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Methyl 2-(2-carboxy-3-hydroxy-5-methylphenoxy)-5-hydroxy-3-methoxybenzoate

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Key indicators

Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.004 Å
R factor = 0.063
wR factor = 0.172
Data-to-parameter ratio = 11.8

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

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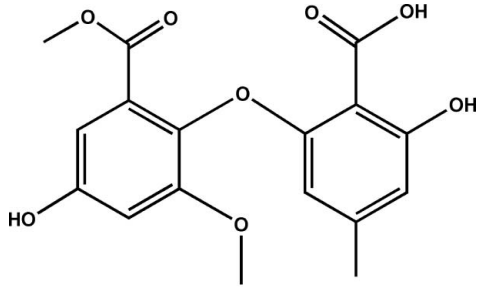
In the title compound, $C_{17}H_{16}O_8$, intermolecular O—H···O hydrogen bonds link adjacent molecules to form a chain. There are also intramolecular hydrogen bonds which stabilize the molecular conformation.

Comment

5,6′-Dihydroxy-3-methoxy-4′-methyl-2,2′-oxydibenzoic acid 1-methyl ester, was isolated from phoma *sp*., a soil fungus that was found in the Shaxi River, in Fujian Province, China. It was found that the compound shows inhibitory activity to ETA receptors (Pairet *et al.*, 1995; Ogawa *et al.*, 1995), and no cytotoxicity to KB and Raji cancer cell lines. The crystal structure shows that adjacent molecules are linked by a short hydrogen bond involving the carboxylic acid group and the hydroxy group (Table 1). There are also intramolecular hydrogen bonds (Table 1) which stabilize the molecular conformation. The dihedral angle between the two benzene rings is 79.10 (8)°. Bond lengths and angles in the title compound, (I), are in agreement with the values reported for related compounds (Hargreaves *et al.*, 2002).



(I)

Experimental

The title compound was isolated from phoma *sp*., which was found in the Shaxi River, in Fujian Province, China. Crystals were grown from a solution in ethyl acetate. The molecular formula of (I) was deduced from the high-resolution FT–ICR mass spectrum as $C_{17}H_{16}O_8$, showing an accurate mass at m/z 347.0765 $[M - H]^-$.

Crystal data

$C_{17}H_{16}O_8$
M_r = 348.30
Monoclinic, $P2_1/c$
a = 4.9176 (15) Å
b = 18.048 (5) Å
c = 17.532 (5) Å
β = 93.004 (6)°
V = 1553.8 (8) Å^3
Z = 4
D_x = 1.489 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 273 (2) K
Chunk, colourless
0.31 × 0.28 × 0.18 mm

Data collection

Bruker APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.964, T_{max} = 0.979
7510 measured reflections
2731 independent reflections
2220 reflections with $I > 2\sigma(I)$
R_{int} = 0.052
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.172
S = 1.07
2731 reflections
232 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0674P)^2 + 0.9562P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.008
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4···O7^{i}	0.82	2.09	2.882 (3)	161
O6—H6···O5	0.82	1.90	2.607 (3)	144
O8—H8···O7	0.82	1.84	2.560 (3)	146

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

All H atoms were placed in geometrically idealized positions and treated as riding on their parent atoms, with C—H = 0.93 (aromatic) and 0.96 Å (CH_3), O—H = 0.82 Å, and U_{iso}(H) = 1.2U_{eq} (aromatic) or 1.5U_{eq} (methyl C,O).

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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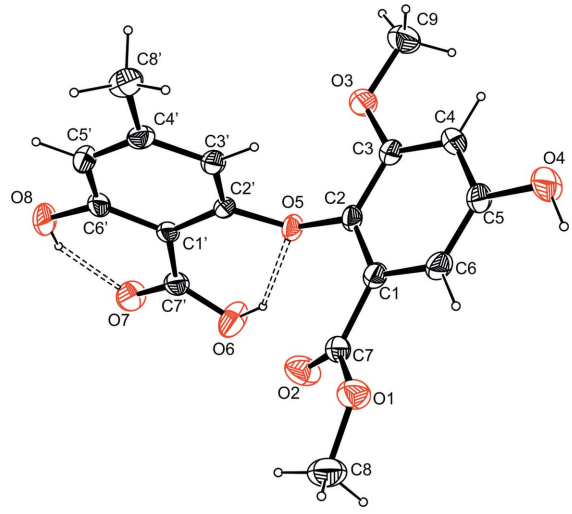

Figure 1
The molecular structure of $C_{16}H_{17}O_8$ with the atom labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radius. Hydrogen bonds are shown as dashed lines.

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