**N-[2-(3,4-Dimethoxyphenyl)-2-(phenylsulfanyl)ethyl]-2-(2-fluorophenyl)acetamide**

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The title compound, \( \text{C}_{24}\text{H}_{24}\text{FNO}_{3}\text{S} \), is an intermediate in the synthesis of fluorine containing isoquinoline alkaloids, which crystallizes in the triclinic space group \( \text{P} \) with one molecule in the asymmetric unit. The structure presents a racemic mixture of enantiomers. The \( \text{C}—\text{S}—\text{C}—\text{C} \) torsion angle between the benzene ring system and the sulfonyl benzene ring is \( 178.5 \, (1) \)°. In the crystal, \( \text{N}—\text{H}···\text{O} \) hydrogen bonds between neighboring molecules form chains of molecules along the \( \text{a} \)-axis direction.

**Structure description**

Sulfur- and fluorine-containing molecules play important roles in medicinal chemistry. Sulfur-containing compounds often show a variety of biological activities and serve important functions in applications in the pharmaceutical industry (Bernardi *et al.*, 1985). A variety of sulfur-containing molecules have been isolated from natural sources and play major roles in drug discovery and development. The role of fluorine in drug design and development is expanding rapidly, as more is learned about the unique properties associated with this unusual element and how to deploy it in the pharmaceutical industry. The introduction of fluorine into a molecule can influence conformation, \( \text{pK}_a \), intrinsic potency, membrane permeability, metabolic pathways, and pharmacokinetic properties (Gillis *et al.*, 2015). Various sulfur- and fluorine-containing molecules have been studied for their applications in medicinal chemistry, with those containing a sulfone group emerging with promising results. Some examples are the recently reported thiochroman-4-one derivatives (Vargas *et al.*, 2017), in which structure–activity relationships have been studied and it has been found that the vinyl sulfone and fluorine moieties play important roles in the biological activity of the molecules (Fig. 1). The literature also reveals that these types of compounds also serve as neuroprotective agents (Woo *et al.*, 2014), exhibit...
Continuing our interest in developing new sulfur- and fluorine-containing C17 S1 C7 C1biologically active alkaloids, we report here the synthesis and characterization of the title compound (Fig. 2) as a racemic mixture. The torsion angle between the benzene ring system and the sulfonyl benzene ring is $178.5^\circ (1)$. The C11—C10—C9 angle is [117.8 (2)] is slightly widened in comparison to an $sp^3$-hybridized carbon atom; this is probably due to an attractive interaction between the fluorine on the benzene ring and the hydrogen atoms on the benzyl carbon. In the crystal, N—H···O hydrogen bonds between neighbouring molecules form chains of molecules along the a-axis direction (Table 1; Fig. 3).

Synthesis and crystallization

The title compound was synthesized by the oxidation of N-(2-(3,4-dimethoxyphenyl)-2-(phenylthio)ethyl)-2-(2-fluorophenyl)acetamide (0.229 g, 0.54 mmol) treated with NaIO4 (0.264, 1.23 mmol) in water (6 ml). The reaction mixture was stirred for 2 h in reflux and then was allowed to cool down at room temperature prior to extractions with DCM (3 x 20 ml). The solvent in the combined organic layer was removed under vacuum and purified by flash chromatography on silica gel (DCM/MeOH 95:5) to give a pale-yellow solid in 67% yield (0.163 g, 0.36 mmol).

Table 2

| Crystal data               | C24H24FNO5S |
|----------------------------|-------------|
| Chemical formula           | C$_2$H$_2$FNO$_5$S |
| M$_r$                      | 457.50      |
| Crystal system, space group| Triclinic, $P\bar{1}$ |
| Temperature (K)            | 293         |
| a, b, c (Å)                | 8.3751 (3), 9.7640 (4), 15.3592 (5) |
| $\alpha, \beta, \gamma (^\circ)$ | 97.676 (3), 93.885 (3), 115.319 (4) |
| V (Å$^3$)                  | 1141.48 (8) |
| Z                          | 2           |
| Radiation type             | Cu Kα       |
| $\mu$ (mm$^{-1}$)          | 1.68        |
| Crystal size (mm)          | 0.21 x 0.12 x 0.07 |

Data collection

Diffractometer                 | Rigaku SuperNova, Dual, Cu at zero, AtlasS2 |
Absorption correction          | Multi-scan (CrysAlis PRO; Rigaku OD, 2015) |
$T_{min}$, $T_{max}$           | 0.816, 1.000 |
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 14171, 4663, 4030 |
$R_{int}$                     | 0.022       |
$\langle \sin \theta \lambda \rangle_{max}$ (Å$^{-1}$) | 0.631       |

Refinement

$R[F^2 > 2\sigma(F^2)], wR(F^2), S$ | 0.052, 0.151, 1.08 |
No. of reflections              | 4663        |
No. of parameters               | 291         |
H-atom treatment               | H-atom parameters constrained |
$\Delta f_{max}$, $\Delta f_{min}$ (e Å$^{-3}$) | 0.37, −0.30 |

Computer programs: CrysAlis PRO (Rigaku OD, 2015), SIR2004 (Barlu et al., 2007), SHELXL (Sheldrick, 2015), Mercury (Macrae et al., 2020) and pubICIF (Westrip, 2010).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.
Funding information
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full crystallographic data

IUCrData (2021). 6, x201663  [https://doi.org/10.1107/S2414314620016636]

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Crystal data
C_{24}H_{24}FNO_{5}S  
Mr = 457.50  
Triclinic, P\bar{1}  
a = 8.3751 (3) Å  
b = 9.7640 (4) Å  
c = 15.3592 (5) Å  
α = 97.676 (3)°  
β = 93.885 (3)°  
γ = 115.319 (4)°  
V = 1114.18 (8) Å^3  
Z = 2  
F(000) = 480  
\(D_x\) = 1.364 Mg m\(^{-3}\)  
Cu Kα radiation, \(λ = 1.54184 \text{ Å}\)  
Cell parameters from 6250 reflections  
\(\theta\) = 2.9–76.6°  
\(\mu\) = 1.68 mm\(^{-1}\)  
\(T\) = 293 K  
Irregular, translucent intense colourless  
0.21 × 0.12 × 0.07 mm

Data collection
Rigaku SuperNova, Dual, Cu at zero, AtlasS2 diffractometer  
Radiation source: micro-focus sealed X-ray tube, SuperNova (Cu) X-ray Source  
Mirror monochromator  
Detector resolution: 5.1980 pixels mm\(^{-1}\)  
\(ω\) scans  
Absorption correction: multi-scan  
(CrysAlisPro; Rigaku OD, 2015)

Refinement
Refinement on \(F^2\)  
Least-squares matrix: full  
\(R[F^2 > 2\sigma(F^2)] = 0.052\)  
wR\((F^2)\) = 0.151  
\(S = 1.08\)  
4663 reflections  
291 parameters  
0 restraints  
Primary atom site location: structure-invariant direct methods  
Hydrogen site location: inferred from neighbouring sites  
H-atom parameters constrained  
\(w = 1/[\sigma^2(F_o^2) + (0.0751P)^2 + 0.4124P]\)  
where \(P = (F_o^2 + 2F_c^2)/3\)  
\((\Delta/\sigma)_{max} = 0.001\)  
\(\Delta \rho_{max} = 0.37 \text{ e Å}^{-3}\)  
\(\Delta \rho_{min} = -0.30 \text{ e Å}^{-3}\)
Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. The C-bound H atoms were placed in calculated positions and treated as riding: C—H = 0.95–0.99 Å with Uiso(H) = 1.5Ueq(Cmethyl) and 1.2Ueq(C) for other H atoms.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

|       | x       | y       | z       | Uiso*/Ueq |
|-------|---------|---------|---------|-----------|
| S1    | 0.39652 (6) | 0.22548 (6) | 0.61360 (4) | 0.04490 (17) |
| F1    | 0.6743 (4)  | 0.9600 (3)  | 0.84275 (19) | 0.1440 (11)   |
| O1    | 0.4440 (2)  | 0.1166 (2)  | 0.64885 (15) | 0.0685 (5)    |
| O2    | 0.4379 (2)  | 0.2591 (2)  | 0.52804 (11) | 0.0733 (6)    |
| O3    | 0.6887 (3)  | 0.5399 (2)  | 0.93514 (12) | 0.0724 (5)    |
| O4    | 1.24722 (18)| 0.61837 (19)| 0.69344 (11) | 0.0505 (4)    |
| O5    | 1.09028 (19)| 0.4413 (2)  | 0.80129 (10) | 0.0524 (4)    |
| N1    | 0.4765 (2)  | 0.5359 (2)  | 0.83493 (12) | 0.0482 (4)    |
| H1    | 0.421805    | 0.586998    | 0.818120     | 0.058*        |
| C1    | 0.7007 (2)  | 0.4691 (2)  | 0.69245 (13) | 0.0387 (4)    |
| C2    | 0.7860 (3)  | 0.5660 (3)  | 0.63531 (15) | 0.0480 (5)    |
| H2    | 0.720985    | 0.596306    | 0.597378     | 0.058*        |
| C3    | 0.9689 (3)  | 0.6187 (3)  | 0.63396 (15) | 0.0493 (5)    |
| H3    | 1.024558    | 0.683868    | 0.595053     | 0.059*        |
| C4    | 1.0682 (2)  | 0.5755 (2)  | 0.68960 (14) | 0.0416 (4)    |
| C5    | 0.9826 (3)  | 0.4781 (2)  | 0.74848 (13) | 0.0401 (4)    |
| C6    | 0.8009 (2)  | 0.4252 (2)  | 0.74868 (13) | 0.0400 (4)    |
| H6    | 0.744532    | 0.359023    | 0.787008     | 0.048*        |
| C7    | 0.5010 (2)  | 0.4060 (2)  | 0.69177 (13) | 0.0395 (4)    |
| H7    | 0.464425    | 0.478089    | 0.667997     | 0.047*        |
| C8    | 0.4351 (3)  | 0.3881 (3)  | 0.78194 (14) | 0.0443 (5)    |
| H8A   | 0.307058    | 0.324890    | 0.773090     | 0.053*        |
| H8B   | 0.490585    | 0.336217    | 0.813264     | 0.053*        |
| C9    | 0.5952 (3)  | 0.5977 (3)  | 0.90877 (15) | 0.0517 (5)    |
| C10   | 0.6108 (4)  | 0.7481 (3)  | 0.95980 (18) | 0.0684 (7)    |
| H10A  | 0.599310    | 0.736563    | 1.021142     | 0.082*        |
| H10B  | 0.730226    | 0.827165    | 0.958892     | 0.082*        |
| C11   | 0.4797 (4)  | 0.8064 (3)  | 0.92863 (16) | 0.0598 (6)    |
| C12   | 0.5128 (6)  | 0.9088 (4)  | 0.8713 (2)   | 0.0853 (10)   |
| C13   | 0.3893 (8)  | 0.9597 (4)  | 0.8421 (2)   | 0.1011 (14)   |
| H13   | 0.416268    | 1.030105    | 0.803685     | 0.121*        |
| C14   | 0.2253 (7)  | 0.9011 (5)  | 0.8724 (3)   | 0.1040 (13)   |
| H14   | 0.139973    | 0.931991    | 0.853658     | 0.125*        |
| C15   | 0.1876 (6)  | 0.8014 (5)  | 0.9281 (3)   | 0.0930 (11)   |
| H15   | 0.076739    | 0.762740    | 0.947768     | 0.112*        |
| C16   | 0.3134 (4)  | 0.7560 (4)  | 0.9562 (2)   | 0.0728 (8)    |
| H16   | 0.285373    | 0.687787    | 0.995874     | 0.087*        |
### Atomic displacement parameters ($\AA^2$)

|     | $U^{11}$  | $U^{22}$  | $U^{33}$  | $U^{12}$  | $U^{13}$  | $U^{23}$  |
|-----|-----------|-----------|-----------|-----------|-----------|-----------|
| S1  | 0.0308 (2) | 0.0492 (3) | 0.0513 (3) | 0.0168 (2) | 0.00980 (19) | −0.0007 (2) |
| F1  | 0.155 (2) | 0.1078 (18) | 0.128 (2) | 0.0098 (17) | 0.0651 (18) | 0.0350 (16) |
| O1  | 0.0445 (9) | 0.0507 (9) | 0.1138 (16) | 0.0277 (8) | 0.0078 (9) | 0.0042 (9) |
| O2  | 0.0508 (10) | 0.0919 (14) | 0.0495 (10) | 0.0093 (9) | 0.0176 (8) | −0.0057 (9) |
| O3  | 0.0679 (12) | 0.0981 (15) | 0.0585 (11) | 0.0487 (11) | −0.0068 (9) | 0.0035 (10) |
| O4  | 0.0292 (7) | 0.0595 (9) | 0.0602 (9) | 0.0132 (6) | 0.0144 (6) | 0.0205 (7) |
| O5  | 0.0329 (7) | 0.0771 (11) | 0.0533 (9) | 0.0249 (7) | 0.0114 (6) | 0.0270 (8) |
| N1  | 0.0403 (9) | 0.0568 (11) | 0.0489 (10) | 0.0267 (8) | 0.0018 (7) | −0.0023 (8) |
| C1  | 0.0294 (9) | 0.0432 (10) | 0.0413 (10) | 0.0145 (8) | 0.0053 (7) | 0.0057 (8) |
| C2  | 0.0393 (10) | 0.0534 (12) | 0.0534 (12) | 0.0199 (9) | 0.0061 (9) | 0.0189 (10) |
| C3  | 0.0398 (11) | 0.0536 (12) | 0.0552 (12) | 0.0164 (9) | 0.0138 (9) | 0.0239 (10) |
| C4  | 0.0288 (9) | 0.0451 (10) | 0.0465 (11) | 0.0115 (8) | 0.0105 (8) | 0.0080 (8) |
| C5  | 0.0311 (9) | 0.0493 (11) | 0.0390 (10) | 0.0166 (8) | 0.0069 (7) | 0.0088 (8) |
| C6  | 0.0316 (9) | 0.0484 (11) | 0.0404 (10) | 0.0161 (8) | 0.0112 (7) | 0.0121 (8) |
| C7  | 0.0314 (9) | 0.0442 (10) | 0.0438 (10) | 0.0180 (8) | 0.0066 (7) | 0.0062 (8) |
| C8  | 0.0333 (9) | 0.0504 (11) | 0.0499 (11) | 0.0197 (8) | 0.0105 (8) | 0.0045 (9) |
| C9  | 0.0410 (11) | 0.0665 (14) | 0.0448 (12) | 0.0226 (10) | 0.0062 (9) | 0.0053 (10) |
| C10 | 0.0630 (16) | 0.0700 (17) | 0.0566 (15) | 0.0229 (13) | −0.0015 (12) | −0.0123 (12) |
| C11 | 0.0762 (17) | 0.0491 (13) | 0.0452 (12) | 0.0237 (12) | 0.0045 (11) | −0.0052 (10) |
| C12 | 0.112 (3) | 0.0577 (16) | 0.0650 (18) | 0.0184 (17) | 0.0204 (17) | 0.0056 (13) |
| C13 | 0.174 (5) | 0.0602 (19) | 0.067 (2) | 0.053 (2) | −0.006 (2) | 0.0107 (15) |
| C14 | 0.144 (4) | 0.094 (3) | 0.085 (3) | 0.075 (3) | −0.010 (3) | −0.011 (2) |
| C15 | 0.099 (3) | 0.106 (3) | 0.087 (2) | 0.063 (2) | 0.0086 (19) | 0.001 (2) |
| C16 | 0.082 (2) | 0.0758 (19) | 0.0651 (17) | 0.0404 (16) | 0.0142 (14) | 0.0053 (14) |
| C17 | 0.0301 (9) | 0.0480 (11) | 0.0444 (11) | 0.0151 (8) | 0.0050 (8) | −0.0017 (8) |
|    | C18  |     | C19  |     | C20  |     | C21  |     | C22  |     | C23  |     | C24  |     |
|----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|
| 0.0417 (12) | 0.0467 (12) | 0.0840 (17) | 0.0176 (10) | 0.0137 (11) | 0.0130 (12) |
| 0.0440 (13) | 0.0555 (15) | 0.115 (2) | 0.0125 (11) | 0.0274 (14) | 0.0172 (15) |
| 0.0325 (11) | 0.0645 (16) | 0.096 (2) | 0.0165 (11) | 0.0112 (12) | −0.0084 (14) |
| 0.0452 (13) | 0.0781 (18) | 0.0735 (17) | 0.0341 (13) | −0.0057 (11) | 0.0041 (14) |
| 0.0416 (11) | 0.0683 (15) | 0.0540 (13) | 0.0228 (11) | 0.0021 (9) | 0.0127 (11) |
| 0.0491 (13) | 0.102 (2) | 0.0669 (16) | 0.0323 (14) | 0.0147 (12) | 0.0473 (16) |
| 0.0403 (12) | 0.0674 (16) | 0.0872 (19) | 0.0164 (11) | 0.0290 (12) | 0.0344 (14) |

**Geometric parameters (Å, °)**

|    |    |    | C1—O4  |    | C5—O5  |    | C2—O1  |    | N1—H1  |    | C1—C2  |    | C3—H2  |    | C2—C3  |    | C4—C5  |    | C5—C6  |    | C6—H6  |    | C7—H7  |    | C7—C8  |    | C8—H8A |    | C8—H8B |    | C9—C10 |    | C10—H10A |    |
|----|----|----|--------|----|--------|----|--------|----|--------|----|--------|----|--------|----|--------|----|--------|----|--------|----|--------|----|--------|----|--------|----|--------|----|--------|----|
| S1—O1 | 1.4378 (19) | C10—H10B | 0.9700 |
| S1—O2 | 1.4264 (18) | C10—C11 | 1.515 (4) |
| S1—C7 | 1.813 (2) | C11—C12 | 1.372 (4) |
| S1—C17 | 1.765 (2) | C11—C16 | 1.382 (4) |
| F1—C12 | 1.353 (5) | C12—C13 | 1.398 (6) |
| O3—C9 | 1.221 (3) | C13—H13 | 0.9300 |
| O4—C4 | 1.367 (2) | C13—C14 | 1.385 (6) |
| O4—C24 | 1.428 (3) | C14—H14 | 0.9300 |
| O5—C5 | 1.363 (2) | C14—C15 | 1.332 (6) |
| O5—C23 | 1.423 (3) | C15—H15 | 0.9300 |
| N1—H1 | 0.8600 | C15—C16 | 1.371 (5) |
| N1—C8 | 1.443 (3) | C16—H16 | 0.9300 |
| N1—C9 | 1.338 (3) | C17—C18 | 1.386 (3) |
| C1—C2 | 1.380 (3) | C17—C22 | 1.377 (3) |
| C1—C6 | 1.394 (3) | C18—H18 | 0.9300 |
| C1—C7 | 1.513 (2) | C18—C19 | 1.387 (3) |
| C2—H2 | 0.9300 | C19—H19 | 0.9300 |
| C2—C3 | 1.394 (3) | C19—C20 | 1.371 (4) |
| C3—H3 | 0.9300 | C20—H20 | 0.9300 |
| C3—C4 | 1.379 (3) | C20—C21 | 1.358 (4) |
| C4—C5 | 1.403 (3) | C21—H21 | 0.9300 |
| C5—C6 | 1.383 (3) | C21—C22 | 1.393 (3) |
| C6—H6 | 0.9300 | C22—H22 | 0.9300 |
| C7—H7 | 0.9800 | C23—H23A | 0.9600 |
| C7—C8 | 1.530 (3) | C23—H23B | 0.9600 |
| C8—H8A | 0.9700 | C23—H23C | 0.9600 |
| C8—H8B | 0.9700 | C24—H24A | 0.9600 |
| C9—C10 | 1.518 (4) | C24—H24B | 0.9600 |
| C10—H10A | 0.9700 | C24—H24C | 0.9600 |

|    | O1—S1—C7 | 107.85 (11) | C11—C10—H10B | 107.9 |
|----|----------|--------------|----------------|------|
| O1—S1—C17 | 107.54 (11) | C12—C11—C10 | 124.0 (3) |
| O2—S1—O1 | 119.44 (13) | C12—C11—C16 | 115.0 (3) |
| O2—S1—C7 | 107.41 (11) | C16—C11—C10 | 121.0 (3) |
| O2—S1—C17 | 108.68 (11) | F1—C12—C11 | 116.5 (4) |
| C17—S1—C7 | 105.03 (9) | F1—C12—C13 | 120.1 (4) |
| C4—O4—C24 | 117.09 (18) | C11—C12—C13 | 123.3 (4) |
| C5—O5—C23 | 117.34 (16) | C12—C13—H13 | 121.3 |
C8—N1—H1 118.2 C14—C13—C12 117.4 (3)
C9—N1—H1 118.2 C14—C13—H13 121.3
C9—N1—C8 123.6 (2) C13—C14—H14 119.4
C2—C1—C6 118.69 (18) C15—C14—C13 121.2 (4)
C2—C1—C7 120.93 (18) C15—C14—H14 119.4
C6—C1—C7 120.33 (17) C14—C15—H15 120.2
C1—C2—H2 119.7 C14—C15—C16 119.6 (4)
C1—C2—C3 120.55 (19) C16—C15—H15 120.2
C3—C2—H2 119.7 C11—C16—H16 118.3
C2—C3—H3 119.6 C15—C16—C11 123.5 (3)
C4—C3—C2 120.83 (19) C15—C16—H16 118.3
C4—C3—H3 119.6 C18—C17—S1 118.95 (18)
O4—C4—C3 125.98 (18) C22—C17—S1 120.22 (17)
O4—C4—C5 115.10 (18) C22—C17—C18 120.8 (2)
C3—C4—C5 118.92 (18) C17—C18—H18 120.5
O5—C5—C4 124.92 (18) C17—C18—C19 119.0 (2)
O5—C5—C6 115.25 (17) C19—C18—H18 120.5
C6—C5—C4 119.83 (18) C18—C19—H19 120.0
C5—C6—H6 119.4 C20—C19—H19 120.1 (3)
C6—C5—C1 121.17 (18) C20—C19—C18 120.0
C5—C6—C1 119.4 C19—C20—H20 119.6
O4—C23—H23A 109.5
O4—C23—H23B 109.5
O4—C23—H23C 109.5
N1—C8—C7 111.25 (18) C17—C22—H22 120.5
N1—C8—H8A 109.4 C21—C22—H22 120.5
N1—C8—H8B 109.4 O5—C23—H23A 109.5
C7—C8—H8A 109.4 O5—C23—H23B 109.5
C7—C8—H8B 109.4 O5—C23—H23C 109.5
H8A—C8—H8B 108.0 H23A—C23—H23B 109.5
O3—C9—N1 123.5 (2) H23A—C23—H23C 109.5
O3—C9—C10 120.3 (2) H23B—C23—H23C 109.5
N1—C9—C10 116.2 (2) O4—C24—H24A 109.5
C9—C10—H10A 107.9 O4—C24—H24B 109.5
C9—C10—H10B 107.9 O4—C24—H24C 109.5
H10A—C10—H10B 107.2 H24A—C24—H24B 109.5
C11—C10—C9 117.8 (2) H24A—C24—H24C 109.5
C11—C10—H10A 107.9 H24B—C24—H24C 109.5

| Hydrogen-bond geometry (Å, º) |
|-----------------------------|
| \( D—H···A \) | \( D—H \) | \( H···A \) | \( D···A \) | \( D—H···A \) |
| N1—H1···O4i 0.86 | 2.46 | 3.207 (2) | 145 |

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|       |       |       |       |
|-------|-------|-------|-------|
| N1—H1···O5i | 0.86  | 2.50  | 2.945 (3) | 113 |

Symmetry code: (i) \(-x, y, z\).