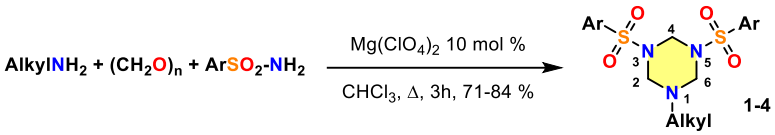
crystals

MDPI

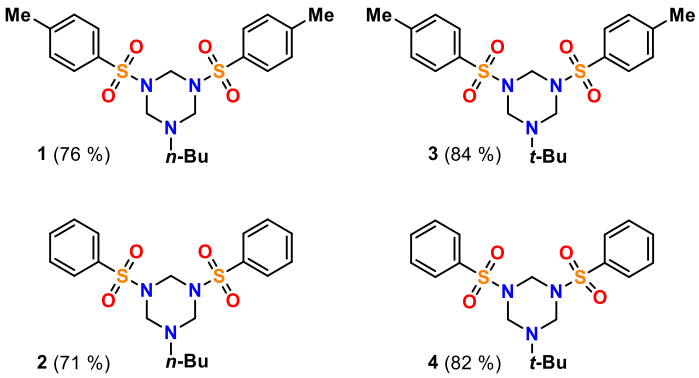
Supplementary information for the paper

Method for preparation of 1,3,5–triazinanes (1–4).



To a solution of 1.57 mmol of the corresponding sulphonamide in chloroform (5 mL), 90 mg (3.00 mmol) of paraformaldehyde (based on formaldehyde) and 36 mg (0.157 mmol) of $Mg(ClO_4)_2$ were added, followed by the addition of 0.8 mmol of appropriate amine. The reaction mixture was further stirred under reflux for 3 h, cooled to r.t, and filtered through a fritted glass filter with a thin layer of silica gel. The filtrate was concentrated to approximately 0.5–0.7 mL under reduced pressure, and diethyl ether (5 mL) was added to the residue. The obtained solution was cooled to −20 °C, and formed solids were filtered off, washed with a small amount of cold ethanol, dried on air, and additionally dried in a vacuum desiccator over P_2O_5.

Conditions for crystal growth were $CHCl_3$–hexane, open vessel, 1:1, r.t for compound **1** and $CDCl_3$, open NMR tube, r.t for compounds **2–4**.



1–Butyl–3,5–ditosyl–1,3,5–triazinane (1). Yield 76 %, m.p. 129–130 °C, white powder. ^{1}H NMR (600.2 MHz, $CDCl_3$) δ 7.69 (d, *J*~8.4 Hz, 4H$_{arom.}$), 7.31 (d, *J*~8.4 Hz, 4H$_{arom.}$), 4.76 (s, 2H, CH_2), 4.20 (s, 4H, 2CH_2), 2.42 (s, 6H, 2CH_3), 2.20–2.14 (m, 2H, CH_2), 1.24–1.17 (m, 2H, CH_2), 1.07 (dq, *J*~14.5, 7.4 Hz, 2H, CH_2), 0.79 (t, *J*~7.4 Hz, 3H, CH_3). ^{13}C NMR (150.9 MHz, $CDCl_3$) δ 144.06 (2C$_{quat.}$), 136.16 (2C$_{quat.}$), 129.95 (4CH$_{arom.}$), 127.26 (4CH$_{arom.}$), 65.66 (2CH_2), 60.96 (CH_2), 50.08 (CH_2), 29.56 (CH_2), 21.63 (2CH_3), 20.07 (CH_2), 13.83 (CH_3). IR (KBr): 3080, 3030 (HC=), 2952, 2940, 2865 (alkyl), 1356, 1236 (SO_2N). MS (ESI): *m*/*z* = 452.2 [M + H$^+$]. Anal. Calcd for $C_{21}H_{29}N_3O_4S_2$: C, 55.85; H, 6.47; N, 9.30; S, 14.20. Found: C, 56.11; H, 6.30; N, 9.19; S, 14.17.

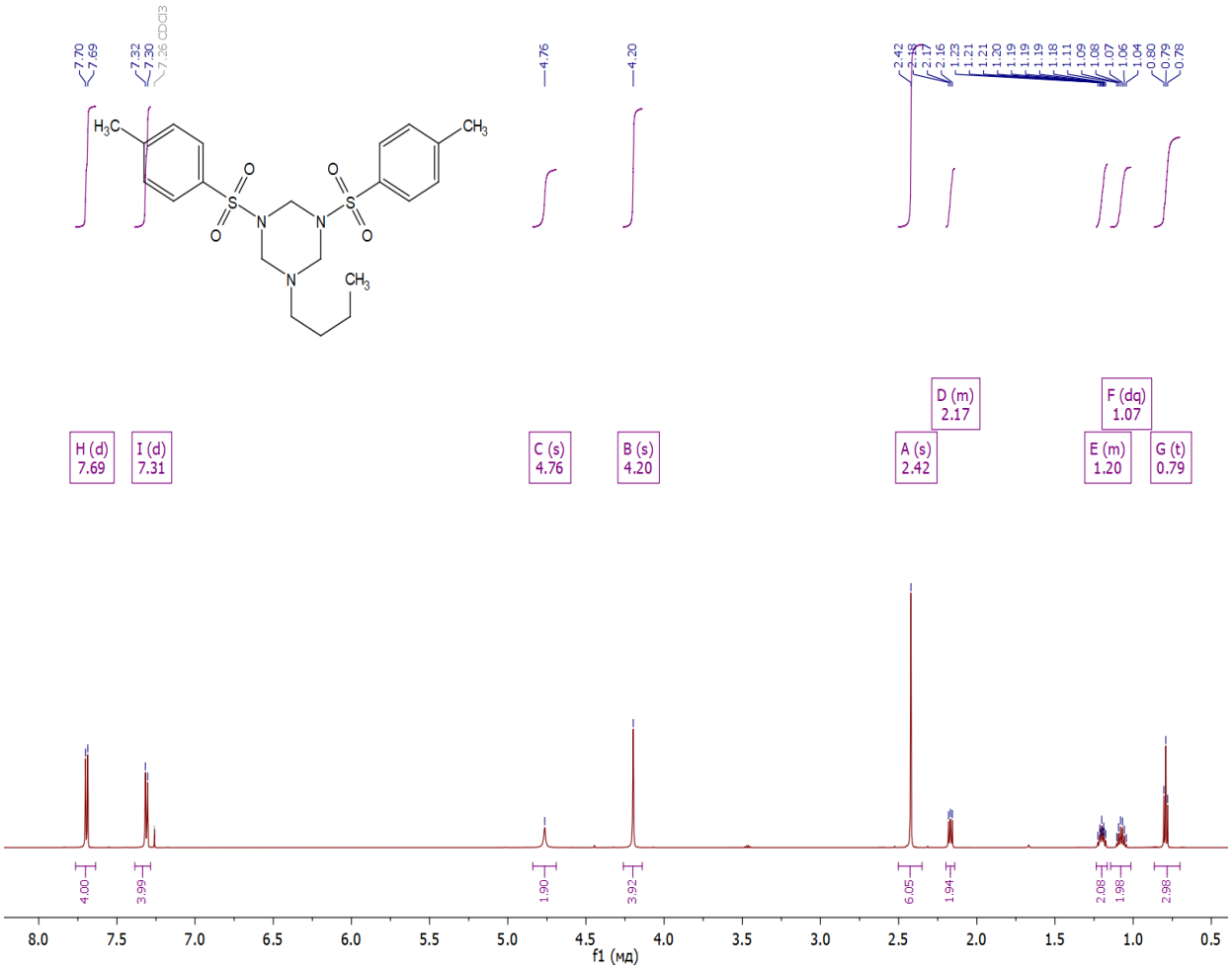
1–Butyl–3,5–*bis*(phenylsulfonyl)–1,3,5–triazinane (2). Yield 71 %, m.p. 116–117 °C, white powder. ^{1}H NMR (600.2 MHz, $CDCl_3$) δ 7.85–7.79 (m, 4H$_{arom.}$), 7.62–7.57 (m, 2H$_{arom.}$), 7.54–7.50 (m, 4H$_{arom.}$), 4.82 (s, 2H, CH_2), 4.24 (s, 4H, 2CH_2), 2.21–2.11 (m, 2H, CH_2), 1.23–1.15 (m, 2H, CH_2), 1.08 (dq, *J*~14.4, 7.3 Hz, 2H, CH_2), 0.80 (t, *J*~7.3 Hz, 3H, CH_3). ^{13}C NMR (150.9 MHz, $CDCl_3$) δ 139.21 (2C$_{quat.}$), 133.21 (2CH$_{arom.}$), 129.41 (4CH$_{arom.}$), 127.22 (4CH$_{arom.}$), 65.71 (CH_2), 60.94 (2CH_2), 50.06 (CH_2), 29.54 (CH_2), 20.06 (CH_2), 13.89 (CH_3). IR (KBr): 3083, 3060 (HC=), 2959, 2928, 2855 (alkyl), 1344, 1161 (SO_2N). MS (ESI): *m*/*z* = 424.1 [M + H$^+$]. Anal. Calcd for $C_{19}H_{25}N_3O_4S_2$: C, 53.88; H, 5.95; N, 9.92; S, 15.14. Found: C, 54.00; H, 6.21; N, 9.89; S, 15.27.

1–(*tert*–Butyl)–3,5–ditosyl–1,3,5–triazinane (3). Yield 84 %, m.p. 213–214 °C, white powder. ^{1}H NMR (600.2 MHz, $CDCl_3$) δ 7.65 (d, *J*~8.1 Hz, 4H$_{arom.}$), 7.30 (d, *J*~8.1 Hz, 4H$_{arom.}$),

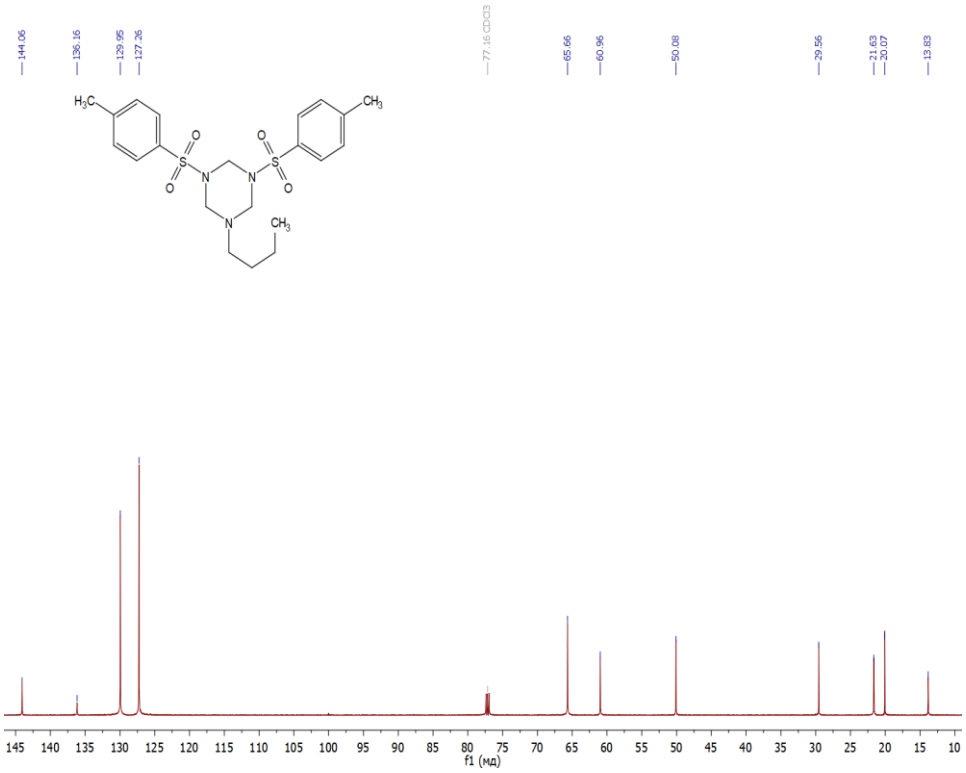
4.55 (s, 2H, CH_2), 4.16 (s, 4H, $2CH_2$), 2.42 (s, 6H, $2CH_3$), 1.08 (s, 9H, $3CH_3$). ^{13}C NMR (150.9 MHz, $CDCl_3$) δ 144.05 ($2C_{quat.}$), 135.42 ($2C_{quat.}$), 129.86 ($4H_{arom.}$), 127.59 ($4H_{arom.}$), 62.51 ($2CH_2$), 61.20 (CH_2), 54.50 ($C_{quat.}$), 27.85 ($3CH_3$), 21.68 ($2CH_3$). IR (KBr): 3067, 3046, 3030 (HC=), 2974, 2925, 2873 (CH_2), 1338, 1156 (SO_2N). MS (ESI): *m*/*z* = 452.2 [M + H^+]. Anal. Calcd for $C_{21}H_{29}N_3O_4S_2$: C, 55.85; H, 6.47; N, 9.30; S, 14.20. Found: C, 56.11; H, 6.30; N, 9.19; S, 14.17.

1–(*tert*–Butyl)–3,5–bis(phenylsulfonyl)–1,3,5–triazinane (4). Yield 82 %, m.p. 165–166 °C, white powder. ^1H NMR (600.2 MHz, $CDCl_3$) δ 7.83–7.74 (m, $4H_{arom.}$), 7.61–7.55 (m, $2H_{arom.}$), 7.56–7.48 (m, $4H_{arom.}$), 4.61 (s, 2H, CH_2), 4.16 (s, 4H, $2CH_2$), 1.06 (s, 9H, $3CH_3$).^{13}C NMR (150.9 MHz, $CDCl_3$) δ 138.43 ($2C_{quat.}$), 133.21 ($2CH_{arom.}$), 129.28 ($4CH_{arom.}$), 127.56 ($4CH_{arom.}$), 62.51 ($2CH_2$), 61.09 (CH_2), 54.38 ($C_{quat.}$), 27.64 ($3CH_3$). IR (KBr): 3066 (HC=), 2967, 2927, 2899, 2864 (alkyl), 1338, 1169 (SO_2N). MS (ESI): *m*/*z* = 424.1 [M + H^+]. Anal. Calcd for $C_{19}H_{25}N_3O_4S_2$: C, 53.88; H, 5.95; N, 9.92; S, 15.14. Found: C, 54.08; H, 6.13; N, 9.99; S, 14.87.

*1–Butyl–3,5–ditosyl–1,3,5–triazinane (**1**)*

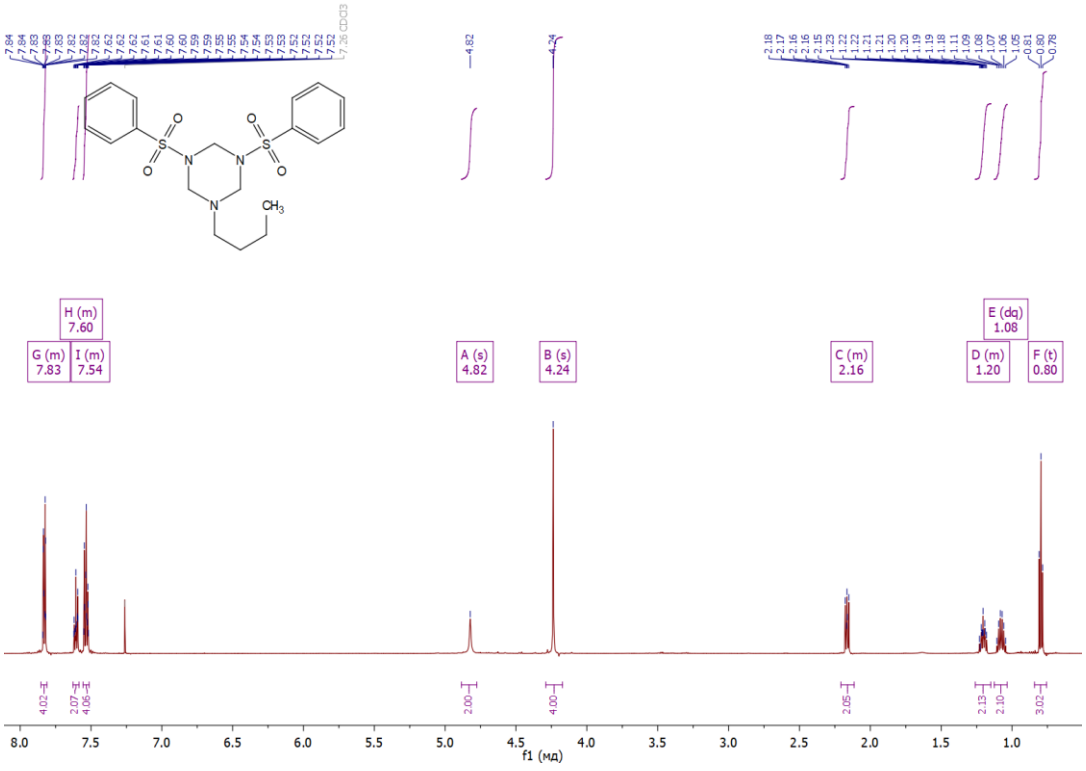


^1H NMR spectrum of compound (**1**).

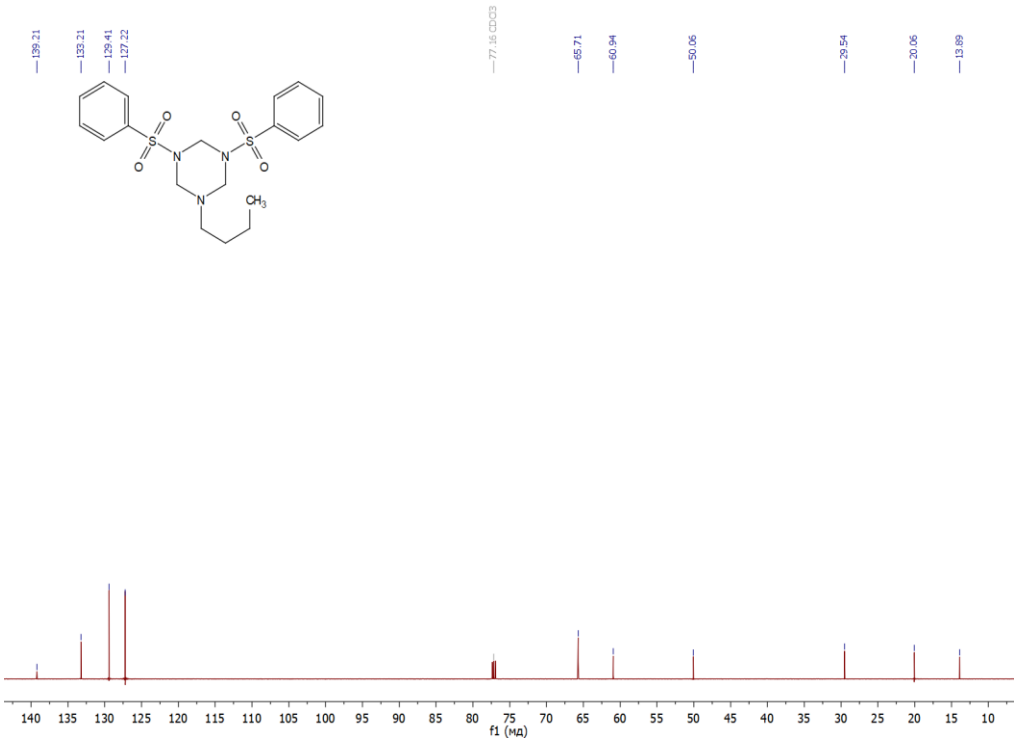


^{13}C NMR spectrum of compound (**1**).

*1 −Butyl−3,5−bis(phenylsulfonyl)−1,3,5−triazinane (**2**)*



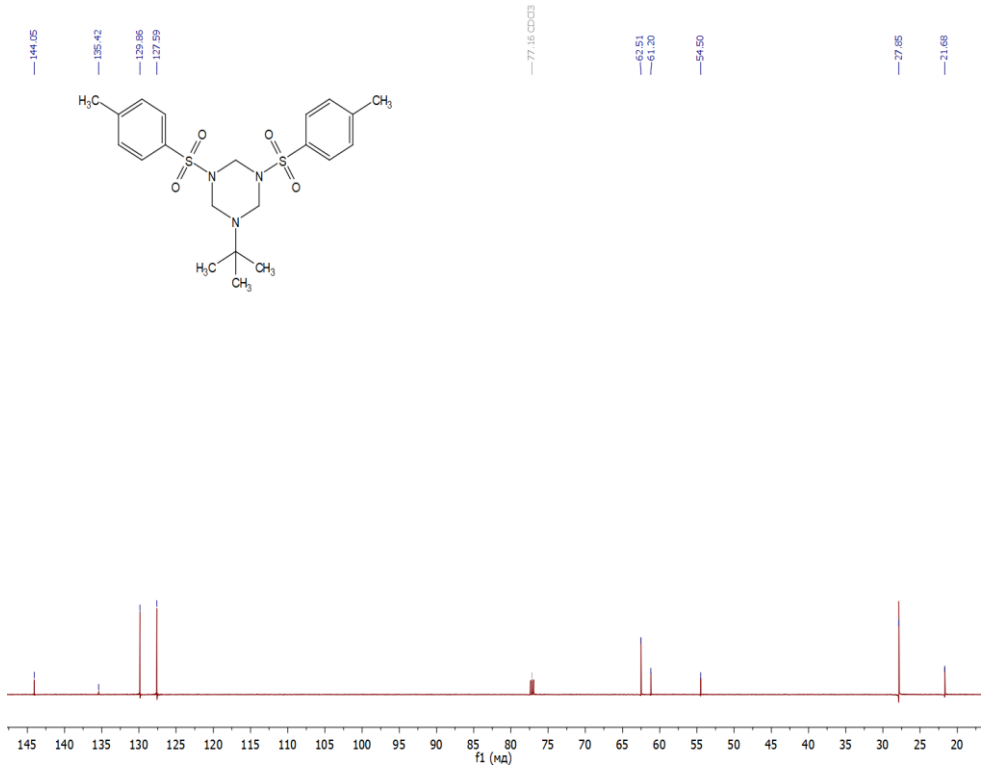
^{1}H NMR spectrum of compound (**2**).



^{13}C NMR spectrum of compound (**2**).

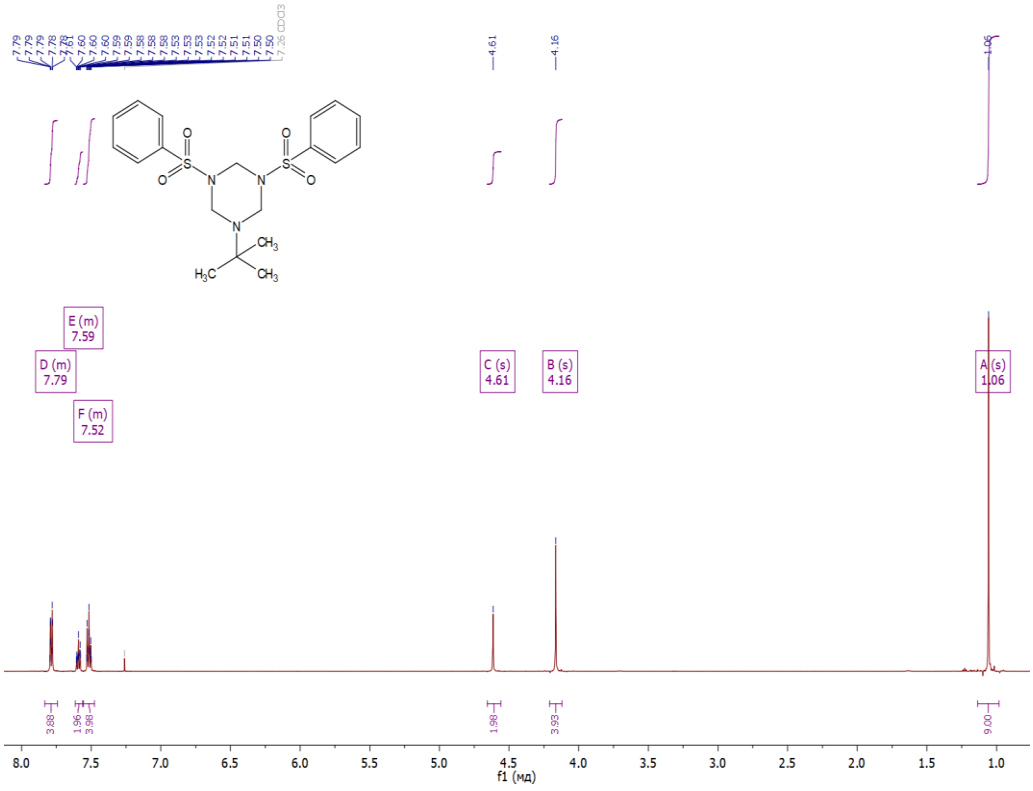
*1–(tert–Butyl)–3,5–ditosyl–1,3,5–triazinane (**3**)*

^{1}H NMR spectrum of compound (**3**).

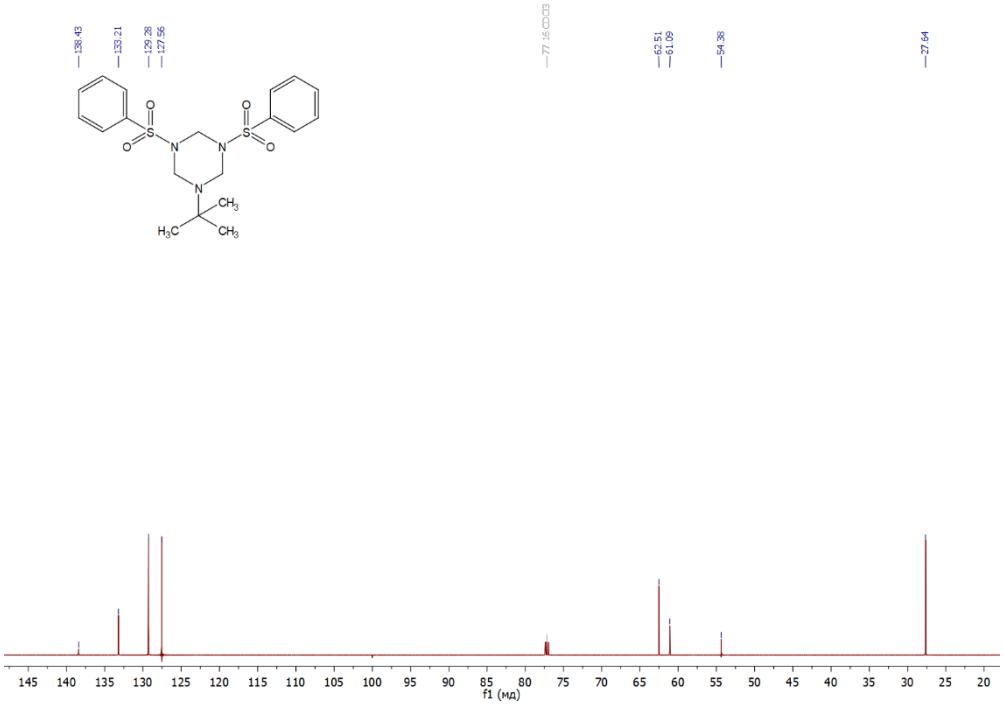


^{13}C NMR spectrum of compound (**3**).

*1–(tert–Butyl)–3,5–bis(phenylsulfonyl)–1,3,5–triazinane (**4**)*



^{1}H NMR spectrum of compound (**4**).



^{13}C NMR spectrum of compound (**4**).

XRD experimental part

The X−ray diffraction data were collected on a Bruker Kappa Apex II automatic four-circle diffractometer equipped with an area detector (Mo−Kα sealed−tube X−ray source, λ = 0.71073 Å, graphite monochromator) at 100 K for all compounds.

The data frames were collected using the program APEX2 and processed using the program SAINT routine within APEX2. The unit cell parameters were refined over the whole dataset.[1] The data were corrected for absorption on the multi-scan technique as implemented in SADABS.[2] The structures were solved by direct methods using SHELXS and refined by full-matrix least squares on F^2 using SHELXL software.[3] in the anisotropic approximation for all non-hydrogen atoms. Hydrogen atoms on carbon were calculated in ideal positions with isotropic displacement parameters set to 1.2×Ueq (CH groups) or 1.5×Ueq (CH3 groups) of the attached atoms. Tables and pictures for structures were generated using Olex2 as GUI.[4] Crystallographic data and structural refinements are summarized in Table 1. The low quality (R_1, wR_2 and R_{int} are high) of structure **3** can be explained by the pseudo-merohedral twinning that was included into the refinement.

X−ray diffraction experiments were performed at the Center for Shared Use of Physical Methods of Investigation at the Frumkin Institute of Physical Chemistry and Electrochemistry, RAS (CKP FMI IPCE RAS). Atomic coordinates for compounds **1**−**4**, have been deposited with the Cambridge Crystallographic Data Centre (CCDC numbers are 1992667 (**1**), 1992668 (**2**), 1992669 (**3**), and 1992670 (**4**)). The supplementary crystallographic data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

1. SAINT-Plus, Version 7.68., Bruker AXS Inc., Madison, Wisconsin, USA.
2. SADABS, Madison, Wisconsin (USA): Bruker AXS, 2008.
3. Sheldrick, G. M. Acta Crystallogr. Sect. C Struct. Chem. **2015**, 71, 3–8.
4. Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H. *J. Appl. Cryst.* **2009**, *42*, 339–341.

Table S1. Data and structure refinement for **1–4.**

Identification code	Compound 1	Compound 2	Compound 3	Compound 4
CCDC number	1992667	1992668	1992669	1992670
Empirical formula	$C_{21}H_{29}N_3O_4S_2$	$C_{19}H_{25}N_3O_4S_2$	$C_{21}H_{29}N_3O_4S_2$	$C_{19}H_{25}N_3O_4S_2$
Formula weight	451.59	423.54	451.59	423.54
Temperature/K	100(2)	100(2)	100(2)	100(2)
Crystal system	monoclinic	monoclinic	monoclinic	orthorhombic
Space group	$P2_1/c$	$P2_1/n$	$P2_1/n$	$P2_12_12_1$
a/Å	13.2871(4)	8.4284(2)	5.955(4)	10.7298(3)
b/Å	10.3261(3)	25.9248(8)	15.378(12)	11.1010(3)
c/Å	15.9595(4)	9.5601(3)	23.915(19)	16.9303(5)
α/°	90	90	90	90
β/°	90.511(2)	106.639(1)	90.968(16)	90
γ/°	90	90	90	90
Volume/$Å^3$	2189.62(11)	2001.46(10)	2190(3)	2016.59(10)
Z	4	4	4	4
$\rho_{calc}g/cm^3$	1.370	1.406	1.370	1.395
μ/mm^{-1}	0.276	0.297	0.276	0.295
F(000)	960.0	896.0	960.0	896.0
Crystal size/mm^3	0.440 × 0.360 × 0.320	0.400 × 0.320 ×− 0.260	0.500 × 0.180 × 0.030	0.420 × 0.400 × 0.360
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	7.126 to 59.998	7.392 to 59.994	8.476 to 55	8.16 to 69.998
Index ranges	$-18 \le h \le 18$, $-14 \le k \le 14$, $-20 \le l \le 22$	$-6 \le h \le 11$, $-35 \le k \le 36$, $-13 \le l \le 13$	$-4 \le h \le 7$, $-19 \le k \le 19$, $-31 \le l \le 31$	$-17 \le h \le 16$, $-17 \le k \le 16$, $-19 \le l \le 27$
Reflections collected	33914	28404	14104	35553
Independent reflections	6383 [R_{int} = 0.0390, R_{sigma} = 0.0303]	5835 [R_{int} = 0.0351, R_{sigma} = 0.0280]	4940 [R_{int} = 0.1432, R_{sigma} = 0.1883]	8855 [R_{int} = 0.0303, R_{sigma} = 0.0303]
Data/restraints/parameters	6383/0/273	5835/0/253	4940/6/274	8855/0/253
Goodness-of-fit on F^2	1.029	1.035	1.049	1.042
Final R indexes [I>=2σ (I)]	R_1 = 0.0350, wR_2 = 0.0877	R_1 = 0.0334, wR_2 = 0.0824	R_1 = 0.1398, wR_2 = 0.3472	R_1 = 0.0283, wR_2 = 0.0698
Final R indexes [all data]	R_1 = 0.0457, wR_2 = 0.0939	R_1 = 0.0423, wR_2 = 0.0873	R_1 = 0.2253, wR_2 = 0.4075	R_1 = 0.0316, wR_2 = 0.0715
Largest diff. peak/hole / e $Å^{-3}$	0.38/−0.37	0.39/−0.37	0.94/−0.55	0.36/−0.28

Table S2. Selected distances (Å), angles (°) and torsion angles (°) for compounds **1–4**.

Compound	1	2	3	4
N(1) ─ C(2)	1.4470(15)	1.4421(15)	1.449(12)	1.4351(16)
N(1) ─ C(6)	1.4483(18)	1.4464(15)	1.451(13)	1.4417(15)
N(3) ─ C(4)	1.4834(17)	1.4642(15)	1.461(13)	1.4663(16)
N(3) ─ C(2)	1.4967(16)	1.4902(16)	1.498(15)	1.4948(17)
N(5) ─ C(4)	1.4526(15)	1.4477(15)	1.475(12)	1.4642(16)
N(5) ─ C(6)	1.4764(17)	1.4762(15)	1.484(14)	1.5048(16)
S(1) ─ O(1)	1.4316(10)	1.4277(10)	1.400(10)	1.4336(11)
S(1) ─ O(2)	1.4363(10)	1.4311(10)	1.453(8)	1.4353(10)
S(1) ─ N(3)	1.6416(10)	1.6304(10)	1.629(10)	1.6396(11)
S(1) ─ C(11)	1.7577(12)	1.7548(12)	1.785(11)	1.7637(14)
S(2) ─ O(4)	1.4313(11)	1.4331(9)	1.441(7)	1.4352(10)
S(2) ─ O(3)	1.4332(10)	1.4338(9)	1.443(10)	1.4370(10)
S(2) ─ N(5)	1.6316(11)	1.6139(10)	1.629(9)	1.6376(11)
S(2) ─ C(21)	1.7583(13)	1.7699(12)	1.781(11)	1.7644(12)
C(2)─N(1)─C(6)	109.29(10)	110.32(10)	108.9(8)	109.98(10)
C(4)─N(3)─C(2)	111.19(10)	110.75(10)	113.0(9)	109.75(10)
C(4)─N(5)─C(6)	113.89(10)	113.61(10)	114.2(9)	112.20(10)
O(1)─S(1)─O(2)	119.95(6)	120.84(6)	119.4(6)	120.28(7)
O(1)─S(1)─N(3)	106.63(5)	105.76(6)	109.6(5)	106.53(6)
O(2)─S(1)─N(3)	106.07(6)	106.51(6)	105.6(5)	105.77(6)
O(1)─S(1)─C(11)	108.22(6)	107.46(6)	108.4(5)	108.20(7)
O(2)─S(1)─C(11)	108.32(6)	108.09(6)	106.8(5)	108.31(6)
N(3)─S(1)─C(11)	106.98(6)	107.53(6)	106.3(5)	107.04(6)
O(4)─S(2)─O(3)	120.64(7)	120.69(6)	119.9(6)	120.10(6)
O(4)─S(2)─N(5)	107.86(6)	107.28(6)	105.5(5)	106.83(6)
O(3)─S(2)─N(5)	106.62(6)	106.07(5)	106.5(5)	106.18(6)
O(4)─S(2)─C(21)	106.90(6)	107.55(6)	108.5(5)	107.54(6)
O(3)─S(2)─C(21)	107.92(6)	106.21(6)	107.5(5)	108.13(6)
N(5)─S(2)─C(21)	106.06(6)	108.64(6)	108.5(5)	107.47(6)
C(6)─N(1)─C(2)─N(3)	−59.21(13)	−57.06(13)	−56.2(11)	58.31(13)
C(4)─N(3)─C(2)─N(1)	61.16(13)	61.61(12)	58.3(11)	−63.26(13)
C(6)─N(5)─C(4)─N(3)	53.50(14)	56.29(13)	53.5(12)	−58.56(13)
C(2)─N(3)─C(4)─N(5)	−56.35(13)	−59.23(12)	−53.9(13)	61.23(12)
C(2)─N(1)─C(6)─N(5)	56.06(14)	53.41(13)	55.1(11)	−54.43(13)
C(4)─N(5)─C(6)─N(1)	−55.03(15)	−54.73(13)	−56.3(11)	56.49(13)
C(7)─N(1)─C(2)─N(3)	66.88(14)	72.05(12)	82.3(11)	−81.49(13)
C(7)─N(1)─C(6)─N(5)	−71.18(13)	−75.61(13)	−84.5(10)	86.37(13)
S(1)─N(3)─C(2)─N(1)	−162.11(9)	−157.38(8)	−117.6(9)	159.19(8)
S(1)─N(3)─C(4)─N(5)	166.92(8)	159.03(8)	122.2(9)	−160.14(8)
S(2)─N(5)─C(6)─N(1)	113.72(11)	131.40(10)	158.0(7)	−165.39(8)
S(2)─N(5)─C(4)─N(3)	−115.18(11)	−129.48(9)	−160.0(9)	162.55(8)
C(11)─S(1)─N(3)─C(2)	−68.33(10)	−65.49(10)	−97.5(9)	70.22(10)
C(21)─S(2)─N(5)─C(6)	84.57(11)	−104.98(11)	76.1(8)	−60.68(10)

Table S3. Hydrogen bonds for compounds **1–4**.

1						
D	**H**	**A**	**d(D–H)/Å**	**d(H–A)/Å**	**d(D–A)/Å**	**D–H–A/°**
C(17)	H(17C)	O(1)[1]	0.98	2.51	3.449(2)	160.7
C(15)	H(15A)	O(1)[1]	0.95	2.62	3.469(2)	148.7
C(27)	H(27C)	O(4)[2]	0.98	2.67	3.631(2)	168.2
C(25)	H(25A)	N(1)[3]	0.95	2.55	3.445(2)	156.2
2						
C(13)	H(13A)	O(1)[4]	0.95	2.50	3.112(2)	122.6
C(10)	H(10B)	O(1)[5]	0.98	2.48	3.415(2)	159.7
C(14)	H(14A)	O(2)[6]	0.95	2.52	3.354(2)	146.6
C(26)	H(26A)	O(4)[7]	0.95	2.66	3.326(2)	127.7
3						
C(2)	H(2B)	O(1)[8]	0.99	2.54	3.180(13)	122.1
C(6)	H(6A)	O(3)[8]	0.99	2.39	3.350(13)	162.0
C(10)	H(10B)	O(3)[9]	0.98	2.53	3.507(14)	175.0
C(10)	H(10C)	O(2)	0.98	2.52	3.431(14)	155.1
C(15)	H(15A)	O(4)[10]	0.95	2.48	3.393(13)	161.5
C(17)	H(17C)	O(4)[4]	0.98	2.50	3.441(17)	161.4
4						
C(6)	H(6A)	O(3)[11]	0.99	2.59	3.538(2)	159.8
C(12)	H(12)	O(3)[12]	0.95	2.58	3.230(2)	125.7
C(16)	H(16)	O(4)[13]	0.95	2.66	3.527(2)	152.6
C(26)	H(26)	O(4)[13]	0.95	2.39	3.312(2)	163.4
C(24)	H(24)	O(2)[14]	0.95	2.60	3.421(2)	145.6

[1] + X,3/2 − Y,−1/2 + Z; [2] 2−X,2−Y,2−Z; [3] 2−X,1/2 + Y,3/2 − Z; [4] −1/2 + X,3/2−Y,1/2 + Z; [5] 1 + X, + Y,1 + Z; [6] −1 + X, + Y, + Z ; [7] 2 − X,1 − Y,1 − Z; [8] −1 + X, + Y, + Z; [9] 3/2 − X,−1/2 + Y,1/2 − Z; [10] 3/2−X,1/2 + Y,1/2 − Z; [11] 1/2 + X,3/2−Y,1 − Z; [12] 1/2 − X,1−Y,1/2 + Z; [13] −1/2 + X,3/2 − Y,1 − Z; [14] + X,1 + Y, + Z.

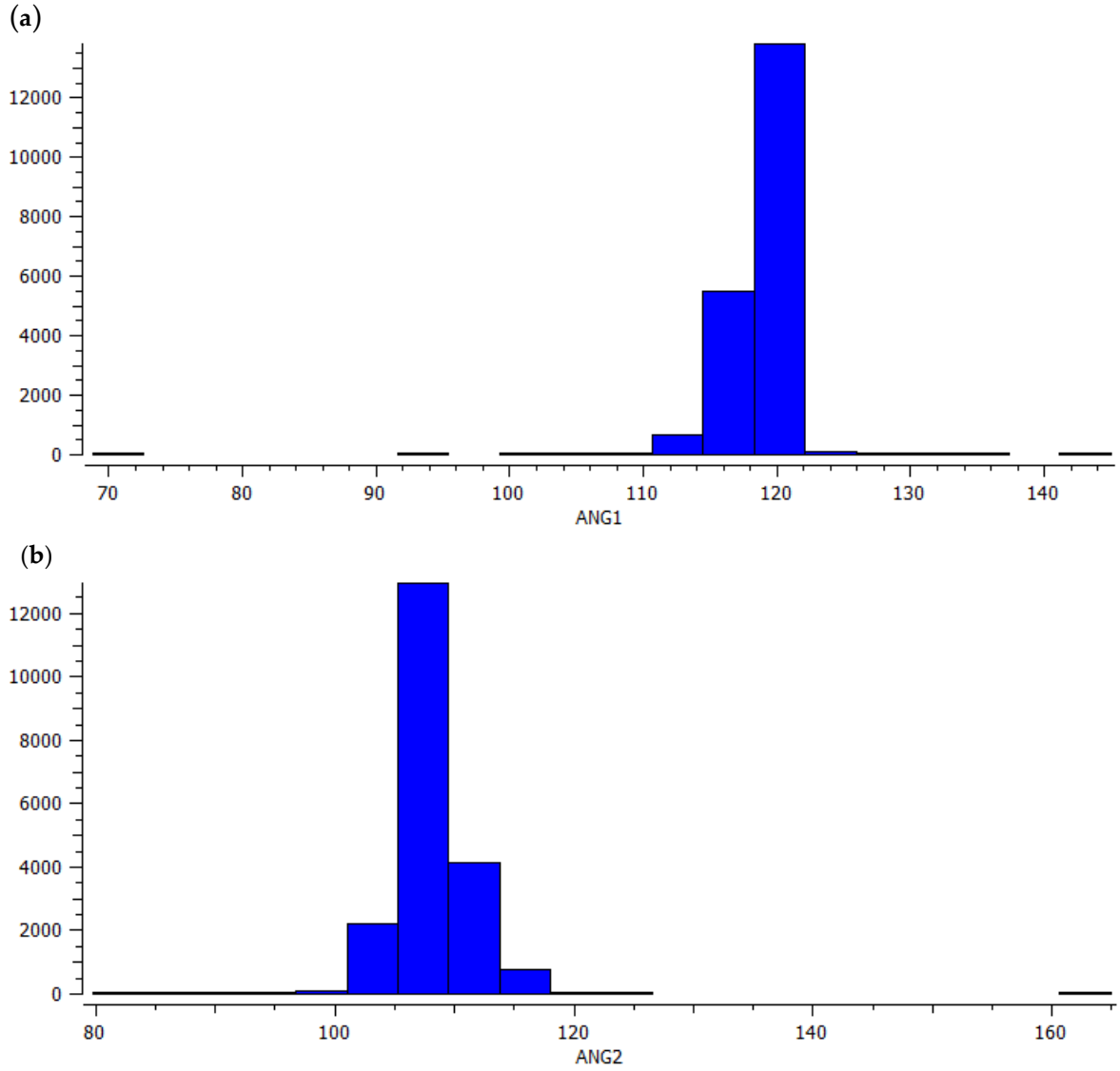
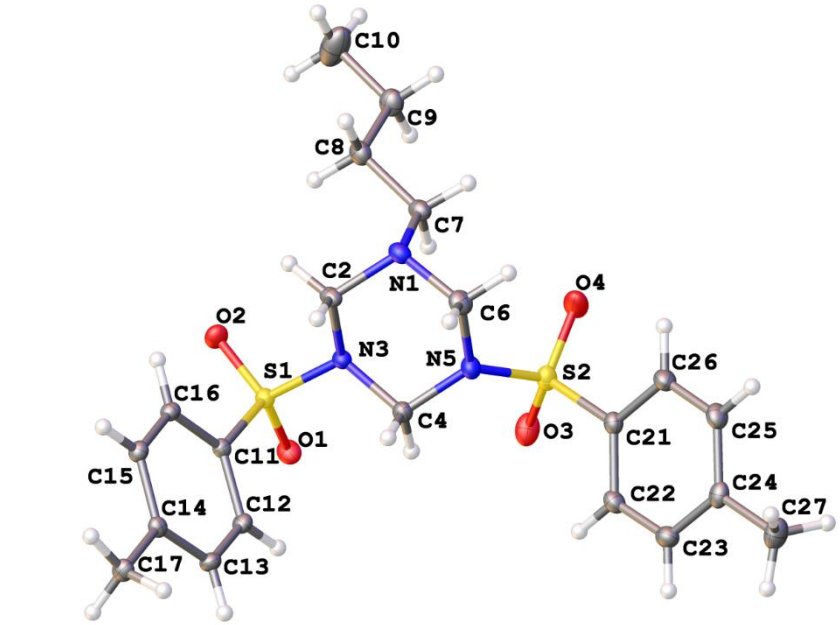


Figure S1. Histogram of O–S–O angle in N−sulfamides (**a**), N–S–O angle in N−sulfamides (**b**) according CSD analysis.

1. (100K) $C_{21}H_{29}N_3O_4S_2$ (CCDC number 1992667)



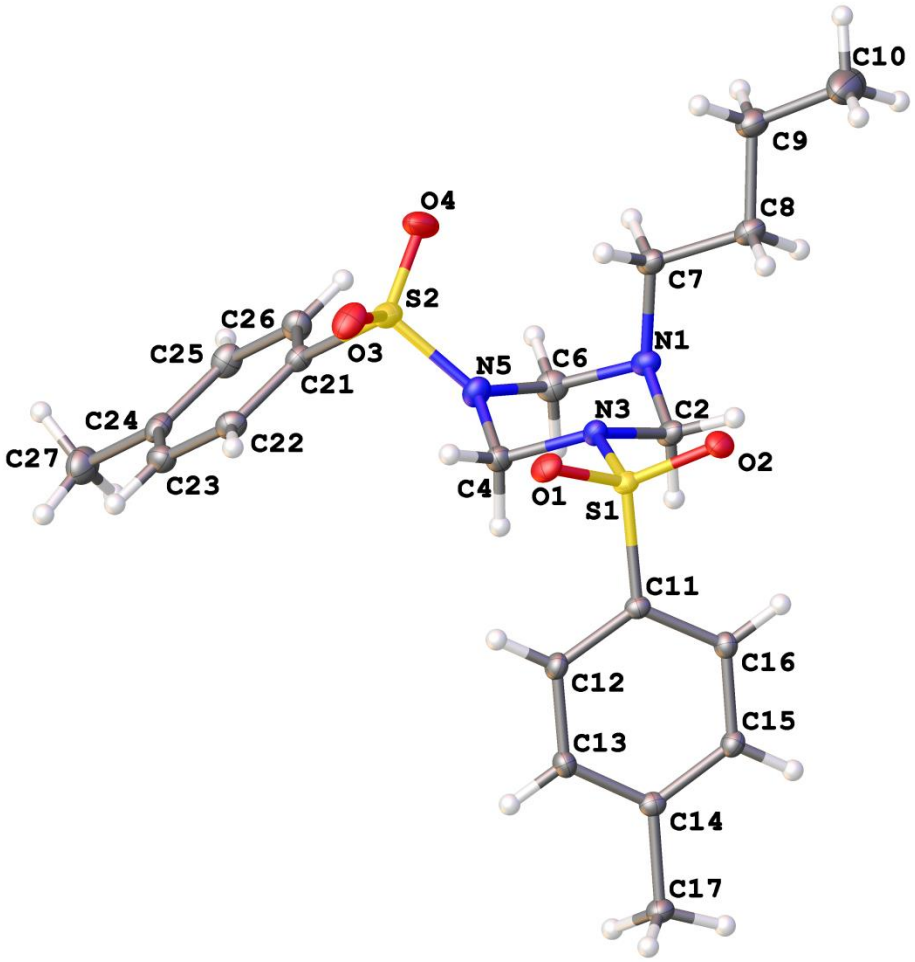


Table S4. Bond Lengths for **1**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
S(1)	O(1)	1.4316(10)	C(8)	C(9)	1.5239(19)
S(1)	O(2)	1.4363(10)	C(9)	C(10)	1.511(2)
S(1)	N(3)	1.6416(10)	C(11)	C(16)	1.3916(17)
S(1)	C(11)	1.7577(12)	C(11)	C(12)	1.3943(17)
S(2)	O(3)	1.4313(11)	C(12)	C(13)	1.3874(17)
S(2)	O(4)	1.4332(10)	C(13)	C(14)	1.3951(17)
S(2)	N(5)	1.6316(11)	C(14)	C(15)	1.3951(17)
S(2)	C(21)	1.7583(13)	C(14)	C(17)	1.5035(17)
N(1)	C(2)	1.4470(15)	C(15)	C(16)	1.3911(17)
N(1)	C(6)	1.4483(18)	C(21)	C(22)	1.3898(18)
N(1)	C(7)	1.4725(17)	C(21)	C(26)	1.3904(17)
N(3)	C(4)	1.4834(17)	C(22)	C(23)	1.3865(19)
N(3)	C(2)	1.4967(16)	C(23)	C(24)	1.3961(18)
N(5)	C(4)	1.4526(15)	C(24)	C(25)	1.3903(19)
N(5)	C(6)	1.4764(17)	C(24)	C(27)	1.5088(19)
C(7)	C(8)	1.5162(19)	C(25)	C(26)	1.3871(19)

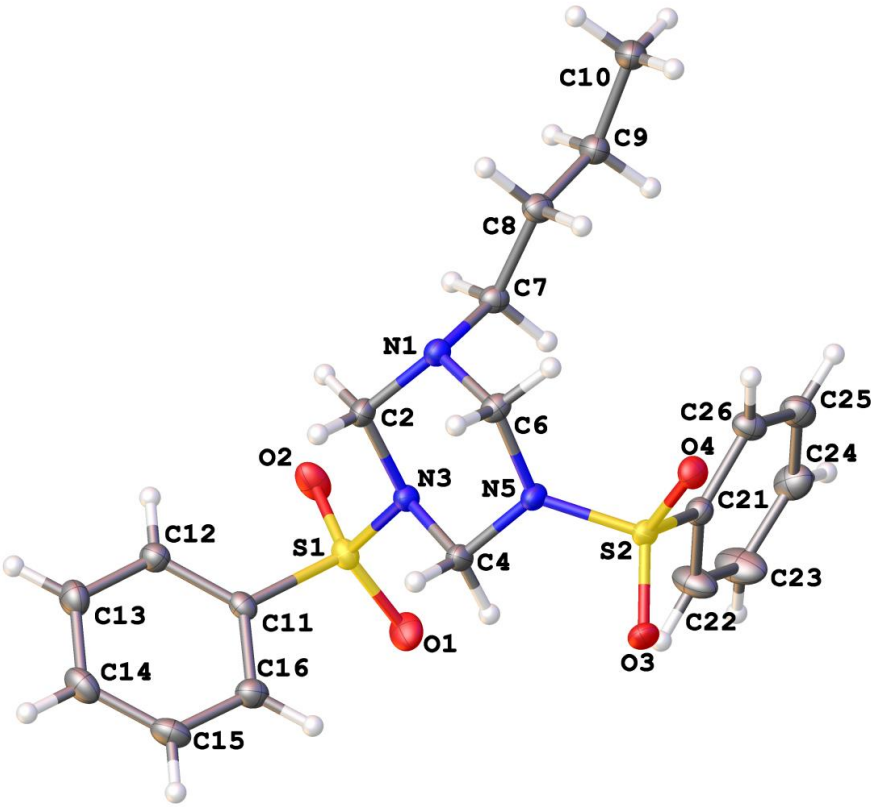
Table S5. Bond Angles for **1**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O(1)	S(1)	O(2)	119.95(6)	N(1)	C(7)	C(8)	113.98(10)
O(1)	S(1)	N(3)	106.63(5)	C(7)	C(8)	C(9)	109.94(11)
O(2)	S(1)	N(3)	106.07(6)	C(10)	C(9)	C(8)	114.10(12)
O(1)	S(1)	C(11)	108.22(6)	C(16)	C(11)	C(12)	120.98(11)
O(2)	S(1)	C(11)	108.32(6)	C(16)	C(11)	S(1)	120.00(9)
N(3)	S(1)	C(11)	106.98(6)	C(12)	C(11)	S(1)	118.96(9)
O(3)	S(2)	O(4)	120.64(7)	C(13)	C(12)	C(11)	119.02(11)
O(3)	S(2)	N(5)	106.62(6)	C(12)	C(13)	C(14)	121.07(12)
O(4)	S(2)	N(5)	107.86(6)	C(13)	C(14)	C(15)	118.93(11)
O(3)	S(2)	C(21)	107.92(6)	C(13)	C(14)	C(17)	120.13(11)
O(4)	S(2)	C(21)	106.90(6)	C(15)	C(14)	C(17)	120.93(11)
N(5)	S(2)	C(21)	106.06(6)	C(16)	C(15)	C(14)	120.86(12)
C(2)	N(1)	C(6)	109.29(10)	C(15)	C(16)	C(11)	119.13(11)
C(2)	N(1)	C(7)	113.97(10)	C(22)	C(21)	C(26)	120.65(12)
C(6)	N(1)	C(7)	111.95(10)	C(22)	C(21)	S(2)	119.49(10)
C(4)	N(3)	C(2)	111.19(10)	C(26)	C(21)	S(2)	119.86(10)
C(4)	N(3)	S(1)	116.50(8)	C(23)	C(22)	C(21)	119.09(12)
C(2)	N(3)	S(1)	116.51(8)	C(22)	C(23)	C(24)	121.26(12)
C(4)	N(5)	C(6)	113.89(10)	C(25)	C(24)	C(23)	118.56(12)
C(4)	N(5)	S(2)	122.86(9)	C(25)	C(24)	C(27)	120.72(12)
C(6)	N(5)	S(2)	122.23(9)	C(23)	C(24)	C(27)	120.72(13)
N(1)	C(2)	N(3)	109.87(10)	C(26)	C(25)	C(24)	121.01(12)
N(5)	C(4)	N(3)	107.68(10)	C(25)	C(26)	C(21)	119.44(12)
N(1)	C(6)	N(5)	112.02(11)				

Table S6. Torsion Angles for **1**.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O(1)	S(1)	N(3)	C(4)	−49.51(10)	N(3)	S(1)	C(11)	C(16)	88.50(10)
O(2)	S(1)	N(3)	C(4)	−178.43(9)	O(1)	S(1)	C(11)	C(12)	25.96(11)
C(11)	S(1)	N(3)	C(4)	66.10(10)	O(2)	S(1)	C(11)	C(12)	157.46(9)
O(1)	S(1)	N(3)	C(2)	176.05(9)	N(3)	S(1)	C(11)	C(12)	−88.59(10)
O(2)	S(1)	N(3)	C(2)	47.13(10)	C(16)	C(11)	C(12)	C(13)	0.57(18)
C(11)	S(1)	N(3)	C(2)	−68.33(10)	S(1)	C(11)	C(12)	C(13)	177.63(9)
O(3)	S(2)	N(5)	C(4)	7.16(12)	C(11)	C(12)	C(13)	C(14)	0.58(18)
O(4)	S(2)	N(5)	C(4)	138.07(11)	C(12)	C(13)	C(14)	C(15)	−1.13(18)
C(21)	S(2)	N(5)	C(4)	−107.69(11)	C(12)	C(13)	C(14)	C(17)	179.23(11)
O(3)	S(2)	N(5)	C(6)	−160.59(10)	C(13)	C(14)	C(15)	C(16)	0.54(18)
O(4)	S(2)	N(5)	C(6)	−29.67(12)	C(17)	C(14)	C(15)	C(16)	−179.82(11)
C(21)	S(2)	N(5)	C(6)	84.57(11)	C(14)	C(15)	C(16)	C(11)	0.57(18)
C(6)	N(1)	C(2)	N(3)	−59.21(13)	C(12)	C(11)	C(16)	C(15)	−1.14(18)
C(7)	N(1)	C(2)	N(3)	66.88(14)	S(1)	C(11)	C(16)	C(15)	−178.17(9)
C(4)	N(3)	C(2)	N(1)	61.16(13)	O(3)	S(2)	C(21)	C(22)	−26.95(12)
S(1)	N(3)	C(2)	N(1)	−162.11(9)	O(4)	S(2)	C(21)	C(22)	−158.10(11)
C(6)	N(5)	C(4)	N(3)	53.50(14)	N(5)	S(2)	C(21)	C(22)	87.00(11)
S(2)	N(5)	C(4)	N(3)	−115.18(11)	O(3)	S(2)	C(21)	C(26)	152.99(11)
C(2)	N(3)	C(4)	N(5)	−56.35(13)	O(4)	S(2)	C(21)	C(26)	21.84(13)
S(1)	N(3)	C(4)	N(5)	166.92(8)	N(5)	S(2)	C(21)	C(26)	−93.06(11)
C(2)	N(1)	C(6)	N(5)	56.06(14)	C(26)	C(21)	C(22)	C(23)	−0.07(19)
C(7)	N(1)	C(6)	N(5)	−71.18(13)	S(2)	C(21)	C(22)	C(23)	179.86(10)
C(4)	N(5)	C(6)	N(1)	−55.03(15)	C(21)	C(22)	C(23)	C(24)	0.5(2)
S(2)	N(5)	C(6)	N(1)	113.72(11)	C(22)	C(23)	C(24)	C(25)	−0.6(2)
C(2)	N(1)	C(7)	C(8)	60.00(14)	C(22)	C(23)	C(24)	C(27)	179.57(13)
C(6)	N(1)	C(7)	C(8)	−175.33(11)	C(23)	C(24)	C(25)	C(26)	0.1(2)
N(1)	C(7)	C(8)	C(9)	170.46(11)	C(27)	C(24)	C(25)	C(26)	179.98(13)
C(7)	C(8)	C(9)	C(10)	176.58(14)	C(24)	C(25)	C(26)	C(21)	0.3(2)
O(1)	S(1)	C(11)	C(16)	−156.95(10)	C(22)	C(21)	C(26)	C(25)	−0.4(2)
O(2)	S(1)	C(11)	C(16)	−25.45(11)	S(2)	C(21)	C(26)	C(25)	179.70(10)

2. (100K) $C_{19}H_{25}N_3O_4S_2$ (CCDC number 1992668)



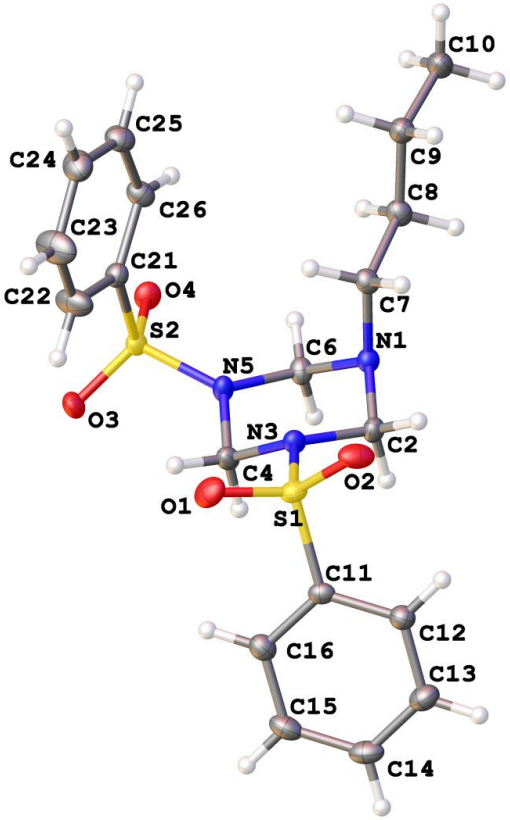


Table S7. Bond Lengths for **2**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
S(1)	O(2)	1.4277(10)	C(7)	C(8)	1.5157(17)
S(1)	O(1)	1.4311(10)	C(8)	C(9)	1.5194(18)
S(1)	N(3)	1.6304(10)	C(9)	C(10)	1.5229(18)
S(1)	C(11)	1.7548(12)	C(11)	C(12)	1.3867(17)
S(2)	O(3)	1.4331(9)	C(11)	C(16)	1.3895(17)
S(2)	O(4)	1.4338(9)	C(12)	C(13)	1.3859(18)
S(2)	N(5)	1.6139(10)	C(13)	C(14)	1.384(2)
S(2)	C(21)	1.7699(12)	C(14)	C(15)	1.385(2)
N(1)	C(2)	1.4421(15)	C(15)	C(16)	1.3895(19)
N(1)	C(6)	1.4464(15)	C(21)	C(26)	1.3863(17)
N(1)	C(7)	1.4696(16)	C(21)	C(22)	1.3865(18)
N(3)	C(4)	1.4642(15)	C(22)	C(23)	1.387(2)
N(3)	C(2)	1.4902(16)	C(23)	C(24)	1.385(2)
N(5)	C(4)	1.4477(15)	C(24)	C(25)	1.384(2)
N(5)	C(6)	1.4762(15)	C(25)	C(26)	1.3876(18)

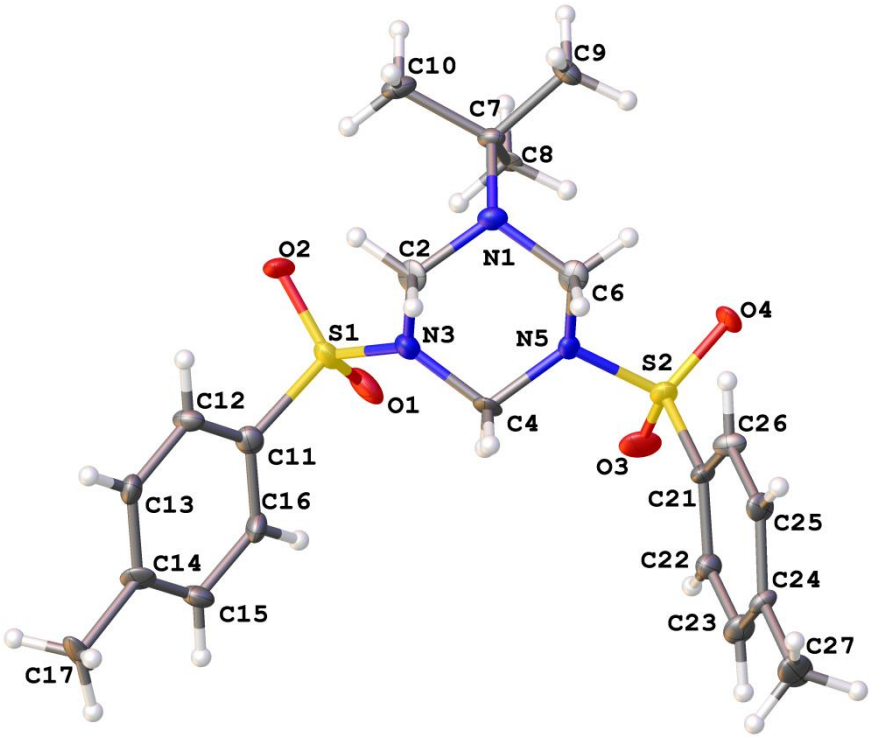
Table S8. Bond Angles for **2**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O(2)	S(1)	O(1)	120.84(6)	N(5)	C(4)	N(3)	106.98(9)
O(2)	S(1)	N(3)	106.51(6)	N(1)	C(6)	N(5)	111.71(10)
O(1)	S(1)	N(3)	105.76(6)	N(1)	C(7)	C(8)	111.32(10)
O(2)	S(1)	C(11)	108.09(6)	C(7)	C(8)	C(9)	112.93(11)
O(1)	S(1)	C(11)	107.46(6)	C(8)	C(9)	C(10)	111.30(12)
N(3)	S(1)	C(11)	107.53(6)	C(12)	C(11)	C(16)	121.51(11)
O(3)	S(2)	O(4)	120.69(6)	C(12)	C(11)	S(1)	119.19(9)
O(3)	S(2)	N(5)	107.28(6)	C(16)	C(11)	S(1)	119.29(10)
O(4)	S(2)	N(5)	106.07(5)	C(13)	C(12)	C(11)	118.98(12)
O(3)	S(2)	C(21)	106.21(6)	C(14)	C(13)	C(12)	120.16(13)
O(4)	S(2)	C(21)	107.55(6)	C(13)	C(14)	C(15)	120.48(12)
N(5)	S(2)	C(21)	108.64(6)	C(14)	C(15)	C(16)	120.13(13)
C(2)	N(1)	C(6)	110.32(10)	C(11)	C(16)	C(15)	118.74(12)
C(2)	N(1)	C(7)	113.61(10)	C(26)	C(21)	C(22)	120.87(12)
C(6)	N(1)	C(7)	113.76(10)	C(26)	C(21)	S(2)	119.64(10)
C(4)	N(3)	C(2)	110.75(10)	C(22)	C(21)	S(2)	119.42(10)
C(4)	N(3)	S(1)	117.50(8)	C(21)	C(22)	C(23)	119.10(13)
C(2)	N(3)	S(1)	119.20(8)	C(24)	C(23)	C(22)	120.28(14)
C(4)	N(5)	C(6)	113.61(10)	C(25)	C(24)	C(23)	120.29(13)
C(4)	N(5)	S(2)	120.37(8)	C(24)	C(25)	C(26)	119.84(13)
C(6)	N(5)	S(2)	125.73(8)	C(21)	C(26)	C(25)	119.56(12)
N(1)	C(2)	N(3)	110.13(9)				

Table S9. Torsion Angles for **2**.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O(2)	S(1)	N(3)	C(4)	−171.36(9)	O(2)	S(1)	C(11)	C(12)	−16.87(12)
O(1)	S(1)	N(3)	C(4)	−41.63(10)	O(1)	S(1)	C(11)	C(12)	−148.78(10)
C(11)	S(1)	N(3)	C(4)	72.96(10)	N(3)	S(1)	C(11)	C(12)	97.76(10)
O(2)	S(1)	N(3)	C(2)	50.19(10)	O(2)	S(1)	C(11)	C(16)	163.86(10)
O(1)	S(1)	N(3)	C(2)	179.92(9)	O(1)	S(1)	C(11)	C(16)	31.95(12)
C(11)	S(1)	N(3)	C(2)	−65.49(10)	N(3)	S(1)	C(11)	C(16)	−81.51(11)
O(3)	S(2)	N(5)	C(4)	−32.89(11)	C(16)	C(11)	C(12)	C(13)	−0.21(19)
O(4)	S(2)	N(5)	C(4)	−163.11(9)	S(1)	C(11)	C(12)	C(13)	−179.46(10)
C(21)	S(2)	N(5)	C(4)	81.53(11)	C(11)	C(12)	C(13)	C(14)	0.3(2)
O(3)	S(2)	N(5)	C(6)	140.60(10)	C(12)	C(13)	C(14)	C(15)	0.1(2)
O(4)	S(2)	N(5)	C(6)	10.38(12)	C(13)	C(14)	C(15)	C(16)	−0.5(2)
C(21)	S(2)	N(5)	C(6)	−104.98(11)	C(12)	C(11)	C(16)	C(15)	−0.23(19)
C(6)	N(1)	C(2)	N(3)	−57.06(13)	S(1)	C(11)	C(16)	C(15)	179.02(10)
C(7)	N(1)	C(2)	N(3)	72.05(12)	C(14)	C(15)	C(16)	C(11)	0.6(2)
C(4)	N(3)	C(2)	N(1)	61.61(12)	O(3)	S(2)	C(21)	C(26)	−151.69(10)
S(1)	N(3)	C(2)	N(1)	−157.38(8)	O(4)	S(2)	C(21)	C(26)	−21.20(12)
C(6)	N(5)	C(4)	N(3)	56.29(13)	N(5)	S(2)	C(21)	C(26)	93.20(11)
S(2)	N(5)	C(4)	N(3)	−129.48(9)	O(3)	S(2)	C(21)	C(22)	25.29(13)
C(2)	N(3)	C(4)	N(5)	−59.23(12)	O(4)	S(2)	C(21)	C(22)	155.78(12)
S(1)	N(3)	C(4)	N(5)	159.03(8)	N(5)	S(2)	C(21)	C(22)	−89.82(12)
C(2)	N(1)	C(6)	N(5)	53.41(13)	C(26)	C(21)	C(22)	C(23)	−0.5(2)
C(7)	N(1)	C(6)	N(5)	−75.61(13)	S(2)	C(21)	C(22)	C(23)	−177.44(13)
C(4)	N(5)	C(6)	N(1)	−54.73(13)	C(21)	C(22)	C(23)	C(24)	2.3(3)
S(2)	N(5)	C(6)	N(1)	131.40(10)	C(22)	C(23)	C(24)	C(25)	−2.0(3)
C(2)	N(1)	C(7)	C(8)	154.52(10)	C(23)	C(24)	C(25)	C(26)	0.0(2)
C(6)	N(1)	C(7)	C(8)	−78.14(13)	C(22)	C(21)	C(26)	C(25)	−1.5(2)
N(1)	C(7)	C(8)	C(9)	−178.08(10)	S(2)	C(21)	C(26)	C(25)	175.39(10)
C(7)	C(8)	C(9)	C(10)	175.90(11)	C(24)	C(25)	C(26)	C(21)	1.8(2)

3 (100K) $C_{21}H_{29}N_3O_4S_2$ (CCDC number 1992669)



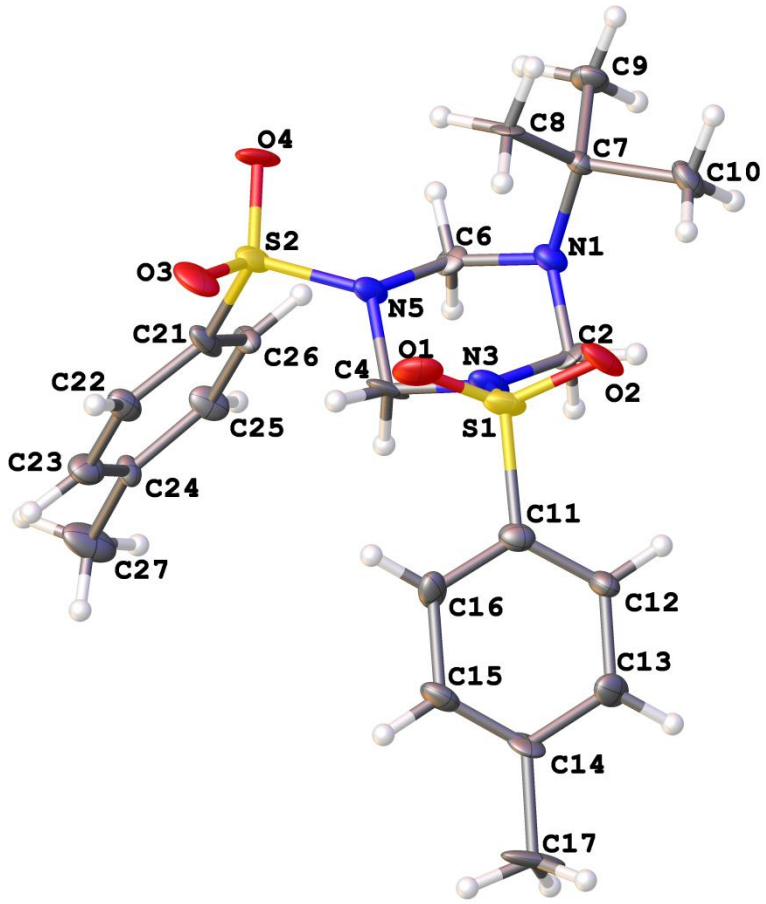


Table S10. Bond Lengths for **3**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
S(1)	O(1)	1.400(10)	C(7)	C(9)	1.553(13)
S(1)	O(2)	1.453(8)	C(7)	C(10)	1.554(14)
S(1)	N(3)	1.629(10)	C(11)	C(12)	1.338(15)
S(1)	C(11)	1.785(11)	C(11)	C(16)	1.389(15)
S(2)	O(4)	1.441(7)	C(12)	C(13)	1.407(14)
S(2)	O(3)	1.443(10)	C(13)	C(14)	1.397(15)
S(2)	N(5)	1.629(9)	C(14)	C(15)	1.346(17)
S(2)	C(21)	1.781(11)	C(14)	C(17)	1.519(14)
N(1)	C(2)	1.449(12)	C(15)	C(16)	1.420(15)
N(1)	C(6)	1.451(13)	C(21)	C(26)	1.395(16)
N(1)	C(7)	1.513(13)	C(21)	C(22)	1.396(14)
N(3)	C(4)	1.461(13)	C(22)	C(23)	1.391(14)
N(3)	C(2)	1.498(15)	C(23)	C(24)	1.380(16)
N(5)	C(4)	1.475(12)	C(24)	C(25)	1.419(14)
N(5)	C(6)	1.484(14)	C(24)	C(27)	1.534(15)
C(7)	C(8)	1.492(15)	C(25)	C(26)	1.380(14)

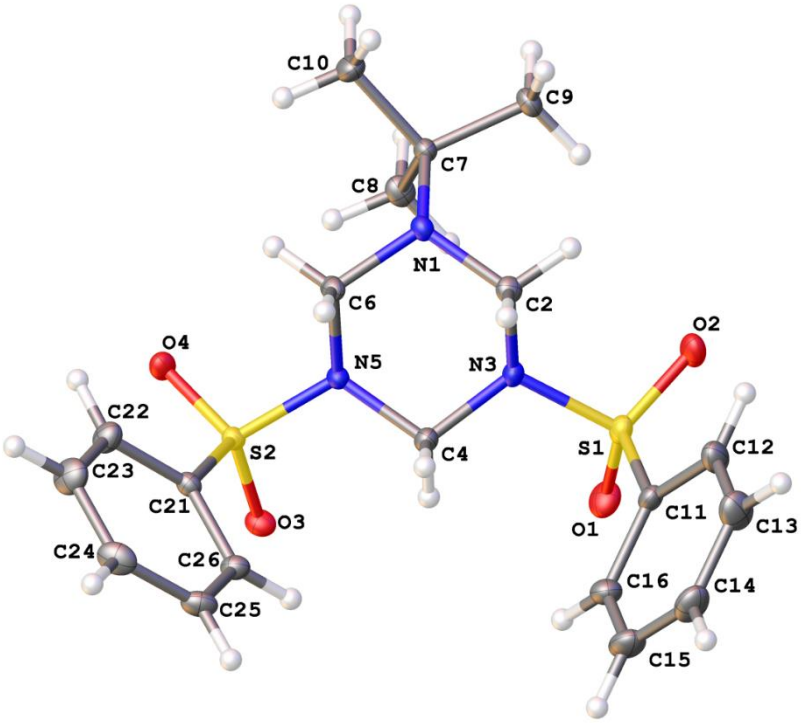
Table S11. Bond Angles for **3**.

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
O(1)	S(1)	O(2)	119.4(6)	C(8)	C(7)	C(9)	110.3(9)
O(1)	S(1)	N(3)	109.6(5)	N(1)	C(7)	C(9)	105.8(8)
O(2)	S(1)	N(3)	105.6(5)	C(8)	C(7)	C(10)	111.5(9)
O(1)	S(1)	C(11)	108.4(5)	N(1)	C(7)	C(10)	107.1(8)
O(2)	S(1)	C(11)	106.8(5)	C(9)	C(7)	C(10)	106.0(8)
N(3)	S(1)	C(11)	106.3(5)	C(12)	C(11)	C(16)	122.0(10)
O(4)	S(2)	O(3)	119.9(6)	C(12)	C(11)	S(1)	120.6(8)
O(4)	S(2)	N(5)	105.5(5)	C(16)	C(11)	S(1)	117.4(8)
O(3)	S(2)	N(5)	106.5(5)	C(11)	C(12)	C(13)	120.0(10)
O(4)	S(2)	C(21)	108.5(5)	C(14)	C(13)	C(12)	119.3(11)
O(3)	S(2)	C(21)	107.5(5)	C(15)	C(14)	C(13)	120.1(10)
N(5)	S(2)	C(21)	108.5(5)	C(15)	C(14)	C(17)	120.9(11)
C(2)	N(1)	C(6)	108.9(8)	C(13)	C(14)	C(17)	119.0(11)
C(2)	N(1)	C(7)	119.6(8)	C(14)	C(15)	C(16)	121.0(10)
C(6)	N(1)	C(7)	117.1(8)	C(11)	C(16)	C(15)	117.7(11)
C(4)	N(3)	C(2)	113.0(9)	C(26)	C(21)	C(22)	120.0(10)
C(4)	N(3)	S(1)	120.9(9)	C(26)	C(21)	S(2)	120.7(8)
C(2)	N(3)	S(1)	126.0(7)	C(22)	C(21)	S(2)	119.2(10)
C(4)	N(5)	C(6)	114.2(9)	C(23)	C(22)	C(21)	119.6(11)
C(4)	N(5)	S(2)	117.2(7)	C(24)	C(23)	C(22)	120.9(10)
C(6)	N(5)	S(2)	119.3(6)	C(23)	C(24)	C(25)	119.3(9)
N(1)	C(2)	N(3)	112.0(8)	C(23)	C(24)	C(27)	121.5(10)
N(3)	C(4)	N(5)	107.0(8)	C(25)	C(24)	C(27)	119.2(10)
N(1)	C(6)	N(5)	111.9(8)	C(26)	C(25)	C(24)	119.9(10)
C(8)	C(7)	N(1)	115.6(8)	C(25)	C(26)	C(21)	120.3(10)

Table S12. Torsion Angles for **3**.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O(1)	S(1)	N(3)	C(4)	−30.1(10)	O(2)	S(1)	C(11)	C(12)	−35.1(10)
O(2)	S(1)	N(3)	C(4)	−159.9(8)	N(3)	S(1)	C(11)	C(12)	77.3(10)
C(11)	S(1)	N(3)	C(4)	86.9(9)	O(1)	S(1)	C(11)	C(16)	16.7(10)
O(1)	S(1)	N(3)	C(2)	145.5(9)	O(2)	S(1)	C(11)	C(16)	146.6(9)
O(2)	S(1)	N(3)	C(2)	15.7(10)	N(3)	S(1)	C(11)	C(16)	−101.0(9)
C(11)	S(1)	N(3)	C(2)	−97.5(9)	C(16)	C(11)	C(12)	C(13)	1.9(16)
O(4)	S(2)	N(5)	C(4)	175.3(8)	S(1)	C(11)	C(12)	C(13)	−176.3(8)
O(3)	S(2)	N(5)	C(4)	46.8(9)	C(11)	C(12)	C(13)	C(14)	−0.7(16)
C(21)	S(2)	N(5)	C(4)	−68.6(9)	C(12)	C(13)	C(14)	C(15)	−1.0(16)
O(4)	S(2)	N(5)	C(6)	−40.0(9)	C(12)	C(13)	C(14)	C(17)	177.2(10)
O(3)	S(2)	N(5)	C(6)	−168.5(7)	C(13)	C(14)	C(15)	C(16)	1.4(16)
C(21)	S(2)	N(5)	C(6)	76.1(8)	C(17)	C(14)	C(15)	C(16)	−176.8(10)
C(6)	N(1)	C(2)	N(3)	−56.2(11)	C(12)	C(11)	C(16)	C(15)	−1.5(16)
C(7)	N(1)	C(2)	N(3)	82.3(11)	S(1)	C(11)	C(16)	C(15)	176.7(8)
C(4)	N(3)	C(2)	N(1)	58.3(11)	C(14)	C(15)	C(16)	C(11)	−0.2(16)
S(1)	N(3)	C(2)	N(1)	−117.6(9)	O(4)	S(2)	C(21)	C(26)	49.6(10)
C(2)	N(3)	C(4)	N(5)	−53.9(13)	O(3)	S(2)	C(21)	C(26)	−179.3(9)
S(1)	N(3)	C(4)	N(5)	122.2(9)	N(5)	S(2)	C(21)	C(26)	−64.5(9)
C(6)	N(5)	C(4)	N(3)	53.5(12)	O(4)	S(2)	C(21)	C(22)	−128.6(9)
S(2)	N(5)	C(4)	N(3)	−160.0(9)	O(3)	S(2)	C(21)	C(22)	2.5(10)
C(2)	N(1)	C(6)	N(5)	55.1(11)	N(5)	S(2)	C(21)	C(22)	117.3(9)
C(7)	N(1)	C(6)	N(5)	−84.5(10)	C(26)	C(21)	C(22)	C(23)	1.7(16)
C(4)	N(5)	C(6)	N(1)	−56.3(11)	S(2)	C(21)	C(22)	C(23)	179.9(8)
S(2)	N(5)	C(6)	N(1)	158.0(7)	C(21)	C(22)	C(23)	C(24)	0.5(16)
C(2)	N(1)	C(7)	C(8)	−79.6(11)	C(22)	C(23)	C(24)	C(25)	−2.6(15)
C(6)	N(1)	C(7)	C(8)	55.6(12)	C(22)	C(23)	C(24)	C(27)	179.0(10)
C(2)	N(1)	C(7)	C(9)	158.0(9)	C(23)	C(24)	C(25)	C(26)	2.7(15)
C(6)	N(1)	C(7)	C(9)	−66.8(11)	C(27)	C(24)	C(25)	C(26)	−179.0(10)
C(2)	N(1)	C(7)	C(10)	45.2(12)	C(24)	C(25)	C(26)	C(21)	−0.5(15)
C(6)	N(1)	C(7)	C(10)	−179.6(9)	C(22)	C(21)	C(26)	C(25)	−1.6(15)
O(1)	S(1)	C(11)	C(12)	−165.0(9)	S(2)	C(21)	C(26)	C(25)	−179.8(8)

4. (100K) $C_{19}H_{25}N_3O_4S_2$ (CCDC number 1992670)



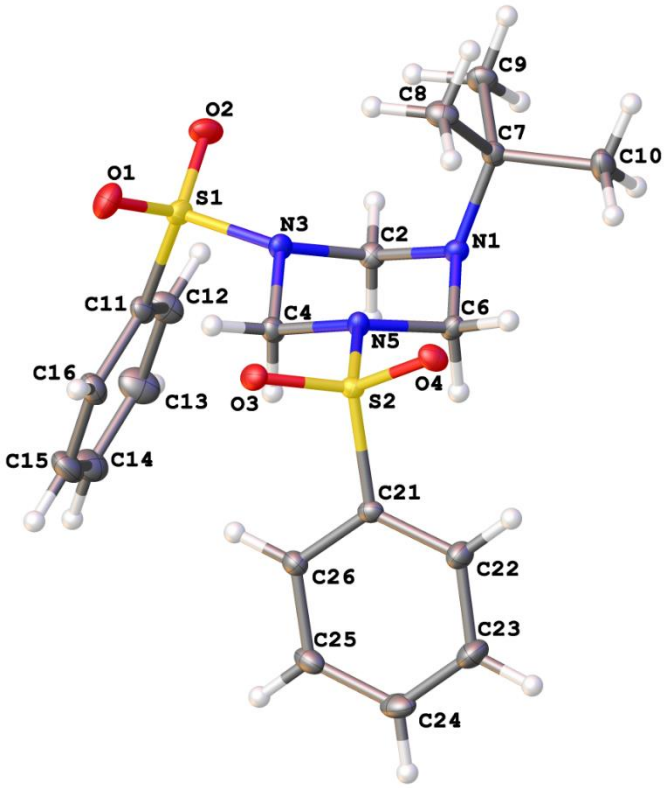


Table S13. Bond Lengths for **4**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
S(1)	O(1)	1.4336(11)	C(7)	C(9)	1.5283(17)
S(1)	O(2)	1.4353(10)	C(7)	C(10)	1.5318(19)
S(1)	N(3)	1.6396(11)	C(7)	C(8)	1.5336(19)
S(1)	C(11)	1.7637(14)	C(11)	C(12)	1.385(2)
S(2)	O(4)	1.4352(10)	C(11)	C(16)	1.3966(19)
S(2)	O(3)	1.4370(10)	C(12)	C(13)	1.390(2)
S(2)	N(5)	1.6376(11)	C(13)	C(14)	1.395(2)
S(2)	C(21)	1.7644(12)	C(14)	C(15)	1.383(2)
N(1)	C(2)	1.4351(16)	C(15)	C(16)	1.391(2)
N(1)	C(6)	1.4417(15)	C(21)	C(22)	1.3907(18)
N(1)	C(7)	1.4967(16)	C(21)	C(26)	1.3939(17)
N(3)	C(4)	1.4663(16)	C(22)	C(23)	1.397(2)
N(3)	C(2)	1.4948(17)	C(23)	C(24)	1.385(2)
N(5)	C(4)	1.4642(16)	C(24)	C(25)	1.391(2)
N(5)	C(6)	1.5048(16)	C(25)	C(26)	1.3879(18)

Table S14. Bond Angles for **4**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O(1)	S(1)	O(2)	120.28(7)	N(1)	C(6)	N(5)	111.04(9)
O(1)	S(1)	N(3)	106.53(6)	N(1)	C(7)	C(9)	109.35(10)
O(2)	S(1)	N(3)	105.77(6)	N(1)	C(7)	C(10)	106.79(10)
O(1)	S(1)	C(11)	108.20(7)	C(9)	C(7)	C(10)	107.70(11)
O(2)	S(1)	C(11)	108.31(6)	N(1)	C(7)	C(8)	113.50(10)
N(3)	S(1)	C(11)	107.04(6)	C(9)	C(7)	C(8)	108.83(11)
O(4)	S(2)	O(3)	120.10(6)	C(10)	C(7)	C(8)	110.51(12)
O(4)	S(2)	N(5)	106.83(6)	C(12)	C(11)	C(16)	121.41(13)
O(3)	S(2)	N(5)	106.18(6)	C(12)	C(11)	S(1)	119.46(11)
O(4)	S(2)	C(21)	107.54(6)	C(16)	C(11)	S(1)	119.11(11)
O(3)	S(2)	C(21)	108.13(6)	C(11)	C(12)	C(13)	119.19(14)
N(5)	S(2)	C(21)	107.47(6)	C(12)	C(13)	C(14)	120.07(15)
C(2)	N(1)	C(6)	109.98(10)	C(15)	C(14)	C(13)	120.10(15)
C(2)	N(1)	C(7)	119.45(10)	C(14)	C(15)	C(16)	120.57(14)
C(6)	N(1)	C(7)	117.19(10)	C(15)	C(16)	C(11)	118.66(14)
C(4)	N(3)	C(2)	109.75(10)	C(22)	C(21)	C(26)	121.63(11)
C(4)	N(3)	S(1)	116.48(9)	C(22)	C(21)	S(2)	119.20(10)
C(2)	N(3)	S(1)	118.78(8)	C(26)	C(21)	S(2)	119.16(10)
C(4)	N(5)	C(6)	112.20(10)	C(21)	C(22)	C(23)	118.67(13)
C(4)	N(5)	S(2)	115.84(8)	C(24)	C(23)	C(22)	120.11(13)
C(6)	N(5)	S(2)	117.59(8)	C(23)	C(24)	C(25)	120.60(13)
N(1)	C(2)	N(3)	110.61(10)	C(26)	C(25)	C(24)	120.08(13)
N(5)	C(4)	N(3)	106.05(10)	C(25)	C(26)	C(21)	118.89(12)

Table S15. Torsion Angles for **4**.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O(1)	S(1)	N(3)	C(4)	51.01(11)	C(6)	N(1)	C(7)	C(8)	−52.44(14)
O(2)	S(1)	N(3)	C(4)	−179.91(9)	O(1)	S(1)	C(11)	C(12)	147.92(12)
C(11)	S(1)	N(3)	C(4)	−64.57(11)	O(2)	S(1)	C(11)	C(12)	16.01(14)
O(1)	S(1)	N(3)	C(2)	−174.20(9)	N(3)	S(1)	C(11)	C(12)	−97.62(12)
O(2)	S(1)	N(3)	C(2)	−45.12(11)	O(1)	S(1)	C(11)	C(16)	−33.93(13)
C(11)	S(1)	N(3)	C(2)	70.22(10)	O(2)	S(1)	C(11)	C(16)	−165.84(11)
O(4)	S(2)	N(5)	C(4)	−168.89(9)	N(3)	S(1)	C(11)	C(16)	80.53(12)
O(3)	S(2)	N(5)	C(4)	−39.59(10)	C(16)	C(11)	C(12)	C(13)	0.1(2)
C(21)	S(2)	N(5)	C(4)	75.94(10)	S(1)	C(11)	C(12)	C(13)	178.25(12)
O(4)	S(2)	N(5)	C(6)	54.49(10)	C(11)	C(12)	C(13)	C(14)	−0.5(3)
O(3)	S(2)	N(5)	C(6)	−176.21(9)	C(12)	C(13)	C(14)	C(15)	0.4(3)
C(21)	S(2)	N(5)	C(6)	−60.68(10)	C(13)	C(14)	C(15)	C(16)	0.1(3)
C(6)	N(1)	C(2)	N(3)	58.31(13)	C(14)	C(15)	C(16)	C(11)	−0.4(2)
C(7)	N(1)	C(2)	N(3)	−81.49(13)	C(12)	C(11)	C(16)	C(15)	0.3(2)
C(4)	N(3)	C(2)	N(1)	−63.26(13)	S(1)	C(11)	C(16)	C(15)	−177.77(11)
S(1)	N(3)	C(2)	N(1)	159.19(8)	O(4)	S(2)	C(21)	C(22)	−9.77(12)
C(6)	N(5)	C(4)	N(3)	−58.56(13)	O(3)	S(2)	C(21)	C(22)	−140.84(11)
S(2)	N(5)	C(4)	N(3)	162.55(8)	N(5)	S(2)	C(21)	C(22)	104.93(11)
C(2)	N(3)	C(4)	N(5)	61.23(12)	O(4)	S(2)	C(21)	C(26)	169.66(10)
S(1)	N(3)	C(4)	N(5)	−160.14(8)	O(3)	S(2)	C(21)	C(26)	38.59(12)
C(2)	N(1)	C(6)	N(5)	−54.43(13)	N(5)	S(2)	C(21)	C(26)	−75.64(11)
C(7)	N(1)	C(6)	N(5)	86.37(13)	C(26)	C(21)	C(22)	C(23)	−1.3(2)
C(4)	N(5)	C(6)	N(1)	56.49(13)	S(2)	C(21)	C(22)	C(23)	178.12(11)
S(2)	N(5)	C(6)	N(1)	−165.39(8)	C(21)	C(22)	C(23)	C(24)	1.7(2)
C(2)	N(1)	C(7)	C(9)	−37.16(15)	C(22)	C(23)	C(24)	C(25)	−0.8(2)
C(6)	N(1)	C(7)	C(9)	−174.15(11)	C(23)	C(24)	C(25)	C(26)	−0.7(2)
C(2)	N(1)	C(7)	C(10)	−153.42(11)	C(24)	C(25)	C(26)	C(21)	1.1(2)
C(6)	N(1)	C(7)	C(10)	69.59(13)	C(22)	C(21)	C(26)	C(25)	−0.1(2)
C(2)	N(1)	C(7)	C(8)	84.55(13)	S(2)	C(21)	C(26)	C(25)	−179.52(10)