Supporting Information for article

Bisthiadiazoleamines: Synthesis, Characterization and Properties

Yu. V. Suvorova, E. A. Petukhova, M. V. Dmitriev, E. A. Danilova, V. V. Aleksandriiskii

Yuliya V. Suvorova, Ekaterina A. Petukhova, Elene A. Danilova, Viktor V. Aleksandriiskii

Research Institute of Macroheterocycles, Ivanovo State University of Chemistry and Technology, Sheremetevsky av., 7, Ivanovo, Russia, 153000

E-mail: yuliya_butina@mail.ru

Maksim V. Dmitriev

Department of Organic Chemistry, Perm State University, Bukireva st., 15, Perm, Russia, 614068

E-mail: maxperm@yandex.ru

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Table S1. Hydrogen-bond geometry (, º).

D—H···*A* [a]	*D*—H, Å	H···*A*, Å	*D*···*A*, Å	*D*—H···*A*, °
N1—H1*A*···Cl2^{i}	0.89(3)	2.27(3)	3.127(2)	161(2)
N1—H1*B*···O1*W*	0.83(2)	2.03(2)	2.850(3)	177(2)
N2—H2···Cl1	0.86(3)	2.24(3)	3.0959(17)	174(3)
N5—H5···Cl2^{ii}	0.83(2)	2.19(2)	3.0208(17)	176(3)
N6—H6*A*···Cl1^{iii}	0.88(3)	2.48(3)	3.249(2)	146(2)
N6—H6*B*···O1*W*^{iv}	0.76(3)	2.28(3)	2.944(3)	146(3)
O1*W*—H1*WA*···Cl1	0.92(2)	2.24(2)	3.121(2)	161(3)
O1*W*—H1*WB*···Cl1^{i}	0.89(2)	2.31(2)	3.2042(19)	178(3)

[a] Symmetry codes: (i) *x*, −*y*+1/2, *z*−1/2; (ii) −*x*, −*y*+1, −*z*+1; (iii) *x*−1, *y*, *z*; (iv) *x*−1, −*y*+1/2, *z*−1/2.

Table S2. Crystal data, data collection and structure refinement details for **1**.

Crystal data	
Chemical formula	$(C_5H_8N_6S_2)^{2+}\cdot H_2O\cdot 2(Cl)^{1-}$
M_r	305.21
Crystal system, space group	monoclinic, $P2_1/c$
Temperature (K)	295.15
a, b, c (Å)	12.2591(17), 11.8547(16), 8.6170(12)
α, β, γ (°)	90, 97.318(15), 90
V (Å^3)	1242.1(3)
Z	4
Radiation type	Mo $K\alpha$ radiation, λ = 0.71073 Å
μ (mm^{-1})	0.848
Crystal size (mm)	0.55 × 0.30 × 0.25
Data collection	
Diffractometer	Xcalibur Ruby (Agilent technologies)
Absorption correction	Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm[1]
T_{min}, T_{max}	0.663, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	6068, 2920, 2557
R_{int}	0.034
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.689
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.0395, 0.1042, 1.098
No. of reflections	2920
No. of parameters	178
No. of restraints	4
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.32, −0.54

Table S3. Atom coordinates for **1**.

Atom	X	Y	Z
N	-0.274080	2.159785	-5.083987
C	-0.806124	2.062630	-7.473184
S	-3.054453	-0.299036	-8.242633
C	-3.079093	-0.972874	-4.980034
N	-1.566732	0.445730	-3.636828
N	-4.463089	-2.923845	-3.976989
H	-6.145406	-3.305347	-4.793842
H	-4.515977	-2.884665	-2.064568
C	0.333872	3.804584	-9.406610
H	1.176127	2.737605	-10.966406
H	1.846395	4.833400	-8.438617
N	-3.794488	7.436063	-13.647378
C	-4.541767	8.796519	-11.725269
S	-3.161619	7.938427	-8.816869
C	-1.522764	5.606789	-10.580796
N	-2.087032	5.612824	-12.963999
N	-6.361190	10.637140	-11.906443
H	-6.203027	12.132616	-10.730734
H	-6.755445	11.109482	-13.708491

Table S4. Atom coordinates for **2**.

Atom	X	Y	Z
N	-0.664895	2.964798	-15.605497
C	-3.013258	2.996052	-14.922750
S	-5.038607	1.444412	-17.110464
C	-2.275354	0.891180	-18.893592
N	-0.216726	1.786183	-17.871961
N	-2.293477	-0.504752	-21.082815
H	-3.820954	-0.321068	-22.212946
H	-0.625340	-0.420184	-22.017299
C	-1.855557	5.174766	-10.829501
H	-0.626395	6.455638	-11.886973
H	-0.690522	3.579049	-10.228125
N	-4.253865	6.749151	-4.503243
C	-4.685897	9.059553	-5.255733
S	-3.816811	9.647088	-8.417580
C	-2.859145	6.424886	-8.493228
N	-3.203544	5.276790	-6.357856
N	-5.577388	10.929211	-3.687363
H	-6.718082	12.242148	-4.474761
H	-6.232109	10.236210	-2.027662
C	-3.999322	4.220486	-12.560098
H	-5.174472	2.876718	-11.507597
H	-5.246498	5.797011	-13.066771

Table S5. Atom coordinates for **3**.

Atom	X	Y	Z
N	-1.443895	-1.189905	-4.428444
C	-1.315440	0.051677	-2.324757
S	0.090885	-1.734149	0.157352
C	0.412855	-4.163194	-2.101930
N	-0.451460	-3.585615	-4.338220
N	1.351328	-6.507463	-1.494729
H	2.759126	-6.564917	-0.206858
H	1.674534	-7.588430	-3.040704
C	-1.619146	4.488442	-6.384780
H	-0.877698	2.707101	-7.130090
H	0.012161	5.548923	-5.651893
N	-5.663420	8.332996	-10.560776
C	-3.943795	8.173655	-12.319468
S	-1.253938	6.413207	-11.445541
C	-2.801870	5.980540	-8.490350
N	-4.979070	7.090791	-8.386045
N	-4.121807	9.394718	-14.610252
H	-3.385370	8.480143	-16.116778
H	-5.883705	10.075775	-14.924480
C	-3.484166	3.935018	-4.230838
H	-4.370883	5.702893	-3.630011
H	-5.001554	2.722807	-4.938259
C	-2.248359	2.704698	-1.908324
H	-0.669183	3.876525	-1.238678
H	-3.622053	2.675657	-0.343955

Table S6. Atom coordinates for **4**.

Atom	X	Y	Z
N	0.427379	-0.262011	-4.452548
C	-0.886991	0.182235	-2.432215
S	-2.705719	-2.465032	-1.446895
C	-1.368497	-4.047217	-4.057960
N	0.185150	-2.667796	-5.387933
N	-2.037209	-6.473237	-4.701026
H	-2.395513	-7.677164	-3.263141
H	-0.904486	-7.207918	-6.057740
C	-2.102548	6.164656	-5.658090
H	-0.501755	4.897509	-6.011183
H	-1.355000	7.759768	-4.552463
N	-5.819025	8.327324	-11.145698
C	-3.717864	8.902008	-12.300410
S	-0.968181	8.260138	-10.534317
C	-3.059713	7.157678	-8.141370
N	-5.414826	7.353885	-8.773322
N	-3.635026	10.052968	-14.632548
H	-2.192896	9.544201	-15.776863
H	-5.339140	10.027121	-15.504911
C	-4.151859	4.778676	-4.135090
H	-5.873233	5.923186	-4.118693
H	-4.641287	3.024743	-5.120940
C	-3.378260	4.207412	-1.396959
H	-3.139473	5.986409	-0.355364
H	-4.935073	3.200794	-0.467861
C	-0.916238	2.667988	-1.073635
H	-0.576538	2.361056	0.947863
H	0.703738	3.731078	-1.786441

Table S7. Atom coordinates for **5**.

Atom	X	Y	Z
N	-4.971736	-0.415020	0.595333
C	-4.882773	-1.805204	-1.418513
S	-3.053669	-4.592450	-0.998783
C	-2.579875	-3.525708	2.119266
N	-3.681395	-1.375816	2.625894
N	-1.055990	-4.783015	3.810024
H	-1.095492	-6.690892	3.738360
H	-1.219387	-4.084221	5.584934
C	-2.254285	3.254748	-10.307364
H	-4.176914	3.920364	-9.914353
H	-2.415154	1.622300	-11.570411
N	1.556364	6.900035	-14.834319
C	1.252045	8.915497	-13.445801
S	-0.607323	8.429237	-10.723961
C	-0.850068	5.239076	-11.762307
N	0.337044	4.827187	-13.864538
N	2.157017	11.260277	-14.110113
H	2.712628	12.400179	-12.682660
H	3.412369	11.171258	-15.552500
C	-0.932709	2.461236	-7.830623
H	1.000376	1.874138	-8.289538
H	-0.762368	4.105223	-6.575295
C	-2.273056	0.304418	-6.418689
H	-2.465698	-1.330548	-7.687535
H	-1.044294	-0.312187	-4.867268
C	-4.874973	1.007728	-5.348956
H	-6.152455	1.557776	-6.886327
H	-4.698768	2.652483	-4.099732
C	-6.178122	-1.138864	-3.861046
H	-8.104481	-0.549191	-3.385030
H	-6.339354	-2.826610	-5.040630

Table S8. Atom coordinates for **6**.

Atom	X	Y	Z
N	0.650322	0.164735	-2.190109
C	-0.893762	0.055782	-4.117783
S	-2.290050	-2.984304	-4.497152
C	-0.540114	-3.845583	-1.801285
N	0.852754	-2.024825	-0.861889
N	-0.532182	-6.255753	-0.861433
H	-2.132481	-7.280095	-1.033408
H	0.323633	-6.395167	0.843608
N	-5.181354	6.466018	-12.614469
C	-3.789155	8.287467	-11.675350
S	-2.039094	7.427321	-8.979183
C	-3.434457	4.386708	-9.357933
N	-4.978299	4.276895	-11.285732
N	-3.797983	10.697390	-12.615709
H	-2.198643	11.723101	-12.442911
H	-4.653486	10.836276	-14.320951
C	-2.946417	2.241785	-7.745690
H	-3.994765	0.565846	-8.308943
C	-1.381565	2.201104	-5.729657
H	-0.333140	3.876975	-5.156211

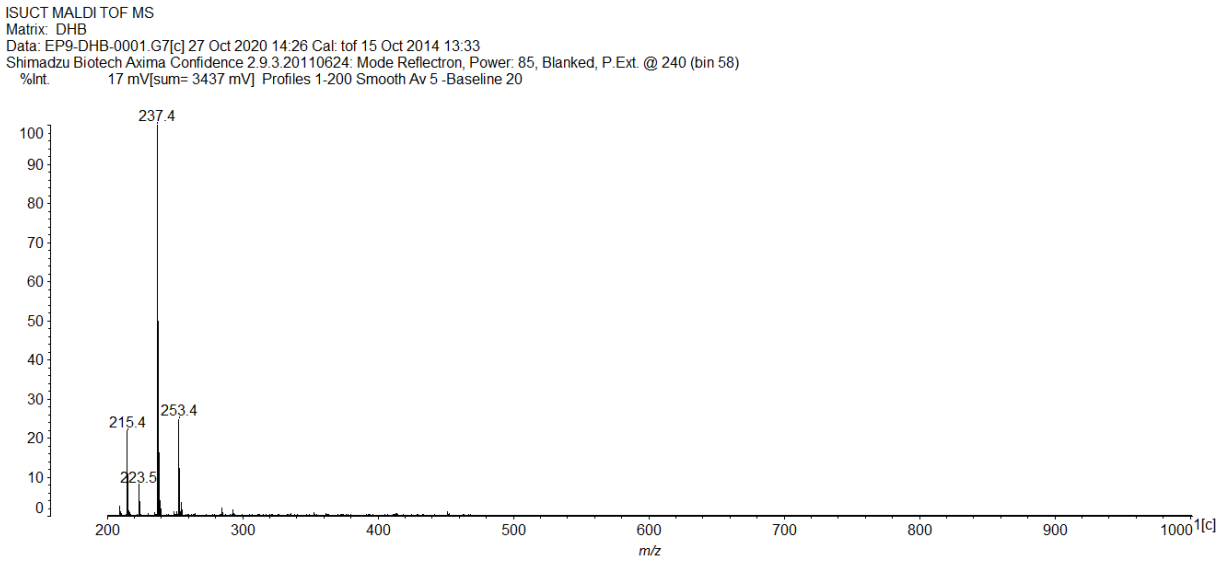

Figure S1. Mass-spectrum of bis(5-amino-1,3,4-thiadiazole)methane **1**.

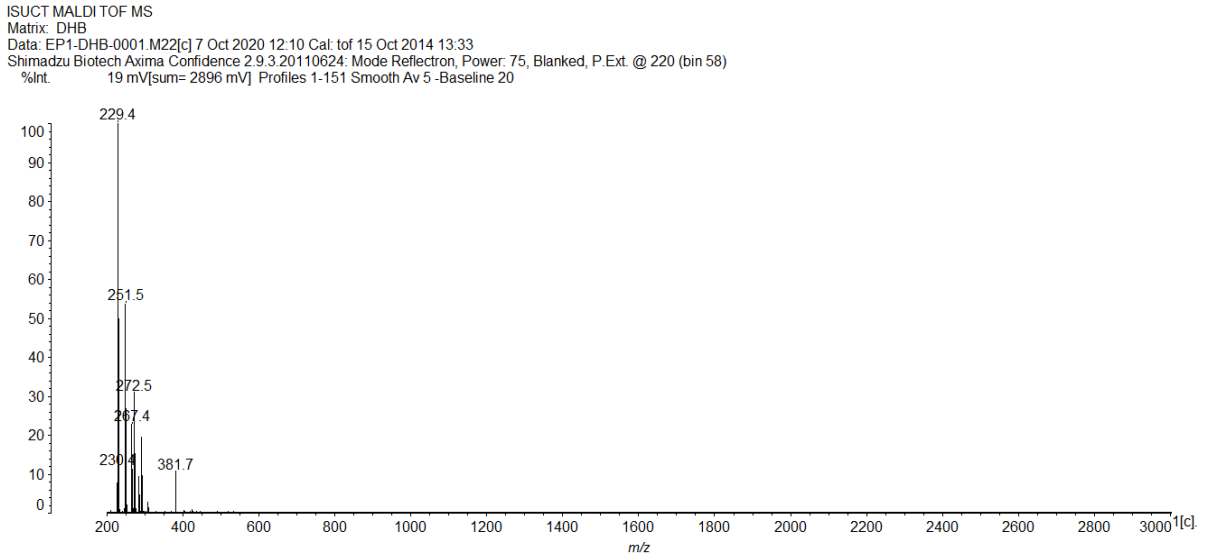

Figure S2. Mass-spectrum of bis(5-amino-1,3,4-thiadiazole)ethane **2**.

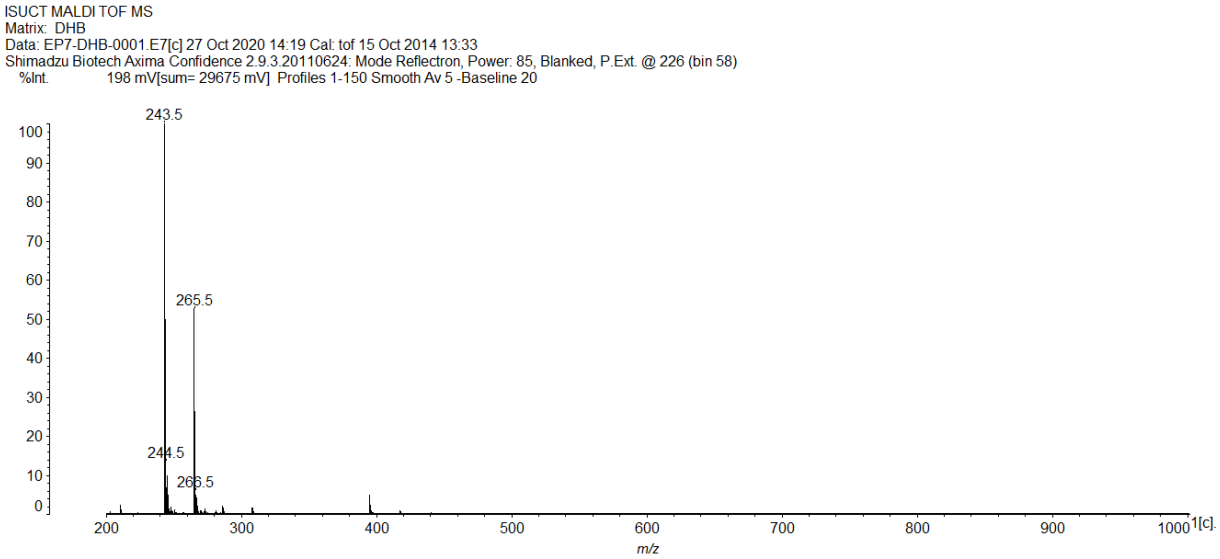

Figure S3. Mass-spectrum of bis(5-amino-1,3,4-thiadiazole)propane **3**.

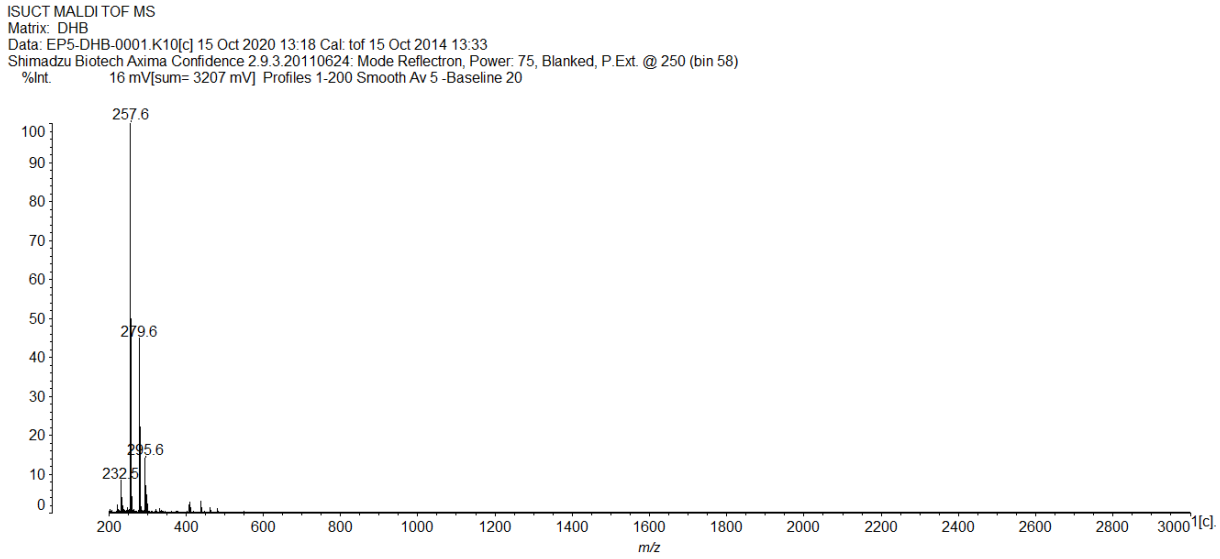

Figure S4. Mass-spectrum of bis(5-amino-1,3,4-thiadiazole)butane **4**.

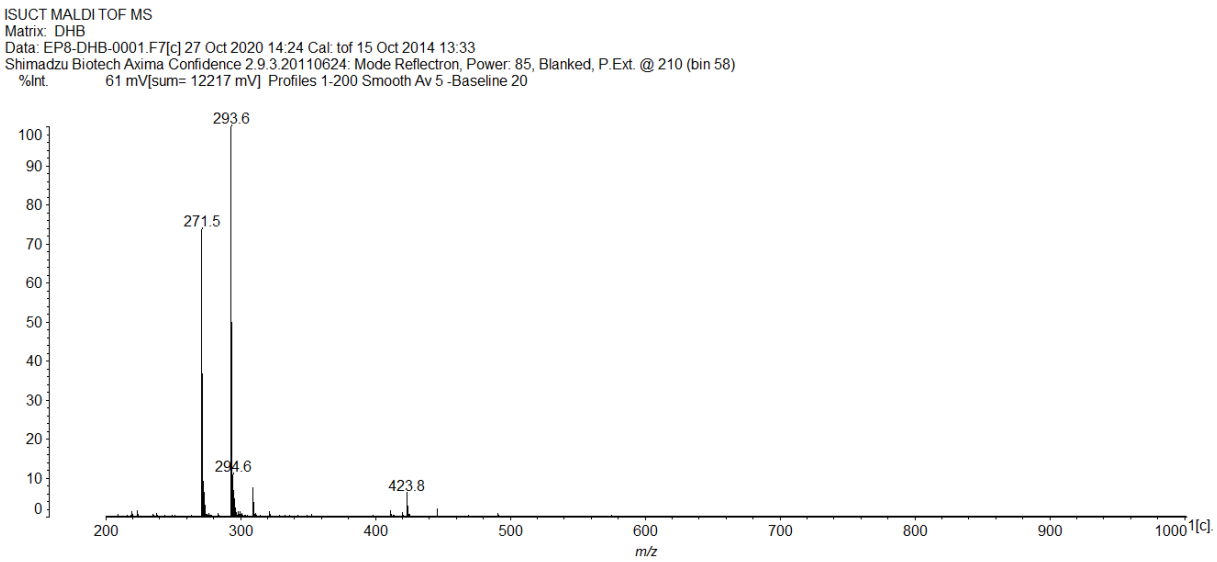

Figure S5. Mass-spectrum of bis(5-amino-1,3,4-thiadiazole)pentane **5**.

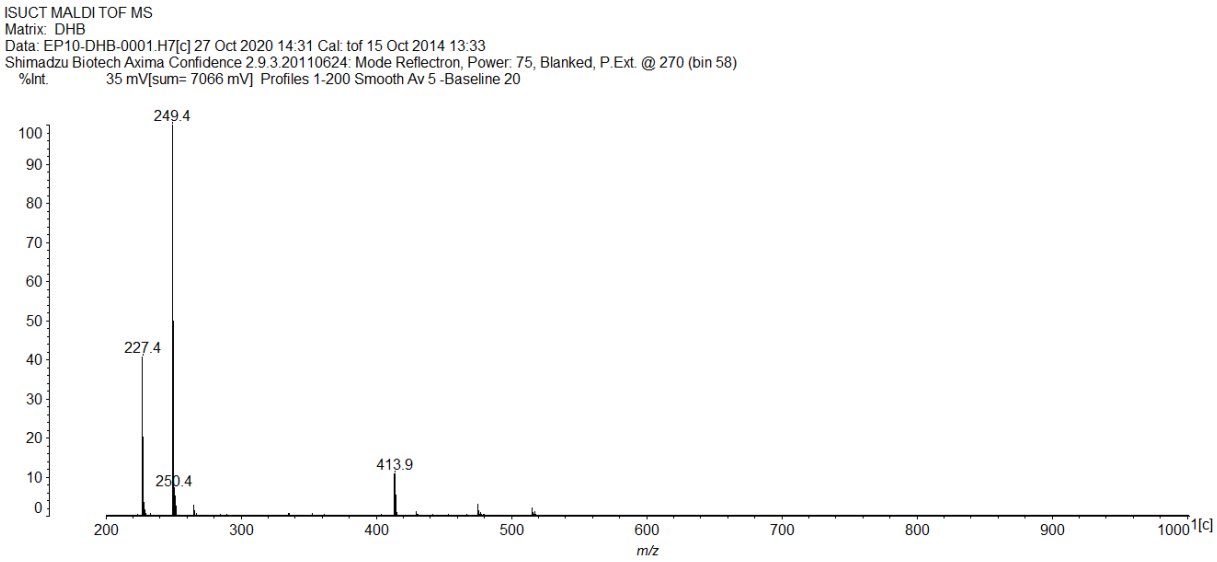

Figure S6. Mass-spectrum of bis(5-amino-1,3,4-thiadiazole)ethene **6**.

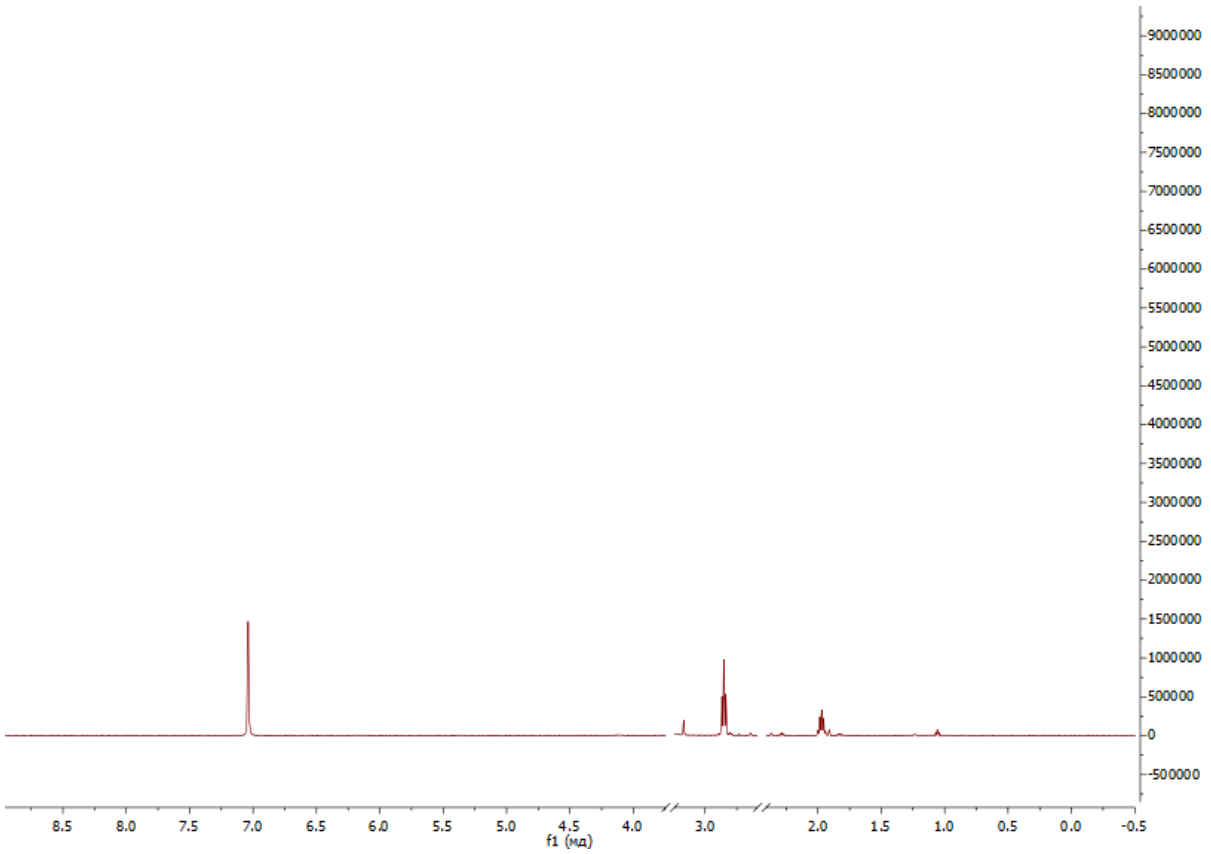

Figure S7. ^{1}H NMR spectrum of bis(5-amino-1,3,4-thiadiazole)propane **3** ([D_6]DMSO).

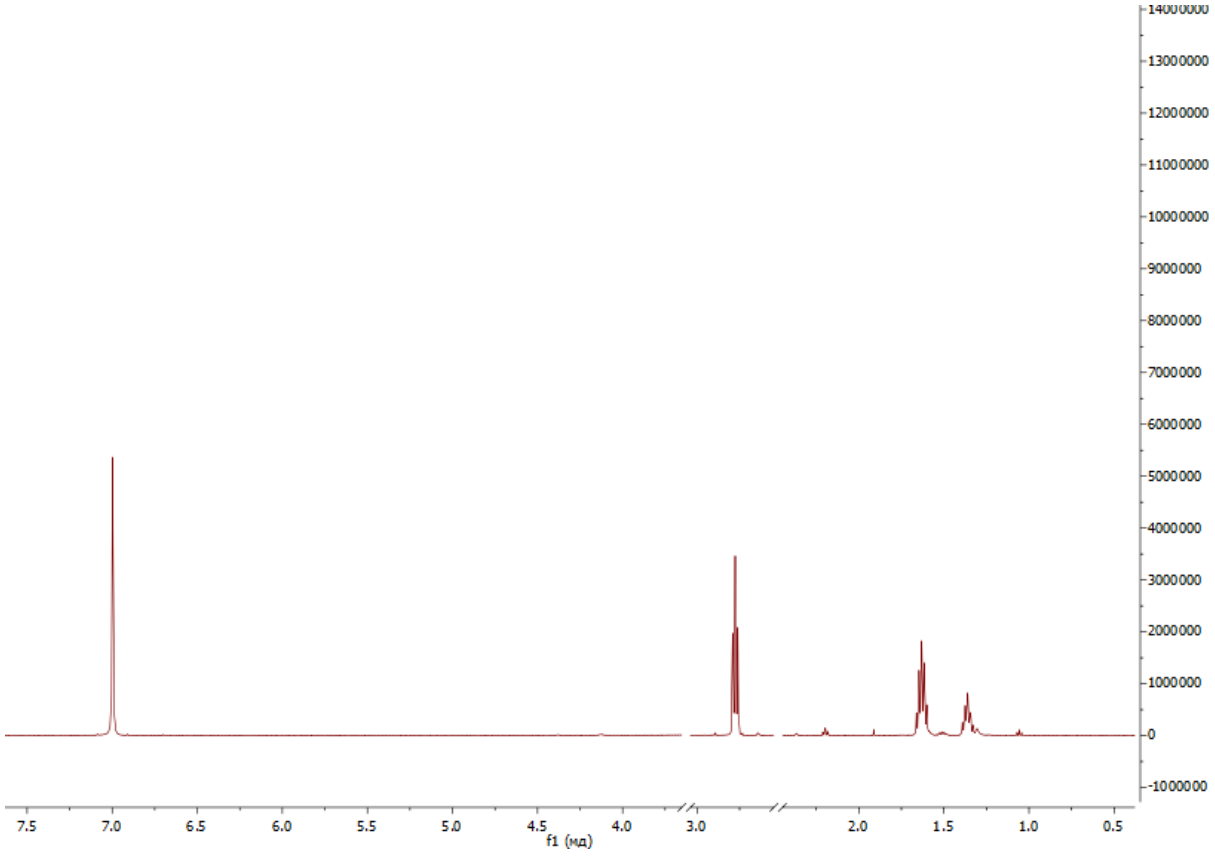

Figure S8. ^{1}H NMR spectrum of bis(5-amino-1,3,4-thiadiazole)pentane **5** ([D_6]DMSO).

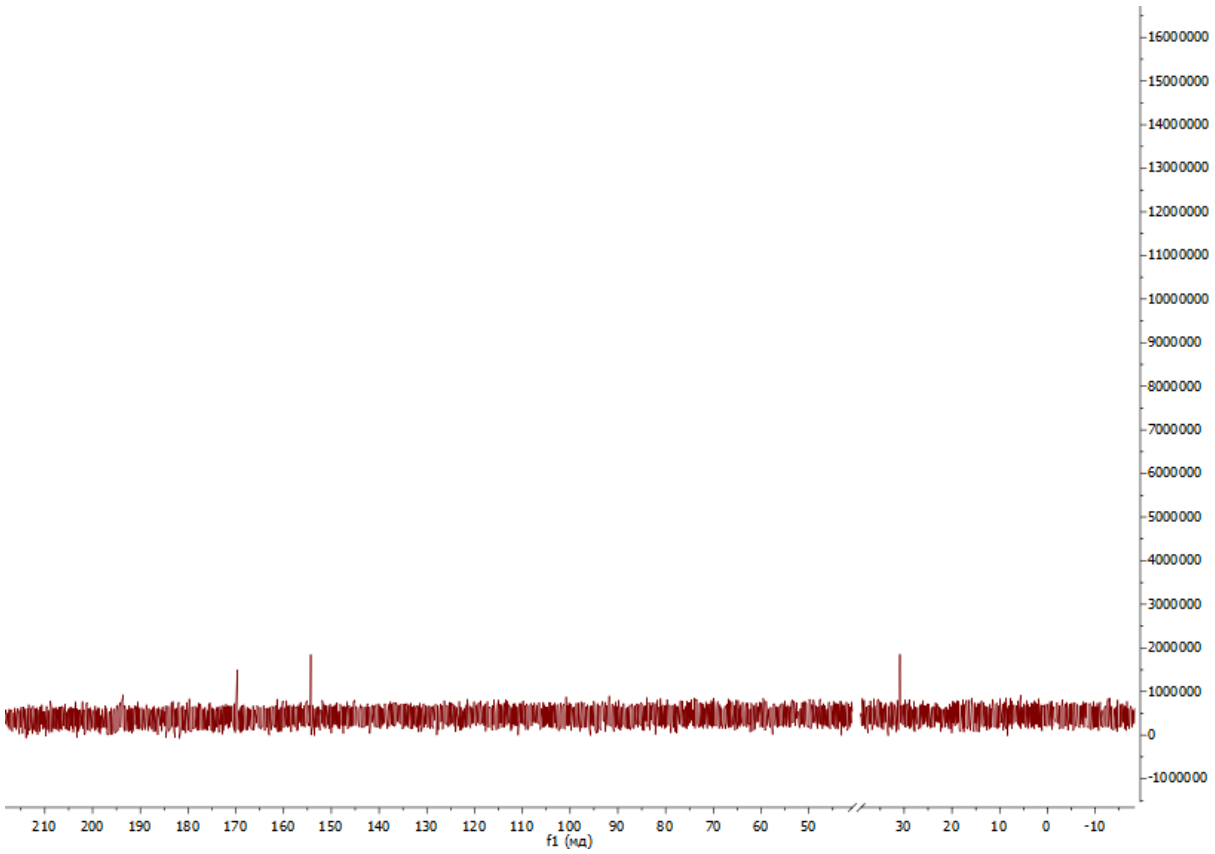

Figure S9. ^{13}C NMR spectrum of bis(5-amino-1,3,4-thiadiazole)methane **1** ([D_6]DMSO).

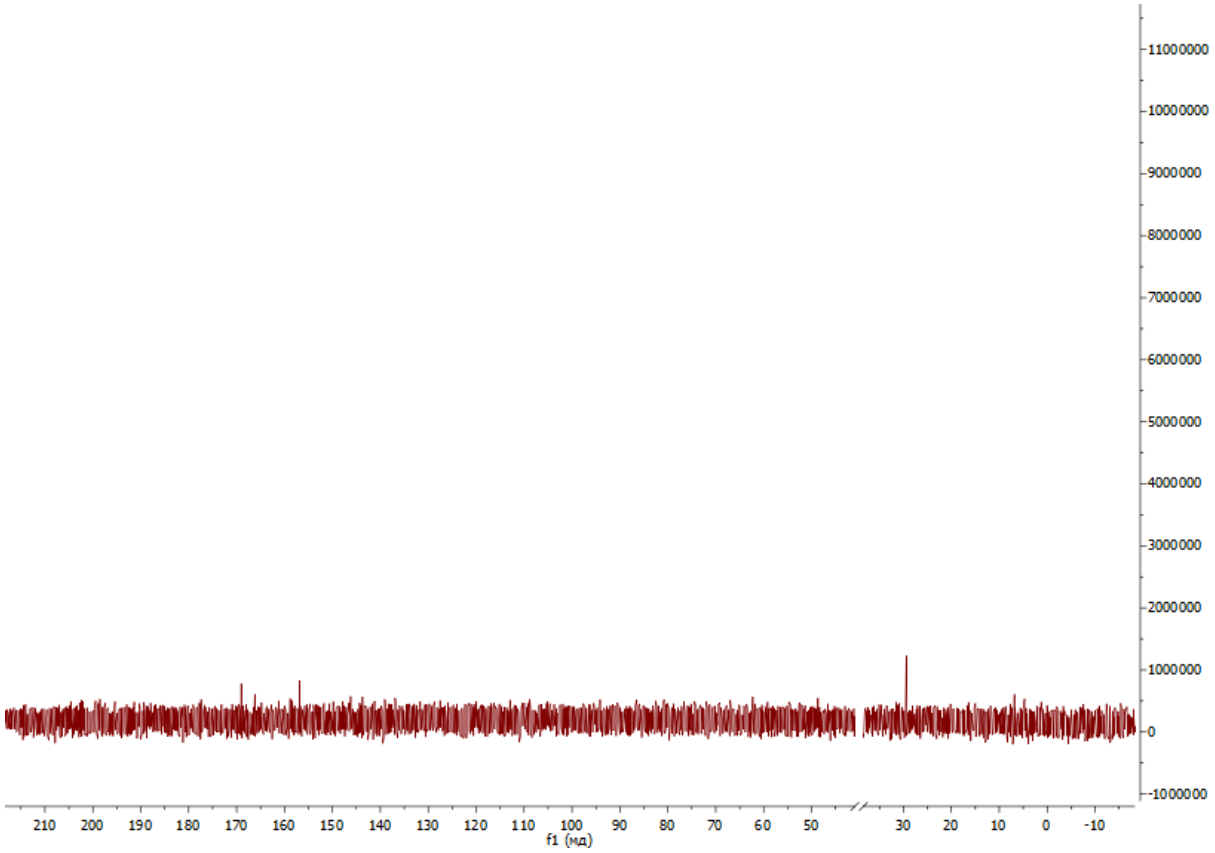

Figure S10. ^{13}C NMR spectrum of bis(5-amino-1,3,4-thiadiazole)ethane **2** ([D_6]DMSO).

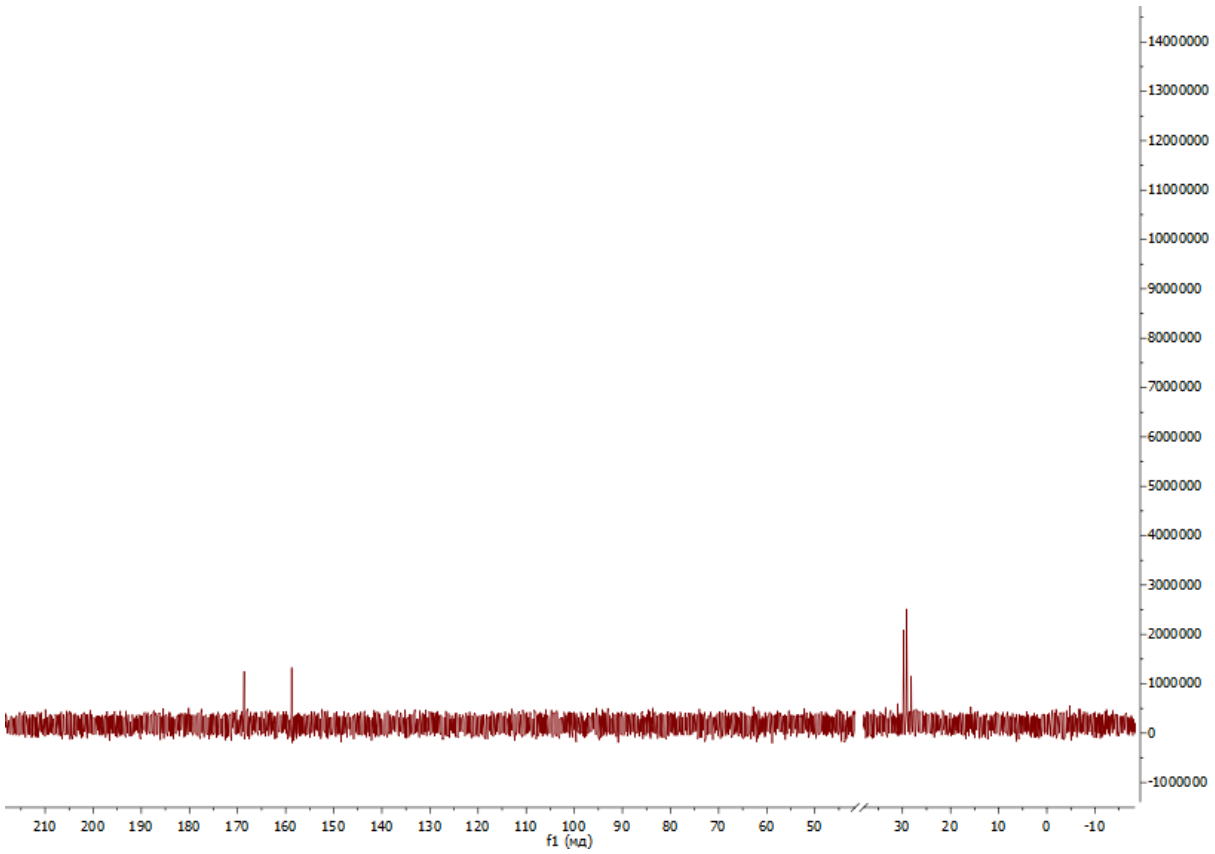

Figure S11. ^{13}C NMR spectrum of bis(5-amino-1,3,4-thiadiazole)pentane **5** ([D_6]DMSO).

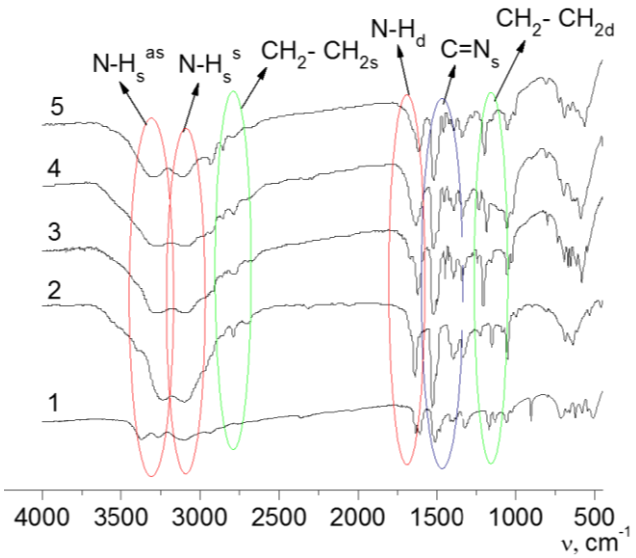

Figure S12. IR spectra (KBr): bis(5-amino-1,3,4-thiadiazole-2-yl): -methane **1**, -ethane **2**, -propane **3**, -butane **4**, -pentane **5**.

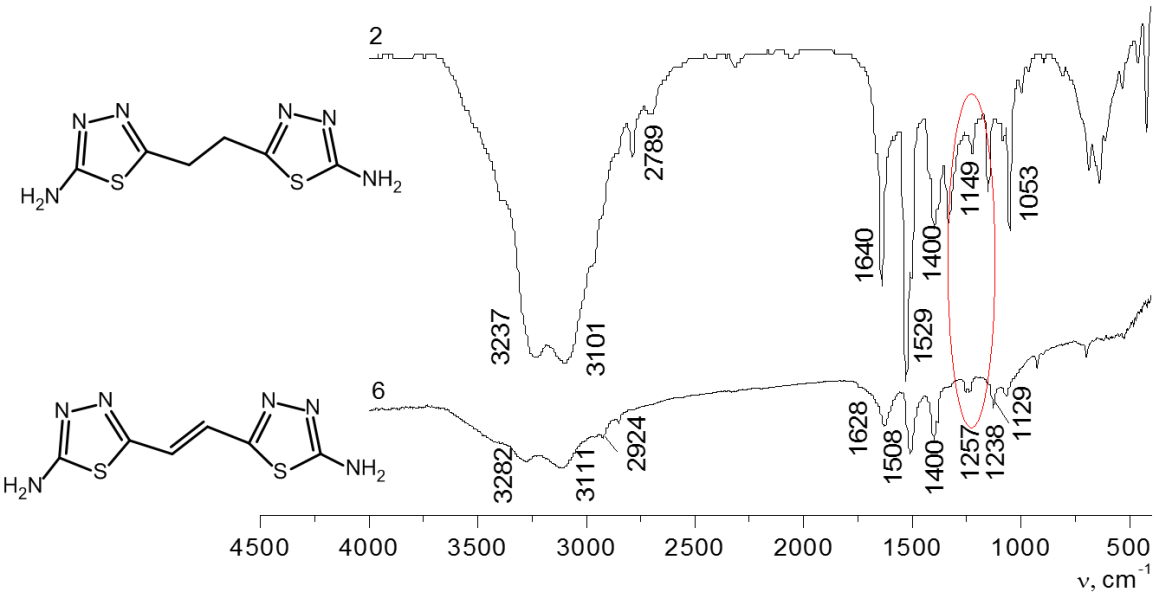

Figure S13. IR spectra (KBr): bis(5-amino-1,3,4-thiadiazole-2-yl): -ethane **2** и -ethene **6.**

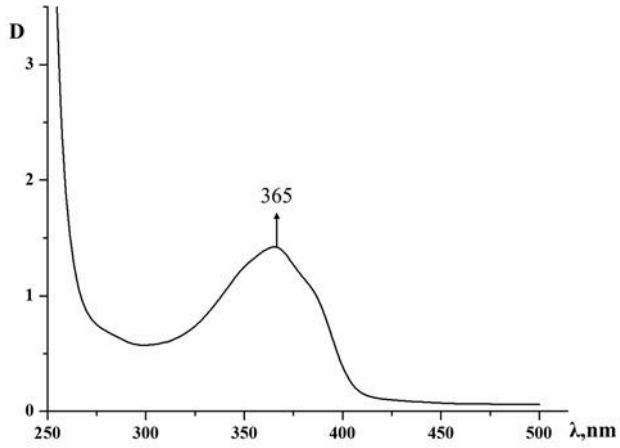

Figure S14. UV-Vis spectrum of bis(5-amino-1,3,4-thiadiazole-2-yl)ethene **6** (DMSO, c = $3.01 \cdot 10^{-4}$ mol/L.

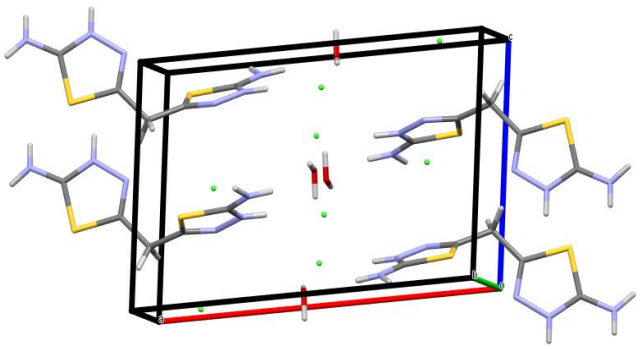

Figure S15. Fragment of crystal packing of **1**.