Supporting information

Synthesis, properties and spatial structure of 4-[(3,5-dimethyl-1,2-oxazol-4-yl)sulfonyl]cytisine

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Experimental

General Information

FTIR spectra were obtained with an Agilent Cary 630 spectrophotometer in a thin sample layer on a crystal attachment. ^{1}H and ^{13}C NMR spectra were recorded on JNM-ECA Jeol 400 spectrometer (fre-quency 399.78 and 100.53 MHz, respectively) with using of CDCl3 solvent. The chemical shifts have been measured relative to signals of residual protons or carbon atoms of deuterated chloroform.

Chromato-mass spectrometric studies were carried out on a Trace GC Ultra chromatograph with a DSQ II mass-selective detector in the electron ionization mode (70 eV) on a Thermo TR-5 MS quartz capillary column, 15 m long, 0.25 mm inner diameter, with a film thickness of the stationary phase of 0.25 μm. Splitless input mode was used. Carrier gas discharge 20 ml/min. The velocity of the carrier gas (helium) is 1 ml/min. Evaporator temperature 200°C, transition chamber temperature 200°C, ion source temperature 200°C. The temperature of the column thermostat was changed according to the program: from 15 (5 min delay) to 220°C at a rate of 20°C per minute, to 290° at a rate of 15° per minute. The total analysis time was 30 min. The volume of the injected sample is 1 μl. Chromatograms were recorded in TIC mode. The range of mass scanning is 30 - 450 amu.
Melting points were determined using a Stuart SMP10 hot bench. Monitoring of the reaction course and the purity of the products was carried out by TLC on Sorbfil plates and visualized using iodine vapor or UV light.

Experimental Procedures

3,5-Dimethylisoxazole-4-sulfonyl chloride (1). To a cooled mixture of 33.8 mL of a chlorosulfonic acid and 4.06 mL of thionyl chloride, 5 mL of 3,5-dimethylisoxazole has been slowly added under stirring. A reaction mixture under stirring has been slowly heated to 120-130°C for 4 h.

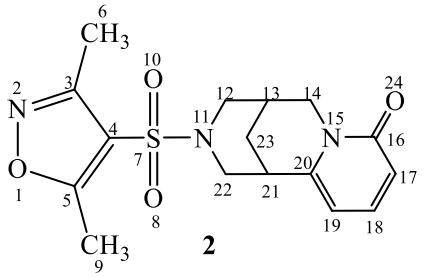
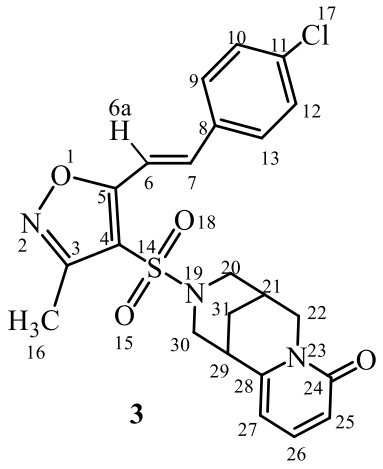
The reaction mixture has been cooled to a room temperature and poured over 100 g of ice (be careful when added to ice, a reaction mixture can react vigorously with water).

The precipitated white residue has been filtered, washed with water and dissolved in 30 ml of chloroform. Solution has been washed with 40 ml of potassium carbonate 5% solution and dried over calcium chloride. Product (9) has been obtained as the white crystals. Its yield has been 2.28 g, m.p. 40-2°C.

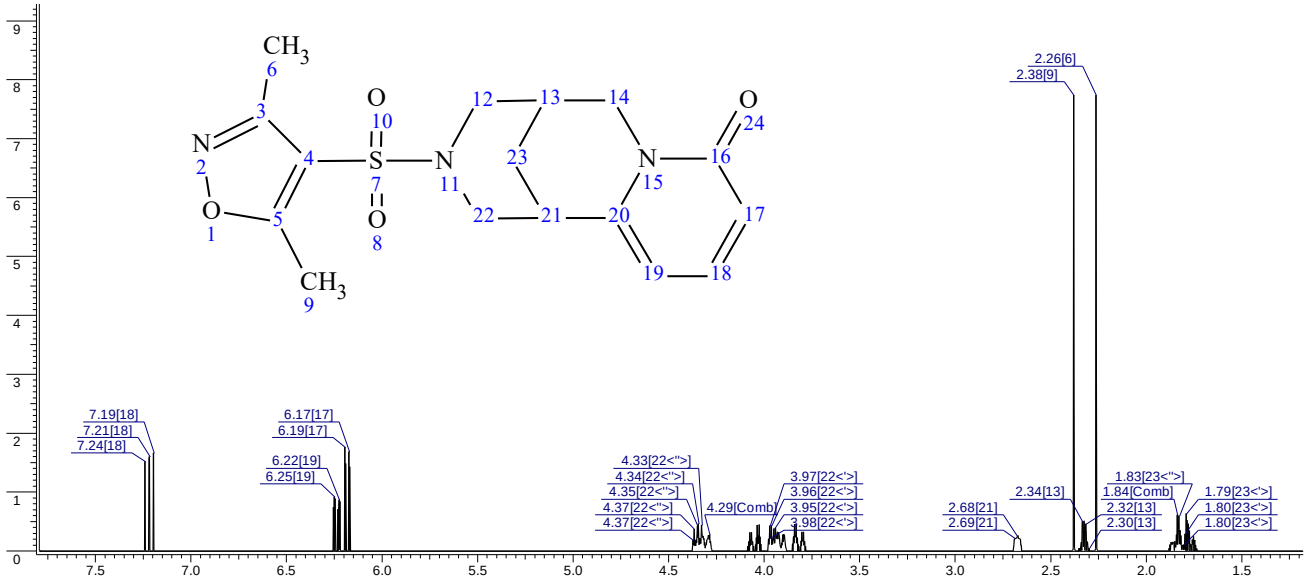
4-[(3,5-dimethyl-1,2-oxazol-4-yl)sulfonyl]cytisine (2). To a solution of 1.9 g (0.01 mol) of cytisine and 1.18 g (0.015 mol) of pyridine in 3 ml of dry acetonitrile, 1.95 g (0.01 mol) of sulfochloride 2 in 10 ml of dry acetonitrile has been added at a room temperature. A color of a reaction mixture has been light yellow, and its residue has been yellow. A reaction mixture has been stirred for 1 h at 40°C. Then a reaction mixture has been cooled. A yellow residue has been filtered and washed with acetonitrile. Then a solvent has been distilled with using a rotary evaporator. A residue has been thick yellow oil. Then 20 ml of a 5% solution of potassium carbonate has been added to a residue. After grinding, the thick oil has been a yellowish powder. The yield of product 2 has been 83%, m.p. 141-142°C.

4-[(3-methyl-5-{(4-chlorophenyl)ethenyl}-1,2-oxazol-4-yl)sulfonyl]cytisine (3). To a solution of 0.91 g of sulfonamide 2 and 0.56 g of 4-chlorobenzaldehyde in 20 ml of ethanol, 2 ml of a 40% aqueous solution of potassium hydroxide has been added at a room temperature. A color of a reaction mixture has been cloudy, and then has become light yellow. A reaction mixture has been stirred and heated for 1 h at 60-70°C. Then, a reaction mixture has been cooled to a room temperature and added 15% hydrochloric acid solution to pH≤3. A residue has been filtered and washed with water. The residue was a hygroscopic substance, light yellow color, m.p. 217-219°C.

Spectroscopic and physical data

 **2** Chemical Formula: $C_{16}H_{19}N_3O_4S$ Molecular Weight: 349,41	**4-[(3,5-dimethyl-1,2-oxazol-4-yl)sulfonyl]-cytisine (2).** Yield: 83%; yellowish powder, mp. 141-142 °C (2-PrOH). ^{1}H NMR (399.78 MHz, DMSO-d_6, δ, ppm, *J*/ Hz): 1.76-1.85 m (2H, H-23ax,23eq), 2.49 s (4H, H-9,9,9,13), 2.83 d (1H, H-12ax, 2J 11.4 Hz), 2.92 d (1H, H-12eq, 2J 11.4 Hz), 3.22 s (1H, H-21), 3.56 d (1H, H-22ax, 2J 10.8 Hz), 3.61 d (1H, H-22eq, 2J 10.8 Hz), 3.73-3.83 m (2H, H-14ax,14eq) ppm. 6.30 br. s (1H, H-17), 6.36 d (1H, H-19, 3J 9.2 Hz), 7.43 t (1H, 2J 6.6 Hz) ppm. H-6,6,6 2.12 ppm, H-9,9,9 2.49 ppm. ^{13}C NMR (100.53 MHz, DMSO-d_6) δ ppm 24.07 (C-23), 26.59 (C-13), 33.60 (C-21), 49.70 (C-14), 51.20 (C-22), 52.61 (C-12), 106.91 (C-19), 115.90 (C-17), 140.37 (C-18), 150.60 (C-20) и 162.45 (C-16) м.д.. 11.04 (C-6), 12.95 (C-9), 113.30 (C-4), 158.21 (C-3) и 174.45 (C-5).
 **3** Chemical Formula: $C_{23}H_{22}ClN_3O_4S$ Molecular Weight: 471,96	**4-[(3-methyl-5-{(4-chlorophenyl)ethenyl}-1,2-oxazol-4-yl)sulfonyl]cytisine (3).** Yield: 76%; Hygroscopic substance, light yellow color, mp 217-219 °C (2-PrOH). ^{1}H NMR (399.78 MHz, DMSO-d_6, δ, ppm, *J*/ 1.74-1.77 m (2H, H-31ax,31eq), 2.45 s (1H, H-21), 2.81 d (1H, H-20ax, 2J 11.6 Hz), 2.91 d (1H, H-20eq, 2J 11.6 Hz), 3.17 s (1H, H-29), 3.29-3.83 m (H-22ax,22eq,30ax,30eq) ppm. 6.15-6.17 m (1H, H-27), 6.22-6.24 m (1H, H-25), 7.30-7.33 m (1H, H-26) ppm. H-16,16,16 - 2.50 s, H-10,12 - 7.46-7.49, H-9,13 - 7.69-7.71 ppm. ^{13}C NMR (100.53 MHz, DMSO-d6) δ ppm 24.12 (C-31), 26.75 (C-21), 33.87 (C-29), 49.27 (C-30), 51.07 (C-22), 52.80 (C-20), 105.65 (C-27), 117.13 (C-25), 140.08 (C-26), 150.11 (C-28) и 162.62 (C-24), 13.01 (C-16), 112.57 (C-4), 129.58 (C-6), 130.28 и 131.64 (C-9,10,12,13), 133.96 (C-11), 138.52 (C-7,8), 150.11 (C-3), 158.52 (C-5).

Copies of NMR Spectra of Products



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17	1	6.18	0.16

Group	nH	Shift	Error
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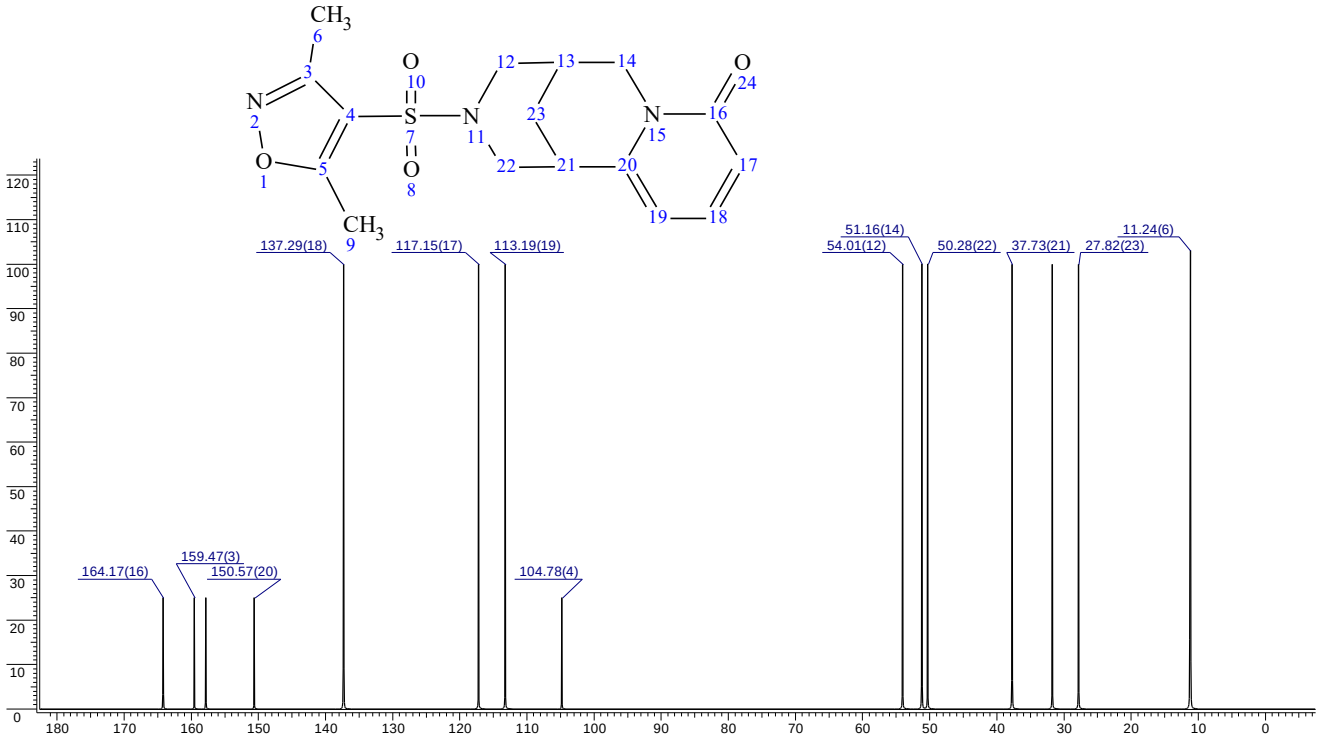
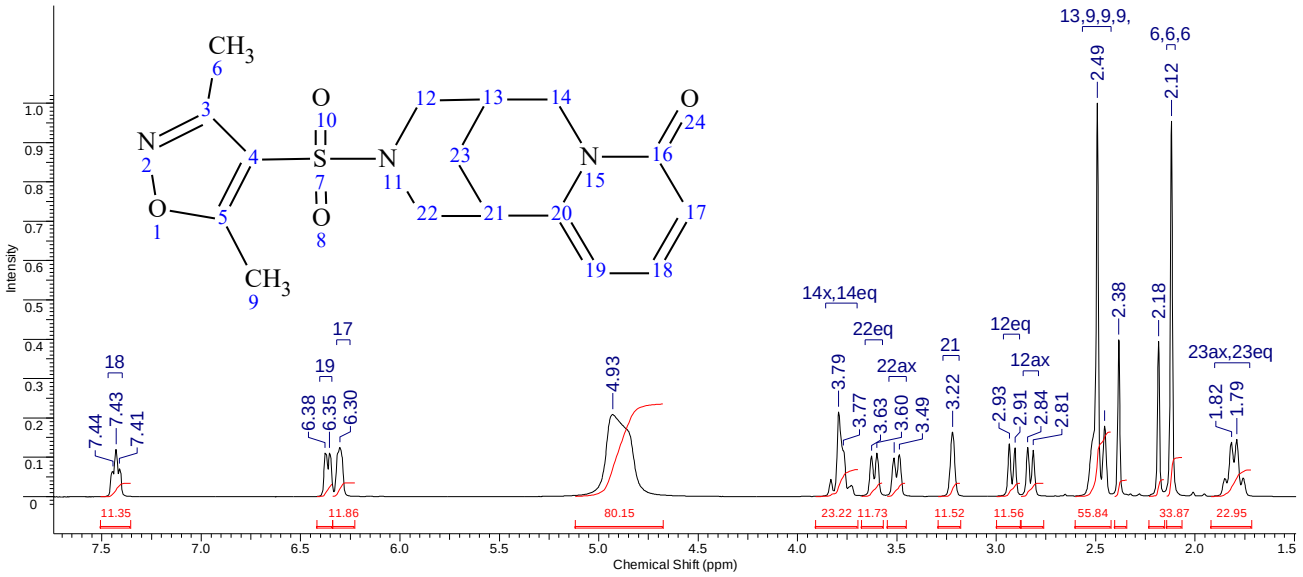


Carbon No.	CHn	Chem. Shifts	Conf. Limits
3	C	159.47	6.5
4	C	104.78	13.2
5	C	157.8	6.5
6	CH_3	11.24	2.9
9	CH_3	11.17	2.1
12	CH_2	54.01	1.7
13	CH	31.72	3.2
14	CH_2	51.16	1.1

Carbon No.	CHn	Chem. Shifts	Conf. Limits
16	C	164.17	2.5
17	CH	117.15	2.7
18	CH	137.29	1.4
19	CH	113.19	1.7
20	C	150.57	1
21	CH	37.73	4.4
22	CH_2	50.28	5.8
23	CH_2	27.82	5.3



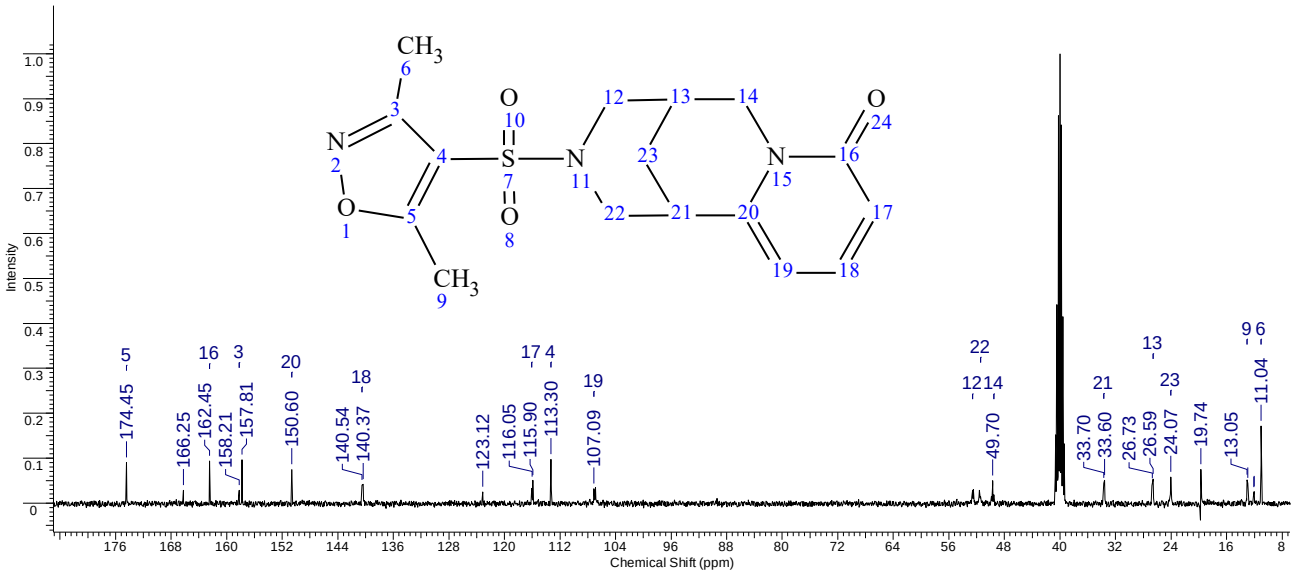
No.	(ppm)	(Hz)	Height
1	1.79	715.7	0.1453
2	1.82	726.3	0.1379
3	2.12	847.2	0.9546
4	2.18	872.8	0.3948
5	2.38	953.0	0.3988
6	2.45	981.4	0.1787
7	2.49	996.0	1.0000
8	2.81	1124.7	0.1171
9	2.84	1136.1	0.1251
10	2.91	1161.8	0.1235
11	2.93	1172.8	0.1339
12	3.22	1287.3	0.1637
13	3.49	1394.4	0.1066

No.	(ppm)	(Hz)	Height
14	3.51	1405.0	0.0976
15	3.60	1439.3	0.1106
16	3.63	1450.3	0.1028
17	3.77	1506.6	0.1168
18	3.79	1516.2	0.2145
19	4.93	1970.5	0.2085
20	6.30	2519.6	0.1246
21	6.35	2540.2	0.1100
22	6.38	2549.4	0.1107
23	7.41	2962.9	0.0703
24	7.43	2969.8	0.1198
25	7.44	2976.2	0.0634

No.	Annotation	(ppm)
1	23ax,23eq	[1.72 .. 1.90]
2	6,6,6	[2.10 .. 2.14]
3	13,9,9,9,	[2.42 .. 2.57]
4	12ax	[2.79 .. 2.86]
5	12eq	[2.88 .. 2.96]
6	21	[3.19 .. 3.27]
7	22ax	[3.45 .. 3.54]
8	22eq	[3.57 .. 3.66]
9	14x,14eq	[3.70 .. 3.86]
10	17	[6.25 .. 6.32]
11	19	[6.34 .. 6.40]
12	18	[7.40 .. 7.47]

No.	(ppm)	Value	Absolute Value
1	[6.34 .. 6.42]	11.168	1.09728e+1
2	[7.36 .. 7.51]	11.354	1.11557e+1
3	[3.45 .. 3.55]	11.492	1.12911e+1
4	[3.18 .. 3.29]	11.517	1.13161e+1
5	[2.76 .. 2.87]	11.548	1.13464e+1
6	[2.88 .. 3.00]	11.563	1.13607e+1
7	[3.57 .. 3.68]	11.731	1.15266e+1
8	[6.23 .. 6.34]	11.861	1.16539e+1

No.	(ppm)	Value	Absolute Value
9	[2.34 .. 2.40]	14.147	1.39000e+1
10	[2.15 .. 2.23]	14.747	1.44893e+1
11	[1.71 .. 1.92]	22.950	2.25498e+1
12	[3.70 .. 3.91]	23.218	2.28124e+1
13	[2.07 .. 2.14]	33.871	3.32797e+1
14	[2.42 .. 2.60]	55.839	5.48642e+1
15	[4.67 .. 5.12]	80.147	7.87480e+1



No.	(ppm)	(Hz)	Height
1	11.04	1110.0	0.1713
2	12.02	1208.8	0.0255
3	12.11	1217.4	0.0234
4	12.95	1301.7	0.0442
5	13.05	1312.3	0.0518
6	19.74	1984.2	0.0748
7	24.07	2419.3	0.0577
8	26.59	2673.3	0.0535
9	26.73	2686.7	0.0435
10	33.60	3377.8	0.0509
11	33.70	3387.4	0.0441
12	49.70	4995.7	0.0499
13	107.09	10765.6	0.0320

No.	(ppm)	(Hz)	Height
14	113.30	11389.6	0.0970
15	115.90	11651.3	0.0510
16	116.05	11665.6	0.0474
17	123.12	12376.8	0.0251
18	140.37	14110.7	0.0415
19	140.54	14127.9	0.0396
20	150.60	15139.1	0.0752
21	157.81	15863.7	0.0959
22	158.21	15904.0	0.0287
23	162.45	16330.5	0.0934
24	166.25	16712.0	0.0280
25	174.45	17536.2	0.0897

No.	Annotation	(ppm)
1	6	11.04
2	9	13.05
3	23	24.07
4	13	26.59
5	21	33.70
6	14	49.53
7	22	51.45
8	12	52.61

No.	Annotation	(ppm)
9	19	107.09
10	4	113.30
11	17	116.07
12	18	140.54
13	20	150.60
14	3	158.21
15	16	162.45
16	5	174.45

Fig. S1. ^{1}H (399.78 MHz, DMSO-d6) and ^{13}C (100.53 MHz, DMSO-d6) NMR Spectra of **2**

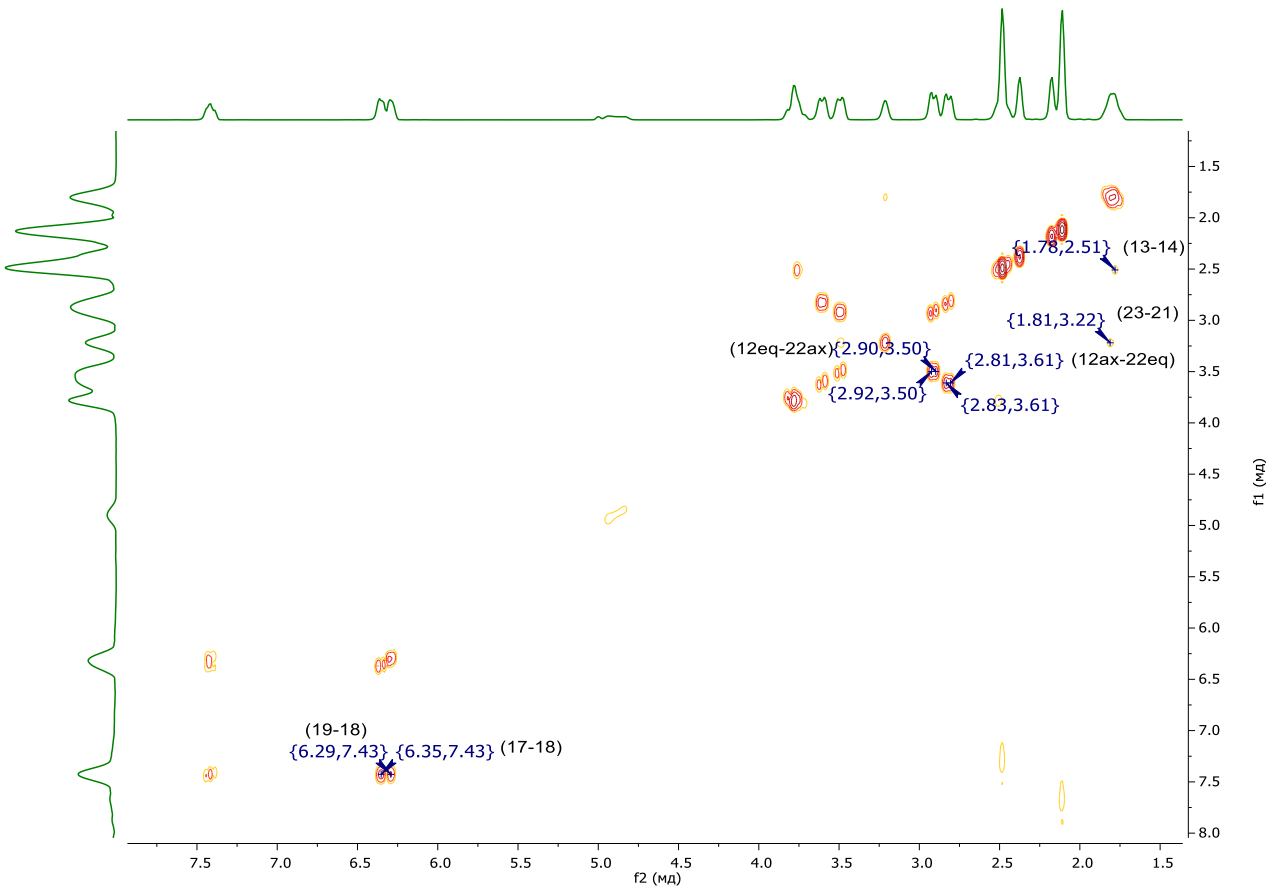


Fig. S2. Cosy of **2** in_DMSO

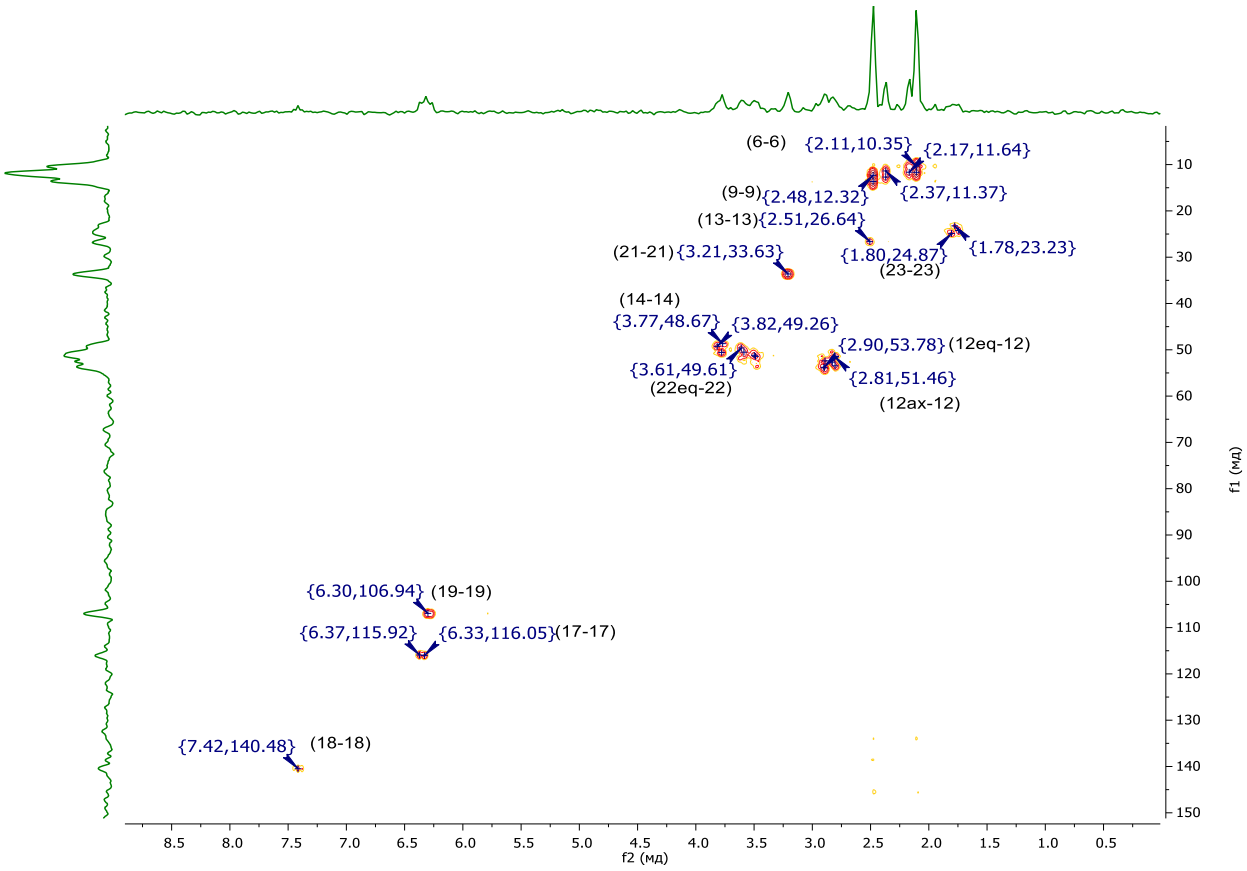


Fig. S3 Hmqc of **2** in_DMSO

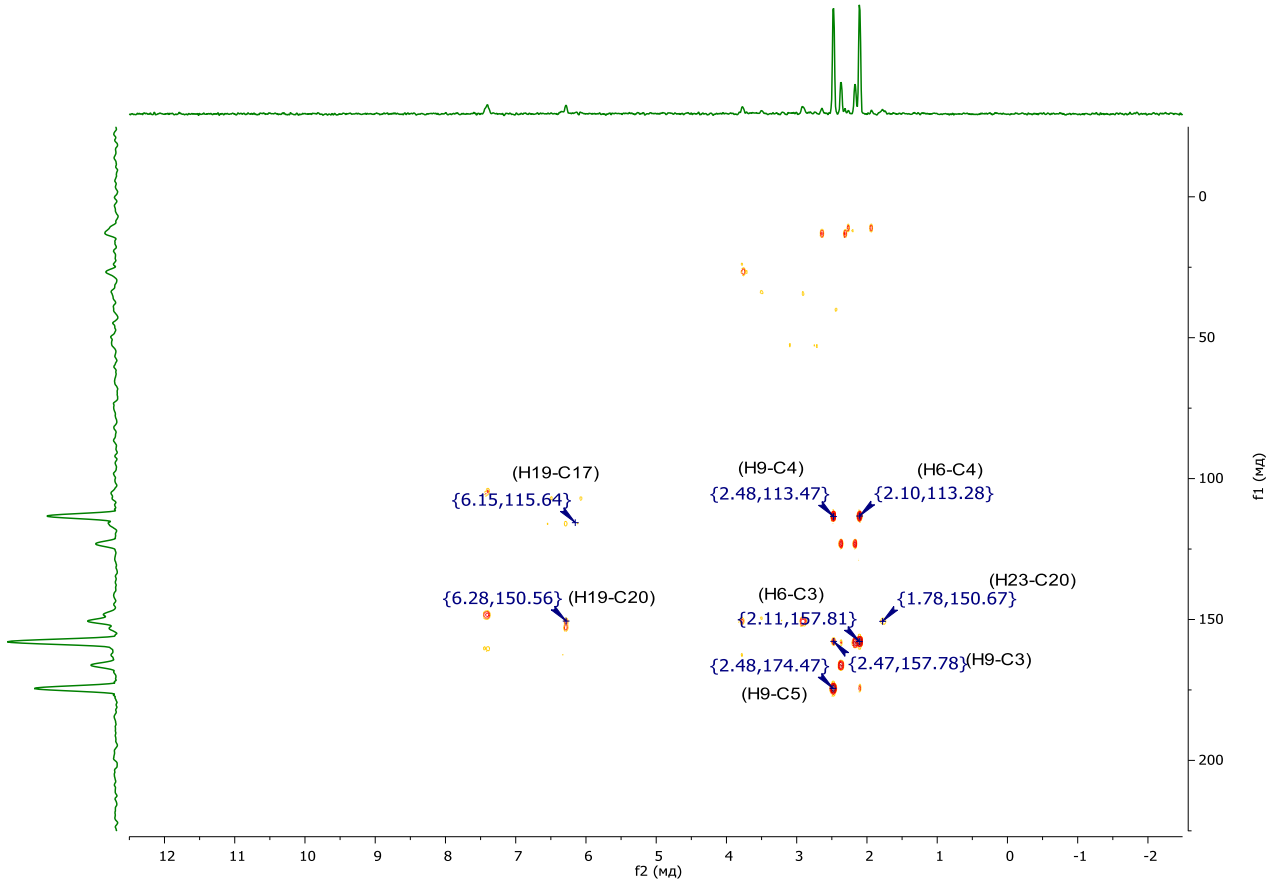
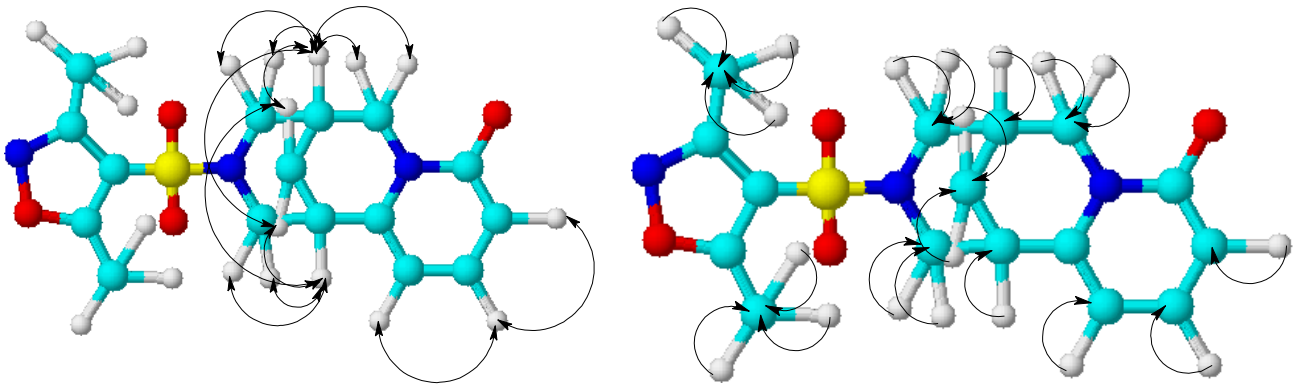
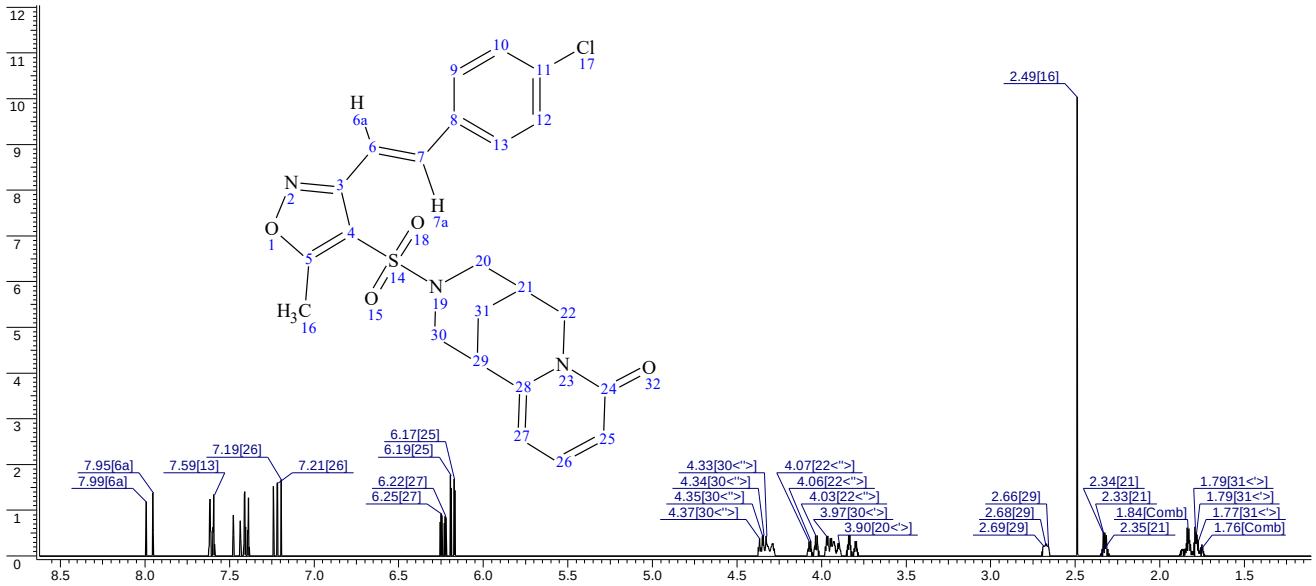


Fig. S4. Hmbc of **2** in_DMSO



a b

Fig. S5. The structural correlations in COSY (a) and HMQC (b) spectra of compound **2**



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7a	1	7.46	0.27
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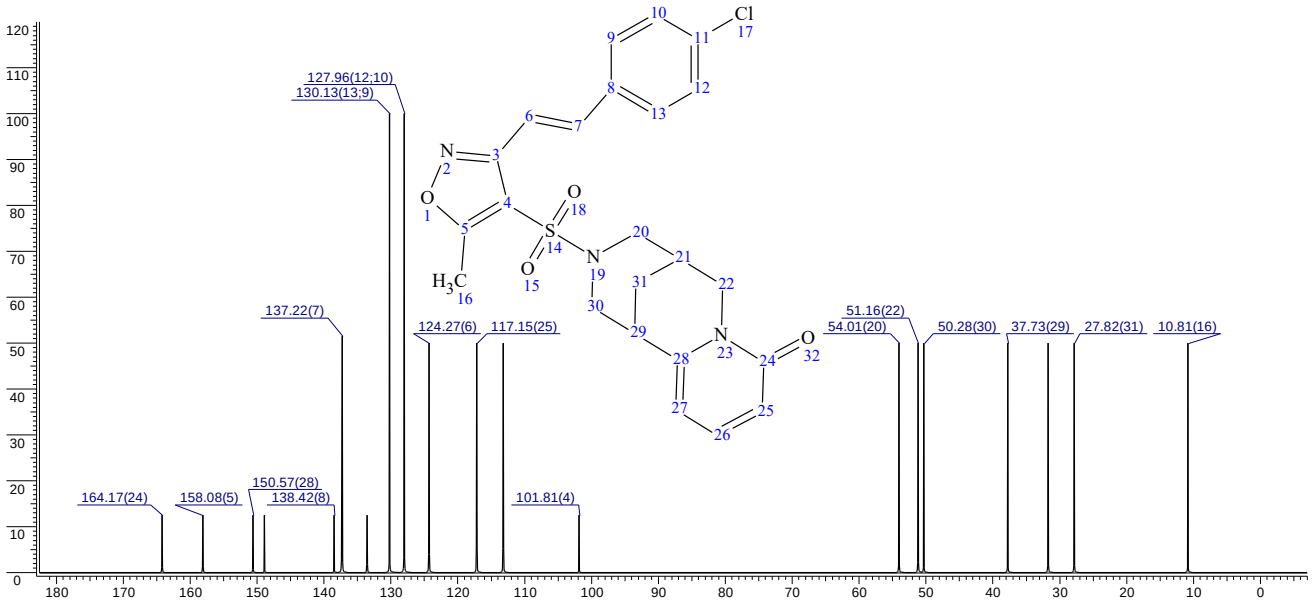
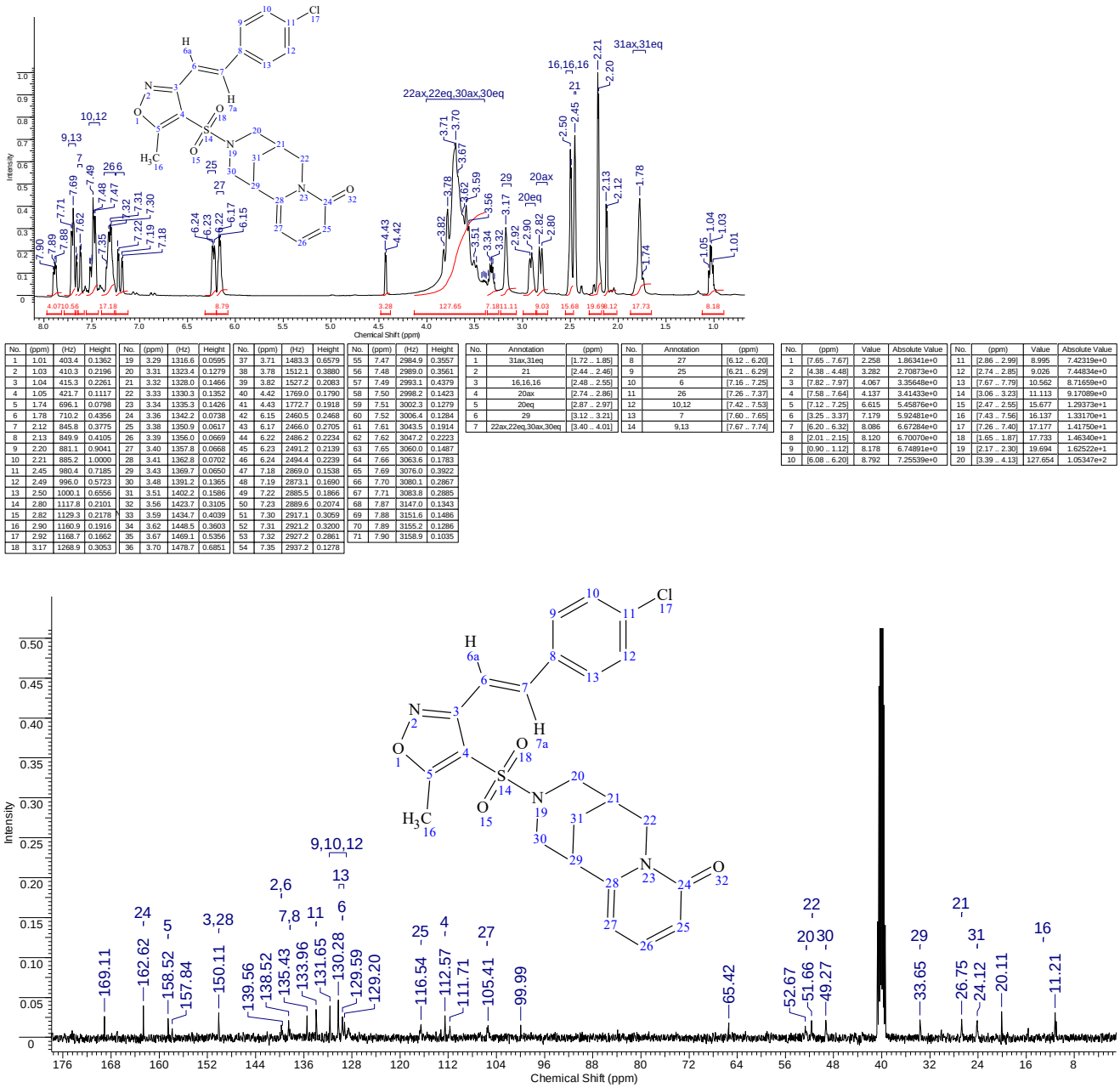
10	1	7.40	0.05
12	1	7.40	0.05
13	1	7.60	0.07
16	3	2.49	0.29
20<">	1	4.30	0.45
20<'>	1	3.91	0.44
21	1	2.33	0.26

Group	nH	Shift	Error
22<">	1	4.05	0.07
22<'>	1	3.82	0.04
25	1	6.18	0.16
26	1	7.22	0.11
27	1	6.24	0.22
29	1	2.67	0.20
30<">	1	4.35	0.45
30<'>	1	3.95	0.44
31<">	1	1.84	0.44
31<'>	1	1.77	0.44



Carbon No.	CHn	Chem. Shifts	Conf. Limits
3	C	148.83	6.7
4	C	101.81	13.2
5	C	158.08	6.5
6	CH	124.27	5.1
7	CH	137.22	3.1
8	C	138.42	1.1
9	CH	130.13	0.7
10	CH	127.96	1
11	C	133.54	1.3
12	CH	127.96	1
13	CH	130.13	0.7
16	CH_3	10.81	2

Carbon No.	CHn	Chem. Shifts	Conf. Limits
20	CH_2	54.01	1.7
21	CH	31.72	3.2
22	CH_2	51.16	1.1
24	C	164.17	2.5
25	CH	117.15	2.7
26	CH	137.29	1.4
27	CH	113.19	1.7
28	C	150.57	1
29	CH	37.73	4.4
30	CH_2	50.28	5.8
31	CH_2	27.82	5.3



No.	(ppm)	(Hz)	Height
1	1.01	403.4	0.1362
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3	1.04	415.3	0.2261
4	1.05	421.7	0.1117
5	1.74	696.1	0.0798
6	1.78	710.2	0.4356
7	2.12	845.8	0.3775
8	2.13	849.9	0.4105
9	2.20	881.1	0.9041
10	2.21	885.2	1.0000
11	2.45	980.4	0.7185
12	2.49	996.0	0.5723
13	2.50	1000.1	0.6556
14	2.80	1117.8	0.2101
15	2.82	1129.3	0.2178
16	2.90	1160.9	0.1916
17	2.92	1168.7	0.1662
18	3.17	1268.9	0.3053

No.	(ppm)	(Hz)	Height
19	3.29	1316.6	0.0595
20	3.31	1323.4	0.1279
21	3.32	1328.0	0.1466
22	3.33	1330.3	0.1352
23	3.34	1335.3	0.1426
24	3.36	1342.2	0.0738
25	3.38	1350.9	0.0617
26	3.39	1356.0	0.0669
27	3.40	1357.8	0.0668
28	3.41	1362.8	0.0702
29	3.43	1369.7	0.0650
30	3.48	1391.2	0.1365
31	3.51	1402.2	0.1586
32	3.56	1423.7	0.3105
33	3.59	1434.7	0.4039
34	3.62	1448.5	0.3603
35	3.67	1469.1	0.5356
36	3.70	1478.7	0.6851

No.	(ppm)	(Hz)	Height
37	3.71	1483.3	0.6579
38	3.78	1512.1	0.3880
39	3.82	1527.2	0.2083
40	4.42	1769.0	0.1790
41	4.43	1772.7	0.1918
42	6.15	2460.5	0.2468
43	6.17	2466.0	0.2705
44	6.22	2486.2	0.2234
45	6.23	2491.2	0.2139
46	6.24	2494.4	0.2239
47	7.18	2869.0	0.1538
48	7.19	2873.1	0.1690
49	7.22	2885.5	0.1866
50	7.23	2889.6	0.2074
51	7.30	2917.1	0.3059
52	7.31	2921.2	0.3200
53	7.32	2927.2	0.2861
54	7.35	2937.2	0.1278

No.	(ppm)	(Hz)	Height
55	7.47	2984.9	0.3557
56	7.48	2989.0	0.3561
57	7.49	2993.1	0.4379
58	7.50	2998.2	0.1423
59	7.51	3002.3	0.1279
60	7.52	3006.4	0.1284
61	7.61	3043.5	0.1914
62	7.62	3047.2	0.2223
63	7.65	3060.0	0.1487
64	7.66	3063.6	0.1783
65	7.69	3076.0	0.3922
66	7.70	3080.1	0.2867
67	7.71	3083.8	0.2885
68	7.87	3147.0	0.1343
69	7.88	3151.6	0.1486
70	7.89	3155.2	0.1286
71	7.90	3158.9	0.1035

No.	Annotation	(ppm)
1	31ax,31eq	[1.72 .. 1.85]
2	21	[2.44 .. 2.46]
3	16,16,16	[2.48 .. 2.55]
4	20ax	[2.74 .. 2.86]
5	20eq	[2.87 .. 2.97]
6	29	[3.12 .. 3.21]
7	22ax,22eq,30ax,30eq	[3.40 .. 4.01]

No.	Annotation	(ppm)
8	27	[6.12 .. 6.20]
9	25	[6.21 .. 6.29]
10	6	[7.16 .. 7.25]
11	26	[7.26 .. 7.37]
12	10,12	[7.42 .. 7.53]
13	7	[7.60 .. 7.65]
14	9,13	[7.67 .. 7.74]

No.	(ppm)	Value	Absolute Value
1	[7.65 .. 7.67]	2.258	1.86341e+0
2	[4.38 .. 4.48]	3.282	2.70873e+0
3	[7.82 .. 7.97]	4.067	3.35648e+0
4	[7.58 .. 7.64]	4.137	3.41433e+0
5	[7.12 .. 7.25]	6.615	5.45876e+0
6	[3.25 .. 3.37]	7.179	5.92481e+0
7	[6.20 .. 6.32]	8.086	6.67284e+0
8	[2.01 .. 2.15]	8.120	6.70070e+0
9	[0.90 .. 1.12]	8.178	6.74891e+0
10	[6.08 .. 6.20]	8.792	7.25539e+0

No.	(ppm)	Value	Absolute Value
11	[2.86 .. 2.99]	8.995	7.42319e+0
12	[2.74 .. 2.85]	9.026	7.44834e+0
13	[7.67 .. 7.79]	10.562	8.71659e+0
14	[3.06 .. 3.23]	11.113	9.17089e+0
15	[2.47 .. 2.55]	15.677	1.29373e+1
16	[7.43 .. 7.56]	16.137	1.33170e+1
17	[7.26 .. 7.40]	17.177	1.41750e+1
18	[1.65 .. 1.87]	17.733	1.46340e+1
19	[2.17 .. 2.30]	19.694	1.62522e+1
20	[3.39 .. 4.13]	127.654	1.05347e+2

No.	(ppm)	(Hz)	Height
1	11.21	1127.3	0.0309
2	20.11	2021.5	0.0324
3	24.12	2425.1	0.0210
4	26.75	2688.6	0.0227
5	33.65	3382.6	0.0218
6	49.27	4952.5	0.0216
7	51.66	5193.1	0.0209
8	52.67	5294.7	0.0141
9	65.42	6576.2	0.0179
10	99.99	10051.6	0.0153
11	105.41	10596.0	0.0150
12	111.71	11229.5	0.0143
13	112.57	11315.8	0.0271
14	116.54	11715.5	0.0164

No.	(ppm)	(Hz)	Height
15	129.20	12988.3	0.0188
16	129.59	13026.7	0.0260
17	130.28	13096.6	0.0467
18	131.65	13233.7	0.0392
19	133.96	13466.6	0.0349
20	135.43	13614.2	0.0271
21	138.52	13924.7	0.0212
22	139.56	14029.2	0.0088
23	150.11	15090.2	0.0305
24	157.84	15866.6	0.0111
25	158.52	15935.6	0.0235
26	162.62	16347.7	0.0399
27	169.11	16999.5	0.0264

No.	Annotation	(ppm)
1	16	13.14
2	31	24.12
3	21	26.75
4	29	33.65
5	30	49.27
6	22	51.52
7	20	52.54
8	27	105.57
9	4	112.57
10	25	116.54

No.	Annotation	(ppm)
11	9,10,12	[128.92 .. 131.75]
12	13	[129.32 .. 130.13]
13	6	129.59
14	11	133.96
15	7,8	138.31
16	2,6	139.70
17	3,28	150.11
18	5	158.52
19	24	162.62

Fig. S6. ^{1}H (399.78 MHz, DMSO-d6) and ^{13}C (100.53 MHz, DMSO-d6) NMR Spectra of **3**

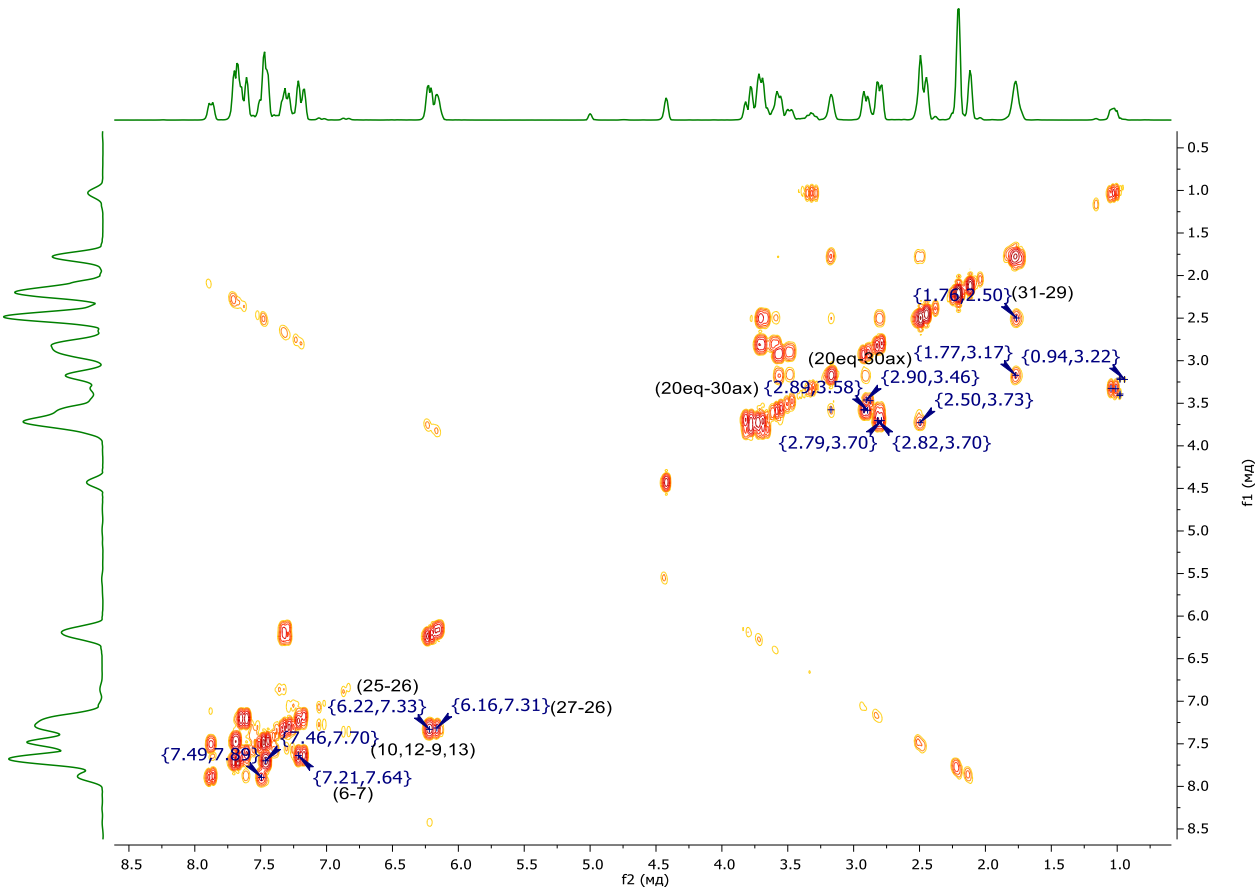


Fig. S7. Cosy of **3** in_DMSO

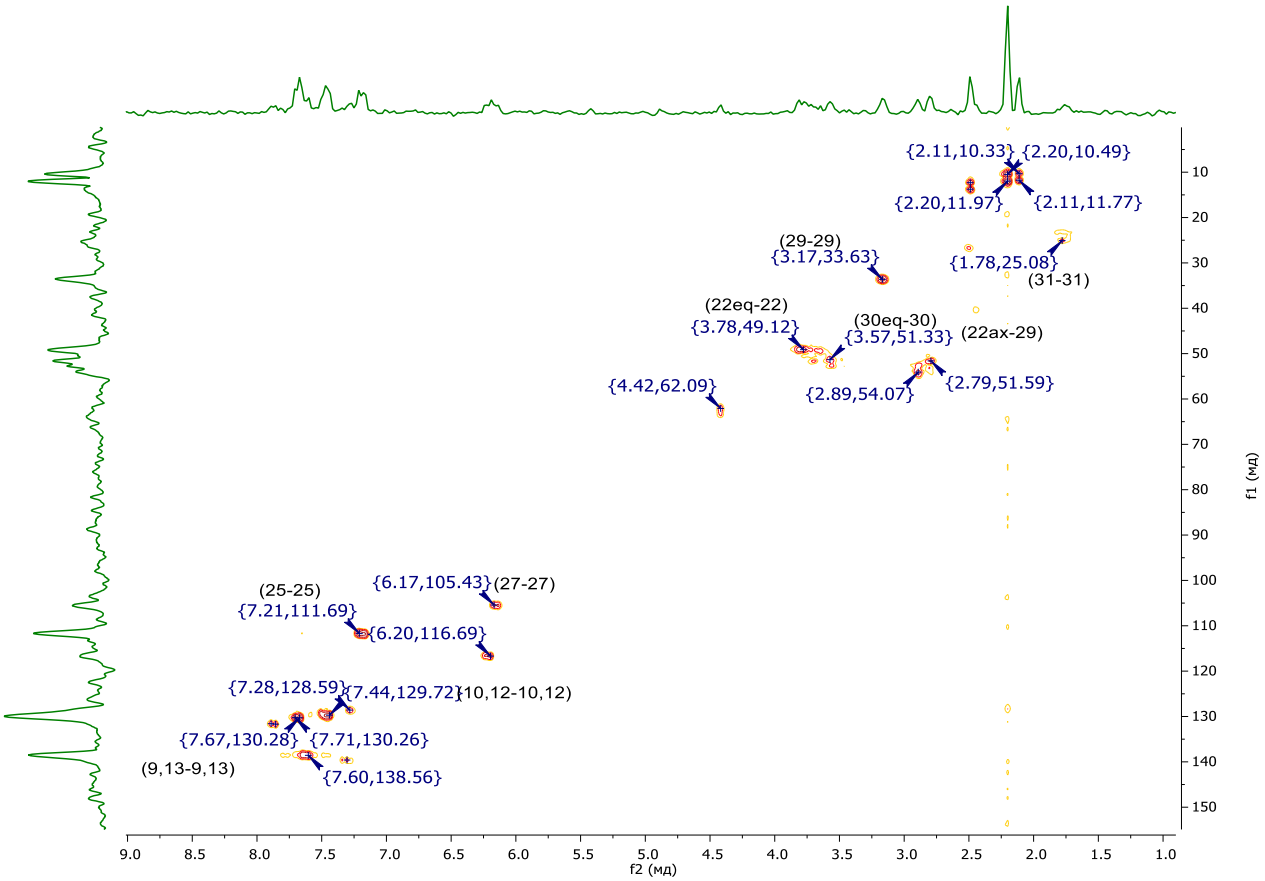


Fig. S8 Hmqc of **3** in_DMSO

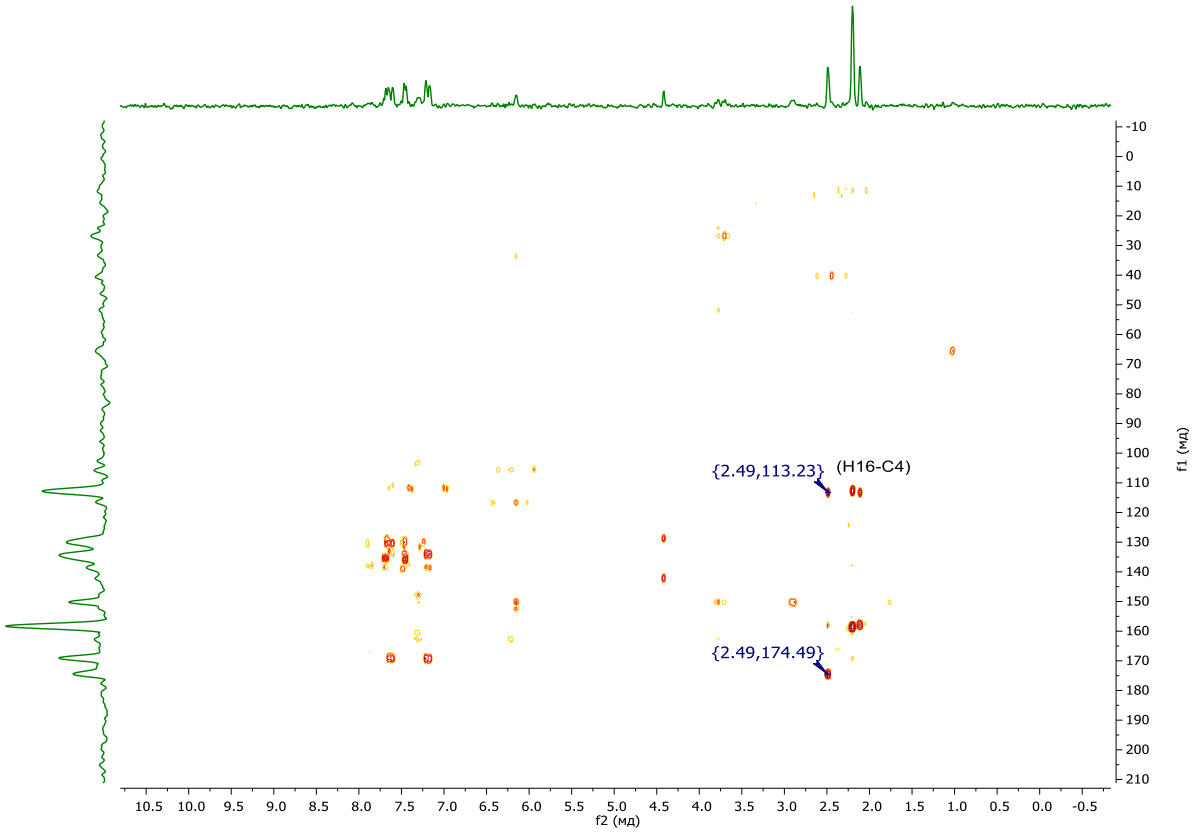
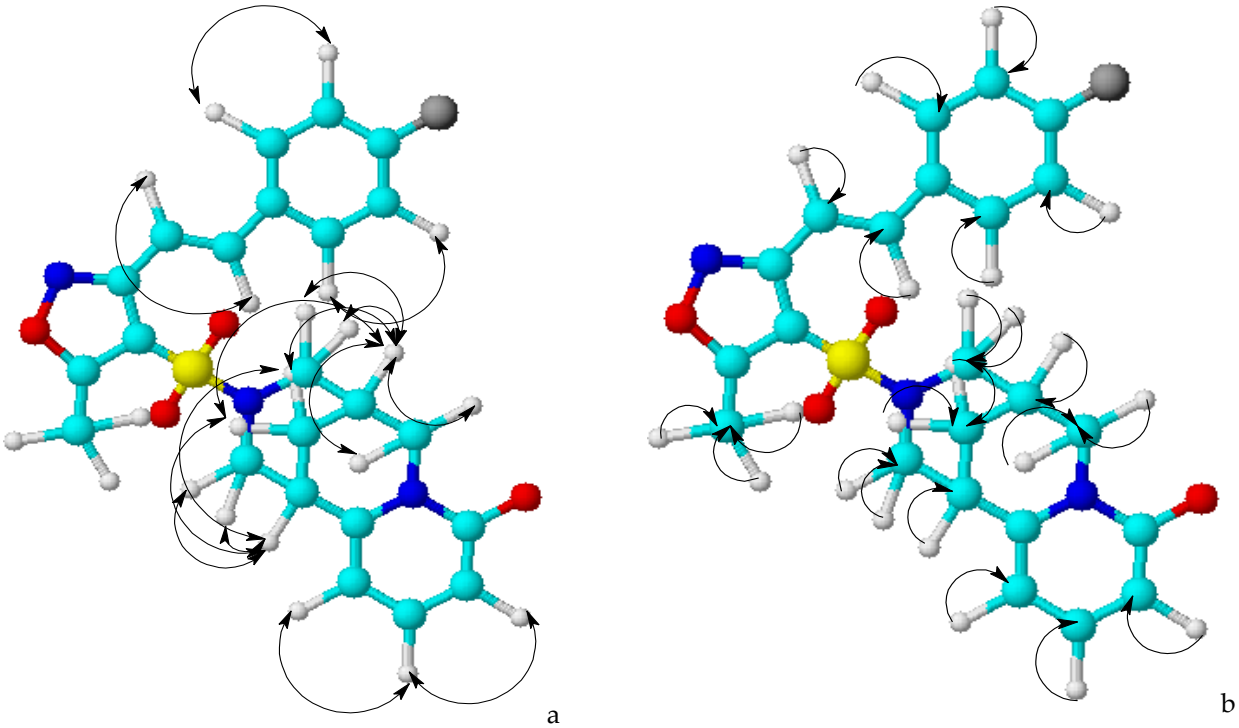


Fig. S9. Hmbc of **3** in_DMSO



a b

Fig. S10. The structural correlations in COSY (a) and HMQC (b) spectra of compound **3**

Copies of MS Spectra of Products

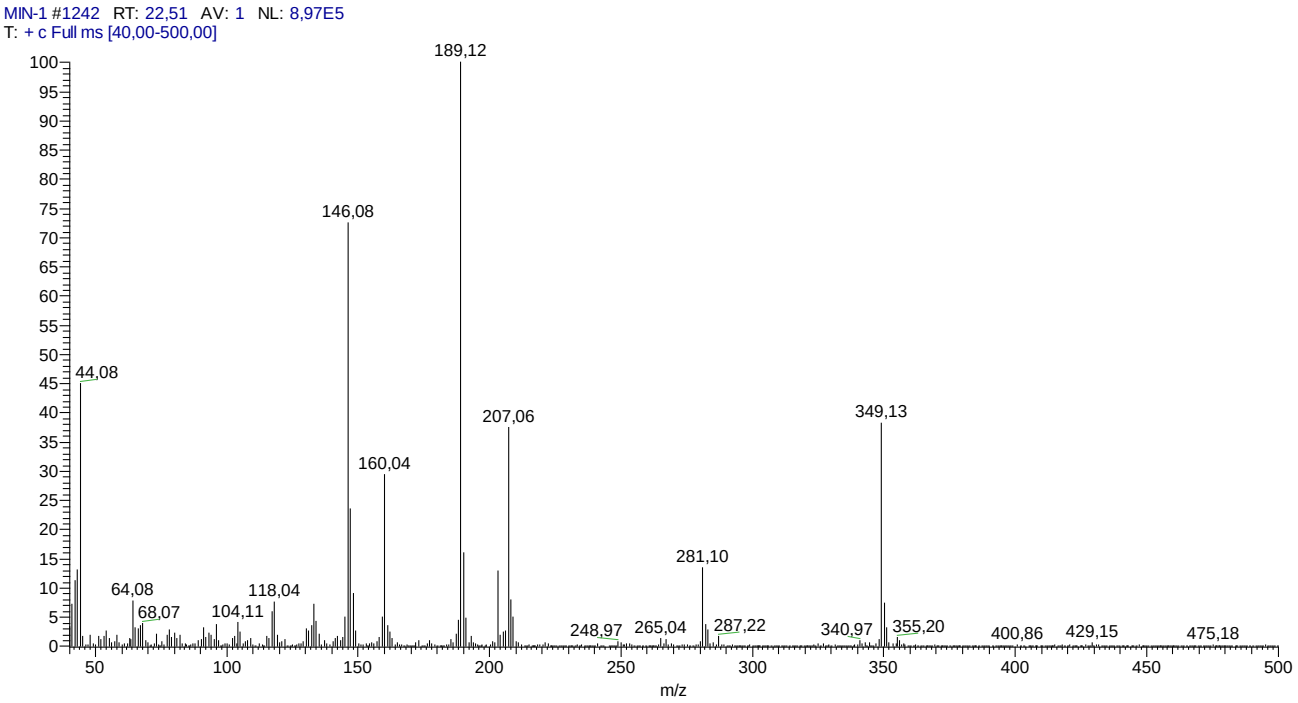


Fig. S11. Mass spectrum of **2**

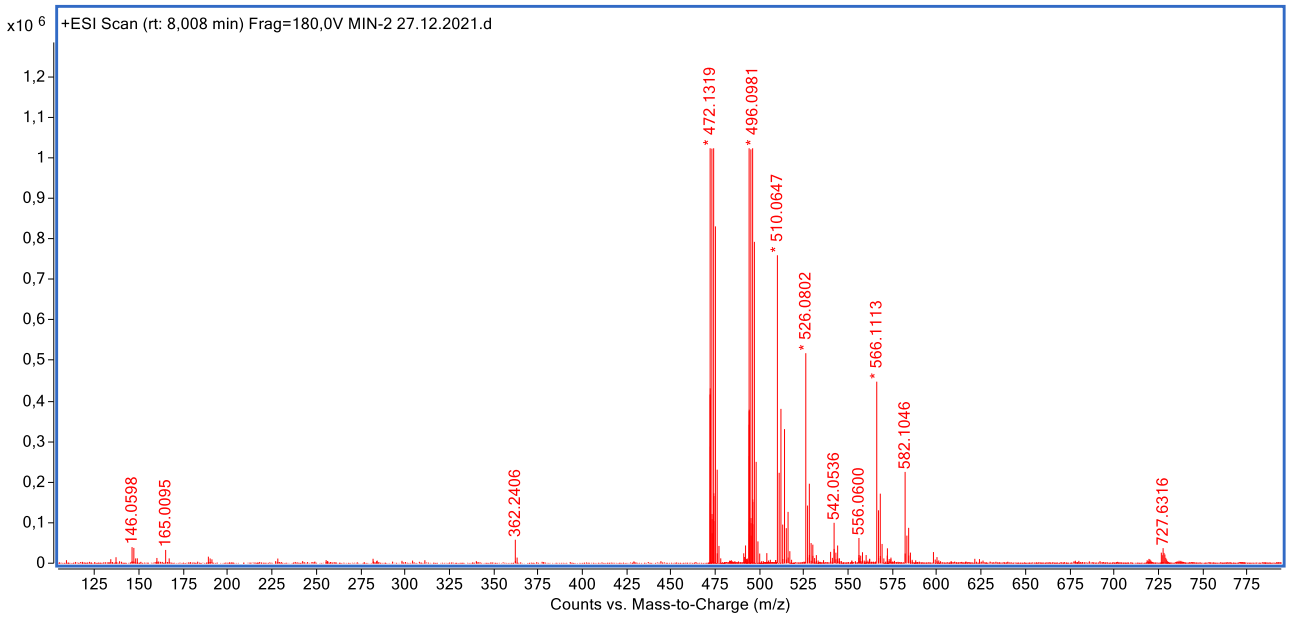


Fig. S12. Mass spectrum of **3**

X-Ray Structural Study of Product 2

The cell parameters and intensities of 8569 pictures (3147 independent, Rint = 0.029) have been measured on Bruker KARRA APEX2 CCD (MoKα) diffractometer, graphite monochromator, φ,θ-scanning, 2.721°< θ < 25.990°) at a temperature of 296 K.

Crystals 2 has been monoclinic, a space group P21, a = 6.6291(3) Å, b = 8.9064(5) Å, c = 13.9604(7) Å, β = 98.093(2)°, V= 816.03(7) A3, Z= 2 (C16H19N3O4S), M = 349.40 g/mol, dcalc.= 1.422 g/cm3, μ = 0.225 mm-1. The array of measured intensities has been processed. Ab-sorption corrections have been performed using the SAINT [24] and SADABS pro-grams included in APEX2 software package (multiscan, Tmin = 0.871, Tmax = 0.904).

Structure has been decoded with a direct method. Positions of the non-hydrogen atoms have been clarified in the anisotropic approximation by the full matrix MNA. Hydrogen atoms have been placed in the geometrically calculated positions. Their posi-tions have been refined in the isotropic approximation with the fixed positional and thermal parameters (a “rider” model). Calculations have used 2944 independent pictures with I>2σ(I). The number of the refined parameters has been 219. Final divergence factors have been R1 = 0.0317, wR2 = 0.0749 for pictures with I>2σ(I), R1= 0.0359, wR2 = 0.0784 for all pictures, GOOF = 0.990. The residual density peaks: Δρ = 0.184 e/A3 and -0.214 e/A3. Structure has been decoded and refined with using the programs of SHELXT-2014/5 and SHELXL-2018/3. The X-ray diffraction data in the form of a CIF file has been deposited in the Cambridge Crystallographic Data Center (CCDC 2168324).

Table 1. Bond lengths (d, Å) in molecule **2**

Bond	d	Bond	d
S(1)-O(3)	1.424(2)	C(9)-C(13)	1.523(4)
S(1)-O(2)	1.427(2)	C(9)-H(9A)	0.9800
S(1)-N(12)	1.634(2)	C(10)-H(10A)	0.9700
S(1)-C(4')	1.749(3)	C(10)-H(10B)	0.9700
O(1)-C(2)	1.231(3)	C(11)-N(12)	1.472(4)
N(1)-C(6)	1.372(3)	C(11)-H(11A)	0.9700
N(1)-C(2)	1.400(3)	C(11)-H(11B)	0.9700
N(1)-C(10)	1.487(3)	N(12)-C(13)	1.484(3)
C(2)-C(3)	1.427(4)	C(13)-H(13A)	0.9700
C(3)-C(4)	1.348(5)	C(13)-H(13B)	0.9700
C(3)-H(3B)	0.9300	O(1')-C(5')	1.334(4)
C(4)-C(5)	1.396(4)	O(1')-N(2')	1.418(4)
C(4)-H(4A)	0.9300	N(2')-C(3')	1.304(4)
C(5)-C(6)	1.362(4)	C(3')-C(4')	1.412(4)
C(5)-H(5A)	0.9300	C(3')-C(6')	1.475(6)
C(6)-C(7)	1.500(4)	C(4')-C(5')	1.372(4)
C(7)-C(8)	1.526(4)	C(5')-C(7')	1.480(5)
C(7)-C(11)	1.532(4)	C(6')-H(6'A)	0.9600
C(7)-H(7A)	0.9800	C(6')-H(6'B)	0.9600
C(8)-C(9)	1.515(5)	C(6')-H(6'C)	0.9600
C(8)-H(8A)	0.9700	C(7')-H(7'A)	0.9600
C(8)-H(8B)	0.9700	C(7')-H(7'B)	0.9600
C(9)-C(10)	1.512(4)	C(7')-H(7'C)	0.9600

Table 2. Bond angles (ω, deg.) in molecule **2**

Angle	ω	Angle	ω
O(3)-S(1)-O(2)	120.01(14)	N(1)-C(10)-H(10A)	108.6
O(3)-S(1)-N(12)	107.74(13)	C(9)-C(10)-H(10A)	108.6
O(2)-S(1)-N(12)	107.29(13)	N(1)-C(10)-H(10B)	108.6
O(3)-S(1)-C(4')	106.65(14)	C(9)-C(10)-H(10B)	108.6
O(2)-S(1)-C(4')	107.25(14)	H(10A)-C(10)-H(10B)	107.6
N(12)-S(1)-C(4')	107.31(12)	N(12)-C(11)-C(7)	108.9(2)
C(6)-N(1)-C(2)	123.0(2)	N(12)-C(11)-H(11A)	109.9
C(6)-N(1)-C(10)	123.5(2)	C(7)-C(11)-H(11A)	109.9
C(2)-N(1)-C(10)	113.4(2)	N(12)-C(11)-H(11B)	109.9
O(1)-C(2)-N(1)	119.6(3)	C(7)-C(11)-H(11B)	109.9
O(1)-C(2)-C(3)	124.8(3)	H(11A)-C(11)-H(11B)	108.3
N(1)-C(2)-C(3)	115.6(3)	C(11)-N(12)-C(13)	113.4(2)
C(4)-C(3)-C(2)	121.2(3)	C(11)-N(12)-S(1)	117.54(17)
C(4)-C(3)-H(3B)	119.4	C(13)-N(12)-S(1)	115.02(19)
C(2)-C(3)-H(3B)	119.4	N(12)-C(13)-C(9)	109.5(2)
C(3)-C(4)-C(5)	120.8(3)	N(12)-C(13)-H(13A)	109.8
C(3)-C(4)-H(4A)	119.6	C(9)-C(13)-H(13A)	109.8
C(5)-C(4)-H(4A)	119.6	N(12)-C(13)-H(13B)	109.8
C(6)-C(5)-C(4)	120.1(3)	C(9)-C(13)-H(13B)	109.8
C(6)-C(5)-H(5A)	120.0	H(13A)-C(13)-H(13B)	108.2
C(4)-C(5)-H(5A)	120.0	C(5')-O(1')-N(2')	108.7(2)
C(5)-C(6)-N(1)	119.3(2)	C(3')-N(2')-O(1')	106.7(3)
C(5)-C(6)-C(7)	122.0(2)	N(2')-C(3')-C(4')	110.1(3)
N(1)-C(6)-C(7)	118.7(2)	N(2')-C(3')-C(6')	118.5(3)
C(6)-C(7)-C(8)	110.9(2)	C(4')-C(3')-C(6')	131.4(3)
C(6)-C(7)-C(11)	111.1(2)	C(5')-C(4')-C(3')	105.9(3)
C(8)-C(7)-C(11)	109.8(2)	C(5')-C(4')-S(1)	126.7(2)
C(6)-C(7)-H(7A)	108.3	C(3')-C(4')-S(1)	127.4(2)
C(8)-C(7)-H(7A)	108.3	O(1')-C(5')-C(4')	108.6(3)
C(11)-C(7)-H(7A)	108.3	O(1')-C(5')-C(7')	117.0(3)
C(9)-C(8)-C(7)	106.5(2)	C(4')-C(5')-C(7')	134.4(3)
C(9)-C(8)-H(8A)	110.4	C(3')-C(6')-H(6'A)	109.5
C(7)-C(8)-H(8A)	110.4	C(3')-C(6')-H(6'B)	109.5
C(9)-C(8)-H(8B)	110.4	H(6'A)-C(6')-H(6'B)	109.5
C(7)-C(8)-H(8B)	110.4	C(3')-C(6')-H(6'C)	109.5
H(8A)-C(8)-H(8B)	108.6	H(6'A)-C(6')-H(6'C)	109.5
C(10)-C(9)-C(8)	111.1(2)	H(6'B)-C(6')-H(6'C)	109.5
C(10)-C(9)-C(13)	112.2(2)	C(5')-C(7')-H(7'A)	109.5
C(8)-C(9)-C(13)	110.4(2)	C(5')-C(7')-H(7'B)	109.5
C(10)-C(9)-H(9A)	107.6	H(7'A)-C(7')-H(7'B)	109.5
C(8)-C(9)-H(9A)	107.6	C(5')-C(7')-H(7'C)	109.5
C(13)-C(9)-H(9A)	107.6	H(7'A)-C(7')-H(7'C)	109.5
N(1)-C(10)-C(9)	114.4(2)	H(7'B)-C(7')-H(7'C)	109.5

Table 3. Torsion angles (τ, deg.) in molecule **2**

Angle	τ	Angle	τ
C(6)-N(1)-C(2)-O(1)	179.4(2)	O(3)-S(1)-N(12)-C(11)	168.7(2)
C(10)-N(1)-C(2)-O(1)	1.6(4)	O(2)-S(1)-N(12)-C(11)	38.1(2)
C(6)-N(1)-C(2)-C(3)	-0.9(4)	C(4')-S(1)-N(12)-C(11)	-76.8(2)
C(10)-N(1)-C(2)-C(3)	-178.7(2)	O(3)-S(1)-N(12)-C(13)	-53.9(2)
O(1)-C(2)-C(3)-C(4)	-178.3(3)	O(2)-S(1)-N(12)-C(13)	175.6(2)
N(1)-C(2)-C(3)-C(4)	2.0(4)	C(4')-S(1)-N(12)-C(13)	60.6(2)
C(2)-C(3)-C(4)-C(5)	-1.2(5)	C(11)-N(12)-C(13)-C(9)	-56.2(3)
C(3)-C(4)-C(5)-C(6)	-0.9(5)	S(1)-N(12)-C(13)-C(9)	164.5(2)
C(4)-C(5)-C(6)-N(1)	1.9(4)	C(10)-C(9)-C(13)-N(12)	-66.1(3)
C(4)-C(5)-C(6)-C(7)	-177.7(3)	C(8)-C(9)-C(13)-N(12)	58.4(3)
C(2)-N(1)-C(6)-C(5)	-1.1(4)	C(5')-O(1')-N(2')-C(3')	-0.2(4)
C(10)-N(1)-C(6)-C(5)	176.5(3)	O(1')-N(2')-C(3')-C(4')	0.4(4)
C(2)-N(1)-C(6)-C(7)	178.6(2)	O(1')-N(2')-C(3')-C(6')	178.5(4)
C(10)-N(1)-C(6)-C(7)	-3.8(3)	N(2')-C(3')-C(4')-C(5')	-0.4(4)
C(5)-C(6)-C(7)-C(8)	-148.2(3)	C(6')-C(3')-C(4')-C(5')	-178.2(4)
N(1)-C(6)-C(7)-C(8)	32.1(3)	N(2')-C(3')-C(4')-S(1)	178.4(2)
C(5)-C(6)-C(7)-C(11)	89.3(3)	C(6')-C(3')-C(4')-S(1)	0.6(6)
N(1)-C(6)-C(7)-C(11)	-90.3(3)	O(3)-S(1)-C(4')-C(5')	29.7(3)
C(6)-C(7)-C(8)-C(9)	-60.9(3)	O(2)-S(1)-C(4')-C(5')	159.4(3)
C(11)-C(7)-C(8)-C(9)	62.3(3)	N(12)-S(1)-C(4')-C(5')	-85.6(3)
C(7)-C(8)-C(9)-C(10)	63.5(3)	O(3)-S(1)-C(4')-C(3')	-148.9(3)
C(7)-C(8)-C(9)-C(13)	-61.6(3)	O(2)-S(1)-C(4')-C(3')	-19.1(3)
C(6)-N(1)-C(10)-C(9)	5.7(4)	N(12)-S(1)-C(4')-C(3')	95.9(3)
C(2)-N(1)-C(10)-C(9)	-176.5(2)	N(2')-O(1')-C(5')-C(4')	0.0(3)
C(8)-C(9)-C(10)-N(1)	-36.3(3)	N(2')-O(1')-C(5')-C(7')	-179.3(3)
C(13)-C(9)-C(10)-N(1)	87.8(3)	C(3')-C(4')-C(5')-O(1')	0.3(3)
C(6)-C(7)-C(11)-N(12)	63.2(3)	S(1)-C(4')-C(5')-O(1')	-178.6(2)
C(8)-C(7)-C(11)-N(12)	-59.9(3)	C(3')-C(4')-C(5')-C(7')	179.3(4)
C(7)-C(11)-N(12)-C(13)	56.9(3)	S(1)-C(4')-C(5')-C(7')	0.5(5)
C(7)-C(11)-N(12)-S(1)	-164.97(18)		