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1-(3,4-Dimethoxyphenyl)-4-(3,4,5-trimethoxyphenyl)perhydrofuro[3,4-*c*]furan

Li Zhang, Yang Lu* and Qi-Tai Zheng

Institute of Materia Medica, Chinese Academy of Medical Sciences and Peking Union Medical College, 1 Xiannong tan Street, Beijing 100050, People's Republic of China

Correspondence e-mail: luy@imm.ac.cn

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The title compound, $C_{23}H_{28}O_7$, is a furofuran derivative. In this structure, both furan rings adopt envelope conformations, and both benzene rings are planar.

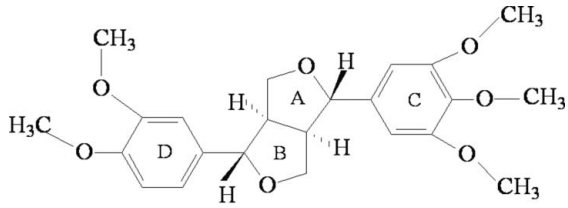
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.004 Å
R factor = 0.052
wR factor = 0.154
Data-to-parameter ratio = 9.7

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

Comment

The title compound, (I), which is also known as magnolin, was extracted from *Flos magnoliae* with ethyl acetate (Fang *et al.*, 2002) and recrystallized from ethanol. As a result of interest in the anti-inflammatory and anti-allergenic effects of (I) (Li *et al.*, 2002), we report its crystal stucture here (Fig. 1 and Table 1).



(I)

Bond lengths and angles within the molecule are normal (Allen *et al.*, 1987) and both furan rings (*A* and *B*) adopt envelope conformations. The flap atom of ring *A* is O1, at a distance of 0.503 (6) Å; the flap atom of ring *B* is O2, at a distance of 0.591 (6) Å. The dihedral angle between the planes through the four atoms of rings *A* and *B* is 119.6 (1)°. The torsion angle linking rings *A* and *C* is O1—C1—C7—C8 is 7.3 (4)°, and the torsion angle between rings *B* and *D* is C5—C4—C16—C17 of −96.4 (3)°.

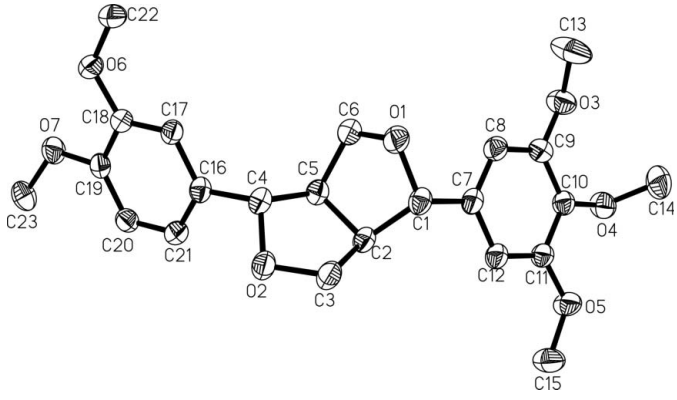


Figure 1
A view of the molecular structure of magnolin, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted.

Experimental

The title compound was prepared according to the procedure for extracting *Flos magnoliae* (Fang *et al.*, 2002). Crystals suitable for data collection were obtained by slow evaporation of an ethanol solution at 283 K over a period of two weeks.

Crystal data

$C_{23}H_{28}O_7$
M_r = 416.45
Orthorhombic, $P2_12_12_1$
a = 8.2890 (17) Å
b = 8.3880 (17) Å
c = 30.875 (6) Å
V = 2146.7 (7) Å^3
Z = 4
D_x = 1.289 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 295 (2) K
Needle, colourless
0.60 × 0.15 × 0.15 mm

Data collection

MAC DIP 2030K diffractometer
ω scans
Absorption correction: none
6431 measured reflections
2648 independent reflections
2560 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 27.3°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.154
S = 1.16
2648 reflections
272 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0795P)^2 + 0.5714P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997)
Extinction coefficient: 0.035 (4)

Table 1
Selected torsion angles (°).

O1—C1—C2—C3	−92.8 (3)	C13—O3—C9—C8	41.0 (6)
C4—C5—C6—O1	88.4 (3)	C5—C4—C16—C17	−96.4 (3)
O1—C1—C7—C8	7.3 (4)	C22—O6—C18—C17	1.5 (5)

In the absence of significant anomalous dispersion effects, Friedel pairs were merged and the absolute configuration was assigned arbitrarily. The methyl H atoms were constrained to an ideal geometry, with C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C). All other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.92–0.98 Å and U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *DENZO* (Otwinowski & Minor, 1997); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); 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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