Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(*E*)-1-[4-(Hexyloxy)phenyl]-3-(3-hydroxyphenyl)prop-2-en-1-one

Zainab Ngaini,[a] Siti Muhaini Haris Fadzillah,[a] Hasnain Hussain,[b] Ibrahim Abdul Razak[c]*‡ and Hoong-Kun Fun[c]§

[a]Department of Chemistry, Faculty of Resource Science and Technology, Universiti Malaysia Sarawak, 94300 Kota Samarahan, Sarawak, Malaysia, [b]Department of Molecular Biology, Faculty of Resource Science and Technology, Universiti Malaysia Sarawak, 94300 Kota Samarahan, Sarawak, Malaysia, and [c]X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia
Correspondence e-mail: arazaki@usm.my

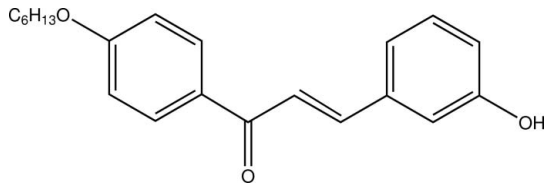
Received 16 November 2010; accepted 17 November 2010

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.060; wR factor = 0.188; data-to-parameter ratio = 22.7.

There are two molecules in the asymmetric unit of the title compound, $C_{21}H_{24}O_3$, in which the dihedral angles between the aromatic rings are 6.4 (1) and 7.0 (1)°. The enone moiety of both molecules adopts an *s–cis* configuration. In the crystal, intermolecular O—H···O and C—H···O interactions to the same acceptor O atom generate $R_2^1(6)$ ring motifs and further C—H···O interactions generate $R_2^2(8)$ ring motifs. Topologically, the $R_2^1(6)$ and $R_2^2(8)$ ring motifs are arranged alternately, forming [001] chains of molecules. The crystal structure is further stabilized by C—H···π interactions.

Related literature

For general background to the biological properties of chalcone derivatives, see: Bhat *et al.* (2005); Xue *et al.* (2004); Satyanarayana *et al.* (2004); Zhao *et al.* (2005); Yayli *et al.* (2006). For related structures, see: Razak, Fun, Ngaini, Rahman *et al.* (2009); Razak, Fun, Ngaini, Fadzillah *et al.* (2009*a*,*b*); Ngaini, Fadzillah *et al.* (2009); Ngaini, Rahman *et al.* (2009); Razak *et al.* (2009*a*,*b*). For hydrogen-bond motifs, see: Bernstein *et al.* (1995). For the stability of the temperature controller used in the data collection, see: Cosier & Glazer (1986). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{21}H_{24}O_3$
M_r = 324.40
Triclinic, $P\overline{1}$
a = 7.6053 (3) Å
b = 13.7328 (5) Å
c = 17.3769 (7) Å
α = 105.226 (2)°
β = 93.740 (2)°
γ = 93.038 (2)°
V = 1742.80 (12) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 100 K
0.77 × 0.44 × 0.12 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.940, T_{max} = 0.990
36519 measured reflections
10044 independent reflections
6371 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.188
S = 1.04
10044 reflections
443 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.66 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

*Cg*1 and *Cg*3 are the centroids of the C1*A*–C6*A* and C1*B*–C6*B* rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
O1*B*—H1*OB*···O2*A*^{i}	0.86 (3)	1.92 (3)	2.773 (2)	171 (2)
C1*B*—H1*BA*···O2*A*^{i}	0.93	2.50	3.196 (2)	132
O1*A*—H1*OA*···O2*B*^{ii}	0.92 (3)	1.85 (3)	2.763 (2)	175 (3)
C1*A*—H1*AA*···O2*B*^{ii}	0.93	2.50	3.214 (2)	133
C12*B*—H12*B*···O3*A*^{iii}	0.93	2.56	3.483 (2)	175
C12*A*—H12*A*···O3*B*^{iv}	0.93	2.56	3.487 (2)	174
C16*A*—H16*A*···*Cg*1^{v}	0.97	2.80	3.653 (2)	147
C16*B*—H16*C*···*Cg*3^{vi}	0.97	2.73	3.595 (2)	149
C17*B*—H17*C*···*Cg*3^{vii}	0.97	2.74	3.640 (2)	154

Symmetry codes: (i) $x+1, y+1, z-1$; (ii) $x-1, y-1, z+1$; (iii) $x, y+1, z$; (iv) $x, y-1, z$; (v) $-x+1, -y, -z+1$; (vi) $-x+2, -y+2, -z$; (vii) $-x+1, -y+2, -z$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

HKF and IAR thank the Malaysian Government and Universiti Sains Malaysia (USM) for the Research University grant No. 1001/PFIZIK/811151. ZN and HH thank Universiti Malaysia Sarawak (UMS) for the Geran Penyelidikan Dana Khas Inovasi, grant No. DI/01/2007 (01) and Fundamental Research grant No: FRGS/01(03)/608/2006(41). SMHF thanks the Malaysian Government and UMS for providing a scholarship for postgraduate studies.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5741).

‡ Thomson Reuters ResearcherID: A-5599-2009.
§ Additional correspondence, e-mail: hkfun@usm.my. Thomson Reuters ResearcherID: A-3561-2009.