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1-(2-Methoxyphenyl)-4-[2-(2-methoxyphenylsulfanyl)benzoyl]piperazine

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Key indicators

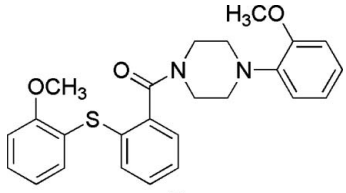
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.005 Å
R factor = 0.051
wR factor = 0.117
Data-to-parameter ratio = 16.6

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

The title compound, $C_{25}H_{26}N_2O_3S$, was synthesized from 2-(2-methoxyphenylsulfanyl)benzoic chloride and 1-(2-methoxyphenyl)piperazine. The piperazine ring exhibits a chair conformation.

Comment

Substituted diphenyl sulfide derivatives are a class of compounds which display high *in vitro* and *in vivo* affinities for serotonin transporter (SERT), high selectivity for dopamine transporter sites (DAT) and partial selectivity over norepinephrine transporter sites (NET), and have been described as potent and selective SERT ligands.



(I)

The title compound, (I), was synthesized from 2-(2-methoxyphenylsulfanyl)benzoic chloride and 1-(2-methoxyphenyl)piperazine. The molecular structure of the title compound is illustrated in Fig. 1. The piperazine ring is in a normal chair conformation.

Experimental

2-(2-Methoxyphenylsulfanyl)benzoic chloride (8 mmol), triethylamine (20 mmol) and 1-(2-methoxyphenyl)piperazine (8 mmol) in

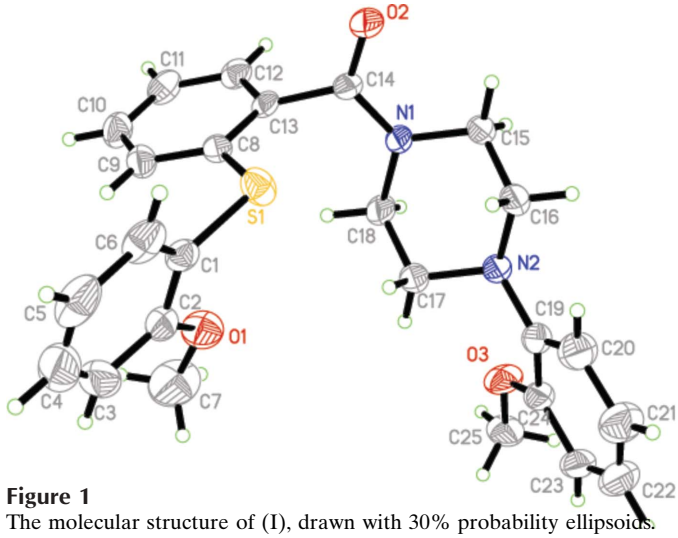


Figure 1
The molecular structure of (I), drawn with 30% probability ellipsoids.

$CHCl_3$ (60 ml) were stirred at room temperature for 3–4.5 h. After cooling to room temperature, the mixture was washed with 2 *M* NaOH. The organic layer was evaporated *in vacuo* to dryness to give a sticky yellow oil, which solidified at room temperature (Mehta & Brieaddy, 1997; Wilson & Howie, 1999; Younes *et al.*, 2000). After recrystallization from 60% aqueous ethanol (50–70 ml), the title compound was obtained as a white crystalline solid. Crystals of (I) suitable for X-ray analysis were grown by slow evaporation of an absolute methanol solution at room temperature over 15 d.

Crystal data

$C_{25}H_{26}N_2O_3S$
M_r = 434.54
Monoclinic, $P2_1/c$
a = 12.483 (3) Å
b = 16.535 (3) Å
c = 12.504 (3) Å
β = 117.451 (3)°
V = 2290.3 (8) Å^3
Z = 4
D_x = 1.260 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1945 reflections
θ = 2.2–21.5°
μ = 0.17 mm^{-1}
T = 294 (2) K
Block, colourless
0.40 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.935, T_{max} = 0.983
12787 measured reflections
4695 independent reflections
2189 reflections with $I > 2\sigma(I)$
R_{int} = 0.059
θ_{max} = 26.4°
$h = -15 \rightarrow 15$
$k = -16 \rightarrow 20$
$l = -13 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.117
S = 1.03
4695 reflections
282 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.04P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

All H atoms were positioned geometrically and refined as riding, with C—H distances in the range 0.93–0.98 Å and with U_{iso}(H) = 1.2 U_{eq}(C).

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

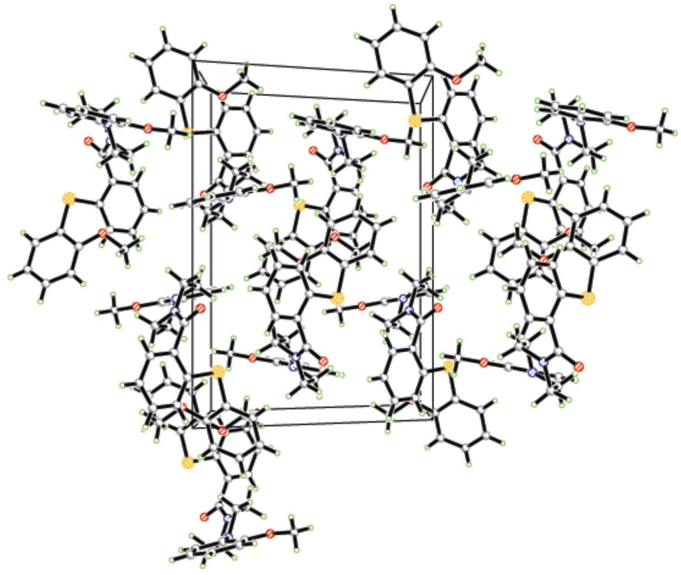


Figure 2
The crystal structure of (I), viewed along the *a* axis

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