A One-Pot Intramolecular Tandem Michael-Aldol Annulation Reaction for the Synthesis of Enantiopure Pentacyclic Terpenes

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Supporting Information

¹H and ¹³C NMR spectra of compounds ¹⁴, ⁸, (-)-⁹, (-)-⁶, (-)-¹⁰, (+)-¹¹, (-)-⁴, and (+)-⁵…..S1-S17
Single-crystal X-ray data of compound (-)-⁶…………………………………………………………………..S18-S81
Single-crystal X-ray data of compound (+)-¹¹…………………………………………………………..S81-S94
Single-crystal X-ray data of compound (+)-⁵……………………………………………………………..S94-S115
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The diagram shows a chemical structure with labels Me, Me, and O. The spectrum graph includes peak assignments for various chemical shifts (δ ppm) ranging from 0.0 to 7.5.
C:\NMR_nuts_2008\DATA\jyl-7-035-13C.fid

Std Carbon experiment
Mar 1 2012

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Hz per Pt 1stD = 0.74 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 10559.8418 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP = -284.66
B = 195.66
C = 0.00
The image shows a chemical structure with labels "Me" at each carbon and oxygen atoms. The compound does not have a specific name or structure described in the text provided. The text includes details about an NMR experiment, such as pulse length, recycle delay, solvent details, and spectral parameters. The NMR spectrum is also shown, providing a graphical representation of the chemical's resonance peaks.
(-)-6

C:\NMR_nuts _2008\data\jyl-8-027-A.fid

Std Proton parameters
May 22 2012

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SOLVENT: cdcl3

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SW2 = 1.00 Hz

Hz per Pt 2ndD = 1.00 Hz

O1  = 2399.7371 Hz

O2  = -0.5000 Hz

LB1 = 0.00      Hz

TP    A = -247.71

B =  90.97

C =   0.00

"
S17
X-ray Crystallographic Study for (-)-6 [code name v32e].

A complete set of unique reflections was collected with monochromated CuKα radiation for a single-domain crystal of (-)-6. A total of 2774 1.0°-wide ω- or φ-scan frames with counting times of 6-30 seconds were collected on a Bruker Platinum 135 CCD area detector. X-rays were provided by a Bruker MicroStar microfocus rotating anode operating at 45kV and 60 mA and equipped with Helios high-brilliance multilayer x-ray optics. Preliminary lattice constants were obtained with the Bruker program SMART. Integrated reflection intensities were produced using the Bruker program SAINT. The data set was corrected empirically for variable absorption effects using equivalent reflections. The Bruker software package SHELXTL was used to solve the structure using “direct methods” techniques. All stages of weighted full-matrix least-squares refinement were conducted using Fo² data with the SHELXTL v2014 software package.

The final structural model incorporated anisotropic thermal parameters for all nonhydrogen atoms and isotropic thermal parameters for all hydrogen atoms. Hydrogen atoms were fixed at idealized riding-model sp²- or sp³-hybridized positions with C-H bond lengths of 0.95 – 1.00 Å. The methyl groups were
placed at idealized “staggered” positions (with a C-H bond length of 0.98 Å). Isotropic thermal parameters of the idealized hydrogen atoms were fixed at values 1.2 (non-methyl) or 1.5 (methyl) times the equivalent isotropic thermal parameter of the carbon atom to which they are covalently bonded. The relevant crystallographic and structure refinement data are given in Tables S1.

The asymmetric unit of (-)-6 contains three crystallographically-independent molecules. The first independent molecule (atom labels have an A) is ordered but mild restraints had to be applied to the metrical parameters for the terminal ketone groups for the second (atoms labels have a B) and third (atom labels have a C or D) molecules. The terminal ketone group for the second molecule had minor disorder about a common site but the terminal ketone group for the third molecule had 50/50 disorder between two preferred orientations (labeled C and D). One orientation (labeled C) of the terminal ketone for the third molecule is near a crystallographic twofold axis in the unit cell and is occupied (50% of the time) whenever the D orientation of the terminal ketone is occupied by the C2-related third molecule. Both orientations for this disordered terminal ketone moiety in the third molecule and a single orientation for the second molecule were restrained to have nearly idealized geometries by using a free variable for the respective C15-C16, C16-C17, C17-C22, C19-C20, C20-C21 and C21-C22 bond lengths. This free variable refined to a final value of 1.500(5) Å. The remaining bond lengths and angles for each of these disordered groups were restrained to be multiples of this free variable that were consistent with sp²- or sp³-hybridization. The C15, C16, C17 and O4 atoms for the second and third molecules were also mildly restrained to be flat. Mild restraints were also applied to the anisotropic thermal parameters of disordered carbon C22D.

**Table S1.** Crystal data and structure refinement for C30H48O4.

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<td></td>
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Z 12

Density (calculated) 1.147 Mg/m³

Absorption coefficient 0.576 mm⁻¹

F(000) 3120

Crystal size 0.540 x 0.140 x 0.040 mm³

Theta range for data collection 2.342 to 68.479°.

Index ranges -46<=h<=46, -7<=k<=4, -42<=l<=37

Reflections collected 30565

Independent reflections 10714 [R(int) = 0.0489]

Completeness to theta = 66.000° 99.2 %

Absorption correction Multi-scan

Max. and min. transmission 0.7531 and 0.5355

Refinement method Full-matrix least-squares on F²

Data / restraints / parameters 10714 / 47 / 925

Goodness-of-fit on F² 1.085

Final R indices [I>2sigma(I)] R1 = 0.0768, wR2 = 0.2320

R indices (all data) R1 = 0.0890, wR2 = 0.2452

Absolute structure parameter -0.18(15)

Extinction coefficient n/a

Largest diff. peak and hole 0.502 and -0.409 e.Å⁻³
Table 2. Atomic coordinates ($x \times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for C30H48O4. $U(eq)$ is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

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Table 3. Bond lengths [Å] and angles [°] for C30H48O4.

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C(20A)-C(28A)  1.509(8)
C(20A)-C(21A)  1.526(7)
C(20A)-C(27A)  1.534(8)
C(21A)-C(22A)  1.529(9)
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O(1B)-C(29B)    1.437(6)
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O(2B)-C(30B)    1.428(8)
O(3B)-C(14B)    1.248(6)
O(4B)-C(16B)    1.170(12)
C(1B)-C(2B)     1.526(6)
C(1B)-C(10B)    1.538(5)
C(1B)-H(1BA)    0.9900
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C(2B)-H(2BA)    0.9900
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C(4B)-C(23B)  1.539(6)
C(4B)-C(5B)  1.551(6)
C(4B)-C(24B)  1.556(6)
C(5B)-C(6B)  1.531(6)
C(5B)-C(10B)  1.572(5)
C(5B)-H(5B)  1.0000
C(6B)-C(7B)  1.508(7)
C(6B)-H(6BA)  0.9900
C(6B)-H(6BB)  0.9900
C(7B)-C(8B)  1.534(6)
C(7B)-H(7BA)  0.9900
C(7B)-H(7BB)  0.9900
C(8B)-C(14B)  1.512(7)
C(8B)-C(26B)  1.547(6)
C(8B)-C(9B)  1.570(5)
C(9B)-C(11B)  1.530(6)
C(9B)-C(10B)  1.539(6)
C(9B)-H(9B)  1.0000
C(10B)-C(25B)  1.540(5)
C(11B)-C(12B)  1.519(7)
C(11B)-H(11C)  0.9900
C(11B)-H(11D)  0.9900
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C(12B)-H(12C)  0.9900
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C(13B)-C(18B)  1.312(9)
C(13B)-C(14B)  1.494(7)
C(15B)-C(16B)  1.482(11)
C(15B)-H(15D)  0.9800
C(15B)-H(15E)  0.9800
C(15B)-H(15F)  0.9800
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C(17B)-C(22B)  1.543(10)
C(17B)-H(17C)  0.9900
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C(22B)-H(22C)  0.9900
C(22B)-H(22D)  0.9900
C(23B)-H(23D)  0.9800
\begin{align*}
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\text{C}(23\text{B})-\text{H}(23\text{F}) & \quad 0.9800 \\
\text{C}(24\text{B})-\text{H}(24\text{D}) & \quad 0.9800 \\
\text{C}(24\text{B})-\text{H}(24\text{E}) & \quad 0.9800 \\
\text{C}(24\text{B})-\text{H}(24\text{F}) & \quad 0.9800 \\
\text{C}(25\text{B})-\text{H}(25\text{D}) & \quad 0.9800 \\
\text{C}(25\text{B})-\text{H}(25\text{E}) & \quad 0.9800 \\
\text{C}(25\text{B})-\text{H}(25\text{F}) & \quad 0.9800 \\
\text{C}(26\text{B})-\text{H}(26\text{D}) & \quad 0.9800 \\
\text{C}(26\text{B})-\text{H}(26\text{E}) & \quad 0.9800 \\
\text{C}(26\text{B})-\text{H}(26\text{F}) & \quad 0.9800 \\
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\text{C}(28\text{B})-\text{H}(28\text{F}) & \quad 0.9800 \\
\text{C}(29\text{B})-\text{C}(30\text{B}) & \quad 1.510(9) \\
\text{C}(29\text{B})-\text{H}(29\text{C}) & \quad 0.9900 \\
\text{C}(29\text{B})-\text{H}(29\text{D}) & \quad 0.9900 \\
\text{C}(30\text{B})-\text{H}(30\text{C}) & \quad 0.9900 \\
\text{C}(30\text{B})-\text{H}(30\text{D}) & \quad 0.9900 \\
\text{O}(1\text{C})-\text{C}(29\text{C}) & \quad 1.427(7) \\
\text{O}(1\text{C})-\text{C}(3\text{C}) & \quad 1.432(5) \\
\text{O}(2\text{C})-\text{C}(3\text{C}) & \quad 1.420(6)
\end{align*}
O(2C)-C(30C)  1.433(7)
O(3C)-C(14C)  1.222(5)
O(4C)-C(16C)  1.229(19)
C(1C)-C(2C)  1.528(6)
C(1C)-C(10C)  1.541(5)
C(1C)-H(1CA)  0.9900
C(1C)-H(1CB)  0.9900
C(2C)-C(3C)  1.521(6)
C(2C)-H(2CA)  0.9900
C(2C)-H(2CB)  0.9900
C(3C)-C(4C)  1.546(6)
C(4C)-C(24C)  1.543(6)
C(4C)-C(23C)  1.547(6)
C(4C)-C(5C)  1.551(6)
C(5C)-C(6C)  1.536(5)
C(5C)-C(10C)  1.562(5)
C(5C)-H(5C)  1.0000
C(6C)-C(7C)  1.520(6)
C(6C)-H(6CA)  0.9900
C(6C)-H(6CB)  0.9900
C(7C)-C(8C)  1.532(6)
C(7C)-C(14C)  1.532(6)
C(7C)-C(26C)  1.545(6)
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O(1A)-C(3A)-C(2A) 110.2(4)
O(2A)-C(3A)-C(2A) 109.0(4)
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C(13A)-C(18A)-C(19A)  127.9(5)
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C(10B)-C(1B)-H(1BA) 108.8
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C(1B)-C(2B)-C(3B) 111.9(3)
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C(8B)-C(7B)-H(7BB) 108.9
H(7BA)-C(7B)-H(7BB) 107.7
C(14B)-C(8B)-C(7B) 108.9(4)
C(14B)-C(8B)-C(26B) 103.9(4)
C(7B)-C(8B)-C(26B) 109.6(4)
C(14B)-C(8B)-C(9B) 109.6(4)
C(7B)-C(8B)-C(9B) 109.3(4)
C(26B)-C(8B)-C(9B) 115.3(3)
C(11B)-C(9B)-C(10B) 116.3(3)
C(11B)-C(9B)-C(8B) 109.3(4)
C(10B)-C(9B)-C(8B) 115.5(3)
C(11B)-C(9B)-H(9B) 104.8
C(10B)-C(9B)-H(9B) 104.8
C(8B)-C(9B)-H(9B) 104.8
C(1B)-C(10B)-C(9B) 108.8(3)
C(1B)-C(10B)-C(25B) 115.7(3)
C(9B)-C(10B)-C(25B) 112.2(4)
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H(15E)-C(15B)-H(15F) 109.5
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O(4B)-C(16B)-C(17B) 122.2(15)
C(15B)-C(16B)-C(17B) 113.3(13)
C(16B)-C(17B)-C(22B) 106.1(10)
C(16B)-C(17B)-H(17C) 110.5
C(16B)-C(17B)-H(17D) 110.5
H(17C)-C(17B)-H(17D) 108.7
C(13B)-C(18B)-C(19B) 128.9(7)
C(13B)-C(18B)-H(18B) 115.6
C(19B)-C(18B)-H(18B) 115.6
C(20B)-C(19B)-C(18B) 114.4(8)
C(20B)-C(19B)-H(19C) 108.7
C(18B)-C(19B)-H(19C) 108.7
C(20B)-C(19B)-H(19D) 108.7
C(18B)-C(19B)-H(19D) 108.7
H(19C)-C(19B)-H(19D) 107.6
C(28B)-C(20B)-C(19B) 118.1(9)
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C(19B)-C(20B)-C(21B) 114.3(7)
C(28B)-C(20B)-C(27B) 106.8(11)
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C(8B)-C(26B)-H(26D) 109.5
C(8B)-C(26B)-H(26E) 109.5
H(26D)-C(26B)-H(26E) 109.5
C(8B)-C(26B)-H(26F) 109.5
H(26D)-C(26B)-H(26F) 109.5
H(26E)-C(26B)-H(26F) 109.5
C(20B)-C(27B)-H(27D) 109.5
C(20B)-C(27B)-H(27E) 109.5
H(27D)-C(27B)-H(27E) 109.5
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H(27D)-C(27B)-H(27F) 109.5
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C(20B)-C(28B)-H(28D) 109.5
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H(28D)-C(28B)-H(28E) 109.5
C(20B)-C(28B)-H(28F) 109.5
H(28D)-C(28B)-H(28F) 109.5
H(28E)-C(28B)-H(28F) 109.5
O(1B)-C(29B)-C(30B) 102.2(5)
O(1B)-C(29B)-H(29C)  111.3
C(30B)-C(29B)-H(29C)  111.3
O(1B)-C(29B)-H(29D)  111.3
C(30B)-C(29B)-H(29D)  111.3
H(29C)-C(29B)-H(29D)  109.2
O(2B)-C(30B)-C(29B)  106.2(4)
O(2B)-C(30B)-H(30C)  110.5
C(29B)-C(30B)-H(30C)  110.5
O(2B)-C(30B)-H(30D)  110.5
C(29B)-C(30B)-H(30D)  110.5
H(30C)-C(30B)-H(30D)  108.7
C(29C)-O(1C)-C(3C)  107.7(4)
C(3C)-O(2C)-C(30C)  106.3(4)
C(2C)-C(1C)-C(10C)  112.9(3)
C(2C)-C(1C)-H(1CA)  109.0
C(10C)-C(1C)-H(1CA)  109.0
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C(10C)-C(1C)-H(1CB)  109.0
H(1CA)-C(1C)-H(1CB)  107.8
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C(1C)-C(2C)-H(2CA)  109.2
C(3C)-C(2C)-H(2CB)  109.2
C(1C)-C(2C)-H(2CB)  109.2
H(2CA)-C(2C)-H(2CB)  107.9
O(2C)-C(3C)-O(1C) 106.6(4)
O(2C)-C(3C)-C(2C) 110.1(4)
O(1C)-C(3C)-C(2C) 108.0(4)
O(2C)-C(3C)-C(4C) 109.7(3)
O(1C)-C(3C)-C(4C) 109.7(3)
C(2C)-C(3C)-C(4C) 112.5(4)
C(24C)-C(4C)-C(3C) 110.0(4)
C(24C)-C(4C)-C(23C) 106.8(4)
C(3C)-C(4C)-C(23C) 108.7(4)
C(24C)-C(4C)-C(5C) 114.3(4)
C(3C)-C(4C)-C(5C) 108.1(3)
C(23C)-C(4C)-C(5C) 108.8(3)
C(6C)-C(5C)-C(4C) 115.0(3)
C(6C)-C(5C)-C(10C) 110.1(3)
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C(10C)-C(5C)-H(5C) 104.3
C(7C)-C(6C)-C(5C) 111.4(3)
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C(6C)-C(7C)-C(8C) 113.2(3)
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C(6C)-C(7C)-H(7CB) 108.9
C(8C)-C(7C)-H(7CB) 108.9
H(7CA)-C(7C)-H(7CB) 107.8
C(14C)-C(8C)-C(7C) 109.4(3)
C(14C)-C(8C)-C(26C) 104.2(4)
C(7C)-C(8C)-C(26C) 109.4(3)
C(14C)-C(8C)-C(9C) 109.1(3)
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C(9C)-C(11C)-H(11G) 109.4
C(12C)-C(11C)-H(11H) 109.4
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C(18C)-C(13C)-C(14C) 117.4(4)
C(12C)-C(13C)-C(14C) 117.3(4)
O(3C)-C(14C)-C(13C) 121.8(4)
O(3C)-C(14C)-C(8C) 120.5(4)
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C(15C)#1-C(15C)-C(16C) 108(3)
C(15C)#1-C(15C)-H(15G) 84.0
C(16C)-C(15C)-H(15G) 111.2
C(15C)#1-C(15C)-H(15H) 112.7
C(16C)-C(15C)-H(15H) 123.9
H(15G)-C(15C)-H(15H) 109.5
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O(4C)-C(16C)-C(17C) 120(2)
C(15C)-C(16C)-C(17C) 111(2)
C(16C)-C(17C)-C(22C) 110.4(17)
C(16C)-C(17C)-H(17G) 109.6
C(22C)-C(17C)-H(17G) 109.6
C(16C)-C(17C)-H(17H) 109.6
C(22C)-C(17C)-H(17H) 109.6
H(17G)-C(17C)-H(17H) 108.1
C(13C)-C(18C)-C(19C) 128.3(5)
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C(19C)-C(18C)-H(18C) 115.9
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C(18C)-C(19C)-H(19H) 108.4
C(20C)-C(19C)-H(19H) 108.4
H(19G)-C(19C)-H(19H) 107.4
C(28C)-C(20C)-C(21C) 110.6(6)
C(28C)-C(20C)-C(27C) 109.8(6)
C(21C)-C(20C)-C(27C) 109.5(5)
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C(22C)-C(21C)-C(20C)  125.5(9)
C(22D)-C(21C)-C(20C)  123.6(8)
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C(20C)-C(21C)-H(21G)  105.9
C(22C)-C(21C)-H(21H)  105.9
C(20C)-C(21C)-H(21H)  105.9
H(21G)-C(21C)-H(21H)  106.3
C(21C)-C(22C)-C(17C)  111.8(14)
C(21C)-C(22C)-H(22G)  109.3
C(17C)-C(22C)-H(22G)  109.3
C(21C)-C(22C)-H(22H)  109.3
C(17C)-C(22C)-H(22H)  109.3
H(22G)-C(22C)-H(22H)  107.9
C(4C)-C(23C)-H(23J)  109.5
C(4C)-C(23C)-H(23K)  109.5
H(23J)-C(23C)-H(23K)  109.5
C(4C)-C(23C)-H(23L)  109.5
H(23J)-C(23C)-H(23L)  109.5
H(23K)-C(23C)-H(23L)  109.5
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C(4C)-C(24C)-H(24K)  109.5
H(24J)-C(24C)-H(24K)  109.5
C(4C)-C(24C)-H(24L)  109.5
H(24J)-C(24C)-H(24L)  109.5
H(24K)-C(24C)-H(24L)  109.5
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C(30C)-C(29C)-H(29G) 110.6
O(1C)-C(29C)-H(29H) 110.6
C(30C)-C(29C)-H(29H) 110.6
H(29G)-C(29C)-H(29H) 108.8
O(2C)-C(30C)-C(29C) 103.7(5)
O(2C)-C(30C)-H(30G) 111.0
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H(30G)-C(30C)-H(30H) 109.0
C(16D)-C(15D)-H(15J) 109.5
C(16D)-C(15D)-H(15K) 109.5
H(15J)-C(15D)-H(15K) 109.5
C(16D)-C(15D)-H(15L) 109.5
H(15J)-C(15D)-H(15L) 109.5
H(15K)-C(15D)-H(15L) 109.5
O(4D)-C(16D)-C(17D) 124.9(18)
O(4D)-C(16D)-C(15D) 121.6(18)
C(17D)-C(16D)-C(15D) 113.2(8)
C(16D)-C(17D)-C(22D) 116.6(13)
C(16D)-C(17D)-H(17E) 108.1
C(22D)-C(17D)-H(17E) 108.1
C(16D)-C(17D)-H(17F) 108.1
C(22D)-C(17D)-H(17F) 108.1
H(17E)-C(17D)-H(17F)  107.3
C(21C)-C(22D)-C(17D)  114.6(13)
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C(17D)-C(22D)-H(22F)  108.6
H(22E)-C(22D)-H(22F)  107.6

Symmetry transformations used to generate equivalent atoms:

#1  -x+1,y,-z
Table 4. Anisotropic displacement parameters (Å² x 10³) for C30H48O4. The anisotropic displacement factor exponent takes the form: 

\[-2\pi^2 \left[ h^2 a^* a^* U_{11} + \ldots + 2 h k a^* b^* U_{12} \right] \]

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Table 6. Torsion angles [°] for C30H48O4.

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C(6B)-C(7B)-C(8B)-C(9B) -49.3(5)
C(14B)-C(8B)-C(9B)-C(11B) -56.6(5)
C(7B)-C(8B)-C(9B)-C(11B) -175.9(4)
C(26B)-C(8B)-C(9B)-C(11B) 60.1(5)
C(14B)-C(8B)-C(9B)-C(10B) 169.9(4)
C(7B)-C(8B)-C(9B)-C(10B) 50.6(5)
C(26B)-C(8B)-C(9B)-C(10B) -73.3(5)
C(2B)-C(1B)-C(10B)-C(9B) 167.3(3)
C(2B)-C(1B)-C(10B)-C(25B) -71.0(5)
C(2B)-C(1B)-C(10B)-C(5B) 52.5(5)
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C(1C)-C(2C)-C(3C)-C(4C) 56.8(5)
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C(10C)-C(9C)-C(11C)-C(12C) -165.8(3)
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C(12C)-C(13C)-C(14C)-O(3C) 149.6(4)
C(18C)-C(13C)-C(14C)-C(8C) 144.1(5)
C(12C)-C(13C)-C(14C)-C(8C) -35.9(6)
C(7C)-C(8C)-C(14C)-O(3C) -21.0(5)
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C(9C)-C(8C)-C(14C)-O(3C) -140.4(4)
C(7C)-C(8C)-C(14C)-C(13C) 164.4(4)
C(26C)-C(8C)-C(14C)-C(13C) -78.6(4)
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C(15C)#1-C(15C)-C(16C)-O(4C) 96(3)
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C(12C)-C(13C)-C(18C)-C(19C) 3.6(9)
C(14C)-C(13C)-C(18C)-C(19C) -176.3(5)
C(13C)-C(18C)-C(19C)-C(20C) -103.9(7)
C(18C)-C(19C)-C(20C)-C(28C) -56.5(7)
C(18C)-C(19C)-C(20C)-C(21C) -177.5(5)
C(18C)-C(19C)-C(20C)-C(27C) 63.6(7)
C(28C)-C(20C)-C(21C)-C(22C) 54.2(14)
C(27C)-C(20C)-C(21C)-C(22C) -67.0(13)
C(19C)-C(20C)-C(21C)-C(22C) 174.8(12)
C(28C)-C(20C)-C(21C)-C(22D) -175.5(14)
C(27C)-C(20C)-C(21C)-C(22D) 63.4(15)
C(19C)-C(20C)-C(21C)-C(22D) -54.8(15)
C(20C)-C(21C)-C(22C)-C(17C) 175.3(12)
C(16C)-C(17C)-C(22C)-C(21C) -174.8(16)
C(3C)-O(1C)-C(29C)-C(30C) 15.1(6)
C(3C)-O(2C)-C(30C)-C(29C) 32.1(6)
O(1C)-C(29C)-C(30C)-O(2C) -28.8(7)
O(4D)-C(16D)-C(17D)-C(22D) 169(5)
C(15D)-C(16D)-C(17D)-C(22D) -5(4)
C(20C)-C(21C)-C(22D)-C(17D) 178.6(11)
C(16D)-C(17D)-C(22D)-C(21C) -82(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y,-z
Table 7. Hydrogen bonds for C30H48O4 [Å and °].

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Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y,-z
#2 -x+1,y,-z+1
#3 -x+1,y+1,-z

Single-crystal X-ray data for compound (+)-11:

Table 1 Crystal data and structure refinement for jl1301m.

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<td>Temperature/K</td>
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Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for j11301m. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{ij} tensor.

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Experimental

Single crystals of C$_{30}$H$_{46}$O$_3$ [jl1301m] were [1]. A suitable crystal was selected and [1] on a 'Bruker APEX-II CCD' diffractometer. The crystal was kept at 119.99 K during data collection. Using Olex2 [1], the structure was solved with the ShelXS [2] structure solution program using Direct Methods and refined with the XL [3] refinement package using Least Squares minimisation.


Crystal structure determination of [jl1301m]

Crystal Data for C$_{30}$H$_{46}$O$_3$ (M = 454.67 g/mol): monoclinic, space group P2$_1$ (no. 4), a = 6.1638(15) Å, b = 25.051(6) Å, c = 16.398(4) Å, β = 100.462(14)°, V = 2489.9(11) Å$^3$, Z = 4, T = 119.99 K, μ(MoKα) = 0.076 mm$^{-1}$, Dcalc = 1.213 g/cm$^3$, 22871 reflections measured (2.526° ≤ 2θ ≤ 60.284°), 12175 unique ($R_{int} = 0.1037$, $R_{sigma} = 0.2181$) which were used in all calculations. The final $R_1$ was 0.0949 (I > 2σ(I)) and $wR_2$ was 0.2716 (all data).

Refinement model description

Number of restraints - 1, number of constraints - unknown.

Details:
1. Twinned data refinement
   Scales: 0.918(3)
   0.082(3)
2. Fixed Uiso
   At 1.2 times of:
   All C(H) groups, All C(H,H) groups
At 1.5 times of:
All C(H,H,H) groups
3.a Ternary CH refined with riding coordinates:
  C5(H5), C9(H9), C13(H13), C17(H17), C18(H18), C5(H5), C9(H9),
  C13(H13),
  C17(H17), C18(H18)
3.b Secondary CH2 refined with riding coordinates:
  C1(H1A,H1B), C2(H2A,H2B), C6(H6A,H6B), C7(H7A,H7B), C11(H11A,H11B),
  C12(H12A,
  H12B), C19(H19A,H19B), C21(H21A,H21B), C22(H22A,H22B),
  C29(H29A,H29B),
  C30(H30A,H30B), C1(H1A,H1B), C2(H2A,H2B), C6(H6A,H6B), C7(H7A,H7B),
  C11(H11A,
  H11B), C12(H12A,H12B), C19(H19A,H19B), C21(H21A,H21B),
  C22(H22A,H22B),
  C29(H29A,H29B), C30(H30A,H30B)
3.c Aromatic/amide H refined with riding coordinates:
  C15(H15), C15(H15)
3.d Idealised Me refined as rotating group:
  C26(H26A,H26B,
  H26C), C27(H27A,H27B,H27C), C28(H28A,H28B,H28C), C23(H23A,H23B,H23C),
  C24(H24A,
  C27(H27A,H27B,H27C),
  C28(H28A,H28B,H28C)

Single-crystal X-ray data for compound (+)-5:
Table 1. Crystal data and structure refinement for jl1202m.

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<th>Identification code</th>
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<tr>
<td></td>
<td>$b = 18.3571(16)$ Å, $\beta = 100.925(4)^\circ$.</td>
</tr>
<tr>
<td></td>
<td>$c = 11.4738(10)$ Å, $\gamma = 90^\circ$.</td>
</tr>
<tr>
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<tr>
<td>Z</td>
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<tr>
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<tr>
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<tr>
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<td>Independent reflections</td>
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<td>Full-matrix least-squares on F²</td>
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<td>Data / restraints / parameters</td>
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Table 2. Atomic coordinates ($x \times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for j1l202m. $U(eq)$ is defined as one third of the trace of the orthogonalized $U_{ij}$ tensor.

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Table 3. Bond lengths [Å] and angles [°] for jl1202m.

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C(28)-H(28C)  0.9800
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C(29)-O(30A)  1.276(3)
C(29)-O(30B)  1.591(6)
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H(1A)-C(1)-H(1B) 107.7
C(3)-C(2)-C(1) 111.24(15)
C(3)-C(2)-H(2A) 109.4
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O(3B)-C(3)-C(4) 109.68(15)
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Symmetry transformations used to generate equivalent atoms:
Table 4. Anisotropic displacement parameters (Å² x 10³) for jil1202m. The anisotropic displacement factor exponent takes the form: -2π²[ h² a*2 U^11 + ... + 2 h k a* b* U^12 ]

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Table 5. Hydrogen coordinates ($x \times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for j11202m.

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References

[S1] Data Collection:  SMART Software in APEX2 v2014.11-0 Suite. Bruker-AXS, 5465 E. Cheryl Parkway, Madison, WI 53711-5373 USA.
[S2] Data Reduction:  SAINT Software in APEX2 v2014.11-0 Suite. Bruker-AXS, 5465 E. Cheryl Parkway, Madison, WI 53711-5373 USA.