Synthesis, Molecular Structure and Applications of 2-Hydroxylamin-4,5-dihydroimidazolinium-O-sulfonate to the Synthesis of Novel Heterocyclic Ring Systems.

Franciszek Sączewski,[a*] Jarosław Sączewski[a] and Maria Gdaniec[b]

[a] Department of Chemical Technology of Drugs, Medical University of Gdańsk, Poland

[b] Faculty of Chemistry, A. Mickiewicz University, 60-780 Poznań, Poland

saczew@amg.gda.pl

Table of Contents:

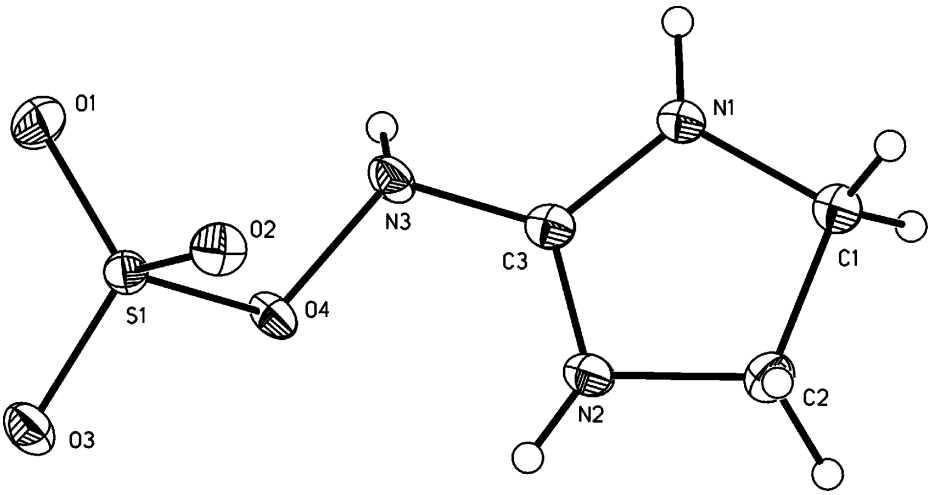


Figure S1. ORTEP drawing of the molecule **1** with the atom labeling scheme. Ellipsoids are drawn at 50% probability level

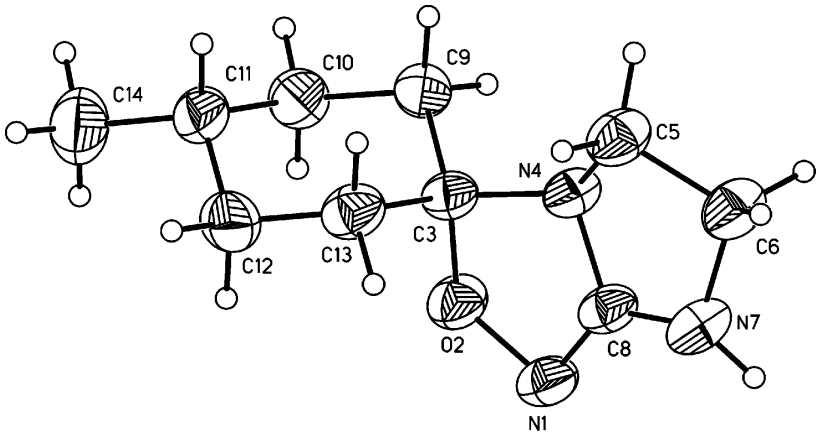


Figure S2. ORTEP drawing of the molecule **7** with the atom labeling scheme. Ellipsoids are drawn at 50% probability level.

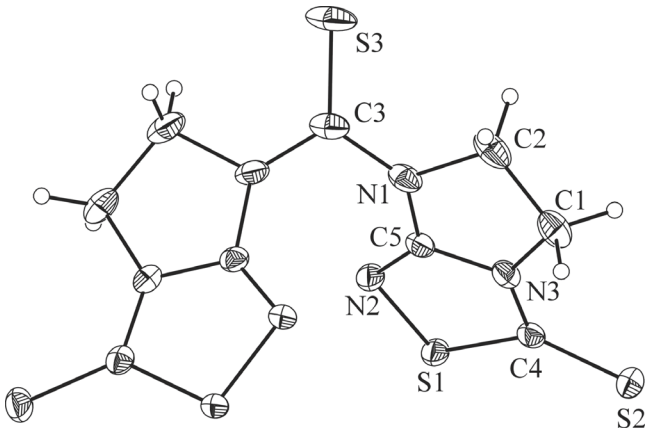


Figure S3. ORTEP drawing of the molecule **11** with the atom labeling scheme. Ellipsoids are drawn at 50% probability level.

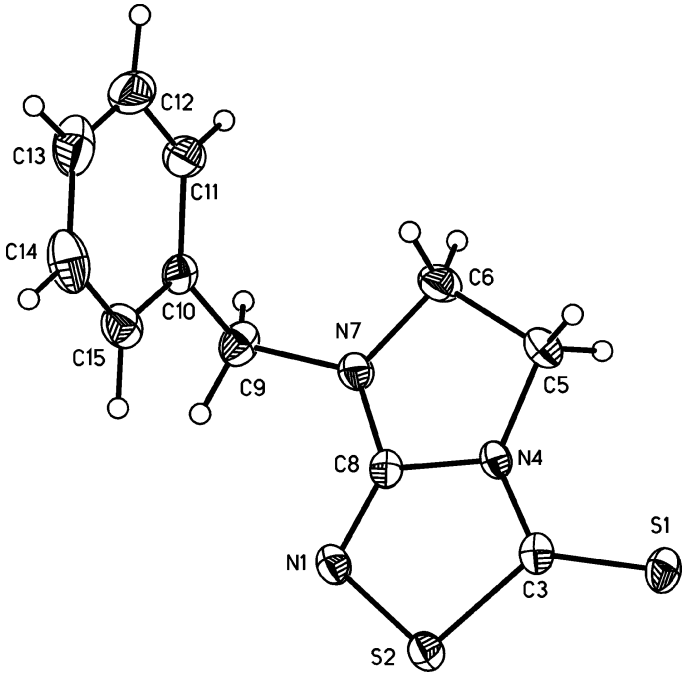


Figure S4. ORTEP drawing of the molecule **13** with the atom labeling scheme. Ellipsoids are drawn at 50% probability level.

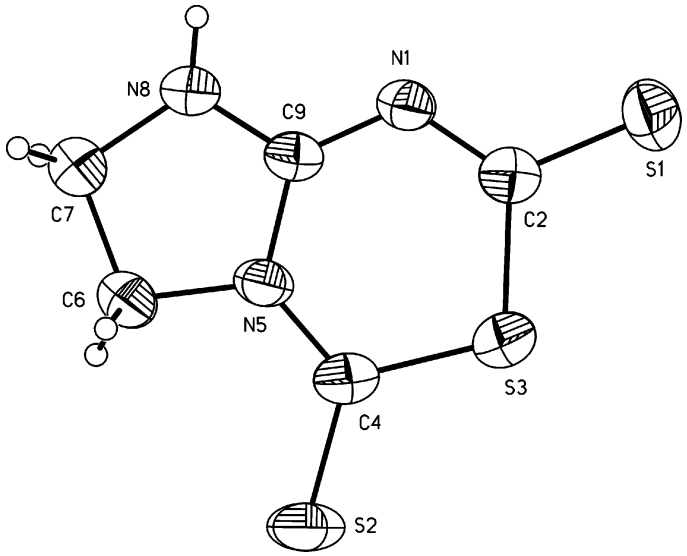


Figure S5. ORTEP drawing of the molecule **16** with the atom labeling scheme. Ellipsoids are drawn at 50% probability level.

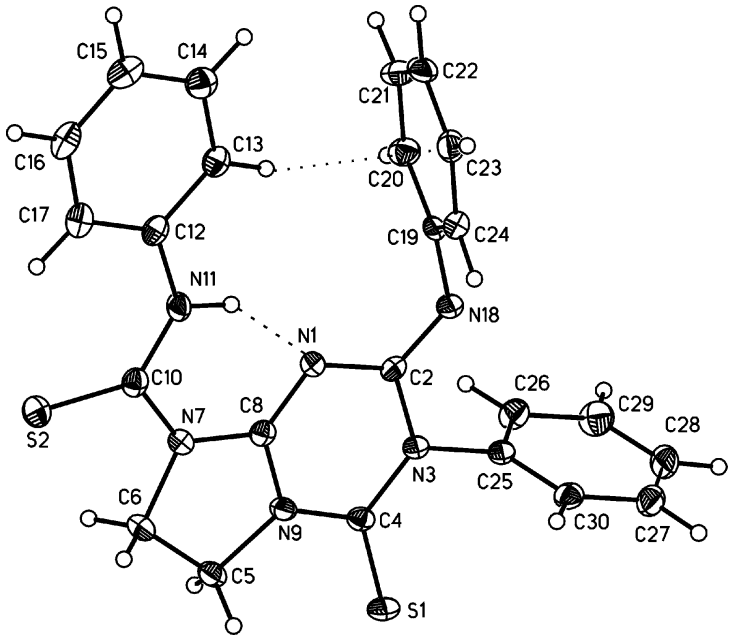


Figure S6. ORTEP drawing of the molecule **17** with the atom labeling scheme. Ellipsoids are drawn at 50% probability level.

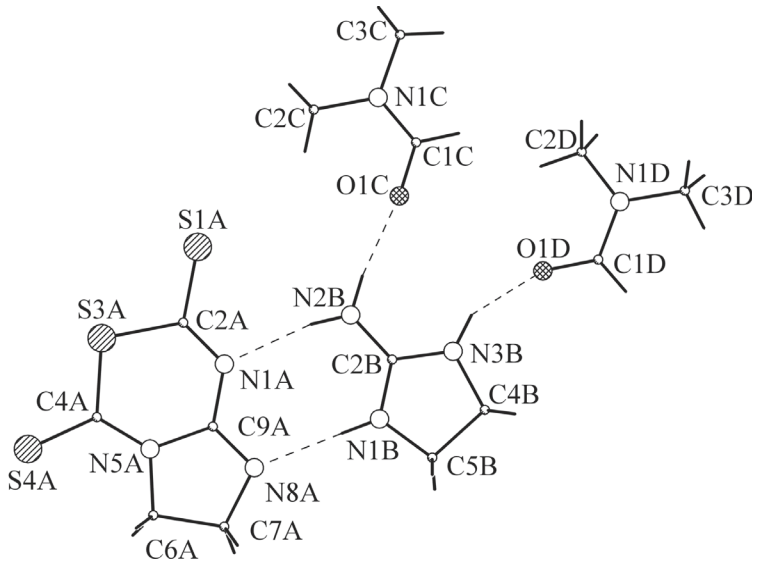
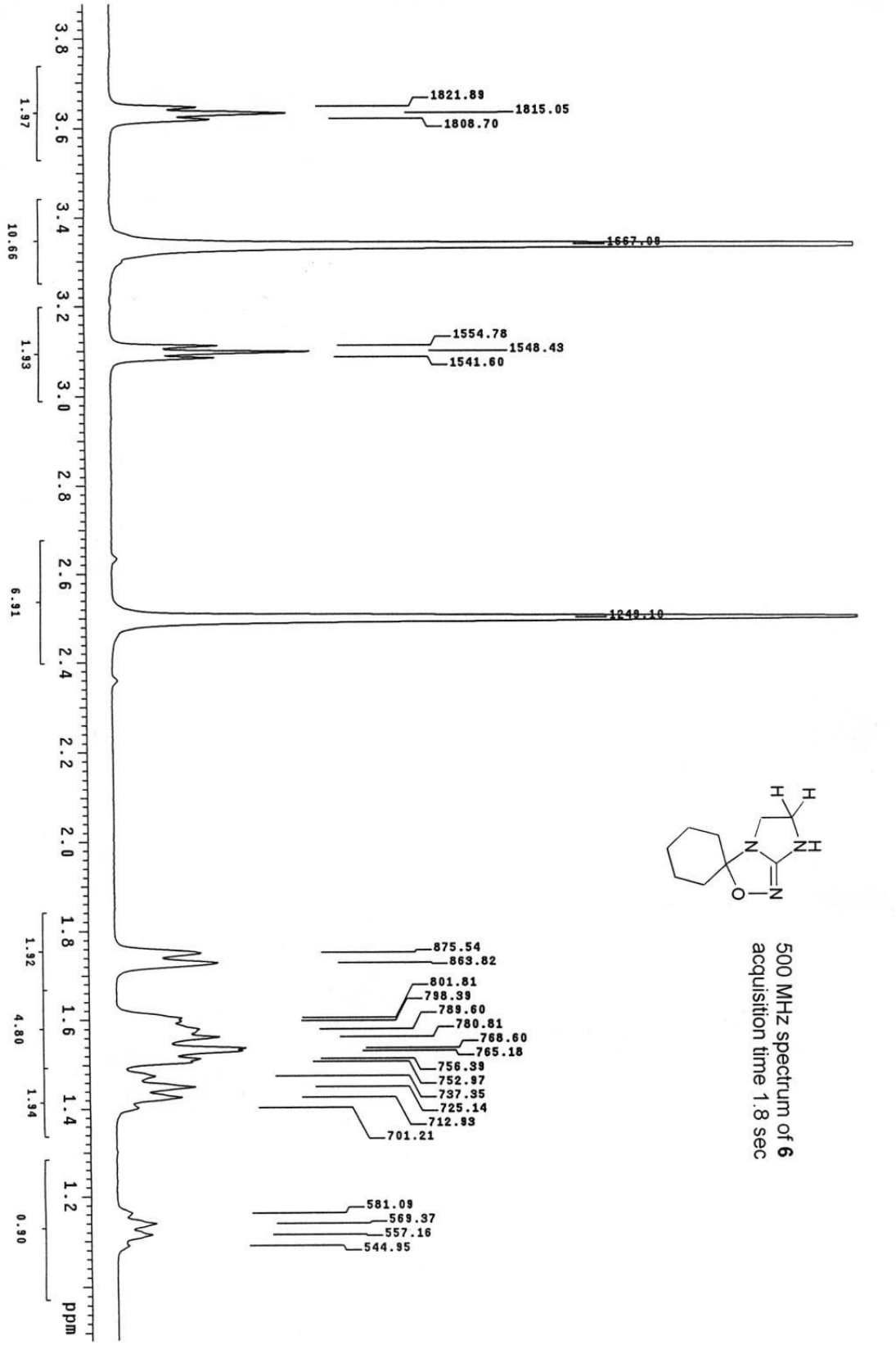
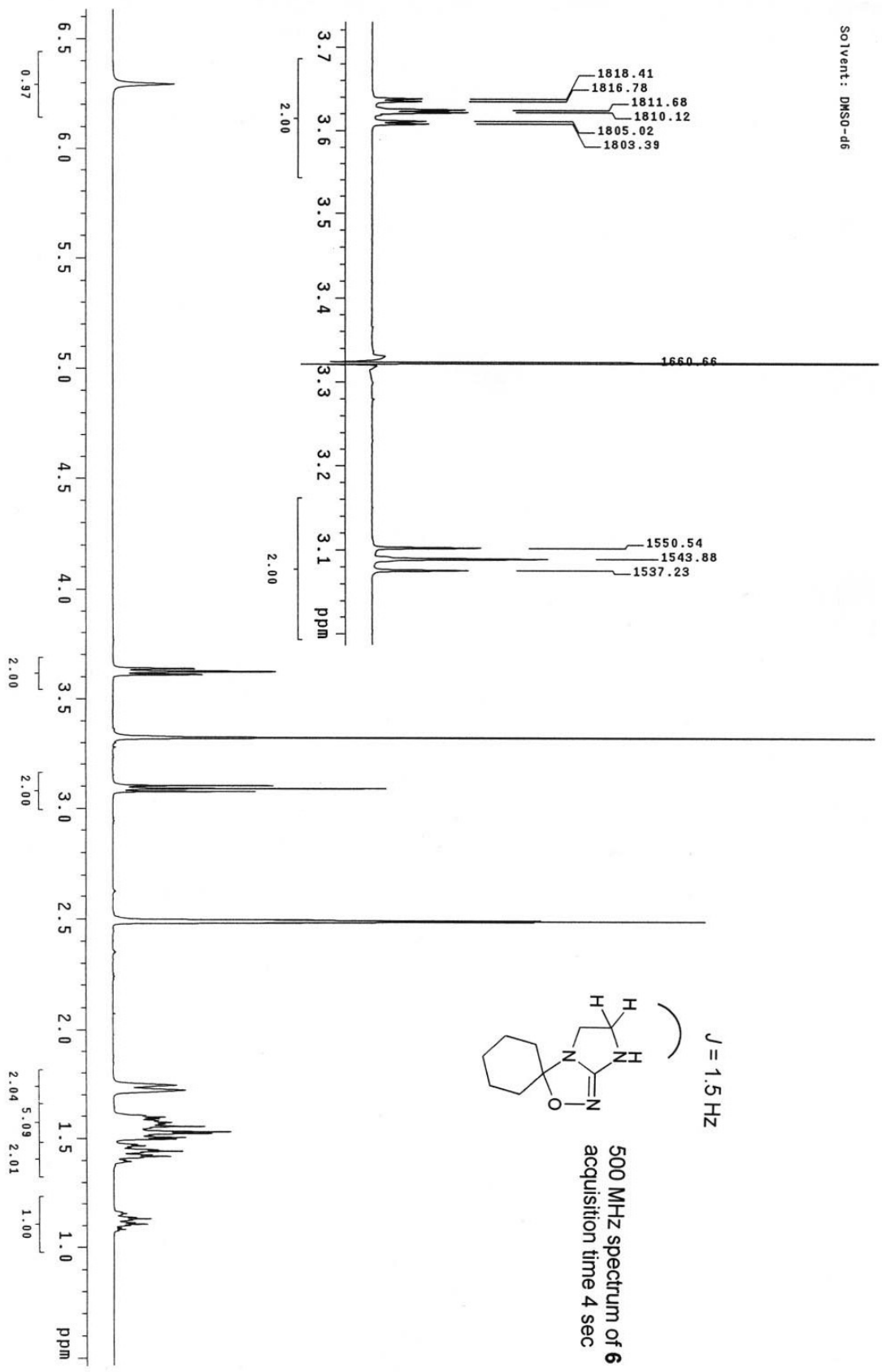


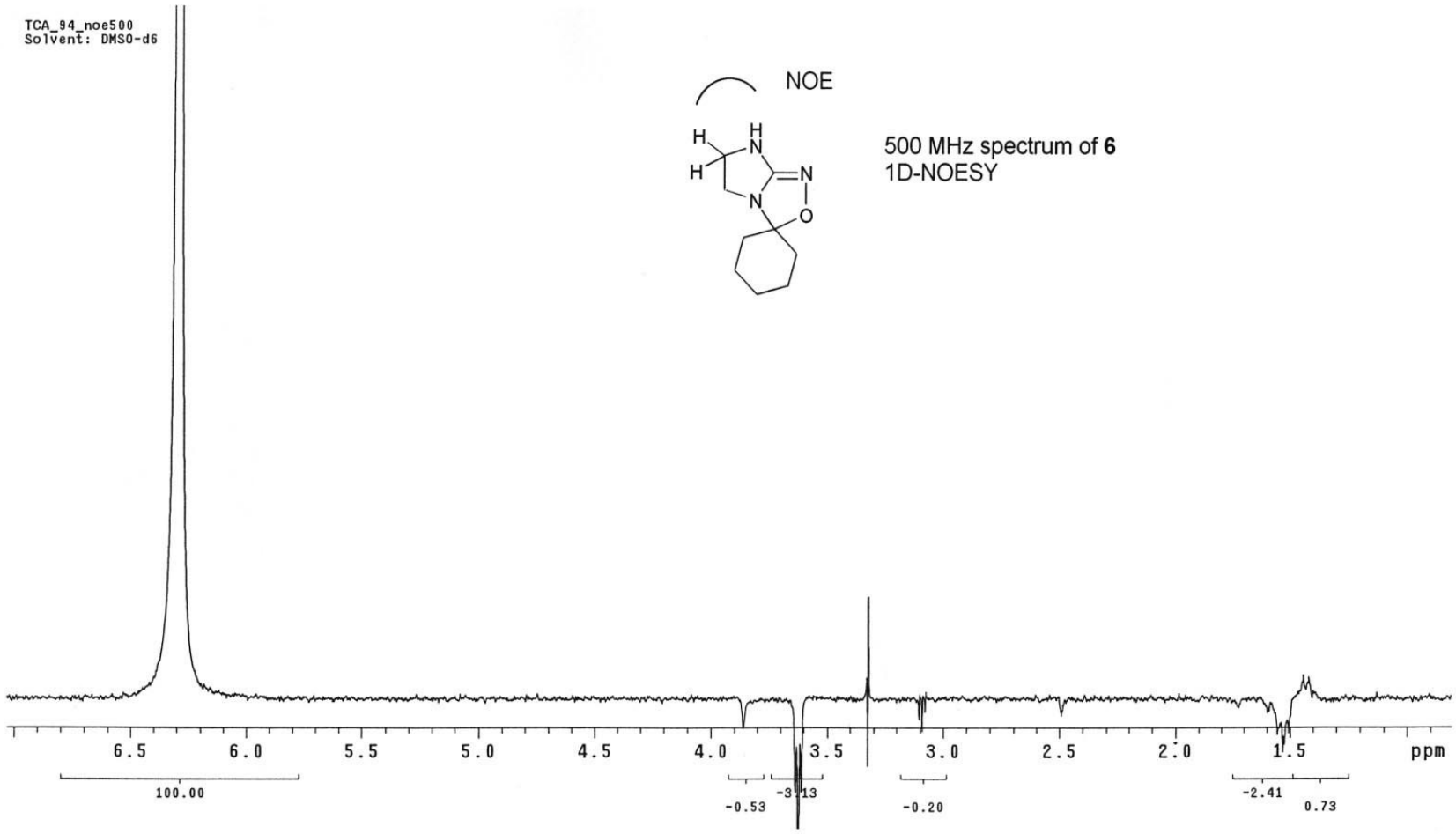
Fig. S7 Asymmetric part of the unit cell in **15** consisting of the deprotonated molecule of **16**, 2-aminoimidazolinium cation and two DMF molecules. The structure was solved on a twinned crystal and refined to R_1 value of 0.20.

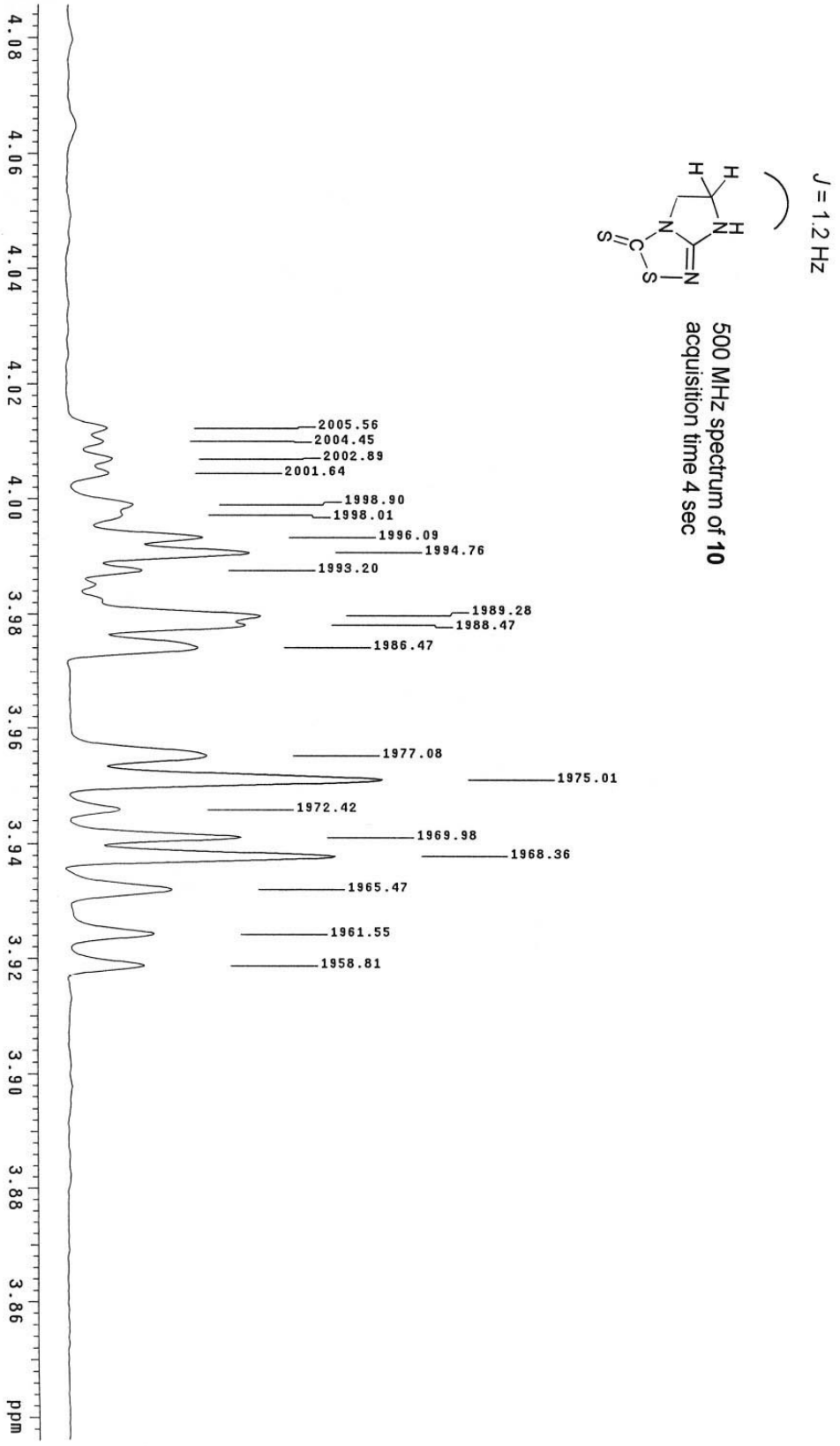
Table S8**.** Selected Theoretical and Experimental Bond Distances (Å) and Bond Angels (deg) for zwitterionic compound **1**.

Bond Angle	**B3LYP/6-31G^{xx}**	**HF/6-31G^{xx}**	**MP2/6-31G****	**Experimental**
S1O4	1.834	1.7207	1.7207	1.6600
N3O4	1.379	1.2551	1.3551	1.4176
N3C3	1.340	1.3144	1.3144	1.3556
N2C3	1.331	1.3222	1.3329	1.3180
N1C3	1.357	1.3229	1.32222	1.3198
C3N3O4	118.13	118.23	118.23	112.54 (10)
C3N1C1	108.84	109.85	109.39	110.34
C3N2C2	109.34	109.39	109.85	110.23 (11)
N2C3N1	112.27	111.67	111.61	112.85 (12)
N2C3N3	124.57	124.81	123.42	124.96 (12)
N1C3N3	123.13	123.42	124.81	122.09 (12)

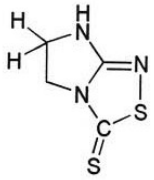

1821.89
1815.05
1808.70
1667.08
1554.78
1548.43
1541.60
1249.19
875.54
863.82
801.81
798.39
789.60
780.81
768.60
765.18
756.39
752.97
737.35
725.14
712.93
701.21
581.09
569.37
557.16
544.95
1.97
10.66
1.93
6.91
1.92
4.80
1.94
0.90
ppm
500 MHz spectrum of 6
acquisition time 1.8 sec


Solvent: DMSO-d6
1818.41
1816.78
1811.68
1810.12
1805.02
1803.39
1660.66
1550.54
1543.88
1537.23
ppm
J = 1.5 Hz
500 MHz spectrum of 6
acquisition time 4 sec

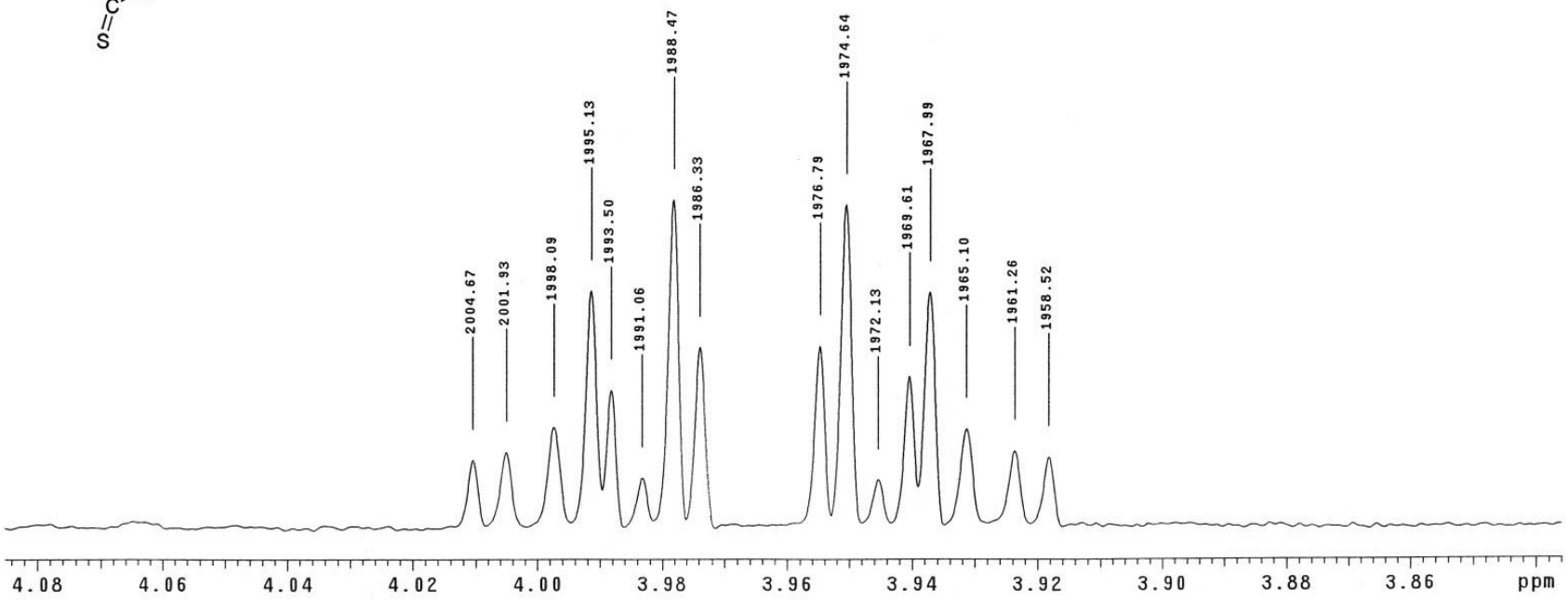

TCA_94_noe500
Solvent: DMSO-d6
NOE
H
H
N
N
N
O
500 MHz spectrum of 6
1D-NOESY
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm
100.00
-0.53
-3.13
-0.20
-2.41
0.73

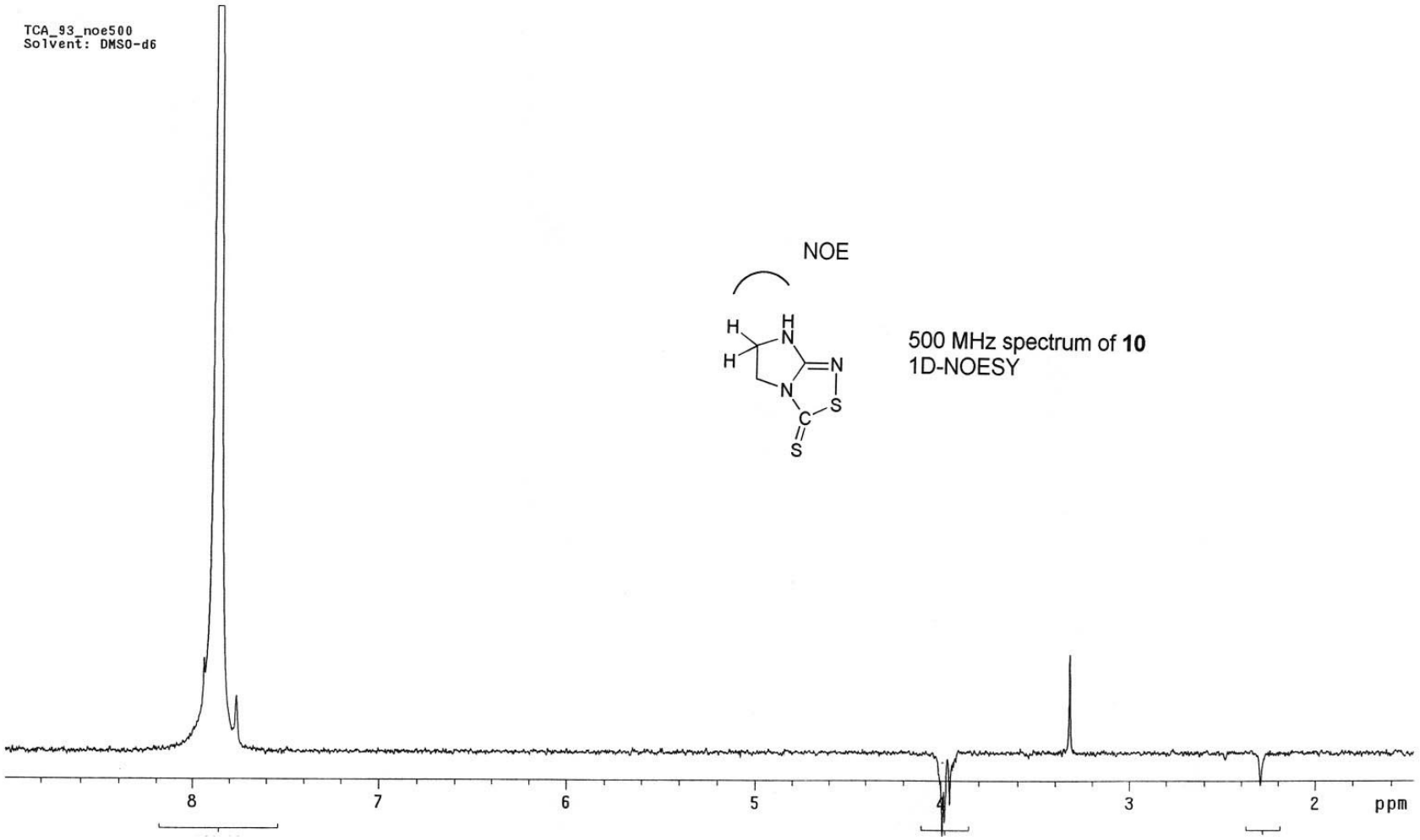

500 MHz spectrum of 10
acquisition time 4 sec
J = 1.2 Hz
2005.56
2004.45
2002.89
2001.64
1998.90
1998.01
1996.09
1994.76
1993.20
1989.28
1988.47
1986.47
1977.08
1975.01
1972.42
1969.98
1968.36
1965.47
1961.55
1958.81
4.08
4.06
4.04
4.02
4.00
3.98
3.96
3.94
3.92
3.90
3.88
3.86
ppm

TCA_93_dec
Solvent: DMSO-d6



500 MHz spectrum of **10**
acquisition time 4 sec
N-H proton decopuled





500 MHz spectrum of **10**
1D-NOESY