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4-[4-(Benzhydryloxy)piperidin-1-yl]-1-(4-*tert*-butylphenyl)butan-1-one

Jing Cheng,* Zhongzhen Zhou and Guangfu Yang

Key Laboratory of Pesticides & Chemical Biology, Ministry of Education, College of Chemistry, Central China Normal University, Wuhan 430079, People's Republic of China

Correspondence e-mail: mdchengjing@126.com

Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.005 Å
R factor = 0.058
wR factor = 0.139
Data-to-parameter ratio = 15.4

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

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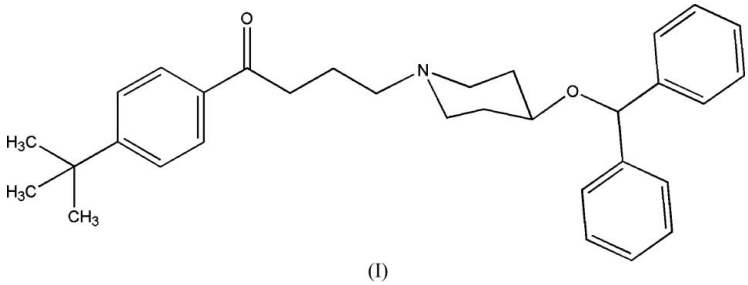
In the title compound, $C_{32}H_{39}NO_2$, the piperidine ring has a chair conformation. C—H···O and C—H···N intermolecular interactions are present, as well as intramolecular C—H···O interactions.

Comment

The title compound, (I), is an orally active and selective H1-receptor antagonist. To our knowledge, its crystal structure has not been reported. In this paper, we present the X-ray crystallographic analysis of (I).



(I)

As shown in Fig. 1, the piperidine ring is in a chair conformation. It is bound to the two phenyl rings *via* an O bridge. Fig. 2 shows the packing arrangement, in which molecules are linked by intermolecular C—H···N and C—H···O interactions. An intramolecular C—H···O interaction is observed in the crystal structure (see Table 2 for details). No π–π stacking interactions in the crystal structure.

Experimental

The title compound was synthesized according to Soto *et al.* (1985). Crystals suitable for data collection were obtained by slow evaporation of an ethanol solution at room temperature.

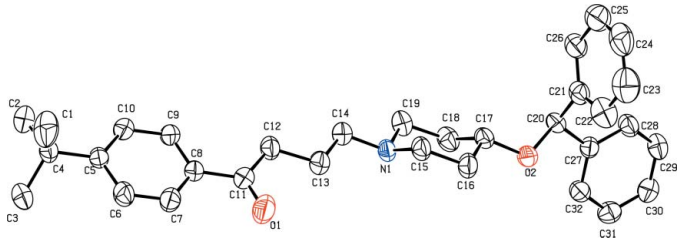


Figure 1
View of the molecule of (I), showing the atom-labelling scheme, with displacement ellipsoids drawn at the 50% probability level. H atoms are represented by circles of arbitrary size.

Crystal data

$C_{32}H_{39}NO_2$
M_r = 469.64
Monoclinic, $P2_1/c$
a = 16.611 (2) Å
b = 10.9820 (13) Å
c = 16.728 (2) Å
β = 113.542 (2)°
V = 2797.5 (6) Å^3
Z = 4
D_x = 1.115 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 973 reflections
θ = 2.3–19.9°
μ = 0.07 mm^{-1}
T = 292 (2) K
Plate, colourless
0.24 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: none
14531 measured reflections
4916 independent reflections
1820 reflections with $I > 2\sigma(I)$
R_{int} = 0.082
θ_{max} = 25.0°
$h = -11 \rightarrow 19$
$k = -11 \rightarrow 13$
$l = -19 \rightarrow 19$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.139
S = 0.81
4916 reflections
319 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0418P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C3—C4	1.525 (4)	C15—N1	1.465 (4)
C11—O1	1.230 (4)	C20—O2	1.426 (3)
C10—C5—C4	124.3 (3)	C27—C20—C21	113.4 (3)
O1—C11—C8	119.0 (4)	C20—O2—C17	113.3 (2)
C2—C4—C5—C6	−162.9 (3)	C13—C14—N1—C15	−65.6 (4)
C21—C20—C27—C32	144.9 (3)	C16—C17—O2—C20	−152.4 (3)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C31—H31···N1^{i}	0.93	2.59	3.522 (4)	175
C20—H20···O1^{ii}	0.98	2.54	3.507 (5)	169
C32—H20···O2	0.93	2.38	2.724 (4)	101

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

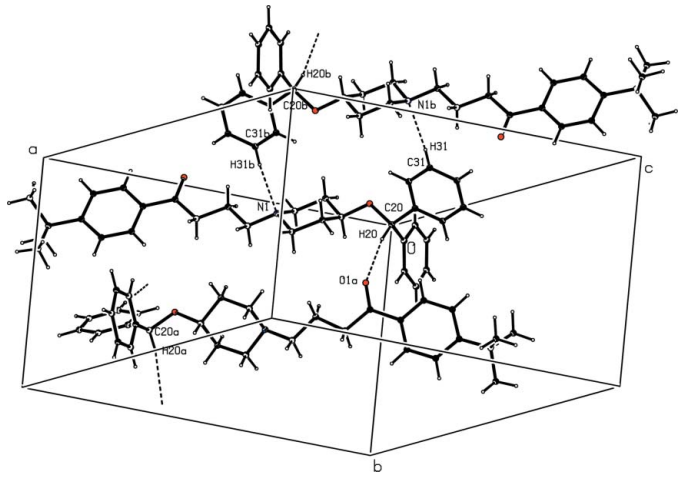


Figure 2
The intermolecular interactions (dashed lines) in the crystal structure of (I).

H atoms were placed at calculated positions and treated as riding atoms (C—H = 0.93 and 0.98 Å), with U_{iso} values set equal to 1.2 (for CH) or 1.5 (for CH and CH_3) times U_{eq} of the parent atom.

Data collection: *SMART* (Bruker, 1997); 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, 2001); software used to prepare material for publication: *SHELXTL*.

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