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1-(1,5-Dimethylhexyl)-3a,5b,12a,14a-tetramethyl-2,3,3a,4,5,5a,5b,11,12,13,-14,14a-dodecahydro-1*H*,12a*H*-cyclopenta[1,2]phenanthro[7,8-*b*]indole

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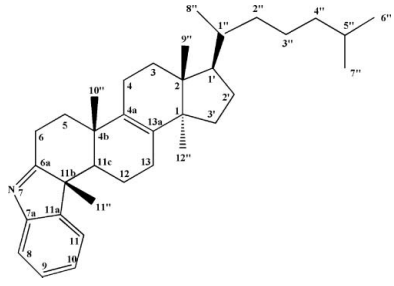
Key indicators: single-crystal X-ray study; T = 170 K; mean σ(C–C) = 0.006 Å; R factor = 0.075; wR factor = 0.176; data-to-parameter ratio = 11.0.

The title compound, $C_{35}H_{51}N$, is a semi-synthesized derivative obtained from 4α,14α-dimethyl-5α-cholest-8-en-3β-ol, a major triterpene isolated from *Euphorbia officinarum* latex. The molecular structure was established by ^{1}H and ^{13}C NMR spectroscopy and confirmed as having the β stereochemistry at the new C11b stereocenter by single-crystal X-ray diffraction. The planar indole group is folded over the extended tetracyclic perhydrocyclopentanephenanthrene triterpene skeleton. There are no π–π interactions between the indole ring systems.

Related literature

For related literature, see: Auhmani *et al.* (2005); Mazoir *et al.* (2006); Mazoir, Giorgi & Auhmani (2005); Mazoir, Giorgi & Benharrei (2005).



Experimental

Crystal data

$C_{35}H_{51}N$
M_r = 485.77
Orthorhombic, $P2_12_12_1$
a = 6.563 (2) Å
b = 18.668 (4) Å
c = 23.930 (7) Å
V = 2931.9 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.06 mm^{-1}
T = 170 (2) K
0.20 × 0.15 × 0.10 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: none
16251 measured reflections
3625 independent reflections
3234 reflections with $I > 2\sigma(I)$
R_{int} = 0.071

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.075
$wR(F^2)$ = 0.176
S = 1.14
3625 reflections
330 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Data collection: *COLLECT* (Nonius 2000); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2320).

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supplementary materials

Acta Cryst. (2007). E**63**, o4911 [**doi:10.1107/S1600536807053913**]

1-(1,5-Dimethylhexyl)-3a,5b,12a,14a-tetramethyl-2,3,3a,4,5,5a,5b,11,12,13,14,14a-dodecahydro-1*H*,12a*H*-cyclopenta[1,2]phenanthro[7,8-*b*]indole

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Comment

The title compound (II) (Scheme 1) was obtained by transformation of the natural triterpene: 4α,14α-dimethyl-5α-cholest-8-en-3β-ol(I) (Scheme1). In the course of the reaction the α stereochemistry at C4 in (I) changes to β at the C11*b* in (II), because the new C11*a*—C11*b* bond is preferably developed through the less crowdy α face of (I). However, that of the remaining stereocenters remains unchanged. The above-mentioned, together with the known absolute stereochemistry of (I) allows us to assign the absolute configuration of (II) as 1(*R*),1'(*R*),1"(*R*),2(*R*),4 b(S),C11*b*(*R*), C11*c*(*R*). For structural details of related hemisynthesized derivatives from moroccan natural products, see:Auhmani *et al.* (2005); Mazoir, Giorgi & Benharrei (2005); Mazoir, Giorgi & Auhmani (2005); Mazoir *et al.* (2006).

Experimental

The oxidation of the natural triterpene 4α,14α-dimethyl-5α-cholest-8-en-3β-ol, during 1 h with 3 equivalents of chromic anhydride (CrO_3) in acetone at 273 K followed by heating under reflux with 1 equivalent of phenylhydrazine in the presence of acetic acid afforded, after chromatographic purification on silica gel column, the title compound, with an overall 92% yield. Crystals were obtained by evaporation from methanol solution at 277 K. Spectroscopic analysis: ^{1}H NMR (500 MHz, CDCl3, δ (p.p.m.): 7.60 (H8,d,J=7.7 Hz),7.33 (H9,t, J1=15.1 Hz; J2=7.6 Hz),7.18 (H10,t, J1=14.8; J2=7.4 Hz, 7.43 (H11,d, J=7.4 Hz), 0.85 (H6", d, J =2.3 Hz), 0.86 (H7",J=2.3 Hz), 0.87 (H8", d, J=6.3 Hz), 0.72 (H9", s), 1.31 (H10", s), 1.33 (H11", s), 0.75 (H12", s);^{13}C NMR (125 MHz, CDCl3, δ (p.p.m.): 49.3 (C1), 44.3 (C2),25.7 (C3), 27.9 (C4),135.2 (C4a), 36.3 (C4b), 39.4 (C5), 40.8 (C6), 192.2 (C6a),154.5 (C7a), 127.9 (C8), 123.4 (C9), 120.7 (C10), 124.8 (C11), 147.9 (C11*a*),57.6 (C11*b*), 50.4 (C11*c*), 21.6 (C12), 20.1 (C13), 133.2 (C13*a*), 51.4 (C1'),25.6 (C2'), 23.9 (C3'), 35.3 (C1"), 30.7 (C2"), 30.8 (C3"),34.6 (C4"),28.0 (C5"), 22.4 (C6"), 22.7 (C7"), 19.0 (C8"),15.6 (C9"), 18.6 (C10"),24.1 (C11"), 16.2 (C12").

Refinement

The lack of suitable anomalous scatters did not allow us to reliably determine the absolute structure according to the Flack parameters and, therefore, 2641 Friedels pairs were merged before the final refinement. However, the absolute configuration of the title compound could be assigned by comparation with the known stereochemistry of the starting compound. H-atoms were positioned geometrically and refined using a riding model with C—H =0.95–0.99 Å and with U_{iso} (H) = 1.2 (1.5 for methyl groups) times U_{eq} (C).

Figures

Fig. 1. The molecular structure of the title compound, (II), with the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probabity level. H-atoms are represented by circles of arbitrary size.

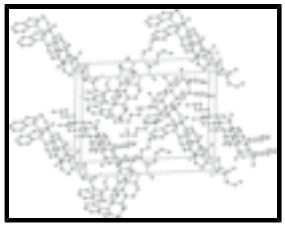

Fig. 2. The packing of (II), viewed down the *a* axis.

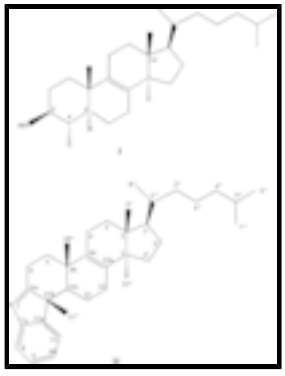

Fig. 3. The structures of (I) and (II).

1-(1,5-Dimethylhexyl)-3a,5 b,12*a*,14*a*-tetramethyl- 2,3,3a,4,5,5a,5 b,11,12,13,14,14*a*-dodecahydro- 1H,12aH-cyclopentano[1,2]phenantreno[7,8-*b*]indole

Crystal data

$C_{35}H_{51}N$	F_{000} = 1072
	D_x = 1.101 Mg m^{-3}
M_r = 485.77	D_m = not performed Mg m^{-3} D_m measured by not measured
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2ac 2ab	Cell parameters from 2013 reflections
a = 6.563 (2) Å	θ = 3.4–27.0º
b = 18.668 (4) Å	μ = 0.06 mm^{-1}
c = 23.930 (7) Å	*T* = 170 (2) K
V = 2931.9 (14) Å^3	Block, colourless
Z = 4	0.20 × 0.15 × 0.10 mm

Data collection

Enraf-Nonius KappaCCD diffractometer	3625 independent reflections
Radiation source: fine-focus sealed tube	3234 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.071
Detector resolution: 9 pixels mm^{-1}	θ_{max} = 27.0º
T = 170(2) K	θ_{min} = 3.4º
φ and ω scans	*h* = 0→8
Absorption correction: none	*k* = 0→23
16251 measured reflections	*l* = 0→30

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0624P)^2 + 2.356P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.075$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.176$	$\Delta\rho_{max} = 0.37$ e Å^{-3}
$S = 1.14$	$\Delta\rho_{min} = -0.26$ e Å^{-3}
3625 reflections	Extinction correction: none
330 parameters	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	
Hydrogen site location: inferred from neighbouring sites	

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.7821 (5)	0.11990 (16)	0.13819 (14)	0.0218 (7)
C1'	0.7970 (6)	0.05385 (18)	0.05148 (14)	0.0265 (8)
H1'	0.6820	0.0226	0.0608	0.032*
C1"	0.8396 (7)	0.0449 (2)	−0.01160 (15)	0.0355 (9)
H1"	0.9563	0.0753	−0.0213	0.043*
C2	0.7460 (5)	0.12964 (18)	0.07411 (14)	0.0235 (7)
C2'	0.9805 (6)	0.0304 (2)	0.08873 (16)	0.0345 (9)
H2'1	0.9611	−0.0183	0.1018	0.041*
H2'2	1.1063	0.0324	0.0675	0.041*
C2"	0.8968 (8)	−0.0333 (2)	−0.02462 (17)	0.0458 (11)
H2"1	0.9809	−0.0515	0.0056	0.055*
H2"2	0.7731	−0.0617	−0.0255	0.055*
C3	0.5296 (6)	0.15825 (19)	0.06657 (15)	0.0276 (8)
H3A	0.4328	0.1220	0.0783	0.033*
H3B	0.5058	0.1682	0.0273	0.033*
C3'	0.9900 (6)	0.08280 (19)	0.13891 (16)	0.0298 (8)
H3'1	1.0106	0.0571	0.1737	0.036*
H3'2	1.0992	0.1173	0.1342	0.036*
C3"	1.0112 (11)	−0.0440 (3)	−0.08002 (19)	0.0670 (16)
H3"1	0.9258	−0.0268	−0.1103	0.080*
H3"2	1.1334	−0.0147	−0.0795	0.080*
C4	0.4946 (6)	0.22715 (19)	0.10081 (15)	0.0295 (8)
H4A	0.5169	0.2677	0.0762	0.035*
H4B	0.3525	0.2283	0.1119	0.035*
C4"	1.0700 (14)	−0.1188 (4)	−0.0919 (3)	0.114 (3)
H4"1	0.9463	−0.1463	−0.0978	0.136*
H4"2	1.1358	−0.1380	−0.0588	0.136*
C4A	0.6224 (5)	0.23830 (17)	0.15256 (14)	0.0211 (7)

C4B	0.5965 (5)	0.31121 (17)	0.18229 (15)	0.0226 (7)
C5	0.3720 (5)	0.33502 (19)	0.18046 (16)	0.0270 (8)
H5A	0.2867	0.2956	0.1928	0.032*
H5B	0.3354	0.3460	0.1421	0.032*
C5"	1.2102 (14)	−0.1319 (6)	−0.1415 (3)	0.138 (4)
H5"	1.2279	−0.1840	−0.1418	0.165*
C6	0.3279 (5)	0.40146 (18)	0.21742 (16)	0.0286 (8)
H6A	0.4003	0.4428	0.2030	0.034*
H6B	0.1832	0.4120	0.2172	0.034*
C6"	1.1121 (13)	−0.1172 (4)	−0.1936 (3)	0.100 (2)
H6"1	0.9720	−0.1318	−0.1916	0.150*
H6"2	1.1793	−0.1432	−0.2229	0.150*
H6"3	1.1192	−0.0668	−0.2012	0.150*
C6A	0.3964 (5)	0.38538 (17)	0.27494 (16)	0.0263 (8)
N7	0.2790 (5)	0.37794 (17)	0.31774 (14)	0.0311 (7)
C7"	1.4140 (13)	−0.1051 (8)	−0.1367 (4)	0.207 (7)
H7"1	1.4693	−0.1185	−0.1010	0.310*
H7"2	1.4126	−0.0538	−0.1398	0.310*
H7"3	1.4966	−0.1249	−0.1659	0.310*
C7A	0.4075 (6)	0.3549 (2)	0.36270 (17)	0.0335 (9)
C8	0.3491 (7)	0.3450 (3)	0.41768 (19)	0.0468 (11)
H8	0.2149	0.3517	0.4290	0.056*
C8"	0.6588 (8)	0.0684 (2)	−0.04728 (17)	0.0475 (11)
H8"1	0.6824	0.0551	−0.0855	0.071*
H8"2	0.6430	0.1194	−0.0448	0.071*
H8"3	0.5372	0.0454	−0.0340	0.071*
C9	0.4993 (9)	0.3248 (3)	0.4551 (2)	0.0585 (14)
H9	0.4650	0.3174	0.4924	0.070*
C9"	0.8963 (6)	0.18492 (19)	0.04933 (16)	0.0328 (9)
H9"1	0.8606	0.1945	0.0111	0.049*
H9"2	1.0323	0.1661	0.0509	0.049*
H9"3	0.8894	0.2285	0.0705	0.049*
C10	0.6972 (9)	0.3154 (3)	0.4385 (2)	0.0584 (14)
H10	0.7943	0.3017	0.4648	0.070*
C10"	0.7275 (6)	0.36513 (18)	0.14958 (17)	0.0324 (9)
H10A	0.8691	0.3552	0.1559	0.049*
H10B	0.6969	0.4128	0.1620	0.049*
H10C	0.6982	0.3610	0.1104	0.049*
C11	0.7561 (7)	0.3259 (2)	0.38344 (18)	0.0472 (11)
H11	0.8911	0.3202	0.3725	0.057*
C11"	0.7645 (6)	0.4297 (2)	0.27791 (18)	0.0353 (9)
H11A	0.7225	0.4673	0.3027	0.053*
H11B	0.7605	0.4467	0.2401	0.053*
H11C	0.9009	0.4152	0.2870	0.053*
C11A	0.6074 (6)	0.3450 (2)	0.34519 (16)	0.0319 (9)
C11B	0.6194 (5)	0.36520 (18)	0.28420 (16)	0.0265 (8)
C11C	0.6612 (5)	0.30024 (17)	0.24441 (15)	0.0215 (7)
H11D	0.5745	0.2614	0.2584	0.026*
C12	0.8779 (5)	0.2720 (2)	0.24856 (17)	0.0301 (8)

H12A	0.9156	0.2670	0.2876	0.036*
H12B	0.9709	0.3059	0.2314	0.036*
C12"	0.6261 (6)	0.06843 (19)	0.16539 (15)	0.0312 (8)
H12C	0.6580	0.0626	0.2043	0.047*
H12D	0.6320	0.0227	0.1471	0.047*
H12E	0.4915	0.0880	0.1617	0.047*
C13	0.8958 (6)	0.19978 (18)	0.21951 (16)	0.0291 (8)
H13A	1.0366	0.1927	0.2085	0.035*
H13B	0.8617	0.1625	0.2462	0.035*
C13A	0.7632 (5)	0.19075 (17)	0.16878 (14)	0.0219 (7)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0261 (17)	0.0158 (15)	0.0235 (18)	0.0017 (13)	−0.0030 (15)	0.0042 (13)
C1'	0.0300 (18)	0.0262 (17)	0.0232 (18)	−0.0008 (15)	0.0027 (15)	0.0029 (15)
C1"	0.049 (2)	0.035 (2)	0.0226 (19)	−0.0009 (18)	0.0076 (18)	0.0043 (16)
C2	0.0292 (18)	0.0235 (17)	0.0177 (17)	0.0007 (15)	0.0008 (15)	0.0046 (13)
C2'	0.040 (2)	0.0307 (19)	0.033 (2)	0.0076 (17)	0.0022 (19)	−0.0001 (17)
C2"	0.069 (3)	0.042 (2)	0.027 (2)	0.007 (2)	0.007 (2)	−0.0063 (18)
C3	0.0302 (19)	0.0292 (19)	0.0235 (18)	0.0036 (16)	−0.0053 (16)	−0.0018 (15)
C3'	0.0344 (19)	0.0257 (19)	0.0293 (19)	0.0106 (16)	−0.0040 (17)	−0.0010 (15)
C3"	0.100 (4)	0.069 (3)	0.032 (2)	0.004 (3)	0.015 (3)	0.001 (2)
C4	0.0250 (17)	0.034 (2)	0.030 (2)	0.0078 (16)	−0.0034 (17)	0.0008 (16)
C4"	0.146 (7)	0.141 (7)	0.054 (4)	0.076 (6)	0.011 (4)	−0.029 (4)
C4A	0.0159 (15)	0.0235 (16)	0.0238 (17)	−0.0012 (13)	0.0024 (14)	0.0057 (14)
C4B	0.0190 (15)	0.0188 (16)	0.0299 (19)	0.0026 (14)	0.0021 (15)	0.0042 (14)
C5	0.0238 (17)	0.0271 (18)	0.0302 (19)	0.0035 (15)	0.0000 (16)	0.0010 (15)
C5"	0.120 (7)	0.247 (11)	0.047 (4)	0.095 (8)	0.023 (4)	0.004 (5)
C6	0.0212 (17)	0.0212 (16)	0.043 (2)	0.0043 (14)	0.0004 (16)	−0.0004 (16)
C6"	0.110 (6)	0.131 (6)	0.060 (4)	0.014 (5)	0.008 (4)	−0.020 (4)
C6A	0.0221 (16)	0.0161 (15)	0.041 (2)	0.0011 (14)	−0.0001 (17)	−0.0086 (15)
N7	0.0189 (14)	0.0336 (17)	0.0410 (19)	0.0001 (13)	0.0028 (14)	−0.0116 (15)
C7"	0.063 (5)	0.42 (2)	0.136 (8)	0.021 (9)	−0.006 (5)	−0.174 (11)
C7A	0.036 (2)	0.0294 (19)	0.035 (2)	−0.0015 (17)	0.0002 (18)	−0.0100 (17)
C8	0.044 (2)	0.058 (3)	0.039 (2)	−0.001 (2)	0.005 (2)	−0.014 (2)
C8"	0.069 (3)	0.051 (3)	0.023 (2)	0.006 (2)	−0.001 (2)	0.0003 (19)
C9	0.078 (4)	0.066 (3)	0.032 (2)	−0.001 (3)	0.001 (3)	−0.010 (2)
C9"	0.039 (2)	0.0298 (19)	0.029 (2)	−0.0013 (18)	0.0099 (18)	0.0056 (16)
C10	0.065 (3)	0.072 (3)	0.038 (3)	0.016 (3)	−0.018 (2)	−0.010 (2)
C10"	0.0327 (19)	0.0241 (18)	0.040 (2)	0.0006 (16)	0.0047 (18)	0.0024 (16)
C11	0.043 (2)	0.060 (3)	0.039 (2)	0.014 (2)	−0.010 (2)	−0.014 (2)
C11"	0.0231 (18)	0.0301 (19)	0.053 (2)	−0.0044 (16)	−0.0004 (18)	−0.0173 (19)
C11A	0.0335 (19)	0.0299 (19)	0.032 (2)	−0.0002 (16)	−0.0063 (17)	−0.0128 (16)
C11B	0.0189 (16)	0.0249 (17)	0.036 (2)	0.0045 (14)	−0.0020 (16)	−0.0053 (16)
C11C	0.0180 (15)	0.0169 (15)	0.0296 (19)	0.0001 (13)	−0.0028 (14)	−0.0013 (14)
C12	0.0211 (17)	0.034 (2)	0.036 (2)	0.0048 (16)	−0.0061 (17)	−0.0050 (17)
C12"	0.046 (2)	0.0252 (18)	0.0226 (18)	−0.0024 (17)	0.0074 (18)	0.0029 (15)

C13	0.0267 (17)	0.0274 (18)	0.033 (2)	0.0084 (15)	−0.0051 (17)	0.0008 (16)
C13A	0.0175 (15)	0.0237 (16)	0.0244 (18)	−0.0019 (14)	0.0012 (14)	0.0029 (14)

Geometric parameters (Å, °)

C1—C13A	1.517 (5)	C6—H6B	0.9700
C1—C3'	1.530 (5)	C6"—H6"1	0.9600
C1—C12"	1.548 (5)	C6"—H6"2	0.9600
C1—C2	1.562 (5)	C6"—H6"3	0.9600
C1'—C1"	1.544 (5)	C6A—N7	1.289 (5)
C1'—C2	1.552 (5)	C6A—C11B	1.527 (5)
C1'—C2'	1.561 (5)	N7—C7A	1.433 (5)
C1'—H1'	0.9800	C7"—H7"1	0.9600
C1"—C8"	1.526 (6)	C7"—H7"2	0.9600
C1"—C2"	1.540 (6)	C7"—H7"3	0.9600
C1"—H1"	0.9800	C7A—C8	1.383 (6)
C2—C3	1.528 (5)	C7A—C11A	1.389 (6)
C2—C9"	1.546 (5)	C8—C9	1.385 (7)
C2'—C3'	1.550 (5)	C8—H8	0.9300
C2'—H2'1	0.9700	C8"—H8"1	0.9600
C2'—H2'2	0.9700	C8"—H8"2	0.9600
C2"—C3"	1.537 (6)	C8"—H8"3	0.9600
C2"—H2"1	0.9700	C9—C10	1.370 (8)
C2"—H2"2	0.9700	C9—H9	0.9300
C3—C4	1.542 (5)	C9"—H9"1	0.9600
C3—H3A	0.9700	C9"—H9"2	0.9600
C3—H3B	0.9700	C9"—H9"3	0.9600
C3'—H3'1	0.9700	C10—C11	1.388 (7)
C3'—H3'2	0.9700	C10—H10	0.9300
C3"—C4"	1.478 (8)	C10"—H10A	0.9600
C3"—H3"1	0.9700	C10"—H10B	0.9600
C3"—H3"2	0.9700	C10"—H10C	0.9600
C4—C4A	1.510 (5)	C11—C11A	1.385 (6)
C4—H4A	0.9700	C11—H11	0.9300
C4—H4B	0.9700	C11"—C11B	1.543 (5)
C4"—C5"	1.522 (9)	C11"—H11A	0.9600
C4"—H4"1	0.9700	C11"—H11B	0.9600
C4"—H4"2	0.9700	C11"—H11C	0.9600
C4A—C13A	1.339 (4)	C11A—C11B	1.509 (5)
C4A—C4B	1.545 (5)	C11B—C11C	1.566 (5)
C4B—C10"	1.538 (5)	C11C—C12	1.520 (5)
C4B—C5	1.540 (5)	C11C—H11D	0.9800
C4B—C11C	1.559 (5)	C12—C13	1.522 (5)
C5—C6	1.550 (5)	C12—H12A	0.9700
C5—H5A	0.9700	C12—H12B	0.9700
C5—H5B	0.9700	C12"—H12C	0.9600
C5"—C6"	1.429 (10)	C12"—H12D	0.9600
C5"—C7"	1.433 (13)	C12"—H12E	0.9600
C5"—H5"	0.9800	C13—C13A	1.503 (5)

C6—C6A	1.479 (5)	C13—H13A	0.9700
C6—H6A	0.9700	C13—H13B	0.9700
C13A—C1—C3'	117.5 (3)	H6A—C6—H6B	108.4
C13A—C1—C12"	106.5 (3)	C5"—C6"—H6"1	109.5
C3'—C1—C12"	107.7 (3)	C5"—C6"—H6"2	109.5
C13A—C1—C2	111.1 (3)	H6"1—C6"—H6"2	109.5
C3'—C1—C2	101.5 (3)	C5"—C6"—H6"3	109.5
C12"—C1—C2	112.6 (3)	H6"1—C6"—H6"3	109.5
C1"—C1'—C2	118.6 (3)	H6"2—C6"—H6"3	109.5
C1"—C1'—C2'	112.8 (3)	N7—C6A—C6	125.4 (3)
C2—C1'—C2'	102.9 (3)	N7—C6A—C11B	115.5 (3)
C1"—C1'—H1'	107.3	C6—C6A—C11B	118.5 (3)
C2—C1'—H1'	107.3	C6A—N7—C7A	106.1 (3)
C2'—C1'—H1'	107.3	C5"—C7"—H7"1	109.5
C8"—C1"—C2"	110.4 (4)	C5"—C7"—H7"2	109.5
C8"—C1"—C1'	112.0 (3)	H7"1—C7"—H7"2	109.5
C2"—C1"—C1'	110.1 (3)	C5"—C7"—H7"3	109.5
C8"—C1"—H1"	108.1	H7"1—C7"—H7"3	109.5
C2"—C1"—H1"	108.1	H7"2—C7"—H7"3	109.5
C1'—C1"—H1"	108.1	C8—C7A—C11A	122.1 (4)
C3—C2—C9"	108.3 (3)	C8—C7A—N7	126.2 (4)
C3—C2—C1'	118.6 (3)	C11A—C7A—N7	111.6 (3)
C9"—C2—C1'	109.7 (3)	C7A—C8—C9	117.1 (4)
C3—C2—C1	107.3 (3)	C7A—C8—H8	121.5
C9"—C2—C1	110.9 (3)	C9—C8—H8	121.5
C1'—C2—C1	101.7 (3)	C1"—C8"—H8"1	109.5
C3'—C2'—C1'	107.2 (3)	C1"—C8"—H8"2	109.5
C3'—C2'—H2'1	110.3	H8"1—C8"—H8"2	109.5
C1'—C2'—H2'1	110.3	C1"—C8"—H8"3	109.5
C3'—C2'—H2'2	110.3	H8"1—C8"—H8"3	109.5
C1'—C2'—H2'2	110.3	H8"2—C8"—H8"3	109.5
H2'1—C2'—H2'2	108.5	C10—C9—C8	121.5 (5)
C3"—C2"—C1"	114.6 (4)	C10—C9—H9	119.3
C3"—C2"—H2"1	108.6	C8—C9—H9	119.3
C1"—C2"—H2"1	108.6	C2—C9"—H9"1	109.5
C3"—C2"—H2"2	108.6	C2—C9"—H9"2	109.5
C1"—C2"—H2"2	108.6	H9"1—C9"—H9"2	109.5
H2"1—C2"—H2"2	107.6	C2—C9"—H9"3	109.5
C2—C3—C4	111.5 (3)	H9"1—C9"—H9"3	109.5
C2—C3—H3A	109.3	H9"2—C9"—H9"3	109.5
C4—C3—H3A	109.3	C9—C10—C11	121.4 (5)
C2—C3—H3B	109.3	C9—C10—H10	119.3
C4—C3—H3B	109.3	C11—C10—H10	119.3
H3A—C3—H3B	108.0	C4B—C10"—H10A	109.5
C1—C3'—C2'	104.0 (3)	C4B—C10"—H10B	109.5
C1—C3'—H3'1	111.0	H10A—C10"—H10B	109.5
C2'—C3'—H3'1	111.0	C4B—C10"—H10C	109.5
C1—C3'—H3'2	111.0	H10A—C10"—H10C	109.5
C2'—C3'—H3'2	111.0	H10B—C10"—H10C	109.5

H3'1—C3'—H3'2	109.0	C11A—C11—C10	117.9 (4)
C4"—C3"—C2"	114.5 (5)	C11A—C11—H11	121.0
C4"—C3"—H3"1	108.6	C10—C11—H11	121.0
C2"—C3"—H3"1	108.6	C11B—C11"—H11A	109.5
C4"—C3"—H3"2	108.6	C11B—C11"—H11B	109.5
C2"—C3"—H3"2	108.6	H11A—C11"—H11B	109.5
H3"1—C3"—H3"2	107.6	C11B—C11"—H11C	109.5
C4A—C4—C3	117.9 (3)	H11A—C11"—H11C	109.5
C4A—C4—H4A	107.8	H11B—C11"—H11C	109.5
C3—C4—H4A	107.8	C11—C11A—C7A	120.0 (4)
C4A—C4—H4B	107.8	C11—C11A—C11B	131.8 (4)
C3—C4—H4B	107.8	C7A—C11A—C11B	107.9 (3)
H4A—C4—H4B	107.2	C11A—C11B—C6A	98.7 (3)
C3"—C4"—C5"	117.3 (7)	C11A—C11B—C11"	108.7 (3)
C3"—C4"—H4"1	108.0	C6A—C11B—C11"	112.6 (3)
C5"—C4"—H4"1	108.0	C11A—C11B—C11C	113.8 (3)
C3"—C4"—H4"2	108.0	C6A—C11B—C11C	105.7 (3)
C5"—C4"—H4"2	108.0	C11"—C11B—C11C	115.9 (3)
H4"1—C4"—H4"2	107.2	C12—C11C—C4B	111.2 (3)
C13A—C4A—C4	122.0 (3)	C12—C11C—C11B	113.1 (3)
C13A—C4A—C4B	121.8 (3)	C4B—C11C—C11B	115.5 (3)
C4—C4A—C4B	116.0 (3)	C12—C11C—H11D	105.3
C10"—C4B—C5	109.4 (3)	C4B—C11C—H11D	105.3
C10"—C4B—C4A	106.3 (3)	C11B—C11C—H11D	105.3
C5—C4B—C4A	110.3 (3)	C11C—C12—C13	110.4 (3)
C10"—C4B—C11C	114.8 (3)	C11C—C12—H12A	109.6
C5—C4B—C11C	109.0 (3)	C13—C12—H12A	109.6
C4A—C4B—C11C	107.1 (3)	C11C—C12—H12B	109.6
C4B—C5—C6	113.2 (3)	C13—C12—H12B	109.6
C4B—C5—H5A	108.9	H12A—C12—H12B	108.1
C6—C5—H5A	108.9	C1—C12"—H12C	109.5
C4B—C5—H5B	108.9	C1—C12"—H12D	109.5
C6—C5—H5B	108.9	H12C—C12"—H12D	109.5
H5A—C5—H5B	107.8	C1—C12"—H12E	109.5
C6"—C5"—C7"	115.1 (9)	H12C—C12"—H12E	109.5
C6"—C5"—C4"	112.2 (7)	H12D—C12"—H12E	109.5
C7"—C5"—C4"	116.4 (8)	C13A—C13—C12	115.1 (3)
C6"—C5"—H5"	103.7	C13A—C13—H13A	108.5
C7"—C5"—H5"	103.7	C12—C13—H13A	108.5
C4"—C5"—H5"	103.7	C13A—C13—H13B	108.5
C6A—C6—C5	108.2 (3)	C12—C13—H13B	108.5
C6A—C6—H6A	110.1	H13A—C13—H13B	107.5
C5—C6—H6A	110.1	C4A—C13A—C13	124.0 (3)
C6A—C6—H6B	110.1	C4A—C13A—C1	119.7 (3)
C5—C6—H6B	110.1	C13—C13A—C1	116.1 (3)
C2—C1'—C1"—C8"	−59.5 (5)	C6A—N7—C7A—C11A	−2.9 (4)
C2'—C1'—C1"—C8"	−179.8 (3)	C11A—C7A—C8—C9	0.1 (6)
C2—C1'—C1"—C2"	177.3 (4)	N7—C7A—C8—C9	−177.8 (4)
C2'—C1'—C1"—C2"	56.9 (5)	C7A—C8—C9—C10	0.4 (8)

C1"—C1'—C2—C3	79.7 (4)
C2'—C1'—C2—C3	−155.0 (3)
C1"—C1'—C2—C9"	−45.5 (4)
C2'—C1'—C2—C9"	79.9 (3)
C1"—C1'—C2—C1	−163.0 (3)
C2'—C1'—C2—C1	−37.6 (3)
C13A—C1—C2—C3	−61.1 (3)
C3'—C1—C2—C3	173.2 (3)
C12"—C1—C2—C3	58.3 (4)
C13A—C1—C2—C9"	57.1 (4)
C3'—C1—C2—C9"	−68.6 (3)
C12"—C1—C2—C9"	176.5 (3)
C13A—C1—C2—C1'	173.7 (3)
C3'—C1—C2—C1'	48.0 (3)
C12"—C1—C2—C1'	−66.9 (3)
C1"—C1'—C2'—C3'	143.0 (3)
C2—C1'—C2'—C3'	14.0 (4)
C8"—C1"—C2"—C3"	75.7 (5)
C1'—C1"—C2"—C3"	−160.1 (4)
C9"—C2—C3—C4	−65.0 (4)
C1'—C2—C3—C4	169.2 (3)
C1—C2—C3—C4	54.9 (4)
C13A—C1—C3'—C2'	−160.1 (3)
C12"—C1—C3'—C2'	79.7 (4)
C2—C1—C3'—C2'	−38.8 (3)
C1'—C2'—C3'—C1	15.6 (4)
C1"—C2"—C3"—C4"	178.7 (6)
C2—C3—C4—C4A	−26.4 (4)
C2"—C3"—C4"—C5"	−171.2 (6)
C3—C4—C4A—C13A	0.4 (5)
C3—C4—C4A—C4B	174.4 (3)
C13A—C4A—C4B—C10"	93.4 (4)
C4—C4A—C4B—C10"	−80.7 (4)
C13A—C4A—C4B—C5	−148.2 (3)
C4—C4A—C4B—C5	37.8 (4)
C13A—C4A—C4B—C11C	−29.7 (4)
C4—C4A—C4B—C11C	156.2 (3)
C10"—C4B—C5—C6	−72.6 (4)
C4A—C4B—C5—C6	170.9 (3)
C11C—C4B—C5—C6	53.6 (4)
C3"—C4"—C5"—C6"	−68.2 (12)
C3"—C4"—C5"—C7"	67.3 (12)
C4B—C5—C6—C6A	−55.2 (4)
C5—C6—C6A—N7	−112.6 (4)
C5—C6—C6A—C11B	58.1 (4)
C6—C6A—N7—C7A	173.5 (3)
C11B—C6A—N7—C7A	2.6 (4)
C6A—N7—C7A—C8	175.1 (4)
C8—C9—C10—C11	0.1 (8)
C9—C10—C11—C11A	−1.1 (8)
C10—C11—C11A—C7A	1.5 (6)
C10—C11—C11A—C11B	175.2 (4)
C8—C7A—C11A—C11	−1.1 (6)
N7—C7A—C11A—C11	177.1 (3)
C8—C7A—C11A—C11B	−176.1 (4)
N7—C7A—C11A—C11B	2.1 (4)
C11—C11A—C11B—C6A	−174.7 (4)
C7A—C11A—C11B—C6A	−0.5 (4)
C11—C11A—C11B—C11"	−57.1 (5)
C7A—C11A—C11B—C11"	117.1 (3)
C11—C11A—C11B—C11C	73.8 (5)
C7A—C11A—C11B—C11C	−112.0 (3)
N7—C6A—C11B—C11A	−1.4 (4)
C6—C6A—C11B—C11A	−173.0 (3)
N7—C6A—C11B—C11"	−116.0 (4)
C6—C6A—C11B—C11"	72.4 (4)
N7—C6A—C11B—C11C	116.5 (3)
C6—C6A—C11B—C11C	−55.1 (4)
C10"—C4B—C11C—C12	−60.6 (4)
C5—C4B—C11C—C12	176.3 (3)
C4A—C4B—C11C—C12	57.1 (3)
C10"—C4B—C11C—C11B	70.0 (4)
C5—C4B—C11C—C11B	−53.0 (4)
C4A—C4B—C11C—C11B	−172.3 (3)
C11A—C11B—C11C—C12	−72.1 (4)
C6A—C11B—C11C—C12	−179.3 (3)
C11"—C11B—C11C—C12	55.2 (4)
C11A—C11B—C11C—C4B	158.2 (3)
C6A—C11B—C11C—C4B	50.9 (4)
C11"—C11B—C11C—C4B	−74.6 (4)
C4B—C11C—C12—C13	−60.9 (4)
C11B—C11C—C12—C13	167.2 (3)
C11C—C12—C13—C13A	34.0 (4)
C4—C4A—C13A—C13	179.3 (3)
C4B—C4A—C13A—C13	5.6 (5)
C4—C4A—C13A—C1	−6.4 (5)
C4B—C4A—C13A—C1	179.9 (3)
C12—C13—C13A—C4A	−6.9 (5)
C12—C13—C13A—C1	178.5 (3)
C3'—C1—C13A—C4A	153.6 (3)
C12"—C1—C13A—C4A	−85.6 (4)
C2—C1—C13A—C4A	37.4 (4)
C3'—C1—C13A—C13	−31.6 (4)
C12"—C1—C13A—C13	89.2 (4)
C2—C1—C13A—C13	−147.8 (3)

Fig. 1

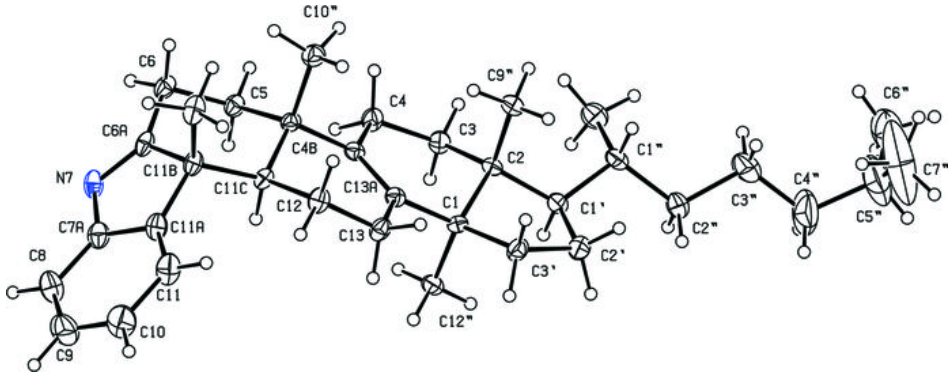
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Fig. 2

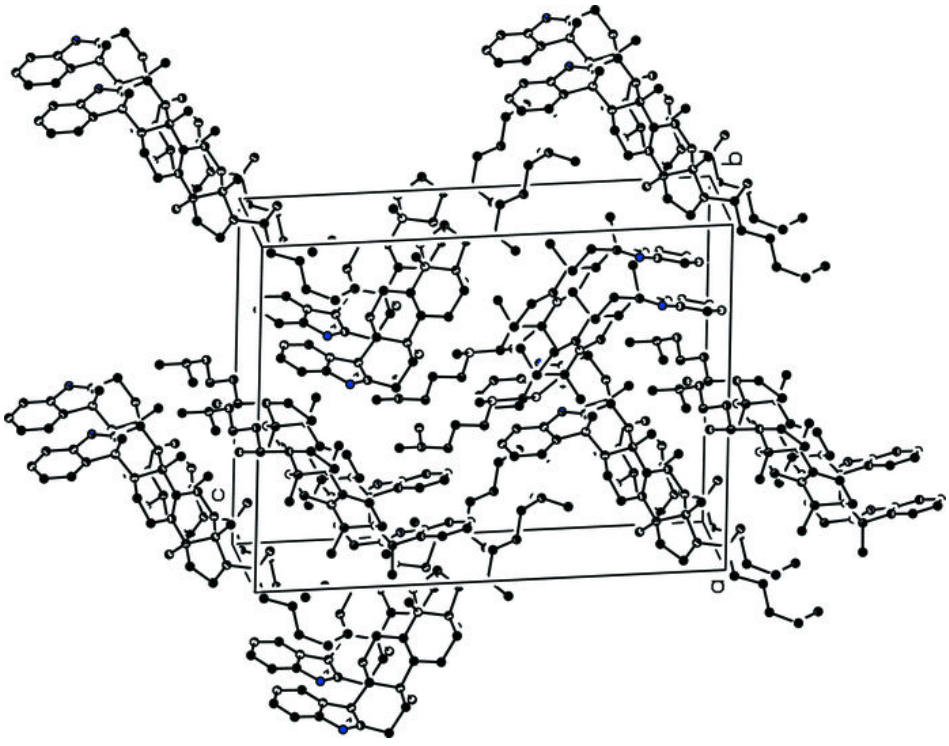
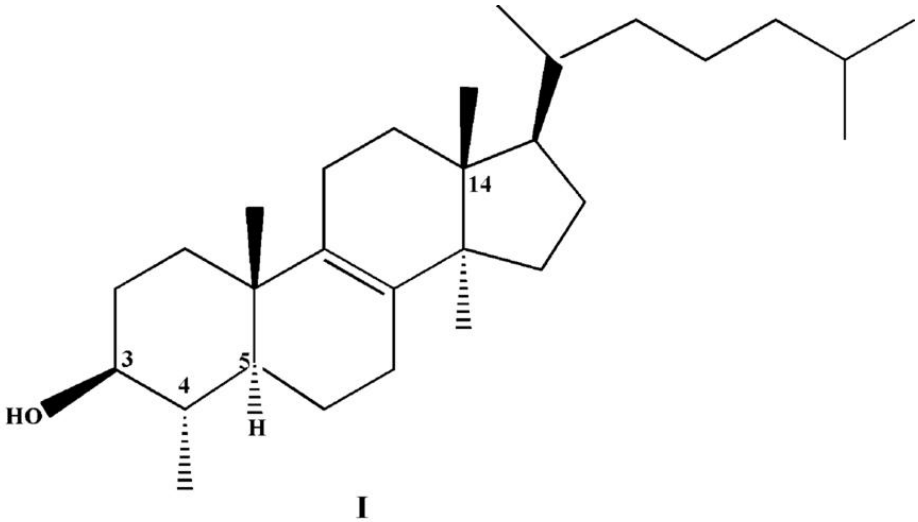


Fig. 3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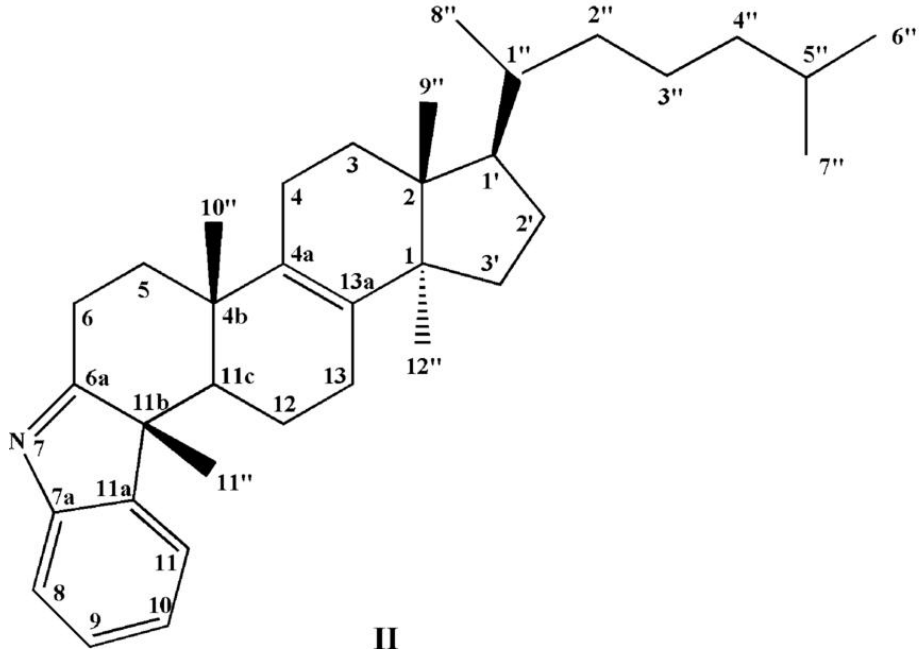
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