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Ethyl (*E*)-4-(2-hydroxy-1-naphthyl)-2-methyl-2-butenoate

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The structure determination of the title compound, $C_{17}H_{18}O_3$, shows an *E* conformation about the C═C bond. Molecules associate *via* O—H···O interactions leading to the formation of chains.

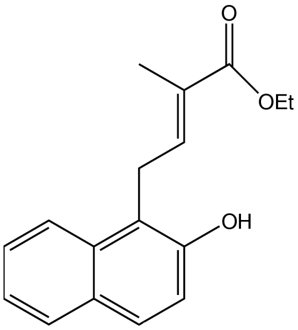
Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.002 Å
R factor = 0.037
wR factor = 0.135
Data-to-parameter ratio = 18.2

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

The title compound, (I), was one of the isomers prepared from the reaction between the ylide Ph_3P═C(Me)C(O)OEt and 2-(2-naphthyl)acetaldehyde (Haselgrove *et al.*, 1999). The structure analysis shows (I) to be the uncyclized (E)-butenoate (Fig. 1). The side chain, while not coplanar with the aromatic portion of the molecule, is effectively planar as seen in the sequence of torsion angles of −178.6 (1), 0.8 (1), 179.97 (8) and 179.10 (8)° for C4—C3—C2—C1, C3—C2—C1—O12, C2—C1—O12—C13 and C1—O12—C13—C14, respectively. The only two torsion angles in the molecule with 'non-trivial' values are those describing the overall conformation of the ethylbutenoate group relative to the naphthalene moiety, namely C2′—C1′—C4—C3 and C1′—C4—C3—C2, which are 94.6 (1) and 130.4 (1)°, respectively.



(I)

The major intermolecular interaction in the lattice occurs between the O—H2′ and translationally related carbonyl O11 atoms, such that O—H2′ is 0.92 Å, H2′···O11^{i} is 1.84 Å, O2′···O11^{i} is 2.751 (2) Å and the angle at H2′ is 174°; symmetry code: (i) $1 + x, y, z$. This association leads to the formation of chains along the *a* axis.

Experimental

The title compound was prepared according to the literature procedure of Haselgrove *et al.* (1999). Crystals were obtained from the slow

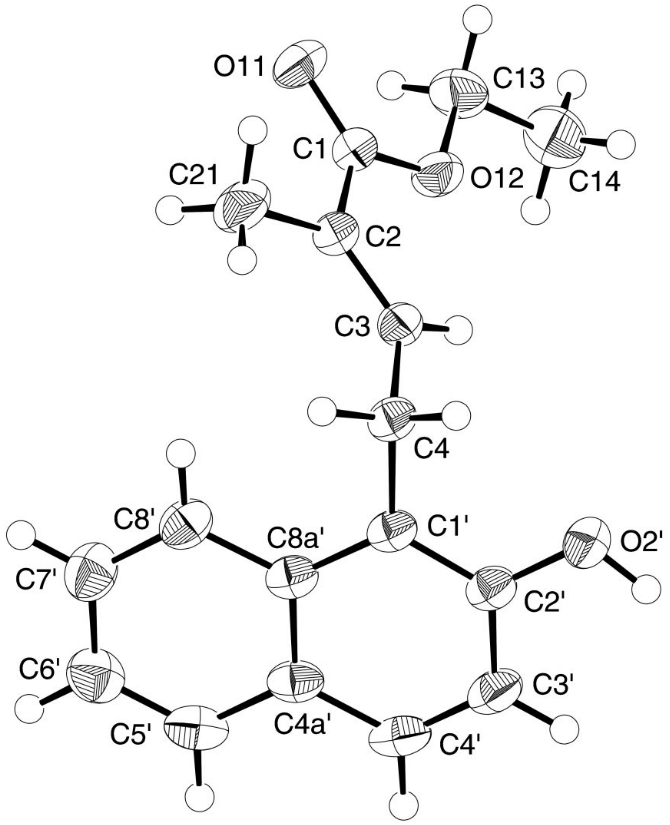


Figure 1
The molecular structure and crystallographic numbering scheme for (I). Displacement ellipsoids are shown at the 50% probability level (Johnson, 1976).

evaporation of a dichloromethane solution of the compound (m.p. 369–370 K).

Crystal data

$C_{17}H_{18}O_3$
$M_r = 270.33$
Monoclinic, $P2_1/n$
$a = 9.273$ (2) Å
$b = 4.877$ (2) Å
$c = 31.976$ (5) Å
$\beta = 92.76$ (2)°
$V = 1444.5$ (7) Å^3
$Z = 4$

$D_x = 1.243$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 12.2$–14.9°
$\mu = 0.08$ mm^{-1}
$T = 173$ K
Block, pale yellow
0.40 × 0.31 × 0.16 mm

Data collection

Rigaku AFC-7*R* diffractometer
ω scans
3930 measured reflections
3318 independent reflections
2254 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.041$
$\theta_{\rm max} = 27.5°$

$h = 0 \rightarrow 12$
$k = 0 \rightarrow 6$
$l = -41 \rightarrow 41$
3 standard reflections
every 400 reflections
intensity decay: 0.3%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.135$
$S = 0.82$
3318 reflections
182 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0918P)^2 + 0.5393P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.21$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.17$ e Å^{-3}

The C-bound H atoms were placed in their geometrically calculated positions and included in the final refinement in the riding model approximation with an overall displacement parameter. The O—H atom was located from a difference map but was not refined.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1996); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1997); program(s) used to solve structure: *SIR*97 (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); software used to prepare material for publication: *SHELXL*97.

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