Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1,6-Dihydroxy-3-hydroxymethyl-8-methoxyanthracene-9,10-dione monohydrate

Wen-Liang Wang, Wei Sun, Qian-Qun Gu and Wei-Ming Zhu*

Key Laboratory of Marine Drugs of the Ministry of Education of China, School of Medicine and Pharmacy, Ocean University of China, 266003 Qingdao, People's Republic of China
Correspondence e-mail: weimingzhu@ouc.edu.cn

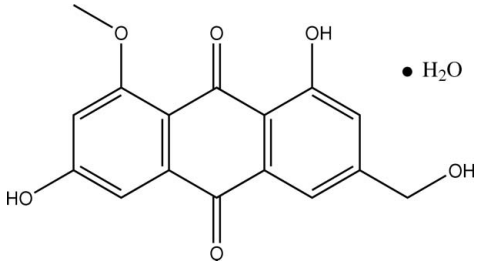
Received 16 November 2007; accepted 14 December 2007

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.055; wR factor = 0.099; data-to-parameter ratio = 11.6.

The title compound, $C_{16}H_{12}O_6\cdot H_2O$, isolated from the halotolerant fungus *Aspergillus variecolor* B-17, is also known as questinol monohydrate. In the crystal structure, O—H···O hydrogen bonds link the molecules, forming a three-dimensional network. π–π stacking interactions consolidate the supramolecular structure [the shortest interplanar distances are 3.456 (3), 3.366 (4) and 3.382 (4) Å].

Related literature

For general background, see: Stickings & Mahmoodian (1962); Slater *et al.* (1971); Kimura *et al.* (1983); Arai *et al.* (1989); Nielsen *et al.* (2004); Wang *et al.* (2007).



Experimental

Crystal data

$C_{16}H_{12}O_6\cdot H_2O$
M_r = 318.27
Monoclinic, $P2_1/c$
a = 11.3317 (11) Å
b = 16.7515 (19) Å
c = 7.2193 (9) Å
β = 95.453 (2)°
V = 1364.2 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 298 (2) K
0.18 × 0.14 × 0.05 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.978, T_{max} = 0.994
7003 measured reflections
2404 independent reflections
1108 reflections with $I > 2\sigma(I)$
R_{int} = 0.090

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.099
S = 1.01
2404 reflections
208 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 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—H1···O6	0.82	1.82	2.525 (3)	144
O2—H2···O5^{i}	0.82	2.38	2.945 (3)	127
O2—H2···O6^{i}	0.82	2.16	2.919 (3)	154
O4—H4···O7^{ii}	0.82	1.85	2.665 (3)	170
O7—H7*A*···O1	0.85	2.03	2.878 (3)	176
O7—H7*B*···O2^{iii}	0.85	1.94	2.771 (3)	165

Symmetry codes: (i) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$; (ii) $x+1, y, z$; (iii) $x, -y+\frac{3}{2}, z-\frac{1}{2}$.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* (Siemens, 1994) and *CAMERON* (Watkin *et al.*, 1993); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

This work was supported by the Chinese National Natural Science Fund (grant Nos. 30470196 and 30670219).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2051).

References

Arai, K., Aoki, Y. & Yamamoto, Y. (1989). *Chem. Pharm. Bull.* **37**, 621–625.
Bruker (2002). *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Kimura, Y., Kozawa, M., Baba, K. & Hata, K. (1983). *Planta Med.* **48**, 164–168.
Nielsen, K. F., Holm, G., Uttrup, L. P. & Nielsen, P. A. (2004). *Int. Biodeter. Biodegr.* **54**, 325–336.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (2003). *SADABS*. Version 2.10. University of Göttingen, Germany.
Siemens (1994). *XP*. Version 5.03. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Slater, G. P., Haskins, R. H. & Hogge, L. R. (1971). *Can. J. Microbiol.* **17**, 1576–1579.
Stickings, C. E. & Mahmoodian, A. (1962). *Chem. Ind. (London)*, **40**, 1718–1719.
Wang, W. L., Zhu, T. J., Tao, H. W., Lu, Z. Y., Fang, Y. C., Gu, Q. Q. & Zhu, W. M. (2007). *J. Antibiot.* **60**, 603–607.
Watkin, D. M., Pearce, L. & Prout, C. K. (1993). *CAMERON*. Chemical Crystallography Laboratory, University of Oxford, England.

  doi:10.1107/S1600536807066986

supplementary materials

Acta Cryst. (2008). E**64**, o332 [**doi:10.1107/S1600536807066986**]

1,6-Dihydroxy-3-hydroxymethyl-8-methoxyanthracene-9,10-dione monohydrate

W.-L. Wang, W. Sun, Q.-Q. Gu and W.-M. Zhu

Comment

Questinol was first isolated from the metabolites of Penicillium frequentans (Stickings & Mahmoodian, 1962). This compound and related derivatives arise from their biological activities (Slater et al., 1971; Kimura et al., 1983; Arai et al., 1989; Nielsen et al., 2004). We isolated the title compound (I) as a part of our ongoing study characterizing bioactive metabolites from various halotolerant microorganism (Wang et al., 2007). This was the first report about the X-ray crystallographic study of the title compound.

As shown in Fig. 1, crystal water connected with questinol by a O—H···O hydrogen bond. There is an intramolecular hydrogen bond between a hydroxyl O1 and carbonyl oxygen atom O6. The three six-membered rings adopt a planar conformation with the maximum deviation being 0.070 (3) Å (for atom C13).

In the crystal structure, O—H···O hydrogen bonds (Table 1, Fig. 2) link the molecules to form a three-dimensional network. A supramolecular structure is consolidated by three types (Symmetry codes: (iii) x, 3/2 − y, z − 1/2; (iv) X, 3/2-Y, z + 1/2; (v) 2-X, 1-Y, 2-Z) of π-π stacking interactions (Fig. 3). The shortest interplanar distances for these π-π stacking interactions are 3.456 (3) Å, 3.366 (4) Å and 3.382 (4) Å, respectively.

Experimental

The isolated halotolerant fugal strain *Aspergillus variecolor* B-17, was isolated from the sediments collected in Jilantai salt field, Alashan, Inner Mongolia, China. The working strain was cultured under static conditions at 303 K for 45 days in thirty 1000-ml conical flasks containing the liquid medium (300 ml/flask) composed of maltose (20 g/*L*), mannitol (20 g/*L*), glucose (10 g/*L*), monosodium glutamate (10 g/*L*), NH_4Cl (10 g/*L*), $MgSO_4$ (10 g/*L*), yeast extract paste (3 g/*L*), maize paste (3 g/*L*), Na_{Cl} (120 g/*L*) and K_{Cl} (5 g/*L*) after adjusting its pH to 7.0. The fermented whole broth (9 liters) was filtered through cheese cloth to separate into supernatant and mycelia. The mycelia was extracted three times with acetone and the acetone solution was concentrated under reduced pressure to afford crude extract (7.8 g). The crude extract, which was subjected to chromatography over silica gel column using a stepwise gradient elution of $CHCl_3$—MeOH, to yield four fractions (Fr.1-Fr.4). Fr.3 was subjected to chromatographing on a silica gel column eluting with $CHCl_3$—MeOH (93:7), to afford sixteen subfractions (Fr.3–1-Fr.3–16). The title compound (9 mg) was purified by extensive preparative HPLC using MeOH-H_2O from Fr.3–3 and Fr.3–4. The single crystals were obtained by slow evaporation of $CHCl_3$—MeOH (1:1) solution at 299 K.

Refinement

Water H atoms were found in a difference Fouier map and were treated as riding, with fixed U_{iso}(H) = 1.2U_{eq}. The other H atoms were positioned geometrically and allowed to ride on their parent atoms at distances of 0.93–0.97 (C—H) and 0.82 Å (O—H), and with U_{iso}(H) values of 1.2U_{eq}(C) and 1.5U_{eq}(C_{methyl}, $O_{hydroxyl}$).

Figures

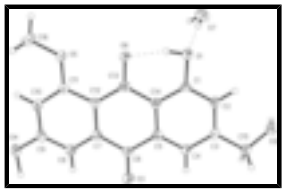


Fig. 1. The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering but for non-H atoms. Dashed lines indicate hydrogen bonds.

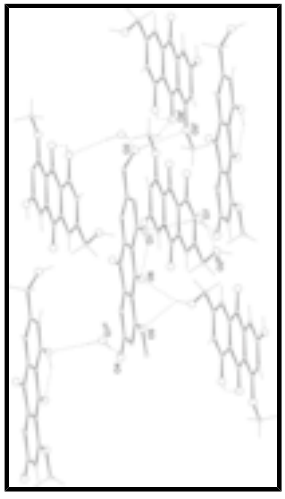


Fig. 2. The packing diagram for (I). The H-bonds are shown as dotted lines; H atoms not involved in hydrogen bonding were omitted for clarity. [Symmetry codes: (i) 1 − *x*, 1/2 + *y*, 3/2 − *z*; (ii) 1 + *x*, *y*, *z*; (iii) *x*, 3/2 − *y*, *z* − 1/2.]

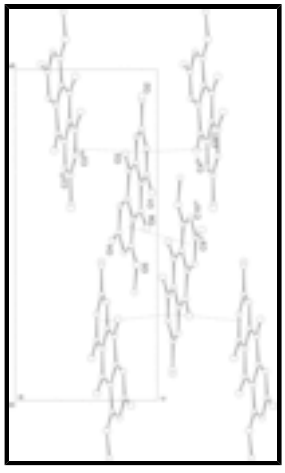


Fig. 3. A view showing the π-π stacking interactions, viewed down the *a* axis. H atoms and H_2O molecules have been omitted for clarity. [Symmetry codes: (iii) *x*, 3/2 − *y*, *z* − 1/2; (iv) *x*, 3/2 − *y*, *z* + 1/2; (v) 2 − *x*, 1 − *y*, 2 − *z*.]

1,6-Dihydroxy-3-hydroxymethyl-8-methoxyanthracene-9,10-dione monohydrate

Crystal data

$C_{16}H_{12}O_6 \cdot H_2O$	F_{000} = 664
M_r = 318.27	D_x = 1.550 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P2ybc	Cell parameters from 901 reflections
a = 11.3317 (11) Å	θ = 2.2–25.2º
b = 16.7515 (19) Å	μ = 0.12 mm^{-1}

c = 7.2193 (9) Å	T = 298 (2) K
β = 95.453 (2)º	Flake, yellow
V = 1364.2 (3) Å^3	0.18 × 0.14 × 0.05 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	2404 independent reflections
Radiation source: fine-focus sealed tube	1108 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.090
T = 298(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.8º
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)	$h = -13 \rightarrow 10$
T_{min} = 0.978, T_{max} = 0.994	$k = -19 \rightarrow 19$
7003 measured reflections	$l = -8 \rightarrow 7$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.055	H-atom parameters constrained
$wR(F^2)$ = 0.099	$w = 1/[\sigma^2(F_o^2) + (0.0163P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.01	$(\Delta/\sigma)_{max} < 0.001$
2404 reflections	$\Delta\rho_{max}$ = 0.23 e Å^{-3}
208 parameters	$\Delta\rho_{min}$ = −0.24 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

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	0.47014 (19)	0.62825 (13)	0.9624 (3)	0.0409 (7)

H1	0.4927	0.5828	0.9423	0.061*
O2	0.4486 (2)	0.91888 (13)	0.8924 (3)	0.0452 (7)
H2	0.4215	0.9337	0.7887	0.068*
O3	0.9454 (2)	0.74461 (14)	0.7759 (4)	0.0548 (8)
O4	1.1510 (2)	0.48495 (14)	0.6863 (3)	0.0489 (7)
H4	1.1898	0.5246	0.6644	0.073*
O5	0.77278 (19)	0.40952 (13)	0.8557 (3)	0.0446 (7)
O6	0.6237 (2)	0.52178 (13)	0.9245 (3)	0.0419 (7)
O7	0.2909 (2)	0.61113 (14)	0.6547 (3)	0.0609 (8)
H7A	0.3423	0.6145	0.7481	0.073*
H7B	0.3279	0.6016	0.5601	0.073*
C1	0.5559 (3)	0.6817 (2)	0.9249 (4)	0.0302 (9)
C2	0.5248 (3)	0.76155 (18)	0.9251 (4)	0.0316 (9)
H2A	0.4486	0.7763	0.9485	0.038*
C3	0.6068 (3)	0.8194 (2)	0.8904 (4)	0.0303 (9)
C4	0.7203 (3)	0.79692 (18)	0.8534 (4)	0.0314 (9)
H4A	0.7757	0.8358	0.8308	0.038*
C5	0.7514 (3)	0.7171 (2)	0.8500 (4)	0.0290 (8)
C6	0.8705 (3)	0.6940 (2)	0.8020 (4)	0.0334 (9)
C7	0.9000 (3)	0.60779 (19)	0.7896 (4)	0.0294 (9)
C8	1.0101 (3)	0.5876 (2)	0.7384 (4)	0.0363 (9)
H8	1.0626	0.6274	0.7094	0.044*
C9	1.0428 (3)	0.5076 (2)	0.7301 (4)	0.0351 (9)
C10	0.9635 (3)	0.4471 (2)	0.7656 (4)	0.0366 (10)
H10	0.9851	0.3939	0.7549	0.044*
C11	0.8527 (3)	0.4668 (2)	0.8167 (4)	0.0334 (9)
C12	0.8161 (3)	0.54798 (19)	0.8292 (4)	0.0285 (8)
C13	0.7004 (3)	0.5714 (2)	0.8841 (4)	0.0304 (9)
C14	0.6699 (3)	0.65733 (19)	0.8854 (4)	0.0278 (8)
C15	0.5733 (3)	0.90622 (19)	0.8933 (4)	0.0393 (9)
H15A	0.6132	0.9309	1.0036	0.047*
H15B	0.6010	0.9324	0.7856	0.047*
C16	0.8055 (3)	0.3271 (2)	0.8389 (5)	0.0564 (12)
H16A	0.8225	0.3165	0.7135	0.085*
H16B	0.7413	0.2936	0.8694	0.085*
H16C	0.8746	0.3160	0.9226	0.085*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0374 (16)	0.0249 (15)	0.0619 (17)	−0.0027 (12)	0.0123 (13)	−0.0018 (12)
O2	0.0414 (16)	0.0392 (16)	0.0558 (17)	0.0107 (13)	0.0084 (13)	0.0035 (12)
O3	0.0387 (17)	0.0291 (16)	0.100 (2)	−0.0081 (13)	0.0226 (15)	0.0001 (14)
O4	0.0384 (16)	0.0398 (17)	0.0711 (19)	0.0066 (13)	0.0182 (14)	0.0000 (13)
O5	0.0337 (15)	0.0244 (15)	0.0771 (19)	0.0011 (13)	0.0122 (14)	−0.0005 (14)
O6	0.0333 (15)	0.0244 (15)	0.0702 (18)	−0.0049 (12)	0.0167 (13)	0.0007 (12)
O7	0.0491 (18)	0.073 (2)	0.0616 (18)	−0.0052 (15)	0.0096 (14)	−0.0054 (15)
C1	0.029 (2)	0.029 (2)	0.032 (2)	−0.0075 (18)	0.0036 (18)	−0.0010 (16)

C2	0.033 (2)	0.025 (2)	0.038 (2)	0.0050 (18)	0.0069 (18)	0.0032 (16)
C3	0.039 (2)	0.022 (2)	0.030 (2)	0.0024 (19)	0.0027 (18)	−0.0010 (15)
C4	0.033 (2)	0.023 (2)	0.039 (2)	−0.0027 (18)	0.0053 (17)	0.0039 (17)
C5	0.028 (2)	0.030 (2)	0.030 (2)	−0.0011 (18)	0.0053 (17)	0.0013 (16)
C6	0.033 (2)	0.027 (2)	0.041 (2)	−0.0038 (19)	0.0032 (18)	−0.0011 (17)
C7	0.029 (2)	0.028 (2)	0.032 (2)	−0.0014 (18)	0.0073 (17)	0.0002 (16)
C8	0.036 (2)	0.032 (2)	0.043 (2)	−0.001 (2)	0.0117 (18)	0.0018 (18)
C9	0.028 (2)	0.042 (3)	0.036 (2)	0.009 (2)	0.0072 (18)	−0.0001 (18)
C10	0.034 (2)	0.031 (2)	0.045 (2)	0.0034 (18)	0.0025 (19)	−0.0053 (17)
C11	0.028 (2)	0.031 (2)	0.040 (2)	−0.0017 (19)	0.0008 (18)	−0.0001 (17)
C12	0.024 (2)	0.027 (2)	0.035 (2)	0.0004 (18)	0.0047 (17)	−0.0012 (16)
C13	0.029 (2)	0.034 (2)	0.028 (2)	−0.0038 (19)	−0.0002 (17)	−0.0044 (17)
C14	0.030 (2)	0.026 (2)	0.027 (2)	0.0021 (17)	0.0045 (17)	−0.0017 (15)
C15	0.042 (2)	0.035 (2)	0.041 (2)	0.002 (2)	0.0071 (19)	−0.0018 (18)
C16	0.061 (3)	0.020 (2)	0.089 (3)	0.003 (2)	0.013 (2)	0.002 (2)

Geometric parameters (Å, °)

O1—C1	1.368 (3)	C4—H4A	0.9300
O1—H1	0.8200	C5—C14	1.403 (4)
O2—C15	1.428 (3)	C5—C6	1.476 (4)
O2—H2	0.8200	C6—C7	1.486 (4)
O3—C6	1.227 (3)	C7—C8	1.376 (4)
O4—C9	1.349 (3)	C7—C12	1.428 (4)
O4—H4	0.8200	C8—C9	1.394 (4)
O5—C11	1.367 (4)	C8—H8	0.9300
O5—C16	1.439 (4)	C9—C10	1.394 (4)
O6—C13	1.256 (3)	C10—C11	1.382 (4)
O7—H7A	0.8500	C10—H10	0.9300
O7—H7B	0.8500	C11—C12	1.428 (4)
C1—C2	1.382 (4)	C12—C13	1.460 (4)
C1—C14	1.409 (4)	C13—C14	1.481 (4)
C2—C3	1.381 (4)	C15—H15A	0.9700
C2—H2A	0.9300	C15—H15B	0.9700
C3—C4	1.390 (4)	C16—H16A	0.9600
C3—C15	1.504 (4)	C16—H16B	0.9600
C4—C5	1.383 (4)	C16—H16C	0.9600
C1—O1—H1	109.5	O4—C9—C10	117.0 (3)
C15—O2—H2	109.5	C8—C9—C10	120.9 (3)
C9—O4—H4	109.5	C11—C10—C9	119.6 (3)
C11—O5—C16	118.3 (3)	C11—C10—H10	120.2
H7A—O7—H7B	107.3	C9—C10—H10	120.2
O1—C1—C2	116.6 (3)	O5—C11—C10	121.7 (3)
O1—C1—C14	122.1 (3)	O5—C11—C12	116.9 (3)
C2—C1—C14	121.3 (3)	C10—C11—C12	121.4 (3)
C3—C2—C1	120.1 (3)	C11—C12—C7	116.9 (3)
C3—C2—H2A	119.9	C11—C12—C13	123.2 (3)
C1—C2—H2A	119.9	C7—C12—C13	119.9 (3)
C2—C3—C4	119.7 (3)	O6—C13—C12	123.0 (3)

C2—C3—C15	120.0 (3)	O6—C13—C14	118.3 (3)
C4—C3—C15	120.3 (3)	C12—C13—C14	118.6 (3)
C5—C4—C3	120.5 (3)	C5—C14—C1	117.5 (3)
C5—C4—H4A	119.8	C5—C14—C13	122.3 (3)
C3—C4—H4A	119.8	C1—C14—C13	120.2 (3)
C4—C5—C14	120.9 (3)	O2—C15—C3	113.2 (3)
C4—C5—C6	119.9 (3)	O2—C15—H15A	108.9
C14—C5—C6	119.2 (3)	C3—C15—H15A	108.9
O3—C6—C5	121.0 (3)	O2—C15—H15B	108.9
O3—C6—C7	120.0 (3)	C3—C15—H15B	108.9
C5—C6—C7	119.0 (3)	H15A—C15—H15B	107.7
C8—C7—C12	121.3 (3)	O5—C16—H16A	109.5
C8—C7—C6	118.0 (3)	O5—C16—H16B	109.5
C12—C7—C6	120.8 (3)	H16A—C16—H16B	109.5
C7—C8—C9	119.9 (3)	O5—C16—H16C	109.5
C7—C8—H8	120.0	H16A—C16—H16C	109.5
C9—C8—H8	120.0	H16B—C16—H16C	109.5
O4—C9—C8	122.1 (3)		
O1—C1—C2—C3	179.3 (3)	O5—C11—C12—C7	179.6 (3)
C14—C1—C2—C3	−1.6 (5)	C10—C11—C12—C7	−1.0 (5)
C1—C2—C3—C4	0.7 (5)	O5—C11—C12—C13	1.2 (5)
C1—C2—C3—C15	−179.2 (3)	C10—C11—C12—C13	−179.5 (3)
C2—C3—C4—C5	0.4 (5)	C8—C7—C12—C11	1.2 (5)
C15—C3—C4—C5	−179.8 (3)	C6—C7—C12—C11	−179.0 (3)
C3—C4—C5—C14	−0.6 (5)	C8—C7—C12—C13	179.7 (3)
C3—C4—C5—C6	177.2 (3)	C6—C7—C12—C13	−0.5 (4)
C4—C5—C6—O3	4.5 (5)	C11—C12—C13—O6	−0.1 (5)
C14—C5—C6—O3	−177.7 (3)	C7—C12—C13—O6	−178.4 (3)
C4—C5—C6—C7	−176.9 (3)	C11—C12—C13—C14	−177.7 (3)
C14—C5—C6—C7	1.0 (4)	C7—C12—C13—C14	3.9 (4)
O3—C6—C7—C8	−3.5 (5)	C4—C5—C14—C1	−0.2 (5)
C5—C6—C7—C8	177.8 (3)	C6—C5—C14—C1	−178.0 (3)
O3—C6—C7—C12	176.7 (3)	C4—C5—C14—C13	−179.6 (3)
C5—C6—C7—C12	−2.0 (4)	C6—C5—C14—C13	2.6 (4)
C12—C7—C8—C9	−2.0 (5)	O1—C1—C14—C5	−179.6 (3)
C6—C7—C8—C9	178.2 (3)	C2—C1—C14—C5	1.3 (5)
C7—C8—C9—O4	−177.9 (3)	O1—C1—C14—C13	−0.2 (4)
C7—C8—C9—C10	2.7 (5)	C2—C1—C14—C13	−179.3 (3)
O4—C9—C10—C11	178.0 (3)	O6—C13—C14—C5	177.2 (3)
C8—C9—C10—C11	−2.5 (5)	C12—C13—C14—C5	−5.1 (4)
C16—O5—C11—C10	−1.2 (4)	O6—C13—C14—C1	−2.2 (4)
C16—O5—C11—C12	178.1 (3)	C12—C13—C14—C1	175.5 (3)
C9—C10—C11—O5	−178.9 (3)	C2—C3—C15—O2	−13.1 (4)
C9—C10—C11—C12	1.7 (5)	C4—C3—C15—O2	167.1 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O6	0.82	1.82	2.525 (3)	144

O2—H2···O5^{i}	0.82	2.38	2.945 (3)	127
O2—H2···O6^{i}	0.82	2.16	2.919 (3)	154
O4—H4···O7^{ii}	0.82	1.85	2.665 (3)	170
O7—H7A···O1	0.85	2.03	2.878 (3)	176
O7—H7B···O2^{iii}	0.85	1.94	2.771 (3)	165

Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+3/2; (ii) *x*+1, *y*, *z*; (iii) *x*, −*y*+3/2, *z*−1/2.

Fig. 1

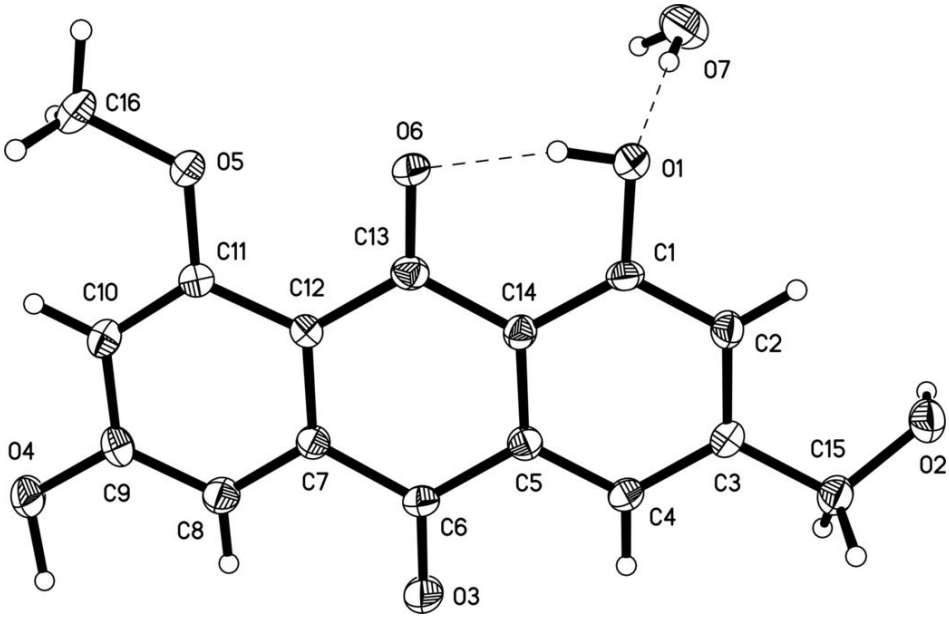

O7
C16
O6
O5
O1
C13
C11
C1
C10
C12
C14
C2
O4
C15
O2
C9
C7
C5
C3
C8
C6
C4
O3

Fig. 2

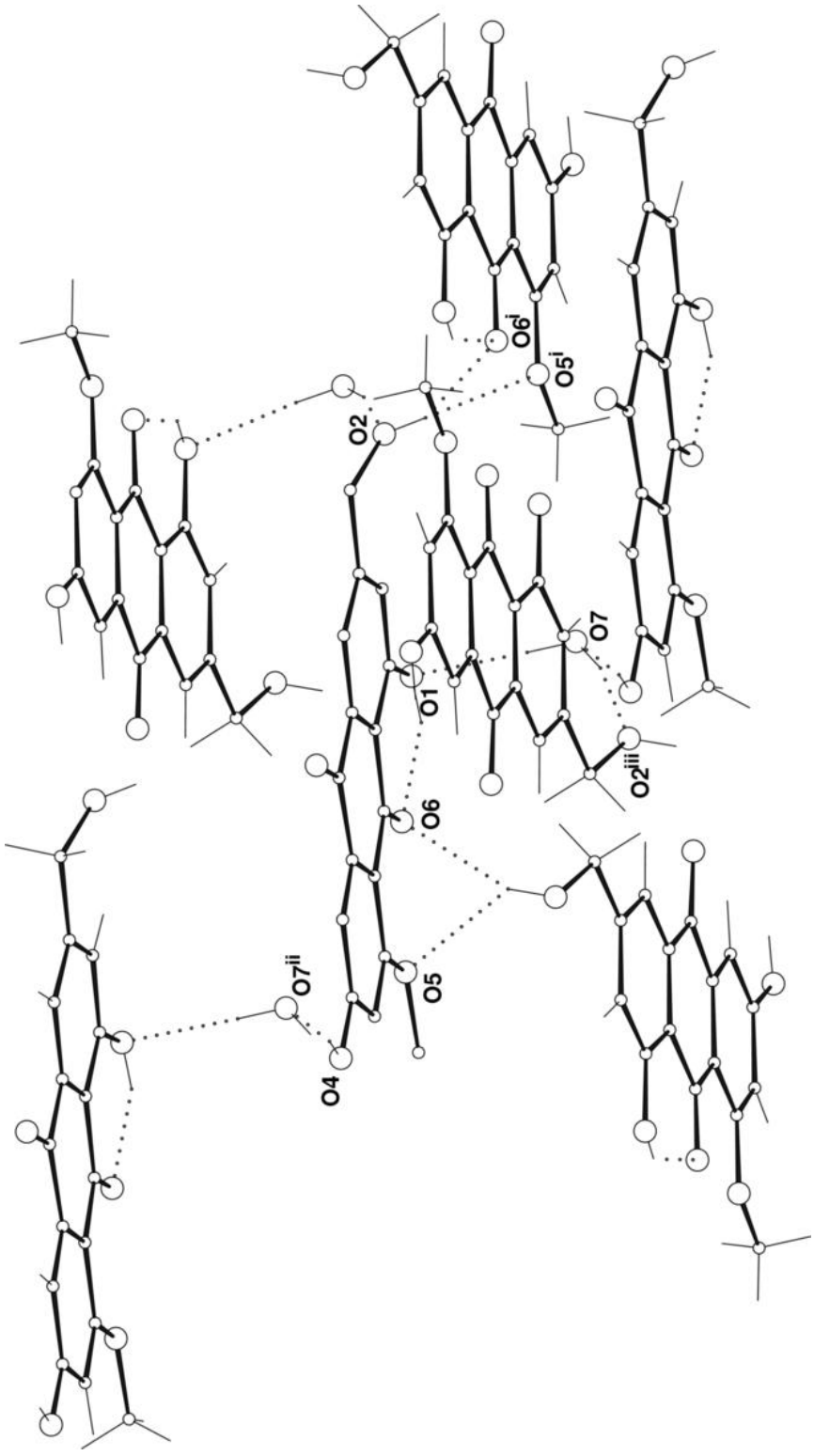


Fig. 3