) at 0-5°. The reaction mixture was stirred at 0-5°C for 2hrs, water was added to the reaction mixture at 0-5°C. The precipitated product was filtered, washed with water, and dried to yield the title compound as white solid (4.75g, 98.7%).

20 ¹H NMR (400 MHz in CDCl₃), δ : 0.92(d, J =6.99Hz, 3H), 1.04(s, 3H), 1.29-1.36(m, 1H), 1.44(s, 3H), 1.41-1.82(m, 4H), 2.12-2.94(m, 6H), 3.19(s, 1H), 3.55-3.65(m, 1H), 6.11(s, 1H), 6.14(dd, J_1 =10.09Hz; J_2 =1.68Hz, 1H), 6.60(d, J =10.06Hz, 1H).

Example 2

25 **9,11-Epoxy-17 α -[(2-furanylcarbonyl)oxy] 16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carboxylic acid**

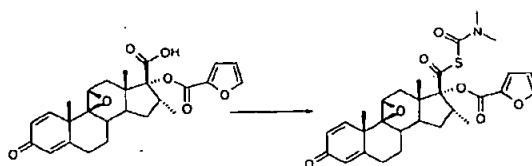


To suspension of 9,11-epoxy-17 α -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carboxylic acid (4.5g, 0.012mol) in acetone (25ml) at 10-15°C was added sequentially triethylamine (5.3ml, 0.038mol) and 2-furoyl chloride (4.96g, 0.038mol). After stirring for 4 hrs at 25-30°C, diethylamine (2.63ml, 0.025mol) was added dropwise at 10-15°C and then stirred at ambient temperature for 1hr. Thereafter the reaction mixture was acidified to pH 1.0-1.5 at 0-5°C, the precipitated product was filtered, washed with water, and dried to yield the title compound as white solid (5.96g, 99%).

¹H NMR (400 MHz in CDCl₃+DMSO-d₆), δ : 0.98(d, J =7.09Hz, 3H), 1.07(s, 3H), 1.25-1.48(m, 2H), 1.46(s, 3H), 1.66-1.81(m, 3H), 2.02-2.74(m, 6H), 3.26(s, 1H), 3.26-3.32(m, 1H), 6.19(s, 1H), 6.22(dd, J_1 =10.13Hz, J_2 =1.76Hz, 1H), 6.53(dd, J_1 =3.44Hz, J_2 =1.61Hz, 1H), 6.64(d, J =10.04Hz, 1H), 7.15(d, J =3.37Hz, 1H), 7.62(d, J =0.81Hz, 1H).

Example 3

17 β -[(*N,N*-Dimethylcarbamoyl)thio]carbonyl-9,11-epoxy-17 α -[(2-furanylcabonyl)oxy]-16 α -methyl-3-oxoandrosta-1,4-diene



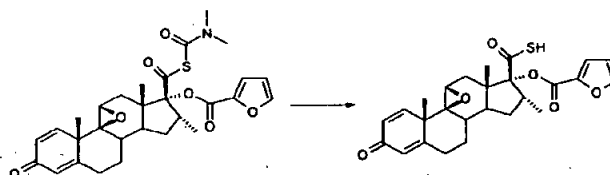
A solution of 9,11-epoxy-17 α -[(2-furanylcabonyl)oxy] 16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carboxylic acid (7.0g, 0.0129mol) and *N,N*-dimethylthiocarbamoyl chloride (2.74g, 0.0259mol) in tetrahydrofuran (35ml) was cooled to 10 to 15°C and treated with triethylamine (2.86g, 0.0283mol) and tetrabutylammonium iodide (0.5g). The reaction mixture was then warmed to ambient temperature, stirred for 4hrs and then added *N,N*-dimethylacetamide (21ml) followed by water (140ml). The resultant mixture was cooled to 0°C, the product filtered, washed with water and dried to yield the title compound as light yellow solid. (6.6g, 79.1%).

¹H NMR (400 MHz in CDCl₃+DMSO-d₆), δ 1.01(d, J =7.11Hz, 3H), 1.15(s, 3H), 1.41-1.49(m, 2H), 1.46(s, 3H), 1.72-1.87(m, 3H), 2.19-2.73(m, 6H), 3.06(s, 3H), 3.16(s, 3H), 3.30(s, 1H), 3.30-3.32(m, 1H), 6.19(s, 1H), 6.22(dd, J_1 =10.02Hz, J_2 =1.74Hz, 1H), 6.58(dd, J_1 =3.51Hz, J_2 =1.68Hz, 1H), 6.64(d, J =10.09Hz, 1H), 7.22(d, J =3.51Hz), 7.67(d, J =0.90Hz, 1H).

5

Example 4

9,11-Epoxy-17 α -[(2-furanylcarbonyl)oxy]-17 α -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioic acid

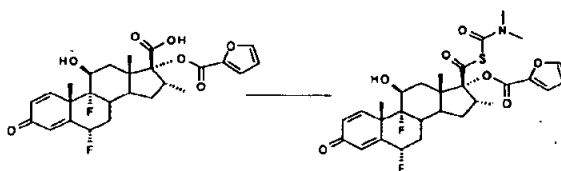


10 A suspension of 17 β -[(*N,N*-dimethylcarbamoyl)thio]carbonyl-9,11-epoxy-17 α -[(2-furanylcarbonyl)oxy]-16 α -methyl-3-oxoandrosta-1,4-diene (5.0g, 0.0106 mol) and potassium carbonate (2.94g, 0.0213mol) in methanol (25ml) was stirred at ambient temperature for 5hrs under a blanket of nitrogen. Thereafter, water was added to the reaction mixture and the resultant clear solution was washed with toluene. The aqueous layer containing the product was
15 charcoalized and then acidified with 2N HCl until pH was 1.5 to 2.0. The precipitated product was filtered, washed with water, and dried to yield the title compound as an off-white solid (3.6g, 83%).

¹H NMR (400 MHz in CDCl₃), δ 1.01(d, J =7.11Hz, 3H), 1.12(s, 3H), 1.36-1.48(m, 2H), 1.46(s, 3H), 1.72-1.81(m, 3H), 2.18-2.69(m, 6H), 3.28-3.31(m, 1H), 3.31(s, 1H), 6.21(s, 1H), 6.25(dd, J_1 =10.08Hz, J_2 =1.76Hz, 1H), 6.55(dd, J_1 =3.48Hz, J_2 =1.61Hz, 1H), 6.63(d, J =10.06Hz, 1H),
20 7.23(dd, J_1 =3.45Hz, J_2 =0.58Hz, 1H), 7.64(d, J =0.97Hz, 1H).

Example 5

25 **17 β -[(*N,N*-Dimethylcarbamoyl)thio]carbonyl-6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene**

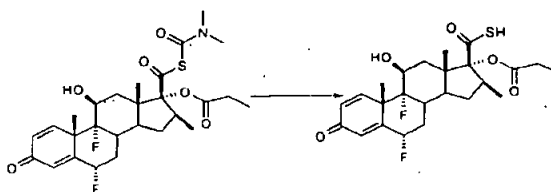


To a solution of 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carboxylic acid (12.3g, 0.025mol) and *N,N*-dimethylthiocarbamoyl chloride (9.29g, 0.075mol) in tetrahydrofuran (60ml) was added triethylamine (10.48ml, 0.075mol) at 10-15°C and tetrabutylammonium iodide (0.92g) and the mixture stirred for 4hrs at ambient temperature. Dimethylacetamide (37ml) and water (310ml) were added to the reaction mixture and stirred for 2hrs at 0°C. The solid obtained was filtered, washed with water and dried to yield the title compound as a white solid (14.3g, 99%).

¹H NMR (400 MHz in CDCl₃+DMSO-d₆), δ : 1.00(d, J =7.10Hz, 3H), 1.19(s, 3H), 1.30-1.36(m, 1H), 1.54(s, 3H), 1.63-2.00(m, 3H), 2.22-2.60(m, 4H), 3.03(s, 3H), 3.16(s, 3H), 3.31-3.36(m, 1H), 4.29(d, J = 8.91Hz, 1H), 5.39(br-s, 1H), 5.43-5.59(m, 1H), 6.22(s, 1H), 6.27(dd, J_1 =10.15Hz, J_2 =1.75Hz, 1H), 6.60(dd, J_1 =3.49Hz, J_2 =1.70Hz, 1H), 7.15(d, J =3.46Hz, 1H), 7.26(d, J =9.85Hz, 1H), 7.80(d, J =0.92Hz, 1H).

Example 6

6 α ,9 α -Difluoro-11 β -hydroxy-16 β -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioic acid



A suspension of 17 β -[(*N,N*-dimethylcarbamoyl)thio]carbonyl-6 α ,9 α -difluoro-11 β -hydroxy-16 β -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene (5.0g, 9.27 mmol) in 75ml diethylamine was heated under reflux for 8hrs. The cooled reaction mixture was poured in to ice-water acidified with 2N HCl to pH 2 and extracted with ethyl acetate. The ethyl acetate extract was washed with

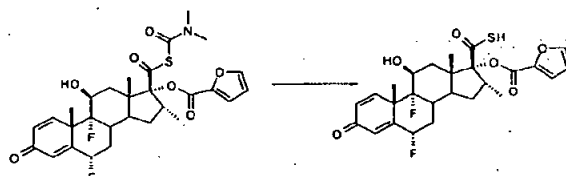
water, dried, and concentrated *in vacuo*. The residue obtained was crystallized from ethyl acetate to give the title compound as light yellow solid (3.2g, 73.7%)

¹H NMR (400 MHz in CDCl₃), δ: 1.06(s, 3H), 1.16(t, *J*=7.52Hz, 3H), 1.20-1.25(m, 1H), 1.39(d, *J*=7.23Hz, 3H), 1.54(s, 3H), 1.67-2.05(m, 4H), 2.22-2.80(m, 4H), 2.39(q, *J*=7.69Hz, 2H),
5 4.45(br-d, *J*=7.69Hz, 1H), 5.30-5.50(m, 1H), 6.38(d, *J*=9.93Hz, 1H), 6.43(s, 1H), 7.15(dd, *J*=10.17Hz, 1H).

In an analogous manner was prepared 6α,9α-difluoro-17α-[(2-furanylcarbonyl)oxy]-11β-hydroxy-16β-methyl-3-oxoandrosta-1,4-diene-17β-carbothioic acid.

10 Example 7

6α,9α-Difluoro-17α-[(2-furanylcarbonyl)oxy]-11β-hydroxy-16α-methyl-3-oxoandrosta-1,4-diene-17β-carbothioic acid



A suspension of 17β-[(*N,N*-dimethylcarbamoyl)thio]carbonyl-6α,9α-difluoro-17α-[(2-furanylcarbonyl)oxy]-11β-hydroxy-16α-methyl-3-oxoandrosta-1,4-diene (14.2g, 0.024mol) and
15 potassium carbonate (6.78g, 0.0491mol) in methanol (70ml) was stirred at ambient temperature for 6hrs under a blanket of nitrogen. Thereafter, water was added to the reaction mixture and the resultant clear solution was washed with toluene. The aqueous layer containing the product was charcoalized and then acidified with 2N HCl until pH was 1.5 to 2.0. The precipitated product
20 was filtered, washed with water, and dried to yield the title compound as white solid (11.8g, 94.8%).

¹H NMR (400 MHz in CDCl₃+DMSO-d₆), δ: 1.03(d, *J*=7.17Hz, 3H), 1.20(s, 3H), 1.31-1.37(m, 1H), 1.56(s, 3H), 1.73-2.03(m, 3H), 2.28-2.59(m, 4H), 3.37-3.42(m, 1H), 4.35-4.38(br-d, 1H),
4.89(d, *J*=1.22Hz, 1H), 5.34-5.51(m, 1H), 6.34(dd, *J*₁=10.06Hz, *J*₂=1.88Hz, 1H), 6.39(s, 1H),
25 6.53(dd, *J*₁=3.45Hz, *J*₂=1.73Hz, 1H), 7.14(dd, *J*₁=3.28Hz, *J*₂=0.49Hz, 1H), 7.25(dd, *J*₁=10.12Hz, *J*₂=1.30Hz, 1H), 7.63(dd, *J*₁=1.73Hz, *J*₂=0.63Hz, 1H).

The following 17 β -carbothioic acids were prepared by an analogous method to example 7:

- 9 α -Fluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioic acid.
- 5
- 6 α ,9 α -Difluoro-11 β -hydroxy-16 α -methyl-17 α -[(3-methyl-2-furanylcarbonyl)oxy]-3-oxoandrosta-1,4-diene-17 β -carbothioic acid.
- 6 α ,9 α -Difluoro-17 α -[(3-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioic acid.
- 10
- 6 α ,9 α -Difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -[(2-thienylcarbonyl)oxy]-androsta-1,4-diene-17 β -carbothioic acid.
- 15
- 17 α -[(5-Chloro-2-thienylcarbonyl)oxy]-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioic acid.
- 17 α -Cyclopropylcarbonyloxy-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioic acid.
- 20
- 17 α -Cyclobutylcarbonyloxy-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioic acid.
- 17 α -Cyclopentylcarbonyloxy-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioic acid.
- 25
- 17 α -Cyclohexylcarbonyloxy-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioic acid.

- 17 α -Cyclohexylmethylcarbonyloxy-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioic acid.
- 5 9 α -Fluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioic acid.
- 9 α -Fluoro-11 β -hydroxy-16 β -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioic acid.
- 10 6 α ,9 α -Difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioic acid.
- 6 α ,9 α -Difluoro-11 β -hydroxy-16 β -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioic acid.
- 15 17 α -Butyryloxy-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioic acid.
- 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -valeryloxyandrosta-1,4-diene-17 β -carbothioic acid.
- 20 6 α ,9 α -Difluoro-11 β -hydroxy-16 α -methyl-17 α -(2-methylpropionyl)oxy-3-oxoandrosta-1,4-diene-17 β -carbothioic acid.
- 25 17 α -Dichloroacetoxo-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioic acid.
- 6 α ,9 α -Difluoro-11 β -hydroxy-17 α -(methoxymethylcarbonyl)oxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioic acid.
- 30

163

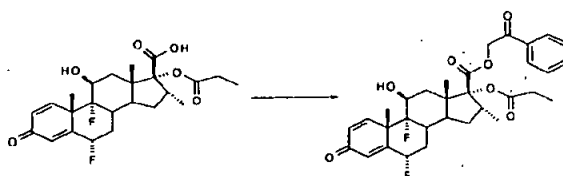
6 α ,9 α -Difluoro-17 α -(ethoxymethylcarbonyl)oxy-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioic acid.

17 α -(Ethoxycarbonyl)oxy-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioic acid.

6 α ,9 α -Difluoro-17 α -(ethoxycarbonyl)oxy-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioic acid.

10 **Example 8- Compound IA.44**

2-Phenyl-2-oxoethyl 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carboxylate



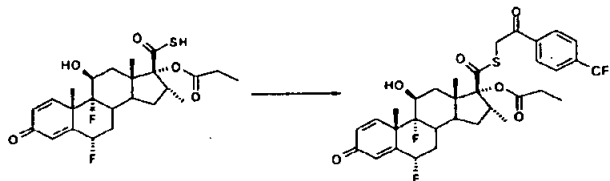
2-Bromo-1-phenylethanone (0.438g, 2.2mmol) and sodium iodide (50mg) were added to a stirred mixture of 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxy-androsta-1,4-diene-17 β -carboxylic acid (1.0g, 2.20mmol) and anhydrous potassium carbonate (0.360g, 2.6mmol) in acetone (15ml). The mixture was stirred under a blanket of nitrogen at 25 to 30°C for 8hrs, then poured into water and extracted with ethyl acetate. The organic layer was washed twice with water, dried, and concentrated *in vacuo*. The residue was purified by column chromatography (40% ethyl acetate in hexane) to yield the title compound as a white solid.

The following compounds were prepared in a manner similar to example 8 using an appropriate carboxylic acid of formula II and compound of formula III-A:

IA.1, IA.2, IA.4, IA.5, IA.7 to IA.10, IA.12, IA.15 to IA.19, IA.21, IA.23 to 25, IA.28 to 30, IA.32, IA.33, IA.36, IA.37, IA.42, IA.46, IA.48, IA.50, IA.52, IA.54, IA.57, IA.60, IA.62 to 25 IA.67, IA.71, IA.72, IA.74, IA.76, IA.77, IA.80, IA.82, IA.84, IA.87, IA.91, IA.103, IA.115, IA.118, IA.121, IA.133.

Example 9- Compound IA.38

***S*-[2-Oxo-2-(4-trifluoromethylphenyl)ethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate**



5

A mixture of 2-bromo-1-(4-trifluoromethylphenyl)ethan-1-one (0.569g, 2.13mmol), 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioic acid (1.0g, 2.13mmol) and anhydrous potassium carbonate (0.295g, 2.13mmol) in acetone (25ml) was stirred under a blanket of nitrogen at 25 to 30°C for 3hrs. The reaction mixture was then poured into water and extracted with ethyl acetate. The organic layer was washed with water, dried, and concentrated *in vacuo*. The residue was purified by column chromatography (40% ethyl acetate in hexane) to yield the title compound as a white solid.

10

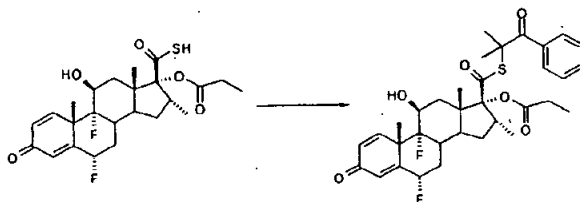
The following compounds were prepared in a manner similar to example 9 using an appropriate thioic acid of formula II and compound of formula III-A:

15 IA.3, IA.6, IA.11, IA.13, IA.14, IA.20, IA.22, IA.26, IA.27, IA.31, IA.34, IA.35, IA.39, IA.40, IA.43, IA.45, IA.47, IA.49, IA.51, IA.53, IA.55, IA.56, IA.58, IA.59, IA.61, IA.63, IA.68 to IA.70, IA.73, IA.75, IA.78, IA.79, IA.81, IA.83, IA.85, IA.86, IA.88 to IA.90, IA.92 to IA.102, IA.104 to IA.108, IA.110 to IA.114, IA.116, IA.117, IA.119, IA.120, IA.122 to IA.124, IA.126 to IA.132, IA.134 to IA.186, IA.198.

20

Example 10- Compound IA.59

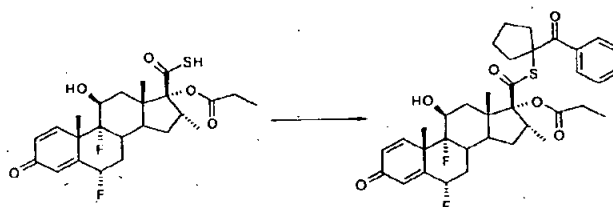
***S*-[1,1-Dimethyl-2-oxo-2-phenylethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate**



- 2-Bromo-2-methyl-1-phenyl-propan-1-one (0.483g, 2.13mmol) was added to a stirred mixture of 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioic acid (1.0g, 2.13mmol) and anhydrous potassium carbonate (0.295g, 2.13mmol) in acetone (20ml) and the mixture was stirred under a blanket of nitrogen at 25 to 30°C for 3hrs.
- 5 The reaction mixture was then poured into water and extracted with ethyl acetate. The organic layer was washed with water, dried, and concentrated *in vacuo*. The residue was purified by column chromatography (40% ethyl acetate in hexane) to yield the title compound as a white solid.
- 10 The following compounds were prepared in a manner similar to example 10 using an appropriate thioic acid of formula II and compound of formula III-A:
IA.109, IA.187 to IA.197.

Example 11- Compound IA-1.2

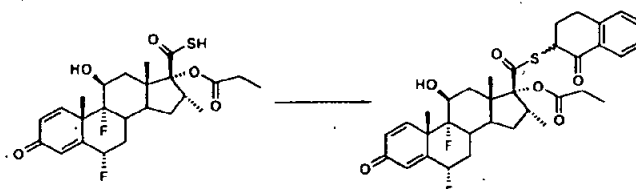
- 15 **S-(1-Benzoylcyclopentyl) 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate**



- (1-Bromocyclopentyl) phenyl methanone (0.539g, 2.13mmol) was added to a stirred mixture of 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioic acid (1.0g, 2.13mmol) and anhydrous potassium carbonate (0.295g, 2.13mmol) in acetone (25ml), and the mixture was stirred under a blanket of nitrogen at 25 to 30°C for 3hrs.
- 20 The reaction mixture was then poured into water and extracted with ethyl acetate. The organic layer was washed with water, dried, and concentrated *in vacuo*. The residue was purified by column chromatography (35% ethyl acetate in hexane) to yield the title compound as a white solid.
- 25 The compound IA-1.1 was prepared in a manner similar to example 11.

Example 12- Compound IA-2.1

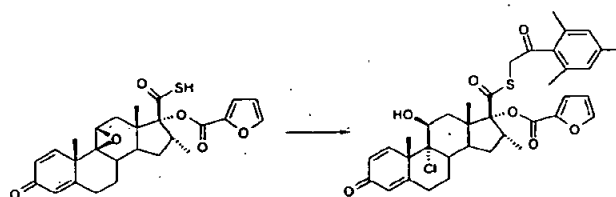
***S*-(1-Oxo-1,2,3,4-tetrahydronaphthalen-2-yl) 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-17 α -propionyloxy-3-oxoandrosta-1,4-diene-17 β -carbothioate**



- 5 2-Bromo-1-tetralone (0.395g, 1.75mmol) was added to a stirred mixture of 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioic acid (0.500g, 1.06mmol) and anhydrous potassium carbonate (0.161g, 1.17mmol) in acetone (10ml) and the mixture was stirred under a blanket of nitrogen at 25 to 30°C for 3hrs. The reaction mixture was then poured into water and extracted with ethyl acetate. The organic layer was washed with
10 water, dried, and concentrated *in vacuo*. The residue was purified by column chromatography (40% ethyl acetate in hexane) to yield the title compound as a white solid.

Example 13- Compound IA.41

- 15 ***S*-[2-Oxo-2-(2,4,6-Trimethylphenyl)ethyl] 9 α -chloro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate**

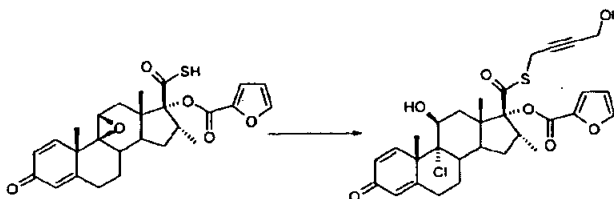


- 2-Bromo-1-(2,4,6-trimethylphenyl)ethanone (0.287g, 1.13mmol) was added to a stirred mixture of 9,11-epoxy-17 α -[(2-furanylcarbonyl)oxy]-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioic acid (0.600g, 1.28mmol) and anhydrous potassium carbonate (0.194g, 1.40mmol) in acetone (25ml) and the mixture was stirred under a blanket of nitrogen at 25 to 30°C for 2.5hrs. The reaction mixture was then poured into water and extracted with ethyl acetate. The organic layer was washed with water, dried, and concentrated *in vacuo*. The crude solid was dissolved in glacial acetic acid (10ml) and concentrated hydrochloric acid (1ml) was added at 10-15°C. The mixture was stirred at 15-20°C for 30 min, poured into ice-water (400ml), the product filtered.

washed with water, and finally dried in air oven. The crude solid was purified by column chromatography (35% ethyl acetate in hexane) to yield the title compound as a white solid.

Example 14- Compound IB.45

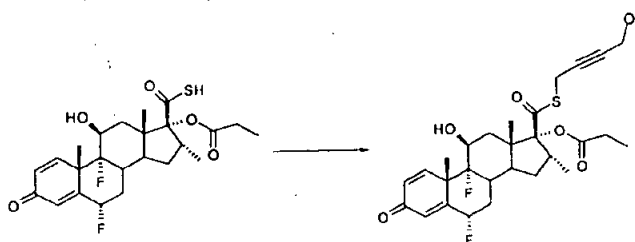
- 5 ***S*-(4-Hydroxy-but-2-ynyl) 9 α -chloro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate**



- 4-(Tetrahydropyran-2-yloxy)-but-2-ynyl toluene-4-sulfonic acid ester (0.727g, 2.24mmol) was added to a stirred mixture of 9,11-epoxy-17 α -[(2-furanylcarbonyl)oxy]-17 α -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioic acid (1.0g, 2.13 mmol) and anhydrous potassium carbonate (0.300g, 2.34mmol) in acetone (20ml) and the mixture was stirred under a blanket of nitrogen at 25 to 30°C for 4hrs. The reaction mixture was then poured into water and extracted with ethyl acetate. The organic layer was washed with water, dried, and concentrated *in vacuo*. The crude solid was dissolve in methanol (15ml) and concentrated hydrochloric acid (4ml) was added at 10-15°C. The mixture was stirred at 25-30 for 30min and then heated at 60°C for 4hrs. The mixture was then cooled and poured in to ice-water. The solid was filtered, washed with water, and dried. The crude solid was purified by column chromatography (3% methanol in dichloromethane) to yield the title compound as a white solid.

20 **Example 15- Compound IB.2**

- S*-(4-Hydroxy-but-2-ynyl) 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate**



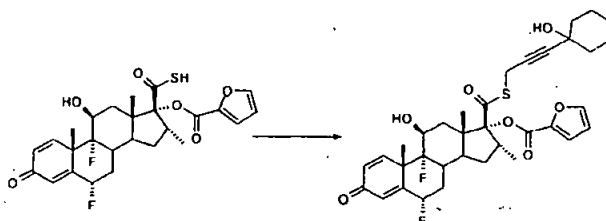
169
4-Chloro-but-2-yne-1-ol (0.169g, 1.62mmol) was added to a stirred mixture of 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioic acid (0.800g, 1.54 mmol) and anhydrous potassium carbonate (0.234g, 1.70 mmol) in acetone (20ml) and the mixture was stirred under a blanket of nitrogen at 25 to 30°C for 3hrs. The reaction mixture was then poured into water and extracted with ethyl acetate. The organic layer was washed with water, dried, and concentrated *in vacuo*. The residue was purified by column chromatography (3% methanol in dichloromethane) to yield the title compound as a white solid.

The following compounds were prepared in a manner similar to example 15 using an appropriate thioic acid of formula II and compound of formula III-B:

IB.1, IB.4, IB.5, IB.7 to IB.11, IB.20 to IB.24, IB.26 to IB.29, IB.38, IB.39, IB.61, IB.62, IB.132.

Example 16- Compound IB.25

15 **S-[3-(1-Hydroxycyclohexyl)prop-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate**

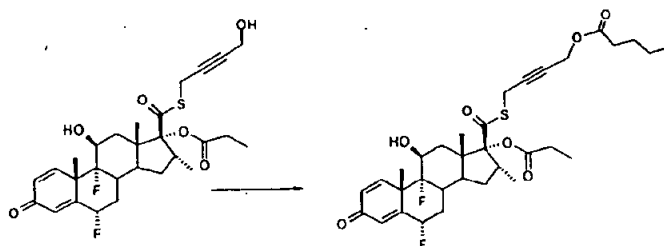


20 4-Methyl-[3-(hydroxycyclohexyl)prop-2-ynyl]benzenesulfonate (0.222g, 0.72mmol) was added to a stirred mixture of 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioic acid (0.350g, 0.688mmol) and anhydrous potassium carbonate (0.104g, 0.756mmol) in acetone (20ml) and the mixture was stirred under a blanket of nitrogen at 25 to 30°C for 3hrs. The reaction mixture was then poured into water and extracted with ethyl acetate. The organic layer was washed with water, dried, and concentrated *in vacuo*. The residue was purified by column chromatography (35% ethyl acetate in hexane) to yield the title compound as a white solid.

Compound IB.40 was prepared in a manner similar to example 16.

Example 17- Compound IB.35

S-[4-*n*-Butylcarbonyloxy-but-2-ynyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate



Valeryl chloride (0.337g, 2.79mmol) was added at 10-15°C in to a stirred mixture of S-(4-hydroxy-but-2-ynyl)6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyl-oxyandrosta-1,4-diene-17 β -carbothioate (0.5g, 0.93mmol) and triethylamine (0.282g, 2.79mmol) in acetone (20ml) and the mixture was stirred under a blanket of nitrogen at 25-30°C for 8hrs. The reaction mixture was then poured into water and extracted with ethyl acetate. The organic layer was washed with water, dried, and concentrated *in vacuo*. The residue was purified by column chromatography (35% ethyl acetate in hexane) to yield the title compound as a white solid.

15

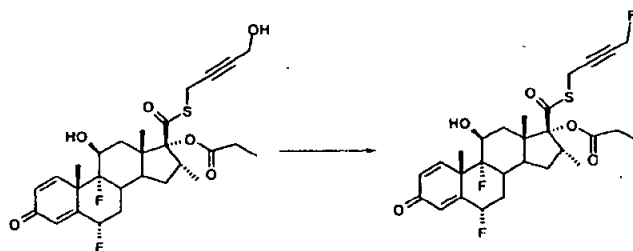
The following compounds were prepared with similar manner to example 17:

IB.31 to IB.37, IB.48 to IB.53, IB.55 to IB.60, IB.67 to IB.73, IB.75 to IB.86, IB.88, IB.92-IB.102, IB.104 to IB.122, IB.124, IB.133, IB.135, IB.148, IB.155, IB.157:

Example 18- Compound IB.3

S-(4-Fluorobut-2-ynyl) 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyl-oxyandrosta-1,4-diene-17 β -carbothioate

20

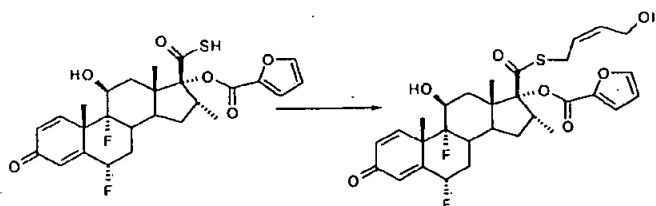


Diethylaminosulfur trifluoride (DAST) (0.151g, 0.93mmol) was added to a stirred solution of *S*-(4-hydroxy-but-2-ynyl) 6α,9α-difluoro-11β-hydroxy-16α-methyl-3-oxo-17α-propionyloxyandrost-1,4-diene-17β-carbothioate (0.450g, 0.783mmol) in dry dichloromethane (20ml) at 25-30°C and the mixture was stirred under a blanket of nitrogen at 25-30°C for 2hrs. The reaction mixture was washed with sodium bicarbonate solution (25ml), water, dried, and concentrated *in vacuo*. The residue was purified by column chromatography (40% ethyl acetate in hexane) to yield the title compound as a white solid.

The compound IB.6 was prepared in a manner similar to example 18.

Example 19- Compound IB.15

S-(4-Hydroxy-(*Z*)-but-2-enyl) 6α,9α-difluoro-17α-[(2-furanylcarbonyl)oxy]-11β-hydroxy-16α-methyl-3-oxoandrost-1,4-diene-17β-carbothioate



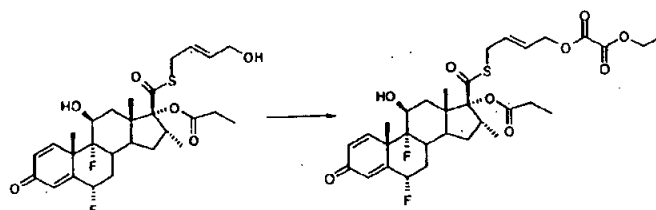
(*Z*)-4-Chloro-but-2-en-1-ol (0.691g, 6.48mmol) was added to a stirred mixture of 6α,9α-difluoro-17α-[(2-furanylcarbonyl)oxy]-11β-hydroxy-16α-methyl-3-oxoandrost-1,4-diene-17β-carbothioic acid (3.0g, 5.87mmol) and anhydrous potassium carbonate (0.895g, 6.48 mmol) in acetone (60ml) and the mixture was stirred under a blanket of nitrogen at 25 to 30°C for 3hrs. The reaction mixture was then poured into water and extracted with ethyl acetate. The organic layer was washed with water, dried, and concentrated *in vacuo*. The residue was purified by

column chromatography (1% methanol in dichloromethane) to yield the title compound as a white solid.

The compounds IB.16, IB.30 were prepared with similar manner to example 19. The compounds IB.13, IB.14, IB.17 were prepared by similar manner using (*E*)-4-bromo-but-2-en-1-ol and an appropriate thioic acid of formula II.

Example 20- Compound IB.44

***S*-[4-(2-Ethoxy-1,2-dioxoethyl)oxy-(*E*)-but-2-enyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate**

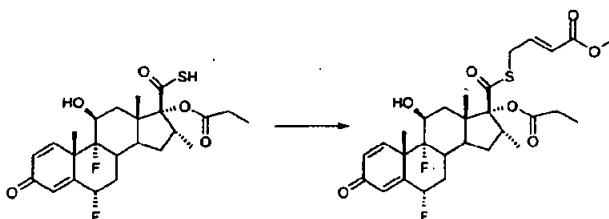


Ethyl oxalyl chloride (0.352g, 2.58mmol) was added at 10-15°C in to a stirred mixture of *S*-(4-hydroxy-(*E*)-but-2-enyl)-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate (0.7g, 1.29mmol) and triethylamine (0.260g, 2.58mmol) in acetone-(20ml) and the mixture was stirred under a blanket of nitrogen at 25-30°C for 8hrs. The reaction mixture was then poured into water and extracted with ethyl acetate. The organic layer was washed with water, dried, and concentrated *in vacuo*. The residue was purified by column chromatography (35% ethyl acetate in hexane) to yield the title compound as a white solid.

The compound IB.46 was prepared in a similar manner to example 20. The compounds IB.47 and IB.54 were prepared from IB.15 and IB.4 respectively, in a similar manner to example 20.

Example 21- Compound IB.42

4-Methoxy-4-oxo-(*E*)-but-2-enyl 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4 diene-17 β -carbothioate



Methyl 4-bromocrotonate (0.191g, 1.06mmol) was added at 25-30°C in to a stirred mixture of 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioic acid (0.5g, 1.06mmol) and anhydrous potassium carbonate (0.146g, 1.06mmol) in *N,N*-dimethylformamide (10ml) and the mixture was stirred under a blanket of nitrogen at 25-30°C for 1.5hrs. The reaction mixture was then poured into water and extracted with ethyl acetate. The organic layer was washed with water, dried, and concentrated *in vacuo*. The residue was purified by column chromatography (40% ethyl acetate in hexane) to yield the title compound as a white solid.

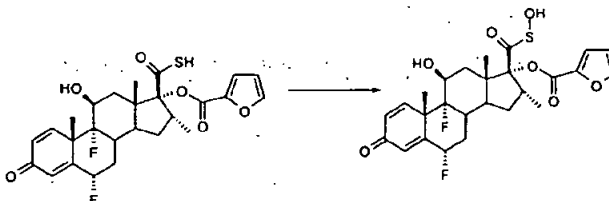
10

Compounds IB.41 and IB.43 were prepared in a manner similar to example 21.

Example 22

6 α ,9 α -Difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbonylsulfenic acid

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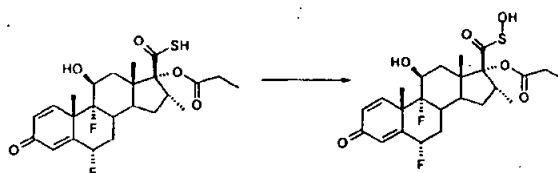
A solution of urea-hydrogen peroxide (2.41g, 0.0256mol) in *N,N*-dimethylformamide was added at 10 to 15°C into a clear solution of 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioic acid (13.0g, 0.0256mol) in *N,N*-dimethylformamide (40ml). The reaction mixture was stirred at 10-15°C for 30min, then poured into ice-water. The solid was filtered, washed with water, and dried at 50-60°C to yield the title compound as white solid (12.0g, 89.48%).

20

¹H NMR (400 MHz in CDCl₃+DMSO-d₆), δ : 1.06(d, J =7.09Hz, 3H), 1.19(s, 3H), 1.33-1.38(m, 1H), 1.55(s, 3H), 1.58-1.98(m, 4H), 2.26-2.52(m, 4H), 3.02-3.06(m, 1H), 4.32-(br-d, J =8.76Hz, 1H), 5.14-5.19(br-s, 1H), 5.38-5.54(m, 1H), 6.29(s, 1H), 6.30(d, J =8.71Hz, 1H), 6.54(dd, J_1 =3.32Hz, J_2 =1.53Hz, 1H), 7.08(d, J =3.37Hz, 1H), 7.27(d, J =10.30Hz, 1H), 7.67(s, 1H).

Example 23

6 α ,9 α -Difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbonylsulfenic acid



10

Hydrogen peroxide (30vol, 60ml) was added to a suspension of 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioic acid (20.0g, 42.68mmol) in methanol (120ml) at 10 to 15°C. The reaction mixture was stirred at ambient temperature for 1hr. Excess peroxide was neutralized with 10% sodium metabisulfite solution, the product was filtered, washed with water, and dried to yield the title compound as white solid (19.9g, 96.22%).

15

¹H NMR (400 MHz in CDCl₃+DMSO-d₆), δ : 0.98(d, J =7.10Hz, 3H), 1.08(t, J =7.55Hz, 3H), 1.12(s, 3H), 1.25-1.33(m, 1H), 1.53(s, 3H), 1.58-1.93(m, 4H), 2.12-2.47(m, 4H), 2.33(q, J =7.57Hz, 2H), 2.95-2.99(m, 1H), 4.24-4.27(br-d, 1H), 5.15(br-s, 1H), 5.36-5.53(m, 1H), 6.26(s, 1H), 6.27(dd, J_1 =10.21Hz, J_2 =1.68Hz, 1H), 7.24(d, J =9.73Hz, 1H).

20

The following 17 β -carbonylsulfenic acids were prepared by an analogous method to example 23:

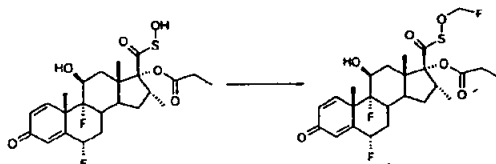
9 α -Fluoro-17 α -[(2-furanylcabonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbonylsulphenic acid.

25

6 α ,9 α -Difluoro-11 β -hydroxy-16 α -methyl-17 α -penatanoyloxy-3-oxoandrosta-1,4-diene-17 β -carbonylsulphenic acid.

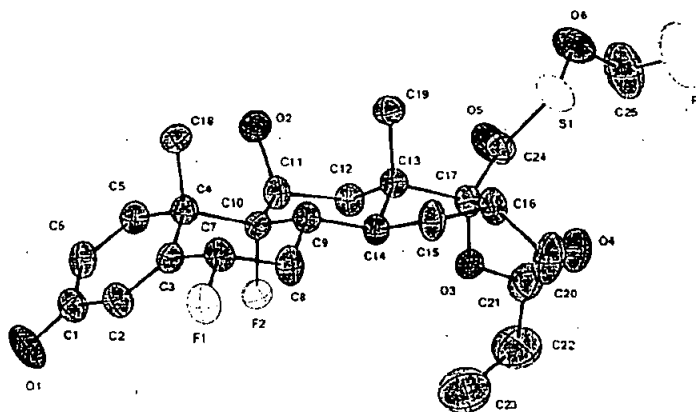
Example 24- Compound IC.3

- 5 6 α ,9 α -Difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbonylsulfenic acid fluoromethyl ester



- Bromofluoromethane (1.5ml) was added at 0°C in to a stirred mixture of 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-17 α -propionyloxy-3-oxoandrosta-1,4-diene-17 β -carbonylsulphenic acid (1.5g, 3.1mmol) and anhydrous potassium carbonate (0.427g, 3.1mmol) in acetone (50ml). The mixture was stirred under a blanket of nitrogen at 5 to 10°C for 1hr. The reaction mixture was then poured into water and extracted with ethyl acetate. The organic layer was washed with water, dried, and concentrated *in vacuo*. The residue was purified by preparative HPLC to yield the title compound as a white solid.

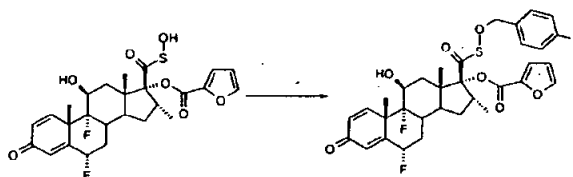
Structure of compound IC.3 was confirmed by single crystal X-Ray as shown below:



The compounds IC.4, IC.11 to IC.14 were prepared in a similar manner to example 24 using appropriate carbonyl sulfenic acid of formula VI and compound of III-C.

Example 25- Compound IC.5

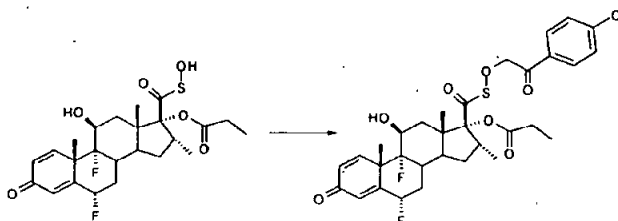
- 5 **6 α ,9 α -Difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbonylsulfenic acid (4-fluorophenyl)methyl ester**



- 4-Fluorobenzyl chloride (0.277g, 1.91mmol) was added at 25-30°C in to a stirred mixture of 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbonylsulfenic acid (1.0g, 1.91mmol) and anhydrous potassium carbonate (0.344g, 2.49mmol) in *N,N*-dimethylformamide (15ml), and the mixture was stirred under a blanket of nitrogen at 25-30°C for 2hrs. The reaction mixture was then poured into water and extracted with ethyl acetate. The organic layer was washed with water, and concentrated *in vacuo*. The residue was purified by crystallization from acetone to yield the title compound as a white solid.
- 15 The compounds IC.1, IC.2, IC.6 to IC.9, IC.15, IC.16, IC.18 to IC.23 were prepared in a manner similar to example 25.

Example 26- Compound IC.10

- 20 **6 α ,9 α -Difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbonylsulfenic acid [2-(4-chlorophenyl)-2-oxoethyl] ester**



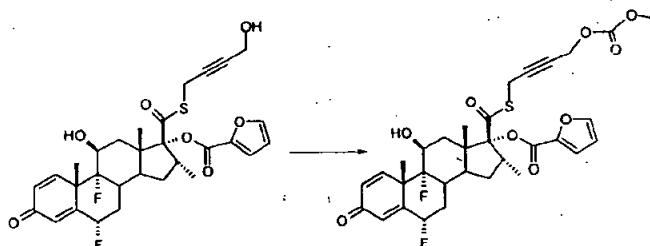
2-Bromo-1-(4-chlorophenyl)ethanone (0.120g, 0.51mmol) was added at 25-30°C in to a stirred mixture of 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-

diene-17 β -carbonylsulfenic acid (0.25g, 0.51mmol) and anhydrous potassium carbonate (0.070g, 0.51mmol) in acetone (20ml) and the mixture was stirred under a blanket of nitrogen at 25-30°C for 2hrs. The reaction mixture was then poured into water and extracted with ethyl acetate. The organic layer was washed with water, dried, and concentrated *in vacuo*. The residue was purified by column chromatography (35% ethyl acetate in hexane) to yield the title compound as a white solid.

Compound IC.17 was prepared in a similar manner to example 26.

Example 27-Compound IB.63

- 10 ***S*-(4-Methoxycarbonyloxy-but-2-ynyl) 6 α ,9 α -difluoro-17 α -[(2-furanylcabonyl)-oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate**

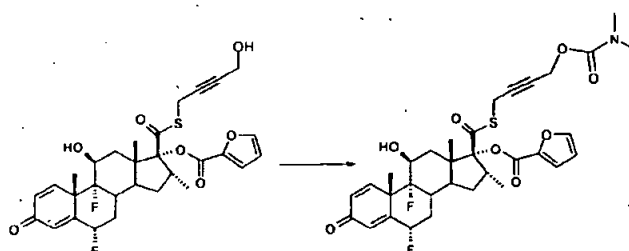


- 15 Methyl chloroformate(0.33g, 3.48mmol) was added at 25-30°C in to a stirred mixture of *S*-(4-hydroxy-but-2-ynyl) 6 α ,9 α -difluoro-17 α -[(2-furanylcabonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate (1.0g, 1.74mmol) and triethylamine (0.70g, 6.96mmol) in dry dichloromethane (30ml). The mixture was stirred at 25 to 30°C for 6hrs, then washed with water and concentrated *in vacuo*. The residue was purified by column chromatography (30% ethyl acetate in hexane) to yield the title compound as a white solid.

- 20 The compounds IB.12, IB.18, IB.19, IB.64 to IB.66, IB.89, IB.91, IB.123, IB.125 to IB.129, IB.131, IB.134, IB.137 to IB.147, IB.149, IB.150, IB.153, IB.154, IB.156 were prepared in a manner similar to example 27.

Example 28-Compound IB.103

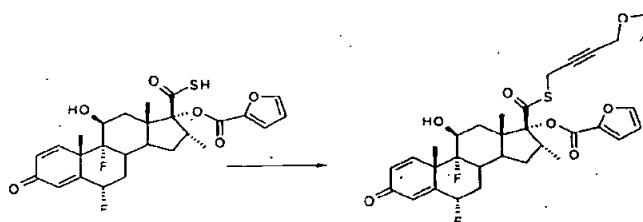
- 25 ***S*-[4-(*N,N*-Dimethylaminocarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcabonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate**



N,N-Dimethylcarbamoyl chloride (0.23g, 2.0mmol) was added at 25-30°C to a stirred mixture of *S*-(4-hydroxy-but-2-ynyl) 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate (1.0g, 1.74mmol) and triethylamine (0.70g, 6.96mmol) in dichloromethane (30ml). The mixture was stirred at 25 to 30°C for 4hrs, then washed with water and concentrated *in vacuo*. The residue was purified by column chromatography (40% ethyl acetate in hexane) to yield the title compound as a white solid. The compounds IB.129 to IB.131 were prepared in a manner similar to example 28.

10 **Example 29- Compound IB.158**

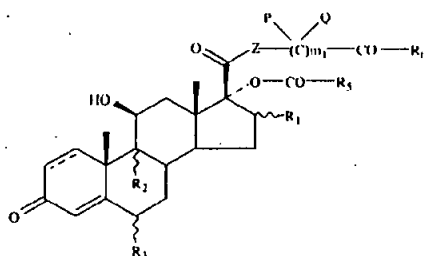
S-[4-Methoxybut-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate.



1-Chloro-4-methoxybut-2-yne (0.086g, 0.72mmol) was added to a stirred mixture of 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioic acid (0.350g, 0.688mmol) and anhydrous potassium carbonate (0.104g, 0.756mmol) in acetone (20ml). The mixture was stirred under a blanket of nitrogen at 25 to 30°C for 3hrs., then poured into water and extracted with ethyl acetate. The organic layer was washed with water, dried, and concentrated *in vacuo*. The residue was purified by column chromatography (35% ethyl acetate in hexane) to yield the title compound as a white solid.

Compounds IB.159, IB.160 were prepared in a manner similar to example 29.

Table 1- Lists the compound of formula I-A which have been synthesized



Formula I-A

Table-1

Table I

| No. | R ₁ | R ₂ | R ₃ | R ₄ | R ₅ | P | Q | m ₁ | Z | Chemical Name |
|-------|---------------------------|----------------|----------------|----------------|--------------------|---|---|----------------|---|--|
| IA.1 | H | H | H | Ethoxy | 4-Chlorophenyl | H | H | I | O | 2-(4-Chlorophenyl)-2-oxoethyl 17 α -ethoxycarbonyloxy-11 β -hydroxy-3-oxoandrosta-1,4-diene-17 β -carboxylate. |
| IA.2 | α -CH ₃ | F | F | Ethyl | 4-Chlorophenyl | H | H | I | O | 2-(4-Chlorophenyl)-2-oxoethyl 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carboxylate |
| IA.3 | α -CH ₃ | F | F | Ethyl | 4-Chlorophenyl | H | H | I | S | S-[2-(4-Chlorophenyl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate. |
| IA.4 | H | H | H | Ethoxy | 4-Fluorophenyl | H | H | I | O | 2-(4-Fluorophenyl)-2-oxoethyl 17 α -ethoxycarbonyloxy-11 β -hydroxy-3-oxoandrosta-1,4-diene-17 β -carboxylate. |
| IA.5 | α -CH ₃ | F | F | Ethyl | 4-Fluorophenyl | H | H | I | O | 2-(4-Fluorophenyl)-2-oxoethyl 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carboxylate. |
| IA.6 | α -CH ₃ | F | F | Ethyl | 4-Fluorophenyl | H | H | I | S | S-[2-(4-Fluorophenyl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate. |
| IA.7 | H | H | H | Ethoxy | 2,4-Difluorophenyl | H | H | I | O | 2-(2,4-Difluorophenyl)-2-oxoethyl 17 α -(ethoxycarbonyloxy-11 β -hydroxy-3-oxoandrosta-1,4-diene-17 β -carboxylate. |
| IA.8 | H | H | H | Ethoxy | 2,4-Dichlorophenyl | H | H | I | O | 2-(2,4-Dichlorophenyl)-2-oxoethyl 17 α -(ethoxycarbonyloxy-11 β -hydroxy-3-oxoandrosta-1,4-diene-17 β -carboxylate. |
| IA.9 | α -CH ₃ | F | F | Ethyl | 2,4-Difluorophenyl | H | H | I | O | 2-(2,4-Difluorophenyl)-2-oxoethyl 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carboxylate. |
| IA.10 | α -CH ₃ | F | F | Ethyl | 2,4-Dichlorophenyl | H | H | I | O | 2-(2,4-Dichlorophenyl)-2-oxoethyl 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carboxylate. |
| IA.11 | α -CH ₃ | F | F | Ethyl | 2,4-Difluorophenyl | H | H | I | S | S-2-[(2,4-Difluorophenyl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate. |
| IA.12 | H | H | H | Ethoxy | 3,4-Dichlorophenyl | H | H | I | O | 2-(3,4-Dichlorophenyl)-2-oxoethyl 17 α -(ethoxycarbonyloxy-11 β -hydroxy-3-oxoandrosta-1,4-diene-17 β -carboxylate. |
| IA.13 | α -CH ₃ | F | F | Ethyl | 2,4-Dichlorophenyl | H | H | I | S | S-[2-(2,4-Dichlorophenyl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate. |
| IA.14 | α -CH ₃ | F | F | Ethyl | 3,4-Dichlorophenyl | H | H | I | S | S-[2-(3,4-Dichlorophenyl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate. |

| No. | R ₁ | R ₂ | R ₃ | R ₄ | R ₅ | P | Q | m ₁ | Z | Chemical Name |
|-------|---------------------------|----------------|----------------|----------------|--------------------------|---|---|----------------|---|---|
| IA.15 | α -CH ₃ | F | F | Ethyl | 3,4-Dichlorophenyl | H | H | 1 | O | 2-(3,4-Dichlorophenyl)-2-oxoethyl 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carboxylate. |
| IA.16 | H | H | H | Ethoxy | 2-Thienyl | H | H | 1 | O | 2-Oxo-2-(thiophen-2-yl)ethyl 17 α -(ethoxycarbonyloxy)-11 β -hydroxy-3-oxoandrosta-1,4-diene-17 β -carboxylate. |
| IA.17 | H | H | H | Ethoxy | 5-Chloro-2-thienyl | H | H | 1 | O | 2-(5-Chlorothiophen-2-yl)-2-oxoethyl 17 α -(ethoxycarbonyloxy)-11 β -hydroxy-3-oxoandrosta-1,4-diene-17 β -carboxylate. |
| IA.18 | α -CH ₃ | F | F | Ethyl | 5-Chloro-2-thienyl | H | H | 1 | O | 2-(5-Chlorothiophen-2-yl)-2-oxoethyl 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carboxylate. |
| IA.19 | H | H | H | Ethoxy | 5-Methyl-2-furyl | H | H | 1 | O | 2-(5-Methylfuran-2-yl)-2-oxoethyl 17 α -(ethoxycarbonyloxy)-11 β -hydroxy-3-oxoandrosta-1,4-diene-17 β -carboxylate. |
| IA.20 | α -CH ₃ | F | F | Ethyl | 5-Chloro-2-thienyl | H | H | 1 | S | S-[2-(5-Chlorothiophen-2-yl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carboxylate. |
| IA.21 | α -CH ₃ | F | F | Ethyl | 5-Methyl-2-furyl | H | H | 1 | O | 2-(5-Methylfuran-2-yl)-2-oxoethyl 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carboxylate. |
| IA.22 | α -CH ₃ | F | F | Ethyl | 5-Methyl-2-furyl | H | H | 1 | S | S-[2-(5-Methylfuran-2-yl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carboxylate. |
| IA.23 | H | H | H | Ethoxy | <i>i</i> -Butyl | H | H | 1 | O | 3,3-Dimethyl-2-oxobutyl 17 α -(ethoxycarbonyloxy)-11 β -hydroxy-3-oxoandrosta-1,4-diene-17 β -carboxylate. |
| IA.24 | H | H | H | Ethoxy | Methyl | H | H | 1 | O | 2-Oxopropyl 17 α -(ethoxycarbonyloxy)-11 β -hydroxy-3-oxoandrosta-1,4-diene-17 β -carboxylate. |
| IA.25 | α -CH ₃ | F | F | Ethyl | <i>i</i> -Butyl | H | H | 1 | O | 3,3-Dimethyl-2-oxobutyl 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carboxylate. |
| IA.26 | α -CH ₃ | F | F | Ethyl | <i>i</i> -Butyl | H | H | 1 | S | S-(3,3-Dimethyl-2-oxobutyl) 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carboxylate. |
| IA.27 | α -CH ₃ | F | F | Ethyl | Methyl | H | H | 1 | S | S-[2-Oxopropyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carboxylate. |
| IA.28 | α -CH ₃ | F | F | Ethyl | Methyl | H | H | 1 | O | 2-Oxopropyl 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carboxylate. |
| IA.29 | H | H | H | Ethoxy | 4-Methoxyphenyl | H | H | 1 | O | 2-(4-Methoxyphenyl)-2-oxoethyl 17 α -(ethoxycarbonyloxy)-11 β -hydroxy-3-oxoandrosta-1,4-diene-17 β -carboxylate. |
| IA.30 | α -CH ₃ | F | F | Ethyl | 4-Methoxyphenyl | H | H | 1 | O | 2-(4-Methoxyphenyl)-2-oxoethyl 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carboxylate. |
| IA.31 | α -CH ₃ | F | F | Ethyl | 4-Methoxyphenyl | H | H | 1 | S | S-[2-(4-Methoxyphenyl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carboxylate. |
| IA.32 | H | H | H | Ethoxy | 1-Adamantyl | H | H | 1 | O | 2-(Adamantan-1-yl)-2-oxoethyl 17 α -(ethoxycarbonyloxy)-11 β -hydroxy-3-oxoandrosta-1,4-diene-17 β -carboxylate. |
| IA.33 | α -CH ₃ | F | F | Ethyl | 1-Adamantyl | H | H | 1 | O | 2-(Adamantan-1-yl)-2-oxoethyl 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carboxylate. |
| IA.34 | α -CH ₃ | F | F | Ethyl | 1-Adamantyl | H | H | 1 | S | S-[2-(Adamantan-1-yl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carboxylate. |
| IA.35 | α -CH ₃ | F | F | Ethyl | 4-Trifluoromethoxyphenyl | H | H | 1 | S | S-[2-Oxo-2-(4-trifluoromethoxyphenyl)ethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carboxylate. |

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| No. | R ₁ | R ₂ | R ₃ | R ₄ | R ₅ | P | Q | m ₁ | Z | Chemical Name |
|-------|---------------------------|----------------|----------------|--------------------|--------------------------|---|---|----------------|---|---|
| IA.36 | α -CH ₃ | F | F | Ethyl | 4-Trifluoromethoxyphenyl | H | H | 1 | O | 2-Oxo-2-(4-trifluoromethoxyphenyl)ethyl 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrost-1,4-diene-17 β -carboxylate. |
| IA.37 | H | H | H | Ethoxy | 4-Trifluoromethoxyphenyl | H | H | 1 | O | 2-Oxo-2-(4-trifluoromethoxyphenyl)ethyl 17 α -(ethoxycarbonyloxy)-11 β -hydroxy-3-oxoandrost-1,4-diene-17 β -carboxylate. |
| IA.38 | α -CH ₃ | F | F | Ethyl | 4-Trifluoromethylphenyl | H | H | 1 | S | S-[2-Oxo-2-(4-trifluoromethylphenyl)ethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrost-1,4-diene-17 β -carbothioate. |
| IA.39 | α -CH ₃ | F | F | 5-Chloro-2-thienyl | 4-Trifluoromethylphenyl | H | H | 1 | S | S-[2-Oxo-2-(4-trifluoromethylphenyl)ethyl] 17 α -[(5-chloro-2-thienyl)carbonyloxy]-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrost-1,4-diene-17 β -carbothioate. |
| IA.40 | α -CH ₃ | F | F | 5-Chloro-2-thienyl | 2,4,6-Trimethylphenyl | H | H | 1 | S | S-[2-Oxo-2-(2,4,6-trimethylphenyl)ethyl] 17 α -[(5-chloro-2-thienyl)carbonyloxy]-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrost-1,4-diene-17 β -carbothioate. |
| IA.41 | α -CH ₃ | Cl | H | 2-Furyl | 2,4,6-Trimethylphenyl | H | H | 1 | S | S-[2-Oxo-2-(2,4,6-trimethylphenyl)ethyl] 9 α -chloro-17 α -[(2-furyl)carbonyloxy]-11 β -hydroxy-16 α -methyl-3-oxoandrost-1,4-diene-17 β -carbothioate. |
| IA.42 | α -CH ₃ | F | F | Ethyl | 4-Methanesulfonylphenyl | H | H | 1 | O | 2-(4-Methanesulfonylphenyl)-2-oxoethyl 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrost-1,4-diene-17 β -carboxylate. |
| IA.43 | α -CH ₃ | F | F | Ethyl | 4-Methanesulfonylphenyl | H | H | 1 | S | S-[2-(4-Methanesulfonylphenyl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrost-1,4-diene-17 β -carbothioate. |
| IA.44 | α -CH ₃ | F | F | Ethyl | Phenyl | H | H | 1 | O | 2-Oxo-2-phenylethyl 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrost-1,4-diene-17 β -carboxylate. |
| IA.45 | α -CH ₃ | F | F | Ethyl | Phenyl | H | H | 1 | S | S-[2-Oxo-2-phenylethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrost-1,4-diene-17 β -carbothioate. |
| IA.46 | α -CH ₃ | F | F | Ethyl | 4-Methylphenyl | H | H | 1 | O | 2-(4-Methylphenyl)-2-oxoethyl 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrost-1,4-diene-17 β -carboxylate. |
| IA.47 | α -CH ₃ | F | F | Ethyl | 4-Methylphenyl | H | H | 1 | S | S-[2-(4-Methylphenyl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrost-1,4-diene-17 β -carbothioate. |
| IA.48 | α -CH ₃ | F | F | Ethyl | 2,6-Dichlorophenyl | H | H | 1 | O | 2-(2,6-Dichlorophenyl)-2-oxoethyl 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrost-1,4-diene-17 β -carboxylate. |
| IA.49 | α -CH ₃ | F | F | Ethyl | 2,6-Dichlorophenyl | H | H | 1 | S | S-[2-(2,6-Dichlorophenyl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrost-1,4-diene-17 β -carbothioate. |
| IA.50 | α -CH ₃ | F | F | Ethyl | 2,3-Dichlorophenyl | H | H | 1 | O | 2-(2,3-Dichlorophenyl)-2-oxoethyl 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrost-1,4-diene-17 β -carboxylate. |
| IA.51 | α -CH ₃ | F | F | Ethyl | 2,3-Dichlorophenyl | H | H | 1 | S | S-[2-(2,3-Dichlorophenyl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrost-1,4-diene-17 β -carbothioate. |
| IA.52 | α -CH ₃ | F | F | Ethyl | 2,6-Difluorophenyl | H | H | 1 | O | 2-(2,6-Difluorophenyl)-2-oxoethyl 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrost-1,4-diene-17 β -carboxylate. |
| IA.53 | α -CH ₃ | F | F | Ethyl | 2,6-Difluorophenyl | H | H | 1 | S | S-[2-(2,6-Difluorophenyl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrost-1,4-diene-17 β -carbothioate. |
| IA.54 | α -CH ₃ | F | F | Ethyl | 2,3-Difluorophenyl | H | H | 1 | O | 2-(2,3-Difluorophenyl)-2-oxoethyl 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrost-1,4-diene-17 β -carboxylate. |
| IA.55 | α -CH ₃ | F | F | Ethyl | 2,3-Difluorophenyl | H | H | 1 | S | S-[2-(2,3-Difluorophenyl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrost-1,4-diene-17 β -carbothioate. |

| No. | R ₁ | R ₂ | R ₃ | R ₅ | R ₆ | P | Q | m | Z | Chemical Name |
|-------|---------------------------|----------------|----------------|--------------------|--------------------------|-----------------|-----------------|---|---|---|
| IA.56 | α -CH ₃ | F | F | 5-Chloro-2-thienyl | 4-Chlorophenyl | H | H | 1 | S | S-[2-(4-Chlorophenyl)-2-oxoethyl] 17 α -[(5-chloro-2-thienyl)carbonyloxy]-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IA.57 | α -CH ₃ | F | F | Ethyl | 2,4,6-Trimethylphenyl | H | H | 1 | O | 2-Oxo-2-(2,4,6-trimethylphenyl)ethyl 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carboxylate. |
| IA.58 | α -CH ₃ | F | F | Ethyl | 2,4,6-Trimethylphenyl | H | H | 1 | S | S-[2-Oxo-2-(2,4,6-trimethylphenyl)ethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate. |
| IA.59 | α -CH ₃ | F | F | Ethyl | Phenyl | CH ₃ | CH ₃ | 1 | S | S-[1,1-Dimethyl-2-oxo-2-phenylethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate. |
| IA.60 | α -CH ₃ | F | F | Ethyl | 2-Thienyl | H | H | 1 | O | 2-Oxo-2-(thiophen-2-yl)ethyl 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carboxylate. |
| IA.61 | α -CH ₃ | F | F | Ethyl | 2-Thienyl | H | H | 1 | S | S-[2-Oxo-2-(thiophen-2-yl)ethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate. |
| IA.62 | α -CH ₃ | F | F | Ethyl | 3,4-Difluorophenyl | H | H | 1 | O | 2-(3,4-Difluorophenyl)-2-oxoethyl 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carboxylate. |
| IA.63 | α -CH ₃ | F | F | Ethyl | 3,4-Difluorophenyl | H | H | 1 | S | S-[2-(3,4-Difluorophenyl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate. |
| IA.64 | α -CH ₃ | F | F | Ethyl | 2-Furyl | H | H | 1 | O | 2-(Furan-2-yl)-2-oxoethyl 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carboxylate. |
| IA.65 | α -CH ₃ | F | F | Dichloromethyl | 4-Fluorophenyl | H | H | 1 | O | 2-(4-Fluorophenyl)-2-oxoethyl 17 α -dichloromethylcarbonyloxy-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carboxylate. |
| IA.66 | α -CH ₃ | F | F | Dichloromethyl | 2,4-Difluorophenyl | H | H | 1 | O | 2-(2,4-Difluorophenyl)-2-oxoethyl 17 α -dichloromethylcarbonyloxy-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carboxylate. |
| IA.67 | α -CH ₃ | F | F | Ethyl | 2-Benzofuryl | H | H | 1 | O | 2-(Benzofuran-2-yl)-2-oxoethyl 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carboxylate. |
| IA.68 | α -CH ₃ | F | F | Ethyl | 2-Furyl | H | H | 1 | S | S-[2-(Furan-2-yl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate. |
| IA.69 | α -CH ₃ | F | F | Ethyl | 2-Benzofuryl | H | H | 1 | S | S-[2-(Benzofuran-2-yl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate. |
| IA.70 | α -CH ₃ | F | F | Ethyl | 4- <i>t</i> -Butylphenyl | H | H | 1 | S | S-[2-(4- <i>t</i> -Butylphenyl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate. |
| IA.71 | α -CH ₃ | F | F | Ethyl | 7-Methoxy-2-benzofuryl | H | H | 1 | O | 2-(7-Methoxybenzofuran-2-yl)-2-oxoethyl 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carboxylate. |
| IA.72 | α -CH ₃ | F | F | Ethyl | 4- <i>t</i> -Butylphenyl | H | H | 1 | O | 2-(4- <i>t</i> -Butylphenyl)-2-oxoethyl 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carboxylate. |
| IA.73 | α -CH ₃ | F | F | Ethyl | 7-Methoxy-2-benzofuryl | H | H | 1 | S | S-[2-(7-Methoxybenzofuran-2-yl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate. |
| IA.74 | α -CH ₃ | F | F | Ethyl | 2-Fluoro-4-methoxyphenyl | H | H | 1 | O | 2-(2-Fluoro-4-methoxyphenyl)-2-oxoethyl 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carboxylate. |

| No. | R ₁ | R ₂ | R ₃ | R ₄ | R ₅ | P | Q | m ₁ | Z | Chemical Name |
|-------|---|----------------|----------------|----------------|--------------------------------|---|---|----------------|---|--|
| IA.75 | α -C ₆ H ₅ | F | F | Ethyl | 2-Fluoro-4-methoxyphenyl | H | H | I | S | 5-[2-(2-Fluoro-4-methoxyphenyl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate. |
| IA.76 | α -C ₆ H ₅ | F | F | Ethyl | 2-Methoxyphenyl | H | H | I | O | 2-(2-Methoxyphenyl)-2-oxoethyl 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carboxylate. |
| IA.77 | α -C ₆ H ₅ | F | F | Ethyl | 2,4-Dimethoxyphenyl | H | H | I | O | 2-(2,4-Dimethoxyphenyl)-2-oxoethyl 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carboxylate. |
| IA.78 | α -C ₆ H ₅ | F | F | Ethyl | 2,4-Dimethoxyphenyl | H | H | I | S | 5-[2-(2,4-Dimethoxyphenyl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate. |
| IA.79 | α -C ₆ H ₅ | F | F | Ethyl | 2-Methoxyphenyl | H | H | I | S | 5-[2-(2-Methoxyphenyl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate. |
| IA.80 | α -C ₆ H ₅ | F | F | Ethyl | 2-Trifluoromethylphenyl | H | H | I | O | 2-Oxy-2-(2-trifluoromethylphenyl)ethyl 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carboxylate. |
| IA.81 | α -C ₆ H ₅ | F | F | Ethyl | 2-Trifluoromethylphenyl | H | H | I | S | 5-[2-Oxy-2-(2-trifluoromethylphenyl)ethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate. |
| IA.82 | α -C ₆ H ₅ | F | F | 2-Furyl | 4-Fluorophenyl | H | H | I | O | 2-(4-Fluorophenyl)-2-oxoethyl 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IA.83 | α -C ₆ H ₅ | F | F | 2-Furyl | 4-Fluorophenyl | H | H | I | S | 5-[2-(4-Fluorophenyl)-2-oxoethyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IA.84 | α -C ₆ H ₅ | F | F | 2-Furyl | 2,4-Difluorophenyl | H | H | I | O | 2-(2,4-Difluorophenyl)-2-oxoethyl 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carboxylate. |
| IA.85 | α -C ₆ H ₅ | F | F | 2-Furyl | 2,4-Difluorophenyl | H | H | I | S | 5-[2-(2,4-Difluorophenyl)-2-oxoethyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IA.86 | α -C ₆ H ₅ | F | H | Ethyl | 4-Fluorophenyl | H | H | I | S | 5-[2-(4-Fluorophenyl)-2-oxoethyl] 9 α -fluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate. |
| IA.87 | α -C ₆ H ₅ | F | H | Ethyl | 4-Fluorophenyl | H | H | I | O | 2-(4-Fluorophenyl)-2-oxoethyl 9 α -fluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carboxylate. |
| IA.88 | α -C ₆ H ₅ | F | F | Ethyl | 3,5-Bis(trifluoromethyl)phenyl | H | H | I | S | 5-[2-[3,5-Bis(trifluoromethyl)phenyl]-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate. |
| IA.89 | α -C ₆ H ₅ | F | F | Ethyl | 3-Trifluoromethylphenyl | H | H | I | S | 5-[2-Oxy-2-(3-trifluoromethyl)phenylethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate. |
| IA.90 | α -C ₆ H ₅ | F | F | Ethyl | 4-Isobutylphenyl | H | H | I | S | 5-[2-(4-Isobutylphenyl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate. |
| IA.91 | β -C ₆ H ₅ | F | H | Ethyl | 4-Fluorophenyl | H | H | I | O | 2-(4-Fluorophenyl)-2-oxoethyl 9 α -fluoro-11 β -hydroxy-16 β -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carboxylate. |
| IA.92 | α -C ₆ H ₅ | F | F | Ethyl | 4-Ethylphenyl | H | H | I | S | 5-[2-(4-Ethylphenyl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate. |

| No. | R ₁ | R ₂ | R ₃ | R ₄ | R ₅ | P | Q | m ₁ | Z | Chemical Name |
|--------|---|----------------|----------------|----------------|-------------------------|-----------------|-----------------|----------------|---|---|
| IA.93 | α -C ₆ H ₅ | F | F | Ethyl | 4-(Cyclohexylphenyl) | H | H | 1 | S | S-[2-(4-(Cyclohexylphenyl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrost-1,4-diene-17 β -carbothioate. |
| IA.94 | β -C ₆ H ₅ | F | H | Ethyl | 2,4-Difluorophenyl | H | H | 1 | S | S-[2-(2,4-Difluorophenyl)-2-oxoethyl] 9 α -fluoro-11 β -hydroxy-16 β -methyl-3-oxo-17 α -propionyloxyandrost-1,4-diene-17 β -carbothioate. |
| IA.95 | α -C ₆ H ₅ | F | F | Ethyl | 4-Isopropylphenyl | H | H | 1 | S | S-[2-(4-Isopropylphenyl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrost-1,4-diene-17 β -carbothioate. |
| IA.96 | α -C ₆ H ₅ | F | F | Ethyl | 4-Cyclopentyl-oxyphenyl | H | H | 1 | S | S-[2-(4-Cyclopentyl-oxyphenyl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrost-1,4-diene-17 β -carbothioate. |
| IA.97 | α -C ₆ H ₅ | F | H | Ethyl | 4-Methylsulfonylphenyl | H | H | 1 | S | S-[2-(4-Methylsulfonylphenyl)-2-oxoethyl] 9 α -fluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrost-1,4-diene-17 β -carbothioate. |
| IA.98 | α -C ₆ H ₅ | F | H | Ethyl | 2,4-Difluorophenyl | H | H | 1 | S | S-[2-(2,4-Difluorophenyl)-2-oxoethyl] 9 α -fluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrost-1,4-diene-17 β -carbothioate. |
| IA.99 | β -C ₆ H ₅ | F | H | Ethyl | 4-Methylsulfonylphenyl | H | H | 1 | S | S-[2-(4-Methylsulfonylphenyl)-2-oxoethyl] 9 α -fluoro-11 β -hydroxy-16 β -methyl-3-oxo-17 α -propionyloxyandrost-1,4-diene-17 β -carbothioate. |
| IA.100 | α -C ₆ H ₅ | F | H | Ethyl | 4-Chlorophenyl | H | H | 1 | S | S-[2-(4-Chlorophenyl)-2-oxoethyl] 9 α -fluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrost-1,4-diene-17 β -carbothioate. |
| IA.101 | β -C ₆ H ₅ | F | H | Ethyl | 4-Chlorophenyl | H | H | 1 | S | S-[2-(4-Chlorophenyl)-2-oxoethyl] 9 α -fluoro-11 β -hydroxy-16 β -methyl-3-oxo-17 α -propionyloxyandrost-1,4-diene-17 β -carbothioate. |
| IA.102 | α -C ₆ H ₅ | F | F | Ethoxy | 4-Trifluoromethylphenyl | H | H | 1 | S | S-[2-Oxo-2-(4-trifluoromethylphenyl)ethyl] 6 α ,9 α -difluoro-17 α -(ethoxycarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrost-1,4-diene-17 β -carbothioate. |
| IA.103 | α -C ₆ H ₅ | F | F | Cyclopropyl | 4-Fluorophenyl | H | H | 1 | O | 2-(4-Fluorophenyl)-2-oxoethyl] 17 α -cyclopropylcarbonyloxy-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrost-1,4-diene-17 β -carboxylate. |
| IA.104 | α -C ₆ H ₅ | F | F | Cyclopropyl | 2,4-Difluorophenyl | H | H | 1 | S | S-[2-(2,4-Difluorophenyl)-2-oxoethyl] 17 α -cyclopropylcarbonyloxy-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrost-1,4-diene-17 β -carbothioate. |
| IA.105 | α -C ₆ H ₅ | F | F | Ethoxy | 4-Chlorophenyl | H | H | 1 | S | S-[2-(4-Chlorophenyl)-2-oxoethyl] 6 α ,9 α -difluoro-17 α -(ethoxycarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrost-1,4-diene-17 β -carbothioate. |
| IA.106 | α -C ₆ H ₅ | F | F | Cyclopropyl | 4-Chlorophenyl | H | H | 1 | S | S-[2-(4-Chlorophenyl)-2-oxoethyl] 17 α -cyclopropylcarbonyloxy-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrost-1,4-diene-17 β -carbothioate. |
| IA.107 | β -C ₆ H ₅ | F | H | Ethyl | 4-Methoxyphenyl | H | H | 1 | S | S-[2-(4-Methoxyphenyl)-2-oxoethyl] 9 α -fluoro-11 β -hydroxy-16 β -methyl-3-oxo-17 α -propionyloxyandrost-1,4-diene-17 β -carbothioate. |
| IA.108 | α -C ₆ H ₅ | F | H | Ethyl | 4-Trifluoromethylphenyl | H | H | 1 | S | S-[2-Oxo-2-(4-trifluoromethylphenyl)-2-oxoethyl] 9 α -fluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrost-1,4-diene-17 β -carbothioate. |
| IA.109 | α -C ₆ H ₅ | F | F | Ethyl | 4-Methoxyphenyl | CH ₃ | CH ₃ | 1 | S | S-[1,1-Dimethyl-2-(4-methoxyphenyl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrost-1,4-diene-17 β -carbothioate. |
| IA.110 | α -C ₆ H ₅ | F | F | Ethoxy | 4-Fluorophenyl | H | H | 1 | S | S-[2-(4-Fluorophenyl)-2-oxoethyl] 6 α ,9 α -difluoro-17 α -(ethoxycarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrost-1,4-diene-17 β -carbothioate. |

| No. | R ₁ | R ₂ | R ₃ | R ₄ | R ₅ | P | Q | m ₁ | Z | Chemical Name |
|--------|---------------------------|----------------|----------------|----------------|-------------------------|-----------------|-----------------|----------------|---|--|
| IA.111 | β -CH ₃ | F | H | Ethyl | 4-Trifluoromethylphenyl | H | H | 1 | S | S-[2-Oxo-2-(4-trifluoromethylphenyl)-2-oxoethyl] 9 α -fluoro-11 β -hydroxy-16 β -methyl-3-oxo-17 α -propionyloxyandrost-1,4-diene-17 β -carbothioate. |
| IA.112 | α -CH ₃ | F | F | Cyclohexyl | 4-Trifluoromethylphenyl | H | H | 1 | S | S-[2-Oxo-2-(4-trifluoromethylphenyl)ethyl] 17 α -cyclohexylcarbonyloxy-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrost-1,4-diene-17 β -carbothioate. |
| IA.113 | α -CH ₃ | F | F | Cyclohexyl | 4-Chlorophenyl | H | H | 1 | S | S-[2-(4-Chlorophenyl)-2-oxoethyl] 17 α -cyclohexylcarbonyloxy-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrost-1,4-diene-17 β -carbothioate. |
| IA.114 | α -CH ₃ | F | F | Cyclohexyl | 2,4-Difluorophenyl | H | H | 1 | S | S-[2-(2,4-Difluorophenyl)-2-oxoethyl] 17 α -cyclohexylcarbonyloxy-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrost-1,4-diene-17 β -carbothioate. |
| IA.115 | α -CH ₃ | F | F | Cyclohexyl | 4-Fluorophenyl | H | H | 1 | O | 2-(4-Fluorophenyl)-2-oxoethyl 17 α -cyclohexylcarbonyloxy-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrost-1,4-diene-17 β -carboxylate. |
| IA.116 | α -CH ₃ | F | F | Cyclohexyl | 4-Methoxyphenyl | H | H | 1 | S | S-[2-(4-Methoxyphenyl)-2-oxoethyl] 17 α -cyclohexylcarbonyloxy-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrost-1,4-diene-17 β -carbothioate. |
| IA.117 | α -CH ₃ | F | F | Cyclopentyl | 4-Chlorophenyl | H | H | 1 | S | S-[2-(4-Chlorophenyl)-2-oxoethyl] 17 α -cyclopentylcarbonyloxy-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrost-1,4-diene-17 β -carbothioate. |
| IA.118 | α -CH ₃ | F | F | Cyclopentyl | 4-Fluorophenyl | H | H | 1 | O | S-[2-(4-Fluorophenyl)-2-oxoethyl] 17 α -cyclopentylcarbonyloxy-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrost-1,4-diene-17 β -carboxylate. |
| IA.119 | α -CH ₃ | F | F | Isopropyl | 4-Trifluoromethylphenyl | H | H | 1 | S | S-[2-Oxo-2-(4-trifluoromethylphenyl)ethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-17 α -(2-methylpropionyloxy)-3-oxoandrost-1,4-diene-17 β -carbothioate. |
| IA.120 | α -CH ₃ | F | F | Cyclopentyl | 2,4-Difluorophenyl | H | H | 1 | S | S-[2-(2,4-Difluorophenyl)-2-oxoethyl] 17 α -cyclopentylcarbonyloxy-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrost-1,4-diene-17 β -carbothioate. |
| IA.121 | α -CH ₃ | F | F | Isopropyl | 4-Fluorophenyl | H | H | 1 | O | 2-(4-Fluorophenyl)-2-oxoethyl 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-17 α -(2-methylpropionyloxy)-3-oxoandrost-1,4-diene-17 β -carboxylate. |
| IA.122 | α -CH ₃ | F | F | Isopropyl | 4-Methoxyphenyl | H | H | 1 | S | S-[2-(4-Methoxyphenyl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-17 α -(2-methylpropionyloxy)-3-oxoandrost-1,4-diene-17 β -carbothioate. |
| IA.123 | α -CH ₃ | F | F | Isopropyl | 2,4-Difluorophenyl | H | H | 1 | S | S-[2-(2,4-Difluorophenyl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-17 α -(2-methylpropionyloxy)-3-oxoandrost-1,4-diene-17 β -carbothioate. |
| IA.124 | α -CH ₃ | F | F | 2-Furyl | 4-Trifluoromethylphenyl | H | H | 1 | S | S-[2-Oxo-2-(4-trifluoromethylphenyl)ethyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrost-1,4-diene-17 β -carbothioate. |
| IA.125 | α -CH ₃ | F | F | Ethyl | 4-Chlorophenyl | CH ₃ | CH ₃ | 1 | S | S-[1,1-Dimethyl-2-(4-chlorophenyl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrost-1,4-diene-17 β -carbothioate. |
| IA.126 | α -CH ₃ | F | F | Ethoxy | 4-Methoxyphenyl | H | H | 1 | S | S-[2-(4-Methoxyphenyl)-2-oxoethyl] 6 α ,9 α -difluoro-17 α -(ethoxycarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrost-1,4-diene-17 β -carbothioate. |

| No. | R ₁ | R ₂ | R ₃ | R ₄ | R ₅ | P | Q | m | Z | Chemical Name |
|--------|---------------------------|----------------|----------------|----------------|-------------------------|---|---|---|---|--|
| IA.127 | α -CH ₃ | F | F | 2-Furyl | 4-Methoxyphenyl | H | H | 1 | S | S-[2-(4-Methoxyphenyl)-2-oxoethyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrost-1,4-diene-17 β -carbothioate. |
| IA.128 | α -CH ₃ | F | F | n-Butyl | 4-Trifluoromethylphenyl | H | H | 1 | S | S-[2-Oxo-2-(4-trifluoromethylphenyl)ethyl] 17 α -n-butylcarbonyloxy-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrost-1,4-diene-17 β -carbothioate. |
| IA.129 | α -CH ₃ | F | F | n-Butyl | 4-Chlorophenyl | H | H | 1 | S | S-[2-(4-Chlorophenyl)-2-oxoethyl] 17 α -n-butylcarbonyloxy-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrost-1,4-diene-17 β -carbothioate. |
| IA.130 | α -CH ₃ | F | F | n-Butyl | 2,4-Difluorophenyl | H | H | 1 | S | S-[2-(2,4-Difluorophenyl)-2-oxoethyl] 17 α -n-butylcarbonyloxy-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrost-1,4-diene-17 β -carbothioate. |
| IA.131 | α -CH ₃ | F | F | n-Butyl | 4-Fluorophenyl | H | H | 1 | S | S-[2-(4-Fluorophenyl)-2-oxoethyl] 17 α -n-butylcarbonyloxy-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrost-1,4-diene-17 β -carbothioate. |
| IA.132 | α -CH ₃ | F | F | Isopropyl | 4-Chlorophenyl | H | H | 1 | S | S-[2-(4-Chlorophenyl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-17 α -(2-methylpropionyloxy)-3-oxoandrost-1,4-diene-17 β -carbothioate. |
| IA.133 | α -CH ₃ | F | F | Cyclobutyl | 4-Fluorophenyl | H | H | 1 | O | S-[2-(4-Fluorophenyl)-2-oxoethyl] 17 α -cyclobutylcarbonyloxy-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrost-1,4-diene-17 β -carboxylate. |
| IA.134 | α -CH ₃ | F | F | Cyclopentyl | 4-Trifluoromethylphenyl | H | H | 1 | S | S-[2-Oxo-2-(4-trifluoromethylphenyl)ethyl] 17 α -cyclopentylcarbonyloxy-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrost-1,4-diene-17 β -carbothioate. |
| IA.135 | α -CH ₃ | F | F | Cyclobutyl | 4-Chlorophenyl | H | H | 1 | S | S-[2-(4-Chlorophenyl)-2-oxoethyl] 17 α -cyclobutylcarbonyloxy-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrost-1,4-diene-17 β -carbothioate. |
| IA.136 | α -CH ₃ | F | F | Cyclobutyl | 4-Trifluoromethylphenyl | H | H | 1 | S | S-[2-Oxo-2-(4-trifluoromethylphenyl)ethyl] 17 α -cyclobutylcarbonyloxy-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrost-1,4-diene-17 β -carbothioate. |
| IA.137 | α -CH ₃ | F | F | Cyclobutyl | 2,4-Difluorophenyl | H | H | 1 | S | S-[2-(2,4-Difluorophenyl)-2-oxoethyl] 17 α -cyclobutylcarbonyloxy-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrost-1,4-diene-17 β -carbothioate. |
| IA.138 | α -CH ₃ | F | F | Cyclobutyl | 4-Methoxyphenyl | H | H | 1 | S | S-[2-(4-Methoxyphenyl)-2-oxoethyl] 17 α -cyclobutylcarbonyloxy-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrost-1,4-diene-17 β -carbothioate. |
| IA.139 | α -CH ₃ | F | H | 2-Furyl | 4-Trifluoromethylphenyl | H | H | 1 | S | S-[2-Oxo-2-(4-trifluoromethylphenyl)ethyl] 9 α -fluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrost-1,4-diene-17 β -carbothioate. |
| IA.140 | α -CH ₃ | F | H | 2-Furyl | 2,4-Difluorophenyl | H | H | 1 | S | S-[2-(2,4-Difluorophenyl)-2-oxoethyl] 9 α -fluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrost-1,4-diene-17 β -carbothioate. |
| IA.141 | α -CH ₃ | F | H | 2-Furyl | 4-Chlorophenyl | H | H | 1 | S | S-[2-(4-Chlorophenyl)-2-oxoethyl] 9 α -fluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrost-1,4-diene-17 β -carbothioate. |
| IA.142 | α -CH ₃ | F | H | 2-Furyl | 4-Methoxyphenyl | H | H | 1 | S | S-[2-(4-Methoxyphenyl)-2-oxoethyl] 9 α -fluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrost-1,4-diene-17 β -carbothioate. |
| IA.143 | α -CH ₃ | F | H | 2-Furyl | 4-Fluorophenyl | H | H | 1 | S | S-[2-(4-Fluorophenyl)-2-oxoethyl] 9 α -fluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrost-1,4-diene-17 β -carbothioate. |

SUBSTITUTE SHEET (RULE 26)

| No. | R ₁ | R ₂ | R ₃ | R ₄ | R ₅ | P | Q | m ₁ | Z | Chemical Name |
|--------|---------------------------|----------------|----------------|------------------|-------------------------|---|---|----------------|---|--|
| IA.144 | <i>α</i> -CH ₃ | F | F | Isopropyl | 2,4,6-Trimethylphenyl | H | H | 1 | S | S-[2-Oxo-2-(2,4,6-trimethylphenyl)ethyl] 6 <i>α</i> ,9 <i>α</i> -difluoro-11 <i>β</i> -hydroxy-16 <i>α</i> -methyl-17 <i>α</i> -(2-methylpropionyloxy)-3-oxoandrosta-1,4-diene-17 <i>β</i> -carbothioate. |
| IA.145 | <i>α</i> -CH ₃ | F | F | Cyclohexyl | 2,4,6-Trimethylphenyl | H | H | 1 | S | S-[2-Oxo-2-(2,4,6-trimethylphenyl)ethyl] 17 <i>α</i> -cyclohexylcarbonyloxy-6 <i>α</i> ,9 <i>α</i> -difluoro-11 <i>β</i> -hydroxy-16 <i>α</i> -methyl-3-oxoandrosta-1,4-diene-17 <i>β</i> -carbothioate. |
| IA.146 | <i>α</i> -CH ₃ | F | F | Cyclopentyl | 2,4,6-Trimethylphenyl | H | H | 1 | S | S-[2-Oxo-2-(2,4,6-trimethylphenyl)ethyl] 17 <i>α</i> -cyclopentylcarbonyloxy-6 <i>α</i> ,9 <i>α</i> -difluoro-11 <i>β</i> -hydroxy-16 <i>α</i> -methyl-3-oxoandrosta-1,4-diene-17 <i>β</i> -carbothioate. |
| IA.147 | <i>α</i> -CH ₃ | F | F | Cyclobutyl | 2,4,6-Trimethylphenyl | H | H | 1 | S | S-[2-Oxo-2-(2,4,6-trimethylphenyl)ethyl] 17 <i>α</i> -cyclobutylcarbonyloxy-6 <i>α</i> ,9 <i>α</i> -difluoro-11 <i>β</i> -hydroxy-16 <i>α</i> -methyl-3-oxoandrosta-1,4-diene-17 <i>β</i> -carbothioate. |
| IA.148 | <i>α</i> -CH ₃ | F | F | Cyclohexylmethyl | 2,4,6-Trimethylphenyl | H | H | 1 | S | S-[2-Oxo-2-(2,4,6-trimethylphenyl)ethyl] 17 <i>α</i> -cyclohexylmethylcarbonyloxy-6 <i>α</i> ,9 <i>α</i> -difluoro-11 <i>β</i> -hydroxy-16 <i>α</i> -methyl-3-oxoandrosta-1,4-diene-17 <i>β</i> -carbothioate. |
| IA.149 | <i>α</i> -CH ₃ | F | F | 2-Thienyl | 2,4,6-Trimethylphenyl | H | H | 1 | S | S-[2-Oxo-2-(2,4,6-trimethylphenyl)ethyl] 6 <i>α</i> ,9 <i>α</i> -difluoro-11 <i>β</i> -hydroxy-16 <i>α</i> -methyl-3-oxo-17 <i>α</i> -(2-thienylcarbonyloxy)androsta-1,4-diene-17 <i>β</i> -carbothioate. |
| IA.150 | <i>α</i> -CH ₃ | F | F | Cyclohexylmethyl | 2,4-Difluorophenyl | H | H | 1 | S | S-[2-(2,4-Difluorophenyl)-2-oxoethyl] 17 <i>α</i> -cyclohexylmethylcarbonyloxy-6 <i>α</i> ,9 <i>α</i> -difluoro-11 <i>β</i> -hydroxy-16 <i>α</i> -methyl-3-oxoandrosta-1,4-diene-17 <i>β</i> -carbothioate. |
| IA.151 | <i>α</i> -CH ₃ | F | F | Cyclohexylmethyl | 4-Chlorophenyl | H | H | 1 | S | S-[2-(4-Chlorophenyl)-2-oxoethyl] 17 <i>α</i> -cyclohexylmethylcarbonyloxy-6 <i>α</i> ,9 <i>α</i> -difluoro-11 <i>β</i> -hydroxy-16 <i>α</i> -methyl-3-oxoandrosta-1,4-diene-17 <i>β</i> -carbothioate. |
| IA.152 | <i>α</i> -CH ₃ | F | F | Cyclohexylmethyl | 4-Trifluoromethylphenyl | H | H | 1 | S | S-[2-Oxo-2-(4-trifluoromethylphenyl)ethyl] 17 <i>α</i> -cyclohexylmethylcarbonyloxy-6 <i>α</i> ,9 <i>α</i> -difluoro-11 <i>β</i> -hydroxy-16 <i>α</i> -methyl-3-oxoandrosta-1,4-diene-17 <i>β</i> -carbothioate. |
| IA.153 | <i>α</i> -CH ₃ | F | F | Cyclohexylmethyl | 4-Methoxyphenyl | H | H | 1 | S | S-[2-(4-Methoxyphenyl)-2-oxoethyl] 17 <i>α</i> -cyclohexylmethylcarbonyloxy-6 <i>α</i> ,9 <i>α</i> -difluoro-11 <i>β</i> -hydroxy-16 <i>α</i> -methyl-3-oxoandrosta-1,4-diene-17 <i>β</i> -carbothioate. |
| IA.154 | <i>α</i> -CH ₃ | F | F | <i>n</i> -Butyl | 2,4,6-Trimethylphenyl | H | H | 1 | S | S-[2-Oxo-2-(2,4,6-trimethylphenyl)ethyl] 17 <i>α</i> - <i>n</i> -butylcarbonyloxy-6 <i>α</i> ,9 <i>α</i> -difluoro-11 <i>β</i> -hydroxy-16 <i>α</i> -methyl-3-oxoandrosta-1,4-diene-17 <i>β</i> -carbothioate. |
| IA.155 | <i>α</i> -CH ₃ | F | F | Ethoxy | 2,4,6-Trimethylphenyl | H | H | 1 | S | S-[2-Oxo-2-(2,4,6-trimethylphenyl)ethyl] 6 <i>α</i> ,9 <i>α</i> -difluoro-17 <i>α</i> -(ethoxycarbonyloxy)-11 <i>β</i> -hydroxy-16 <i>α</i> -methyl-3-oxoandrosta-1,4-diene-17 <i>β</i> -carbothioate. |
| IA.156 | <i>α</i> -CH ₃ | F | F | 2-Furyl | 2,4,6-Trimethylphenyl | H | H | 1 | S | S-[2-Oxo-2-(2,4,6-trimethylphenyl)ethyl] 6 <i>α</i> ,9 <i>α</i> -difluoro-17 <i>α</i> -(2-furylcarbonyloxy)-11 <i>β</i> -hydroxy-16 <i>α</i> -methyl-3-oxoandrosta-1,4-diene-17 <i>β</i> -carbothioate. |
| IA.157 | <i>α</i> -CH ₃ | F | F | 2-Furyl | 4-Chlorophenyl | H | H | 1 | S | S-[2-(4-Chlorophenyl)-2-oxoethyl] 6 <i>α</i> ,9 <i>α</i> -difluoro-17 <i>α</i> -(2-furylcarbonyloxy)-11 <i>β</i> -hydroxy-16 <i>α</i> -methyl-3-oxoandrosta-1,4-diene-17 <i>β</i> -carbothioate. |
| IA.158 | <i>β</i> -CH ₃ | F | F | Ethyl | 4-Chlorophenyl | H | H | 1 | S | S-[2-(4-Chlorophenyl)-2-oxoethyl] 6 <i>α</i> ,9 <i>α</i> -difluoro-11 <i>β</i> -hydroxy-16 <i>β</i> -methyl-3-oxo-17 <i>α</i> -propionyloxyandrosta-1,4-diene-17 <i>β</i> -carbothioate. |
| IA.159 | <i>α</i> -CH ₃ | F | F | 2-Thienyl | 4-Trifluoromethylphenyl | H | H | 1 | S | S-[2-Oxo-2-(4-trifluoromethylphenyl)ethyl] 6 <i>α</i> ,9 <i>α</i> -difluoro-17 <i>α</i> -(2-thienylcarbonyloxy)-11 <i>β</i> -hydroxy-16 <i>α</i> -methyl-3-oxoandrosta-1,4-diene-17 <i>β</i> -carbothioate. |
| IA.160 | <i>α</i> -CH ₃ | F | F | Ethyl | 3-Nitrophenyl | H | H | 1 | S | S-[2-(3-Nitrophenyl)-2-oxoethyl] 6 <i>α</i> ,9 <i>α</i> -difluoro-11 <i>β</i> -hydroxy-16 <i>α</i> -methyl-3-oxo-17 <i>α</i> -propionyloxyandrosta-1,4-diene-17 <i>β</i> -carbothioate. |

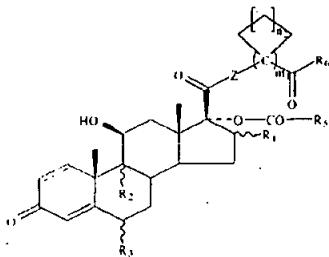
SUBSTITUTE SHEET (RULE 26)

| No. | R ₁ | R ₂ | R ₃ | R ₄ | R ₅ | P | Q | m ₁ | Z | Chemical Name |
|--------|---------------------------|----------------|----------------|----------------|-------------------------|---|---|----------------|---|--|
| IA.161 | α -CH ₃ | F | F | Ethyl | 3,4-Dimethylphenyl | H | H | 1 | S | S-[2-(3,4-Dimethylphenyl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrost-1,4-diene-17 β -carbothioate. |
| IA.162 | β -CH ₃ | F | F | Ethyl | 4-Trifluoromethylphenyl | H | H | 1 | S | S-[2-Oxo-2-(4-trifluoromethylphenyl)ethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 β -methyl-3-oxo-17 α -propionyloxyandrost-1,4-diene-17 β -carbothioate. |
| IA.163 | α -CH ₃ | F | F | n-Propyl | 4-Trifluoromethylphenyl | H | H | 1 | S | S-[2-Oxo-2-(4-trifluoromethylphenyl)ethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propylcarbonyloxyandrost-1,4-diene-17 β -carbothioate. |
| IA.164 | α -CH ₃ | F | F | n-Propyl | 4-Chlorophenyl | H | H | 1 | S | S-[2-(4-Chlorophenyl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -n-propylcarbonyloxyandrost-1,4-diene-17 β -carbothioate. |
| IA.165 | α -CH ₃ | F | F | n-Propyl | 2,4-Difluorophenyl | H | H | 1 | S | S-[2-(2,4-Difluorophenyl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -n-propylcarbonyloxyandrost-1,4-diene-17 β -carbothioate. |
| IA.166 | α -CH ₃ | F | F | n-Propyl | 4-Fluorophenyl | H | H | 1 | S | S-[2-(4-Fluorophenyl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -n-propylcarbonyloxyandrost-1,4-diene-17 β -carbothioate. |
| IA.167 | α -CH ₃ | F | F | n-Propyl | 4-Methoxyphenyl | H | H | 1 | S | S-[2-(4-Methoxyphenyl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -n-propylcarbonyloxyandrost-1,4-diene-17 β -carbothioate. |
| IA.168 | α -CH ₃ | F | F | 2-Furyl | 3-Chlorophenyl | H | H | 1 | S | S-[2-(3-Chlorophenyl)-2-oxoethyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrost-1,4-diene-17 β -carbothioate. |
| IA.169 | β -CH ₃ | F | F | 2-Furyl | 4-Trifluoromethylphenyl | H | H | 1 | S | S-[2-Oxo-2-(4-trifluoromethylphenyl)ethyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 β -methyl-3-oxoandrost-1,4-diene-17 β -carbothioate. |
| IA.170 | α -CH ₃ | F | F | 2-Furyl | 3,5-Dimethoxyphenyl | H | H | 1 | S | S-[2-(3,5-Dimethoxyphenyl)-2-oxoethyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrost-1,4-diene-17 β -carbothioate. |
| IA.171 | α -CH ₃ | F | F | 2-Furyl | 4-Nitrophenyl | H | H | 1 | S | S-[2-(4-Nitrophenyl)-2-oxoethyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrost-1,4-diene-17 β -carbothioate. |
| IA.172 | α -CH ₃ | F | F | Methoxymethyl | 4-Trifluoromethylphenyl | H | H | 1 | S | S-[2-Oxo-2-(4-trifluoromethylphenyl)ethyl] 6 α ,9 α -difluoro-11 β -hydroxy-17 α -(methoxymethylcarbonyloxy)-16 α -methyl-3-oxoandrost-1,4-diene-17 β -carbothioate. |
| IA.173 | α -CH ₃ | F | F | Methoxymethyl | 2,4,6-Trimethylphenyl | H | H | 1 | S | S-[2-Oxo-2-(2,4,6-trimethylphenyl)ethyl] 6 α ,9 α -difluoro-11 β -hydroxy-17 α -(methoxymethylcarbonyloxy)-16 α -methyl-3-oxoandrost-1,4-diene-17 β -carbothioate. |
| IA.174 | α -CH ₃ | F | F | Ethyl | 3-Chloro-4-fluorophenyl | H | H | 1 | S | S-[2-(3-Chloro-4-fluorophenyl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrost-1,4-diene-17 β -carbothioate. |
| IA.175 | β -CH ₃ | F | F | 2-Furyl | 2,4,6-Trimethylphenyl | H | H | 1 | S | S-[2-Oxo-2-(2,4,6-trimethylphenyl)ethyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 β -methyl-3-oxoandrost-1,4-diene-17 β -carbothioate. |
| IA.176 | α -CH ₃ | F | F | Ethoxymethyl | 2,4,6-Trimethylphenyl | H | H | 1 | S | S-[2-Oxo-2-(2,4,6-trimethylphenyl)ethyl] 6 α ,9 α -difluoro-17 α -(ethoxymethylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrost-1,4-diene-17 β -carbothioate. |
| IA.177 | α -CH ₃ | F | F | Ethoxymethyl | 4-Trifluoromethylphenyl | H | H | 1 | S | S-[2-Oxo-2-(4-trifluoromethylphenyl)ethyl] 6 α ,9 α -difluoro-17 α -(ethoxymethylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrost-1,4-diene-17 β -carbothioate. |

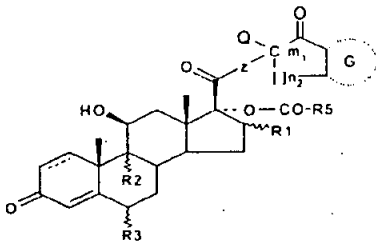
| No. | R ₁ | R ₂ | R ₃ | R ₄ | R ₅ | P | Q | m ₁ | Z | Chemical Name |
|--------|---------------------------|----------------|----------------|------------------|-------------------------|-----------------|-----------------|----------------|---|---|
| IA.179 | α -CH ₃ | F | F | 2-Furyl | 2-Naphthyl | H | H | I | S | S-[2-(Naphthalen-2-yl)-2-oxoethyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IA.180 | α -CH ₃ | F | F | 2-Furyl | 1-Naphthyl | H | H | I | S | S-[2-(Naphthalen-1-yl)-2-oxoethyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IA.181 | α -CH ₃ | F | F | 3-Methyl-2-furyl | 4-Trifluoromethylphenyl | H | H | I | S | S-[2-Oxo-2-(4-trifluoromethylphenyl)ethyl] 6 α ,9 α -difluoro-11 β -hydroxy-17 α -[(3-methyl-2-furyl)-carbonyloxy]-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IA.182 | α -CH ₃ | F | F | 3-Methyl-2-furyl | 2,4,6-Trimethylphenyl | H | H | I | S | S-[2-Oxo-2-(2,4,6-trimethylphenyl)ethyl] 6 α ,9 α -difluoro-11 β -hydroxy-17 α -[(3-methyl-2-furyl)-carbonyloxy]-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IA.183 | α -CH ₃ | F | F | 2-Furyl | 3-Nitro-4-methoxyphenyl | H | H | I | S | S-[2-(3-Nitro-4-methoxyphenyl)-2-oxoethyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IA.184 | α -CH ₃ | F | F | 2-Furyl | 3,4-Dimethylphenyl | H | H | I | S | S-[2-(3,4-Dimethylphenyl)-2-oxoethyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IA.185 | α -CH ₃ | F | F | 3-Furyl | 4-Trifluoromethylphenyl | H | H | I | S | S-[2-Oxo-2-(4-trifluoromethylphenyl)ethyl] 6 α ,9 α -difluoro-17 α -(3-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IA.186 | α -CH ₃ | F | F | 3-Furyl | 2,4,6-Trimethylphenyl | H | H | I | S | S-[2-Oxo-2-(2,4,6-trimethylphenyl)ethyl] 6 α ,9 α -difluoro-17 α -(3-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IA.187 | α -CH ₃ | F | F | Ethyl | 4-Trifluoromethylphenyl | CH ₃ | CH ₃ | I | S | S-[1,1-Dimethyl-2-oxo-2-(4-trifluoromethylphenyl)ethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate. |
| IA.188 | α -CH ₃ | F | F | Ethyl | 4-Fluorophenyl | CH ₃ | CH ₃ | I | S | S-[1,1-Dimethyl-2-(4-fluorophenyl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate. |
| IA.189 | α -CH ₃ | F | H | Ethyl | Phenyl | CH ₃ | CH ₃ | I | S | S-[1,1-Dimethyl-2-phenyl-2-oxoethyl] 9 α -fluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate. |
| IA.190 | α -CH ₃ | F | F | Cyclohexyl | Phenyl | CH ₃ | CH ₃ | I | S | S-[1,1-Dimethyl-2-phenyl-2-oxoethyl] 17 α -cyclohexylcarbonyloxy-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IA.191 | α -CH ₃ | F | F | Cyclopentyl | Phenyl | CH ₃ | CH ₃ | I | S | S-[1,1-Dimethyl-2-phenyl-2-oxoethyl] 17 α -cyclopentylcarbonyloxy-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IA.192 | α -CH ₃ | F | F | Isopropyl | Phenyl | CH ₃ | CH ₃ | I | S | S-[1,1-Dimethyl-2-phenyl-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-17 α -(2-methylpropionyloxy)-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IA.193 | α -CH ₃ | F | F | Cyclobutyl | Phenyl | CH ₃ | CH ₃ | I | S | S-[1,1-Dimethyl-2-phenyl-2-oxoethyl] 17 α -cyclobutylcarbonyloxy-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IA.194 | α -CH ₃ | F | H | 2-Furyl | Phenyl | CH ₃ | CH ₃ | I | S | S-[1,1-Dimethyl-2-phenyl-2-oxoethyl] 9 α -fluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |

| No. | R ₁ | R ₂ | R ₃ | R ₄ | R ₅ | P | Q | m ₁ | Z | Chemical Name |
|--------|---------------------------|----------------|----------------|--------------------|-------------------------|-----------------|-----------------|----------------|---|--|
| IA.195 | α -CH ₃ | F | F | Cyclohexylmethyl | Phenyl | CH ₃ | CH ₃ | 1 | S | S-[1,1-Dimethyl-2-phenyl-2-oxoethyl] 17 α -cyclohexylmethylcarbonyloxy-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IA.196 | α -CH ₃ | F | F | 2-Furyl | 4-Fluorophenyl | CH ₃ | CH ₃ | 1 | S | S-[1,1-Dimethyl-2-(4-fluorophenyl)-2-oxoethyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IA.197 | α -CH ₃ | F | F | 2-Furyl | 4-Trifluoromethylphenyl | CH ₃ | CH ₃ | 1 | S | S-[1,1-Dimethyl-2-oxo-2-(4-trifluoromethylphenyl)ethyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IA.198 | α -CH ₃ | F | F | 5-Chloro-2-thienyl | 3,4-Dimethylphenyl | H | H | 1 | S | S-[2-(3,4-Dimethylphenyl)-2-oxoethyl] 17 α -(5-chloro-2-thienylcarbonyloxy)-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |

5 Table 2- Lists the compound of formula I-A-1 and Table-3 lists the compound of formula I-A-2 which have been synthesized



Formula I-A-1



Formula I-A-2

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Table 2

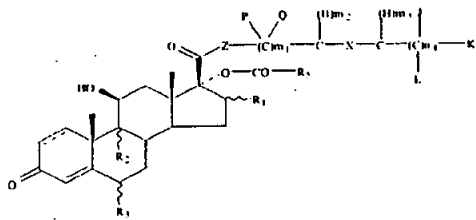
| Sr. No | R ₁ | R ₂ | R ₃ | R ₄ | R ₅ | n ₁ | m ₁ | Z | Chemical Name |
|--------|---------------------------|----------------|----------------|----------------|----------------|----------------|----------------|---|--|
| IA-1.1 | α -CH ₃ | F | F | Ethyl | 4-Fluorophenyl | 2 | 1 | S | S-[1-(4-Fluorobenzoyl)cyclopentyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxy-androsta-1,4-diene-17 β -carbothioate. |
| IA-1.2 | α -CH ₃ | F | F | Ethyl | Phenyl | 2 | 1 | S | S-[1-Benzoylcyclopentyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate. |

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Table 3

| Sr. No | R ₁ | R ₂ | R ₃ | R ₄ | n ₁ | Q | G | m ₁ | Z | Chemical Name |
|--------|---------------------------|----------------|----------------|----------------|----------------|---|--------|----------------|---|--|
| IA-2.1 | α -CH ₃ | F | F | Ethyl | 2 | H | Phenyl | 1 | S | S-(1-oxo-1,2,3,4-tetrahydronaphthalen-2-yl) 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate. |

Table 4- Lists the compound of formula I-B which have been synthesized



Formula I-B

| Table-4 | | | | | | | | | | | | | | | |
|---------|-------------------|----------------|----------------|----------------|---|---|----|----|---|---|----------------|----------------|----------------|----------------|---|
| Sr. No | R ₁ | R ₂ | R ₃ | R ₄ | P | Q | J | K | Z | X | m ₁ | m ₂ | m ₃ | n ₁ | Chemical Name |
| IB.1 | α-CH ₃ | F | F | Ethyl | H | H | H | H | O | = | 1 | 0 | 0 | 1 | OH
4-Hydroxy-but-2-ynyl 6α,9α-difluoro-11β-hydroxy-16α-methyl-3-oxo-17α-propionyloxyandrosta-1,4-diene-17β-carboxylate. |
| IB.2 | α-CH ₃ | F | F | Ethyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OH
S-(4-Hydroxy-but-2-ynyl) 6α,9α-difluoro-11β-hydroxy-16α-methyl-3-oxo-17α-propionyloxyandrosta-1,4-diene-17β-carbothioate. |
| IB.3 | α-CH ₃ | F | F | Ethyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | F
S-(4-Fluoro-but-2-ynyl) 6α,9α-difluoro-11β-hydroxy-16α-methyl-3-oxo-17α-propionyloxyandrosta-1,4-diene-17β-carbothioate. |
| IB.4 | α-CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OH
S-(4-Hydroxy-but-2-ynyl) 6α,9α-difluoro-17α-[(2-furanylcarbonyloxy)-11β-hydroxy-16α-methyl-3-oxoandrosta-1,4-diene-17β-carbothioate. |
| IB.5 | α-CH ₃ | F | H | Ethyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OH
S-(4-Hydroxy-but-2-ynyl) 9α-fluoro-11β-hydroxy-16α-methyl-3-oxo-17α-propionyloxyandrosta-1,4-diene-17β-carbothioate. |
| IB.6 | α-CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | F
S-(4-Fluoro-but-2-ynyl) 6α,9α-difluoro-17α-[(2-furanylcarbonyloxy)-11β-hydroxy-16α-methyl-3-oxoandrosta-1,4-diene-17β-carbothioate. |
| IB.7 | α-CH ₃ | F | F | Isopropyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OH
S-(4-Hydroxy-but-2-ynyl) 6α,9α-difluoro-11β-hydroxy-16α-methyl-17α-(2-methyl-propionyloxy)-3-oxoandrosta-1,4-diene-17β-carbothioate. |
| IB.8 | α-CH ₃ | F | F | Cyclobutyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OH
S-(4-Hydroxy-but-2-ynyl) 17α-cyclobutylcarbonyloxy-6α,9α-difluoro-11β-hydroxy-16α-methyl-3-oxoandrosta-1,4-diene-17β-carbothioate. |
| IB.9 | α-CH ₃ | F | H | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OH
S-(4-Hydroxy-but-2-ynyl) 9α-fluoro-17α-[(2-furanylcarbonyloxy)-11β-hydroxy-16α-methyl-3-oxoandrosta-1,4-diene-17β-carbothioate. |
| IB.10 | α-CH ₃ | F | F | 2-Thienyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OH
S-(4-Hydroxy-but-2-ynyl) 6α,9α-difluoro-11β-hydroxy-16α-methyl-3-oxo-17α-[(2-thienylcarbonyloxy)-androsta-1,4-diene-17β-carbothioate. |
| IB.11 | α-CH ₃ | F | F | Ethyl | H | H | -- | -- | S | = | 1 | 0 | 1 | 0 | --
S-(Prop-2-ynyl) 6α,9α-difluoro-11β-hydroxy-16α-methyl-3-oxo-17α-propionyl-oxyandrosta-1,4-diene-17β-carbothioate. |

| Sr. No | R ₁ | R ₂ | R ₃ | R ₄ | P | Q | J | K | Z | X | m ₁ | m ₂ | m ₃ | m ₄ | I | Chemical Name |
|--------|---------------------------|----------------|----------------|--------------------|---|---|---------------------------------|---|---|-------|----------------|----------------|----------------|----------------|--|---|
| BB.12 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | 1,4-Dioxo-spiro[4.5]decan-2-ylmethoxycarbonyloxy | S-[4-(1,4-Dioxo-spiro[4.5]decan-2-ylmethoxycarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanyl-carbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| BB.13 | α -CH ₃ | F | F | Ethyl | H | H | H | H | S | = (E) | 1 | 1 | 1 | 1 | OH | S-[4-(1-Hydroxy-(E)-but-2-enyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyl-oxyandrosta-1,4-diene-17 β -carbothioate. |
| BB.14 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = (E) | 1 | 1 | 1 | 1 | OH | S-[4-(1-Hydroxy-(E)-but-2-enyl] 6 α ,9 α -difluoro-17 α -(2-furanyl-carbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| BB.15 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = (Z) | 1 | 1 | 1 | 1 | OH | S-[4-(1-Hydroxy-(Z)-but-2-enyl] 6 α ,9 α -difluoro-17 α -(2-furanyl-carbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| BB.16 | α -CH ₃ | F | F | 2-Thienyl | H | H | H | H | S | = (Z) | 1 | 1 | 1 | 1 | OH | S-[4-(1-Hydroxy-(Z)-but-2-enyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -(2-thienyl-carbonyloxy)-androsta-1,4-diene-17 β -carbothioate. |
| BB.17 | α -CH ₃ | F | F | 2-Thienyl | H | H | H | H | S | = (E) | 1 | 1 | 1 | 1 | OH | S-[4-(1-Hydroxy-(E)-but-2-enyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -(2-thienyl-carbonyloxy)-androsta-1,4-diene-17 β -carbothioate. |
| BB.18 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | 1,4-Dioxo-spiro[4.4]nonan-2-ylmethoxycarbonyloxy | S-[4-(1,4-Dioxo-spiro[4.4]nonan-2-ylmethoxycarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanyl-carbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| BB.19 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCO-O(CH ₃)-ONO ₂ | S-(4-(4-Nitroxybutyloxycarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanyl-carbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| BB.20 | α -CH ₃ | F | F | 5-Chloro-2-Thienyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OH | S-[4-Hydroxy-but-2-ynyl] 17 α -[(5-chloro-2-thienyl-carbonyloxy)-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| BB.21 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | H | S-[But-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanyl-carbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| BB.22 | α -CH ₃ | F | F | 3-Methyl-2-furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OH | S-[4-Hydroxy-but-2-ynyl] 6 α ,9 α -difluoro-11 β -hydroxy-17 α -[(3-methyl-2-furanyl)-carbonyloxy]-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| BB.23 | α -CH ₃ | F | F | Ethoxy-methyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OH | S-[4-Hydroxy-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(ethoxymethyl-carbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| BB.24 | α -CH ₃ | F | F | Methoxy-methyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OH | S-[4-Hydroxy-but-2-ynyl] 6 α ,9 α -difluoro-11 β -hydroxy-17 α -(methoxymethyl-carbonyloxy)-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| BB.25 | α -CH ₃ | F | F | 2-Furyl | H | H | (CH ₂) ₆ | | S | = | 1 | 0 | 0 | 1 | OH | S-[3-(1-Hydroxycyclohexyl)prop-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanyl-carbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |

SUBSTITUTE SHEET (RULE 26)

| Sr. No | R ₁ | R ₂ | R ₃ | R ₄ | P | Q | J | K | Z | X | m ₁ | m ₂ | m ₃ | n ₁ | L | Chemical Name |
|--------|---------------------------|----------------|----------------|------------------|---|---|-----------------|-----------------|---|-------|----------------|----------------|----------------|----------------|---|---|
| IB.26 | α -CH ₃ | F | F | Cyclohexylmethyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OH | S-[4-Hydroxy-but-2-ynyl] 17 α -cyclohexylmethylcarbonyloxy-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.27 | α -CH ₃ | F | F | n-Butyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OH | S-[4-Hydroxy-but-2-ynyl] 17 α -n-butylcarbonyloxy-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.28 | α -CH ₃ | F | F | Ethyl | H | H | -- | -- | O | = | 1 | 0 | 1 | 0 | -- | Prop-2-ynyl 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carboxylate. |
| IB.29 | α -CH ₃ | F | F | Cyclopentyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OH | S-[4-Hydroxy-but-2-ynyl] 17 α -cyclopentylcarbonyloxy-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.30 | α -CH ₃ | F | F | Ethyl | H | H | H | H | S | = (Z) | 1 | 1 | 1 | 1 | OH | S-[4-Hydroxy-(Z)-but-2-ynyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate. |
| IB.31 | α -CH ₃ | F | F | Ethyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | (KOC ₂ H ₅) ₃ | S-[4-Propionyloxy-but-2-ynyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate. |
| IB.32 | α -CH ₃ | F | F | Ethyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCOCH ₃ | S-[4-Acetoxy-but-2-ynyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate. |
| IB.33 | α -CH ₃ | F | F | Ethyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCO-n-C ₃ H ₇ | S-[4-n-Propylcarbonyloxy-but-2-ynyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate. |
| IB.34 | α -CH ₃ | F | F | Ethyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCO-CH(CH ₃) ₂ | S-[4-(2-Methylpropionyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate. |
| IB.35 | α -CH ₃ | F | F | Ethyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCO-n-C ₄ H ₉ | S-[4-n-Butylcarbonyloxy-but-2-ynyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate. |
| IB.36 | α -CH ₃ | F | F | Ethyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCO-cyclobutyl | S-[4-Cyclobutylcarbonyloxy-but-2-ynyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate. |
| IB.37 | α -CH ₃ | F | F | Ethyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCO-n-C ₅ H ₁₁ | S-[4-n-Pentylcarbonyloxy-but-2-ynyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate. |
| IB.38 | β -CH ₃ | F | H | Ethyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OH | S-[4-Hydroxy-but-2-ynyl] 9 α -fluoro-11 β -hydroxy-16 β -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate. |
| IB.39 | β -CH ₃ | F | F | Ethyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OH | S-[4-Hydroxy-but-2-ynyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 β -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate. |
| IB.40 | α -CH ₃ | F | F | 2-Furyl | H | H | CH ₃ | CH ₃ | S | = | 1 | 0 | 0 | 1 | OH | S-[4-Hydroxy-4-methyl-pent-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |

| Sr. No | R ₁ | R ₂ | R ₃ | R ₄ | P | Q | J | K | Z | X | m ₁ | m ₂ | m ₃ | n ₁ | I | Chemical Name |
|--------|---------------------------|----------------|----------------|----------------|---|---|---|---|---|----------|----------------|----------------|----------------|----------------|---|--|
| IB.41 | α -CH ₃ | F | F | Ethyl | H | H | | | O | =
(E) | 1 | 1 | 1 | 1 | OCH ₃ | 4-Methoxy-4-oxo-(E)-but-2-enyl 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carboxylate. |
| IB.42 | α -CH ₃ | F | F | Ethyl | H | H | | O | S | =
(E) | 1 | 1 | 1 | 1 | OCH ₃ | S-[4-Methoxy-4-oxo-(E)-but-2-enyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate. |
| IB.43 | - | H | H | Ethoxy | H | H | | O | O | =
(E) | 1 | 1 | 1 | 1 | OCH ₃ | 4-Methoxy-4-oxo-(E)-but-2-enyl 17 α -tetraoxycarbonyloxy-11 β -hydroxy-3-oxoandrosta-1,4-diene-17 β -carboxylate. |
| IB.44 | α -CH ₃ | F | F | Ethyl | H | H | H | H | S | =
(E) | 1 | 1 | 1 | 1 | OC(=O)OC ₂ H ₅ | S-[4-(2-Ethoxy-1,2-dioxoethyl)oxy-(E)-but-2-enyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate. |
| IB.45 | α -CH ₃ | Cl | H | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OH | S-[4-(Hydroxy-but-2-ynyl)] 9 α -chloro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.46 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | =
(E) | 1 | 1 | 1 | 1 | OC(=O)OC ₂ H ₅ | S-[4-(2-Ethoxy-1,2-dioxoethyl)oxy-(E)-but-2-enyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.47 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | =
(Z) | 1 | 1 | 1 | 1 | OC(=O)OC ₂ H ₅ | S-[4-(2-Ethoxy-1,2-dioxoethyl)oxy-(Z)-but-2-enyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.48 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | (S)-(-)-2-Acetoxypropionyl-ony | S-[4-((S)-(-)-2-Acetoxypropionyl)oxy] but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.49 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCO-
n-C ₃ H ₇ | S-[4-n-Propylcarbonyloxy-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.50 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCO-
CH(CH ₃) ₂ | S-[4-(2-Methylpropionyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.51 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCO-
C(CH ₃) ₃ | S-[4-(2,2-Dimethylpropionyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.52 | α -CH ₃ | F | F | Ethyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCO-
C(CH ₃) ₃ | S-[4-(2,2-Dimethylpropionyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate. |
| IB.53 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | =
(Z) | 1 | 1 | 1 | 1 | OCO-
n-C ₃ H ₇ | S-[4-n-Propylcarbonyloxy-(Z)-but-2-enyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.54 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OC(=O)OC ₂ H ₅ | S-[4-(2-Ethoxy-1,2-dioxoethyl)oxy-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.55 | α -CH ₃ | F | F | 2-Thienyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCO-
n-C ₃ H ₇ | S-[4-n-Propylcarbonyloxy-but-2-ynyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -(2-thienylcarbonyloxy)androsta-1,4-diene-17 β -carbothioate. |

| Sr. No | R ₁ | R ₂ | R ₃ | R ₄ | P | Q | J | K | Z | X | m ₁ | m ₂ | m ₃ | n ₁ | L | Chemical Name |
|--------|---------------------------|----------------|----------------|----------------|---|---|---|---|---|----------|----------------|----------------|----------------|----------------|--|--|
| IB.56 | α -CH ₃ | F | F | 5-Cl-2-Thienyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCO-
n-C ₃ H ₇ | S-[4-n-Propylcarbonyloxy-but-2-ynyl] 17 α -[(5-chloro-2-thienyl) carbonyl]-oxy]-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-androsta-1,4-diene-17 β -carbothioate. |
| IB.57 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCO-cyclopropyl | S-[4-(4-cyclopropylcarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyl)-oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.58 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCO-cyclobutyl | S-[4-(4-cyclobutylcarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyl)-oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.59 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCO-cyclopentyl | S-[4-(4-cyclopentylcarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyl)-oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.60 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | =
(E) | 1 | 1 | 1 | 1 | OCO-n-C ₃ H ₇ | S-[4-n-Propylcarbonyloxy-(E)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyl)-oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.61 | α -CH ₃ | F | F | 4-Cl-phenyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OH | S-[4-Hydroxy-but-2-ynyl] 17 α -(4-chlorophenyl)carbonyloxy-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.62 | α -CH ₃ | F | F | 3-Cl-phenyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OH | S-[4-Hydroxy-but-2-ynyl] 17 α -(3-chlorophenyl)carbonyloxy-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.63 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCO-OCH ₃ | S-[4-(4-Methoxycarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyl)-oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.64 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCO-OC ₂ H ₅ | S-[4-(4-Ethoxycarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyl)-oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.65 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCO-OC(CH ₃) ₃ | S-[4-(2,2-Dimethylethoxycarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyl)-oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.66 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCO-OCH ₂ CH ₂ CH ₃ | S-[4-(2-Methylpropyloxycarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyl)-oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.67 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCO-(CH ₂) ₃ CH ₂ Cl | S-[4-(3-Chloropropylcarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyl)-oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.68 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | =
(Z) | 1 | 1 | 1 | 1 | OCO-C(CH ₃) ₃ | S-[4-(2,2-Dimethylpropionyloxy)-(Z)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyl)-oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.69 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | =
(E) | 1 | 1 | 1 | 1 | OCO-C(CH ₃) ₃ | S-[4-(2,2-Dimethylpropionyloxy)-(E)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyl)-oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.70 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCOCHCl ₂ | S-[4-Dichloroacetoxy-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyl)-oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |

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| Sr. No. | R ₁ | R ₂ | R ₃ | R ₄ | P | Q | J | K | Z | X | m ₁ | m ₂ | m ₃ | n ₁ | I. | Chemical Name |
|---------|---------------------------|----------------|----------------|----------------|---|---|---|---|---|-------|----------------|----------------|----------------|----------------|---|---|
| IB.71 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | 2-methyl-propyl-carbonyloxy | S-[4-(2-methylpropylcarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanyl-carbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.72 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OC(CH ₃) ₂ -C(CH ₃) ₃ | S-[4-(3,3-dimethylpropylcarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.73 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCO-CH ₂ CH ₃ | S-[4-Propionyloxy-but-2-ynyl] 6 α ,9 α -difluoro-11 β -hydroxy-17 α -(2-furanyl-carbonyloxy)-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.74 | α -CH ₃ | F | F | Cyclobutyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCO-COOCH ₂ CH ₃ | S-[4-(2-Ethoxy-1,2-dioxoethyl-oxy-but-2-ynyl] 17 α -cyclobutylcarbonyloxy-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.75 | α -CH ₃ | F | F | Cyclobutyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCO-CH(CH ₃) ₂ | S-[4-(2-Methylpropionyloxy-but-2-ynyl] 17 α -cyclobutylcarbonyloxy-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.76 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | Adamantyl-carbonyloxy | S-[4-(Adamantylcarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanyl-carbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.77 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCOCH ₂ -CF ₃ | S-[4-(3,3,3-Trifluoropropionyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.78 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCOCH ₂ -OCH ₃ | S-[4-(Methoxyacetyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanyl-carbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.79 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCOCH ₂ -OCH ₂ CH ₃ | S-[4-(Ethoxyacetyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanyl-carbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.80 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCOCH ₂ -CH ₂ COOH | S-[4-(4-Hydroxybutyl-1,4-dione-oxy-but-2-ynyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-17 α -(2-furanylcarbonyloxy)-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.81 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCOCH ₃ | S-[4-Acetoxy-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyl)-oxy-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.82 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = (E) | 1 | 1 | 1 | 1 | OCO-CH(CH ₃) ₂ | S-[4-(2-Methylpropionyloxy-(E)-but-2-enyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.83 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = (Z) | 1 | 1 | 1 | 1 | OCO-CH(CH ₃) ₂ | S-[4-(2-Methylpropionyloxy-(Z)-but-2-enyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.84 | α -CH ₃ | F | F | Cyclobutyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCO-C(CH ₃) ₃ | S-[4-(2,2-Dimethylpropionyloxy)-but-2-ynyl] 17 α -cyclobutylcarbonyloxy-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |

| Sr. No | R ₁ | R ₂ | R ₃ | R ₄ | P | Q | J | K | Z | X | m ₁ | m ₂ | m ₃ | n ₁ | I. | Chemical Name |
|--------|--|----------------|----------------|--------------------|---|---|---|---|---|---|----------------|----------------|----------------|----------------|---|--|
| IB.85 | α -C ₁₁ H ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | 2,2-Dimethyl-butylcarbonyloxy | S-[4-(2,2-Dimethylbutylcarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.86 | α -C ₁₁ H ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | (1S)-Camphanlylcarbonyloxy | S-[4-(1S)-Camphanlylcarbonyloxy-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.87 | α -C ₁₁ H ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCONH-C(CH ₃) ₃ | S-[4-(1,1-Dimethylethylcarbamoyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.88 | α -C ₁₁ H ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCO(CH ₃) ₂ -COOC ₂ H ₅ | S-[4-(4-Ethoxybutyl-1,4-dioneoxy-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.89 | α -C ₁₁ H ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | Menthylcarbonyloxy | S-[4-Menthylcarbonyloxy-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.90 | α -C ₁₁ H ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCOCH ₂ NH-COCH ₃ | S-[4-Acetamidocetoxy-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.91 | α -C ₁₁ H ₃ | F | F | 5-Chloro-2-Thienyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCOOC ₂ H ₅ -CH(CH ₃) ₂ | S-[4-(2-Methylpropyloxybutyl-1,4-dioneoxy)-but-2-ynyl] 17 α -[(5-chloro-2-thienylcarbonyloxy)-oxy]-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.92 | α -C ₁₁ H ₃ | F | F | 5-Chloro-2-Thienyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCO-CH(CH ₃) ₂ | S-[4-(2-Methylpropyloxybutyl-1,4-dioneoxy)-but-2-ynyl] 17 α -[(5-chloro-2-thienylcarbonyloxy)-oxy]-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.93 | α -C ₁₁ H ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCOCH=CH-COOC ₂ H ₅ | S-[4-(4-Ethoxy-2-but-2-en-1,4-dioneoxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.94 | α -C ₁₁ H ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCO(CH ₃) ₂ -COOCH ₃ | S-[4-(4-Methoxybutyl-1,4-dioneoxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.95 | α -C ₁₁ H ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCO(CH ₃) ₂ -COOCH ₂ -CH ₃ | S-[4-(4-Isopropoxybutyl-1,4-dioneoxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.96 | α -C ₁₁ H ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCO(CH ₃) ₂ -COOCH ₂ CH ₂ -CH ₃ | S-[4-(4-Isobutoxybutyl-1,4-dioneoxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.97 | α -C ₁₁ H ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCO(CH ₃) ₂ -COO(CH ₂) ₂ -CH ₃ | S-[4-(4-n-Butyloxybutyl-1,4-dioneoxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.98 | α -C ₁₁ H ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | 3-Chloro-2,2-dimethyl-propionyloxy | S-[4-(3-Chloro-2,2-dimethylpropionyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |

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| Sr. No | R ₁ | R ₂ | R ₃ | R ₄ | P | Q | J | K | Z | X | m ₁ | m ₂ | m ₃ | n ₁ | I | Chemical Name |
|--------|---------------------------|----------------|----------------|----------------|---|---|---|---|---|---|----------------|----------------|----------------|----------------|---|---|
| IB.99 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCOCH=CH-COOCH ₂ CH(CH ₃) ₂ | S-[4-(4-Isobutyloxy-(Z)-but-2-en-1,4-dione)oxy-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.100 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCOCH=CH-COOCH ₃ | S-[4-(4-Methoxy-(E)-but-2-en-1,4-dione)oxy-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.101 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCO-CH ₂ CH(CH ₃) ₂ | S-[4-(3-Methyl-1-oxobutyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.102 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCO-CH(CH ₃) ₂ | S-[4-(2-Ethyl-1-oxobutyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.103 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCOS(CH ₃) ₂ | S-[4-(N,N-Dimethylaminoacetyl)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.104 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCO-C(CH ₃) ₂ | S-[4-(2-Chloro-2-methylpropionyl)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.105 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCO(CH ₃) ₂ -CH(CH ₃) ₂ | S-[4-(4-Methyl-1-oxopentyl)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.106 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCO(CH ₃) ₂ -COOCH ₂ F | S-[4-(4-Fluoromethoxy-1,4-dioxo-2-butyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.107 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCOCH=CH-COOCH ₂ F | S-[4-(4-Fluoromethoxy-1,4-dioxo-(Z)-but-2-en)oxy-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.108 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OC(OCH ₂ -COOCH ₃) ₂ | S-[4-(3-Methoxypropyl-1,3-dione)oxy-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.109 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCOC(CH ₃) ₂ -COOCH ₃ | S-[4-(3-Methoxy-2,2-dimethylpropyl-1,3-dione)oxy-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.110 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OC(OCH(OH)-CH ₃) ₂ | S-[4-(2-Hydroxy-2-methylpropionyl)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.111 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCOCF(CH ₃) ₂ | S-[4-(2-Fluoro-2-methylpropionyl)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |

SUBSTITUTE SHEET (RULE 26)

| Sr. No | R ₁ | R ₂ | R ₃ | R ₄ | P | Q | J | K | Z | X | m ₁ | m ₂ | m ₃ | n ₁ | L | Chemical Name |
|--------|---------------------------|----------------|----------------|----------------|---|---|---|---|---|---|----------------|----------------|----------------|----------------|--|--|
| IB.112 | <i>α</i> -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCOCH=CH-COOCH ₃ | S-[4-(4-Methoxy-(Z)-but-2-en-1,4-dione)-oxy-but-2-ynyl] 6 <i>α</i> ,9 <i>α</i> -difluoro-17 <i>α</i> -(2-furanylcarbonyloxy)-11 <i>β</i> -hydroxy-16 <i>α</i> -methyl-3-oxoandrosta-1,4-diene-17 <i>β</i> -carbothioate. |
| IB.113 | <i>α</i> -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCOCH=CH-COOCH ₃ | S-[4-(4-Ethoxy-(E)-but-2-en-1,4-dione)-oxy-but-2-ynyl] 6 <i>α</i> ,9 <i>α</i> -difluoro-17 <i>α</i> -(2-furanylcarbonyloxy)-11 <i>β</i> -hydroxy-16 <i>α</i> -methyl-3-oxoandrosta-1,4-diene-17 <i>β</i> -carbothioate. |
| IB.114 | <i>α</i> -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCOCH=CH-COOCH ₃ -CH(CH ₃) ₂ | S-[4-(4-Isobutyloxy-1,4-dioxo-(E)-but-2-en)-oxy-but-2-ynyl] 6 <i>α</i> ,9 <i>α</i> -difluoro-17 <i>α</i> -(2-furanylcarbonyloxy)-11 <i>β</i> -hydroxy-16 <i>α</i> -methyl-3-oxoandrosta-1,4-diene-17 <i>β</i> -carbothioate. |
| IB.115 | <i>α</i> -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCOCH=CH-COOCH ₃ -CH ₃ | S-[4-(4-n-butyloxy-1,4-dioxo-(E)-but-2-en)-oxy-but-2-ynyl] 6 <i>α</i> ,9 <i>α</i> -difluoro-17 <i>α</i> -(2-furanylcarbonyloxy)-11 <i>β</i> -hydroxy-16 <i>α</i> -methyl-3-oxoandrosta-1,4-diene-17 <i>β</i> -carbothioate. |
| IB.116 | <i>α</i> -CH ₃ | Cl | H | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCOCH=CH-CH ₃ | S-[4-(2-Methylpropionyloxy)-but-2-ynyl] 9 <i>α</i> -chloro-17 <i>α</i> -(2-furanylcarbonyloxy)-11 <i>β</i> -hydroxy-16 <i>α</i> -methyl-3-oxoandrosta-1,4-diene-17 <i>β</i> -carbothioate. |
| IB.117 | <i>α</i> -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | 2-(S)-Methylbutyryloxy | S-[4-(2-(S)-methylbutyryloxy)-but-2-ynyl] 6 <i>α</i> ,9 <i>α</i> -difluoro-17 <i>α</i> -(2-furanylcarbonyloxy)-11 <i>β</i> -hydroxy-16 <i>α</i> -methyl-3-oxoandrosta-1,4-diene-17 <i>β</i> -carbothioate. |
| IB.118 | <i>α</i> -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCO-(2-Furyl) | S-[4-(furan-2-ylcarbonyloxy)-but-2-ynyl] 6 <i>α</i> ,9 <i>α</i> -difluoro-17 <i>α</i> -(2-furanylcarbonyloxy)-11 <i>β</i> -hydroxy-16 <i>α</i> -methyl-3-oxoandrosta-1,4-diene-17 <i>β</i> -carbothioate. |
| IB.119 | <i>α</i> -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCOCH=CH-COOCH ₃ -CH ₃ | S-[4-(4-Isopropoxy-1,4-dioxo-(E)-but-2-en)-oxy-but-2-ynyl] 6 <i>α</i> ,9 <i>α</i> -difluoro-17 <i>α</i> -(2-furanylcarbonyloxy)-11 <i>β</i> -hydroxy-16 <i>α</i> -methyl-3-oxoandrosta-1,4-diene-17 <i>β</i> -carbothioate. |
| IB.120 | <i>α</i> -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | 3-Hydroxy-2,2-dimethyl-Propionyl-oxy | S-[4-(3-Hydroxy-2,2-dimethyl-propionyl-oxy)-but-2-ynyl] 6 <i>α</i> ,9 <i>α</i> -difluoro-17 <i>α</i> -(2-furanylcarbonyloxy)-11 <i>β</i> -hydroxy-16 <i>α</i> -methyl-3-oxoandrosta-1,4-diene-17 <i>β</i> -carbothioate. |
| IB.121 | <i>α</i> -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCO-CH=CH ₂ | S-[4-Acryloyloxy-but-2-ynyl] 6 <i>α</i> ,9 <i>α</i> -difluoro-17 <i>α</i> -(2-furanylcarbonyloxy)-11 <i>β</i> -hydroxy-16 <i>α</i> -methyl-3-oxoandrosta-1,4-diene-17 <i>β</i> -carbothioate. |
| IB.122 | <i>α</i> -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCOC(OH)-C ₃ H ₅ | S-[4-(1-Ethyl-1-hydroxypropylcarbonyloxy)-but-2-ynyl] 6 <i>α</i> ,9 <i>α</i> -difluoro-17 <i>α</i> -(2-furanylcarbonyloxy)-11 <i>β</i> -hydroxy-16 <i>α</i> -methyl-3-oxoandrosta-1,4-diene-17 <i>β</i> -carbothioate. |
| IB.123 | <i>α</i> -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCOOCH ₂ -cyclopropyl | S-[4-(Cyclopropylmethyloxycarbonyloxy)-but-2-ynyl] 6 <i>α</i> ,9 <i>α</i> -difluoro-17 <i>α</i> -(2-furanylcarbonyloxy)-11 <i>β</i> -hydroxy-16 <i>α</i> -methyl-3-oxoandrosta-1,4-diene-17 <i>β</i> -carbothioate. |
| IB.124 | <i>α</i> -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCOC=C-COOCH ₃ | S-[4-(4-Methoxybut-2-yno-1,4-dione)-oxy-but-2-ynyl] 6 <i>α</i> ,9 <i>α</i> -difluoro-17 <i>α</i> -(2-furanylcarbonyloxy)-11 <i>β</i> -hydroxy-16 <i>α</i> -methyl-3-oxoandrosta-1,4-diene-17 <i>β</i> -carbothioate. |

| Sr. No | R ₁ | R ₂ | R ₃ | R ₄ | P | Q | J | K | Z | X | m ₁ | m ₂ | m ₃ | n ₁ | L | Chemical Name |
|---------|---------------------------|----------------|----------------|----------------|---|---|---|---|---|---|----------------|----------------|----------------|----------------|---|--|
| III.125 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OC(O)-cyclopentyl | S-[4-(Cyclopentylloxycarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanyl-carbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| III.126 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OC(O)-CH ₂ -cyclopentyl | S-[4-(Cyclopentylmethyloxycarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanyl-carbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| III.127 | α -CH ₃ | Cl | H | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OC(O)-CH ₂ -CH(CH ₃) ₂ | S-[4-(2-Methylpropyloxycarbonyloxy)-but-2-ynyl] 9 α -chloro-17 α -(2-furanyl-carbonyloxy)-11 β -hydroxy-16 β -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| III.128 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | 2,2-Dimethyl-1,3-dioxolan-4-yl-methoxy-carbonyloxy | S-[4-(2,2-Dimethyl-1,3-dioxolan-4-yl-methoxycarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanyl-carbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| III.129 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OC(=O)N(C ₂ H ₅) ₂ | S-[4-(N,N-Diethylaminocarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanyl-carbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| III.130 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | Piperidin-1-ylcarbonyloxy | S-[4-(Piperidin-1-ylcarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanyl-carbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| III.131 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | 4-Methyl-piperazine-1-yl-carbonyloxy | S-[4-(4-Methyl-piperazine-1-yl-carbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanyl-carbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| III.132 | β -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OH | S-(4-Hydroxy-but-2-ynyl) 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyl)-oxy]-11 β -hydroxy-16 β -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| III.133 | β -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OC(=O)CH ₂ (CH ₃) ₂ | S-[4-(2-Methylpropyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyl)-oxy]-11 β -hydroxy-16 β -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| III.134 | β -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OC(=O)OCH ₂ -CH(CH ₃) ₂ | S-[4-(2-Methylpropyloxycarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanyl-carbonyloxy)-11 β -hydroxy-16 β -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| III.135 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OC(=O)CCl ₂ -CH ₃ | S-[4-(2,2-Dichloropropionyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanyl-carbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| III.136 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | N(C ₂ H ₅) ₂ | S-[4-(N,N-Diethylamino)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyl)-oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| III.137 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OC(=O)OCH ₂ (CH ₃) ₂ | S-[4-(Isopropyloxycarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanyl-carbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |

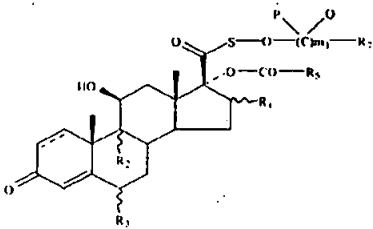
| Sr. No | R ₁ | R ₂ | R ₃ | R ₄ | P | Q | J | K | Z | X | m ₁ | m ₂ | m ₃ | m ₄ | I | Chemical Name |
|---------|---------------------------|----------------|----------------|----------------|---|---|---|---|---|---|----------------|----------------|----------------|----------------|--|--|
| III.138 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OC(OOCCH ₃) ₂ C(H)=C(CH ₃) ₂ | S-[4-(3-Methylbut-2-enoxycarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| III.139 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OC(OO-(CH ₂) ₆ CH ₃) ₂ | S-[4-(<i>n</i> -Hexyloxycarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| III.140 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OC(OOCCH ₂ -cyclohexyl) ₂ | S-[4-(Cyclohexyloxycarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| III.141 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OC(OO-cyclohexyl) ₂ | S-[4-(Cyclohexyloxycarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| III.142 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OC(OO-(CH ₂) ₈ CH ₃) ₂ | S-[4-(<i>n</i> -Octyloxycarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| III.143 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OC(OOCCH ₂ -C(CH ₃) ₃) ₂ | S-[4-(2,2-Dimethylpropyloxycarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| III.144 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OC(OOCCH ₂ -cyclobutyl) ₂ | S-[4-(Cyclobutylmethyloxycarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| III.145 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OC(OOCCH ₂ -(furan-2-yl)) ₂ | S-[4-(2-Methylfuryloxycarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| III.146 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OC(OO-(CH ₂) ₄ CH ₃) ₂ | S-[4-(<i>n</i> -Butyloxycarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| III.147 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OC(OO-(CH ₂) ₅ CH ₃) ₂ | S-[4-(<i>n</i> -Pentyloxycarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| III.148 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | 2,2-Dimethyl-3-fluoro-propionyl-oxy | S-[4-(2,2-Dimethyl-3-fluoro-propionyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| III.149 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | (S)-2,2-Dimethyl-1,3-dioxolan-4-yl-methoxy-carbonyloxy | S-[4-((S)-2,2-Dimethyl-1,3-dioxolan-4-yl-methoxycarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| III.150 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | (R)-2,2-Dimethyl-1,3-dioxolan-4-yl-methoxy-carbonyloxy | S-[4-((R)-2,2-Dimethyl-1,3-dioxolan-4-yl-methoxycarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |

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| Sr. No | R ₁ | R ₂ | R ₃ | R ₄ | P | Q | J | K | Z | X | m ₁ | m ₂ | m ₃ | n ₁ | I. | Chemical Name |
|--------|---------------------------|----------------|----------------|----------------|---|---|---|---|---|---|----------------|----------------|----------------|----------------|--|---|
| IB.151 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | (Morpholin-4-yl)-carbonyloxy | S-[4-(Morpholin-4-yl)carbonyloxy-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanyl-carbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.152 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | 2,2-Dimethyl-1,3-dioxolan-4-ylmethyl carbamoyloxy | S-[4-(2,2-Dimethyl-1,3-dioxolan-4-yl-methylcarbamoyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.153 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCOO(CH ₂) ₂ -cyclopentyl | S-[4-(2-Cyclopentylethoxycarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.154 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCOO-(CH ₂) ₂ -CH(CH ₃) ₂ | S-[4-(Isobutoxycarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.155 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OC'CO(CH ₂) ₂ -ONO ₂ | S-[4-(3-Nitroxypropylcarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.156 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | 2,2,7,7-Tetramethyltetrahydro-bis[1,3]dioxolo[4,5-b:4',5'-d]pyran-5-yl methoxy carbonyloxy | S-[4-(2,2,7,7-Tetramethyltetrahydro-bis[1,3]dioxolo[4,5-b:4',5'-d]pyran-5-yl methoxycarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.157 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCO(CH ₂) ₂ -ONO ₂ | S-[4-(4-Nitroxybutylcarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.158 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCH ₃ | S-(4-Methoxy-but-2-ynyl) 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.159 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCH ₂ CH ₃ | S-(4-Ethoxy-but-2-ynyl) 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |
| IB.160 | α -CH ₃ | F | F | 2-Furyl | H | H | H | H | S | = | 1 | 0 | 0 | 1 | OCH ₂ CH-(CH ₃) ₂ | S-[4-Isobutoxy-but-2-ynyl] 6 α ,9 α -difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate. |

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Table 5- Lists the compound of formula I-C which have been synthesized



Formula I-C

Table-5

| Sr. No | R ₁ | R ₂ | R ₃ | R ₄ | m ₁ | R ₇ | P | Q | Chemical Name |
|--------|---------------------------|----------------|----------------|---------------------------------|----------------|--------------------------|---|---|---|
| IC.1 | α -CH ₃ | F | F | Ethyl | 1 | 4-Fluoro-phenyl | H | H | 6 α ,9 α -Difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbonylsulfenic acid (4-fluorophenyl)methyl ester. |
| IC.2 | α -CH ₃ | F | F | Ethyl | 1 | 3,4-Dichloro-phenyl | H | H | 6 α ,9 α -Difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbonylsulfenic acid (3,4-dichlorophenyl)methyl ester. |
| IC.3 | α -CH ₃ | F | F | Ethyl | 1 | F | H | H | 6 α ,9 α -Difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbonylsulfenic acid fluoromethyl ester. |
| IC.4 | α -CH ₃ | F | F | 2-Furyl | 1 | F | H | H | 6 α ,9 α -Difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbonylsulfenic acid fluoromethyl ester. |
| IC.5 | α -CH ₃ | F | F | 2-Furyl | 1 | 4-Fluoro-phenyl | H | H | 6 α ,9 α -Difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbonylsulfenic acid (4-fluorophenyl)methyl ester. |
| IC.6 | α -CH ₃ | F | F | 2-Furyl | 1 | 4-Trifluoro-methylphenyl | H | H | 6 α ,9 α -Difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbonylsulfenic acid (4-trifluoromethylphenyl)methyl ester. |
| IC.7 | α -CH ₃ | F | F | 2-Furyl | 1 | 4-Chloro-phenyl | H | H | 6 α ,9 α -Difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbonylsulfenic acid (4-chlorophenyl)methyl ester. |
| IC.8 | α -CH ₃ | F | F | Ethyl | 1 | 4-Trifluoro-methylphenyl | H | H | 6 α ,9 α -Difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbonylsulfenic acid (4-trifluoromethylphenyl)methyl ester. |
| IC.9 | α -CH ₃ | F | H | 2-Furyl | 1 | 4-Fluoro-phenyl | H | H | 9 α -Fluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbonylsulfenic acid (4-fluorophenyl)methyl ester. |
| IC.10 | α -CH ₃ | F | F | Ethyl | 1 | 4-Chlorophenyl-carbonyl | H | H | 6 α ,9 α -Difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbonylsulfenic acid [2-(4-chlorophenyl)-2-oxoethyl] ester. |
| IC.11 | α -CH ₃ | F | H | 2-Furyl | 1 | F | H | H | 9 α -Fluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbonylsulfenic acid fluoromethyl ester. |
| IC.12 | α -CH ₃ | F | F | n-C ₄ H ₉ | 1 | F | H | H | 17 α -n-Butylcarbonyloxy-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbonylsulfenic acid fluoromethyl ester. |
| IC.13 | α -CH ₃ | F | F | Ethyl | 1 | H | H | H | 6 α ,9 α -Difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbonylsulfenic acid methyl ester. |
| IC.14 | α -CH ₃ | F | F | 2-Furyl | 1 | H | H | H | 6 α ,9 α -Difluoro-17 α -(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbonylsulfenic acid methyl ester. |
| IC.15 | α -CH ₃ | F | F | Ethyl | 1 | Phcnyl | H | H | 6 α ,9 α -Difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbonylsulfenic acid phenylmethyl ester. |

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| Sr. No | R ₁ | R ₂ | R ₃ | R ₄ | m ₁ | R ₇ | P | Q | Chemical Name |
|--------|---------------------------|----------------|----------------|----------------|----------------|---------------------------------|---|---|--|
| IC-16 | α -CH ₃ | F | F | 2-Furyl | 1 | Phenyl | H | H | 6 α ,9 α -Difluoro-17 α -[(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbonylsulfenic acid phenylmethyl ester. |
| IC-17 | α -CH ₃ | F | F | Ethyl | 1 | 2,4,6-Tri-methylphenyl-carbonyl | H | H | 6 α ,9 α -Difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbonylsulfenic acid [2-(2,4,6-trimethylphenyl)-2-oxoethyl] ester. |
| IC-18 | α -CH ₃ | F | F | Ethyl | 1 | 4-Chloro-phenyl | H | H | 6 α ,9 α -Difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbonylsulfenic acid (4-chlorophenyl)methyl ester. |
| IC-19 | α -CH ₃ | F | F | 2-Furyl | 1 | 3,4-Dichloro-phenyl | H | H | 6 α ,9 α -Difluoro-17 α -[(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbonylsulfenic acid (3,4-dichlorophenyl)methyl ester. |
| IC-20 | α -CH ₃ | F | F | 2-Furyl | 1 | 2,4-Dichloro-phenyl | H | H | 6 α ,9 α -Difluoro-17 α -[(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbonylsulfenic acid (2,4-dichlorophenyl)methyl ester. |
| IC-21 | α -CH ₃ | F | F | 2-Furyl | 1 | 3-Chloro-phenyl | H | H | 6 α ,9 α -Difluoro-17 α -[(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbonylsulfenic acid (3-chlorophenyl)methyl ester. |
| IC-22 | α -CH ₃ | F | F | 2-Furyl | 1 | 2,4,6-Trifluoro-phenyl | H | H | 6 α ,9 α -Difluoro-17 α -[(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbonylsulfenic acid (2,4,6-trifluorophenyl)methyl ester. |
| IC-23 | α -CH ₃ | F | F | 2-Furyl | 1 | 3-(Trifluoromethyl) phenyl | H | H | 6 α ,9 α -Difluoro-17 α -[(2-furanylcarbonyloxy)-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbonylsulfenic acid (3-trifluoromethylphenyl)methyl ester. |

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Table-6: Spectral data for the synthesized compounds

| Comp. No | ¹ H-NMR (δ ppm), MASS (EI / ES+, m/z) |
|----------|--|
| IA-1 | 1.19 (s, 3H), 1.29 (t, 3H, J=7.1Hz), 1.45 (s, 3H), 1.55-1.54 (m, 1H), 1.66-1.73 (m, 3H), 1.81-1.84 (m, 1H), 1.95-2.24 (m, 6H), 2.32-2.36 (m, 1H), 2.56-2.62 (m, 1H), 2.9-3.0 (m, 1H), 4.1-4.2 (q, 2H, J=7.1), 4.51 (br, d, 1H, J=2.51Hz), 5.07 (d, 1H, J=16.4Hz), 5.62 (d, 1H, J=16.4Hz), 6.17 (s, 1H), 6.27 (dd, 1H, J ₁ =10.1Hz, J ₂ =1.8Hz); 7.27 (d, 1H, J=10.4Hz), 7.47 (d, 2H, J=6.9Hz), 7.84 (d, 2H, J=6.9Hz). MASS (ES+): 592.9(M+Na) ⁺ . |
| IA-2 | 0.96 (d, 3H, J=7.16Hz), 1.11-1.15 (m, 3H), 1.24 (s, 3H), 1.55 (s, 3H), 1.67 (s, 2H), 1.71-1.89 (m, 3H), 2.25-2.40 (m, 6H), 3.3-3.4 (m, 1H), 4.42 (br, 1H), 4.95 (d, 1H, J=16.6Hz), 5.69 (d, 1H, J=16.6Hz), 5.3-5.37 & 5.43-5.49 (m, 1H), 6.38 (dd, 1H, J ₁ =10.14Hz, J ₂ =1.81Hz), 6.45 (s, 1H), 7.16 (dd, 1H, J ₁ =10.1Hz, J ₂ =1.8 Hz), 7.49 (d, 2H, J=8.8Hz), 7.56 (d, 2H, J=8.6Hz). MASS (ES+): 627.0(M+Na) ⁺ . |
| IA-3 | 0.99 (d, 3H, J=7.14Hz), 1.11-1.14 (m, 6H), 1.53 (s, 3H), 1.62 (s, 2H), 1.7-1.91 (m, 4H), 2.21-2.29 (m, 2H), 2.34-2.38 (m, 4H), 3.35-3.42 (m, 1H), 4.3 (d, 1H, J=16.5Hz), 4.41 (br, 1H), 4.48 (d, 1H, J=16.5Hz), 5.30-5.35 & 5.42-5.47 (m, 1H), 6.38 (dd, 1H, J ₁ =10.15Hz, J ₂ =1.75Hz), 6.43 (s, 1H), 7.12 (d, 1H, J=10.15Hz), 7.47 (d, 2H, J=8.5Hz), 7.9 (d, 2H, J=8.5Hz). MASS (ES+): 643.1(M+Na) ⁺ . |
| IA-4 | 1.16 (d, 1H, J=3.30Hz), 1.20 (s, 3H), 1.29 (t, 3H, J=7.10Hz), 1.48 (s, 3H), 1.54 (m, 2H), 1.70 (m, 1H), 1.83 (m, 2H), 1.96-2.22 (m, 5H), 2.34 (m, 1H), 2.59 (m, 1H), 2.95 (m, 1H), 4.16 (q, 2H, J=7.00Hz), 4.52 (br, 1H), 5.08 (d, 1H, J=16.32Hz), 5.63 (d, 1H, J=16.32Hz), 6.02 (s, 1H), 6.27 (dd, 1H, J ₁ =10.59Hz, J ₂ =1.67Hz), 7.17 (dd, 2H, J ₁ =J ₂ =8.55Hz), 7.28 (d, 1H, J=10.19Hz), 7.94 (dd, 2H, J ₁ =8.76, J ₂ =5.31). MASS (EI) : 554. |
| IA-5 | 0.96 (s, 3H), 1.13 (t, 3H, J=7.55Hz), 1.24 (s, 3H), 1.30 (m, 1H), 1.55 (s, 3H), 1.82 (m, 2H), 2.05 (m, 2H), 2.20 (br, 1H), 2.25-2.50 (m, 6H), 3.35 (m, 1H), 4.41 (d, 1H, J=8.52Hz), 5.00 (d, 1H, J=16.53), 5.33 & 5.46 (m, 1H), 5.69 (d, 1H, J=16.53Hz), 6.38 (1H, dd, J ₁ =10.15Hz, J ₂ =1.64Hz), 6.44 (s, 1H), 7.18 (dd, 2H, J ₁ =J ₂ =8.50Hz), 7.95 (dd, 2H, J ₁ =8.70Hz, J ₂ =5.30Hz). MASS (ES+): 611.1(M+Na) ⁺ . |
| IA-6 | 0.99 (d, 3H, J=7.15Hz), 1.13 (m, 6H), 1.25 (s, 1H), 1.33 (m, 1H), 1.53 (s, 3H), 1.86 (m, 3H), 2.26 (m, 2H), 2.39 (m, 4H), 3.39 (m, 1H), 4.32 (d, 1H, J=16.48Hz), 4.41 (d, 1H, J=8.92Hz), 4.48 (d, 1H, J=16.49Hz), 5.32 & 5.44 (m, 1H), 6.38 (dd, 1H, J ₁ =10.15Hz, J ₂ =1.69Hz), 6.44 (s, 1H), 7.12 (dd, 1H, J ₁ =10.19Hz, J ₂ =0.95Hz), 7.17 (dd, 2H, J ₁ =J ₂ =8.50Hz), 8.05 (dd, 2H, J ₁ =10.26Hz, J ₂ =5.35Hz). MASS (ES+): 627.1(M+Na) ⁺ . |
| IA-7 | 1.38 (dd, 2H, J ₁ =11.44Hz, J ₂ =3.21Hz), 1.21 (s, 3H), 1.29 (t, 3H, J=7.11Hz), 1.48 (s, 3H), 1.52 (m, 1H), 1.66-1.84 (m, 2H), 1.95-2.25 (m, 6H), 2.32-2.36 (m, 1H), 2.91-2.98 (m, 1H), 4.16 (q, 2H, J=7.14Hz), 4.52 (s, 1H), 5.00 (dd, 1H, J ₁ =17.35Hz, J ₂ =11z3.61), 5.48 (dd, 1H, J ₁ =17.35Hz, J ₂ =3.61Hz), 6.02 (s, 1H), 6.22 (dd, 1H, J ₁ =10.09Hz, J ₂ =1.731Hz), 6.92 (t, 1H, J=6.67Hz), 7.00 (1H, t, J=6.67Hz), 7.29 (1H, d, J=10.15Hz), 8.01 (dd, 1H, J ₁ =8.25Hz, J ₂ =6.75Hz). MASS (ES+): 595.1(M+Na) ⁺ . |

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| Comp. No | ¹ H-NMR (δ ppm), MASS (EI / ES+, m/z) |
|----------|---|
| IA.8 | 1.13 (s, 3H), 1.16 (dd, 2H, J ₁ =11.37Hz, J ₂ =3.21Hz), 1.28 (t, 3H, J=7.13Hz), 1.47 (s, 3H), 1.50-1.52 (m, 1H), 1.64-1.68 (m, 1H), 1.80-1.83 (m, 1H), 1.91-2.20 (m, 6H), 2.33 (dd, 1H, J ₁ =13.36Hz, J ₂ =2.801Hz), 2.53-2.61 (m, 1H), 2.88-2.95 (m, 1H), 4.14 (q, 2H, J=7.121Hz), 4.51 (s, 1H), 5.00 (d, 1H, J=16.75Hz), 5.41 (d, 1H, J=16.75Hz), 6.02 (s, 1H), 6.26 (dd, 1H, J ₁ =10.01, J ₂ =1.781Hz), 7.27 (d, 1H, J=10.091Hz), 7.36 (dd, 1H, J ₁ =8.38Hz, J ₂ =1.931Hz), 7.47 (d, 1H, J=1.89Hz), 7.62 (d, 1H, J=8.37Hz). MASS (ES+): 627.0(M+Na) ⁺ . |
| IA.9 | 0.96 (d, 3H, J=7.14Hz), 1.14 (t, 3H, J=7.571Hz), 1.26 (s, 3H), 1.29-1.34 (m, 3H), 1.56 (s, 3H), 1.71-1.88 (m, 4H), 2.02-2.05 (m, 1H), 2.25-2.50 (m, 6H), 3.33-3.38 (m, 1H), 4.42 (d, 1H, J=8.87Hz), 4.92 (dd, 1H, J ₁ =17.59Hz, J ₂ =3.07Hz), 5.35 & 5.46 (m, 1H), 5.56 (dd, 1H, J ₁ =17.59Hz, J ₂ =3.071Hz), 6.38 (dd, 1H, J ₁ =10.14Hz, J ₂ =1.701Hz), 6.44 (s, 1H), 6.90-7.04 (m, 1H), 7.15 (d, 1H, J=10.121Hz), 8.00 (dd, 1H, J ₁ =15.04Hz, J ₂ =8.43Hz). MASS (ES+): 629.0(M+Na) ⁺ . |
| IA.10 | 0.94 (d, 3H, J=6.91Hz), 1.12 (t, 3H, J=7.51Hz), 1.18 (s, 3H), 1.24-1.32 (m, 2H), 1.55 (s, 3H), 1.71-1.96 (m, 4H), 2.27-2.48 (m, 5H), 3.32 (s, 1H), 4.40 (d, 1H, J=7.181Hz), 4.90 (d, 1H, J=16.85Hz), 5.33 (m, 0.5H), 5.46 (d, 1.5H, J=16.871Hz), 6.38 (d, 1H, J=10.071Hz), 6.44 (s, 1H), 7.15 (d, 1H, J=9.95Hz), 7.37 (d, 1H, J=8.30Hz), 7.49 (s, 1H), 7.64 (d, 1H, J=8.33). MASS (ES+): 661.0(M+Na) ⁺ . |
| IA.11 | 0.98 (d, 3H, J=7.13Hz), 1.10-1.13 (m, 6H), 1.26-1.35 (m, 2H), 1.54 (s, 3H), 1.72-2.01 (m, 4H), 2.23-2.46 (m, 5H), 3.37 (m, 1H), 4.92 (dd, 1H, J ₁ =17.43Hz, J ₂ =2.691Hz), 4.43 (dd, 2H, J ₁ =17.44Hz, J ₂ =2.76Hz), 5.33 & 5.45 (m, 1H), 6.37 (dd, 1H, J ₁ =10.13Hz, J ₂ =1.731Hz), 6.43 (s, 1H), 6.89-7.01 (m, 2H), 7.16 (dd, 1H, J ₁ =10.14Hz, J ₂ =1.05Hz), 7.94 (dd, 1H, J ₁ =15.09Hz, J ₂ =8.50Hz). MASS (ES+): 645.0(M+Na) ⁺ . |
| IA.12 | 1.15 (d, 1H, J=3.26Hz), 1.17 (s, 4H), 1.29 (t, 3H, J=7.13Hz), 1.48 (s, 3H), 1.51-1.54 (m, 1H), 1.66-1.73 (m, 2H), 1.81-1.84 (m, 1H), 1.95-2.22 (m, 5H), 2.34 (dd, 1H, J ₁ =13.41Hz, J ₂ =2.71Hz), 2.56-2.62 (m, 1H), 2.90-2.97 (m, 1H), 4.15 (q, 2H, J=7.15Hz), 4.52 (s, 1H), 5.06 (d, 1H, J=16.43Hz), 5.56 (d, 1H, J=16.43Hz), 6.02 (s, 1H), 6.27 (dd, 1H, J ₁ =10.08Hz, J ₂ =1.701Hz), 7.29 (d, 1H, J=10.08Hz), 7.59 (d, 1H, J=8.341Hz), 7.73 (dd, 1H, J ₁ =8.35Hz, J ₂ =1.92Hz), 7.99 (d, 1H, J=1.88Hz). MASS (ES+): 627.0(M+Na) ⁺ . |
| IA.13 | 0.97 (d, 3H, J=7.16Hz), 1.05 (s, 3H), 1.12 (t, 3H, J=7.58Hz), 1.28-1.35 (m, 2H), 1.53 (s, 3H), 1.72-1.94 (m, 3H), 2.24-2.42 (m, 6H), 3.35 (m, 1H), 4.21 (d, 1H, J=16.84Hz), 4.34 (d, 1H, J=6.84Hz), 5.32 & 5.44 (m, 1H), 6.38 (dd, 1H, J ₁ =10.14Hz, J ₂ =1.78Hz), 6.43 (s, 1H), 7.11 (dd, 1H, J ₁ =10.12Hz, J ₂ =1.22Hz), 7.35 (dd, 1H, J ₁ =8.34Hz, J ₂ =1.92Hz), 7.46 (d, 1H, J=8.33Hz). MASS (ES+): 677.0(M+Na) ⁺ . |
| IA.14 | 0.99 (3H, d, J=7.10Hz), 1.10 (s, 3H), 1.12 (t, 3H, J=7.57Hz), 1.33 (m, 1H), 1.53 (s, 3H), 1.73-1.97 (m, 5H), 2.20-2.46 (m, 5H), 3.37 (m, 1H), 4.28 (d, 2H, J=16.38Hz), 4.41 (d, 2H, J=15.93Hz), 5.32 & 5.44 (m, 1H), 6.36 (d, 1H, J=10.14Hz), 6.43 (s, 1H), 7.13 (d, 1H, J=10.14Hz), 7.58 (d, 1H, J=8.35Hz), 7.83 (dd, 1H, J ₁ =8.23Hz, J ₂ =1.66Hz), 8.08 (d, 1H, J=1.71Hz). MASS (ES+): 677.0(M+Na) ⁺ . |
| IA.15 | 0.96 (d, 3H, J=7.10Hz), 1.13 (t, 3H, J=7.56Hz), 1.22 (s, 3H), 1.26-1.33 (m, 2H), 1.55 (s, 3H), 1.71-1.90 (m, 3H), 2.00 (d, 1H, J=14.88Hz), 2.27-2.50 (m, 5H), 3.34 (m, 1H), 4.41 (d, 1H, J=8.73Hz), 4.96 (d, 1H, J=16.66Hz), 5.33 & 5.45 (m, 1H), 5.64 (d, 1H, J=16.59Hz), 6.38 (d, 1H, J=10.14Hz), 6.44 (s, 1H), 7.14 (d, 1H, J=10.14Hz), 7.59 (d, 1H, J=8.35Hz), 8.01 (s, 1H). |
| IA.16 | 1.15 (m, 2H), 1.19 (s, 3H), 1.29 (t, 3H, J=7.13Hz), 1.61 (s, 3H), 1.66-1.84 (m, 2H), 1.95-2.22 (m, 6H), 2.32-2.36 (m, 1H), 2.55-2.63 (m, 2H), 2.92-2.98 (m, 1H), 4.15 (q, 2H, J=7.04Hz), 4.51 (br, 1H), 5.00 (d, 1H, J=16.00Hz), 5.58 (d, 1H, J=16.00Hz), 6.02 (s, 1H), 6.27 (dd, 1H, J ₁ =10.09Hz, J ₂ =1.74Hz), 7.18 (t, 1H, J=3.94Hz), 7.29 (s, 1H), 7.72 (d, 1H, J=4.92Hz), 7.75 (d, 1H, J=3.82Hz). MASS (ES+): 565.1(M+Na) ⁺ . |
| IA.17 | 1.16 (s, 3H), 1.19 (m, 2H), 1.28 (t, 3H, J=7.13Hz), 1.45 (m, 2H), 1.47 (s, 3H), 1.67-2.38 (m, 6H), 2.51-2.67 (m, 1H), 2.88-3.00 (m, 1H), 4.14 (q, 2H, J ₁ =14.24Hz, J ₂ =7.11Hz), 4.51 (br, 1H), 4.94 (d, 1H, J=15.95Hz), 5.49 (d, 1H, J=15.98Hz), 6.02 (s, 1H), 6.27 (dd, 1H, J ₁ =10.07Hz, J ₂ =1.72Hz), 7.00 (d, 1H, J=4.08Hz), 7.27 (d, 1H, J=9.96Hz), 7.54 (d, 1H, J=4.09Hz). MASS (ES+): 599.0(M+Na) ⁺ . |
| IA.18 | 0.95 (d, 3H, J=7.14Hz), 1.13 (t, 3H, J=7.56Hz), 1.20 (s, 3H), 1.26-1.36 (m, 1H), 1.54 (s, 3H), 1.77-2.04 (m, 4H), 2.25-2.43 (m, 6H), 3.30-3.37 (m, 1H), 4.40 (d, 1H, J=9.64Hz), 4.85 (d, 1H, J=16.19Hz), 5.28 & 5.51 (m, 1H), 5.56 (d, 1H, J=16.17Hz), 6.35-6.44 (m, 2H), 7.00 (d, 1H, J=4.09Hz), 7.14 (d, 1H, J=10.02 Hz), 7.54 (d, 1H, J=4.08Hz). MASS (ES+): 633.0(M+Na) ⁺ . |
| IA.19 | 1.17 (m, 2H), 1.18 (s, 3H), 1.28 (t, 3H, J=7.11Hz), 1.47 (s, 5H), 1.70-2.38 (m, 8H), 2.41 (s, 3H), 2.51-2.66 (m, 1H), 2.88-3.01 (m, 1H), 4.15 (q, 2H, J ₁ =14.21Hz, J ₂ =7.09Hz), 4.49 (br, 1H), 4.89 (d, 1H, J=16.20Hz), 5.49 (d, 1H, J=16.21Hz), 6.02 (s, 1H), 6.21 (dd, 1H, J ₁ =3.51Hz, J ₂ =1.72Hz), 7.19 (d, 1H, J=3.46Hz), 7.28 (d, 1H, J=9.26Hz). MASS (EI): 540. |
| IA.20 | 0.99 (d, 3H, J=7.35Hz), 1.10-1.16 (m, 6H), 1.21-1.38 (m, 1H), 1.53 (s, 3H), 1.69-2.02 (m, 4H), 2.16-2.49 (m, 6H), 3.34-3.46 (m, 1H), 4.17 (d, 1H, J=16.03Hz), 4.35 (d, 1H, J=16.01Hz), 4.43 (br, 1H), 5.28 & 5.51 (m, 1H), 6.37 (d, 1H, J=10.33Hz), 6.99 (d, 1H, J=4.03Hz), 7.16 (d, 1H, J=10.03Hz), 7.65 (d, 1H, J=4.04Hz). MASS (ES+): 649.0 (M+Na) ⁺ . |
| IA.21 | 0.95 (d, 3H, J=7.13Hz), 1.13 (t, 3H, J=7.56Hz), 1.22 (s, 3H), 1.54 (s, 3H), 1.70-1.88 (m, 2H), 2.03-2.08 (m, 1H), 2.25-2.51 (m, 8H), 2.40 (s, 3H), 3.30-3.38 (m, 1H), 4.39 (d, 1H, J=8.28Hz), 4.80 (d, 1H, J=16.31Hz), 5.28 & 5.50 (m, 1H), 5.52 (d, 1H, J=16.33Hz), 6.21 (d, 1H, J=2.99Hz), 6.37 (dd, 1H, J ₁ =10.12 Hz, J ₂ =1.77Hz), 6.43 (s, 1H), 7.15-7.20 (m, 2H). MASS (EI): 574. |
| IA.22 | 0.98 (d, 3H, J=7.13Hz), 1.09-1.16 (m, 6H), 1.22-1.37 (m, 1H), 1.53 (s, 3H), 1.69-2.56 (m, 10H), 2.41 (s, 3H), 3.36-3.43 (m, 1H), 4.12 (d, 1H, J=16.31Hz), 4.33 (d, 1H, J=16.33Hz), 4.43 (br, 1H), 5.28 & 5.52 (m, 1H), 6.21 (d, 1H, J=3.12Hz), 6.34-6.43 (m, 2H), 7.18 (dd, 1H, J ₁ =10.04Hz, J ₂ =1.03Hz), 7.27 (d, 1H, J=3.60Hz). MASS (ES+): 613.1(M+Na) ⁺ . |
| IA.23 | 1.17 (s, 3H), 1.20 (s, 1H), 1.21 (s, 9H), 1.28 (t, 3H, J=7.12Hz), 1.43 (s, 1H), 1.47 (s, 3H), 1.63-2.97 (m, 12H), 4.14 (q, 2H, J ₁ =14.26Hz, J ₂ =7.12Hz), 4.49 (br, 1H), 4.63 (d, 1H, J=16.68Hz), 5.23 (d, 1H, J=16.69Hz), 6.01 (s, 1H), 6.27 (dd, 1H, J ₁ =10.10Hz, J ₂ =1.84Hz), 7.27 (d, 1H, J=9.73Hz). MASS (EI): 516. |
| IA.24 | 1.13 (s, 3H), 1.18-1.25 (m, 3H), 1.28 (t, 3H, J=7.12Hz), 1.47 (s, 3H), 1.55-2.16 (m, 8H), 2.18 (s, 3H), 2.36-2.96 (m, 3H), 4.14 (q, 2H, J=7.13Hz), 4.50 (d, 1H, J=16.83Hz), 4.51 (m, 1H), 4.92 (d, 1H, J=16.84 Hz), 6.02 (s, 1H), 6.26 (dd, 1H, J ₁ =10.09Hz, J ₂ =1.82Hz), 7.28 (d, 1H, J=10.10Hz). MASS (EI): 474. |
| IA.25 | 0.94 (d, 3H, J=7.171Hz), 1.12 (t, 3H, J=7.56Hz), 1.21 (s, 12H), 1.26-1.29 (m, 1H), 1.54 (s, 3H), 1.77-2.41 (m, 10H), 3.28-3.35 (m, 1H), 4.38 (br, 1H), 4.54 (d, 1H, J=16.98Hz), 5.28 & 5.52 (m, 1H), 5.30 (d, 1H, J=16.91Hz), 6.38 (dd, 1H, J ₁ =10.10Hz, J ₂ =1.73Hz), 6.43 (s, 1H), 7.17 (dd, 1H, J ₁ =10.05 Hz, J ₂ =1.10Hz). MASS (ES+): 573.2 (M+Na) ⁺ . |
| IA.26 | 0.98 (d, 3H, J=7.12Hz), 1.12 (s, 3H), 1.12 (t, 3H, J=7.54Hz), 1.24 (s, 9H), 1.23-1.34 (m, 1H), 1.54 (s, 3H), 1.75-2.50 (m, 10H), 3.34-3.42 (m, 1H), 3.89 (d, 1H, J=17.40Hz), 4.14 (d, 1H, J=17.38Hz), 4.38-4.42 (br, 1H), 5.28 & 5.52 (m, 1H), 6.37 (dd, 1H, J ₁ =10.20Hz, J ₂ =1.64Hz), 6.43 (s, 1H), 7.17 (d, 1H, J=9.96 Hz). MASS (ES+): 589.1 (M+Na) ⁺ . |
| IA.27 | 0.99 (d, 3H, J=7.13Hz), 1.10 (s, 3H), 1.12 (t, 3H, J=7.55Hz), 1.20-1.39 (m, 2H), 1.53 (s, 3H), 1.69-1.97 (m, 4H), 2.22-2.42 (m, 8H), 3.33-3.40 (m, 1H), 3.72 (d, 1H, J=16.52Hz), 3.83 (d, 1H, J=16.51Hz), 4.40 (br, 1H), 5.28 & 5.50 (m, 1H), 6.38 (dd, 1H, J ₁ =10.08Hz, J ₂ =1.28Hz), 6.43 (s, 1H), 7.13 (dd, 1H, J ₁ =10.08 Hz, J ₂ =1.37Hz). MASS (ES+): 547.1(M+Na) ⁺ . |

SUBSTITUTE SHEET (RULE 26)

| Comp. No | ¹ H-NMR (δ ppm), MASS (EI / ES+, m/z) |
|----------|---|
| IA.28 | 0.94 (d, 3H, J=7.12Hz), 1.12 (t, 3H, J=7.58Hz), 1.17 (s, 3H), 1.24-1.35 (m, 1H), 1.55 (s, 3H), 1.70-1.95 (m, 3H), 2.18 (s, 3H), 2.24-2.42 (m, 7H), 3.30 (m, 1H), 4.39 (br, 1H), 4.43 (d, 1H, J=17.04Hz), 4.96 (d, 1H, J=17.04Hz), 5.28 & 5.52 (m, 1H), 6.37 (dd, 1H, J=10.10Hz, J ₂ =1.79Hz), 6.42 (s, 1H), 7.17 (dd, 1H, J ₁ =10.07Hz, J ₂ =1.11Hz). MASS (ES+): 531.1 (M+Na) ⁺ . |
| IA.29 | 1.15 (d, J=3.31Hz, 3H), 1.21 (s, 3H), 1.29 (t, J=7.08, 3H), 1.48 (s, 3H), 1.71-2.38 (m, 6H), 2.58 (m, 1H), 2.97 (m, 1H), 3.89 (s, 3H), 4.16 (q, J=7.07Hz, 2H), 4.51 (d, 1H), 5.05 (d, J=16.2Hz, 1H), 5.60 (d, J=16.2Hz, 1H), 6.02 (s, 1H), 6.27 (dd, J ₁ =10.11Hz, J ₂ =1.83Hz, 1H), 6.90 (d, J=8.9Hz, 2H), 7.28 (d, J=10.3Hz, 1H), 7.88 (d, J=8.9Hz, 2H). |
| IA.30 | 0.96 (d, J=7.1Hz, 3H), 1.13 (t, J=7.5Hz, 3H), 1.25 (s, 3H), 1.55 (s, 3H), 1.70-1.88 (m, 2H), 2.08 (d, J=15.9Hz, 1H), 2.26-2.46 (m, 7H), 2.56 (m, 1H), 3.34 (m, 1H), 3.38 (s, 3H), 4.40 (d, J=8.63Hz, 1H), 4.97 (d, J=16.4Hz, 1H), 5.42 (m, 1H), 5.70 (d, J=16.42, Hz, 1H), 6.37 (dd, J ₁ =10.1Hz, J ₂ =1.76Hz, 1H), 6.43 (s, 1H), 6.95 (d, J=10.9Hz, 2H), 7.175 (dd, J ₁ =10.1Hz, J ₂ =1.03Hz, 1H), 7.88 (d, J=8.89Hz, 1H). MASS (ES+): 623.1 (M+Na) ⁺ . |
| IA.31 | 0.98 (d, J=6.2Hz, 3H), 1.11 (s, 3H), 1.13 (t, J=7.3Hz, 3H), 1.22-1.37 (m, 2H), 1.53 (s, 3H), 1.69-2.27 (m, 3H), 2.37 (q, J=7.52Hz, 2H), 2.15-2.35 (m, 4H), 3.40 (m, 1H), 3.88 (s, 3H), 4.30 (d, J=16.5Hz, 1H), 4.39 (bd, 1H), 4.52 (d, J=16.5Hz, 1H), 5.25-5.60 (m, 1H), 6.38 (dd, J ₁ =10.10Hz, J ₂ =1.7Hz, 1H), 6.42 (s, 1H), 6.95 (d, J=8.8Hz, 2H), 7.16 (d, J=10Hz, 1H), 7.98 (d, J=8.89Hz, 2H). MASS (ES+): 639.1 (M+Na) ⁺ . |
| IA.32 | 1.16 (s, 6H), 1.26 (t, J=7.07Hz, 3H), 1.47 (s, 3H), 1.54-2.36 (m, 24H), 2.57 (m, 1H), 2.90 (t, J=11.31Hz, 1H), 4.13 (q, J=7.14Hz, 2H), 4.49 (d, J=1.39Hz, 1H), 4.60 (d, J=16.61Hz, 1H), 5.21 (d, J=16.70Hz, 1H), 6.01 (s, 1H), 6.26 (dd, J ₁ =1.64Hz, J ₂ =10.82Hz, 1H), 7.27 (d, J=3.22Hz, 1H). MASS (ES+): 617.2 (M+Na) ⁺ . |
| IA.33 | 0.935 (d, J=7.11Hz, 3H), 1.11 (t, J=7.66Hz, 3H), 1.20-1.34 (m, 3H), 1.54 (s, 3H), 1.66-1.94 (m, 14H), 2.05 (d, J=4.87Hz, 6H), 2.18-2.51 (m, 6H), 3.30 (m, 1H), 4.38 (d, J=8.13Hz, 1H), 4.51 (d, J=16.91Hz, 1H), 5.25 (d, J=17.23Hz, 1H), 5.40-5.60 (m, 1H), 6.37 (dd, J ₁ =1.73Hz, J ₂ =10.09Hz, 1H), 6.42 (s, 1H), 7.15 (d, J=9.01Hz, 1H). MASS (ES+): 651.2 (M+Na) ⁺ . |
| IA.34 | 0.97 (d, J=7.14Hz, 3H), 1.12 (t, J=7.57Hz, 6H), 1.22-1.36 (m, 2H), 1.52 (s, 3H), 1.71 (s, 6H), 1.82-1.91 (m, 9H), 2.06 (s, 3H), 2.21-2.26 (m, 4H), 2.35 (q, J=7.15Hz, 2H), 3.39 (m, 1H), 3.84 (d, J=17.48Hz, 1H), 4.11 (d, J=17.49Hz, 1H), 4.40 (d, J=7.69Hz, 1H), 5.40-5.60 (m, 1H), 6.35 (d, J=1.81Hz, 1H), 6.41 (d, J=6.48Hz, 1H), 7.16 (dd, J ₁ =1.21Hz, J ₂ =10.06Hz, 1H). MASS (ES+): 667.1 (M+Na) ⁺ . |
| IA.35 | 0.99 (d, J=7.06Hz, 3H), 1.12 (t, J=7.44Hz, 6H), 1.22-1.38 (m, 2H), 1.53 (s, 3H), 1.69-2.02 (m, 3H), 2.16-2.38 (m, 6H), 3.38 (m, 1H), 4.30 (d, J=16.50Hz, 1H), 4.39 (s, 1H), 4.48 (d, J=16.51Hz, 1H), 5.20-5.50 (m, 1H), 6.345 (d, J=1.69Hz, 1H), 6.41 (d, J=4.53Hz, 1H), 7.16 (d, J=10.03Hz, 1H), 7.31 (d, J=8.31Hz, 2H), 8.06 (d, J=8.87Hz, 2H). MASS (ES+): 693.1 (M+Na) ⁺ . |
| IA.36 | 0.96 (d, J=7.02Hz, 3H), 1.12 (t, J=7.50Hz, 3H), 1.24-1.36 (m, 4H), 1.55 (s, 3H), 1.64-2.07 (m, 3H), 2.26-2.58 (m, 6H), 3.31-3.38 (m, 1H), 4.41 (d, J=8.22Hz, 1H), 5.03 (d, J=16.58Hz, 1H), 5.40 (m, 1H), 5.65 (d, J=16.59Hz, 1H), 6.35 (d, J=1.62Hz, 1H), 6.42 (d, J=5.32Hz, 1H), 7.17 (d, J=9.99Hz, 1H), 7.32 (d, J=8.23Hz, 2H), 7.97 (d, J=8.76Hz, 2H). MASS (ES+): 677.0 (M+Na) ⁺ . |
| IA.37 | 0.88-1.32 (m, 10H), 1.48 (s, 3H), 1.53-2.37 (m, 7H), 2.51-3.01 (m, 2H), 4.15 (q, J=7.13Hz, 2H), 4.52 (d, J=2.46Hz, 1H), 5.08 (d, J=16.41Hz, 1H), 5.64 (d, J=16.41Hz, 1H), 6.02 (s, 1H), 6.28 (dd, J ₁ =1.78Hz, J ₂ =10.07Hz, 1H), 7.26 (s, 1H), 7.33 (d, J=8.60Hz, 2H), 7.97 (d, J=8.84Hz, 2H). MASS (ES+): 643.1 (M+Na) ⁺ . |
| IA.38 | 1.00 (d, J=7.18Hz, 3H), 1.05-1.50 (m, 8H), 1.53 (s, 3H), 1.69-2.42 (m, 9H), 3.38 (m, 1H), 4.32 (d, J=16.14Hz, 1H), 4.40 (s, 1H), 4.50 (d, J=16.10Hz, 1H), 5.30 (m, 1H), 6.38 (dd, J ₁ =1.67Hz, J ₂ =10.12Hz, 1H), 6.43 (s, 1H), 7.12 (d, J=10.05Hz, 1H), 7.76 (d, J=8.21Hz, 2H), 8.12 (d, J=8.08Hz, 2H). MASS (ES+): 677.1 (M+Na) ⁺ . |
| IA.39 | 1.06 (d, J=7.12Hz, 3H), 1.17 (s, 3H), 1.36-1.41 (m, 1H), 1.55 (s, 3H), 1.72-2.01 (m, 4H), 2.28-2.49 (m, 4H), 3.43-3.48 (m, 1H), 4.38 (d, J=16.56Hz, 1H), 4.47 (d, J=10.79Hz, 1H), 4.52 (d, J=16.65Hz, 1H), 5.32-5.49 (m, 1H), 6.41 (d, J=10.13Hz, J ₂ =1.79Hz, 1H), 6.46 (s, 1H), 6.93 (d, J=4.18Hz, 1H), 7.14 (d, J=10.19Hz, J ₂ =1.16Hz, 1H), 7.52 (d, J=4.00Hz, 1H), 7.77 (d, J=8.24Hz, 2H), 8.12 (d, J=8.13Hz, 2H). MASS (ES+): 743.5 |
| IA.40 | 1.05 (d, J=7.15Hz, 3H), 1.11 (s, 3H), 1.34-1.40 (m, 1H), 1.54 (s, 3H), 1.77-2.01 (m, 4H), 2.25 (s, 6H), 2.28 (s, 3H), 2.28-2.50 (m, 4H), 3.45-3.50 (m, 1H), 4.09 (d, J=17.76Hz, 1H), 4.29 (d, J=17.83Hz, 1H), 4.43 (d, J=8.40Hz, 1H), 5.32-5.48 (m, 1H), 6.40 (dd, J ₁ =10.15Hz, J ₂ =1.79Hz, 1H), 6.46 (s, 1H), 6.85 (s, 2H), 6.93 (d, J=4.09Hz, 1H), 7.14 (dd, J ₁ =10.11Hz, J ₂ =1.00Hz, 1H), 7.52 (d, J=4.07Hz, 1H). MASS (ES+): 717.5 |
| IA.41 | 1.06 (d, J=7.16Hz, 3H), 1.10 (s, 3H), 1.29-1.35 (m, 1H), 1.67 (s, 3H), 1.77-1.92 (m, 4H), 2.25 (s, 6H), 2.28 (s, 3H), 2.42-2.87 (m, 5H), 3.45-3.48 (m, 1H), 4.07 (d, J=17.54Hz, 1H), 4.31 (d, J=17.68Hz, 1H), 4.59 (s, 1H), 6.11 (s, 1H), 6.36 (dd, J ₁ =10.09Hz, J ₂ =1.74Hz, 1H), 6.49 (dd, J ₁ =3.45Hz, J ₂ =1.67Hz, 1H), 6.85 (s, 2H), 7.17 (d, J=3.45Hz, 1H), 7.20 (d, J=10.13Hz, 1H), 7.58 (d, J=0.8Hz, 1H). MASS (ES+): 687.5 (M+Na) ⁺ . |
| IA.42 | 0.96 (d, J=7.10Hz, 3H), 1.13 (t, J=7.35Hz, 2H), 1.22-1.34 (m, 4H), 1.55 (s, 3H), 1.64-2.04 (m, 7H), 2.17-2.51 (m, 4H), 3.10 (s, 3H), 3.34 (m, 1H), 4.41 (d, J=8.44Hz, 1H), 5.02 (d, J=16.63Hz, 1H), 5.44 (m, 1H), 5.70 (d, J=16.73Hz, 1H), 6.38 (d, J=10.14Hz, 1H), 6.44 (s, 1H), 7.14 (d, J=10.14Hz, 1H), 8.09 (s, 4H). MASS (ES+): 671.0 (M+Na) ⁺ . |
| IA.43 | 0.99 (d, J=7.11Hz, 3H), 1.12 (t, J=7.54Hz, 3H), 1.24-1.52 (m, 4H), 1.72-1.90 (m, 8H), 2.23-2.43 (m, 6H), 3.10 (s, 3H), 3.35 (m, 1H), 4.36 (d, J=16.36Hz, 1H), 4.40 (d, 1H), 4.43 (d, J=16.19Hz, 1H), 5.40 (m, 1H), 6.37 (d, J=10.14Hz, 1H), 6.43 (s, 1H), 7.11 (d, J=10.09Hz, 1H), 8.04 (d, J=8.32Hz, 2H), 8.17 (d, J=8.33Hz, 2H). MASS (ES+): 687.0 (M+Na) ⁺ . |
| IA.44 | 0.90 (d, J=7.14Hz, 3H), 1.13 (t, J=7.56Hz, 3H), 1.24-1.33 (m, 3H), 1.70-2.08 (m, 8H), 2.25-2.42 (m, 6H), 3.36 (m, 1H), 4.41 (d, J=8.98Hz, 1H), 5.02 (d, J=16.63Hz, 1H), 5.40 (m, 1H), 5.75 (d, J=16.64Hz, 1H), 6.38 (dd, J ₁ =1.52Hz, J ₂ =10.13Hz, 1H), 6.44 (s, 1H), 7.12 (d, J=10.09Hz, 1H), 7.50 (t, J=7.73Hz, 2H), 7.63 (t, J=7.38Hz, 1H), 7.91 (d, J=7.47Hz, 2H). MASS (ES+): 593.1 (M+Na) ⁺ . |
| IA.45 | 1.00 (d, J=7.12Hz, 3H), 1.13 (t, J=7.67Hz, 6H), 1.14-1.35 (m, 3H), 1.67-2.00 (m, 6H), 2.23-2.44 (m, 5H), 3.40 (m, 1H), 4.35 (d, J=16.72Hz, 1H), 4.40 (d, J=9.27 Hz, 1H), 4.53 (d, J=16.82Hz, 1H), 5.40 (m, 1H), 6.38 (dd, J ₁ =1.22Hz, J ₂ =10.10Hz, 1H), 6.43 (s, 1H), 7.12 (d, J=10.05Hz, 1H), 7.49 (t, J=7.71Hz, 2H), 7.61 (t, J=7.43Hz, 1H), 8.01 (d, J=Hz, 2H). MASS (ES+): 609.1 (M+Na) ⁺ . |
| IA.46 | 0.96 (d, J=7.11Hz, 3H), 1.13 (t, J=7.55Hz, 3H), 1.24 (s, 3H), 1.27-2.09 (m, 8H), 2.24-2.40 (m, 6H), 2.43 (s, 3H), 3.36 (m, 1H), 4.41 (d, J=8.93Hz, 1H), 5.00 (d, J=16.55Hz, 1H), 5.40 (m, 1H), 5.73 (d, J=16.56Hz, 1H), 6.37 (dd, J ₁ =10.18Hz, J ₂ =1.37Hz, 1H), 6.44 (s, 1H), 7.15 (d, J=10.15Hz, 1H), 7.29 (d, J=8.01Hz, 2H), 7.80 (d, J=8.08Hz, 2H). MASS (ES+): 607.1 (M+Na) ⁺ . |
| IA.47 | 0.99 (d, J=7.15Hz, 3H), 1.12 (t, J=7.49Hz, 6H), 1.29-2.00 (m, 8H), 2.20-2.42 (m, 6H), 2.42 (s, 3H), 3.40 (m, 1H), 4.34 (d, J=16.63Hz, 1H), 4.40 (d, J=8.60Hz, 1H), 4.52 (d, J=16.61Hz, 1H), 5.40 (m, 1H), 6.37 (dd, J ₁ =10.17Hz, J ₂ =Hz, 1H), 6.43 (s, 1H), 7.13 (d, J=10.15Hz, 1H), 7.28 (d, J=8.05Hz, 2H), 7.90 (d, J=8.17Hz, 2H). MASS (ES+): 623.1 (M+Na) ⁺ . |

SUBSTITUTE SHEET (RULE 26)

| Comp. No | ¹ H-NMR (δ ppm), MASS (EI / ES+, m/z) |
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| IA.48 | 0.93(d, J=7.14Hz, 3H), 1.11(t, J=7.56Hz, 3H), 1.15(s, 3H), 1.25-1.84(m, 8H), 2.21-2.38(m, 6H), 3.32(m, 1H), 4.34(d, J=8.93Hz, 1H), 4.81(d, J=17.90Hz, 1H), 5.40(m, 1H), 5.41(d, J=17.68Hz, 1H), 6.38(d, d, J ₁ =10.17Hz, J ₂ =1.49Hz, 1H), 6.43(s, 1H), 7.11(d, J=10.07Hz, 1H), 7.36(d, J=2.95Hz, 3H). MASS (ES+): 661.0 (M+Na) ⁺ . |
| IA.49 | 0.98(d, J=7.13Hz, 3H), 1.07(s, 3H), 1.12(t, J=7.55Hz, 3H), 1.25-2.01(m, 8H), 2.23-2.43(m, 6H), 3.40(m, 1H), 4.25(d, J=17.50Hz, 1H), 4.42(d, J=8.45Hz, 1H), 4.45(d, J=17.57Hz, 1H), 5.40(m, 1H), 6.39(d, J=10.15Hz, 1H), 6.43(s, 1H), 7.13(d, J=10.11Hz, 1H), 7.26-7.36(m, 3H). MASS (ES+): 677.0 (M+Na) ⁺ . |
| IA.50 | 0.93(d, J=7.14Hz, 3H), 1.08(s, 3H), 1.12(t, J=7.53Hz, 3H), 1.26-1.80(m, 8H), 2.24-2.38(m, 6H), 3.29(m, 1H), 4.39(d, J=8.69Hz, 1H), 4.85(d, J=19.97Hz, 1H), 5.36(d, J=17.05Hz, 1H), 5.40(m, 1H), 6.38(d, d, J ₁ =10.10Hz, J ₂ =1.50Hz, 1H), 6.43(s, 1H), 7.13(d, J=10.14Hz, 1H), 7.33(t, J=7.90Hz, 1H), 7.47(d, d, J ₁ =7.60Hz, J ₂ =1.21Hz, 1H), 7.62(d, d, J ₁ =7.38Hz, J ₂ =1.11Hz, 1H). MASS (ES+): 661.0 (M+Na) ⁺ . |
| IA.51 | 0.97(d, J=7.13Hz, 3H), 1.01(s, 3H), 1.12(t, J=7.55Hz, 3H), 1.29-1.95(m, 8H), 2.24-2.40(m, 6H), 3.35(m, 1H), 4.17(d, J=16.89Hz, 1H), 4.32(d, J=16.88Hz, 1H), 4.41(d, J=8.19Hz, 1H), 5.40(m, 1H), 6.38(d, d, J ₁ =10.04Hz, J ₂ =1.50Hz, 1H), 6.43(s, 1H), 7.13(d, J=10.14Hz, 1H), 7.31(d, J=7.89Hz, 1H), 7.53(dd, J ₁ =7.62Hz, J ₂ =1.15Hz, 1H), 7.58(dd, J ₁ =8.01Hz, J ₂ =1.19Hz, 1H). MASS (ES+): 677.0 (M+Na) ⁺ . |
| IA.52 | 0.94(d, J=7.16Hz, 3H), 1.12(t, J=7.55Hz, 3H), 1.19(s, 3H), 1.25-1.97(m, 8H), 2.17-2.41(m, 6H), 3.34(m, 1H), 4.39(d, J=8.73Hz, 1H), 4.81(d, J=17.22Hz, 1H), 5.38(m, 1H), 5.42(d, J=17.55Hz, 1H), 6.38(d, d, J ₁ =10.13Hz, J ₂ =1.37Hz, 1H), 6.43(s, 1H), 7.02(d, J=8.53Hz, 2H), 7.15(d, J=10.17Hz, 1H), 7.47-7.51(m, 1H). MASS (ES+): 629.1 (M+Na) ⁺ . |
| IA.53 | 0.97(d, J=7.13Hz, 3H), 1.07(s, 3H), 1.10(t, J=7.54Hz, 3H), 1.16-1.95(m, 8H), 2.22-2.44(m, 6H), 3.36(m, 1H), 4.17(d, J=16.90Hz, 1H), 4.29(d, J=16.88Hz, 1H), 4.40(d, J=8.72Hz, 1H), 5.40(m, 1H), 6.37(dd, J ₁ =10.16Hz, J ₂ =1.46Hz, 1H), 6.43(s, 1H), 6.98(t, J=8.34Hz, 2H), 7.13(d, J=9.90Hz, 1H), 7.44(d, J=7.62Hz, 1H). MASS (ES+): 645.0 (M+Na) ⁺ . |
| IA.54 | 0.96(d, J=7.13Hz, 3H), 1.13(t, J=7.55Hz, 3H), 1.24(s, 3H), 1.25-1.99(m, 8H), 2.17-2.43(m, 6H), 3.35(m, 1H), 4.42(d, J=8.41Hz, 1H), 4.95(dd, J ₁ =17.53Hz, J ₂ =2.75Hz, 1H), 5.40(m, 1H), 5.57(dd, J ₁ =17.55Hz, J ₂ =2.80Hz, 1H), 6.38(d, d, J ₁ =10.10Hz, J ₂ =1.06Hz, 1H), 6.44(s, 1H), 7.15(d, J=10.15Hz, 1H), 7.22(d, d, J ₁ =10.05Hz, J ₂ =5.61Hz, 1H), 7.43(d, d, J ₁ =16.25Hz, J ₂ =8.85Hz, 1H), 7.69(t, J=7.42Hz, 1H). MASS (ES+): 629.1 (M+Na) ⁺ . |
| IA.55 | 0.98(d, J=7.08Hz, 3H), 1.10-1.14(m, 6H), 1.24-1.99(m, 8H), 2.23-2.43(m, 6H), 3.36(m, 1H), 4.29(dd, J ₁ =17.37Hz, J ₂ =1.85Hz, 1H), 4.43(d, d, J ₁ =17.25Hz, J ₂ =2.03Hz, 2H), 5.40(m, 1H), 6.38(d, J=10.14Hz, 1H), 6.43(s, 1H), 7.13(d, J=10.11Hz, 1H), 7.21(dd, J ₁ =12.35Hz, J ₂ =7.93Hz, 1H), 7.40(d, J=8.21Hz, 1H), 7.63(t, J=6.40Hz, 1H). MASS (ES+): 645.1 (M+Na) ⁺ . |
| IA.56 | 1.06(d, J=7.11Hz, 3H), 1.17(s, 3H), 1.35-1.41(m, 1H), 1.54(s, 3H), 1.77-2.03(m, 4H), 2.28-2.49(m, 4H), 3.43-3.49(m, 1H), 4.34(d, 1H, J=16.58Hz), 4.47(d, J=6.32Hz, 1H), 4.50(d, J=16.57Hz, 1H), 5.32-5.49(m, 1H), 6.40(dd, J ₁ =10.19Hz, J ₂ =1.84Hz, 1H), 6.46(s, 1H), 6.92(d, J=3.95Hz, 1H), 7.14(dd, J ₁ =10.12Hz, J ₂ =1.10Hz, 1H), 7.47(d, J=8.60Hz, 2H), 7.52(d, J=4.06Hz, 1H), 7.95(d, J=8.60Hz, 2H). MASS (ES+): 731.5 (M+Na) ⁺ . |
| IA.57 | 0.93(d, J=7.11Hz, 3H), 1.07(s, 3H), 1.11(t, J=7.54Hz, 3H), 1.25-1.82(m, 8H), 2.25(s, 9H), 2.22-2.37(m, 6H), 3.31(m, 1H), 4.27(d, J=8.71Hz, 1H), 4.55(d, J=17.82Hz, 1H), 5.33(d, J=17.85Hz, 1H), 5.40(m, 1H), 6.38(d, d, J ₁ =10.14Hz, J ₂ =1.44Hz, 1H), 6.43(s, 1H), 6.87(s, 2H), 7.11(d, J=9.94Hz, 1H). MASS (ES+): 611.3 (M+H) ⁺ . |
| IA.58 | 0.98(d, J=7.07Hz, 3H), 1.03(s, 3H), 1.12(t, J=7.53Hz, 3H), 1.25-1.95(m, 8H), 2.25(s, 9H), 2.22-2.41(m, 6H), 3.40(m, 1H), 4.05(d, J=17.72Hz, 1H), 4.28(d, J=17.74Hz, 1H), 4.38(d, J=8.06Hz, 1H), 5.41(m, 1H), 6.38(d, J=10.17Hz, 1H), 6.43(s, 1H), 6.85(s, 2H), 7.12(d, J=10.13Hz, 1H). MASS (ES+): 651.1 (M+Na) ⁺ . |
| IA.59 | 0.44(s, 3H), 0.95(d, J=7.02Hz, 3H), 1.08(t, J=7.53Hz, 3H), 1.22-1.75(m, 15H), 2.17-2.32(m, 6H), 3.15(m, 1H), 4.29(d, J=6.81Hz, 1H), 5.40(m, 1H), 6.35(dd, J ₁ =10.11Hz, J ₂ =1.43Hz, 1H), 6.40(s, 1H), 7.05(d, J=9.98Hz, 1H), 7.36(t, J=7.70Hz, 2H), 7.46(t, J=7.20Hz, 1H), 7.95(d, J=7.43Hz, 2H). MASS (ES+): 637.1 (M+Na) ⁺ . |
| IA.60 | 0.96(d, J=7.10Hz, 3H), 1.13(t, J=7.56Hz, 3H), 1.23-2.06(m, 11H), 2.17-2.49(m, 6H), 3.35(m, 1H), 4.40(d, J=8.55Hz, 1H), 4.93(d, J=16.21Hz, 1H), 5.39(m, 1H), 5.64(d, J=16.21Hz, 1H), 6.38(d, d, J ₁ =10.18Hz, J ₂ =1.30Hz, 1H), 6.43(s, 1H), 7.15(d, J=10.22Hz, 1H), 7.18(t, J=4.56Hz, 1H), 7.73(d, J=4.96Hz, 1H), 7.75(d, J=3.66Hz, 1H). MASS (ES+): 599.2 (M+Na) ⁺ . |
| IA.61 | 0.99(d, J=7.11Hz, 3H), 1.11-1.14(m, 6H), 1.25-1.96(m, 8H), 2.17-2.41(m, 6H), 3.39(m, 1H), 4.27(d, J=16.28Hz, 1H), 4.41(d, J=13.26Hz, 1H), 4.44(d, J=16.48Hz, 1H), 5.42(m, 1H), 6.38(dd, J ₁ =10.16Hz, J ₂ =1.46Hz, 1H), 6.43(s, 1H), 7.13(d, J=9.66Hz, 1H), 7.17(t, J=4.16Hz, 1H), 7.71(d, J=4.90Hz, 1H), 7.86(d, J=3.51Hz, 1H). MASS (ES+): 615.2 (M+Na) ⁺ . |
| IA.62 | 0.96(d, J=7.11Hz, 3H), 1.13(t, J=7.54Hz, 3H), 1.23(s, 3H), 1.25-2.03(m, 8H), 2.24-2.42(m, 6H), 3.34(m, 1H), 4.40-4.42(m, 1H), 4.97(d, J=16.57Hz, 1H), 5.40(m, 1H), 5.64(d, J=16.56Hz, 1H), 6.37(d, d, J ₁ =10.15Hz, 1H), 6.44(s, 1H), 7.14(d, J=10.11Hz, 1H), 7.33-7.26(m, 1H), 7.68-7.79(m, 2H). MASS (ES+): 629.2 (M+Na) ⁺ . |
| IA.63 | 0.99(d, J=7.09Hz, 3H), 1.11(t, J=7.80Hz, 6H), 1.25-1.93(m, 8H), 2.17-2.44(m, 6H), 3.36(m, 1H), 4.18-4.38(m, 3H), 4.40(d, J=16.10Hz, 1H), 5.38(m, 1H), 6.33(d, J=10.07Hz, 1H), 6.39(s, 1H), 7.20(d, J=10.05Hz, 1H), 7.28-7.32(m, 1H), 7.79-7.85(m, 1H). MASS (ES+): 625.1 (M+Na) ⁺ . |
| IA.64 | 0.95(d, J=7.13Hz, 3H), 1.13(t, J=7.56Hz, 3H), 1.22(s, 3H), 1.25-2.05(m, 8H), 2.24-2.49(m, 6H), 3.32-3.37(m, 1H), 4.40(d, J=8.68Hz, 1H), 4.86(d, J=16.63Hz, 1H), 5.32-5.48(m, 1H), 5.58(d, J=16.63Hz, 1H), 6.38(d, d, J ₁ =10.13Hz, J ₂ =1.29Hz, 1H), 6.43(s, 1H), 6.60(d, d, J ₁ =3.19Hz, J ₂ =1.29Hz, 1H), 7.14(d, J=10.16Hz, 1H), 7.27(d, J=3.65Hz, 1H), 7.63(s, 1H). MASS (ES+): 583.2 (M+Na) ⁺ . |
| IA.65 | 1.03(d, J=7.10Hz, 3H), 1.25-1.95(m, 10H), 2.07(d, J=14.85Hz, 1H), 2.28-2.51(m, 4H), 3.41-3.44(m, 1H), 4.44(d, J=8.26Hz, 1H), 5.02(d, J=16.48Hz, 1H), 5.32-5.49(m, 1H), 5.73(d, J=16.48Hz, 1H), 5.97(s, 1H), 6.38(d, J=10.19Hz, 1H), 6.44(s, 1H), 7.13-7.21(m, 3H), 7.93(d, d, J ₁ =8.18Hz, J ₂ =5.45Hz, 2H). MASS (ES+): 641.2 (M+H) ⁺ . |
| IA.66 | 1.03(d, J=7.12Hz, 3H), 1.25-2.07(m, 11H), 2.28-2.52(m, 4H), 3.41-3.44(m, 1H), 4.44(d, J=8.40Hz, 1H), 4.93(d, d, J ₁ =17.51Hz, J ₂ =3.47Hz, 1H), 5.32-5.49(m, 1H), 5.67(d, d, J ₁ =17.49Hz, J ₂ =3.40Hz, 1H), 5.96(s, 1H), 6.38(d, d, J ₁ =10.16Hz, J ₂ =1.38Hz, 1H), 6.44(s, 1H), 6.91-6.97(m, 1H), 7.01-7.05(m, 1H), 7.15(d, J=10.12Hz, 1H), 8.01(d, d, J ₁ =14.98Hz, J ₂ =8.29Hz, 1H). MASS (ES+): 683.1 (M+Na) ⁺ . |
| IA.67 | 0.97(d, J=7.10Hz, 3H), 1.14(t, J=7.53Hz, 3H), 1.24-2.05(m, 8H), 2.27-2.44(m, 6H), 3.32-3.36(m, 1H), 4.40(d, J=8.07Hz, 1H), 5.00(d, J=16.85Hz, 1H), 5.20-5.60(m, 1H), 5.72(d, J=16.81Hz, 1H), 6.38(d, d, J ₁ =10.11Hz, J ₂ =1.74Hz, 1H), 6.44(s, 1H), 7.15(d, J=10.06Hz, 1H), 7.31-7.39(m, 1H), 7.49-7.59(m, 3H), 7.74(d, J=7.85Hz, 1H). MASS (ES+): 633.2 (M+Na) ⁺ . |
| IA.68 | 0.99(d, J=7.11Hz, 3H), 1.13(d, J=7.32Hz, 6H), 1.25-1.99(m, 8H), 2.23-2.45(m, 6H), 3.38(m, 1H), 4.19(d, J=16.55Hz, 1H), 4.36(d, J=16.90Hz, 1H), 4.40(d, J=13.09Hz, 1H), 5.39(m, 1H), 6.38(dd, J ₁ =10.15Hz, J ₂ =1.46Hz, 1H), 6.43(s, 1H), 7.13(d, J=10.16Hz, 1H), 7.33(d, J=3.51Hz, 1H), 7.64(s, 1H). MASS (ES+): 599.1 (M+Na) ⁺ . |

SUBSTITUTE SHEET (RULE 26)

| Comp. No | ¹ H-NMR (δ ppm), MASS (EI / ES+, m/z) |
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| IA.69 | 0.99(d, J=7.07Hz, 3H), 1.13(t, J=7.22Hz, 6H), 1.25-1.93(m, 8H), 2.00-2.48(m, 6H), 3.35-3.42(m, 1H), 4.27-4.52(m, 3H), 5.25-5.52(m, 1H), 6.34-6.40(m, 1H), 6.43(s, 1H), 7.13(d, J=9.96Hz, 1H), 7.33(t, J=6.94Hz, 1H), 7.47-7.76(m, 4H). MASS (ES+): 649.1 (M+Na) ⁺ . |
| IA.70 | 0.95(d, J=7.18Hz, 3H), 1.09-1.16(m, 6H), 1.25-1.30(m, 2H), 1.34(s, 9H), 1.42-1.95(m, 6H), 2.17-2.43(m, 6H), 3.37-3.44(m, 1H), 4.28-4.49(m, 2H), 4.53(d, J=16.72Hz, 1H), 5.20-5.60(m, 1H), 6.37(dd, J ₁ =10.12Hz, J ₂ =1.73Hz, 1H), 6.43(s, 1H), 7.13(d, J=10.19Hz, 1H), 7.50(d, J=8.52Hz, 2H), 7.95(d, J=8.52Hz, 2H). MASS (ES+): 665.2 (M+Na) ⁺ . |
| IA.71 | 0.96(d, J=7.11Hz, 3H), 1.14(t, J=7.52Hz, 3H), 1.24-1.36(m, 5H), 1.55-2.07(m, 6H), 2.20-2.46(m, 6H), 3.32-3.39(m, 1H), 4.02(s, 3H), 4.40(d, J=9.33Hz, 1H), 5.02(d, J=16.95Hz, 1H), 5.20-5.60(m, 1H), 5.74(d, J=16.94Hz, 1H), 6.37(d, J ₁ =10.13Hz, J ₂ =1.73Hz, 1H), 6.44(s, 1H), 6.97(d, J ₁ =6.86Hz, J ₂ =1.97Hz, 1H), 7.13-7.28(m, 3H), 7.56(s, 1H). MASS (ES+): 663.2 (M+Na) ⁺ . |
| IA.72 | 0.96(d, J=7.11Hz, 3H), 1.14(t, J=7.52Hz, 3H), 1.24-1.30(m, 6H), 1.34(s, 8H), 1.42-1.92(m, 6H), 2.11-2.54(m, 6H), 3.30-3.41(m, 1H), 4.41(d, J=9.37Hz, 1H), 5.00(d, J=16.55Hz, 1H), 5.26-5.53(m, 1H), 5.74(d, J=16.56Hz, 1H), 6.38(d, J ₁ =10.12Hz, J ₂ =1.67Hz, 1H), 6.44(s, 1H), 7.15(d, J=10.03Hz, 1H), 7.50(d, J=8.48Hz, 2H), 7.85(d, J=8.47Hz, 2H). MASS (ES+): 649.2 (M+Na) ⁺ . |
| IA.73 | 1.00(d, J=7.18Hz, 3H), 1.05-1.50(m, 8H), 1.53(s, 3H), 1.69-2.42(m, 9H), 3.38(m, 1H), 4.32(d, J=16.14Hz, 1H), 4.40(s, 1H), 4.50(d, J=16.10Hz, 1H), 5.30(m, 1H), 6.38(dd, J ₁ =1.67Hz, J ₂ =10.12Hz, 1H), 6.43(s, 1H), 7.12(d, J=10.05Hz, 1H), 7.76(d, J=8.21Hz, 2H), 8.12(d, J=8.08Hz, 2H). MASS (ES+): 679.1 (M+Na) ⁺ . |
| IA.74 | 0.96(d, J=7.10Hz, 3H), 1.13(t, J=7.54Hz, 3H), 1.25-1.99(m, 8H), 2.11-2.43(m, 6H), 3.30-3.50(m, 1H), 3.88(s, 3H), 4.40(d, J=9.28Hz, 1H), 4.85(d, J ₁ =17.50Hz, J ₂ =3.72Hz, 1H), 5.20-5.60(m, 1H), 5.60(d, J ₁ =17.50Hz, J ₂ =3.65Hz, 1H), 6.37(d, J ₁ =10.11Hz, J ₂ =1.74Hz, 1H), 6.44(s, 1H), 6.65(d, J ₁ =13.13Hz, J ₂ =2.25Hz, 1H), 6.79(d, J ₁ =8.90Hz, J ₂ =2.35Hz, 1H), 7.15(d, J ₁ =10.14Hz, J ₂ =1.04Hz, 1H), 7.91(t, J=8.54Hz, 1H). MASS (ES+): 641.2 (M+Na) ⁺ . |
| IA.75 | 0.99(d, J=7.17Hz, 3H), 1.09-1.16(m, 6H), 1.25-1.97(m, 8H), 2.05-2.44(m, 6H), 3.30-3.50(m, 1H), 3.87(s, 3H), 4.25-4.54(m, 3H), 5.20-5.60(m, 1H), 6.38(dd, J ₁ =10.09Hz, J ₂ =1.73Hz, 1H), 6.43(s, 1H), 6.65(dd, J ₁ =13.18Hz, J ₂ =2.35Hz, 1H), 6.77(dd, J ₁ =8.40Hz, J ₂ =2.38Hz, 1H), 7.14(d, J=9.05Hz, 1H), 7.89(t, J=8.67Hz, 1H). MASS (ES+): 657.1 (M+Na) ⁺ . |
| IA.76 | 0.96(d, J=7.15Hz, 3H), 1.15(t, J=7.60Hz, 3H), 1.25-1.94(m, 8H), 2.04-2.43(m, 6H), 3.33-3.41(m, 1H), 3.95(s, 3H), 4.41(d, J=8.47Hz, 1H), 4.97(d, J=17.66Hz, 1H), 5.20-5.60(m, 1H), 5.65(d, J=17.71Hz, 1H), 6.34-6.44(m, 2H), 6.98-7.08(m, 2H), 7.15(d, J=10.01Hz, 1H), 7.52(t, J=6.82Hz, 1H), 7.89(dd, J ₁ =7.79Hz, J ₂ =1.66Hz, 1H). MASS (ES+): 623.2 (M+Na) ⁺ . |
| IA.77 | 0.96(d, J=7.13Hz, 3H), 1.13(t, J=7.55Hz, 3H), 1.24-2.43(m, 17H), 3.31-3.40(m, 1H), 3.87(s, 3H), 3.92(s, 3H), 4.41(d, J=9.87Hz, 1H), 4.88(d, J=17.64Hz, 1H), 5.20-5.68(m, 2H), 6.34-6.59(m, 4H), 7.17(d, J ₁ =10.11Hz, J ₂ =0.97Hz, 1H), 7.92(d, J=8.80Hz, 1H). MASS (ES+): 635.2 (M+Na) ⁺ . |
| IA.78 | 0.98(d, J=7.16Hz, 3H), 1.09-1.16(m, 6H), 1.25-1.88(m, 8H), 2.05-2.41(m, 6H), 3.36-3.45(m, 1H), 3.86(s, 3H), 3.93(s, 3H), 4.30-4.61(m, 3H), 5.20-5.60(m, 1H), 6.34-6.57(m, 4H), 7.15(dd, J ₁ =10.05Hz, J ₂ =1.00Hz, 1H), 7.85(d, J=8.73Hz, 1H). MASS (ES+): 669.1 (M+Na) ⁺ . |
| IA.79 | 0.97(d, J=7.16Hz, 3H), 1.09-1.25(m, 6H), 1.29-1.96(m, 8H), 2.03-2.41(m, 6H), 3.36-3.43(m, 1H), 3.95(s, 3H), 4.31-4.60(m, 3H), 5.20-5.60(m, 1H), 6.35-6.45(m, 2H), 6.97-7.05(m, 2H), 7.14(d, J=9.89Hz, 1H), 7.46-7.55(m, 1H), 7.77(dd, J ₁ =7.71Hz, J ₂ =1.58Hz, 1H). MASS (ES+): 639.1 (M+Na) ⁺ . |
| IA.80 | 0.95(d, J=7.16Hz, 3H), 1.08-1.18(m, 6H), 1.22-1.93(m, 8H), 2.19-2.41(m, 6H), 3.28-3.37(m, 1H), 4.39(d, J=8.09Hz, 1H), 4.73(d, J=17.18Hz, 1H), 5.22-5.53(m, 2H), 6.38(d, J ₁ =10.09Hz, J ₂ =1.78Hz, 1H), 6.43(s, 1H), 7.14(d, J ₁ =10.07Hz, J ₂ =1.16Hz, 1H), 7.63-7.88(m, 4H). MASS (ES+): 661.1 (M+Na) ⁺ . |
| IA.81 | 0.99(d, J=7.15Hz, 3H), 1.09-1.17(m, 6H), 1.25-2.02(m, 8H), 2.17-2.44(m, 6H), 3.34-3.41(m, 1H), 4.11(d, J=17.43Hz, 1H), 4.30(d, J=17.42Hz, 1H), 4.41(d, J=9.75Hz, 1H), 5.20-5.60(m, 1H), 6.38(dd, J ₁ =10.11Hz, J ₂ =1.74Hz, 1H), 6.43(s, 1H), 7.13(dd, J ₁ =10.13Hz, J ₂ =1.07Hz, 1H), 7.60-7.88(m, 4H). MASS (ES+): 677.1 (M+Na) ⁺ . |
| IA.82 | 1.03(d, J=7.07Hz, 3H), 1.25-1.79(m, 7H), 1.79-2.55(m, 8H), 3.41-3.45(m, 1H), 4.45(d, J=8.28Hz, 1H), 4.98(d, J=16.58Hz, 1H), 5.34-5.50(m, 1H), 5.79(d, J=16.48Hz, 1H), 6.40(d, J ₁ =10.16Hz, J ₂ =1.38Hz, 1H), 6.46(s, 1H), 6.51(s, 1H), 7.14-7.19(m, 4H), 7.60(s, 1H), 7.93(d, J ₁ =8.55Hz, J ₂ =3.55Hz, 2H). MASS (ES+): 649.1 (M+Na) ⁺ . |
| IA.83 | 1.07(d, J=6.86Hz, 3H), 1.17(s, 3H), 1.38-1.92(m, 6H), 1.95-2.54(m, 6H), 3.47(m, 1H), 4.31(d, J=16.60Hz, 1H), 4.45-4.67(m, 2H), 5.32-5.49(m, 1H), 6.39-6.51(m, 3H), 7.14-7.19(m, 4H), 7.59(s, 1H), 8.05(dd, J ₁ =8.14Hz, J ₂ =5.42Hz, 2H). MASS (ES+): 665.1 (M+Na) ⁺ . |
| IA.84 | 1.03(d, J=7.08Hz, 3H), 1.25-1.66(m, 7H), 1.76-2.56(m, 8H), 3.41-3.45(m, 1H), 4.45(d, J=8.26Hz, 1H), 4.90(d, J ₁ =17.59Hz, J ₂ =3.07Hz, 1H), 5.34-5.51(m, 1H), 5.65(d, J ₁ =17.61Hz, J ₂ =3.17Hz, 1H), 6.41(d, J ₁ =10.05Hz, J ₂ =1.50Hz, 1H), 6.46(s, 1H), 6.51(d, J ₁ =3.20Hz, J ₂ =1.52Hz, 1H), 6.90-7.04(m, 2H), 7.13-7.19(m, 2H), 7.59(s, 1H), 7.99(d, J ₁ =15.08Hz, J ₂ =8.28Hz, 1H). MASS (ES+): 683.1 (M+Na) ⁺ . |
| IA.85 | 1.06(d, J=7.02Hz, 3H), 1.19(s, 3H), 1.36-1.66(m, 6H), 1.71-2.55(m, 6H), 3.44-3.48(m, 1H), 4.31(d, J=17.67Hz, 1H), 4.46-4.50(m, 2H), 5.33-5.66(m, 1H), 6.41(dd, J ₁ =10.18Hz, J ₂ =0.81Hz, 1H), 6.45(s, 1H), 6.50(d, J=1.54Hz, 1H), 6.89-7.01(m, 2H), 7.12-7.17(m, 2H), 7.59(s, 1H), 7.95(dd, J ₁ =15.16Hz, J ₂ =8.35Hz, 1H). MASS (ES+): 683.1 (M+Na) ⁺ . |
| IA.86 | 0.96(d, J=7.14Hz, 3H), 1.11(s, 3H), 1.12(t, J=7.53Hz, 3H), 1.24-1.34(m, 1H), 1.54(s, 3H), 1.59-1.64(m, 1H), 1.75-1.98(m, 4H), 2.13-2.61(m, 7H), 3.37(m, 1H), 4.36(d, J=11.18Hz), 4.42(d, J=8.71Hz), 4.49(d, J=16.46Hz), 6.34(s, 1H), 6.34(d, J ₁ =10.12Hz, J ₂ =1.79Hz, 1H), 7.11-7.23(m, 3H), 8.01(m, 2H). MASS (ES+): 609.1 (M+Na) ⁺ . |
| IA.87 | 0.94(d, J=7.09Hz, 3H), 1.12(t, J=7.54Hz, 3H), 1.24(s, 3H), 1.27-1.31(m, 1H), 1.57(s, 3H), 1.59-1.62(m, 1H), 1.81-1.87(m, 2H), 1.97-2.03(m, 2H), 2.15-2.23(m, 1H), 2.34-2.46(m, 6H), 2.60-2.66(m, 1H), 3.30-3.36(m, 1H), 4.41(d, J=8.85Hz, 1H), 4.98(d, J=16.51Hz, 1H), 5.09(d, J=16.54Hz, 1H), 6.13(s, 1H), 6.34(d, J ₁ =9.98Hz, J ₂ =1.40Hz, 1H), 7.17(t, J=8.50Hz, 2H), 7.23(d, J=10.14Hz, 1H), 7.95(dd, J ₁ =8.58Hz, J ₂ =5.36Hz, 2H). MASS (ES+): 593.2 (M+Na) ⁺ . |
| IA.88 | 0.98(d, J=6.7Hz, 3H), 1.09(m, 6H), 1.31-1.35(m, 2H), 1.54(s, 3H), 1.71-1.84(m, 1H), 1.87-2.00(m, 2H), 2.20-2.33(m, 6H), 2.88(s, 1H), 3.30(m, 1H), 4.39(d, J=31.8Hz), 4.47(d, J=31.7Hz), 5.31-5.48(m, 1H), 6.36(d, J=10.1Hz), 6.41(s, 1H), 7.21(d, J=10.0), 8.10(s, 1H), 8.44(s, 2H). MASS (ES+): 745.1 (M+Na) ⁺ . |
| IA.89 | 0.99(d, J=6.91Hz, 3H), 1.10(m, 5H), 1.32(m, 1H), 1.54(s, 3H), 1.80(m, 2H), 2.20-2.48(m, 7H), 3.21(m, 1H), 3.38(m, 1H), 4.36-4.47(m, 3H), 5.32-5.48(m, 1H), 6.36(d, J=10.0Hz), 6.41(s, 1H), 7.22(d, J=10.0Hz), 7.65(t, J=7.7Hz), 7.85(d, J=7.6Hz), 8.19(d, J=7.81Hz), 8.24(s, 1H). MASS (ES+): 677.1 (M+Na) ⁺ . |
| IA.90 | 0.90(d, J=6.4Hz, 6H), 0.99(d, 3H, J=6.7Hz), 1.12(s, 3H), 1.30-1.34(m, 1H), 1.52(s, 3H), 1.72-1.89(m, 3H), 1.91-2.19(m, 4H), 2.25-2.47(m, 7H), 2.53(m, 3H), 3.40(m, 1H), 4.36(d, J=17.0Hz), 4.51(d, J=16.5Hz), 5.30-5.50(m, 1H), 6.37(d, J=10.0Hz, 6.43(s, 1H), 7.17(d, J=10.0Hz), 7.25(d, 2H, J=7.8Hz), 7.91(d, 2H, J=7.8Hz). MASS (ES+): 665.2 (M+Na) ⁺ . |

SUBSTITUTE SHEET (RULE 26)

| Comp. No | ¹ H-NMR (δ ppm), MASS (EI / ES+, m/z) |
|----------|---|
| IA.91 | 1.11(t, J=7.57Hz, 3H), 1.18(s, 3H), 1.23-1.25(m, 1H), 1.43(d, J=7.34Hz, 3H), 1.58(s, 3H), 1.61-1.64(m, 1H), 1.91-2.07(m, 4H), 2.13-2.22(m, 2H), 2.29-2.55(m, 7H), 2.61-2.66(m, 1H), 4.43(d, J=8.38Hz, 1H), 4.88(d, J=16.49Hz, 1H), 5.68(d, J=16.41Hz, 1H), 6.14(s, 1H), 6.35(d, J ₁ =10.12Hz, J ₂ =1.44Hz, 1H), 7.17(t, J=8.52Hz, 2H), 7.25(d, J=9.93Hz, 1H), 7.92(dd, J ₁ =8.67Hz, J ₂ =5.31Hz, 2H). MASS (ES+): 593.2(M+Na) ⁺ |
| IA.92 | 0.99(d, 3H, J=6.95Hz), 1.06-1.14(m, 6H), 1.26(t, 3H, J=7.52), 1.30-1.34(m, 1H), 1.52(s, 3H), 1.72-1.96(m, 4H), 2.0-2.28(m, 2H), 2.34-2.44(m, 4H), 2.72(q, 2H, J ₁ =15.05Hz, J ₂ =7.51Hz), 3.39-3.42(m, 1H), 4.33-4.41(m, 2H), 4.52(1H, d, J=16.60Hz), 5.25-5.50(m, 1H), 6.37(1H, d, J=10.09Hz), 6.43(s, 1H), 7.13(d, 1H, J=10.07Hz), 7.31(d, 2H, J=7.92Hz), 7.93(d, 2H, J=8.00Hz). MASS (ES+): 637.1(M+Na) ⁺ |
| IA.93 | 0.99(d, J=7.0Hz, 3H), 1.11-1.50(m, 5H), 1.26-1.48(m, 7H), 1.52(s, 3H), 1.67(s, 3H), 1.70-1.80(m, 2H), 1.87-2.00(m, 6H), 2.20-2.45(m, 3H), 2.57(m, 1H), 3.38-3.42(m, 1H), 4.32(d, 1H, J=16.7Hz), 4.40(d, 1H, J=8.01Hz), 4.54(d, 1H, J=16.7Hz), 5.30-5.47(m, 1H), 6.38(d, 1H, J ₁ =10.01Hz, J ₂ =1.00Hz), 6.43(s, 1H), 7.13(d, 1H, J=5.05Hz), 7.32(d, 2H, J=8.13Hz), 7.94(d, 2H, J=8.12Hz). MASS (ES+): 691.2(M+Na) ⁺ |
| IA.94 | 0.99(s, 3H), 1.14(t, J=7.53Hz, 3H), 1.22-1.29(m, 1H), 1.36(d, J=7.31Hz, 3H), 1.56(s, 3H), 1.63-2.11(m, 6H), 2.25-2.65(m, 7H), 4.01(d, d, J ₁ =17.65Hz, J ₂ =3.11Hz, 1H), 4.47(d, d, J ₁ =17.62Hz, J ₂ =3.11Hz, 1H), 4.49(d, J=7.05Hz, 1H), 6.13(s, 1H), 6.34(d, d, J ₁ =10.11Hz, J ₂ =1.81Hz, 1H), 6.86-7.04(m, 2H), 7.22(d, J=10.18Hz, 1H), 7.87-7.98(m, 1H). MASS (ES+): 627.1(M+Na) ⁺ |
| IA.95 | 0.99(d, J=7.08Hz, 6H), 1.11-1.15(m, 5H), 1.27(d, 6H, J=6.8Hz), 1.52(s, 3H), 1.67(s, 3H), 1.72-1.89(m, 3H), 1.99(d, 1H, J=14.47Hz), 2.37(q, 2H), 2.96-2.99(m, 1H), 3.39-3.42(m, 1H), 4.32(d, 1H, J=16.63Hz), 4.40(d, 1H, J=8.64Hz), 4.54(d, 1H, J=16.71Hz), 5.30-5.47(m, 1H), 6.37(d, 1H, J=10.01Hz), 6.43(s, 1H), 7.14(d, 1H, J=10.01Hz), 7.34(d, 2H, J=8.17Hz), 7.94(d, 2H, J=8.11Hz). MASS (ES+): 651.1(M+Na) ⁺ |
| IA.96 | 0.83-0.95(m, 1H), 0.99(d, 3H, J=7.0Hz), 1.11(d, 3H, J=4.13Hz), 1.26-1.34(m, 2H), 1.65-1.69(m, 2H), 1.72-2.08(m, 1H), 2.14-2.32(m, 2H), 2.36(q, 2H, J ₁ =15.04, J ₂ =7.58), 3.39-3.42(m, 1H), 4.32(d, 1H, J=16.43Hz), 4.40(1H, d, J=8.26Hz), 4.49(d, 1H, J=16.4Hz), 5.30-5.46(m, 1H), 6.37(d, 1H, J=9.92Hz), 6.43(s, 1H), 6.90(d, 2H, J=8.71Hz), 7.13(d, 1H, J=10.04Hz), 7.95(d, 2H, J=8.71Hz). MASS (ES+): 693.1(M+Na) ⁺ |
| IA.97 | 0.94(d, J=7.11Hz, 3H), 1.04(s, 3H), 1.11(t, J=7.55Hz, 3H), 1.21-1.44(m, 1H), 1.54(s, 3H), 1.75-2.04(m, 4H), 2.12-2.41(m, 7H), 3.1(s, 3H), 3.29-3.33(m, 1H), 4.34(d, J=16.23, 1H), 4.44(d, J=16.35, 1H), 6.12(s, 1H), 6.34(d, d, J ₁ =10.12Hz, J ₂ =1.77Hz, 1H), 7.19(d, J=10.15Hz, 1H), 8.06(d, J=8.59Hz, 2H), 8.18(d, J=8.62Hz, 2H). MASS (ES+): 669.1(M+Na) ⁺ |
| IA.98 | 0.97(d, J=7.14Hz, 3H), 1.11(t, J=7.54Hz, 3H), 1.13(s, 3H), 1.21-1.45(m, 1H), 1.55(s, 3H), 1.60-2.07(m, 5H), 2.17-2.68(m, 7H), 3.31-3.41(m, 1H), 4.22(dd, J ₁ =17.96Hz, J ₂ =3.50Hz, 1H), 4.40-4.42(d, 1H), 4.43(dd, J ₁ =17.47Hz, J ₂ =2.98Hz, 1H), 6.13(s, 1H), 6.35(d, d, J ₁ =10.13Hz, J ₂ =1.83Hz, 1H), 6.86-7.03(m, 2H), 7.21(d, J=10.16Hz, 1H), 7.89-8.01(m, 1H). MASS (ES+): 627.1(M+Na) ⁺ |
| IA.99 | 0.94(s, 3H), 1.12(t, J=7.54Hz, 3H), 1.20-1.29(m, 1H), 1.37(d, J=7.28Hz, 3H), 1.55(s, 3H), 1.60-1.95(m, 6H), 2.25-2.46(m, 7H), 3.1(s, 3H), 4.00(d, J=16.59Hz, 1H), 4.42(d, J=9.05Hz, 1H), 4.53(d, J=16.61Hz, 1H), 6.12(s, 1H), 6.35(d, d, J ₁ =10.12Hz, J ₂ =1.75Hz, 1H), 7.19(d, J=10.15Hz, 1H), 8.07(d, J=6.69Hz, 2H), 8.13(d, J=8.73Hz, 2H). MASS (ES+): 669.0(M+Na) ⁺ |
| IA.100 | 0.98(d, J=7.10Hz, 3H), 1.11(s, 3H), 1.11(t, J=7.46Hz, 3H), 1.27-1.33(m, 1H), 1.54(s, 3H), 1.57-1.65(m, 4H), 2.14-2.41(m, 7H), 2.61-2.63(m, 1H), 3.35-3.37(m, 1H), 4.30(d, 1H, J=16.48Hz), 4.40(d, 1H, J=8.83Hz), 4.47(d, 1H, J=16.47Hz), 6.13(s, 1H), 6.34(d, d, J ₁ =10.13Hz, J ₂ =1.45Hz, 1H), 7.20(d, J=10.15Hz, 1H), 7.47(d, J=8.5Hz, 2H), 7.95(d, J=8.5Hz, 2H). MASS (ES+): 625.1(M+Na) ⁺ |
| IA.101 | 0.97(s, 3H), 1.14(t, J=7.50Hz, 3H), 1.18-1.27(m, 1H), 1.38(d, J=7.26Hz, 3H), 1.56(s, 3H), 1.60-1.64(m, 1H), 1.89-2.29(m, 6H), 2.35-2.47(m, 1H), 2.59-2.64(m, 1H), 3.97(d, J=16.8Hz, 1H), 4.45(d, J=8.17Hz, 1H), 4.55(d, J=16.82Hz, 1H), 6.13(s, 1H), 6.35(d, J ₁ =10.18Hz, 1H), 7.22(d, J=10.13Hz, 1H), 7.47(d, J=8.37Hz, 2H), 7.92(d, J=8.38Hz, 2H). MASS (ES+): 625.1(M+Na) ⁺ |
| IA.102 | 1.05-1.15(m, 6H), 1.22-1.52(m, 9H), 1.76-2.47(m, 8H), 3.34-3.41(m, 1H), 4.07-4.16(m, 2H), 4.16-4.56(m, 3H), 5.23-5.48(m, 1H), 6.36(d, J ₁ =11.36Hz, 1H), 6.42(s, 1H), 7.11(d, J=9.95Hz, 1H), 7.76(d, J=8.11Hz, 2H), 8.11(d, J=8.12Hz, 2H). MASS (ES+): 693.5(M+Na) ⁺ |
| IA.103 | 0.87(m, 4H), 0.96(d, J=6.88Hz, 3H), 1.24(s, 3H), 1.29-1.35(m, 1H), 1.55(s, 3H), 1.61-1.66(m, 1H), 1.81-2.09(m, 2H), 2.28-2.50(m, 6H), 3.31-3.36(m, 1H), 4.42(d, J=8.86Hz, 1H), 4.97(d, J=16.53Hz, 1H), 5.32-5.48(m, 1H), 5.69(d, J=16.53Hz, 1H), 6.38(d, d, J ₁ =10.17Hz, J ₂ =1.46Hz, 1H), 6.44(s, 1H), 7.16(d, J=8.50Hz, 2H), 7.23(t, J=8.64Hz, 3H), 7.94(dd, J ₁ =8.60Hz, J ₂ =5.35Hz, 2H). MASS (ES+): 623.0(M+Na) ⁺ |
| IA.104 | 0.86-0.96(m, 4H), 0.98(d, J=7.35Hz, 3H), 1.12(s, 3H), 1.31-1.36(m, 1H), 1.53(s, 3H), 1.60-1.65(m, 1H), 1.70-2.03(m, 5H), 2.22-2.29(m, 2H), 2.39-2.45(m, 2H), 3.35-3.39(m, 1H), 4.26(d, J=17.62Hz, 1H), 4.42(d, J=8.24Hz, 1H), 4.43(d, J=17.30Hz, 1H), 5.31-5.47(m, 1H), 6.38(d, d, J ₁ =10.11Hz, J ₂ =1.09Hz, 1H), 6.43(s, 1H), 6.89-6.94(m, 1H), 6.96-7.01(m, 1H), 7.14(d, J=10.14Hz, 1H), 7.95(dd, J ₁ =15.13Hz, J ₂ =8.38Hz, 1H). MASS (ES+): 657.5(M+Na) ⁺ |
| IA.105 | 1.07(d, J=7.14Hz, 3H), 1.10(s, 3H), 1.27(t, J=7.60Hz, 3H), 1.32-1.97(m, 8H), 2.23-2.44(m, 4H), 3.36-3.42(m, 1H), 4.09-4.14(m, 2H), 4.30(d, J=16.57Hz, 1H), 4.40(d, J=8.43Hz, 1H), 4.51(d, J=16.58Hz, 1H), 5.20-5.60(m, 1H), 6.36(dd, J ₁ =10.15Hz, J ₂ =1.20Hz, 1H), 6.42(s, 1H), 7.12(d, J=10.14Hz, 1H), 7.47(d, J=8.52Hz, 2H), 7.95(d, J=8.54Hz, 2H). MASS (ES+): 659.4(M+Na) ⁺ |
| IA.106 | 0.87-0.97(m, 4H), 0.99(d, J=7.12Hz, 3H), 1.00(s, 3H), 1.31-1.36(m, 1H), 1.53(s, 3H), 1.62-1.66(m, 1H), 1.77-2.01(m, 3H), 2.25-2.42(m, 4H), 3.36-3.39(m, 1H), 4.28(d, J=16.54Hz, 1H), 4.42(d, J=14.05Hz, 1H), 4.46(d, J=16.73Hz, 1H), 5.30-5.48(m, 1H), 6.38(d, d, J ₁ =9.63Hz, J ₂ =1.85Hz, 1H), 6.43(s, 1H), 7.14(d, J=10.10Hz, 1H), 7.46(d, J=8.51Hz, 2H), 7.94(d, J=8.53Hz, 2H). MASS (ES+): 655.2(M+Na) ⁺ |
| IA.107 | 0.98(s, 3H), 1.14(t, J=7.56Hz, 3H), 1.20-1.27(m, 1H), 1.38(d, J=7.23Hz, 3H), 1.56(s, 3H), 1.60-1.65(m, 1H), 1.91-1.98(m, 3H), 2.04-2.30(m, 2H), 2.36-2.66(m, 7H), 3.88(s, 3H), 3.97(d, 1H, J=16.74Hz), 4.44(d, 1H, J=8.41Hz), 4.58(d, 1H, J=16.74Hz), 6.13(s, 1H), 6.35(d, J ₁ =10.07Hz, 1H), 6.95(d, J=8.74Hz, 2H), 7.24(d, J=10.33Hz, 1H), 7.97(d, J=8.74Hz, 2H). MASS (ES+): 621.3(M+Na) ⁺ |
| IA.108 | 0.98(d, J=7.15Hz, 3H), 1.11(s, 3H), 1.11(t, J=7.56Hz, 3H), 1.27-1.33(m, 1H), 1.54(s, 3H), 1.57-1.94(m, 5H), 2.13-2.17(m, 1H), 2.32-2.41(m, 5H), 2.62-2.63(m, 1H), 3.33-3.38(m, 1H), 4.33(d, 1H, J=16.52Hz), 4.41(d, 1H, J=9.09Hz), 4.49(d, 1H, J=16.49Hz), 6.13(s, 1H), 6.34(d, d, J ₁ =10.12Hz, J ₂ =1.81Hz, 1H), 7.21(d, J=10.12Hz, 1H), 7.76(d, J=8.25Hz, 2H), 8.12(d, J=8.14Hz, 2H). MASS (ES+): 659.3(M+Na) ⁺ |
| IA.109 | 0.53(s, 3H), 0.93(d, J=6.88Hz, 3H), 1.07(t, J=7.52Hz, 3H), 1.12-1.90(m, 14H), 2.07-2.42(m, 6H), 3.14-3.17(m, 1H), 3.84(s, 3H), 4.28(d, J=7.12Hz, 1H), 5.25-5.42(m, 1H), 6.34(dd, J ₁ =10.14Hz, J ₂ =1.19Hz, 1H), 6.40(s, 1H), 6.87(d, J=8.84Hz, 2H), 7.03(d, J=10.07Hz, 1H), 8.02(d, J=8.80Hz, 2H). MASS (ES+): 667.3(M+Na) ⁺ |

SUBSTITUTE SHEET (RULE 26)

| Comp. No | ¹ H-NMR (δ ppm), MASS (EI/ES+, m/z) |
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| IA.110 | 1.07(d, J=7.20Hz, 3H), 1.11(s, 3H), 1.27(t, J=7.12Hz, 3H), 1.33-1.39(m, 1H), 1.52(s, 3H), 1.74-1.98(m, 6H), 2.33-2.45(m, 4H), 3.36-3.42(m, 1H), 4.08-4.14(m, 2H), 4.31(d, J=16.55Hz, 1H), 4.41(d, J=8.80Hz, 1H), 4.52(d, J=16.55Hz, 1H), 5.29-5.46(m, 1H), 6.37(dd, J ₁ =10.15Hz, J ₂ =1.75Hz, 1H), 6.42(s, 1H), 7.13(dd, J ₁ =10.15Hz, J ₂ =1.05Hz, 1H), 7.17-7.19(m, 2H), 8.03-8.07(m, 2H). MASS (ES+): 643.2 (M+Na) ⁺ . |
| IA.111 | 0.97(s, 3H), 1.13(t, J=7.55Hz, 3H), 1.15-1.29(m, 1H), 1.38(d, J=7.33Hz, 3H), 1.56(s, 3H), 1.58-1.66(m, 1H), 1.88-2.14(m, 5H), 2.17-2.30(m, 1H), 2.35-2.64(m, 5H), 4.01(d, J=16.84Hz, 1H), 4.45(d, J=8.23Hz, 1H), 4.57(d, J=16.84Hz, 1H), 6.13(s, 1H), 6.35(d, d, J ₁ =10.12Hz, J ₂ =1.77Hz, 1H), 7.22(d, J=10.13Hz, 1H), 7.77(d, J=8.24Hz, 2H), 8.09(d, J=8.14Hz, 2H). MASS (ES+): 659.2 (M+Na) ⁺ . |
| IA.112 | 0.97(d, J=7.05Hz, 3H), 1.10(s, 3H), 1.12-1.48(m, 7H), 1.53(s, 3H), 1.71-2.01(m, 8H), 2.20-2.43(m, 5H), 3.36-3.39(m, 1H), 4.30(d, J=16.59Hz, 1H), 4.43(d, J=8.27Hz, 1H), 4.51(d, J=16.56Hz, 1H), 5.31-5.47(m, 1H), 6.38(d, d, J ₁ =10.12Hz, J ₂ =1.33Hz, 1H), 6.44(s, 1H), 7.16(d, J=10.07Hz, 1H), 7.76(d, J=8.15Hz, 1H), 8.11(d, J=8.08Hz). MASS (ES+): 731.2 (M+Na) ⁺ . |
| IA.113 | 0.96(d, J=7.05Hz, 3H), 1.12(s, 3H), 1.15-1.45(m, 6H), 1.53(s, 3H), 1.58-1.66(m, 1H), 1.72-2.0(m, 8H), 2.20-2.44(m, 5H), 3.36-3.40(m, 1H), 4.28(d, J=16.54Hz, 1H), 4.43(d, J=8.81Hz, 1H), 4.48(d, J=16.56Hz, 1H), 5.31-5.47(m, 1H), 6.38(d, d, J ₁ =10.15Hz, J ₂ =1.46Hz, 1H), 6.44(s, 1H), 7.14(d, J=10.06Hz, 1H), 7.46(d, J=8.53Hz, 2H), 7.94(d, J=8.54Hz, 2H). MASS (ES+): 697.2 (M+Na) ⁺ . |
| IA.114 | 0.96(d, J=7.05Hz, 3H), 1.12(s, 3H), 1.17-1.48(m, 6H), 1.53(s, 3H), 1.58-1.65(m, 1H), 1.71-2.06(m, 8H), 2.20-2.43(m, 5H), 3.36-3.39(m, 1H), 4.27(d, J=17.51Hz, 1H), 4.24-4.45(m, 2H), 5.31-5.47(m, 1H), 6.38(dd, J ₁ =10.12Hz, J ₂ =1.43Hz, 1H), 6.44(s, 1H), 6.89-7.01(m, 2H), 7.14(d, J=10.11Hz, 1H), 7.94(dd, J ₁ =15.1Hz, J ₂ =8.41Hz, 1H). MASS (ES+): 699.2 (M+Na) ⁺ . |
| IA.115 | 0.94(d, J=7.07Hz, 3H), 1.24(s, 3H), 1.28-1.46(m, 5H), 1.55(s, 3H), 1.61-2.06(m, 10H), 2.24-2.50(m, 5H), 3.32-3.37(m, 1H), 4.42(d, J=8.32Hz, 1H), 4.96(d, J=16.52Hz, 1H), 5.32-5.48(m, 1H), 5.68(d, J=16.53Hz, 1H), 6.38(d, d, J ₁ =10.12Hz, J ₂ =1.30Hz, 1H), 6.44(s, 1H), 7.17(d, J=9.91Hz, 1H), 7.16-7.19(m, 2H), 7.94(dd, J ₁ =8.62Hz, J ₂ =5.31Hz, 2H). MASS (ES+): 665.5 (M+Na) ⁺ . |
| IA.116 | 0.96(d, J=7.14Hz, 3H), 1.10(s, 3H), 1.14-1.43(m, 6H), 1.53(s, 3H), 1.62-2.06(m, 10H), 2.23-2.45(m, 4H), 3.38-3.42(m, 1H), 3.88(s, 3H), 4.27(d, J=16.51Hz, 1H), 4.42(d, J=8.73Hz, 1H), 4.53(d, J=16.53Hz, 1H), 5.31-5.47(m, 1H), 6.38(d, d, J ₁ =10.11Hz, J ₂ =1.66Hz, 1H), 6.44(s, 1H), 6.95(d, J=8.90Hz, 2H), 7.15(d, J=10.10Hz, 1H), 7.99(d, J ₁ =8.89Hz, J ₂ =5.31Hz, 2H). MASS (ES+): 693.2 (M+Na) ⁺ . |
| IA.117 | 0.98(d, J=7.03Hz, 3H), 1.10(s, 3H), 1.24-1.34(m, 1H), 1.53(s, 3H), 1.55-1.68(m, 2H), 1.73-2.04(m, 9H), 2.20-2.41(m, 4H), 2.74-2.78(m, 1H), 3.36-3.40(m, 1H), 4.27(d, J=16.55Hz, 1H), 4.41(d, J=7.75Hz, 1H), 4.49(d, J=16.55Hz, 1H), 5.30-5.47(s, 1H), 6.37(d, d, J ₁ =10.15Hz, 1H), 6.43(s, 1H), 7.13(d, J=10.12Hz, 1H), 7.47(d, J=8.36Hz, 1H), 7.95(d, J=8.36Hz, 2H). MASS (ES+): 661.2 |
| IA.118 | 0.96(d, J=7.08Hz, 3H), 1.24(s, 3H), 1.24-1.33(m, 1H), 1.55(s, 3H), 1.56-1.92(m, 9H), 2.022.50(m, 5H), 2.73-2.81(m, 1H), 3.32-3.36(m, 1H), 4.42(d, J=7.77Hz, 1H), 4.97(d, J=16.51Hz, 1H), 5.32-5.48(m, 1H), 5.68(d, J=16.56Hz, 1H), 6.38(d, d, J ₁ =10.08Hz, J ₂ =1.22Hz, 1H), 6.44(s, 1H), 7.14-7.19(m, 3H), 7.93-7.96(m, 2H). MASS (ES+): 629.3 |
| IA.119 | 0.98(d, J=6.93Hz, 3H), 1.10(s, 3H), 1.16(t, J=6.88Hz, 6H), 1.31-1.35(m, 1H), 1.53(s, 3H), 1.58-2.01(m, 4H), 2.21-2.62(m, 5H), 3.36-3.38(m, 1H), 4.31(d, J=16.58Hz), 4.42(d, J=7.40Hz, 1H), 4.51(d, J=16.58Hz, 1H), 5.30-5.47(m, 1H), 6.38(d, J=10.15Hz, 1H), 6.43(s, 1H), 7.13(d, J=10.11Hz, 1H), 7.76(d, J=7.98Hz, 2H), 8.11(d, J=7.91Hz, 2H). MASS (ES+): 669.2 |
| IA.120 | 0.98(d, J=7.12Hz, 3H), 1.12(s, 3H), 1.29-1.35(m, 1H), 1.53(s, 3H), 1.56-1.66(m, 5H), 1.70-2.00(m, 7H), 2.20-2.40(m, 4H), 2.73-2.77(m, 1H), 3.35-3.40(m, 1H), 4.26(d, d, J ₁ =17.47Hz, J ₂ =2.37Hz, 1H), 4.42(d, J=5.81Hz, 1H), 4.54(d, d, J ₁ =17.35Hz, J ₂ =2.61Hz, 1H), 5.31-5.47(m, 1H), 6.38(d, d, J ₁ =10.14Hz, J ₂ =1.38Hz, 1H), 6.43(s, 1H), 6.89-7.01(m, 1H), 7.13(d, J=10.09Hz, 1H), 7.94(dd, J ₁ =15.10Hz, J ₂ =8.46Hz, 2H). MASS (ES+): 663.3 |
| IA.121 | 0.95(d, J=7.14Hz, 3H), 1.16(d, J=7.00Hz, 6H), 1.22(s, 3H), 1.28-1.34(m, 1H), 1.55(s, 3H), 1.74-2.18(m, 4H), 2.28-2.57(m, 4H), 2.58-2.62(m, 1H), 2.30-2.38(m, 1H), 3.30-3.38(m, 1H), 4.42(d, J=8.92Hz, 1H), 4.97(d, J=16.51Hz, 1H), 5.32-5.49(m, 1H), 5.69(d, J=16.53Hz, 1H), 6.38(d, d, J ₁ =10.13Hz, J ₂ =1.75Hz, 1H), 6.44(s, 1H), 7.14-7.20(m, 3H), 7.93-7.97(m, 2H). MASS (ES+): 603.3 |
| IA.122 | 0.98(d, J=7.14Hz, 3H), 1.11(s, 3H), 1.16(d, J=2.98Hz, 3H), 1.17(d, J=3.00Hz, 3H), 1.31-1.34(m, 1H), 1.53(s, 3H), 1.71-2.03(m, 3H), 2.24-2.42(m, 4H), 2.57-2.61(m, 1H), 3.40-3.43(m, 1H), 3.88(s, 3H), 4.28(d, J=16.49Hz, 1H), 4.42(d, J=8.74Hz, 1H), 4.54(d, J=16.50Hz, 1H), 5.30-5.47(m, 1H), 6.37(d, d, J ₁ =10.13Hz, J ₂ =1.77Hz, 1H), 6.43(s, 1H), 6.95(d, J=8.89Hz, 2H), 7.14(dd, J ₁ =10.18Hz, J ₂ =1.12Hz, 2H), 7.99(d, J=8.87Hz, 2H). MASS (ES+): 653.3 |
| IA.123 | 0.97(d, J=7.14Hz, 3H), 1.13(s, 3H), 1.16(d, d, J ₁ =6.99Hz, J ₂ =3.08Hz, 6H), 1.29-1.33(m, 3H), 1.53(s, 3H), 1.73-2.02(m, 4H), 2.23-2.47(m, 4H), 2.55-2.62(m, 1H), 3.36-3.41(m, 1H), 4.28(d, d, J ₁ =17.54Hz, J ₂ =2.63Hz, 1H), 4.42(d, 1H), 4.44(d, d, J ₁ =17.54Hz, J ₂ =2.90Hz, 1H), 5.31-5.48(m, 1H), 6.38(d, d, J ₁ =10.13Hz, J ₂ =1.79Hz, 1H), 6.44(s, 1H), 6.89-7.01(m, 2H), 7.13(d, d, J ₁ =10.10Hz, J ₂ =1.16Hz, 1H), 7.92-7.98(m, 1H). MASS (ES+): 637.3 |
| IA.124 | 1.07(d, J=7.13Hz, 3H), 1.17(s, 3H), 1.33-1.41(m, 1H), 1.55(s, 3H), 1.73-2.04(m, 3H), 2.28-2.54(m, 5H), 3.43-3.48(m, 1H), 4.35(d, J=16.65Hz, 1H), 4.46(d, J=8.34Hz, 1H), 4.54(d, J=16.65Hz, 1H), 5.33-5.49(m, 1H), 6.41(dd, J ₁ =10.12Hz, J ₂ =1.69Hz, 1H), 6.42(s, 1H), 6.51(dd, J ₁ =3.46Hz, J ₂ =1.69Hz, 1H), 7.09-7.21(m, 2H), 7.59(d, J=0.72Hz, 1H), 7.77(d, J=8.25Hz, 2H), 8.72(d, J=8.18Hz, 2H). MASS (ES+): 693.3 |
| IA.125 | 0.59(s, 3H), 0.93(d, J=6.99Hz, 3H), 1.07(t, J=7.54Hz, 3H), 1.21-1.88(m, 14H), 2.09-2.36(m, 6H), 3.13-3.17(m, 1H), 4.31(d, J=7.52Hz, 1H), 5.27-5.42(m, 1H), 6.35(dd, J ₁ =10.08Hz, J ₂ =1.16Hz, 1H), 6.41(s, 1H), 7.07(d, J=10.11Hz, 1H), 7.36(d, J=8.47Hz, 2H), 7.29(d, J=8.49Hz, 2H). MASS (ES+): 649.2 |
| IA.126 | 1.07(d, J=7.12Hz, 3H), 1.11(s, 3H), 1.16-1.87(m, 11H), 1.90-2.09(m, 2H), 2.13-2.44(m, 4H), 3.38-3.42(m, 1H), 4.06-4.19(m, 2H), 4.31(d, J=16.58Hz, 1H), 4.40(d, J=8.68Hz, 1H), 4.55(d, J=16.55Hz, 1H), 5.29-5.47(m, 1H), 6.37(dd, J ₁ =10.17Hz, J ₂ =1.45Hz, 1H), 6.42(s, 1H), 6.96(d, J=8.81Hz, 2H), 7.13(d, J=10.19Hz, 1H), 8.00(d, J=8.83Hz, 2H). MASS (ES+): 633 |
| IA.127 | 1.07(d, J=7.06Hz, 3H), 1.17(s, 3H), 1.23-2.10(m, 8H), 2.17-2.53(m, 4H), 3.46-3.50(m, 1H), 3.88(s, 3H), 4.31(d, J=16.63Hz, 1H), 4.45(d, J=8.39Hz, 1H), 4.57(d, J=16.60Hz, 1H), 5.32-5.49(m, 1H), 6.40(dd, J ₁ =10.14Hz, J ₂ =1.36Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.11Hz, J ₂ =1.47Hz, 1H), 6.96(d, J=8.82Hz, 2H), 7.13-7.21(m, 2H), 7.59(s, 1H), 8.00(d, J=8.80Hz, 2H). MASS (ES+): 655.2 |
| IA.128 | 0.88(t, J=Hz, 3H), 0.99(d, J=Hz, 3H), 1.11(s, 3H), 1.22-1.32(m, 4H), 1.53-1.97(m, 8H), 2.20-2.46(m, 6H), 3.36-3.40(m, 1H), 4.33(d, J=Hz, 1H), 4.41(d, J=Hz, 1H), 4.49(d, J=Hz, 1H), 5.30-5.47(m, 1H), 6.38(dd, J ₁ =Hz, J ₂ =Hz, 1H), 6.43(s, 1H), 7.13(dd, J ₁ =Hz, J ₂ =Hz, 1H), 7.76(d, J=Hz, 2H), 8.12(d, J=Hz, 2H). MASS (ES+): 683.2 |
| IA.129 | 0.88(t, J=7.32Hz, 3H), 0.99(d, J=7.10Hz, 3H), 1.11(s, 3H), 1.19-1.32(m, 4H), 1.48-1.97(m, 8H), 2.20-2.48(m, 6H), 3.36-3.40(m, 1H), 4.30(d, J=16.53Hz, 1H), 4.41(d, J=7.86Hz, 1H), 4.47(d, J=16.56Hz, 1H), 5.30-5.47(m, 1H), 6.38(dd, J ₁ =10.12Hz, J ₂ =1.53Hz, 1H), 6.43(s, 1H), 7.13(d, J=10.02Hz, 1H), 7.47(d, J=8.48Hz, 2H), 7.95(d, J=8.48Hz, 2H). MASS (ES+): 649.3 |

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| Comp. No | ¹ H-NMR (δ ppm), MASS (EI / ES+, m/z) |
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| IA.130 | 0.88(t, J=7.32Hz, 3H), 0.98(d, J=7.11Hz, 3H), 1.13(s, 3H), 1.18-1.42(m, 4H), 1.45-1.99(m, 8H), 2.20-2.46(m, 6H), 3.36-3.39(m, 1H), 4.30(d, J=17.38Hz, 1H), 4.41-4.46(m, 2H), 5.30-5.47(m, 1H), 6.38(dd, J ₁ =10.13Hz, J ₂ =1.55Hz, 1H), 6.43(s, 1H), 6.89-6.95(m, 1H), 6.97-7.01(m, 1H), 7.13(d, J=9.99Hz, 1H), 7.92-7.98(m, 1H). MASS (ES+): 651.4 |
| IA.131 | 0.88(t, J=7.35Hz, 3H), 0.99(d, J=7.12Hz, 3H), 1.11(s, 3H), 1.21-1.38(m, 3H), 1.45-1.99(m, 9H), 2.20-2.46(m, 6H), 3.36-3.40(m, 1H), 4.31(d, J=16.51Hz, 1H), 4.41(d, J=7.65Hz, 1H), 4.49(d, J=16.50Hz, 1H), 5.30-5.47(m, 1H), 6.38(dd, J ₁ =10.12Hz, J ₂ =1.69Hz, 1H), 6.43(s, 1H), 7.12-7.18(m, 3H), 8.03-8.06(m, 2H). MASS (ES+): 633.4 |
| IA.132 | 0.98(d, J=7.04Hz, 3H), 1.11(s, 3H), 1.16(d, J=5.6Hz, 6H), 1.30-1.35(m, 1H), 1.53(s, 3H), 1.73-2.01(m, 4H), 2.21-2.60(m, 5H), 3.37-3.40(m, 1H), 4.28(d, J=16.48Hz, 1H), 4.42(d, J=7.47Hz, 1H), 4.48(d, J=16.59Hz, 1H), 5.30-5.47(m, 1H), 6.38(d, J=10.17Hz, 1H), 6.43(s, 1H), 7.13(d, J=10.11Hz, 1H), 7.473(d, J=8.33Hz, 2H), 7.95(d, J=8.39Hz, 2H). MASS (ES+): 635.2 |
| IA.133 | 0.96(d, J=7.13Hz, 3H), 1.24(s, 3H), 1.27-1.33(m, 1H), 1.55(s, 3H), 1.75-2.06(m, 6H), 2.19-2.38(m, 8H), 3.13-3.19(m, 1H), 3.33-3.37(m, 1H), 4.41(d, J=9.04Hz, 1H), 5.00(d, J=16.54Hz, 1H), 5.31-5.48(m, 1H), 5.71(d, J=16.57Hz, 1H), 6.38(dd, J ₁ =10.15Hz, J ₂ =1.70Hz, 1H), 6.44(s, 1H), 7.15(d, J ₁ =9.99Hz, J ₂ =1.10Hz, 1H), 7.18(t, J=8.54Hz, 2H), 7.94-7.97(m, 2H). MASS (ES+): 615.1 |
| IA.134 | 0.98(d, J=7.16Hz, 3H), 1.10(s, 3H), 1.30-1.36(m, 1H), 1.53(s, 3H), 1.53-1.98(m, 12H), 2.23-2.42(m, 4H), 2.72-2.80(m, 1H), 3.36-3.40(m, 1H), 4.33(d, J=16.54Hz, 1H), 4.42(d, J=8.83Hz, 1H), 4.49(d, J=16.53Hz, 1H), 5.30-5.47(m, 1H), 6.38(dd, J ₁ =10.14Hz, J ₂ =1.61Hz, 1H), 6.43(s, 1H), 7.12(d, J ₁ =10.19Hz, J ₂ =1.24Hz, 1H), 7.76(d, J=8.27Hz, 2H), 8.11(d, J=8.14Hz, 2H). MASS (ES+): 695.3 |
| IA.135 | 0.99(d, J=7.13Hz, 3H), 1.11(s, 3H), 1.25-1.32(m, 1H), 1.52(s, 3H), 1.72-2.04(m, 6H), 2.18-2.40(m, 8H), 3.14-3.16(m, 1H), 4.31(d, J=16.5Hz, 1H), 4.41(d, J=8.48Hz, 1H), 4.48(d, J=16.52Hz, 1H), 6.37(dd, J ₁ =10.12Hz, J ₂ =1.72Hz, 1H), 6.43(s, 1H), 7.12(d, J ₁ =10.12Hz, J ₂ =0.81Hz, 1H), 7.47(d, J=8.57Hz, 2H), 7.95(d, J=8.59Hz, 2H). MASS (ES+): 647.2 |
| IA.136 | 0.99(d, J=7.12Hz, 3H), 1.10(s, 3H), 1.29-1.35(m, 1H), 1.53(s, 3H), 1.76-1.99(m, 6H), 2.17-2.45(m, 8H), 3.12-3.21(m, 1H), 3.35-3.41(m, 1H), 4.33(d, J ₁ =16.59Hz, 4.41(d, J=8.63Hz, 1H), 4.51(d, J=16.56Hz, 1H), 5.30-5.47(m, 1H), 6.37(dd, J ₁ =10.16Hz, J ₂ =1.61Hz, 1H), 6.43(s, 1H), 7.13(d, J ₁ =10.18Hz, J ₂ =0.73Hz, 1H), 7.77(d, J=8.24Hz, 2H), 8.12(d, J=8.14Hz, 2H). MASS (ES+): 681.2 |
| IA.137 | 0.98(d, J=7.13Hz, 3H), 1.12(s, 3H), 1.29-1.35(m, 1H), 1.53(s, 3H), 1.70-2.00(m, 5H), 2.16-2.45(m, 7H), 3.13-3.18(m, 1H), 3.36-3.41(m, 1H), 4.29(d, J ₁ =17.52Hz, J ₂ =2.62Hz, 1H), 4.41(d, J=9.87Hz, 1H), 4.45(d, J ₁ =17.67Hz, J ₂ =2.71Hz, 1H), 5.31-5.47(m, 1H), 6.37(dd, J ₁ =10.13Hz, J ₂ =1.71Hz, 1H), 6.43(s, 1H), 6.89-7.02(m, 2H), 7.14(d, J=10.13Hz, 1H), 7.92-7.98(m, 1H). MASS (ES+): 649.3 |
| IA.138 | 0.96(d, J=7.16Hz, 3H), 1.11(s, 3H), 1.29-1.34(m, 1H), 1.52(s, 3H), 1.84-2.04(m, 6H), 2.17-2.39(m, 8H), 3.14-3.19(m, 1H), 3.38-3.43(m, 1H), 3.88(s, 3H), 4.30(d, J=16.51Hz, 1H), 4.40(d, J=8.92Hz, 1H), 4.53(d, J=16.51Hz, 1H), 5.30-5.47(m, 1H), 6.37(dd, J ₁ =10.13Hz, J ₂ =1.74Hz, 1H), 6.43(s, 1H), 6.96(d, J=8.85Hz, 2H), 7.14(d, J=10.11Hz, 1H), 7.99(d, J=8.85Hz, 2H). MASS (ES+): 643.3 |
| IA.139 | 1.06(d, J=7.12Hz, 3H), 1.17(s, 3H), 1.33-1.38(m, 1H), 1.56(s, 3H), 1.60-1.99(m, 5H), 2.29-2.65(m, 4H), 3.41-3.46(m, 1H), 4.35(d, 1H), J=16.58Hz), 4.46(d, J=8.88Hz), 4.53(d, J=16.55Hz), 6.15(s, 1H), 6.37(dd, J ₁ =10.13Hz, J ₂ =1.68Hz, 1H), 6.49(dd, J ₁ =3.42Hz, J ₂ =1.65Hz, 1H), 7.12(d, J=3.47Hz, 1H), 7.22(d, J=10.12Hz, 1H), 7.58(d, J=1.48Hz, 1H), 7.76(d, J=8.35Hz, 2H), 8.12(d, J=8.26Hz, 2H). MASS (ES+): 675.3 |
| IA.140 | 1.05(d, J=7.1Hz, 3H), 1.19(s, 3H), 1.32-1.37(m, 1H), 1.57(s, 3H), 1.60-2.02(m, 5H), 2.29-2.67(m, 5H), 3.42-3.47(m, 1H), 4.31(dd, J ₁ =17.52Hz, J ₂ =2.24Hz, 1H), 4.46(d, J=8.89Hz, 1H), 4.47(dd, 1H), 6.15(s, 1H), 6.37(dd, J ₁ =10.11Hz, J ₂ =1.09Hz, 1H), 6.48(dd, J ₁ =3.04Hz, J ₂ =1.33Hz, 1H), 6.88-7.01(m, 2H), 7.12(d, J=3.45Hz, 1H), 7.23(d, J=10.12Hz, 1H), 7.58(d, J=8.35Hz, 2H), 7.95(d, J ₁ =15.1Hz, J ₂ =8.46Hz, 1H). MASS (ES+): 643.2 |
| IA.141 | 1.05(d, J=7.09Hz, 3H), 1.17(s, 3H), 1.25-1.38(m, 1H), 1.56(s, 3H), 1.60-2.00(m, 5H), 2.29-2.65(m, 4H), 3.43-3.45(m, 1H), 4.32(d, 1H), J=16.52Hz), 4.45(d, 1H, J=9.02Hz), 4.50(d, 1H, J=16.61Hz), 6.15(s, 1H), 6.37(dd, J ₁ =10.07Hz, J ₂ =0.81Hz, 1H), 6.49(d, J=3.33Hz, 1H), 7.12(d, J=3.43Hz, 1H), 7.22(d, J=10.12Hz, 1H), 7.47(d, J=8.40Hz, 2H), 7.58(s, 1H), 7.95(d, J=8.45Hz, 2H). MASS (ES+): 641.3 |
| IA.142 | 1.06(d, J=7.12Hz, 3H), 1.18(s, 3H), 1.31-1.37(m, 1H), 1.56(s, 3H), 1.60-2.04(m, 4H), 2.29-2.65(m, 5H), 3.44-3.48(m, 1H), 3.88(s, 3H), 4.33(d, J=16.64Hz, 1H), 4.45(d, J=8.94Hz, 1H), 4.54(d, J=16.50Hz, 1H), 6.15(s, 1H), 6.36(dd, J ₁ =10.11Hz, J ₂ =1.73Hz, 1H), 6.49(dd, J ₁ =3.46Hz, J ₂ =1.70Hz, 1H), 6.95(d, J=8.89Hz, 2H), 7.12(d, J=13.39Hz, 1H), 7.23(d, J=10.15Hz, 1H), 7.58(s, 1H), 7.99(d, J ₁ =8.66Hz, J ₂ =8.66Hz, 2H). MASS (ES+): 637.4 |
| IA.143 | 1.05(d, J=7.12Hz, 3H), 1.18(s, 3H), 1.25-1.35(m, 1H), 1.57(s, 3H), 1.63-1.99(m, 5H), 2.03-2.64(m, 5H), 3.45(m, 1H), 4.32(d, J=16.52, 1H), 4.45(d, J=9.01, 1H), 4.53(d, J=16.54, 1H), 6.15(s, 1H), 6.37(dd, J ₁ =10.11Hz, J ₂ =1.75Hz, 1H), 6.49(dd, J ₁ =3.47Hz, J ₂ =1.71Hz, 1H), 7.12-7.25(m, 4H), 7.58(d, J=0.81Hz, 1H), 8.03-8.07(m, 2H). MASS (ES+): 647.2 (M+Na) ⁺ |
| IA.144 | 0.96(d, J=7.17Hz, 3H), 1.04(s, 3H), 1.15(d, J=3.84Hz, 3H), 1.17(d, J=3.86Hz, 3H), 1.28-1.34(m, 1H), 1.52(s, 3H), 1.76-1.89(m, 4H), 2.25(s, 6H), 2.28(s, 3H), 2.22-2.41(m, 4H), 2.55-2.62(m, 1H), 3.38-3.43(m, 1H), 4.03(d, J=17.76Hz, 1H), 4.30(d, J=17.79Hz, 1H), 4.37(d, J=8.81Hz, 1H), 5.30-5.47(m, 1H), 6.37(dd, J ₁ =10.14Hz, J ₂ =1.86Hz, 1H), 6.43(s, 1H), 6.85(s, 2H), 7.12(dd, J ₁ =10.13Hz, J ₂ =1.29Hz, 1H). MASS (ES+): 643.5 |
| IA.145 | 0.95(d, J=7.15Hz, 3H), 1.02(s, 3H), 1.20-1.42(m, 8H), 1.52(s, 3H), 1.72-1.89(m, 6H), 2.25(s, 6H), 2.28(s, 3H), 2.25-2.41(m, 5H), 3.37-3.43(m, 1H), 4.02(d, J=17.62Hz, 1H), 4.30(d, J=17.83Hz, 1H), 4.38(d, J=8.83Hz, 1H), 5.30-5.47(m, 1H), 6.38(dd, J ₁ =10.14Hz, J ₂ =1.86Hz, 1H), 6.44(s, 1H), 6.85(s, 2H), 7.13(dd, J ₁ =10.14Hz, J ₂ =1.39Hz, 1H). MASS (ES+): 705.3 (M + Na) ⁺ |
| IA.146 | 0.96(d, J=7.16Hz, 3H), 1.03(s, 3H), 1.25-1.34(m, 1H), 1.52(s, 3H), 1.54-1.69(m, 4H), 1.76-1.89(m, 7H), 2.25(s, 6H), 2.28(s, 3H), 2.27-2.80(m, 1H), 3.37-3.43(m, 1H), 4.03(d, J=17.77Hz, 1H), 4.30(d, J=17.77Hz, 1H), 4.37(d, J=8.7Hz, 1H), 5.30-5.47(m, 1H), 6.37(dd, J ₁ =10.14Hz, J ₂ =1.82Hz, 1H), 6.43(s, 1H), 6.85(s, 2H), 7.12(dd, J ₁ =10.14Hz, J ₂ =1.12Hz, 1H). MASS (ES+): 669.4 |
| IA.147 | 0.97(d, J=7.17Hz, 3H), 1.02(s, 3H), 1.28-1.34(m, 1H), 1.52(s, 3H), 1.72-1.97(m, 6H), 2.18-2.23(m, 5H), 2.26(s, 6H), 2.28(s, 3H), 2.30-2.43(m, 2H), 3.12-3.20(m, 1H), 3.38-3.43(m, 1H), 4.06(d, J=17.72Hz, 1H), 4.29(d, J=17.72Hz, 1H), 4.37(d, J=8.92Hz, 1H), 5.30-5.47(m, 1H), 6.38(dd, J ₁ =10.15Hz, J ₂ =1.87Hz, 1H), 6.43(s, 1H), 6.85(s, 2H), 7.11(dd, J ₁ =10.13Hz, J ₂ =1.27Hz, 1H). MASS (ES+): 655.4 |
| IA.148 | 0.91-0.94(m, 2H), 0.98(d, J=7.11Hz, 3H), 1.03(s, 3H), 1.09-1.26(m, 5H), 1.52(s, 3H), 1.65-1.75(m, 8H), 1.83-1.93(m, 2H), 2.17-2.22(m, 3H), 2.25(s, 6H), 2.28(s, 3H), 2.34-2.38(m, 1H), 3.37-3.41(m, 1H), 4.06(d, J=17.78Hz, 1H), 4.27(d, J=17.79Hz, 1H), 4.27(d, J=9.08Hz, 1H), 5.30-5.46(m, 1H), 6.38(dd, J ₁ =10.14Hz, J ₂ =1.85Hz, 1H), 6.43(s, 1H), 6.85(s, 2H), 7.12(d, J ₁ =10.12Hz, J ₂ =1.20Hz, 1H). MASS (ES+): 719.4 (M+Na) ⁺ |

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| Comp. No | ¹ H-NMR (δ ppm), MASS (EI / ES+, m/z) |
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| IA.149 | 1.07(d, J=7.13Hz, 3H), 1.20(s, 3H), 1.35-1.40(m, 1H), 1.56(s, 3H), 1.72-1.98(m, 3H), 2.25(s, 6H), 2.28(s, 3H), 2.32-2.44(m, 4H), 3.44-3.49(m, 1H), 4.13(d, J=17.69Hz, 1H), 4.23(d, J=17.69Hz, 1H), 4.40(d, J=8.86Hz, 1H), 4.53-4.55(m, 1H), 5.34-5.51(m, 1H), 6.36(dd, J ₁ =10.10Hz, J ₂ =1.79Hz, 1H), 6.41(s, 1H), 6.86(s, 2H), 7.10(dd, J ₁ =4.94Hz, J ₂ =3.81Hz, 1H), 7.25(dd, J ₁ =10.12Hz, J ₂ =1.05Hz, 1H), 7.58(dd, J ₁ =4.98Hz, J ₂ =1.15Hz, 1H), 7.73(dd, J ₁ =3.65Hz, J ₂ =1.16Hz, 1H). MASS (ES+): 683.9 |
| IA.150 | 0.88-0.94(m, 2H), 0.99(d, J=7.10Hz, 3H), 1.13(s, 3H), 1.17-1.35(m, 4H), 1.53(s, 3H), 1.64-1.98(m, 10H), 2.17-2.46(m, 6H), 3.35-3.39(m, 1H), 4.30(dd, J ₁ =15.16Hz, J ₂ =2.50Hz, 1H), 4.40(d, 1H), 4.42(d, J ₁ =17.58Hz, J ₂ =2.47Hz, 1H), 5.31-5.45(m, 1H), 6.38(dd, J ₁ =10.13Hz, J ₂ =1.65Hz, 1H), 6.43(s, 1H), 6.89-7.01(m, 2H), 7.13(dd, J ₁ =10.11Hz, J ₂ =1.11Hz, 1H), 7.92-7.98(m, 1H). MASS (ES+): 691.5 |
| IA.141 | 0.91-0.97(m, 2H), 0.99(d, J=7.15Hz, 3H), 1.11(s, 3H), 1.13-1.35(m, 4H), 1.52(s, 3H), 1.61-1.95(m, 9H), 2.19-2.40(m, 6H), 3.35-3.40(m, 1H), 4.33(d, J=16.41Hz, 1H), 4.41(d, J=12.88Hz, 1H), 4.45(d, J=16.53Hz, 1H), 5.30-5.47(m, 1H), 6.38(dd, J ₁ =10.12Hz, J ₂ =1.80Hz, 1H), 6.43(s, 1H), 7.13(dd, J ₁ =10.14Hz, J ₂ =1.27Hz, 1H), 7.46(d, J=8.55Hz, 2H), 7.94(d, J=8.61Hz, 2H). MASS (ES+): 711.3 (M+Na) ⁺ |
| IA.152 | 0.91-0.97(m, 2H), 1.00(d, J=7.13Hz, 3H), 1.11(s, 3H), 1.13-1.36(m, 4H), 1.53(s, 3H), 1.61-1.91(m, 10H), 2.20-2.45(m, 6H), 3.34-3.40(m, 1H), 4.35(d, J=16.56Hz, 1H), 4.41(d, J=8.94Hz, 1H), 4.48(d, J=16.54Hz, 1H), 5.30-5.47(m, 1H), 6.38(dd, J ₁ =10.15Hz, J ₂ =1.87Hz, 1H), 6.43(s, 1H), 7.12(dd, J ₁ =10.13Hz, J ₂ =1.26Hz, 1H), 7.76(d, J=8.28Hz, 2H), 8.11(d, J=8.16Hz, 2H). MASS (ES+): 723.1 |
| IA.153 | 0.91-0.97(m, 2H), 1.00(d, J=7.11Hz, 3H), 1.12(s, 3H), 1.09-1.36(m, 4H), 1.52(s, 3H), 1.61-1.87(m, 10H), 2.20-2.39(m, 6H), 3.37-3.42(m, 1H), 3.88(s, 3H), 4.34(d, J=16.49Hz, 1H), 4.40(d, J=9.19Hz, 1H), 4.48(d, J=16.43Hz, 1H), 5.30-5.47(m, 1H), 6.37(dd, J ₁ =10.14Hz, J ₂ =1.76Hz, 1H), 6.43(s, 1H), 6.95(d, J=8.87Hz, 2H), 7.13(dd, J ₁ =10.13Hz, J ₂ =1.02Hz, 1H), 7.99(d, J=8.89Hz, 2H). MASS (ES+): 707.3 (M+Na) ⁺ |
| IA.154 | 0.89(t, J=7.34Hz, 3H), 0.97(d, J=7.10Hz, 3H), 1.03(s, 3H), 1.25-1.96(m, 8H), 2.09-2.40(m, 15H), 3.38-3.42(m, 1H), 4.05(d, J=17.80Hz, 1H), 4.29(d, J=17.72Hz, 1H), 4.39(d, J=7.99Hz, 1H), 5.30-5.47(m, 1H), 6.39(dd, J ₁ =10.10Hz, J ₂ =1.65Hz, 1H), 6.43(s, 1H), 6.85(s, 2H), 7.13(d, J=10.07Hz, 1H). MASS (ES+): 657.3 |
| IA.155 | 1.03(s, 3H), 1.06(d, J=7.19Hz, 3H), 1.26(t, J=7.09Hz, 3H), 1.32-1.94(m, 10H), 2.22-2.44(m, 12H), 3.37-3.42(m, 1H), 4.04-4.18(m, 3H), 4.30(d, J=17.74Hz, 1H), 4.36-4.38(m, 1H), 5.30-5.45(m, 1H), 6.37(dd, J ₁ =10.14Hz, J ₂ =1.67Hz, 1H), 6.42(s, 1H), 6.86(s, 2H), 7.12(d, J=10.21Hz, 1H). MASS (ES+): 645.1 |
| IA.156 | 1.06(d, J=7.19Hz, 3H), 1.11(s, 3H), 1.25-1.97(m, 8H), 2.25(s, 6H), 2.28(s, 3H), 2.30-2.53(m, 3H), 3.46-3.51(m, 1H), 4.07(d, J=17.84Hz, 1H), 4.31(dd, J ₁ =17.82Hz, 1H), 5.34-5.46(m, 1H), 6.41(dd, J ₁ =10.14Hz, J ₂ =1.87Hz, 1H), 6.51(dd, J ₁ =3.50Hz, J ₂ =1.73Hz, 1H), 6.85(s, 2H), 7.12-7.16(m, 2H), 7.59(d, J=1.01Hz, 1H). MASS (ES+): 667.3 |
| IA.157 | 1.07(d, J=7.10Hz, 3H), 1.17(s, 3H), 1.21-2.03(m, 8H), 2.17-2.55(m, 4H), 3.45-3.48(m, 1H), 4.32(d, J=16.56Hz, 1H), 4.46(d, J=8.46Hz, 1H), 4.51(d, J=15.90Hz, 1H), 5.7-5.49(m, 1H), 6.40(dd, J ₁ =10.14Hz, J ₂ =1.70Hz, 1H), 6.45(s, 1H), 6.51(dd, J ₁ =3.44Hz, J ₂ =1.67Hz, 1H), 7.13-7.16(m, 2H), 7.47(d, J=8.56Hz, 2H), 7.59(s, 1H), 7.96(d, J=8.59Hz, 2H). MASS (ES+): 659.5 |
| IA.158 | 0.97(s, 3H), 1.14(t, J=7.54Hz, 3H), 1.19-1.25(m, 1H), 1.38(d, J=7.35Hz, 3H), 1.54(s, 3H), 1.92-2.14(m, 4H), 2.26-2.48(m, 5H), 3.97(d, J=16.90Hz, 1H), 4.45(d, J=8.33Hz, 1H), 4.56(d, J=16.89Hz, 1H), 5.31-5.48(m, 1H), 6.38(dd, J ₁ =10.14Hz, J ₂ =1.85Hz, 1H), 6.44(s, 1H), 7.14(dd, J ₁ =10.12Hz, J ₂ =1.22Hz, 1H), 7.47(d, J=8.60Hz, 2H), 7.93(d, J=8.59Hz, 2H). MASS (ES+): 643.3 (M+Na) ⁺ |
| IA.159 | 1.08(d, J=7.14Hz, 3H), 1.17(s, 3H), 1.37-1.42(m, 1H), 1.55(s, 3H), 1.78-1.94(m, 4H), 2.00-2.57(m, 4H), 3.44-3.49(m, 1H), 4.37(d, J=16.62Hz, 1H), 4.47(d, J=6.55Hz, 1H), 4.53(d, J=16.57Hz, 1H), 5.33-5.55(m, 1H), 6.40(dd, J ₁ =10.15Hz, J ₂ =1.80Hz, 1H), 6.46(s, 1H), 7.11(d, J=4.95Hz, J ₂ =3.87Hz, 1H), 7.15(d, J=10.14Hz, 1H), 7.58(dd, J ₁ =5.02Hz, J ₂ =1.10Hz, 1H), 7.74(d, J=3.85Hz, J ₂ =1.12Hz, 1H), 7.76(d, J=8.39Hz, 2H), 8.10(d, J=8.23Hz, 2H). MASS (ES+): 709.3 |
| IA.160 | 0.99(d, J=7.10Hz, 3H), 1.09(s, 3H), 1.11(t, J=7.59Hz, 3H), 1.31-1.36(m, 1H), 1.53(s, 3H), 1.72-1.97(m, 4H), 2.23-2.44(m, 6H), 3.32-3.37(m, 1H), 4.38-4.48(m, 3H), 5.30-5.47(m, 1H), 6.38(d, J ₁ =10.14Hz, J ₂ =1.5Hz, 1H), 6.43(s, 1H), 7.13(d, J=10.08Hz, 1H), 7.72(t, J=7.99Hz, 1H), 8.34(d, J=7.78Hz, 1H), 8.46(d, J=8.17Hz, 1H), 8.82(s, 1H). MASS (ES+): 654.3 (M+Na) ⁺ |
| IA.161 | 0.99(d, J=7.16Hz, 3H), 1.12(t, J=7.58Hz, 3H), 1.13(s, 3H), 1.31-1.35(m, 1H), 1.52(s, 3H), 1.76-2.01(m, 3H), 2.23-2.45(m, 6H), 2.32(s, 3H), 2.33(s, 3H), 3.38-3.43(m, 1H), 4.34(d, J=16.65Hz, 1H), 4.39-4.41(m, 1H), 4.52(d, J=16.66Hz, 1H), 5.30-5.47(m, 1H), 6.37(dd, J ₁ =10.14Hz, J ₂ =1.81Hz, 1H), 6.43(s, 1H), 7.13(dd, J ₁ =10.13Hz, J ₂ =1.23Hz, 1H), 7.24(d, J=7.86Hz, 1H), 7.74(dd, J ₁ =8.51Hz, J ₂ =1.38Hz, 1H), 7.77(s, 1H). MASS (ES+): 615.4 |
| IA.162 | 0.97(s, 3H), 1.14(t, J=7.51Hz, 3H), 1.21-1.27(m, 1H), 1.38(d, J=7.37Hz, 3H), 1.54(s, 3H), 1.73-2.12(m, 5H), 2.26-2.50(m, 6H), 4.01(d, 1H), J=16.98Hz), 4.46(d, J=8.09Hz, 1H), 4.58(d, J=16.98Hz, 1H), 5.31-5.48(m, 1H), 6.38(dd, J ₁ =10.11Hz, J ₂ =1.78Hz, 1H), 6.44(s, 1H), 7.13(dd, J ₁ =10.17Hz, J ₂ =1.27Hz, 1H), 7.77(d, J=8.35Hz, 2H), 8.09(d, J=8.05Hz, 2H). MASS (ES+): 655.4 |
| IA.163 | 0.93(t, J=7.36Hz, 3H), 1.00(d, J=7.20Hz, 3H), 1.11(s, 3H), 1.25-1.97(m, 10H), 2.20-2.41(m, 6H), 3.35-3.39(m, 1H), 4.33(d, J=16.58Hz, 1H), 4.41(d, J=8.84Hz, 1H), 4.50(d, J=16.57Hz, 1H), 5.30-5.47(m, 1H), 6.38(dd, J ₁ =10.14Hz, J ₂ =1.81Hz, 1H), 6.43(s, 1H), 7.12(dd, J ₁ =10.12Hz, J ₂ =1.17Hz, 1H), 7.76(d, J=8.29Hz, 2H), 8.12(d, J=8.12Hz, 2H). MASS (ES+): 669.3 |
| IA.164 | 0.94(t, J=7.40Hz, 3H), 0.99(d, J=7.15Hz, 3H), 1.11(s, 3H), 1.24-1.98(m, 10H), 2.22-2.41(m, 6H), 3.36-3.40(m, 1H), 4.29(d, J=16.51Hz, 1H), 4.41(d, J=8.74Hz, 1H), 4.47(d, J=16.54Hz, 1H), 5.30-5.47(m, 1H), 6.37(dd, J ₁ =10.12Hz, J ₂ =1.75Hz, 1H), 6.43(s, 1H), 7.13(dd, J ₁ =10.12Hz, J ₂ =1.14Hz, 1H), 7.46-7.48(m, 2H), 7.95(d, J=8.61Hz, 2H). MASS (ES+): 635.3 |
| IA.165 | 0.94(t, J=7.39Hz, 3H), 0.99(d, J=7.16Hz, 3H), 1.13(s, 3H), 1.22-2.01(m, 10H), 2.20-2.45(m, 6H), 3.36-3.40(m, 1H), 4.30(d, J=16.52Hz, 1H), 4.28(dd, J ₁ =17.53Hz, J ₂ =2.68Hz), 4.42-4.47(m, 2H), 5.30-5.47(m, 1H), 6.38(dd, J ₁ =10.14Hz, J ₂ =1.76Hz, 1H), 6.43(s, 1H), 6.89-7.01(m, 2H), 7.12-7.15(m, 1H), 7.92-7.98(m, 1H). MASS (ES+): 637.3 |
| IA.166 | 0.94(t, J=7.36Hz, 3H), 0.99(d, J=7.16Hz, 3H), 1.11(s, 3H), 1.24-1.99(m, 10H), 2.20-2.41(m, 6H), 3.37-3.41(m, 1H), 4.30(d, J=16.52Hz, 1H), 4.41(d, J=8.86Hz, 1H), 4.49(d, J=16.51Hz, 1H), 5.30-5.47(m, 1H), 6.38(dd, J ₁ =10.14Hz, J ₂ =1.74Hz, 1H), 6.43(s, 1H), 7.12-7.18(m, 3H), 8.03-8.06(m, 2H). MASS (ES+): 619.4 |
| IA.167 | 1.07(d, J=7.15Hz, 3H), 1.16(s, 3H), 1.35-1.41(m, 1H), 1.55(s, 3H), 1.74-2.03(m, 4H), 2.28-2.55(m, 1H), 3.38-3.43(m, 1H), 3.88(s, 3H), 4.30(d, J=16.44Hz, 1H), 4.41(d, J=9.06Hz, 1H), 4.52(d, J=16.51Hz, 1H), 5.30-5.47(m, 1H), 6.38(dd, J ₁ =10.15Hz, J ₂ =1.85Hz, 1H), 6.43(s, 1H), 6.94-6.97(m, 2H), 7.13(dd, J ₁ =10.12Hz, J ₂ =1.21Hz, 1H), 7.98-8.00(m, 2H). MASS (ES+): 631.3 |
| IA.168 | 1.07(d, J=7.15Hz, 3H), 1.16(s, 3H), 1.35-1.41(m, 1H), 1.55(s, 3H), 1.74-2.03(m, 4H), 2.28-2.55(m, 1H), 3.38-3.43(m, 1H), 3.43-3.48(m, 1H), 4.33(d, J=16.67Hz, 1H), 4.46(d, J=11.14Hz, 1H), 4.49(d, J=16.89Hz, 1H), 5.32-5.49(m, 1H), 6.40(dd, J ₁ =10.14Hz, J ₂ =1.69Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.47Hz, J ₂ =1.69Hz, 1H), 7.13(d, J=2.81Hz, 1H), 7.14(dd, J ₁ =9.98Hz, J ₂ =1.20Hz, 1H), 7.45(t, J=7.89Hz, 1H), 7.57(dd, J ₁ =1.86Hz, J ₂ =0.89Hz, 1H), 7.59(m, 1H), 7.88-7.91(m, 1H), 7.98(t, J=1.75Hz, 1H). MASS (ES+): 681.3 (M+Na) ⁺ |

SUBSTITUTE SHEET (RULE 26)

| Comp. No | ¹ H-NMR (δ ppm), MASS (EI / ES+, m/z) |
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| IA.169 | 1.03(s, 3H), 1.13-1.36(m, 1H), 1.43(d, J=7.23Hz, 3H), 1.56(s, 3H), 1.77-2.23(m, 5H), 2.31-2.67(m, 4H), 3.97(d, 1H, J=17.00Hz), 4.53(d, J=7.38Hz, 1H), 4.62(d, J=17.03Hz, 1H), 5.24-5.57(m, 1H), 6.41(d, J=10.09Hz, 1H), 6.44 (s, 1H), 6.53(dd, J ₁ =3.24Hz, J ₂ =1.49Hz, 1H), 7.17 (d, J=9.71Hz, 1H), 7.20(d, J=3.03Hz, 1H), 7.62(s, 1H), 7.76(d, J=8.15Hz, 2H), 8.09(d, J=8.09Hz, 2H). MASS (ES+) : 693.2 |
| IA.170 | 1.07(d, J=7.13Hz, 3H), 1.17(s, 3H), 1.35-1.41(m, 1H), 1.54(s, 3H), 1.76-2.04(m, 4H), 2.28-2.54(m, 4H), 3.45-3.50(m, 1H), 3.83(s, 3H), 4.36(d, 1H, J=16.61Hz), 4.45(d, J=8.19Hz, 1H), 4.51(d, J=16.68Hz, 1H), 5.32-5.49(m, 1H), 6.39(dd, J ₁ =10.15Hz, J ₂ =1.84Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.50Hz, J ₂ =1.70Hz, 1H), 6.68(t, J=2.27Hz, 1H), 7.13-7.17(m, 4H), 7.59 (m, 1H). MASS (ES+) : 685.2 |
| IA.171 | 1.07(d, J=7.12Hz, 3H), 1.17(s, 3H), 1.34-1.42(m, 1H), 1.55(s, 3H), 1.73-1.99(m, 4H), 2.28-2.55(m, 4H), 3.41-3.47(m, 1H), 4.35(d, 1H, J=16.49Hz), 4.46(d, J=8.61Hz, 1H), 4.52(d, J=16.49Hz, 1H), 5.33-5.49(m, 1H), 6.40(dd, J ₁ =10.12Hz, J ₂ =1.73Hz, 1H), 6.45(s, 1H), 6.51(dd, J ₁ =3.47Hz, J ₂ =1.71Hz, 1H), 7.13(d, J=3.46Hz, 1H), 7.14(d, J=10.8Hz, 1H), 7.59-7.60(m, 1H), 8.17(d, J=8.81Hz, 2H), 8.34(d, J=8.72Hz, 2H). MASS (ES+) : 692.3 (M+Na) ⁺ |
| IA.172 | 1.03(d, J=7.16Hz, 3H), 1.13(s, 3H), 1.33-1.38(m, 1H), 1.52(s, 3H), 1.66-1.96(m, 4H), 2.18-2.38(m, 4H), 3.36-3.43(m, 1H), 3.41(s, 3H), 4.05(s, 2H), 4.35(d, 1H, J=16.67Hz), 4.40(d, J=9.01Hz, 1H), 4.49(d, J=16.66Hz, 1H), 5.30-5.47(m, 1H), 6.37(dd, J ₁ =10.12Hz, J ₂ =1.73Hz, 1H), 6.43(s, 1H), 7.11(dd, J ₁ =10.11Hz, J ₂ =1.01Hz, 1H), 7.77(d, J=8.33Hz, 2H), 8.11(d, J=8.18Hz, 2H). MASS (ES+) : 693.3 (M + Na) ⁺ |
| IA.173 | 1.01(d, J=7.14Hz, 3H), 1.07(s, 3H), 1.31-1.35(m, 1H), 1.52(s, 3H), 1.75-1.95(m, 4H), 2.19-2.35(m, 4H), 2.25(s, 6H), 2.28(s, 3H), 3.41(s, 3H), 3.41-3.49(m, 1H), 4.05(s, 3H), 4.07(d, J=13.34Hz, 1H), 4.27(d, J=17.85Hz, 1H), 4.37(d, J=8.64Hz, 1H), 5.30-5.46(m, 1H), 6.37(dd, J ₁ =10.13Hz, J ₂ =1.65Hz, 1H), 6.43(s, 1H), 6.86(s, 2H), 7.12(d, J ₁ =10.09Hz, 1H). MASS (ES+) : 667.2(M+Na) ⁺ |
| IA.174 | 0.99(d, J=7.00Hz, 3H), 1.10-1.14(m, 6H), 1.22-1.97(m, 8H), 2.20-2.45(m, 6H), 3.35-3.39(m, 1H), 4.27(d, J=16.36Hz, 1H), 4.40-4.45(m, 2H), 5.30-5.47(m, 1H), 6.37(dd, J ₁ =10.14Hz, J ₂ =1.74Hz, 1H), 6.43(s, 1H), 7.13(dd, J ₁ =10.15Hz, J ₂ =0.90Hz, 1H), 7.24-7.28(m, 1H), 7.91-7.95(m, 1H), 8.08-8.10(m, 1H). MASS (ES+) : 639.4 |
| IA.175 | 0.91(s, 3H), 1.25-1.27(m, 1H), 1.44(d, J=7.23Hz, 3H), 1.55(s, 3H), 1.74-2.17(m, 4H), 2.23(s, 6H), 2.28(s, 3H), 2.31-2.58(m, 4H), 3.69(d, J=17.64Hz, 1H), 4.43(d, J=17.63Hz, 1H), 4.46(d, J=11.28Hz, 1H), 5.32-5.48(m, 1H), 6.40(dd, J ₁ =10.11Hz, J ₂ =1.68Hz, 1H), 6.44(s, 1H), 6.52(dd, J ₁ =3.63Hz, J ₂ =1.51Hz, 1H), 6.85(s, 2H), 7.16(dd, J ₁ =10.15Hz, J ₂ =0.99Hz, 1H), 7.19(d, J=3.31Hz, 1H), 7.61(d, J=0.79Hz, 1H). MASS (ES+) : 667.1 |
| IA.176 | 1.01(d, J=7.14Hz, 3H), 1.06(s, 3H), 1.21(d, J=7.00Hz, 3H), 1.32-1.36(m, 1H), 1.52(s, 3H), 1.75-1.94(m, 4H), 2.25(s, 6H), 2.28(s, 3H), 2.29-2.36(m, 4H), 3.35-3.45(m, 1H), 3.54(q, J=7.02Hz, 2H), 4.06(d, J=17.75Hz, 1H), 4.09(s, 2H), 4.26(d, J=17.82Hz, 1H), 4.36(d, J=8.94Hz, 1H), 5.29-5.47(m, 1H), 6.37(dd, J ₁ =10.14Hz, J ₂ =1.78Hz, 1H), 6.43(s, 1H), 6.86(s, 2H), 7.10(dd, J ₁ =10.11Hz, J ₂ =0.82Hz, 1H). MASS (ES+) : 659.1 |
| IA.177 | 1.03(d, J=7.13Hz, 3H), 1.13(s, 3H), 1.21(t, J=7.00Hz, 3H), 1.32-1.37(m, 1H), 1.52(s, 3H), 1.68-1.95(m, 4H), 2.20-2.45(m, 4H), 3.38-3.43(m, 1H), 3.54(qd, J ₁ =6.98Hz, J ₂ =1.49Hz, 2H), 4.09(s, 2H), 4.25(d, J=16.66Hz, 1H), 4.40(d, J=10.48Hz, 1H), 4.49(d, J=16.63Hz, 1H), 5.30-5.46(m, 1H), 6.37(dd, J ₁ =10.15Hz, J ₂ =1.72Hz, 1H), 6.43 (s, 1H), 7.11(dd, J ₁ =10.11Hz, J ₂ =0.73Hz, 1H), 7.77(d, J=8.28Hz, 2H), 8.11(d, J=8.15Hz, 2H). MASS (ES+) : 685.1 |
| IA.178 | 1.07(d, J=7.12Hz, 3H), 1.19(s, 3H), 1.31-1.40(m, 1H), 1.55(s, 3H), 1.77-2.06(m, 4H), 2.21-2.54(m, 4H), 2.37(s, 6H), 3.46-3.50(m, 1H), 4.35(d, J=16.85Hz, 1H), 4.45(d, J=8.6Hz, 1H), 4.56(d, J=16.77Hz, 1H), 5.32-5.49(m, 1H), 6.39(dd, J ₁ =10.15Hz, J ₂ =1.71Hz, 1H), 6.43(s, 1H), 6.50(dd, J ₁ =3.43Hz, J ₂ =1.68Hz, 1H), 7.13(s, 1H), 7.14(s, 1H), 7.16(dd, J ₁ =11.79Hz, J ₂ =0.67Hz, 1H), 7.24(s, 1H), 7.59(s, 1H), 7.61(s, 1H). MASS (ES+) : 653.1 |
| IA.179 | 1.08(d, J=7.11Hz, 3H), 1.16(s, 3H), 1.33-1.41(s, 1H), 1.53(s, 3H), 1.71-2.04(m, 4H), 2.28-2.51(m, 4H), 3.46-3.51(m, 1H), 4.44(d, J=8.45Hz, 1H), 4.53(d, J=16.43Hz, 1H), 4.69(d, J=16.48Hz, 1H), 5.31-5.48(m, 1H), 6.39(dd, J ₁ =10.15Hz, J ₂ =1.84Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.48Hz, J ₂ =1.69Hz, 1H), 7.13(s, 1H), 7.14(dd, J ₁ =8.47Hz, J ₂ =1.99Hz, 1H), 7.56-7.65(m, 3H), 7.87-8.04(m, 4H), 8.58(s, 1H). MASS (ES+) : 675.1 |
| IA.180 | 0.98(s, 3H), 1.06(d, J=7.15Hz, 3H), 1.33-1.39(m, 1H), 1.51(s, 3H), 1.71-1.93(m, 4H), 2.35-2.49(m, 4H), 3.42-3.47(m, 1H), 4.37(d, J=13.12Hz, 1H), 4.39(d, J=4.87Hz, 1H), 4.59(d, J=16.48Hz, 1H), 5.30-5.47(m, 1H), 6.37(dd, J ₁ =10.12Hz, J ₂ =1.80Hz, 1H), 6.44(s, 1H), 6.50(dd, J ₁ =3.14Hz, J ₂ =1.36Hz, 1H), 7.11(dd, J ₁ =6.33Hz, J ₂ =1.21Hz, 1H), 7.13(s, 1H), 7.52-7.61(m, 4H), 7.89(dd, J ₁ =8.54Hz, J ₂ =1.43Hz, 1H), 8.02(d, J=8.22Hz, 1H), 8.07(dd, J ₁ =7.22Hz, J ₂ =0.94Hz, 1H), 8.49(d, J=8.42Hz, 1H). MASS (ES+) : 674.9 |
| IA.181 | 1.06(d, J=7.10Hz, 3H), 1.16(s, 3H), 1.34-1.42(m, 1H), 1.54(s, 3H), 1.65-2.02(m, 4H), 2.29(s, 3H), 2.24-2.61(m, 4H), 3.44-3.49(m, 1H), 4.37(d, 1H, J=16.53Hz), 4.44(d, J=8.48Hz, 1H), 4.53(d, J=16.5Hz, 1H), 5.31-5.48(m, 1H), 6.34(d, J=1.44Hz, 1H), 6.38(dd, J ₁ =10.12Hz, J ₂ =1.75Hz, 1H), 6.44 (s, 1H), 7.13(dd, J ₁ =10.11Hz, J ₂ =1.05Hz, 1H), 7.44 (d, J=1.43Hz, 1H), 7.76(d, J=8.26Hz, 2H), 8.12(d, J=8.13Hz, 2H). MASS (ES+) : 707.2 |
| IA.182 | 1.05(d, J=7.13Hz, 3H), 1.09(s, 3H), 1.36-1.43(m, 1H), 1.54(s, 3H), 1.75-2.00(m, 4H), 2.26(s, 6H), 2.28(s, 3H), 2.30(s, 3H), 2.41-2.60(m, 4H), 3.47-3.50(m, 1H), 4.09(d, J=17.81Hz, 1H), 4.32(d, J=17.76Hz, 1H), 4.41(d, J=8.28Hz, 1H), 5.32-5.48(m, 1H), 6.34(d, J=1.21Hz, 1H), 6.38(dd, J ₁ =10.16Hz, J ₂ =1.66Hz, 1H), 6.44(s, 1H), 6.85(s, 2H), 7.14(d, J=10.11Hz), 7.43(d, J=1.18Hz, 1H). MASS (ES+) : 681.1 |
| IA.183 | 1.07(d, J=7.10Hz, 3H), 1.12(s, 3H), 1.32-1.42(m, 1H), 1.54(s, 3H), 1.73-2.00(m, 4H), 2.27-2.53(m, 4H), 3.40-3.44(m, 1H), 4.05(s, 3H), 4.39(s, 2H), 4.46(d, J=8.45Hz, 1H), 5.32-5.48(m, 1H), 6.40(dd, J ₁ =10.12Hz, J ₂ =1.68Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.44Hz, J ₂ =1.68Hz, 1H), 7.13(s, 1H), 7.15(dd, J ₁ =11.15Hz, J ₂ =0.94Hz, 1H), 7.19(d, J=8.88Hz, 1H), 7.59(d, J=0.69Hz, 1H), 8.22(dd, J ₁ =8.81Hz, J ₂ =2.16Hz, 1H), 8.49(d, J=2.15Hz, 1H). MASS (ES+) : 700.1 |
| IA.184 | 1.07(d, J=7.16Hz, 3H), 1.18(s, 3H), 1.32-1.40(m, 1H), 1.55(s, 3H), 1.73-2.08(m, 4H), 2.25-2.43(m, 4H), 2.32(s, 3H), 2.32 (s, 3H), 3.46-3.51(m, 1H), 4.34(d, J=16.73Hz, 1H), 4.45(d, J=8.08Hz, 1H), 4.57(d, J=16.76Hz, 1H), 5.32-5.49(m, 1H), 6.39(dd, J ₁ =10.14Hz, J ₂ =1.82Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.53Hz, J ₂ =1.74Hz, 1H), 7.13(dd, J ₁ =3.63Hz, J ₂ =0.62Hz, 1H), 7.16(dd, J ₁ =10.14Hz, J ₂ =1.18Hz, 1H), 7.24(d, J=7.87Hz, 1H), 7.59(m, 1H), 7.74(dd, J ₁ =8.69Hz, J ₂ =1.66Hz, 1H), 7.77(s, 1H). MASS (ES+) : 653.5 (M+H) ⁺ |
| IA.185 | 1.05(d, J=7.17Hz, 3H), 1.16(s, 3H), 1.14-1.40(m, 1H), 1.54(s, 3H), 1.72-2.03(m, 4H), 2.29-2.48(m, 4H), 3.42-3.47(m, 1H), 4.35(d, 1H, J=16.60Hz), 4.46(d, J=8.55Hz, 1H), 4.53(d, J=16.65Hz, 1H), 5.32-5.49(m, 1H), 6.39(dd, J ₁ =10.14Hz, J ₂ =1.84Hz, 1H), 6.45 (s, 1H), 6.65(d, J=1.52Hz, 1H), 7.13 (dd, J ₁ =10.12Hz, J ₂ =1.21Hz, 1H), 7.42(t, J=1.70Hz, 1H), 7.76(d, J=8.27Hz, 2H), 7.97(d, J=0.75Hz, 1H), 8.12(d, J=8.08Hz, 2H). MASS (ES+) : 693.2 (M+H) ⁺ |

| Comp. No | ¹ H-NMR (δ ppm), MASS (EI / ES+, m/z) - |
|----------|--|
| IA.186 | 1.04(d, J=7.12Hz, 3H), 1.10(s, 3H), 1.33-1.38(m, 1H), 1.54(s, 3H), 1.75-2.04(m, 4H), 2.25(s, 6H), 2.28(s, 3H), 2.17-2.46(m, 4H), 3.46-3.49(m, 1H), 4.09(d, J=17.58Hz, 1H), 4.30(d, J=17.79Hz, 1H), 4.42(d, J=7.85Hz, 1H), 5.32-5.48(m, 1H), 6.40(dd, J ₁ =10.12Hz, J ₂ =1.70Hz, 1H), 6.45(s, 1H), 6.65(d, J=1.50Hz, 1H), 6.85(s, 2H), 7.13(dd, J ₁ =10.09Hz, J ₂ =0.79Hz, 1H), 7.42(t, J=1.40Hz, 1H), 7.97(s, 1H). MASS (ES+): 667.1(M+H) ⁺ |
| IA.187 | 0.44(s, 3H), 0.95(d, J=7.02Hz, 3H), 1.08(t, J=7.53Hz, 3H), 1.22-1.75(m, 15H), 2.17-2.32(m, 6H), 3.15(m, 1H), 4.29(d, J=6.81Hz, 1H), 5.40(m, 1H), 6.35(dd, J ₁ =10.11Hz, J ₂ =1.43Hz, 1H), 6.40(s, 1H), 7.05(d, J=9.98Hz, 1H), 7.36(t, J=7.70Hz, 2H), 7.46(t, J=7.20Hz, 1H), 7.95(d, J=7.43Hz, 2H). MASS (ES+): 705.4(M+Na) ⁺ |
| IA.188 | 0.60(s, 3H), 0.93(d, J=7.04Hz, 3H), 1.06(t, J=7.54Hz, 3H), 1.10-1.89(m, 14H), 2.09-2.36(m, 6H), 3.14-3.17(m, 1H), 4.30(d, J=7.66Hz, 1H), 5.26-5.43(m, 1H), 6.34(dd, J ₁ =10.14Hz, J ₂ =1.67Hz, 1H), 6.41(s, 1H), 7.06(m, 3H), 8.02-8.05(m, 2H). MASS (ES+): 655.5(M+Na) ⁺ |
| IA.199 | 0.42(s, 3H), 0.93(d, J=7.14Hz, 3H), 1.08(t, J=7.57Hz, 3H), 1.20-1.25(m, 1H), 1.49(s, 3H), 1.51-1.79(m, 4H), 1.75(s, 6H), 1.80-2.37(m, 7H), 3.31(m, 1H), 4.28(d, J=8.59Hz, 1H), 6.10(s, 1H), 6.31(d, J ₁ =10.12Hz, J ₂ =1.80Hz, 1H), 7.13(d, J=10.14Hz, 1H), 7.38(t, J=7.53Hz, 2H), 7.45-7.47(m, 1H), 7.95-7.97(m, 1H). MASS (ES+): 619.6(M+Na) ⁺ |
| IA.190 | 0.44(s, 3H), 0.82-1.15(m, 2H), 0.92(d, J=6.92Hz, 3H), 1.21-1.42(m, 8H), 1.48(s, 3H), 1.52-1.84(m, 6H), 1.71(s, 6H), 2.10-2.29(m, 5H), 3.14-3.17(m, 1H), 4.40(d, J=7.44Hz, 1H), 5.24-5.44(m, 1H), 6.35(d, J=9.7Hz, 1H), 6.41(s, 1H), 7.07(d, J=10.11Hz, 1H), 7.37(t, J=7.54Hz, 2H), 7.46(t, J=7.28Hz, 1H), 7.95(d, J=7.61Hz, 2H). MASS (ES+): 691.6(M+Na) ⁺ |
| IA.191 | 0.44(s, 3H), 0.93(d, J=7.07Hz, 3H), 1.23-1.25(m, 1H), 1.47(s, 3H), 1.52-1.83(m, 12H), 1.74(s, 6H), 2.19-2.25(m, 4H), 2.67-2.71(m, 1H), 3.13-3.17(m, 1H), 4.30(d, J=7.27Hz, 1H), 5.25-5.42(m, 1H), 6.34(d, J ₁ =10.19Hz, J ₂ =1.75Hz, 1H), 6.41(s, 1H), 7.06(d, J=10.22Hz, 1H), 7.37(t, J=7.57Hz, 2H), 7.46(t, J=7.34Hz), 7.95(d, 2H, J=7.22Hz). MASS (ES+): 655.2 |
| IA.192 | 0.45(s, 3H), 0.93(d, J=7.14Hz, 3H), 1.11(d, J=6.96Hz, 3H), 1.21-1.26(m, 1H), 1.48(s, 3H), 1.55-1.75(m, 4H), 1.75(d, J=1.51Hz, 6H), 2.10-2.27(m, 4H), 2.47-2.52(m, 1H), 3.13-3.18(m, 1H), 4.30(d, J=7.45Hz, 1H), 5.25-5.42(m, 1H), 6.34(d, J ₁ =10.13Hz, J ₂ =1.77Hz, 1H), 6.41(s, 1H), 7.06(dd, J ₁ =10.13Hz, J ₂ =1.06Hz, 1H), 7.37(t, J=7.59Hz, 2H), 7.47(t, J=7.59Hz, 2H), 7.47(t, J=7.35Hz, 1H), 7.95(d, J=7.28Hz, 2H). MASS (ES+): 629.2 |
| IA.193 | 0.45(s, 3H), 0.94(d, J=7.06Hz, 3H), 1.16-1.26(m, 2H), 1.47(s, 3H), 1.55-1.96(m, 5H), 1.7(Two s, 6H), 2.09-2.29(m, 8H), 3.06-3.17(m, 2H), 4.28(d, J=7.88Hz, 1H), 5.25-5.43(m, 1H), 6.33(dd, J ₁ =10.13Hz, J ₂ =1.66Hz, 1H), 6.40(s, 1H), 7.05(d, J=10.13Hz, 1H), 7.38(t, J=7.58Hz, 2H), 7.47(t, J=7.83Hz, 1H), 7.96(d, J=8.66Hz, 2H). MASS (ES+): 641.5 |
| IA.194 | 0.5(s, 3H), 1.0(d, J=6.97Hz, 3H), 1.22-1.28(m, 1H), 1.51(s, 3H), 1.41-1.74(m, 5H), 1.77(s, 3H), 1.78(s, 3H), 2.15-2.60(m, 5H), 3.19-3.33(m, 1H), 4.33(d, J=8.07Hz, 1H), 6.12(s, 1H), 6.35(d, J=10.10Hz, 1H), 6.46(d, J=3.25Hz, 1H), 7.04(d, J=3.27Hz, 1H), 7.16(d, J=1.10Hz, 1H), 7.38(t, J=7.57Hz, 2H), 7.47(t, J=7.30Hz, 1H), 7.56(s, 1H), 7.95(d, J=7.71Hz, 2H). MASS (ES+): 635.4 |
| IA.195 | 0.44(s, 3H), 0.88-0.91(m, 2H), 0.94(d, J=7.11Hz, 3H), 1.09-1.36(m, 5H), 1.47(s, 3H), 1.52-1.73(m, 8H), 1.74(s, 6H), 2.12-2.22(m, 6H), 3.13-3.16(m, 1H), 5.29(d, J=8.09Hz, 1H), 5.25-5.42(m, 1H), 6.35(dd, J ₁ =10.12Hz, J ₂ =1.79Hz, 1H), 6.40(s, 3H), 7.06(dd, J ₁ =10.14Hz, J ₂ =1.36Hz, 1H), 7.37(t, J=7.54Hz, 2H), 7.44-7.47(m, 1H), 7.95(dd, J ₁ =8.31Hz, J ₂ =1.23Hz, 2H). MASS (ES+): 683.4 |
| IA.196 | 0.66(s, 3H), 1.02(d, J=7.03Hz, 3H), 1.10-1.43(m, 2H), 1.50(s, 3H), 1.54-1.82(m, 9H), 2.22-2.41(m, 4H), 3.22-3.25(m, 1H), 4.34(d, J=6.85Hz, 1H), 5.28-5.45(m, 1H), 6.38(dd, J ₁ =10.17Hz, J ₂ =1.68Hz, 1H), 6.43(s, 1H), 6.47(dd, J ₁ =3.39Hz, J ₂ =1.86Hz, 1H), 7.03-7.09(m, 4H), 7.56(s, 1H), 8.01-8.01(m, 2H). MASS (ES+): 671.3 |
| IA.197 | 0.58(s, 3H), 1.02(d, J=7.09Hz, 3H), 1.08-1.37(m, 3H), 1.50(s, 3H), 1.61-1.80(m, 8H), 2.22-2.38(m, 4H), 3.20-3.25(m, 1H), 4.34-4.36(m, 1H), 5.28-5.48(m, 1H), 6.39(dd, J ₁ =10.12Hz, J ₂ =1.77Hz, 1H), 6.43(s, 1H), 6.48(dd, J ₁ =3.47Hz, J ₂ =1.71Hz, 1H), 7.05(d, J=3.34Hz, 1H), 7.09(dd, J ₁ =10.12Hz, J ₂ =1.07Hz, 1H), 7.57(t, J=0.85Hz, 1H), 7.65(d, J=8.33Hz, 2H), 8.01(d, J=8.21Hz, 2H). MASS (ES+): 721.2 |
| IA.198 | 1.05(d, J=7.15Hz, 3H), 1.17(s, 3H), 1.34-1.39(m, 1H), 1.55(s, 3H), 1.74-1.92(m, 4H), 2.09-2.50(m, 4H), 2.32(s, 3H), 2.33(s, 3H), 3.45-3.49(m, 1H), 4.32(d, J=16.76Hz, 1H), 4.46(d, J=8.58Hz, 1H), 4.59(d, J=16.79Hz, 1H), 5.32-5.49(m, 1H), 6.40(dd, J ₁ =10.12Hz, J ₂ =1.65Hz, 1H), 6.46(s, 1H), 6.93(d, J=4.02Hz, 1H), 7.17(d, J=10.13Hz, 1H), 7.24(d, J=7.93Hz, 1H), 7.53(dd, J=3.95Hz, 1H), 7.75(d, J=7.93Hz, 1H), 7.78(s, 1H). MASS (ES+): 703.7 |
| IA-1.1 | 0.33(s, 3H), 0.92(d, J=7.14Hz, 3H), 1.07(t, J=7.55Hz, 3H), 1.17-1.88(m, 12H), 2.08-2.30(m, 8H), 2.66-2.63(m, 2H), 3.10-3.13(m, 1H), 4.28-4.30(m, 1H), 5.25-5.41(m, 1H), 6.36(dd, J ₁ =10.13Hz, J ₂ =1.77Hz, 1H), 6.40(s, 1H), 7.03-7.07(m, 3H), 7.94-7.97(m, 2H). MASS (ES+): 660.5 |
| IA-1.2 | 0.15(s, 3H), 0.91(d, J=7.10Hz, 3H), 1.08(t, J=7.68Hz, 3H), 1.17-1.88(m, 12H), 2.04-2.31(m, 8H), 2.63-2.67(m, 2H), 3.05-3.15(m, 1H), 4.26(d, J=7.89Hz, 1H), 5.23-5.39(m, 1H), 6.35(dd, J ₁ =10.11Hz, J ₂ =1.47Hz, 1H), 6.39(s, 1H), 7.05(d, J=10.11Hz, 2H), 7.36-7.39(m, 2H), 7.45-7.49(m, 2H), 7.90(d, J=7.49Hz, 2H). MASS (ES+): 663.0(M+Na) ⁺ |
| IB.1 | 0.94(d, J=7.16Hz, 3H), 1.10(s, 3H), 1.12(t, J=7.53Hz, 3H), 1.23-1.35(m, 1H), 1.53(s, 3H), 1.69-1.85(m, 3H), 2.17-2.49(m, 7H), 3.29-3.36(m, 1H), 4.30-4.40(m, 3H), 4.55(d, J=15.48, 1H), 5.04(d, J=15.46, 1H), 5.27-5.52(m, 1H), 6.37(d, J ₁ =10.11Hz, J ₂ =1.69Hz, 1H), 6.43(s, 1H), 7.13(d, J=10.10Hz, 1H). MASS (ES+): 543.5(M+Na) ⁺ |
| IB.2 | 0.97(d, J=6.99Hz, 3H), 1.11(s, 3H), 1.12(t, J=7.33Hz, 3H), 1.29-1.33(m, 1H), 1.53(s, 3H), 1.70-1.98(m, 3H), 2.17-2.54(m, 7H), 3.33-3.34(m, 1H), 3.67(d, J=14.69, 1H), 3.74(d, J=16.44, 1H), 4.19(s, 2H), 4.32(d, J=7.28, 1H), 4.59(s, 1H), 5.31-5.48(m, 1H), 6.33(d, J=10.16Hz, 1H), 6.37(s, 1H), 7.22(d, J=10.02Hz, 1H). MASS (ES+): 559.5(M+Na) ⁺ |
| IB.3 | 0.99(d, J=7.10Hz, 3H), 1.10(s, 3H), 1.12(t, J=7.59Hz, 3H), 1.31-1.36(m, 1H), 1.52(s, 3H), 1.70-1.91(m, 4H), 2.19-2.45(m, 6H), 3.33-3.37(m, 1H), 3.72-3.78(m, 2H), 4.41(d, J=6.54, 1H), 4.94(d, J=47.47Hz, 2H), 5.30-5.47(m, 1H), 6.38(d, J=10.13Hz, 1H), 6.43(s, 1H), 7.12(d, J=10.13Hz, 1H). MASS (ES+): 561.2(M+Na) ⁺ |
| IB.4 | 1.02(d, J=7.08Hz, 3H), 1.13(s, 3H), 1.32-1.37(m, 1H), 1.55(s, 3H), 1.66-2.02(m, 4H), 2.07-2.32(m, 4H), 3.38-3.41(m, 1H), 3.70(d, J=16.32, 1H), 3.78(d, J=16.35Hz, 1H), 1.12-4.15(m, 2H), 4.33(d, J=6.37, 1H), 4.88(t, J=5.92, 1H), 5.14(m, 1H), 5.36-5.53(m, 1H), 6.29-6.32(m, 2H), 6.54(dd, J ₁ =3.47Hz, J ₂ =1.72Hz, 1H), 7.11(d, J=3.46, 1H), 7.25(d, J=10.45Hz, 1H), 7.66(m, 1H). MASS (ES+): 597.5(M+Na) ⁺ |
| IB.5 | 0.98(d, J=7.03Hz, 3H), 1.11(s, 3H), 1.12(t, J=7.72Hz, 3H), 1.27-1.33(m, 1H), 1.54(s, 3H), 1.78-1.88(m, 5H), 2.04-2.31(m, 2H), 2.33-2.63(m, 6H), 3.31-3.34(m, 1H), 3.66(d, J=16.48, 1H), 3.74(d, J=16.56, 1H), 4.24(s, 2H), 4.40(d, J=8.44, 1H), 6.13(s, 1H), 6.35(d, J=10.06Hz, 1H), 7.20(d, J=10.07Hz, 1H). MASS (ES+): 541.6(M+Na) ⁺ |

SUBSTITUTE SHEET (RULE 26)

| Comp. No | ¹ H-NMR (δ ppm), MASS (EI / ES+, m/z) |
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| IB.6 | 1.07(d, J=7.08Hz, 3H), 1.15(s, 3H), 1.32-1.41(m, 1H), 1.54(s, 3H), 1.58-1.95(m, 5H), 2.29-2.53(m, 3H), 3.41-3.45(m, 1H), 3.75(dd, J ₁ =15.74Hz, J ₂ =5.95Hz, 1H), 3.83(dd, J ₁ =16.61Hz, J ₂ =6.93Hz, 1H), 4.46(d, J=8.11Hz, 1H), 4.94(d, J=47.47Hz, 2H), 5.32-5.49(m, 1H), 6.40(dd, J ₁ =10.11Hz, J ₂ =1.43Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.14Hz, J ₂ =1.5Hz, 1H), 7.12(s, 1H), 7.14(d, J=10.36Hz, 1H), 7.59(s, 1H). MASS (ES+): 599.5 (M+Na) ⁺ . |
| IB.7 | 0.95(d, J=7.14Hz, 3H), 1.10(s, 3H), 1.14(d, J=4.89Hz, 3H), 1.16(d, J=4.92Hz, 3H), 1.23-1.33(m, 1H), 1.53(s, 3H), 1.68-2.00(m, 3H), 2.16-2.29(m, 2H), 2.54-2.62(m, 2H), 3.32-3.36(m, 1H), 3.64-3.78(m, 2H), 4.15-4.17(m, 2H), 4.30-4.33(m, 1H), 4.72(t, J=5.89, 1H), 4.99(t, J=2.77, 1H), 5.34-5.50(m, 1H), 6.31(d, J ₁ =12.18Hz, J ₂ =1.97Hz, 1H), 6.32(s, 1H), 7.24(d, J=10.03Hz, 1H). MASS (ES+): 551.2 |
| IB.8 | 0.99(d, J=7.31Hz, 3H), 1.11(s, 3H), 1.27-1.35(m, 1H), 1.52(s, 3H), 1.72-1.99(m, 7H), 2.04-2.37(m, 8H), 3.14-3.18(m, 1H), 3.33-3.36(m, 1H), 3.65-3.77(m, 2H), 4.24 (d, J=2.11, 2H), 4.39 (d, J=8.66, 1H), 5.28-5.48(m, 1H), 6.37 (dd, J ₁ =10.12Hz, J ₂ =1.60Hz, 1H), 6.43 (s, 1H), 7.12 (d, J=10.18Hz, 1H). MASS (ES+): 564.3 |
| IB.9 | 1.02(d, J=7.10Hz, 3H), 1.16(s, 3H), 1.13-1.36(m, 1H), 1.57(s, 3H), 1.60-2.00(m, 4H), 2.24-2.66(m, 6H), 3.38-3.42(m, 1H), 3.70(d, J=16.38, 1H), 3.78(d, J=16.39, 1H), 4.15-4.17(m, 2H), 4.34-4.37(m, 1H), 4.73(t, J=5.85, 1H), 4.78(s, 1H), 6.09(s, 1H), 6.29(dd, J ₁ =10.10Hz, J ₂ =1.45Hz, 1H), 6.52(dd, J ₁ =3.33Hz, J ₂ =1.60Hz, 1H), 7.11(d, J=3.43Hz, 1H), 7.32(d, J=10.12Hz, 1H), 7.63(s, 1H). MASS (ES+): 557.3 |
| IB.10 | 1.03(d, J=6.98Hz, 3H), 1.13(s, 3H), 1.33-1.37(m, 1H), 1.55(s, 3H), 1.62-1.98(m, 3H), 2.24-2.54(m, 4H), 3.3-(m, 1H), 3.71(d, J=16.40, 1H), 3.79(d, J=16.39Hz, 1H), 4.08(d, J=7.17Hz, 1H), 4.12(d, J=5.83Hz, 2H), 4.99(t, J=5.92, 1H), 5.27(s, 1H), 5.40-5.56(m, 1H), 6.28(s, 1H), 6.29(d, J=13.05Hz, 1H), 7.14(t, J=4.33Hz, 1H), 7.27(d, J=10.03, 1H), 7.71(m, 2H). MASS (ES+): 591.4 |
| IB.11 | 0.99(d, J=7.15Hz, 3H), 1.09(s, 3H), 1.12(t, J=7.66Hz, 3H), 1.30-1.36(m, 1H), 1.52(s, 3H), 1.64-1.90(m, 4H), 2.18-2.44(m, 7H), 3.34-3.38(m, 1H), 3.65(dd, J ₁ =16.57Hz, J ₂ =2.60Hz, 1H), 3.71(dd, J ₁ =16.58Hz, J ₂ =2.58Hz, 1H), 4.41(d, J=7.42, 1H), 5.30-5.47(m, 1H), 6.37(dd, J ₁ =10.14Hz, J ₂ =1.54Hz, 1H), 6.43(s, 1H), 7.12(d, J=10.05Hz, 1H). MASS (ES+): 507.3 |
| IB.12 | 1.06(d, J=7.11Hz, 3H), 1.18(s, 3H), 1.35-1.61(m, 1H), 1.55(s, 3H), 1.80-1.97(m, 3H), 2.39-2.60(m, 5H), 3.43-3.46(m, 1H), 3.70-3.82(m, 3H), 4.06-4.33(m, 4H), 4.45(d, J=7.47Hz, 1H), 4.69-4.71(m, 2H), 5.32-5.49(m, 1H), 6.39(d, J=10.13Hz, 1H), 6.45(s, 1H), 6.50(d, J ₁ =3.26Hz, J ₂ =1.48Hz, 1H), 7.13(d, J=3.42Hz, 1H), 7.16(d, J=10.32Hz, 1H), 7.59(s, 1H). MASS (ES+): 773.2 |
| IB.13 | 0.70(d, J=7.16Hz, 3H), 1.07(s, 3H), 1.11(t, J=7.53Hz, 3H), 1.25-1.35(m, 1H), 1.53(s, 3H), 1.70-2.03(m, 3H), 2.18-2.60(m, 7H), 3.34-3.37(m, 1H), 3.56-3.60(m, 2H), 4.04(d, J=3.79Hz, 2H), 4.28(d, J=9.37Hz, 1H), 4.93(s, 1H), 5.32-5.51(m, 1H), 5.63-5.81(m, 1H), 5.80-5.88(m, 1H), 6.30(dd, J ₁ =10.12Hz, J ₂ =1.88Hz, 1H), 6.33(s, 1H), 7.24(d, J=9.87Hz, 1H). MASS (ES+): 539.2 |
| IB.14 | 1.04(d, J=7.10Hz, 3H), 1.12(s, 3H), 1.12-1.37(m, 1H), 1.55(s, 3H), 1.70-1.95(m, 4H), 2.29-2.59(m, 4H), 3.40-3.44(m, 1H), 3.55-3.68(m, 2H), 4.02(d, J=4.19Hz, 1H), 4.23(br-s, 1H), 4.33(br-d, J=10.86Hz, 1H), 5.07-5.09(m, 1H), 5.36-5.53(m, 1H), 5.65-5.71(m, 1H), 5.81-5.87(m, 1H), 6.31(dd, J ₁ =10.68Hz, J ₂ =1.76Hz, 1H), 6.33(s, 1H), 6.53(dd, J ₁ =3.46Hz, J ₂ =1.75Hz, 1H), 7.10(d, J=3.47Hz, 1H), 7.26(d, J=10.00Hz, 1H), 7.64(d, J=1.37Hz, 1H). MASS (ES+): 599.3(M+Na) ⁺ |
| IB.15 | 1.02(d, J=7.10Hz, 3H), 1.10(s, 3H), 1.31-1.38(m, 1H), 1.54(s, 3H), 1.65-1.96(m, 3H), 2.26-2.53(m, 4H), 3.38-3.41(m, 1H), 3.64(d, J=7.8Hz, 2H), 4.16(d, J=5.94Hz, 2H), 4.29(b, d, 1H), 4.48(bs, 1H), 5.27(m, 1H), 5.40-5.57(m, 2H), 5.62-5.69(m, 1H), 6.26(s, 1H), 6.28(dd, J ₁ =10.12Hz, J ₂ =1.79Hz, 1H), 6.56(dd, J ₁ =3.47Hz, J ₂ =1.72Hz, 1H), 7.10(d, J=3.48Hz, 1H), 7.26(d, J=10.10Hz, 1H), 7.72(d, J=1.51Hz, 1H). MASS (ES+): 599.3(M+Na) ⁺ |
| IB.16 | 1.03(d, J=7.09Hz, 3H), 1.11(s, 3H), 1.31-1.37(m, 1H), 1.55(s, 3H), 1.65-2.01(m, 4H), 2.28-2.58(m, 4H), 3.36-3.41(m, 1H), 3.64(d, J=7.76Hz, 2H), 4.16(m, 2H), 3.31(d, J=6.77Hz, 1H), 4.49(t, J=5.37Hz, 1H), 5.28(m, 1H), 5.41-5.57(m, 2H), 5.64-5.69(m, 1H), 6.26(s, 1H), 6.29(dd, J ₁ =10.11Hz, J ₂ =1.82Hz, 1H), 7.14(t, J=4.36Hz, 1H), 7.27(dd, J ₁ =10.11Hz, J ₂ =0.74Hz, 1H), 7.70-7.71(m, 2H). MASS (ES+): 615.0(M+Na) ⁺ |
| IB.17 | 1.04(d, J=7.11Hz, 3H), 1.12(s, 3H), 1.32-1.38(m, 1H), 1.55(s, 3H), 1.60-1.99(m, 4H), 2.29-2.59(m, 4H), 3.39-3.43(m, 1H), 3.56-3.67(m, 2H), 4.00(d, J=5.11Hz, 1H), 4.22(dd, J ₁ =4.85Hz, J ₂ =0.81Hz, 1H), 4.32(d, J=6.73Hz, 1H), 4.43(t, J=5.49Hz, 1H), 5.21-5.22(m, 1H), 5.39-5.56(m, 1H), 5.63-5.70(m, 1H), 5.83(d, J ₁ =15.27Hz, J ₂ =5.03Hz, 1H), 6.29(s, 1H), 6.30(dd, J ₁ =10.58Hz, J ₂ =1.77Hz, 1H), 7.13(dd, J ₁ =4.87Hz, J ₂ =3.87Hz, 1H), 7.27(d, J=9.68Hz, 1H), 7.67(dd, J ₁ =4.97Hz, J ₂ =0.99Hz, 1H), 7.70(dd, J ₁ =3.70Hz, J ₂ =1.05Hz, 1H). MASS (ES+): 592.7 |
| IB.18 | 1.06(d, J=7.11Hz, 3H), 1.18(s, 3H), 1.35-1.41(m, 1H), 1.55(s, 3H), 1.67-1.97(m, 1H), 2.28-2.56(m, 5H), 3.44(m, 1H), 3.66-3.81(m, 3H), 3.99-4.31(m, 4H), 4.45(d, J=7.88Hz, 1H), 4.65-4.75(m, 2H), 5.32-5.49(m, 1H), 6.39(dd, J ₁ =10.15Hz, J ₂ =1.29Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.34Hz, J ₂ =1.69Hz, 1H), 7.13(d, J=3.45Hz, 1H), 7.16(d, J=10.13Hz, 1H), 7.59(d, J=0.66Hz, 1H). MASS (ES+): 759.1 |
| IB.19 | 1.06(d, J=7.05Hz, 3H), 1.18(s, 3H), 1.36-1.41(m, 1H), 1.54(s, 3H), 1.74-1.97(m, 7H), 2.29-2.50(m, 5H), 3.42-3.45(m, 1H), 3.72-3.74(m, 2H), 4.20(t, J=5.74Hz, 2H), 4.44-4.47(m, 1H), 4.48(t, J=5.90Hz, 2H), 4.65-4.74(m, 2H), 5.33-5.50(m, 1H), 6.40(dd, J ₁ =10.14Hz, J ₂ =1.52Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.22Hz, J ₂ =1.48Hz, 1H), 7.13-7.16(m, 2H), 7.59(s, 1H). MASS (ES+): 736.1 |
| IB.20 | 1.03(d, J=7.10Hz, 3H), 1.15(s, 3H), 1.33-1.39(m, 1H), 1.55(s, 3H), 1.60-2.00(m, 4H), 2.25-2.60(m, 4H), 3.30-3.42(m, 1H), 3.71(d, J=16.35Hz, 1H), 3.78(d, J ₁ =16.38Hz, J ₂ =1.86Hz, 1H), 4.15-4.17(m, 2H), 4.36(d, J=9.1Hz, 1H), 4.71(t, J=5.90, 1H), 5.03(d, J=2.42Hz, 1H), 5.16-5.52(m, 1H), 6.34(dd, J ₁ =10.97Hz, J ₂ =1.70Hz, 1H), 6.36(s, 1H), 6.97(d, J=13.05Hz, 1H), 7.26(d, J=10.17Hz, 1H), 7.52(s, 1H). MASS (ES+): 647.0(M+Na) ⁺ |
| IB.21 | 1.06(d, J=7.13Hz, 3H), 1.14(s, 3H), 1.35-1.40(m, 1H), 1.54(s, 3H), 1.79(t, J=2.34Hz, 3H), 1.73-1.96(m, 4H), 2.28-2.54(m, 4H), 3.41-3.46(m, 1H), 3.66(dd, J ₁ =16.08Hz, J ₂ =2.46Hz, 1H), 3.73(dd, J ₁ =16.12Hz, J ₂ =2.45Hz, 1H), 4.45(d, J=8.43Hz, 1H), 5.32-5.48(m, 1H), 6.40(d, J=10.71Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.21Hz, J ₂ =1.11Hz, 1H), 7.11(d, J=3.39, 1H), 7.13(d, J=9.96Hz, 1H), 7.58(m, 1H). MASS (ES+): 559.5 |
| IB.22 | 1.06(d, J=7.10Hz, 3H), 1.17(s, 3H), 1.36-1.43(m, 1H), 1.53(s, 3H), 1.56-1.96(m, 4H), 2.30(s, 3H), 2.38-2.58(m, 4H), 3.41-3.45(m, 1H), 3.70(d, J=16.56, 1H), 3.79(d, J=16.56Hz, 1H), 4.22(d, J=14.06, 1H), 4.27(d, J=15.99Hz, 1H), 4.42(d, J=8.53, 1H), 5.31-5.48(m, 1H), 6.34(d, J=0.96, 1H), 6.38(dd, J ₁ =10.16Hz, J ₂ =1.43Hz, 1H), 6.44(s, 1H), 7.14(d, J=10.21Hz, 1H), 7.44(s, 1H). MASS (ES+): MASS (ES+): 589.3 |
| IB.23 | 1.03(d, J=7.10Hz, 3H), 1.12(s, 3H), 1.21(t, J=6.99Hz, 3H), 1.32-1.37(m, 1H), 1.52(s, 3H), 1.66-1.92(m, 4H), 2.17-2.45(m, 5H), 3.35-3.38(m, 1H), 3.54(q, J=6.98Hz, 2H), 3.69(d, J=14.78Hz, 1H), 3.73(d, J=14.72Hz, 1H), 4.09(s, 2H), 4.19-4.28 (m, 2H), 4.39 (d, J=8.39Hz, 1H), 5.30-5.46(m, 1H), 6.37(dd, J ₁ =10.13Hz, J ₂ =1.65Hz, 1H), 6.43(s, 1H), 7.13 (dd, J ₁ =10.07Hz, J ₂ =0.65Hz, 1H). MASS (ES+): 567.1 |

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| Comp. No | ¹ H-NMR (δ ppm), MASS (EI / ES+, m/z) |
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| IB.24 | 1.03(d, J=7.11Hz, 3H), 1.12(s, 3H), 1.32-1.38(m, 1H), 1.52(s, 3H), 1.68-1.93(m, 5H), 2.16-2.32(m, 4H), 3.35-3.39(m, 1H), 3.41(s, 3H), 3.71-3.73(m, 2H), 4.05(s, 2H), 4.23(t, J=2.22, 1H), 4.25(t, J=2.23, 1H), 4.39(d, J=8.92, 1H), 5.30-5.47(m, 1H), 6.37(dd, J ₁ =10.17Hz, J ₂ =1.78Hz, 1H), 6.43(s, 1H), 7.14(d, J=10.13Hz, 1H). MASS (ES+): 553.2 |
| IB.25 | 1.07(d, J=7.15Hz, 3H), 1.18(s, 3H), 1.28-1.42(m, 1H), 1.46-1.67(m, 10H), 1.54(s, 3H), 1.74-2.02(m, 9H), 2.28-2.50(m, 1H), 3.40-3.46(m, 1H), 3.70(d, J=16.45Hz, 1H), 3.78(d, J=16.43Hz, 1H), 4.44(d, J=8.82Hz, 1H), 5.32-5.49(m, 1H), 6.39(dd, J ₁ =10.13Hz, J ₂ =1.66Hz, 1H), 6.45(s, 1H), 6.49(dd, J ₁ =3.42Hz, J ₂ =1.66Hz, 1H), 7.12(d, J=3.71Hz, 1H), 7.14(d, J=12.28Hz, 1H), 7.59(s, 1H). MASS (ES+): 643.3 |
| IB.26 | 0.89-0.94(m, 2H), 1.0(d, J=7.14Hz, 3H), 1.12(s, 3H), 1.08-1.36(m, 4H), 1.52(s, 3H), 1.61-1.91(m, 10H), 2.16-2.44(m, 7H), 3.31-3.35(m, 1H), 3.65-3.76(m, 2H), 4.19-4.28(m, 2H), 4.40(d, J=8.88, 1H), 5.30-5.47(m, 1H), 6.38(d, J ₁ =10.12Hz, J ₂ =1.78Hz, 1H), 6.43(s, 1H), 7.14(d, J ₁ =10.12Hz, J ₂ =1.31Hz, 1H). MASS (ES+): 605.5 |
| IB.27 | 0.89(t, J=7.32Hz, 3H), 0.99(d, J=7.11Hz, 3H), 1.11(s, 3H), 1.34(q, J=7.53Hz, 2H), 1.52(s, 3H), 1.55-1.59(m, 2H), 1.73-2.04(m, 4H), 2.22-2.37(m, 7H), 3.34(m, 1H), 3.69-3.73(m, 2H), 4.24(d, J=1.36Hz, 2H), 4.40(d, J=8.57, 1H), 5.30-5.48(m, 1H), 6.38(dd, J ₁ =10.13Hz, J ₂ =1.70Hz, 1H), 6.43(s, 1H), 7.13(d, J=10.12Hz, 1H). MASS (ES+): 565.3 |
| IB.28 | 0.94(d, J=7.17Hz, 3H), 1.08(s, 3H), 1.12(t, J=7.58Hz, 3H), 1.27-1.32(m, 1H), 1.53(s, 3H), 1.64-1.83(m, 4H), 2.22-2.48(m, 7H), 3.30-3.34(m, 1H), 4.40(d, J=7.59, 1H), 4.60(d, J ₁ =15.58Hz, J ₂ =1.63Hz, 1H), 4.84(d, J ₁ =15.60Hz, J ₂ =2.18Hz, 1H), 5.30-5.47(m, 1H), 6.37(d, J ₁ =10.17Hz, J ₂ =1.46Hz, 1H), 6.43(s, 1H), 7.12(d, J=10.10Hz, 1H). MASS (ES+): 491.2 |
| IB.29 | 0.99(d, J=7.12Hz, 3H), 1.12(s, 3H), 1.31-1.36(m, 1H), 1.52(s, 3H), 1.54-1.70(m, 5H), 1.73-1.92(m, 6H), 2.18-2.38(m, 6H), 2.72-2.80(m, 1H), 3.32-3.37(m, 1H), 3.64-3.76(m, 2H), 4.24(s, 2H), 4.41(d, J=8.75, 1H), 5.31-5.47(m, 1H), 6.38(d, J ₁ =10.16Hz, J ₂ =1.64Hz, 1H), 6.44(s, 1H), 7.14(d, J=10.17Hz, 1H). MASS (ES+): 577.2 |
| IB.30 | 0.99(d, J=7.17Hz, 3H), 1.06(s, 3H), 1.11(t, J=7.59Hz, 3H), 1.30-1.35(m, 1H), 1.52(s, 3H), 1.72-2.04(m, 4H), 2.17-2.43(m, 7H), 3.31-3.36(m, 1H), 3.57(dd, J ₁ =13.64Hz, J ₂ =7.49Hz, 1H), 3.73(dd, J ₁ =13.86Hz, J ₂ =8.50Hz, 1H), 4.21(dd, J ₁ =12.64Hz, J ₂ =6.89Hz, 1H), 4.33(dd, J ₁ =12.89Hz, J ₂ =8.13Hz, 1H), 4.37(d, J=10.81Hz, 1H), 5.30-5.46(m, 1H), 5.52-5.59(m, 1H), 5.73-5.79(m, 1H), 6.37(dd, J ₁ =10.14Hz, J ₂ =1.74Hz, 1H), 6.43(s, 1H), 7.22(dd, J ₁ =10.10Hz, J ₂ =1.03Hz, 1H). MASS (ES+): 539.3 |
| IB.31 | 0.98(d, J=7.11Hz, 3H), 1.10-1.17(m, 6H), 1.15(s, 3H), 1.30-1.36(m, 1H), 1.54(s, 3H), 1.73-1.90(m, 3H), 2.20-2.44(m, 8H), 3.03(d, J=2.56Hz, 1H), 3.34-3.38(m, 1H), 3.68(dd, 2H), 4.40(d, J=8.47, 1H), 4.55(d, J=15.41Hz, 1H), 7.72(d, J=15.4Hz, 1H), 5.31-5.49(m, 1H), 6.36(dd, J ₁ =10.11Hz, J ₂ =1.62Hz, 1H), 6.43(s, 1H), 7.16(d, J=10.11Hz, 1H). MASS (ES+): 615.5 (M+Na) ⁺ |
| IB.32 | 0.98(d, J=7.1Hz, 3H), 1.12(t, J=7.49Hz, 3H), 1.13(s, 3H), 1.20-1.36(m, 1H), 1.54(s, 3H), 1.70-1.93(m, 3H), 2.10(s, 3H), 2.19-2.42(m, 6H), 2.88(s, 1H), 3.34-3.37(m, 1H), 3.64(d, J=16.77, 1H), 3.72(d, J=16.82, 1H), 4.41-1.12(d, J=8.07Hz, 1H), 4.56(d, J=15.4Hz, 1H), 4.69-1.12(d, J=15.4Hz, 1H), 5.30-5.47(m, 1H), 6.38(dd, J ₁ =10.12Hz, J ₂ =1.50Hz, 1H), 6.43(s, 1H), 7.17(d, J=10.15Hz, 1H). MASS (ES+): 601.0 (M+Na) ⁺ |
| IB.33 | 0.97(t, J=7.74Hz, 3H), 0.98(d, J=7.44Hz, 3H), 1.12(t, J=7.64Hz, 3H), 1.15(s, 3H), 1.30-1.36(m, 1H), 1.54(s, 3H), 1.66(q, J=7.42Hz, 2H), 1.70-1.94(m, 4H), 2.19-2.46(m, 8H), 3.01(d, J=2.63Hz, 1H), 3.33-3.38(m, 1H), 3.64(d, J=16.88Hz, 1H), 3.72(d, J=16.75Hz, 1H), 4.40(d, J=8.68Hz, 1H), 4.53(t, J ₁ =15.38Hz, J ₂ =1.70Hz, 1H), 4.72(dd, J ₁ =15.39Hz, J ₂ =1.62Hz, 1H), 5.31-5.48(m, 1H), 6.37(dd, J ₁ =10.12Hz, J ₂ =1.77Hz, 1H), 6.43(s, 1H), 7.16(dd, J ₁ =10.15Hz, J ₂ =1.26Hz, 1H). MASS (ES+): 607.5 |
| IB.34 | 0.98(d, J=7.15Hz, 3H), 1.12(t, J=7.59Hz, 3H), 1.16(s, 3H), 1.18(d, J=7.00Hz, 3H), 1.19(d, J=6.96Hz, 3H), 1.30-1.36(m, 1H), 1.54(s, 3H), 1.70-1.94(m, 4H), 2.19-2.48(m, 4H), 2.36(q, J=7.55Hz, 2H), 2.56-2.63(m, 1H), 3.11(d, J=3.05Hz, 1H), 3.33-3.37(m, 1H), 3.65(d, J=16.93Hz, 1H), 3.71(d, J=17.26Hz, 1H), 4.40(d, J=8.83Hz, 1H), 4.53(t, J ₁ =15.38Hz, J ₂ =1.72Hz, 1H), 4.73(dd, J ₁ =15.36Hz, J ₂ =1.61Hz, 1H), 5.31-5.48(m, 1H), 6.37(dd, J ₁ =10.12Hz, J ₂ =1.79Hz, 1H), 6.43(s, 1H), 7.16(dd, J ₁ =10.12Hz, J ₂ =1.17Hz, 1H). MASS (ES+): 607.7 |
| IB.35 | 0.93(t, J=7.31Hz, 3H), 0.98(d, J=7.15Hz, 3H), 1.12(t, J=7.71Hz, 3H), 1.15(s, 3H), 1.25-1.41(m, 3H), 1.54(s, 3H), 1.55-1.94(m, 6H), 2.19-2.46(m, 8H), 3.03(d, J=2.91Hz, 1H), 3.33-3.38(m, 1H), 3.64(d, J=16.76Hz, 1H), 3.72(d, J=16.71Hz, 1H), 4.40(d, J=8.90Hz, 1H), 4.53(t, J ₁ =15.40Hz, J ₂ =1.75Hz, 1H), 4.71(dd, J ₁ =15.41Hz, J ₂ =1.43Hz, 1H), 5.31-5.48(m, 1H), 6.37(dd, J ₁ =10.13Hz, J ₂ =1.78Hz, 1H), 6.43(s, 1H), 7.16(dd, J ₁ =10.11Hz, J ₂ =1.19Hz, 1H). MASS (ES+): 621.5 |
| IB.36 | 0.98(d, J=7.18Hz, 3H), 1.12(t, J=7.59Hz, 3H), 1.15(s, 3H), 1.25-1.36(m, 1H), 1.55(s, 3H), 1.73-2.04(m, 6H), 2.20-2.47(m, 10H), 3.16-3.20(m, 2H), 3.34-3.37(m, 1H), 3.68(2d, 2H), 4.41(d, J=8.64Hz, 1H), 4.54(t, J ₁ =15.38Hz, J ₂ =1.74Hz, 1H), 4.72(t, J ₁ =15.37Hz, J ₂ =1.66Hz, 1H), 5.33-5.45(m, 1H), 6.37(dd, J ₁ =10.16Hz, J ₂ =1.81Hz, 1H), 6.43(s, 1H), 7.16(qd, J ₁ =10.10Hz, J ₂ =1.26Hz, 1H). MASS (ES+): 619.7 |
| IB.37 | 0.91(t, J=6.86Hz, 3H), 0.98(d, J=7.15Hz, 3H), 1.12(t, J=7.59Hz, 3H), 1.15(s, 3H), 1.25-1.36(m, 3H), 1.54(s, 3H), 1.61-1.94(m, 6H), 2.19-2.38(m, 8H), 3.05(d, J=3.03Hz, 1H), 3.34-3.38(m, 1H), 3.64(d, J=16.70Hz, 1H), 3.72(d, J=16.93Hz, 1H), 4.40(d, J=8.58Hz, 1H), 4.52(d, J=15.37Hz, 1H), 4.72(d, J=15.39Hz, 1H), 5.31-5.47(m, 1H), 6.37(dd, J ₁ =10.14Hz, J ₂ =1.75Hz, 1H), 6.43(s, 1H), 7.16(dd, J ₁ =10.63Hz, J ₂ =1.04Hz, 1H). MASS (ES+): 634.8 |
| IB.38 | 1.07(s, 3H), 1.14(t, J=7.53Hz, 3H), 1.21-1.28(m, 1H), 1.42(d, J=7.27Hz, 3H), 1.55(s, 3H), 1.60-1.65(m, 1H), 1.90-2.00(m, 5H), 2.26-2.42(m, 7H), 2.61-2.71(m, 1H), 3.36(d, J=16.65, 1H), 3.80(d, J=16.65, 1H), 4.26(m, 2H), 4.40(d, J=8.38, 1H), 6.14(s, 1H), 6.35(dd, J ₁ =10.06Hz, J ₂ =1.39Hz, 1H), 7.24(d, J=10.23Hz, 1H). MASS (ES+): 541.6 (M+Na) ⁺ |
| IB.39 | 1.06(s, 3H), 1.15(t, J=7.54Hz, 3H), 1.21-1.29(m, 1H), 1.43(d, J=7.35Hz, 3H), 1.53(s, 3H), 1.70-2.06(m, 6H), 2.27-2.41(m, 6H), 3.35(d, J ₁ =16.67, J ₂ =2.34, 1H), 3.81(d, J ₁ =16.67, J ₂ =2.08, 1H), 4.25-4.28(m, 2H), 4.40(d, J=8.32Hz, 1H), 5.31-5.48(m, 1H), 6.37(dd, J ₁ =10.12Hz, J ₂ =1.77Hz, 1H), 6.44(s, 1H), 7.16(dd, J ₁ =10.12Hz, J ₂ =1.16Hz, 1H). MASS (ES+): 559.2 (M+Na) ⁺ |
| IB.40 | 1.04(d, J=7.13Hz, 3H), 1.16(s, 3H), 1.25-1.39(m, 2H), 1.43(s, 3H), 1.44(s, 3H), 1.55(s, 3H), 1.72-1.94(m, 3H), 2.28-2.51(m, 4H), 3.39-3.44(m, 1H), 3.67(d, J=16.29Hz, 1H), 3.75(d, J=16.24Hz, 1H), 4.60(s, 1H), 4.98-4.99(m, 1H), 5.37-5.50(m, 1H), 6.32-6.35(m, 2H), 6.53(dd, J ₁ =3.41Hz, J ₂ =1.65Hz, 1H), 7.12(d, J=3.48Hz, 1H), 7.26(d, J=10.03Hz, 1H), 7.64(s, 1H). MASS (ES+): 625.0 (M+Na) ⁺ |
| IB.41 | 0.96(d, 3H, J=7.16Hz), 1.06(s, 3H), 1.12(t, 3H, J=7.57Hz), 1.26-1.34(m, 1H), 1.53(s, 3H), 1.71-1.91(m, 3H), 2.24-2.39(m, 6H), 3.30-3.35(m, 1H), 3.76(s, 3H), 4.41(m, 1H), 4.71(1H, ddd, J ₁ =15.93Hz, J ₂ =4.75Hz, J ₃ =1.81Hz), 4.84(ddd, 1H, J ₁ =16.00Hz, J ₂ =4.75Hz, J ₃ =1.82Hz), 5.34 & 5.46(m, 1H), 6.03(d, 1H, J=15.77Hz), 6.37(dd, 1H, J ₁ =10.15Hz, J ₂ =1.78Hz), 6.44(s, 1H), 6.93-6.97(m, 1H), 7.12(dd, J ₁ =10.13Hz, J ₂ =1.18Hz). MASS (ES+): 573.1 (M+Na) ⁺ |
| IB.42 | 1.00(d, 3H, J=7.15Hz), 1.06(s, 3H), 1.12(t, 3H, J=7.56Hz), 1.30-1.35(m, 1H), 1.52(s, 3H), 1.73-1.87(m, 4H), 2.22-2.40(m, 6H), 3.34-3.36(m, 1H), 3.71(d, 2H, J=7.09Hz), 3.74(s, 3H), 4.40(d, 1H, J=8.85Hz), 5.32 & 5.44(m, 1H), 6.02(d, 1H, J=15.46Hz), 6.38(dd, 1H, J ₁ =10.15Hz, J ₂ =1.79Hz), 6.43(s, 1H), 6.85-6.89(m, 1H), 7.12(dd, 1H, J ₁ =10.15Hz, J ₂ =1.18Hz). MASS (ES+): 589.1 (M+Na) ⁺ |

SUBSTITUTE SHEET (RULE 26)

| Comp. No | ¹ H-NMR (δ ppm), MASS (EI / ES+, m/z) |
|----------|---|
| IB.43 | 1.03 (s, 3H), 1.15-1.23 (m, 3H), 1.27 (t, 3H, J=7.12Hz), 1.45 (s, 3H), 1.47-1.55 (m, 1H), 1.63-1.70 (m, 2H), 1.80-1.87 (m, 1H), 1.93-2.00 (m, 1H), 2.09-2.16 (m, 3H), 2.32-2.36 (m, 1H), 2.53-2.61 (m, 1H), 2.91-2.98 (m, 1H), 3.76 (s, 3H), 4.13 (d of q, 2H, J ₁ =14.22Hz, J ₂ =7.10Hz, J ₃ =2.13Hz), 4.51 (s, 1H), 4.79 (d, 1H, J=1.62Hz), 4.80 (d, 1H, J=1.62Hz), 6.02 (s, 1H), 6.06 (d, 1H, J=15.77Hz), 6.27 (dd, 1H, J ₁ =10.09Hz, J ₂ =1.75Hz), 6.94 (d of t, 1H, J ₁ =15.76Hz, J ₂ =4.71Hz), 7.23 (d, 1H, J=10.11Hz). MASS (EI) : 516 |
| IB.44 | 0.99(d, J=7.13Hz, 3H), 1.09(s, 3H), 1.11(t, J=7.38Hz, 3H), 1.29-1.35(m, 1H), 1.39(t, J=7.18Hz, 3H), 1.53(s, 3H), 1.72-1.89(m, 3H), 2.20-2.50(m, 6H), 3.12-3.37(m, 1H), 3.52(d, J=13.42Hz, 1H), 3.62(dd, J ₁ =15.97Hz, J ₂ =4.53Hz, 1H), 4.37(q, J=7.15Hz, 2H), 4.38-4.40(m, 1H), 4.70-4.82(m, 1H), 5.30-5.47(m, 1H), 5.82-5.83(m, 2H), 6.37(dd, J ₁ =10.13Hz, J ₂ =1.77Hz, 1H), 6.43(s, 1H), 7.15(dd, J ₁ =10.12Hz, J ₂ =1.18Hz, 1H). |
| IB.45 | 1.04(d, J=7.06Hz, 3H), 1.16(s, 3H), 1.29-1.34(m, 1H), 1.68(s, 3H), 1.71-1.97(m, 4H), 2.37-2.70(m, 5H), 3.38-3.41(m, 1H), 3.70(d, J=16.35, 1H), 3.79(d, J=16.32Hz, 1H), 4.15-4.16(m, 2H), 4.53(d, J=2.4Hz, 1H), 4.74(t, J=5.94, 1H), 5.03(d, J=3.67Hz, 1H), 6.05(s, 1H), 6.28(dd, J ₁ =10.07Hz, J ₂ =1.27Hz, 1H), 6.53(dd, J ₁ =3.15Hz, J ₂ =1.47Hz, 1H), 7.18(d, J=3.35, 1H), 7.31(d, J=10.11Hz, 1H), 7.63(br-s, 1H). MASS (ES+): 595.4(M+Na) ⁺ . |
| IB.46 | 1.07(d, J=7.16Hz, 3H), 1.15(s, 3H), 1.35-1.38(m, 1H), 1.39(t, J=7.14Hz, 3H), 1.56(s, 3H), 1.76-1.97(m, 3H), 2.28-2.50(m, 5H), 3.40-3.44(m, 1H), 3.55(dd, J ₁ =14.06Hz, J ₂ =2.91Hz, 1H), 3.65(dd, J ₁ =15.79Hz, J ₂ =4.86Hz, 1H), 4.36(q, J=7.17Hz, 2H), 4.43(d, J=9.21Hz, 1H), 4.70-4.83(m, 1H), 5.32-5.49(m, 1H), 5.83-5.85(m, 2H), 6.39(dd, J ₁ =10.13Hz, J ₂ =1.82Hz, 1H), 6.45(s, 1H), 6.48(dd, J ₁ =3.49Hz, J ₂ =1.73Hz, 1H), 7.11(dd, J ₁ =3.49Hz, J ₂ =0.64Hz, 1H), 7.18(dd, J ₁ =10.11Hz, J ₂ =1.20Hz, 1H), 7.57(dd, J ₁ =1.6Hz, J ₂ =0.70Hz, 1H). |
| IB.47 | 1.06(d, J=7.13Hz, 3H), 1.12(s, 3H), 1.34-1.38(m, 1H), 1.38(t, J=7.16Hz, 3H), 1.55(s, 3H), 1.77-1.98(m, 3H), 2.25-2.48(m, 5H), 3.42-3.45(m, 1H), 3.63(dd, J ₁ =13.76Hz, J ₂ =7.57Hz, 1H), 3.76(dd, J ₁ =13.79Hz, J ₂ =8.48Hz, 1H), 4.36(q, J=7.17Hz, 2H), 4.43(d, J=8.99Hz, 1H), 4.95-5.05(m, 2H), 5.31-5.50(m, 1H), 5.67-5.71(m, 1H), 5.77-5.81(m, 1H), 6.39(dd, J ₁ =10.14Hz, J ₂ =1.55Hz, 1H), 6.45(s, 1H), 6.49(dd, J ₁ =3.32Hz, J ₂ =1.55Hz, 1H), 7.11(dd, J ₁ =3.48Hz, 1H), 7.16(d, J=10.14Hz, 1H), 7.58(s, 1H). |
| IB.48 | 1.05(d, J=7.15Hz, 3H), 1.17(s, 3H), 1.37-1.40(m, 1H), 1.49(d, J=7.07Hz, 3H), 1.55(s, 3H), 1.77-1.99(m, 4H), 2.13(s, 3H), 2.17-2.48(m, 4H), 3.42-3.46(m, 1H), 3.67(d, J=16.90, 1H), 3.77(d, J=16.82Hz, 1H), 4.44(d, J=8.50Hz, 1H), 4.64(t, J=15.4Hz, J ₂ =1.87Hz, 1H), 4.78(t, J ₁ =15.41Hz, J ₂ =1.86Hz, 1H), 5.09(q, J=6.37Hz, 1H), 5.32-5.51(m, 1H), 6.39(dd, J ₁ =10.12Hz, J ₂ =1.78Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.49Hz, J ₂ =1.73Hz, 1H), 7.12(dd, J ₁ =3.47Hz, J ₂ =0.49Hz, 1H), 7.16(dd, J ₁ =10.14Hz, J ₂ =1.31Hz, 1H), 7.59(d, J=0.75Hz, 1H). MASS (ES+): 689.0 |
| IB.49 | 0.97(t, J=7.47Hz, 3H), 0.98(d, J=7.44Hz, 3H), 1.12(t, J=7.64Hz, 3H), 1.15(s, 3H), 1.30-1.36(m, 1H), 1.54(s, 3H), 1.66(q, J=7.42Hz, 2H), 1.70-1.94(m, 4H), 2.19-2.46(m, 8H), 3.01(d, J=2.63Hz, 1H), 3.33-3.38(m, 1H), 3.64(d, J=16.88Hz, 1H), 3.72(d, J=16.75Hz, 1H), 4.40(d, J=8.68Hz, 1H), 4.53(t, J=15.38Hz, J ₂ =1.70Hz, 1H), 4.72(dd, J ₁ =15.39Hz, J ₂ =1.62Hz, 1H), 5.31-5.48(m, 1H), 6.37(dd, J ₁ =10.12Hz, J ₂ =1.77Hz, 1H), 6.43(s, 1H), 7.16(dd, J ₁ =10.15Hz, J ₂ =1.26Hz, 1H). MASS (ES+): 607.5 |
| IB.50 | 1.06(d, J=7.16Hz, 3H), 1.17(d, J=2.39Hz, 3H), 1.18(d, J=2.37Hz, 3H), 1.21(s, 3H), 1.35-1.41(m, 1H), 1.56(s, 3H), 1.77-2.00(m, 3H), 2.29-2.62(m, 5H), 3.21(d, J=2.62Hz, 1H), 3.42-3.49(m, 1H), 3.67(d, J=16.86Hz, 1H), 4.44(d, J=8.50Hz, 1H), 4.45(d, J=16.81Hz, 1H), 4.52(d, J=15.45Hz, 1H), 4.74(d, J=15.33Hz, 1H), 5.33-5.50(m, 1H), 6.40(dd, J ₁ =10.05Hz, J ₂ =1.65Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.50Hz, J ₂ =1.69Hz, 1H), 7.13(dd, J ₁ =3.56Hz, J ₂ =0.57Hz, 1H), 7.19(dd, J ₁ =0.75Hz, J ₂ =0.22Hz, 1H), 7.58(s, 1H). MASS (ES+): 667.0(M+Na) ⁺ . |
| IB.51 | 1.06(d, J=7.16Hz, 3H), 1.21(s, 9H), 1.22(s, 3H), 1.35-1.41(m, 1H), 1.56(s, 3H), 1.77-2.00(m, 1H), 2.29-2.53(m, 1H), 3.27(d, J=3.09Hz, 1H), 3.42-3.47(m, 1H), 3.67(d, J=16.88Hz, 1H), 3.74(d, J=16.89Hz, 1H), 4.45(d, J=8.56Hz, 1H), 4.50(d, J=15.35Hz, 1H), 4.75(t, J=15.40Hz, 1H), 5.33-5.40(m, 1H), 6.40(dd, J ₁ =10.19Hz, J ₂ =1.84Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.51Hz, J ₂ =1.68Hz, 1H), 7.14(d, J=3.43Hz, 1H), 7.17(dd, J ₁ =15.12Hz, J ₂ =0.99Hz, 1H), 7.58(d, J=0.98Hz, 1H). MASS (ES+): 680.9(M+Na) ⁺ . |
| IB.52 | 0.98(d, J=7.14Hz, 3H), 1.12(t, J=7.56Hz, 3H), 1.17(s, 3H), 1.22(s, 9H), 1.30-1.36(m, 1H), 1.54(s, 3H), 1.73-1.95(m, 3H), 2.21-2.40(m, 6H), 3.20(d, J=3.29Hz, 1H), 3.34-3.38(m, 1H), 3.68(br-s, 2H), 4.40(d, J=8.77Hz, 1H), 4.50(d, J=14.59Hz, 1H), 4.74(d, J=15.33Hz, 1H), 5.30-5.50(m, 1H), 6.37(dd, J ₁ =10.12Hz, J ₂ =1.77Hz, 1H), 6.43(s, 1H), 7.15(dd, J ₁ =10.09Hz, J ₂ =1.04Hz, 1H). MASS (ES+): 643.0(M+Na) ⁺ . |
| IB.53 | 0.94(d, J=7.45Hz, 3H), 1.06(d, J=7.18Hz, 3H), 1.12(s, 3H), 1.34-1.40(m, 1H), 1.55(s, 3H), 1.66(t, J=7.41Hz, 2H), 1.77-2.05(m, 3H), 2.30(t, J=7.45Hz, 2H), 2.35-2.48(m, 4H), 3.43-3.47(m, 1H), 3.66(d, J=7.79Hz, 1H), 3.43(d, J=9.05Hz, 1H), 4.76-4.79(m, 2H), 5.59-5.72(m, 1H), 6.39(dd, J ₁ =10.17Hz, J ₂ =1.80Hz, 1H), 6.45(s, 1H), 6.49(dd, J ₁ =3.48Hz, J ₂ =1.81Hz, 1H), 7.12(d, J=3.42Hz, 1H), 7.17(dd, J ₁ =10.08Hz, J ₂ =1.02Hz, 1H), 7.58(d, J=0.93Hz, 1H). MASS (ES+): 669.0(M+Na) ⁺ . |
| IB.54 | 1.06(d, 3H, J=7.14Hz), 1.21(s, 3H), 1.38-1.41(m, 1H), 1.39(t, 3H, J=7.15Hz), 1.56(s, 3H), 1.77-1.96(m, 3H), 2.28-2.64(m, 5H), 3.37-3.45(m, 1H), 3.72(br-s, 2H), 4.38(q, J=7.12Hz, 2H), 4.46(d, J=8.96Hz, 1H), 4.79(d, J=15.27Hz, 1H), 4.89(d, J=15.31Hz, 1H), 5.32-5.51(m, 1H), 6.40(dd, J ₁ =10.14Hz, J ₂ =1.77Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.47Hz, J ₂ =1.69Hz, 1H), 7.12(d, J=3.25Hz, 1H), 7.19(dd, J ₁ =10.11Hz, J ₂ =0.85Hz, 1H), 7.58(d, J=0.72Hz, 1H). |
| IB.55 | 0.96(t, J=7.42Hz, 3H), 1.07(d, J=7.18Hz, 3H), 1.21(s, 3H), 1.36-1.42(m, 1H), 1.56(s, 3H), 1.65(q, J=7.43Hz, 2H), 1.70-2.02(m, 3H), 2.29-2.53(m, 6H), 3.09(d, J=2.87Hz, 1H), 3.43-3.47(m, 1H), 3.67(d, J=16.68Hz, 1H), 3.77(d, J=16.66Hz, 1H), 4.46(d, J=8.60Hz, 1H), 4.53(d, J=18.41Hz, 1H), 4.73(d, J=15.35Hz, 1H), 5.33-5.50(m, 1H), 6.40(dd, J ₁ =10.17Hz, J ₂ =1.81Hz, 1H), 6.46(s, 1H), 7.10(dd, J ₁ =4.83Hz, J ₂ =3.94Hz, 1H), 7.19(dd, J ₁ =10.10Hz, J ₂ =1.02Hz, 1H), 7.57(dd, J ₁ =5.01Hz, J ₂ =1.05Hz, 1H), 7.75(dd, J ₁ =3.71Hz, J ₂ =1.03Hz, 1H). MASS (ES+): 682.9(M+Na) ⁺ . |
| IB.56 | 0.96(t, J=7.40Hz, 3H), 1.05(d, J=7.16Hz, 3H), 1.21(s, 3H), 1.37-1.40(m, 1H), 1.56(s, 3H), 1.66(q, J=7.42Hz, 2H), 1.78-2.0(m, 3H), 2.28-2.41(m, 6H), 3.11(d, J=3.03Hz, 1H), 3.38-3.45(m, 1H), 3.71(d, J=11.09Hz, 1H), 4.46(d, J=8.70Hz, 1H), 4.52(d, J=15.37Hz, 1H), 4.74(d, J=15.34Hz, 1H), 6.42(dd, J ₁ =10.18Hz, J ₂ =1.82Hz, 1H), 6.46(s, 1H), 6.94(d, J=4.09Hz, 1H), 7.19(dd, J ₁ =10.09Hz, J ₂ =1.06Hz, 1H), 7.54(d, J=4.07Hz, 1H). MASS (ES+): 716.9(M+Na) ⁺ . |
| IB.57 | 0.92-1.03(m, 4H), 1.05(d, J=7.26Hz, 3H), 1.19(s, 3H), 1.35-1.40(m, 1H), 1.56(s, 3H), 1.61-1.98(m, 4H), 2.28-2.51(m, 4H), 3.06(d, J=2.41Hz, 1H), 3.43-3.46(m, 1H), 3.66(d, J=16.84Hz, 1H), 3.77(d, J=16.84Hz, 1H), 4.44(d, J=8.44Hz, 1H), 4.55(d, J=16.23Hz, 1H), 4.70(d, J=14.68Hz, 1H), 5.33-5.50(m, 1H), 6.40(dd, J ₁ =10.15Hz, J ₂ =1.79Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.47Hz, J ₂ =1.65Hz, 1H), 7.13(d, J=3.3Hz, 1H), 7.18(dd, J ₁ =10.10Hz, J ₂ =1.04Hz, 1H), 7.59(d, J=0.83Hz, 1H). MASS (ES+): 693.0(M+Na) ⁺ . |
| IB.58 | 1.06(d, J=7.14Hz, 3H), 1.21(s, 3H), 1.35-1.41(m, 1H), 1.57(s, 3H), 1.77-2.04(m, 5H), 2.21-2.53(m, 8H), 3.15-3.21(m, 2H), 3.42-3.47(m, 1H), 3.67(d, J=16.81Hz, 1H), 3.75(d, J=17.06Hz, 1H), 4.45(d, J=8.61Hz, 1H), 4.43(d, J=15.33Hz, 1H), 4.73(d, J=15.39Hz, 1H), 5.33-5.50(m, 1H), 6.40(dd, J ₁ =10.14Hz, J ₂ =1.82Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.47Hz, J ₂ =1.60Hz, 1H), 7.13(d, J=3.26Hz, 1H), 7.18(dd, J ₁ =10.18Hz, J ₂ =1.26Hz, 1H), 7.58(d, J=1.71Hz, 1H). MASS (ES+): 678.9(M+Na) ⁺ . |

| Comp. No | ¹ H-NMR (δ ppm), MASS (EI / ES+, m/z) |
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| IB.59 | 1.06(d, J=7.16Hz, 3H), 1.21(s, 3H), 1.35-1.41(m, 1H), 1.56(s, 3H), 1.62-1.9(m, 1H), 2.28-2.51(m, 4H), 2.73-2.81(m, 1H), 3.17(d, J=2.84Hz, 1H), 3.42-3.49(m, 1H), 3.66(d, J=16.87Hz, 1H), 3.75(d, J=16.86Hz, 1H), 4.44(d, J=8.46Hz, 1H), 4.51(d, J=15.31Hz, 1H), 4.74(d, J=15.33Hz, 1H), 5.33-5.50(m, 1H), 6.40(dd, J ₁ =10.18Hz, J ₂ =1.82Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.48Hz, J ₂ =1.79Hz, 1H), 7.13(d, J=3.41Hz, 1H), 7.17(dd, J ₁ =10.08Hz, J ₂ =1.08Hz, 1H), 7.59(d, J=1.89Hz, 1H). MASS (ES+) : 693.0(M+Na) ⁺ |
| IB.60 | 0.95(t, J=7.38Hz, 3H), 1.06(d, J=7.18Hz, 3H), 1.12(s, 3H), 1.34-1.40(m, 1H), 1.55(s, 3H), 1.64(q, J=7.44Hz, 2H), 1.74-1.94(m, 3H), 2.30(t, J=7.46Hz, 2H), 2.36-2.50(m, 4H), 2.72(s, 1H), 3.42-3.47(m, 1H), 3.53(dd, J ₁ =14.08Hz, J ₂ =6.92Hz, 1H), 3.67(dd, J ₁ =14.01Hz, J ₂ =5.33Hz, 1H), 4.42(d, J=8.53Hz, 1H), 4.50(dd, J ₁ =13.23Hz, J ₂ =4.74Hz, 1H), 4.62(dd, J ₁ =13.20Hz, J ₂ =5.70Hz, 1H), 5.32-5.49(m, 1H), 5.67-5.81(m, 2H), 6.39(dd, J ₁ =10.19Hz, J ₂ =1.80Hz, 1H), 6.45(s, 1H), 6.49(dd, J ₁ =3.49Hz, J ₂ =1.56Hz, 1H), 7.12(d, J=3.42Hz, 1H), 7.16(dd, J ₁ =10.15Hz, J ₂ =1.02Hz, 1H), 7.58(d, J=0.79Hz, 1H). MASS (ES+) : 669.0(M+Na) ⁺ |
| IB.61 | 1.03(d, J=7.12Hz, 3H), 1.19(s, 3H), 1.25-1.42(m, 2H), 1.55(s, 3H), 1.65-1.96(m, 3H), 2.21-2.46(m, 4H), 3.45(m, 1H), 3.71(d, J=16.51Hz, 1H), 3.79(d, J=16.46Hz, 1H), 4.20-4.30(m, 2H), 4.46(d, J=8.42Hz, 1H), 5.30-5.50(m, 1H), 6.42(dd, J ₁ =10.05Hz, J ₂ =1.80Hz, 1H), 6.47(s, 1H), 7.15(dd, J ₁ =10.15Hz, J ₂ =1.21Hz, 1H), 7.43(d, J=8.59Hz, 2H), 7.86(d, J=8.55Hz, 2H). MASS (ES+) : 640.9(M+Na) ⁺ |
| IB.62 | 1.03(d, J=7.05Hz, 3H), 1.20(s, 3H), 1.22-1.93(m, 8H), 2.29-2.51(m, 4H), 3.44-3.50(m, 1H), 3.71(d, J=16.42Hz, 1H), 3.80(d, J=16.52Hz, 1H), 4.26-4.32(m, 2H), 4.46(d, J=8.81Hz, 1H), 5.33-5.50(m, 1H), 6.40-6.42(m, 1H), 6.46(s, 1H), 7.16(dd, J=10.15Hz, 1H), 7.39(d, J=7.91Hz, 1H), 7.55(d, J=7.56Hz, 1H), 7.79(d, J=7.76Hz, 1H), 7.91(s, 1H). MASS (ES+) : 640.9(M+Na) ⁺ |
| IB.63 | 1.06(d, J=7.14Hz, 3H), 1.19(s, 3H), 1.36-1.41(m, 1H), 1.55(s, 3H), 1.74-1.99(m, 3H), 2.17-2.51(m, 5H), 3.42-3.46(m, 1H), 3.69(d, J=16.73Hz, 1H), 3.76(d, J=16.91Hz, 1H), 3.81(s, 3H), 4.45(d, J=8.63Hz, 1H), 4.66(dd, J ₁ =15.52Hz, J ₂ =1.70Hz, 1H), 4.73(d, J=15.49Hz, J ₂ =1.71Hz, 1H), 5.33-5.49(m, 1H), 6.40(dd, J ₁ =10.12Hz, J ₂ =1.72Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.48Hz, J ₂ =1.68Hz, 1H), 7.14(d, J=3.43Hz, 1H), 7.16(dd, J ₁ =10.09Hz, J ₂ =0.99Hz, 1H), 7.59(d, J=0.92Hz, 1H). MASS (ES+) : 654.9 (M + Na) ⁺ |
| IB.64 | 1.06(d, J=7.16Hz, 3H), 1.19(s, 3H), 1.33(t, J=7.05Hz, 3H), 1.36-1.41(m, 1H), 1.55(s, 3H), 1.74-1.99(m, 3H), 2.28-2.50(m, 4H), 2.56(d, J=1.85Hz, 1H), 3.42-3.47(m, 1H), 3.69(d, J=16.88Hz, 1H), 3.76(d, J=16.88Hz, 1H), 4.22(q, J=7.13Hz, 2H), 4.44(d, J=8.65Hz, 1H), 4.65(d, J=15.49Hz, 1H), 4.72(d, J=15.41Hz, 1H), 5.33-5.49(m, 1H), 6.40(dd, J ₁ =10.13Hz, J ₂ =1.63Hz, 1H), 6.45(s, 1H), 6.51(dd, J ₁ =3.44Hz, J ₂ =1.69Hz, 1H), 7.14(d, J=3.50Hz, 1H), 7.16(d, J=10.20Hz, 1H), 7.59(d, J=0.87Hz, 1H). MASS (ES+) : 669.1(M + Na) ⁺ |
| IB.65 | 1.06(d, J=7.19Hz, 3H), 1.20(s, 3H), 1.34-1.43(m, 1H), 1.50(s, 9H), 1.55(s, 3H), 1.62-1.99(m, 3H), 2.28-2.54(m, 5H), 3.43-3.48(m, 1H), 3.68(d, J=16.70Hz, 1H), 3.77(d, J=16.65Hz, 1H), 4.44(d, J=8.51Hz, 1H), 4.57-4.68(m, 2H), 5.33-5.49(m, 1H), 6.40(dd, J ₁ =10.06Hz, J ₂ =1.79Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.48Hz, J ₂ =1.78Hz, 1H), 7.11-7.14(m, 2H), 7.59(d, J=1.00Hz, 1H). MASS (ES+) : 697.0(M + Na) ⁺ |
| IB.66 | 0.96(d, J=6.74Hz, 6H), 1.06(d, J=7.13Hz, 3H), 1.19(s, 3H), 1.35-1.41(m, 1H), 1.55(s, 3H), 1.74-2.00(m, 4H), 2.28-2.52(m, 5H), 3.43-3.46(m, 1H), 3.69(d, J=16.80Hz, 1H), 3.77(d, J=16.79Hz, 1H), 3.93(d, J=6.72Hz, 2H), 4.44(d, J=8.62Hz, 1H), 4.66(d, J=15.49Hz, 1H), 4.71(d, J=15.48Hz, 1H), 5.33-5.49(m, 1H), 6.40(dd, J ₁ =10.18Hz, J ₂ =1.48Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.36Hz, J ₂ =1.59Hz, 1H), 7.13-7.16(m, 2H), 7.59(s, 1H). MASS (ES+) : 697.0(M + Na) ⁺ |
| IB.67 | 1.06(d, J=7.14Hz, 3H), 1.19(s, 3H), 1.35-1.41(m, 1H), 1.55(s, 3H), 1.77-2.14(m, 5H), 2.28-2.72(m, 5H), 2.55(t, J=7.26Hz, 2H), 3.42-3.47(m, 1H), 3.59(t, J=6.37Hz, 2H), 3.64(d, J=16.76Hz, 1H), 3.76(d, J=16.58Hz, 1H), 4.46(d, J=8.65Hz, 1H), 4.58(d, J=15.39Hz, 1H), 4.73(d, J=15.40Hz, 1H), 5.33-5.49(m, 1H), 6.40(dd, J ₁ =10.14Hz, J ₂ =1.64Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.4Hz, J ₂ =1.57Hz, 1H), 7.13(d, J=3.45Hz, 1H), 7.18(d, J=9.98Hz, 1H), 7.59(d, J=0.75Hz, 1H). MASS (ES+) : 679.0 |
| IB.68 | 1.05(d, J=7.14Hz, 3H), 1.12(s, 3H), 1.19(s, 9H), 1.34-1.40(m, 1H), 1.55(s, 3H), 1.71-2.06(m, 3H), 2.27-2.52(m, 4H), 3.42-3.47(m, 1H), 3.63(d, J=11.76Hz, 1H), 3.68(d, J=11.84Hz, 1H), 4.43(d, J=9.20Hz, 1H), 4.74(dd, J ₁ =13.06Hz, J ₂ =6.26Hz, 1H), 4.79(dd, J ₁ =13.58Hz, J ₂ =6.06Hz, 1H), 5.32-5.49(m, 1H), 5.55-5.74(m, 1H), 6.39(dd, J ₁ =10.19Hz, J ₂ =1.41Hz, 1H), 6.45(s, 2H), 6.49(dd, J ₁ =15.49Hz, J ₂ =1.53Hz, 1H), 7.12(d, J=3.45Hz, 1H), 7.15(d, J=10.17Hz, 1H), 7.58(s, 1H). MASS (ES+) : 683.0(M+Na) ⁺ |
| IB.69 | 1.06(d, J=7.15Hz, 3H), 1.13(s, 3H), 1.20(s, 9H), 1.34-1.42(m, 1H), 1.55(s, 3H), 1.71-1.95(m, 3H), 2.17-2.53(m, 4H), 2.81(s, 1H), 3.42-3.49(m, 1H), 3.54(dd, J ₁ =14.17Hz, J ₂ =7.36Hz, 1H), 3.67(dd, J ₁ =14.01Hz, J ₂ =5.52Hz, 1H), 4.42(d, J=8.46Hz, 1H), 4.50(dd, J ₁ =13.61Hz, J ₂ =4.34Hz, 1H), 4.62(dd, J ₁ =13.51Hz, J ₂ =5.59Hz, 1H), 5.32-5.49(m, 1H), 5.64-5.80(m, 2H), 6.39(dd, J ₁ =10.18Hz, J ₂ =1.77Hz, 1H), 6.45(s, 1H), 6.49(dd, J ₁ =3.43Hz, J ₂ =1.80Hz, 1H), 7.12(d, J=3.31Hz, 1H), 7.15(dd, J ₁ =10.24Hz, J ₂ =0.78Hz, 1H), 7.58(d, J=0.85Hz, 1H). MASS (ES+) : 683.1(M+Na) ⁺ |
| IB.70 | 1.06(d, 3H, J=7.16Hz), 1.19(s, 3H), 1.36-1.42(m, 1H), 1.56(s, 3H), 1.77-1.96(m, 3H), 2.29-2.52(m, 5H), 3.41-3.45(m, 1H), 3.70(d, 1H, J=16.78Hz), 3.77(d, J=16.93Hz, 1H), 4.46(d, J=8.62Hz, 1H), 4.77(d, J=15.30Hz, 1H), 4.89(d, J=15.31Hz, 1H), 5.33-5.50(m, 1H), 5.99(s, 1H), 6.40(dd, J ₁ =10.16Hz, J ₂ =1.75Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.47Hz, J ₂ =1.67Hz, 1H), 7.12(d, J=3.41Hz, 1H), 7.17(d, J=10.19Hz, 1H), 7.59(s, 1H). MASS (ES+) : 597.2 [(M+Na) ⁺ of IB.4] |
| IB.71 | 0.92(q, J=4.52Hz, 3H), 1.06(d, J=7.11Hz, 3H), 1.15(dd, 3H), 1.22(s, 3H), 1.22(s, 3H), 1.35-1.41(m, 1H), 1.56(s, 3H), 1.46-2.00(m, 5H), 2.29-2.53(m, 5H), 3.22-3.26(dd, 1H), 3.40-3.50(m, 1H), 3.66(d, J=16.58Hz, 1H), 3.75(d, J=16.83Hz, 1H), 4.45(d, J=8.39Hz, 1H), 4.48-4.53(m, 1H), 5.33-5.50(m, 1H), 6.40(dd, J ₁ =10.15Hz, J ₂ =1.71Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.39Hz, J ₂ =1.67Hz, 1H), 7.13(d, J=3.49Hz, 1H), 7.19(d, J=10.13Hz, 1H), 7.58(s, 1H). MASS (ES+) : 659.3 |
| IB.72 | 1.03(s, 9H), 1.05(d, J=7.35Hz, 3H), 1.20(s, 3H), 1.35-1.40(m, 1H), 1.56(s, 3H), 1.72-2.03(m, 3H), 2.20(d, J=13.11Hz, 1H), 2.24(d, J=13.16Hz, 1H), 2.29-2.54(m, 4H), 3.07(s, 1H), 3.44-3.48(m, 1H), 3.63(d, J=16.81Hz, 1H), 3.78(d, J=16.84Hz, 1H), 4.44(d, J=8.47Hz, 1H), 4.50(d, J=15.41Hz, 1H), 4.73(d, J=15.35Hz, 1H), 5.33-5.50(m, 1H), 6.40(dd, J ₁ =10.17Hz, J ₂ =1.78Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.45Hz, J ₂ =1.78Hz, 1H), 7.14(d, J=3.37Hz, 1H), 7.18(dd, J ₁ =9.63Hz, J ₂ =1.07Hz, 1H), 7.59(s, 1H). MASS (ES+) : 673.3 |
| IB.73 | 1.06(d, J=7.17Hz, 3H), 1.15(t, J=7.57Hz, 3H), 1.20(s, 3H), 1.35-1.41(m, 1H), 1.56(s, 3H), 1.74-2.00(m, 3H), 2.28-2.52(m, 6H), 3.10(d, J=2.84Hz, 1H), 3.42-3.46(m, 1H), 3.66(d, J=16.80Hz, 1H), 3.75(d, J=16.82Hz, 1H), 4.45(d, J=8.54Hz, 1H), 4.54(d, J=15.48Hz, 1H), 4.73(d, J=15.38Hz, 1H), 5.33-5.40(m, 1H), 6.40(dd, J ₁ =10.11Hz, J ₂ =1.76Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.49Hz, J ₂ =1.65Hz, 1H), 7.13(d, J=3.35Hz, 1H), 7.18(dd, J ₁ =10.06Hz, J ₂ =1.04Hz, 1H), 7.59(d, J=0.80Hz, 1H). MASS (ES+) : 631.3 |
| IB.74 | 0.98(d, J=7.10Hz, 3H), 1.16(s, 3H), 1.30-1.36(m, 1H), 1.40(t, J=7.12Hz, 3H), 1.54(s, 3H), 1.73-1.99(m, 5H), 2.10-2.47(m, 8H), 2.61(m, 1H), 3.11-3.19(m, 1H), 3.31-3.35(m, 1H), 3.67(d, J=16.90Hz, 1H), 3.73(d, J=16.78Hz, 1H), 4.36-4.41(m, 3H), 4.79 (d, J=15.23Hz, 1H), 4.88 (d, J=15.28Hz, 1H), 5.31-5.48(m, 1H), 6.38(d, J ₁ =10.17Hz, 1H), 6.43(s, 1H), 7.17 (d, J=10.05Hz, 1H). MASS (ES+) : 585.22 [(M+Na) ⁺ of IB.08] |

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| Comp. No | ¹ H-NMR (δ ppm), MASS (EI / ES+, m/z) |
|----------|---|
| 113.75 | 0.98(d, J=7.18Hz, 3H), 1.10(s, 3H), 1.18(d, J=3.67Hz, 3H), 1.20(d, J=3.71Hz, 3H), 1.29-1.35(m, 1H), 1.54(s, 3H), 1.70-1.99(m, 5H), 2.16-2.61(m, 9H), 3.12(d, J=3.61Hz, 1H), 3.12-3.20(m, 1H), 3.33-3.38(m, 1H), 3.65(d, J=16.64Hz, 1H), 3.72(d, J=16.26Hz, 1H), 4.40(d, J=8.93, 1H), 4.52(d, J=15.32, 1H), 4.73(d, J=15.33Hz, 1H), 5.31-5.48(m, 1H), 6.37(dd, J ₁ =10.09Hz, J ₂ =1.77Hz, 1H), 6.43(s, 1H), 7.16(d, J ₁ =10.10Hz, J ₂ =1.10Hz, 1H). MASS (ES+): 633.25 |
| 113.76 | 1.06(d, J=7.17Hz, 3H), 1.22(s, 3H), 1.35-1.41(m, 1H), 1.57(s, 3H), 1.67-2.03(m, 1H), 2.29-2.53(m, 4H), 3.31(d, J=3.06Hz, 1H), 3.45(m, 1H), 3.67(d, J=16.78Hz, 1H), 3.73(d, J=17.10Hz, 1H), 4.45(d, J=7.42Hz, 1H), 4.48(d, J=15.47Hz, 1H), 4.73(d, J=15.40Hz, 1H), 5.33-5.40(m, 1H), 6.40(dd, J ₁ =10.07Hz, J ₂ =1.79Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.47Hz, J ₂ =1.81Hz, 1H), 7.14(d, J=3.28Hz, 1H), 7.18(dd, J ₁ =10.07Hz, J ₂ =1.07Hz, 1H), 7.58(d, J=0.97Hz, 1H). MASS (ES+): 737.4 |
| 113.77 | 1.06(d, J=7.12Hz, 3H), 1.19(s, 3H), 1.25-1.43(m, 2H), 1.55(s, 3H), 1.74-1.97(m, 3H), 2.28-2.50(m, 4H), 3.24(q, J=10.07Hz, 2H), 3.42-3.45(m, 1H), 3.68(d, J=16.80Hz, 1H), 3.76(d, J=16.82Hz, 1H), 4.45(d, J=8.56Hz, 1H), 4.65(d, J=15.34Hz, 1H), 4.83(d, J=15.37Hz, 1H), 5.33-5.49(m, 1H), 6.41(dd, J ₁ =10.14Hz, J ₂ =1.72Hz, 1H), 6.41(s, 1H), 6.51(dd, J ₁ =3.42Hz, J ₂ =1.62Hz, 1H), 7.13(d, J=3.42Hz, 1H), 7.16(d, J=10.14Hz, 1H), 7.59(s, 1H). MASS (ES+): 707.13(M + Na) ⁺ |
| 113.78 | 1.06(d, J=7.14Hz, 3H), 1.23(s, 3H), 1.35-1.41(m, 1H), 1.57(s, 3H), 1.77-1.99(m, 3H), 2.28-2.53(m, 4H), 3.11(s, 1H), 3.39-3.45(m, 1H), 3.45(s, 3H), 3.67(d, J=17.19Hz, 1H), 3.73(d, J=16.96Hz, 1H), 4.03(d, J=16.48Hz, 1H), 4.10(d, J=16.55Hz, 1H), 4.43(d, J=8.74Hz, 1H), 4.58(d, J=15.30Hz, 1H), 4.58(d, J=15.33Hz, 1H), 5.33-5.50(m, 1H), 6.39(dd, J ₁ =10.14Hz, J ₂ =1.71Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.41Hz, J ₂ =1.76Hz, 1H), 7.12(d, J=3.55Hz, 1H), 7.17(dd, J ₁ =10.19Hz, J ₂ =0.74Hz, 1H), 7.58(d, J=0.71Hz, 1H). MASS (ES+): 647.24 |
| 113.79 | 1.06(d, J=7.16Hz, 3H), 1.23(s, 3H), 1.27(l, J=7.04Hz, 3H), 1.35-1.41(m, 1H), 1.56(s, 3H), 1.73-1.99(m, 3H), 2.28-2.53(m, 4H), 3.17(s, 1H), 3.39-3.42(m, 1H), 3.57(dd, J ₁ =7.03Hz, J ₂ =2.38Hz, 1H), 3.60(dd, J ₁ =4.44Hz, J ₂ =2.44Hz, 1H), 3.65(d, J=16.18Hz, 1H), 3.73(d, J=16.94Hz, 1H), 4.07(d, J=16.64Hz, 1H), 4.14(d, J=16.63Hz, 1H), 4.43(d, J=8.74Hz, 1H), 4.56(d, J=15.41Hz, 1H), 4.85(d, J=15.30Hz, 1H), 5.33-5.50(m, 1H), 6.38(dd, J ₁ =10.11Hz, J ₂ =1.72Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.49Hz, J ₂ =1.65Hz, 1H), 7.12(d, J=3.37Hz, 1H), 7.17(d, J=10.17Hz, 1H), 7.58(d, J=1.57Hz, 1H). MASS (ES+): 661.22 |
| 113.80 | 1.05(d, J=7.10Hz, 3H), 1.18(s, 3H), 1.25-1.42(m, 2H), 1.55(s, 3H), 1.71-2.00(m, 3H), 2.17-2.51(m, 4H), 2.62-2.68(m, 4H), 3.43-3.49(m, 1H), 3.68(d, J=16.72Hz, 1H), 3.75(d, J=16.78Hz, 1H), 4.45(d, J=8.41Hz, 1H), 4.58(d, J=15.45Hz, 1H), 4.74(d, J=15.45Hz, 1H), 5.33-5.49(m, 1H), 6.42(dd, J ₁ =10.09Hz, J ₂ =1.58Hz, 1H), 6.45(s, 1H), 6.51(dd, J ₁ =3.41Hz, J ₂ =1.69Hz, 1H), 7.14(d, J=3.41Hz, 1H), 7.22(d, J=10.04Hz, 1H), 7.59(s, 1H). MASS (ES+): 697.16(M+Na) ⁺ |
| 113.81 | 1.06(d, J=7.17Hz, 3H), 1.18(s, 3H), 1.35-1.41(m, 1H), 1.56(s, 3H), 1.77-1.99(m, 3H), 2.09(s, 3H), 2.28-2.51(m, 4H), 2.91(d, 1H), J=2.60Hz), 3.42-3.47(m, 1H), 3.66(d, J=16.74Hz, 1H), 3.76(d, J=16.78Hz, 1H), 4.46(d, J=8.63Hz, 1H), 4.56(d, J=15.46Hz, 1H), 4.56(d, J=15.46Hz, 1H), 4.70(d, J=15.39Hz, J ₂ =1.65Hz, 1H), 5.32-5.50(m, 1H), 6.39(dd, J ₁ =10.07Hz, J ₂ =1.79Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.53Hz, J ₂ =1.68Hz, 1H), 7.14(d, J=3.37Hz, 1H), 7.20(dd, J ₁ =10.18Hz, J ₂ =1.23Hz, 1H), 7.59(d, J=0.86Hz, 1H). MASS (ES+): 617.1 |
| 113.82 | 1.06(d, J=7.18Hz, 3H), 1.13(s, 3H), 1.16(d, J=1.26Hz, 3H), 1.18(d, J=1.30Hz, 3H), 1.34-1.43(m, 1H), 1.55(s, 3H), 1.77-1.95(m, 3H), 2.28-2.53(m, 4H), 2.53-2.80(m, 1H), 2.81(m, 1H), 3.43-3.48(m, 1H), 3.54(dd, J ₁ =14.12Hz, J ₂ =7.29Hz, 1H), 3.66(dd, J ₁ =14.07Hz, J ₂ =5.43Hz, 1H), 4.43(d, J=8.57Hz, 1H), 4.50(dd, J ₁ =13.32Hz, J ₂ =4.52Hz, 1H), 4.62(dd, J ₁ =13.25Hz, J ₂ =5.69Hz, 1H), 5.32-5.49(m, 1H), 5.65-5.80(m, 2H), 6.39(dd, J ₁ =10.15Hz, J ₂ =1.79Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.46Hz, J ₂ =1.64Hz, 1H), 7.11(d, J=3.43Hz, 1H), 7.16(dd, J ₁ =10.03Hz, J ₂ =0.93Hz, 1H), 7.58(d, J=0.86Hz, 1H). MASS (ES+): 647.1 |
| 113.83 | 1.06(d, J=7.17Hz, 3H), 1.12(s, 3H), 1.16(d, J=6.98Hz, 6H), 1.34-1.40(m, 1H), 1.55(s, 3H), 1.77-2.06(m, 3H), 2.28-2.59(m, 5H), 3.42-3.47(m, 1H), 3.66(d, J=7.82Hz, 2H), 4.44(d, J=9.08Hz, 1H), 4.75-4.79(m, 2H), 5.34-5.47(m, 1H), 5.58-5.72(m, 2H), 6.39(dd, J ₁ =10.16Hz, J ₂ =1.79Hz, 1H), 6.45(s, 1H), 6.49(dd, J ₁ =3.41Hz, J ₂ =1.82Hz, 1H), 7.12(d, J=3.19Hz, 1H), 7.16(dd, J ₁ =10.08Hz, J ₂ =1.06Hz, 1H), 7.58(br-s, 1H). MASS (ES+): 647.1 |
| 113.84 | 0.98(d, J=7.15Hz, 3H), 1.17(s, 3H), 1.22(s, 9H), 1.27-1.38(m, 1H), 1.54(s, 3H), 1.70-1.99(m, 5H), 2.17-2.50(m, 8H), 3.12-3.18(m, 1H), 3.21(d, J=3.24Hz, 1H), 3.35-3.38(m, 1H), 3.65(d, J=16.86Hz, 1H), 3.65(d, J=16.86Hz, 1H), 3.72(d, J=17.02Hz, 1H), 4.39(d, J=8.61Hz, 1H), 4.51(d, J=15.31Hz, 1H), 4.73(d, J=15.33Hz, 1H), 5.31-5.48(m, 1H), 6.37(dd, J ₁ =10.11Hz, J ₂ =1.61Hz, 1H), 6.43(s, 1H), 7.15(d, J=10.16Hz, 1H). MASS (ES+): 647.1 |
| 113.85 | 0.86(l, J=7.46Hz, 3H), 1.05(d, J=7.15Hz, 3H), 1.17(s, 6H), 1.23(s, 3H), 1.35-1.41(m, 1H), 1.56(s, 3H), 1.73-2.01(m, 3H), 2.29-2.56(m, 4H), 3.36(br-s, 1H), 3.43-3.49(m, 1H), 4.40(d, 1H), 4.48(d, J=15.37Hz, 1H), 4.76(d, J=15.31Hz, 1H), 5.34-5.50(m, 1H), 6.40(dd, J ₁ =10.17Hz, J ₂ =1.72Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.44Hz, J ₂ =1.67Hz, 1H), 7.13(d, J=3.37Hz, 1H), 7.17(dd, J ₁ =10.07Hz, J ₂ =0.60Hz, 1H), 7.58(s, 1H). MASS (ES+): 673.26 |
| 113.86 | 0.96(s, 3H), 1.06(d, J=5.33Hz, 3H), 1.07(s, 3H), 1.13(s, 3H), 1.25(s, 3H), 1.35-1.41(m, 1H), 1.56(s, 3H), 1.69-2.13(m, 6H), 2.28-2.57(m, 5H), 3.10(s, 1H), 3.39-3.42(m, 1H), 3.66(d, J=16.62Hz, 1H), 3.73(d, J=17.10Hz, 1H), 4.53(d, J=8.29Hz, 1H), 4.64(d, J=15.20Hz, 1H), 4.92(d, J=15.23Hz, 1H), 5.33-5.50(m, 1H), 6.41(dd, J ₁ =10.07Hz, J ₂ =1.78Hz, 1H), 6.44(s, 1H), 6.49(dd, J ₁ =3.51Hz, J ₂ =1.70Hz, 1H), 7.12(d, J=3.41Hz, 1H), 7.29(dd, J ₁ =10.04Hz, J ₂ =0.99Hz, 1H), 7.58(d, J=0.95Hz, 1H). MASS (ES+): 777.18(M+Na) ⁺ |
| 113.87 | 1.06(d, J=7.15Hz, 3H), 1.23(s, 3H), 1.33(s, 9H), 1.33-1.38(m, 1H), 1.56(s, 3H), 1.77-2.08(m, 3H), 2.29-2.53(m, 4H), 3.47(m, 1H), 3.61(d, J=16.75Hz, 1H), 3.80(d, J=16.80Hz, 1H), 4.38(d, J=16.03Hz, 1H), 4.44(d, J=8.47Hz, 1H), 4.72(d, J=15.70Hz, 1H), 4.78(s, 1H), 5.33-5.49(m, 1H), 6.39(dd, J ₁ =10.09Hz, J ₂ =1.72Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.45Hz, J ₂ =1.62Hz, 1H), 7.14(m, 2H), 7.59(d, J=0.74Hz, 1H). MASS (ES+): 696.20(M+Na) ⁺ |
| 113.88 | 1.06(d, J=7.17Hz, 3H), 1.18(s, 3H), 1.35-1.41(m, 2H), 1.55(s, 3H), 1.77-1.96(m, 3H), 2.17-2.47(m, 4H), 3.42-3.46(m, 1H), 3.66(d, J=16.77Hz, 1H), 3.76(d, J=16.80Hz, 1H), 4.15(q, J=7.15Hz, 2H), 4.45(d, J=8.67Hz, 1H), 4.59(d, J=15.47Hz, 1H), 4.73(d, J=15.36Hz, 1H), 5.32-5.49(m, 1H), 6.40(dd, J ₁ =10.09Hz, J ₂ =1.75Hz, 1H), 6.41(s, 1H), 6.51(dd, J ₁ =3.46Hz, J ₂ =1.81Hz, 1H), 7.13(d, J=3.36Hz, 1H), 7.20(dd, J ₁ =10.14Hz, J ₂ =1.08Hz, 1H), 7.59(s, 1H). MASS (ES+): 725.18(M + Na) ⁺ |
| 113.89 | 0.78(d, J=6.98Hz, 3H), 0.88(d, J=7.03Hz, 3H), (d, J=6.41Hz, 3H), 1.02-1.10(m, 5H), 1.20(s, 3H), 1.30-1.49(m, 3H), 1.55(s, 3H), 1.69-2.00(m, 7H), 2.28-2.51(m, 4H), 2.59(s, 1H), 3.42-3.46(m, 1H), 3.69(d, J=16.56Hz, 1H), 3.76(d, J=16.91Hz, 1H), 4.42(d, J=8.58Hz, 1H), 4.59(d, J=10.91Hz, J ₂ =4.39Hz, 1H), 4.62(d, J=15.52Hz, 1H), 4.72(d, J=15.41Hz, 1H), 5.32-5.49(m, 1H), 6.46(dd, J ₁ =10.18Hz, J ₂ =1.81Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.47Hz, J ₂ =1.78Hz, 1H), 7.12-7.14(m, 2H), 7.59(s, 1H). MASS (ES+): 779.32(M + Na) ⁺ |

| Comp. No | ¹ H-NMR (δ ppm), MASS (EI / ES+, m/z) |
|----------|---|
| IB.90 | 1.06(d, J=7.14Hz, 3H), 1.17(s, 3H), 1.34-1.40(m, 1H), 1.55(s, 3H), 1.76-1.97(m, 3H), 2.06(s, 3H), 2.28-2.54(m, 4H), 3.41-3.46(m, 1H), 3.67-3.75(m, 2H), 4.00(dd, J ₁ =18.22Hz, J ₂ =5.46Hz, 1H), 4.09(dd, J ₁ =18.22Hz, J ₂ =5.84Hz, 1H), 4.41(d, J=5.81Hz, 1H), 4.71(s, 2H), 5.32-5.49(m, 1H), 6.11(s, 1H), 6.39(dd, J ₁ =10.16Hz, J ₂ =1.79Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.45Hz, J ₂ =1.77Hz, 1H), 7.12(d, J=3.51Hz, 1H), 7.19(dd, J ₁ =10.09Hz, J ₂ =0.96Hz, 1H), 7.58(d, J=0.90Hz, 1H). MASS (ES+) : 696.13(M+Na) ⁺ |
| IB.91 | 0.96(d, J=6.72Hz, 3H), 1.05(d, J=7.15Hz, 3H), 1.19(s, 3H), 1.35-1.41(m, 1H), 1.55(s, 3H), 1.78-2.02(m, 4H), 2.30-2.63(m, 5H), 3.41-3.45(m, 1H), 3.70(d, J=16.81Hz, 1H), 3.76(d, J=16.76Hz, 1H), 3.93(d, J=6.80Hz, 2H), 4.44-4.46(m, 1H), 4.66(d, J=15.53Hz, 1H), 4.71(d, J=15.50Hz, 1H), 5.33-5.49(m, 1H), 6.40(dd, J ₁ =10.13Hz, J ₂ =1.67Hz, 1H), 6.46(s, 1H), 6.94(d, J=4.00Hz, 1H), 7.15(d, J=10.22Hz, 1H), 7.53(d, J=4.01Hz, 1H). MASS (ES+) : 747.0(M+Na) ⁺ |
| IB.92 | 1.05(d, J=7.14Hz, 3H), 1.18(d, J=6.98Hz, 3H), 1.19(d, J=7.13Hz, 3H), 1.22(s, 3H), 1.35-1.41(m, 1H), 1.56(s, 3H), 1.78-2.00(m, 3H), 2.28-2.63(m, 5H), 3.23(d, J=3.19Hz, 1H), 3.40-3.45(m, 1H), 3.67-3.75(m, 2H), 3.45-3.47(m, 1H), 3.49-3.77(m, 2H), 5.33-5.50(m, 1H), 6.41(dd, J ₁ =10.15Hz, J ₂ =1.79Hz, 1H), 6.46(s, 1H), 6.93(d, J=4.0Hz, 1H), 7.18(dd, J ₁ =10.14Hz, J ₂ =1.08Hz, 1H), 7.53(d, J=4.08Hz, 1H). MASS (ES+) : 717.12(M+Na) ⁺ |
| IB.93 | 1.06(d, J=7.16Hz, 3H), 1.17(s, 3H), 1.33(t, J=7.12Hz, 3H), 1.36-1.40(m, 1H), 1.55(s, 3H), 1.71-1.97(m, 3H), 2.28-2.48(m, 4H), 2.71(s, 1H), 3.42-3.48(m, 1H), 3.68(d, J=16.79Hz, 1H), 3.77(d, J=16.60Hz, 1H), 4.25-4.30(m, 2H), 4.44(m, 1H), 4.68(d, J=15.47Hz, 1H), 4.81(d, J=15.45Hz, 1H), 5.32-5.49(m, 1H), 6.21(d, J=12.01Hz, 1H), 6.32(d, J=11.98Hz, 1H), 6.40(dd, J ₁ =10.10Hz, J ₂ =1.75Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.47Hz, J ₂ =1.75Hz, 1H), 7.13(d, J=3.42Hz, 1H), 7.19(dd, J ₁ =10.25Hz, J ₂ =0.81Hz, 1H), 7.59(d, J=0.88Hz, 1H). MASS (ES+) : 723.22(M+Na) ⁺ |
| IB.94 | 1.06(d, J=7.17Hz, 3H), 1.18(s, 3H), 1.35-1.41(m, 1H), 1.56(s, 3H), 1.74-1.99(m, 3H), 2.28-2.47(m, 4H), 2.63-2.69(m, 4H), 2.93(s, 1H), 3.43-3.47(m, 1H), 3.66(d, J=16.86Hz, 1H), 3.70(s, 3H), 3.76(d, J=17.21Hz, 1H), 4.45(d, J=8.60Hz, 1H), 4.59(d, J=15.38Hz, 1H), 4.68(d, J=15.45Hz, 1H), 5.33-5.50(m, 1H), 6.41(dd, J ₁ =10.15Hz, J ₂ =1.76Hz, 1H), 6.46(s, 1H), 6.51(dd, J ₁ =3.45Hz, J ₂ =1.64Hz, 1H), 7.13(d, J=3.43Hz, 1H), 7.19(d, J=9.97Hz, 1H), 7.59(d, J=0.73Hz, 1H). MASS (ES+) : 711.19(M+Na) ⁺ |
| IB.95 | 1.06(d, J=7.07Hz, 3H), 1.18(s, 3H), 1.23(d, J=6.20Hz, 3H), 1.246(d, J=6.25Hz, 3H), 1.35-1.41(m, 1H), 1.56(s, 3H), 1.74-2.00(m, 3H), 2.28-2.51(m, 4H), 2.58-2.67(m, 4H), 3.00(s, 1H), 3.43-3.47(m, 1H), 3.65(d, J=16.97Hz, 1H), 3.76(d, J=17.57Hz, 1H), 4.46(d, J=8.05Hz, 1H), 4.59(d, J=15.43Hz, 1H), 4.72(d, J=15.40Hz, 1H), 4.96-5.06(m, 1H), 5.33-5.49(m, 1H), 6.41(dd, J ₁ =10.20Hz, J ₂ =1.24Hz, 1H), 6.46(s, 1H), 6.51(dd, J ₁ =3.13Hz, J ₂ =1.24Hz, 1H), 7.13(d, J=3.33Hz, 1H), 7.19(d, J=10.11Hz, 1H), 7.59(s, 1H). MASS (ES+) : 739.31(M+Na) ⁺ |
| IB.96 | 0.92(d, J=6.64Hz, 6H), 1.06(d, J=6.64Hz, 3H), 1.18(s, 3H), 1.36-1.41(m, 1H), 1.56(s, 3H), 1.74-2.06(m, 4H), 2.29-2.51(m, 4H), 2.66-2.69(m, 4H), 2.99(s, 1H), 3.43-3.45(m, 1H), 3.66(d, J=16.76Hz, 1H), 3.77(d, J=16.64Hz, 1H), 3.88(d, J=6.57Hz, 2H), 4.46(d, J=6.66Hz, 1H), 4.59(d, J=15.40Hz, 1H), 4.73(d, J=15.33Hz, 1H), 5.33-5.49(m, 1H), 6.41(d, J=10.11Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =2.62Hz, J ₂ =1.21Hz, 1H), 7.13(d, J=3.43Hz, 1H), 7.19(d, J=10.11Hz, 1H), 7.59(s, 1H). MASS (ES+) : 753.35(M+Na) ⁺ |
| IB.97 | 0.92(t, J=7.32Hz, 3H), 1.05(d, J=7.15Hz, 3H), 1.18(s, 3H), 1.20-1.38(m, 5H), 1.40-1.62(m, 4H), 1.77-2.00(m, 3H), 2.25-2.50(m, 4H), 2.61-2.69(m, 4H), 2.97(s, 1H), 3.42-3.47(m, 1H), 3.65(d, J=16.71Hz, 1H), 3.76(d, J=16.87Hz, 1H), 4.10(t, J=6.71Hz, 2H), 4.45(d, J=8.59Hz, 1H), 4.59(d, J=15.45Hz, 1H), 4.72(d, J=15.43Hz, 1H), 5.32-5.49(m, 1H), 6.39(dd, J ₁ =10.16Hz, J ₂ =1.78Hz, 1H), 6.46(s, 1H), 6.50(dd, J ₁ =3.74Hz, J ₂ =1.47Hz, 1H), 7.13(d, J=3.44Hz, 1H), 7.19(dd, J ₁ =10.10Hz, J ₂ =0.91Hz, 1H), 7.59(d, J=1.08Hz, 1H). MASS (ES+) : 753.18(M+Na) ⁺ |
| IB.98 | 1.06(d, J=7.12Hz, 3H), 1.21(s, 3H), 1.31(s, 6H), 1.35-1.41(m, 1H), 1.56(s, 3H), 1.77-2.01(m, 3H), 2.29-2.53(m, 4H), 2.91(d, J=2.26Hz, 1H), 3.43-3.47(m, 1H), 3.58-3.64(m, 2H), 3.66(d, J=17.24Hz, 1H), 3.76(d, J=16.76Hz, 1H), 4.45-4.47(m, 1H), 4.57(d, J=15.36Hz, 1H), 4.78(d, J=15.36Hz, 1H), 5.34-5.50(m, 1H), 6.40(dd, J ₁ =10.15Hz, J ₂ =1.46Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.28Hz, J ₂ =1.48Hz, 1H), 7.14(d, J=3.49Hz, 1H), 7.18(dd, J ₁ =10.12Hz, 1H), 7.59(s, 1H). MASS (ES+) : 715.02(M+Na) ⁺ |
| IB.99 | 0.94(d, J=6.70Hz, 6H), 1.06(d, J=7.12Hz, 3H), 1.17(s, 3H), 1.25-1.40(m, 1H), 1.55(s, 3H), 1.73-1.99(m, 4H), 2.28-2.46(m, 4H), 2.73(s, 1H), 3.43-3.47(m, 1H), 3.67(d, J=16.91Hz, 1H), 3.78(d, J=17.01Hz, 1H), 3.99(d, J=6.69Hz, 2H), 4.44(d, J=8.42Hz, 1H), 4.67(d, J=15.51Hz, 1H), 4.81(d, J=15.46Hz, 1H), 5.32-5.49(m, 1H), 6.22(d, J=12.05Hz, 1H), 6.34(d, J=12.03Hz, 1H), 6.39(dd, J ₁ =10.13Hz, J ₂ =1.65Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.57Hz, J ₂ =1.85Hz, 1H), 7.13(d, J=3.44Hz, 1H), 7.19(d, J=10.20Hz, 1H), 7.59(d, J=0.67Hz, 1H). MASS (ES+) : 751.16(M+Na) ⁺ |
| IB.100 | 1.06(d, J=7.15Hz, 3H), 1.16(s, 3H), 1.25-1.41(m, 1H), 1.56(s, 3H), 1.77-1.96(m, 3H), 2.28-2.49(m, 4H), 2.71(s, 1H), 3.41-3.45(m, 1H), 3.67(d, J=16.72Hz, 1H), 3.77(d, J=16.87Hz, 1H), 3.82(s, 3H), 4.46(m, 1H), 4.74(d, J=15.44Hz, 1H), 4.80(d, J=15.44Hz, 1H), 5.32-5.49(m, 1H), 6.42(dd, J ₁ =10.16Hz, J ₂ =1.79Hz, 1H), 6.46(s, 1H), 6.50(dd, J ₁ =3.45Hz, J ₂ =1.76Hz, 1H), 6.86(d, J=15.85Hz, 1H), 6.90(d, J=15.82Hz, 1H), 7.13(d, J=3.51Hz, 1H), 7.20(dd, J ₁ =10.00Hz, J ₂ =1.00Hz, 1H), 7.59(d, J=0.73Hz, 1H). MASS (ES+) : 709.11(M+Na) ⁺ |
| IB.101 | 0.96(d, J=6.59Hz, 6H), 1.05(d, J=7.115Hz, 3H), 1.20(s, 3H), 1.35-1.41(m, 1H), 1.56(s, 3H), 1.77-2.01(m, 3H), 2.052-1.2(m, 1H), 2.21-2.52(m, 6H), 3.07(d, J=2.84Hz, 1H), 3.43-3.47(m, 1H), 3.65(d, J=16.86Hz, 1H), 3.77(d, J=16.79Hz, 1H), 4.45(d, J=8.63Hz, 1H), 4.52(d, J=15.42Hz, 1H), 4.73(d, J=15.34Hz, 1H), 5.33-5.48(m, 1H), 6.40(dd, J ₁ =10.12Hz, J ₂ =1.71Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.43Hz, J ₂ =1.61Hz, 1H), 7.13(d, J=3.43Hz, 1H), 7.19(dd, J ₁ =10.19Hz, 1H), 7.58(d, J=0.85Hz, 1H). MASS (ES+) : 681.0(M+Na) ⁺ |
| IB.102 | 0.90(q, J=7.40Hz, 3H), 1.05(d, J=7.14Hz, 3H), 1.23(s, 3H), 1.35-1.41(m, 1H), 1.50-1.65(m, 4H), 1.57(s, 3H), 1.77-2.01(m, 3H), 2.21-2.55(m, 5H), 3.31(d, J=2.47Hz, 1H), 3.44-3.47(m, 1H), 3.64(d, J=16.73Hz, 1H), 3.76(d, J=16.70Hz, 1H), 4.43-4.46(m, 1H), 4.49(d, J=15.39Hz, 1H), 4.78(d, J=15.38Hz, 1H), 5.34-5.50(m, 1H), 6.40(dd, J ₁ =10.08Hz, J ₂ =1.62Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.37Hz, J ₂ =1.57Hz, 1H), 7.13(d, J=3.45Hz, 1H), 7.19(dd, J ₁ =10.16Hz, 1H), 7.59(s, 1H). MASS (ES+) : 695.0(M+Na) ⁺ |
| IB.103 | 1.05(d, J=7.18Hz, 3H), 1.23(s, 3H), 1.34-1.40(m, 1H), 1.56(s, 3H), 1.77-2.08(m, 3H), 2.17-2.53(m, 4H), 2.92(s, 6H), 3.44-3.48(m, 1H), 3.64(d, J=16.62Hz, 1H), 3.76(d, J=16.16Hz, 1H), 4.01(d, J=3.45Hz, 1H), 4.41-4.43(m, 1H), 4.49(d, J=15.61Hz, 1H), 4.76(d, J=15.59Hz, 1H), 5.33-5.50(m, 1H), 6.39(dd, J ₁ =10.11Hz, J ₂ =1.75Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.47Hz, J ₂ =1.74Hz, 1H), 7.14(d, J=3.40Hz, 1H), 7.18(dd, J ₁ =10.16Hz, J ₂ =0.91Hz, 1H), 7.59(s, 1H). MASS (ES+) : 668.0(M+Na) ⁺ |
| IB.104 | 1.06(d, J=7.12Hz, 3H), 1.21(s, 3H), 1.35-1.41(m, 1H), 1.56(s, 3H), 1.79(s, 3H), 1.80(s, 3H), 1.80-1.98(m, 3H), 2.28-2.52(m, 4H), 2.70(d, J=2.16Hz, 1H), 3.42-3.46(m, 1H), 3.67-3.77(m, 2H), 3.44-3.46(m, 1H), 4.62-4.85(m, 2H), 5.33-5.49(m, 1H), 6.39(dd, J ₁ =10.15Hz, J ₂ =1.70Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.44Hz, J ₂ =1.71Hz, 1H), 7.12(dd, J=3.42Hz, 1H), 7.16(dd, J ₁ =10.07Hz, J ₂ =0.93Hz, 1H), 7.58(s, 1H). MASS (ES+) : 670.0 |

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| Comp. No. | ¹ H-NMR (δ ppm), MASS (EI / ES+, m/z) |
|-----------|--|
| IB.105 | 0.90(d, J=6.31Hz, 3H), 0.91(d, J=6.24Hz, 3H), 1.06(d, J=7.14Hz, 3H), 1.20(s, 3H), 1.35-1.41(m, 1H), 1.47-1.59(m, 3H), 1.56(s, 3H), 1.77-2.00(m, 3H), 2.29-2.52(m, 4H), 2.35(t, J=7.72Hz, 2H), 3.10(d, J=2.65Hz, 1H), 3.43-3.46(m, 1H), 3.65(d, J=16.80Hz, 1H), 3.77(d, J=16.81Hz, 1H), 4.44-4.46(m, 1H), 4.53(d, J=15.38Hz, 1H), 4.71(d, J=15.33Hz, 1H), 5.33-5.50(m, 1H), 6.39(dd, J ₁ =10.16Hz, J ₂ =1.74Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.43Hz, J ₂ =1.77Hz, 1H), 7.13(d, J=3.60Hz, 1H), 7.18(dd, J ₁ =10.22Hz, J ₂ =0.72Hz, 1H), 7.59(s, 1H). MASS (ES+): 673.0 |
| IB.106 | 1.06(d, J=7.18Hz, 3H), 1.17(s, 3H), 1.35-1.41(m, 1H), 1.55(s, 3H), 1.74-1.97(m, 3H), 2.28-2.48(m, 4H), 2.65(s, 1H), 2.69-2.77(m, 4H), 3.43-3.47(m, 1H), 3.67(d, J=16.80Hz, 1H), 3.76(d, J=16.76Hz, 1H), 4.45(d, J=8.68Hz, 1H), 4.61(d, J=15.48Hz, 1H), 4.74(d, J=15.38Hz, 1H), 5.32-5.49(m, 1H), 5.71(d, J=50.60Hz, 2H), 6.41(dd, J ₁ =10.18Hz, J ₂ =1.81Hz, 1H), 6.45(s, 1H), 6.51(dd, J ₁ =3.49Hz, J ₂ =1.64Hz, 1H), 7.13(d, J=3.29Hz, 1H), 7.18(dd, J ₁ =10.16Hz, J ₂ =0.91Hz, 1H), 7.59(d, J=0.79Hz, 1H). MASS (ES+): 729.28(M+Na) ⁺ |
| IB.106 | 1.06(d, J=7.17Hz, 3H), 1.17(s, 3H), 1.25-1.41(m, 1H), 1.54(s, 3H), 1.77-1.98(m, 3H), 2.28-2.49(m, 5H), 3.42-3.47(m, 1H), 3.69(d, J=16.78Hz, 1H), 3.78(d, J=16.84Hz, 1H), 4.44(d, J=8.74Hz, 1H), 4.66(d, J=17.09Hz, 1H), 4.84(d, J=17.31Hz, 1H), 5.32-5.49(m, 1H), 5.78(dd, J ₁ =50.72Hz, J ₂ =1.89Hz, 1H), 5.82(dd, J ₁ =50.31Hz, J ₂ =1.91Hz, 1H), 6.34(d, J=12.00Hz, 1H), 6.38(d, J=12.14Hz, 1H), 6.39(dd, J ₁ =3.46Hz, J ₂ =1.60Hz, 1H), 6.45(s, 1H), 6.51(dd, J ₁ =3.46Hz, J ₂ =1.60Hz, 1H), 7.13(d, J=3.42Hz, 1H), 7.17(d, J=10.16Hz, 1H), 7.59(d, J=0.84Hz, 1H). MASS (ES+): 727.26(M+Na) ⁺ |
| IB.108 | 1.06(d, J=7.15Hz, 3H), 1.19(s, 3H), 1.25-1.41(m, 1H), 1.55(s, 3H), 1.74-1.97(m, 3H), 2.29-2.50(m, 4H), 2.81(s, 1H), 3.43(m, 3H), 3.68(d, J=17.09Hz, 1H), 3.75(d, J=16.15Hz, 1H), 3.77(s, 3H), 4.46(d, J=8.71Hz, 1H), 4.62(d, J=15.45Hz, 1H), 4.80(d, J=15.32Hz, 1H), 5.33-5.50(m, 1H), 6.41(dd, J ₁ =10.09Hz, J ₂ =1.69Hz, 1H), 6.45(s, 1H), 6.51(dd, J ₁ =3.43Hz, J ₂ =1.69Hz, 1H), 7.13(d, J=3.39Hz, 1H), 7.18(d, J=10.15Hz, 1H), 7.59(d, J=0.88Hz, 1H). MASS (ES+): 697.29(M+Na) ⁺ |
| IB.109 | 1.06(d, J=7.15Hz, 3H), 1.21(s, 3H), 1.37-1.41(m, 1H), 1.44(s, 3H), 1.45(s, 3H), 1.56(s, 3H), 1.77-1.97(m, 3H), 2.29-2.52(m, 4H), 3.05(d, J=2.12Hz, 1H), 3.42-3.47(m, 3H), 2.71-3.75(m, 5H), 4.46(d, J=8.69Hz, 1H), 4.62(d, J=15.42Hz, 1H), 4.74(d, J=15.43Hz, 1H), 5.33-5.50(m, 1H), 6.41(dd, J ₁ =10.15Hz, J ₂ =1.76Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.48Hz, J ₂ =1.64Hz, 1H), 7.13(d, J=3.41Hz, 1H), 7.18(dd, J ₁ =10.12Hz, J ₂ =0.95Hz, 1H), 7.59(d, J=0.88Hz, 1H). MASS (ES+): 725.30(M+Na) ⁺ |
| IB.110 | 1.06(d, J=7.15Hz, 3H), 1.18(s, 1H), 1.35-1.42(m, 1H), 1.15(s, 3H), 1.47(s, 3H), 1.55(s, 3H), 1.59-1.98(m, 3H), 2.17-2.51(m, 4H), 3.88(m, 1H), 2.97(s, 1H), 3.39-3.45(m, 1H), 3.72(s, 2H), 4.43-4.45(m, 1H), 4.64-4.81(m, 2H), 5.33-5.49(m, 1H), 6.39(d, J=10.16Hz, 1H), 6.39(d, J=1.75Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.45Hz, J ₂ =1.76Hz, 1H), 7.13(d, J=3.44Hz, 1H), 7.17(dd, J ₁ =10.12Hz, J ₂ =0.76Hz, 1H), 7.58(d, J=0.90Hz, 1H). MASS (ES+): 683.10(M+Na) ⁺ |
| IB.111 | 1.06(d, J=7.13Hz, 3H), 1.23(s, 3H), 1.36-1.41(m, 1H), 1.56(d, J=21.29Hz, 3H), 1.62(d, J=21.37Hz, 3H), 1.77-1.99(m, 3H), 2.28-2.53(m, 4H), 2.95(s, 1H), 3.39-3.43(m, 1H), 3.67(d, J=16.95Hz, 1H), 3.74(d, J=16.49Hz, 1H), 4.44(d, J=8.03Hz, 1H), 4.60(d, J=15.23Hz, 1H), 4.86(d, J=15.34Hz, 1H), 5.33-5.50(m, 1H), 6.39(dd, J ₁ =10.11Hz, J ₂ =1.63Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.35Hz, J ₂ =1.50Hz, 1H), 7.12(d, J=3.42Hz, 1H), 7.19(d, J=10.13Hz, 1H), 7.58(s, 1H). MASS (ES+): 685.10(M+Na) ⁺ |
| IB.112 | 1.06(d, J=7.15Hz, 3H), 1.17(s, 3H), 1.35-1.40(m, 1H), 1.55(s, 3H), 1.76-1.97(m, 3H), 2.28-2.47(m, 4H), 2.71(s, 1H), 3.42-3.47(m, 1H), 3.69(d, J=16.76Hz, 1H), 3.78(d, J=16.97Hz, 1H), 3.82(s, 3H), 4.44(d, J=8.22Hz, 1H), 4.69(d, J=15.50Hz, 1H), 4.82(d, J=15.54Hz, 1H), 5.30-5.60(m, 1H), 6.23(d, J=11.91Hz, 1H), 6.33(d, J=12.06Hz, 1H), 6.40(dd, J ₁ =10.14Hz, J ₂ =1.58Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.31Hz, J ₂ =1.51Hz, 1H), 7.13(d, J=3.47Hz, 1H), 7.19(d, J=10.14Hz, 1H), 7.59(s, 1H). MASS (ES+): 687.73 |
| IB.113 | 1.06(d, J=7.12Hz, 3H), 1.16(s, 3H), 1.32(t, 3H), 1.35-1.42(m, 2H), 1.56(s, 3H), 1.72-1.97(m, 3H), 2.28-2.48(m, 4H), 2.86(s, 1H), 3.42-3.45(m, 1H), 3.68(d, J=16.77Hz, 1H), 3.77(d, J=16.62Hz, 1H), 4.26(q, J=7.07Hz, 2H), 4.46(d, J=8.36Hz, 1H), 4.75(d, J=15.39Hz, 1H), 4.80(d, J=15.39Hz, 1H), 5.30-5.49(m, 1H), 6.41(dd, J ₁ =10.14Hz, J ₂ =1.76Hz, 1H), 6.46(s, 1H), 6.50(dd, J ₁ =3.45Hz, J ₂ =1.76Hz, 1H), 6.85(d, J=15.75Hz, 1H), 6.90(d, J=15.90Hz, 1H), 7.13(d, J=3.74Hz, 1H), 7.20(dd, J ₁ =10.19Hz, J ₂ =0.84Hz, 1H), 7.59(d, J=0.87Hz, 1H). MASS (ES+): 701.0 |
| IB.114 | 0.90(d, J=6.72Hz, 6H), 1.06(d, J=7.13Hz, 3H), 1.17(s, 3H), 1.25-1.41(m, 1H), 1.56(s, 3H), 1.74-2.00(m, 4H), 2.28-2.49(m, 4H), 2.86(s, 1H), 3.42-3.45(m, 1H), 3.68(d, J=16.76Hz, 1H), 3.78(d, J=16.83Hz, 1H), 4.00(d, J=6.70Hz, 2H), 4.46(d, J=8.56Hz, 1H), 4.75(d, J=15.47Hz, 1H), 4.80(d, J=15.38Hz, 1H), 5.30-5.49(m, 1H), 6.41(dd, J ₁ =10.15Hz, J ₂ =1.80Hz, 1H), 6.46(s, 1H), 6.50(dd, J ₁ =3.50Hz, J ₂ =1.73Hz, 1H), 6.85(d, J=15.79Hz, 1H), 6.92(d, J=15.93Hz, 1H), 7.13(d, J=3.32Hz, 1H), 7.20(dd, J ₁ =10.12Hz, J ₂ =0.96Hz, 1H), 7.59(d, J=0.90Hz, 1H). MASS (ES+): 729.1 |
| IB.115 | 0.95(t, J=7.37Hz, 6H), 1.06(d, J=7.10Hz, 3H), 1.17(s, 3H), 1.36-1.45(m, 3H), 1.56(s, 3H), 1.67-1.97(m, 7H), 2.28-2.51(m, 4H), 2.82(s, 1H), 3.42-3.45(m, 1H), 3.72(d, J=16.78Hz, 1H), 3.77(d, J=16.74Hz, 1H), 4.22(t, J=6.67Hz, 2H), 4.47(d, J=8.32Hz, 1H), 4.75(d, J=15.54Hz, 1H), 4.79(d, J=15.52Hz, 1H), 5.33-5.49(m, 1H), 6.41(dd, J ₁ =10.13Hz, J ₂ =1.66Hz, 1H), 6.46(s, 1H), 6.50(dd, J ₁ =3.33Hz, J ₂ =1.52Hz, 1H), 6.84(d, J=15.81Hz, 1H), 6.90(d, J=15.77Hz, 1H), 7.13(d, J=3.40Hz, 1H), 7.20(d, J=10.18Hz, 1H), 7.59(s, 1H). MASS (ES+): 729.1 |
| IB.116 | 1.06(d, J=7.16Hz, 3H), 1.18(d, J=7.07Hz, 3H), 1.19(d, J=6.98Hz, 3H), 1.23(s, 3H), 1.31-1.36(m, 1H), 1.62(s, 3H), 1.75-2.04(m, 4H), 2.17-2.82(m, 6H), 3.19(s, 1H), 3.41-3.45(m, 1H), 3.65-3.75(m, 1H), 4.53(d, J=15.43Hz, 1H), 4.63(s, 1H), 4.73(d, J=15.42Hz, 1H), 6.11(s, 1H), 6.38(dd, J ₁ =10.04Hz, J ₂ =1.72Hz, 1H), 6.49(dd, J ₁ =3.43Hz, J ₂ =1.62Hz, 1H), 7.18(d, J=3.35Hz, 1H), 7.24(d, J=10.57Hz, 1H), 7.58(d, J=0.75Hz, 1H). MASS (ES+): 665.1(M+Na) ⁺ |
| IB.117 | 0.91(t, J=7.48Hz, 3H), 1.05(d, J=7.13Hz, 3H), 1.15(d, 3H, J=7.02Hz), 1.22(s, 3H), 1.38-2.00(m, 6H), 1.56(s, 3H), 2.28-2.46(m, 5H), 3.41(d, J=3.09Hz), 3.45(m, 1H), 3.68-3.73(m, 2H), 4.44-4.46(m, 1H), 4.51(d, J=15.29Hz, 1H), 4.75(d, J=15.38Hz, 1H), 5.33-5.52(m, 1H), 6.40(dd, J ₁ =10.18Hz, J ₂ =1.78Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.46Hz, J ₂ =1.61Hz, 1H), 7.13(d, J=3.32Hz, 1H), 7.18(d, J=10.03Hz, 1H), 7.22-7.25(m, 2H), 7.57(d, J=0.83Hz, 1H), 7.61(d, J=0.85Hz, 1H). MASS (ES+): 669.1 |
| IB.118 | 1.05(d, J=7.15Hz, 3H), 1.20(s, 3H), 1.35-1.40(m, 1H), 1.59(s, 3H), 1.77-2.00(m, 3H), 2.28-2.52(m, 4H), 3.12(d, J=2.71Hz, 1H), 3.41-3.45(m, 1H), 3.68(d, J=16.77Hz, 1H), 3.75(d, J=16.87Hz, 1H), 4.48-4.50(m, 1H), 4.75-4.96(m, 2H), 5.33-5.50(m, 1H), 6.41(dd, J ₁ =10.08Hz, J ₂ =1.70Hz, 1H), 6.46(s, 1H), 6.49(dd, J ₁ =3.44Hz, J ₂ =1.76Hz, 1H), 6.55(dd, J ₁ =3.51Hz, J ₂ =1.65Hz, 1H), 7.11(d, J=3.34Hz, 1H), 7.22-7.25(m, 2H), 7.57(d, J=0.83Hz, 1H), 7.61(d, J=0.85Hz, 1H). MASS (ES+): 669.1 |
| IB.119 | 1.06(d, J=7.12Hz, 3H), 1.17(s, 3H), 1.30(d, J=6.20Hz, 6H), 1.36-1.41(m, 1H), 1.56(s, 3H), 1.72-1.97(m, 3H), 2.28-2.50(m, 4H), 2.82(s, 1H), 3.42-3.45(m, 1H), 3.67(d, J=16.71Hz, 1H), 3.76(d, J=16.51Hz, 1H), 4.46(d, J=8.56Hz, 1H), 4.74(d, J=15.47Hz, 1H), 4.79(d, J=15.41Hz, 1H), 5.08-5.13(m, 1H), 5.33-5.49(m, 1H), 6.41(dd, J ₁ =10.16Hz, J ₂ =1.58Hz, 1H), 6.46(s, 1H), 6.50(dd, J ₁ =3.36Hz, J ₂ =1.62Hz, 1H), 6.83(d, J=15.87Hz, 1H), 6.88(d, J=15.76Hz, 1H), 7.13(d, J=3.39Hz, 1H), 7.20(d, J=10.29Hz, 1H), 7.58(s, 1H). MASS (ES+): 715.1 |

SUBSTITUTE SHEET (RULE 26)

| Comp. No | ¹ H-NMR (δ ppm), MASS (EI / ES+, m/z) |
|----------|--|
| III.120 | 1.03(d, 3H, J=7.05Hz), 1.15(s, 3H), 1.16(s, 6H), 1.33-1.39(m, 1H), 1.55(s, 1H), 1.67-2.00(m, 3H), 2.29-2.59(m, 4H), 3.39-3.49(m, 1H), 3.51(d, 1H, J=4.81Hz), 3.54(d, 1H, J=11.65Hz), 3.71(d, 1H, J=16.53Hz), 3.77(d, 1H, J=16.53Hz), 4.73(t, 1H, J=5.86Hz), 4.33-4.35(m, 1H), 4.64(d, 1H, J=15.64Hz), 4.68(d, 1H, J=15.66Hz), 5.07(s, 1H), 5.37-5.53(m, 1H), 6.31-6.33(m, 1H), 6.33(s, 1H), 6.54(dd, 1H, J ₁ =3.41Hz, J ₂ =1.58Hz), 7.12(d, 1H, J=3.37Hz), 7.26(d, 1H, J=10.30Hz), 7.66(s, 1H). MASS (ES+) : 697.07(M+Na) ⁺ |
| III.121 | 1.05(d, 3H, J=7.11Hz), 1.18(s, 3H), 1.35-1.40(m, 1H), 1.56(s, 1H), 1.73-2.00(m, 3H), 2.28-2.55(m, 4H), 3.01(d, 1H, J=2.36Hz), 3.42-3.46(m, 1H), 3.66(d, 1H, J=16.75Hz), 3.77(d, 1H, J=16.77Hz), 4.46(d, 1H, J=8.20Hz), 4.67(d, 1H, J=15.43Hz), 4.78(d, 1H, J=15.43Hz), 5.33-5.49(m, 1H), 5.92(d, 1H, J=10.35Hz), 6.12(dd, 1H, J ₁ =17.32Hz, J ₂ =10.52Hz), 6.39-6.46(m, 1H), 6.43(d, 1H, J=13.31Hz), 6.50(dd, 1H, J ₁ =3.27Hz, J ₂ =1.52Hz), 7.12(d, 1H, J=3.39Hz), 7.19(d, 1H, J=10.12Hz), 7.58(s, 1H). MASS (ES+) : 629.05 |
| III.122 | 0.86(t, J=6.57Hz, 6H), 1.06(d, J=7.13Hz, 3H), 1.16(s, 3H), 1.27-1.41(m, 1H), 1.55(s, 3H), 1.61-1.98(m, 8H), 2.29-2.51(m, 4H), 3.38-3.42(m, 1H), 3.64-3.79(m, 3H), 4.36(d, J=6.47Hz, 1H), 4.68-4.82(m, 3H), 5.35-5.51(m, 1H), 6.35(dd, J ₁ =10.15Hz, J ₂ =1.67Hz, 1H), 6.38(s, 1H), 6.52(dd, J ₁ =3.40Hz, J ₂ =1.68Hz, 1H), 7.12(d, J=3.46Hz, 1H), 7.27(d, J=9.97Hz, 1H), 7.62(s, 1H). MASS (ES+) : 689.1 |
| III.123 | 0.30-0.34(m, 2H), 0.60-0.64(m, 2H), 1.06(d, J=7.15Hz, 3H), 1.19(s, 3H), 1.36-1.41(m, 1H), 1.55(s, 3H), 1.64-1.99(m, 4H), 2.29-2.51(m, 4H), 2.61(s, 1H), 3.42-3.47(m, 1H), 3.69(d, J=16.73Hz, 1H), 3.77(d, J=16.72Hz, 1H), 3.99(d, J=7.39Hz, 2H), 4.44(d, J=8.47Hz, 1H), 4.65-4.74(m, 2H), 5.33-5.49(m, 1H), 6.41(dd, J ₁ =10.13Hz, J ₂ =1.66Hz, 1H), 6.46(s, 1H), 6.51(dd, J ₁ =3.43Hz, J ₂ =1.68Hz, 1H), 7.13-7.17(m, 2H), 7.59(s, 1H). MASS (ES+) : 673.0 |
| III.124 | 1.05(d, J=7.07Hz, 3H), 1.15(s, 3H), 1.29-1.41(m, 1H), 1.54(s, 3H), 1.72-2.00(m, 3H), 2.28-2.50(m, 4H), 2.76(s, 3H), 3.39-3.43(m, 1H), 3.73(d, J=16.53Hz, 1H), 3.79(d, J=16.54Hz, 1H), 4.16(m, 2H), 4.36(d, J=6.03Hz, 1H), 4.93(s, 1H), 5.35-5.51(m, 1H), 6.35(d, J=10.19Hz, 1H), 6.37(s, 1H), 6.52(dd, J ₁ =3.09Hz, J ₂ =1.32Hz, 1H), 7.12(d, J=3.40Hz, 1H), 7.27(d, J=10.15Hz, 1H), 7.62(s, 1H). MASS (ES+) : 707.1(M+Na) ⁺ |
| III.125 | 1.06(d, J=7.13Hz, 3H), 1.20-1.42(m, 8H), 1.55(s, 3H), 1.71-2.00(m, 7H), 2.28-2.49(m, 4H), 2.66(s, 1H), 3.43-3.47(m, 1H), 3.69(d, J=17.44Hz, 1H), 3.76(d, J=16.97Hz, 1H), 4.44(d, J=8.32Hz, 1H), 4.63(d, J=15.47Hz, 1H), 4.70(d, J=15.45Hz, 1H), 5.05-5.09(m, 1H), 5.33-5.49(m, 1H), 6.40(dd, J ₁ =10.14Hz, J ₂ =1.48Hz, 1H), 6.46(s, 1H), 6.51(dd, J ₁ =3.32Hz, J ₂ =1.53Hz, 1H), 7.13-7.16(m, 2H), 7.59(s, 1H). MASS (ES+) : 687.1 |
| III.126 | 1.06(d, J=7.07Hz, 3H), 1.20-1.99(m, 15H), 2.20-2.49(m, 5H), 2.60(s, 1H), 3.44(m, 1H), 3.69(d, J=16.73Hz, 1H), 3.77(d, J=16.67Hz, 1H), 4.04(d, J=7.15Hz, 2H), 4.44(d, J=7.91Hz, 1H), 4.64-4.73(m, 2H), 5.33-5.49(m, 1H), 6.40(d, J=10.02Hz, 1H), 6.46(s, 1H), 6.50(m, 1H), 7.13-7.17(m, 2H), 7.59(s, 1H). MASS (ES+) : 701.1 |
| III.127 | 1.06(d, J=7.16Hz, 3H), 1.17(d, J=2.39Hz, 3H), 1.18(d, J=2.37Hz, 3H), 1.21(s, 3H), 1.35-1.41(m, 1H), 1.56(s, 3H), 1.77-2.00(m, 3H), 2.29-2.62(m, 5H), 3.21(d, J=2.62Hz, 1H), 3.42-3.49(m, 1H), 3.67(d, J=16.86Hz, 1H), 3.75(d, J=16.81Hz, 1H), 4.45(d, J=8.59Hz, 1H), 4.52(d, J=15.45Hz, 1H), 4.74(d, J=15.33Hz, 1H), 5.33-5.50(m, 1H), 6.40(dd, J ₁ =10.05Hz, J ₂ =1.65Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.50Hz, J ₂ =1.69Hz, 1H), 7.13(dd, J ₁ =3.56Hz, J ₂ =0.57Hz, 1H), 7.19(dd, J ₁ =0.75Hz, J ₂ =0.22Hz, 1H), 7.58(s, 1H). MASS (ES+) : 673.1 |
| III.128 | 1.06(d, J=7.12Hz, 3H), 1.18(s, 3H), 1.35(s, 3H), 1.38-1.41(m, 1H), 1.43(s, 3H), 1.55(s, 3H), 1.80-1.97(m, 3H), 2.40-2.64(m, 5H), 3.39-3.50(m, 1H), 3.71-3.83(m, 3H), 4.07-4.33(m, 4H), 4.44(d, J=8.59Hz, 1H), 4.69-4.72(m, 2H), 5.31-5.51(m, 1H), 6.40(dd, J ₁ =10.17Hz, J ₂ =1.73Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.47Hz, J ₂ =1.64Hz, 1H), 7.13(d, J=3.43Hz, 1H), 7.16(d, J=10.04Hz, 1H), 7.59(s, 1H). MASS (ES+) : 733.0 |
| III.129 | 1.05(d, J=7.13Hz, 3H), 1.12-1.14(m, 6H), 1.24(s, 3H), 1.35-1.39(m, 1H), 1.56(s, 3H), 1.80-2.11(m, 3H), 2.30-2.42(m, 4H), 3.19-3.35(m, 4H), 3.43-3.52(m, 1H), 3.60-3.82(m, 2H), 4.12(d, J=3.12Hz, 1H), 4.42(d, J=8.25Hz, 1H), 4.48(d, J=15.61Hz, 1H), 4.76(d, J=15.96Hz, 1H), 5.32-5.52(m, 1H), 6.39(dd, J ₁ =10.12Hz, J ₂ =1.75Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.47Hz, J ₂ =1.67Hz, 1H), 7.14(d, J=3.39Hz, 1H), 7.16(dd, J ₁ =10.13Hz, J ₂ =0.97Hz, 1H), 7.58(d, J=0.78Hz, 1H). MASS (ES+) : 674.1 |
| III.130 | 1.05(d, J=7.17Hz, 3H), 1.22(s, 3H), 1.34-1.40(m, 1H), 1.56(s, 3H), 1.56-1.60(m, 6H), 1.77-2.07(m, 3H), 2.28-2.42(m, 4H), 3.40-3.49(m, 5H), 3.62-3.82(m, 2H), 3.86(d, J=3.25Hz, 1H), 3.42(d, J=8.41Hz, 1H), 4.52(d, J=15.61Hz, 1H), 4.74(d, J=15.58Hz, 1H), 5.32-5.51(m, 1H), 6.39(dd, J ₁ =10.11Hz, J ₂ =1.68Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.41Hz, J ₂ =1.58Hz, 1H), 7.13(d, J=3.41Hz, 1H), 7.18(d, J=10.00Hz, 1H), 7.59(d, J=0.74Hz, 1H). MASS (ES+) : 686.1 |
| III.131 | 1.05(d, J=7.11Hz, 3H), 1.20(s, 3H), 1.34-1.40(m, 1H), 1.55(s, 3H), 1.77-2.04(m, 3H), 2.30(s, 3H), 2.39-2.53(m, 8H), 3.48(m, 5H), 3.64(d, J=15.98Hz, 1H), 3.66(s, 1H), 3.77(d, J=17.39Hz, 1H), 4.42(d, J=8.06Hz, 1H), 4.57(d, J=15.59Hz, 1H), 4.73(d, J=15.61Hz, 1H), 5.32-5.49(m, 1H), 6.39(dd, J ₁ =10.15Hz, J ₂ =1.22Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.11Hz, J ₂ =1.26Hz, 1H), 7.14(d, J=3.49Hz, 1H), 7.17(d, J=10.13Hz, 1H), 7.59(s, 1H). MASS (ES+) : 701.1 |
| III.132 | 1.12(s, 3H), 1.29-1.34(m, 1H), 1.48(d, J=7.34Hz, 3H), 1.55(s, 3H), 1.74-2.16(m, 4H), 2.33-2.81(m, 4H), 3.35(t, d, J ₁ =16.65Hz, J ₂ =2.31Hz, 1H), 3.82(t, d, J ₁ =16.66Hz, J ₂ =1.98Hz, 1H), 4.26(m, 2H), 4.46(d, J=8.42, 1H), 5.32-5.49(m, 1H), 6.39(dd, J ₁ =10.13Hz, J ₂ =1.75Hz, 1H), 6.44(s, 1H), 6.51(dd, J ₁ =3.50Hz, J ₂ =1.65Hz, 1H), 7.17-7.19(m, 1H), 7.61(s, 1H). MASS (ES+) : 575.1 |
| III.133 | 1.14(s, 3H), 1.19(d, J=6.97Hz, 3H), 1.25-1.32(m, 1H), 1.48(d, J=7.33Hz, 3H), 1.58(s, 3H), 1.75-2.15(m, 4H), 2.33-2.62(m, 5H), 3.20(dd, J ₁ =17.13Hz, J ₂ =0.74Hz, 1H), 3.84-3.90(m, 2H), 4.40(m, 2H), 4.72(dd, J ₁ =15.25Hz, J ₂ =1.33Hz, 1H), 5.33-5.51(m, 1H), 6.40(dd, J ₁ =10.13Hz, J ₂ =1.69Hz, 1H), 6.44(s, 1H), 6.51(dd, J ₁ =3.43Hz, J ₂ =1.57Hz, 1H), 7.18-7.20(m, 2H), 7.61(d, J=0.73Hz, 1H). MASS (ES+) : 645.0 |
| III.134 | 1.06(d, J=7.16Hz, 3H), 1.17(d, J=2.39Hz, 3H), 1.18(d, J=2.37Hz, 3H), 1.21(s, 3H), 1.35-1.41(m, 1H), 1.56(s, 3H), 1.77-2.00(m, 3H), 2.29-2.62(m, 5H), 3.21(d, J=2.62Hz, 1H), 3.42-3.49(m, 1H), 3.67(d, J=16.86Hz, 1H), 3.75(d, J=16.81Hz, 1H), 4.45(d, J=8.59Hz, 1H), 4.52(d, J=15.45Hz, 1H), 4.74(d, J=15.33Hz, 1H), 5.33-5.50(m, 1H), 6.40(dd, J ₁ =10.05Hz, J ₂ =1.65Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.50Hz, J ₂ =1.69Hz, 1H), 7.13(dd, J ₁ =3.56Hz, J ₂ =0.57Hz, 1H), 7.19(dd, J ₁ =0.75Hz, J ₂ =0.22Hz, 1H), 7.58(s, 1H). MASS (ES+) : 675.0 |
| III.135 | 1.06(d, J=7.12Hz, 3H), 1.19(s, 3H), 1.36-1.41(m, 1H), 1.55(s, 3H), 1.77-1.97(m, 3H), 2.32(s, 3H), 2.29-2.49(m, 5H), 3.41-3.58(m, 1H), 3.73-3.75(m, 2H), 4.45(d, J=8.67Hz, 1H), 4.77(d, J=15.28Hz, 1H), 4.98(d, J=15.27Hz, 1H), 5.31-5.50(m, 1H), 6.40(dd, J ₁ =10.15Hz, J ₂ =1.65Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.39Hz, J ₂ =1.64Hz, 1H), 7.12(d, J=3.45Hz, 1H), 7.15(dd, J ₁ =9.90Hz, 1H), 7.59(s, 1H). MASS (ES+) : 699.0 |
| III.136 | 1.05(t, J=7.09Hz, 6H), 1.05(d, J=6.67Hz, 3H), 1.34-1.40(m, 1H), 1.55(s, 3H), 1.76-2.02(m, 3H), 2.28-2.62(m, 4H), 2.56(q, J=7.22Hz, 2H), 3.26-3.39(m, 3H), 3.44-3.47(m, 1H), 3.63(d, J=16.46Hz, 1H), 3.85(d, J=16.45Hz, 1H), 4.42(d, J=8.63Hz, 1H), 5.30-5.81(m, 1H), 6.39(dd, J ₁ =10.17Hz, J ₂ =1.45Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.30Hz, J ₂ =1.61Hz, 1H), 7.14(d, J=3.21Hz, 1H), 7.15(d, J=9.85Hz, 1H), 7.59(s, 1H). MASS (ES+) : 630.1 |

SUBSTITUTE SHEET (RULE 26)

| Comp. No | ¹ H-NMR (δ ppm), MASS (EI / ES+, m/z) |
|----------|--|
| IB.137 | 1.06(d, J=7.13Hz, 3H), 1.20(s, 3H), 1.32(d, J=6.25Hz, 3H), 1.32(d, J=6.13Hz, 3H), 1.35-1.39(m, 1H), 1.55(s, 3H), 1.71-1.99(m, 3H), 2.28-2.49(m, 4H), 2.53(s, 1H), 3.42-3.46(m, 1H), 3.69(d, J=16.80Hz, 1H), 3.76(d, J=16.64Hz, 1H), 4.44(d, J=8.28Hz, 1H), 4.64(d, J=15.56Hz, 1H), 4.70(d, J=15.45Hz, 1H), 4.82-4.90(m, 1H), 5.33-5.49(m, 1H), 6.41(dd, J ₁ =10.17Hz, J ₂ =1.38Hz, 1H), 6.46(s, 1H), 6.50(dd, J ₁ =3.26Hz, J ₂ =1.44Hz, 1H), 7.13-7.16(m, 2H), 7.59(s, 1H). MASS (ES+): 661.1 |
| IB.138 | 1.06(d, J=7.13Hz, 3H), 1.20(s, 3H), 1.35-1.41(m, 1H), 1.55(s, 3H), 1.72(s, 1H), 1.76(s, 3H), 1.74-1.98(m, 3H), 2.28-2.53(m, 5H), 3.42-3.46(m, 1H), 3.69(d, J=16.85Hz, 1H), 3.76(d, J=16.94Hz, 1H), 4.43(d, J=8.85Hz, 1H), 4.64-4.68(m, 3H), 5.33-5.49(m, 1H), 6.39(dd, J ₁ =10.11Hz, J ₂ =1.71Hz, 1H), 6.46(s, 1H), 6.50(dd, J ₁ =3.45Hz, J ₂ =1.71Hz, 1H), 7.13-7.16(m, 2H), 7.59(d, J=0.83Hz, 1H). MASS (ES+): 687.1 |
| IB.139 | 0.87(t, J=6.15Hz, 3H), 1.06(d, J=7.15Hz, 3H), 1.19(s, 3H), 1.28-1.40(m, 1H), 1.55(s, 3H), 1.64-1.99(m, 5H), 2.28-2.59(m, 5H), 3.43-3.46(m, 1H), 3.69(d, J=16.84Hz, 1H), 3.76(d, J=16.70Hz, 1H), 4.14(t, J=6.75Hz, 1H), 4.44(d, J=8.29Hz, 1H), 4.65(d, J=15.47Hz, 1H), 4.65(d, J=15.48Hz, 1H), 5.32-5.49(m, 1H), 6.40(dd, J ₁ =10.13Hz, J ₂ =1.66Hz, 1H), 6.46(s, 1H), 6.50(dd, J ₁ =3.42Hz, J ₂ =1.70Hz, 1H), 7.13-7.16(m, 2H), 7.59(s, 1H). MASS (ES+): 703.1 |
| IB.140 | 0.94-1.02(m, 2H), 1.06(d, J=7.14Hz, 3H), 1.19(s, 3H), 1.23-1.41(m, 3H), 1.55(s, 3H), 1.66-1.99(m, 9H), 2.29-2.49(m, 4H), 2.58(d, J=2.05Hz, 1H), 3.43-3.46(m, 1H), 3.68(d, J=16.65Hz, 1H), 3.77(d, J=16.93Hz, 1H), 3.97(d, J=6.45Hz, 2H), 4.44(d, J=8.23Hz, 1H), 4.65(d, J=15.56Hz, 1H), 4.71(d, J=15.48Hz, 1H), 5.33-5.49(m, 1H), 6.40(dd, J ₁ =10.16Hz, J ₂ =1.50Hz, 1H), 6.46(s, 1H), 6.51(dd, J ₁ =3.33Hz, J ₂ =1.61Hz, 1H), 7.13-7.16(m, 2H), 7.59(s, 1H). MASS (ES+): 715.2 |
| IB.141 | 1.06(d, J=7.13Hz, 3H), 1.20(s, 3H), 1.25-1.52(m, 7H), 1.55(s, 3H), 1.73-1.99(m, 7H), 2.29-2.53(m, 4H), 2.63(s, 1H), 3.43-3.47(m, 1H), 3.68(d, J=16.79Hz, 1H), 3.77(d, J=16.71Hz, 1H), 4.44(d, J=8.52Hz, 1H), 4.56-4.62(m, 1H), 4.64(d, J=15.48Hz, 1H), 4.70(d, J=15.53Hz, 1H), 5.33-5.50(m, 1H), 6.40(dd, J ₁ =10.11Hz, J ₂ =1.71Hz, 1H), 6.46(s, 1H), 6.50(dd, J ₁ =3.45Hz, J ₂ =1.58Hz, 1H), 7.13-7.16(m, 2H), 7.59(d, J=0.91Hz, 1H). MASS (ES+): 701.1 |
| IB.142 | 0.88(m, 9H), 0.94-1.25(m, 14H), 1.38-1.41(m, 1H), 1.49-1.72(m, 6H), 1.78-1.99(m, 3H), 2.28-2.55(m, 5H), 3.43-3.46(m, 1H), 3.68(d, J=17.42Hz, 1H), 3.76(d, J=16.72Hz, 1H), 4.17(m, 2H), 4.44(d, J=7.54Hz, 1H), 4.64(d, J=15.74Hz, 1H), 4.76(d, J=15.62Hz, 1H), 5.33-5.49(m, 1H), 6.40(d, J=10.10Hz, 1H), 6.46(s, 1H), 6.50(m, 1H), 7.13-7.16(m, 2H), 7.59(m, 1H). MASS (ES+): 745.1 |
| IB.143 | 0.96(s, 9H), 1.06(d, J=7.05Hz, 3H), 1.19(s, 3H), 1.25-1.40(m, 7H), 1.55(s, 3H), 1.74-1.99(m, 3H), 2.30-2.56(m, 5H), 3.44(m, 1H), 3.68(d, J=16.89Hz, 1H), 3.79(d, J=17.24Hz, 1H), 3.85(s, 2H), 4.45(d, J=7.73Hz, 1H), 4.67(d, J=15.98Hz, 1H), 4.71(d, J=15.98Hz, 1H), 5.33-5.49(m, 1H), 6.40(d, J=10.09Hz, 1H), 6.46(s, 1H), 6.50-6.51(m, 1H), 7.13-7.16(m, 2H), 7.59(s, 1H). MASS (ES+): 689.1 |
| IB.144 | 1.06(d, J=7.16Hz, 3H), 1.19(s, 3H), 1.25-1.39(m, 1H), 1.55(s, 3H), 1.76-2.10(m, 9H), 2.28-2.67(m, 6H), 3.43-3.47(m, 1H), 3.67-3.79(m, 2H), 4.12(d, J=8.32Hz, 1H), 4.65-4.75(m, 2H), 5.33-5.50(m, 1H), 6.40(dd, J ₁ =10.11Hz, J ₂ =1.64Hz, 1H), 6.46(s, 1H), 6.51(dd, J ₁ =3.45Hz, J ₂ =1.60Hz, 1H), 7.13-7.17(m, 2H), 7.59(m, 1H). MASS (ES+): 687.1 |
| IB.145 | 1.06(d, J=7.07Hz, 3H), 1.19(s, 3H), 1.36-1.41(m, 1H), 1.54(s, 3H), 1.70-1.94(m, 3H), 2.17-2.49(m, 5H), 3.44(m, 1H), 3.68(d, J=16.70Hz, 1H), 3.76(d, J=16.66Hz, 1H), 4.42(d, J=7.94Hz, 1H), 4.70(s, 2H), 5.13(s, 2H), 5.32-5.49(m, 1H), 6.38-6.50(m, 5H), 7.12-7.14(m, 2H), 7.43(s, 1H), 7.59(s, 1H). MASS (ES+): 699.1 |
| IB.146 | 0.94(t, J=7.29Hz, 3H), 1.06(d, J=7.15Hz, 3H), 1.19(s, 3H), 1.25-1.43(m, 3H), 1.55(s, 3H), 1.61-1.99(m, 5H), 2.28-2.49(m, 4H), 2.59(s, 1H), 3.44-3.47(m, 1H), 3.68-3.79(m, 2H), 4.15(t, J=6.69Hz, 1H), 4.44(d, J=8.63Hz, 1H), 4.65(d, J=15.51Hz, 1H), 4.71(d, J=15.47Hz, 1H), 5.33-5.49(m, 1H), 6.40(dd, J ₁ =10.14Hz, J ₂ =1.59Hz, 1H), 6.46(s, 1H), 6.50(dd, J ₁ =3.39Hz, J ₂ =1.60Hz, 1H), 7.13-7.17(m, 2H), 7.59(s, 1H). MASS (ES+): 675.1 |
| IB.147 | 0.90(t, J=6.86Hz, 3H), 1.06(d, J=7.11Hz, 3H), 1.19(s, 3H), 1.33-1.43(m, 5H), 1.55(s, 3H), 1.65-1.99(m, 5H), 2.28-2.53(m, 4H), 2.60(s, 1H), 3.42-3.47(m, 1H), 3.69(d, J=16.86Hz, 1H), 3.76(d, J=16.62Hz, 1H), 4.15(t, J=6.78Hz, 2H), 4.44(d, J=8.38Hz, 1H), 4.66(d, J=15.54Hz, 1H), 4.71(d, J=15.39Hz, 1H), 5.33-5.49(m, 1H), 6.40(dd, J ₁ =10.08Hz, J ₂ =1.55Hz, 1H), 6.46(s, 1H), 6.50(dd, J ₁ =3.36Hz, J ₂ =1.74Hz, 1H), 7.13-7.17(m, 2H), 7.59(s, 1H). MASS (ES+): 689.2 |
| IB.148 | 1.06(d, J=7.17Hz, 3H), 1.20(s, 3H), 1.24-1.25(m, 6H), 1.35-1.41(m, 1H), 1.56(s, 3H), 1.77-1.98(m, 3H), 2.28-2.52(m, 4H), 2.82(s, 1H), 3.42-3.46(m, 1H), 3.67(d, J=16.93Hz, 1H), 3.75(d, J=16.87Hz, 1H), 4.33(dd, J ₁ =13.35Hz, J ₂ =8.87Hz, 1H), 4.45(dd, J ₁ =13.22Hz, J ₂ =8.77Hz, 1H), 4.42-4.48(m, 1H), 4.58(d, J=15.35Hz, 1H), 4.78(d, J=15.36Hz, 1H), 5.31-5.49(m, 1H), 6.40(dd, J ₁ =10.12Hz, J ₂ =1.68Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.43Hz, J ₂ =1.64Hz, 1H), 7.12(d, J=3.44Hz, 1H), 7.17(dd, J=10.21Hz, 1H), 7.58(d, J=0.71Hz, 1H). MASS (ES+): 677.1 |
| IB.149 | 1.06(d, J=7.10Hz, 3H), 1.18(s, 3H), 1.36(s, 3H), 1.38-1.43(m, 1H), 1.43(s, 3H), 1.55(s, 3H), 1.77-1.98(m, 3H), 2.28-2.55(m, 5H), 3.43-3.46(m, 1H), 3.66-3.83(m, 3H), 4.07-4.36(m, 4H), 4.44(d, J=7.86Hz, 1H), 4.67(d, J=15.48Hz, 1H), 4.73(d, J=15.48Hz, 1H), 5.32-5.49(m, 1H), 6.39(d, J=10.08Hz, 1H), 6.45(s, 1H), 6.50(d, J=1.59Hz, 1H), 7.13(d, J=3.39Hz, 1H), 7.15(d, J=10.24Hz, 1H), 7.59(s, 1H). MASS (ES+): 733.1 |
| IB.150 | 1.06(d, J=7.08Hz, 3H), 1.18(s, 3H), 1.35(s, 3H), 1.38-1.43(m, 1H), 1.43(s, 3H), 1.55(s, 3H), 1.77-1.97(m, 3H), 2.28-2.49(m, 5H), 3.42-3.46(m, 1H), 3.69(d, J=16.77Hz, 1H), 3.77(d, J=15.45Hz, 1H), 3.80(d, J=5.40Hz, 1H), 3.82(d, J=5.56Hz, 1H), 4.08(d, J=6.42Hz, 1H), 4.10(d, J=6.85Hz, 1H), 4.18(d, J=5.35Hz, 2H), 4.32(m, 1H), 4.45(d, J=7.55Hz, 2H), 4.70(m, 1H), 5.31-5.51(m, 1H), 6.39(d, J=10.13Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.47Hz, J ₂ =1.52Hz, 1H), 7.12(d, J=3.44Hz, 1H), 7.14(d, J=10.15Hz, 1H), 7.59(s, 1H). MASS (ES+): 733.1 |
| IB.151 | 1.05(d, J=7.11Hz, 3H), 1.20(s, 3H), 1.35-1.40(m, 1H), 1.54(s, 3H), 1.77-2.03(m, 3H), 2.28-2.52(m, 4H), 3.39(d, J=72.79Hz, 1H), 3.39-3.46(m, 5H), 3.67-3.80(m, 6H), 4.42(d, J=8.10Hz, 1H), 4.59(d, J=15.59Hz, 1H), 4.74(d, J=15.59Hz, 1H), 7.14(d, J=2.57Hz, 1H), 7.16(d, J=10.25Hz, 1H), 7.59(s, 1H). MASS (ES+): 688.1 |
| IB.152 | 1.05(d, J=7.10Hz, 3H), 1.20(s, 3H), 1.34(s, 3H), 1.34-1.40(m, 1H), 1.43(s, 3H), 1.55(s, 3H), 1.77-2.03(m, 3H), 2.28-2.53(m, 4H), 3.23-3.30(m, 1H), 3.37-3.45(m, 3H), 3.63-3.79(m, 3H), 4.02-4.24(m, 2H), 4.43(d, J=7.99Hz, 1H), 4.53(d, J=15.80Hz, 1H), 4.70(d, J=15.61Hz, 1H), 5.15(s, 1H), 5.33-5.49(m, 1H), 6.39(dd, J ₁ =10.16Hz, J ₂ =1.42Hz, 1H), 6.45(s, 1H), 6.50(d, J=3.31Hz, J ₂ =1.54Hz, 1H), 7.14(d, J=3.39Hz, 1H), 7.18(d, J=9.90Hz, 1H), 7.59(s, 1H). MASS (ES+): 732.1 |

| Comp. No. | ¹ H-NMR (δ ppm), MASS (EI / ES+, m/z) |
|-----------|---|
| III.153 | 1.06(d, J=7.12Hz, 3H), 1.09(m, 2H), 1.20(s, 3H), 1.36-1.41(m, 1H), 1.51-1.99(m, 15H), 2.29-2.49(m, 4H), 2.64(d, J=1.80Hz, 1H), 3.43-3.47(m, 1H), 3.69(d, J=16.81Hz, 1H), 3.76(d, J=16.88Hz, 1H), 4.17(t, J=6.97Hz, 2H), 4.44(d, J=8.65Hz, 1H), 4.65(d, J=15.48Hz, 1H), 4.71(d, J=15.44Hz, 1H), 5.33-5.49(m, 1H), 6.40(dd, J ₁ =10.13Hz, J ₂ =1.56Hz, 1H), 6.46(s, 1H), 6.51(dd, J ₁ =3.37Hz, J ₂ =1.53Hz, 1H), 7.13-7.17(m, 2H), 7.59(d, J=0.70Hz, 1H). MASS (ES+): 715.1 |
| III.154 | 0.93(d, J=6.53Hz, 6H), 1.06(d, J=7.11Hz, 3H), 1.20(m, 2H), 1.35-1.41(m, 1H), 1.55(s, 3H), 1.57-1.66(m, 2H), 1.66-1.99(m, 4H), 2.29-2.49(m, 4H), 2.57(s, 1H), 3.43-3.46(m, 1H), 3.69(d, J=16.54Hz, 1H), 3.77(d, J=16.68Hz, 1H), 4.19(t, J=6.87Hz, 2H), 4.44(d, J=8.08Hz, 1H), 4.65(d, J=15.53Hz, 1H), 4.71(d, J=15.51Hz, 1H), 5.33-5.49(m, 1H), 6.40(d, J=10.11Hz, 1H), 6.46(s, 1H), 6.50(dd, J ₁ =3.10Hz, J ₂ =1.63Hz, 1H), 7.13-7.17(m, 2H), 7.59(s, 1H). MASS (ES+): 689.1 |
| III.155 | 1.06(d, J=7.08Hz, 3H), 1.17(s, 3H), 1.36-1.40(m, 1H), 1.55(s, 3H), 1.74-2.11(m, 5H), 2.29-2.63(m, 6H), 3.44(m, 1H), 3.67(d, J=16.71Hz, 1H), 3.76(d, J=16.62Hz, 1H), 4.45(d, J=8.31Hz, 1H), 4.51(t, J=6.24Hz, 2H), 4.61(d, J=15.49Hz, 1H), 4.73(d, J=15.42Hz, 1H), 4.40(d, J=11.18Hz, 1H), 5.33-5.50(m, 1H), 6.40(d, J=11.18Hz, 1H), 6.45(s, 1H), 6.50(m, 1H), 7.13(d, J=3.30Hz, 1H), 7.17(d, J=10.24Hz, 1H), 7.59(s, 1H). MASS (ES+): 706.1 |
| III.156 | 1.05(d, J=7.06Hz, 3H), 1.19(s, 3H), 1.31(s, 3H), 1.33(s, 3H), 1.37-1.41(m, 1H), 1.44(s, 3H), 1.50(s, 3H), 1.55(s, 3H), 1.77-2.00(m, 3H), 2.28-2.50(m, 4H), 2.68(s, 1H), 3.45(m, 1H), 3.66(d, J=13.96Hz, 1H), 3.77(d, J=16.58Hz, 1H), 4.05(t, J=5.83Hz, 1H), 4.24-4.34(m, 4H), 4.46(d, J=7.50Hz, 1H), 4.62(dd, J ₁ =7.80Hz, J ₂ =2.15Hz, 1H), 4.69(s, 2H), 5.33-5.49(m, 1H), 5.52(d, J=4.93Hz, 1H), 6.38(d, J=10.13Hz, 1H), 6.45(s, 1H), 6.50(dd, J ₁ =3.19Hz, J ₂ =1.47Hz, 1H), 7.13(d, J=3.18Hz, 1H), 7.18(d, J=10.10Hz, 1H), 7.59(s, 1H). MASS (ES+): 861.1 |
| III.157 | 1.06(d, J=7.08Hz, 3H), 1.17(s, 3H), 1.36-1.40(m, 1H), 1.55(s, 3H), 1.74-2.11(m, 5H), 2.29-2.63(m, 6H), 3.44(m, 1H), 3.67(d, J=16.71Hz, 1H), 3.76(d, J=16.62Hz, 1H), 4.45(d, J=8.31Hz, 1H), 4.51(t, J=6.24Hz, 2H), 4.61(d, J=15.49Hz, 1H), 4.73(d, J=15.42Hz, 1H), 4.40(d, J=11.18Hz, 1H), 5.33-5.50(m, 1H), 6.40(d, J=11.18Hz, 1H), 6.45(s, 1H), 6.50(m, 1H), 7.13(d, J=3.30Hz, 1H), 7.17(d, J=10.24Hz, 1H), 7.59(s, 1H). MASS (ES+): 720.1 |
| III.158 | 1.06(d, J=7.14Hz, 3H), 1.16(s, 3H), 1.35-1.41(m, 1H), 1.55(s, 3H), 1.77-1.97(m, 3H), 2.12-2.51(m, 5H), 3.36(s, 3H), 3.43-3.47(m, 1H), 3.71(d, J=16.48Hz, 1H), 3.83(d, J=16.48Hz, 1H), 4.05(d, J=15.61Hz, 1H), 4.10(d, J=15.58Hz, 1H), 4.44(d, J=8.60Hz, 1H), 5.34-5.47(m, 1H), 6.41(dd, J ₁ =10.16Hz, J ₂ =1.69Hz, 1H), 6.46(s, 1H), 6.51(dd, J ₁ =3.44Hz, J ₂ =1.75Hz, 1H), 7.13(d, J=3.40Hz, 1H), 7.15(d, J=10.20Hz, 1H), 7.59(d, J=0.86Hz, 1H). MASS (ES+): 589.1 |
| III.159 | 1.06(d, J=7.16Hz, 3H), 1.16(s, 3H), 1.22(t, J=7.01Hz, 3H), 1.36-1.41(m, 1H), 1.54(s, 3H), 1.71-2.00(m, 3H), 2.28-2.51(m, 4H), 3.42-3.46(m, 1H), 3.46-3.59(m, 2H), 3.70(d, J=16.51Hz, 1H), 3.83(d, J=16.49Hz, 1H), 4.07-4.17(m, 2H), 4.44(d, J=8.80Hz, 1H), 5.32-5.49(m, 1H), 6.41(dd, J ₁ =10.12Hz, J ₂ =1.68Hz, 1H), 6.46(s, 1H), 6.51(dd, J ₁ =3.43Hz, J ₂ =1.63Hz, 1H), 7.13-7.16(m, 2H), 7.59(s, 1H). MASS (ES+): 603.1 |
| III.160 | 0.91(d, J=6.70Hz, 6H), 1.06(d, J=7.07Hz, 3H), 1.15(s, 3H), 1.25-1.41(m, 1H), 1.54(s, 3H), 1.67-1.97(m, 5H), 2.28-2.53(m, 4H), 3.22-3.28(m, 2H), 3.42-3.46(m, 1H), 3.71(d, J=16.42Hz, 1H), 3.84(d, J=16.45Hz, 1H), 4.06-4.16(m, 2H), 4.44(d, J=7.72Hz, 1H), 5.32-5.49(m, 1H), 6.39-6.41(m, 1H), 6.46(s, 1H), 6.51(dd, J ₁ =3.19Hz, J ₂ =1.44Hz, 1H), 7.12-7.15(m, 2H), 7.59(s, 1H). MASS (ES+): 631.1 |
| IC.1 | 1.03(d, J=7.07Hz, 3H), 1.13(d, J=7.68Hz, 3H), 1.15(s, 3H), 1.20-1.89(m, 8H), 2.15-2.44(m, 6H), 2.85-2.88(m, 1H), 4.30-4.33(m, 1H), 4.82(s, 2H), 5.30-5.47(m, 1H), 6.34(dd, J ₁ =10.13Hz, J ₂ =1.17Hz, 2H), 6.38(s, 1H), 7.05(dd, J=8.67Hz, 2H), 7.21(d, J=10.17Hz, 1H), 7.43-7.47(m, 2H). MASS (ES+): 615.5 (M+Na ⁺). |
| IC.2 | 1.03(d, J=7.01Hz, 3H), 1.11-1.14(m, 6H), 1.32-1.89(m, 8H), 2.20-2.44(m, 6H), 2.80-2.84(m, 1H), 4.40(d, J=8.11Hz, 1H), 4.78(d, J=11.17Hz, 1H), 4.4-4.81(d, J=11.19Hz, 1H), 5.32-5.49(m, 1H), 6.37(d, J=10.14Hz, 1H), 7.10(d, J=10.15Hz, 1H), 7.29(d, J=8.19Hz, 1H), 7.44(d, J=8.19Hz, 1H). 7.57(s, 1H). MASS (ES+): 665.4 (M+Na ⁺). |
| IC.3 | 1.03(d, J=7.09Hz, 3H), 1.12(t, J=7.50Hz, 3H), 1.16(s, 3H), 1.16-1.95(m, 8H), 2.20-2.40(m, 6H), 2.78-2.84(m, 1H), 4.41(d, J=8.70Hz, 1H), 5.28-5.48(m, 1H), 5.39(d, J=50.31Hz, J ₂ =2.66Hz, 1H), 5.51(d, J=49.30Hz, J ₂ =2.61Hz, 1H), 6.37(dd, J ₁ =10.15Hz, J ₂ =1.74Hz, 1H), 6.43(s, 1H), 7.10(dd, J ₁ =10.12Hz, J ₂ =1.11Hz, 1H). MASS (ES+): 517.2 |
| IC.4 | 1.11(d, J=7.09Hz, 3H), 1.21(s, 3H), 1.24-1.97(m, 8H), 2.28-2.50(m, 4H), 2.86-2.90(m, 1H), 4.45-4.47(m, 1H), 5.30-5.52(m, 1H), 5.41(d, J ₁ =53.67Hz, J ₂ =2.34Hz, 1H), 5.56(d, J ₁ =52.24Hz, J ₂ =2.33Hz, 1H), 6.39(d, J ₁ =10.13Hz, J ₂ =1.77Hz, 1H), 6.45(s, 1H), 6.51(d, J ₁ =3.50Hz, J ₂ =1.72Hz, 1H), 7.12-7.15(m, 2H), 7.60(d, J=0.88Hz, 1H). MASS (ES+): 555.2 |
| IC.5 | 1.10(d, J=7.17Hz, 3H), 1.21(s, 1H), 1.25-1.38(m, 2H), 1.55(s, 1H), 1.85-1.99(m, 3H), 2.16-2.59(m, 4H), 2.88-2.93(m, 1H), 4.83(d, J=10.67Hz, 1H), 4.83(d, J=10.69Hz, 1H), 5.03-5.09(m, 1H), 6.31-6.35(m, 2H), 6.54(dd, J ₁ =3.47Hz, J ₂ =1.71Hz, 1H), 7.03-7.07(m, 2H), 7.26(d, J=10.03Hz, 1H), 7.45-7.49(m, 2H), 7.65(d, J=0.82Hz, 1H). MASS (ES+): 631.2 |
| IC.6 | 1.12(d, J=7.07Hz, 3H), 1.21(s, 3H), 1.26-1.48(m, 1H), 1.53(s, 3H), 1.59-1.96(m, 4H), 2.28-2.52(m, 4H), 2.82-2.86-2.89(m, 1H), 4.44-4.46(m, 1H), 4.93(d, J=11.263Hz, 1H), 5.03(d, J=11.24Hz, 1H), 5.32-5.48(m, 1H), 6.39(dd, J ₁ =10.11Hz, J ₂ =1.68Hz, 1H), 6.45(s, 1H), 6.52(dd, J ₁ =3.41Hz, J ₂ =1.70Hz, 1H), 7.11(d, J=5.71Hz, 1H), 7.13(s, 1H), 7.58-7.64(m, 4H). MASS (ES+): 681.3 |
| IC.7 | 1.09(d, J=6.89Hz, 3H), 1.20(s, 3H), 1.25-1.50(m, 1H), 1.55(s, 3H), 1.60-2.03(m, 4H), 2.16-2.52(m, 4H), 2.92-3.13(m, 1H), 4.32(m, 1H), 4.83(d, J=10.85Hz, 1H), 4.87(d, J=10.88Hz, 1H), 5.13-5.51(m, 1H), 6.30-6.33(m, 2H), 6.55(s, 1H), 7.13(s, 1H), 7.26(d, J=10.22Hz, 1H), 7.33-7.58(m, 4H), 7.58-7.77(m, 1H). MASS (ES+): 647.2 |
| IC.8 | 0.99(d, J=7.09Hz, 3H), 1.09(t, J=7.52Hz, 3H), 1.12(s, 3H), 1.22-1.88(m, 8H), 2.13-2.55(m, 6H), 2.82-2.86(m, 1H), 4.25-4.27(m, 1H), 4.89(s, 2H), 4.96-4.98(m, 1H), 5.30-5.50(m, 1H), 6.26-6.29(m, 2H), 7.21(dd, J ₁ =10.03Hz, J ₂ =1.05Hz, 1H), 7.56(d, J=8.26Hz, 2H), 7.61(d, J=8.30Hz, 2H). MASS (ES+): 643.0 |
| IC.9 | 1.05(d, J=7.09Hz, 3H), 1.18(s, 1H), 1.20-1.87(m, 8H), 2.19-2.56(m, 4H), 2.58-2.70(m, 1H), 2.86-2.90(m, 1H), 4.30-4.32(m, 1H), 4.80(d, J=10.70Hz, 1H), 4.85(d, J=10.70Hz, 1H), 4.92-4.94(m, 1H), 6.05(m, 1H), 6.25(dd, J ₁ =10.13Hz, J ₂ =1.77Hz, 1H), 6.51(dd, J ₁ =3.45Hz, J ₂ =1.70Hz, 1H), 7.00-7.02(m, 2H), 7.29(d, J=10.11Hz, 1H), 7.43-7.46(m, 2H), 7.63(d, J=0.85Hz, 1H). MASS (ES+): 613.0 |
| IC.10 | 1.00(d, J=7.06Hz, 3H), 1.07(t, J=7.54Hz, 3H), 1.15(s, 3H), 1.25-1.92(m, 8H), 2.16-2.44(m, 6H), 2.81-2.84(m, 1H), 4.41(d, J=8.51Hz, 1H), 5.10(d, J=16.55Hz, 1H), 5.21(d, J=16.64Hz, 1H), 5.30-5.46(m, 1H), 6.38(dd, J ₁ =10.13Hz, J ₂ =1.69Hz, 1H), 7.14(d, J=10.13Hz, 1H), 7.46(d, J=8.54Hz, 2H), 7.85(d, J=8.58Hz, 2H). MASS (ES+): 637.1 |

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| Comp. No | ¹ H-NMR (δ ppm), MASS (EI / ES+, m/z) |
|----------|--|
| IC-11 | 1.10(d, J=7.08Hz, 3H), 1.22(s, 3H), 1.25-1.94(m, 8H), 2.27-2.65(m, 5H), 2.80-2.92(m, 1H), 4.45-4.56(m, 1H), 5.41 (dd, J ₁ =52.28Hz, J ₂ =2.31Hz, 1H), 5.56 (dd, J ₁ =53.72Hz, J ₂ =2.34Hz, 1H), 6.15(s, 1H), 6.37(dd, J ₁ =10.13Hz, J ₂ =1.82Hz, 1H), 6.50(dd, J ₁ =3.48Hz, J ₂ =1.70Hz, 1H), 7.12(d, J=3.40Hz, 1H), 7.21(d, J=10.12Hz, 1H), 7.59(d, J=0.86Hz, 1H). MASS(ES+): 537.1 |
| IC-12 | 0.89(t, J=7.31Hz, 3H), 1.03(d, J=7.07Hz, 3H), 1.16(s, 3H), 1.25-1.91(m, 12H), 2.17-2.44(m, 6H), 2.80-2.84(m, 1H), 4.1-4.33 (m, 1H), 5.30-5.58(m, 3H), 6.38(dd, J ₁ =10.13Hz, J ₂ =1.69Hz, 1H), 6.43(s, 1H), 7.11(dd, J=10.12Hz, J ₂ =0.98 Hz). MASS(ES+): 537.1 |
| IC-13 | 1.02(d, J=7.08Hz, 3H), 1.12(t, J=7.70Hz, 3H), 1.15(s, 3H), 1.32-1.37(m, 1H), 1.52(s, 3H), 1.68-1.92(m, 4H), 2.22-2.39(m, 4H), 2.76-2.81(m, 1H), 3.84(s, 3H), 4.40-4.42(m, 1H), 5.29-5.47(m, 1H), 6.38(dd, J ₁ =10.12Hz, J ₂ =1.79Hz, 1H), 6.43(s, 1H), 7.12(dd, J ₁ =10.14Hz, J ₂ =1.32Hz, 1H). MASS(ES+): 499.0 |
| IC-14 | 1.08(d, J=7.08Hz, 3H), 1.20(s, 3H), 1.29-1.40(m, 1H), 1.55(s, 3H), 1.59-2.00(m, 4H), 2.27-2.51(m, 4H), 2.88-2.92(m, 1H), 3.85(s, 3H), 4.33-4.35 (m, 1H), 4.95-4.97(m, 1H), 5.34-5.51(m, 3H), 6.33(dd, J ₁ =10.10Hz, J ₂ =1.85Hz, 1H), 6.36(s, 1H), 6.52(dd, J ₁ =3.49Hz, J ₂ =1.72 Hz, 1H), 7.11(dd, J ₁ =3.48Hz, J ₂ =0.53Hz, 1H), 7.26(dd, J ₁ =10.05Hz, J ₂ =0.96Hz, 1H), 7.62-7.63(m, 1H). MASS(ES+): 537.0 |
| IC-15 | 1.04(d, J=7.09Hz, 3H), 1.11-1.15(m, 6H), 1.34-1.85(m, 8H), 2.20-2.39(m, 6H), 2.80-2.90(m, 1H), 4.38(d, J=8.66Hz, 1H), 4.86(d, J=10.78Hz, 1H), 4.92(d, J=10.77Hz, 1H), 5.27-5.49(m, 1H), 6.36(dd, J ₁ =10.14Hz, J ₂ =1.80Hz, 1H), 6.43(s, 1H), 7.09(dd, J ₁ =10.13Hz, J ₂ =1.20Hz, 1H), 7.35-7.45(m, 5H). MASS(ES+): 575.0 |
| IC-16 | 1.08(d, J=7.08Hz, 3H), 1.20(s, 3H), 1.22-1.97(m, 8H), 2.26-2.54(m, 4H), 2.91-2.95(m, 1H), 4.31(d, J=6.59Hz, 1H), 4.85(d, J=10.66Hz, 1H), 4.88(d, J=10.66Hz, 1H), 5.24-5.56(m, 1H), 6.28-6.31(m, 2H), 6.56(dd, J ₁ =3.39Hz, J ₂ =1.64Hz, 1H), 7.31(d, J=3.45Hz, 1H), 7.18-7.46(m, 6H), 7.72(s, 1H). MASS(ES+): 613.0 |
| IC-17 | 0.99(d, J=7.07Hz, 3H), 1.09(t, J=7.51Hz, 3H), 1.14(s, 3H), 1.19-1.96(m, 8H), 2.09-2.47(m, 12H), 2.77-2.81(m, 1H), 4.40(d, J=6.30Hz, 1H), 4.74(d, J=18.25Hz, 1H), 4.82(d, J=18.27Hz, 1H), 5.30-5.46(m, 1H), 6.38(dd, J ₁ =10.15Hz, J ₂ =1.79Hz, 1H), 6.43(s, 1H), 6.84(s, 2H), 7.12(d, J=9.89Hz, 1H). MASS(ES+): 645.3 |
| IC-18 | 1.03(d, J=7.09Hz, 3H), 1.14(s, 3H), 1.13(t, J=7.54Hz, 3H), 1.25-1.89(m, 8H), 2.17-2.40(m, 6H), 2.81-2.83(m, 1H), 4.38-4.41(m, 1H), 4.81(d, J=10.91Hz, 1H), 4.88(d, J=10.91Hz, 1H), 5.25-5.50(m, 1H), 6.35(d, J ₁ =10.13Hz, J ₂ =1.65Hz), 6.43(s, 1H), 7.10(d, J ₁ =10.10Hz, J ₂ =0.67Hz, 1H), 7.34(d, J=8.40Hz, 2H), 7.40(d, J=8.39Hz, 2H). MASS(ES+): 609.0 |
| IC-19 | 1.10(d, J=7.04Hz, 3H), 1.21(s, 3H), 1.30-1.96(m, 8H), 2.29-2.54(m, 4H), 2.90-2.93(m, 1H), 4.33-4.36(m, 1H), 4.82(d, J=11.11Hz, 1H), 4.87(d, J=11.10Hz, 1H), 4.95-4.98(m, 1H), 5.36-5.51(m, 1H), 6.33(dd, J ₁ =10.13Hz, J ₂ =1.75Hz, 1H), 7.14(d, J=3.45Hz, 1H), 7.25(d, J=10.09Hz, 1H), 7.32(dd, J ₁ =8.22Hz, J ₂ =1.89Hz, 1H), 7.44-7.46(m, 1H), 7.64(s, 1H). MASS(ES+): 680.9 |
| IC-20 | 1.09(d, J=7.00Hz, 3H), 1.20(s, 3H), 1.30-2.02(m, 8H), 2.26-2.53(m, 4H), 2.91-2.95(m, 1H), 4.32(d, J=6.99Hz, 1H), 4.97(d, J=11.64Hz, 1H), 5.03(d, J=11.59Hz, 1H), 5.37-5.54(m, 1H), 6.31-6.32(m, 2H), 6.56(dd, J ₁ =3.28Hz, J ₂ =1.56Hz, 1H), 7.13(d, J=3.41Hz, 1H), 7.18-7.31(m, 2H), 7.42(d, J=1.43Hz, 1H), 7.58(d, J=8.25Hz, 1H), 7.70(s, 1H). MASS(ES+): 681.5 |
| IC-21 | 1.11(d, J=6.97Hz, 3H), 1.22(s, 3H), 1.25-1.96(m, 8H), 2.28-2.58(m, 4H), 2.90-3.95(m, 1H), 4.36(m, 1H), 4.83-4.88(m, 3H), 5.30-5.55(m, 1H), 6.34(d, J ₁ =10.10Hz, J ₂ =1.68Hz, 1H), 6.38(m, 1H), 6.53(d, J ₁ =3.39Hz, J ₂ =1.65Hz, 1H), 7.13(d, J=3.43Hz, 1H), 7.124-7.42(m, 4H), 7.50(s, 1H), 7.63(s, 1H). MASS(ES+): 647.7 |
| IC-22 | 1.09(d, J=7.04Hz, 3H), 1.20(s, 3H), 1.25-1.97(m, 8H), 2.03-2.57(m, 4H), 2.89-2.93(m, 1H), 4.33(d, J=6.78Hz, 1H), 4.95(d, J=10.92Hz, 1H), 5.05(d, J=10.89Hz, 1H), 5.12(m, 1H), 5.30-5.30(m, 1H), 6.30-6.33(m, 2H), 6.54(dd, J ₁ =3.39Hz, J ₂ =1.63Hz, 1H), 6.74-6.78(m, 2H), 7.11(d, J=3.36Hz, 1H), 7.26(d, J=10.07Hz, 1H), 7.66(s, 1H). MASS(ES+): 667.0 |
| IC-23 | 1.10(d, J=7.05Hz, 3H), 1.22(s, 3H), 1.36-1.42(m, 1H), 1.55(s, 3H), 1.72-2.00(m, 4H), 2.29-2.52(m, 4H), 2.87-2.92(m, 1H), 4.32-4.35(m, 1H), 4.93(d, J=11.04Hz, 1H), 4.97(d, J=11.07Hz, 1H), 5.05-5.06(m, 1H), 5.30-5.52(m, 1H), 6.33(dd, J ₁ =10.09Hz, J ₂ =1.88Hz, 1H), 6.35(s, 1H), 6.54(dd, J ₁ =3.49Hz, J ₂ =1.72Hz, 1H), 7.13(d, J=3.39Hz, 1H), 7.26(dd, J ₁ =10.07Hz, J ₂ =1.01Hz, 1H), 7.51-7.69(m, 4H), 7.74(s, 1H). MASS(ES+): 681.5 |

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Example 30 : Pharmacological Activity:**(a) Steroid Receptor Binding Assays:**

The steroid receptor binding assay were performed by MDS Pharma Services at their Taipei
5 (Taiwan) pharmacology laboratory.

(i) Glucocorticoid Receptor Binding Assay

The activity of test compounds on glucocorticoid receptor was assessed using radioligand
binding assays. The Human HeLa cells transfected with glucocorticoid receptors were
10 incubated with [³H]dexamethasone at 25 °C for 2hrs in RPMI-1640, 10nM HEPES, pH 7.2
incubation medium, in the absence or presence of test compounds at 3nM and/or 10nM
concentration. Free [³H]dexamethasone was removed from the medium by centrifugation and
concentration of receptor bound ligand was determined in the supernatant by liquid scintillation
counting.

15 Dexamethasone as reference compound was tested concurrently as an integral part of each assay
to ensure the validity of the results obtained. The % inhibition was evaluated using a single
concentration of test compound and the corresponding radiolabeled ligand. Results are presented
as the percent inhibition of specific binding. The values are average of duplicate determinations
20 for each concentration.

Table 7: Glucocorticoid Receptor binding (*in vitro*) screen

| Compound No. | Glucocorticoid receptor binding
% inhibition |
|--------------|---|
| IA.143 | 58 ^b |
| IA.161 | 55 ^b |
| IA.157 | 56 ^b |
| IA.159 | 36 ^b |
| IA.168 | 40 ^a |
| IB.2 | 55 ^a |
| IB.4 | 88 ^b |
| IB.6 | 92 ^b |
| IB.7 | 82 ^b |
| IB.8 | 93 ^b |

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| Compound No. | Glucocorticoid receptor binding
% inhibition |
|------------------------|---|
| IB.10 | 82 ^b |
| IB.13 | 79 ^b |
| IB.14 | 85 ^b |
| IB.15 | 83 ^b |
| IB.50 | 74 ^b |
| IB.51 | 67 ^b |
| IB.54 | 82 ^b |
| IB.66 | 72 ^b |
| IB.67 | 77 ^b |
| IB.70 | 43 ^a |
| IB.73 | 45 ^a |
| IB.88 | 46 ^a |
| IB.100 | 45 ^a |
| IB.101 | 45 ^a |
| IB.103 | 78 ^b |
| IB.104 | 72 ^b |
| IB.105 | 42 ^a |
| IC.3 | 72 ^c |
| IC.4 | 73 ^b |
| IC.5 | 75 ^c |
| IC.7 | 41 ^b |
| Fluticasone propionate | 88 ^b |
| Budesonide | 85 ^b |

^a %Inhibition at 3nM; ^b % Inhibition at 10nM; ^c % Inhibition at 100nM.

(b) Croton oil ear edema

- 5 Mice (male, CD-1) were made into different groups. Test compounds were dissolved in pyridine-water-acetone (4:2:14) solution 10μl of compound or vehicle solution was applied to the left ear of the mice. The right ear of each mouse was applied simultaneously with 10μl of pyridine-water: acetone (4:2:14) solution. After 2hrs of compound or vehicle application, 10μl of croton oil solution was applied to the left ear of all animals. After 6hr of croton oil treatment the
- 10 animals were sacrificed; ears were excised and weighed separately.

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Table 8: Croton oil Ear Edema Screen

| Compound No. | Mean % Inhibition |
|------------------------|--------------------|
| IA.3 | 45.31 ^a |
| IA.56 | 34.59 ^a |
| IA.184 | 49.06 ^a |
| IA.185 | 49.06 ^a |
| IB.20 | 61.49 ^a |
| IB.33 | 76.16 ^a |
| IB.34 | 64.39 ^a |
| IB.35 | 60.18 ^a |
| IB.37 | 57.12 ^a |
| IB.44 | 75.19 ^a |
| IB.46 | 75.97 ^a |
| IB.49 | 71.82 ^a |
| IB.52 | 78.12 ^a |
| IB.53 | 71.19 ^a |
| IB.55 | 74.78 ^a |
| IB.57 | 74.43 ^a |
| IB.64 | 72.75 ^a |
| IB.73 | 76.24 ^a |
| IB.77 | 71.71 ^a |
| IB.81 | 77.75 ^a |
| IB.98 | 73.71 ^b |
| IB.102 | 73.63 ^b |
| IB.112 | 66.94 ^b |
| IB.138 | 72.48 ^b |
| IB.150 | 77.76 ^b |
| IB.159 | 66.02 ^b |
| IC.13 | 41.79 ^a |
| IC.14 | 61.46 ^a |
| Fluticasone propionate | 81.09 ^a |
| Dexamethasone | 50.05 ^a |

^a Inhibition at 1.6µg; ^b Inhibition at 0.5µg

(c) Cotton pellet granuloma

SD rats were used for assessing anti-inflammatory activity of test compound using cotton pellet granuloma method. Sterilized cotton pellets weighing 20mg were prepared. Test compounds were dissolved in acetone so as to get the required quantity for each cotton pellet in 500µl.

5 Different pellets were impregnated with 500µl of acetone to contain required quantity of test compounds and allowed to dry. Vehicle control pellets were impregnated with 500µl acetone. Rats were made into different groups. Two cotton pellets were surgically implanted into the scapular region of each rat. On sixth day of such implantation, pellets along with granuloma were taken out. Thymus gland was also separated from each animal and weighed. The pellets

10 with granuloma were dried for 20 hrs at 60°C and weighed. Mean weights of dry granuloma and thymus, body weight gain/100g body weights were calculated.

Table 9: Cotton pellet granuloma test

| Compound No. | Dose (mcg) | Mean % Inhibition of Granuloma | Thymus wt.* (% Decrease) |
|--------------|------------|--------------------------------|--------------------------|
| IA.3 | 1000 | 74.76 | -11.72 |
| IA.6 | 1000 | 61.25 | -6.95 |
| IA.11 | 1000 | 61.36 | -4.72 |
| IA.13 | 1000 | 62.52 | 6.46 |
| IA.14 | 1000 | 70.74 | -13.26 |
| IA.20 | 1000 | 67.57 | 0.73 |
| IA.27 | 10 | 31.28 | 8.71 |
| | 1000 | 69.84 | 11.74 |
| IA.28 | 1000 | 73.73 | 13.5 |
| IA.35 | 1000 | 67.16 | -11.43 |
| IA.36 | 1000 | 70.74 | -13.26 |
| IA.38 | 10 | 67.17 | -1.28 |
| IA.42 | 1000 | 65.63 | -1.33 |
| IA.43 | 10 | 27.72 | -0.55 |
| | 1000 | 72.03 | 1.47 |
| IA.44 | 1000 | 71.79 | 4.58 |
| IA.45 | 1000 | 80.06 | -4.46 |
| IA.58 | 10 | 59.00 | 6.00 |
| IA.59 | 1000 | 76.86 | -2.51 |
| IA.122 | 3 | 37.29 | 2.25 |
| IA.136 | 10 | 37.74 | 4.44 |
| | 1000 | 67.79 | 2.14 |

| Compound No. | Dose (mcg) | Mean % Inhibition of Granuloma | Thymus wt.* (% Decrease) |
|------------------------|------------|--------------------------------|--------------------------|
| IA.137 | 1000 | 65.58 | 1.59 |
| IA.138 | 1000 | 66.16 | 15.45 |
| IA.140 | 1000 | 62.54 | -36.16 |
| IA.141 | 1000 | 63.1 | -18.26 |
| IA.142 | 10 | 45.36 | -8.43 |
| IA.197 | 1000 | 79.04 | -8.89 |
| IB.5 | 10 | 39.79 | -0.39 |
| IB.7 | 1000 | 78.82 | 14.89 |
| IB.16 | 3 | 68.92 | -11.06 |
| | 1000 | 77.36 | -11.65 |
| IB.163 | 3 | 45.8 | -5.44 |
| | 10 | 76.13 | 13.77 |
| IC.6 | 1000 | 84.96 | 10.96 |
| IC.8 | 3 | 45.15 | 3.38 |
| IC.9 | 3 | 34.3 | 2.51 |
| Fluticasone propionate | 1000 | 75.03 | 82.36 |
| Dexamethasone | 1000 | 44.73 | 68.66 |

* In all the compounds (other than the reference compounds) the thymus weight change and the body weight gain were statistically insignificant when compared with vehicle control

5

(d) Sephadex-Induced Lung Edema in the SD Rat

Sephadex G-200 was prepared in sterile saline (10mg/ml) and allowed to swell for at least 3 days at room temperature. Test compounds were prepared as suspensions by grinding and sonicating the solid in chilled saline. All the compounds were administered intratracheally at 24hrs and 2hrs prior to intratracheal administration of Sephadex (5 mg/kg) under light ether anesthesia. Vehicle control animals were administered vehicle instead of Sephadex. At 24hr after Sephadex instillation, lung and thymus were excised from individual animals and weighed. Wet weight of lung and thymus was corrected for 100g of initial body weight. The percentage increase in lung weight caused by Sephadex and its inhibitions by the compounds, were calculated. The percentage inhibitions of thymus compared to vehicle control group were also calculated.

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Table 10: Sephadex-Induced Lung Edema in the SD Rat

| Compound No. | Dose (mcg/kg) | Mean % inhibition* | |
|--------------|---------------|--------------------|--------|
| | | Lung edema | Thymus |
| IA.168 | 3000 | 95.3 | 9.2 |
| IB.15 | 1000 | 70.3 | 4.5 |
| IB.15 | 3000 | 71.1 | 6.4 |
| IB.51 | 3000 | 120.5 | 29.8 |
| IB.54 | 3000 | 110.4 | 29.7 |
| IB.64 | 1000 | 86.4 | 2.0 |
| IB.64 | 3000 | 104.6 | 20.0 |
| IB.67 | 3000 | 121.8 | 33.4 |
| IB.79 | 3000 | 99.3 | 15.2 |
| IB.94 | 3000 | 99.7 | 8.1 |
| IB.100 | 3000 | 120.8 | 36.0 |
| IB.101 | 3000 | 114.8 | 8.9 |
| IB.150 | 3000 | 106.2 | 18.0 |
| Budesonide | 3000 | 119.38 | 67.08 |

* In all the compounds (other than the reference compounds) the body weight gain was statistically insignificant when compared with vehicle control

5

Table 10a: Therapeutic Index for Compounds in Sephadex Lung Edema model in SD Rat

| Comp No. | ED50 Lung edema (mg/kg, i.t.) | ED ₅₀ Thymus (mg/kg, i.t.) | Therapeutic index
ED ₅₀ Thymus involution/
ED ₅₀ Lung edema |
|------------------------|-------------------------------|---------------------------------------|---|
| IB.51 | 0.641 | 13.31 | 20.76 |
| IB.67 | 0.232 | 8.84 | 38.10 |
| IB.70 | 0.323 | 7.67 | 23.75 |
| IB.88 | 0.300 | 4.09 | 13.63 |
| Budesonide | 0.101 | 0.68 | 6.73 |
| Fluticasone propionate | 0.086 | 0.36 | 4.18 |

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(e) Liver Glycogen Deposition in Rats

Male Sprague Dawley rats, weighing 190-220g were bilaterally adrenalectomized and maintained on 0.9% saline solution throughout the experiment. On day 5th and 6th of adrenalectomy, animals were made into different groups, test compounds prepared in cold saline (sonicated for 30min) were instilled intratracheally 2 doses @ 3mg/kg, 24hrs apart. At 15hrs after the last treatment, animals were sacrificed and livers were excised and weighed. The glycogen content of the livers was determined by anthrone method. Briefly, a weighed quantity of liver tissue was homogenized with 5% trichloroacetic acid, supernatant mixed with ethanol and kept overnight for precipitation. The glycogen thus extracted was estimated as glucose generated after acid hydrolysis by addition of anthrone reagent at 620nm. Glycogen content was expressed as mg/100g liver.

Table 11: Liver Glycogen Deposition in Rats

| Comp No. | Dose (mg/kg) | Glycogen content (mg/100g liver) | % Inhibition of thymus |
|------------------------|--------------|----------------------------------|------------------------|
| IA.3 | 3 | -13.6 | -2.42 |
| IB.4 | 3 | -5.77 | -9.68 |
| IB.50 | 3 | 6.67 | 5.48 |
| IC.3 | 3 | -11.34 | -2.43 |
| Fluticasone propionate | 3 | 1514.65 | 70.17 |
| Mometasone furoate | 3 | 1117.32 | 43.51 |
| Budesonide | 3 | 552.77 | 65.02 |

(f) Assessment of Systemic Activity by i.v. Route of Administration

For assessing systemic side effect on i.v. administration, cotton pellet granuloma assay (blank cotton pellet) in male SD rats was undertaken. Sterilized cotton pellets weighing 20mg were surgically implanted into the scapular region on both sides. Starting from next day of implantation, compounds dissolved in Pharmasolve (Pharmasolve 66.67% in saline) or vehicle were administered intravenously at 1.6mg/kg dose for 3 successive days. On fifth day of implantation, pellets along with granuloma were taken out. The thymus gland was also separated from each animal and weighed. The pellets with granuloma were dried for 20hrs at 60°C and

weighed. Mean weights of dry granuloma and thymus and body weight gain/100g body weights were compared with vehicle control groups.

The compounds of formula I of present invention did not induce any significant thymus and body weight gain suppression by i.v. administration. Further, there was no significant cotton pellet granuloma inhibition by i.v. route of administration, thus clearly indicating lack of systemic activity and hence excellent systemic safety profile for the compounds of formula I.

Table 12: Activity by i.v. Routes of Administration

| Comp No. | Dose mcg (for 3 days), i.v. | Mean Inhibition of Granuloma (%) | Mean Thymus wt. Decrease (%)* |
|------------------------|-----------------------------|----------------------------------|-------------------------------|
| IA.3 | 1600 | 3.98 | 6.37 |
| IA.11 | 1600 | 16.65 | -17.88 |
| IA.89 | 1600 | 15.90 | 6.54 |
| IC.3 | 1600 | 12.09 | -10.38 |
| IC.5 | 1600 | -22.20 | 1.67 |
| IA.143 | 1600 | -3.01 | 5.51 |
| Fluticasone propionate | 1600 | 55.62 | 75.71 |

*The body weight gain in all the compounds was statistically not significant when compared with vehicle control

Conclusion

The compounds of formula I of the present invention have potent binding to the glucocorticoid receptor *in vitro*. In the *in vivo* models, which include croton oil induced ear edema, cotton pellet induced granuloma, and Sephadex induced lung edema screens, the compounds of the present invention exhibit significant anti-inflammatory activity. In the cotton pellet granuloma, the thymus involution and the body weight gain due to the compounds was either absent or insignificant even at dose levels as high as 100-1000mcg per pellet. Similar behaviour was once again observed in the case Sephadex induced lung edema models even when the compounds were administered at very high doses, clearly demonstrating that these compounds do not cause any adverse systemic effects following local administration. The absence or non-significance of the systemic side effects was further confirmed by measurement of hepatic glycogen deposition

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in rats after intratracheal administration, and by measurement of thymus and body weight gain suppression following i.v. administration.

Thus the compounds of formula I described in the present invention are potent anti-inflammatory glucocorticoids having insignificant or no noteworthy systemic activity even at doses
5 significantly higher than therapeutic doses. Due to non-significant systemic effects, the compounds of the present invention have high therapeutic index for anti-inflammatory activity vs systemic side effects, a property which is highly desirable for therapies using glucocorticoids.

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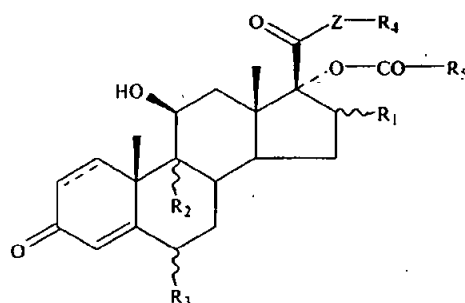
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WE CLAIM

1. 11 β -hydroxyandrost-4-ene-3-one, compound of formula I, and physiologically acceptable salt thereof:



Formula I

- 10 --- represents single or double bond and

~~~~~ represents α or β -configuration.

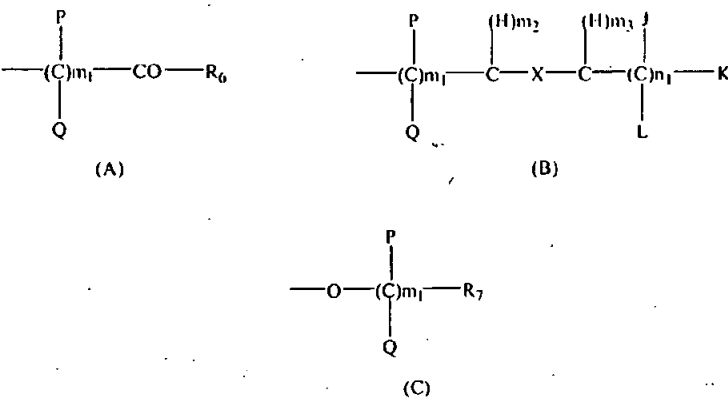
wherein

Z represents O or S;

- 15 R_1 represents hydrogen or methyl which may be either in α or β -configuration, or methylene;
 R_2 and R_3 are the same or different and each independently represents hydrogen, halogen or a methyl group;

- R_5 represents a group selected from (C₁-C₁₀)-alkyl, (C₃-C₁₃)-cycloalkyl, -O-(C₁-C₁₀)-alkyl, aryl or heterocyclic ring wherein the ring or ring system is unsubstituted or substituted by one or more halogen, -OH, (C₁-C₃)-alkyl, -O-(C₁-C₃)-alkyl, (C₃-C₁₃)-cycloalkyl; wherein the alkyl or cycloalkyl groups can optionally contain one or more unsaturations and/or can have one or more hetero atom incorporated therein and optionally in each case have one or more hydrogen atoms replaced by halogen, -OH, (C₁-C₃)-alkyl, -O-(C₁-C₃)-alkyl, (C₃-C₁₃)-cycloalkyl; and

R₄ represents moiety selected from a group consisting of A, B and C, with a proviso that when R₄ represents moiety (C), Z is S;



5

wherein

m₁ is 1, 2 or 3;

m₂ is 0 or 1;

m₃ is 0 or 1;

10

n₁ is 0, 1 or 2;

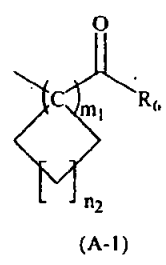
R₆ represents a group selected from (C₁-C₈)-alkyl, (C₃-C₁₃)-cycloalkyl, aryl and a heterocyclic radical, where the ring or ring system is unsubstituted or substituted by one or more substituents selected from (C₁-C₈)-alkyl, (C₃-C₁₃)-cycloalkyl, halogen, O-(C₁-C₈)-alkyl, O-(C₃-C₁₃)-cycloalkyl, OCO-(C₁-C₃)-alkyl, S(O)₀₋₂(C₁-C₈)-alkyl, COO-(C₁-C₈)-alkyl, -OCO-O-(C₁-C₃)-alkyl, -OCO-CO-O-(C₁-C₃)-alkyl, CONH₂, CONH-(C₁-C₈)-alkyl, CON-[(C₁-C₈)-alkyl]₂, -NHCO-(C₁-C₈)-alkyl, N-(C₁-C₈)-alkyl-CO-(C₁-C₈)-alkyl, -NHCO-O-(C₁-C₈)-alkyl, -N-(C₁-C₈)-alkyl-CO-O-(C₁-C₈)-alkyl, -NHCONH-(C₁-C₈)-alkyl, -N-(C₁-C₈)-alkyl-CONH-(C₁-C₈)-alkyl, -NHCONH-SO₂-(C₁-C₈)-alkyl, -N-(C₁-C₈)-alkyl-CONH-SO₂-(C₁-C₈)-alkyl, -NO₂, -CN; wherein the alkyl or cycloalkyl groups can optionally contain one or more unsaturations and/or can have one or more hetero atom incorporated therein and optionally, in each case have one or more hydrogen atoms replaced by halogen, -OH, (C₁-C₃)-alkyl, -OCO-(C₁-C₃)-alkyl or (C₃-C₁₃)-cycloalkyl;

20

with a proviso that when R₄ represents moiety A wherein R₆ represents (C₃-C₁₃)-cycloalkyl optionally containing one or more hetero atom incorporated therein, the hetero atom is not nitrogen;

P and Q are independently selected from hydrogen and C₁ to C₃ alkyl;

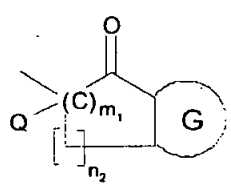
- 5 or P and Q can be joined together with the carbon atom to which they are attached to form (C₃-C₈)-cycloalkyl as represented by moiety (A-1):



wherein m₁ is 1 and n₂ is 0, 1, 2, 3, 4 or 5 and R₆ is an aryl as defined above;

- 10 or P and R₆ can be joined together to form a cyclic system as represented by moiety (A-2):

(A-2)



wherein m₁ is 1 and n₂ is 0, 1, 2, 3 or 4 and ring G is an aryl as defined above;

X represents either a double bond or a triple bond; and

J, K and L are independently selected from a group consisting of hydrogen, halogen,

- 15 (C₁-C₁₀)-alkyl, (C₃-C₁₃)-cycloalkyl, -OH, -O-(C₁-C₁₀)-alkyl, -O-(C₃-C₁₃)-cycloalkyl, -OCO-(C₁-C₁₀)-alkyl, -OCO-(C₃-C₁₃)-cycloalkyl, -OCO-CO-O-(C₁-C₁₀)-alkyl, -OCO-CO-O-(C₃-C₁₃)-cycloalkyl, -OCO-O-(C₁-C₁₀)-alkyl, -OCO-O-(C₃-C₁₃)-cycloalkyl, -OCO-NH-(C₁-C₁₀)-alkyl, -OCO-NH-(C₃-C₁₃)-cycloalkyl, -OCO-N-[(C₁-C₁₀)-alkyl]₂, -OCO-N-[(C₃-C₁₃)-cycloalkyl]₂, -OCO-NHSO₂-(C₁-C₁₀)-alkyl, -OCO-NHSO₂-(C₃-C₁₃)-cycloalkyl, -NH₂, -NH-(C₁-C₈)-alkyl, -N-[(C₁-C₈)-alkyl]₂, -NO₂ and -CN;
- 20

wherein the alkyl or cycloalkyl groups can optionally contain one or more unsaturations and/or can have one or more hetero atom incorporated therein and optionally, in each case have one or more hydrogen atoms replaced by halogen, -OH, (C₁-C₃)-alkyl,

-O-(C₁-C₃)-alkyl, -OCO-(C₁-C₃)-alkyl, -COOH, -COO-(C₁-C₃)-alkyl,

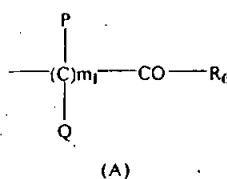
5 -COO-(C₁-C₅)-haloalkyl, -NHCO-(C₁-C₈)-alkyl, -ONO₂, -NH-(C₁-C₈)-alkyl, -N-[(C₁-C₈)-alkyl]₂, -NO₂, -CN, (C₃-C₁₃)-cycloalkyl, aryl or heterocyclic radical;

or J and K can be joined together with the carbon atom to which they are attached to represent a (C₃-C₁₃)-cycloalkyl or -CO- group and L is as defined above;

or J, K and L are absent when n₁ is 0;

10 R₇ represents a group selected from hydrogen, halogen, aryl and CO-aryl, wherein the ring or ring system is unsubstituted or substituted as defined above;

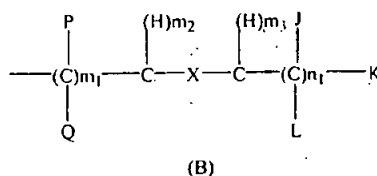
2. 11β-hydroxyandrosta-4-ene-3-one, compound of formula I, and physiologically acceptable salt thereof, as claimed in claim 1, wherein R₄ represents moiety (A).



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wherein m₁, P, Q and R₆ are as defined in claim 1.

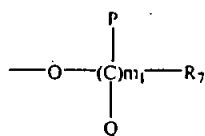
3. 11β-hydroxyandrosta-4-ene-3-one, compound of formula I, and physiologically acceptable salt thereof, as claimed in claim 1, wherein R₄ represents moiety (B).



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wherein m₁, m₂, m₃, n₁, P, Q, J, K, L and X are as defined in claim 1.

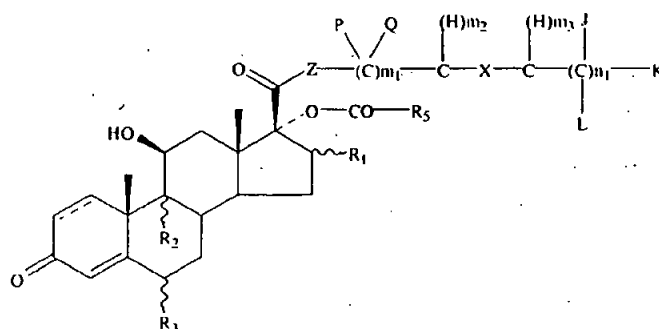
4. 11β-hydroxyandrosta-4-ene-3-one, compound of formula I, and physiologically acceptable salt thereof, as claimed in claim 1, wherein R₄ represents moiety (C).



(C)

wherein m_1 , P, Q and R_7 are as defined in claim 1.

- 5 5. 11β -hydroxyandrost-4-ene-3-one, compound of formula I-B, and physiologically acceptable salt thereof:



Formula I-B

10 wherein

Z represents O or S;

R_1 represents hydrogen or methyl which may be either in α or β -configuration, or methylene;

R_2 and R_3 are the same or different and each independently represents hydrogen, halogen or a methyl group;

R_5 represents a group selected from (C_1-C_{10}) -alkyl, (C_3-C_{13}) -cycloalkyl,

-O- (C_1-C_{10}) -alkyl, aryl or heterocyclic ring wherein the ring or ring system is unsubstituted or substituted by one or more halogen, -OH, (C_1-C_3) -alkyl, -O- (C_1-C_3) -alkyl, (C_3-C_{13}) -cycloalkyl; wherein the alkyl or cycloalkyl groups can optionally contain one or more

20 unsaturations and/or can have one or more hetero atom incorporated therein and optionally in

each case have one or more hydrogen atoms replaced by halogen, -OH, (C₁-C₃)-alkyl, -O-(C₁-C₃)-alkyl, (C₃-C₁₃)-cycloalkyl; and

m₁ is 1;

m₂ is 0 or 1;

5 m₃ is 0 or 1;

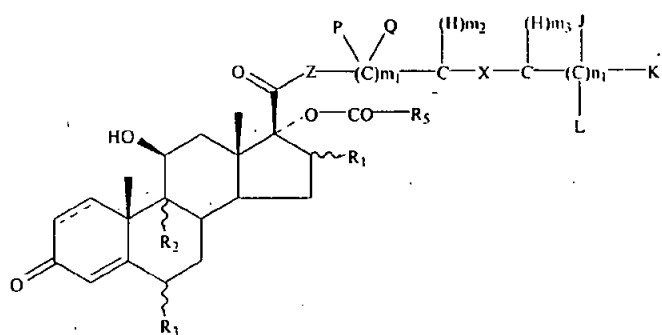
n₁ is 0, 1 or 2;

P and Q are hydrogen;

X represents either a double bond or a triple bond; and

J, K and L are independently selected from a group consisting of hydrogen, halogen, (C₁-C₁₀)-alkyl, (C₃-C₁₃)-cycloalkyl, -OH, -O-(C₁-C₁₀)-alkyl, -O-(C₃-C₁₃)-cycloalkyl, -OCO-(C₁-C₁₀)-alkyl, -OCO-(C₃-C₁₃)-cycloalkyl, -OCO-CO-O-(C₁-C₁₀)-alkyl, -OCO-CO-O-(C₃-C₁₃)-cycloalkyl, -OCO-O-(C₁-C₁₀)-alkyl, -OCO-O-(C₃-C₁₃)-cycloalkyl, -OCO-NH-(C₁-C₁₀)-alkyl, -OCO-NH-(C₃-C₁₃)-cycloalkyl, -OCO-N-[(C₁-C₁₀)-alkyl]₂, -OCO-N-[(C₃-C₁₃)-cycloalkyl]₂, -OCO-NHSO₂-(C₁-C₁₀)-alkyl, -OCO-NHSO₂-(C₃-C₁₃)-cycloalkyl, -NH₂, -NH-(C₁-C₈)-alkyl, -N-[(C₁-C₈)-alkyl]₂, -NO₂ and -CN.

6. 11 β -hydroxyandrosta-4-ene-3-one, compound of formula I-B, and physiologically acceptable salt thereof:



Formula I-B

wherein

Z represents S;

R₁ represents hydrogen or methyl which may be either in α or β -configuration, or methylene;

R₂ and R₃ are the same or different and each independently represents hydrogen, halogen or a methyl group;

R₅ represents a group selected from (C₁-C₁₀)-alkyl, (C₃-C₁₃)-cycloalkyl,

-O-(C₁-C₁₀)-alkyl, aryl or heterocyclic ring wherein the ring or ring system is unsubstituted or substituted by one or more halogen, -OH, (C₁-C₃)-alkyl, -O-(C₁-C₃)-alkyl, (C₃-C₁₃)-cycloalkyl; wherein the alkyl or cycloalkyl groups can optionally contain one or more unsaturations and/or can have one or more hetero atom incorporated therein and optionally in each case have one or more hydrogen atoms replaced by halogen, -OH, (C₁-C₃)-alkyl, -O-(C₁-C₃)-alkyl, (C₃-C₁₃)-cycloalkyl; and

m₁ is 1;

m₂ is 0;

m₃ is 0;

n_i is 0, 1 or 2;

P and Q are hydrogen;

X represents a triple bond, and

J, K and L are independently selected from a group consisting of hydrogen, halogen, (C₁-C₁₀)-alkyl, (C₃-C₁₃)-cycloalkyl, -OH, -O-(C₁-C₁₀)-alkyl, -O-(C₃-C₁₃)-cycloalkyl, -OCO-(C₁-C₁₀)-alkyl, -OCO-(C₃-C₁₃)-cycloalkyl, -OCO-CO-O-(C₁-C₁₀)-alkyl, -OCO-CO-O-(C₃-C₁₃)-cycloalkyl, -OCO-O-(C₁-C₁₀)-alkyl, -OCO-O-(C₃-C₁₃)-cycloalkyl, -OCO-NH-(C₁-C₁₀)-alkyl, -OCO-NH-(C₃-C₁₃)-cycloalkyl, -OCO-N-[(C₁-C₁₀)-alkyl]₂, -OCO-N-[(C₃-C₁₃)-cycloalkyl]₂, -OCO-NHSO₂-(C₁-C₁₀)-alkyl, -OCO-NHSO₂-(C₃-C₁₃)-cycloalkyl, -NH₂, -NH-(C₁-C₈)-alkyl, -N-[(C₁-C₈)-alkyl]₂, -NO₂ and -CN.

7. 1 β -Hydroxyandrosta-4-ene-3-one as claimed in claim 1 selected from the group consisting of

S-[2-(4-Chlorophenyl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate,

2-(4-Fluorophenyl)-2-oxoethyl 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carboxylate,

S-[2-(4-Fluorophenyl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate,

5 *S*-[2-(2,4-Difluorophenyl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate,

S-[2-(2,4-Dichlorophenyl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate,

10 *S*-[2-(3,4-Dichlorophenyl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate,

S-[2-(5-Chlorothiophen-2-yl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carboxylate,

15 *S*-[2-Oxopropyl]6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate,

20 2-Oxopropyl 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-dien-17 β -carboxylate,

S-[2-(4-Methoxyphenyl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate,

25 *S*-[2-Oxo-2-(4-trifluoromethoxyphenyl)ethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate,

S-[2-Oxo-2-(4-trifluoromethylphenyl)ethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate,

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2-(4-Methanesulphonylphenyl)-2-oxoethyl 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carboxylate,

5 S-[2-(4-Methanesulphonylphenyl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate,

2-Oxo-2-phenylethyl 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carboxylate,

10 S-[2-Oxo-2-phenylethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate,

S-[2-Oxo-2-(2,4,6-trimethylphenyl)ethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate,

15 S-[1,1-Dimethyl-2-oxo-2-phenylethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate,

20 S-[2-(4-Methoxyphenyl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-17 α -(2-methylpropionyloxy)-3-oxoandrosta-1,4-diene-17 β -carbothioate,

S-[2-Oxo-2-(4-trifluoromethylphenyl)ethyl] 17 α -cyclobutylcarbonyloxy-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,

25 S-[2-(2,4-Difluorophenyl)-2-oxoethyl] 17 α -cyclobutylcarbonyloxy-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,

S-[2-(4-Methoxyphenyl)-2-oxoethyl] 17 α -cyclobutylcarbonyloxy-6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,

S-[2-(2,4-Difluorophenyl)-2-oxoethyl] 9 α -fluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate.

5 *S*-[2-(4-Chlorophenyl)-2-oxoethyl] 9 α -fluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,

S-[2-(4-Methoxyphenyl)-2-oxoethyl] 9 α -fluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,

10 *S*-[2-(4-Fluorophenyl)-2-oxoethyl] 9 α -fluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,

S-[2-(4-Chlorophenyl)-2-oxoethyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,

15 *S*-[2-Oxo-2-(4-trifluoromethylphenyl)ethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -[(2-thienylcarbonyl)oxy]androsta-1,4-diene-17 β -carbothioate,

20 *S*-[2-(3,4-Dimethylphenyl)-2-oxoethyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate,

S-[2-(3-Chlorophenyl)-2-oxoethyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,

25 *S*-[2-Oxo-2-(4-trifluoromethylphenyl)ethyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 β -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate.

S-(4-Hydroxy-but-2-ynyl) 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,

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S-(4-*n*-Propylcarbonyloxy-but-2-ynyl) 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate,

5 *S*-[4-(2-Ethoxy-1,2-dioxoethyl)-(E)-but-2-enyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate,

S-[4-(2-Ethoxy-1,2-dioxoethyl)oxy-(E)-but-2-enyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate.,

10 *S*-[4-*n*-Propylcarbonyloxy-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,

S-[4-(2-Methylpropionyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,

15 *S*-[4-(2,2-Dimethylpropionyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,

20 *S*-[4-(2,2-Dimethylpropionyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate,

S-[4-*n*-Propylcarbonyloxy-(Z)-but-2-enyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,

25 *S*-[4-(2-Ethoxy-1,2-dioxoethyl)oxy-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate.

S-[4-*n*-Propylcarbonyloxy-but-2-ynyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -[(2-thienylcarbonyl)oxy]androsta-1,4-diene-17 β -carbothioate,

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- S*-[(4-Cyclopropylcarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,
- 5 *S*-[(4-Cyclobutylcarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,
- S*-[(4-Cyclopentylcarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,
- 10 *S*-[4-*n*-Propylcarbonyloxy-(*E*)-but-2-enyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,
- S*-[(4-Methoxycarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,
- 15 *S*-[(4-Ethoxycarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,
- S*-[4-(2,2-Dimethylethyloxy)carbonyloxy]-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,
- 20 *S*-[4-(2-Methylpropyloxy)carbonyloxy]-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,
- 25 *S*-[4-(3-Chloropropylcarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,
- S*-[4-Dichloroacetoxy-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,
- 30

SUBSTITUTE SHEET (RULE 26)

245

- S*-[4-(2-Methylpropylcarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)-oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,
- 5 *S*-[4-(3,3-Dimethylpropylcarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,
- S*-(4-Propionyloxy-but-2-ynyl) 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,
- 10 *S*-[4-(3,3,3-Trifluoropropionyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)-oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,
- S*-[4-(Methoxyacetyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,
- 15 *S*-[4-(Ethoxyacetyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,
- S*-(4-Acetoxy-but-2-ynyl) 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,
- 20 *S*-[4-(2,2-Dimethylbutylcarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)-oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,
- 25 *S*-[4-((1*S*)-Camphanylcarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)-oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,
- S*-[4-(4-Ethoxybutyl-1,4-dione)oxy-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)-oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,
- 30

- S*-[4-(4-Ethoxy-(*Z*)-but-2-en-1,4-dione)oxy-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate.
- 5 *S*-[4-(4-Methoxybutyl-1,4-dione)oxy-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate.
- S*-[4-(4-Isopropoxybutyl-1,4-dione)oxy-but-2-ynyl] 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-17 α -[(2-furanylcarbonyl)oxy]-3-oxoandrosta-1,4-diene-17 β -carbothioate.
- 10 *S*-[4-(4-Isobutyloxybutyl-1,4-dione)oxy-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate.
- S*-[4-(4-*n*-Butyloxybutyl-1,4-dione)oxy-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate.
- 15 *S*-[4-(3-Chloro-2,2-dimethylpropionyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate.
- S*-[4-(4-Methoxy-(*E*)-but-2-en-1,4-dione)oxy-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate.
- 20 *S*-[4-(3-Methyl-1-oxobutyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate.
- S*-[4-(2-Ethyl-1-oxobutyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate.
- 25 *S*-[4-(*N,N*-Dimethylaminocarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate.
- 30

S-[4-(2-Chloro-2-methylpropionyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanyl-carbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,

S-[4-(4-Methyl-1-oxopentyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)oxy]-
11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,

S-[4-(2-Hydroxy-2-methylpropionyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanyl-carbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,

S-[4-(2-Fluoro-2-methylpropionyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanyl-carbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,

S-[4-(4-Methoxy-(*Z*)-but-2-en-1,4-dione)oxy-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanyl-carbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,

S-[4-(4-Ethoxy-(*E*)-but-2-en-1,4-dione)oxy-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanyl-carbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,

S-[4-(4-Isobutyloxy-(*E*)-but-2-en-1,4-dione)oxy-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,

S-(4-Acryloyloxy-but-2-ynyl) 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,

S-[4-(Cyclopentylmethyloxycarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanyl-carbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,

S-[4-(3-Methylbut-2-enoxycarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanyl-carbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,

- S*-[4-(*n*-Pentyloxy-carbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,
- 5 *S*-[4-(2,2-Dimethyl-3-fluoropropionyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,
- 10 *S*-[4-((*S*)-2,2-Dimethyl-1,3-dioxolan-4-yl-methoxycarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,
- S*-[4-(*R*)-2,2-Dimethyl-1,3-dioxolan-4-yl-methoxycarbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,
- 15 *S*-[4-(Isoamyloxy-carbonyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,
- S*-(4-Ethoxy-but-2-ynyl) 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate,
- 20 6 α ,9 α -Difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbonylsulfenic acid fluoromethyl ester,
- 25 6 α ,9 α -Difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbonylsulfenic acid fluoromethyl ester,
- 6 α ,9 α -Difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbonylsulfenic acid (4-fluorophenyl)methyl ester.

- 6 α ,9 α -Difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbonylsulfenic acid (4-trifluoromethylphenyl)methyl ester,
- 5 6 α ,9 α -Difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbonylsulfenic acid (4-chlorophenyl)methyl ester,
- 6 α ,9 α -Difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbonylsulfenic acid (4-trifluoromethylphenyl)methyl ester,
- 10 9 α -Fluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbonylsulfenic acid (4-fluorophenyl)methyl ester,
- 6 α ,9 α -Difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,4-diene-17 β -carbonylsulfenic acid methyl ester,
- 15 6 α ,9 α -Difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbonylsulfenic acid methyl ester,
- 20 S-[4-(4-Methyl-1-oxopentyloxy)-but-2-ynyl] 6 α ,9 α -difluoro-17 α -[(2-furanylcarbonyl)oxy]-11 β -hydroxy-16 α -methyl-3-oxoandrosta-1,4-diene-17 β -carbothioate.

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Industria y Comercio

REGISTRARÍA

SUPERINTENDENCIA DE INDUSTRIA Y COMERCIO

DIVISION DE NUEVAS CREACIONES

TARJETA ARCHIVO TEMATICO

PATENTE DE INVENCION ____ PCT ____ MODELO DE UTILIDAD ____ DISEÑO INDUSTRIAL

| | | |
|--|--|-----------------------------------|
| N° de solicitud: (22) Fecha de solicitud: | | FIGURA CARACTERISTICA
6 x 6 cm |
| Clasificación Internacional : | | |
| Solicitante(s)
UN PHARMACEUTICAL INDUSTRIES LIMITED | | |
| Inventor(es) <u>PATEL, Jiten Ranchhodbhai; PATEL, Gopalkumar Chimanlal;</u>
<u>HEIH, Gaurav Sanjivkumar; SHAH Samir Rameshchandra; MANDHANE,</u>
<u>anjay Nandlal; CHITTURI, Trinadha Rao; THENNATT, Rajamannar.</u> | | |
| Agente: <u>JOSE LUIS REYES VILLAMIZAR</u> | | |
| Prioridad (31) No. Prioridad 32) Fecha (33) Pais
X 131/MUM/06 27.01.2006 INDIA | | |
| Fecha inicio fase nacional: 26.08.2008 | | |
| Datos relativos a la presentación de la solíc. PCT Fecha: 07.09.2007 | | |
| Fecha de presentación de la solicitud: 29.01.2007 No. Publicación : WO 2007/099548 A2 | | |
| No. de solicitud PCT/ IN2007/000039 | | |
| Titulo:
NOVEDOSAS 11 β -HIDROXIANDROSTA-4-EN-3-ONAS | | |

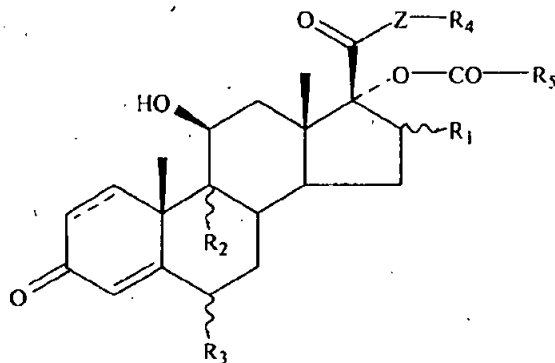
Resumen:

VER RESPALDO

CONTINUA AL RESPALDO ...

RESUMEN:

La presente invención se refiere a análogos anti-inflamatorios y antialérgicos novedosos de las 11β -hidroxiandrosta-4-en-3-onas, representados como fórmula I y su sal fisiológicamente aceptable, que tienen efectos sistémicos insignificantes o no dignos de mención con múltiplos de una dosis eficaz.



Fórmula I

SECRETARÍA DE INDUSTRIA Y COMERCIO

PATENTE

☒

MODELO DE UTILIDAD

☐

DISEÑO INDUSTRIAL

☐

SOLICITANTE/S. RAZON SOCIAL O APELLIDOS Y NOMBRES SUN PHARMACEUTICAL INDUSTRIES LIMITED

DOMICILIO Acme Plaza, Andherikurla Road, Andheri (east), Mumbai 400 059 (IN)

APODERADO JOSE LUIS REYES VILLAMIZAR

TITULO NOVEDOSAS 11~~8~~-HIDROXIANDROSTA-4-EN-3-ONAS

CLASIFICACION

EXPEDIENTE No. _____ FECHA DE SOLICITUD _____ ROLLO MICROFILM _____

CERTIFICADO No. _____ FECHA DE CONCESION _____ VIGENCIA DESDE _____ HASTA _____

PRORROGA _____ CAMBIO DE NOMBRE _____

TRASPASO A

INVENTOR (ES) PATEL, Jiten Ranchhodbhai; PATEL, Gopalkumar Chimanlal; SHETH, Gaurav Sanjivkumar;
 OTROS SHAH, Samir Rameshchandra; MANDHANE, Sanjay Nandlal; CHITTURI, Trinadha Rao; THENNATI, Rajamannar.

SUPERINTENDENCIA DE INDUSTRIA Y COMERCIO

NIT : 800176089-2

RECIBO OFICIAL DE CAJA : 08 - 67.910
FECHA : AGOSTO 26 DE 2008



**** CONSIGNACION ****

| DEPOSITANTE | TIPO PAGO | BANCO | CUENTA | No. PAGO | FECHA PGO | Vr. PAGO |
|---------------------------|--------------|-----------------|-------------|----------|------------|--------------|
| REYES Y REYES ABOGADOS | CONSIGNACION | BANCO DE BOGOTA | 062754387 | 4276215 | 26/08/2008 | 286,000.00 |
| REYES Y REYES ABOGADOS | CONSIGNACION | BANCO DE BOGOTA | 062754387 | 4276225 | 26/08/2008 | 99,000.00 |
| REYES Y REYES ABOGADOS | CONSIGNACION | BANCO DE BOGOTA | 062754387 | 4276230 | 26/08/2008 | 460,000.00 |
| REYES Y REYES ABOGADOS | CONSIGNACION | BANCO DE BOGOTA | 062754387 | 4276241 | 26/08/2008 | 420,000.00 |
| REYES Y REYES ABOGADOS | CONSIGNACION | BANCO DE BOGOTA | 062754387 | 4276252 | 26/08/2008 | 641,000.00 |
| ...MAS INFORMACION NO IMP | | | TOTAL | | | 1,969,000.00 |

**** C O N C E P T O ****

| CANT. | CONCEPTO | TOTAL CONCEPTO |
|-------|-------------------------------------|----------------|
| 1 | 50005-01-01 SOLICITUDES | |
| | 1 TRAMITES DE SOL. DE PATENTE DE IN | 501,000.00 |
| | TOTAL : | \$ 501,000.00 |

SON: QUINIENTOS UN MIL PESOS

RESPONSABLE : _____

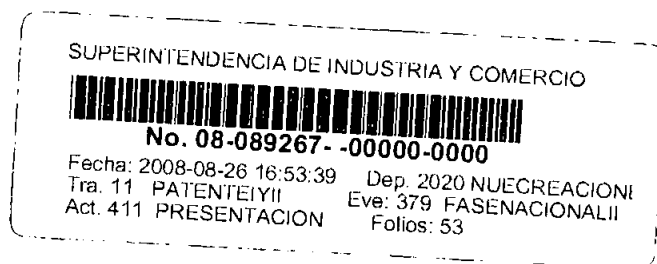
RECIBO DE CAJA APLICADO AL EXPEDIENTE No. _____

253

SUPERINTENDENCIA DE INDUSTRIA Y COMERCIO

NIT : 800176089-2

RECIBO OFICIAL DE CAJA : 08 - 67,911
FECHA : AGOSTO 26 DE 2008



**** CONSIGNACION ****

| DEPOSITANTE | TIPO PAGO | BANCO | CUENTA | No. PAGO | FECHA PGO | Vr. PAGO |
|---------------------------|--------------|-----------------|-------------|----------|------------|--------------|
| REYES Y REYES ABOGADOS | CONSIGNACION | BANCO DE BOGOTA | 062754387 | 4276215 | 26/08/2008 | 286,000.00 |
| REYES Y REYES ABOGADOS | CONSIGNACION | BANCO DE BOGOTA | 062754387 | 4276225 | 26/08/2008 | 99,000.00 |
| REYES Y REYES ABOGADOS | CONSIGNACION | BANCO DE BOGOTA | 062754387 | 4276230 | 26/08/2008 | 460,000.00 |
| REYES Y REYES ABOGADOS | CONSIGNACION | BANCO DE BOGOTA | 062754387 | 4276241 | 26/08/2008 | 420,000.00 |
| REYES Y REYES ABOGADOS | CONSIGNACION | BANCO DE BOGOTA | 062754387 | 4276252 | 26/08/2008 | 641,000.00 |
| ...MAS INFORMACION NO IMP | | | TOTAL | | | 1,969,000.00 |

**** C O N C E P T O ****

| CANT. | RENTISTICO | CONCEPTO | TOTAL CONCEPTO |
|-------|-------------|--------------------------------------|----------------|
| 1 | 50005-01-01 | SOLICITUDES | |
| | | 82 INVOCACION DE UNA PRIORIDAD EN NU | 140,000.00 |
| | | TOTAL : | 140,000.00 |

SON: CIENTO CUARENTA MIL PESOS

RESPONSABLE : _____

RECIBO DE CAJA APLICADO AL EXPEDIENTE No. _____

34

SUPLENTENDENCIA DE INDUSTRIA Y COMERCIO



No 08 089267 00000 0000

Fecha 2008 08 26 16 53 39 Dep 2020 NUECLACIONI
Tri 11 PATENTEIYII Lva 379 PASL NACIONALII
Act 411 PRESENTACION Folia 53



Industria y Comercio
SUPERINTENDENCIA

REQUISITOS MINIMOS PARA ADMISION A TRAMITE PCT

PATENTE DE INVENCION

☒

MODELO DE UTILIDAD ☐

- ◆ Indicación de que se solicita la concesión de una patente ☒
- ◆ Datos de identificación del solicitante o de la persona que presenta la solicitud ☒
- ◆ Descripción de la invención ☐
- ◆ Dibujos de ser estos pertinentes ☒
- ◆ Comprobante de pago de las tasas establecidas ☒

COMPLETA ☐

INCOMPLETA ☐

- DISEÑO INDUSTRIAL ☐

- ◆ Indicación de que se solicita el registro de Diseño Industrial ☐
- ◆ Datos de identificación del solicitante o de la persona que presenta la solicitud ☐
- ◆ Representación gráfica y fotográfica del Diseño Industrial o muestra del material que incorpora el diseño ☐
- ◆ Comprobante de pago de las tasas establecidas ☐

COMPLETA ☐

INCOMPLETA ☐

ESQUEMA DE TRAZADO ☐

- ◆ Indicación de que se solicita el registro de un Esquema de Trazado ☐
- ◆ Datos de identificación del solicitante o de la persona que presenta la solicitud ☐
- ◆ Representación gráfica del esquema trazado ☐
- ◆ Comprobante de pago de las tasas establecidas ☐

COMPLETA ☐

INCOMPLETA ☐

SIRY

Firma Responsable

Fecha Agosto 26-08

Carrera 13 No 27 00 Piso 5, 7 y 10
Commutador 3 82 08 40
Fax 350 52 20
E-mail info@sic.gov.co
www.sic.gov.co

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REPUBLICA DE COLOMBIA
SUPERINTENDENCIA DE INDUSTRIA Y COMERCIO

Bogotá,
2020

Doctor(a)
REYES VILLAMIZAR JOSE LUIS

| | | |
|------------|----------------------------|-------------------|
| REFERENCIA | Radicación No. | 8 89267 |
| | Solicitud internacional | PCT/IN2007/000039 |
| | Fecha inicio fase nacional | 27/08/2008 |
| | Trámite | 11 |
| | Evento | 379 |
| | Actuación | 430 |
| | Oficio No. | |

11317

Como resultado del examen de forma, realizado con fundamento en el artículo 38 de la Decisión 486 de la Comisión de la Comunidad Andina, artículo 27 del Tratado de Cooperación en Materia de Patentes (PCT), regla 51 bis del Reglamento y Circular Única de la Superintendencia de Industria y Comercio, se le comunica que:

1. Si fuere el caso, el solicitante debe adjuntar la traducción de los anexos del reporte de examen preliminar internacional (Art. 36.2.b) del tratado PCT.
2. La solicitud no contiene el poder debidamente otorgado, con el lleno de los requisitos exigidos por los artículos 63 y subsiguientes del Código de Procedimiento Civil. Adicionalmente, deberá presentar el documento que acredita la existencia y representación legal de la sociedad solicitante, cuando ésta fuere persona jurídica.
3. La solicitud no contiene la copia del documento en que consta la cesión del derecho a la patente del inventor al solicitante o a su causante, conforme a lo establecido por el artículo 26 literal k) de la Decisión 486 de la Comisión de la Comunidad Andina. Cuando se trate de documentos otorgados en el extranjero, estos deberán legalizarse de conformidad con lo dispuesto por los artículos 259 y 260 del Código de Procedimiento Civil. Cuando se trate de las declaraciones a que hace referencia la Regla 4.17 ii) del Tratado de Cooperación en Materia de Patentes PCT., el alcance de las tales declaraciones se determinará según indiquen claramente una cesión de derechos del inventor al solicitante o su causante, de conformidad con lo dispuesto en el numeral 5.2.15 del Capítulo Quinto, Título X de la Circular Única de Superintendencia de Industria y Comercio.

En cumplimiento de lo dispuesto por el artículo 39 de la Decisión 486, se le requiere para que dentro del término de dos meses siguientes a la fecha de notificación del presente oficio, complete los requisitos anteriormente enunciados. En caso de no dar cumplimiento al presente requerimiento, la solicitud se considerará abandonada y perderá su prelación.

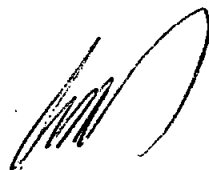
Notifíquese el presente oficio conforme a lo dispuesto en el numeral 5.2, literal e), del capítulo quinto del título primero de la Circular Única No.10 de 2001.

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REPUBLICA DE COLOMBIA
SUPERINTENDENCIA DE INDUSTRIA Y COMERCIO

Radicación No.: 8 89267


ALIX CARMENZA CESPEDES DE VERGEL
Jefe de la división de Nuevas Creaciones

El anterior requerimiento fue notificado por fijación en lista de
fecha 05 SET. 2008
adpall