ЖУРНАЛ СТРУКТУРНОЙ ХИМИИ

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SUPPLEMENTARY MATERIALS TO:

SYNTHESIS, CHARACTERIZATION, CRYSTAL STRUCTURE, AND DFT STUDY OF 3-BROMO-*N*-(3-FLUOROPHENYL)BENZENESULFONAMIDE

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Contents:

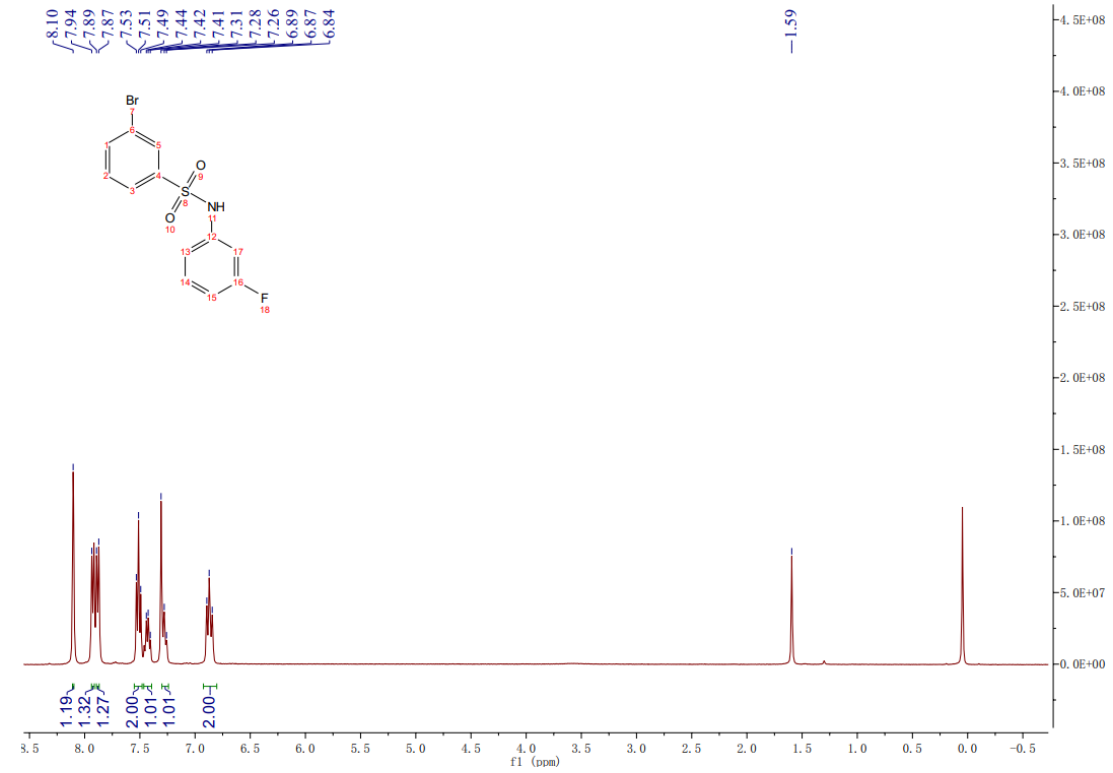

Figure S1. ^{1}H NMR of **1**.

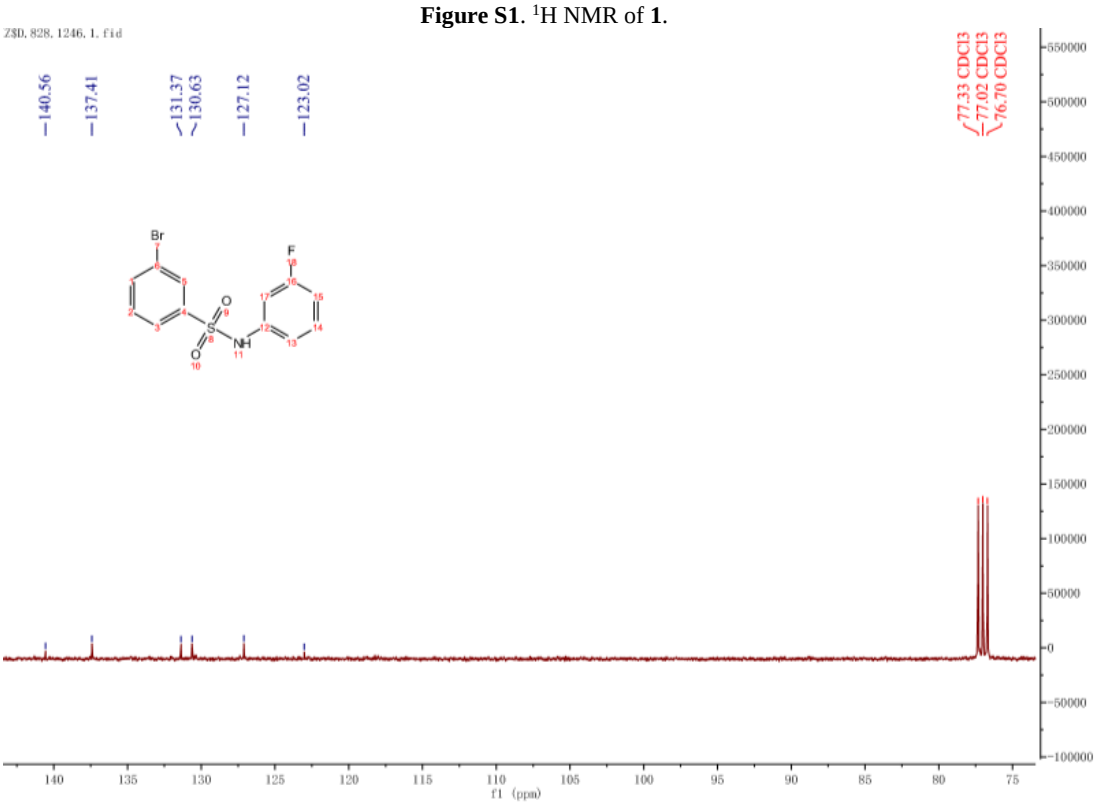

Figure S2. ^{13}C NMR of **1**.

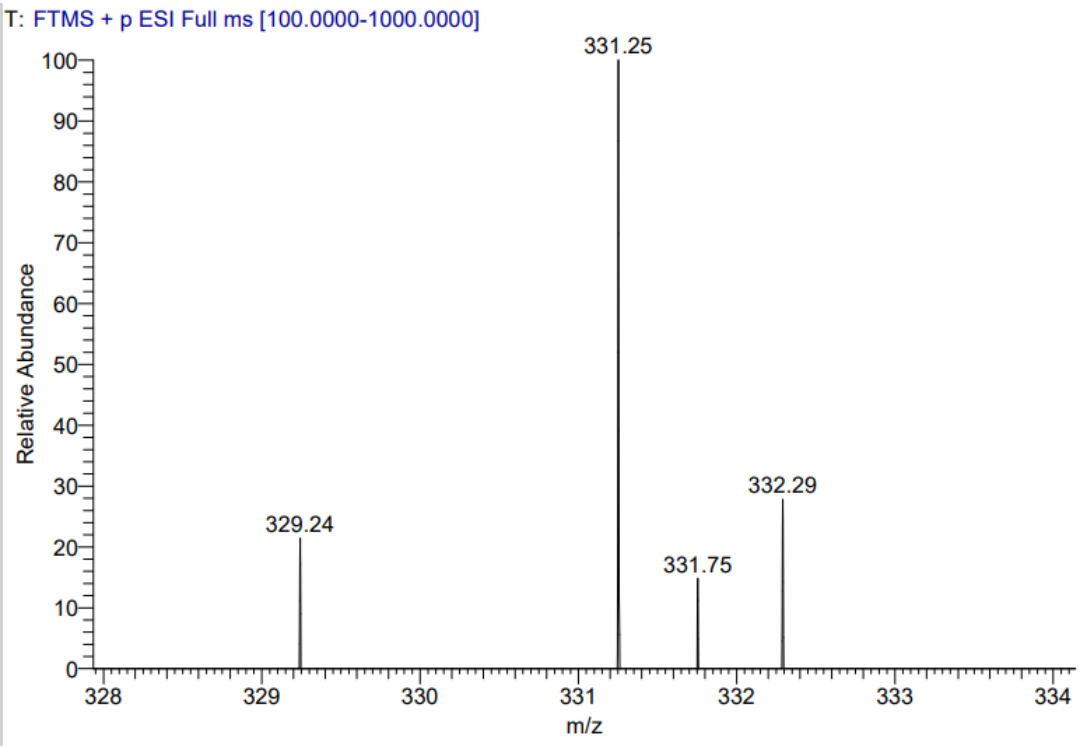

Figure S3. MS of **1**.

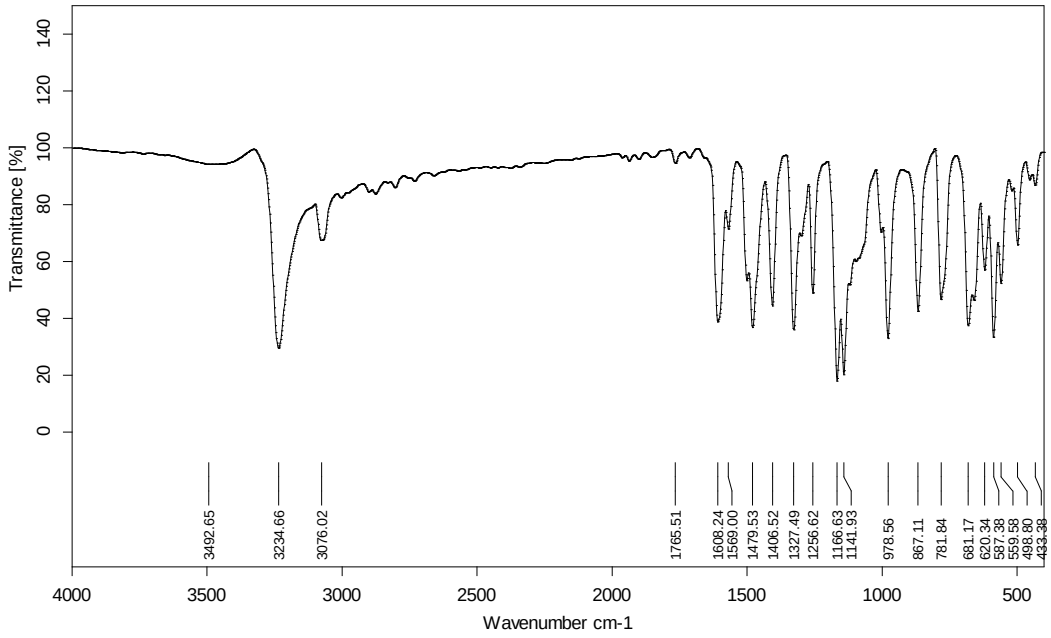

Figure S4. IR of **1**.

Table S1. Crystallographic characteristics, the X-ray data collection and structure-refinement parameters for **1**.

Compound	**1**
CCDC	1980901
Molecular formula	$C_{12}H_9BrFNO_2S$
Molecular weight	330.17
Crystal system	Monoclinic
Space group	$P2_1$ / c
a(Å)	8.8797(3)
b(Å)	8.6251(3)
c(Å)	16.4081(6)
α (°)	90
β (°)	92.6370(10)
γ (°)	90
V (Å^3)	1255.34(8)
Z	4
N(param)refined	167
μ (mm^{-1})	3.445
Radiation λ (Å)	0.71073
Ranges/indices (*h, k, l*)	$-11 \le h \le 11, -11 \le k \le 11, -21 \le l \le 21$
θ limit (°)	4.97 - 55.058
$N(hkl)_{measured}$, $N(hkl)_{unique}$	14838 / 2878 [R(int) = 0.0427]
$N(hkl)_{gt}$	2451
Diffractometer	Bruker APEX II
Scan mode	φ - ω
Programs	SHELXL-2014/7

Table S2. Bond distances, bond angles and torsion angles for compound **1** and conformer **1-3**.

Bond distance (Å)	**Exp.[a]**	**Calcd.[b]**	**Difference**
Br(1)-C(1)	1.899(2)	1.9140	0.0150
S(1)-O(2)	1.4363(15)	1.4423	0.0060
S(1)-O(1)	1.4282(16)	1.4441	0.0159
S(1)-N(1)	1.6291(17)	1.6853	0.0562
S(1)-C(5)	1.768(2)	1.7927	0.0247
F(1)-C(9)	1.356(3)	1.3522	-0.0038
N(1)-C(7)	1.423(3)	1.4201	-0.0029
C(6)-C(1)	1.375(3)	1.3860	0.0110
C(6)-C(5)	1.390(3)	1.3923	0.0023
C(1)-C(2)	1.387(3)	1.3898	0.0028
C(5)-C(4)	1.389(3)	1.3900	0.0010
C(7)-C(8)	1.388(3)	1.3963	0.0083
C(7)-C(12)	1.381(3)	1.3965	0.0155
C(4)-C(3)	1.382(3)	1.3904	0.0084
C(8)-C(9)	1.378(3)	1.3827	0.0047
C(2)-C(3)	1.391(3)	1.3905	-0.0005
C(9)-C(10)	1.364(4)	1.3824	0.0184
C(12)-C(11)	1.392(4)	1.3892	-0.0028
C(10)-C(11)	1.372(4)	1.3918	0.0198
Torsion angle (°)	**Exp.[a]**	**Calcd.[b]**	**Difference**
C(6)-C(5)-S(1)-O(1)	39.62	23.7219	-15.8981
C(6)-C(5)-S(1)-O(2)	170.00	158.17167	-11.8283

C(4)-C(5)-S(1)-O(1)	-139.29	-156.82516	-17.5352
C(4)-C(5)-S(1)-O(2)	-8.48	-22.39568	-13.9157
Br(1)-C(1)-C(6)-C(5)	-179.38	179.76247	359.1425
Br(1)-C(1)-C(2)-C(3)	179.46	-179.29202	-358.752
C(7)-N(1)-S(1)-O(1)	-172.93	-175.00921	-2.07921
C(7)-N(1)-S(1)-O(2)	58.45	53.68339	-4.76661
N(1)-C(7)-C(8)-C(9)	179.20	176.73180	-2.4682
N(1)-C(7)-C(12)-C(11)	178.83	-177.89290	-356.723
C(7)-C(8)-C(9)-F(1)	-179.90	-179.45665	0.44335
C(11)-C(10)-C(9)-F(1)	-179.59	179.96191	359.5519
C(9)-C(8)-C(7)-N(1)	178.83	176.73180	-2.0982
C(11)-C(12)-C(7)-N(1)	179.71	-177.89290	-357.603
C(12)-C(7)-N(1)-S(1)	-39.25	-57.05106	-17.8011
C(8)-C(7)-N(1)-S(1)	142.68	125.77734	-16.9027
C(4)-C(5)-S(1)-N(1)	107.27	92.33421	-14.9358
C(6)-C(5)-S(1)-N(1)	-73.82	-87.09844	-13.2784
C(3)-C(4)-C(5)-S(1)	178.58	-178.78006	-357.36
C(1)-C(6)-C(5)-S(1)	-179.23	178.77001	358

Bond angle (°)	**Exp.[a]**	**Calcd.[b]**	**Difference**
Br(1)-C(1)-C(6)	118.79	119.22345	0.4334
Br(1)-C(1)-C(2)	25.23	119.47957	94.2496
C(6)-C(5)-S(1)	118.06	118.58824	0.5282
C(4)-C(5)-S(1)	33.89	119.74606	85.8561
C(5)-S(1)-O(1)	109.35	108.07716	-1.2728
C(5)-S(1)-O(2)	107.04	107.47633	0.4363
O(2)-S(1)-N(1)	108.03	107.33968	-0.6903
O(1)-S(1)-N(1)	105.08	103.70180	-1.3782
S(1)-N(1)-C(7)	125.19	123.98112	-1.2089
N(1)-C(7)-C(12)	122.65	121.03420	-1.6158
N(1)-C(7)-C(8)	117.00	118.93277	1.9328
C(8)-C(9)-F(1)	117.51	118.20405	0.6940
C(10)-C(9)-F(1)	119.13	119.09133	-0.0387
O(1)-S(1)-O(2)	119.51	122.79080	3.2808

a: Experimental geometry parameters for compound **1**; b: Calculated geometry parameters for conformer **1**-**3**.

TABLE 1. Hydrogen Bond Geometry of Compound 1