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Loureirin A

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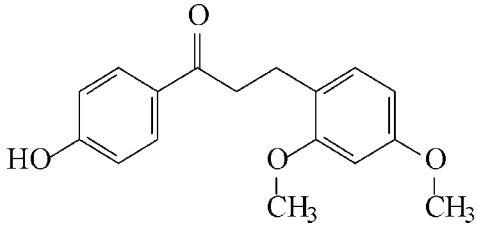
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.004 Å; R factor = 0.057; wR factor = 0.189; data-to-parameter ratio = 12.5.

The asymmetric unit of the title compound [systematic name: 3-(2,4-dimethoxyphenyl)-1-(4-hydroxyphenyl)propan-1-one], $C_{17}H_{18}O_4$, contains two independent molecules; these have different conformations with respect to the relative orientation of the aromatic ring planes. The dihedral angles formed by the dimethoxyphenyl and hydroxyphenyl rings in the two molecules are 19.61 (10) and 66.37 (9)°. In the crystal structure, intermolecular O—H···O hydrogen-bonding interactions link the molecules into one-dimensional chains running parallel to the c axis.

Related literature

For the extraction of the components of *Sanguis draxonis* see: Zhou *et al.* (2001). For the crystal structure of loureirin B see: Lu *et al.* (2006).



Experimental

Crystal data

$C_{17}H_{18}O_4$
M_r = 286.31
Triclinic, $P\overline{1}$
a = 8.1750 (7) Å
b = 12.8971 (8) Å
c = 15.2410 (6) Å
α = 73.509 (10)°
β = 86.259 (12)°
γ = 74.206 (10)°
V = 1482.5 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 295 (2) K
0.20 × 0.20 × 0.10 mm

Data collection

MAC DIP 2030K diffractometer
Absorption correction: none
10182 measured reflections
5366 independent reflections
3408 reflections with $I > 2\sigma(I)$
R_{int} = 0.049

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.189
S = 1.02
5366 reflections
431 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···O2A^{i}	0.82 (4)	1.96 (4)	2.733 (3)	155 (5)
O1A—H1B···O2^{ii}	0.79 (4)	1.96 (4)	2.732 (3)	166 (5)
C5—H5A···O3	1.03 (3)	2.60 (4)	3.609 (4)	168 (3)
C8—H8B···O3	0.97	2.57	3.120 (4)	116

Symmetry codes: (i) $-x+2, -y+1, -z+1$; (ii) $-x+1, -y+1, -z+2$.

Data collection: *DENZO* (Otwinowski & Minor, 1997); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2161).

References

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supplementary materials

Acta Cryst. (2007). E**63**, o3927 [**doi:10.1107/S1600536807035520**]

Loureirin A

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Comment

We have recently published the crystal structure of loureirin B (Lu *et al.*, 2006). As a continuation of our studies on the components of *Sanguis draxonis*, we report here the crystal structure of loureirin A, which was crystallized from a DMF:water (1:1 *v*/*v*) solution.

In the asymmetric unit of the title compound there are two independent molecules (Fig. 1) with different conformations. The main difference between the two molecules relates to the relative orientation of the aromatic ring planes, as indicated by the dihedral angles formed by the dimethoxyphenyl and hydroxyphenyl rings [19.61 (10) and 66.37 (9)°] and by the values of the C4—C7—C8—C9 torsion angles [83.9 (4) and 179.3 (2)°]. In this orientation, intramolecular C—H···O hydrogen bonds stabilizing the conformation are observed only in one molecule (Table 1). In the crystal packing, the molecules are linked by intermolecular O—H···O hydrogen bonding interactions (Table 1) into one-dimensional chains running parallel to the *c* axis (Fig. 2).

Experimental

The title compound was extracted according to the literature method (Zhou *et al.*, 2001) from the herb *Sanguis draxonis*. Colourless block-shaped crystals suitable for X-ray analysis were obtained by slow evaporation of as DMF:water (1:1 *v*/*v*) solution at 298 K over a period of one month.

Refinement

The hydroxy and aromatic H atoms were located in a difference Fourier map and refined freely with U_{iso}(H) = 1.2U_{eq}(C, O). The methyl H atoms were constrained to an ideal geometry with C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C), but each group was allowed to rotate freely about its C—C bond. The methylene H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H = 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C).

Figures

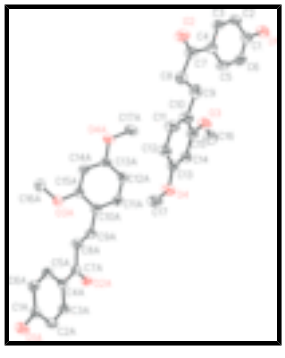
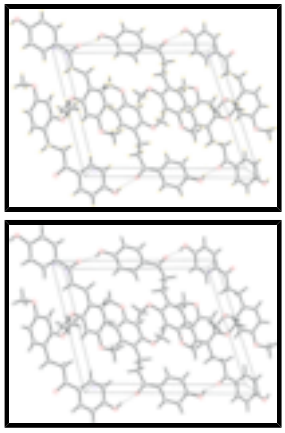


Fig. 1. A view of the asymmetric unit of loureirin A showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are omitted for clarity.
Fig. 2. The molecular packing of loureirin A viewed down the *a* axis. Dashed lines indicate intermolecular C—H···O hydrogen bonding interactions.



3-(2,4-dimethoxyphenyl)-1-(4-hydroxyphenyl)propan-1-one

Crystal data

$C_{17}H_{18}O_4$	$Z = 4$
$M_r = 286.31$	$F_{000} = 608$
Triclinic, $P\overline{1}$	$D_x = 1.283$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.1750$ (7) Å	Cell parameters from 5366 reflections
$b = 12.8971$ (8) Å	$\theta = 2.5$–25.6º
$c = 15.2410$ (6) Å	$\mu = 0.09$ mm^{-1}
$\alpha = 73.509$ (10)º	$T = 295$ (2) K
$\beta = 86.259$ (12)º	Block, colourless
$\gamma = 74.206$ (10)º	0.20 × 0.20 × 0.10 mm
$V = 1482.5$ (2) Å^3	

Data collection

MAC DIP 2030K diffractometer	3408 reflections with $I > 2\sigma(I)$
Radiation source: rotating anode	$R_{int} = 0.049$
Monochromator: graphite	$\theta_{max} = 25.6$º
$T = 295(2)$ K	$\theta_{min} = 2.5$º
ω scans	$h = -9 \rightarrow 9$
Absorption correction: none	$k = -14 \rightarrow 15$
10182 measured reflections	$l = -18 \rightarrow 18$
5366 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.057$	H atoms treated by a mixture of

	independent and constrained refinement
$wR(F^2) = 0.189$	$w = 1/[\sigma^2(F_o^2) + (0.1025P)^2 + 0.2205P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} < 0.001$
5366 reflections	$\Delta\rho_{max} = 0.29$ e Å^{-3}
431 parameters	$\Delta\rho_{min} = -0.20$ e Å^{-3}
3 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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	0.8504 (3)	−0.0889 (2)	0.31936 (15)	0.0893 (8)
H1A	0.895 (6)	−0.045 (4)	0.282 (3)	0.134*
O2	0.6352 (4)	−0.05071 (19)	0.71439 (14)	0.0959 (8)
O3	0.7430 (3)	0.34222 (18)	0.52269 (14)	0.0849 (7)
O4	0.5812 (3)	0.64527 (17)	0.65600 (14)	0.0780 (6)
C1	0.8119 (4)	−0.0571 (3)	0.39738 (19)	0.0663 (8)
C2	0.7716 (4)	−0.1363 (3)	0.4721 (2)	0.0675 (8)
H2A	0.769 (4)	−0.208 (3)	0.463 (2)	0.081*
C3	0.7254 (4)	−0.1091 (2)	0.5530 (2)	0.0663 (8)
H3A	0.694 (4)	−0.162 (3)	0.604 (2)	0.080*
C4	0.7268 (4)	−0.0048 (2)	0.56262 (19)	0.0663 (8)
C5	0.7722 (5)	0.0726 (3)	0.4876 (2)	0.0778 (9)
H5A	0.780 (4)	0.149 (3)	0.493 (2)	0.093*
C6	0.8117 (5)	0.0463 (3)	0.4060 (2)	0.0763 (9)
H6A	0.839 (4)	0.098 (3)	0.358 (2)	0.092*
C7	0.6835 (5)	0.0173 (3)	0.6527 (2)	0.0793 (9)
C8	0.7015 (5)	0.1266 (3)	0.6695 (2)	0.0869 (10)
H8A	0.7163	0.1159	0.7344	0.104*
H8B	0.8000	0.1467	0.6379	0.104*
C9	0.5417 (5)	0.2186 (3)	0.6340 (2)	0.0843 (9)
H9A	0.4440	0.1993	0.6672	0.101*
H9B	0.5248	0.2270	0.5697	0.101*
C10	0.5596 (4)	0.3302 (3)	0.6468 (2)	0.0768 (9)

C11	0.4803 (5)	0.3731 (3)	0.7163 (2)	0.0816 (10)
H11A	0.417 (5)	0.333 (3)	0.759 (2)	0.098*
C12	0.4845 (4)	0.4774 (3)	0.7244 (2)	0.0697 (8)
H12A	0.431 (4)	0.499 (3)	0.776 (2)	0.084*
C13	0.5740 (4)	0.5393 (2)	0.65944 (18)	0.0604 (7)
C14	0.6624 (4)	0.4961 (3)	0.59190 (19)	0.0624 (7)
H14A	0.719 (4)	0.542 (3)	0.550 (2)	0.075*
C15	0.6579 (4)	0.3920 (3)	0.58686 (19)	0.0677 (8)
C16	0.8440 (5)	0.3992 (3)	0.4582 (2)	0.0955 (11)
H16A	0.8976	0.3537	0.4189	0.143*
H16B	0.9295	0.4137	0.4898	0.143*
H16C	0.7734	0.4689	0.4222	0.143*
C17	0.4891 (5)	0.6949 (3)	0.7225 (2)	0.0896 (11)
H17A	0.5032	0.7689	0.7123	0.134*
H17B	0.5311	0.6500	0.7825	0.134*
H17C	0.3707	0.6994	0.7177	0.134*
O1A	0.4963 (3)	1.16103 (19)	1.12874 (15)	0.0815 (7)
H1B	0.468 (6)	1.120 (4)	1.172 (3)	0.122*
O2A	0.9855 (2)	0.99444 (15)	0.83152 (12)	0.0637 (5)
O3A	1.2335 (3)	0.58212 (16)	0.97268 (12)	0.0666 (5)
O4A	1.0914 (3)	0.32784 (16)	0.83785 (14)	0.0760 (6)
C1A	0.5971 (4)	1.1025 (2)	1.07499 (18)	0.0584 (7)
C2A	0.6605 (4)	1.1639 (2)	0.9963 (2)	0.0664 (8)
H2B	0.628 (4)	1.240 (3)	0.981 (2)	0.080*
C3A	0.7646 (4)	1.1097 (2)	0.93961 (19)	0.0613 (7)
H3B	0.807 (4)	1.154 (3)	0.888 (2)	0.074*
C4A	0.8053 (3)	0.9935 (2)	0.95884 (16)	0.0519 (6)
C5A	0.7388 (4)	0.9331 (2)	1.03753 (17)	0.0564 (7)
H5B	0.773 (4)	0.853 (3)	1.0537 (18)	0.068*
C6A	0.6373 (4)	0.9868 (2)	1.09567 (18)	0.0587 (7)
H6B	0.592 (4)	0.944 (2)	1.1526 (19)	0.070*
C7A	0.9191 (3)	0.9379 (2)	0.89583 (17)	0.0534 (6)
C8A	0.9471 (4)	0.8144 (2)	0.90919 (18)	0.0589 (7)
H8C	0.8383	0.7991	0.9059	0.071*
H8D	0.9951	0.7742	0.9698	0.071*
C9A	1.0642 (4)	0.7713 (2)	0.83885 (18)	0.0620 (7)
H9C	1.0288	0.8217	0.7787	0.074*
H9D	1.1784	0.7735	0.8503	0.074*
C10A	1.0694 (3)	0.6541 (2)	0.83781 (17)	0.0550 (7)
C11A	0.9883 (4)	0.6345 (2)	0.76959 (18)	0.0618 (7)
H11B	0.925 (4)	0.699 (3)	0.722 (2)	0.074*
C12A	0.9910 (4)	0.5275 (2)	0.76584 (19)	0.0599 (7)
H12B	0.928 (4)	0.518 (2)	0.719 (2)	0.072*
C13A	1.0773 (4)	0.4372 (2)	0.83321 (17)	0.0574 (7)
C14A	1.1586 (4)	0.4520 (2)	0.90420 (18)	0.0570 (7)
H14B	1.217 (4)	0.389 (3)	0.9520 (19)	0.068*
C15A	1.1545 (3)	0.5599 (2)	0.90622 (16)	0.0519 (6)
C16A	1.3028 (4)	0.4903 (3)	1.04937 (19)	0.0733 (8)
H16D	1.3500	0.5166	1.0923	0.110*

H16E	1.3905	0.4357	1.0293	0.110*
H16F	1.2147	0.4566	1.0782	0.110*
C17A	1.0131 (6)	0.3063 (3)	0.7664 (2)	0.0924 (11)
H17D	1.0336	0.2268	0.7768	0.139*
H17E	1.0601	0.3374	0.7086	0.139*
H17F	0.8928	0.3401	0.7655	0.139*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.1167 (19)	0.0998 (18)	0.0703 (14)	−0.0473 (15)	0.0337 (13)	−0.0426 (13)
O2	0.118 (2)	0.0785 (15)	0.0748 (13)	−0.0372 (15)	0.0304 (14)	−0.0242 (11)
O3	0.1130 (18)	0.0782 (14)	0.0746 (13)	−0.0331 (13)	0.0349 (13)	−0.0389 (11)
O4	0.0961 (16)	0.0659 (13)	0.0831 (13)	−0.0318 (12)	0.0251 (12)	−0.0335 (11)
C1	0.0682 (18)	0.072 (2)	0.0625 (16)	−0.0219 (15)	0.0137 (14)	−0.0250 (14)
C2	0.083 (2)	0.0628 (18)	0.0662 (17)	−0.0297 (16)	0.0144 (15)	−0.0250 (14)
C3	0.082 (2)	0.0545 (17)	0.0628 (16)	−0.0264 (15)	0.0137 (15)	−0.0119 (13)
C4	0.080 (2)	0.0550 (16)	0.0636 (16)	−0.0191 (14)	0.0125 (15)	−0.0170 (13)
C5	0.109 (3)	0.0528 (17)	0.0726 (18)	−0.0291 (17)	0.0264 (18)	−0.0175 (15)
C6	0.099 (2)	0.0647 (19)	0.0604 (17)	−0.0256 (17)	0.0238 (17)	−0.0112 (14)
C7	0.099 (2)	0.0748 (19)	0.0734 (19)	−0.0200 (17)	0.0268 (18)	−0.0228 (16)
C8	0.101 (3)	0.086 (2)	0.0711 (19)	−0.018 (2)	0.0080 (18)	−0.0226 (17)
C9	0.081 (2)	0.076 (3)	0.0724 (19)	−0.0160 (19)	0.0010 (17)	−0.0250 (18)
C10	0.087 (2)	0.0630 (19)	0.088 (2)	−0.0130 (16)	0.0184 (18)	−0.0231 (16)
C11	0.100 (2)	0.067 (2)	0.083 (2)	−0.0328 (18)	0.0380 (19)	−0.0268 (17)
C12	0.079 (2)	0.0667 (19)	0.0702 (18)	−0.0232 (16)	0.0210 (16)	−0.0307 (15)
C13	0.0681 (18)	0.0556 (16)	0.0599 (15)	−0.0184 (13)	0.0074 (13)	−0.0194 (13)
C14	0.0677 (18)	0.0640 (18)	0.0591 (15)	−0.0223 (14)	0.0059 (14)	−0.0189 (13)
C15	0.078 (2)	0.0697 (19)	0.0620 (16)	−0.0219 (15)	0.0143 (15)	−0.0290 (14)
C16	0.110 (3)	0.100 (3)	0.079 (2)	−0.029 (2)	0.033 (2)	−0.036 (2)
C17	0.115 (3)	0.065 (2)	0.092 (2)	−0.0213 (19)	0.033 (2)	−0.0362 (18)
O1A	0.1072 (18)	0.0697 (14)	0.0769 (14)	−0.0298 (13)	0.0361 (13)	−0.0369 (11)
O2A	0.0785 (13)	0.0529 (11)	0.0602 (10)	−0.0220 (9)	0.0176 (9)	−0.0155 (9)
O3A	0.0773 (13)	0.0637 (12)	0.0616 (11)	−0.0219 (10)	0.0006 (9)	−0.0186 (9)
O4A	0.1073 (17)	0.0479 (11)	0.0773 (13)	−0.0210 (11)	−0.0013 (11)	−0.0235 (10)
C1A	0.0665 (17)	0.0570 (16)	0.0572 (14)	−0.0181 (13)	0.0074 (13)	−0.0240 (12)
C2A	0.087 (2)	0.0434 (15)	0.0725 (17)	−0.0185 (15)	0.0161 (15)	−0.0238 (13)
C3A	0.0778 (19)	0.0455 (15)	0.0631 (16)	−0.0210 (13)	0.0066 (14)	−0.0156 (12)
C4A	0.0604 (15)	0.0437 (14)	0.0518 (13)	−0.0146 (12)	0.0011 (11)	−0.0127 (11)
C5A	0.0694 (17)	0.0450 (14)	0.0528 (14)	−0.0155 (13)	0.0048 (12)	−0.0108 (11)
C6A	0.0664 (17)	0.0540 (16)	0.0563 (14)	−0.0182 (13)	0.0083 (13)	−0.0157 (12)
C7A	0.0582 (15)	0.0478 (14)	0.0541 (13)	−0.0159 (12)	0.0000 (12)	−0.0121 (11)
C8A	0.0657 (17)	0.0482 (15)	0.0648 (15)	−0.0161 (13)	0.0127 (13)	−0.0203 (12)
C9A	0.0787 (19)	0.0484 (15)	0.0606 (15)	−0.0200 (14)	0.0144 (14)	−0.0178 (12)
C10A	0.0653 (16)	0.0462 (14)	0.0528 (14)	−0.0142 (12)	0.0169 (12)	−0.0166 (11)
C11A	0.0764 (19)	0.0529 (16)	0.0507 (14)	−0.0118 (14)	0.0081 (13)	−0.0126 (12)
C12A	0.0727 (19)	0.0578 (17)	0.0535 (14)	−0.0195 (14)	0.0037 (13)	−0.0207 (13)
C13A	0.0731 (18)	0.0466 (14)	0.0555 (14)	−0.0193 (13)	0.0161 (13)	−0.0191 (12)

C14A	0.0636 (17)	0.0468 (15)	0.0552 (14)	−0.0103 (12)	0.0100 (13)	−0.0118 (12)
C15A	0.0554 (15)	0.0523 (15)	0.0493 (13)	−0.0141 (12)	0.0113 (11)	−0.0189 (11)
C16A	0.0719 (19)	0.087 (2)	0.0608 (16)	−0.0233 (17)	−0.0011 (14)	−0.0180 (15)
C17A	0.133 (3)	0.069 (2)	0.093 (2)	−0.041 (2)	0.007 (2)	−0.0393 (19)

Geometric parameters (Å, °)

O1—C1	1.356 (3)	O1A—C1A	1.358 (3)
O1—H1A	0.82 (4)	O1A—H1B	0.79 (4)
O2—C7	1.217 (3)	O2A—C7A	1.236 (3)
O3—C15	1.370 (3)	O3A—C15A	1.370 (3)
O3—C16	1.415 (4)	O3A—C16A	1.423 (4)
O4—C13	1.369 (3)	O4A—C13A	1.365 (3)
O4—C17	1.418 (3)	O4A—C17A	1.426 (4)
C1—C6	1.375 (4)	C1A—C6A	1.384 (4)
C1—C2	1.387 (4)	C1A—C2A	1.392 (4)
C2—C3	1.378 (4)	C2A—C3A	1.373 (4)
C2—H2A	0.98 (3)	C2A—H2B	0.91 (3)
C3—C4	1.396 (4)	C3A—C4A	1.390 (4)
C3—H3A	0.96 (3)	C3A—H3B	0.94 (3)
C4—C5	1.393 (4)	C4A—C5A	1.398 (3)
C4—C7	1.482 (4)	C4A—C7A	1.488 (3)
C5—C6	1.376 (4)	C5A—C6A	1.375 (4)
C5—H5A	1.03 (3)	C5A—H5B	0.95 (3)
C6—H6A	0.90 (3)	C6A—H6B	1.00 (3)
C7—C8	1.548 (5)	C7A—C8A	1.501 (3)
C8—C9	1.514 (5)	C8A—C9A	1.514 (3)
C8—H8A	0.9700	C8A—H8C	0.9700
C8—H8B	0.9700	C8A—H8D	0.9700
C9—C10	1.552 (5)	C9A—C10A	1.506 (3)
C9—H9A	0.9700	C9A—H9C	0.9700
C9—H9B	0.9700	C9A—H9D	0.9700
C10—C11	1.377 (4)	C10A—C11A	1.383 (4)
C10—C15	1.398 (4)	C10A—C15A	1.400 (4)
C11—C12	1.395 (4)	C11A—C12A	1.392 (4)
C11—H11A	0.93 (3)	C11A—H11B	0.98 (3)
C12—C13	1.389 (4)	C12A—C13A	1.370 (4)
C12—H12A	0.94 (3)	C12A—H12B	0.96 (3)
C13—C14	1.379 (4)	C13A—C14A	1.389 (4)
C14—C15	1.376 (4)	C14A—C15A	1.392 (4)
C14—H14A	0.93 (3)	C14A—H14B	0.96 (3)
C16—H16A	0.9600	C16A—H16D	0.9600
C16—H16B	0.9600	C16A—H16E	0.9600
C16—H16C	0.9600	C16A—H16F	0.9600
C17—H17A	0.9600	C17A—H17D	0.9600
C17—H17B	0.9600	C17A—H17E	0.9600
C17—H17C	0.9600	C17A—H17F	0.9600
C1—O1—H1A	111 (3)	C1A—O1A—H1B	110 (3)
C15—O3—C16	118.8 (2)	C15A—O3A—C16A	117.1 (2)

C13—O4—C17	117.5 (2)	C13A—O4A—C17A	117.5 (2)
O1—C1—C6	124.3 (3)	O1A—C1A—C6A	122.7 (2)
O1—C1—C2	116.1 (3)	O1A—C1A—C2A	117.2 (2)
C6—C1—C2	119.6 (3)	C6A—C1A—C2A	120.1 (2)
C3—C2—C1	119.6 (3)	C3A—C2A—C1A	120.1 (3)
C3—C2—H2A	123.0 (18)	C3A—C2A—H2B	120.1 (19)
C1—C2—H2A	117.3 (18)	C1A—C2A—H2B	119.8 (19)
C2—C3—C4	121.1 (3)	C2A—C3A—C4A	120.7 (2)
C2—C3—H3A	120.4 (18)	C2A—C3A—H3B	117.1 (18)
C4—C3—H3A	118.5 (18)	C4A—C3A—H3B	122.2 (18)
C5—C4—C3	118.4 (3)	C3A—C4A—C5A	118.6 (2)
C5—C4—C7	123.2 (3)	C3A—C4A—C7A	119.0 (2)
C3—C4—C7	118.4 (2)	C5A—C4A—C7A	122.4 (2)
C6—C5—C4	120.1 (3)	C6A—C5A—C4A	121.0 (3)
C6—C5—H5A	119.3 (18)	C6A—C5A—H5B	119.6 (16)
C4—C5—H5A	120.6 (18)	C4A—C5A—H5B	119.1 (16)
C1—C6—C5	121.2 (3)	C5A—C6A—C1A	119.6 (2)
C1—C6—H6A	120 (2)	C5A—C6A—H6B	121.3 (16)
C5—C6—H6A	119 (2)	C1A—C6A—H6B	119.1 (16)
O2—C7—C4	120.4 (3)	O2A—C7A—C4A	119.6 (2)
O2—C7—C8	119.4 (3)	O2A—C7A—C8A	120.8 (2)
C4—C7—C8	120.2 (3)	C4A—C7A—C8A	119.6 (2)
C9—C8—C7	108.2 (3)	C7A—C8A—C9A	113.0 (2)
C9—C8—H8A	110.1	C7A—C8A—H8C	109.0
C7—C8—H8A	110.1	C9A—C8A—H8C	109.0
C9—C8—H8B	110.1	C7A—C8A—H8D	109.0
C7—C8—H8B	110.1	C9A—C8A—H8D	109.0
H8A—C8—H8B	108.4	H8C—C8A—H8D	107.8
C8—C9—C10	109.1 (3)	C10A—C9A—C8A	114.8 (2)
C8—C9—H9A	109.9	C10A—C9A—H9C	108.6
C10—C9—H9A	109.9	C8A—C9A—H9C	108.6
C8—C9—H9B	109.9	C10A—C9A—H9D	108.6
C10—C9—H9B	109.9	C8A—C9A—H9D	108.6
H9A—C9—H9B	108.3	H9C—C9A—H9D	107.5
C11—C10—C15	117.1 (3)	C11A—C10A—C15A	116.9 (2)
C11—C10—C9	122.3 (3)	C11A—C10A—C9A	121.4 (2)
C15—C10—C9	120.6 (3)	C15A—C10A—C9A	121.7 (3)
C10—C11—C12	122.8 (3)	C10A—C11A—C12A	123.1 (3)
C10—C11—H11A	119 (2)	C10A—C11A—H11B	118.2 (18)
C12—C11—H11A	118 (2)	C12A—C11A—H11B	118.7 (18)
C13—C12—C11	117.9 (3)	C13A—C12A—C11A	118.4 (3)
C13—C12—H12A	124.9 (19)	C13A—C12A—H12B	121.4 (18)
C11—C12—H12A	117.1 (19)	C11A—C12A—H12B	120.1 (18)
O4—C13—C14	115.2 (2)	O4A—C13A—C12A	124.7 (3)
O4—C13—C12	124.2 (2)	O4A—C13A—C14A	114.4 (3)
C14—C13—C12	120.6 (3)	C12A—C13A—C14A	120.9 (3)
C15—C14—C13	119.9 (3)	C13A—C14A—C15A	119.6 (3)
C15—C14—H14A	123.2 (19)	C13A—C14A—H14B	120.8 (17)
C13—C14—H14A	116.8 (19)	C15A—C14A—H14B	119.6 (17)

O3—C15—C14	123.8 (2)	O3A—C15A—C14A	123.5 (2)
O3—C15—C10	114.8 (3)	O3A—C15A—C10A	115.4 (2)
C14—C15—C10	121.3 (3)	C14A—C15A—C10A	121.1 (3)
O3—C16—H16A	109.5	O3A—C16A—H16D	109.5
O3—C16—H16B	109.5	O3A—C16A—H16E	109.5
H16A—C16—H16B	109.5	H16D—C16A—H16E	109.5
O3—C16—H16C	109.5	O3A—C16A—H16F	109.5
H16A—C16—H16C	109.5	H16D—C16A—H16F	109.5
H16B—C16—H16C	109.5	H16E—C16A—H16F	109.5
O4—C17—H17A	109.5	O4A—C17A—H17D	109.5
O4—C17—H17B	109.5	O4A—C17A—H17E	109.5
H17A—C17—H17B	109.5	H17D—C17A—H17E	109.5
O4—C17—H17C	109.5	O4A—C17A—H17F	109.5
H17A—C17—H17C	109.5	H17D—C17A—H17F	109.5
H17B—C17—H17C	109.5	H17E—C17A—H17F	109.5
O1—C1—C2—C3	−177.8 (3)	O1A—C1A—C2A—C3A	179.3 (3)
C6—C1—C2—C3	2.5 (5)	C6A—C1A—C2A—C3A	−0.7 (5)
C1—C2—C3—C4	−3.2 (5)	C1A—C2A—C3A—C4A	1.3 (5)
C2—C3—C4—C5	1.5 (5)	C2A—C3A—C4A—C5A	−0.5 (4)
C2—C3—C4—C7	−177.2 (3)	C2A—C3A—C4A—C7A	−179.8 (3)
C3—C4—C5—C6	1.1 (5)	C3A—C4A—C5A—C6A	−0.9 (4)
C7—C4—C5—C6	179.6 (3)	C7A—C4A—C5A—C6A	178.4 (3)
O1—C1—C6—C5	−179.6 (3)	C4A—C5A—C6A—C1A	1.5 (4)
C2—C1—C6—C5	0.0 (5)	O1A—C1A—C6A—C5A	179.3 (3)
C4—C5—C6—C1	−1.8 (6)	C2A—C1A—C6A—C5A	−0.7 (4)
C5—C4—C7—O2	175.7 (4)	C3A—C4A—C7A—O2A	5.3 (4)
C3—C4—C7—O2	−5.7 (5)	C5A—C4A—C7A—O2A	−174.0 (3)
C5—C4—C7—C8	−5.0 (5)	C3A—C4A—C7A—C8A	−172.6 (3)
C3—C4—C7—C8	173.6 (3)	C5A—C4A—C7A—C8A	8.1 (4)
O2—C7—C8—C9	−96.8 (4)	O2A—C7A—C8A—C9A	1.4 (4)
C4—C7—C8—C9	83.8 (4)	C4A—C7A—C8A—C9A	179.3 (2)
C7—C8—C9—C10	−177.9 (3)	C7A—C8A—C9A—C10A	−168.6 (2)
C8—C9—C10—C11	−102.6 (4)	C8A—C9A—C10A—C11A	105.0 (3)
C8—C9—C10—C15	77.7 (4)	C8A—C9A—C10A—C15A	−74.2 (3)
C15—C10—C11—C12	4.8 (6)	C15A—C10A—C11A—C12A	−1.2 (4)
C9—C10—C11—C12	−174.9 (3)	C9A—C10A—C11A—C12A	179.6 (2)
C10—C11—C12—C13	−0.4 (6)	C10A—C11A—C12A—C13A	0.4 (4)
C17—O4—C13—C14	178.5 (3)	C17A—O4A—C13A—C12A	1.2 (4)
C17—O4—C13—C12	−0.9 (5)	C17A—O4A—C13A—C14A	−179.1 (3)
C11—C12—C13—O4	176.3 (3)	C11A—C12A—C13A—O4A	−179.6 (2)
C11—C12—C13—C14	−3.1 (5)	C11A—C12A—C13A—C14A	0.7 (4)
O4—C13—C14—C15	−177.4 (3)	O4A—C13A—C14A—C15A	179.3 (2)
C12—C13—C14—C15	2.0 (5)	C12A—C13A—C14A—C15A	−0.9 (4)
C16—O3—C15—C14	1.0 (5)	C16A—O3A—C15A—C14A	−8.8 (3)
C16—O3—C15—C10	179.2 (3)	C16A—O3A—C15A—C10A	172.3 (2)
C13—C14—C15—O3	−179.4 (3)	C13A—C14A—C15A—O3A	−178.8 (2)
C13—C14—C15—C10	2.6 (5)	C13A—C14A—C15A—C10A	0.0 (4)
C11—C10—C15—O3	175.9 (3)	C11A—C10A—C15A—O3A	180.0 (2)
C9—C10—C15—O3	−4.4 (5)	C9A—C10A—C15A—O3A	−0.8 (3)

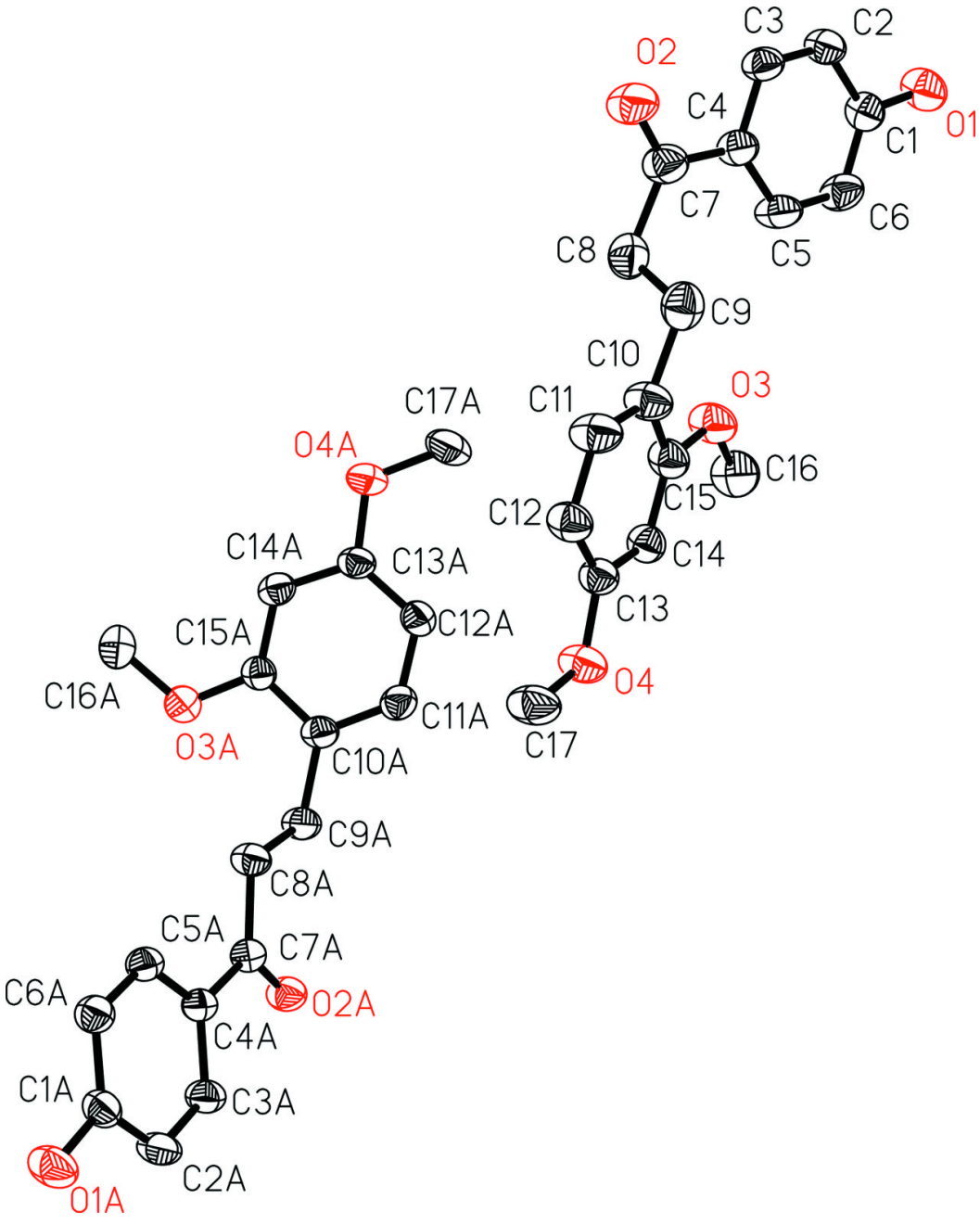
C11—C10—C15—C14	−5.9 (5)	C11A—C10A—C15A—C14A	1.0 (3)
C9—C10—C15—C14	173.8 (3)	C9A—C10A—C15A—C14A	−179.8 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1A···O2A^{i}	0.82 (4)	1.96 (4)	2.733 (3)	155 (5)
O1A—H1B···O2^{ii}	0.79 (4)	1.96 (4)	2.732 (3)	166 (5)
C5—H5A···O3	1.03 (3)	2.60 (4)	3.609 (4)	168 (3)
C8—H8B···O3	0.97	2.57	3.120 (4)	116
C8—H8A···O2A^{iii}	0.97	2.59	3.255 (4)	126
C5A—H5B···O4A^{iv}	0.96 (4)	2.46 (3)	3.322 (3)	150
C17A—H17D···O1^{v}	0.96	2.57	3.317 (5)	135

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

Fig. 1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C10A
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Fig. 2

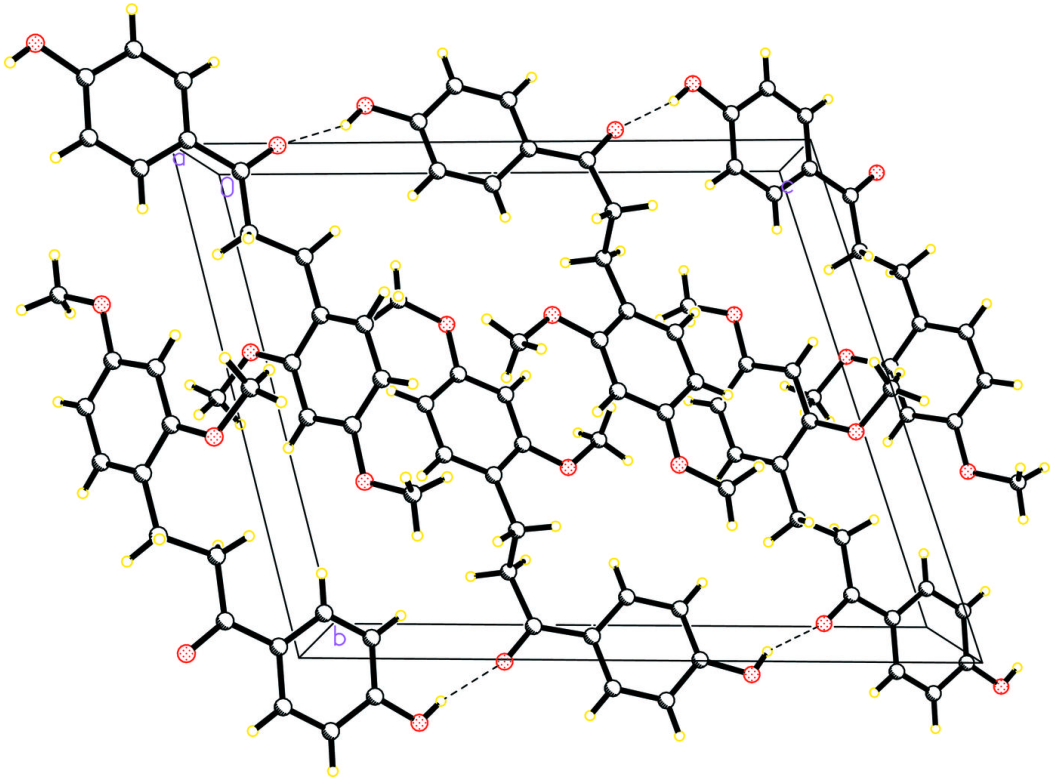

Fig. 3