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9-(3,4-Dimethoxyphenyl)-4-*p*-tolyl-4,5,6,7-tetrahydrofuro[3,4-*b*]quinoline-1,8(3*H*,9*H*)-dione

Shu-Jiang Tu,* Yan Zhang and Run-Hong Jia

Department of Chemistry, Xuzhou Normal University, Xuzhou 221116, People's Republic of China

Correspondence e-mail: laotu2001@263.net

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Key indicators

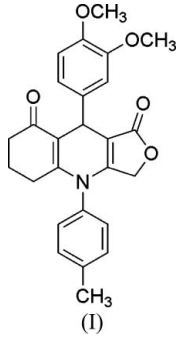
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.060
wR factor = 0.153
Data-to-parameter ratio = 12.9

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

The title compound, $C_{26}H_{25}NO_5$, was synthesized by the reaction of 3,4-dimethoxybenzaldehyde, 3-(*p*-tolylamino)-cyclohex-2-enone and tetronic acid in glacial acetic acid under microwave irradiation. Its molecular structure shows a planar furan ring, a dihydropyridine ring in a flattened envelope conformation and a cyclohexenone ring in an envelope conformation.

Comment

Tetronic acid derivatives and their metabolites are widespread in nature, of which vitamin C and penicillic acid are undoubtedly the most important (Neelakantan & Seshadri, 1959). Natural 4-ylidenetetronic acid derivatives known as pulvinic acids have been found as pigments in lichens and higher fungi (Weinstock *et al.*, 1979). Tetronic acid derivatives are interesting because of their antibiotic, antitumor, anti-coagulant, anti-epileptic, antifungal, and anti-inflammatory properties (Foden & McCormick, 1975). We report here the crystal structure of the title compound, (I).



(I)

The dihydropyridine ring adopts a flattened envelope conformation, with atom C5 deviating from the C1/C4/C6/C11/N1 plane by 0.174 (3) Å. The cyclohexenone ring adopts an envelope conformation (Fig. 1), with atom C9 deviating from the C6/C7/C8/C10/C11 plane by 0.648 (6) Å. The dihedral angles between the C1/C4/C6/C11/N1 plane and the C12–C24 and C19–C24 benzene ring planes are 74.1 (2) and 85.0 (1)°, respectively. The cyclohexenone and the furanone rings make dihedral angles of 6.4 (2) and 4.7 (2)°, respectively, with the central C1/C4/C6/C11/N1 plane.

Experimental

Compound (I) was prepared by the reaction of 3,4-dimethoxybenzaldehyde (1 mmol), 3-(*p*-tolylamino)cyclohex-2-enone (1 mmol) and tetronic acid (1 mmol) in glacial acetic acid (2 ml) under microwave irradiation. Single crystals of (I) suitable for X-ray

diffraction were obtained by slow evaporation of a 95% aqueous ethanol solution (yield 93%; m.p. 499 K).

Crystal data

$C_{26}H_{25}NO_5$	V = 1085 (2) Å^3
M_r = 431.47	Z = 2
Triclinic, $P\overline{1}$	D_x = 1.320 Mg m^{-3}
a = 8.427 (9) Å	Mo $K\alpha$ radiation
b = 11.453 (12) Å	μ = 0.09 mm^{-1}
c = 11.579 (12) Å	T = 298 (2) K
α = 95.909 (14)°	Block, yellow
β = 100.870 (13)°	0.22 × 0.18 × 0.09 mm
γ = 94.902 (15)°	

Data collection

Bruker SMART CCD 1000 area-detector diffractometer	5706 measured reflections
φ and ω scans	3767 independent reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	1874 reflections with $I > 2\sigma(I)$
T_{min} = 0.980, T_{max} = 0.992	R_{int} = 0.031
	θ_{max} = 25.0°

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.060	$w = 1/[\sigma^2(F_o^2) + (0.0634P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.153	$(\Delta/\sigma)_{max} < 0.001$
S = 0.99	$\Delta\rho_{max}$ = 0.20 e Å^{-3}
3767 reflections	$\Delta\rho_{min}$ = −0.19 e Å^{-3}
292 parameters	

H atoms were positioned geometrically and refined as riding, with C—H = 0.93–0.98 Å and U_{iso}(H) = 1.5U_{eq}(methyl C) or 1.2U_{eq}(C,N).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

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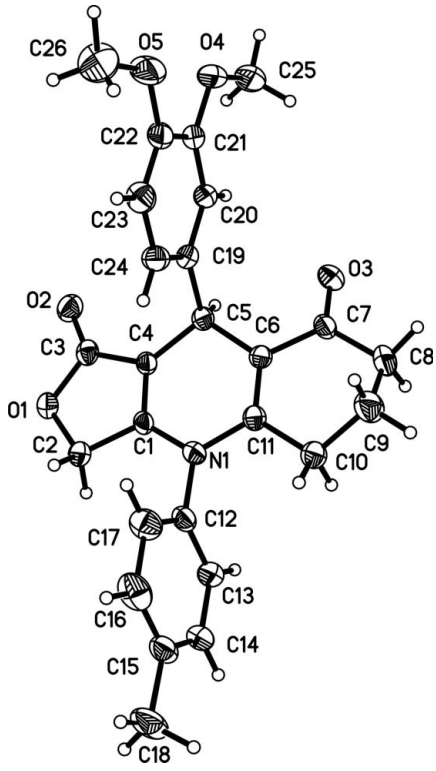

Figure 1
The structure of (I), showing 30% probability displacement ellipsoids.

References

Bruker (1998). *SMART*. Version 5.0/NT. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (1999). *SAINT* (Version 6.01) and *SHELXTL* (Version 6.01/NT). Bruker AXS Inc., Madison, Wisconsin, USA.
Foden, F. R. & McCormick, J. (1975). *J. Med. Chem.* **18**, 199–203.
Neelakantan, S. & Seshadri, T. R. (1959). *Curr. Sci.* **28**, 476–480.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Weinstock, J., Blank, J. E., Oh, H. J. & Sutton, B. M. (1979). *J. Org. Chem.* **44**, 673–676.