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2,8-Dihydroxy-1-(3-methylbut-2-enyl)-9*H*-carbazole-3-carbaldehyde

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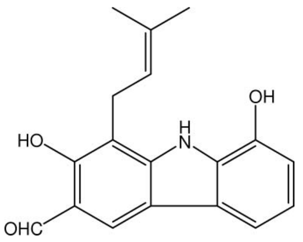
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.044; wR factor = 0.116; data-to-parameter ratio = 14.2.

The title naturally occurring carbazole compound, $C_{18}H_{17}NO_3$, known as heptazoline, was isolated from *Micromelum minutum*. The carbazole ring system is essentially planar. The hydroxy and aldehyde substituent groups lie in the plane of the benzene ring, while the 3-methyl-2-butenyl group is anticlinal, with a dihedral angle of 70.26 (7)° between it and the mean plane of the carbazole. In the crystal structure, an intramolecular O—H⋯O interaction generates an $S(6)$ ring motif, while an intermolecular O—H⋯O interaction forms dimers that link into chains along the [401] direction. The structure is further stabilized by weak intramolecular C—H⋯O interactions and π–π interactions [centroid-to-centroid distances 3.5901 (8) and 3.5899 (8) Å].

Related literature

For background to the biological activity of alkaloids, flavonoids and coumarins, see, for example: Das *et al.* (1984); Ito *et al.* (2000); Nakahara *et al.* (2002); Rahmani *et al.* (2003); Sohrab *et al.* (2004); Tantishaiyakul *et al.* (1986); Tantivatana *et al.* (1983). For related structures, see, for example: Duan *et al.* (2005); Huang *et al.* (2005); Li *et al.* (2006). Bernstein *et al.* (1995) provide information on hydrogen-bond motifs. For reference structural data, see Allen *et al.* (1987).



Experimental

Crystal data

$C_{18}H_{17}NO_3$
M_r = 295.33
Monoclinic, $P2_1/c$
a = 4.7749 (1) Å
b = 18.8511 (6) Å
c = 16.0164 (5) Å
β = 97.931 (2)°
V = 1427.88 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 100.0 (1) K
0.52 × 0.18 × 0.09 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.953, T_{max} = 0.992
15047 measured reflections
3795 independent reflections
2840 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.116
S = 1.10
3795 reflections
267 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O1—H1O1⋯O2	0.95 (2)	1.75 (2)	2.6274 (13)	151.4 (18)
O3—H1O3⋯O2^i	0.96 (2)	1.77 (2)	2.7139 (14)	166.9 (19)
C13—H13B⋯O1	1.011 (16)	2.391 (16)	2.8469 (17)	106.4 (11)

Symmetry code: (i) $x + 2, -y + \frac{1}{2}, z + \frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2348).

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supplementary materials

Acta Cryst. (2007). E**63**, o3964-o3965 [**doi:10.1107/S1600536807042626**]

2,8-Dihydroxy-1-(3-methylbut-2-enyl)-9*H*-carbazole-3-carbaldehyde

H.-K. Fun, S. Laphookhieo, W. Maneerat and S. Chantrapromma

Comment

Plants of the genus Micromelum (Rutaceae) are known to be rich sources of alkaloids (Nakahara *et al.*, 2002), coumarins (Rahmani *et al.*, 2003; Ito *et al.*, 2000; Tantishaiyakul *et al.*, 1986; Tantivatana *et al.*, 1983) and flavonoids (Das *et al.*, 1984; Sohrab *et al.*, 2004). Some of these compounds show anti-cancer activity (Tantishaiyakul *et al.*, 1986; Tantivatana *et al.*, 1983). *Micromelum minutum* known locally in Thailand as "Hat-Sa-Khun", is a small to medium-sized tree or shrub found widespread in South-East Asian countries. The leaves of this plant are traditionally used in the treatment of fever and giddiness and a poultice of the boiled roots is used for ague (Rahmani *et al.*, 2003). In our search for bioactive compounds from Thai medicinal plant, we herein report the crystal structure of the title compound, which was isolated from the stem barks of *M. minutum* collected from Nongkhai province in the northeasthern of Thailand.

In the structure of the title compound (Fig. 1), the carbazole ring system (C1–C12/N1) is essentially planar with the maximum deviation of −0.013 (1) Å for atom N1. The hydroxy and aldehyde substituent groups lie in the plane of the benzene ring and an intramolecular O1—H1O1···O2 hydrogen bond between the aldehyde and one of the hydroxy groups helps maintain the planarity of the structure. The orientation of the 3-methyl-2-butenyl substituent group with respect to the C1–C6 benzene ring is indicated by the torsion angle C2/C1/C13/C14 of 130.72 (13)°, showing an anti-clinal conformation. The dihedral angle between the 3-methyl-2-butenyl group and the mean plane of carbazole is 70.26 (7) Å. Bond lengths and angles in the title compound are within normal ranges (Allen *et al.*, 1987) and comparable to related structures (Duan *et al.*, 2005; Huang *et al.*, 2005; Li *et al.*, 2006). An O1—H1O1···O2 intramolecular interaction generates S(6) ring motif (Bernstein *et al.*, 1995). In addition, the weak C13—H13B···O1 intramolecular interaction generates S(5) ring motif. O3—H1O3···O2 intermolecular interactions connect the molecules into dimers (Fig. 2). These dimers form chains along the [401] direction (Fig. 2). The crystal is stabilized by O—H···O hydrogen bonds and weak C—H···O intramolecular interaction. π–π interactions were also observed with the $Cg_1 \cdots Cg_2$ distances of 3.5901 (8) Å (symmetry code; $1 + x, y, z$) and 3.5899 (8) Å (symmetry code; $-1 + x, y, z$), Cg_1 and Cg_2 are the centroids of C1–C6 and C6–C5–C12–C7–N1 rings.

Experimental

Stem barks of *M. minutum* (12 kg) were extracted with hexane–EtOAc (1:1) over the period of 3 days at room temperature. The mixture was filtered and concentrated under reduced pressure to provide the crude extract (58.3 g). This crude extract was subjected to quick column chromatography (QCC) over silica gel and eluted with a gradient of EtOAc–hexane to afford 60 factions (A1–A60). Fractions A29–A30 (617 mg) was subjected to repeated CC using the gradient of CH_2Cl_2 (70% CH_2Cl_2 in hexane to 100% CH_2Cl_2) to give the title compound (15.2 mg). Colorless block-shaped single crystals of the title compound were obtained by recrystallization from CH_2Cl_2–hexane (2:1 *v*/*v*) solution, Mp 487–489 K.

Refinement

All H atoms were located from the difference map and refined isotropically.

Figures

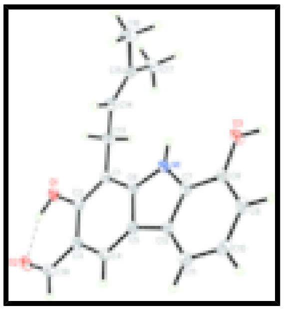

Fig. 1. The asymmetric unit of the title compound, showing 50% probability displacement ellipsoids and the atomic numbering scheme.

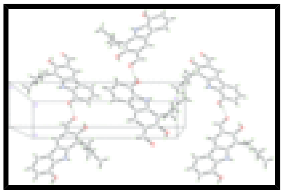

Fig. 2. Crystal packing of the title compound viewed approximately along the *c* axis. O—H···O hydrogen bonds are shown as dashed lines.

2,8-Dihydroxy-1-(3-methylbut-2-enyl)-9*H*-carbazole-3-carbaldehyde

Crystal data

$C_{18}H_{17}NO_3$

$M_r = 295.33$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 4.7749$ (1) Å

$b = 18.8511$ (6) Å

$c = 16.0164$ (5) Å

$\beta = 97.931$ (2)°

$V = 1427.88$ (7) Å^3

$Z = 4$

$F_{000} = 624$

$D_x = 1.374$ Mg m^{-3}

Melting point: 487-489 K

Mo *K*α radiation
λ = 0.71073 Å

Cell parameters from 3795 reflections

θ = 1.7–29.0°

μ = 0.09 mm^{-1}

$T = 100.0$ (1) K

Block, colourless

0.52 × 0.18 × 0.09 mm

Data collection

Bruker APEXII CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

Detector resolution: 8.33 pixels mm^{-1}

$T = 100.0(1)$ K

ω scans

Absorption correction: multi-scan (SADABS; Bruker, 2005)

$T_{min} = 0.953$, $T_{max} = 0.992$

15047 measured reflections

3795 independent reflections

2840 reflections with $I > 2\sigma(I)$

$R_{int} = 0.033$

$\theta_{max} = 29.0°$

$\theta_{min} = 1.7°$

$h = -6 \rightarrow 6$

$k = -24 \rightarrow 25$

$l = -21 \rightarrow 21$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.044$

$wR(F^2) = 0.116$

$S = 1.10$

3795 reflections

267 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0537P)^2 + 0.2314P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.32$ e Å^{-3}

$\Delta\rho_{min} = -0.24$ e Å^{-3}

Extinction correction: none

Special details

Experimental. The low-temparture data was collected with the Oxford Cyrosystem Cobra low-temperature attachment.

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	−0.1526 (2)	0.39677 (5)	0.42061 (6)	0.0216 (2)
H1O1	−0.288 (4)	0.3808 (11)	0.3755 (13)	0.057 (6)*
O2	−0.43458 (19)	0.31436 (5)	0.30620 (6)	0.0224 (2)
O3	1.1123 (2)	0.23309 (6)	0.69986 (6)	0.0229 (2)
H1O3	1.265 (5)	0.2095 (11)	0.7341 (13)	0.059 (6)*
N1	0.6366 (2)	0.28325 (6)	0.58847 (7)	0.0174 (2)
H1N1	0.695 (4)	0.3170 (10)	0.6218 (11)	0.035 (5)*
C1	0.2402 (3)	0.34865 (7)	0.50719 (8)	0.0167 (3)
C2	0.0161 (3)	0.33985 (7)	0.44266 (8)	0.0167 (3)
C3	−0.0384 (3)	0.27355 (7)	0.40085 (8)	0.0174 (3)
C4	0.1316 (3)	0.21427 (7)	0.42481 (8)	0.0173 (3)
H4A	0.093 (3)	0.1682 (8)	0.3955 (10)	0.021 (4)*
C5	0.3561 (3)	0.22080 (7)	0.48859 (7)	0.0164 (3)
C6	0.4046 (3)	0.28848 (7)	0.52797 (7)	0.0162 (3)
C7	0.7370 (3)	0.21414 (7)	0.59080 (8)	0.0175 (3)
C8	0.9687 (3)	0.18691 (8)	0.64334 (8)	0.0189 (3)
C9	1.0343 (3)	0.11657 (8)	0.63314 (8)	0.0218 (3)

H9A	1.198 (3)	0.0965 (8)	0.6684 (10)	0.025 (4)*
C10	0.8714 (3)	0.07462 (8)	0.57257 (9)	0.0230 (3)
H10A	0.923 (3)	0.0249 (9)	0.5670 (10)	0.026 (4)*
C11	0.6392 (3)	0.10177 (8)	0.52068 (8)	0.0202 (3)
H11A	0.524 (3)	0.0717 (8)	0.4791 (9)	0.021 (4)*
C12	0.5716 (3)	0.17311 (7)	0.52989 (8)	0.0174 (3)
C13	0.3057 (3)	0.41821 (8)	0.55191 (8)	0.0211 (3)
H13A	0.480 (3)	0.4407 (8)	0.5317 (10)	0.027 (4)*
H13B	0.147 (3)	0.4527 (9)	0.5336 (10)	0.030 (4)*
C14	0.3473 (3)	0.41179 (8)	0.64689 (8)	0.0213 (3)
H14A	0.218 (3)	0.3766 (9)	0.6707 (10)	0.027 (4)*
C15	0.5236 (3)	0.44972 (8)	0.70103 (8)	0.0210 (3)
C16	0.5300 (4)	0.44116 (10)	0.79470 (9)	0.0302 (4)
H16A	0.462 (4)	0.4849 (10)	0.8203 (11)	0.036 (5)*
H16B	0.399 (3)	0.4005 (9)	0.8061 (10)	0.029 (4)*
H16C	0.730 (4)	0.4325 (10)	0.8242 (12)	0.046 (5)*
C17	0.7187 (3)	0.50577 (9)	0.67578 (9)	0.0258 (3)
H17A	0.727 (4)	0.5072 (9)	0.6130 (12)	0.041 (5)*
H17B	0.652 (4)	0.5541 (10)	0.6914 (11)	0.037 (5)*
H17C	0.913 (4)	0.4996 (10)	0.7068 (11)	0.044 (5)*
C18	−0.2709 (3)	0.26594 (8)	0.33395 (8)	0.0200 (3)
H18A	−0.292 (3)	0.2171 (8)	0.3105 (9)	0.020 (4)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0183 (5)	0.0200 (5)	0.0242 (5)	0.0030 (4)	−0.0051 (4)	0.0011 (4)
O2	0.0174 (5)	0.0263 (6)	0.0214 (5)	0.0001 (4)	−0.0044 (4)	0.0024 (4)
O3	0.0193 (5)	0.0265 (6)	0.0202 (5)	0.0007 (4)	−0.0066 (4)	0.0016 (4)
N1	0.0158 (5)	0.0189 (6)	0.0161 (5)	0.0002 (5)	−0.0026 (4)	−0.0003 (5)
C1	0.0151 (6)	0.0187 (7)	0.0156 (6)	−0.0006 (5)	−0.0002 (5)	0.0012 (5)
C2	0.0146 (6)	0.0180 (7)	0.0171 (6)	0.0010 (5)	0.0009 (5)	0.0029 (5)
C3	0.0141 (6)	0.0228 (7)	0.0147 (6)	−0.0022 (5)	−0.0001 (5)	0.0014 (5)
C4	0.0167 (6)	0.0188 (7)	0.0161 (6)	−0.0023 (5)	0.0013 (5)	−0.0005 (5)
C5	0.0152 (6)	0.0190 (7)	0.0150 (6)	−0.0001 (5)	0.0016 (5)	0.0010 (5)
C6	0.0142 (6)	0.0209 (7)	0.0133 (5)	−0.0015 (5)	0.0008 (5)	0.0010 (5)
C7	0.0160 (6)	0.0203 (7)	0.0164 (6)	0.0007 (5)	0.0029 (5)	0.0022 (5)
C8	0.0162 (6)	0.0252 (8)	0.0148 (6)	0.0001 (5)	0.0003 (5)	0.0024 (5)
C9	0.0188 (7)	0.0268 (8)	0.0194 (6)	0.0057 (6)	0.0018 (5)	0.0063 (6)
C10	0.0266 (7)	0.0204 (8)	0.0224 (6)	0.0057 (6)	0.0052 (6)	0.0024 (6)
C11	0.0215 (7)	0.0212 (8)	0.0176 (6)	0.0008 (6)	0.0021 (5)	0.0007 (5)
C12	0.0150 (6)	0.0218 (7)	0.0152 (5)	0.0007 (5)	0.0017 (5)	0.0025 (5)
C13	0.0234 (7)	0.0194 (8)	0.0190 (6)	0.0003 (6)	−0.0028 (5)	0.0000 (5)
C14	0.0227 (7)	0.0200 (8)	0.0209 (6)	0.0008 (6)	0.0021 (5)	0.0002 (5)
C15	0.0229 (7)	0.0206 (8)	0.0187 (6)	0.0038 (6)	−0.0004 (5)	−0.0017 (5)
C16	0.0418 (10)	0.0292 (9)	0.0188 (7)	−0.0012 (8)	0.0013 (6)	−0.0026 (6)
C17	0.0265 (8)	0.0260 (9)	0.0232 (7)	−0.0029 (6)	−0.0027 (6)	−0.0025 (6)
C18	0.0179 (7)	0.0228 (8)	0.0189 (6)	−0.0032 (6)	0.0011 (5)	0.0009 (5)

Geometric parameters (Å, °)

O1—C2	1.3587 (16)	C9—C10	1.401 (2)
O1—H1O1	0.95 (2)	C9—H9A	0.974 (16)
O2—C18	1.2433 (17)	C10—C11	1.389 (2)
O3—C8	1.3698 (17)	C10—H10A	0.977 (17)
O3—H1O3	0.96 (2)	C11—C12	1.396 (2)
N1—C6	1.3707 (16)	C11—H11A	0.983 (15)
N1—C7	1.3870 (18)	C13—C14	1.5115 (18)
N1—H1N1	0.851 (18)	C13—H13A	1.027 (16)
C1—C2	1.3914 (17)	C13—H13B	1.010 (17)
C1—C6	1.3933 (18)	C14—C15	1.3305 (19)
C1—C13	1.5062 (19)	C14—H14A	1.015 (16)
C2—C3	1.4249 (19)	C15—C17	1.501 (2)
C3—C4	1.4034 (19)	C15—C16	1.5049 (19)
C3—C18	1.4396 (18)	C16—H16A	0.994 (18)
C4—C5	1.3803 (17)	C16—H16B	1.022 (17)
C4—H4A	0.993 (16)	C16—H16C	1.02 (2)
C5—C6	1.4279 (19)	C17—H17A	1.012 (18)
C5—C12	1.4550 (18)	C17—H17B	1.007 (19)
C7—C8	1.3922 (18)	C17—H17C	0.996 (19)
C7—C12	1.4005 (18)	C18—H18A	0.993 (16)
C8—C9	1.377 (2)		

C2—O1—H1O1	105.3 (13)	C9—C10—H10A	118.7 (9)
C8—O3—H1O3	110.8 (12)	C10—C11—C12	117.98 (13)
C6—N1—C7	109.23 (11)	C10—C11—H11A	121.2 (9)
C6—N1—H1N1	123.5 (12)	C12—C11—H11A	120.8 (9)
C7—N1—H1N1	127.0 (12)	C11—C12—C7	119.30 (12)
C2—C1—C6	115.52 (12)	C11—C12—C5	134.97 (12)
C2—C1—C13	123.01 (12)	C7—C12—C5	105.72 (12)
C6—C1—C13	121.47 (11)	C1—C13—C14	113.50 (12)
O1—C2—C1	117.81 (12)	C1—C13—H13A	109.5 (9)
O1—C2—C3	120.49 (11)	C14—C13—H13A	110.5 (9)
C1—C2—C3	121.70 (12)	C1—C13—H13B	108.9 (9)
C4—C3—C2	120.58 (12)	C14—C13—H13B	109.4 (9)
C4—C3—C18	118.80 (12)	H13A—C13—H13B	104.6 (12)
C2—C3—C18	120.61 (12)	C15—C14—C13	126.62 (13)
C5—C4—C3	119.48 (12)	C15—C14—H14A	117.9 (9)
C5—C4—H4A	120.1 (9)	C13—C14—H14A	115.3 (9)
C3—C4—H4A	120.4 (9)	C14—C15—C17	124.27 (13)
C4—C5—C6	117.96 (12)	C14—C15—C16	121.07 (14)
C4—C5—C12	135.20 (13)	C17—C15—C16	114.60 (12)
C6—C5—C12	106.84 (11)	C15—C16—H16A	111.0 (10)
N1—C6—C1	126.95 (12)	C15—C16—H16B	109.2 (9)
N1—C6—C5	108.30 (11)	H16A—C16—H16B	107.9 (13)
C1—C6—C5	124.75 (12)	C15—C16—H16C	111.5 (11)
N1—C7—C8	127.28 (12)	H16A—C16—H16C	106.2 (15)
N1—C7—C12	109.89 (11)	H16B—C16—H16C	110.9 (14)

C8—C7—C12	122.83 (13)	C15—C17—H17A	113.4 (10)
O3—C8—C9	126.08 (12)	C15—C17—H17B	110.0 (10)
O3—C8—C7	116.65 (13)	H17A—C17—H17B	106.3 (14)
C9—C8—C7	117.26 (12)	C15—C17—H17C	110.7 (11)
C8—C9—C10	120.79 (13)	H17A—C17—H17C	109.7 (14)
C8—C9—H9A	118.8 (9)	H17B—C17—H17C	106.5 (14)
C10—C9—H9A	120.4 (9)	O2—C18—C3	125.11 (13)
C11—C10—C9	121.84 (14)	O2—C18—H18A	121.3 (9)
C11—C10—H10A	119.4 (9)	C3—C18—H18A	113.6 (9)

C6—C1—C2—O1	179.32 (11)	C12—C7—C8—O3	179.74 (11)
C13—C1—C2—O1	−1.14 (18)	N1—C7—C8—C9	−178.43 (12)
C6—C1—C2—C3	−0.31 (17)	C12—C7—C8—C9	0.49 (19)
C13—C1—C2—C3	179.23 (12)	O3—C8—C9—C10	−179.66 (12)
O1—C2—C3—C4	−178.56 (11)	C7—C8—C9—C10	−0.48 (19)
C1—C2—C3—C4	1.07 (19)	C8—C9—C10—C11	0.0 (2)
O1—C2—C3—C18	0.72 (18)	C9—C10—C11—C12	0.5 (2)
C1—C2—C3—C18	−179.66 (11)	C10—C11—C12—C7	−0.47 (18)
C2—C3—C4—C5	−1.02 (18)	C10—C11—C12—C5	178.79 (13)
C18—C3—C4—C5	179.70 (11)	N1—C7—C12—C11	179.07 (11)
C3—C4—C5—C6	0.25 (18)	C8—C7—C12—C11	−0.01 (19)
C3—C4—C5—C12	179.63 (13)	N1—C7—C12—C5	−0.38 (14)
C7—N1—C6—C1	178.76 (12)	C8—C7—C12—C5	−179.46 (11)
C7—N1—C6—C5	−1.12 (13)	C4—C5—C12—C11	1.0 (3)
C2—C1—C6—N1	179.65 (11)	C6—C5—C12—C11	−179.62 (14)
C13—C1—C6—N1	0.10 (19)	C4—C5—C12—C7	−179.72 (13)
C2—C1—C6—C5	−0.48 (18)	C6—C5—C12—C7	−0.30 (13)
C13—C1—C6—C5	179.97 (12)	C2—C1—C13—C14	130.72 (13)
C4—C5—C6—N1	−179.59 (10)	C6—C1—C13—C14	−49.76 (17)
C12—C5—C6—N1	0.87 (13)	C1—C13—C14—C15	146.11 (14)
C4—C5—C6—C1	0.52 (19)	C13—C14—C15—C17	−1.1 (2)
C12—C5—C6—C1	−179.02 (11)	C13—C14—C15—C16	175.88 (14)
C6—N1—C7—C8	179.98 (12)	C4—C3—C18—O2	−179.07 (12)
C6—N1—C7—C12	0.94 (14)	C2—C3—C18—O2	1.6 (2)
N1—C7—C8—O3	0.82 (19)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1O1···O2	0.95 (2)	1.75 (2)	2.6274 (13)	151.4 (18)
O3—H1O3···O2^{i}	0.96 (2)	1.77 (2)	2.7139 (14)	166.9 (19)
C13—H13B···O1	1.011 (16)	2.391 (16)	2.8469 (17)	106.4 (11)

Symmetry codes: (i) *x*+2, −*y*+1/2, *z*+1/2.

Fig. 1

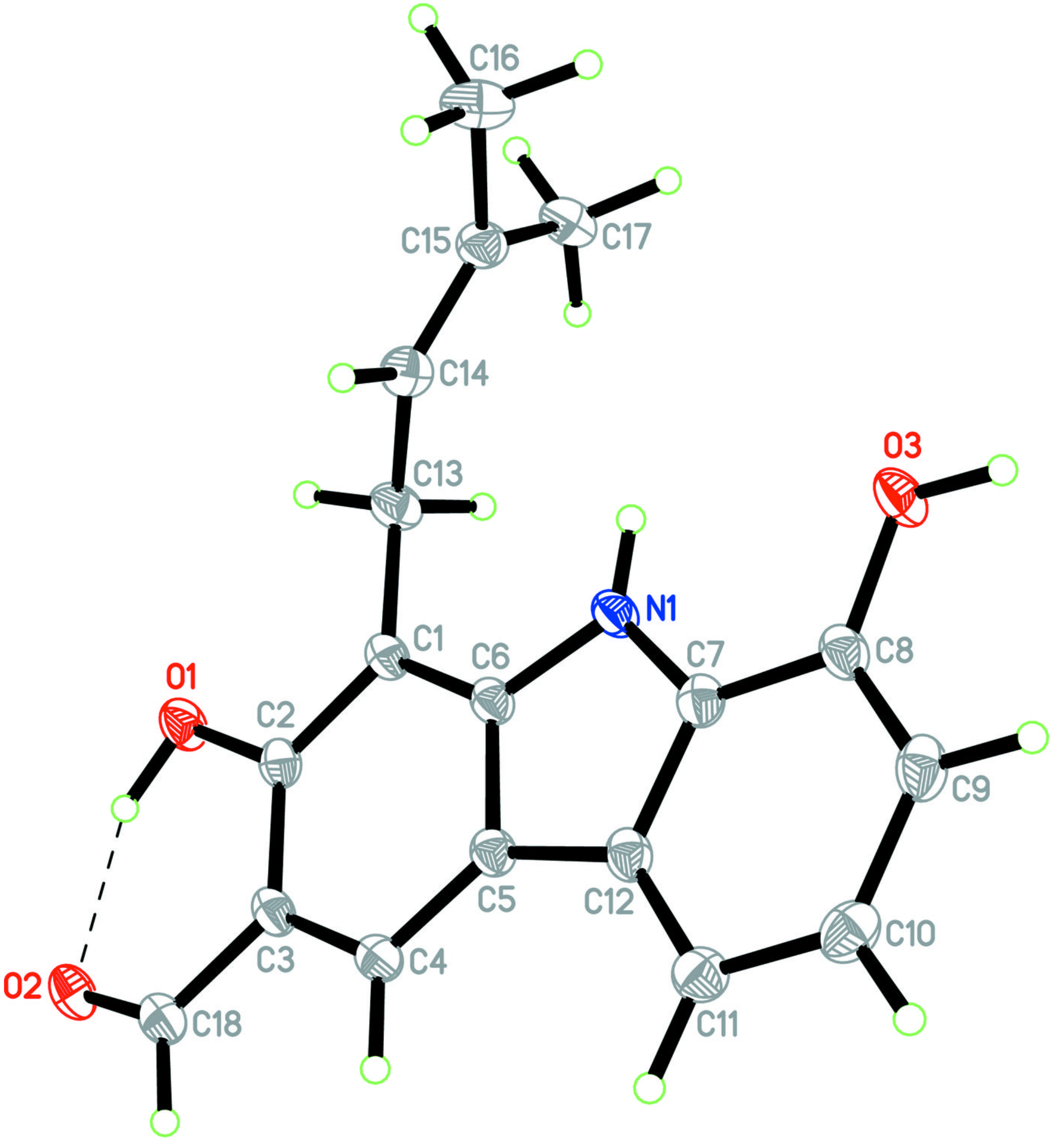
C16
C15
C17
C14
C13
O3
N1
C1
C6
C7
C8
O1
C2
C9
C5
C12
C10
C3
C4
O2
C18
C11

Fig. 2