Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Ethyl *N*-[4-(3-methyl-4,5-dihydrobenzo[*g*]indazol-1-yl)phenylsulfonyl]thiocarbamate ethanol monosolvate

Abdullah M. Asiri,[a,b]‡ Abdulrahman O. Al-Youbi,[a] Hassan M. Faidallah,[a] Seik Weng Ng[c] and Edward R. T. Tiekink[c]*

[a]Chemistry Department, Faculty of Science, King Abdulaziz University, PO Box 80203, Jeddah,Saudi Arabia, [b]Center of Excellence for Advanced Materials Research, King Abdulaziz University, PO Box 80203, Jeddah, Saudi Arabia, and [c]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: Edward.Tiekink@gmail.com

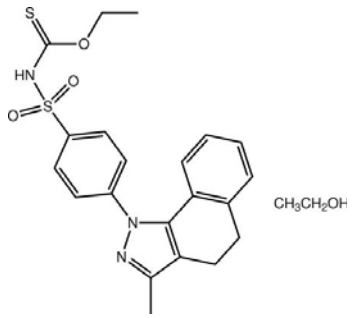
Received 15 August 2011; accepted 19 August 2011

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.007 Å; R factor = 0.087; wR factor = 0.261; data-to-parameter ratio = 17.8.

The title compound, $C_{21}H_{20}N_3O_3S_2{\cdot}CH_3CH_2OH$, comprises two independent organic molecules and two ethanol solvent molecules. The molecules are related by pseudo-mirror symmetry. In both molecules, the N-bound benzene ring is twisted out of the plane of the pyrazole ring [the dihedral angles are 51.4 (3) and 44.1 (3)°, respectively]. Similarly, the benzene ring of the 1,2-dihydronaphthalene residue is inclined with respect to the five-membered ring [dihedral angles 18.3 (3) and 22.2 (3)°]. Overall, each molecule has a flattened U shape. Dimeric aggregates mediated by O—H···N(pyrazole) and amide-N—H···O hydrogen bonds feature in the crystal packing, whereby the ethanol molecules link the independent organic molecules, leading to four-molecule aggregates.

Related literature

For background to the biological activity of species related to the title compound, see: Faidallah *et al.* (2007); Al-Saadi *et al.* (2008).



Experimental

Crystal data

$C_{21}H_{21}N_3O_3S_2{\cdot}C_2H_6O$
M_r = 473.60
Monoclinic, $P2_1/c$
a = 22.673 (2) Å
b = 12.5563 (8) Å
c = 17.3831 (17) Å
β = 110.410 (11)°
V = 4638.1 (7) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.27 mm^{-1}
T = 100 K
0.25 × 0.25 × 0.05 mm

Data collection

Agilent SuperNova Dual diffractometer with Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
T_{min} = 0.786, T_{max} = 1.000
21133 measured reflections
10333 independent reflections
4871 reflections with $I > 2\sigma(I)$
R_{int} = 0.089

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.087
$wR(F^2)$ = 0.261
S = 1.03
10333 reflections
581 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.80 e Å^{-3}
$\Delta\rho_{min}$ = −0.67 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3···O8	0.88	1.82	2.700 (5)	174
N6—H6···O7	0.88	1.88	2.750 (6)	170
O7—H7···N1	0.84	2.03	2.839 (6)	161
O8—H8···N4	0.84	1.98	2.807 (5)	170

Data collection: *CrysAlis PRO* (Agilent, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997), *DIAMOND* (Brandenburg, 2006) and *Qmol* (Gans & Shalloway, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

The authors are grateful to the Center of Excellence for Advanced Materials Research and the Chemistry Department at King Abdulaziz University for providing research facilities. The authors also thank the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2343).

References

Agilent (2010). *CrysAlis PRO*. Agilent Technologies, Yarnton, Oxfordshire, England.
Al-Saadi, M. S., Rostom, S. A. F. & Faidallah, H. M. (2008). *Arch. Pharm. Chem. Life Sci*, **341**, 181–190.
Brandenburg, K. (2006). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Faidallah, H. M., Al-Saadi, M. S., Rostom, S. A. F. & Fahmy, H. T. Y. (2007). *Med. Chem. Res.* **16**, 300–318.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Gans, J. & Shalloway, D. (2001). *J. Mol. Graphics Modell.* **19**, 557–559.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

‡ Additional correspondence author, e-mail: aasiri2@kau.edu.sa.