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2-[(4-Hexyloxyphenyl)iminomethyl]-benzene-1,4-diol

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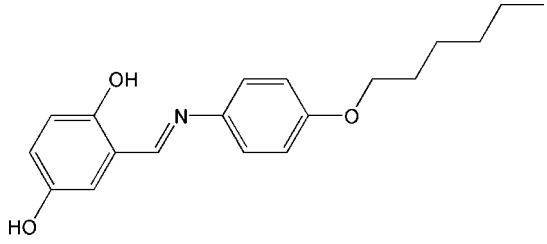
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.052; wR factor = 0.158; data-to-parameter ratio = 14.1.

The title molecule, $C_{19}H_{23}NO_3$, is an amphiphilic molecule with a hydrophobic alkyl chain and polar hydroxy groups. The molecule is almost planar, with a dihedral angle between the aromatic rings of 8.52 (11)°. This conformation is, at least partially, a consequence of a strong intramolecular hydrogen bond between the imine N atom and the *ortho* OH functionality, resulting in an S(6) ring. The molecules are associated in a layered network built *via* O—H···O intermolecular hydrogen bonds involving all the hydroxy groups. The molecules in the layers are arranged in a head-to-head tail-to-tail fashion, and C—H···π interlayer contacts further stabilize the crystal structure.

Related literature

The crystal structure of the title compound is closely related to that of its starting material, 4-(hexyloxy)aniline (Herrera *et al.*, 2005; Herrera, 2006). For related imines as potential precursors for liquid crystalline compounds and polymers, see: Sudhakar *et al.* (2000); Cerrada *et al.* (1996); Wang *et al.* (1996). For the graph-set notation S(6), see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{19}H_{23}NO_3$
M_r = 313.38
Orthorhombic, *Pbca*
a = 7.5559 (10) Å
b = 12.3351 (15) Å
c = 36.597 (4) Å
V = 3411.0 (7) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 296 (2) K
0.60 × 0.54 × 0.16 mm

Data collection

Bruker P4 diffractometer
Absorption correction: none
3894 measured reflections
2996 independent reflections
1762 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
3 standard reflections
every 97 reflections
intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.158
S = 1.03
2996 reflections
212 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

*Cg*1 is the centroid of the C1–C6 ring.

D—H···A	D—H	H···A	D···A	D—H···A
O22—H22···N8	0.82	1.85	2.581 (2)	147
O23—H23···O22^{i}	0.82	2.14	2.933 (2)	162
C6—H6*C*···*Cg*1^{ii}	0.93	2.74	3.433 (2)	132
C14—H14*A*···*Cg*1^{iii}	0.93	2.83	3.536 (2)	134

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

Data collection: *XSCANS* (Siemens, 1996); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXTL-Plus* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL-Plus*; molecular graphics: *SHELXTL-Plus* and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXTL-Plus*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZL2051).

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supplementary materials

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2-[(4-Hexyloxyphenyl)iminomethyl]benzene-1,4-diol

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Comment

Imines or Schiff bases are potential precursors for liquid crystalline compounds (Sudhakar *et al.*, 2000) and polymers (Cerrada *et al.*, 1996; Wang *et al.*, 1996). We are interested in the synthesis and characterization of imines, as well as in the incorporation of reactive functional groups that can undergo radical or condensation polymerization reactions (Herrera, 2006).

The title compound, (I), is such a potential precursors for liquid crystalline materials. It is an amphiphilic molecule with a hydrophobic alkyl-chain and polar hydroxyl groups (Fig. 1), and the hexyloxy chains are in an all-*trans* conformation. The benzene rings bonded to the imine core functionality are almost co-planar, with a dihedral angle of 8.52 (11)°. A strong intramolecular hydrogen bond is observed, involving the imine N atom and the *ortho*-hydroxyl functionality of the benzylidene group, forming an S(6) ring motif (Bernstein *et al.*, 1995). The planar conformation of the molecule is probably a consequence of this contact.

The packing of the molecules in the crystal is partially facilitated by intermolecular O—H···O hydrogen bonds involving the *meta*-hydroxyl functionality of the benzylidene as the H-donor and the *ortho*-hydroxyl group of a neighboring molecules as the acceptor. The resulting crystal structure exhibits a head-to-head tail-to-tail arrangement (Fig. 2). Molecules are thus arranged in layers, and the crystal structure is further stabilized through C—H···π interlayer contacts: C6—H6 and C14—H14 groups in the asymmetric unit are close to the centroids of the C1···C6 rings of symmetry related molecules at positions −1/2 + *x*, *y*, 1/2 − *z* and 3/2 − *x*, −1/2 + *y*, *z*, respectively. H···centroids separations are 2.74 for the former, and 2.82 Å for the latter contact, with corresponding C—H···centroid tilt angles of 132 and 134°.

The arrangement of molecules in the crystal structure of (I) is reminiscent of that stabilized for the starting material, 4-(hexyloxy)aniline (Herrera *et al.*, 2005).

Experimental

To a stirred solution of 2,5-dihydroxybenzaldehyde (0.24 g, 1.76 mmol) in 60 ml of dry ethanol was added 2.10 mmol (0.41 g) of 4-hexyloxyaniline (Herrera *et al.*, 2005) under Ar. The mixture was heated to 325 K for 4 h, and then cooled to room temperature. Ethanol was evaporated, and finally the resulting solid product was recrystallized from petroleum ether, affording thin orange crystals (yield 0.50 g, 91% based on aldehyde; m.p. 389 K). Analysis found: C 72.83, H 7.32, O 15.33, N 4.45%; Calcd. for $C_{19}H_{23}NO_3$: C 72.82, H 7.40, O 15.32, N 4.47%. ^{1}H NMR (400 MHz, DMSO-d_6): δ 0.88 (t, *J* = 6.4 Hz, 3H, CH_3), 1.42–1.30 (m, *J* = 7.2 Hz, 6H, CH_2), 1.71 (m, *J* = 6.8 Hz, 2H, CH_2), 3.97 (t, *J* = 6.8 Hz, 6.4 Hz, 2H, OCH_2), 6.79 (m, *J* = 8.7 Hz, 2H, Ph), 6.99 (m, 3H, Ph), 7.36 (d, *J* = 8.8 Hz, 2H, Ph), 8.82 (s, 1H, N═CH), 9.08 (s, 1H, OH), 12.50 (s, 1H, OH).

Refinement

All C-bonded H atoms were placed in idealized positions and refined using a riding model; C—H bond lengths were set to 0.96 (methyl CH_3 group, considered as a free to rotate rigid group), 0.97 (methylene CH_2 groups) or 0.93 Å (aromatic CH). Hydroxyl H atoms were found in a difference map and refined with a regularized geometry (O—H = 0.82 Å; C—O—H = 109.5°) allowing free rotation about the C—O axis. Isotropic displacement parameters were fixed for all H atoms: U_{iso}(H) = 1.2 U_{eq}(carrier C) for methylene and aromatic H atoms, U_{iso}(H) = 1.5 U_{eq}(carrier atom) for methyl and hydroxyl H atoms.

Figures

Fig. 1. The structure of (I) with displacement ellipsoids for non-H atoms at the 50% probability level.

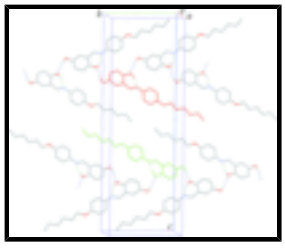

Fig. 2. Part of the crystal structure of (I), showing the hydrogen-bonding scheme (dashed lines). The red molecule corresponds to the asymmetric unit, while the green molecule is related to the asymmetric unit through operator $1 - x$, $1 - y$, $1 - z$.

2-[(4-Hexyloxyphenyl)iminomethyl]benzene-1,4-diol

Crystal data

$C_{19}H_{23}NO_3$	D_x = 1.221 Mg m^{-3}
M_r = 313.38	Melting point: 389 K
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 80 reflections
a = 7.5559 (10) Å	θ = 3.9–12.2º
b = 12.3351 (15) Å	μ = 0.08 mm^{-1}
c = 36.597 (4) Å	*T* = 296 (2) K
V = 3411.0 (7) Å^3	Plate, orange
Z = 8	0.60 × 0.54 × 0.16 mm
F_{000} = 1344	

Data collection

Bruker P4 diffractometer	θ_{max} = 25.0º
Monochromator: graphite	θ_{min} = 2.2º
T = 296(1) K	*h* = −8→1
ω scans	*k* = −14→1
Absorption correction: none	*l* = −43→1
3894 measured reflections	3 standard reflections

2996 independent reflections
1762 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$
every 97 reflections
intensity decay: 1%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.158$
$S = 1.03$
2996 reflections
212 parameters
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0794P)^2 + 0.2325P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.22$ e Å^{-3}
$\Delta\rho_{min} = -0.18$ e Å^{-3}
Extinction correction: SHELXTL-Plus (Sheldrick, 1998), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0027 (6)

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.3979 (3)	0.76235 (16)	0.27705 (6)	0.0461 (6)
C2	0.4892 (3)	0.77627 (16)	0.31019 (6)	0.0449 (6)
C3	0.5559 (3)	0.87943 (16)	0.31853 (6)	0.0483 (6)
H3C	0.6188	0.8897	0.3401	0.058*
C4	0.5297 (3)	0.96557 (16)	0.29535 (6)	0.0489 (6)
C5	0.4367 (3)	0.95043 (18)	0.26302 (6)	0.0497 (6)
H5C	0.4172	1.0088	0.2474	0.060*
C6	0.3732 (3)	0.84884 (16)	0.25397 (6)	0.0513 (6)
H6C	0.3132	0.8389	0.2320	0.062*
C7	0.5198 (3)	0.68504 (18)	0.33457 (6)	0.0502 (6)
H7A	0.5889	0.6948	0.3553	0.060*
N8	0.4534 (2)	0.59150 (14)	0.32798 (5)	0.0502 (5)
C9	0.4813 (3)	0.49935 (17)	0.35029 (6)	0.0480 (6)
C10	0.5530 (4)	0.50164 (19)	0.38539 (6)	0.0607 (7)
H10B	0.5873	0.5674	0.3956	0.073*
C11	0.5733 (4)	0.40725 (19)	0.40491 (6)	0.0645 (7)
H11B	0.6205	0.4099	0.4284	0.077*
C12	0.5246 (3)	0.30830 (19)	0.39013 (6)	0.0550 (6)
C13	0.4544 (3)	0.30473 (18)	0.35534 (6)	0.0567 (7)
H13B	0.4222	0.2389	0.3449	0.068*
C14	0.4327 (3)	0.40059 (17)	0.33616 (6)	0.0550 (6)
H14A	0.3834	0.3980	0.3129	0.066*
O15	0.5508 (3)	0.22029 (13)	0.41222 (5)	0.0722 (6)
C16	0.4815 (4)	0.11738 (18)	0.40096 (7)	0.0617 (7)
H16A	0.5476	0.0896	0.3803	0.074*

H16B	0.3582	0.1243	0.3940	0.074*
C17	0.4999 (4)	0.04240 (19)	0.43334 (7)	0.0651 (7)
H17B	0.6228	0.0413	0.4410	0.078*
H17C	0.4306	0.0711	0.4535	0.078*
C18	0.4411 (4)	−0.07187 (19)	0.42573 (7)	0.0727 (8)
H18A	0.5081	−0.0999	0.4052	0.087*
H18B	0.3172	−0.0710	0.4188	0.087*
C19	0.4643 (4)	−0.1480 (2)	0.45808 (7)	0.0788 (9)
H19A	0.5858	−0.1426	0.4664	0.095*
H19B	0.3892	−0.1226	0.4778	0.095*
C20	0.4251 (6)	−0.2609 (2)	0.45176 (9)	0.1174 (14)
H20A	0.4927	−0.2846	0.4307	0.141*
H20B	0.3008	−0.2669	0.4454	0.141*
C21	0.4617 (5)	−0.3377 (3)	0.48262 (10)	0.1139 (13)
H21A	0.4262	−0.4095	0.4757	0.171*
H21B	0.3964	−0.3154	0.5038	0.171*
H21C	0.5860	−0.3372	0.4881	0.171*
O22	0.3302 (2)	0.66392 (11)	0.26689 (4)	0.0615 (5)
H22	0.3504	0.6192	0.2829	0.092*
O23	0.5998 (3)	1.06534 (11)	0.30460 (4)	0.0687 (6)
H23	0.6040	1.1040	0.2864	0.103*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0512 (14)	0.0380 (12)	0.0490 (12)	0.0011 (11)	−0.0011 (11)	−0.0034 (10)
C2	0.0515 (14)	0.0408 (12)	0.0425 (11)	0.0051 (10)	0.0028 (10)	0.0010 (10)
C3	0.0604 (15)	0.0448 (13)	0.0398 (11)	−0.0015 (12)	0.0009 (11)	−0.0040 (10)
C4	0.0633 (15)	0.0364 (12)	0.0469 (13)	−0.0008 (11)	0.0070 (11)	−0.0047 (10)
C5	0.0583 (15)	0.0404 (12)	0.0505 (13)	0.0051 (12)	0.0014 (11)	0.0039 (10)
C6	0.0588 (14)	0.0479 (13)	0.0471 (12)	0.0034 (13)	−0.0085 (11)	0.0015 (11)
C7	0.0593 (15)	0.0491 (14)	0.0422 (12)	0.0033 (12)	−0.0008 (11)	0.0011 (10)
N8	0.0594 (12)	0.0404 (11)	0.0508 (11)	0.0024 (10)	−0.0006 (9)	0.0041 (8)
C9	0.0561 (14)	0.0418 (12)	0.0460 (13)	0.0032 (11)	−0.0004 (11)	0.0044 (10)
C10	0.0833 (19)	0.0459 (13)	0.0529 (14)	−0.0040 (13)	−0.0095 (13)	0.0008 (11)
C11	0.089 (2)	0.0542 (15)	0.0503 (14)	−0.0056 (14)	−0.0184 (13)	0.0056 (12)
C12	0.0646 (16)	0.0467 (13)	0.0538 (14)	−0.0001 (12)	−0.0026 (12)	0.0097 (11)
C13	0.0730 (17)	0.0445 (13)	0.0527 (14)	−0.0039 (13)	−0.0084 (13)	0.0019 (11)
C14	0.0685 (16)	0.0502 (14)	0.0463 (12)	−0.0027 (13)	−0.0084 (12)	0.0047 (11)
O15	0.1023 (15)	0.0477 (10)	0.0667 (11)	−0.0070 (10)	−0.0228 (10)	0.0171 (8)
C16	0.0777 (18)	0.0459 (14)	0.0614 (15)	−0.0004 (13)	0.0003 (14)	0.0083 (12)
C17	0.0819 (19)	0.0511 (14)	0.0624 (15)	0.0053 (14)	0.0054 (14)	0.0136 (12)
C18	0.093 (2)	0.0542 (15)	0.0706 (17)	−0.0019 (15)	−0.0001 (15)	0.0139 (13)
C19	0.102 (2)	0.0641 (17)	0.0703 (17)	−0.0069 (16)	0.0087 (16)	0.0165 (14)
C20	0.196 (4)	0.0631 (19)	0.093 (2)	−0.014 (2)	−0.020 (3)	0.0166 (17)
C21	0.139 (3)	0.080 (2)	0.123 (3)	−0.007 (2)	−0.014 (2)	0.042 (2)
O22	0.0849 (13)	0.0416 (9)	0.0581 (9)	−0.0041 (9)	−0.0170 (9)	0.0001 (7)
O23	0.1063 (14)	0.0424 (9)	0.0574 (10)	−0.0136 (10)	−0.0045 (11)	−0.0020 (7)

Geometric parameters (Å, °)

C1—O22	1.369 (2)	C13—H13B	0.9300
C1—C6	1.374 (3)	C14—H14A	0.9300
C1—C2	1.406 (3)	O15—C16	1.434 (3)
C2—C3	1.402 (3)	C16—C17	1.510 (3)
C2—C7	1.455 (3)	C16—H16A	0.9700
C3—C4	1.374 (3)	C16—H16B	0.9700
C3—H3C	0.9300	C17—C18	1.504 (3)
C4—O23	1.382 (2)	C17—H17B	0.9700
C4—C5	1.388 (3)	C17—H17C	0.9700
C5—C6	1.382 (3)	C18—C19	1.521 (3)
C5—H5C	0.9300	C18—H18A	0.9700
C6—H6C	0.9300	C18—H18B	0.9700
C7—N8	1.281 (3)	C19—C20	1.443 (4)
C7—H7A	0.9300	C19—H19A	0.9700
N8—C9	1.415 (3)	C19—H19B	0.9700
C9—C14	1.374 (3)	C20—C21	1.500 (4)
C9—C10	1.395 (3)	C20—H20A	0.9700
C10—C11	1.375 (3)	C20—H20B	0.9700
C10—H10B	0.9300	C21—H21A	0.9600
C11—C12	1.385 (3)	C21—H21B	0.9600
C11—H11B	0.9300	C21—H21C	0.9600
C12—O15	1.368 (3)	O22—H22	0.8200
C12—C13	1.380 (3)	O23—H23	0.8200
C13—C14	1.385 (3)		
O22—C1—C6	118.11 (19)	C12—O15—C16	118.69 (18)
O22—C1—C2	121.74 (18)	O15—C16—C17	106.5 (2)
C6—C1—C2	120.1 (2)	O15—C16—H16A	110.4
C3—C2—C1	118.36 (19)	C17—C16—H16A	110.4
C3—C2—C7	120.8 (2)	O15—C16—H16B	110.4
C1—C2—C7	120.8 (2)	C17—C16—H16B	110.4
C4—C3—C2	121.0 (2)	H16A—C16—H16B	108.6
C4—C3—H3C	119.5	C18—C17—C16	113.7 (2)
C2—C3—H3C	119.5	C18—C17—H17B	108.8
C3—C4—O23	118.8 (2)	C16—C17—H17B	108.8
C3—C4—C5	119.7 (2)	C18—C17—H17C	108.8
O23—C4—C5	121.50 (19)	C16—C17—H17C	108.8
C6—C5—C4	120.1 (2)	H17B—C17—H17C	107.7
C6—C5—H5C	119.9	C17—C18—C19	113.6 (2)
C4—C5—H5C	119.9	C17—C18—H18A	108.8
C1—C6—C5	120.6 (2)	C19—C18—H18A	108.8
C1—C6—H6C	119.7	C17—C18—H18B	108.8
C5—C6—H6C	119.7	C19—C18—H18B	108.8
N8—C7—C2	121.3 (2)	H18A—C18—H18B	107.7
N8—C7—H7A	119.4	C20—C19—C18	116.6 (2)
C2—C7—H7A	119.4	C20—C19—H19A	108.1
C7—N8—C9	123.80 (19)	C18—C19—H19A	108.1

C14—C9—C10	117.9 (2)	C20—C19—H19B	108.1
C14—C9—N8	117.09 (19)	C18—C19—H19B	108.1
C10—C9—N8	125.0 (2)	H19A—C19—H19B	107.3
C11—C10—C9	120.3 (2)	C19—C20—C21	116.8 (3)
C11—C10—H10B	119.8	C19—C20—H20A	108.1
C9—C10—H10B	119.8	C21—C20—H20A	108.1
C10—C11—C12	120.9 (2)	C19—C20—H20B	108.1
C10—C11—H11B	119.5	C21—C20—H20B	108.1
C12—C11—H11B	119.5	H20A—C20—H20B	107.3
O15—C12—C13	125.1 (2)	C20—C21—H21A	109.5
O15—C12—C11	115.5 (2)	C20—C21—H21B	109.5
C13—C12—C11	119.4 (2)	H21A—C21—H21B	109.5
C12—C13—C14	119.1 (2)	C20—C21—H21C	109.5
C12—C13—H13B	120.5	H21A—C21—H21C	109.5
C14—C13—H13B	120.5	H21B—C21—H21C	109.5
C9—C14—C13	122.3 (2)	C1—O22—H22	109.5
C9—C14—H14A	118.8	C4—O23—H23	109.5
C13—C14—H14A	118.8		
O22—C1—C2—C3	179.5 (2)	C14—C9—C10—C11	−0.1 (4)
C6—C1—C2—C3	−1.0 (3)	N8—C9—C10—C11	179.5 (2)
O22—C1—C2—C7	1.9 (3)	C9—C10—C11—C12	0.5 (4)
C6—C1—C2—C7	−178.7 (2)	C10—C11—C12—O15	−179.9 (2)
C1—C2—C3—C4	1.4 (3)	C10—C11—C12—C13	−0.1 (4)
C7—C2—C3—C4	179.0 (2)	O15—C12—C13—C14	179.0 (2)
C2—C3—C4—O23	−179.3 (2)	C11—C12—C13—C14	−0.7 (4)
C2—C3—C4—C5	−0.4 (3)	C10—C9—C14—C13	−0.7 (4)
C3—C4—C5—C6	−1.0 (3)	N8—C9—C14—C13	179.7 (2)
O23—C4—C5—C6	177.9 (2)	C12—C13—C14—C9	1.1 (4)
O22—C1—C6—C5	179.2 (2)	C13—C12—O15—C16	−8.2 (4)
C2—C1—C6—C5	−0.3 (4)	C11—C12—O15—C16	171.5 (2)
C4—C5—C6—C1	1.3 (4)	C12—O15—C16—C17	−169.6 (2)
C3—C2—C7—N8	177.1 (2)	O15—C16—C17—C18	−177.2 (2)
C1—C2—C7—N8	−5.3 (3)	C16—C17—C18—C19	178.5 (2)
C2—C7—N8—C9	178.73 (19)	C17—C18—C19—C20	−174.8 (3)
C7—N8—C9—C14	−167.1 (2)	C18—C19—C20—C21	175.2 (3)
C7—N8—C9—C10	13.3 (4)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O22—H22···N8	0.82	1.85	2.581 (2)	147
O23—H23···O22^{i}	0.82	2.14	2.933 (2)	162

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

Fig. 1

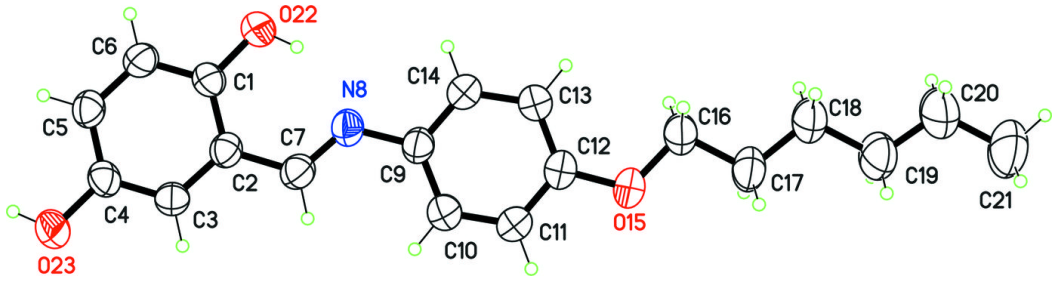
O22
C6
C1
N8
C14
C13
C16
C18
C20
C5
C7
C12
C2
C9
C17
C19
C21
C4
C3
O15
O23
C10
C11

Fig. 2