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1-Benzamido-2-(2-furyl)-3-phenylcyclopropanecarboxylic acid

Wan-Yun Huang, Gui-Fa Su,* Cheng-Xue Pan and Jiang-Ke Qin

College of Chemistry and Chemical Engineering, Guangxi Normal University, Guilin 541004, People's Republic of China

Correspondence e-mail: edward_su75@163.com

Key indicators

Single-crystal X-ray study
T = 284 K
Mean σ(C–C) = 0.003 Å
R factor = 0.047
wR factor = 0.085
Data-to-parameter ratio = 15.2

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

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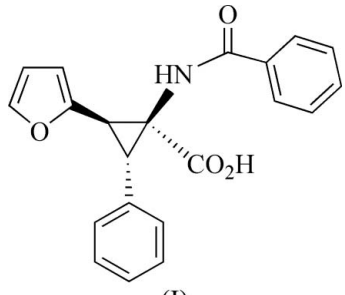
The molecule of the title compound, $C_{21}H_{17}NO_4$, exhibits a *trans* arrangement of the furyl and phenyl substituents on the cyclopropane ring. The crystal structure is stabilized by intermolecular O—H···O hydrogen-bond interactions.

Comment

1-Aminocyclopropanecarboxylic acid and its derivatives (Accs) possess a broad spectrum of biological activities (Park & Kurth, 2002); they have been extensively used as mechanistic probes and enzyme inhibitors as well as in the design and synthesis of conformationally constrained peptidomimetics (Jiménez *et al.*, 2005; Peggion *et al.*, 2003; Casanovas *et al.*, 2003).



(I)

The title compound, (I), is an Acc with a special class of conformationally constrained side-chain residues. Its structure (Fig. 1) is similar to that observed in some diaryl-substituted Accs, which are characterized by a *trans* arrangement of the two substituents on the three-membered ring (Jiménez *et al.*, 2001; Su *et al.*, 2003; Pan *et al.*, 2005). With respect to the cyclopropane ring, the furanyl ring, the phenyl ring and the benzoylamino group form dihedral angles of 65.41 (9), 70.30 (9) and 44.63 (10)°, respectively. The crystal packing is stabilized by O—H···O hydrogen bonds (Table 1).

Experimental

To a 50 ml flask containing 1-benzoylamino-2-furan-2-yl-3-phenylcyclopropanecarboxylic acid methyl ester (Su *et al.*, 2003) (0.90 g, 2.48 mmol) was added a solution of potassium hydroxide (0.06 mol) in anhydrous methanol (30 ml). The reaction mixture was refluxed until completion of the reaction, as monitored by TLC. The solution was then adjusted to pH 3 with a solution of 5% potassium hydrogen sulfate, and filtered after 6 h to obtain a white solid. Colourless crystals suitable for X-ray analysis (0.53 g, 61% yield) were obtained by slow evaporation of a dichloromethane–ethyl acetate (3:1 *v*/*v*) solution.

Crystal data

$C_{21}H_{17}NO_4$
M_r = 347.36
Monoclinic, $P2_1/n$
a = 9.134 (2) Å
b = 10.641 (3) Å
c = 17.696 (5) Å
β = 98.04 (2)°
V = 1703.1 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 284 (2) K
0.58 × 0.46 × 0.18 mm

Data collection

Siemens $P4$ diffractometer
Absorption correction: none
4308 measured reflections
3716 independent reflections
1987 reflections with $I > 2\sigma(I)$
R_{int} = 0.017
3 standard reflections
every 97 reflections
intensity decay: 0.3%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.085
S = 0.99
3716 reflections
244 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3O···O2^{i}	1.00 (2)	1.72 (2)	2.715 (2)	173 (2)

Symmetry code: (i) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$.

The H atoms attached to the N and O atoms were located in a difference Fourier map and refined freely. All other H atoms were positioned geometrically and included in the refinement in the riding-model approximation, with C—H = 0.93–0.98 Å and with U_{iso}(H) = 1.2U_{eq}(C). Refined N—H distance = 0.866 (19) Å.

Data collection: *XSCANS* (Siemens, 1994); cell refinement: *XSCANS*; data reduction: *SHELXTL* (Siemens, 1994); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

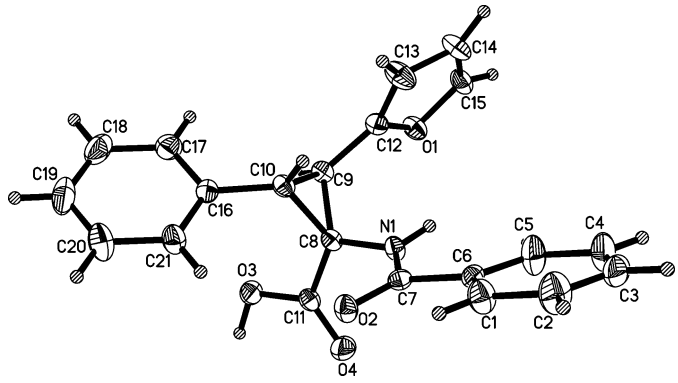


Figure 1
The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as spheres of arbitrary radius.

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