

Supporting Information

Figure S1. ^1H spectrum of compound **2** in $\text{DMSO}-d_6$.

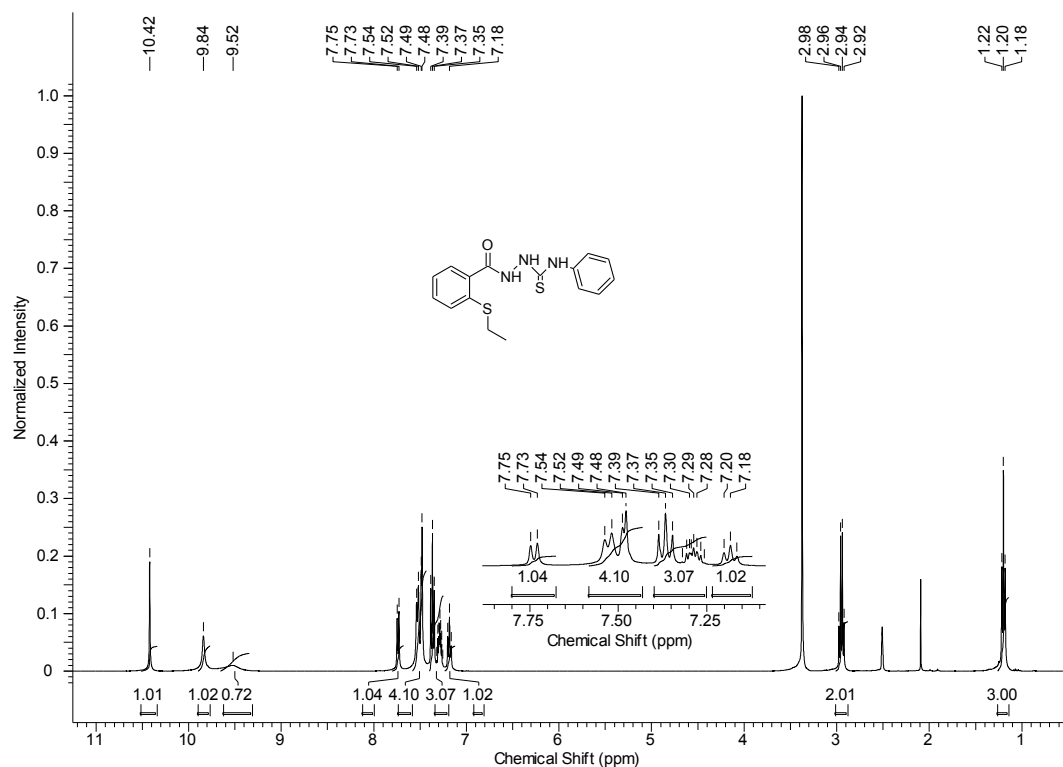


Figure S2. ^{13}C spectrum of compound **2** in $\text{DMSO}-d_6$.

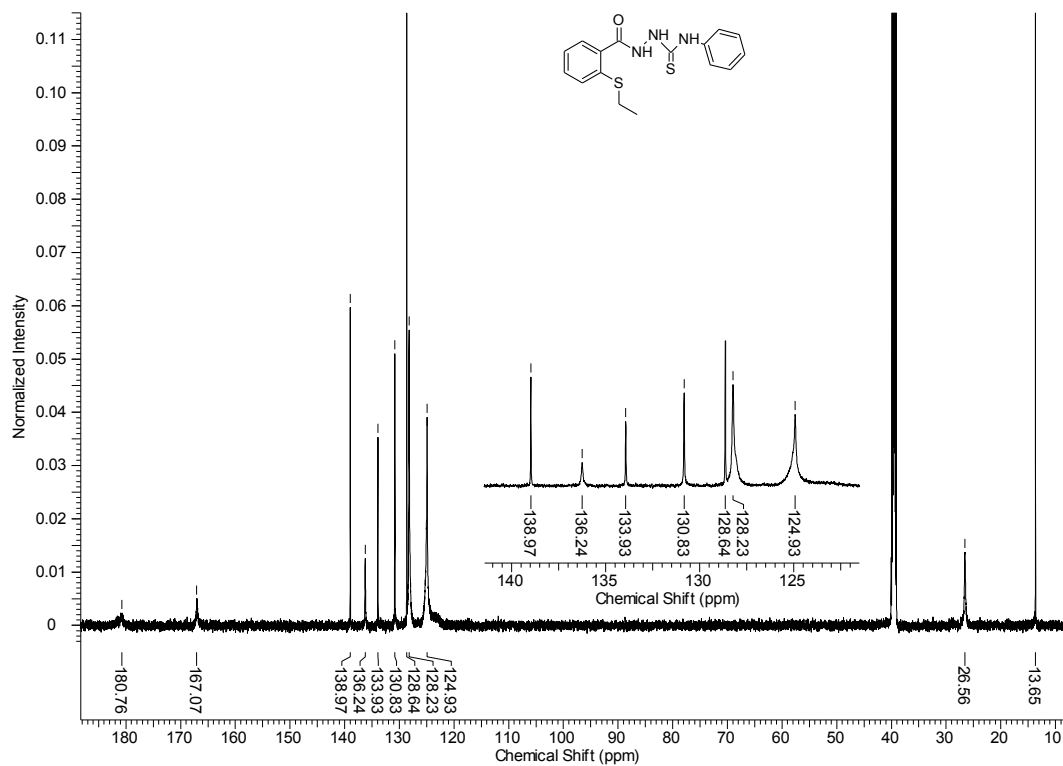


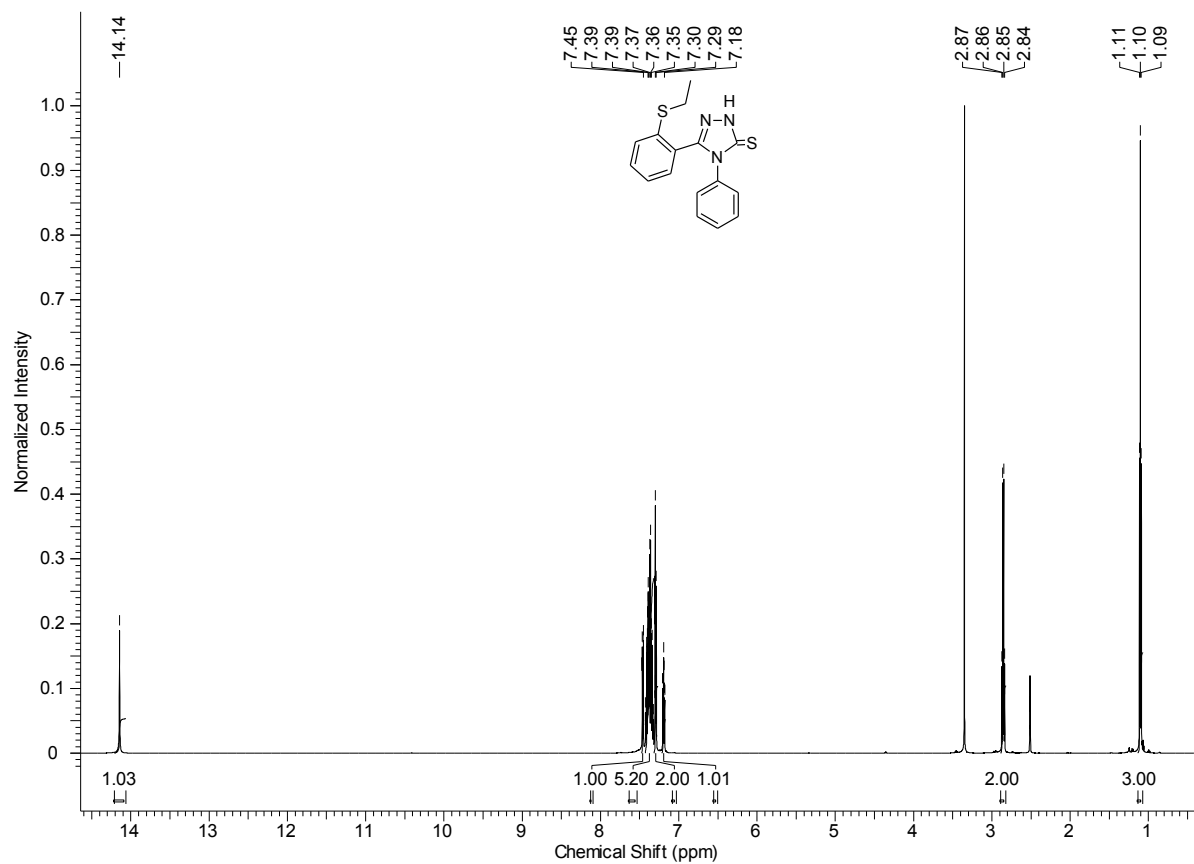
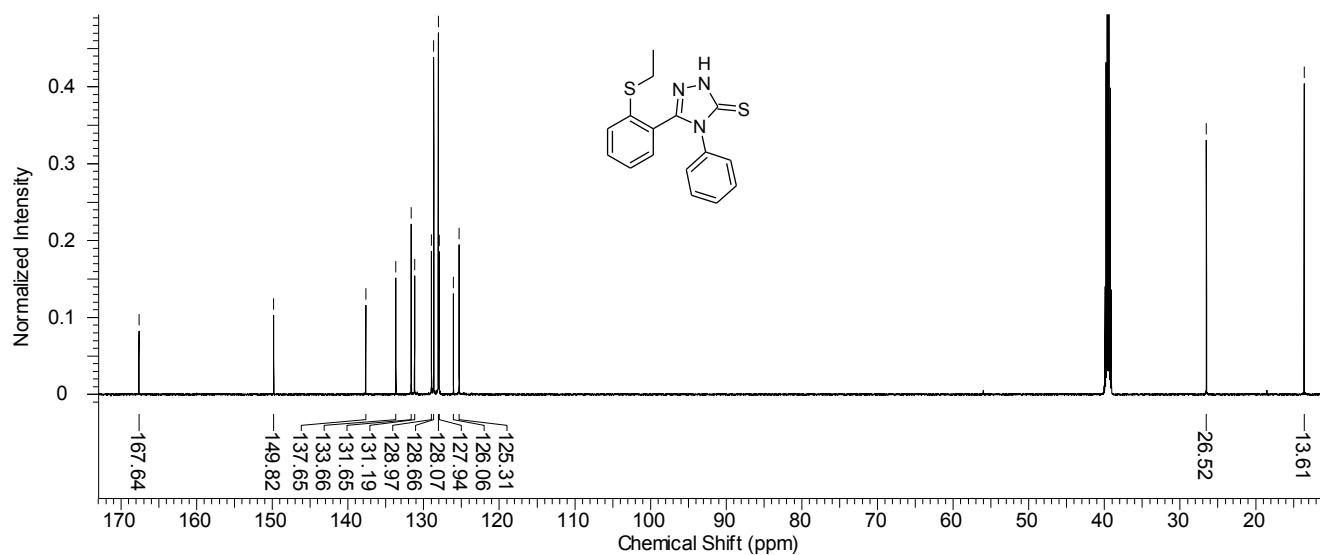
Figure S3. ^1H spectrum of compound 7 in $\text{DMSO}-d_6$.**Figure S4.** ^{13}C spectrum of compound 7 in $\text{DMSO}-d_6$.

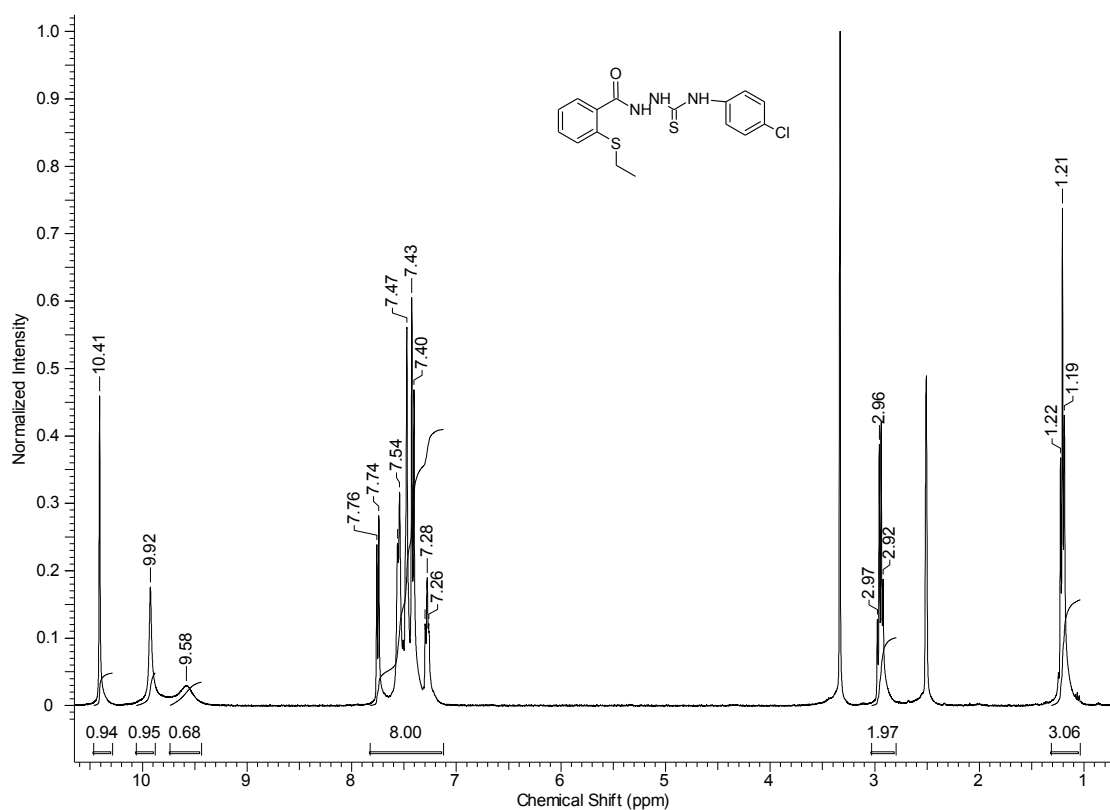
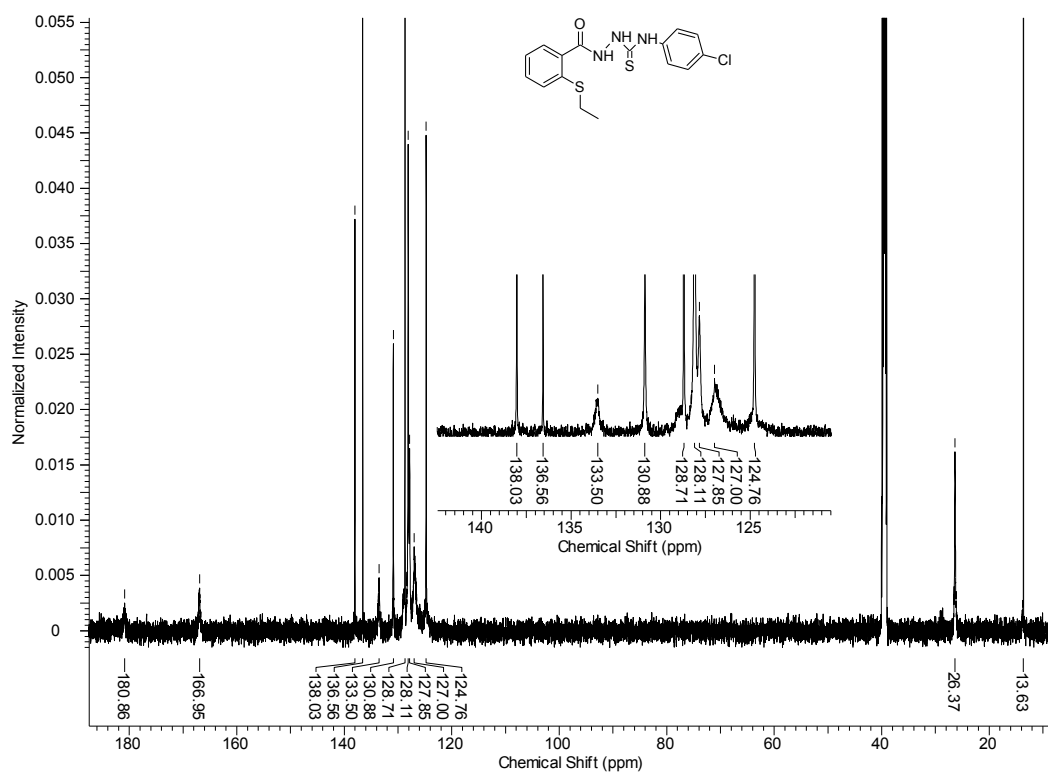
Figure S5. ^1H spectrum of compound **3** in $\text{DMSO}-d_6$.**Figure S6.** ^{13}C spectrum of compound **3** in $\text{DMSO}-d_6$.

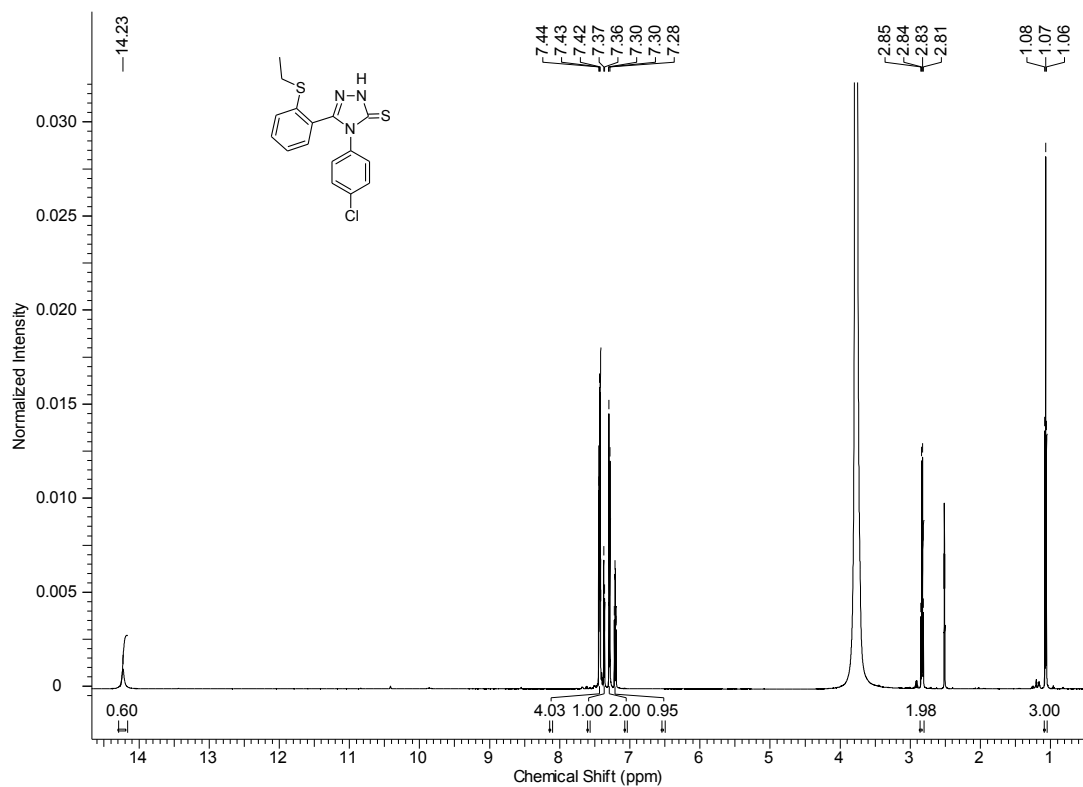
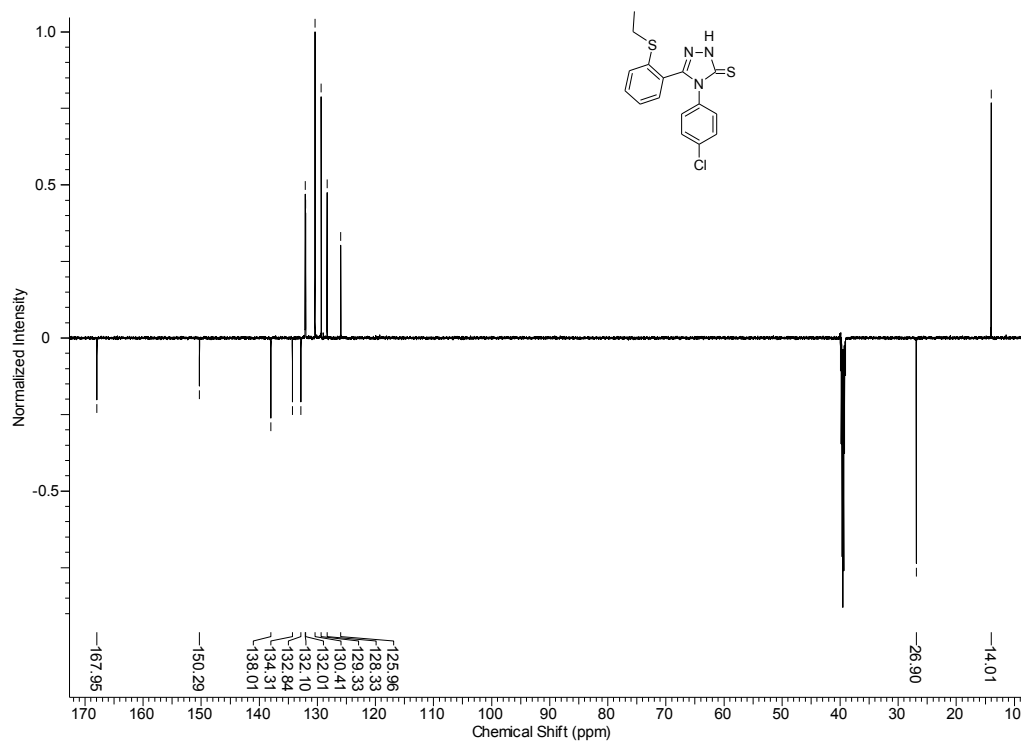
Figure S7. ^1H spectrum of compound **8** in $\text{DMSO}-d_6$.**Figure S8.** ^{13}C (APT) spectrum of compound **8** in $\text{DMSO}-d_6$.

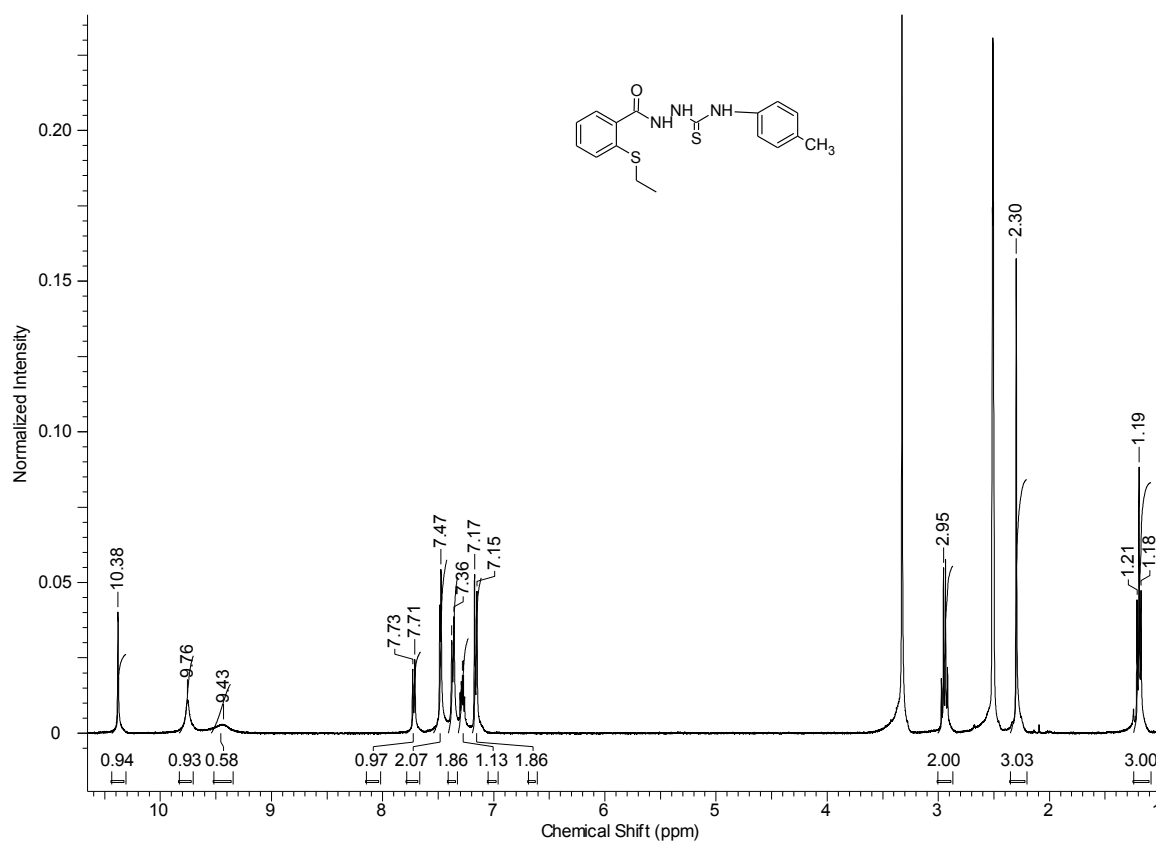
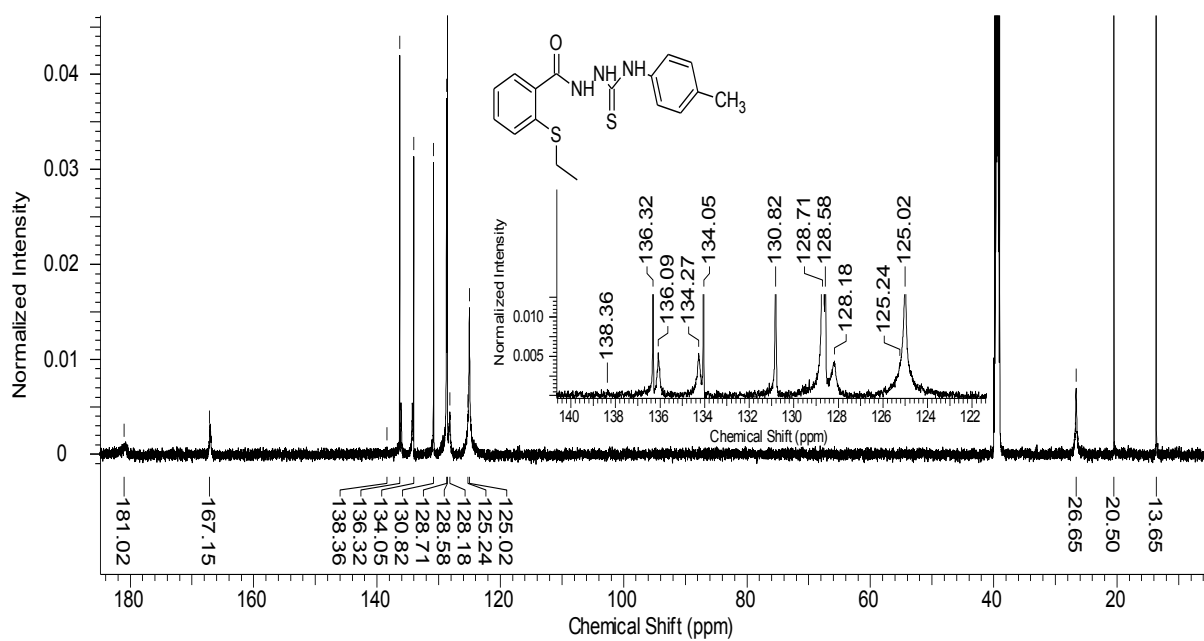
Figure S9. ^1H spectrum of compound **4** in $\text{DMSO}-d_6$.**Figure S10.** ^{13}C spectrum of compound **4** in $\text{DMSO}-d_6$.

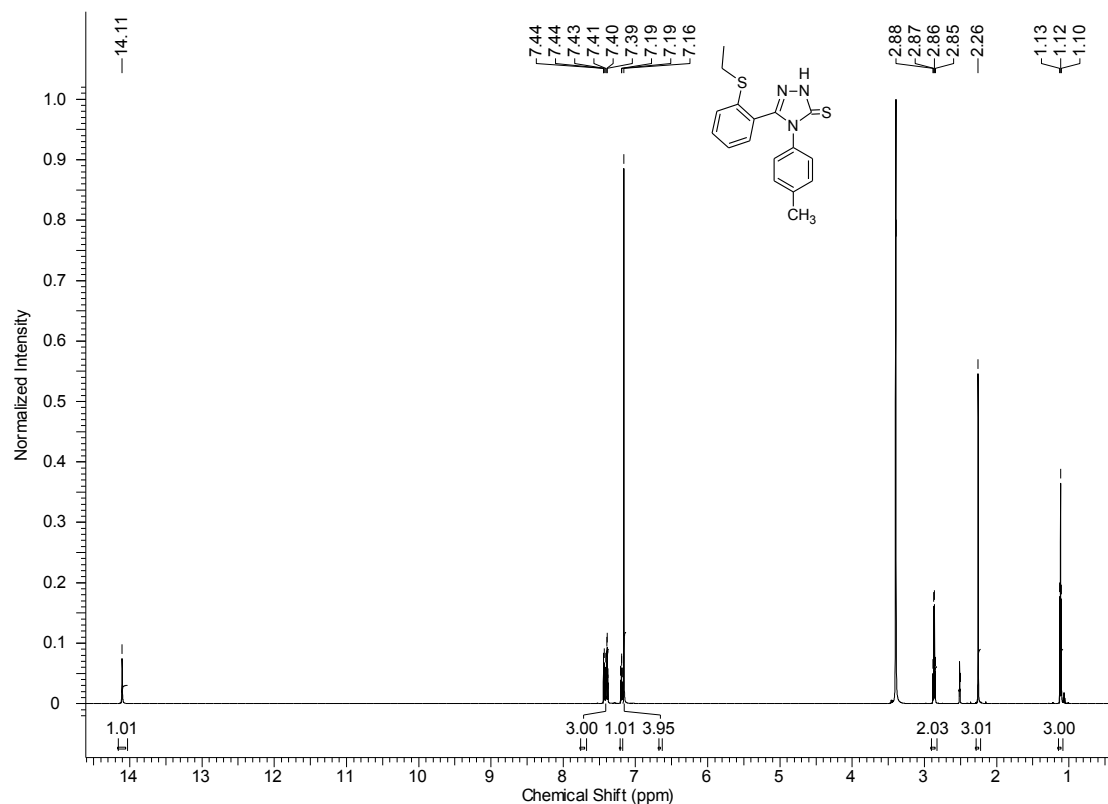
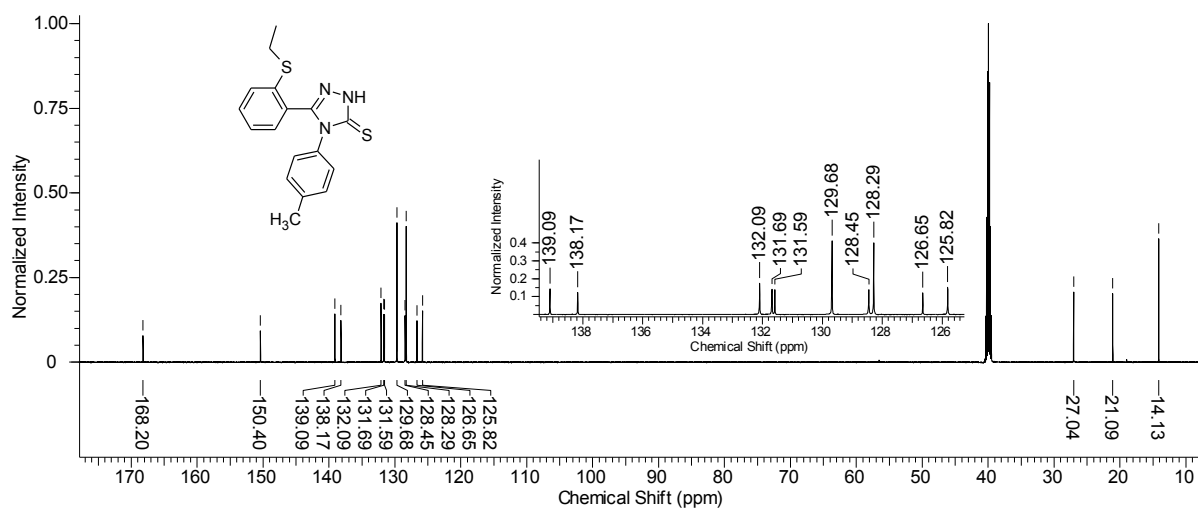
Figure S11. ^1H spectrum of compound **9** in $\text{DMSO-}d_6$.**Figure S12.** ^{13}C spectrum of compound **9** in $\text{DMSO-}d_6$.

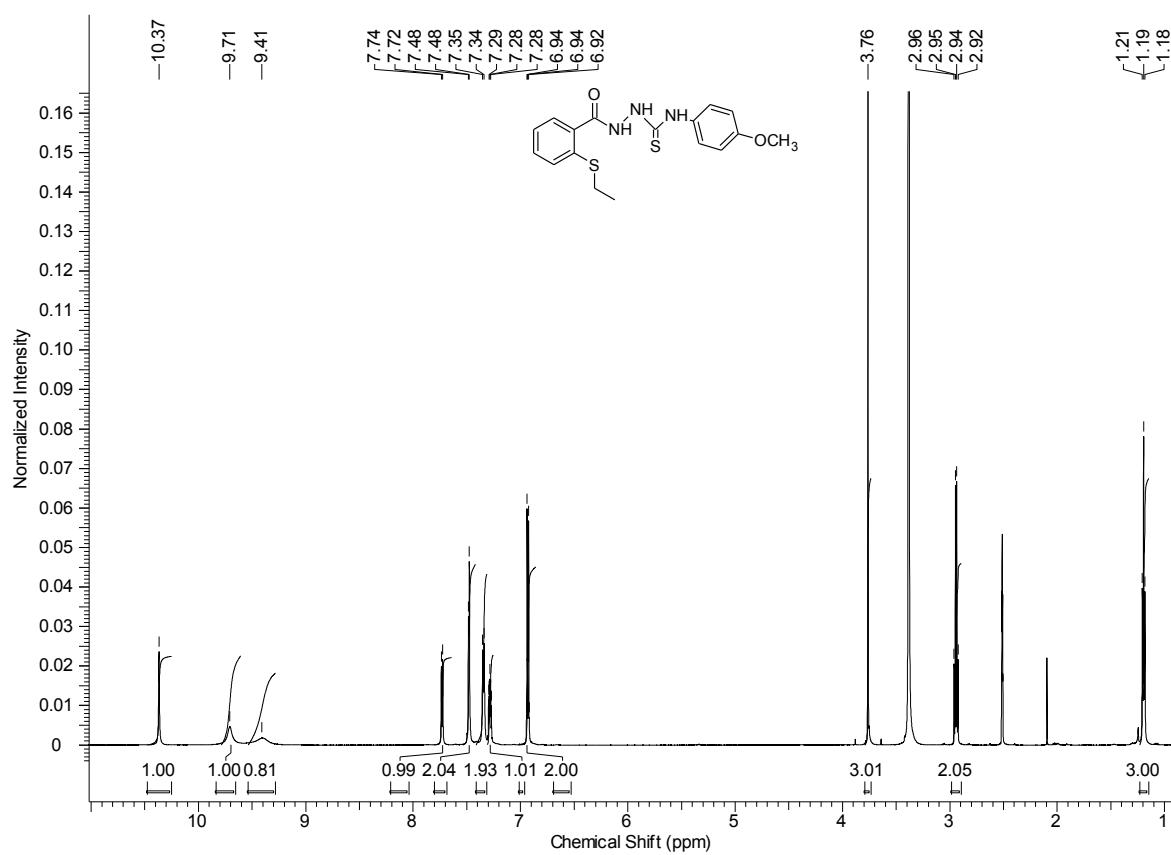
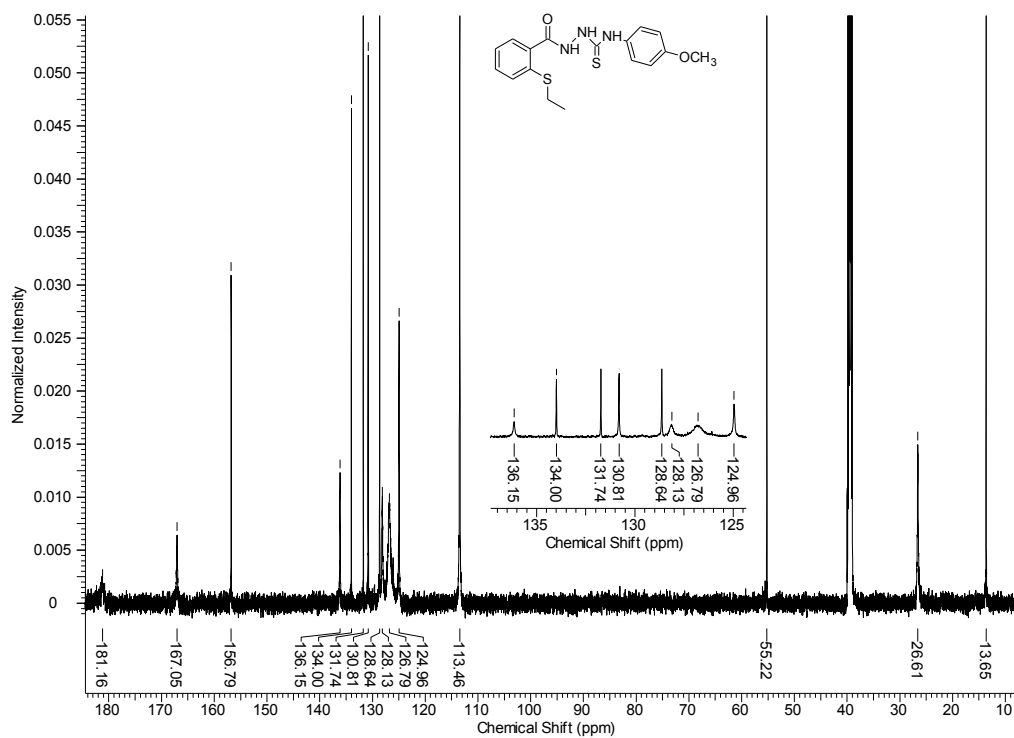
Figure S13. ^1H spectrum of compound **5** in $\text{DMSO}-d_6$.**Figure S14.** ^{13}C spectrum of compound **5** in $\text{DMSO}-d_6$.

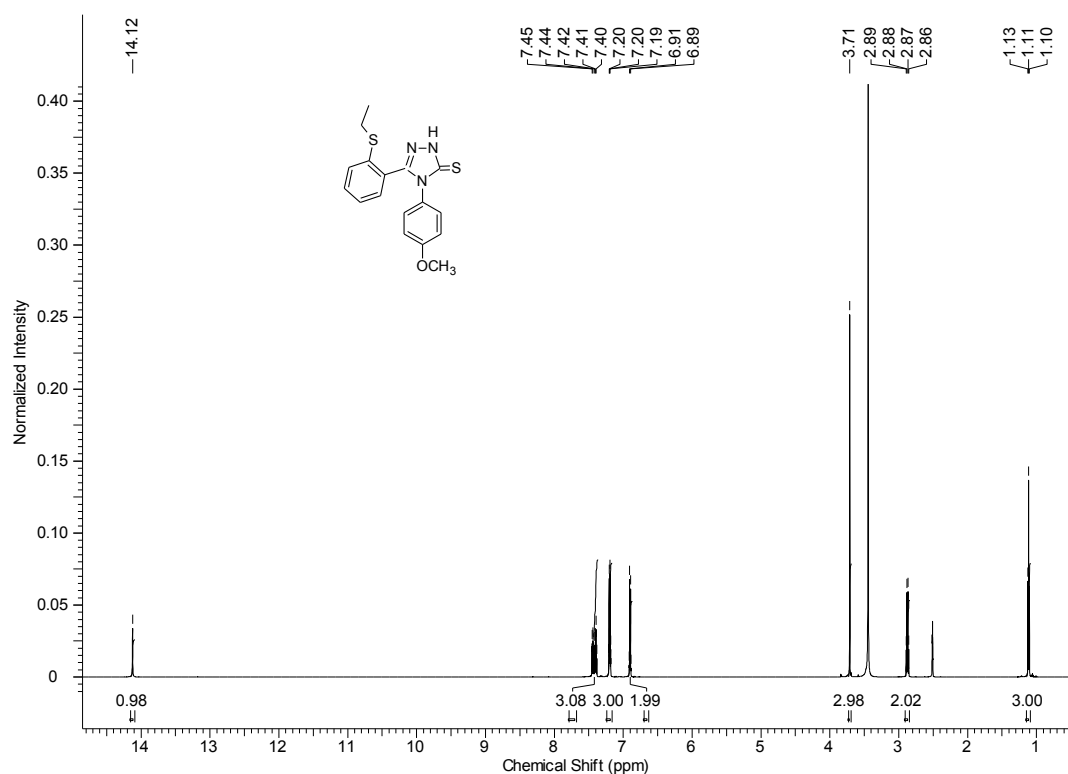
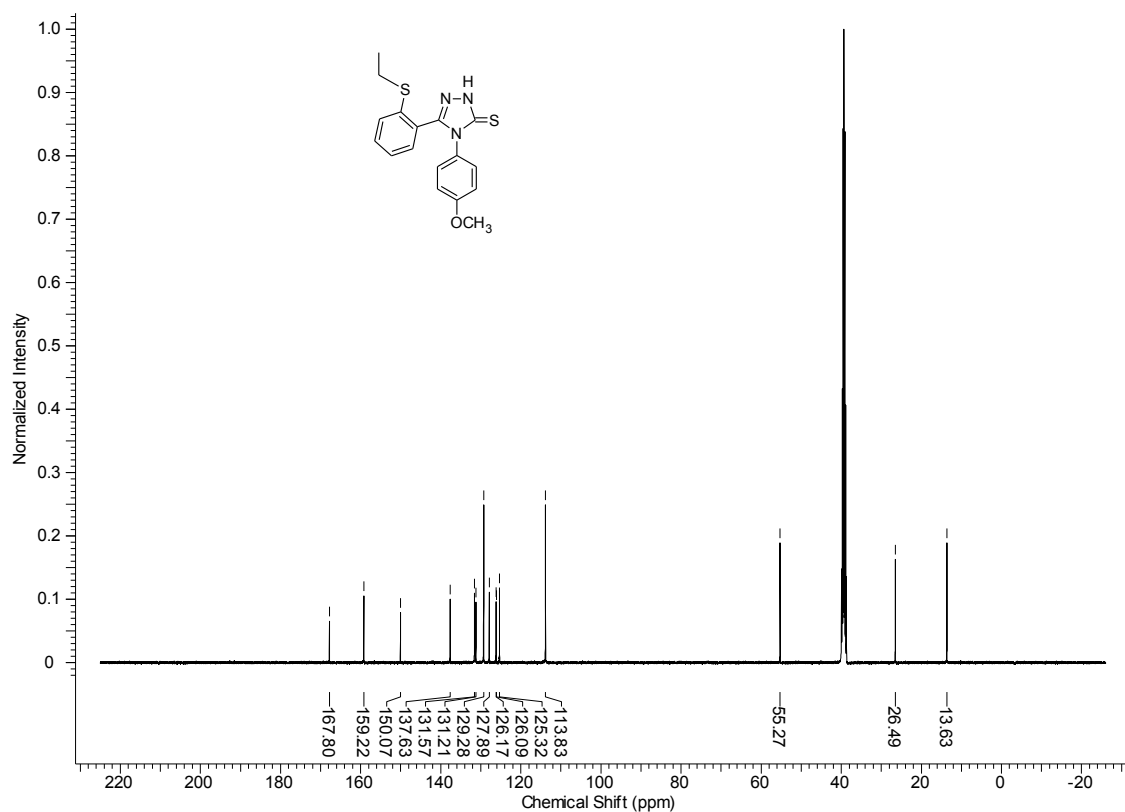
Figure S15. ^1H spectrum of compound **10** in $\text{DMSO}-d_6$.**Figure S16.** ^{13}C spectrum of compound **10** in $\text{DMSO}-d_6$.

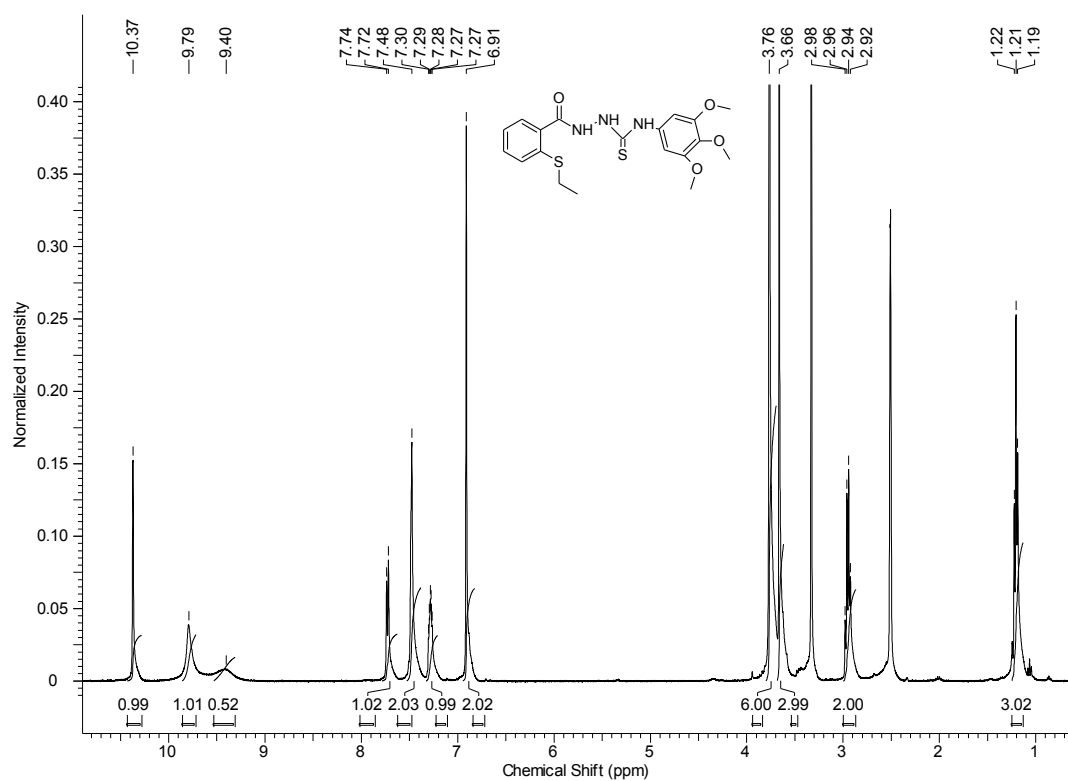
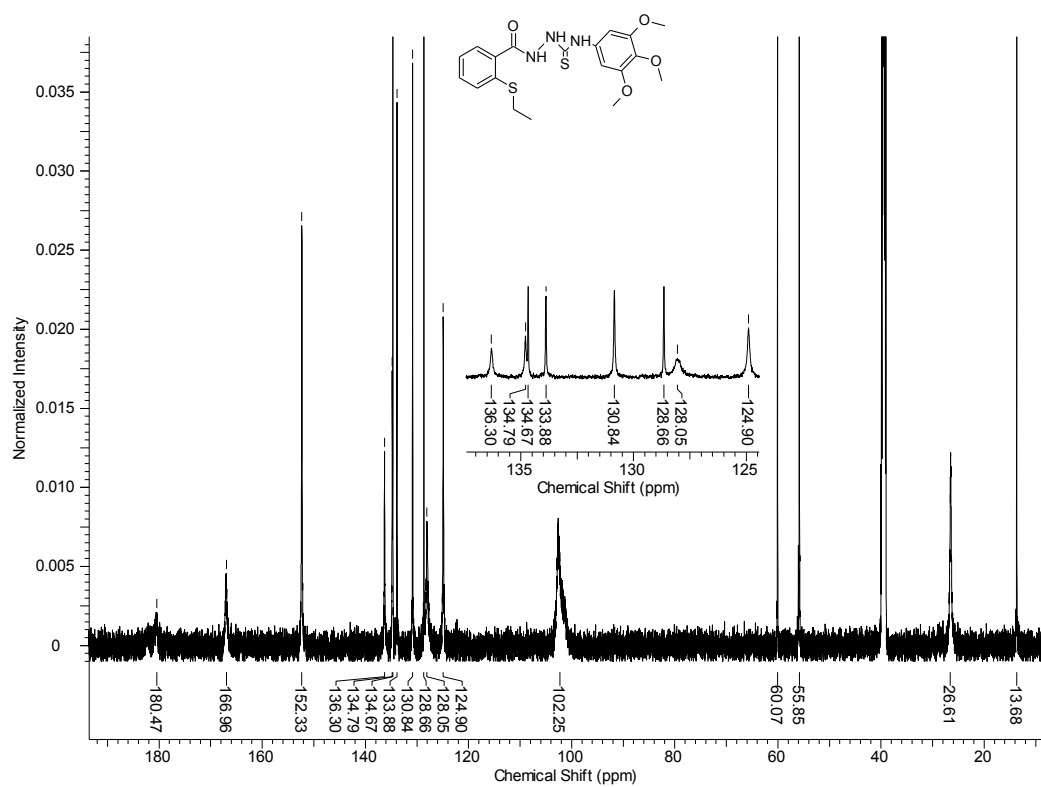
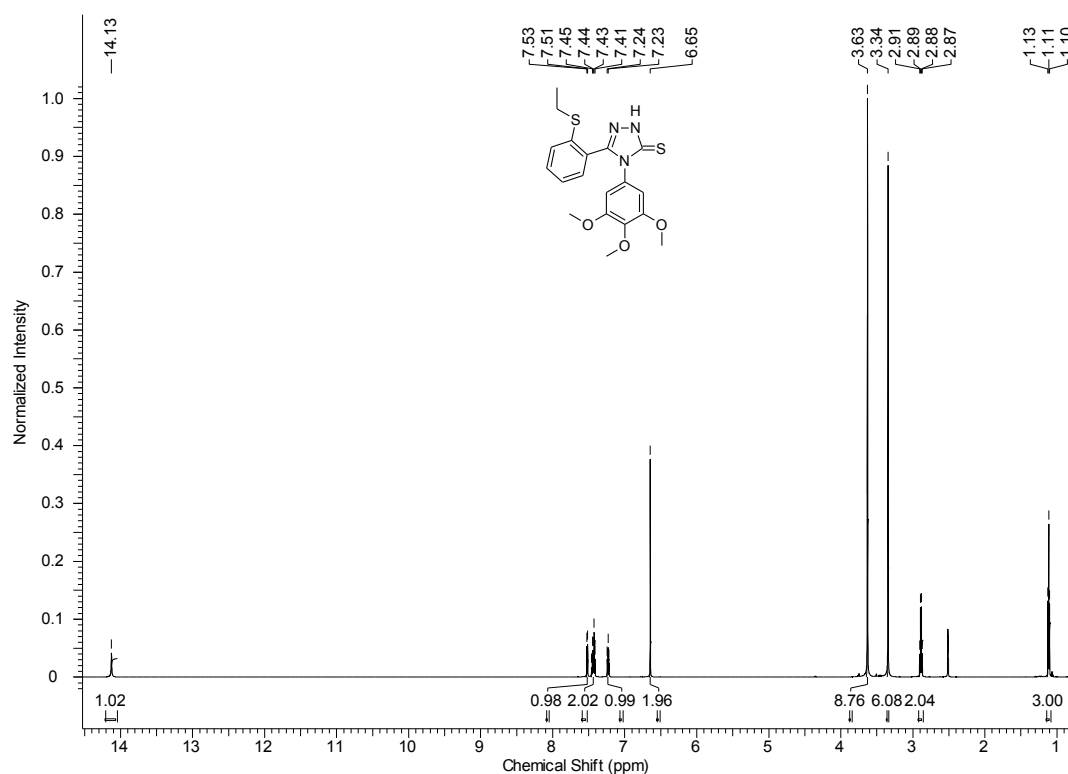
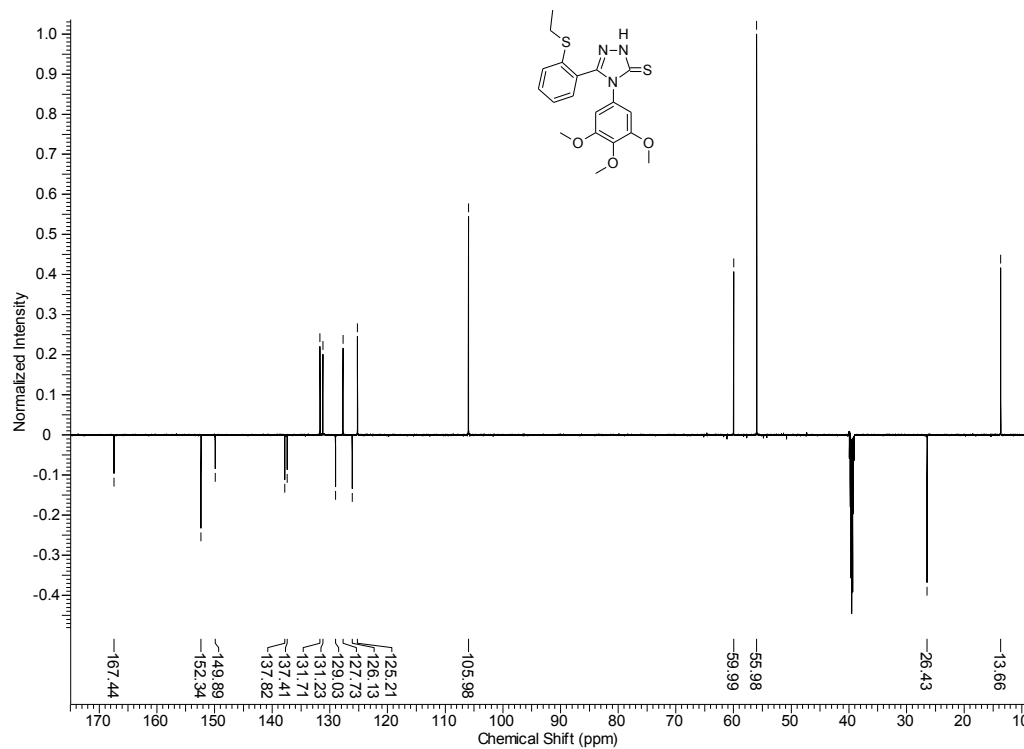
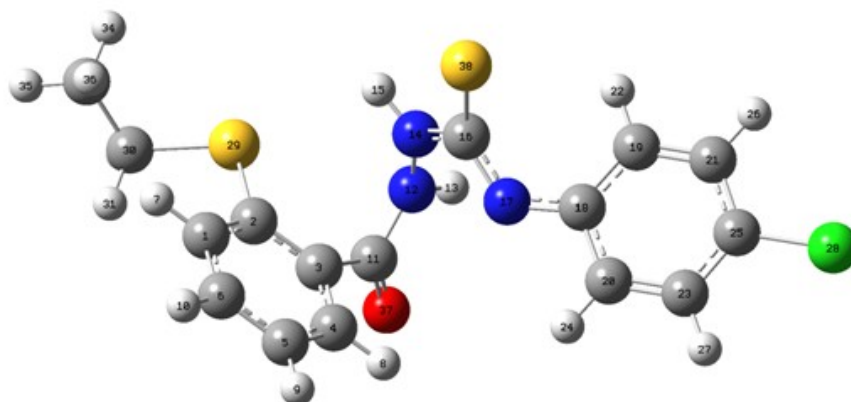
Figure S17. ^1H spectrum of compound **6** in $\text{DMSO}-d_6$.**Figure S18.** ^{13}C spectrum of compound **6** in $\text{DMSO}-d_6$.

Figure S19. ^1H spectrum of compound **11** in $\text{DMSO}-d_6$.**Figure S20.** ^{13}C (APT) spectrum of compound **11** in $\text{DMSO}-d_6$.

Computational Supporting Data

Compound **3r1** [# opt freq ub3lyp/6-31g(d,p)]

Zero-point correction = 0.284468 (Hartree/Particle)

Thermal correction to Energy = 0.306813

Thermal correction to Enthalpy = 0.307757

Thermal correction to Gibbs Free Energy = 0.227641

Sum of electronic and zero-point Energies = -2114.485647

Sum of electronic and thermal Energies = -2114.463302

Sum of electronic and thermal Enthalpies = -2114.462358

Sum of electronic and thermal Free Energies = -2114.542474

	E (Thermal)/KCal/Mol	CV/Cal/Mol-Kelvin	S/Cal/MolKelvin
Total	192.528	82.424	168.619

Mulliken atomic spin densities:

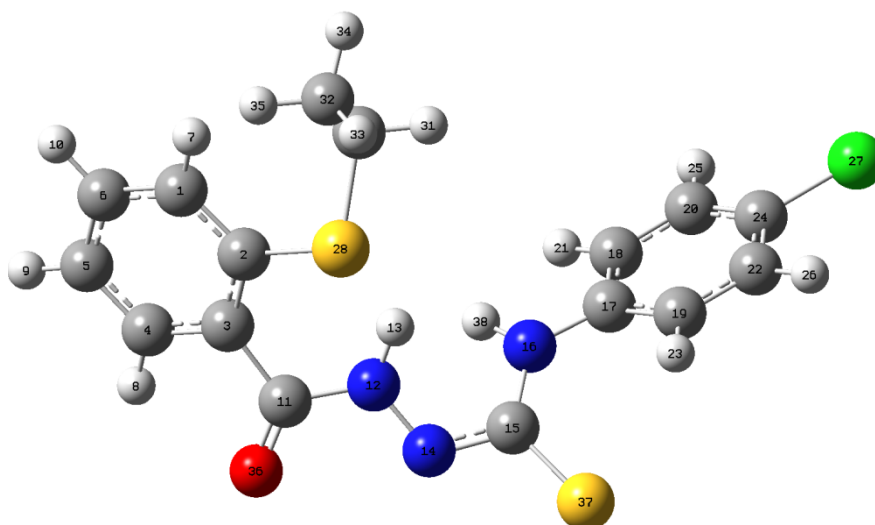
1

1	C	0.009937
2	C	-0.119027
3	C	-0.007243
4	C	-0.006443
5	C	-0.000279
6	C	0.015678
7	H	-0.000625
8	H	-0.001201
9	H	0.001046
10	H	-0.000702
11	C	-0.040618
12	N	0.113716
13	H	0.008464
14	N	-0.037928
15	H	-0.231644

16	C	0.114501
17	N	−0.017897
18	C	0.003119
19	C	−0.028430
20	C	0.017892
21	C	−0.003497
22	H	−0.000117
23	C	0.009474
24	H	−0.002443
25	C	−0.000251
26	H	−0.000077
27	H	0.000351
28	Cl	0.000027
29	S	0.795159
30	C	0.324939
31	H	−0.002150
32	H	−0.020897
33	C	0.006649
34	H	−0.000076
35	H	0.012745
36	H	0.002234
37	O	0.003964
38	S	0.081649

Sum of Mulliken atomic spin densities = 1.00000

Compound **3r2 (radical)** [# opt freq ub3lyp/6-31g(d,p)]



Zero-point correction = 0.284621 (Hartree/Particle)
 Thermal correction to Energy = 0.306865
 Thermal correction to Enthalpy = 0.307809
 Thermal correction to Gibbs Free Energy = 0.227583
 Sum of electronic and zero-point Energies = −2114.478768
 Sum of electronic and thermal Energies = −2114.456524
 Sum of electronic and thermal Enthalpies = −2114.455580
 Sum of electronic and thermal Free Energies = −2114.535806

	E (Thermal)/KCal/Mol	CV/Cal/Mol-Kelvin	S/Cal/MolKelvin
Total	192.560	82.380	168.849

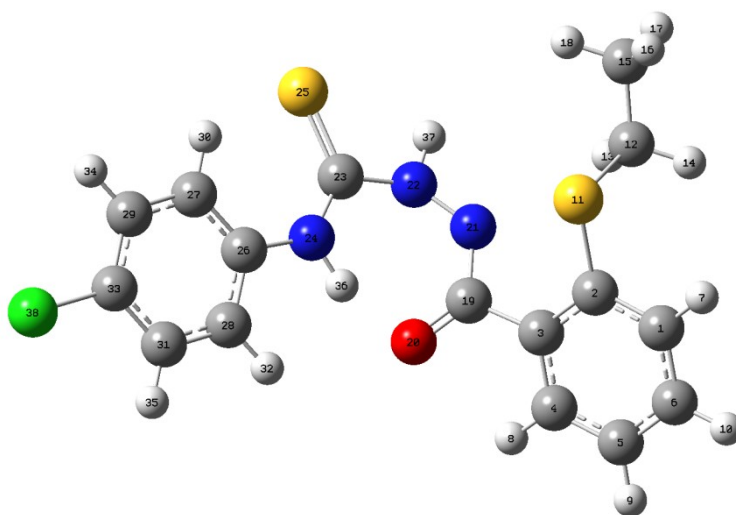
Mulliken atomic spin densities:

1	
1	C −0.003656
2	C 0.006384
3	C −0.004068
4	C 0.006164
5	C −0.002993
6	C 0.007323
7	H 0.000151
8	H −0.000374
9	H 0.000079
10	H −0.000334
11	C −0.005013
12	N 0.136679
13	H −0.005228
14	N 0.483971
15	C −0.103702
16	N 0.010095
17	C −0.006008
18	C 0.009772
19	C 0.008446
20	C −0.004517
21	H −0.000450
22	C −0.005689
23	H −0.000815
24	C 0.010573
25	H 0.000143
26	H 0.000193
27	Cl 0.001282
28	S 0.007054

29 C 0.000593
 30 H 0.000023
 31 H 0.000080
 32 C 0.000295
 33 H −0.000002
 34 H 0.000226
 35 H −0.000011
 36 O 0.078624
 37 S 0.374997
 38 H −0.000239

Sum of Mulliken atomic spin densities = 1.00000

Compound 3r3 (radical) [# opt freq ub3lyp/6-31g(d,p)]



Zero-point correction = 0.286271 (Hartree/Particle)

Thermal correction to Energy = 0.307270

Thermal correction to Enthalpy = 0.307741

Thermal correction to Gibbs Free Energy = 0.230113

Sum of electronic and zero-point Energies = −2114.461291

Sum of electronic and thermal Energies = −2114.439292

Sum of electronic and thermal Enthalpies = −2114.438348

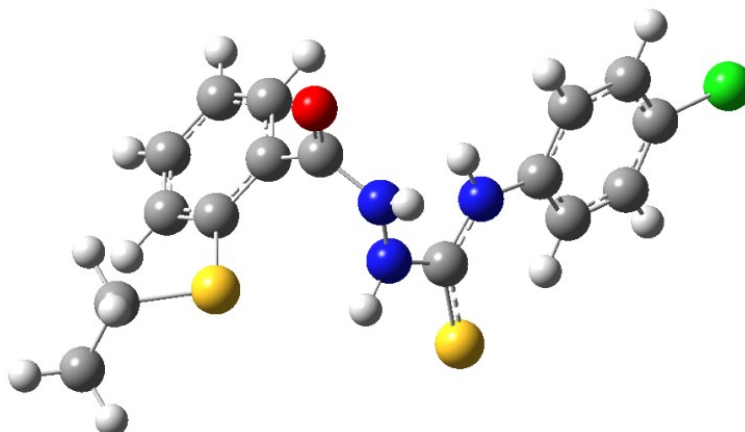
Sum of electronic and thermal Free Energies = −2114.517449

	E (Thermal)/ KCal/Mol	CV/ Cal/Mol-Kelvin	S/ Cal/MolKelvin
Total	193.442	81.329	166.482

Mulliken atomic spin densities:

1		
1	C	−0.001220
2	C	0.000611
3	C	−0.002528
4	C	0.001749
5	C	−0.001823
6	C	0.003473
7	H	−0.000148
8	H	−0.000231
9	H	0.000151
10	H	−0.000177
11	S	0.094268
12	C	−0.003858
13	H	0.002992
14	H	0.000914
15	C	0.000399
16	H	−0.000004
17	H	−0.000092
18	H	−0.000082
19	C	0.005938
20	O	0.149833
21	N	0.397865
22	N	0.237919
23	C	−0.052580
24	N	0.022300
25	S	0.140571
26	C	−0.004957
27	C	0.009213
28	C	0.010456
29	C	−0.006053
30	H	−0.001010
31	C	−0.005108
32	H	−0.000286
33	C	0.011707
34	H	0.000221
35	H	0.000176
36	H	−0.002017
37	H	−0.010171
38	Cl	0.001588

Sum of Mulliken atomic spin densities = 1.00000

Compound 3 (neutral) [opt freq b3lyp/6-31g(d,p)]

Zero-point correction = 0.296816 (Hartree/Particle)

Thermal correction to Energy = 0.318665

Thermal correction to Enthalpy = 0.319609

Thermal correction to Gibbs Free Energy = 0.241849

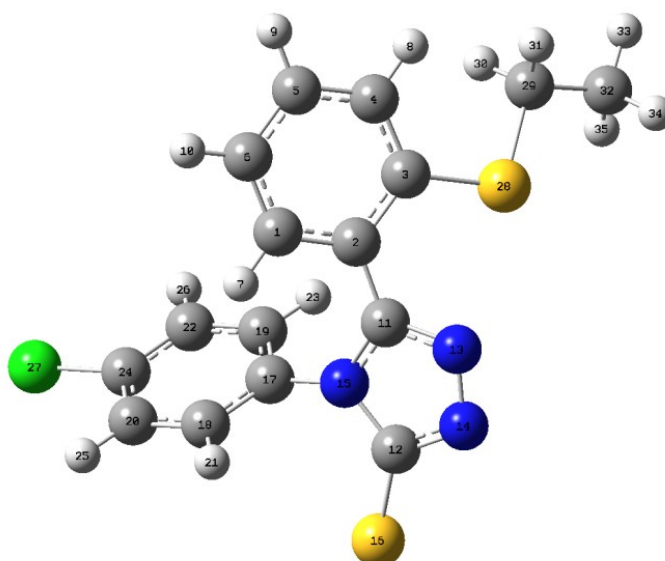
Sum of electronic and zero-point Energies = -2115.146198

Sum of electronic and thermal Energies = -2115.124349

Sum of electronic and thermal Enthalpies = -2115.123405

Sum of electronic and thermal Free Energies = -2115.201165

	E (Thermal)/KCal/Mol	CV/Cal/Mol-Kelvin	S/ Cal/MolKelvin
Total	199.965	81.878	163.660

Compound 8 (radical) [opt freq ub3lyp/6-31g(d,p)]

Zero-point correction = 0.257555 (Hartree/Particle)
 Thermal correction to Energy = 0.277493
 Thermal correction to Enthalpy = 0.278437
 Thermal correction to Gibbs Free Energy = 0.205137
 Sum of electronic and zero-point Energies = −2038.106883
 Sum of electronic and thermal Energies = −2038.086946
 Sum of electronic and thermal Enthalpies = −2038.086001
 Sum of electronic and thermal Free Energies = −2038.159302

	E (Thermal)/KCal/Mol	CV/ Cal/Mol-Kelvin	S/ Cal/Mol-Kelvin
Total	174.129	74.461	154.273

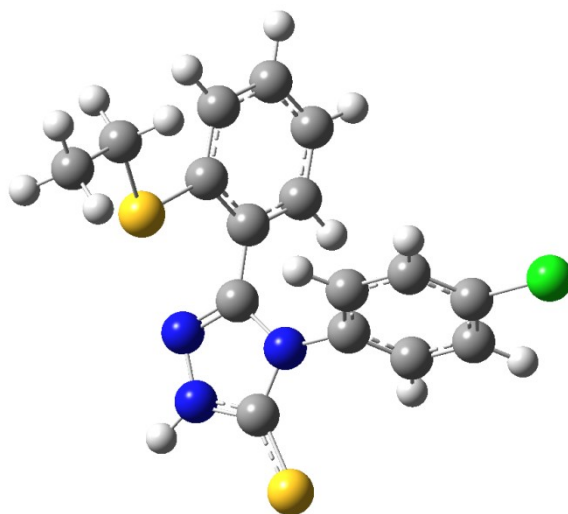
Mulliken atomic spin densities:

1	
1	C −0.010589
2	C 0.021197
3	C −0.023838
4	C 0.022631
5	C −0.009553
6	C 0.020267
7	H 0.000635
8	H −0.000716
9	H 0.000582
10	H −0.000940
11	C 0.161590
12	C −0.064291
13	N 0.016363
14	N 0.210826
15	N 0.009669
16	S 0.641561
17	S 0.002543
18	C 0.000568
19	H −0.000055
20	H 0.000126
21	C 0.000021
22	H −0.000003
23	H 0.000020
24	H −0.000002
25	C −0.000820
26	C 0.001642
27	C 0.000569
28	C −0.000764

29 H -0.000523
 30 C -0.000084
 31 H -0.000099
 32 C 0.001169
 33 H 0.000081
 34 H 0.000039
 35 Cl 0.000179

Sum of Mulliken atomic spin densities = 1.00000

Compound 8 (neutral) [opt freq b3lyp/6-31g(d,p)]



Zero-point correction = 0.270712 (Hartree/Particle)

Thermal correction to Energy = 0.291003

Thermal correction to Enthalpy = 0.291947

Thermal correction to Gibbs Free Energy = 0.217869

Sum of electronic and zero-point Energies = -2038.741688

Sum of electronic and thermal Energies = -2038.721397

Sum of electronic and thermal Enthalpies = -2038.720452

Sum of electronic and thermal Free Energies = -2038.794531

	E (Thermal)/KCal/Mol	CV/ Cal/Mol-Kelvin	S/ Cal/MolKelvin
Total	182.607	75.755	155.911