Supporting Information

A convenient stereoselective access to novel 1,2,4-triazepan-3-ones/thiones via reduction or reductive alkylation of 7-membered cyclic semicarbazones and thiosemicarbazones

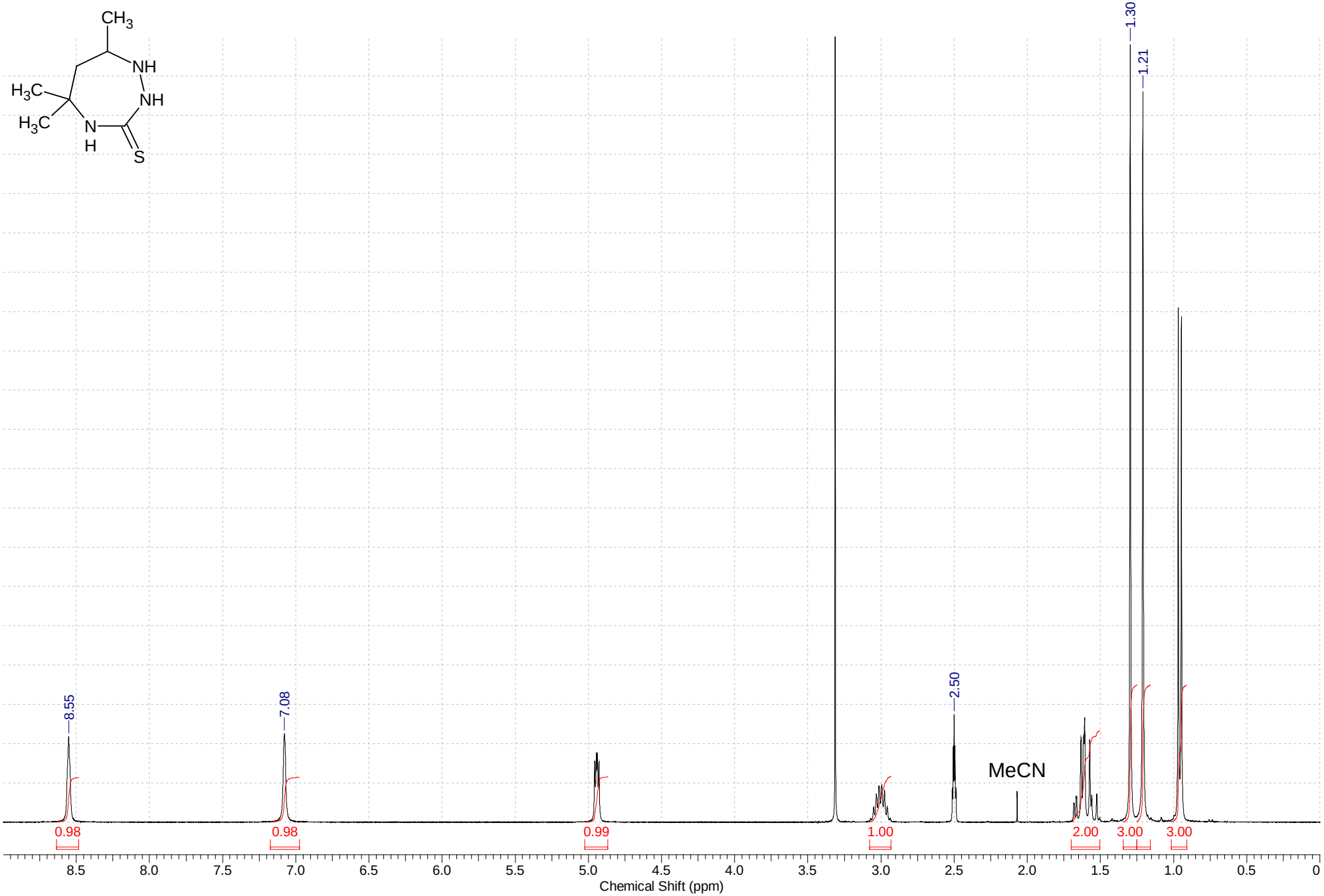
Anastasia A. Fesenko,[a] Mikhail S. Grigoriev[b] and Anatoly D. Shutalev[a,]*

[a] *N. D. Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, 47 Leninsky Ave., 119991 Moscow, Russian Federation*

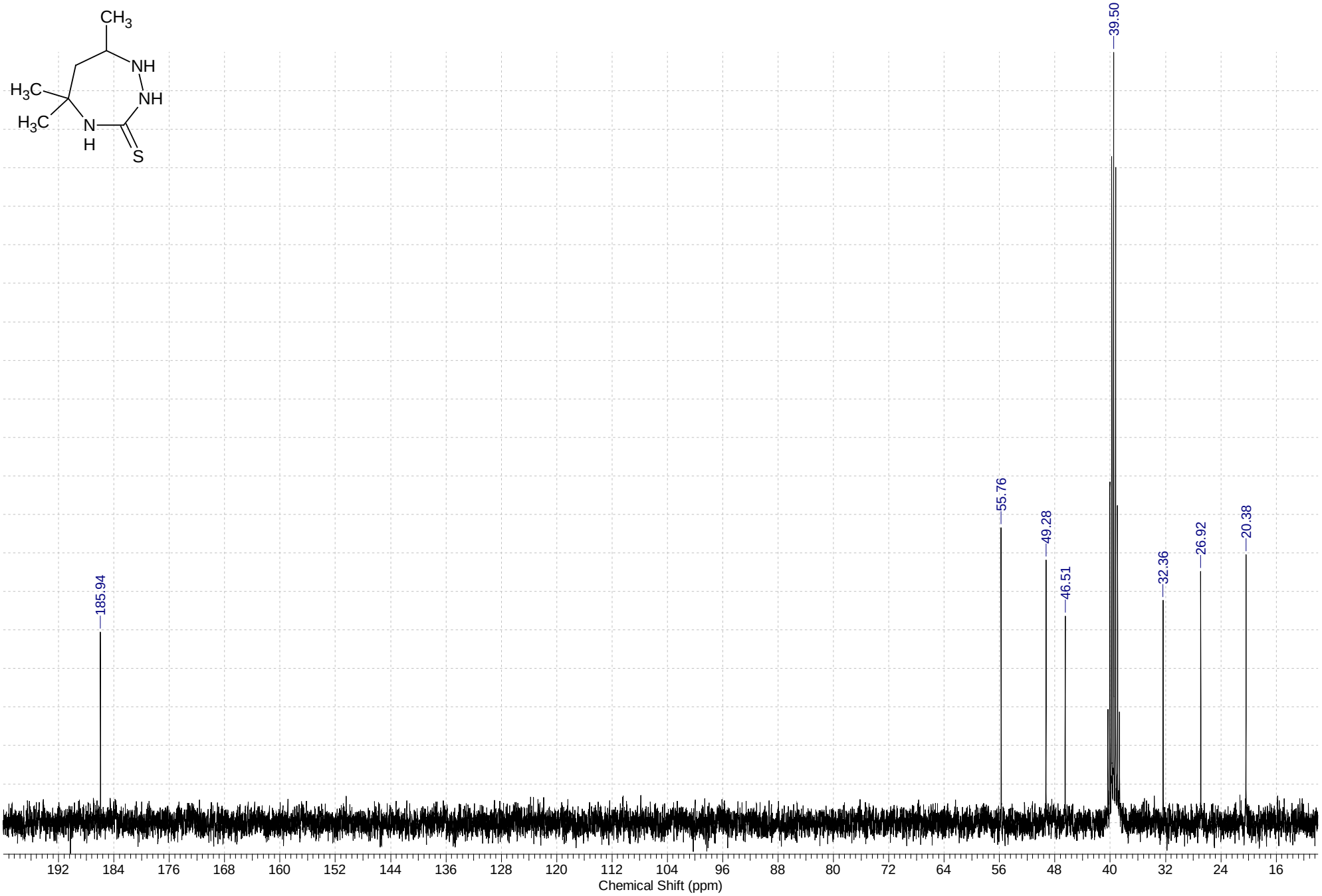
[b] *A. N. Frumkin Institute of Physical Chemistry and Electrochemistry, Russian Academy of Sciences, 31 Leninsky Ave., 119071 Moscow, Russian Federation*

Contents

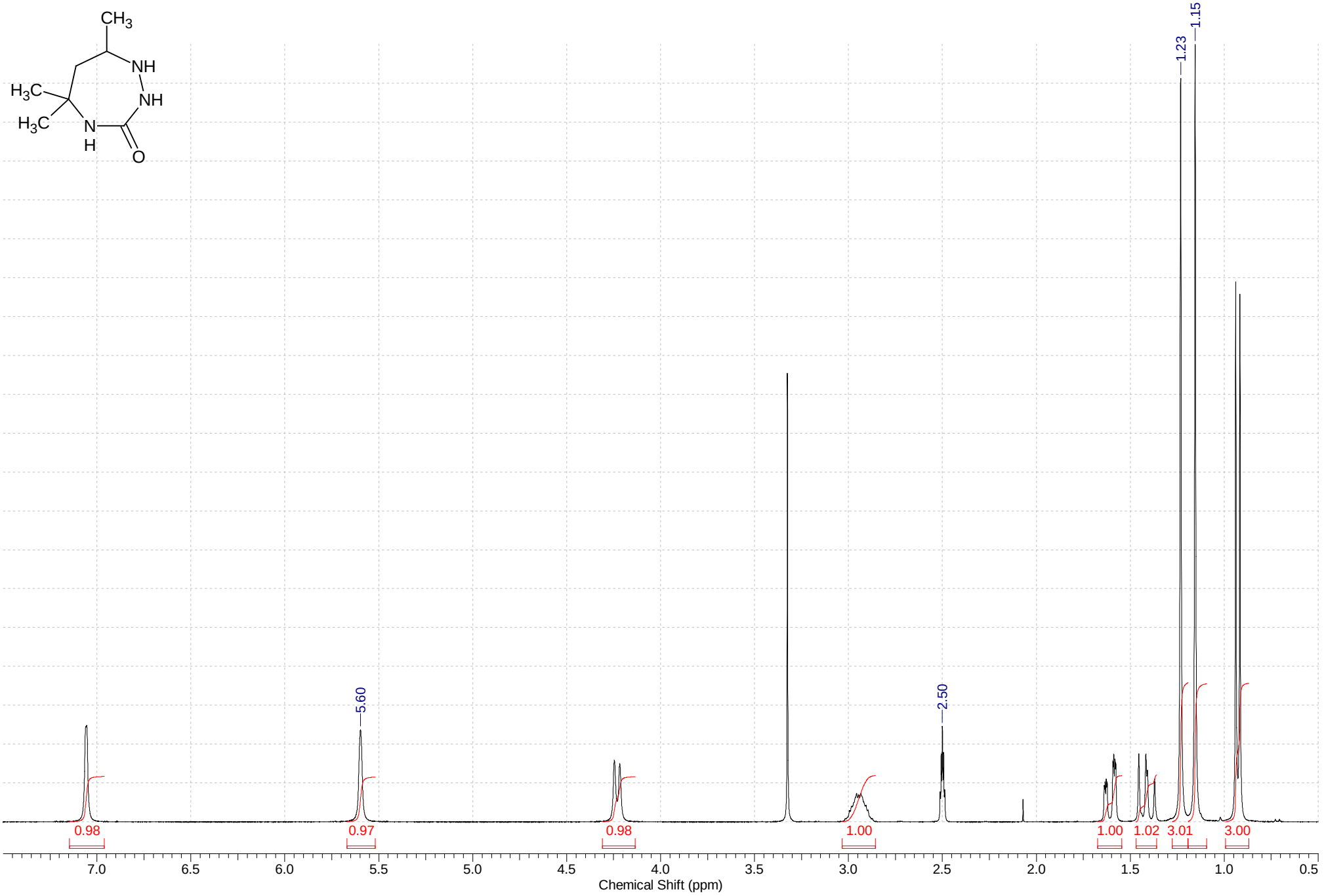
^{1}H NMR spectrum of compound **4a** (DMSO-d_6)



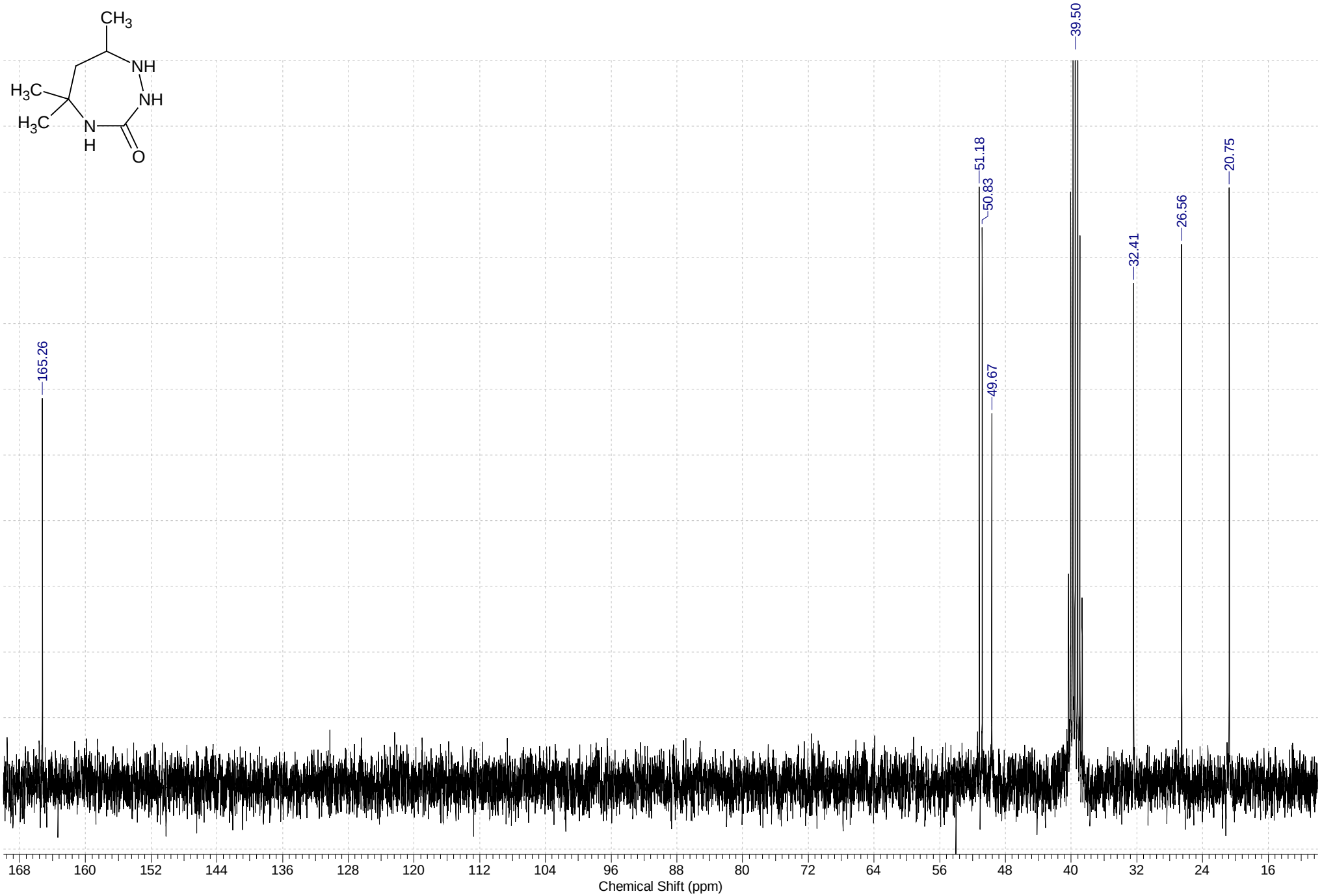
^{13}C NMR spectrum of compound **4a** (DMSO-d_6)



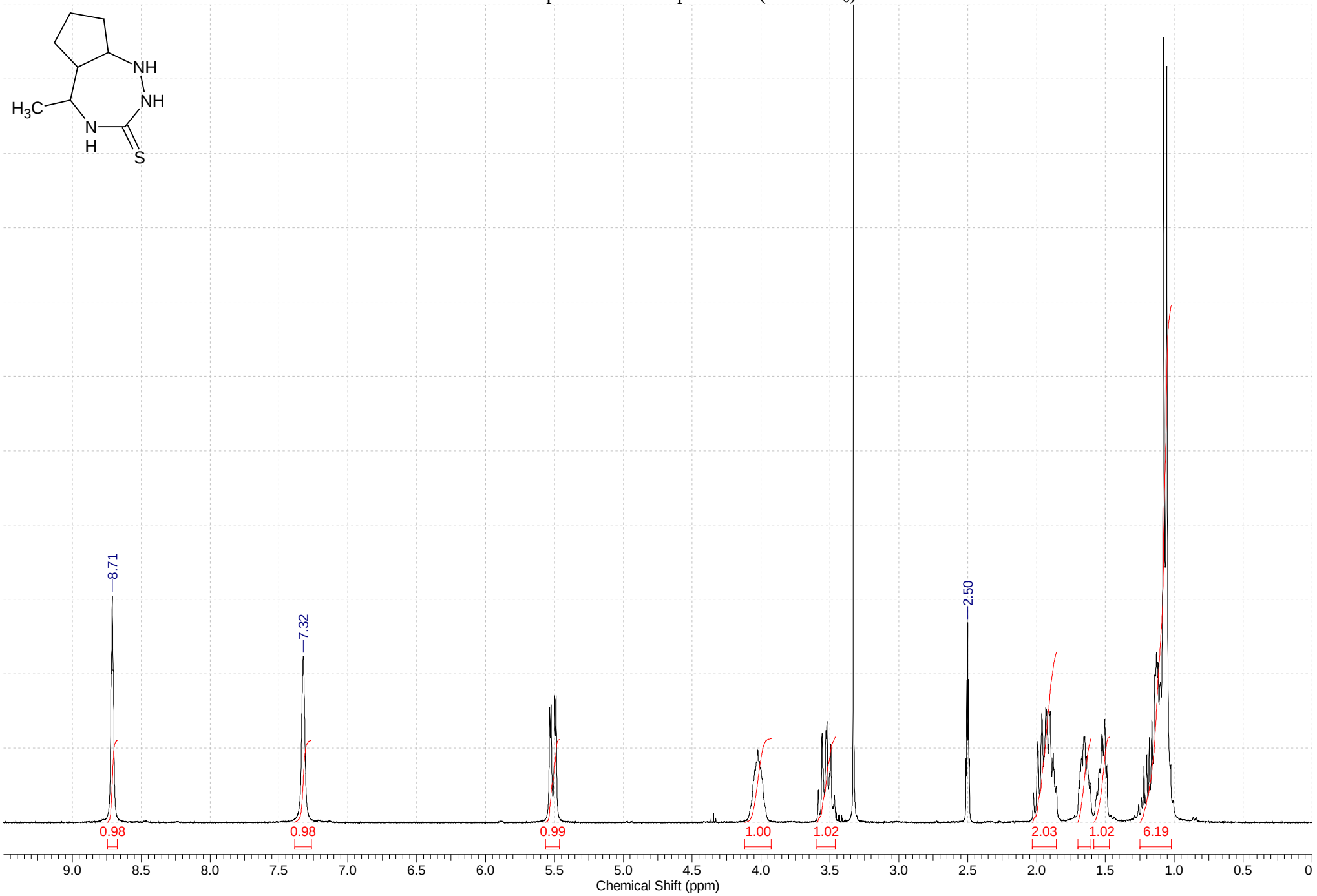
^{1}H NMR spectrum of compound **4b** (DMSO-d_6)



^{13}C NMR spectrum of compound **4b** (DMSO-d_6)



^{1}H NMR spectrum of compound **4c** (DMSO-d_6)



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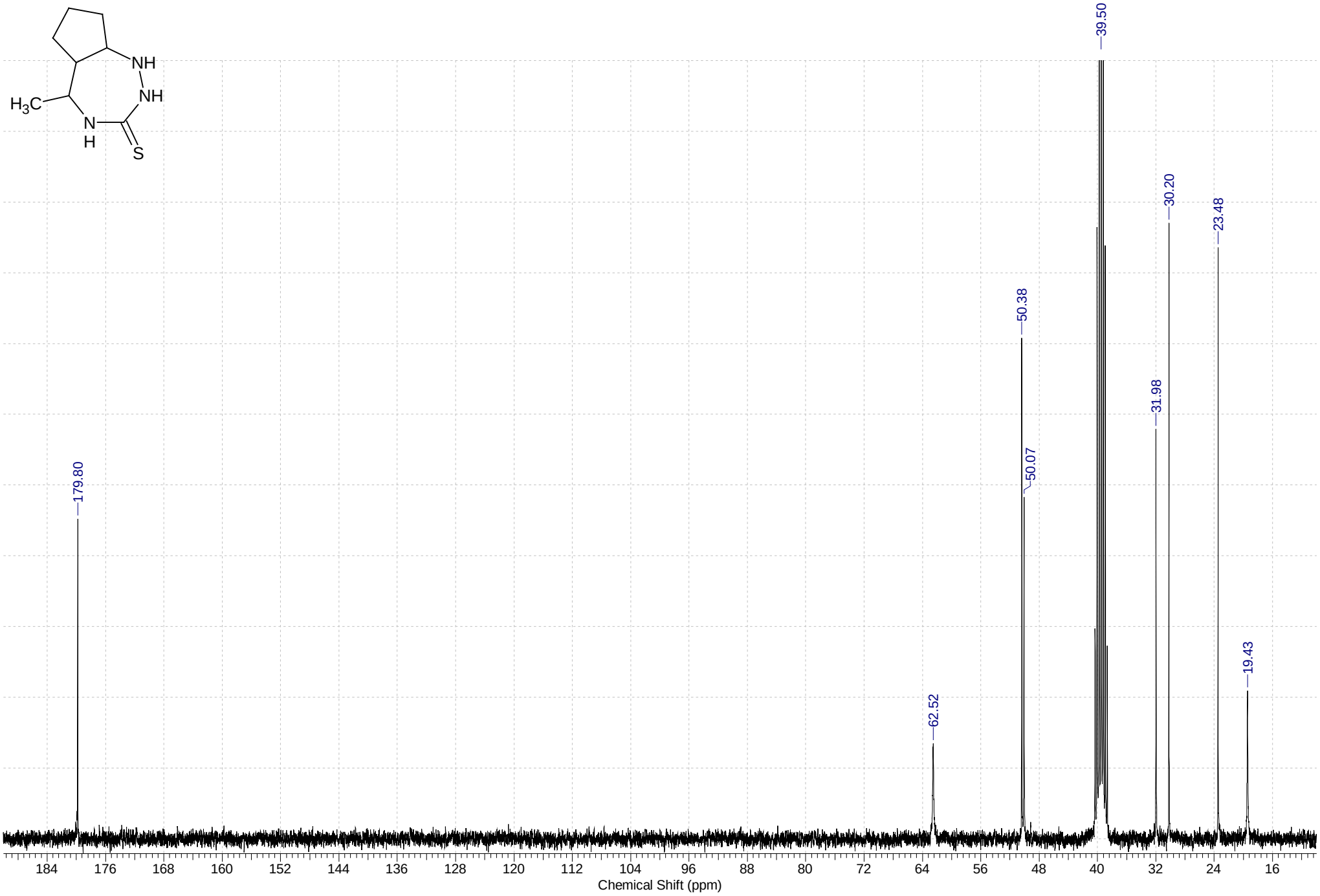
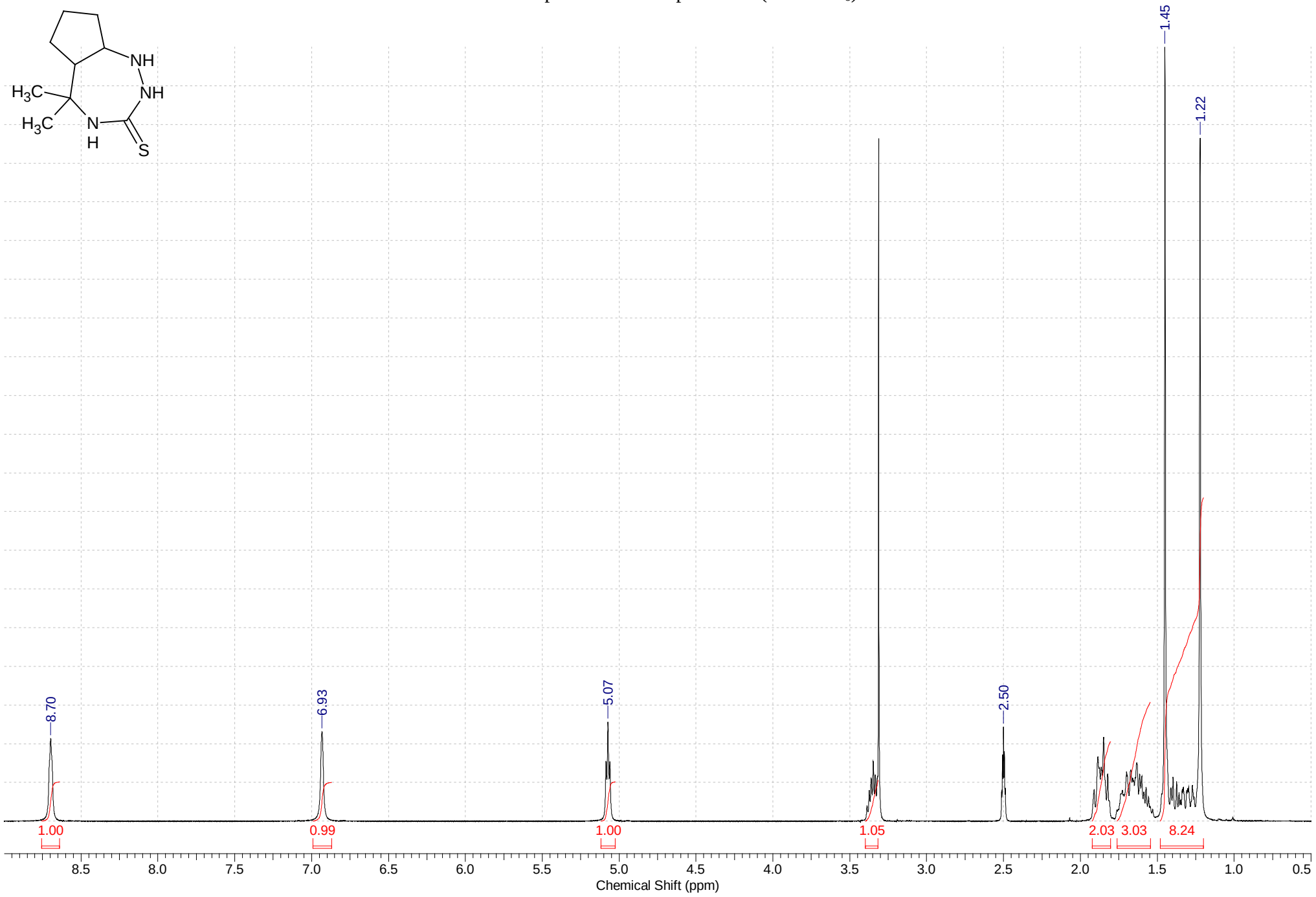


^{1}H NMR spectrum of compound **4d** (DMSO-d_6)



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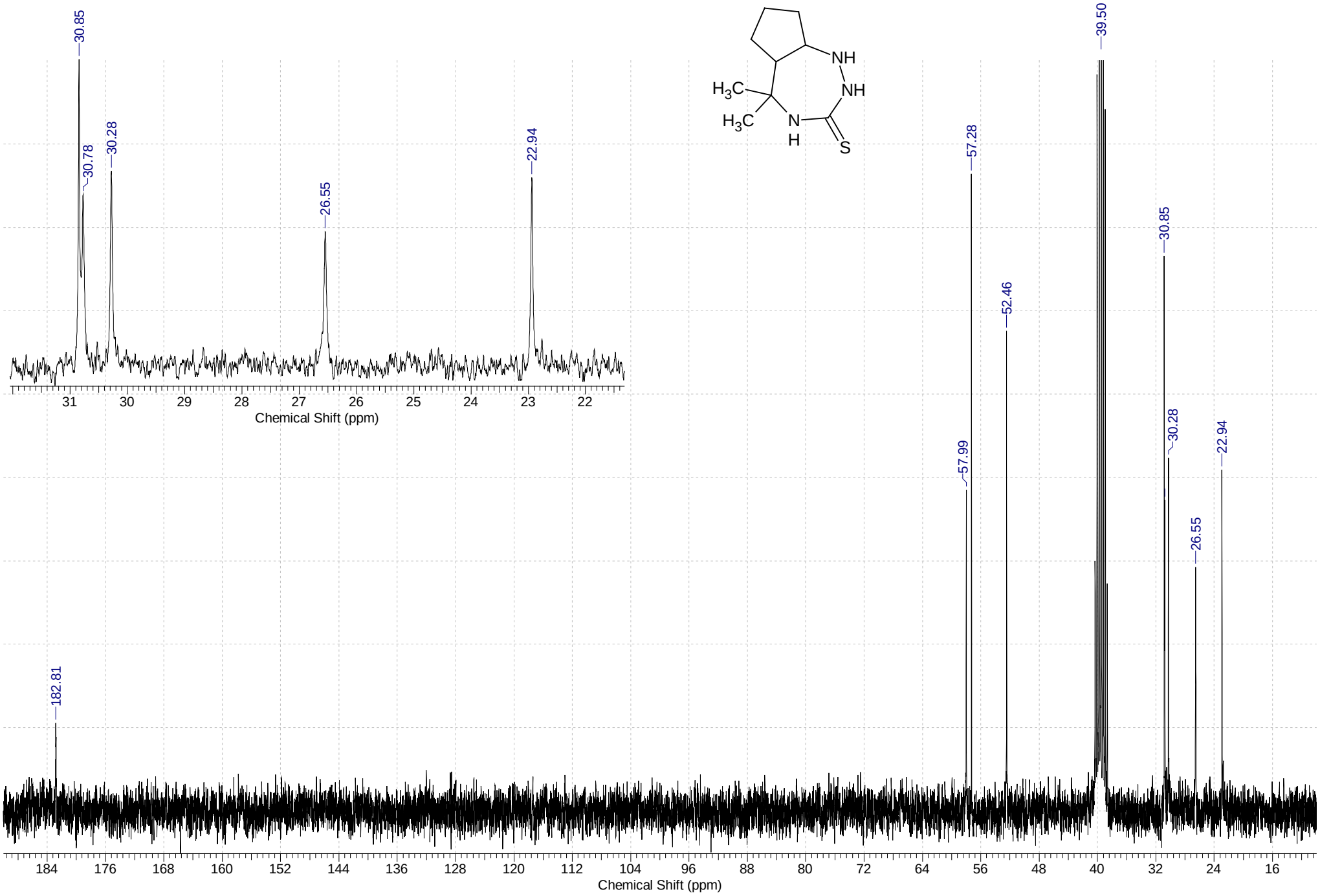

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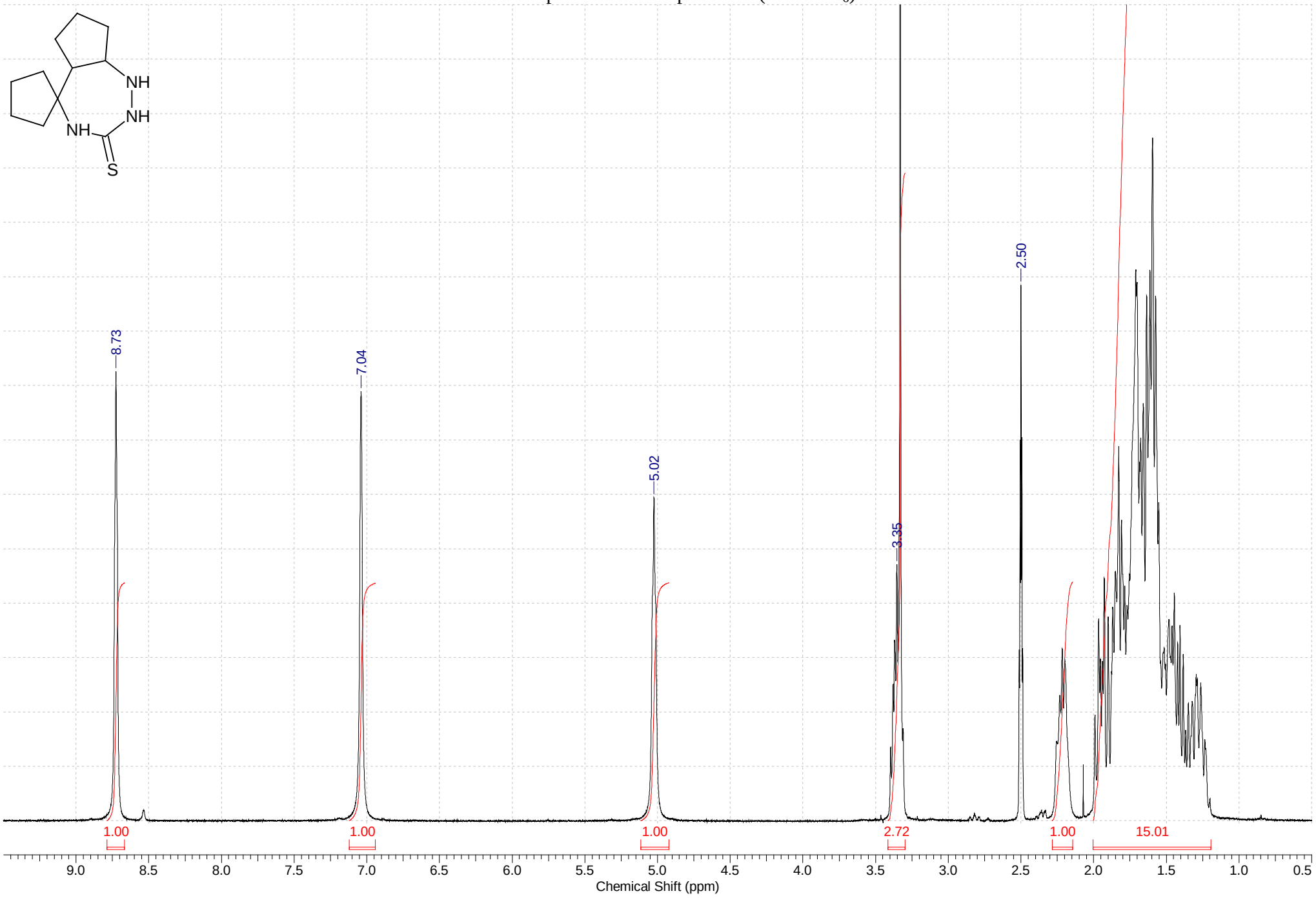

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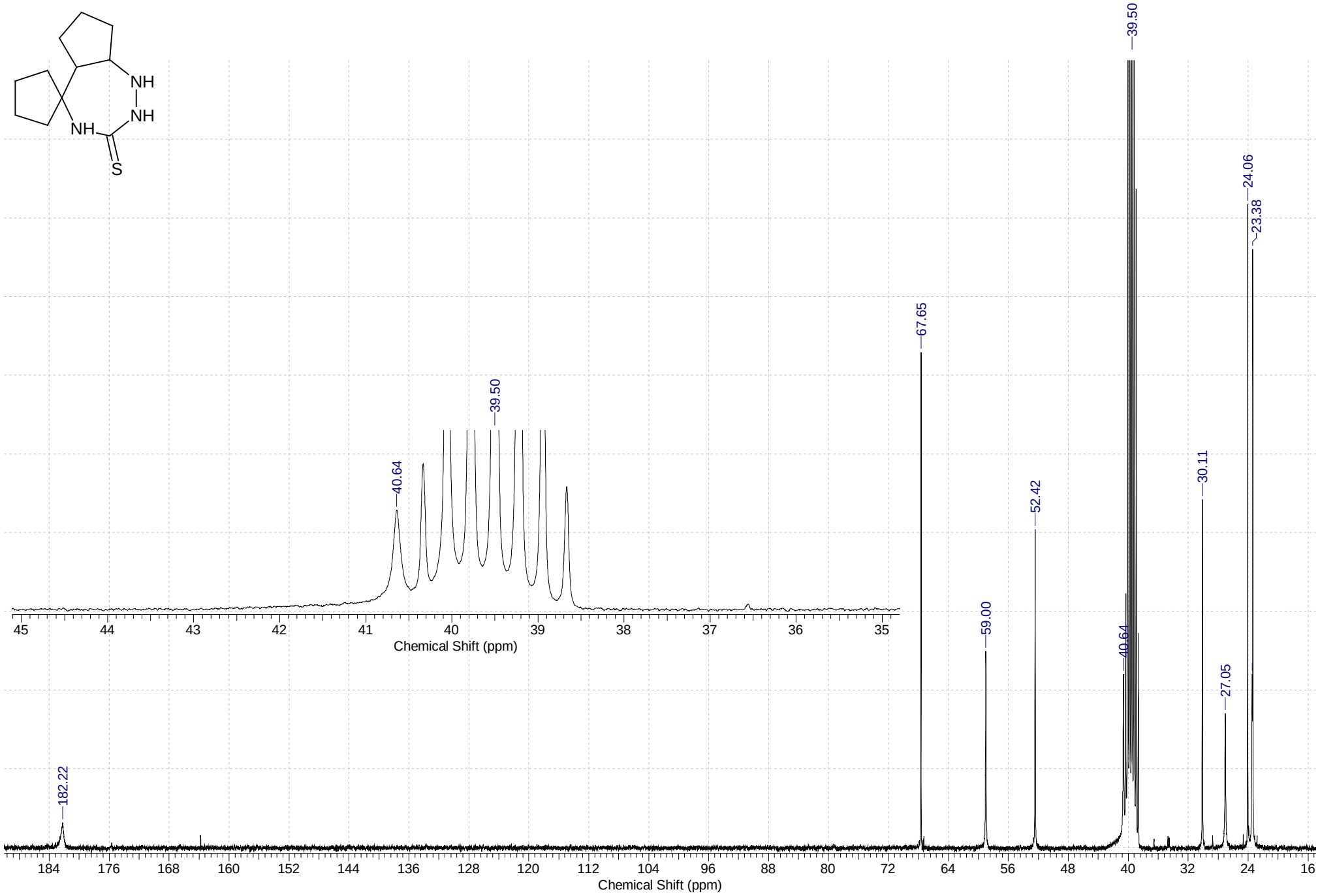

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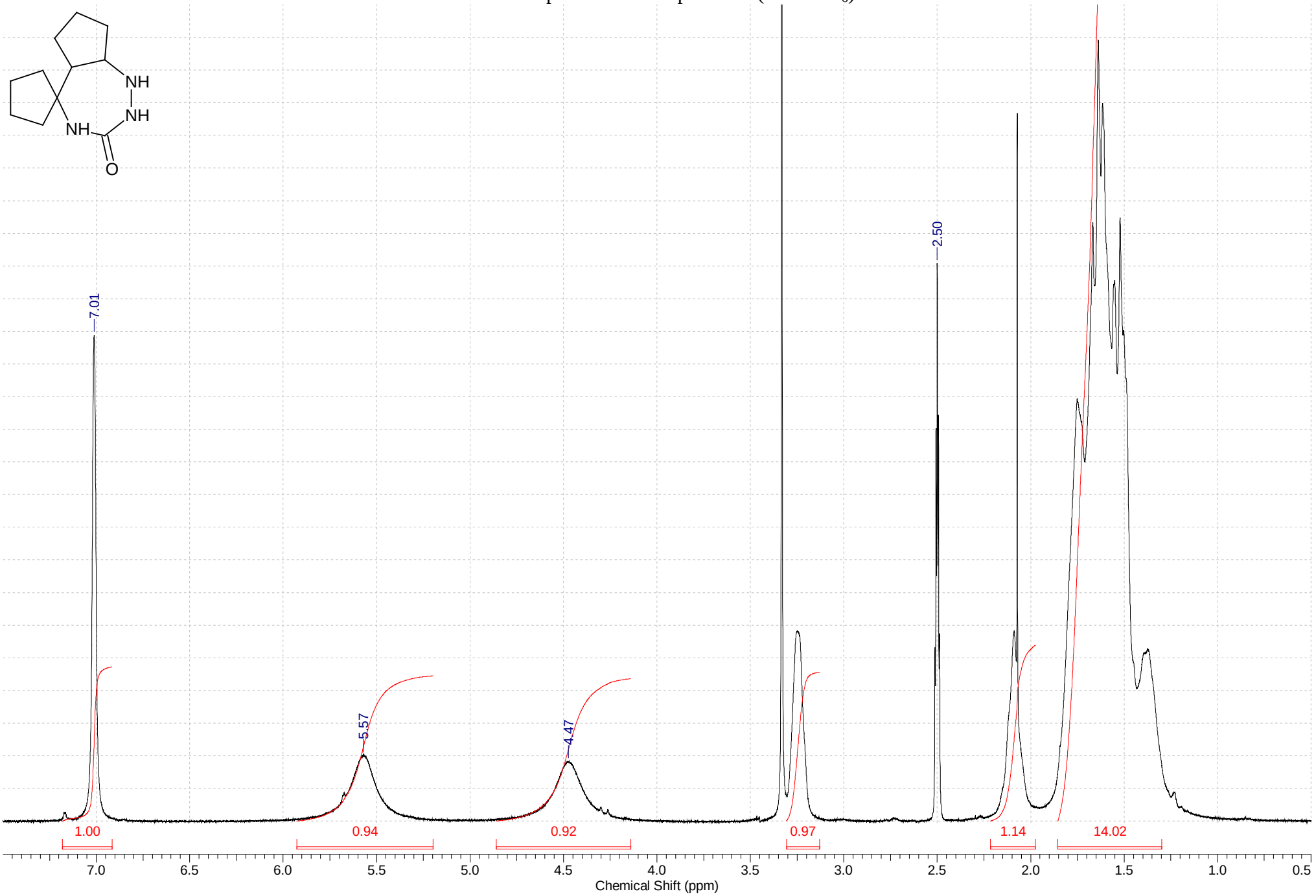

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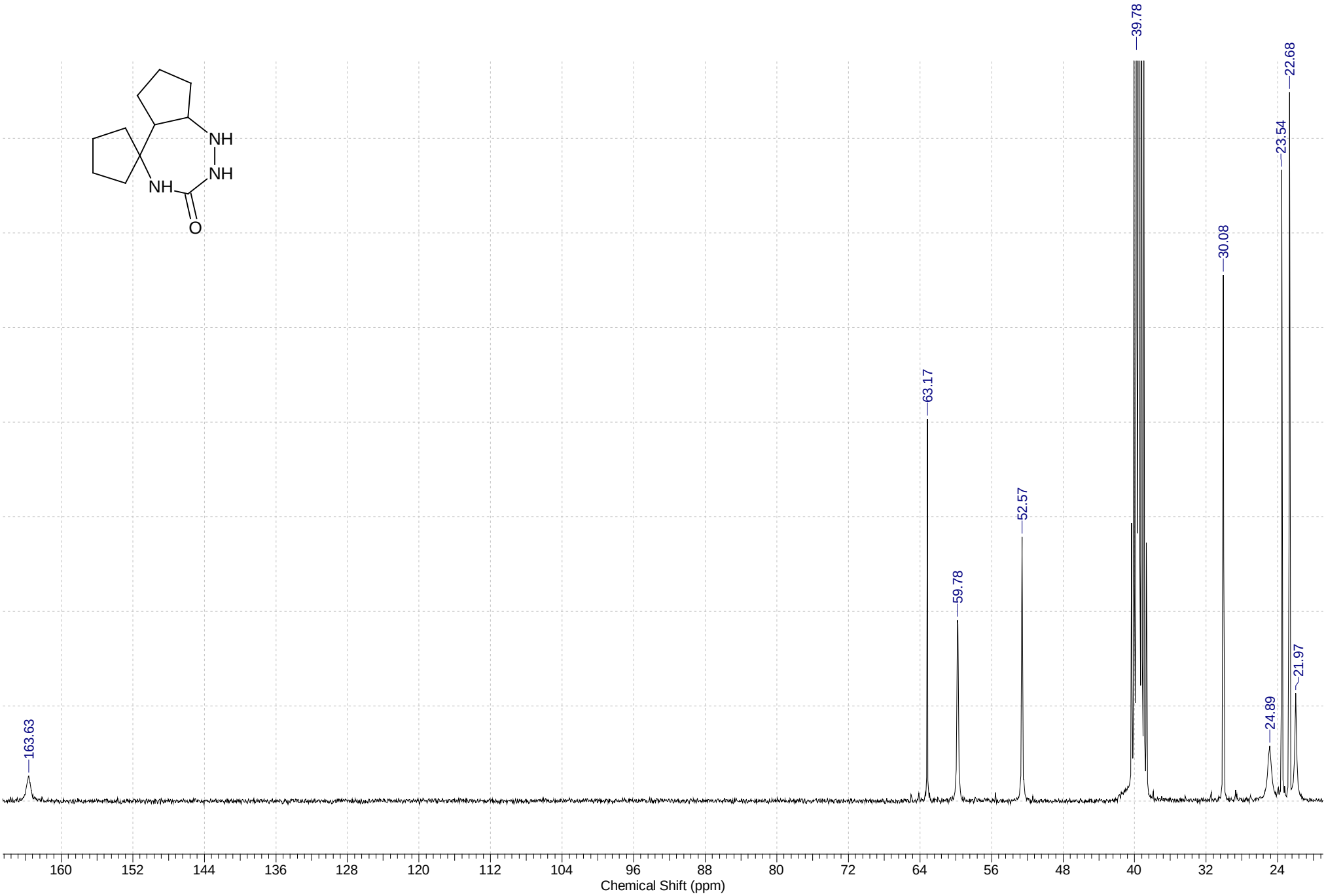

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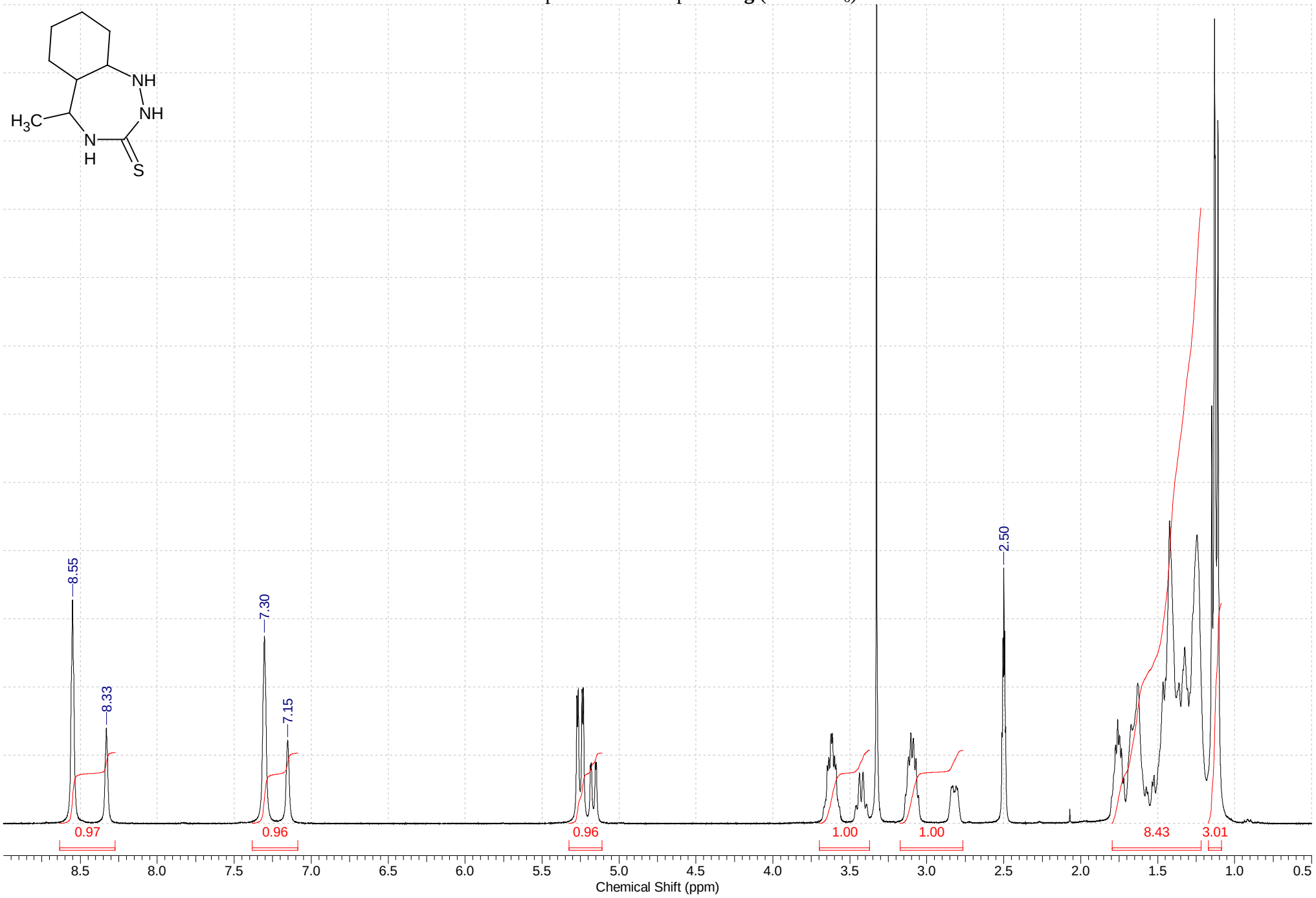

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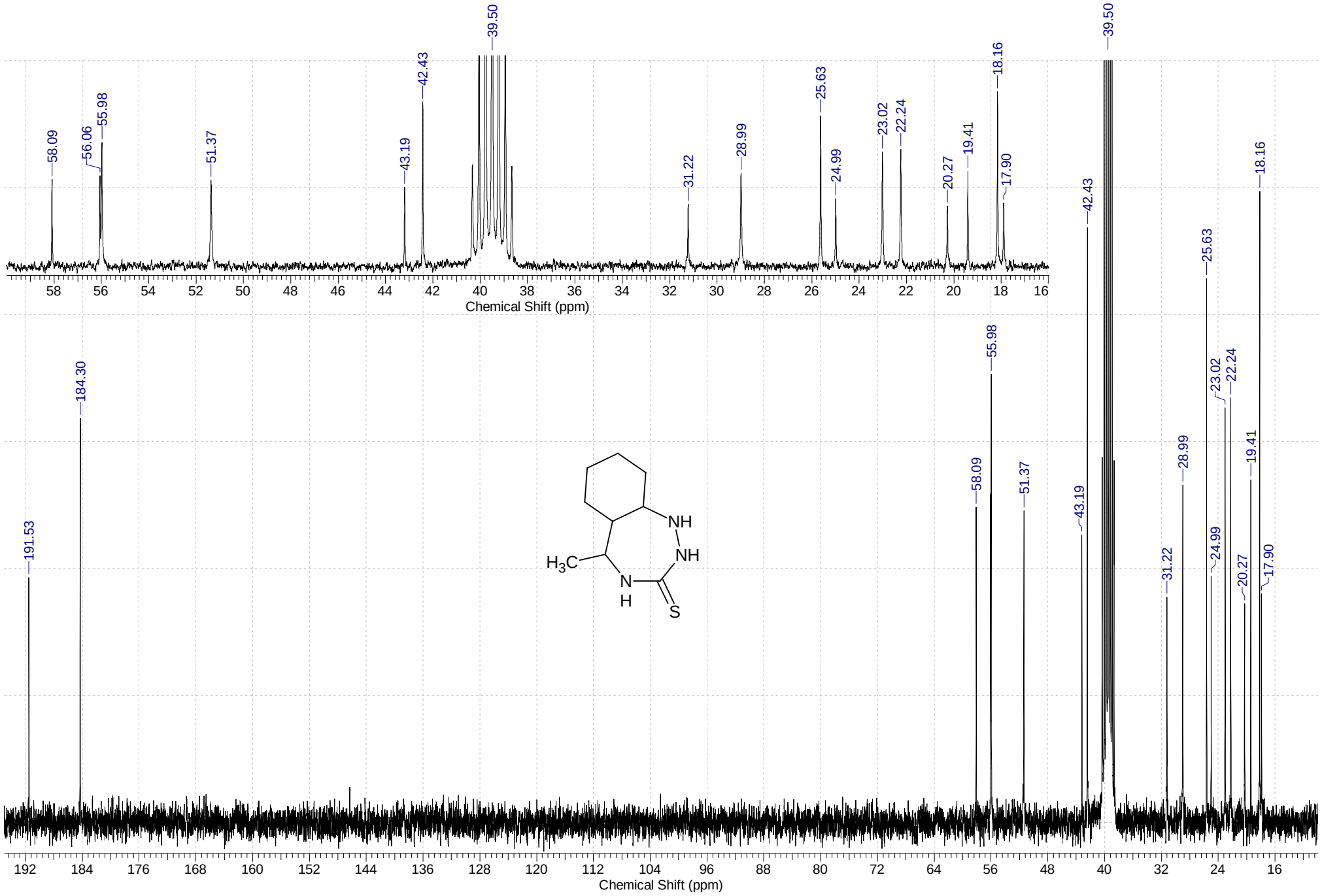

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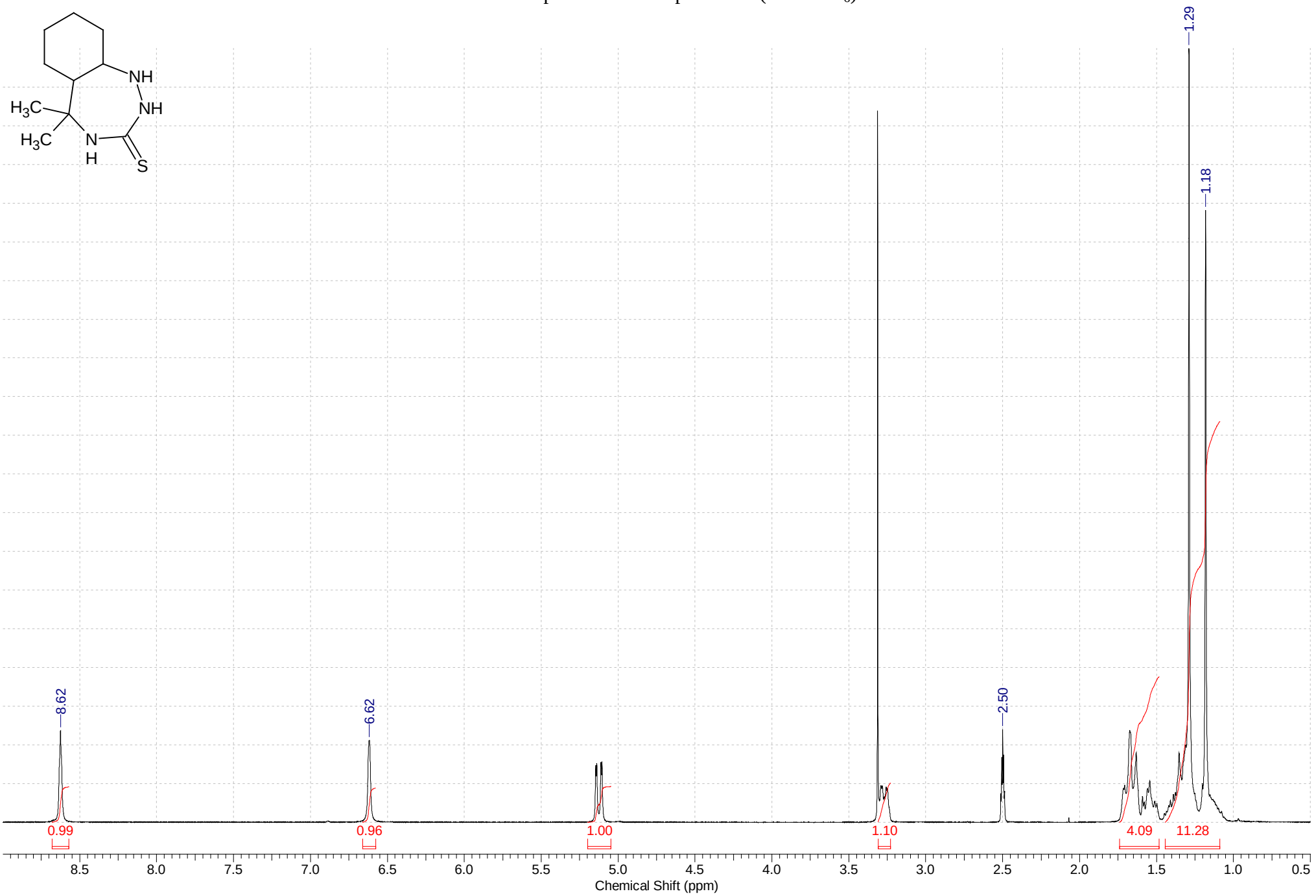

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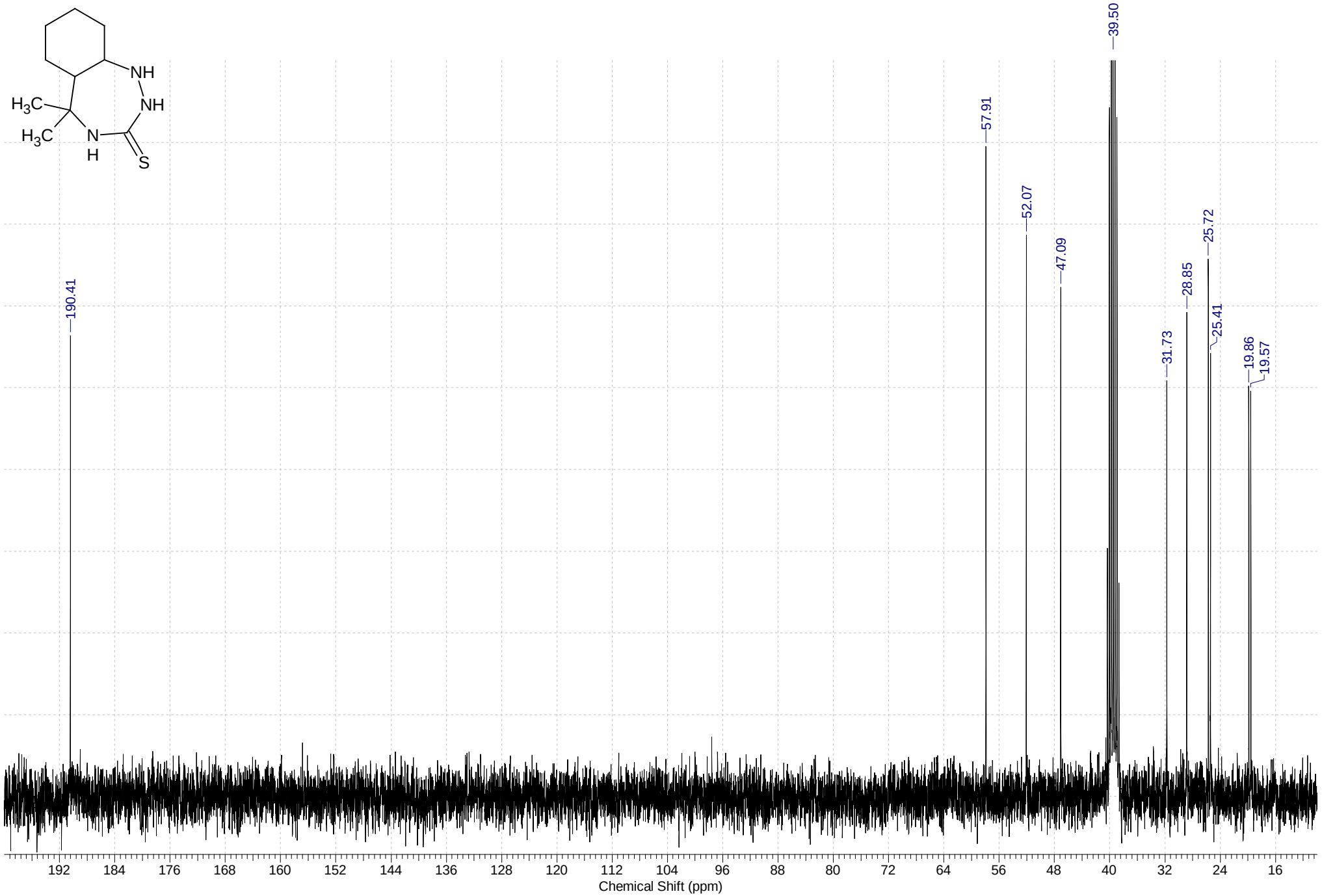

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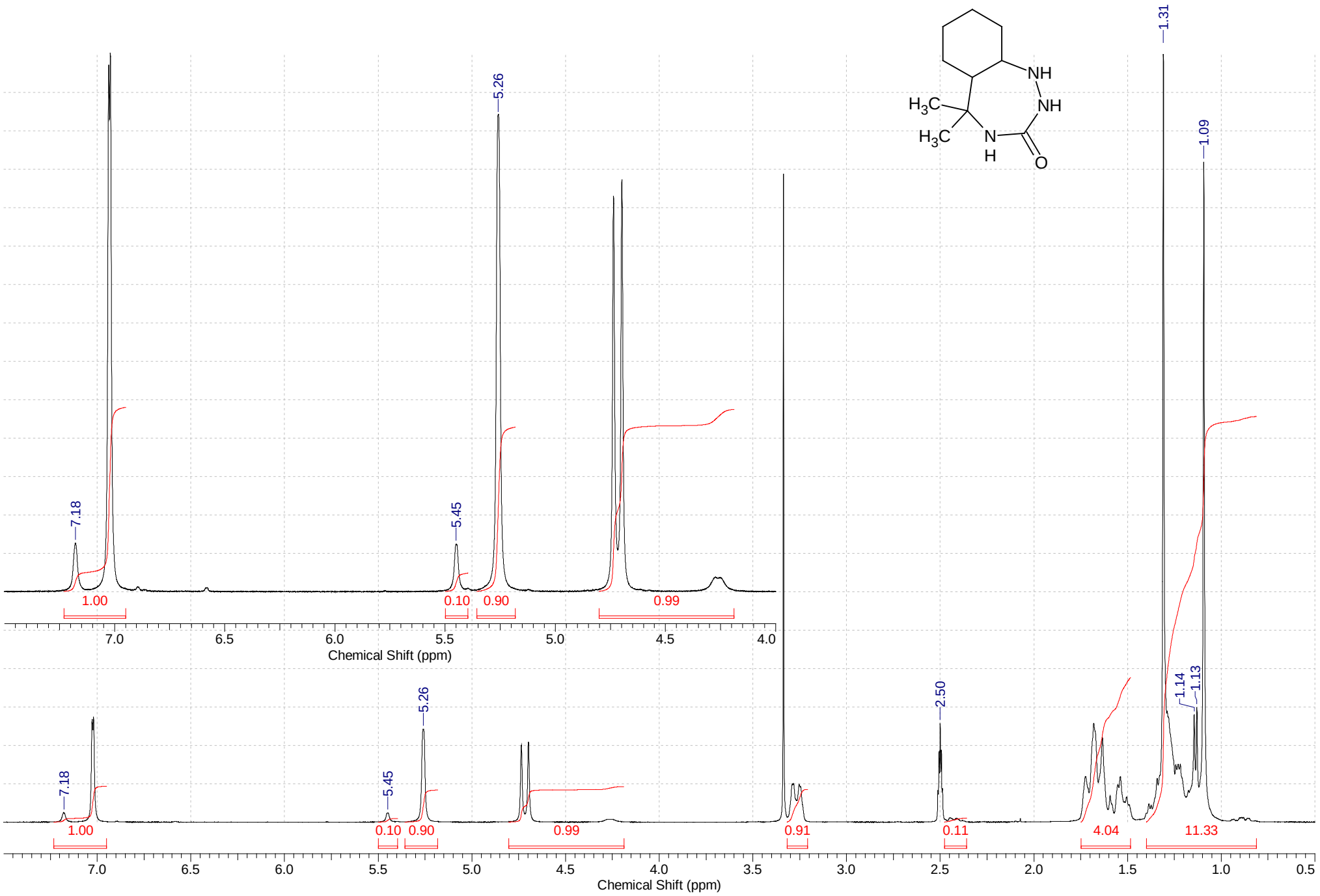

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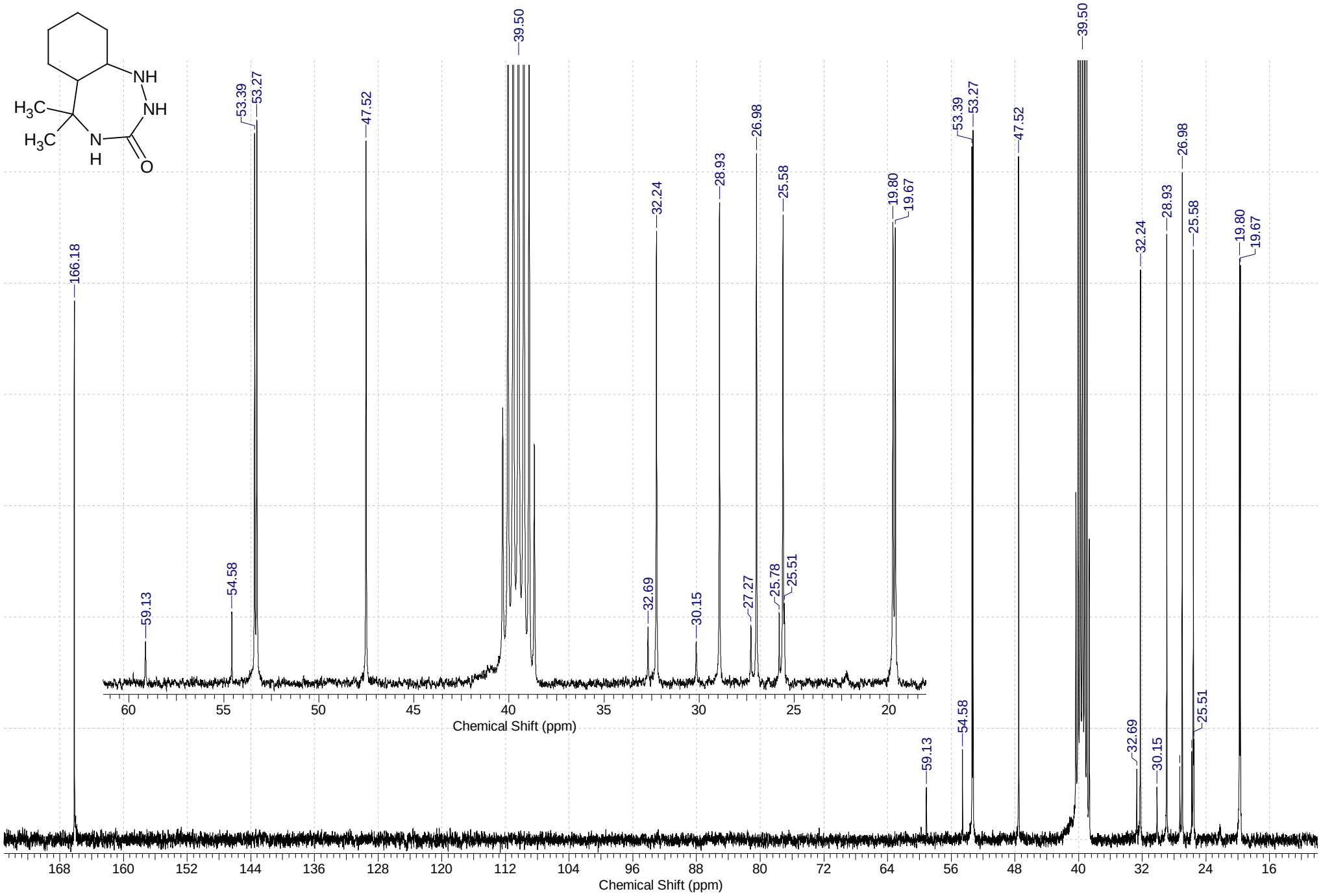

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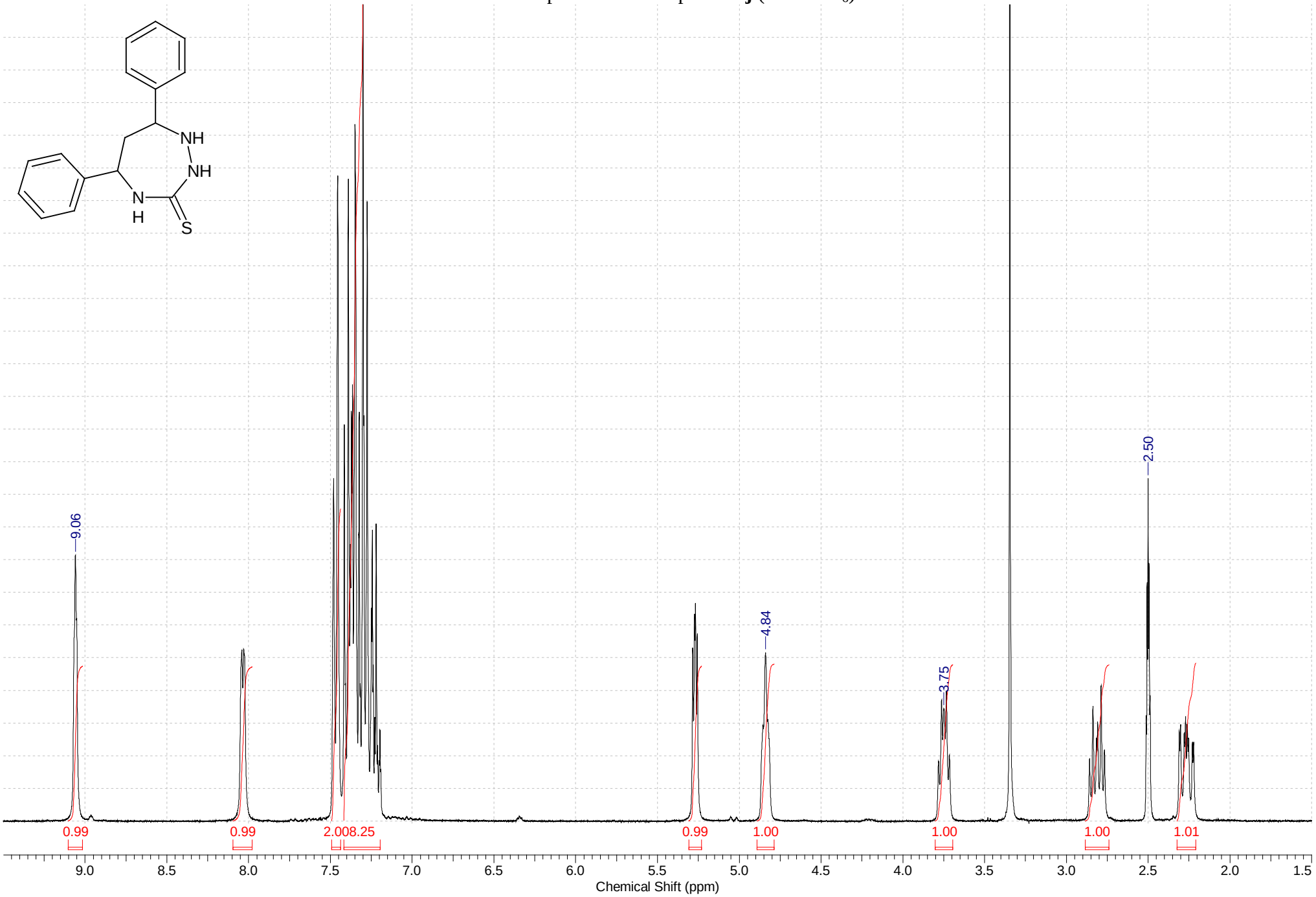

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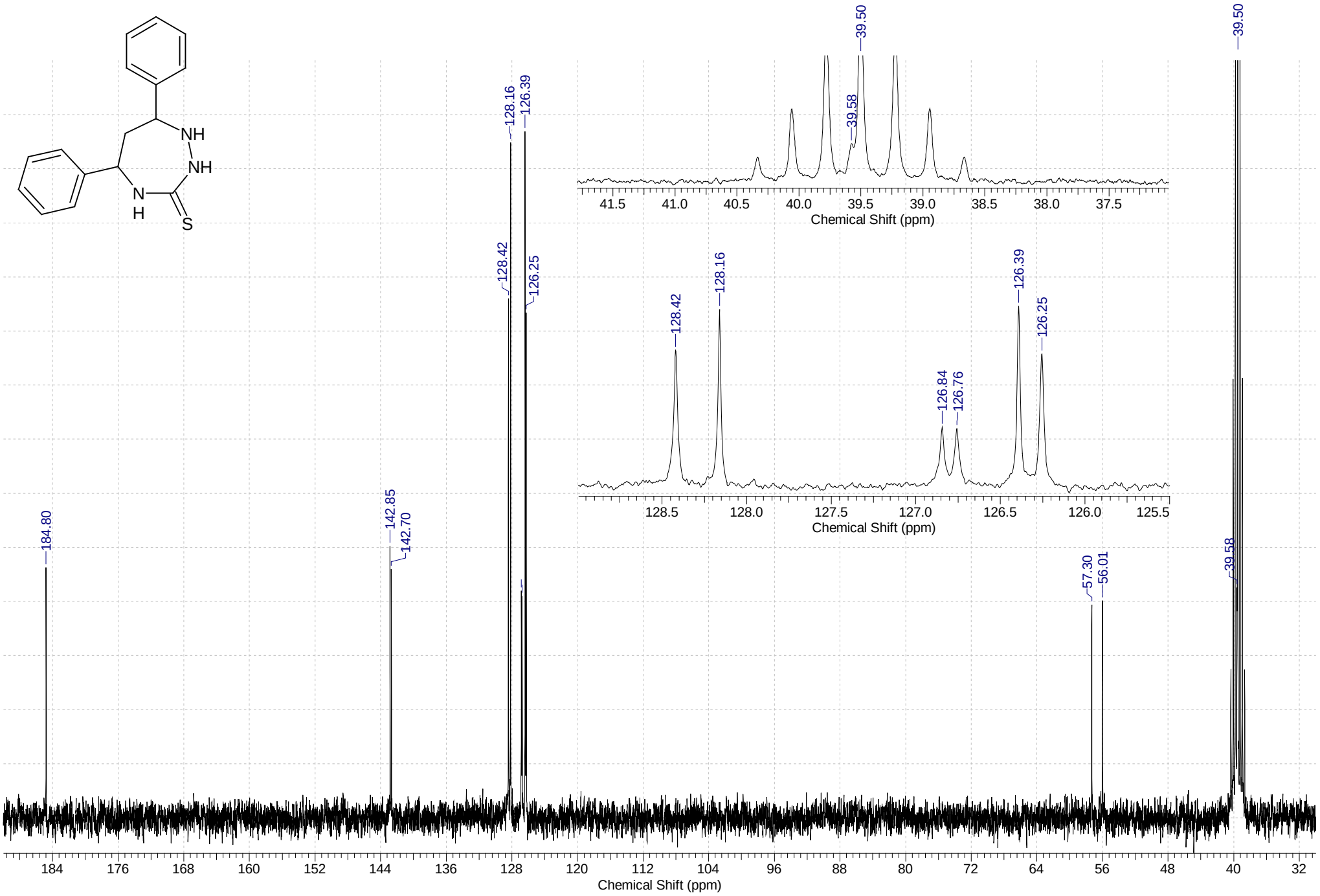

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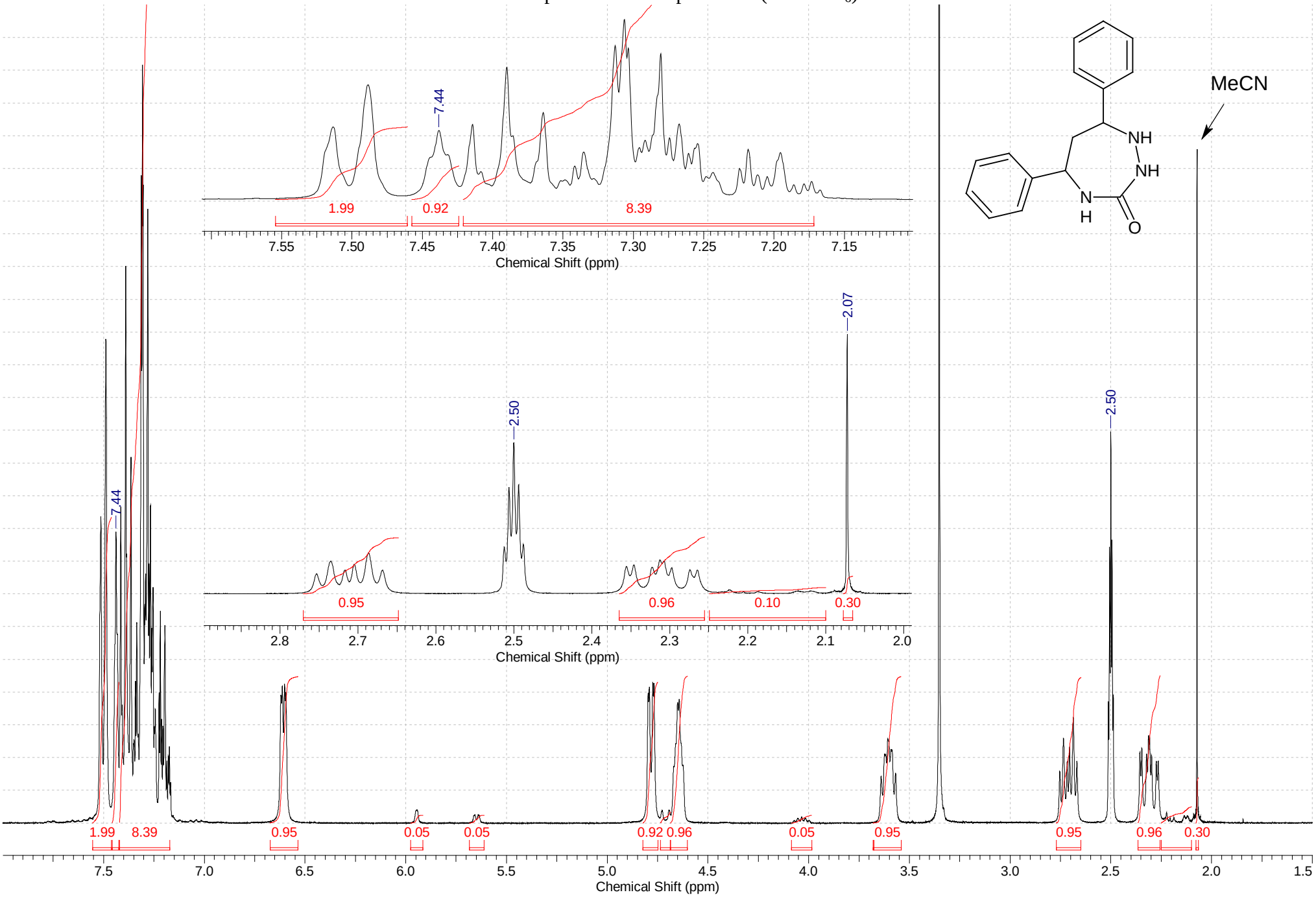

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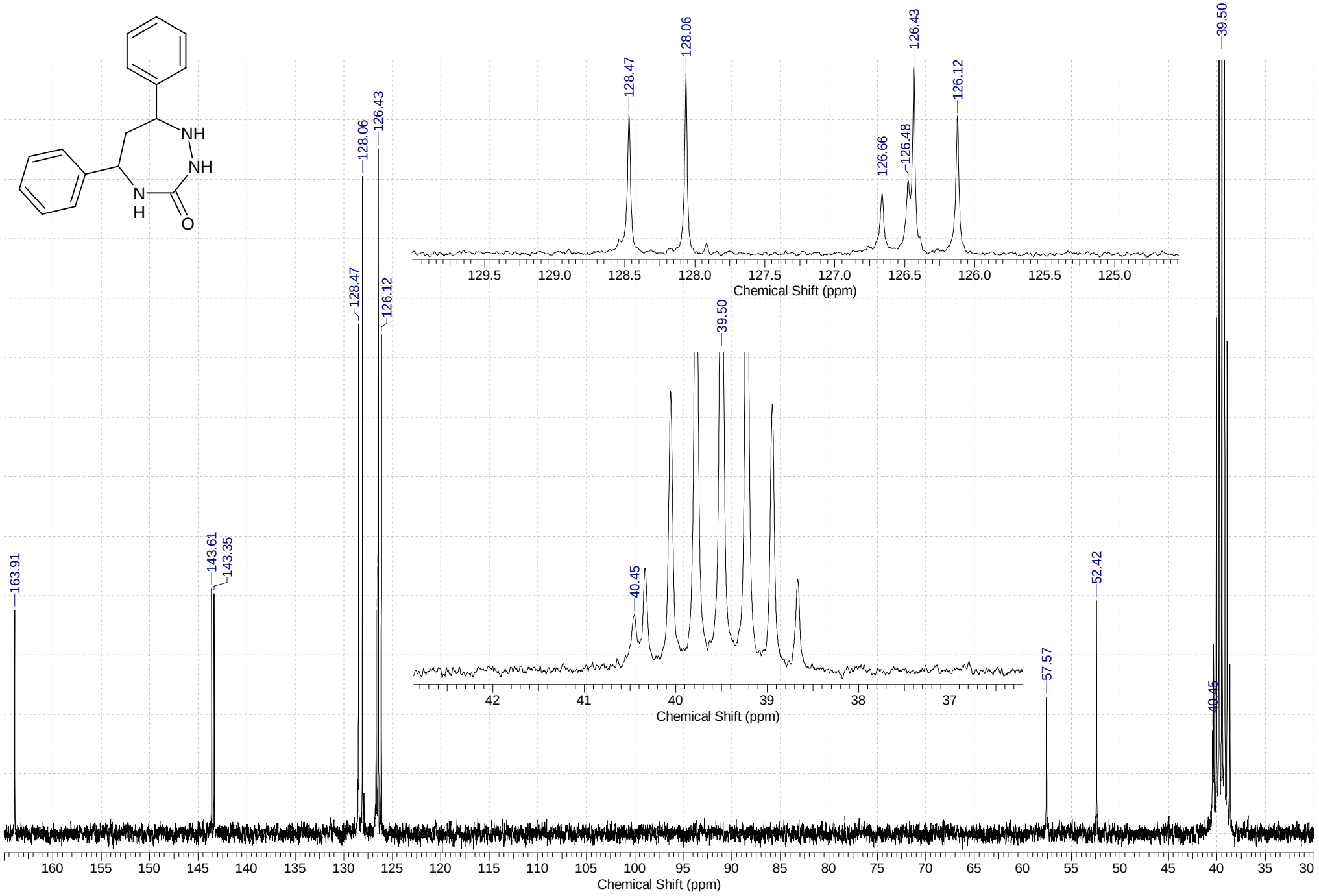
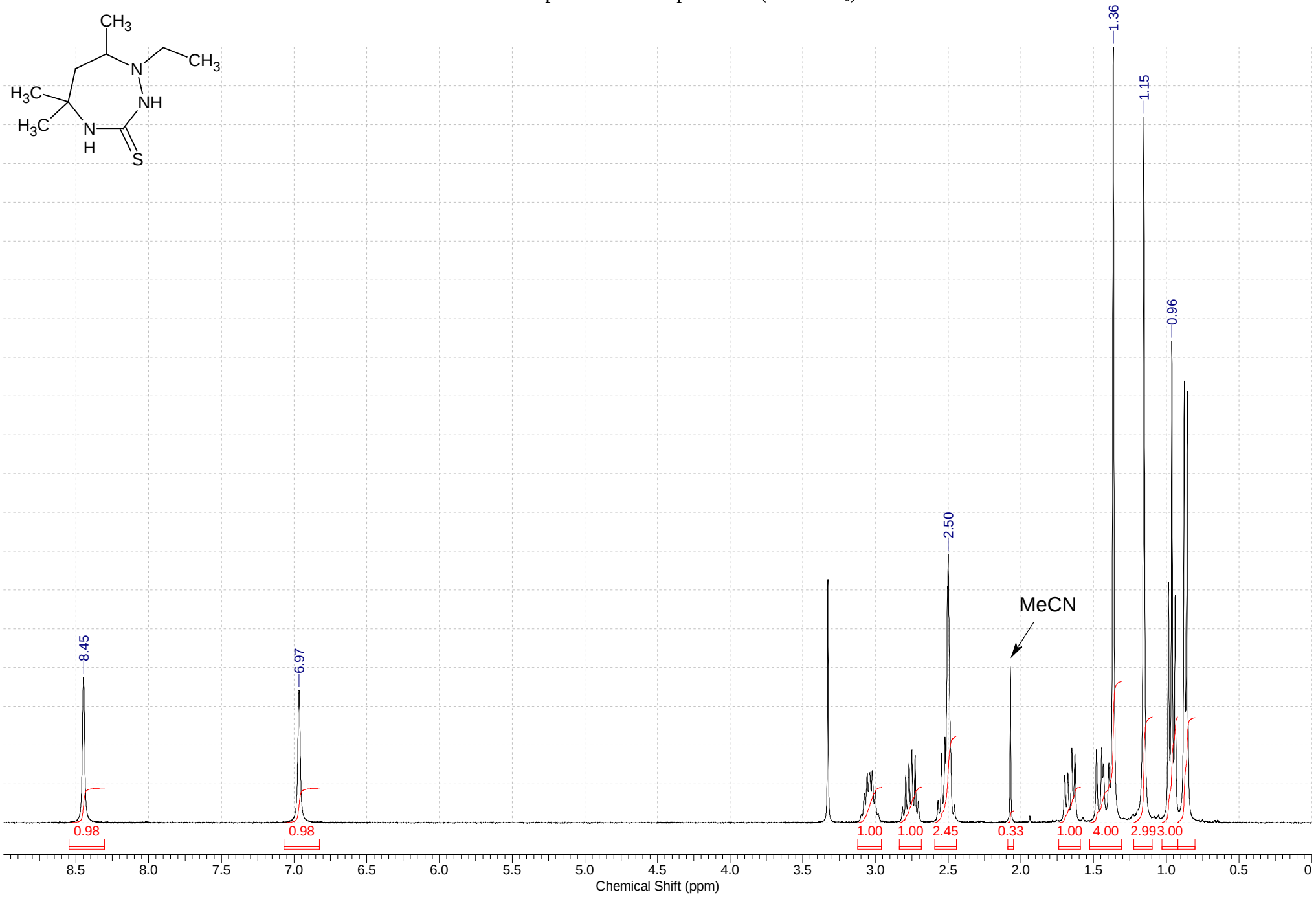
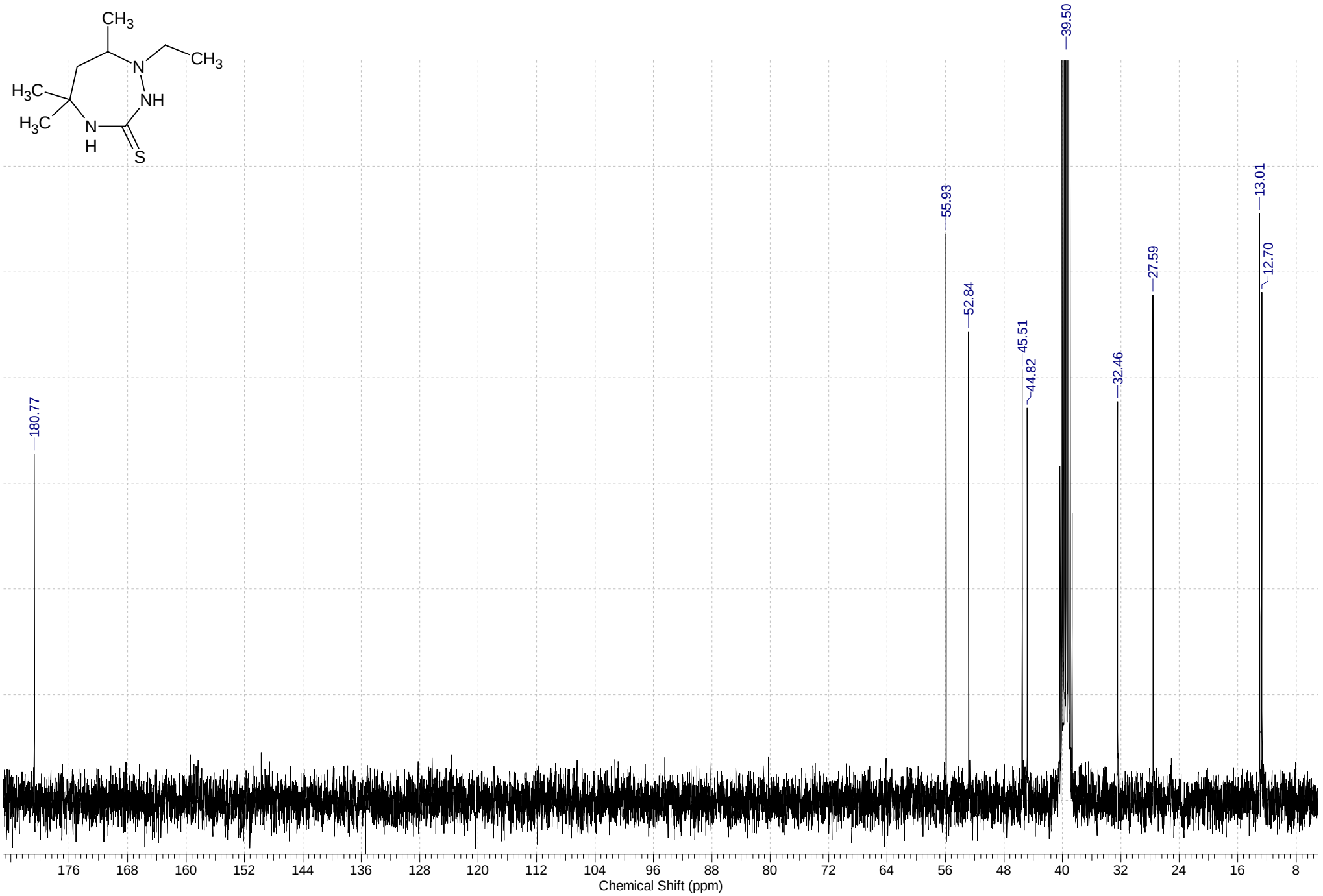


^{1}H NMR spectrum of compound **7a** (DMSO-d_6)



^{13}C NMR spectrum of compound **7a** (DMSO-d_6)



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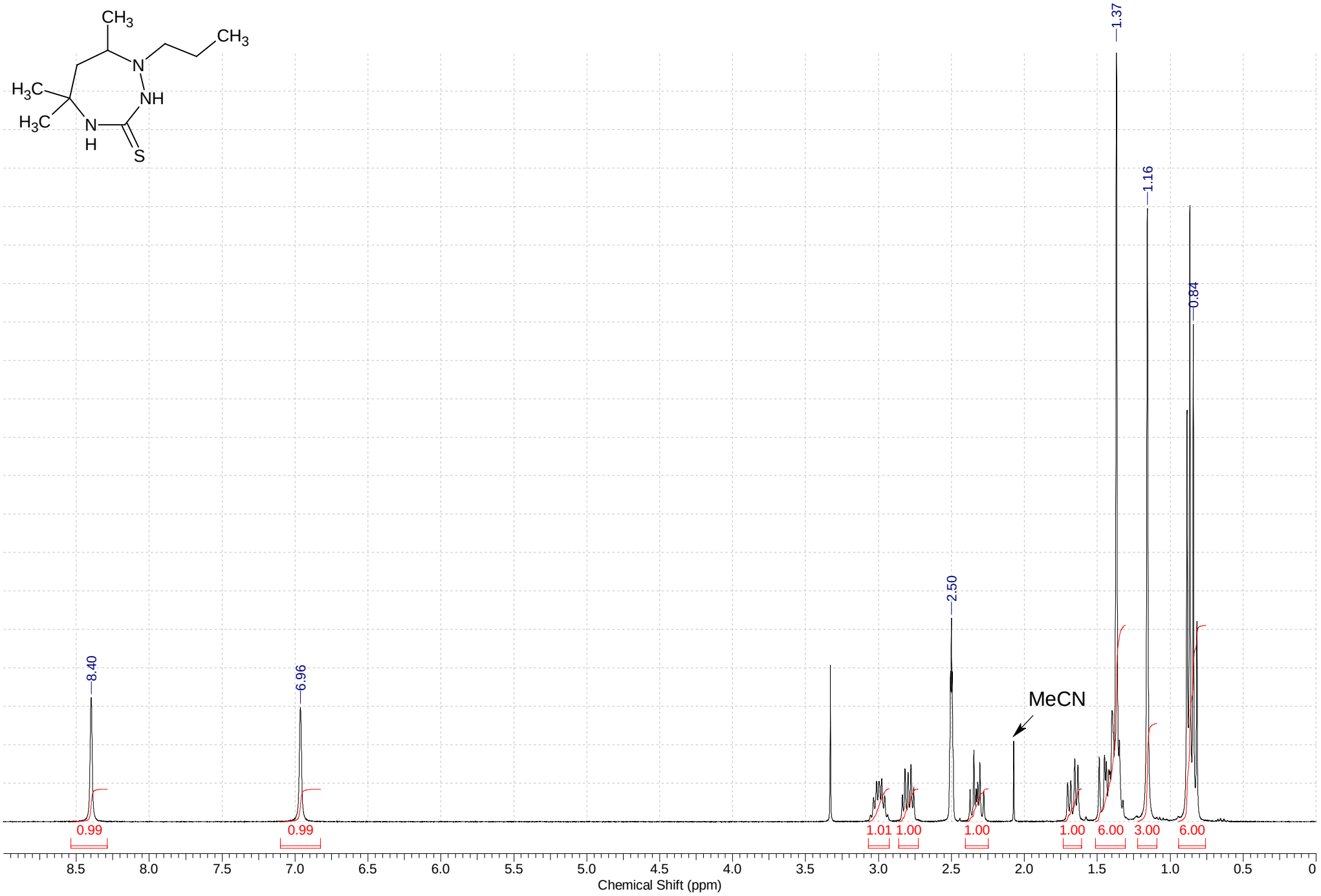

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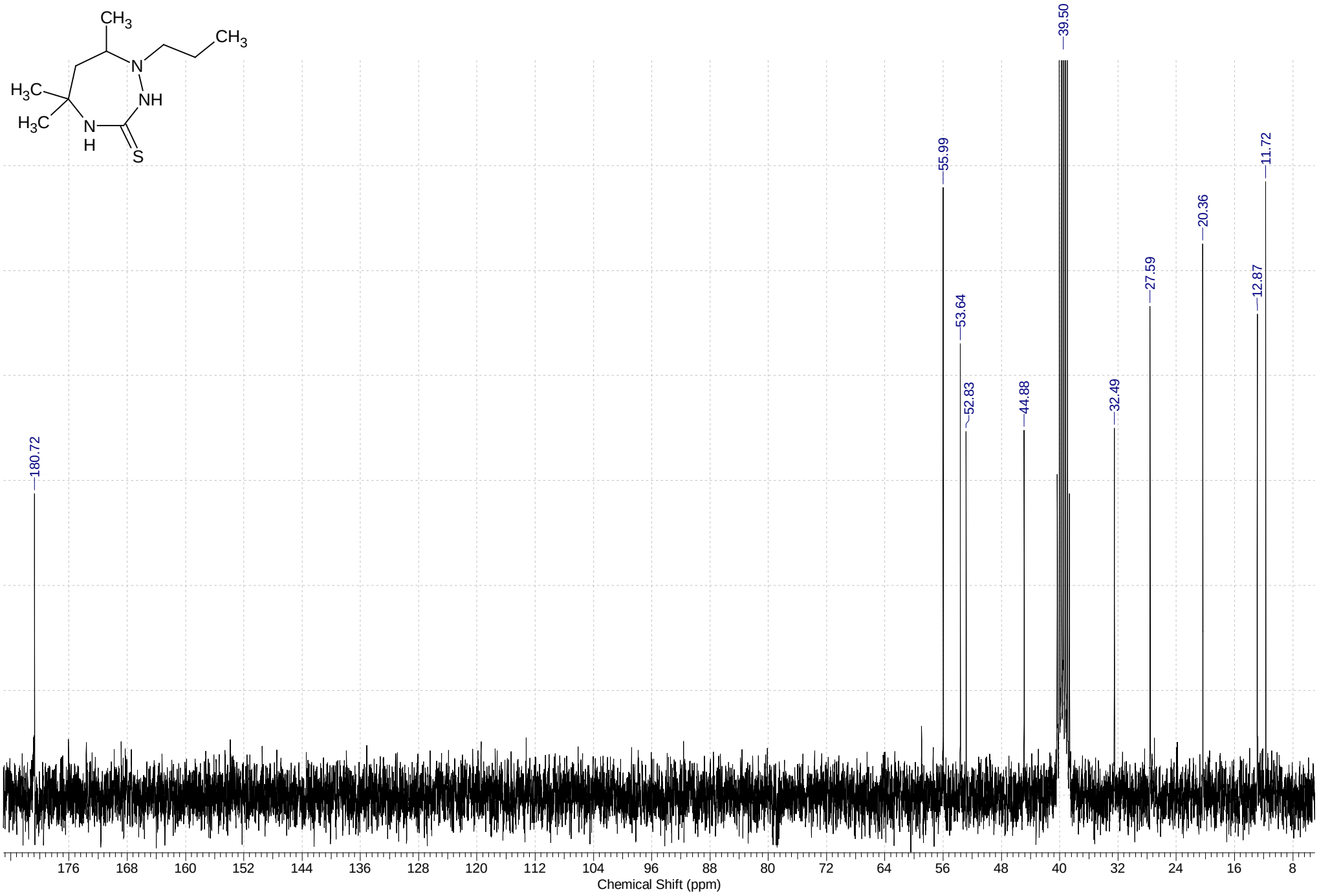

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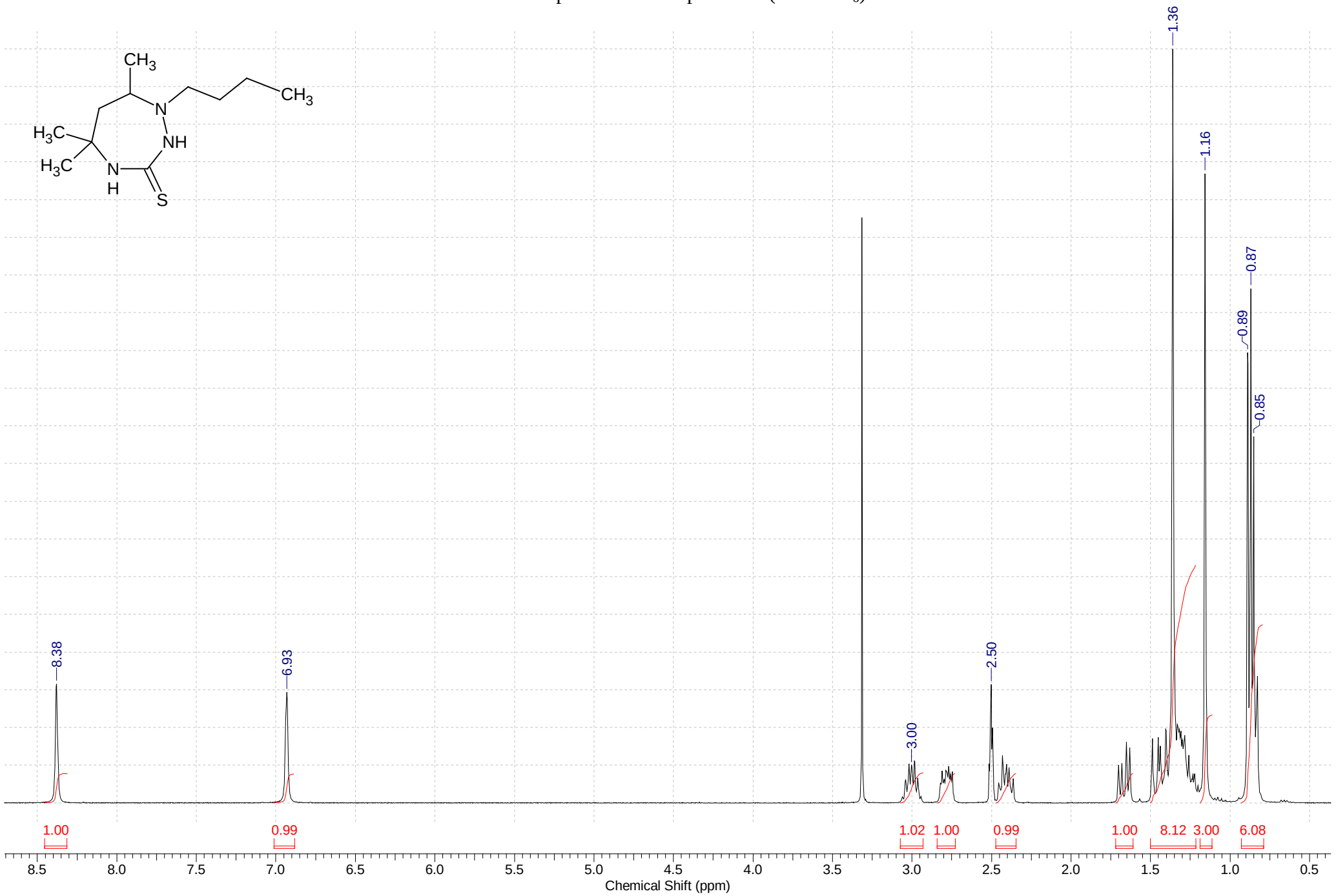
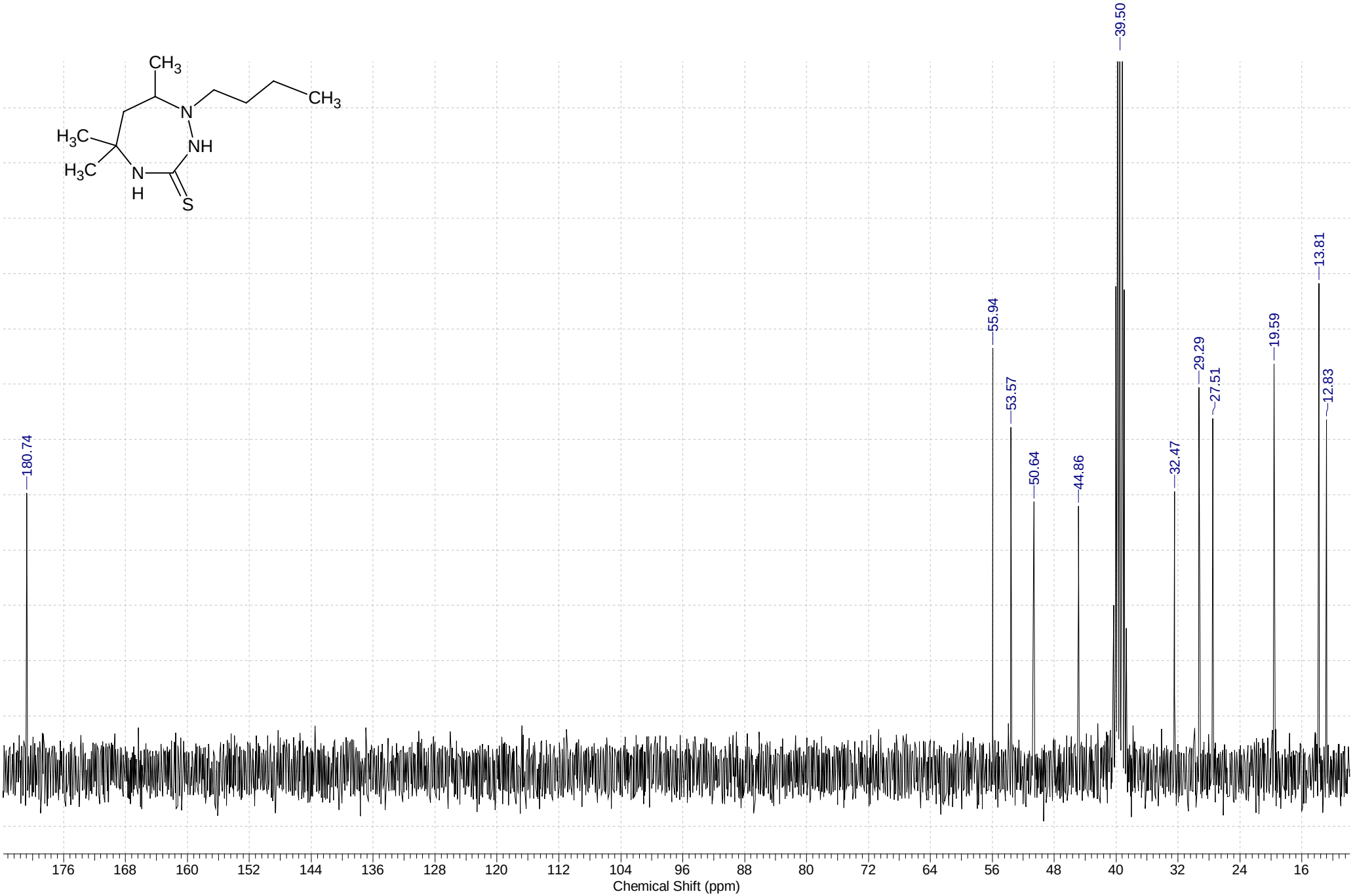


^{13}C NMR spectrum of compound **7c** (DMSO-d_6)



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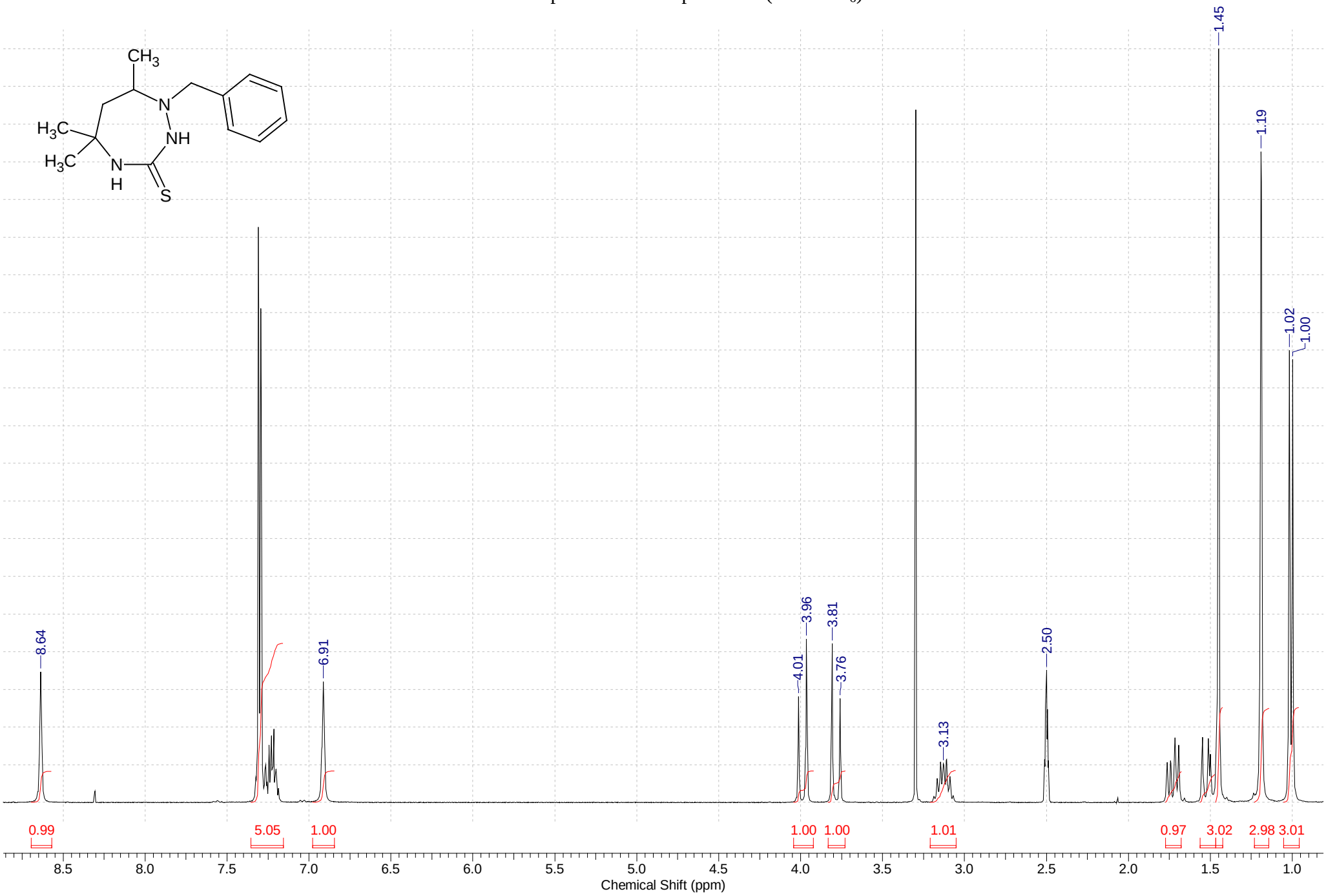
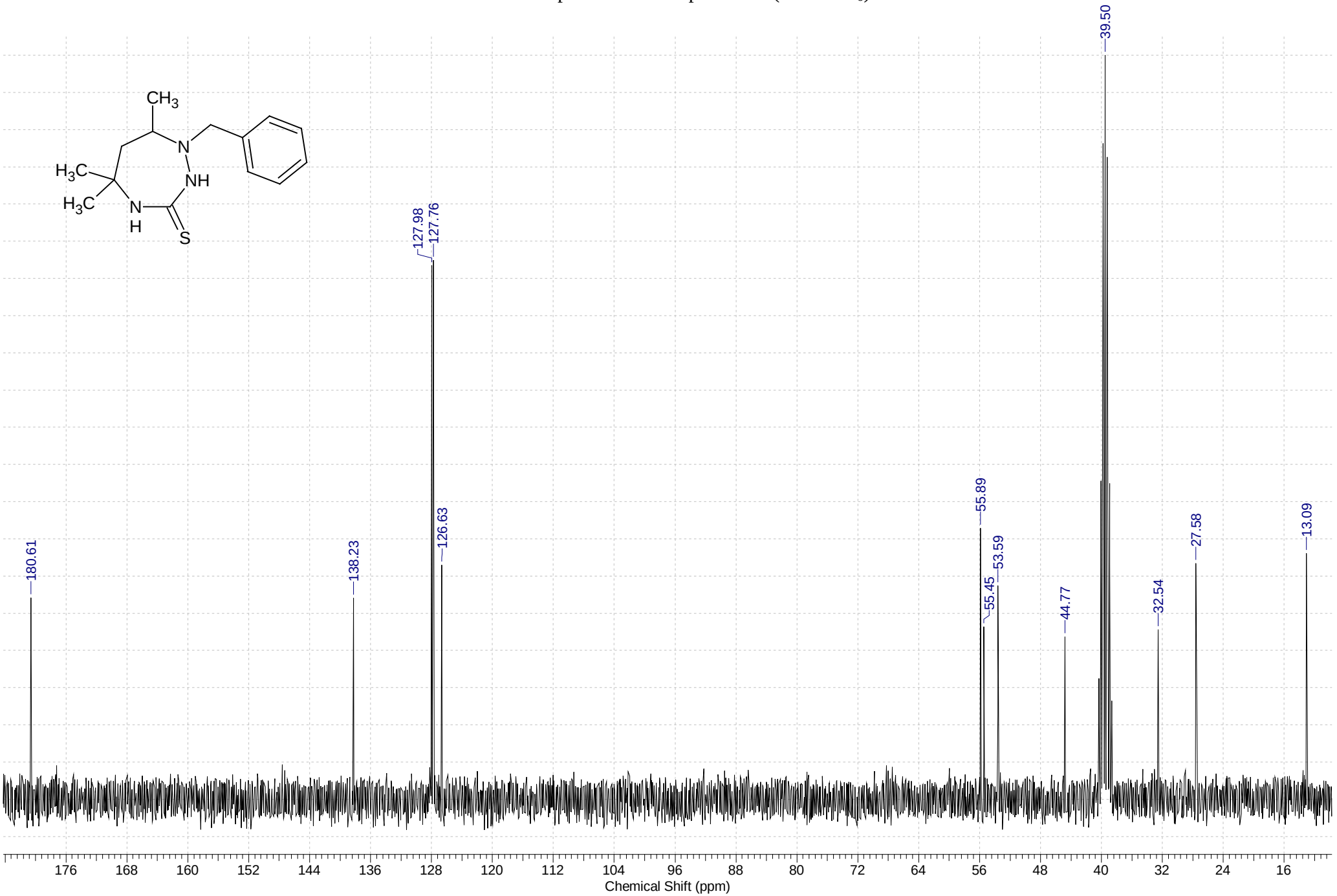


^{13}C NMR spectrum of compound **7d** (DMSO-d_6)



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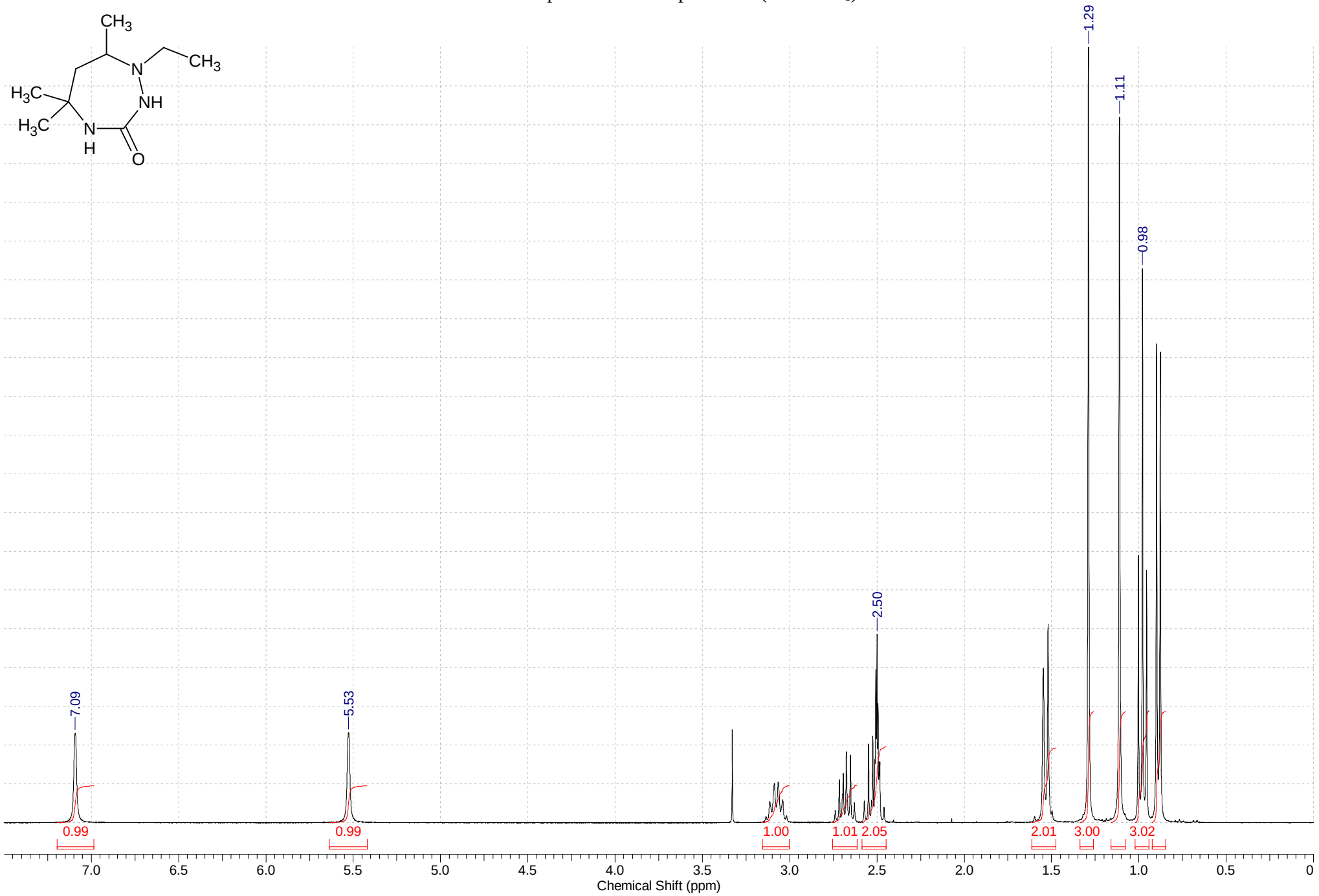

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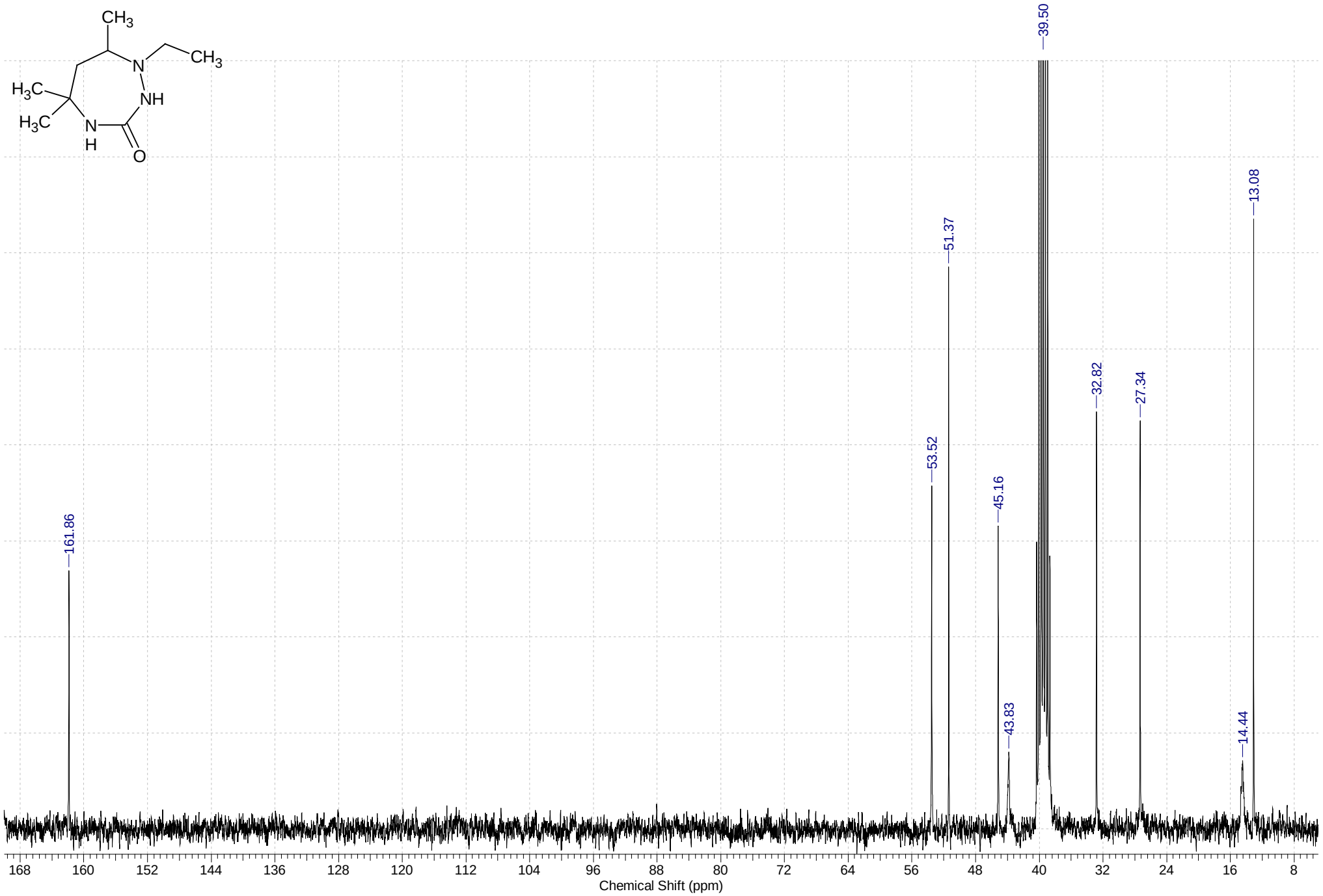

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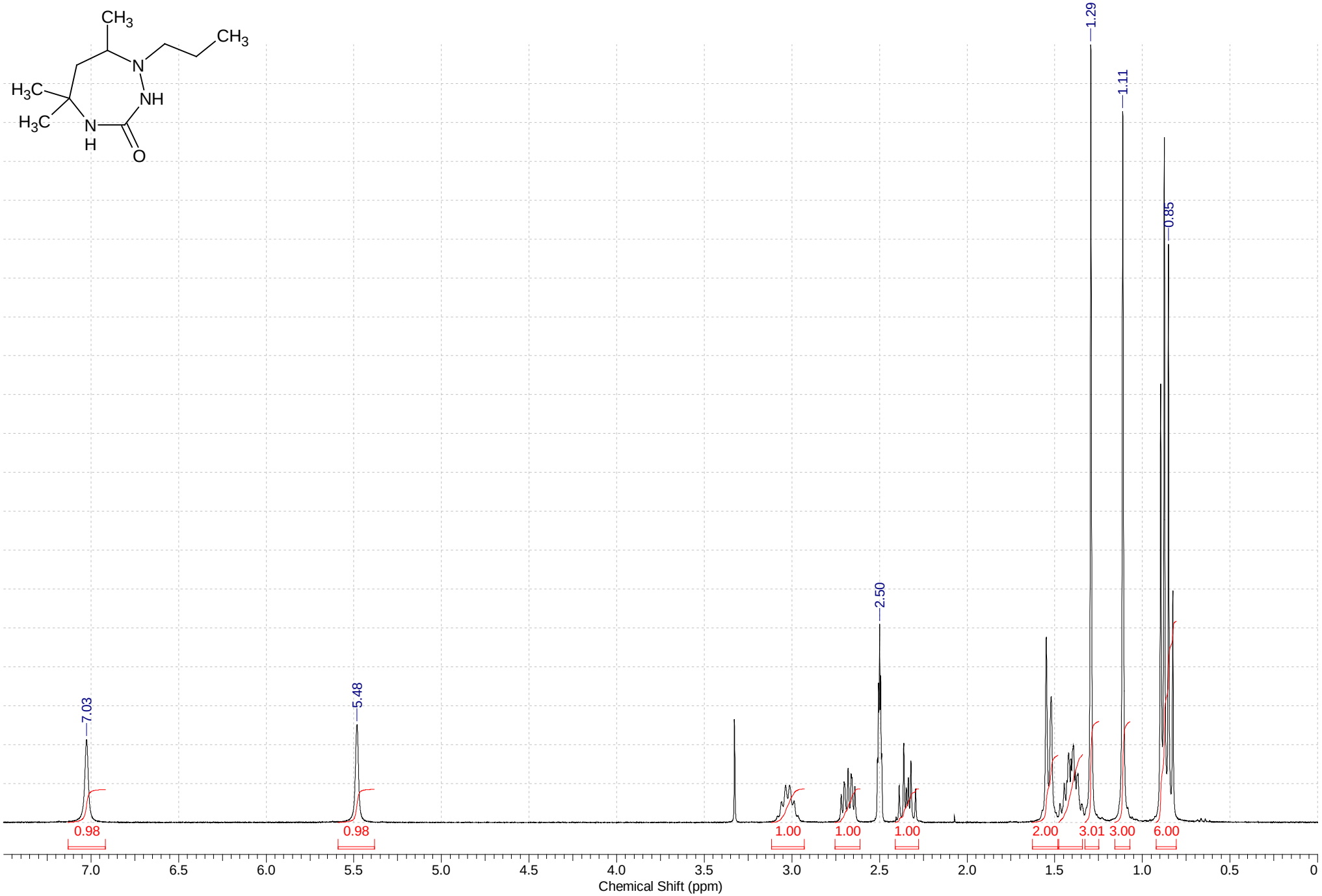

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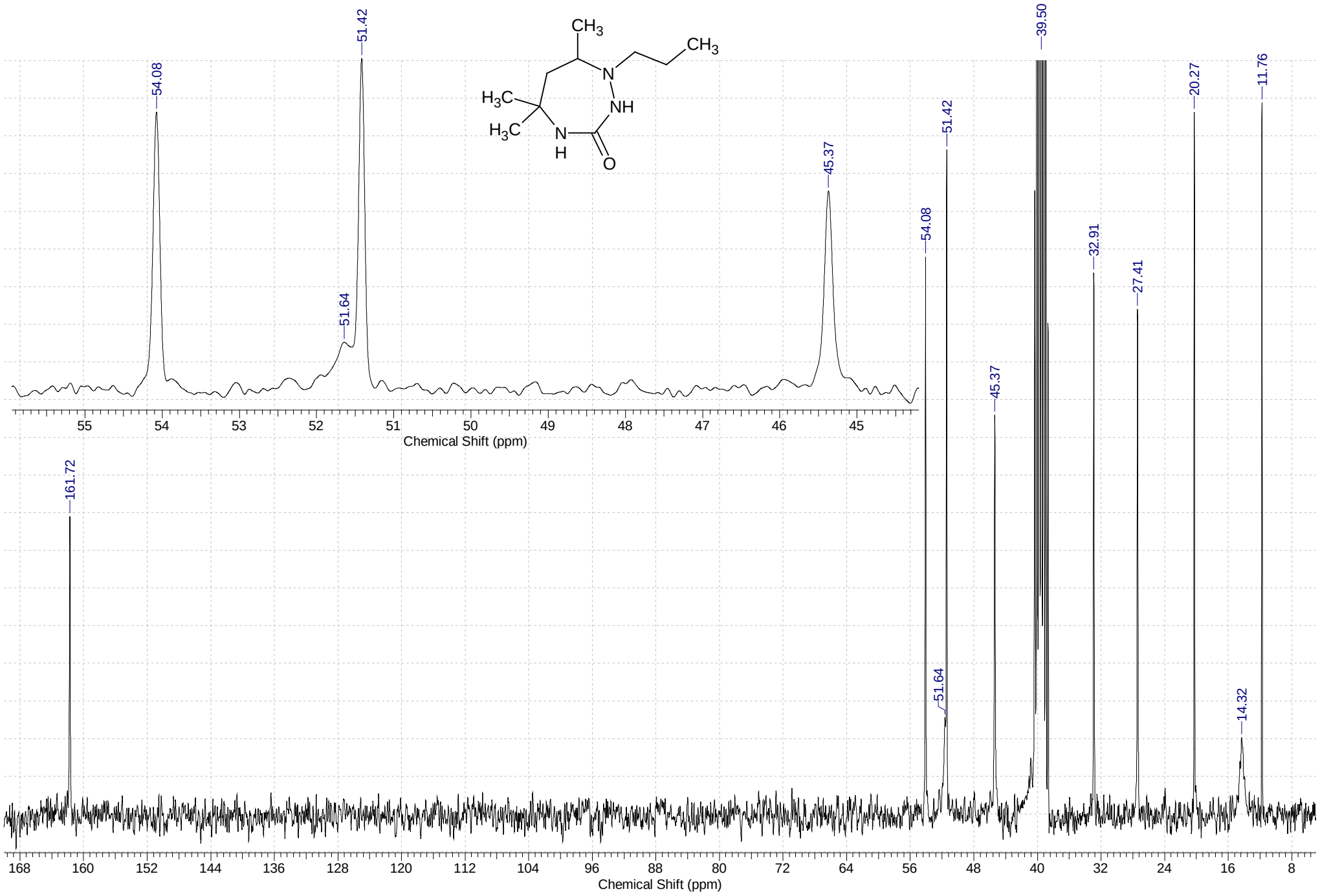

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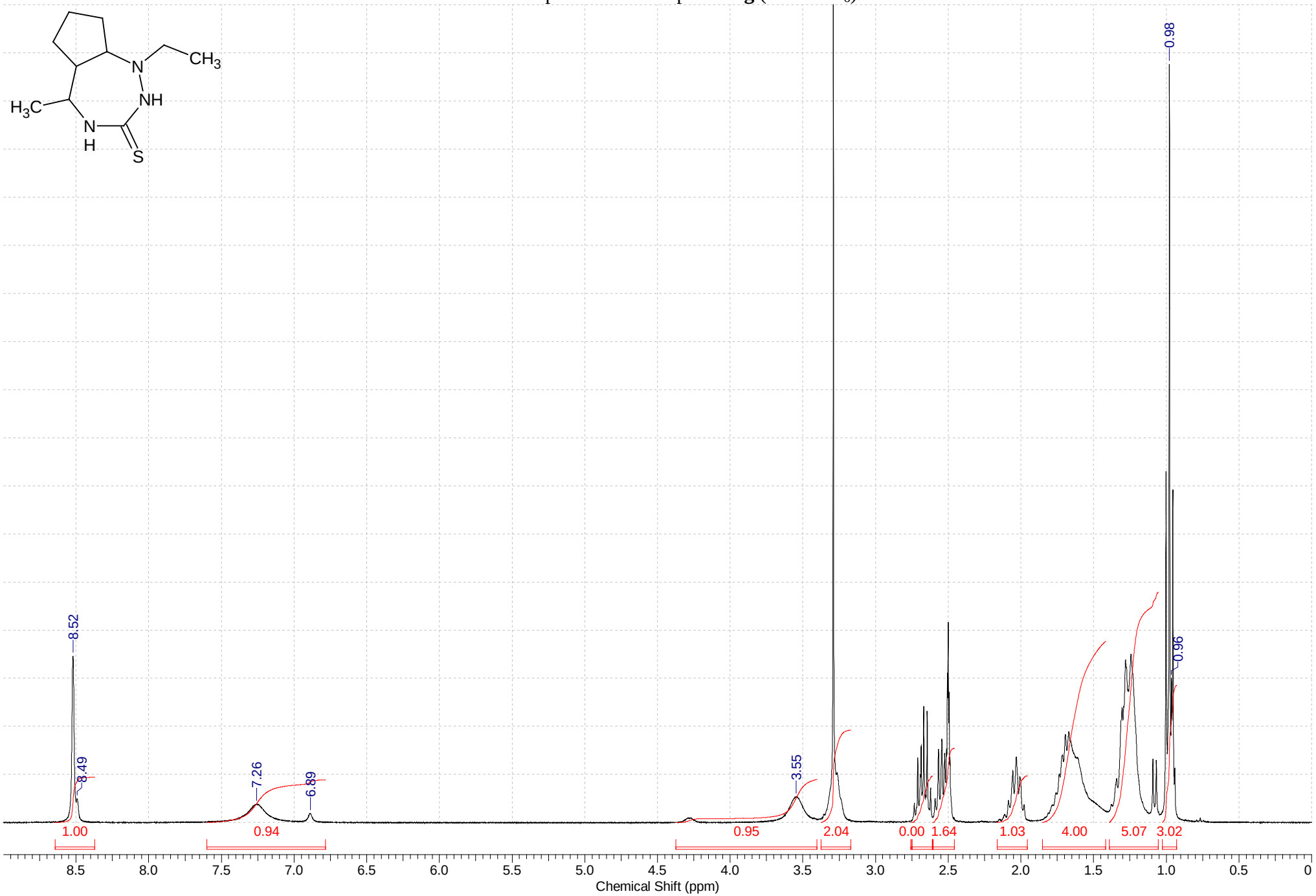

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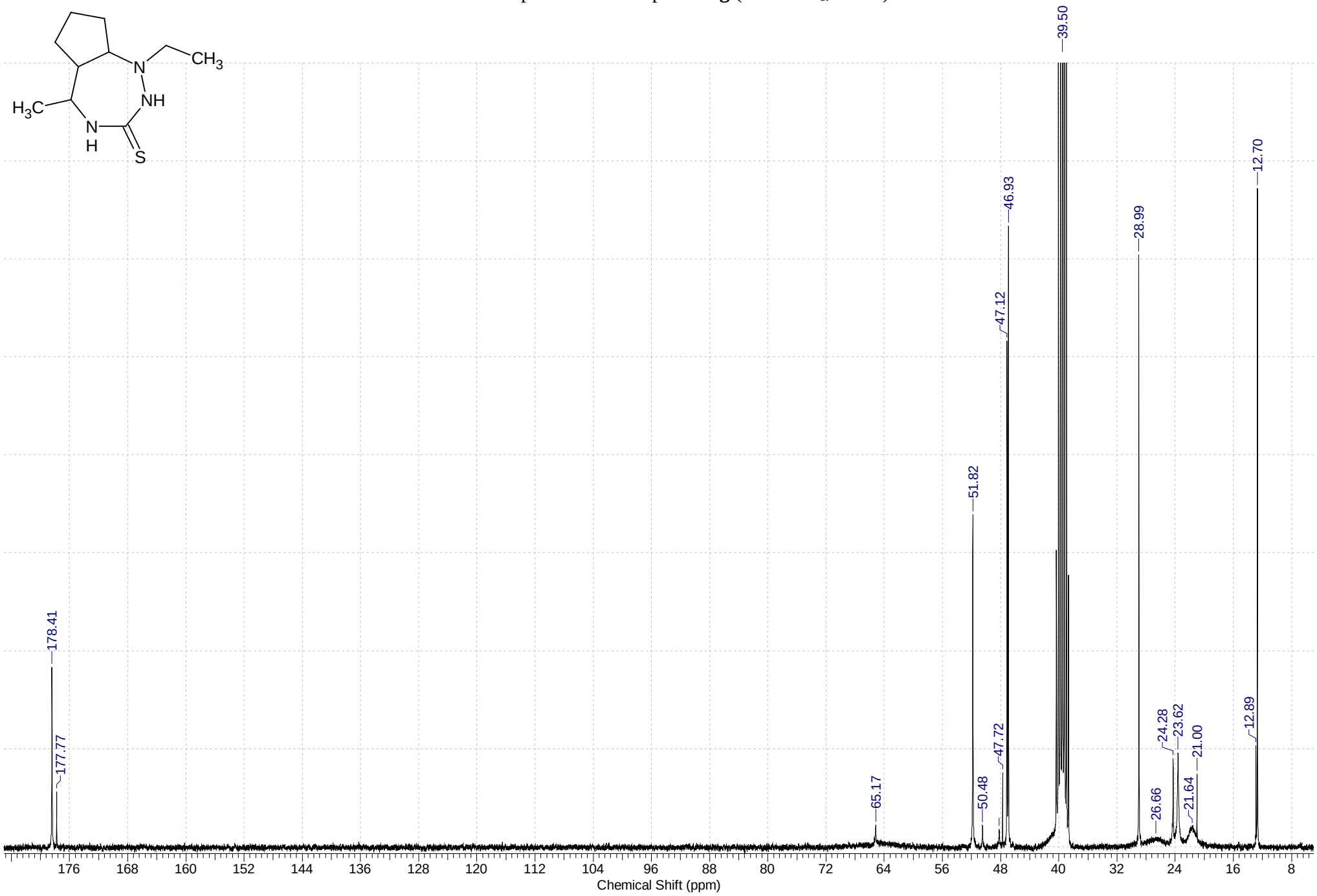

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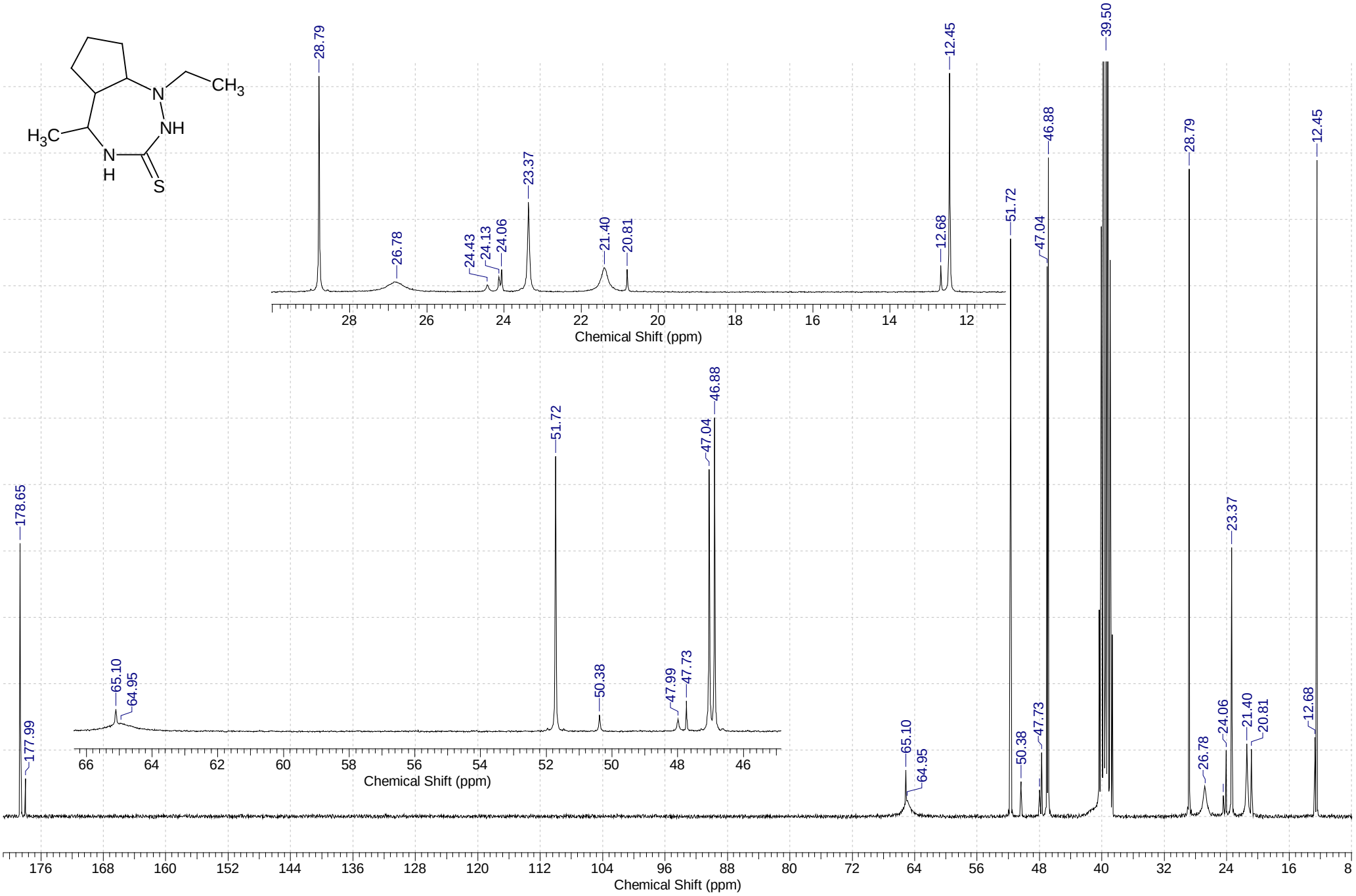

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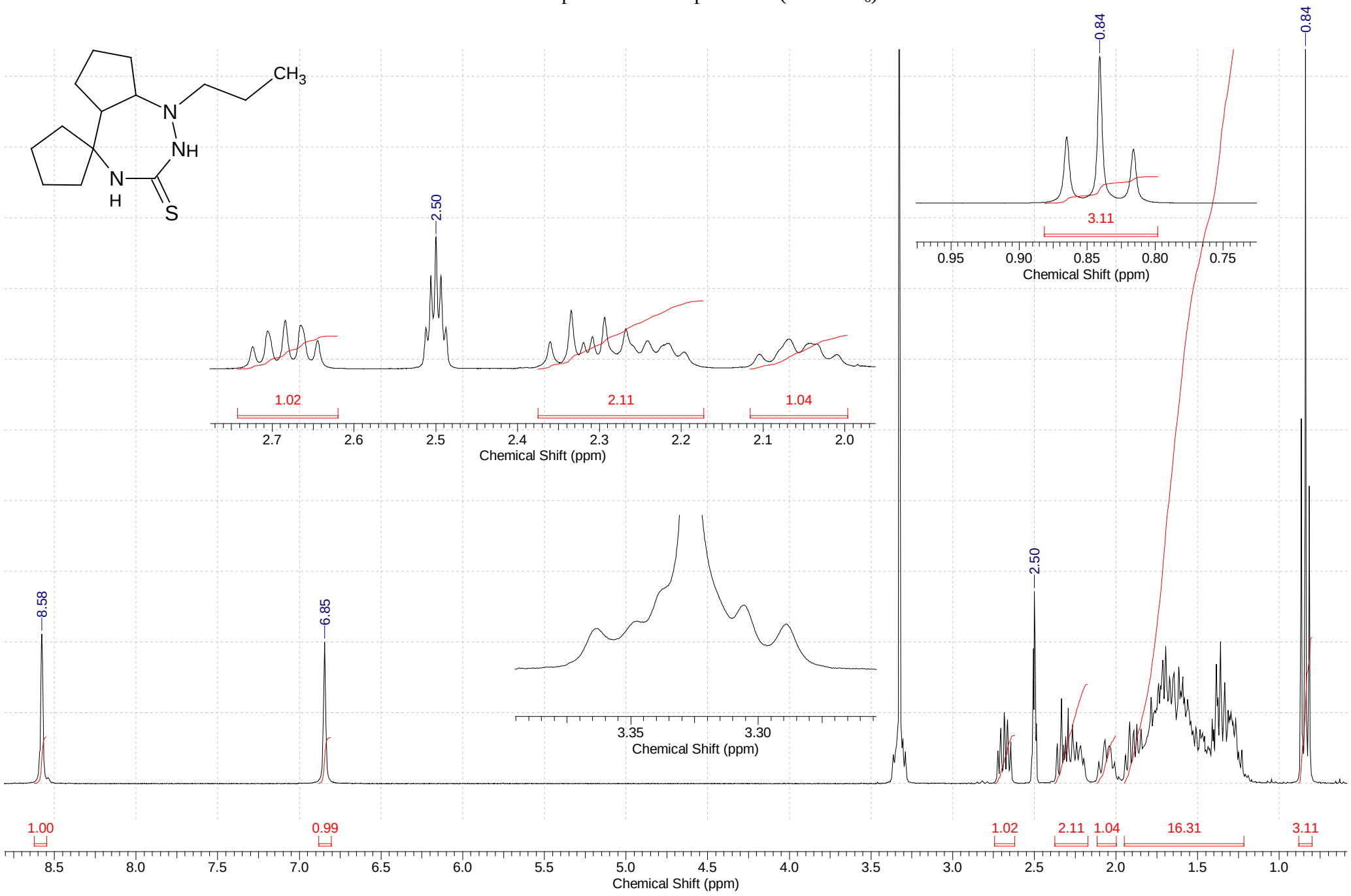

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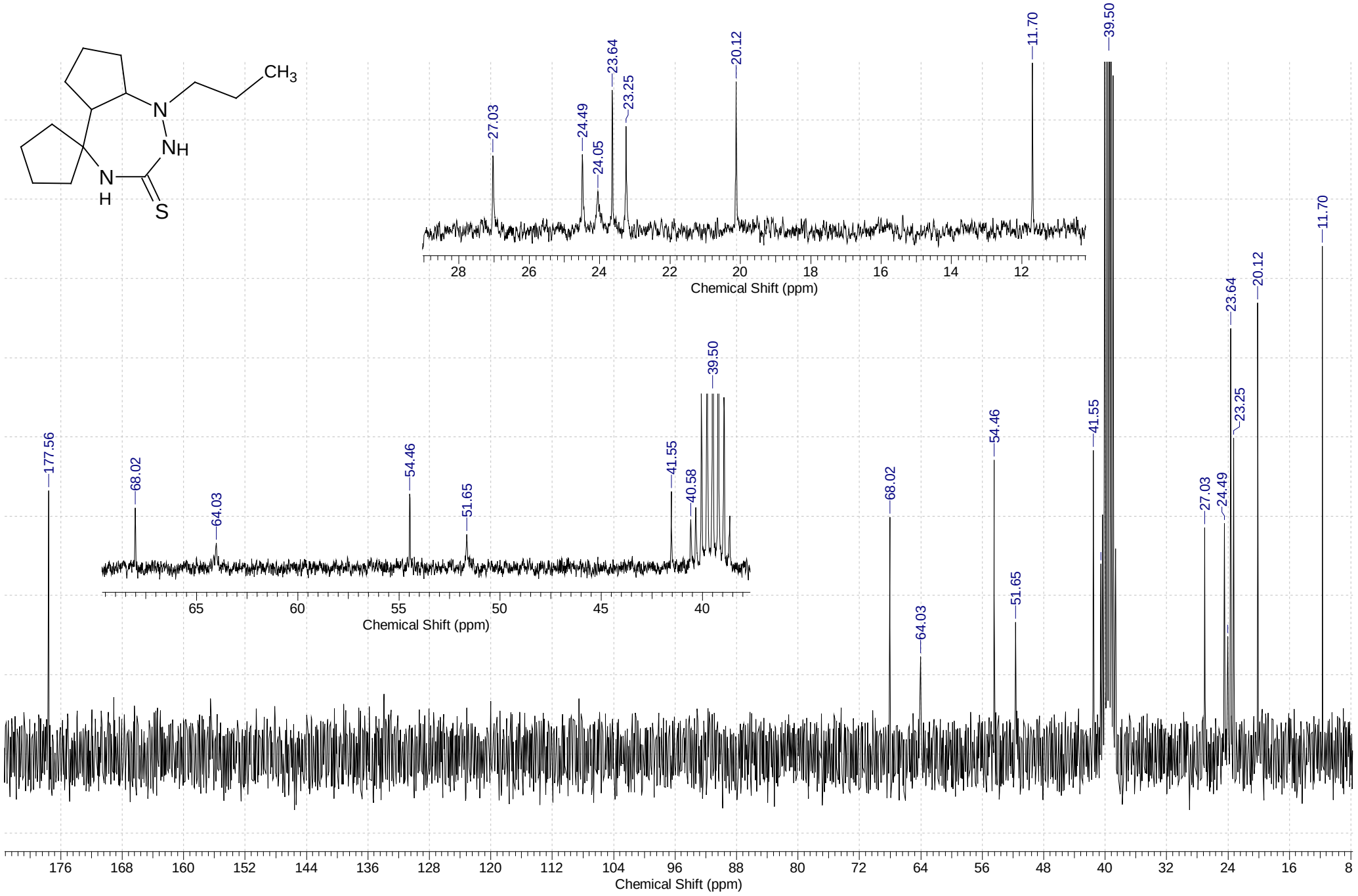

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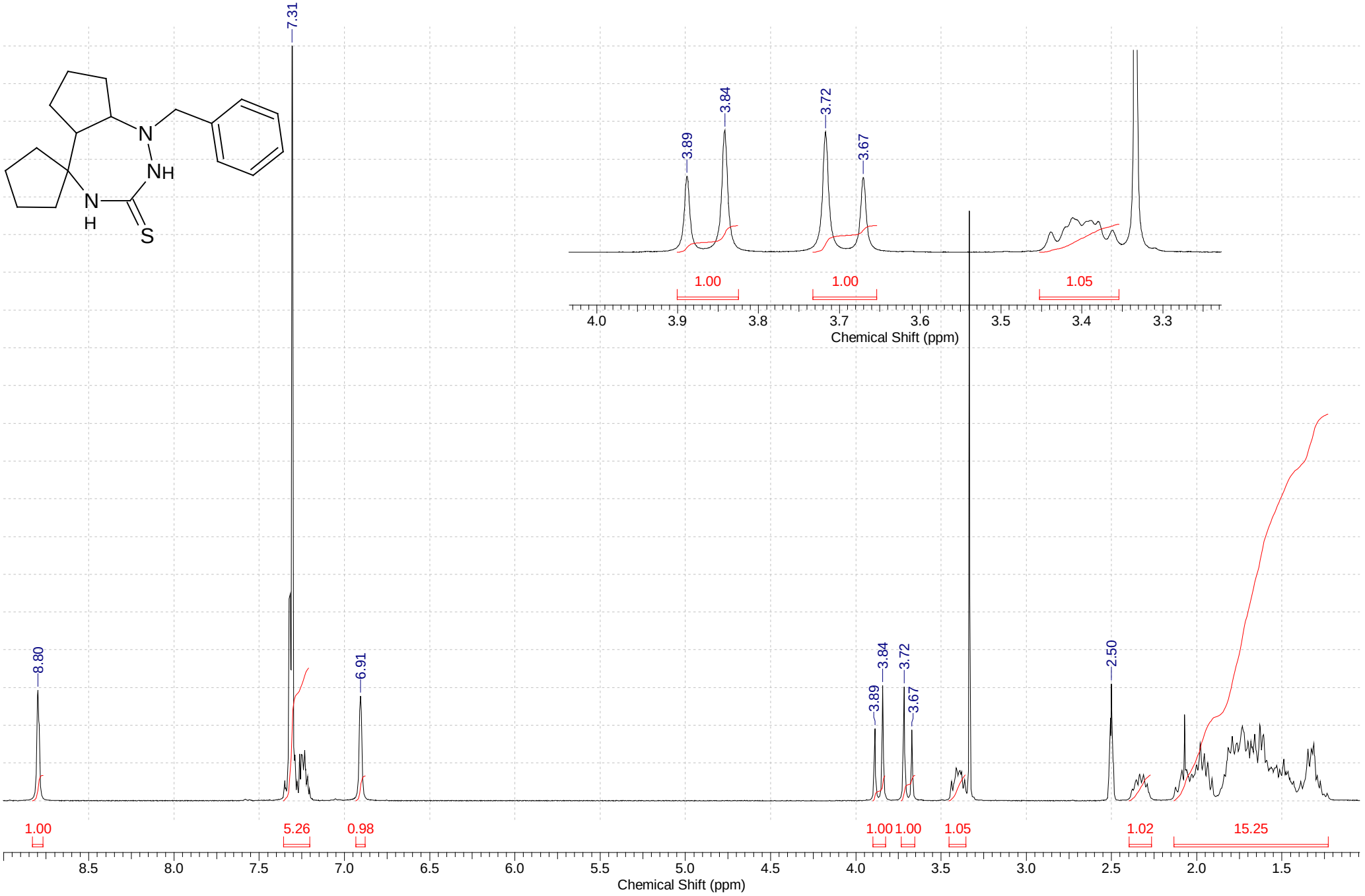

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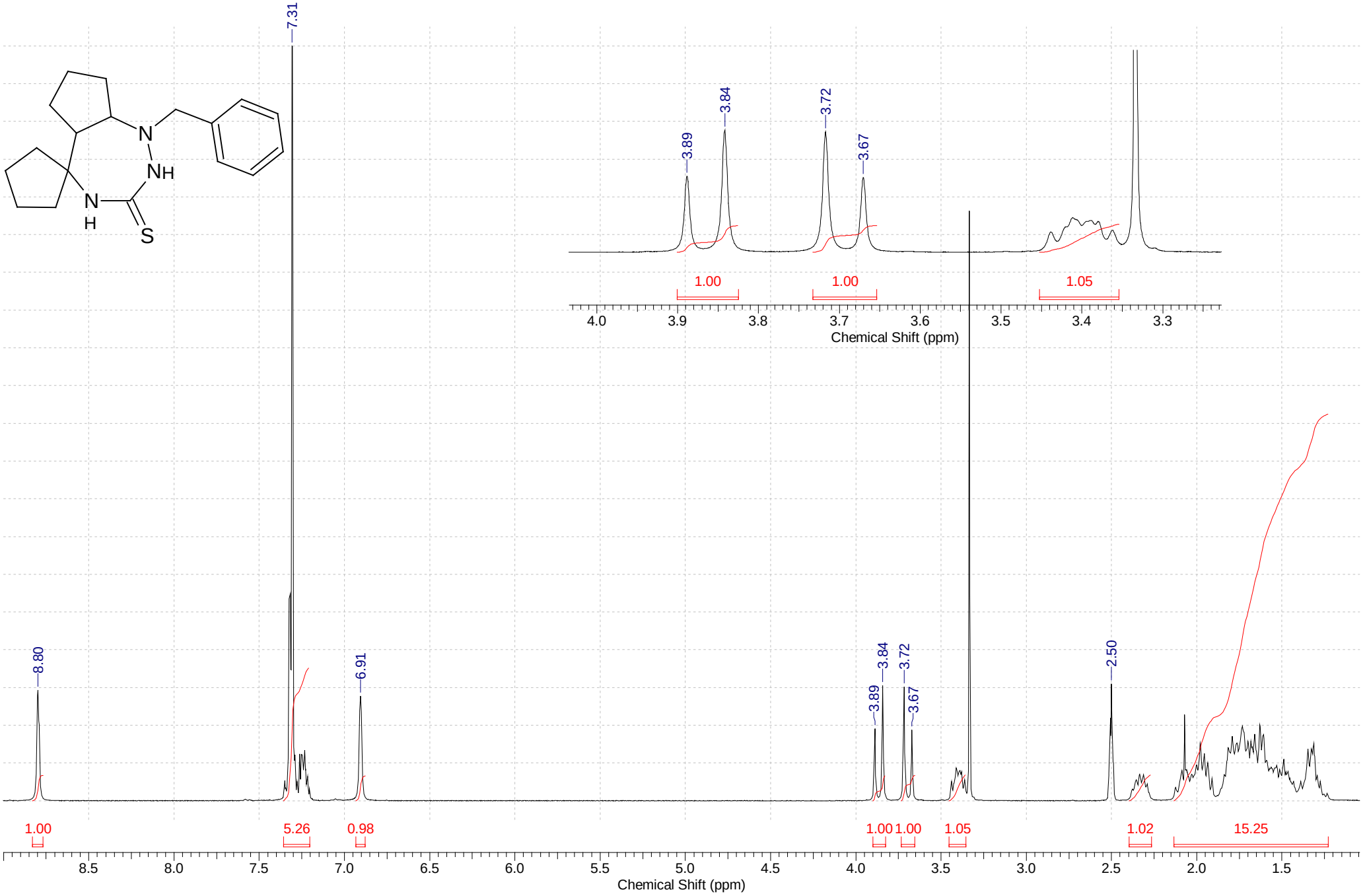

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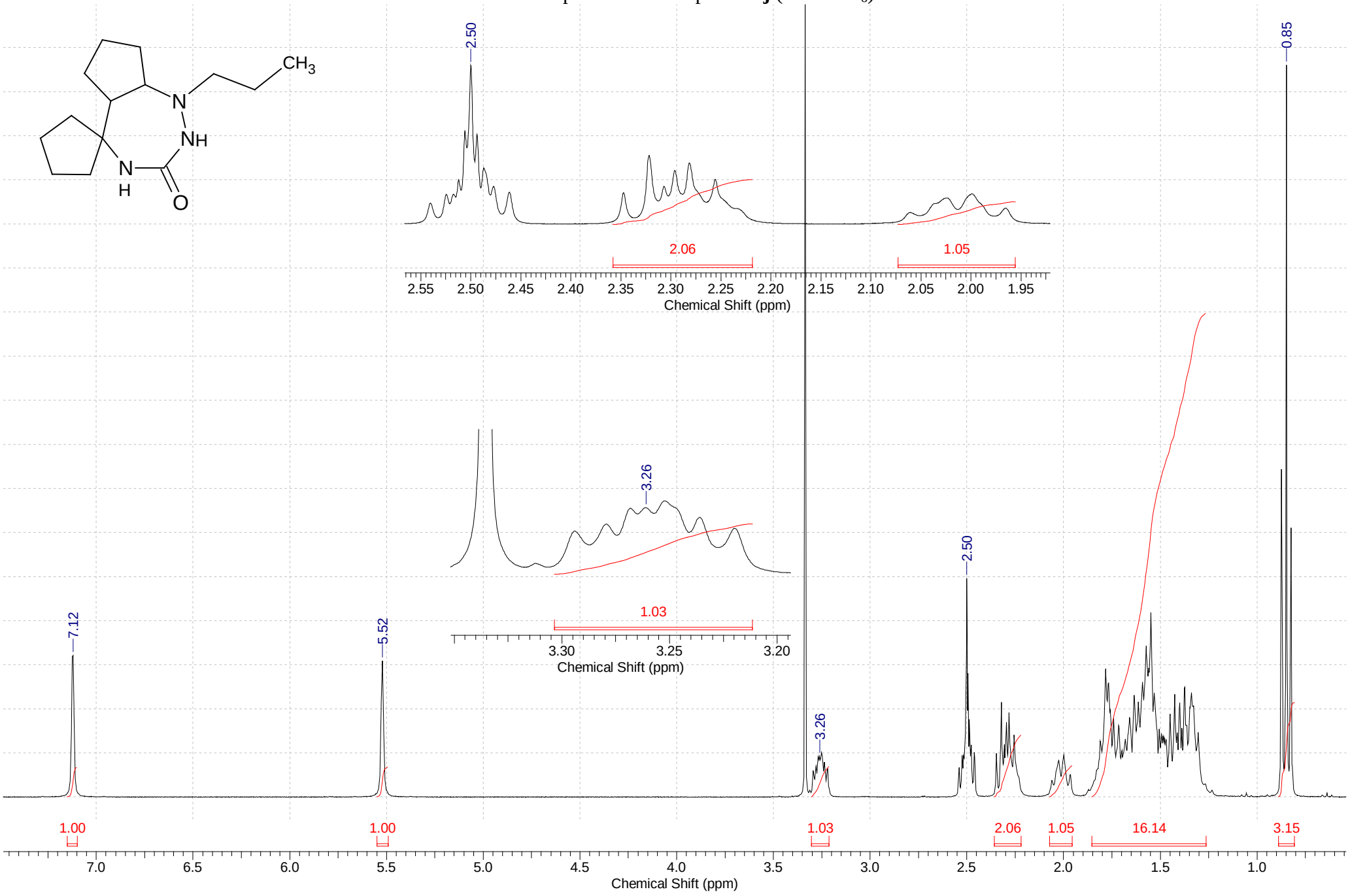

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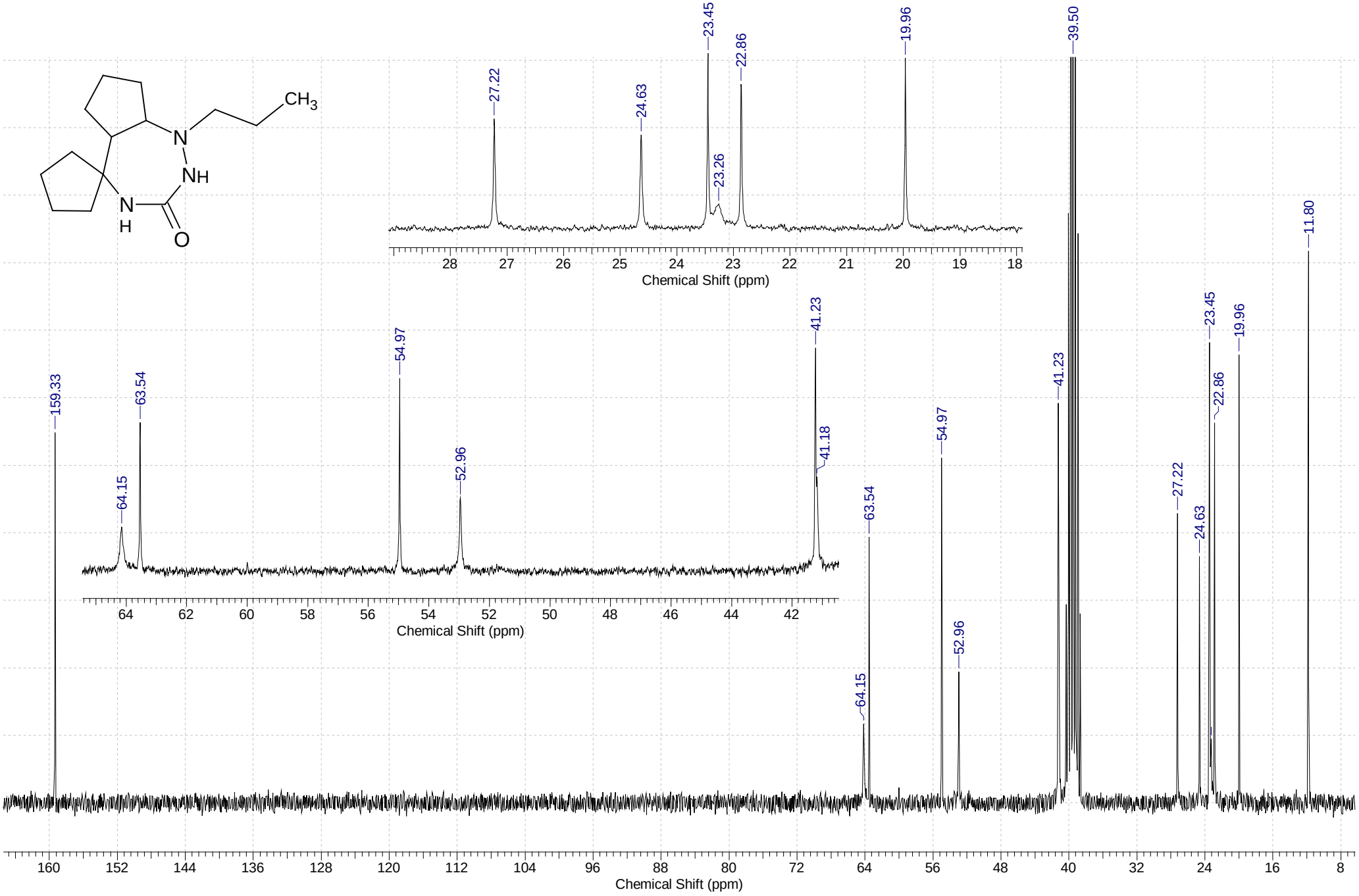

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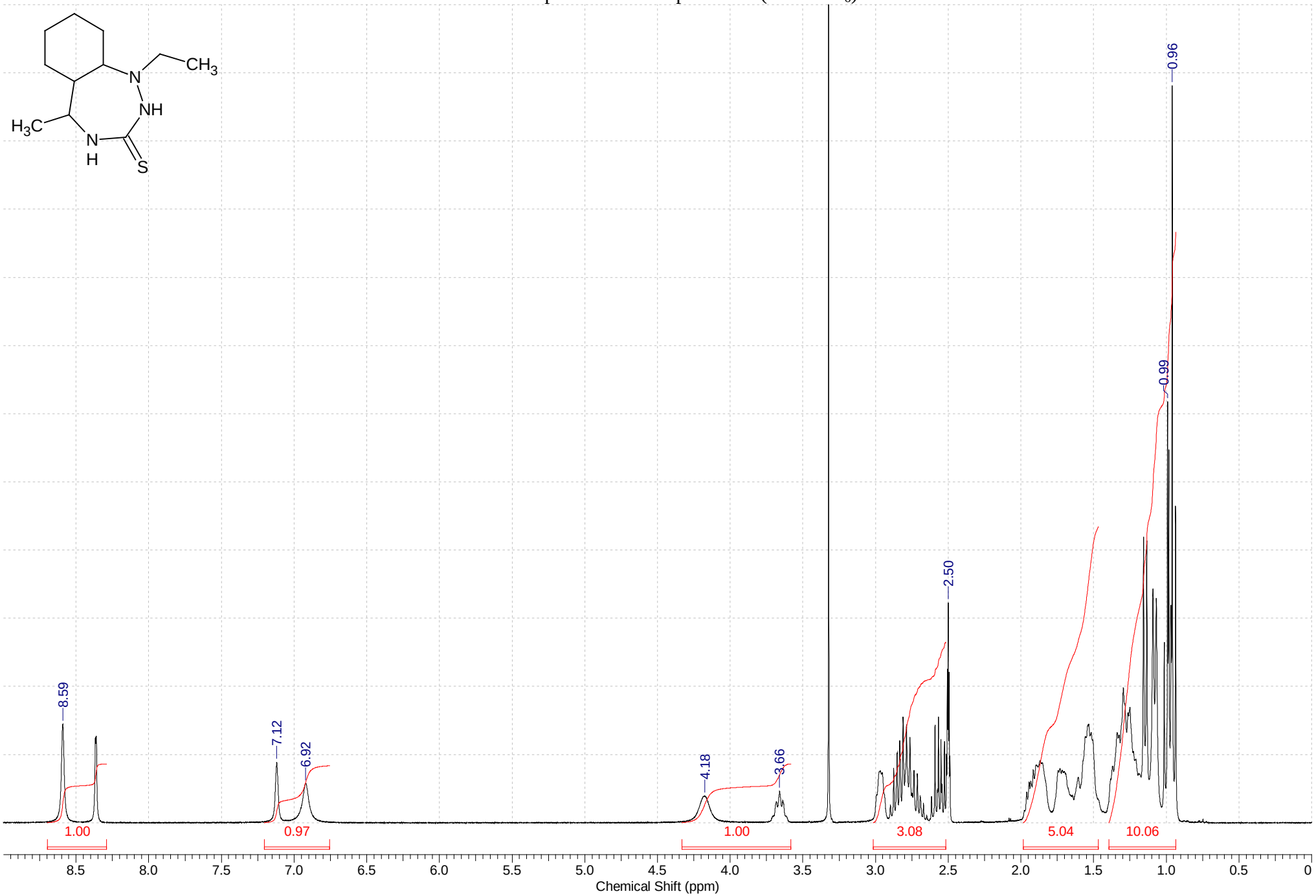

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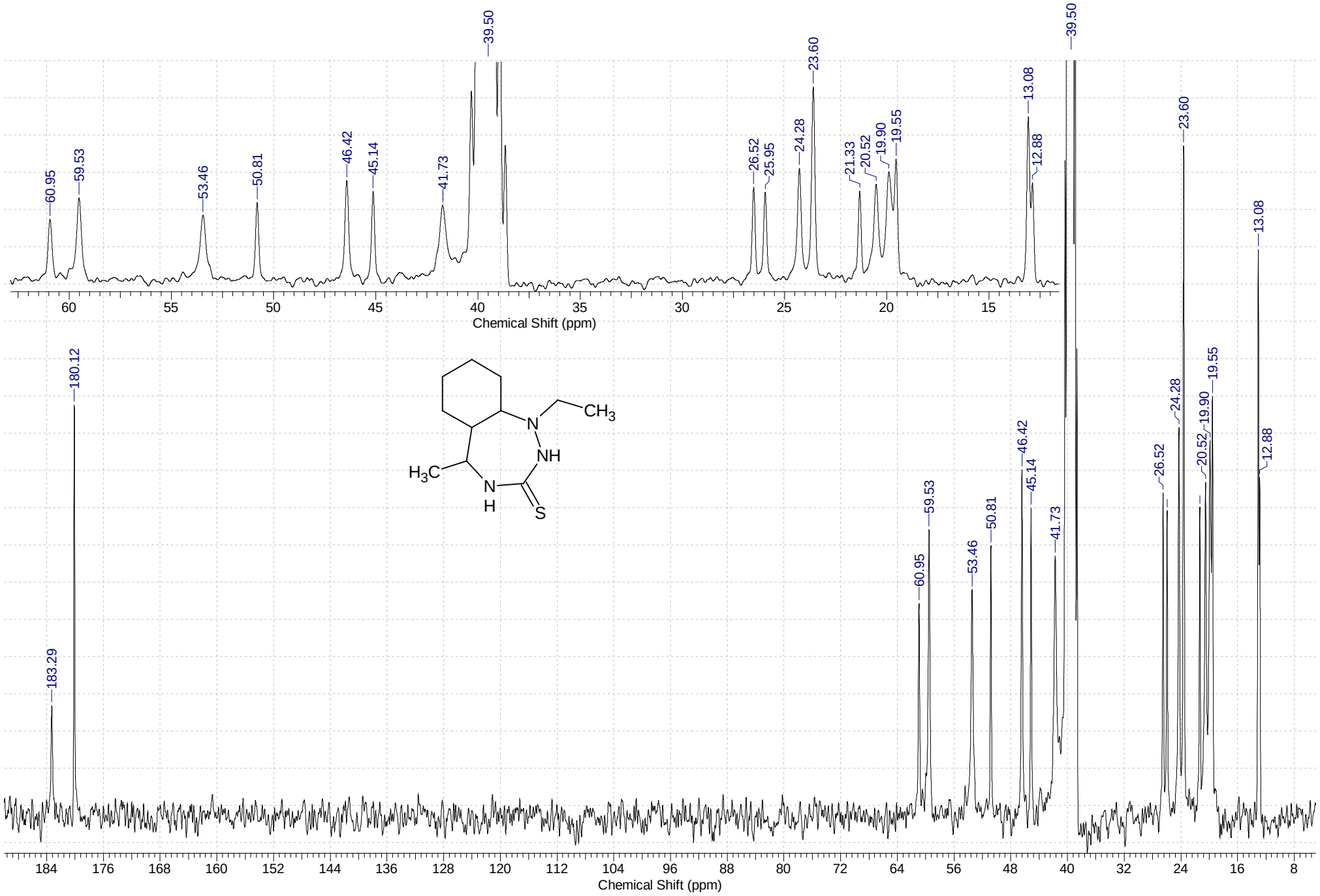

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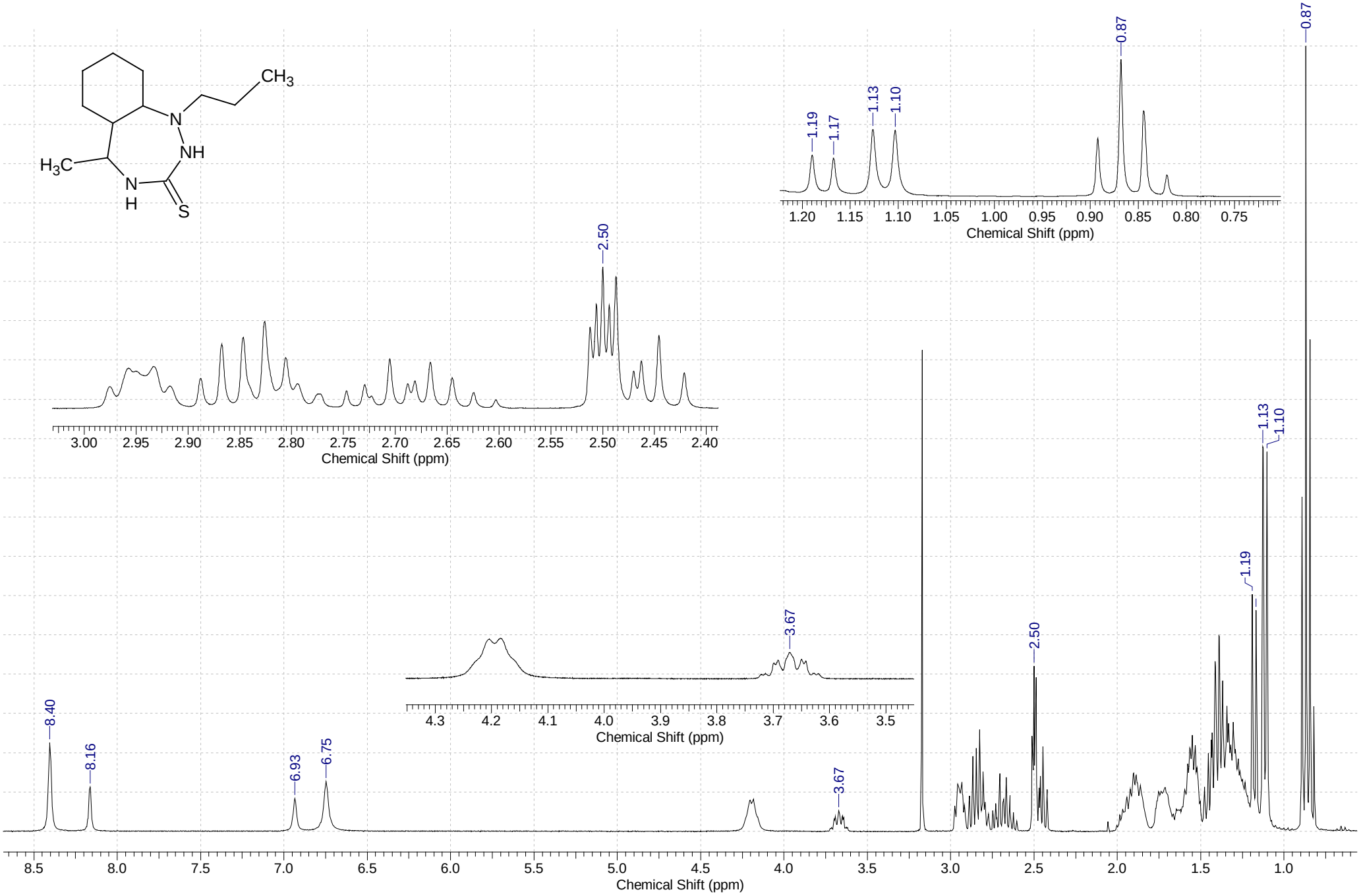

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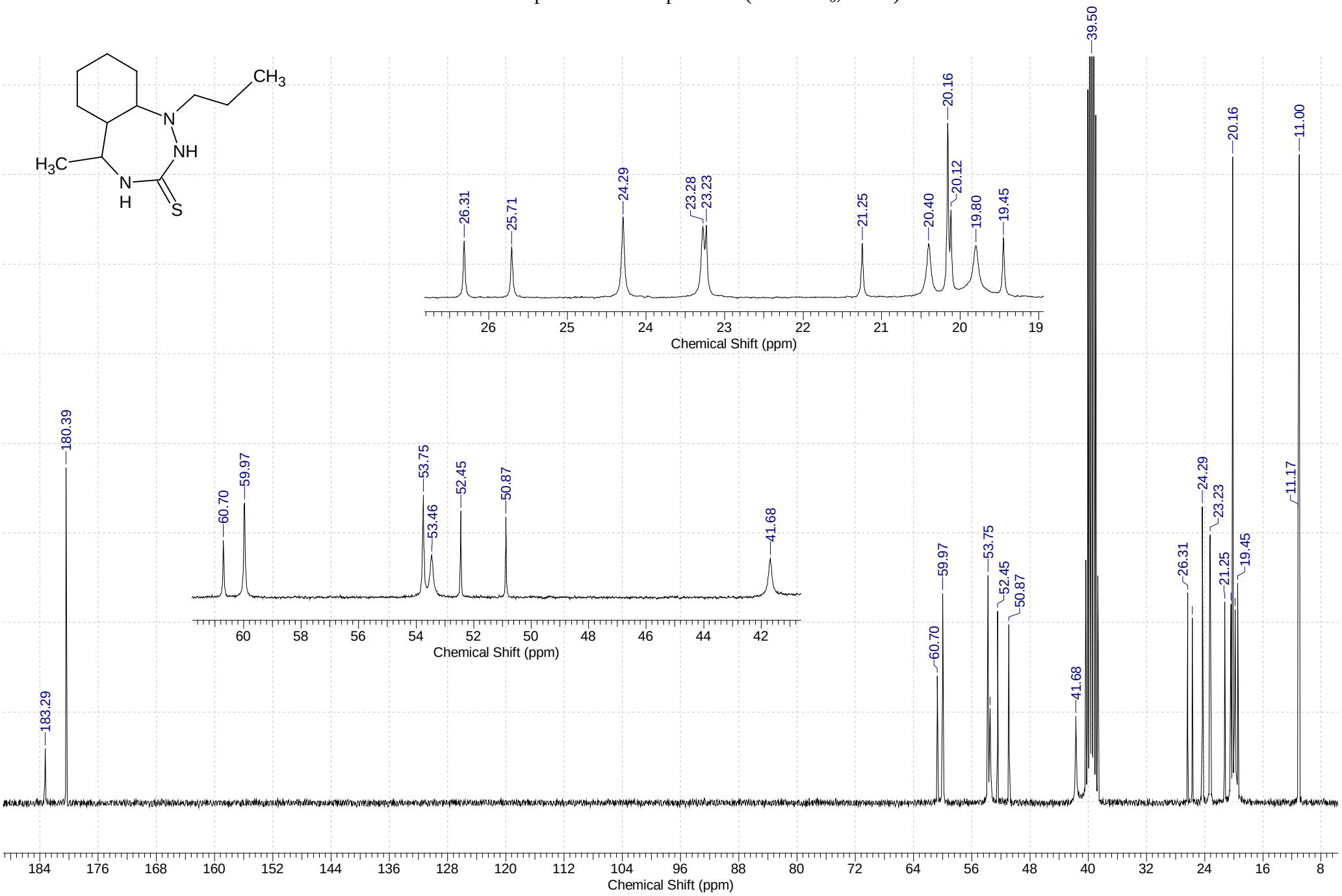
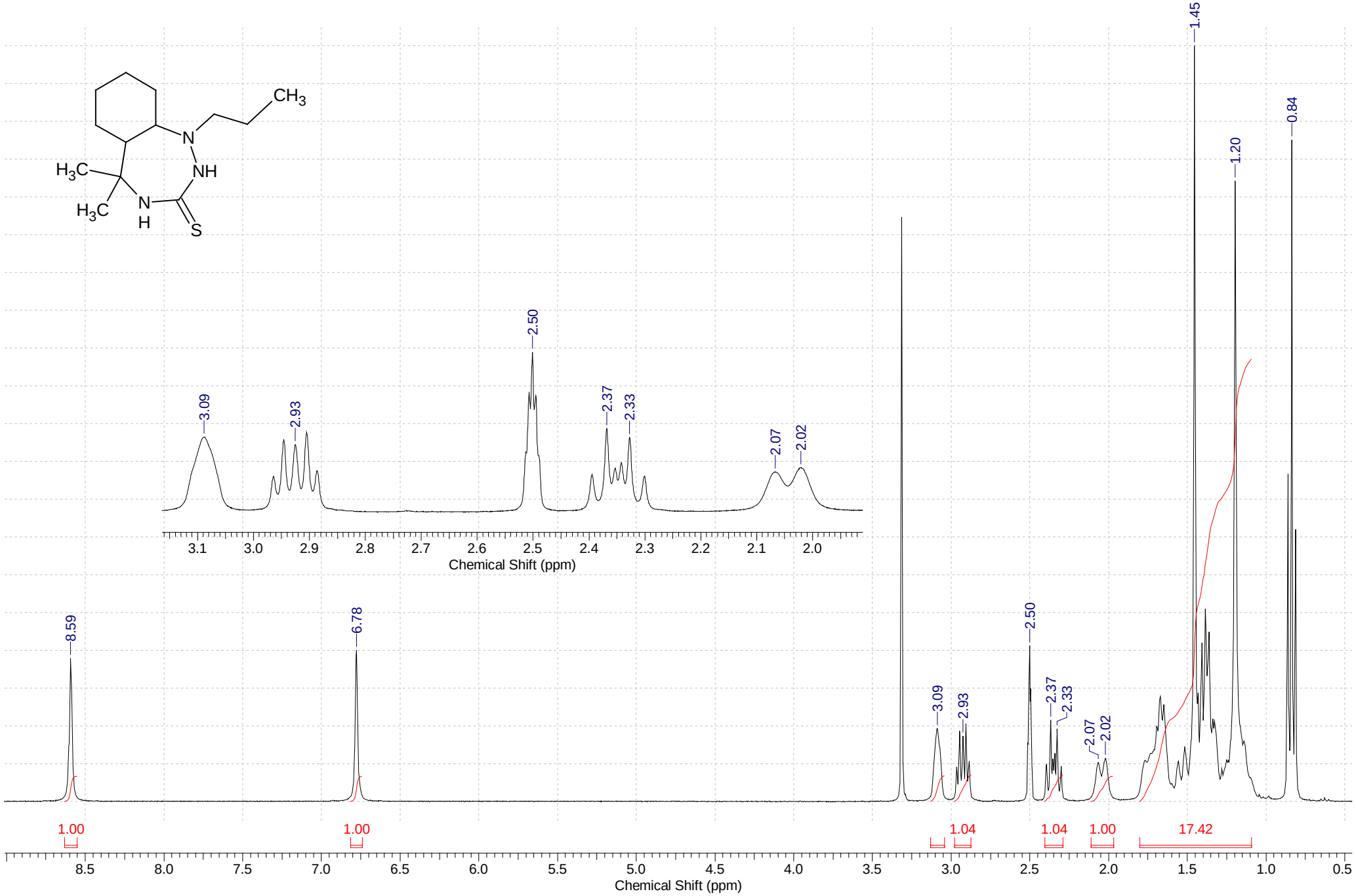


^{1}H NMR spectrum of compound **7m** (DMSO-d_6)



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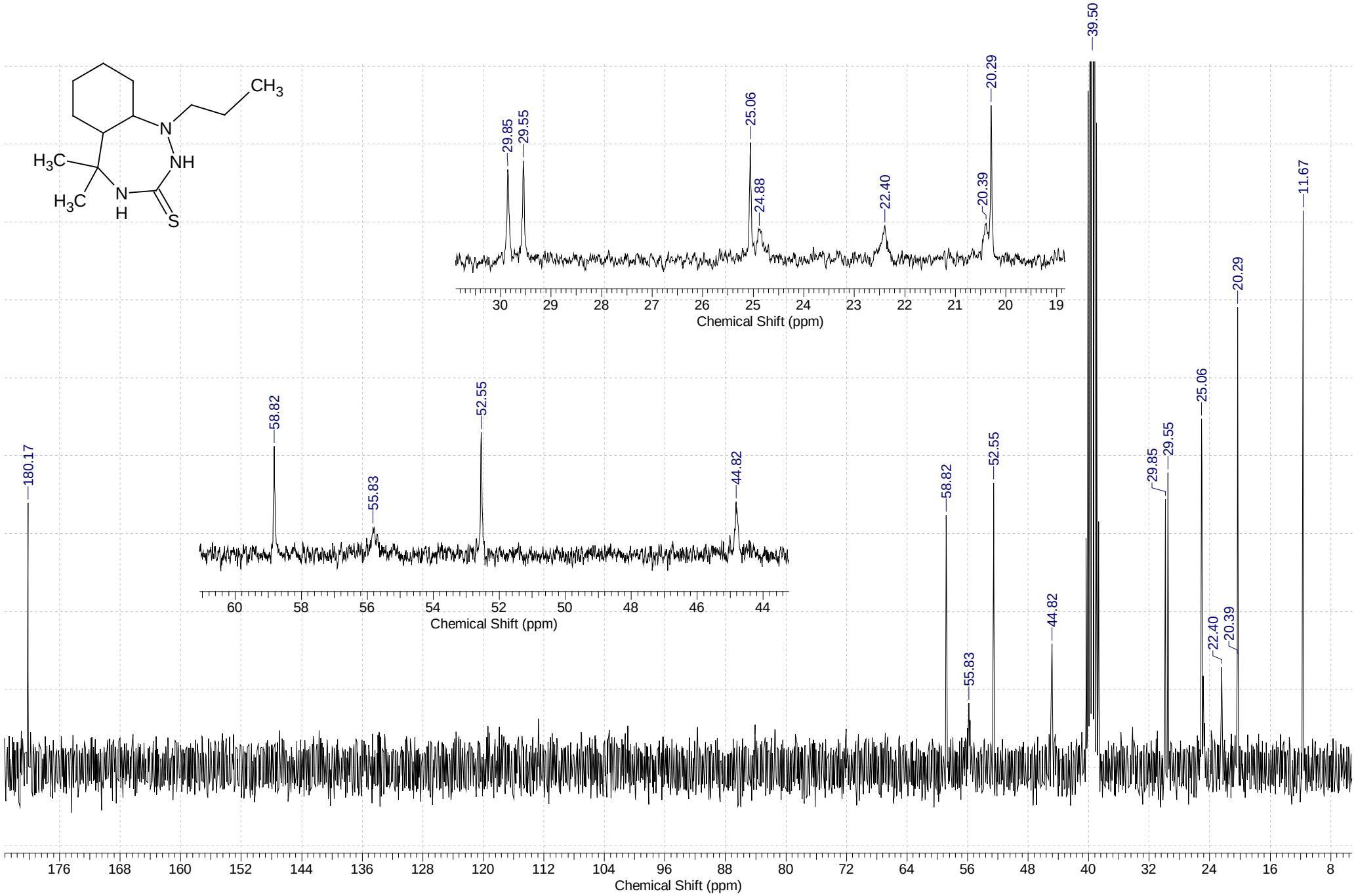

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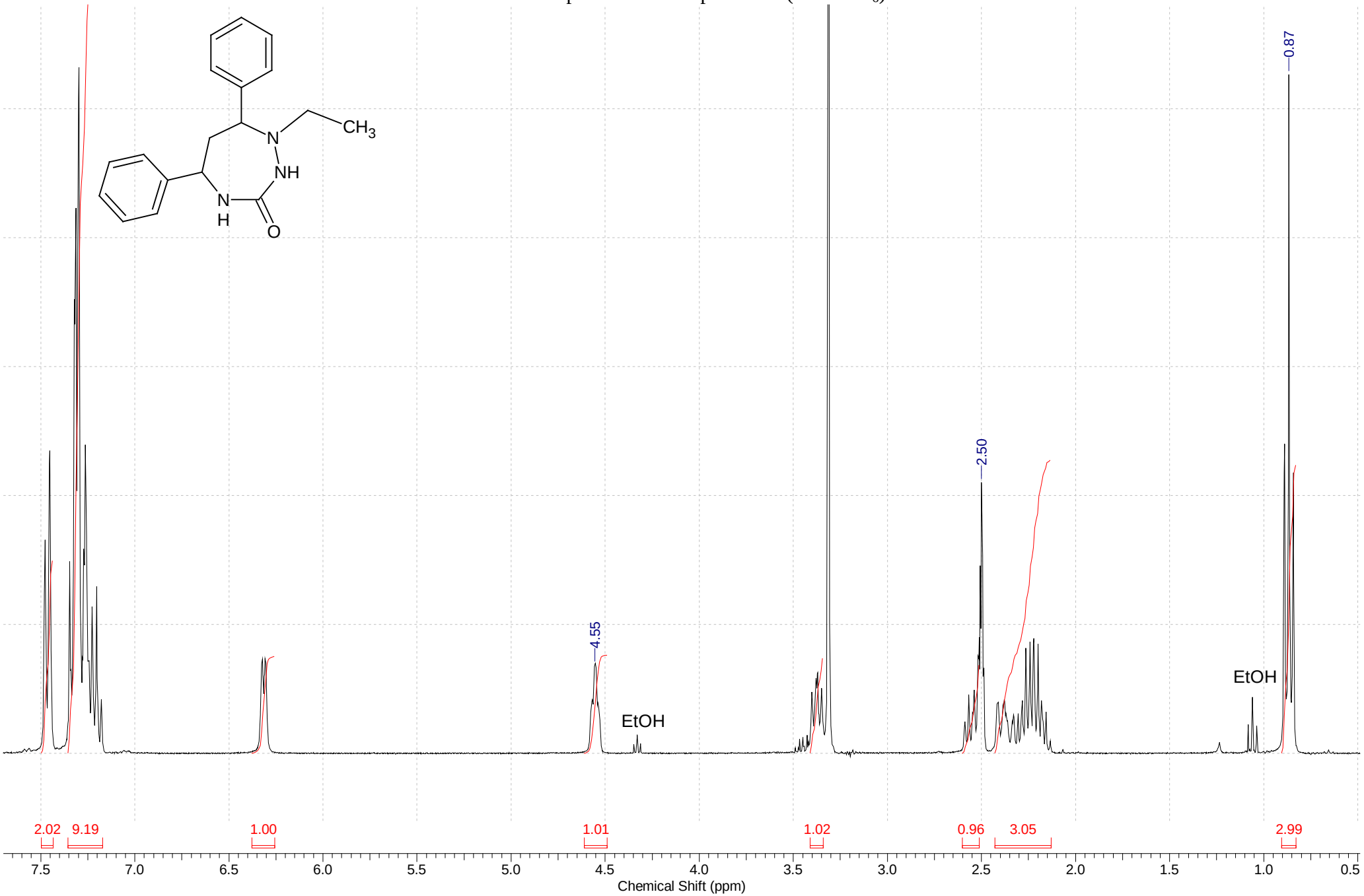

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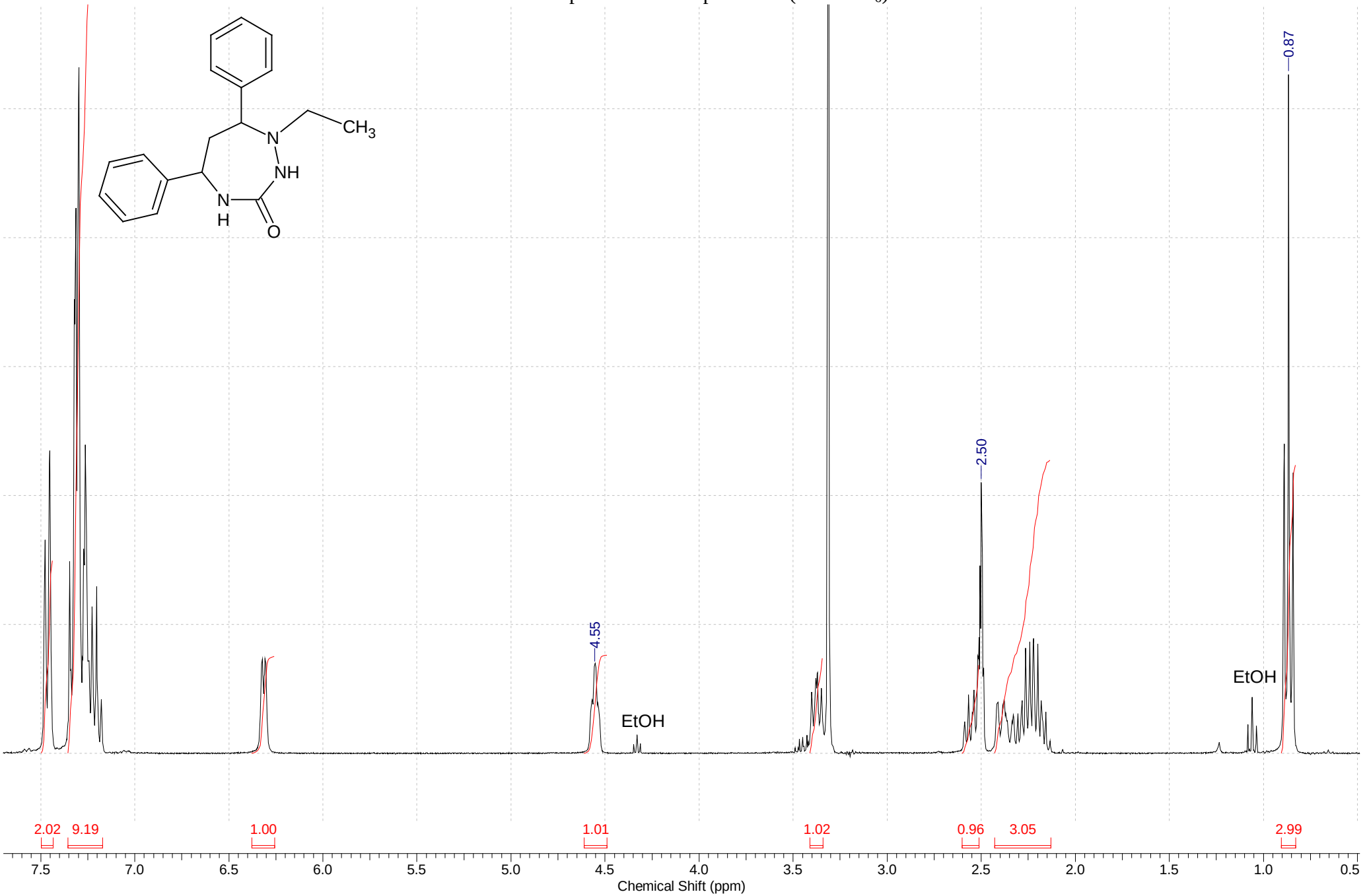
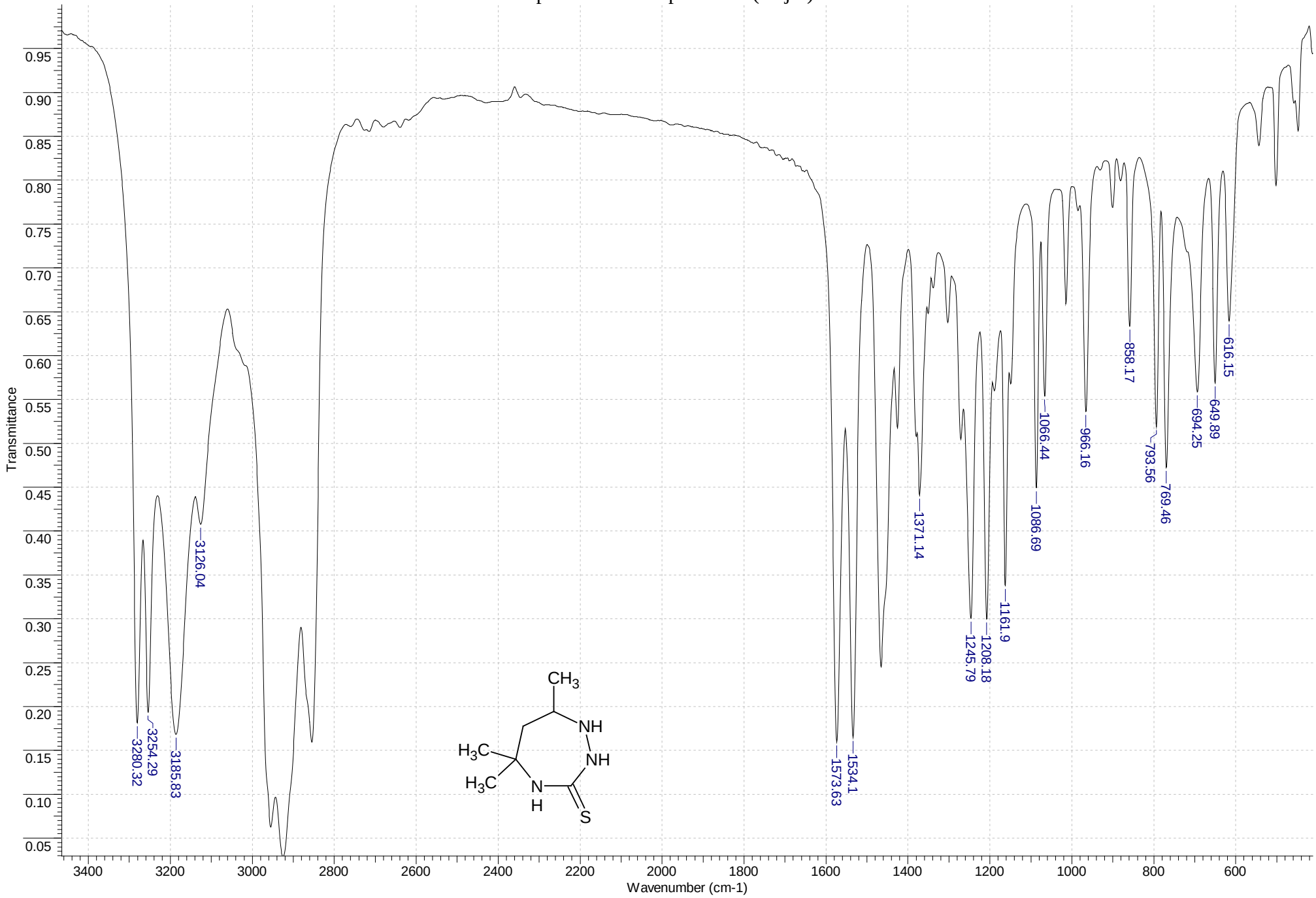
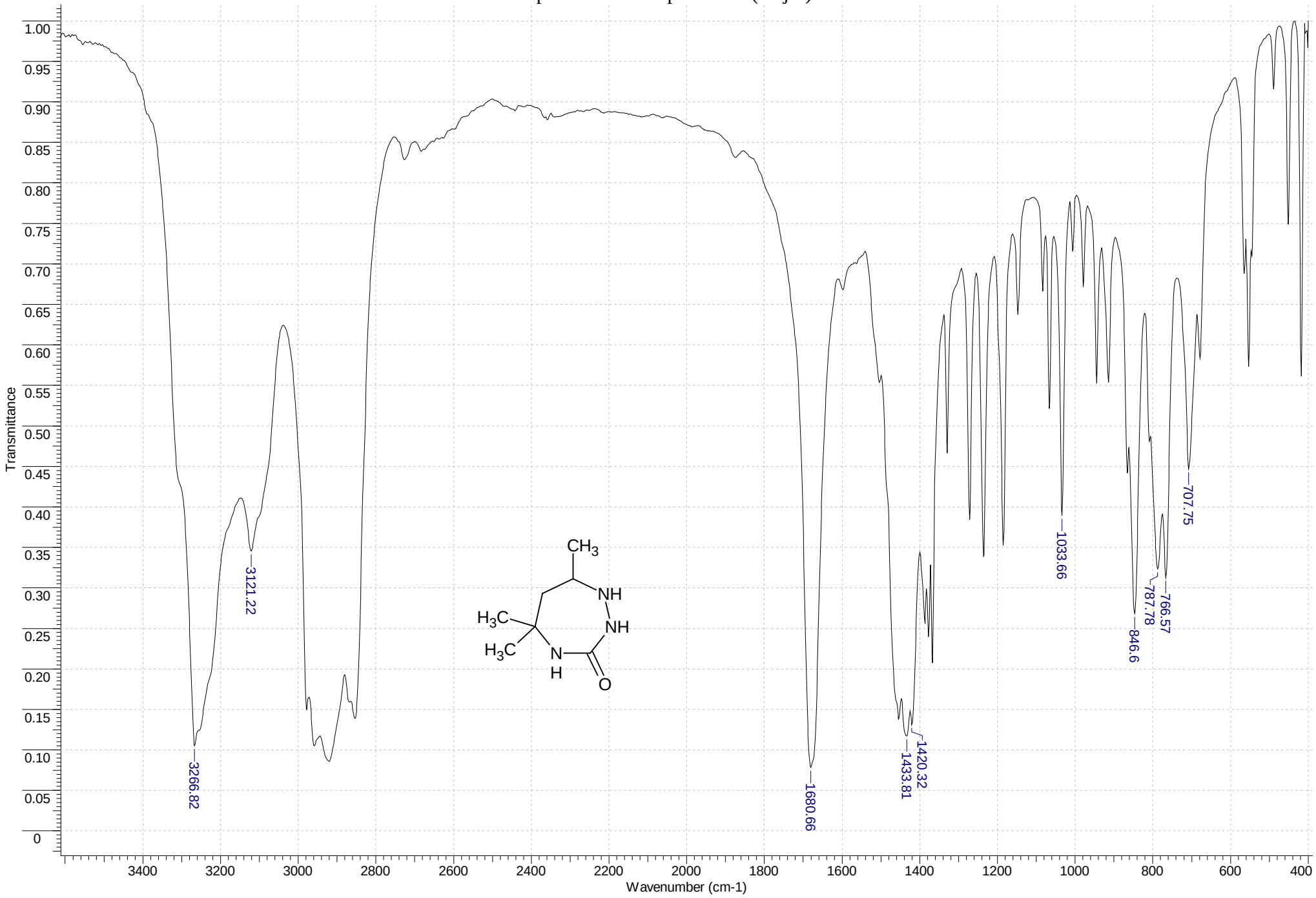


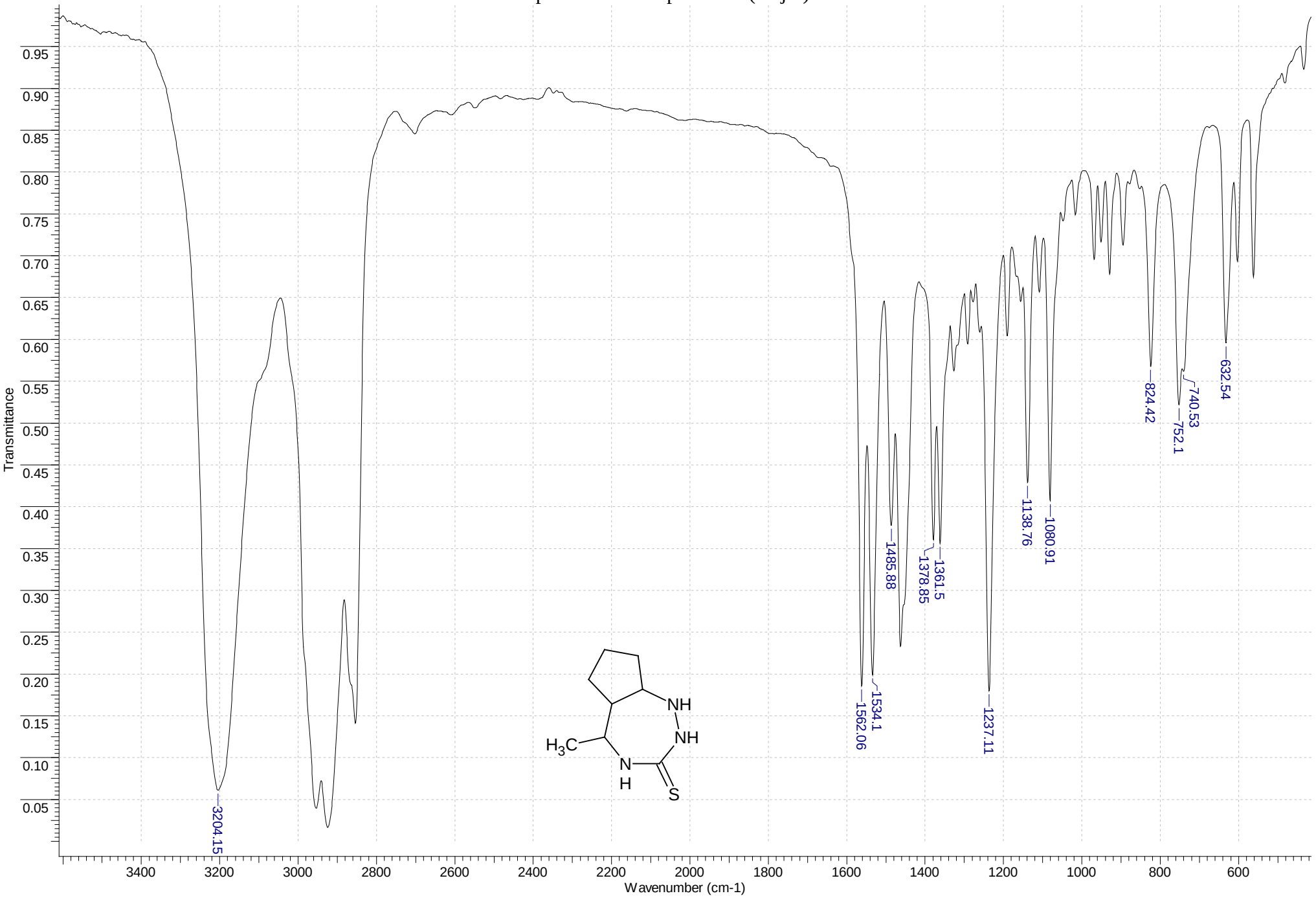
IR spectrum of compound **4a** (Nujol)



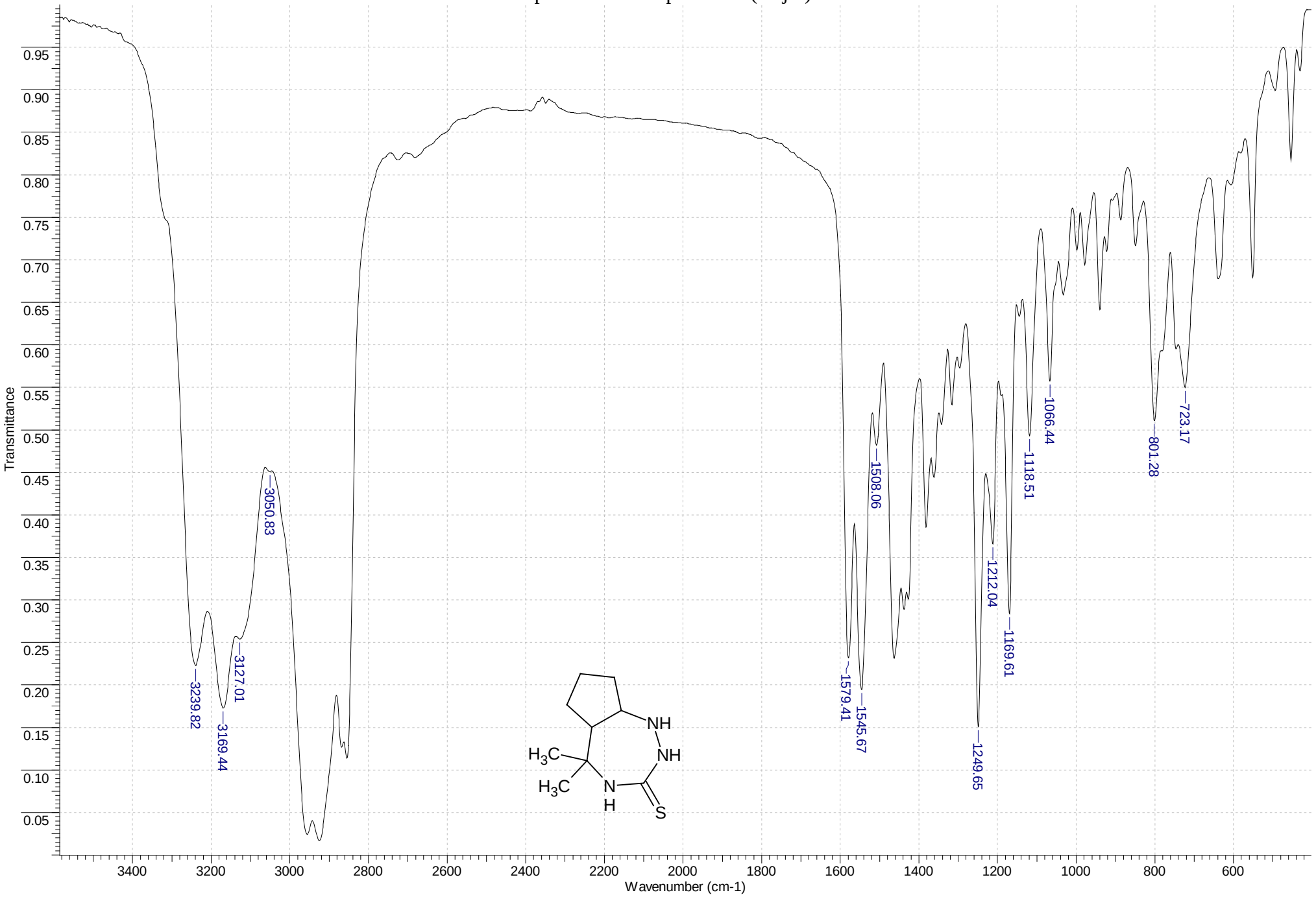
IR spectrum of compound **4b** (Nujol)



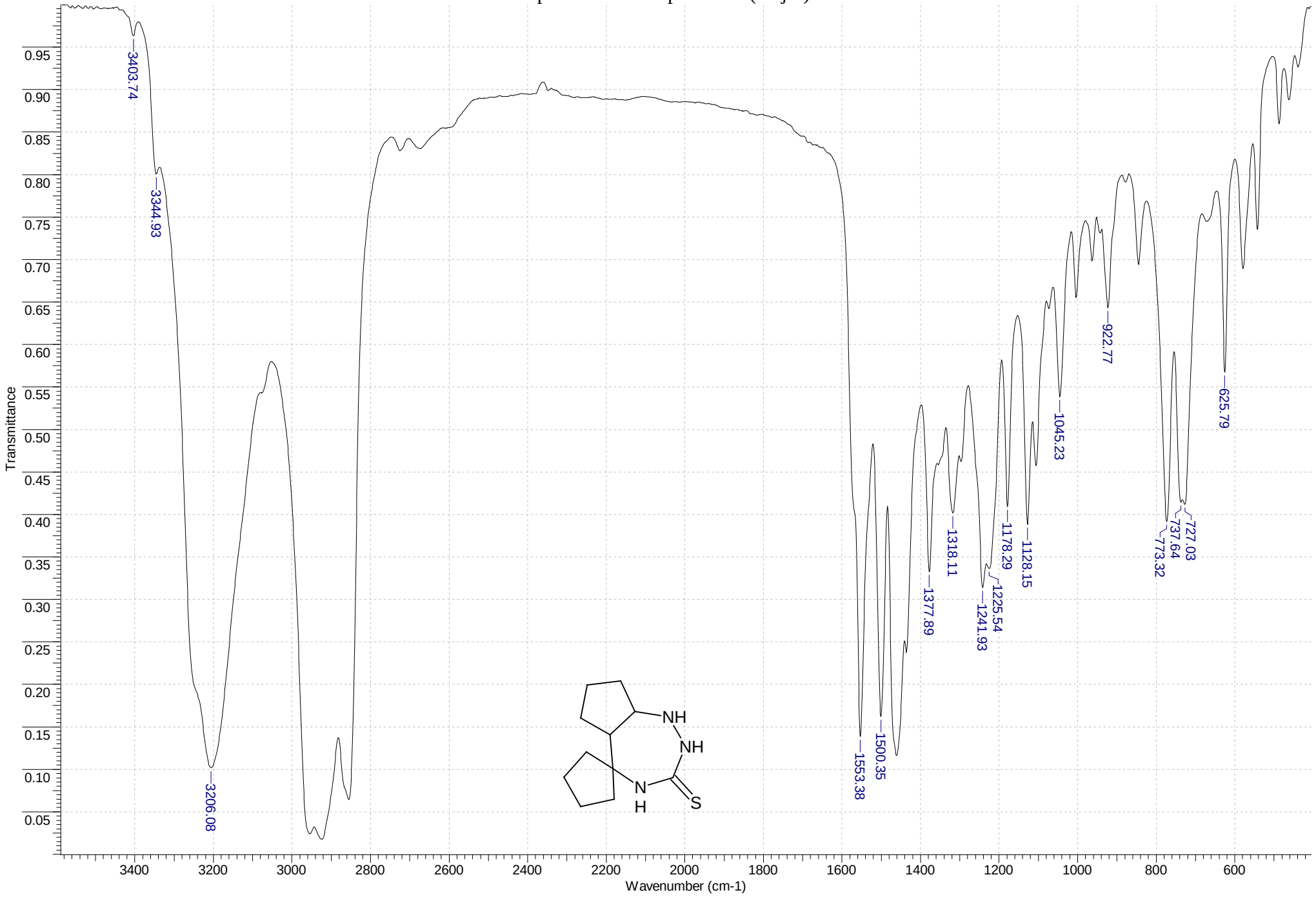
IR spectrum of compound **4c** (Nujol)



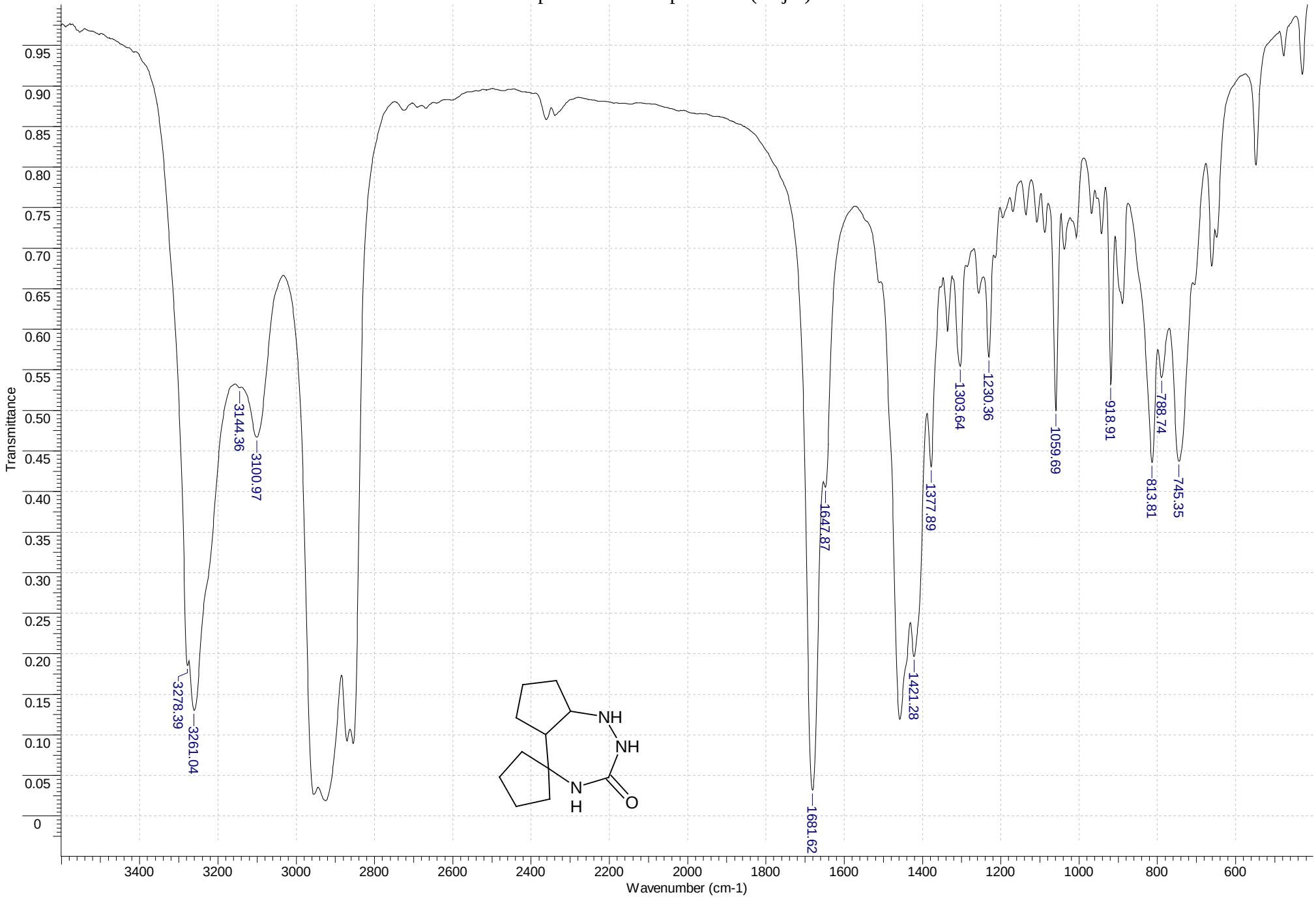
IR spectrum of compound **4d** (Nujol)



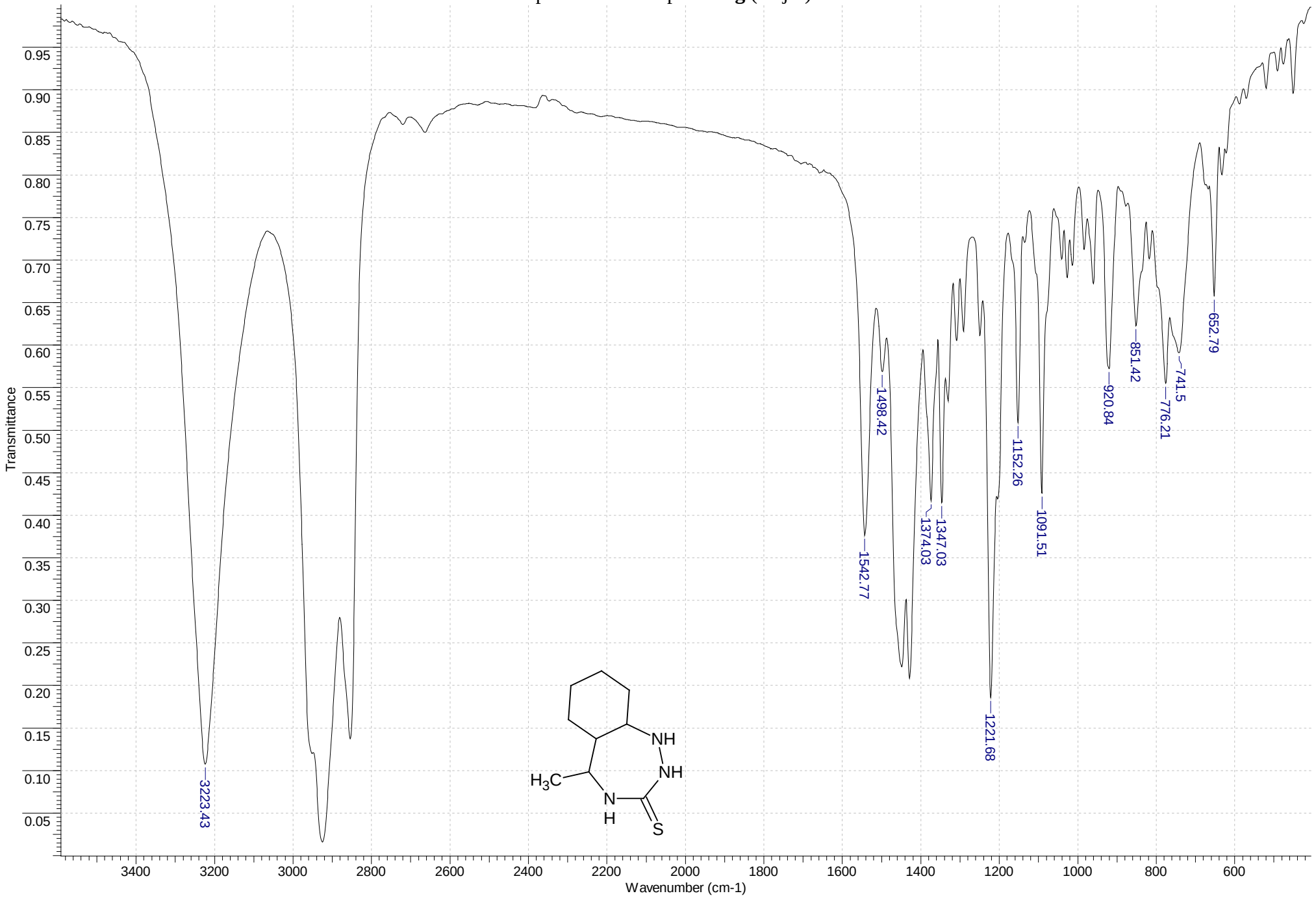
IR spectrum of compound **4e** (Nujol)



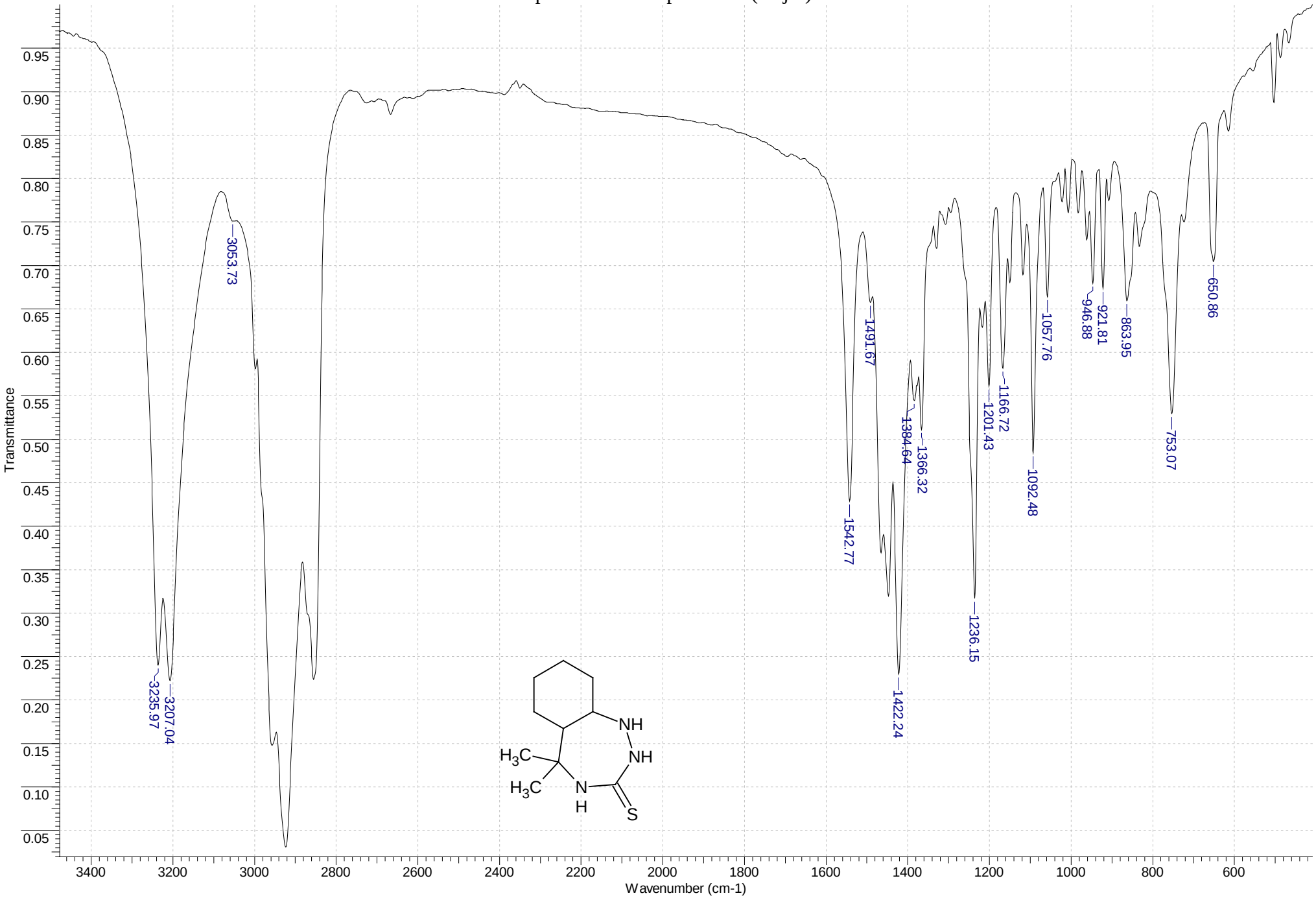
IR spectrum of compound **4f** (Nujol)



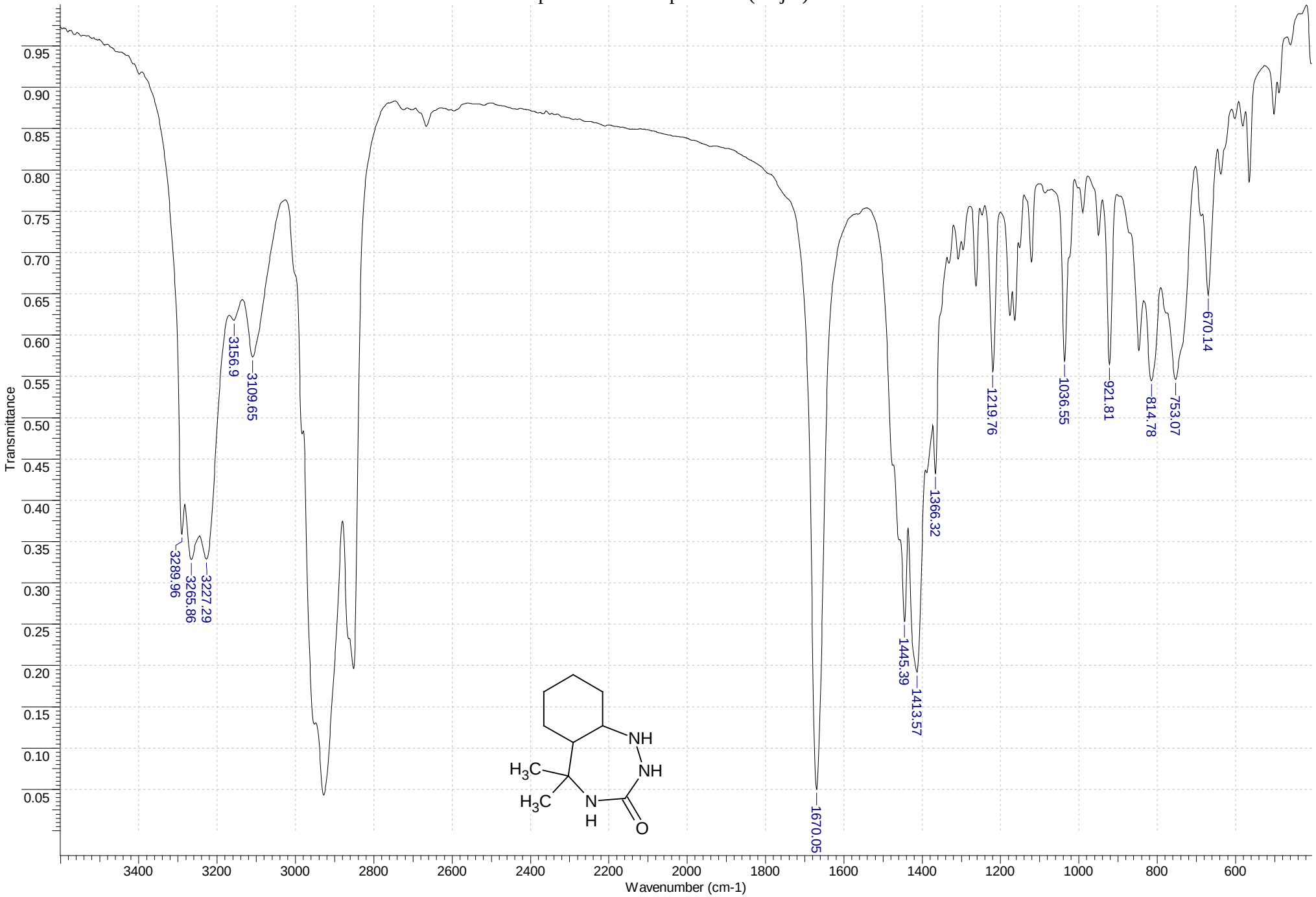
IR spectrum of compound **4g** (Nujol)



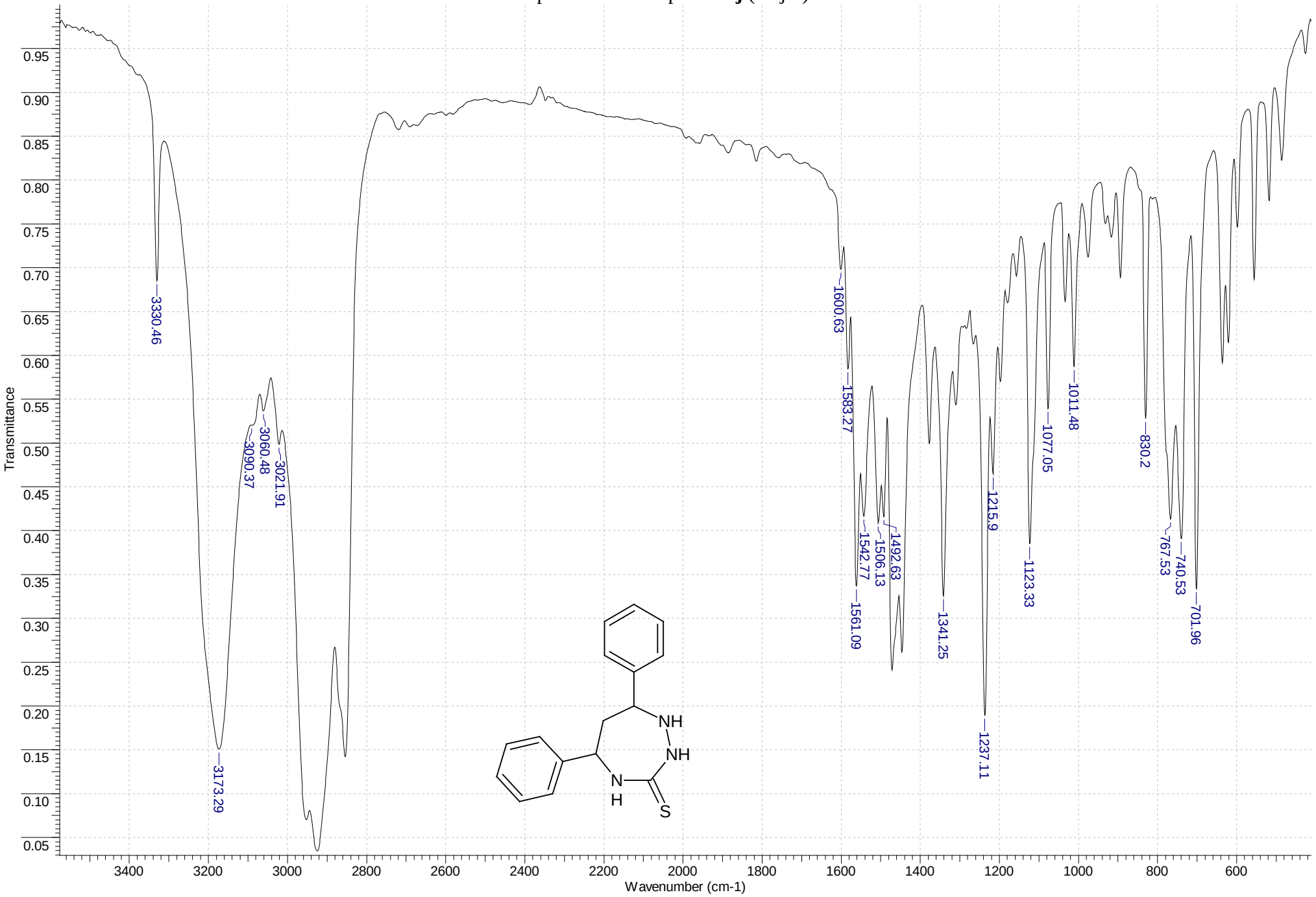
IR spectrum of compound **4h** (Nujol)



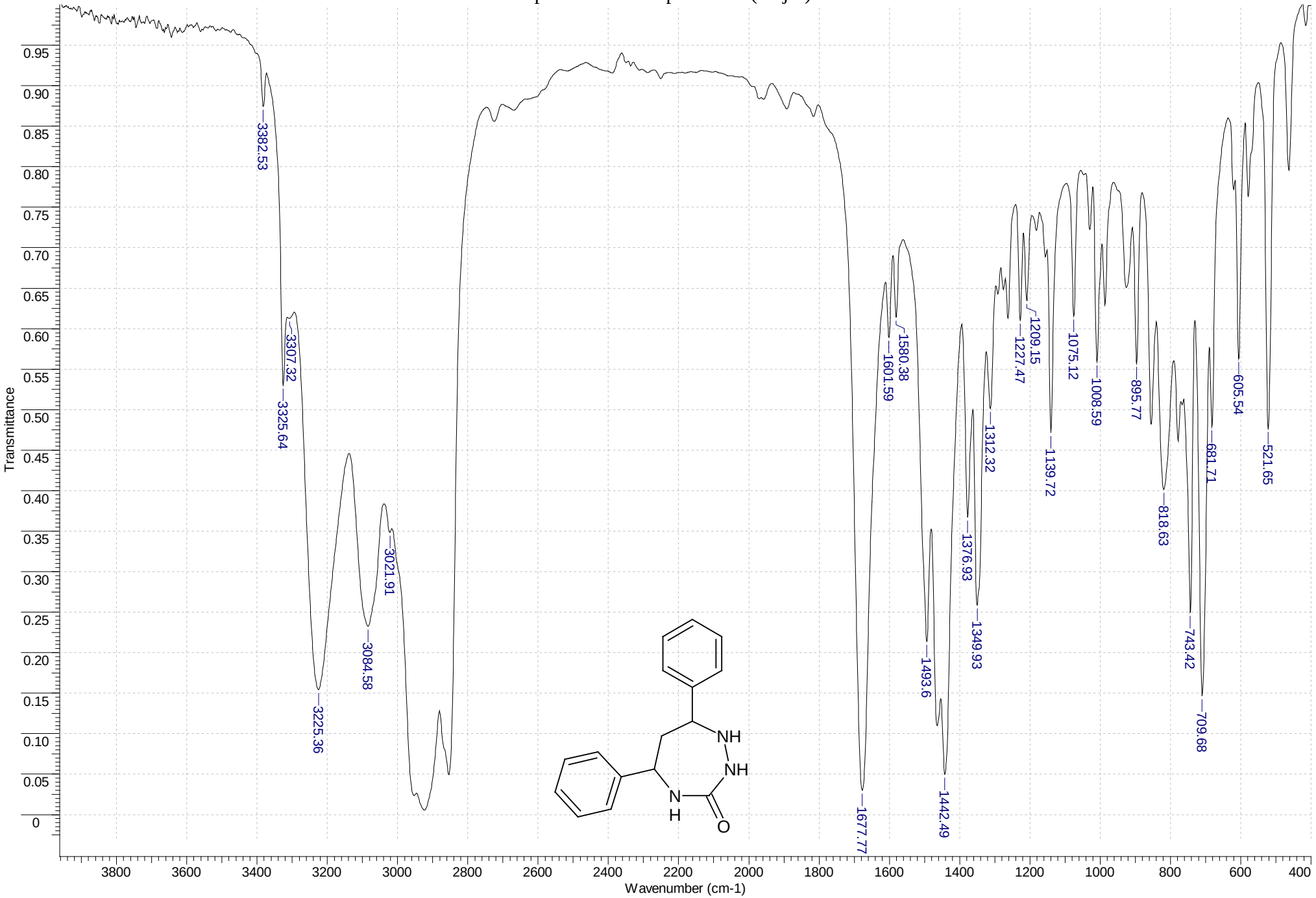
IR spectrum of compound **4i** (Nujol)



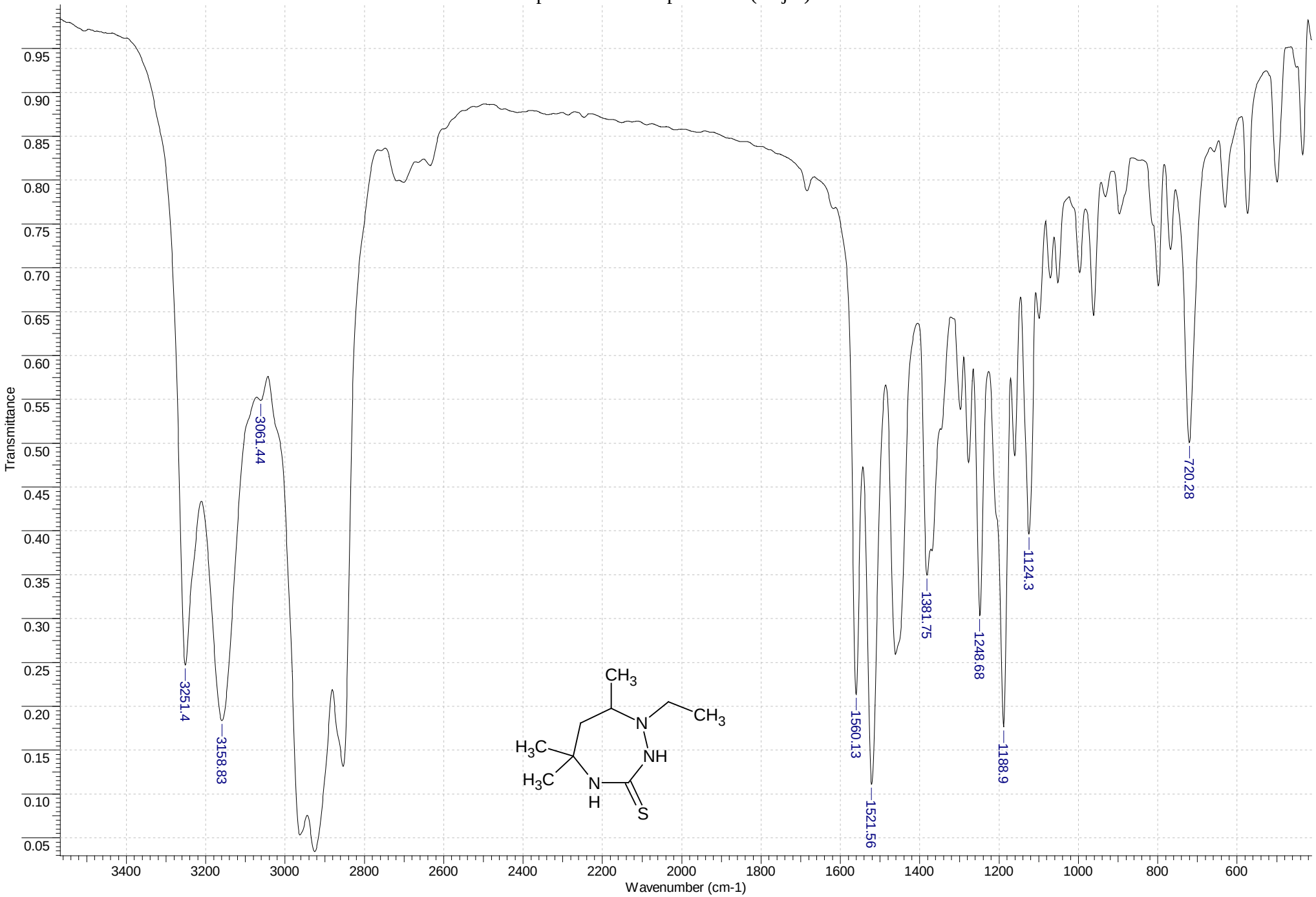
IR spectrum of compound **4j** (Nujol)



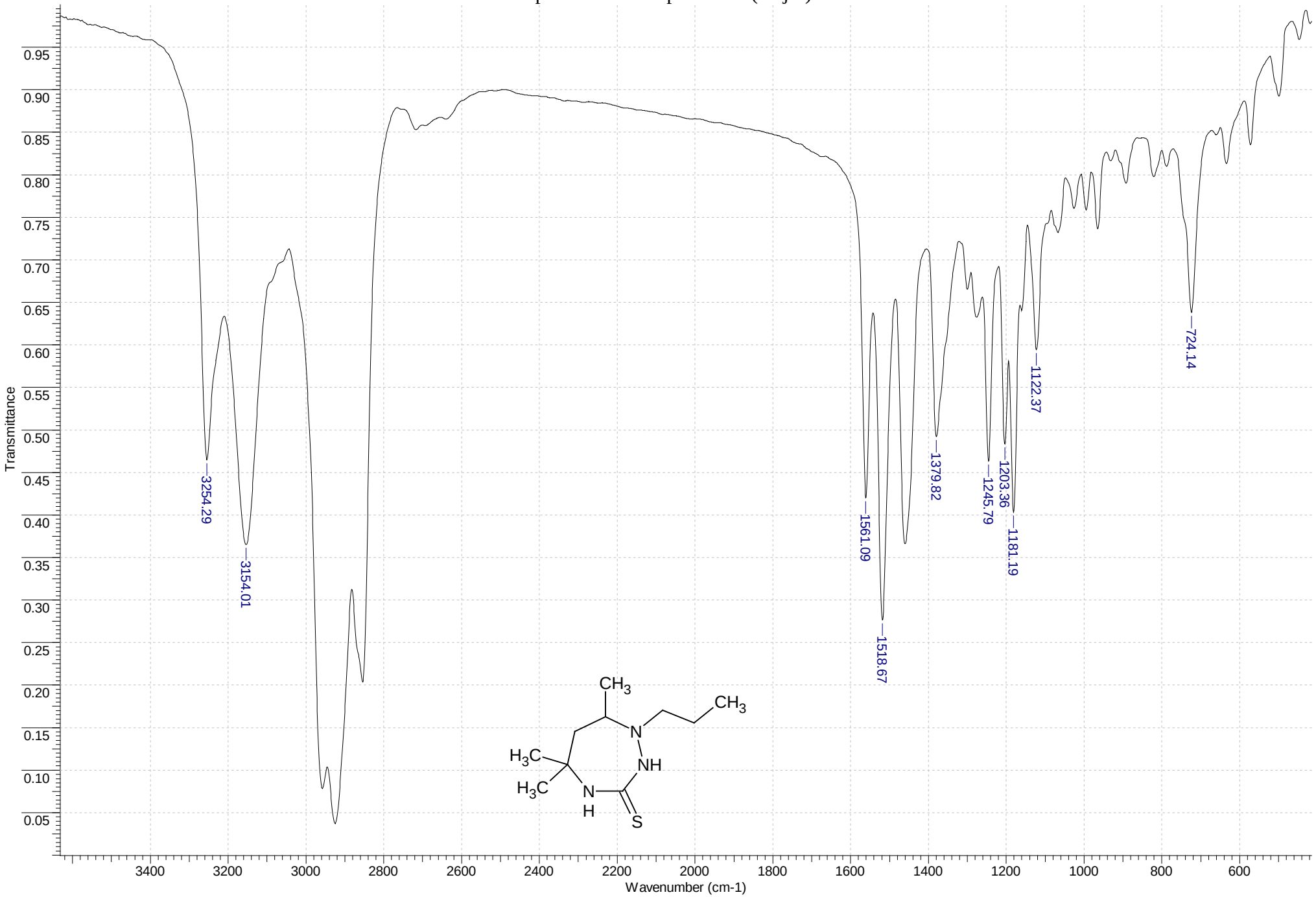
IR spectrum of compound **4k** (Nujol)



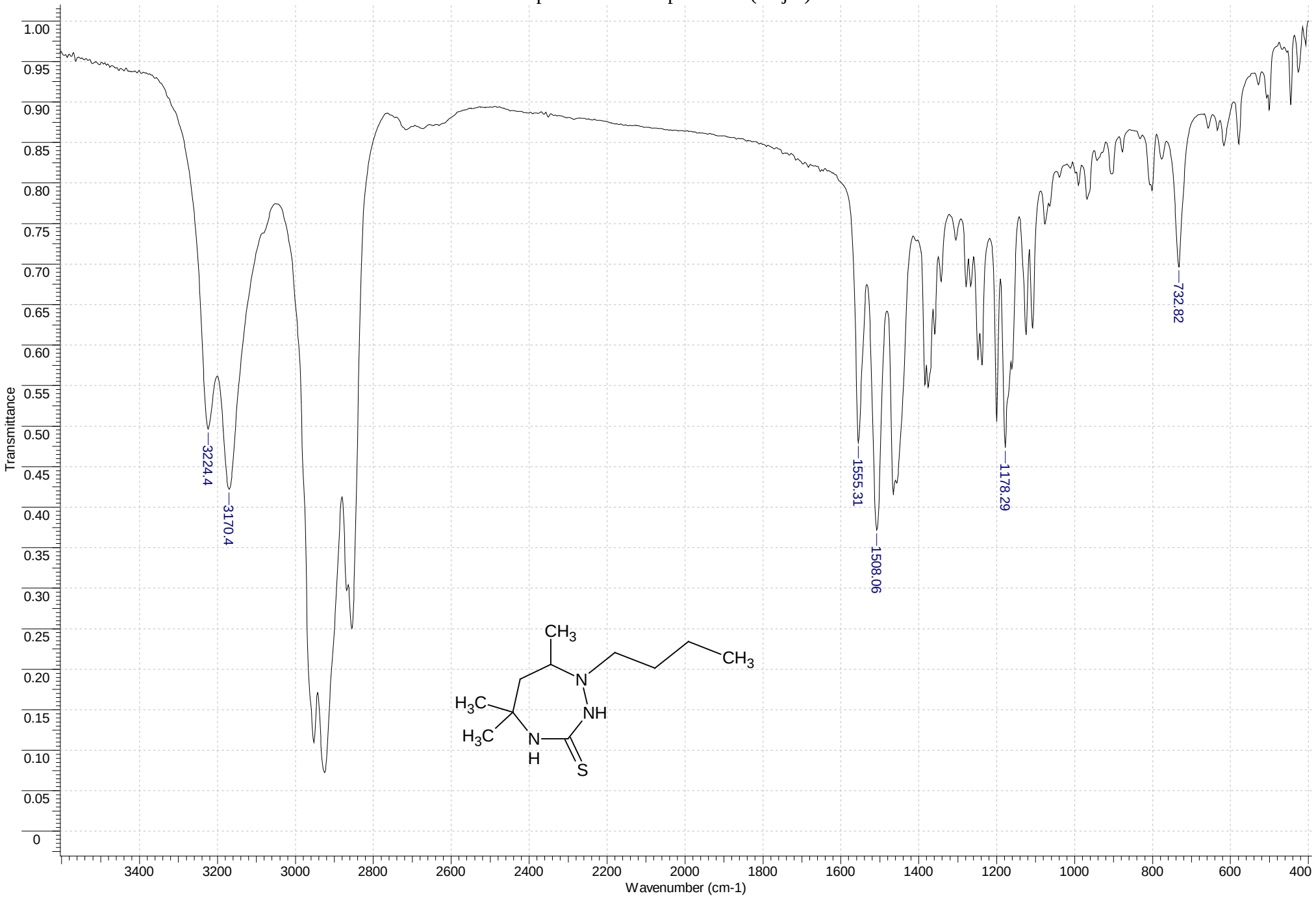
IR spectrum of compound **7a** (Nujol)



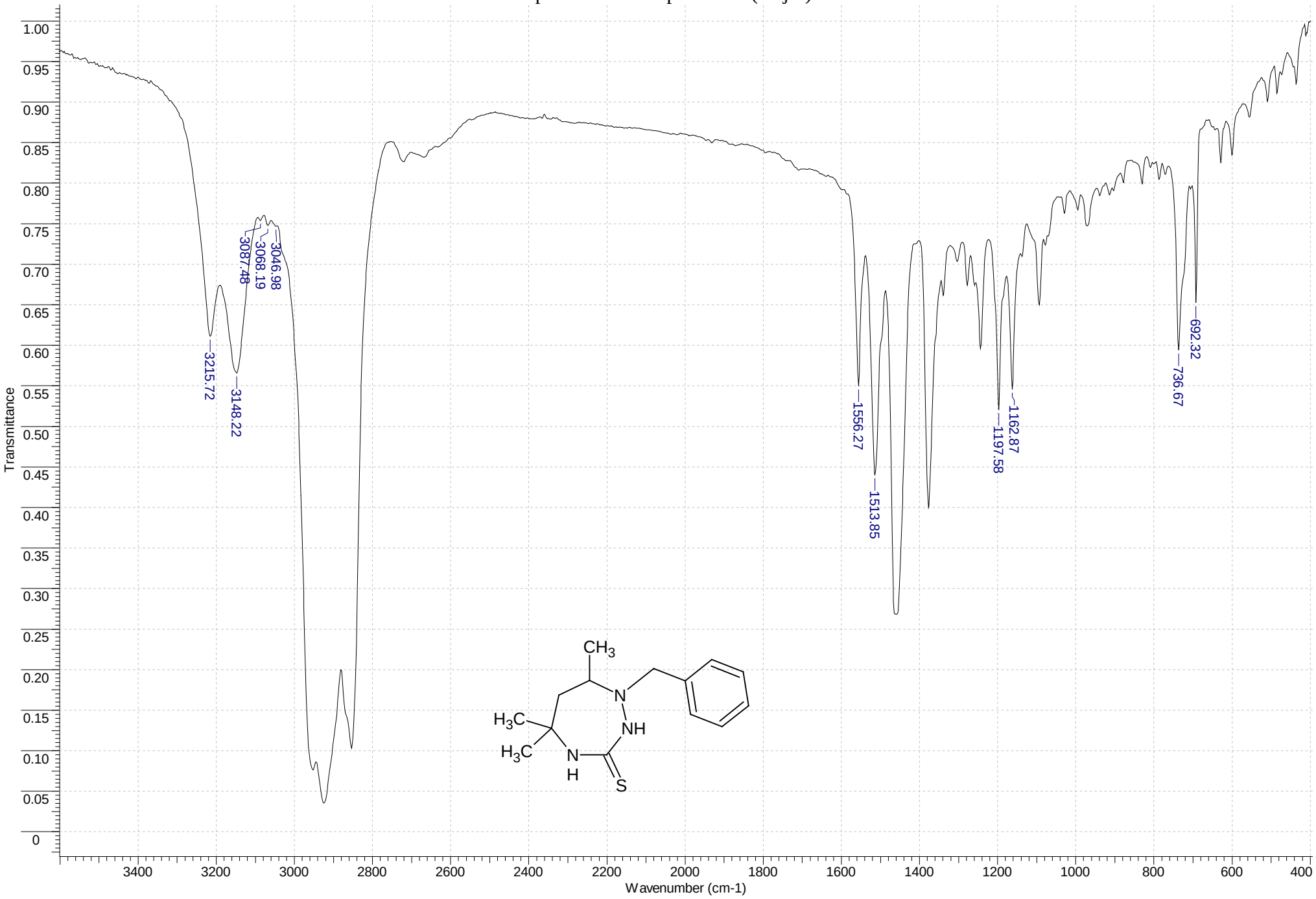
IR spectrum of compound **7b** (Nujol)



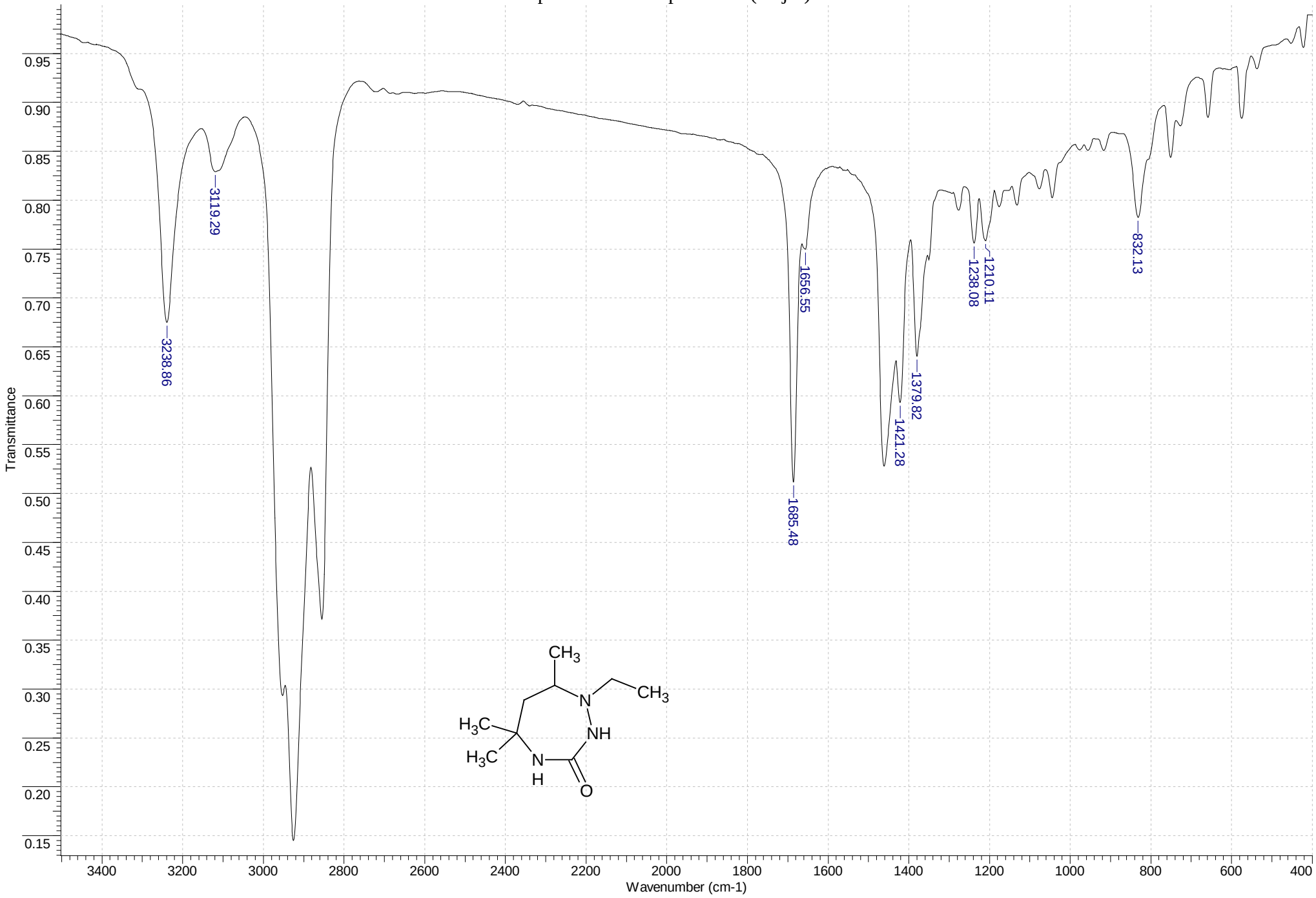
IR spectrum of compound **7c** (Nujol)



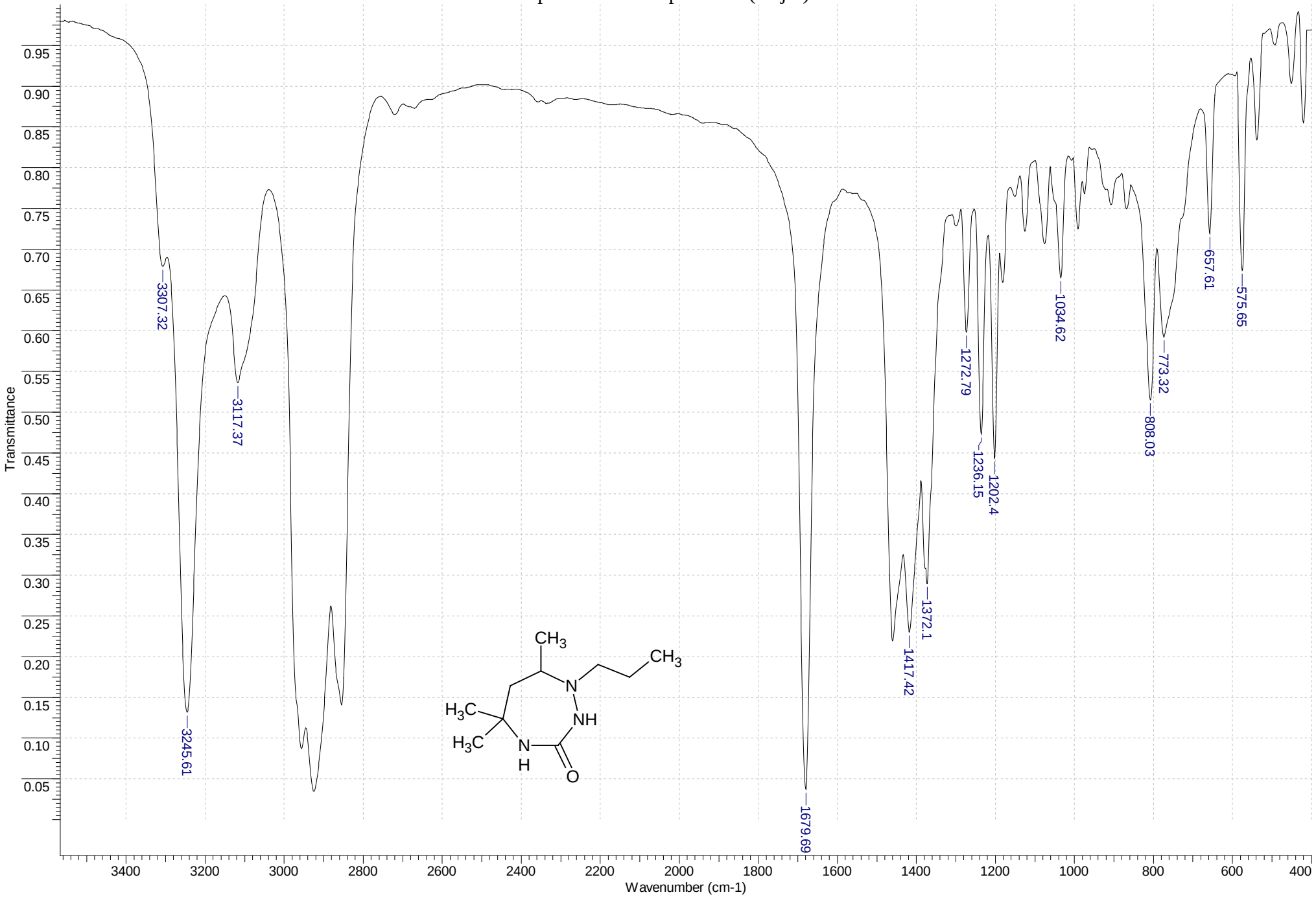
IR spectrum of compound **7d** (Nujol)



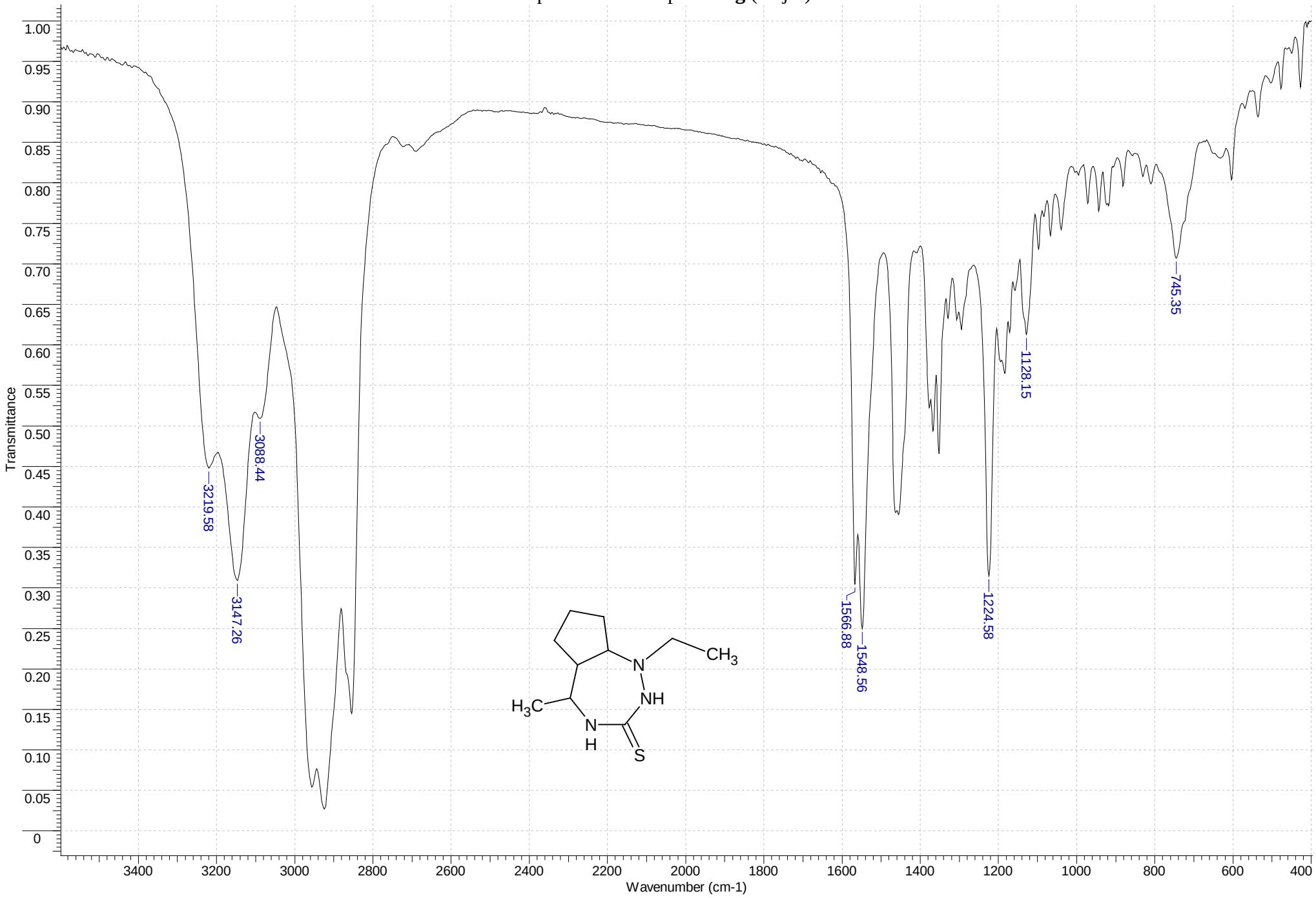
IR spectrum of compound **7e** (Nujol)



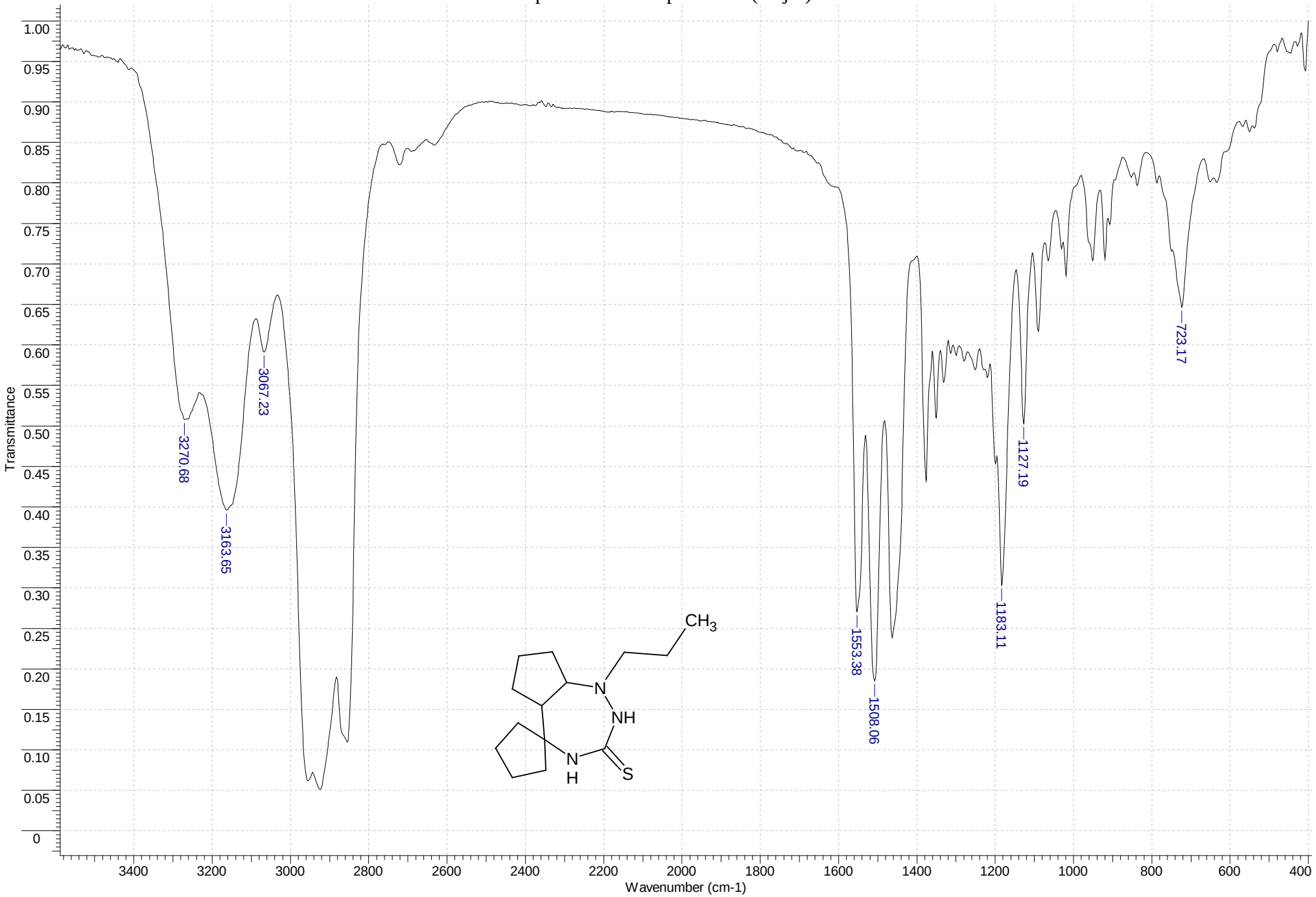
IR spectrum of compound **7f** (Nujol)



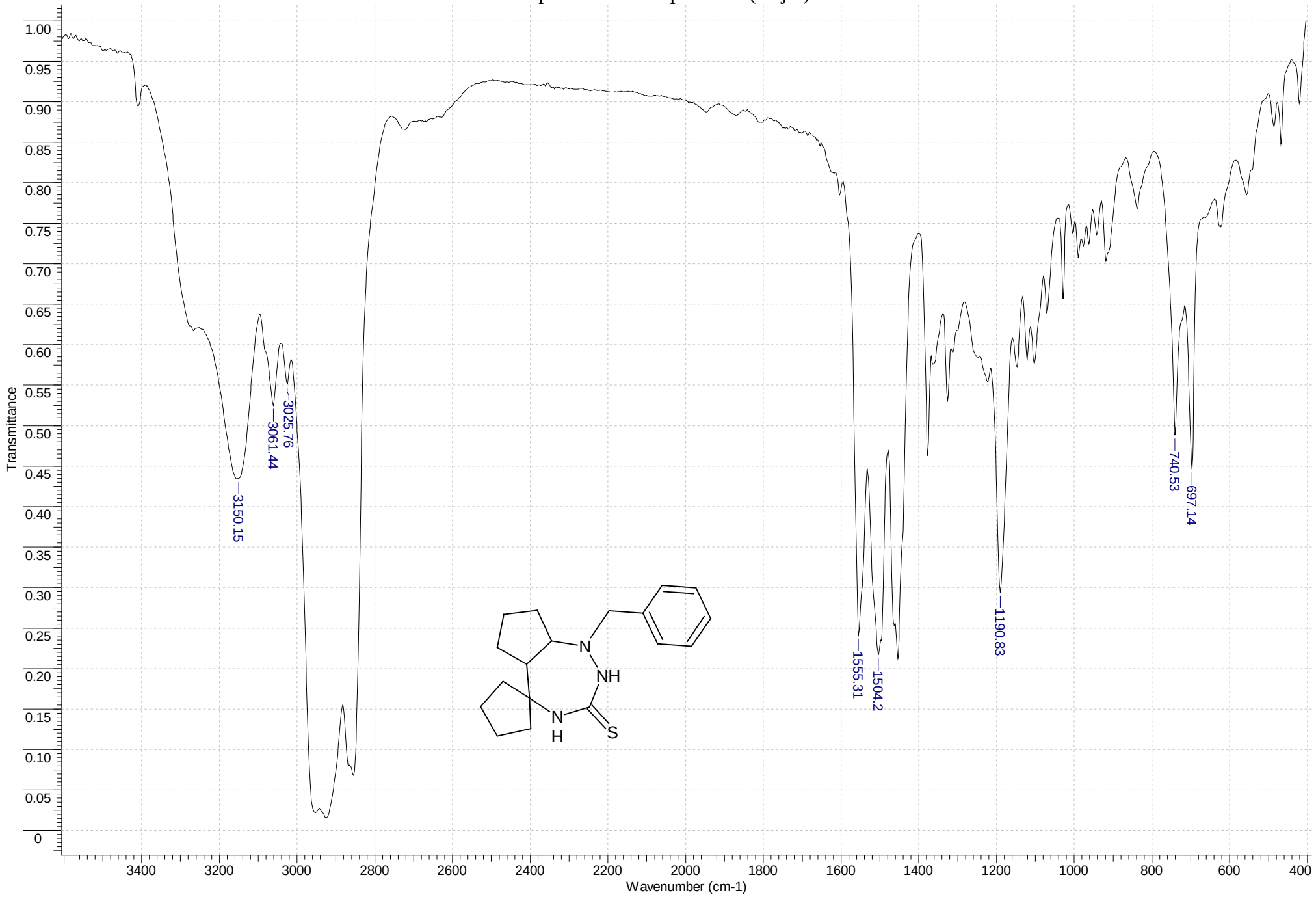
IR spectrum of compound **7g** (Nujol)



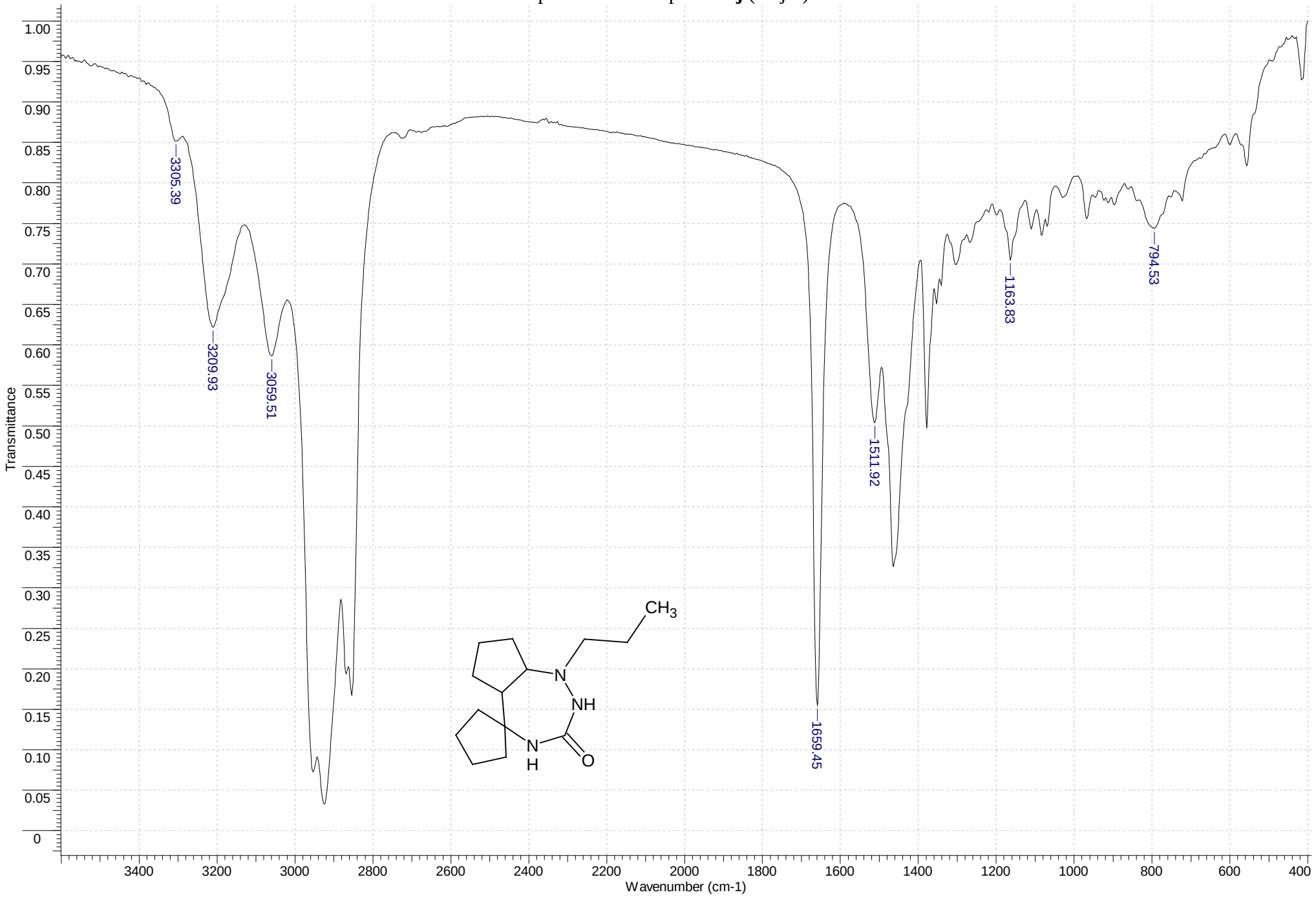
IR spectrum of compound **7h** (Nujol)



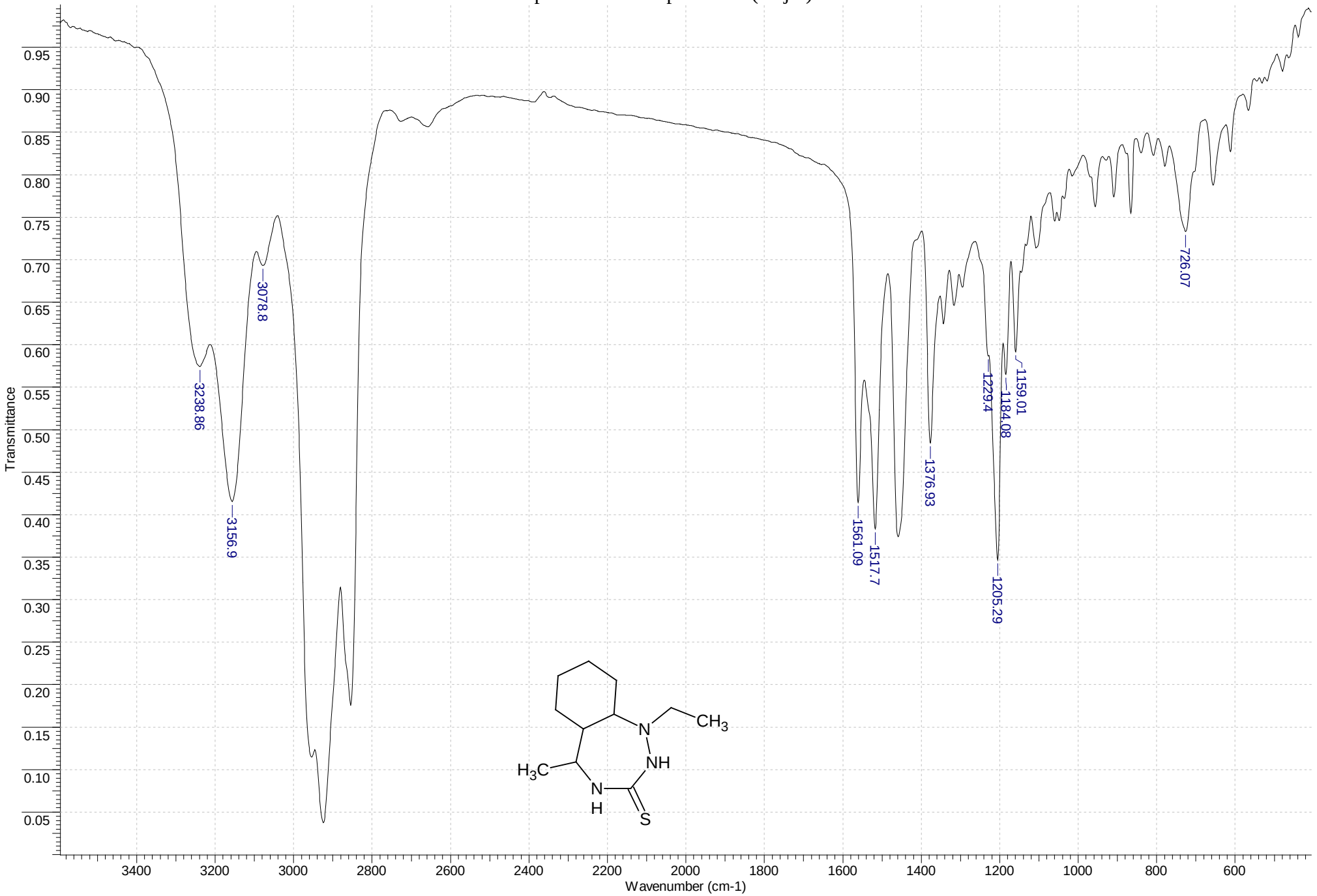
IR spectrum of compound **7i** (Nujol)



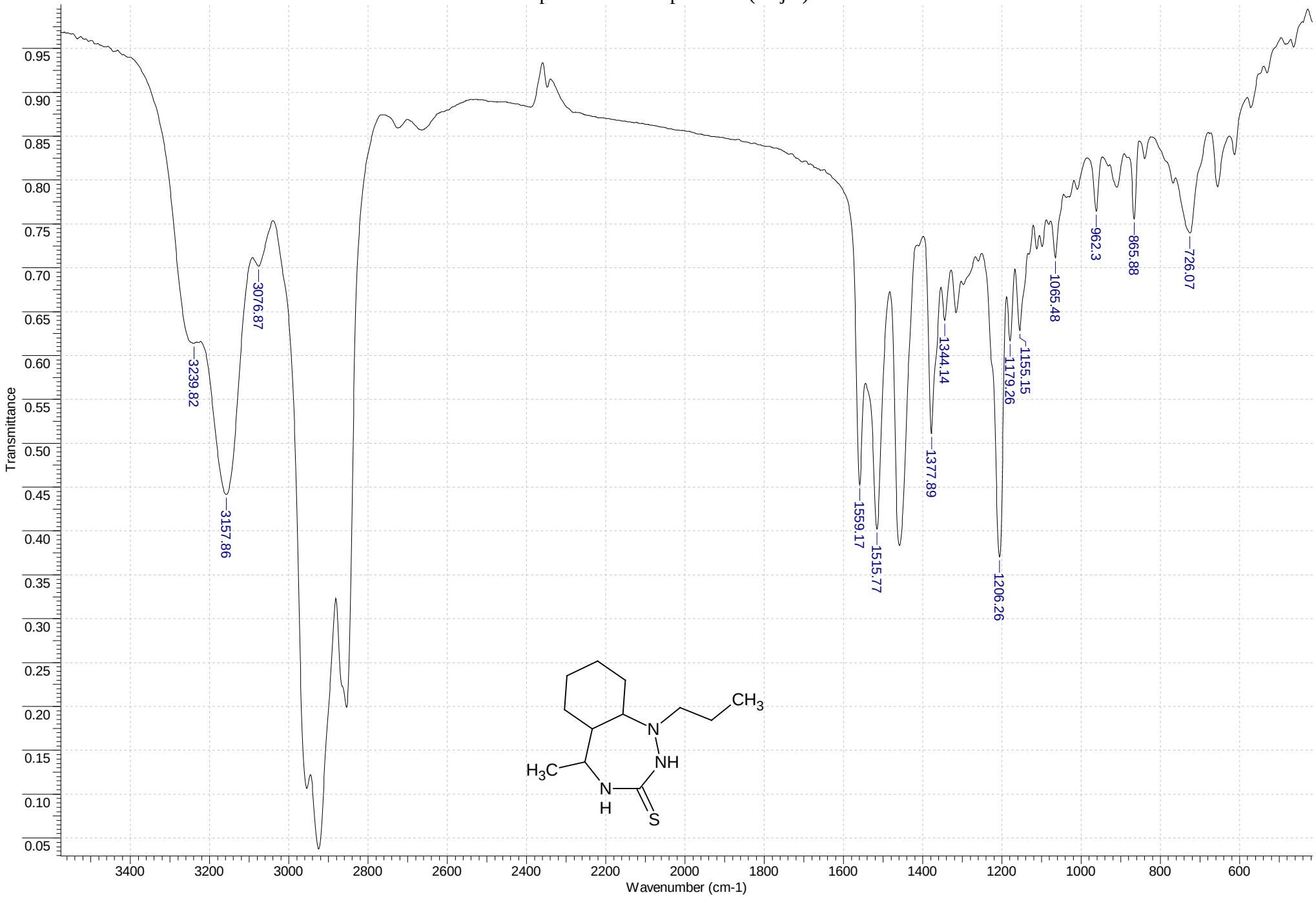
IR spectrum of compound **7j** (Nujol)



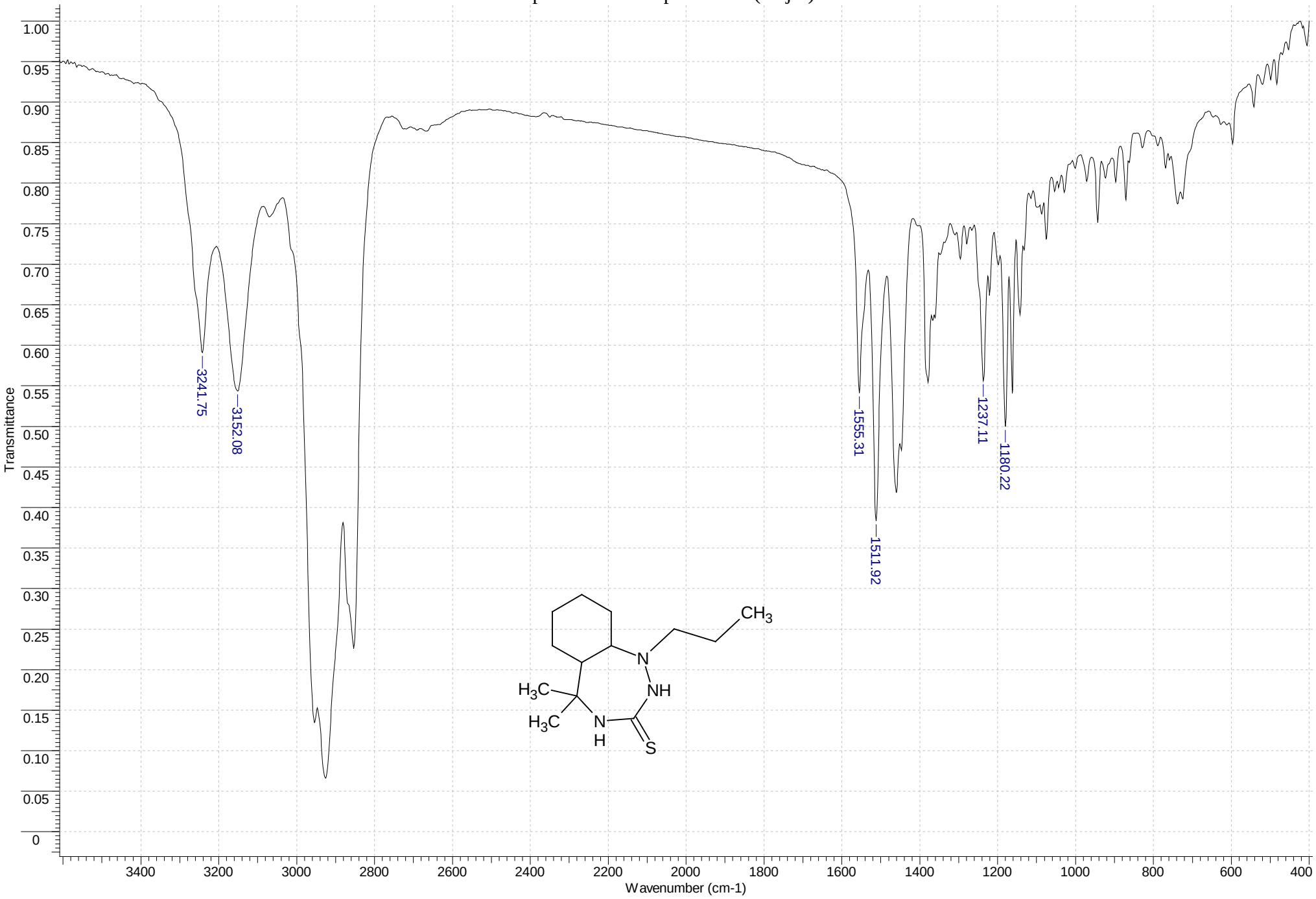
IR spectrum of compound **7k** (Nujol)



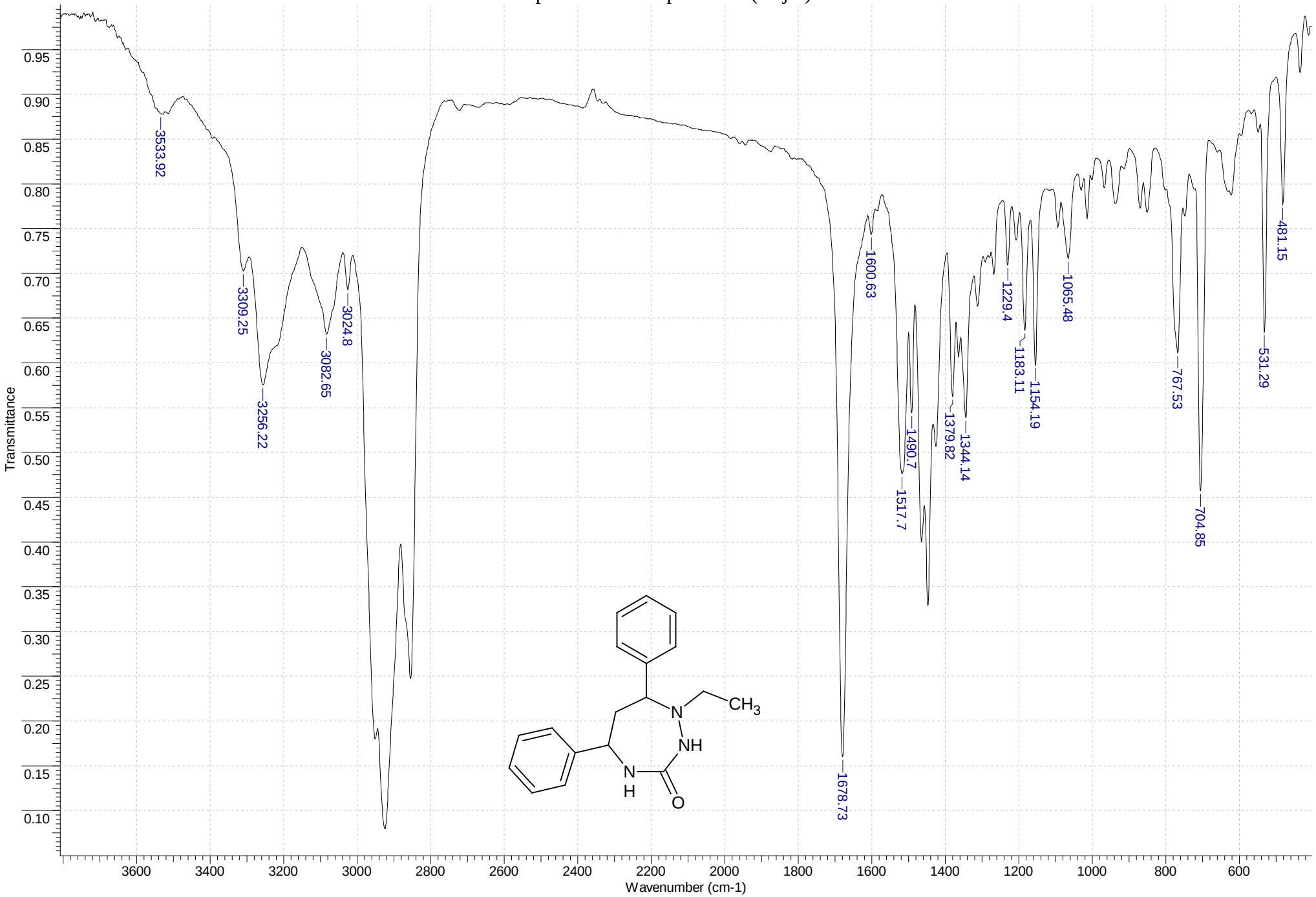
IR spectrum of compound **7l** (Nujol)



IR spectrum of compound **7m** (Nujol)

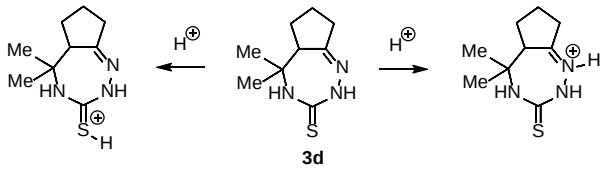


IR spectrum of compound **7n** (Nujol)

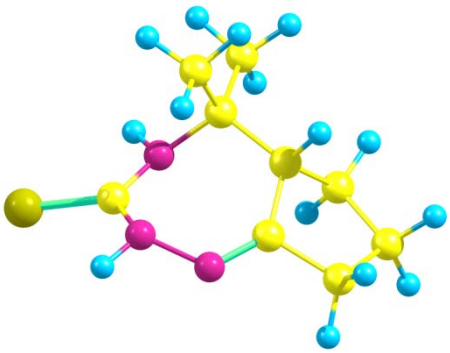


Computational details

The geometry optimizations of all key stationary points were carried out at the B3LYP level of theory using Gaussian 09 suite[1] of quantum chemical programs. Pople's basis sets, 6-311++G(d,p), was employed for geometry optimization. The effect of continuum solvation was incorporated by using the polarizable continuum model (PCM). Enthalpies and Gibbs free energies were obtained by adding unscaled zero-point vibrational energy corrections (ZPVE) and thermal contributions to the energies. All transition states were fully optimized and characterized as a first-order saddle point by harmonic vibrational frequency analysis. One and only one imaginary frequency of the first-order saddle point was subjected to visual inspection to examine whether it represented the desired reaction coordinate. Furthermore, the intrinsic reaction coordinate (IRC) analysis was performed to authenticate that the transition state pertains to the desired reaction coordinate. The IRC calculations were done at the B3LYP/6-311++G(d,p) level of theory.



Data 1: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of 2,4,5,6-tetrahydro-3*H*-1,2,4-triazepine-3-thione **3d** with pseudo axial orientation of the C6-CH_2 bond (MeOH solution)

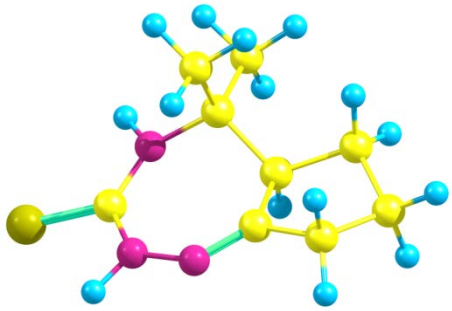


Electronic Energy =	-914.591467195 a.u.
Zero-point correction=	0.239091 (Hartree/Particle)
Thermal correction to Energy=	0.251515
Thermal correction to Enthalpy=	0.252459
Thermal correction to Gibbs Free Energy=	0.200604
Sum of electronic and zero-point Energies=	-914.352376
Sum of electronic and thermal Energies=	-914.339953
Sum of electronic and thermal Enthalpies=	-914.339008
Sum of electronic and thermal Free Energies=	-914.390863

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.047092	1.318934	0.267410
2	6	0	1.321742	0.458643	0.260891
3	6	0	1.161062	-1.043362	0.392003
4	7	0	0.157642	-1.817801	0.538804
5	6	0	0.297727	2.689476	-0.376923
6	7	0	-1.020859	0.666223	-0.546684
7	6	0	-1.754925	-0.398346	-0.160858
8	16	0	-3.382911	-0.589235	-0.618428
9	7	0	-1.159840	-1.351789	0.616730
10	1	0	-1.546451	1.298270	-1.135527
11	1	0	-1.779572	-2.121747	0.824365
12	6	0	2.286833	0.531878	-0.945330
13	6	0	2.527368	-1.664107	0.156013
14	6	0	3.309964	-0.589039	-0.647620
15	1	0	1.913172	0.761349	1.137766
16	1	0	0.549424	2.597236	-1.435215
17	1	0	1.120183	3.197278	0.129720
18	1	0	-0.592270	3.317809	-0.285318
19	1	0	2.760503	1.508803	-1.043923
20	1	0	1.740262	0.324663	-1.870866
21	1	0	3.010515	-1.883766	1.112998
22	1	0	2.422676	-2.608312	-0.378872
23	1	0	4.131080	-0.189528	-0.048249
24	1	0	3.744132	-0.997579	-1.561109
25	6	0	-0.445610	1.526533	1.714451
26	1	0	0.293104	2.104928	2.273674
27	1	0	-1.388265	2.078397	1.717783
28	1	0	-0.598039	0.579880	2.235441

Data 2: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of 2,4,5,6-tetrahydro-3*H*-1,2,4-triazepine-3-thione **3d** with pseudo equatorial orientation of the C6-CH_2 bond (MeOH solution)



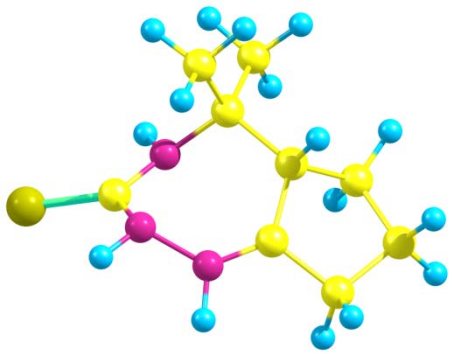
Electronic Energy =	-914.600680112 a.u.
Zero-point correction=	0.238839 (Hartree/Particle)
Thermal correction to Energy=	0.251299
Thermal correction to Enthalpy=	0.252244
Thermal correction to Gibbs Free Energy=	0.200493
Sum of electronic and zero-point Energies=	-914.361841
Sum of electronic and thermal Energies=	-914.349381
Sum of electronic and thermal Enthalpies=	-914.348437
Sum of electronic and thermal Free Energies=	-914.400187

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.129809	1.266393	0.176588
2	6	0	1.097579	0.268933	-0.514202
3	6	0	1.066051	-1.126814	0.078884

4	7	0	0.070218	-1.877297	0.351224
5	6	0	0.299613	1.296746	1.706675
6	7	0	-1.259958	0.878365	-0.157882
7	6	0	-1.888451	-0.303316	-0.094393
8	16	0	-3.589814	-0.385281	-0.322541
9	7	0	-1.241014	-1.478471	0.151353
10	1	0	-1.892690	1.643377	-0.346189
11	1	0	-1.873248	-2.258226	0.250801
12	6	0	2.476667	-1.627342	0.306007
13	6	0	2.598730	0.645159	-0.499284
14	6	0	3.331221	-0.705812	-0.578898
15	1	0	0.769202	0.187475	-1.557970
16	1	0	0.112640	0.317359	2.151521
17	1	0	-0.405047	2.008141	2.143026
18	1	0	1.308745	1.611637	1.980051
19	1	0	2.572888	-2.691488	0.086376
20	1	0	2.738762	-1.483042	1.361564
21	1	0	2.860971	1.321022	-1.313863
22	1	0	2.856813	1.143449	0.439772
23	1	0	4.368745	-0.641293	-0.247424
24	1	0	3.332542	-1.072609	-1.610176
25	6	0	0.321018	2.674592	-0.406591
26	1	0	0.214908	2.667235	-1.494140
27	1	0	-0.416837	3.364042	0.012933
28	1	0	1.310487	3.058002	-0.157204

Data 3: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of N1-protonated 2,4,5,6-tetrahydro-3*H*-1,2,4-triazepine-3-thione **3d** with pseudo axial orientation of the C6-CH_2 bond (MeOH solution)



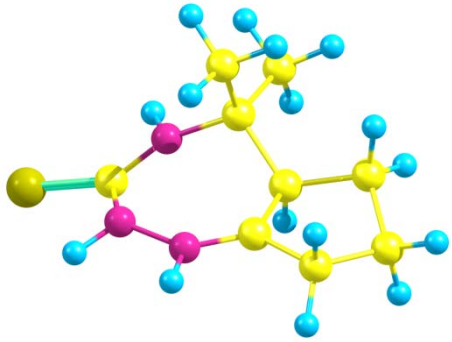
Electronic Energy =	-915.019858161 a.u.
Zero-point correction=	0.252572 (Hartree/Particle)
Thermal correction to Energy=	0.265038
Thermal correction to Enthalpy=	0.265982
Thermal correction to Gibbs Free Energy=	0.214250
Sum of electronic and zero-point Energies=	-914.767286
Sum of electronic and thermal Energies=	-914.754820
Sum of electronic and thermal Enthalpies=	-914.753876
Sum of electronic and thermal Free Energies=	-914.805608

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.068958	1.334808	0.223272
2	6	0	1.326177	0.425035	0.306921
3	6	0	1.131530	-1.059266	0.293376
4	7	0	0.047611	-1.720816	0.519428
5	6	0	0.388101	2.644793	-0.509641
6	7	0	-1.007531	0.668090	-0.580530
7	6	0	-1.807105	-0.326813	-0.159546
8	16	0	-3.395785	-0.552466	-0.620482
9	7	0	-1.225758	-1.203889	0.769960
10	1	0	-1.441824	1.255234	-1.281162
11	1	0	-1.853581	-1.938550	1.072346

12	6	0	2.471341	0.581113	-0.732449
13	6	0	2.390988	-1.766191	-0.125529
14	6	0	3.379019	-0.620269	-0.424167
15	1	0	1.799128	0.607320	1.285339
16	1	0	0.685502	2.470235	-1.544771
17	1	0	1.194996	3.172761	-0.000712
18	1	0	-0.491309	3.293077	-0.503543
19	1	0	2.982043	1.536297	-0.625361
20	1	0	2.073629	0.513305	-1.748839
21	1	0	2.726100	-2.470232	0.640279
22	1	0	2.171713	-2.348830	-1.026525
23	1	0	3.991386	-0.411393	0.455882
24	1	0	4.047943	-0.866855	-1.247586
25	6	0	-0.450217	1.666456	1.636552
26	1	0	0.304127	2.249657	2.169059
27	1	0	-1.362369	2.262189	1.569625
28	1	0	-0.661768	0.772059	2.222974
29	1	0	0.073848	-2.738513	0.475981

Data 4: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of N1-protonated 2,4,5,6-tetrahydro-3*H*-1,2,4-triazepine-3-thione **3d** with pseudo equatorial orientation of the C6-CH_2 bond (MeOH solution)



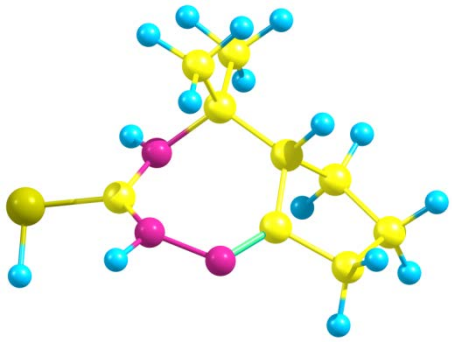
Electronic Energy =	-915.025883452 a.u.
Zero-point correction=	0.252222 (Hartree/Particle)
Thermal correction to Energy=	0.264878
Thermal correction to Enthalpy=	0.265823
Thermal correction to Gibbs Free Energy=	0.214025
Sum of electronic and zero-point Energies=	-914.773662
Sum of electronic and thermal Energies=	-914.761005
Sum of electronic and thermal Enthalpies=	-914.760061
Sum of electronic and thermal Free Energies=	-914.811858

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.115000	1.284853	0.182675
2	6	0	1.143813	0.325256	-0.479603
3	6	0	1.100446	-1.084910	0.016161
4	7	0	0.046207	-1.756151	0.337386
5	6	0	0.189071	1.271919	1.719947
6	7	0	-1.245019	0.888504	-0.260909
7	6	0	-1.919952	-0.253112	-0.101651
8	16	0	-3.575410	-0.393174	-0.405870
9	7	0	-1.288988	-1.391377	0.374109
10	1	0	-1.823659	1.634407	-0.624025
11	1	0	-1.897284	-2.198521	0.430968
12	6	0	2.472368	-1.681417	0.132284
13	6	0	2.648010	0.681134	-0.367740
14	6	0	3.362265	-0.660533	-0.601252
15	1	0	0.887793	0.273712	-1.546802
16	1	0	-0.030920	0.289111	2.141659
17	1	0	-0.536137	1.979568	2.124694
18	1	0	1.181694	1.573110	2.058327

19	1	0	2.518214	-2.701768	-0.252763
20	1	0	2.727571	-1.720553	1.198929
21	1	0	2.933714	1.444302	-1.089717
22	1	0	2.876365	1.057959	0.632544
23	1	0	4.383521	-0.665410	-0.222343
24	1	0	3.395943	-0.893284	-1.668350
25	6	0	0.333948	2.707659	-0.349426
26	1	0	0.292848	2.733947	-1.440755
27	1	0	-0.430875	3.378282	0.048874
28	1	0	1.304916	3.084806	-0.029666
29	1	0	0.167649	-2.710813	0.669887

Data 5: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of S-protonated 2,4,5,6-tetrahydro-3*H*-1,2,4-triazepine-3-thione **3d** with pseudo axial orientation of the C6-CH_2 bond (MeOH solution)



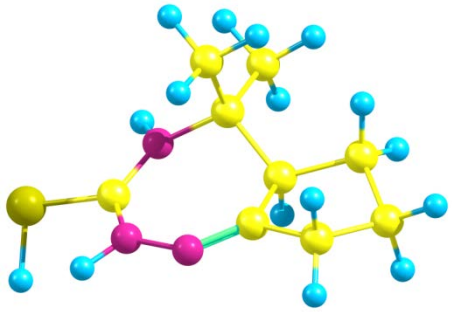
Electronic Energy =	-915.013039694 a.u.
Zero-point correction=	0.248449 (Hartree/Particle)
Thermal correction to Energy=	0.261462
Thermal correction to Enthalpy=	0.262406
Thermal correction to Gibbs Free Energy=	0.209459
Sum of electronic and zero-point Energies=	-914.764591
Sum of electronic and thermal Energies=	-914.751578
Sum of electronic and thermal Enthalpies=	-914.750634
Sum of electronic and thermal Free Energies=	-914.803581

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.096846	1.335132	0.274641
2	6	0	1.356401	0.453669	0.249844
3	6	0	1.191475	-1.045204	0.392837
4	7	0	0.191591	-1.825205	0.547032
5	6	0	0.345124	2.695533	-0.387683
6	7	0	-1.007255	0.686516	-0.511122
7	6	0	-1.683025	-0.387691	-0.131831
8	16	0	-3.381872	-0.477717	-0.584904
9	7	0	-1.128371	-1.353473	0.602219
10	1	0	-1.461848	1.271078	-1.201760
11	1	0	-1.743918	-2.071830	0.957962
12	6	0	2.312111	0.510948	-0.966403
13	6	0	2.551478	-1.672951	0.157445
14	6	0	3.333759	-0.608615	-0.659990
15	1	0	1.960786	0.751199	1.118731
16	1	0	0.585476	2.592684	-1.447432
17	1	0	1.178343	3.197575	0.105804
18	1	0	-0.537459	3.332004	-0.287924
19	1	0	2.785381	1.486238	-1.074570
20	1	0	1.760972	0.295481	-1.886939
21	1	0	3.031285	-1.884741	1.117429
22	1	0	2.437296	-2.622387	-0.365426
23	1	0	4.157570	-0.205525	-0.067765
24	1	0	3.761267	-1.029004	-1.570515
25	6	0	-0.382829	1.546731	1.723964

26	1	0	0.368944	2.120182	2.268851
27	1	0	-1.319011	2.107974	1.736441
28	1	0	-0.533254	0.604944	2.254561
29	1	0	-3.441658	-1.822568	-0.682824

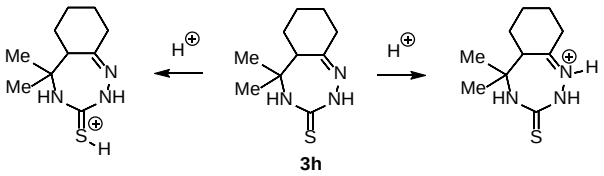
Data 6: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of S-protonated 2,4,5,6-tetrahydro-3*H*-1,2,4-triazepine-3-thione **3d** with pseudo equatorial orientation of the C6-CH_2 bond (MeOH solution)



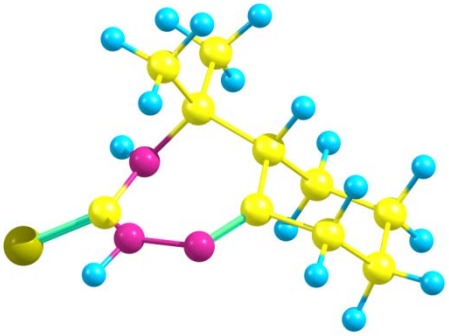
Electronic Energy =	-915.023056185 a.u.
Zero-point correction=	0.248292 (Hartree/Particle)
Thermal correction to Energy=	0.261372
Thermal correction to Enthalpy=	0.262316
Thermal correction to Gibbs Free Energy=	0.209688
Sum of electronic and zero-point Energies=	-914.774764
Sum of electronic and thermal Energies=	-914.761684
Sum of electronic and thermal Enthalpies=	-914.760740
Sum of electronic and thermal Free Energies=	-914.813368

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.168762	1.274908	0.180836
2	6	0	1.138720	0.273178	-0.509296
3	6	0	1.098183	-1.126741	0.070120
4	7	0	0.107660	-1.874692	0.373884
5	6	0	0.304249	1.287705	1.712074
6	7	0	-1.222037	0.881510	-0.178458
7	6	0	-1.805741	-0.297001	-0.080927
8	16	0	-3.568574	-0.299027	-0.298506
9	7	0	-1.212684	-1.456672	0.221283
10	1	0	-1.808938	1.624375	-0.537846
11	1	0	-1.836197	-2.224454	0.426724
12	6	0	2.504187	-1.647586	0.265663
13	6	0	2.640614	0.644802	-0.478021
14	6	0	3.364526	-0.707498	-0.593072
15	1	0	0.823441	0.198242	-1.556994
16	1	0	0.111688	0.305974	2.148518
17	1	0	-0.403797	1.998501	2.141978
18	1	0	1.310373	1.597790	1.998195
19	1	0	2.584508	-2.705764	0.015239
20	1	0	2.765569	-1.538559	1.325361
21	1	0	2.905414	1.339872	-1.274597
22	1	0	2.896562	1.116495	0.474900
23	1	0	4.400157	-0.658059	-0.255142
24	1	0	3.367718	-1.046341	-1.633371
25	6	0	0.362880	2.684923	-0.392452
26	1	0	0.270218	2.686626	-1.481065
27	1	0	-0.375422	3.372230	0.028261
28	1	0	1.351274	3.060574	-0.130140
29	1	0	-3.634230	-1.514238	-0.880453



Data 7: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of 2,4,5,6-tetrahydro-3*H*-1,2,4-triazepine-3-thione **3h** with pseudo axial orientation of the C6-CH_2 bond (MeOH solution)

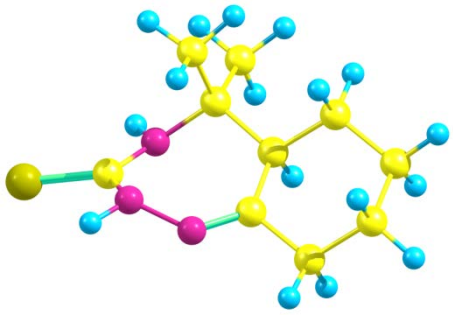


Electronic Energy =	-953.924826402 a.u.
Zero-point correction=	0.268357 (Hartree/Particle)
Thermal correction to Energy=	0.281670
Thermal correction to Enthalpy=	0.282615
Thermal correction to Gibbs Free Energy=	0.229438
Sum of electronic and zero-point Energies=	-953.656469
Sum of electronic and thermal Energies=	-953.643156
Sum of electronic and thermal Enthalpies=	-953.642212
Sum of electronic and thermal Free Energies=	-953.695389

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.341052	1.395648	0.352377
2	6	0	1.025637	0.684015	0.232169
3	6	0	1.047935	-0.763954	0.680551
4	7	0	0.111656	-1.629907	0.816470
5	6	0	-0.274731	2.828520	-0.198582
6	7	0	-1.363299	0.688652	-0.457890
7	6	0	-1.911696	-0.506990	-0.197512
8	16	0	-3.446145	-0.944140	-0.805660
9	7	0	-1.236702	-1.404533	0.580647
10	1	0	-1.937511	1.268587	-1.053544
11	1	0	-1.759037	-2.253497	0.738715
12	6	0	1.707738	0.739519	-1.161306
13	6	0	2.449364	-1.300969	0.857665
14	6	0	3.135781	0.173959	-1.096852
15	6	0	3.186244	-1.237147	-0.498857
16	1	0	1.695684	1.212672	0.922613
17	1	0	-0.112211	2.845695	-1.277496
18	1	0	0.538304	3.377285	0.280051
19	1	0	-1.208491	3.354582	0.015222
20	1	0	1.749209	1.772386	-1.510763
21	1	0	1.106272	0.176465	-1.882756
22	1	0	2.985646	-0.687900	1.591694
23	1	0	2.407135	-2.324457	1.232351
24	1	0	3.753615	0.846115	-0.488757
25	1	0	3.573083	0.171227	-2.099839
26	1	0	2.713758	-1.947619	-1.187049
27	1	0	4.223148	-1.560669	-0.369787
28	6	0	-0.778171	1.457504	1.830993
29	1	0	-0.060774	2.053914	2.399296
30	1	0	-1.758715	1.931535	1.912618
31	1	0	-0.834665	0.469797	2.289532

Data 8: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of 2,4,5,6-tetrahydro-3*H*-1,2,4-triazepine-3-thione **3h** with pseudo equatorial orientation of the C6-CH_2 bond (MeOH solution)

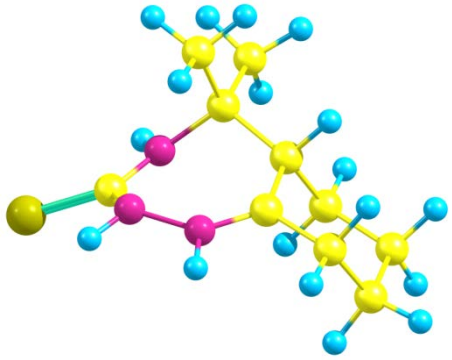


Electronic Energy =	-953.923124429 a.u.
Zero-point correction=	0.268267 (Hartree/Particle)
Thermal correction to Energy=	0.281626
Thermal correction to Enthalpy=	0.282570
Thermal correction to Gibbs Free Energy=	0.228921
Sum of electronic and zero-point Energies=	-953.654857
Sum of electronic and thermal Energies=	-953.641499
Sum of electronic and thermal Enthalpies=	-953.640555
Sum of electronic and thermal Free Energies=	-953.694203

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.279896	1.317982	-0.000107
2	6	0	0.977835	0.487558	-0.365249
3	6	0	0.896729	-1.015741	-0.137243
4	7	0	-0.049526	-1.773251	0.283576
5	6	0	-0.464591	1.509510	1.517882
6	7	0	-1.487011	0.658670	-0.578085
7	6	0	-2.107492	-0.421018	-0.069284
8	16	0	-3.787811	-0.658002	-0.203224
9	7	0	-1.343970	-1.353781	0.570544
10	1	0	-2.122299	1.281427	-1.058374
11	1	0	-1.884989	-2.132464	0.917879
12	6	0	2.159685	-1.774104	-0.507938
13	6	0	2.270357	1.029973	0.306727
14	6	0	3.534362	0.305871	-0.164344
15	6	0	3.432375	-1.191939	0.123214
16	1	0	1.112719	0.602297	-1.449041
17	1	0	-0.455385	0.561782	2.058338
18	1	0	-1.417097	2.007495	1.712189
19	1	0	0.330519	2.137790	1.920875
20	1	0	2.257131	-1.727604	-1.601202
21	1	0	2.024057	-2.822887	-0.240737
22	1	0	2.359210	2.098212	0.099285
23	1	0	2.187251	0.921666	1.392732
24	1	0	4.407604	0.734260	0.336613
25	1	0	3.675197	0.468102	-1.240131
26	1	0	4.305949	-1.725535	-0.262201
27	1	0	3.410360	-1.357067	1.206847
28	6	0	-0.218762	2.691892	-0.687807
29	1	0	-0.130589	2.582838	-1.771942
30	1	0	-1.124582	3.263488	-0.467796
31	1	0	0.629847	3.272854	-0.329106

Data 9: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of N1-protonated 2,4,5,6-tetrahydro-3*H*-1,2,4-triazepine-3-thione **3h** with pseudo axial orientation of the C6-CH_2 bond (MeOH solution)

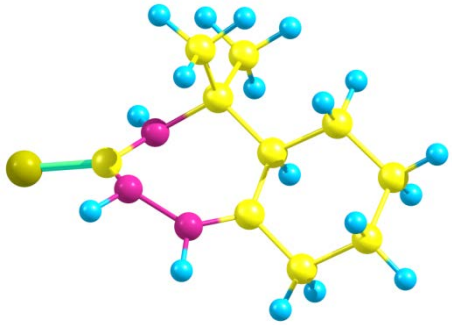


Electronic Energy =	-954.352766309 a.u.
Zero-point correction=	0.282078 (Hartree/Particle)
Thermal correction to Energy=	0.295563
Thermal correction to Enthalpy=	0.296507
Thermal correction to Gibbs Free Energy=	0.243107
Sum of electronic and zero-point Energies=	-954.070689
Sum of electronic and thermal Energies=	-954.057204
Sum of electronic and thermal Enthalpies=	-954.056260
Sum of electronic and thermal Free Energies=	-954.109659

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.343101	1.424642	0.357807
2	6	0	1.032072	0.718695	0.244986
3	6	0	1.076199	-0.709664	0.688400
4	7	0	0.066053	-1.512119	0.823395
5	6	0	-0.268839	2.851187	-0.207676
6	7	0	-1.355699	0.708362	-0.462699
7	6	0	-1.931519	-0.471295	-0.216065
8	16	0	-3.391112	-0.976076	-0.875897
9	7	0	-1.303055	-1.318607	0.694145
10	1	0	-1.852968	1.264864	-1.145269
11	1	0	-1.800012	-2.189712	0.831938
12	6	0	1.710086	0.756554	-1.162550
13	6	0	2.438321	-1.311338	0.833340
14	6	0	3.123242	0.160722	-1.121630
15	6	0	3.144912	-1.257489	-0.546903
16	1	0	1.710398	1.244990	0.926689
17	1	0	-0.101611	2.859102	-1.285663
18	1	0	0.541611	3.402327	0.271552
19	1	0	-1.203331	3.376828	-0.001065
20	1	0	1.763447	1.795201	-1.486665
21	1	0	1.083339	0.219905	-1.880767
22	1	0	2.999094	-0.712215	1.556739
23	1	0	2.387897	-2.334968	1.209236
24	1	0	3.769571	0.809374	-0.520271
25	1	0	3.538392	0.154204	-2.132822
26	1	0	2.641327	-1.950761	-1.227803
27	1	0	4.169164	-1.614195	-0.421513
28	6	0	-0.785766	1.504089	1.833463
29	1	0	-0.074122	2.118022	2.388969
30	1	0	-1.769014	1.972565	1.900174
31	1	0	-0.839782	0.529587	2.319304
32	1	0	0.269669	-2.467966	1.108664

Data 10: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of N1-protonated 2,4,5,6-tetrahydro-3*H*-1,2,4-triazepine-3-thione **3h** with pseudo equatorial orientation of the C6-CH_2 bond (MeOH solution)

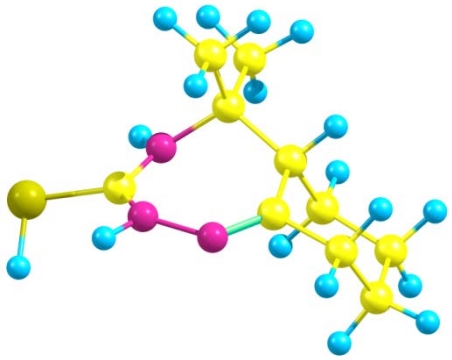


Electronic Energy =	-954.351765548 a.u.
Zero-point correction=	0.281691 (Hartree/Particle)
Thermal correction to Energy=	0.295243
Thermal correction to Enthalpy=	0.296187
Thermal correction to Gibbs Free Energy=	0.242302
Sum of electronic and zero-point Energies=	-954.070074
Sum of electronic and thermal Energies=	-954.056523
Sum of electronic and thermal Enthalpies=	-954.055579
Sum of electronic and thermal Free Energies=	-954.109464

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.278178	1.352383	-0.002262
2	6	0	0.987059	0.515756	-0.345693
3	6	0	0.914684	-0.971220	-0.159755
4	7	0	-0.087198	-1.652807	0.299516
5	6	0	-0.468003	1.593815	1.506802
6	7	0	-1.483835	0.678003	-0.577220
7	6	0	-2.132129	-0.376585	-0.065889
8	16	0	-3.765759	-0.689880	-0.243399
9	7	0	-1.353202	-1.243663	0.705008
10	1	0	-2.066624	1.260246	-1.164587
11	1	0	-1.874988	-2.024549	1.083663
12	6	0	2.120993	-1.768772	-0.565124
13	6	0	2.289279	1.020308	0.349035
14	6	0	3.536336	0.284112	-0.146276
15	6	0	3.408738	-1.221592	0.082810
16	1	0	1.145376	0.628453	-1.426550
17	1	0	-0.476695	0.670315	2.085989
18	1	0	-1.412932	2.113933	1.674156
19	1	0	0.334608	2.225910	1.887456
20	1	0	2.198374	-1.683069	-1.655508
21	1	0	1.979770	-2.827095	-0.334919
22	1	0	2.384535	2.089330	0.156403
23	1	0	2.195248	0.892749	1.430776
24	1	0	4.413124	0.668034	0.381149
25	1	0	3.690954	0.489473	-1.211439
26	1	0	4.259344	-1.760032	-0.339700
27	1	0	3.390268	-1.437614	1.155656
28	6	0	-0.198891	2.703015	-0.732343
29	1	0	-0.112459	2.563042	-1.812653
30	1	0	-1.096473	3.290280	-0.525301
31	1	0	0.657902	3.281150	-0.389134
32	1	0	0.033125	-2.660525	0.379968

Data 11: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of S-protonated 2,4,5,6-tetrahydro-3*H*-1,2,4-triazepine-3-thione **3h** with pseudo axial orientation of the C6-CH_2 bond (MeOH solution)

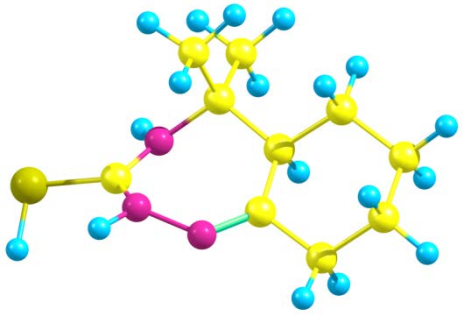


Electronic Energy =	-954.346921929 a.u.
Zero-point correction=	0.277789 (Hartree/Particle)
Thermal correction to Energy=	0.291670
Thermal correction to Enthalpy=	0.292614
Thermal correction to Gibbs Free Energy=	0.238457
Sum of electronic and zero-point Energies=	-954.069133
Sum of electronic and thermal Energies=	-954.055252
Sum of electronic and thermal Enthalpies=	-954.054308
Sum of electronic and thermal Free Energies=	-954.108464

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.293730	1.419686	0.356633
2	6	0	1.060757	0.684467	0.223493
3	6	0	1.081756	-0.756776	0.687070
4	7	0	0.151010	-1.628913	0.835258
5	6	0	-0.225992	2.842193	-0.216037
6	7	0	-1.342178	0.706782	-0.429852
7	6	0	-1.837512	-0.485105	-0.158553
8	16	0	-3.461520	-0.832872	-0.756809
9	7	0	-1.200999	-1.396077	0.582184
10	1	0	-1.836721	1.248410	-1.127888
11	1	0	-1.742686	-2.200024	0.867010
12	6	0	1.725975	0.715203	-1.181279
13	6	0	2.478901	-1.296387	0.866073
14	6	0	3.150587	0.141145	-1.123471
15	6	0	3.199416	-1.259163	-0.502097
16	1	0	1.744349	1.213780	0.898094
17	1	0	-0.068422	2.845876	-1.295580
18	1	0	0.594694	3.388182	0.251245
19	1	0	-1.153869	3.376410	0.000091
20	1	0	1.769101	1.744178	-1.539783
21	1	0	1.113040	0.148689	-1.889999
22	1	0	3.020033	-0.669059	1.582822
23	1	0	2.435548	-2.312153	1.259412
24	1	0	3.780401	0.820385	-0.536944
25	1	0	3.572447	0.117023	-2.132247
26	1	0	2.716947	-1.980716	-1.170888
27	1	0	4.234702	-1.585906	-0.374063
28	6	0	-0.723937	1.491906	1.834707
29	1	0	0.002483	2.090318	2.387426
30	1	0	-1.700329	1.972221	1.920068
31	1	0	-0.777199	0.510374	2.306515
32	1	0	-3.272368	-2.157605	-0.928699

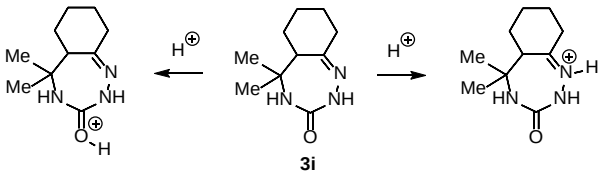
Data 12: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of S-protonated 2,4,5,6-tetrahydro-3*H*-1,2,4-triazepine-3-thione **3h** with pseudo equatorial orientation of the C6-CH_2 bond (MeOH solution)



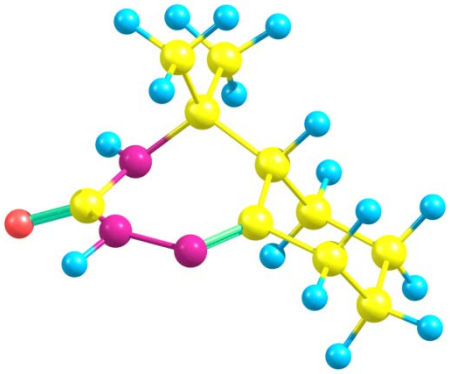
Electronic Energy =	-954.344920803 a.u.
Zero-point correction=	0.277735 (Hartree/Particle)
Thermal correction to Energy=	0.291643
Thermal correction to Enthalpy=	0.292587
Thermal correction to Gibbs Free Energy=	0.238178
Sum of electronic and zero-point Energies=	-954.067186
Sum of electronic and thermal Energies=	-954.053278
Sum of electronic and thermal Enthalpies=	-954.052334
Sum of electronic and thermal Free Energies=	-954.106742

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.230934	1.331710	0.016240
2	6	0	1.009151	0.481466	-0.367867
3	6	0	0.925797	-1.018283	-0.123780
4	7	0	-0.019493	-1.779581	0.297644
5	6	0	-0.407710	1.509160	1.535218
6	7	0	-1.463159	0.683873	-0.540978
7	6	0	-2.033663	-0.407418	-0.063508
8	16	0	-3.783182	-0.540008	-0.205740
9	7	0	-1.325560	-1.356239	0.549638
10	1	0	-2.037048	1.259326	-1.144896
11	1	0	-1.841629	-2.086238	1.021429
12	6	0	2.182032	-1.790018	-0.482931
13	6	0	2.316376	1.028497	0.273827
14	6	0	3.568973	0.289389	-0.201821
15	6	0	3.463728	-1.200104	0.121126
16	1	0	1.122681	0.580202	-1.454850
17	1	0	-0.399174	0.559786	2.072811
18	1	0	-1.351319	2.017986	1.741186
19	1	0	0.398615	2.126081	1.931179
20	1	0	2.262781	-1.764980	-1.577896
21	1	0	2.041798	-2.831737	-0.193398
22	1	0	2.404958	2.090729	0.040897
23	1	0	2.248770	0.943239	1.362470
24	1	0	4.449136	0.724824	0.279502
25	1	0	3.696330	0.429075	-1.282002
26	1	0	4.326763	-1.748649	-0.265321
27	1	0	3.454863	-1.342535	1.207676
28	6	0	-0.173256	2.704724	-0.670577
29	1	0	-0.077143	2.599423	-1.754195
30	1	0	-1.079974	3.273960	-0.450785
31	1	0	0.672398	3.283936	-0.304393
32	1	0	-3.827375	-1.885395	-0.297270



Data 13: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of 2,4,5,6-tetrahydro-3*H*-1,2,4-triazepin-3-one **3i** with pseudo axial orientation of the C6-CH_2 bond (MeOH solution)



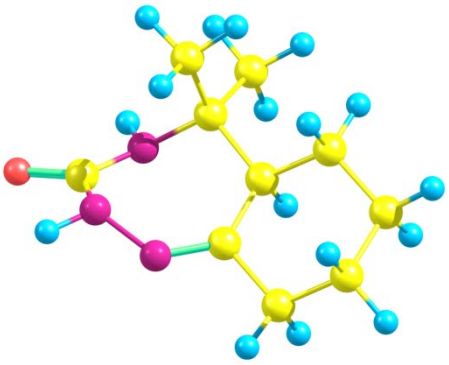
Electronic Energy =	-630.967846508 a.u.
Zero-point correction=	0.270354 (Hartree/Particle)
Thermal correction to Energy=	0.283247
Thermal correction to Enthalpy=	0.284191
Thermal correction to Gibbs Free Energy=	0.232362
Sum of electronic and zero-point Energies=	-630.697492
Sum of electronic and thermal Energies=	-630.684600
Sum of electronic and thermal Enthalpies=	-630.683656
Sum of electronic and thermal Free Energies=	-630.735485

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.871244	1.153502	0.335960
2	6	0	0.602024	0.683384	0.308338
3	6	0	0.824440	-0.793718	0.588401
4	7	0	0.037459	-1.803513	0.526140
5	6	0	-0.986722	2.638830	-0.041825
6	7	0	-1.663390	0.408712	-0.668037
7	6	0	-2.053382	-0.889455	-0.589184
8	7	0	-1.308340	-1.756271	0.204652
9	1	0	-2.295104	0.958344	-1.234190
10	1	0	-1.686210	-2.691949	0.164793
11	6	0	1.406343	1.032770	-0.973004
12	6	0	2.275890	-1.123933	0.859504
13	6	0	2.896251	0.694151	-0.801823
14	6	0	3.123758	-0.761414	-0.377779
15	1	0	1.096737	1.213014	1.133422
16	1	0	-0.727610	2.815901	-1.086728
17	1	0	-0.326003	3.241141	0.584509
18	1	0	-2.011156	2.984653	0.119163
19	1	0	1.307774	2.097140	-1.194852
20	1	0	0.987217	0.485244	-1.823846
21	1	0	2.626950	-0.544227	1.722120
22	1	0	2.371195	-2.183541	1.101402
23	1	0	3.324431	1.361939	-0.043835
24	1	0	3.428083	0.901344	-1.735615
25	1	0	2.848393	-1.432411	-1.199978
26	1	0	4.182759	-0.936466	-0.165637
27	6	0	-1.455341	0.967802	1.752747
28	1	0	-0.910314	1.594635	2.462846
29	1	0	-2.505512	1.269019	1.766614

30	1	0	-1.390716	-0.066039	2.093653
31	8	0	-3.044139	-1.327718	-1.183894

Data 14: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of 2,4,5,6-tetrahydro-3*H*-1,2,4-triazepin-3-one **3i** with pseudo equatorial orientation of the C6-CH_2 bond (MeOH solution)

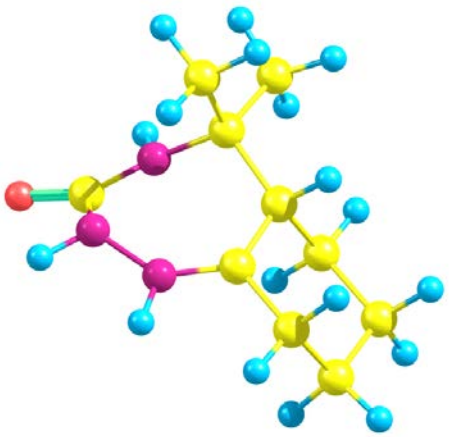


Electronic Energy =	-630.966651623 a.u.
Zero-point correction=	0.270604 (Hartree/Particle)
Thermal correction to Energy=	0.283434
Thermal correction to Enthalpy=	0.284378
Thermal correction to Gibbs Free Energy=	0.232554
Sum of electronic and zero-point Energies=	-630.696047
Sum of electronic and thermal Energies=	-630.683218
Sum of electronic and thermal Enthalpies=	-630.682273
Sum of electronic and thermal Free Energies=	-630.734097

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.745059	1.191673	-0.032264
2	6	0	0.611632	0.509879	-0.353720
3	6	0	0.696949	-1.001520	-0.169870
4	7	0	-0.158335	-1.871187	0.223790
5	6	0	-0.992987	1.372206	1.478927
6	7	0	-1.842145	0.400175	-0.650943
7	6	0	-2.360094	-0.750019	-0.135753
8	7	0	-1.482657	-1.587748	0.542689
9	1	0	-2.562946	0.954865	-1.094234
10	1	0	-1.950101	-2.440070	0.819424
11	6	0	2.045362	-1.590906	-0.547826
12	6	0	1.807281	1.168811	0.388848
13	6	0	3.161658	0.616010	-0.064308
14	6	0	3.225173	-0.896836	0.148860
15	1	0	0.781164	0.670058	-1.427297
16	1	0	-0.904841	0.430793	2.023405
17	1	0	-1.998148	1.769437	1.640354
18	1	0	-0.281079	2.080840	1.904705
19	1	0	2.164011	-1.479206	-1.634304
20	1	0	2.028772	-2.660243	-0.332481
21	1	0	1.778294	2.248864	0.228960
22	1	0	1.700087	1.003353	1.465696
23	1	0	3.964005	1.114851	0.487774
24	1	0	3.317052	0.846500	-1.125659
25	1	0	4.166016	-1.305729	-0.231425
26	1	0	3.193462	-1.117587	1.222536
27	6	0	-0.808149	2.564231	-0.724075
28	1	0	-0.682325	2.461642	-1.805063
29	1	0	-1.773751	3.039951	-0.530336
30	1	0	-0.033253	3.231320	-0.347597
31	8	0	-3.546882	-1.067437	-0.250766

Data 15: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of N1-protonated 2,4,5,6-tetrahydro-3*H*-1,2,4-triazepin-3-one **3i** with pseudo axial orientation of the C6-CH_2 bond (MeOH solution)

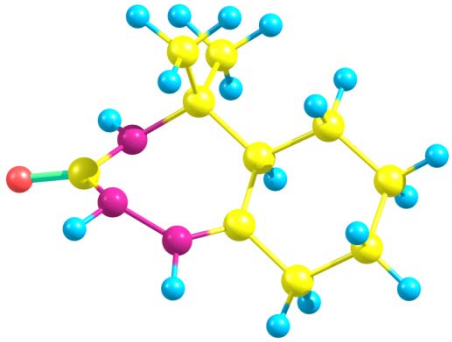


Electronic Energy =	-631.400169715 a.u.
Zero-point correction=	0.283802 (Hartree/Particle)
Thermal correction to Energy=	0.297014
Thermal correction to Enthalpy=	0.297958
Thermal correction to Gibbs Free Energy=	0.245392
Sum of electronic and zero-point Energies=	-631.116368
Sum of electronic and thermal Energies=	-631.103155
Sum of electronic and thermal Enthalpies=	-631.102211
Sum of electronic and thermal Free Energies=	-631.154778

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.880951	1.168343	0.344207
2	6	0	0.601948	0.713170	0.339161
3	6	0	0.849422	-0.743915	0.590579
4	7	0	-0.012982	-1.707909	0.507906
5	6	0	-0.991550	2.653132	-0.036702
6	7	0	-1.647025	0.421844	-0.683757
7	6	0	-2.056169	-0.861363	-0.635541
8	7	0	-1.380711	-1.708533	0.281903
9	1	0	-2.169035	0.974042	-1.351208
10	1	0	-1.727968	-2.658498	0.226907
11	6	0	1.423017	1.078829	-0.939510
12	6	0	2.275737	-1.141425	0.820449
13	6	0	2.906555	0.721779	-0.782384
14	6	0	3.115072	-0.749812	-0.420356
15	1	0	1.090256	1.228030	1.175134
16	1	0	-0.716332	2.832769	-1.076666
17	1	0	-0.344257	3.255620	0.602235
18	1	0	-2.019607	2.991260	0.109190
19	1	0	1.325506	2.150000	-1.113252
20	1	0	0.990289	0.566393	-1.803954
21	1	0	2.639053	-0.597172	1.697654
22	1	0	2.361746	-2.209744	1.029326
23	1	0	3.349365	1.356737	-0.006846
24	1	0	3.431260	0.951024	-1.713609
25	1	0	2.824987	-1.390944	-1.258608
26	1	0	4.165447	-0.956154	-0.204976
27	6	0	-1.490166	0.985888	1.750159
28	1	0	-0.967989	1.633355	2.457788
29	1	0	-2.543334	1.272355	1.735558
30	1	0	-1.422786	-0.038342	2.117985
31	8	0	-2.979145	-1.337131	-1.278069
32	1	0	0.334107	-2.649240	0.679158

Data 16: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of N1-protonated 2,4,5,6-tetrahydro-3*H*-1,2,4-triazepin-3-one **3i** with pseudo equatorial orientation of the C6-CH_2 bond (MeOH solution)

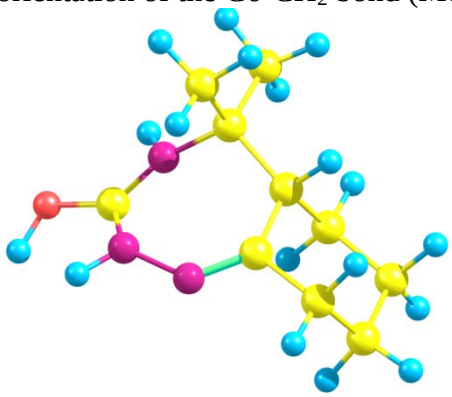


Electronic Energy =	-631.399837691 a.u.
Zero-point correction=	0.284430 (Hartree/Particle)
Thermal correction to Energy=	0.297481
Thermal correction to Enthalpy=	0.298425
Thermal correction to Gibbs Free Energy=	0.246142
Sum of electronic and zero-point Energies=	-631.115408
Sum of electronic and thermal Energies=	-631.102357
Sum of electronic and thermal Enthalpies=	-631.101413
Sum of electronic and thermal Free Energies=	-631.153696

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.748697	1.216450	-0.027989
2	6	0	0.618863	0.541711	-0.337758
3	6	0	0.724087	-0.948520	-0.188527
4	7	0	-0.193359	-1.760459	0.230210
5	6	0	-1.004278	1.421844	1.477395
6	7	0	-1.840486	0.412700	-0.650278
7	6	0	-2.378853	-0.724166	-0.154870
8	7	0	-1.498055	-1.512500	0.633052
9	1	0	-2.500999	0.936033	-1.210517
10	1	0	-1.939928	-2.371241	0.940022
11	6	0	2.029573	-1.578611	-0.582625
12	6	0	1.826949	1.180434	0.413864
13	6	0	3.169449	0.615762	-0.057249
14	6	0	3.219860	-0.900923	0.125723
15	1	0	0.801273	0.697935	-1.409698
16	1	0	-0.924646	0.495953	2.047991
17	1	0	-2.007368	1.828172	1.621453
18	1	0	-0.291086	2.137495	1.887991
19	1	0	2.129762	-1.446552	-1.666223
20	1	0	2.013640	-2.653091	-0.388410
21	1	0	1.796719	2.258360	0.251556
22	1	0	1.715411	1.011637	1.488367
23	1	0	3.977159	1.086738	0.508660
24	1	0	3.328885	0.869734	-1.111247
25	1	0	4.143227	-1.318151	-0.281217
26	1	0	3.194486	-1.152348	1.190915
27	6	0	-0.801273	2.577375	-0.742749
28	1	0	-0.668884	2.460737	-1.821120
29	1	0	-1.765238	3.057605	-0.558196
30	1	0	-0.025563	3.244607	-0.369188
31	8	0	-3.529496	-1.097748	-0.305237
32	1	0	0.048343	-2.747945	0.278570

Data 17: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of O-protonated 2,4,5,6-tetrahydro-3*H*-1,2,4-triazepin-3-one **3i** with pseudo axial orientation of the C6-CH_2 bond (MeOH solution)

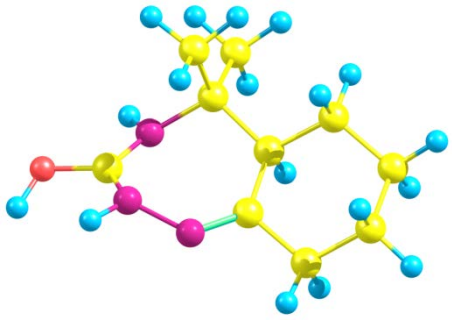


Electronic Energy =	-631.389141542 a.u.
Zero-point correction=	0.283481 (Hartree/Particle)
Thermal correction to Energy=	0.296630
Thermal correction to Enthalpy=	0.297574
Thermal correction to Gibbs Free Energy=	0.245455
Sum of electronic and zero-point Energies=	-631.105661
Sum of electronic and thermal Energies=	-631.092511
Sum of electronic and thermal Enthalpies=	-631.091567
Sum of electronic and thermal Free Energies=	-631.143687

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.818349	1.207678	0.347222
2	6	0	0.640230	0.698388	0.278178
3	6	0	0.855022	-0.762286	0.622862
4	7	0	0.075422	-1.780955	0.593137
5	6	0	-0.927817	2.673728	-0.092814
6	7	0	-1.677038	0.431582	-0.590249
7	6	0	-1.975199	-0.843522	-0.486794
8	7	0	-1.268226	-1.733671	0.215537
9	1	0	-2.251251	0.948338	-1.245776
10	1	0	-1.694725	-2.641624	0.346569
11	6	0	1.408862	0.961757	-1.047986
12	6	0	2.301460	-1.088922	0.903266
13	6	0	2.899076	0.618845	-0.888509
14	6	0	3.125579	-0.807374	-0.374250
15	1	0	1.174210	1.257812	1.055287
16	1	0	-0.696061	2.805128	-1.150401
17	1	0	-0.237491	3.285218	0.489568
18	1	0	-1.940201	3.042468	0.087037
19	1	0	1.310913	2.012404	-1.324940
20	1	0	0.965153	0.370250	-1.855666
21	1	0	2.663156	-0.457012	1.721759
22	1	0	2.393209	-2.132209	1.205982
23	1	0	3.351363	1.332964	-0.190263
24	1	0	3.406885	0.755282	-1.847539
25	1	0	2.833887	-1.530537	-1.144090
26	1	0	4.185423	-0.974879	-0.165093
27	6	0	-1.367488	1.069945	1.780572
28	1	0	-0.791337	1.712654	2.448662
29	1	0	-2.411637	1.386205	1.816149
30	1	0	-1.301964	0.048806	2.158768
31	8	0	-3.077703	-1.228691	-1.111437
32	1	0	-3.097261	-2.179851	-1.293977

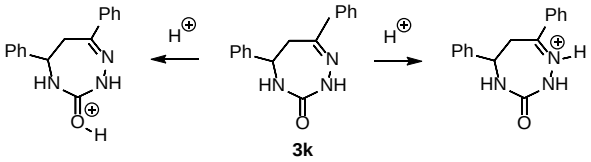
Data 18: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of O-protonated 2,4,5,6-tetrahydro-3*H*-1,2,4-triazepin-3-one **3i** with pseudo equatorial orientation of the C6-CH_2 bond (MeOH solution)



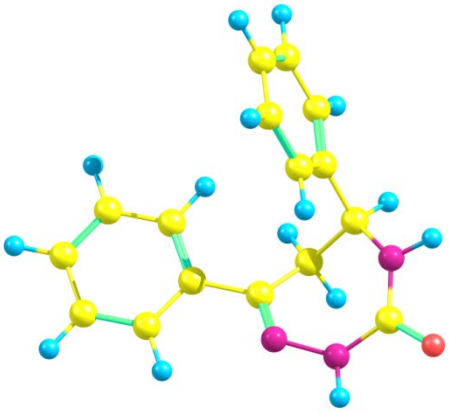
Electronic Energy =	-631.386963177 a.u.
Zero-point correction=	0.283239 (Hartree/Particle)
Thermal correction to Energy=	0.296441
Thermal correction to Enthalpy=	0.297385
Thermal correction to Gibbs Free Energy=	0.244905
Sum of electronic and zero-point Energies=	-631.103725
Sum of electronic and thermal Energies=	-631.090522
Sum of electronic and thermal Enthalpies=	-631.089578
Sum of electronic and thermal Free Energies=	-631.142058

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.670141	1.230963	-0.004990
2	6	0	0.650919	0.498276	-0.361976
3	6	0	0.708615	-1.008130	-0.143297
4	7	0	-0.162639	-1.867309	0.244454
5	6	0	-0.890390	1.398787	1.509544
6	7	0	-1.827356	0.474937	-0.581712
7	6	0	-2.283409	-0.671758	-0.126813
8	7	0	-1.507368	-1.566619	0.486062
9	1	0	-2.493022	1.004017	-1.133110
10	1	0	-1.969317	-2.354492	0.921659
11	6	0	2.041834	-1.644621	-0.492470
12	6	0	1.881792	1.152622	0.329229
13	6	0	3.211629	0.554197	-0.133433
14	6	0	3.247136	-0.946350	0.151839
15	1	0	0.789265	0.624418	-1.443413
16	1	0	-0.815981	0.453134	2.049291
17	1	0	-1.876925	1.828233	1.694611
18	1	0	-0.146279	2.080103	1.921368
19	1	0	2.141290	-1.587853	-1.584597
20	1	0	1.999183	-2.701246	-0.227141
21	1	0	1.869443	2.225233	0.129705
22	1	0	1.796842	1.027404	1.412773
23	1	0	4.033947	1.061356	0.378964
24	1	0	3.346987	0.733556	-1.206733
25	1	0	4.167418	-1.397477	-0.228685
26	1	0	3.232120	-1.116635	1.234341
27	6	0	-0.722650	2.600612	-0.699151
28	1	0	-0.602687	2.497802	-1.780298
29	1	0	-1.678957	3.089131	-0.495647
30	1	0	0.063319	3.253788	-0.324696
31	8	0	-3.577418	-0.894907	-0.284835
32	1	0	-3.807776	-1.835857	-0.252217



Data 19: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of 2,4,5,6-tetrahydro-3*H*-1,2,4-triazepin-3-one **3k** with pseudo axial orientation of the 5-Ph group (MeOH solution)



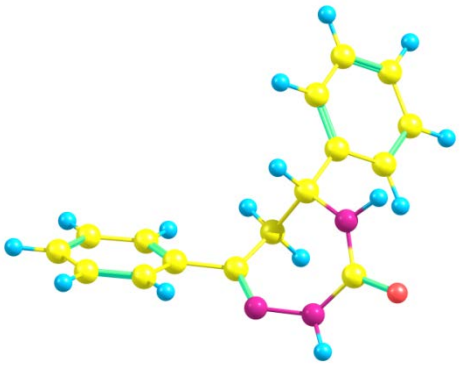
Electronic Energy =	-858.446382726 a.u.
Zero-point correction=	0.283174 (Hartree/Particle)
Thermal correction to Energy=	0.299177
Thermal correction to Enthalpy=	0.300121
Thermal correction to Gibbs Free Energy=	0.237850
Sum of electronic and zero-point Energies=	-858.163209
Sum of electronic and thermal Energies=	-858.147206
Sum of electronic and thermal Enthalpies=	-858.146262
Sum of electronic and thermal Free Energies=	-858.208532

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.712695	0.199699	-1.016268
2	6	0	0.551514	-0.696986	-1.481141
3	6	0	-0.269113	-1.304570	-0.371363
4	7	0	0.209486	-2.206066	0.410489
5	6	0	-1.707037	-0.966296	-0.199258
6	6	0	-2.234026	0.246284	-0.666860
7	6	0	-3.584265	0.551002	-0.495177
8	6	0	-4.433514	-0.353376	0.137753
9	6	0	-3.921541	-1.567225	0.603526
10	6	0	-2.575052	-1.869417	0.439970
11	7	0	1.528473	-2.607192	0.254569
12	6	0	2.702126	-1.849316	0.204006
13	8	0	3.748858	-2.385601	0.582201
14	7	0	2.687295	-0.561002	-0.228800
15	6	0	1.241871	1.458236	-0.293508
16	6	0	0.950265	2.601963	-1.045365
17	6	0	0.479859	3.759801	-0.427745
18	6	0	0.301591	3.790135	0.955581
19	6	0	0.600292	2.658125	1.713211
20	6	0	1.069014	1.499772	1.092846
21	1	0	1.703012	-3.449830	0.785167
22	1	0	3.609510	-0.149668	-0.177776
23	1	0	2.232202	0.524181	-1.923691
24	1	0	-0.073769	-0.123255	-2.161657
25	1	0	0.974654	-1.528079	-2.058909
26	1	0	-1.593382	0.973290	-1.149438
27	1	0	-3.968637	1.497865	-0.856997

28	1	0	-5.484165	-0.118920	0.265475
29	1	0	-4.576322	-2.281152	1.090517
30	1	0	-2.181899	-2.811916	0.798383
31	1	0	1.096269	2.589198	-2.121170
32	1	0	0.261797	4.638334	-1.024590
33	1	0	-0.058421	4.691031	1.439400
34	1	0	0.473014	2.676153	2.789883
35	1	0	1.310423	0.630410	1.692750

Data 20: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of 2,4,5,6-tetrahydro-3*H*-1,2,4-triazepin-3-one **3k** with pseudo equatorial orientation of the 5-Ph group (MeOH solution)



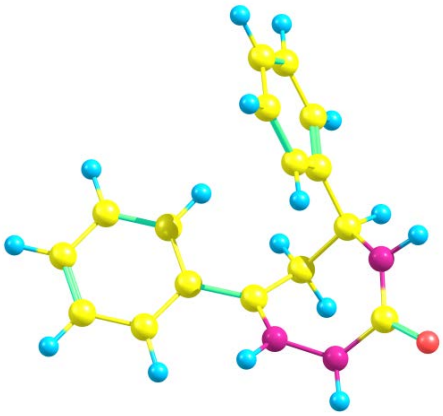
Electronic Energy =	-858.447718105 a.u.
Zero-point correction=	0.283058 (Hartree/Particle)
Thermal correction to Energy=	0.299159
Thermal correction to Enthalpy=	0.300104
Thermal correction to Gibbs Free Energy=	0.237345
Sum of electronic and zero-point Energies=	-858.164661
Sum of electronic and thermal Energies=	-858.148559
Sum of electronic and thermal Enthalpies=	-858.147614
Sum of electronic and thermal Free Energies=	-858.210373

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.972075	0.182460	0.495305
2	6	0	-0.011847	0.012077	-0.696541
3	6	0	1.340815	0.617269	-0.427799
4	7	0	1.528096	1.889344	-0.380045
5	6	0	2.535894	-0.237967	-0.211099
6	6	0	2.650156	-1.504776	-0.804532
7	6	0	3.795376	-2.276864	-0.617945
8	6	0	4.840132	-1.805024	0.175018
9	6	0	4.734041	-0.550760	0.778909
10	6	0	3.594824	0.224279	0.588762
11	7	0	0.429716	2.727489	-0.530761
12	6	0	-0.769736	2.743365	0.185227
13	8	0	-1.353286	3.825039	0.314349
14	7	0	-1.269666	1.602793	0.730902
15	6	0	-2.262765	-0.596996	0.279622
16	6	0	-2.464277	-1.803244	0.956606
17	6	0	-3.619816	-2.554522	0.740673
18	6	0	-4.589349	-2.102923	-0.153623
19	6	0	-4.397707	-0.897085	-0.829816
20	6	0	-3.241609	-0.149204	-0.614883
21	1	0	0.732575	3.677796	-0.695320
22	1	0	-2.113324	1.785535	1.257051
23	1	0	-0.481251	-0.226709	1.383583
24	1	0	0.071244	-1.052480	-0.900466
25	1	0	-0.448911	0.489617	-1.580524
26	1	0	1.859720	-1.889850	-1.436680

27	1	0	3.869084	-3.247660	-1.094576
28	1	0	5.726384	-2.410606	0.326377
29	1	0	5.536801	-0.180261	1.406412
30	1	0	3.508406	1.191439	1.067220
31	1	0	-1.715303	-2.156276	1.658271
32	1	0	-3.764205	-3.486282	1.275845
33	1	0	-5.490040	-2.682931	-0.319708
34	1	0	-5.149008	-0.538361	-1.524363
35	1	0	-3.105247	0.788817	-1.141888

Data 21: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of N1-protonated 2,4,5,6-tetrahydro-3*H*-1,2,4-triazepin-3-one **3k** with pseudo axial orientation of the 5-Ph group (MeOH solution)



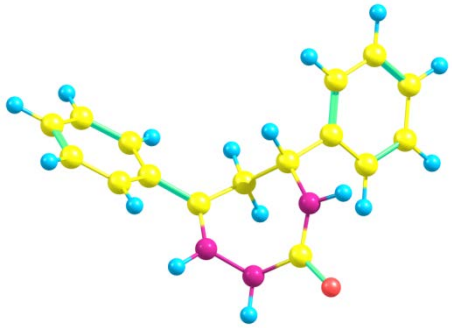
Electronic Energy =	-858.875191098 a.u.
Zero-point correction=	0.296973 (Hartree/Particle)
Thermal correction to Energy=	0.313035
Thermal correction to Enthalpy=	0.313979
Thermal correction to Gibbs Free Energy=	0.252426
Sum of electronic and zero-point Energies=	-858.578218
Sum of electronic and thermal Energies=	-858.562157
Sum of electronic and thermal Enthalpies=	-858.561212
Sum of electronic and thermal Free Energies=	-858.622765

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.703673	0.324775	0.928092
2	6	0	-0.621697	-0.628925	1.494054
3	6	0	0.199948	-1.316884	0.452904
4	7	0	-0.437278	-2.196848	-0.272918
5	6	0	1.618366	-1.078515	0.228844
6	6	0	2.194322	0.142510	0.626073
7	6	0	3.545798	0.380772	0.410382
8	6	0	4.342327	-0.596723	-0.183916
9	6	0	3.785696	-1.820298	-0.566282
10	6	0	2.435991	-2.062250	-0.366160
11	7	0	-1.756636	-2.560611	-0.046476
12	6	0	-2.838474	-1.667995	-0.259002
13	8	0	-3.889454	-2.133676	-0.670965
14	7	0	-2.650397	-0.358111	0.028278
15	6	0	-1.115146	1.564955	0.264728
16	6	0	-0.807129	2.672364	1.062956
17	6	0	-0.233350	3.811973	0.502463
18	6	0	0.031747	3.859507	-0.866334
19	6	0	-0.284577	2.764608	-1.669070
20	6	0	-0.856504	1.622842	-1.107729
21	1	0	-1.957907	-3.484348	-0.409937
22	1	0	-3.476022	0.187213	-0.187003
23	1	0	-2.272482	0.654772	1.801909
24	1	0	0.011818	-0.069101	2.175617

25	1	0	-1.114315	-1.417354	2.075477
26	1	0	1.587788	0.916423	1.076167
27	1	0	3.976723	1.328309	0.708665
28	1	0	5.398358	-0.412145	-0.341184
29	1	0	4.408615	-2.588150	-1.007705
30	1	0	2.038134	-3.034335	-0.632068
31	1	0	-1.022711	2.647114	2.126525
32	1	0	-0.003559	4.663878	1.132023
33	1	0	0.472622	4.747214	-1.305088
34	1	0	-0.091349	2.798072	-2.735194
35	1	0	-1.114820	0.785632	-1.745575
36	1	0	0.023043	-2.681088	-1.039096

Data 22: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of N1-protonated 2,4,5,6-tetrahydro-3*H*-1,2,4-triazepin-3-one **3k** with pseudo equatorial orientation of the 5-Ph group (MeOH solution)



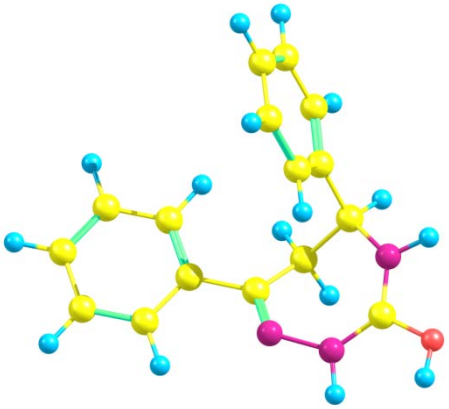
Electronic Energy =	-858.877317421 a.u.
Zero-point correction=	0.296798 (Hartree/Particle)
Thermal correction to Energy=	0.312988
Thermal correction to Enthalpy=	0.313932
Thermal correction to Gibbs Free Energy=	0.251398
Sum of electronic and zero-point Energies=	-858.580519
Sum of electronic and thermal Energies=	-858.564329
Sum of electronic and thermal Enthalpies=	-858.563385
Sum of electronic and thermal Free Energies=	-858.625920

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.929875	0.095286	0.475657
2	6	0	-0.023125	-0.056514	-0.770486
3	6	0	1.329400	0.521848	-0.517883
4	7	0	1.407155	1.823990	-0.498710
5	6	0	2.519941	-0.267839	-0.229667
6	6	0	2.670771	-1.541872	-0.808818
7	6	0	3.827969	-2.275600	-0.582734
8	6	0	4.833170	-1.765326	0.239131
9	6	0	4.682837	-0.512943	0.837400
10	6	0	3.537463	0.235182	0.605624
11	7	0	0.311296	2.651257	-0.657893
12	6	0	-0.767191	2.677772	0.264950
13	8	0	-1.313538	3.751243	0.468904
14	7	0	-1.149474	1.512506	0.837731
15	6	0	-2.257879	-0.615736	0.262427
16	6	0	-2.511878	-1.813345	0.935767
17	6	0	-3.709431	-2.498577	0.730015
18	6	0	-4.663323	-1.987930	-0.148489
19	6	0	-4.417182	-0.789077	-0.819920
20	6	0	-3.220432	-0.106316	-0.616300
21	1	0	0.575912	3.581278	-0.959779
22	1	0	-1.894981	1.656449	1.507296
23	1	0	-0.421508	-0.384166	1.315587

24	1	0	0.053531	-1.117043	-0.989929
25	1	0	-0.477283	0.449214	-1.627454
26	1	0	1.908202	-1.945545	-1.461439
27	1	0	3.944362	-3.247189	-1.046557
28	1	0	5.728339	-2.347459	0.422924
29	1	0	5.451187	-0.126984	1.495681
30	1	0	3.416150	1.182199	1.117892
31	1	0	-1.773847	-2.211438	1.624272
32	1	0	-3.897152	-3.425329	1.259873
33	1	0	-5.595608	-2.517659	-0.307179
34	1	0	-5.157268	-0.385537	-1.501317
35	1	0	-3.043093	0.827129	-1.139156
36	1	0	2.301112	2.293785	-0.369885

Data 23: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of O-protonated 2,4,5,6-tetrahydro-3*H*-1,2,4-triazepin-3-one **3k** with pseudo axial orientation of the 5-Ph group (MeOH solution)



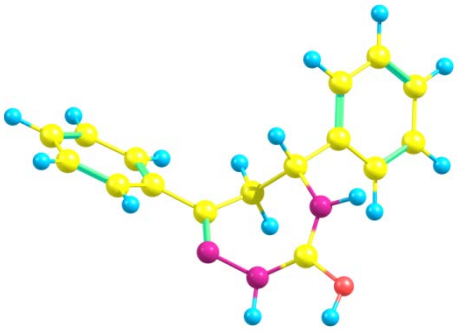
Electronic Energy =	-858.865332207 a.u.
Zero-point correction=	0.296041 (Hartree/Particle)
Thermal correction to Energy=	0.312349
Thermal correction to Enthalpy=	0.313293
Thermal correction to Gibbs Free Energy=	0.250560
Sum of electronic and zero-point Energies=	-858.569291
Sum of electronic and thermal Energies=	-858.552984
Sum of electronic and thermal Enthalpies=	-858.552039
Sum of electronic and thermal Free Energies=	-858.614772

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.651233	0.270586	-1.062882
2	6	0	0.517983	-0.676274	-1.500909
3	6	0	-0.273702	-1.279311	-0.368232
4	7	0	0.236695	-2.115396	0.468202
5	6	0	-1.719648	-0.994699	-0.203706
6	6	0	-2.291420	0.182567	-0.708063
7	6	0	-3.650092	0.439217	-0.535681
8	6	0	-4.458391	-0.480343	0.128820
9	6	0	-3.900497	-1.659772	0.628257
10	6	0	-2.544469	-1.914069	0.468627
11	7	0	1.582574	-2.469541	0.329352
12	6	0	2.662952	-1.702913	0.150925
13	8	0	3.857272	-2.188585	0.455692
14	7	0	2.685728	-0.471390	-0.319825
15	6	0	1.171299	1.498489	-0.300784
16	6	0	0.861310	2.653609	-1.026716
17	6	0	0.373801	3.787056	-0.379199
18	6	0	0.200806	3.780550	1.004806
19	6	0	0.520450	2.637177	1.735323

20	6	0	1.003594	1.500758	1.086892
21	1	0	1.749007	-3.389393	0.717815
22	1	0	3.600321	-0.036353	-0.275105
23	1	0	2.146770	0.614450	-1.973667
24	1	0	-0.130725	-0.130953	-2.181087
25	1	0	0.952070	-1.501223	-2.077450
26	1	0	-1.683407	0.918907	-1.217566
27	1	0	-4.074099	1.358195	-0.922859
28	1	0	-5.516852	-0.283546	0.254252
29	1	0	-4.526084	-2.383315	1.137909
30	1	0	-2.114146	-2.830415	0.850758
31	1	0	1.004809	2.669479	-2.102257
32	1	0	0.138828	4.675445	-0.953979
33	1	0	-0.172208	4.663363	1.511084
34	1	0	0.398360	2.627789	2.812283
35	1	0	1.257371	0.625912	1.673510
36	1	0	3.825570	-2.951148	1.051859

Data 24: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of O-protonated 2,4,5,6-tetrahydro-3*H*-1,2,4-triazepin-3-one **3k** with pseudo equatorial orientation of the 5-Ph group (MeOH solution)

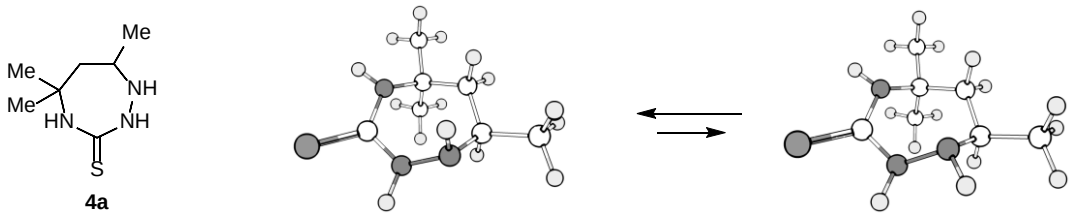


Electronic Energy =	-858.867456719 a.u.
Zero-point correction=	0.296185 (Hartree/Particle)
Thermal correction to Energy=	0.312458
Thermal correction to Enthalpy=	0.313402
Thermal correction to Gibbs Free Energy=	0.251085
Sum of electronic and zero-point Energies=	-858.571272
Sum of electronic and thermal Energies=	-858.554999
Sum of electronic and thermal Enthalpies=	-858.554055
Sum of electronic and thermal Free Energies=	-858.616371

Standard orientation:

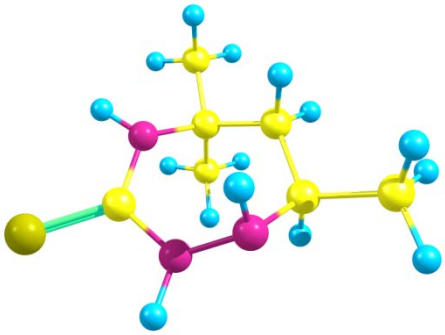
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.966070	0.154457	0.467248
2	6	0	0.011267	0.006568	-0.717172
3	6	0	1.357747	0.611130	-0.418164
4	7	0	1.553295	1.880569	-0.314990
5	6	0	2.547792	-0.246275	-0.207463
6	6	0	2.668337	-1.493071	-0.840666
7	6	0	3.811474	-2.267942	-0.660469
8	6	0	4.840471	-1.819043	0.165679
9	6	0	4.725565	-0.585097	0.808695
10	6	0	3.591440	0.196610	0.623051
11	7	0	0.449573	2.731513	-0.431579
12	6	0	-0.744723	2.661381	0.162420
13	8	0	-1.486878	3.755687	0.262594
14	7	0	-1.303955	1.580667	0.672075
15	6	0	-2.243398	-0.643100	0.263350
16	6	0	-2.460893	-1.794212	1.025200
17	6	0	-3.607522	-2.563299	0.829314
18	6	0	-4.548407	-2.182695	-0.126271

19	6	0	-4.338402	-1.031905	-0.887032
20	6	0	-3.190467	-0.266131	-0.695507
21	1	0	0.728646	3.639283	-0.781683
22	1	0	-2.156893	1.766814	1.187479
23	1	0	-0.475754	-0.205785	1.373115
24	1	0	0.104539	-1.055534	-0.924156
25	1	0	-0.416435	0.480684	-1.605971
26	1	0	1.889863	-1.857344	-1.499042
27	1	0	3.895775	-3.222407	-1.166479
28	1	0	5.724610	-2.428566	0.312475
29	1	0	5.517609	-0.236125	1.460976
30	1	0	3.496719	1.148199	1.129866
31	1	0	-1.733560	-2.090645	1.773551
32	1	0	-3.766899	-3.453245	1.427061
33	1	0	-5.442242	-2.777169	-0.276330
34	1	0	-5.067672	-0.730467	-1.630027
35	1	0	-3.040410	0.626357	-1.293179
36	1	0	-0.980522	4.576953	0.179772



4a

Data 25: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of 5,5,7-trimethyl-1,2,4-triazepane-3-thione with pseudo axial orientation of the N(1)H proton [**4a(H$_{ax}$)**] (the gas phase)



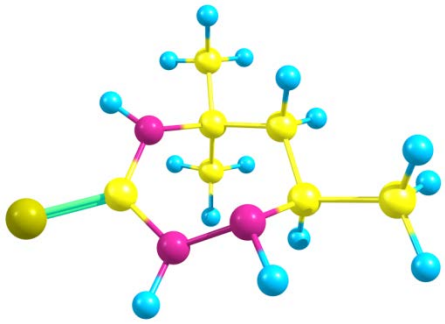
Electronic Energy =	-838.364010815 a.u.
Zero-point correction=	0.227065 (Hartree/Particle)
Thermal correction to Energy=	0.238778
Thermal correction to Enthalpy=	0.239722
Thermal correction to Gibbs Free Energy=	0.190294
Sum of electronic and zero-point Energies=	-838.136946
Sum of electronic and thermal Energies=	-838.125233
Sum of electronic and thermal Enthalpies=	-838.124289
Sum of electronic and thermal Free Energies=	-838.173716

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.400413	1.354569	0.010903
2	6	0	-1.690099	0.565676	-0.293314
3	6	0	-1.777709	-0.865408	0.254749
4	7	0	-0.687578	-1.733527	-0.216893
5	7	0	0.580224	-1.448069	0.334898
6	6	0	1.405563	-0.445635	-0.109331
7	7	0	0.800279	0.687930	-0.579193

8	1	0	-0.624893	-1.700680	-1.234210
9	1	0	1.078766	-2.276426	0.628132
10	1	0	1.501987	1.344051	-0.895572
11	6	0	-3.105019	-1.521799	-0.131838
12	6	0	-0.495260	2.718596	-0.690744
13	6	0	-0.202509	1.568992	1.524311
14	1	0	-1.815520	0.525104	-1.382580
15	1	0	-2.533266	1.145547	0.098582
16	1	0	-1.698171	-0.853786	1.345325
17	1	0	-3.196890	-1.611597	-1.219561
18	1	0	-3.174354	-2.522702	0.297427
19	1	0	-3.950545	-0.927503	0.223605
20	1	0	-0.612775	2.596394	-1.770683
21	1	0	-1.352441	3.279819	-0.313154
22	1	0	0.401740	3.317136	-0.504809
23	1	0	-0.052259	0.626348	2.052012
24	1	0	0.672840	2.196982	1.706539
25	1	0	-1.076132	2.067466	1.954086
26	16	0	3.073382	-0.625026	-0.071578

Data 26: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of 5,5,7-trimethyl-1,2,4-triazepane-3-thione with pseudo equatorial orientation of the N(1)H proton [**4a(H$_{eq}$)**] (the gas phase)



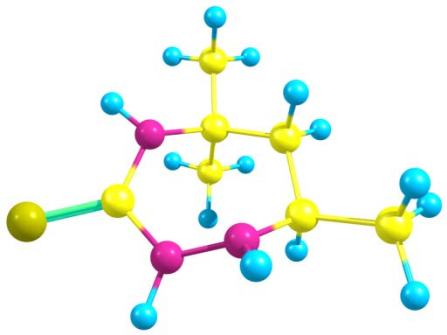
Electronic Energy =	-838.357017150 a.u.
Zero-point correction=	0.226684 (Hartree/Particle)
Thermal correction to Energy=	0.238513
Thermal correction to Enthalpy=	0.239457
Thermal correction to Gibbs Free Energy=	0.189852
Sum of electronic and zero-point Energies=	-838.130333
Sum of electronic and thermal Energies=	-838.118504
Sum of electronic and thermal Enthalpies=	-838.117560
Sum of electronic and thermal Free Energies=	-838.167165

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.392429	1.359735	0.010220
2	6	0	-1.681078	0.567329	-0.298146
3	6	0	-1.781533	-0.856969	0.253669
4	7	0	-0.688316	-1.660311	-0.322112
5	7	0	0.573280	-1.425593	0.325992
6	6	0	1.410731	-0.440305	-0.123428
7	7	0	0.819278	0.704932	-0.567013
8	1	0	-0.883792	-2.646640	-0.186188
9	1	0	1.075505	-2.267875	0.570271
10	1	0	1.521976	1.364807	-0.872343
11	6	0	-3.107826	-1.505283	-0.144312
12	6	0	-0.494368	2.720333	-0.697801
13	6	0	-0.203950	1.582511	1.524273
14	1	0	-1.795718	0.511558	-1.385399
15	1	0	-2.521653	1.150293	0.093841
16	1	0	-1.706840	-0.841950	1.350535
17	1	0	-3.194958	-1.575035	-1.232049
18	1	0	-3.196761	-2.513304	0.273316

19	1	0	-3.948804	-0.917729	0.230112
20	1	0	-0.603832	2.591098	-1.777569
21	1	0	-1.357878	3.277027	-0.327825
22	1	0	0.397018	3.326307	-0.508971
23	1	0	-0.048619	0.642734	2.055716
24	1	0	0.665985	2.217800	1.707415
25	1	0	-1.083089	2.075829	1.948901
26	16	0	3.078405	-0.643264	-0.071542

Data 27: Cartesian coordinates, energy, imaginary frequency of the transition state for the transformation of conformer **4a(H_{ax})** into conformer **4a(H_{eq})** (the gas phase)

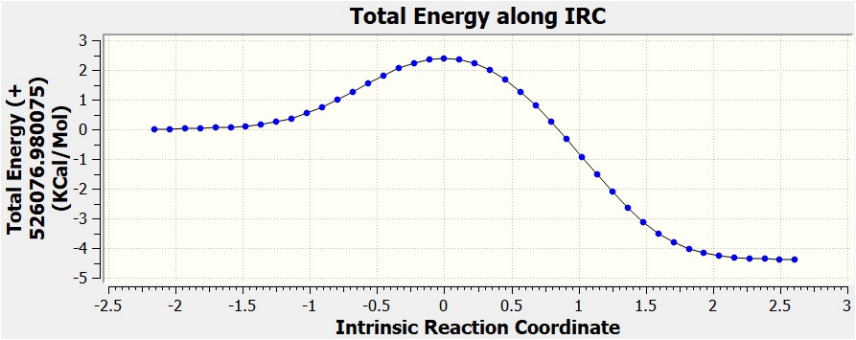


Imaginary Frequency=	-532.6869 cm^{-1}
Electronic Energy =	-838.353177299 a.u.
Zero-point correction=	0.225395 (Hartree/Particle)
Thermal correction to Energy=	0.237039
Thermal correction to Enthalpy=	0.237983
Thermal correction to Gibbs Free Energy=	0.188658
Sum of electronic and zero-point Energies=	-838.127782
Sum of electronic and thermal Energies=	-838.116139
Sum of electronic and thermal Enthalpies=	-838.115194
Sum of electronic and thermal Free Energies=	-838.164519

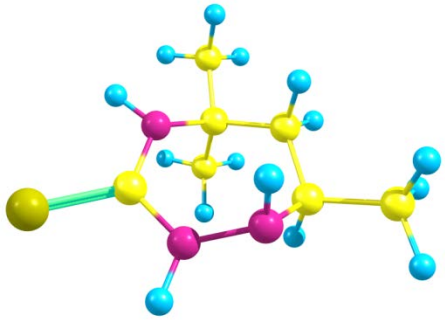
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.366654	1.350075	0.003255
2	6	0	-1.703536	0.614061	-0.242698
3	6	0	-1.806976	-0.825733	0.285307
4	7	0	-0.724802	-1.615568	-0.269726
5	7	0	0.554334	-1.479289	0.230117
6	6	0	1.400213	-0.482010	-0.163492
7	7	0	0.801819	0.657143	-0.632497
8	1	0	-0.897162	-2.426532	-0.839628
9	1	0	0.988692	-2.272055	0.683207
10	1	0	1.513682	1.310744	-0.931410
11	6	0	-3.141568	-1.462961	-0.101175
12	6	0	-0.446433	2.718675	-0.692256
13	6	0	-0.102623	1.556900	1.508254
14	1	0	-1.882496	0.585332	-1.322857
15	1	0	-2.497008	1.221963	0.208052
16	1	0	-1.726676	-0.824348	1.381332
17	1	0	-3.237633	-1.534920	-1.189457
18	1	0	-3.233504	-2.466664	0.322244
19	1	0	-3.975456	-0.861759	0.266996
20	1	0	-0.602241	2.600614	-1.767630
21	1	0	-1.274255	3.303815	-0.286272
22	1	0	0.473004	3.291143	-0.535339
23	1	0	0.025540	0.609112	2.033553
24	1	0	0.806051	2.144958	1.657329
25	1	0	-0.937078	2.092377	1.970188
26	16	0	3.065160	-0.657739	-0.033046

Data 28: The intrinsic reaction coordinate analysis for the transformation of conformer **4a(H_{ax})** into conformer **4a(H_{eq})** (the gas phase)



Data 29: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of 5,5,7-trimethyl-1,2,4-triazepane-3-thione with pseudo axial orientation of the N(1)H proton [**4a(H_{ax})**] (DMSO solution)



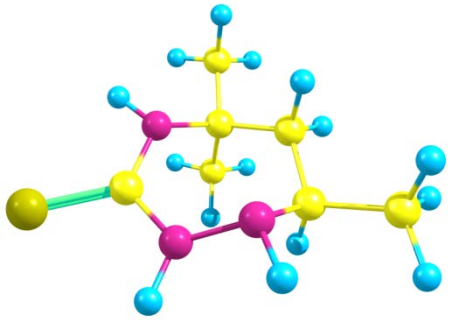
Electronic Energy =	-838.377194927 a.u.
Zero-point correction=	0.226843 (Hartree/Particle)
Thermal correction to Energy=	0.238625
Thermal correction to Enthalpy=	0.239569
Thermal correction to Gibbs Free Energy=	0.189969
Sum of electronic and zero-point Energies=	-838.150352
Sum of electronic and thermal Energies=	-838.138570
Sum of electronic and thermal Enthalpies=	-838.137626
Sum of electronic and thermal Free Energies=	-838.187226

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.428533	1.358322	0.007247
2	6	0	-1.689659	0.535630	-0.315082
3	6	0	-1.760338	-0.884966	0.255816
4	7	0	-0.672077	-1.750639	-0.236454
5	7	0	0.609127	-1.463486	0.283023
6	6	0	1.403289	-0.428673	-0.104888
7	7	0	0.818448	0.716011	-0.526226
8	1	0	-0.627882	-1.712253	-1.254724
9	1	0	1.111431	-2.286480	0.583665
10	1	0	1.511317	1.391270	-0.821424
11	6	0	-3.089825	-1.553836	-0.099783
12	6	0	-0.531572	2.706695	-0.721698
13	6	0	-0.270942	1.598712	1.520774
14	1	0	-1.795794	0.475853	-1.404839
15	1	0	-2.547783	1.105986	0.054044
16	1	0	-1.660065	-0.862224	1.344047
17	1	0	-3.199171	-1.657856	-1.184131
18	1	0	-3.151138	-2.547671	0.347794
19	1	0	-3.928112	-0.955362	0.264044

20	1	0	-0.624065	2.561737	-1.800934
21	1	0	-1.408969	3.252785	-0.370843
22	1	0	0.348598	3.326177	-0.526606
23	1	0	-0.117285	0.667884	2.069224
24	1	0	0.583424	2.251977	1.713288
25	1	0	-1.167574	2.082286	1.916732
26	16	0	3.099379	-0.599914	-0.051629

Data 30: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of 5,5,7-trimethyl-1,2,4-triazepane-3-thione with pseudo equatorial orientation of the N(1)H proton [**4a(H$_{eq}$)**] (DMSO solution)

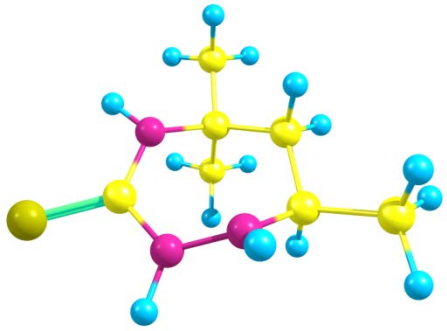


Electronic Energy =	-838.373487326 a.u.
Zero-point correction=	0.226762 (Hartree/Particle)
Thermal correction to Energy=	0.238606
Thermal correction to Enthalpy=	0.239551
Thermal correction to Gibbs Free Energy=	0.189901
Sum of electronic and zero-point Energies=	-838.146726
Sum of electronic and thermal Energies=	-838.134881
Sum of electronic and thermal Enthalpies=	-838.133937
Sum of electronic and thermal Free Energies=	-838.183587

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.396869	1.365077	0.003845
2	6	0	-1.687882	0.574049	-0.281343
3	6	0	-1.771578	-0.851298	0.264565
4	7	0	-0.710063	-1.663103	-0.370312
5	7	0	0.581466	-1.472683	0.206456
6	6	0	1.392456	-0.455035	-0.141397
7	7	0	0.821988	0.699682	-0.570559
8	1	0	-0.915357	-2.648454	-0.238195
9	1	0	1.049022	-2.312914	0.516376
10	1	0	1.531997	1.370555	-0.834210
11	6	0	-3.117029	-1.492844	-0.073380
12	6	0	-0.494227	2.717828	-0.717703
13	6	0	-0.189540	1.597794	1.512988
14	1	0	-1.835817	0.528645	-1.365230
15	1	0	-2.515795	1.154428	0.136967
16	1	0	-1.642808	-0.851922	1.354705
17	1	0	-3.265918	-1.541175	-1.155728
18	1	0	-3.181299	-2.507209	0.330910
19	1	0	-3.931604	-0.908066	0.358135
20	1	0	-0.615402	2.577827	-1.794672
21	1	0	-1.352623	3.278993	-0.343994
22	1	0	0.401617	3.320645	-0.542634
23	1	0	-0.046868	0.661573	2.055627
24	1	0	0.688313	2.226057	1.681999
25	1	0	-1.059840	2.105175	1.936872
26	16	0	3.089166	-0.633429	-0.022592

Data 31: Cartesian coordinates, energy, imaginary frequency of the transition state for the transformation of conformer **4a(H_{ax})** into conformer **4a(H_{eq})** (DMSO solution)

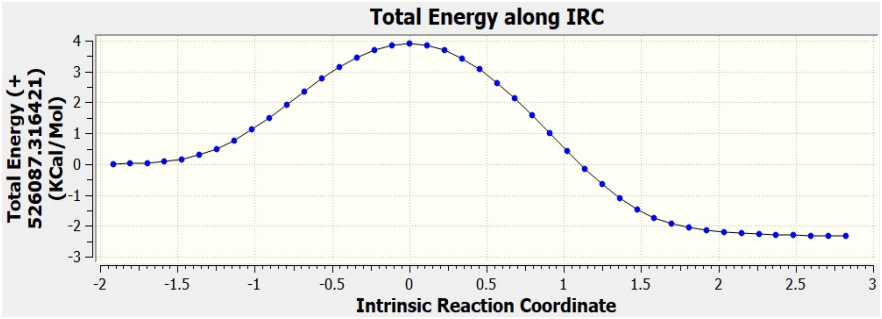


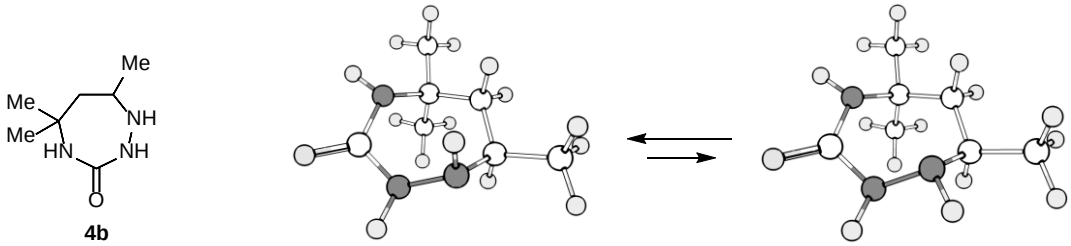
Imaginary Frequency=	-585.9765 cm^{-1}
Electronic Energy =	-838.367258329 a.u.
Zero-point correction=	0.225340 (Hartree/Particle)
Thermal correction to Energy=	0.236988
Thermal correction to Enthalpy=	0.237932
Thermal correction to Gibbs Free Energy=	0.188637
Sum of electronic and zero-point Energies=	-838.141919
Sum of electronic and thermal Energies=	-838.130270
Sum of electronic and thermal Enthalpies=	-838.129326
Sum of electronic and thermal Free Energies=	-838.178621

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.394909	1.357681	-0.001572
2	6	0	-1.710246	0.594338	-0.254737
3	6	0	-1.784411	-0.839835	0.287297
4	7	0	-0.713775	-1.637532	-0.284274
5	7	0	0.584593	-1.510794	0.155851
6	6	0	1.391327	-0.474550	-0.161855
7	7	0	0.809277	0.673668	-0.598399
8	1	0	-0.889047	-2.395170	-0.923442
9	1	0	1.020306	-2.306724	0.604051
10	1	0	1.519105	1.344400	-0.863605
11	6	0	-3.122964	-1.494157	-0.054418
12	6	0	-0.478651	2.711803	-0.722736
13	6	0	-0.152813	1.588933	1.502719
14	1	0	-1.887205	0.555077	-1.334950
15	1	0	-2.515263	1.190647	0.187996
16	1	0	-1.671871	-0.830826	1.378916
17	1	0	-3.253000	-1.571656	-1.138554
18	1	0	-3.186680	-2.496723	0.375175
19	1	0	-3.947939	-0.897883	0.340034
20	1	0	-0.621449	2.573057	-1.797250
21	1	0	-1.319765	3.289463	-0.335135
22	1	0	0.431111	3.298426	-0.564219
23	1	0	-0.021154	0.651317	2.046258
24	1	0	0.741902	2.197559	1.654535
25	1	0	-1.003529	2.116434	1.941676
26	16	0	3.084989	-0.628754	-0.003245

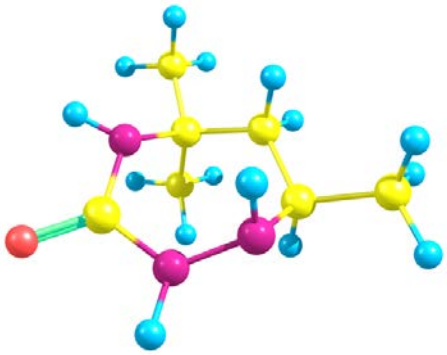
Data 32: The intrinsic reaction coordinate analysis for the transformation of conformer **4a(H_{ax})** into conformer **4a(H_{eq})** (DMSO solution)





4b

Data 33: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of 5,5,7-trimethyl-1,2,4-triazepan-3-one with pseudo axial orientation of the N(1)H proton [**4b(H_{ax})**] (the gas phase)



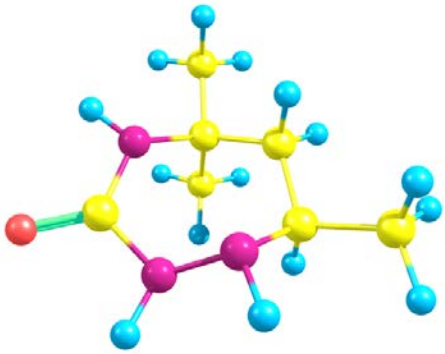
Electronic Energy =	-515.408307115 a.u.
Zero-point correction=	0.229343 (Hartree/Particle)
Thermal correction to Energy=	0.240643
Thermal correction to Enthalpy=	0.241587
Thermal correction to Gibbs Free Energy=	0.193569
Sum of electronic and zero-point Energies=	-515.178965
Sum of electronic and thermal Energies=	-515.167664
Sum of electronic and thermal Enthalpies=	-515.166720
Sum of electronic and thermal Free Energies=	-515.214738

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.549301	1.174650	0.009074
2	6	0	-0.965779	1.085160	-0.272553
3	6	0	-1.713144	-0.145636	0.264443
4	7	0	-1.171925	-1.418876	-0.232782
5	7	0	0.079815	-1.773141	0.312450

6	6	0	1.294418	-1.269825	-0.136749
7	8	0	2.308992	-1.951288	-0.116027
8	7	0	1.280769	0.033682	-0.610165
9	1	0	-1.110974	-1.399696	-1.250033
10	1	0	0.141579	-2.753040	0.552737
11	1	0	2.222692	0.277590	-0.889485
12	6	0	-3.197436	-0.083159	-0.104779
13	6	0	1.088397	2.435989	-0.684915
14	6	0	0.843822	1.260484	1.520302
15	1	0	-1.109217	1.124062	-1.359802
16	1	0	-1.433664	1.986746	0.138699
17	1	0	-1.624585	-0.191670	1.353453
18	1	0	-3.332241	-0.099087	-1.191715
19	1	0	-3.731098	-0.937551	0.315057
20	1	0	-3.653970	0.836076	0.271137
21	1	0	0.914016	2.392759	-1.763090
22	1	0	0.596075	3.327922	-0.291395
23	1	0	2.163636	2.547098	-0.512377
24	1	0	0.539625	0.352193	2.042207
25	1	0	1.914351	1.402771	1.689719
26	1	0	0.313761	2.106507	1.967661

Data 34: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of 5,5,7-trimethyl-1,2,4-triazepan-3-one with pseudo equatorial orientation of the N(1)H proton [**4b(H$_{eq}$)**] (the gas phase)



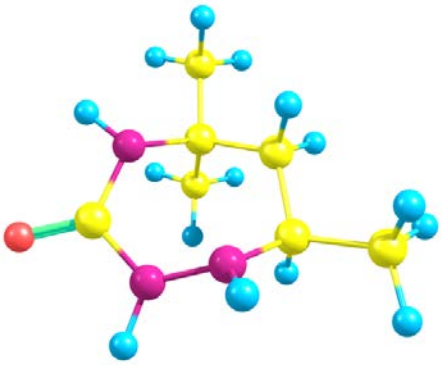
Electronic Energy =	-515.400379015 a.u.
Zero-point correction=	0.229002 (Hartree/Particle)
Thermal correction to Energy=	0.240383
Thermal correction to Enthalpy=	0.241327
Thermal correction to Gibbs Free Energy=	0.193214
Sum of electronic and zero-point Energies=	-515.171377
Sum of electronic and thermal Energies=	-515.159996
Sum of electronic and thermal Enthalpies=	-515.159052
Sum of electronic and thermal Free Energies=	-515.207165

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.580101	1.165224	0.012148
2	6	0	-0.932676	1.091789	-0.296713
3	6	0	-1.717276	-0.103554	0.254024
4	7	0	-1.158013	-1.341980	-0.313121
5	7	0	0.057834	-1.737004	0.363151
6	6	0	1.277866	-1.294614	-0.146791
7	8	0	2.256458	-2.029115	-0.164820
8	7	0	1.317005	0.014184	-0.573916
9	1	0	0.103568	-2.735800	0.518125
10	1	0	2.258153	0.240550	-0.867440
11	6	0	-3.189679	-0.015193	-0.149814
12	6	0	1.140298	2.412739	-0.691160
13	6	0	0.850120	1.272737	1.527132
14	1	0	-1.055947	1.096218	-1.384611
15	1	0	-1.388019	2.009653	0.091322

16	1	0	-1.647634	-0.124803	1.351472
17	1	0	-3.294998	-0.036584	-1.238049
18	1	0	-3.765655	-0.847387	0.267665
19	1	0	-3.633820	0.911749	0.219530
20	1	0	0.981019	2.355341	-1.770869
21	1	0	0.650415	3.314339	-0.316995
22	1	0	2.213766	2.516576	-0.503889
23	1	0	0.535676	0.371786	2.055216
24	1	0	1.918367	1.415554	1.710382
25	1	0	0.314902	2.126156	1.954195
26	1	0	-1.811754	-2.101593	-0.153255

Data 35: Cartesian coordinates, energy, imaginary frequency of the transition state for the transformation of conformer **4b(H$_{ax}$)** into conformer **4b(H$_{eq}$)** (the gas phase)



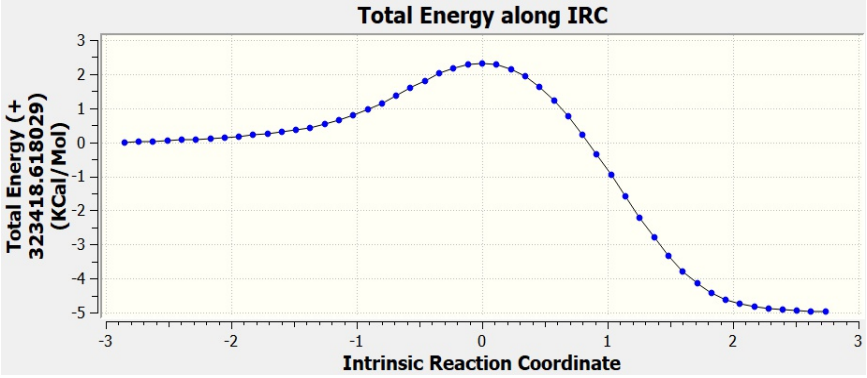
Imaginary Frequency=	-511.2251 cm^{-1}
Electronic Energy =	-515.396659939 a.u.
Zero-point correction=	0.227356 (Hartree/Particle)
Thermal correction to Energy=	0.238701
Thermal correction to Enthalpy=	0.239645
Thermal correction to Gibbs Free Energy=	0.191342
Sum of electronic and zero-point Energies=	-515.169304
Sum of electronic and thermal Energies=	-515.157959
Sum of electronic and thermal Enthalpies=	-515.157015
Sum of electronic and thermal Free Energies=	-515.205318

Standard orientation:

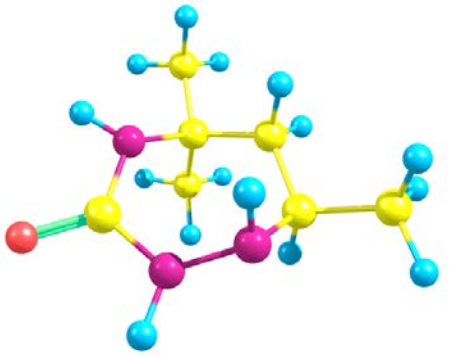
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.557315	1.158203	0.001006
2	6	0	-0.973430	1.112581	-0.227948
3	6	0	-1.723987	-0.127106	0.290031
4	7	0	-1.126677	-1.314679	-0.288136
5	7	0	0.066197	-1.783888	0.219240
6	6	0	1.292588	-1.281639	-0.168936
7	7	0	1.269410	0.019705	-0.655872
8	1	0	-1.667046	-1.960713	-0.837980
9	1	0	0.089042	-2.670257	0.705429
10	1	0	2.215855	0.269391	-0.914789
11	6	0	-3.204231	-0.069263	-0.087184
12	6	0	1.094090	2.424045	-0.687571
13	6	0	0.897187	1.218208	1.504757
14	1	0	-1.155281	1.180055	-1.306049
15	1	0	-1.398465	2.010696	0.235984
16	1	0	-1.644010	-0.177824	1.385607
17	1	0	-3.327859	-0.071841	-1.175084
18	1	0	-3.747777	-0.923518	0.325649
19	1	0	-3.664435	0.843448	0.297192
20	1	0	0.893968	2.395614	-1.761565
21	1	0	0.621796	3.316576	-0.271199
22	1	0	2.174438	2.520711	-0.539119
23	1	0	0.583886	0.312324	2.026400

24	1	0	1.975322	1.330029	1.646565
25	1	0	0.401225	2.070970	1.977862
26	8	0	2.318706	-1.937976	-0.058306

Data 36: The intrinsic reaction coordinate analysis for the transformation of conformer **4b(H_{ax})** into conformer **4b(H_{eq})** (the gas phase)



Data 37: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of 5,5,7-trimethyl-1,2,4-triazepan-3-one with pseudo axial orientation of the N(1)H proton [**4b(H_{ax})**] (DMSO solution)



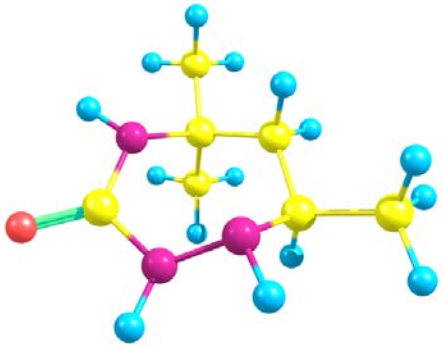
Electronic Energy =	-515.420683514 a.u.
Zero-point correction=	0.228967 (Hartree/Particle)
Thermal correction to Energy=	0.240307
Thermal correction to Enthalpy=	0.241251
Thermal correction to Gibbs Free Energy=	0.193149
Sum of electronic and zero-point Energies=	-515.191716
Sum of electronic and thermal Energies=	-515.180376
Sum of electronic and thermal Enthalpies=	-515.179432
Sum of electronic and thermal Free Energies=	-515.227535

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.537584	1.183895	0.008106
2	6	0	-0.971152	1.069866	-0.288964
3	6	0	-1.709792	-0.156604	0.264222
4	7	0	-1.165704	-1.432219	-0.234661
5	7	0	0.094894	-1.782549	0.297344
6	6	0	1.300271	-1.259076	-0.130136
7	8	0	2.325886	-1.948432	-0.106472
8	7	0	1.301107	0.040170	-0.578259
9	1	0	-1.108558	-1.410282	-1.252212

10	1	0	0.161245	-2.761726	0.539511
11	1	0	2.241179	0.298907	-0.850796
12	6	0	-3.195908	-0.101878	-0.097969
13	6	0	1.070858	2.438893	-0.700833
14	6	0	0.816727	1.294272	1.519829
15	1	0	-1.107299	1.089332	-1.377255
16	1	0	-1.449477	1.972485	0.104798
17	1	0	-1.615002	-0.195042	1.352681
18	1	0	-3.334846	-0.130931	-1.183746
19	1	0	-3.729613	-0.948641	0.338361
20	1	0	-3.647485	0.822178	0.270688
21	1	0	0.903400	2.378764	-1.779210
22	1	0	0.563429	3.328143	-0.321935
23	1	0	2.143105	2.563358	-0.521405
24	1	0	0.516102	0.391721	2.054484
25	1	0	1.883522	1.455381	1.695834
26	1	0	0.269609	2.139787	1.945484

Data 38: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of 5,5,7-trimethyl-1,2,4-triazepan-3-one with pseudo equatorial orientation of the N(1)H proton [**4b(H_{eq})**] (DMSO solution)



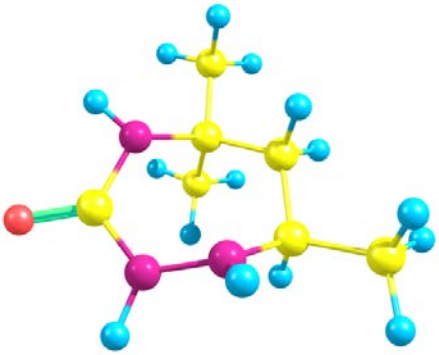
Electronic Energy =	-515.415316032 a.u.
Zero-point correction=	0.228714 (Hartree/Particle)
Thermal correction to Energy=	0.240133
Thermal correction to Enthalpy=	0.241077
Thermal correction to Gibbs Free Energy=	0.192840
Sum of electronic and zero-point Energies=	-515.186602
Sum of electronic and thermal Energies=	-515.175183
Sum of electronic and thermal Enthalpies=	-515.174239
Sum of electronic and thermal Free Energies=	-515.222476

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.575162	1.168751	0.008523
2	6	0	-0.939268	1.097287	-0.282167
3	6	0	-1.713377	-0.107778	0.257881
4	7	0	-1.162322	-1.338826	-0.343877
5	7	0	0.055046	-1.758422	0.302851
6	6	0	1.271344	-1.291691	-0.144002
7	8	0	2.276043	-2.014527	-0.117118
8	7	0	1.313466	0.009301	-0.580764
9	1	0	-1.815777	-2.100023	-0.187033
10	1	0	0.080353	-2.748428	0.507697
11	1	0	2.261566	0.245999	-0.845304
12	6	0	-3.193046	-0.014829	-0.115383
13	6	0	1.134086	2.412181	-0.701579
14	6	0	0.863047	1.272865	1.519352
15	1	0	-1.080967	1.127034	-1.367778
16	1	0	-1.387796	2.006910	0.129491
17	1	0	-1.625278	-0.155768	1.351721
18	1	0	-3.321258	0.001222	-1.201541
19	1	0	-3.754718	-0.863311	0.286466

20	1	0	-3.629357	0.898910	0.293314
21	1	0	0.964759	2.354437	-1.779740
22	1	0	0.645736	3.312405	-0.323310
23	1	0	2.208763	2.514167	-0.522810
24	1	0	0.540242	0.378706	2.054899
25	1	0	1.934462	1.406290	1.690891
26	1	0	0.339901	2.132584	1.946760

Data 39: Cartesian coordinates, energy, imaginary frequency of the transition state for the transformation of conformer **4b(H_{ax})** into conformer **4b(H_{eq})** (DMSO solution)

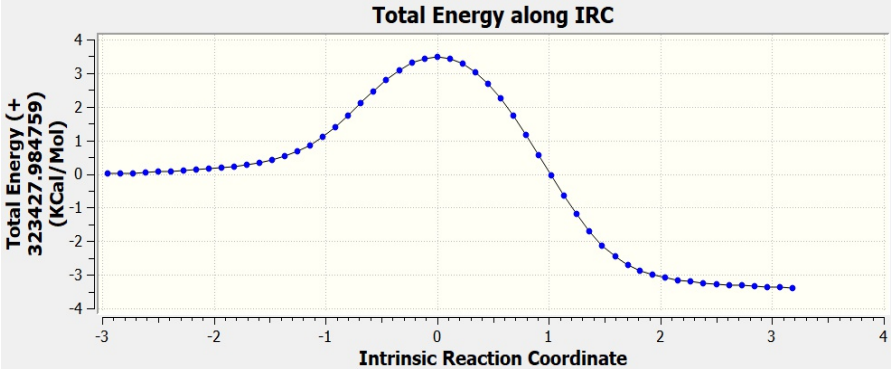


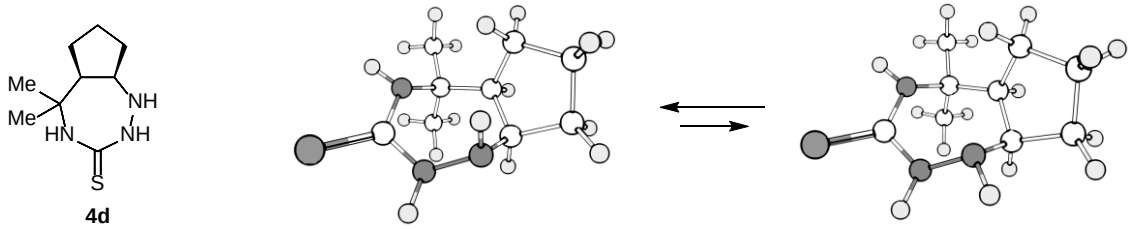
Imaginary Frequency=	-573.7999 cm^{-1}
Electronic Energy =	-515.40972642 a.u.
Zero-point correction=	0.227036 (Hartree/Particle)
Thermal correction to Energy=	0.238381
Thermal correction to Enthalpy=	0.239325
Thermal correction to Gibbs Free Energy=	0.191111
Sum of electronic and zero-point Energies=	-515.182690
Sum of electronic and thermal Energies=	-515.171346
Sum of electronic and thermal Enthalpies=	-515.170401
Sum of electronic and thermal Free Energies=	-515.218616

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.561976	1.162491	-0.003175
2	6	0	-0.966277	1.122500	-0.228289
3	6	0	-1.713559	-0.116510	0.291559
4	7	0	-1.144559	-1.312791	-0.301205
5	7	0	0.049068	-1.818045	0.157100
6	6	0	1.270851	-1.289000	-0.161023
7	7	0	1.272706	0.006149	-0.648066
8	1	0	-1.669217	-1.899891	-0.927653
9	1	0	0.053715	-2.681774	0.685077
10	1	0	2.227405	0.254167	-0.879471
11	6	0	-3.201481	-0.045567	-0.052060
12	6	0	1.112138	2.415451	-0.702984
13	6	0	0.907050	1.226088	1.498194
14	1	0	-1.156868	1.198489	-1.304623
15	1	0	-1.384192	2.019465	0.242001
16	1	0	-1.611693	-0.179402	1.383385
17	1	0	-3.349299	-0.038637	-1.136831
18	1	0	-3.739312	-0.900608	0.365094
19	1	0	-3.642808	0.868087	0.351280
20	1	0	0.907673	2.382845	-1.776089
21	1	0	0.646907	3.312910	-0.290303
22	1	0	2.193355	2.502335	-0.557341
23	1	0	0.583707	0.327948	2.028264
24	1	0	1.986395	1.332117	1.636073
25	1	0	0.418377	2.085963	1.964293
26	8	0	2.308896	-1.945490	-0.011411

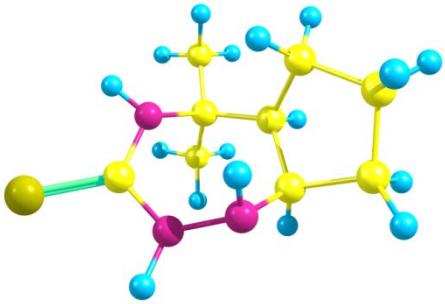
Data 40: The intrinsic reaction coordinate analysis for the transformation of conformer **4b(H$_{ax}$)** into conformer **4b(H$_{eq}$)** (DMSO solution)





4d

Data 41: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of (6*R**,7*S**)-5,5-dimethyl-6,7-trimethylene-1,2,4-triazepane-3-thione with pseudo axial orientation of the N(1)H proton [**4d(H$_{ax}$)**] (the gas phase)



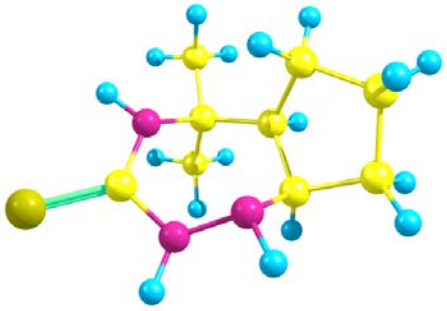
Electronic Energy =	-915.79308559 a.u.
Zero-point correction=	0.263675 (Hartree/Particle)
Thermal correction to Energy=	0.276316
Thermal correction to Enthalpy=	0.277260
Thermal correction to Gibbs Free Energy=	0.225327
Sum of electronic and zero-point Energies=	-915.529410
Sum of electronic and thermal Energies=	-915.516770
Sum of electronic and thermal Enthalpies=	-915.515825
Sum of electronic and thermal Free Energies=	-915.567759

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.034199	1.362638	0.226520
2	6	0	-1.324963	0.623732	0.254213
3	6	0	-1.327051	-0.814453	0.829480
4	7	0	-0.348533	-1.723810	0.216752

5	7	0	1.003305	-1.433093	0.509204
6	6	0	1.735847	-0.490386	-0.169117
7	16	0	3.369281	-0.718422	-0.472896
8	7	0	1.058566	0.626385	-0.575830
9	6	0	-0.128559	2.725366	-0.468534
10	6	0	0.553596	1.598836	1.659978
11	6	0	-2.049070	0.466526	-1.103410
12	6	0	-3.072072	-0.686055	-0.900153
13	6	0	-2.740764	-1.308454	0.483118
14	1	0	-1.969765	1.218519	0.914608
15	1	0	-1.139573	-0.834774	1.904515
16	1	0	-0.467426	-1.762526	-0.793736
17	1	0	1.537490	-2.256021	0.751110
18	1	0	1.678225	1.238533	-1.089453
19	1	0	-0.409121	2.612269	-1.517579
20	1	0	-0.900154	3.314631	0.031608
21	1	0	0.805811	3.292731	-0.421210
22	1	0	0.734770	0.662435	2.188112
23	1	0	1.492999	2.156277	1.635098
24	1	0	-0.173698	2.180515	2.233141
25	1	0	-1.324511	0.211089	-1.882353
26	1	0	-2.532837	1.392944	-1.417134
27	1	0	-4.099916	-0.318391	-0.927827
28	1	0	-2.989448	-1.427054	-1.699313
29	1	0	-2.794198	-2.398524	0.492332
30	1	0	-3.437484	-0.940785	1.240981

Data 42: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of (6*R**,7*S**)-5,5-dimethyl-6,7-trimethylene-1,2,4-triazepane-3-thione with pseudo equatorial orientation of the N(1)H proton [**4d(H$_{eq}$)**] (the gas phase)



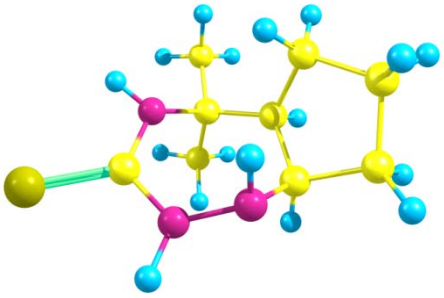
Electronic Energy =	-915.787338452 a.u.
Zero-point correction=	0.263172 (Hartree/Particle)
Thermal correction to Energy=	0.275942
Thermal correction to Enthalpy=	0.276886
Thermal correction to Gibbs Free Energy=	0.224709
Sum of electronic and zero-point Energies=	-915.524167
Sum of electronic and thermal Energies=	-915.511396
Sum of electronic and thermal Enthalpies=	-915.510452
Sum of electronic and thermal Free Energies=	-915.562629

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.044320	1.361921	0.225673
2	6	0	-1.317875	0.623172	0.251562
3	6	0	-1.333647	-0.809931	0.826151
4	7	0	-0.375353	-1.643394	0.084922
5	7	0	0.986789	-1.420734	0.475641
6	6	0	1.738755	-0.490200	-0.189388
7	16	0	3.378923	-0.732606	-0.456048
8	7	0	1.079198	0.639954	-0.575223
9	6	0	-0.126989	2.725875	-0.465681
10	6	0	0.560660	1.598454	1.660967
11	6	0	-2.039295	0.468459	-1.106346

12	6	0	-3.081144	-0.662440	-0.897721
13	6	0	-2.749307	-1.293959	0.479875
14	1	0	-1.956550	1.220289	0.915609
15	1	0	-1.136000	-0.833489	1.905659
16	1	0	-0.563815	-2.624254	0.260402
17	1	0	1.507214	-2.260902	0.686753
18	1	0	1.706138	1.260858	-1.068831
19	1	0	-0.401988	2.612247	-1.515892
20	1	0	-0.904847	3.308335	0.032812
21	1	0	0.803029	3.299864	-0.412741
22	1	0	0.749167	0.661550	2.185818
23	1	0	1.496019	2.162707	1.637557
24	1	0	-0.170748	2.172703	2.236499
25	1	0	-1.313771	0.181261	-1.869178
26	1	0	-2.507281	1.401470	-1.425718
27	1	0	-4.103270	-0.276832	-0.910693
28	1	0	-3.011984	-1.402450	-1.696828
29	1	0	-2.823648	-2.385937	0.478162
30	1	0	-3.437741	-0.934629	1.249453

Data 43: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of (6*R**,7*S**)-5,5-dimethyl-6,7-trimethylene-1,2,4-triazepane-3-thione with pseudo axial orientation of the N(1)H proton [**4d(H$_{ax}$)**] (DMSO solution)



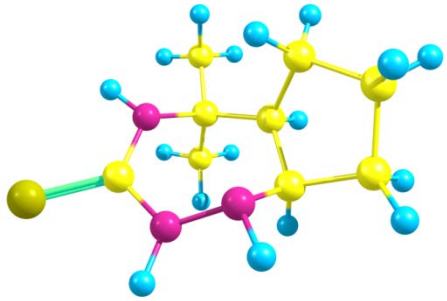
Electronic Energy =	-915.805762525 a.u.
Zero-point correction=	0.263422 (Hartree/Particle)
Thermal correction to Energy=	0.276102
Thermal correction to Enthalpy=	0.277046
Thermal correction to Gibbs Free Energy=	0.225165
Sum of electronic and zero-point Energies=	-915.542340
Sum of electronic and thermal Energies=	-915.529661
Sum of electronic and thermal Enthalpies=	-915.528717
Sum of electronic and thermal Free Energies=	-915.580597

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.019984	1.373391	0.222536
2	6	0	-1.327320	0.618324	0.236677
3	6	0	-1.326665	-0.807361	0.836386
4	7	0	-0.349925	-1.727447	0.228000
5	7	0	1.009005	-1.438416	0.490750
6	6	0	1.729082	-0.481692	-0.159686
7	16	0	3.387521	-0.721873	-0.463602
8	7	0	1.085124	0.644012	-0.543118
9	6	0	-0.142400	2.723686	-0.494667
10	6	0	0.514230	1.628960	1.661038
11	6	0	-2.038248	0.436166	-1.124180
12	6	0	-3.066566	-0.707564	-0.900857
13	6	0	-2.739619	-1.306852	0.494206
14	1	0	-1.983646	1.216589	0.880341
15	1	0	-1.138730	-0.812305	1.911165
16	1	0	-0.479099	-1.780581	-0.780636
17	1	0	1.542285	-2.255367	0.752949

18	1	0	1.695317	1.261029	-1.062328
19	1	0	-0.404417	2.592611	-1.546134
20	1	0	-0.929523	3.307351	-0.013802
21	1	0	0.785013	3.300803	-0.438506
22	1	0	0.695773	0.700555	2.203937
23	1	0	1.444027	2.202513	1.645103
24	1	0	-0.232811	2.204388	2.213188
25	1	0	-1.312571	0.160469	-1.895292
26	1	0	-2.515963	1.358284	-1.457434
27	1	0	-4.091560	-0.333106	-0.932010
28	1	0	-2.985739	-1.462840	-1.686269
29	1	0	-2.798360	-2.396654	0.520366
30	1	0	-3.434620	-0.923167	1.244844

Data 44: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of (6*R**,7*S**)-5,5-dimethyl-6,7-trimethylene-1,2,4-triazepane-3-thione with pseudo equatorial orientation of the N(1)H proton [**4d(H$_{eq}$)**] (DMSO solution)

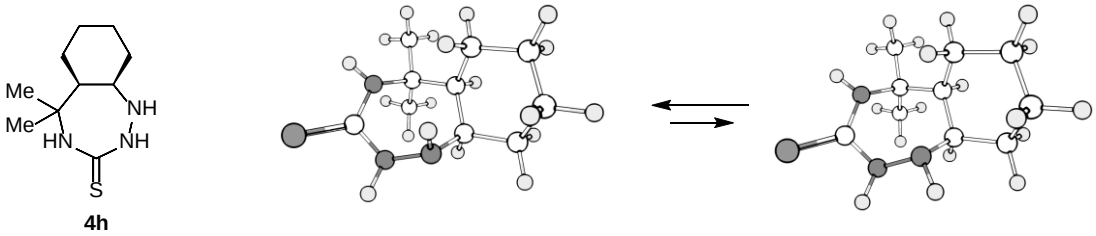


Electronic Energy =	-915.802780978 a.u.
Zero-point correction=	0.263031 (Hartree/Particle)
Thermal correction to Energy=	0.275841
Thermal correction to Enthalpy=	0.276785
Thermal correction to Gibbs Free Energy=	0.224552
Sum of electronic and zero-point Energies=	-915.539750
Sum of electronic and thermal Energies=	-915.526940
Sum of electronic and thermal Enthalpies=	-915.525996
Sum of electronic and thermal Free Energies=	-915.578228

Standard orientation:

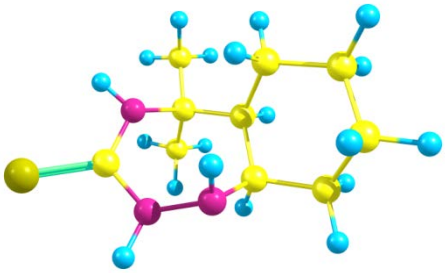
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.041534	1.358865	0.220882
2	6	0	-1.316066	0.619099	0.263106
3	6	0	-1.317815	-0.820631	0.814260
4	7	0	-0.388431	-1.655702	0.029462
5	7	0	0.985223	-1.470676	0.360853
6	6	0	1.728502	-0.499900	-0.205498
7	16	0	3.411518	-0.706511	-0.411153
8	7	0	1.086306	0.635767	-0.582516
9	6	0	-0.130182	2.720605	-0.472451
10	6	0	0.573456	1.592491	1.650321
11	6	0	-2.084006	0.496387	-1.072822
12	6	0	-3.114961	-0.643160	-0.853222
13	6	0	-2.744608	-1.295474	0.504550
14	1	0	-1.933695	1.203597	0.955552
15	1	0	-1.086150	-0.868178	1.884546
16	1	0	-0.581767	-2.636227	0.204854
17	1	0	1.487127	-2.300704	0.643548
18	1	0	1.722750	1.273145	-1.042863
19	1	0	-0.414014	2.605260	-1.519920
20	1	0	-0.904007	3.301726	0.032754
21	1	0	0.801063	3.292692	-0.427564
22	1	0	0.755499	0.655804	2.179450
23	1	0	1.510802	2.153087	1.618054

24	1	0	-0.150955	2.171631	2.228106
25	1	0	-1.391244	0.237100	-1.875719
26	1	0	-2.565279	1.436749	-1.346240
27	1	0	-4.137541	-0.260077	-0.831611
28	1	0	-3.066254	-1.371136	-1.665374
29	1	0	-2.822788	-2.386294	0.492208
30	1	0	-3.404635	-0.939419	1.299323



4h

Data 45: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of (6*R**,7*S**)-5,5-dimethyl-6,7-tetramethylene-1,2,4-triazepane-3-thione with pseudo axial orientation of the N(1)H proton [**4h(H$_{ax}$)**] (the gas phase)



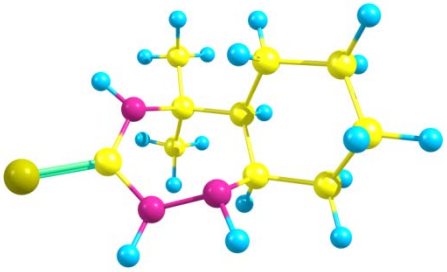
Electronic Energy =	-955.121657937 a.u.
Zero-point correction=	0.293138 (Hartree/Particle)
Thermal correction to Energy=	0.306548
Thermal correction to Enthalpy=	0.307492
Thermal correction to Gibbs Free Energy=	0.254302
Sum of electronic and zero-point Energies=	-954.828520
Sum of electronic and thermal Energies=	-954.815110
Sum of electronic and thermal Enthalpies=	-954.814166
Sum of electronic and thermal Free Energies=	-954.867356

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	3.533652	-0.925057	-0.601268
2	7	0	1.347668	0.614474	-0.549726
3	1	0	2.002033	1.197662	-1.053545
4	7	0	-0.234039	-1.639850	0.209790
5	1	0	-0.403706	-1.637517	-0.792725
6	7	0	1.151975	-1.486047	0.438862
7	1	0	1.621255	-2.362001	0.621157
8	6	0	1.936369	-0.575001	-0.223059
9	6	0	0.392073	1.389892	0.299669
10	6	0	-1.038094	0.764688	0.292679
11	1	0	-1.632122	1.404728	0.959826
12	6	0	-1.087580	-0.661014	0.903760
13	1	0	-0.714572	-0.630555	1.929137
14	6	0	-1.724621	0.784198	-1.089053
15	1	0	-1.752177	1.803423	-1.478744
16	1	0	-1.131410	0.205576	-1.807378
17	6	0	-3.159019	0.236578	-1.035872
18	1	0	-3.778067	0.912198	-0.430950

19	1	0	-3.592092	0.237950	-2.041207
20	6	0	-3.214394	-1.169485	-0.430302
21	1	0	-2.728167	-1.885015	-1.105242
22	1	0	-4.251986	-1.504118	-0.334598
23	6	0	-2.530184	-1.195469	0.942313
24	1	0	-2.514166	-2.208920	1.351430
25	1	0	-3.105260	-0.573515	1.639024
26	6	0	0.937349	1.504574	1.739701
27	1	0	0.248722	2.086639	2.358880
28	1	0	1.080929	0.531509	2.207949
29	1	0	1.903464	2.014581	1.733384
30	6	0	0.365043	2.803452	-0.310269
31	1	0	-0.376021	3.423331	0.199303
32	1	0	1.339939	3.284924	-0.191128
33	1	0	0.124078	2.785522	-1.374180

Data 46: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of (6*R**,7*S**)-5,5-dimethyl-6,7-tetramethylene-1,2,4-triazepane-3-thione with pseudo equatorial orientation of the N(1)H proton [**4h(H$_{eq}$)**] (the gas phase)



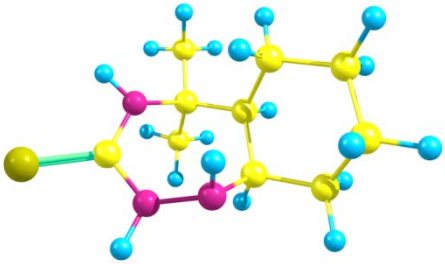
Electronic Energy =	-955.115167272 a.u.
Zero-point correction=	0.292566 (Hartree/Particle)
Thermal correction to Energy=	0.306141
Thermal correction to Enthalpy=	0.307086
Thermal correction to Gibbs Free Energy=	0.253582
Sum of electronic and zero-point Energies=	-954.822601
Sum of electronic and thermal Energies=	-954.809026
Sum of electronic and thermal Enthalpies=	-954.808082
Sum of electronic and thermal Free Energies=	-954.861585

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	3.532391	-0.945080	-0.601746
2	7	0	1.364950	0.626766	-0.543526
3	1	0	2.023015	1.212764	-1.038779
4	7	0	-0.257607	-1.567593	0.112711
5	7	0	1.141839	-1.464783	0.433478
6	1	0	1.599386	-2.356822	0.561077
7	6	0	1.934592	-0.572321	-0.236287
8	6	0	0.399477	1.393357	0.300885
9	6	0	-1.032660	0.767543	0.287811
10	1	0	-1.625140	1.412694	0.951370
11	6	0	-1.094487	-0.649383	0.908237
12	1	0	-0.729117	-0.612697	1.942378
13	6	0	-1.703949	0.774439	-1.099924
14	1	0	-1.716467	1.788377	-1.504071
15	1	0	-1.110659	0.161935	-1.784131
16	6	0	-3.145926	0.249071	-1.048923
17	1	0	-3.761780	0.932982	-0.448998
18	1	0	-3.574844	0.250262	-2.055969
19	6	0	-3.218255	-1.156004	-0.444578
20	1	0	-2.729195	-1.866898	-1.118679
21	1	0	-4.259472	-1.479478	-0.345709
22	6	0	-2.536833	-1.183891	0.929744

23	1	0	-2.539496	-2.198758	1.346838
24	1	0	-3.109335	-0.567041	1.631833
25	6	0	0.939241	1.511296	1.743460
26	1	0	0.246153	2.089895	2.360977
27	1	0	1.086246	0.538860	2.211939
28	1	0	1.902854	2.026067	1.739160
29	6	0	0.367969	2.807462	-0.308370
30	1	0	-0.380589	3.422945	0.195515
31	1	0	1.339226	3.294339	-0.181390
32	1	0	0.135320	2.787403	-1.373856
33	1	0	-0.513649	-2.525693	0.327449

Data 47: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of (6*R**,7*S**)-5,5-dimethyl-6,7-tetramethylene-1,2,4-triazepane-3-thione with pseudo axial orientation of the N(1)H proton [**4h(H$_{ax}$)**] (DMSO solution)



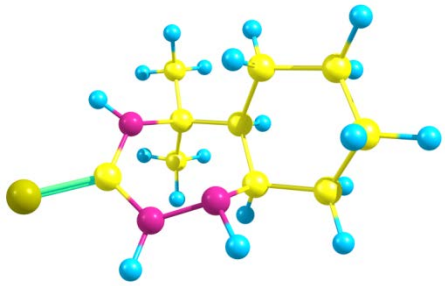
Electronic Energy =	-955.134510184 a.u.
Zero-point correction=	0.292690 (Hartree/Particle)
Thermal correction to Energy=	0.306217
Thermal correction to Enthalpy=	0.307161
Thermal correction to Gibbs Free Energy=	0.253687
Sum of electronic and zero-point Energies=	-954.841820
Sum of electronic and thermal Energies=	-954.828293
Sum of electronic and thermal Enthalpies=	-954.827349
Sum of electronic and thermal Free Energies=	-954.880823

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	3.550926	-0.934654	-0.586955
2	7	0	1.377198	0.626588	-0.517523
3	1	0	2.027205	1.214585	-1.021609
4	7	0	-0.240864	-1.643741	0.216642
5	1	0	-0.423747	-1.653787	-0.783651
6	7	0	1.150820	-1.495463	0.413061
7	1	0	1.618789	-2.367088	0.616751
8	6	0	1.928061	-0.569540	-0.213193
9	6	0	0.381527	1.402730	0.295066
10	6	0	-1.038769	0.761735	0.275246
11	1	0	-1.641564	1.406992	0.927251
12	6	0	-1.086081	-0.651625	0.909137
13	1	0	-0.708945	-0.609806	1.932148
14	6	0	-1.716248	0.757182	-1.111143
15	1	0	-1.740837	1.769762	-1.516572
16	1	0	-1.125549	0.163981	-1.819776
17	6	0	-3.152575	0.214569	-1.049256
18	1	0	-3.768791	0.905387	-0.459612
19	1	0	-3.581964	0.195015	-2.055807
20	6	0	-3.215345	-1.178571	-0.414371
21	1	0	-2.736239	-1.910307	-1.076891
22	1	0	-4.255123	-1.502701	-0.307976
23	6	0	-2.530024	-1.180856	0.958464
24	1	0	-2.522066	-2.185580	1.389897
25	1	0	-3.098426	-0.540794	1.642916
26	6	0	0.905392	1.541272	1.740409

27	1	0	0.197281	2.120082	2.338758
28	1	0	1.052278	0.576989	2.226714
29	1	0	1.862388	2.068019	1.740796
30	6	0	0.353109	2.804384	-0.339916
31	1	0	-0.401807	3.421594	0.150935
32	1	0	1.321555	3.296630	-0.214835
33	1	0	0.126383	2.766127	-1.406061

Data 48: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of (6*R**,7*S**)-5,5-dimethyl-6,7-tetramethylene-1,2,4-triazepane-3-thione with pseudo equatorial orientation of the N(1)H proton [**4h(H$_{eq}$)**] (DMSO solution)

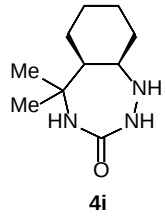


Electronic Energy =	-955.130688501 a.u.
Zero-point correction=	0.292354 (Hartree/Particle)
Thermal correction to Energy=	0.306011
Thermal correction to Enthalpy=	0.306955
Thermal correction to Gibbs Free Energy=	0.253210
Sum of electronic and zero-point Energies=	-954.838335
Sum of electronic and thermal Energies=	-954.824678
Sum of electronic and thermal Enthalpies=	-954.823734
Sum of electronic and thermal Free Energies=	-954.877478

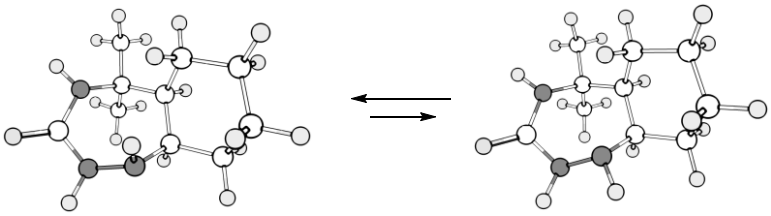
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	3.582937	-0.904393	-0.541930
2	7	0	1.373668	0.627229	-0.550738
3	1	0	2.047515	1.233561	-0.999217
4	7	0	-0.264627	-1.580161	0.035555
5	7	0	1.136859	-1.512709	0.297533
6	1	0	1.584915	-2.393800	0.505870
7	6	0	1.929525	-0.574416	-0.253603
8	6	0	0.391589	1.388391	0.295739
9	6	0	-1.034042	0.755121	0.293065
10	1	0	-1.609960	1.379380	0.988415
11	6	0	-1.075384	-0.674781	0.879438
12	1	0	-0.677631	-0.668483	1.900625
13	6	0	-1.749340	0.802073	-1.072023
14	1	0	-1.775077	1.827799	-1.443544
15	1	0	-1.184294	0.211613	-1.799103
16	6	0	-3.189208	0.275059	-0.983568
17	1	0	-3.778664	0.944116	-0.342735
18	1	0	-3.653648	0.304227	-1.974463
19	6	0	-3.243972	-1.145206	-0.413355
20	1	0	-2.785469	-1.842389	-1.122955
21	1	0	-4.282191	-1.466869	-0.283951
22	6	0	-2.514865	-1.212976	0.934893
23	1	0	-2.501143	-2.238480	1.321663
24	1	0	-3.059864	-0.614073	1.672581
25	6	0	0.940731	1.499872	1.734628
26	1	0	0.251191	2.079170	2.353828
27	1	0	1.081834	0.526824	2.205457
28	1	0	1.904961	2.013472	1.726748
29	6	0	0.355590	2.802016	-0.311591

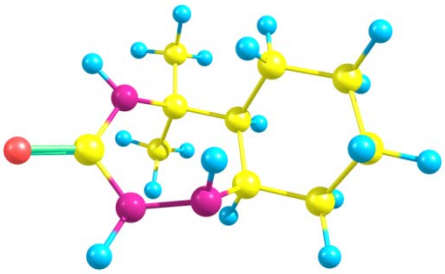
30	1	0	-0.393734	3.410651	0.198400
31	1	0	1.325505	3.291766	-0.187458
32	1	0	0.117944	2.782635	-1.375753
33	1	0	-0.524209	-2.542261	0.228278



4i



Data 49: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of (6*R**,7*S**)-5,5-dimethyl-6,7-tetramethylene-1,2,4-triazepan-3-one with pseudo axial orientation of the N(1)H proton [**4i(H$_{ax}$)**] (the gas phase)



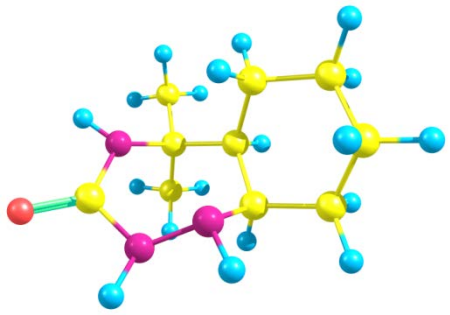
Electronic Energy =	-632.164701422 a.u.
Zero-point correction=	0.295087 (Hartree/Particle)
Thermal correction to Energy=	0.308172
Thermal correction to Enthalpy=	0.309116
Thermal correction to Gibbs Free Energy=	0.257107
Sum of electronic and zero-point Energies=	-631.870657
Sum of electronic and thermal Energies=	-631.857572
Sum of electronic and thermal Enthalpies=	-631.856628
Sum of electronic and thermal Free Energies=	-631.908637

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.664741	0.310829	-0.692935
2	1	0	2.372497	0.819662	-1.205092
3	7	0	-0.220300	-1.710665	0.028745
4	1	0	-0.455093	-1.596010	-0.953882
5	7	0	1.184092	-1.805331	0.154788
6	1	0	1.509601	-2.758419	0.234894
7	6	0	2.064424	-0.982136	-0.501552
8	6	0	0.914427	1.157473	0.284884
9	6	0	-0.598048	0.777248	0.349327
10	1	0	-1.028222	1.447122	1.106839
11	6	0	-0.846431	-0.667631	0.858374
12	1	0	-0.404601	-0.785214	1.849546
13	6	0	-1.363972	1.025268	-0.967005
14	1	0	-1.245064	2.064505	-1.278912
15	1	0	-0.927693	0.420218	-1.770913
16	6	0	-2.863367	0.716914	-0.836827
17	1	0	-3.316360	1.431103	-0.136580
18	1	0	-3.357496	0.873910	-1.800902
19	6	0	-3.114590	-0.707232	-0.331368
20	1	0	-2.803720	-1.433033	-1.093285
21	1	0	-4.184882	-0.874670	-0.175886
22	6	0	-2.352662	-0.960468	0.975624

23	1	0	-2.480612	-1.993783	1.308196
24	1	0	-2.765248	-0.313964	1.759684
25	6	0	1.568171	1.059516	1.680303
26	1	0	1.031900	1.691914	2.393658
27	1	0	1.576512	0.040059	2.064184
28	1	0	2.603979	1.403470	1.632095
29	6	0	1.085601	2.602824	-0.217676
30	1	0	0.496702	3.290213	0.393702
31	1	0	2.133767	2.906703	-0.143931
32	1	0	0.773089	2.714398	-1.256993
33	8	0	3.138737	-1.380335	-0.890638

Data 50: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of (6*R**,7*S**)-5,5-dimethyl-6,7-tetramethylene-1,2,4-triazepan-3-one with pseudo equatorial orientation of the N(1)H proton [**4i(H$_{eq}$)**] (the gas phase)



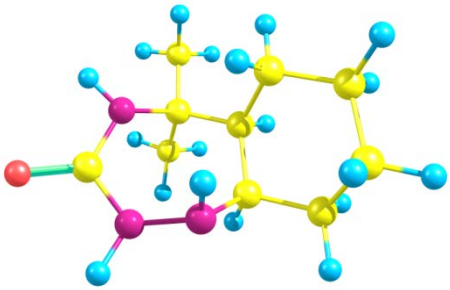
Electronic Energy =	-632.158403824 a.u.
Zero-point correction=	0.294805 (Hartree/Particle)
Thermal correction to Energy=	0.307938
Thermal correction to Enthalpy=	0.308882
Thermal correction to Gibbs Free Energy=	0.256872
Sum of electronic and zero-point Energies=	-631.863599
Sum of electronic and thermal Energies=	-631.850466
Sum of electronic and thermal Enthalpies=	-631.849521
Sum of electronic and thermal Free Energies=	-631.901532

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.684997	0.316874	-0.682611
2	1	0	2.410582	0.809669	-1.185642
3	7	0	-0.250692	-1.635934	-0.025889
4	7	0	1.168839	-1.788741	0.220276
5	1	0	1.459373	-2.756038	0.157171
6	6	0	2.051624	-0.999467	-0.517427
7	6	0	0.932868	1.160395	0.284827
8	6	0	-0.585052	0.787076	0.333134
9	1	0	-1.020655	1.475655	1.070487
10	6	0	-0.858699	-0.639127	0.874491
11	1	0	-0.431357	-0.737803	1.880871
12	6	0	-1.323513	1.000722	-1.003707
13	1	0	-1.182530	2.026344	-1.351770
14	1	0	-0.886594	0.341762	-1.758437
15	6	0	-2.830453	0.727443	-0.884039
16	1	0	-3.281966	1.468192	-0.209913
17	1	0	-3.308720	0.865475	-1.859108
18	6	0	-3.115229	-0.679001	-0.347983
19	1	0	-2.800632	-1.421271	-1.088811
20	1	0	-4.190134	-0.820745	-0.194957
21	6	0	-2.369551	-0.910507	0.971722
22	1	0	-2.530674	-1.933044	1.335882
23	1	0	-2.778876	-0.246750	1.742042
24	6	0	1.570306	1.073562	1.689990
25	1	0	1.017851	1.695152	2.401007
26	1	0	1.593134	0.053083	2.070146

27	1	0	2.600242	1.437320	1.651223
28	6	0	1.106092	2.607811	-0.212368
29	1	0	0.508408	3.293869	0.392158
30	1	0	2.153107	2.911774	-0.121329
31	1	0	0.810713	2.721789	-1.256149
32	8	0	3.102451	-1.457320	-0.946044
33	1	0	-0.653247	-2.544720	0.179204

Data 51: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of (6*R**,7*S**)-5,5-dimethyl-6,7-tetramethylene-1,2,4-triazepan-3-one with pseudo axial orientation of the N(1)H proton [**4i(H$_{ax}$)**] (DMSO solution)



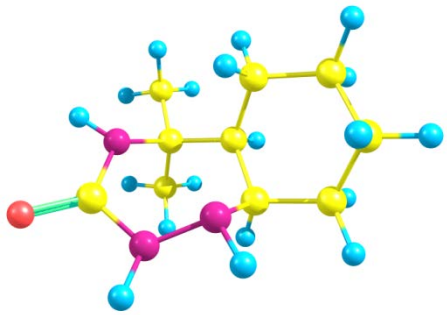
Electronic Energy =	-632.177842319 a.u.
Zero-point correction=	0.294600 (Hartree/Particle)
Thermal correction to Energy=	0.307723
Thermal correction to Enthalpy=	0.308667
Thermal correction to Gibbs Free Energy=	0.256596
Sum of electronic and zero-point Energies=	-631.883243
Sum of electronic and thermal Energies=	-631.870119
Sum of electronic and thermal Enthalpies=	-631.869175
Sum of electronic and thermal Free Energies=	-631.921246

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.681846	0.321295	-0.682317
2	1	0	2.417406	0.829334	-1.156682
3	7	0	-0.228697	-1.718339	0.033126
4	1	0	-0.471789	-1.605214	-0.947398
5	7	0	1.176404	-1.817072	0.152360
6	1	0	1.499732	-2.774023	0.193416
7	6	0	2.070655	-0.981198	-0.490314
8	6	0	0.910221	1.169526	0.277388
9	6	0	-0.597736	0.775282	0.331186
10	1	0	-1.037843	1.451238	1.075846
11	6	0	-0.843444	-0.663124	0.860198
12	1	0	-0.396860	-0.772986	1.850016
13	6	0	-1.360990	1.000002	-0.991571
14	1	0	-1.239822	2.032873	-1.323379
15	1	0	-0.930958	0.377055	-1.784896
16	6	0	-2.861753	0.699257	-0.852067
17	1	0	-3.309305	1.429712	-0.165811
18	1	0	-3.356035	0.836162	-1.819197
19	6	0	-3.118530	-0.712959	-0.315095
20	1	0	-2.817528	-1.455057	-1.065129
21	1	0	-4.188994	-0.868257	-0.148064
22	6	0	-2.350289	-0.943969	0.992153
23	1	0	-2.487745	-1.968451	1.349473
24	1	0	-2.751132	-0.276843	1.764232
25	6	0	1.549531	1.096230	1.681161
26	1	0	0.992468	1.722022	2.383617
27	1	0	1.573774	0.080503	2.075526
28	1	0	2.577405	1.465203	1.639646
29	6	0	1.071712	2.612598	-0.233492
30	1	0	0.468001	3.295385	0.367955
31	1	0	2.116162	2.925364	-0.147803

32	1	0	0.773065	2.715728	-1.277493
33	8	0	3.168358	-1.406351	-0.867917

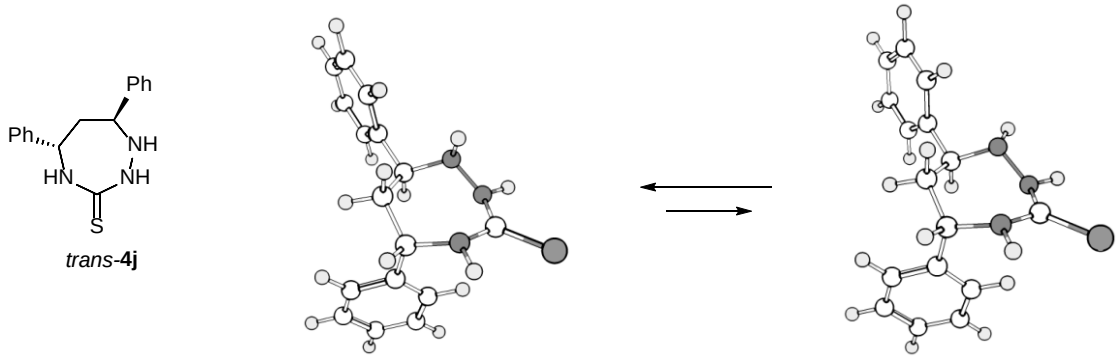
Data 52: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of (6*R**,7*S**)-5,5-dimethyl-6,7-tetramethylene-1,2,4-triazepan-3-one with pseudo equatorial orientation of the N(1)H proton [**4i(H$_{eq}$)**] (DMSO solution)



Electronic Energy =	-632.172253906 a.u.
Zero-point correction=	0.294291 (Hartree/Particle)
Thermal correction to Energy=	0.307504
Thermal correction to Enthalpy=	0.308449
Thermal correction to Gibbs Free Energy=	0.256195
Sum of electronic and zero-point Energies=	-631.877963
Sum of electronic and thermal Energies=	-631.864749
Sum of electronic and thermal Enthalpies=	-631.863805
Sum of electronic and thermal Free Energies=	-631.916059

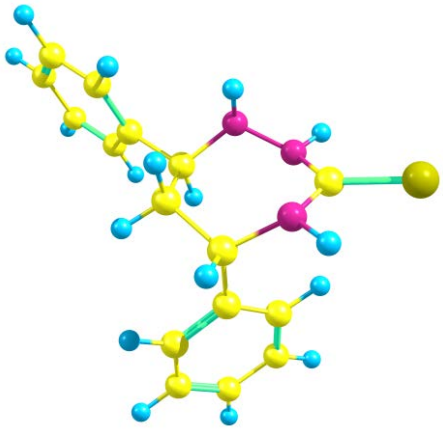
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.693870	0.322689	-0.681281
2	1	0	2.432524	0.831979	-1.149194
3	7	0	-0.240194	-1.642331	-0.066553
4	7	0	1.176717	-1.797551	0.162845
5	1	0	1.471337	-2.764950	0.148297
6	6	0	2.067325	-0.984498	-0.505229
7	6	0	0.919173	1.164638	0.281565
8	6	0	-0.592677	0.775917	0.333224
9	1	0	-1.023568	1.447616	1.087222
10	6	0	-0.849342	-0.659591	0.853624
11	1	0	-0.412354	-0.772841	1.853196
12	6	0	-1.352414	1.015617	-0.987423
13	1	0	-1.223998	2.050697	-1.310495
14	1	0	-0.925990	0.381525	-1.769776
15	6	0	-2.855483	0.728365	-0.849718
16	1	0	-3.297638	1.452003	-0.152042
17	1	0	-3.350034	0.884398	-1.814096
18	6	0	-3.124134	-0.690095	-0.337399
19	1	0	-2.823460	-1.418347	-1.098217
20	1	0	-4.195432	-0.838355	-0.167136
21	6	0	-2.356039	-0.946537	0.964738
22	1	0	-2.502512	-1.977848	1.306821
23	1	0	-2.756800	-0.301763	1.754822
24	6	0	1.557830	1.086499	1.685905
25	1	0	1.004124	1.714709	2.388904
26	1	0	1.575889	0.070292	2.078784
27	1	0	2.587600	1.450430	1.644173
28	6	0	1.082964	2.610227	-0.222333
29	1	0	0.475600	3.290805	0.377993
30	1	0	2.126944	2.922628	-0.128983
31	1	0	0.790460	2.717086	-1.267608
32	8	0	3.160656	-1.420751	-0.890135
33	1	0	-0.633914	-2.556970	0.131609



trans-**4j**

Data 53: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of (5*R**,7*R**)-5,7-diphenyl-1,2,4-triazepane-3-thione with pseudo axial orientation of the N(1)H proton [*trans*-**4j(H$_{ax}$)**] (the gas phase)



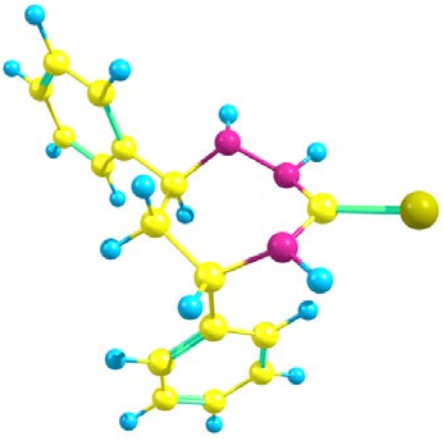
Electronic Energy =	-1182.59254388 a.u.
Zero-point correction=	0.305026 (Hartree/Particle)
Thermal correction to Energy=	0.321824
Thermal correction to Enthalpy=	0.322768
Thermal correction to Gibbs Free Energy=	0.257999
Sum of electronic and zero-point Energies=	-1182.287518
Sum of electronic and thermal Energies=	-1182.270720
Sum of electronic and thermal Enthalpies=	-1182.269776
Sum of electronic and thermal Free Energies=	-1182.334545

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.089086	-0.000149	1.379058
2	6	0	0.447952	0.075212	1.292687
3	6	0	1.044989	-0.243494	-0.085610
4	7	0	0.788081	-1.635142	-0.503552
5	7	0	-0.541045	-1.902494	-0.889772
6	6	0	-1.600594	-2.080055	-0.036682
7	7	0	-1.626829	-1.349161	1.116885
8	1	0	1.069107	-2.288598	0.226069
9	1	0	-0.598991	-2.478752	-1.717384
10	1	0	-2.456032	-1.569599	1.650820
11	1	0	0.863152	-0.616055	2.034119
12	1	0	0.754337	1.080237	1.593296
13	1	0	0.564974	0.383024	-0.840969
14	16	0	-2.833352	-3.154629	-0.426705
15	6	0	2.541749	0.018627	-0.135325
16	6	0	3.423888	-0.591667	0.764013
17	6	0	3.068234	0.875819	-1.105669
18	6	0	4.795234	-0.355391	0.690328
19	6	0	4.438306	1.120790	-1.178198
20	6	0	5.306926	0.504017	-0.280367

21	1	0	3.048752	-1.259774	1.532337
22	1	0	2.399243	1.354640	-1.813232
23	1	0	5.463402	-0.841039	1.392829
24	1	0	4.826044	1.790977	-1.937339
25	1	0	6.373302	0.691179	-0.335653
26	6	0	-1.788722	1.125571	0.604518
27	6	0	-1.564293	2.448237	1.012279
28	6	0	-2.660808	0.898507	-0.462192
29	6	0	-2.177224	3.514355	0.361299
30	6	0	-3.275433	1.967709	-1.116833
31	6	0	-3.034341	3.277086	-0.713094
32	1	0	-0.911703	2.650941	1.855865
33	1	0	-2.882697	-0.109347	-0.787338
34	1	0	-1.991755	4.528422	0.697595
35	1	0	-3.948612	1.768035	-1.942970
36	1	0	-3.514830	4.104829	-1.222166
37	1	0	-1.326170	0.161475	2.435208

Data 54: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of (5*R**,7*R**)-5,7-diphenyl-1,2,4-triazepane-3-thione with pseudo equatorial orientation of the N(1)H proton [*trans*-**4h(H$_{eq}$)**] (the gas phase)



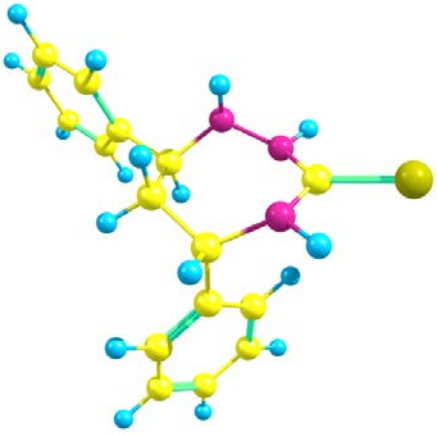
Electronic Energy =	-1182.58894772 a.u.
Zero-point correction=	0.305036 (Hartree/Particle)
Thermal correction to Energy=	0.321829
Thermal correction to Enthalpy=	0.322774
Thermal correction to Gibbs Free Energy=	0.258478
Sum of electronic and zero-point Energies=	-1182.283911
Sum of electronic and thermal Energies=	-1182.267118
Sum of electronic and thermal Enthalpies=	-1182.266174
Sum of electronic and thermal Free Energies=	-1182.330470

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.075471	0.005726	1.366840
2	6	0	0.460062	0.096632	1.257435
3	6	0	1.051792	-0.225454	-0.119690
4	7	0	0.806190	-1.659217	-0.401283
5	7	0	-0.532000	-1.902335	-0.874317
6	6	0	-1.574494	-2.097428	-0.011537
7	7	0	-1.610011	-1.347483	1.125562
8	1	0	1.410549	-1.944447	-1.165668
9	1	0	-0.567227	-2.553847	-1.646174
10	1	0	-2.434995	-1.565099	1.666771
11	1	0	0.899335	-0.588269	1.987727
12	1	0	0.754194	1.110532	1.537950
13	1	0	0.567175	0.398977	-0.881528
14	16	0	-2.797994	-3.188985	-0.395793

15	6	0	2.546039	0.031812	-0.159354
16	6	0	3.438437	-0.773657	0.560360
17	6	0	3.056230	1.092609	-0.914254
18	6	0	4.808190	-0.520828	0.521931
19	6	0	4.425713	1.351274	-0.946142
20	6	0	5.305686	0.543943	-0.228371
21	1	0	3.059024	-1.603428	1.145631
22	1	0	2.376673	1.721191	-1.480798
23	1	0	5.487464	-1.154835	1.080915
24	1	0	4.803746	2.179597	-1.534926
25	1	0	6.371393	0.741297	-0.254668
26	6	0	-1.801375	1.118248	0.595791
27	6	0	-1.585496	2.447320	0.986831
28	6	0	-2.693336	0.870901	-0.449983
29	6	0	-2.225822	3.499901	0.339866
30	6	0	-3.335589	1.926245	-1.100461
31	6	0	-3.102704	3.242363	-0.713686
32	1	0	-0.918136	2.665965	1.814753
33	1	0	-2.908392	-0.142978	-0.760941
34	1	0	-2.046631	4.519204	0.663708
35	1	0	-4.024078	1.710579	-1.909855
36	1	0	-3.604946	4.059390	-1.219145
37	1	0	-1.293668	0.175544	2.425744

Data 55: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of (5*R**,7*R**)-5,7-diphenyl-1,2,4-triazepane-3-thione with pseudo axial orientation of the N(1)H proton [*trans*-**4j(H$_{ax}$)**] (DMSO solution)



Electronic Energy =	-1182.60858876 a.u.
Zero-point correction=	0.304988 (Hartree/Particle)
Thermal correction to Energy=	0.321855
Thermal correction to Enthalpy=	0.322799
Thermal correction to Gibbs Free Energy=	0.258022
Sum of electronic and zero-point Energies=	-1182.304260
Sum of electronic and thermal Energies=	-1182.287393
Sum of electronic and thermal Enthalpies=	-1182.286448
Sum of electronic and thermal Free Energies=	-1182.351225

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.089086	-0.000149	1.379058
2	6	0	0.447952	0.075212	1.292687
3	6	0	1.044989	-0.243494	-0.085610
4	7	0	0.788081	-1.635142	-0.503552
5	7	0	-0.541045	-1.902494	-0.889772
6	6	0	-1.600594	-2.080055	-0.036682
7	7	0	-1.626829	-1.349161	1.116885
8	1	0	1.069107	-2.288598	0.226069
9	1	0	-0.598991	-2.478752	-1.717384

10	1	0	-2.456032	-1.569599	1.650820
11	1	0	0.863152	-0.616055	2.034119
12	1	0	0.754337	1.080237	1.593296
13	1	0	0.564974	0.383024	-0.840969
14	16	0	-2.833352	-3.154629	-0.426705
15	6	0	2.541749	0.018627	-0.135325
16	6	0	3.423888	-0.591667	0.764013
17	6	0	3.068234	0.875819	-1.105669
18	6	0	4.795234	-0.355391	0.690328
19	6	0	4.438306	1.120790	-1.178198
20	6	0	5.306926	0.504017	-0.280367
21	1	0	3.048752	-1.259774	1.532337
22	1	0	2.399243	1.354640	-1.813232
23	1	0	5.463402	-0.841039	1.392829
24	1	0	4.826044	1.790977	-1.937339
25	1	0	6.373302	0.691179	-0.335653
26	6	0	-1.788722	1.125571	0.604518
27	6	0	-1.564293	2.448237	1.012279
28	6	0	-2.660808	0.898507	-0.462192
29	6	0	-2.177224	3.514355	0.361299
30	6	0	-3.275433	1.967709	-1.116833
31	6	0	-3.034341	3.277086	-0.713094
32	1	0	-0.911703	2.650941	1.855865
33	1	0	-2.882697	-0.109347	-0.787338
34	1	0	-1.991755	4.528422	0.697595
35	1	0	-3.948612	1.768035	-1.942970
36	1	0	-3.514830	4.104829	-1.222166
37	1	0	-1.326170	0.161475	2.435208

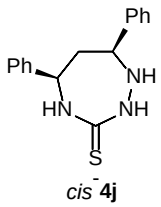
Data 56: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of (5*R**,7*R**)-5,7-diphenyl-1,2,4-triazepane-3-thione with pseudo equatorial orientation of the N(1)H proton [*trans*-**4h(H$_{eq}$)**] (DMSO solution)

Electronic Energy =	-1182.60574412 a.u.
Zero-point correction=	0.304903 (Hartree/Particle)
Thermal correction to Energy=	0.321826
Thermal correction to Enthalpy=	0.322770
Thermal correction to Gibbs Free Energy=	0.257943
Sum of electronic and zero-point Energies=	-1182.301649
Sum of electronic and thermal Energies=	-1182.284726
Sum of electronic and thermal Enthalpies=	-1182.283782
Sum of electronic and thermal Free Energies=	-1182.348608

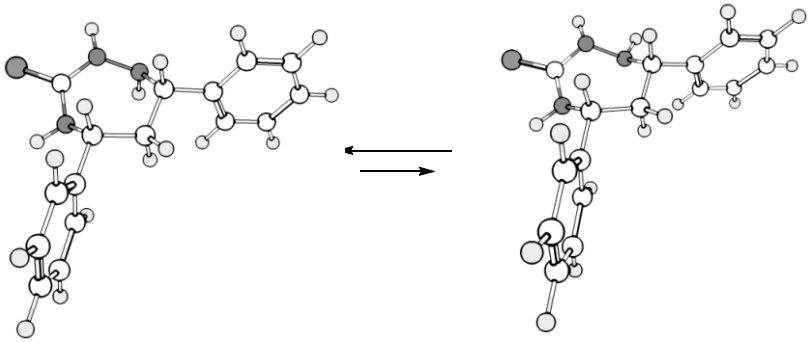
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.075471	0.005726	1.366840
2	6	0	0.460062	0.096632	1.257435
3	6	0	1.051792	-0.225454	-0.119690

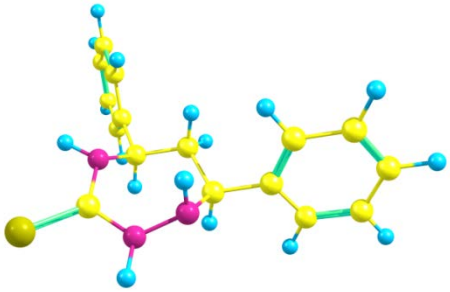
4	7	0	0.806190	-1.659217	-0.401283
5	7	0	-0.532000	-1.902335	-0.874317
6	6	0	-1.574494	-2.097428	-0.011537
7	7	0	-1.610011	-1.347483	1.125562
8	1	0	1.410549	-1.944447	-1.165668
9	1	0	-0.567227	-2.553847	-1.646174
10	1	0	-2.434995	-1.565099	1.666771
11	1	0	0.899335	-0.588269	1.987727
12	1	0	0.754194	1.110532	1.537950
13	1	0	0.567175	0.398977	-0.881528
14	16	0	-2.797994	-3.188985	-0.395793
15	6	0	2.546039	0.031812	-0.159354
16	6	0	3.438437	-0.773657	0.560360
17	6	0	3.056230	1.092609	-0.914254
18	6	0	4.808190	-0.520828	0.521931
19	6	0	4.425713	1.351274	-0.946142
20	6	0	5.305686	0.543943	-0.228371
21	1	0	3.059024	-1.603428	1.145631
22	1	0	2.376673	1.721191	-1.480798
23	1	0	5.487464	-1.154835	1.080915
24	1	0	4.803746	2.179597	-1.534926
25	1	0	6.371393	0.741297	-0.254668
26	6	0	-1.801375	1.118248	0.595791
27	6	0	-1.585496	2.447320	0.986831
28	6	0	-2.693336	0.870901	-0.449983
29	6	0	-2.225822	3.499901	0.339866
30	6	0	-3.335589	1.926245	-1.100461
31	6	0	-3.102704	3.242363	-0.713686
32	1	0	-0.918136	2.665965	1.814753
33	1	0	-2.908392	-0.142978	-0.760941
34	1	0	-2.046631	4.519204	0.663708
35	1	0	-4.024078	1.710579	-1.909855
36	1	0	-3.604946	4.059390	-1.219145
37	1	0	-1.293668	0.175544	2.425744



cis-**4j**



Data 57: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of (5*R**,7*S**)-5,7-diphenyl-1,2,4-triazepane-3-thione with pseudo axial orientation of the N(1)H proton [*cis*-**4j(H$_{ax}$)**] (the gas phase)



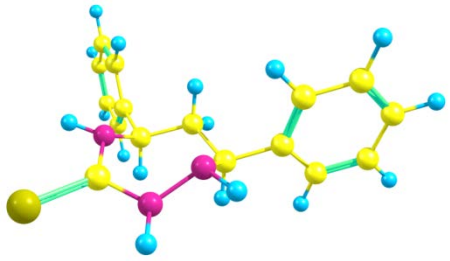
Electronic Energy =	-1182.59717934 a.u.
Zero-point correction=	0.304661 (Hartree/Particle)
Thermal correction to Energy=	0.321597
Thermal correction to Enthalpy=	0.322541
Thermal correction to Gibbs Free Energy=	0.256909
Sum of electronic and zero-point Energies=	-1182.292518

Sum of electronic and thermal Energies= -1182.275582
Sum of electronic and thermal Enthalpies= -1182.274638
Sum of electronic and thermal Free Energies= -1182.340270

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.156481	0.049092	-0.439367
2	6	0	-0.216182	-0.571150	-0.124327
3	6	0	-1.408683	0.319717	-0.508638
4	7	0	-1.385701	1.652483	0.126101
5	7	0	-0.376714	2.519372	-0.350369
6	6	0	0.926408	2.496003	0.086808
7	7	0	1.444382	1.261497	0.368932
8	1	0	-1.315576	1.571642	1.138988
9	1	0	-0.719570	3.453849	-0.525093
10	1	0	2.411022	1.335971	0.656461
11	6	0	2.272341	-0.956839	-0.217555
12	6	0	2.969882	-1.483789	-1.307514
13	6	0	3.977524	-2.428944	-1.119329
14	6	0	4.305418	-2.853644	0.165982
15	6	0	3.619494	-2.329625	1.261156
16	6	0	2.608363	-1.390859	1.070891
17	6	0	-2.742820	-0.342013	-0.203379
18	6	0	-3.060833	-0.788056	1.084690
19	6	0	-4.299070	-1.367683	1.353949
20	6	0	-5.237556	-1.520534	0.334974
21	6	0	-4.930595	-1.085399	-0.952483
22	6	0	-3.694297	-0.498408	-1.215258
23	1	0	1.165236	0.336901	-1.498303
24	1	0	-0.292999	-1.517221	-0.669161
25	1	0	-0.255498	-0.815423	0.941958
26	1	0	-1.367143	0.515650	-1.583764
27	1	0	2.727809	-1.149026	-2.310993
28	1	0	4.509871	-2.825837	-1.976337
29	1	0	5.092501	-3.583998	0.314923
30	1	0	3.871348	-2.652740	2.265017
31	1	0	2.082448	-0.989918	1.930813
32	1	0	-2.342635	-0.687703	1.891839
33	1	0	-4.528941	-1.703139	2.359131
34	1	0	-6.199360	-1.975298	0.543179
35	1	0	-5.653665	-1.199550	-1.752405
36	1	0	-3.467251	-0.152792	-2.218562
37	16	0	1.814586	3.907372	0.241004

Data 58: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of (5*R**,7*S**)-5,7-diphenyl-1,2,4-triazepane-3-thione with pseudo equatorial orientation of the N(1)H proton [*cis*-**4h(H$_{eq}$)**] (the gas phase)



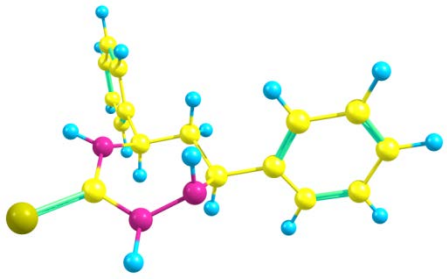
Electronic Energy = -1182.59379646 a.u.
Zero-point correction= 0.304590 (Hartree/Particle)
Thermal correction to Energy= 0.321498
Thermal correction to Enthalpy= 0.322442
Thermal correction to Gibbs Free Energy= 0.257790
Sum of electronic and zero-point Energies= -1182.289207
Sum of electronic and thermal Energies= -1182.272298

Sum of electronic and thermal Enthalpies= -1182.271354
Sum of electronic and thermal Free Energies= -1182.336006

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.161276	0.046573	-0.446937
2	6	0	-0.224060	-0.546768	-0.128795
3	6	0	-1.406716	0.342005	-0.537614
4	7	0	-1.310624	1.627497	0.188310
5	7	0	-0.338408	2.514084	-0.392460
6	6	0	0.959266	2.501083	0.051068
7	7	0	1.477959	1.271146	0.329132
8	1	0	-2.200526	2.110959	0.123740
9	1	0	-0.679224	3.455104	-0.534280
10	1	0	2.448240	1.338417	0.605023
11	6	0	2.253323	-0.978296	-0.193397
12	6	0	2.943372	-1.551421	-1.264579
13	6	0	3.928139	-2.513774	-1.044719
14	6	0	4.239793	-2.909747	0.253792
15	6	0	3.560903	-2.339455	1.330149
16	6	0	2.572742	-1.383233	1.108581
17	6	0	-2.738813	-0.306235	-0.213404
18	6	0	-3.149326	-0.486530	1.114020
19	6	0	-4.372782	-1.087954	1.400847
20	6	0	-5.200412	-1.525448	0.367314
21	6	0	-4.800722	-1.351321	-0.955841
22	6	0	-3.579999	-0.741557	-1.242031
23	1	0	1.180473	0.307319	-1.513490
24	1	0	-0.306235	-1.499228	-0.660734
25	1	0	-0.287314	-0.759577	0.941553
26	1	0	-1.357999	0.518295	-1.622101
27	1	0	2.713824	-1.239158	-2.278261
28	1	0	4.455495	-2.946481	-1.887415
29	1	0	5.008876	-3.653761	0.427388
30	1	0	3.800310	-2.640102	2.344018
31	1	0	2.051148	-0.945326	1.952860
32	1	0	-2.511575	-0.148056	1.922449
33	1	0	-4.678931	-1.217627	2.432959
34	1	0	-6.150515	-1.996688	0.592237
35	1	0	-5.438988	-1.685865	-1.766003
36	1	0	-3.277652	-0.602994	-2.275212
37	16	0	1.847013	3.919260	0.170605

Data 59: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of (5*R**,7*S**)-5,7-diphenyl-1,2,4-triazepane-3-thione with pseudo axial orientation of the N(1)H proton [*cis*-**4j(H$_{ax}$)**] (DMSO solution)



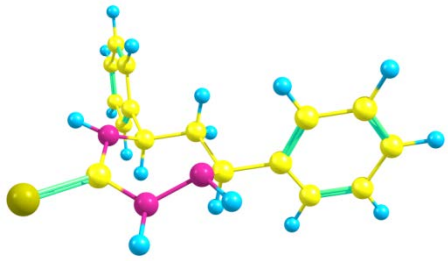
Electronic Energy = -1182.61362280 a.u.
Zero-point correction= 0.304612 (Hartree/Particle)
Thermal correction to Energy= 0.321591
Thermal correction to Enthalpy= 0.322535
Thermal correction to Gibbs Free Energy= 0.257348
Sum of electronic and zero-point Energies= -1182.309010
Sum of electronic and thermal Energies= -1182.292032
Sum of electronic and thermal Enthalpies= -1182.291088

Sum of electronic and thermal Free Energies= -1182.356274

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.146863	0.027257	-0.444117
2	6	0	-0.225249	-0.560420	-0.078520
3	6	0	-1.406035	0.337580	-0.475053
4	7	0	-1.375003	1.663650	0.181950
5	7	0	-0.374565	2.542580	-0.291990
6	6	0	0.940932	2.490568	0.062221
7	7	0	1.481680	1.272675	0.301665
8	1	0	-1.270550	1.562206	1.190294
9	1	0	-0.722082	3.474673	-0.468466
10	1	0	2.454157	1.335629	0.570764
11	6	0	2.258499	-0.980815	-0.210059
12	6	0	2.933962	-1.539812	-1.298677
13	6	0	3.937634	-2.488631	-1.101528
14	6	0	4.281984	-2.883510	0.190223
15	6	0	3.616245	-2.326897	1.283104
16	6	0	2.608849	-1.384458	1.084691
17	6	0	-2.746777	-0.319415	-0.189436
18	6	0	-3.111493	-0.706337	1.106580
19	6	0	-4.351805	-1.294392	1.351460
20	6	0	-5.244235	-1.514555	0.301995
21	6	0	-4.889163	-1.138517	-0.992724
22	6	0	-3.650762	-0.542999	-1.233075
23	1	0	1.134533	0.277563	-1.511003
24	1	0	-0.321137	-1.517550	-0.598927
25	1	0	-0.255946	-0.772200	0.994835
26	1	0	-1.351684	0.541982	-1.547254
27	1	0	2.675905	-1.231018	-2.306208
28	1	0	4.452313	-2.912589	-1.956326
29	1	0	5.064848	-3.617095	0.345675
30	1	0	3.879398	-2.628057	2.290808
31	1	0	2.097699	-0.961692	1.942980
32	1	0	-2.431509	-0.554182	1.937918
33	1	0	-4.618581	-1.584339	2.361640
34	1	0	-6.206604	-1.975993	0.492360
35	1	0	-5.574696	-1.306086	-1.815932
36	1	0	-3.384473	-0.248895	-2.243034
37	16	0	1.853558	3.919838	0.177249

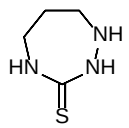
Data 60: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of (5*R**,7*S**)-5,7-diphenyl-1,2,4-triazepane-3-thione with pseudo equatorial orientation of the N(1)H proton [*cis*-**4h(H$_{eq}$)**] (DMSO solution)



Electronic Energy = -1182.61147439 a.u.
Zero-point correction= 0.304486 (Hartree/Particle)
Thermal correction to Energy= 0.321490
Thermal correction to Enthalpy= 0.322434
Thermal correction to Gibbs Free Energy= 0.257523
Sum of electronic and zero-point Energies= -1182.306988
Sum of electronic and thermal Energies= -1182.289984
Sum of electronic and thermal Enthalpies= -1182.289040
Sum of electronic and thermal Free Energies= -1182.353952

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.152294	0.036843	-0.436264
2	6	0	-0.229234	-0.550741	-0.107732
3	6	0	-1.404541	0.353924	-0.495071
4	7	0	-1.314161	1.618486	0.277782
5	7	0	-0.357837	2.540769	-0.249213
6	6	0	0.951695	2.491872	0.077076
7	7	0	1.484142	1.269527	0.334063
8	1	0	-2.206157	2.100694	0.226628
9	1	0	-0.716810	3.465760	-0.440412
10	1	0	2.464482	1.334216	0.573151
11	6	0	2.250092	-0.984765	-0.194866
12	6	0	2.933424	-1.544744	-1.278120
13	6	0	3.923974	-2.505870	-1.074178
14	6	0	4.247249	-2.912594	0.219384
15	6	0	3.573585	-2.355192	1.307012
16	6	0	2.579347	-1.400268	1.101634
17	6	0	-2.742646	-0.298031	-0.201636
18	6	0	-3.141993	-0.575267	1.112786
19	6	0	-4.371991	-1.180127	1.366821
20	6	0	-5.217211	-1.524287	0.311191
21	6	0	-4.827903	-1.253389	-0.999896
22	6	0	-3.600505	-0.640239	-1.252298
23	1	0	1.162438	0.301233	-1.500483
24	1	0	-0.321268	-1.490434	-0.658987
25	1	0	-0.283719	-0.784317	0.958906
26	1	0	-1.350966	0.569313	-1.570254
27	1	0	2.691826	-1.226849	-2.286941
28	1	0	4.444958	-2.930216	-1.924992
29	1	0	5.019735	-3.655977	0.380248
30	1	0	3.820325	-2.665542	2.316116
31	1	0	2.061590	-0.976341	1.955263
32	1	0	-2.492791	-0.315934	1.941071
33	1	0	-4.668693	-1.385795	2.389260
34	1	0	-6.171744	-1.998439	0.509767
35	1	0	-5.478875	-1.515077	-1.826524
36	1	0	-3.306413	-0.427115	-2.274733
37	16	0	1.887079	3.916037	0.122464



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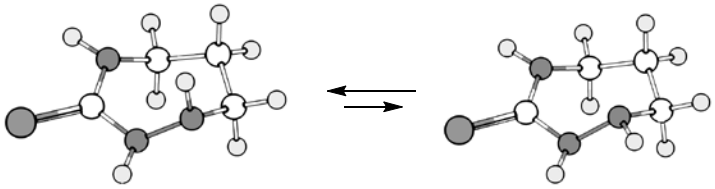
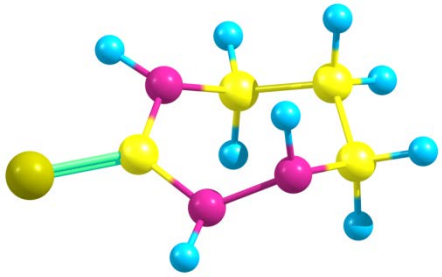


Data 61: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of 1,2,4-triazepane-3-thione with pseudo axial orientation of the N(1)H proton [**8(H$_{ax}$)**] (the gas phase)



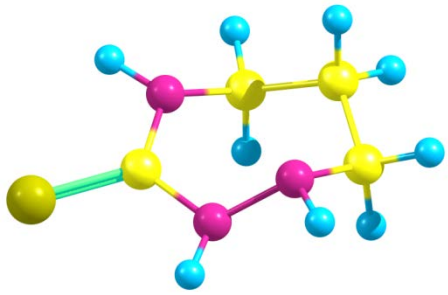
Electronic Energy =	-720.386623293 a.u.
Zero-point correction=	0.144212 (Hartree/Particle)
Thermal correction to Energy=	0.151691

Thermal correction to Enthalpy=	0.152635
Thermal correction to Gibbs Free Energy=	0.111966
Sum of electronic and zero-point Energies=	-720.242412
Sum of electronic and thermal Energies=	-720.234933
Sum of electronic and thermal Enthalpies=	-720.233988
Sum of electronic and thermal Free Energies=	-720.274657

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.036176	1.482765	0.316340
2	6	0	-2.244473	0.679105	-0.162454
3	6	0	-2.155283	-0.805950	0.194383
4	7	0	-0.968984	-1.490563	-0.323486
5	7	0	0.246005	-1.121537	0.299685
6	6	0	0.965723	0.008397	-0.014472
7	7	0	0.235160	1.119247	-0.333626
8	1	0	-0.933089	1.386632	1.405165
9	1	0	-1.193983	2.540087	0.096830
10	1	0	-3.146157	1.106314	0.291501
11	1	0	-2.345773	0.794706	-1.247695
12	1	0	-3.024259	-1.339512	-0.202214
13	1	0	-2.157107	-0.944064	1.279119
14	1	0	0.831613	-1.917436	0.510265
15	1	0	0.840745	1.898846	-0.546035
16	16	0	2.640529	0.005990	0.015122
17	1	0	-0.884464	-1.357353	-1.329679

Data 62: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of 1,2,4-triazepane-3-thione with pseudo equatorial orientation of the N(1)H proton [**8(H_{eq})**] (the gas phase)



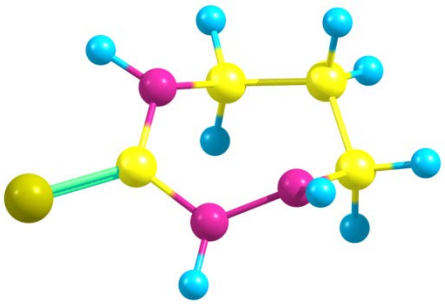
Electronic Energy =	-720.379864631 a.u.
Zero-point correction=	0.143883 (Hartree/Particle)
Thermal correction to Energy=	0.151448
Thermal correction to Enthalpy=	0.152393
Thermal correction to Gibbs Free Energy=	0.111617
Sum of electronic and zero-point Energies=	-720.235982
Sum of electronic and thermal Energies=	-720.228416
Sum of electronic and thermal Enthalpies=	-720.227472
Sum of electronic and thermal Free Energies=	-720.268248

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.027805	1.492682	0.307632
2	6	0	-2.236520	0.689774	-0.176056
3	6	0	-2.163104	-0.788176	0.195121
4	7	0	-0.978063	-1.398815	-0.419250

5	7	0	0.232659	-1.094537	0.299119
6	6	0	0.969894	0.017438	-0.026641
7	7	0	0.253006	1.136632	-0.324763
8	1	0	-0.935025	1.399423	1.398336
9	1	0	-1.188657	2.548686	0.084273
10	1	0	-3.134180	1.127780	0.274342
11	1	0	-2.324224	0.784413	-1.262097
12	1	0	-3.032283	-1.314177	-0.209525
13	1	0	-2.163751	-0.911242	1.288605
14	1	0	-1.059496	-2.408878	-0.404414
15	1	0	0.822736	-1.899467	0.459029
16	1	0	0.858738	1.916784	-0.533149
17	16	0	2.646759	-0.013537	0.013657

Data 63: Cartesian coordinates, energy, imaginary frequency of the transition state for the transformation of conformer **8(H_{ax})** into conformer **8(H_{eq})** (the gas phase)

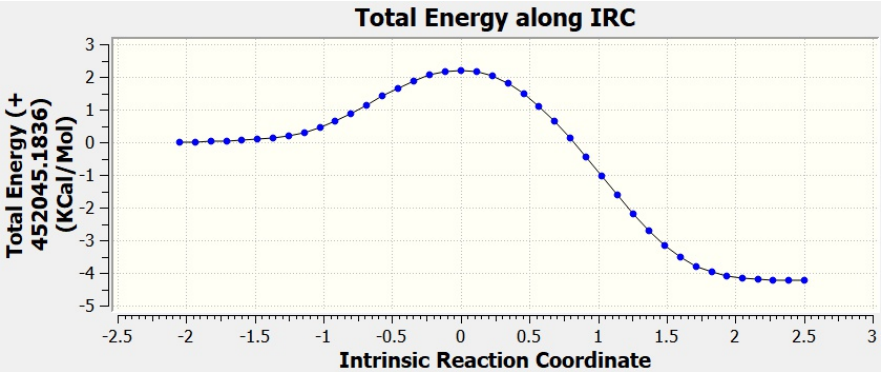


Imaginary Frequency=	-516.1188 cm^{-1}
Electronic Energy =	-720.376318849 a.u.
Zero-point correction=	0.142546 (Hartree/Particle)
Thermal correction to Energy=	0.149942
Thermal correction to Enthalpy=	0.150886
Thermal correction to Gibbs Free Energy=	0.110348
Sum of electronic and zero-point Energies=	-720.233772
Sum of electronic and thermal Energies=	-720.226377
Sum of electronic and thermal Enthalpies=	-720.225433
Sum of electronic and thermal Free Energies=	-720.265970

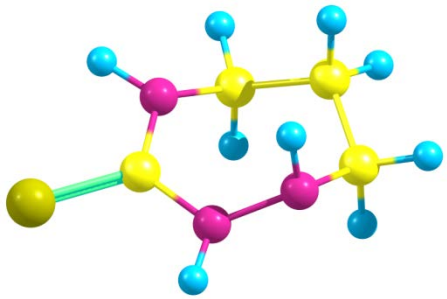
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.005646	1.479854	0.289217
2	6	0	-2.259122	0.700887	-0.119605
3	6	0	-2.171327	-0.786536	0.237605
4	7	0	-0.990790	-1.375969	-0.351056
5	7	0	0.247113	-1.129229	0.213612
6	6	0	0.978842	-0.005428	-0.066155
7	7	0	0.244413	1.099524	-0.401452
8	1	0	-1.038532	-2.140870	-1.001073
9	1	0	0.773473	-1.910936	0.580041
10	1	0	0.852516	1.879521	-0.605587
11	1	0	-2.412401	0.803670	-1.198158
12	1	0	-3.118807	1.155189	0.387587
13	1	0	-2.166491	-0.917418	1.329442
14	16	0	2.650411	0.001603	0.059160
15	1	0	-3.041107	-1.321431	-0.153154
16	1	0	-1.157237	2.537179	0.065132
17	1	0	-0.859630	1.396517	1.375104

Data 64: The intrinsic reaction coordinate analysis for the transformation of conformer **8(H_{eq})** into conformer **8(H_{ax})** (the gas phase)



Data 65: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of 1,2,4-triazepane-3-thione with pseudo axial orientation of the N(1)H proton [**8(H_{ax})**] (DMSO solution)

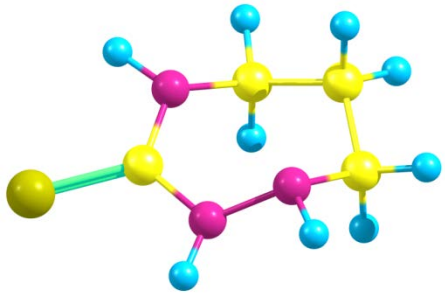


Electronic Energy =	-720.400367971 a.u.
Zero-point correction=	0.144131 (Hartree/Particle)
Thermal correction to Energy=	0.151685
Thermal correction to Enthalpy=	0.152630
Thermal correction to Gibbs Free Energy=	0.111830
Sum of electronic and zero-point Energies=	-720.256237
Sum of electronic and thermal Energies=	-720.248683
Sum of electronic and thermal Enthalpies=	-720.247738
Sum of electronic and thermal Free Energies=	-720.288538

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.061597	1.494889	0.298189
2	6	0	-2.245265	0.665863	-0.189333
3	6	0	-2.154053	-0.802642	0.218672
4	7	0	-0.976931	-1.505457	-0.306941
5	7	0	0.259356	-1.129143	0.270965
6	6	0	0.950218	0.014268	-0.012172
7	7	0	0.244980	1.131848	-0.289196
8	1	0	-0.986824	1.430232	1.390347
9	1	0	-1.215572	2.542711	0.041235
10	1	0	-3.156680	1.101194	0.233533
11	1	0	-2.325985	0.744481	-1.279001
12	1	0	-3.027099	-1.347876	-0.149163
13	1	0	-2.137657	-0.905351	1.307075
14	1	0	0.847722	-1.922179	0.483320
15	1	0	0.839513	1.917283	-0.511489
16	16	0	2.653115	0.006980	0.011568
17	1	0	-0.914908	-1.387176	-1.316880

Data 66: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of 1,2,4-triazepane-3-thione with pseudo equatorial orientation of the N(1)H proton [**8(H_{eq})**] (DMSO solution)

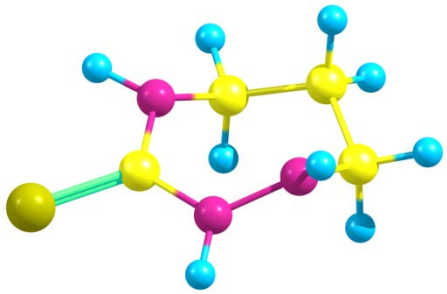


Electronic Energy =	-720.396607895 a.u.
Zero-point correction=	0.143892 (Hartree/Particle)
Thermal correction to Energy=	0.151534
Thermal correction to Enthalpy=	0.152479
Thermal correction to Gibbs Free Energy=	0.111523
Sum of electronic and zero-point Energies=	-720.252716
Sum of electronic and thermal Energies=	-720.245073
Sum of electronic and thermal Enthalpies=	-720.244129
Sum of electronic and thermal Free Energies=	-720.285085

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.034540	1.508579	0.281085
2	6	0	-2.245496	0.690907	-0.158038
3	6	0	-2.153200	-0.774814	0.244341
4	7	0	-1.001488	-1.409939	-0.418117
5	7	0	0.251798	-1.122040	0.211218
6	6	0	0.952662	0.005458	-0.044366
7	7	0	0.252656	1.127207	-0.341145
8	1	0	-0.928848	1.454595	1.371992
9	1	0	-1.187104	2.555039	0.017526
10	1	0	-3.130326	1.135095	0.308531
11	1	0	-2.369055	0.764533	-1.242512
12	1	0	-3.037527	-1.314640	-0.101317
13	1	0	-2.095243	-0.876443	1.336907
14	1	0	-1.095515	-2.418637	-0.372004
15	1	0	0.817589	-1.933295	0.418248
16	1	0	0.860941	1.910120	-0.533970
17	16	0	2.657986	-0.001484	0.043424

Data 67: Cartesian coordinates, energy, imaginary frequency of the transition state for the transformation of conformer **8(H_{ax})** into conformer **8(H_{eq})** (DMSO solution)

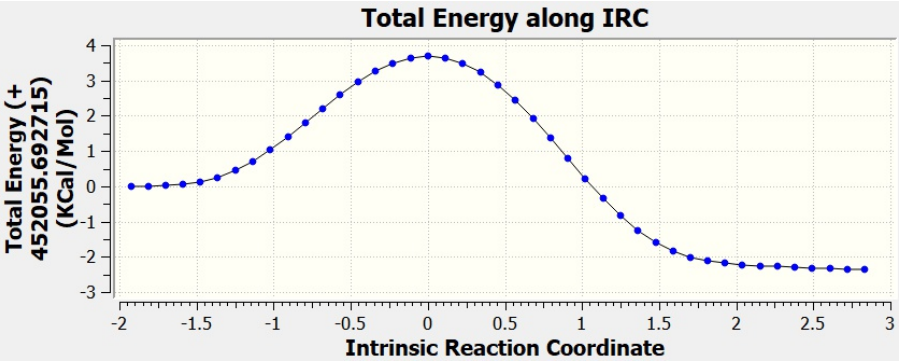


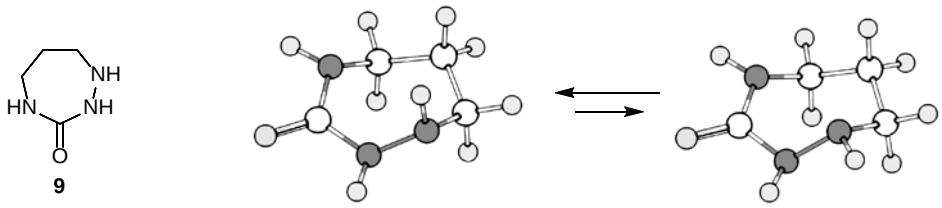
Imaginary Frequency=	-570.7844 cm^{-1}
Electronic Energy =	-720.390699959 a.u.
Zero-point correction=	0.142507 (Hartree/Particle)
Thermal correction to Energy=	0.149960
Thermal correction to Enthalpy=	0.150904
Thermal correction to Gibbs Free Energy=	0.110309
Sum of electronic and zero-point Energies=	-720.248193
Sum of electronic and thermal Energies=	-720.240740
Sum of electronic and thermal Enthalpies=	-720.239796
Sum of electronic and thermal Free Energies=	-720.280391

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.029969	1.495543	0.265683
2	6	0	-2.266810	0.692108	-0.128933
3	6	0	-2.157235	-0.778813	0.276138
4	7	0	-0.998761	-1.400459	-0.326686
5	7	0	0.270857	-1.153757	0.152502
6	6	0	0.959739	-0.009449	-0.071738
7	7	0	0.243330	1.100072	-0.387050
8	1	0	-1.070494	-2.121866	-1.023430
9	1	0	0.800550	-1.935448	0.516250
10	1	0	0.849028	1.884964	-0.581009
11	1	0	-2.424383	0.761678	-1.209648
12	1	0	-3.130614	1.150446	0.365275
13	1	0	-2.111824	-0.870002	1.369973
14	16	0	2.659352	0.015925	0.072135
15	1	0	-3.034385	-1.334104	-0.062852
16	1	0	-1.175502	2.542395	-0.000768
17	1	0	-0.894350	1.449809	1.353784

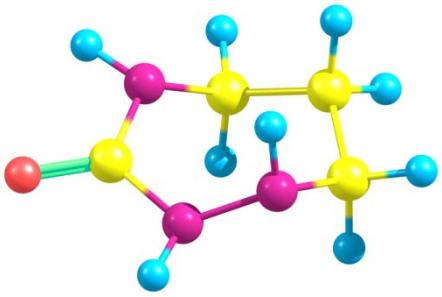
Data 68: The intrinsic reaction coordinate analysis for the transformation of conformer **8(H_{eq})** into conformer **8(H_{ax})** (DMSO solution)





9

Data 69: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of 1,2,4-triazepan-3-one with pseudo axial orientation of the N(1)H proton [**9(H$_{ax}$)**] (the gas phase)

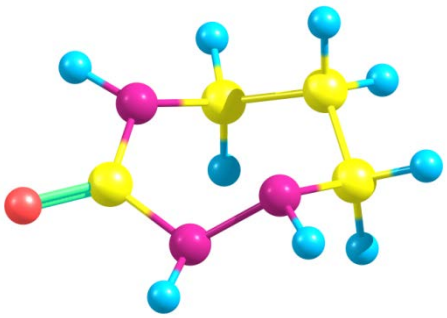


Electronic Energy =	-397.431160427 a.u.
Zero-point correction=	0.146497 (Hartree/Particle)
Thermal correction to Energy=	0.153600
Thermal correction to Enthalpy=	0.154545
Thermal correction to Gibbs Free Energy=	0.115257
Sum of electronic and zero-point Energies=	-397.284663
Sum of electronic and thermal Energies=	-397.277560
Sum of electronic and thermal Enthalpies=	-397.276616
Sum of electronic and thermal Free Energies=	-397.315904

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.638265	1.491551	0.312689
2	6	0	-1.842797	0.678597	-0.161410
3	6	0	-1.753836	-0.808712	0.194384
4	7	0	-0.572356	-1.497871	-0.325727
5	7	0	0.638269	-1.132910	0.304324
6	6	0	1.371737	0.010011	-0.005376
7	8	0	2.592369	0.012355	0.031461
8	7	0	0.628731	1.129276	-0.342725
9	1	0	-0.542472	1.409043	1.403647
10	1	0	-0.807745	2.545484	0.083671
11	1	0	-2.746930	1.101839	0.291902
12	1	0	-1.944284	0.792616	-1.247009
13	1	0	-2.627837	-1.336955	-0.199287
14	1	0	-1.752182	-0.946502	1.279251
15	1	0	1.238997	-1.926676	0.480069
16	1	0	1.252384	1.907610	-0.505162
17	1	0	-0.492424	-1.363445	-1.331592

Data 70: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of 1,2,4-triazepan-3-one with pseudo equatorial orientation of the N(1)H proton [**8(H_{eq})**] (the gas phase)

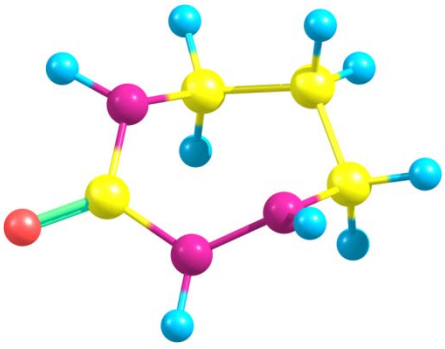


Electronic Energy =	-397.423476035 a.u.
Zero-point correction=	0.146148 (Hartree/Particle)
Thermal correction to Energy=	0.153326
Thermal correction to Enthalpy=	0.154271
Thermal correction to Gibbs Free Energy=	0.114884
Sum of electronic and zero-point Energies=	-397.277328
Sum of electronic and thermal Energies=	-397.270150
Sum of electronic and thermal Enthalpies=	-397.269206
Sum of electronic and thermal Free Energies=	-397.308592

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.622032	1.499623	0.318394
2	6	0	-1.822653	0.701607	-0.196104
3	6	0	-1.771957	-0.780891	0.167586
4	7	0	-0.580161	-1.405906	-0.416184
5	7	0	0.608669	-1.103270	0.353777
6	6	0	1.376131	0.006293	-0.013815
7	8	0	2.597596	-0.039265	-0.017936
8	7	0	0.661452	1.145684	-0.302299
9	1	0	-0.555938	1.401797	1.410502
10	1	0	-0.783115	2.556911	0.099139
11	1	0	-2.730110	1.140970	0.233353
12	1	0	-1.882235	0.802608	-1.283671
13	1	0	-2.638701	-1.292429	-0.261180
14	1	0	-1.801215	-0.907955	1.260559
15	1	0	-0.676221	-2.414336	-0.381070
16	1	0	1.215370	-1.907885	0.445818
17	1	0	1.284742	1.919088	-0.483383

Data 71: Cartesian coordinates, energy, imaginary frequency of the transition state for the transformation of conformer **9(H_{ax})** into conformer **9(H_{eq})** (the gas phase)



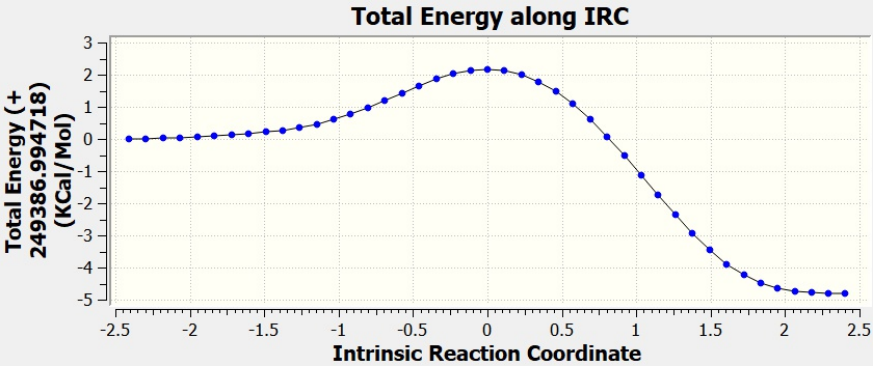
Imaginary Frequency= -502.4061 cm^{-1}

Electronic Energy =	-397.420007566 a.u.
Zero-point correction=	0.144626 (Hartree/Particle)
Thermal correction to Energy=	0.151706
Thermal correction to Enthalpy=	0.152651
Thermal correction to Gibbs Free Energy=	0.113308
Sum of electronic and zero-point Energies=	-397.275381
Sum of electronic and thermal Energies=	-397.268301
Sum of electronic and thermal Enthalpies=	-397.267357
Sum of electronic and thermal Free Energies=	-397.306700

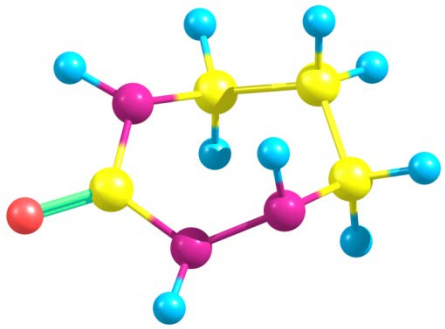
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.602089	1.485328	0.293885
2	6	0	-1.850707	0.706281	-0.135665
3	6	0	-1.780193	-0.786825	0.210937
4	7	0	-0.590532	-1.373234	-0.360182
5	7	0	0.626325	-1.133187	0.252948
6	6	0	1.388951	-0.009809	-0.030043
7	7	0	0.651905	1.108618	-0.387350
8	1	0	-0.630639	-2.155576	-0.989093
9	1	0	1.143305	-1.916121	0.630148
10	1	0	1.279774	1.885240	-0.541457
11	1	0	-1.984966	0.814945	-1.216345
12	1	0	-2.718043	1.160529	0.358770
13	1	0	-1.799541	-0.927209	1.301948
14	8	0	2.605751	-0.010593	0.079433
15	1	0	-2.647019	-1.308954	-0.204090
16	1	0	-0.759177	2.542208	0.068955
17	1	0	-0.479356	1.404451	1.383106

Data 72: The intrinsic reaction coordinate analysis for the transformation of conformer **9(H_{eq})** into conformer **9(H_{ax})** (the gas phase)



Data 73: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of 1,2,4-triazepan-3-one with pseudo axial orientation of the N(1)H proton [**9(H_{ax})**] (DMSO solution)

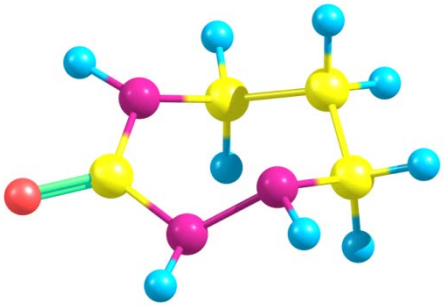


Electronic Energy =	-397.444047686 a.u.
Zero-point correction=	0.146259 (Hartree/Particle)
Thermal correction to Energy=	0.153403
Thermal correction to Enthalpy=	0.154347
Thermal correction to Gibbs Free Energy=	0.114988
Sum of electronic and zero-point Energies=	-397.297789
Sum of electronic and thermal Energies=	-397.290645
Sum of electronic and thermal Enthalpies=	-397.289701
Sum of electronic and thermal Free Energies=	-397.329060

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.653756	1.495684	0.306120
2	6	0	-1.841707	0.670000	-0.180801
3	6	0	-1.754285	-0.807842	0.202955
4	7	0	-0.572763	-1.507284	-0.314301
5	7	0	0.647464	-1.132363	0.298479
6	6	0	1.363699	0.016323	-0.004940
7	8	0	2.598363	0.010997	0.019523
8	7	0	0.636693	1.137176	-0.312609
9	1	0	-0.575367	1.425885	1.398164
10	1	0	-0.819119	2.545021	0.059994
11	1	0	-2.753064	1.097076	0.251505
12	1	0	-1.926982	0.763845	-1.269272
13	1	0	-2.627012	-1.342266	-0.182713
14	1	0	-1.751370	-0.926130	1.290103
15	1	0	1.253882	-1.924573	0.462267
16	1	0	1.248137	1.923082	-0.485593
17	1	0	-0.499469	-1.377607	-1.321626

Data 74: Cartesian coordinates and energies of the optimized geometry for the most stable conformer of 1,2,4-triazepan-3-one with pseudo equatorial orientation of the N(1)H proton [**9(H_{eq})**] (DMSO solution)

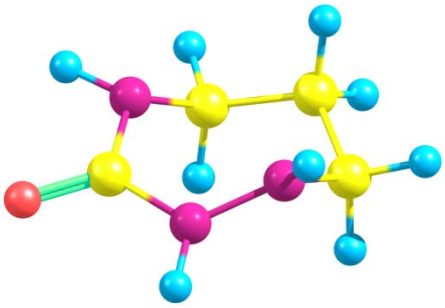


Electronic Energy =	-397.438769423 a.u.
Zero-point correction=	0.146013 (Hartree/Particle)
Thermal correction to Energy=	0.153205
Thermal correction to Enthalpy=	0.154149
Thermal correction to Gibbs Free Energy=	0.114717
Sum of electronic and zero-point Energies=	-397.292756
Sum of electronic and thermal Energies=	-397.285564
Sum of electronic and thermal Enthalpies=	-397.284620
Sum of electronic and thermal Free Energies=	-397.324052

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.627819	1.504633	0.305046
2	6	0	-1.831123	0.699585	-0.184102
3	6	0	-1.767440	-0.778677	0.186512
4	7	0	-0.585669	-1.409061	-0.420863
5	7	0	0.622873	-1.112515	0.315107
6	6	0	1.369007	0.005493	-0.014015
7	8	0	2.604961	-0.024628	0.009826
8	7	0	0.660633	1.138317	-0.314037
9	1	0	-0.549725	1.425370	1.396722
10	1	0	-0.782669	2.557486	0.067172
11	1	0	-2.729453	1.138592	0.262008
12	1	0	-1.918907	0.798558	-1.270418
13	1	0	-2.639048	-1.299904	-0.217278
14	1	0	-1.769617	-0.902540	1.278930
15	1	0	-0.684097	-2.417126	-0.365803
16	1	0	1.213569	-1.925578	0.432110
17	1	0	1.279655	1.918776	-0.484150

Data 75: Cartesian coordinates, energy, imaginary frequency of the transition state for the transformation of conformer **9(H_{ax})** into conformer **9(H_{eq})** (DMSO solution)



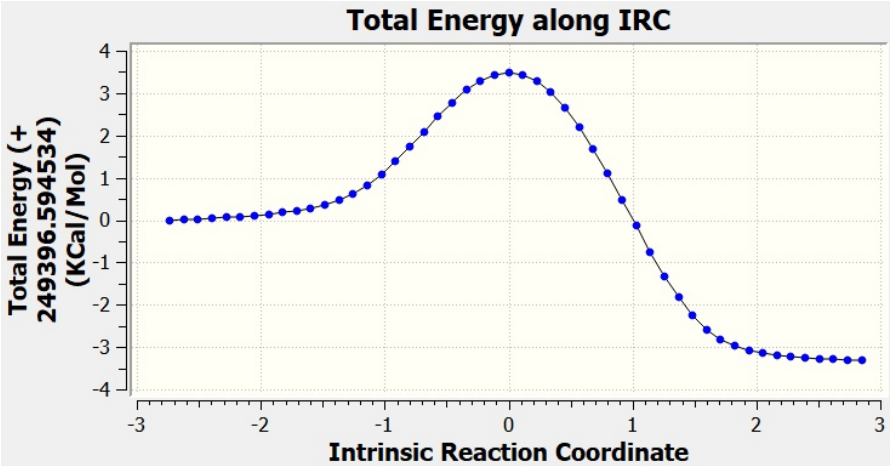
Imaginary Frequency=	-570.7844 cm^{-1}
Electronic Energy =	-397.433219279 a.u.
Zero-point correction=	0.144375 (Hartree/Particle)
Thermal correction to Energy=	0.151499
Thermal correction to Enthalpy=	0.152443
Thermal correction to Gibbs Free Energy=	0.113018
Sum of electronic and zero-point Energies=	-397.288844
Sum of electronic and thermal Energies=	-397.281720
Sum of electronic and thermal Enthalpies=	-397.280776
Sum of electronic and thermal Free Energies=	-397.320201

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.618304	1.492882	0.277122
2	6	0	-1.859028	0.697104	-0.132089
3	6	0	-1.766370	-0.787371	0.237825
4	7	0	-0.590004	-1.388903	-0.347598
5	7	0	0.651446	-1.148972	0.204217
6	6	0	1.377472	-0.006293	-0.030284
7	7	0	0.646150	1.106072	-0.393141
8	1	0	-0.641550	-2.121277	-1.034007
9	1	0	1.161166	-1.924155	0.608403
10	1	0	1.268968	1.890071	-0.534706
11	1	0	-2.010920	0.789653	-1.212320
12	1	0	-2.724172	1.149855	0.365703
13	1	0	-1.754505	-0.906572	1.330552

14	8	0	2.605787	0.014267	0.108172
15	1	0	-2.637961	-1.326073	-0.141850
16	1	0	-0.772679	2.543244	0.026948
17	1	0	-0.490401	1.435801	1.366112

Data 76: The intrinsic reaction coordinate analysis for the transformation of conformer **9(H_{eq})** into conformer **9(H_{ax})** (DMSO solution)



Reference

1. *Gaussian 09, Revision D.01*, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, N. J. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.