Electronic Supplementary Information (ESI) for *New Journal of Chemistry*.

Enantiopure Schiff bases of aminoacid phenylhydrazides: impact of the hydrazide function on their structure and properties

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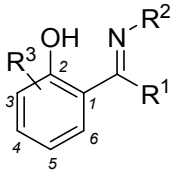
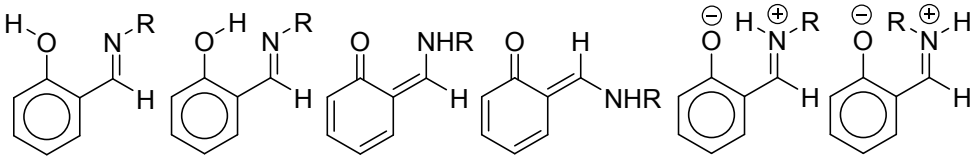
1. Comparison with Schiff bases in the literature





Stereochemistry [a]	*anti-E* [b]	*syn-E* [b]	*Z* [c]	*E* [c]	*E*	*Z*
Form	enol-imine (I)		keto-amine (II)		enolate-iminium (III)	
Electronic charge	no formal				zwitterionic	

Representation of monomeric forms[d]. [a] Representations of localized π-aromatic electrons are possible doubling each I and III drawn forms; [b] the *Z* configuration of enol-imine forms is not reported in literature; [c] *syn* and *anti* conformations could be also defined for the keto-amine forms according to the spatial position of N-H and N-R in regard the oxygen atom; [d] lot of reported studies do not distinguish the forms II and III (mesomeric forms).

Table S1

R^1	R^2	R^3	Physical state	Form	Ref
H	Me	4,6-diOMe	solid	II-Z	27
H	Me, alkyl	4-OMe	solid	II-Z	27
H	Bn	4,6-diOMe	solid	I / II : 1 / 1	27
H	Ph or Bn	4-OMe	solid	I	27
H	Ph	4,6-diOMe	solid	I	27
H	Me	3- or 5- or 6-OMe	solid	I	27
H	Me	3,5-diCl	solid	I / II	18
H	Et	5-NO_2	solid	I / II	24
H	4-HOPh	5-Cl	solid	II	27
H	Ph	3,5-di-*t*-Bu	*i*-Pent	I (from 77 to 297 K)	25
H	Ph	H	*i*-Pent	I (rt) II (<140K)	25
H	4-HOPh	5-Cl	solid	I-syn-E (rt) III-E (<90K)	25
H	Et	5-NO_2	solid	III	18
H	Et	5-NO_2	DMSO or $CDCl_3$	2 forms	18
H	2-(3-HOPy)	H	solid (*t*-BuOH, Tol or *i*-PrOH)	I-E (>100-140°C) II-Z (<100°C)	26
H	2-(3-HOPy)	H	solid (MeOH, MeCN or *n*-PrOH)	I-E	26
H	2-(3-HOPy)	H or 6-OMe	MeOH or DMSO	II-Z	35
H	2-(3-HOPy)	H or 6-OMe	solid	III	35
H	Et	3,5-diNO2	solid	II / III	21
H	Cy	5-NO_2	solid	II / III	21
H	CH_2(1-HO-Cy)	3,5-di-*t*-Bu	solid	I	19
H	(2-$HOCH_2$)Ph	3,5-di-*t*-Bu	solid	I	19
H	PhCH-CHOHPh	H	solid	I	19
H	CH_2(1-HO-Cy)	H	solid	II	19

Me	CH_2CH_2OH	H	solid	II	19
H	MeCH-CHOHPh	5-NO_2	solid	II	19
H	MeCH-CHOHPh	5-Br	solid	II	19
H	(2-$HOCH_2$-4-Cl)Ph	4-NEt_2	solid	I / II	19
H	CH_2(1-HO-Cy)	H	MeOH or EtOH	I major / II minor	19
H	CH_2(1-HO-Cy)	H	Tol or DMF	I very major	19
H	CH_2CH_2OH	H	MeOH or EtOH	I minor / II major	19
H	CH_2CH_2OH	H	Tol or DMF	I very major	19
H	Me or *i*-Pr or *t*-Bu	3-OH	solid	I minor / II major	23
H	4-NO_2Ph	3-OH	solid	II	23
H	(3,4,5-triOMe)Ph	3-OH	solid	I minor / II major	23
H	(4-NMe_2)Ph	3-OH	solid	I major / II minor	23
H	Me or *i*-Pr or *t*-Bu	3-OH	$CDCl_3$ or CCl_4	I	23
H	4-NO_2Ph	3-OH	$CDCl_3$ or CCl_4	I	23
H	(3,4,5-triOMe)Ph	3-OH	$CDCl_3$ or CCl_4	I	23
H	(4-NMe_2)Ph	3-OH	$CDCl_3$ or CCl_4	I	23
H	$CH_2CH_2SO_3^-$ K^+	3-OMe	solid	I-E / II-Z	20
H	$CH_2CH_2SO_3^-$ K^+	3-OMe	MeOH	I / II	20
H	$CH_2CH_2SO_3^-$ K^+	3-OMe	DMSO	I	20

References

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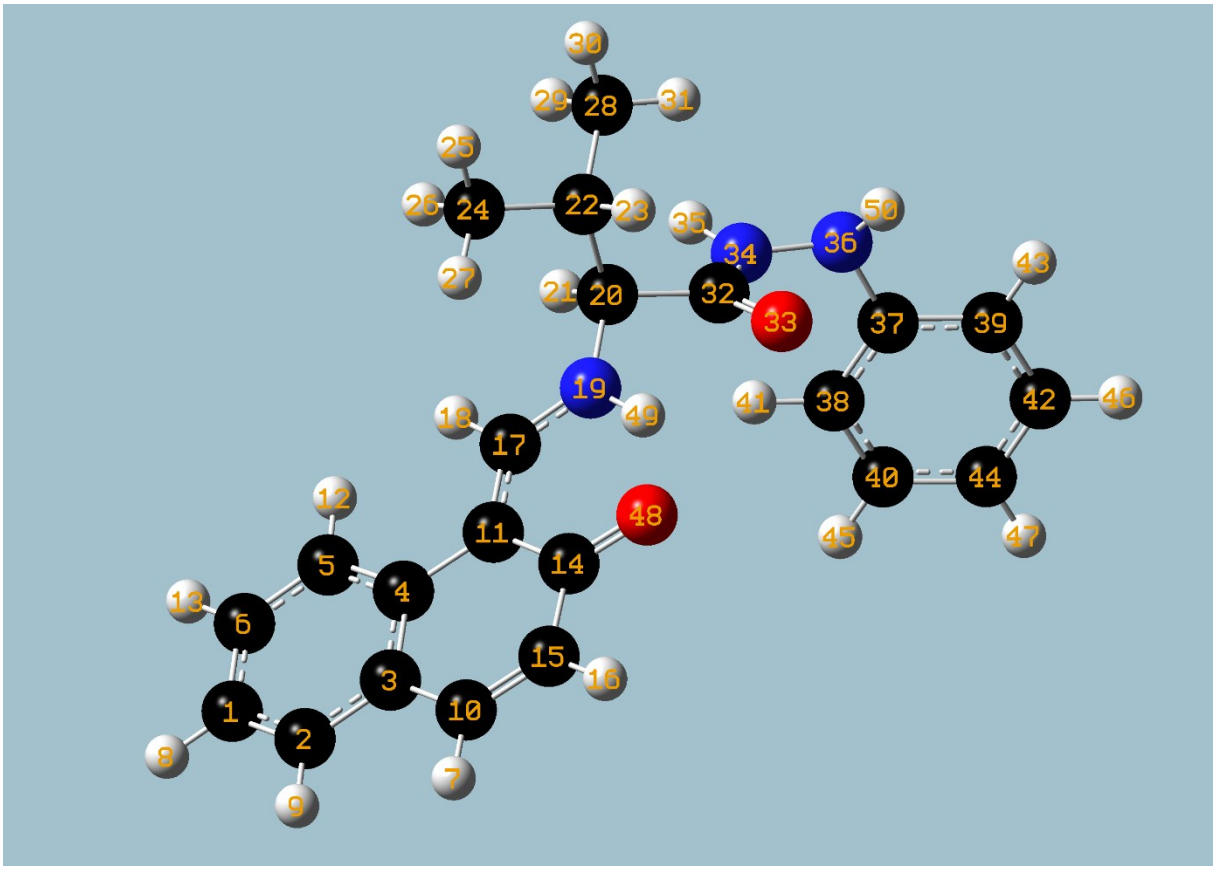
2. Calculation section

a. Labels of 5b for this calculation section



b. Examples of Gaussian input files

Research of transition state

```
%NprocShared=4
%chk=C:\Users\Calculs\TS2a.chk
# BMK/6-31G(2df,2pd) opt=(CalcFC, Tight, TS, noeigentest) gfprint freq

TS

0 1
6   -5.520139   -2.310302   -1.475348
6   -5.521732   -2.030155   -0.123711
6   -4.507262   -1.235739    0.457675
6   -3.459429   -0.709239   -0.351521
6   -3.484052   -1.013249   -1.736048
6   -4.487617   -1.792216   -2.281784
1   -5.328603   -1.362536    2.459673
1   -6.300271   -2.919201   -1.913521
1   -6.306600   -2.418199    0.516315
6   -4.518867   -0.948525    1.867349
6   -2.436610    0.099431    0.280338
1   -2.709676   -0.635376   -2.391070
1   -4.477363   -2.007054   -3.343572
6   -2.477735    0.368068    1.690590
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1   -1.238035    0.512870   -1.507286
7   -0.450762    1.383081    0.183628
6    0.679478    1.976980   -0.486448
1    0.641041    1.725457   -1.557026
6    0.687044    3.518734   -0.332281
1    0.748096    3.718392    0.742053
6   -0.608554    4.124174   -0.891527
1   -0.598753    5.211054   -0.783090
1   -0.713661    3.896855   -1.958268
1   -1.486238    3.738374   -0.370929
6    1.921171    4.122410   -1.023268
1    1.923518    3.887637   -2.093461
1    1.915161    5.210216   -0.927337
1    2.854823    3.757381   -0.588667
6    1.955968    1.390620    0.144432
8    2.205813    1.493253    1.320591
7    2.785784    0.751838   -0.734903
1    2.731333    0.985151   -1.713699
7    4.062217    0.367984   -0.300636
6    4.278845   -1.018101   -0.128393
6    3.491988   -1.985847   -0.760748
6    5.378806   -1.417909    0.644846
6    3.810487   -3.338194   -0.619162
1    2.635852   -1.685811   -1.348003
6    5.683589   -2.768993    0.780508
1    5.989887   -0.666081    1.131141
6    4.903708   -3.740761    0.146753
1    3.192068   -4.078924   -1.111455
1    6.533320   -3.062179    1.384552
1    5.146213   -4.790293    0.249659
8   -1.588849    1.078768    2.264676
1   -0.792481    1.388671    1.353237
1    4.272926    0.890544    0.542288
```

Research of charges

```
%nproc=4
#p MP2/6-31G(2df,2pd) Density=(MP2) pop=CHelp gfprint

Geometry taken from BMK/6-31G(2df,2pd) opt tight checked by freq

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C,0,-4.7638285289,-1.1979220775,0.362992974
C,0,-3.6621766611,-0.6645876502,-0.3600652081
C,0,-3.7203311172,-0.7305894114,-1.77032494
C,0,-4.8141065782,-1.2757321009,-2.4268868643
H,0,-5.6050981899,-1.5922643841,2.3272736532
H,0,-6.7517920329,-2.214706036,-2.2227638328
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H,0,-3.7016064452,-0.6607035647,3.6027578776
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H,0,1.5841408758,5.0950967082,-0.7765050663
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H,0,2.8147429064,1.1856341339,-1.6532033951
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C,0,3.9476710057,-1.7431112772,-0.9413748652
C,0,5.7192212752,-1.0675099395,0.5636414849
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H,0,6.2218719645,-0.2904461999,1.1280303096
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H,0,3.9127488875,-3.821493658,-1.4623530936
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H,0,5.9026448161,-4.4021637145,-0.0928431313
O,0,-1.6035482614,0.3610444264,2.5290358715
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```

c. Charge distribution of 5b (II or III forms)

The charge distribution was performed using the electron density computed in the gas phase at the MP2/6-31G(2df,2pd) level of theory on the gas phase BMK/6-31G(2df,2pd) optimized geometry. Several methods were used:

- Mulliken[53] or natural population[54] analyses,
- electrostatic potential-derived charges using the CHelpG[55] or Merz-Kollman-Singh (MK)[56] schemes.

Table S2

		Atomic charges model				Electric Potential (atomic unit)
				ESP-derived		
Atom N°	Type	Mulliken	Natural	CHelpG Scheme	MK Scheme	
1	C	-0.18281	-0.20288	0.13057	-0.11432	-14.75476
2	C	-0.18100	-0.19227	-0.40073	-0.21046	-14.75598
3	C	0.09983	-0.06999	0.36123	0.11268	-14.74408
4	C	0.08649	-0.03783	-0.07977	0.16048	-14.73703
5	C	-0.20761	-0.18376	-0.05574	-0.20783	-14.75022
6	C	-0.17814	-0.21671	-0.19296	-0.13055	-14.75457
7	H	0.14937	0.20769	0.10662	0.13666	-1.10287
8	H	0.15352	0.21174	0.00913	0.12193	-1.10497
9	H	0.14379	0.20678	0.14617	0.12606	-1.10631
10	C	-0.16584	-0.16312	-0.20244	-0.17805	-14.74742
11	C	-0.16667	-0.23364	-0.30655	-0.38662	-14.75115
12	H	0.13651	0.19712	0.06445	0.12113	-1.09942
13	H	0.14875	0.20743	0.10208	0.11714	-1.10662
14	**C**	**0.30867**	**0.44494**	**0.65741**	**0.57382**	**-14.69080**
15	C	-0.20916	-0.23476	-0.29026	-0.25968	-14.76148
16	H	0.16137	0.21876	0.14558	0.14452	-1.10788
17	C	0.04416	0.13163	0.13689	0.06958	-14.69035
18	H	0.15183	0.18892	0.09563	0.13802	-1.07075
19	**N**	**-0.30522**	**-0.54236**	**-0.31710**	**-0.09717**	**-18.31335**
20	C	-0.14395	-0.10902	0.17619	-0.67300	-14.67482
21	H	0.14945	0.20733	-0.02924	0.19243	-1.06830
22	C	-0.04850	-0.24195	0.45740	0.53356	-14.71736
23	H	0.17047	0.23242	-0.10183	0.01654	-1.10528
24	C	-0.51118	-0.61373	-0.24322	-0.53982	-14.74620
25	H	0.16214	0.22195	0.04625	0.13606	-1.10443
26	H	0.14461	0.20010	0.02974	0.14310	-1.10302
27	H	0.17710	0.22525	0.01756	0.13693	-1.10763
28	C	-0.51384	-0.61605	-0.11898	-0.64911	-14.73889
29	H	0.14430	0.19930	-0.00594	0.15600	-1.09599
30	H	0.16904	0.22626	0.01789	0.16755	-1.09880
31	H	0.16478	0.21523	0.00970	0.16249	-1.09863
32	C	0.42611	0.64605	0.12871	0.67598	-14.63193
33	O	-0.38079	-0.56725	-0.37940	-0.45322	-22.34074
34	N	-0.30310	-0.46033	0.02460	-0.34488	-18.28448
35	H	0.28076	0.39173	0.16399	0.34642	-0.98518
36	N	-0.35252	-0.44548	-0.43865	-0.55351	-18.30733
37	C	0.25426	0.13280	0.38245	0.37285	-14.70745
38	C	-0.19623	-0.23829	-0.07402	-0.15029	-14.74977
39	C	-0.19097	-0.22485	-0.30895	-0.28537	-14.74810
40	C	-0.15993	-0.20032	-0.29570	-0.14749	-14.75039
41	H	0.14376	0.21405	0.03100	0.10092	-1.09707
42	C	-0.16107	-0.20223	-0.17926	-0.07311	-14.74996
43	H	0.15095	0.20994	0.14952	0.15284	-1.09355
44	C	-0.17209	-0.21903	0.09824	-0.16180	-14.75460
45	H	0.15308	0.21011	0.15191	0.13058	-1.10477
46	H	0.15437	0.21113	0.12623	0.11550	-1.10405
47	H	0.15474	0.21109	0.03300	0.12739	-1.10520
48	**O**	**-0.42881**	**-0.59223**	**-0.60417**	**-0.53322**	**-22.37298**
49	**H**	**0.31732**	**0.45723**	**0.34829**	**0.31451**	**-1.01000**
50	H	0.25793	0.38113	0.27651	0.34582	-1.01694

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d. Cartesian coordinates of 5b (II/III forms)

HF/3-21G. gas phase

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.641063	-1.724502	-1.742034
2	6	0	-5.576361	-1.767143	-0.372096
3	6	0	-4.509934	-1.189104	0.317980
4	6	0	-3.475231	-0.547997	-0.379504
5	6	0	-3.562126	-0.518857	-1.779107
6	6	0	-4.619729	-1.092560	-2.443218
7	1	0	-5.273244	-1.749335	2.263640
8	1	0	-6.462983	-2.170599	-2.264319
9	1	0	-6.352958	-2.250642	0.189059
10	6	0	-4.463019	-1.248763	1.767938
11	6	0	-2.373793	0.047353	0.385429
12	1	0	-2.799038	-0.046196	-2.361992
13	1	0	-4.654105	-1.051333	-3.514230
14	6	0	-2.352415	-0.028384	1.837617
15	6	0	-3.472039	-0.716543	2.473974
16	1	0	-3.443195	-0.765450	3.542232
17	6	0	-1.340540	0.696397	-0.238298
18	1	0	-1.347086	0.779690	-1.307270
19	7	0	-0.294130	1.259680	0.351024
20	6	0	0.776537	1.954166	-0.352629
21	1	0	0.636596	1.824537	-1.418325
22	6	0	0.790437	3.460746	-0.004035
23	1	0	0.964161	3.528155	1.063306
24	6	0	-0.556793	4.114619	-0.348932
25	1	0	-0.534077	5.166856	-0.089438
26	1	0	-0.757200	4.036932	-1.414047
27	1	0	-1.369358	3.651497	0.193641
28	6	0	1.932674	4.175603	-0.752426
29	1	0	1.785955	4.103120	-1.826494
30	1	0	1.946353	5.226166	-0.488956
31	1	0	2.902882	3.760554	-0.507391
32	6	0	2.081964	1.323332	0.120801
33	8	0	2.340619	1.218665	1.300666
34	7	0	2.929546	0.929265	-0.865007
35	1	0	2.776839	1.139673	-1.825713
36	7	0	4.178199	0.378282	-0.549689
37	6	0	4.257032	-1.015069	-0.336267
38	6	0	3.259627	-1.886353	-0.742184
39	6	0	5.404095	-1.529797	0.257710
40	6	0	3.409998	-3.249272	-0.555329
41	1	0	2.369848	-1.502674	-1.192579
42	6	0	5.544809	-2.889625	0.441831
43	1	0	6.183679	-0.863348	0.571397
44	6	0	4.548726	-3.762248	0.035581
45	1	0	2.625756	-3.908687	-0.870971
46	1	0	6.434414	-3.267695	0.905450
47	1	0	4.658278	-4.817693	0.181262
48	8	0	-1.442524	0.462750	2.526005
49	1	0	-0.247268	1.169219	1.359911
50	1	0	4.698556	0.949353	0.087344

E(RHF) = -1153.09454269 h
Sum of electronic and thermal Free Energies = -1152.706268 h

HF/6-31G(d). gas phase

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.446669	-1.813373	-1.793811
2	6	0	-5.449891	-1.773062	-0.420261
3	6	0	-4.421936	-1.146588	0.288955
4	6	0	-3.353585	-0.536682	-0.388807
5	6	0	-3.369080	-0.597183	-1.790686
6	6	0	-4.389961	-1.217315	-2.475263
7	1	0	-5.288018	-1.607515	2.224595
8	1	0	-6.241435	-2.297471	-2.331364
9	1	0	-6.254250	-2.230279	0.129671
10	6	0	-4.452195	-1.128458	1.743606
11	6	0	-2.293313	0.115830	0.399860
12	1	0	-2.576003	-0.161428	-2.368485
13	1	0	-4.363755	-1.240531	-3.550463
14	6	0	-2.351127	0.106434	1.862433
15	6	0	-3.502953	-0.556880	2.480867
16	1	0	-3.532739	-0.551549	3.554337
17	6	0	-1.249336	0.761934	-0.211490
18	1	0	-1.222688	0.805459	-1.284044
19	7	0	-0.227785	1.375362	0.370931
20	6	0	0.828402	2.060121	-0.342473
21	1	0	0.629576	1.952944	-1.404430
22	6	0	0.893375	3.561128	0.004960
23	1	0	1.079284	3.627318	1.072130
24	6	0	-0.431931	4.258464	-0.309932
25	1	0	-0.373044	5.309270	-0.046713
26	1	0	-0.665196	4.199708	-1.371010
27	1	0	-1.256595	3.825974	0.242551
28	6	0	2.052410	4.244384	-0.729879
29	1	0	1.937261	4.166158	-1.808939
30	1	0	2.082797	5.299651	-0.482747
31	1	0	3.014432	3.823033	-0.458711
32	6	0	2.141975	1.363148	0.017814
33	8	0	2.564665	1.366299	1.136442
34	7	0	2.771143	0.731672	-1.006680
35	1	0	2.548837	0.964802	-1.947277
36	7	0	4.014002	0.158485	-0.832881
37	6	0	4.043300	-1.191015	-0.407094
38	6	0	2.983242	-2.060264	-0.612799
39	6	0	5.214959	-1.666601	0.172512
40	6	0	3.098329	-3.389113	-0.233688
41	1	0	2.072585	-1.706661	-1.055910
42	6	0	5.317922	-2.992490	0.546075
43	1	0	6.042808	-0.996737	0.329741
44	6	0	4.259710	-3.866277	0.345811
45	1	0	2.265887	-4.051337	-0.392980
46	1	0	6.228536	-3.343027	0.998454
47	1	0	4.340126	-4.896887	0.639793
48	8	0	-1.500284	0.627968	2.562460
49	1	0	-0.195627	1.337769	1.373345
50	1	0	4.580764	0.741719	-0.252608

E(RHF) = -1159.55378850 h
Sum of electronic and thermal Free Energies = -1159.168407 h

HF/6-31+G(d). gas phase

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.417717	-1.824509	-1.806950
2	6	0	-5.428046	-1.784212	-0.431967
3	6	0	-4.406227	-1.150381	0.283518
4	6	0	-3.337253	-0.533930	-0.388667
5	6	0	-3.346498	-0.591480	-1.792750
6	6	0	-4.360379	-1.219208	-2.483759
7	1	0	-5.281758	-1.613249	2.215511
8	1	0	-6.206594	-2.313830	-2.348738
9	1	0	-6.232806	-2.246580	0.113375
10	6	0	-4.446490	-1.129702	1.737720
11	6	0	-2.283767	0.122765	0.406111
12	1	0	-2.555795	-0.147338	-2.367413
13	1	0	-4.329108	-1.240424	-3.558956
14	6	0	-2.354274	0.119991	1.866279
15	6	0	-3.504859	-0.547509	2.481150
16	1	0	-3.543426	-0.539754	3.554669
17	6	0	-1.229814	0.762299	-0.202317
18	1	0	-1.194722	0.793445	-1.275129
19	7	0	-0.212031	1.377465	0.381001
20	6	0	0.837068	2.071381	-0.336639
21	1	0	0.628777	1.967273	-1.397309
22	6	0	0.894281	3.571766	0.014382
23	1	0	1.090178	3.640021	1.079928
24	6	0	-0.439922	4.258345	-0.287753
25	1	0	-0.385208	5.310184	-0.026158
26	1	0	-0.684318	4.197913	-1.346634
27	1	0	-1.257044	3.822142	0.273468
28	6	0	2.039011	4.265065	-0.733176
29	1	0	1.908969	4.192656	-1.811248
30	1	0	2.066125	5.319597	-0.480792
31	1	0	3.008094	3.849229	-0.478621
32	6	0	2.157683	1.374936	0.003386
33	8	0	2.613651	1.397096	1.109733
34	7	0	2.751336	0.714813	-1.025146
35	1	0	2.503653	0.930954	-1.963740
36	7	0	3.992164	0.129069	-0.877407
37	6	0	4.018769	-1.210867	-0.421574
38	6	0	2.950071	-2.077977	-0.596216
39	6	0	5.194713	-1.681665	0.156262
40	6	0	3.060379	-3.401046	-0.188853
41	1	0	2.035568	-1.729100	-1.035995
42	6	0	5.294003	-3.001552	0.557350
43	1	0	6.028808	-1.014559	0.292079
44	6	0	4.226715	-3.874045	0.387997
45	1	0	2.221393	-4.060582	-0.323652
46	1	0	6.207377	-3.347971	1.007575
47	1	0	4.303881	-4.898533	0.703931
48	8	0	-1.507594	0.651299	2.569006
49	1	0	-0.191902	1.362972	1.384993
50	1	0	4.586443	0.718153	-0.331409

E(RHF) = -1159.58366680 h
Sum of electronic and thermal Free Energies = -1159.198884 h

HF/6-31G(d.p). gas phase

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.431141	-1.802249	-1.795023
2	6	0	-5.432156	-1.764766	-0.421719
3	6	0	-4.403538	-1.138741	0.286877
4	6	0	-3.337150	-0.526607	-0.391773
5	6	0	-3.354932	-0.584305	-1.793767
6	6	0	-4.376354	-1.203987	-2.477199
7	1	0	-5.265637	-1.604174	2.223877
8	1	0	-6.226591	-2.286118	-2.332273
9	1	0	-6.235418	-2.223967	0.128834
10	6	0	-4.431078	-1.123408	1.741437
11	6	0	-2.276287	0.125205	0.396011
12	1	0	-2.563356	-0.146826	-2.372744
13	1	0	-4.352261	-1.225247	-3.552857
14	6	0	-2.331530	0.112832	1.858184
15	6	0	-3.481122	-0.552437	2.477953
16	1	0	-3.509016	-0.549248	3.551758
17	6	0	-1.233526	0.773738	-0.215096
18	1	0	-1.208735	0.819049	-1.288538
19	7	0	-0.214006	1.386054	0.370475
20	6	0	0.841790	2.072370	-0.341767
21	1	0	0.639628	1.974258	-1.404800
22	6	0	0.913804	3.570410	0.015552
23	1	0	1.111877	3.627214	1.081719
24	6	0	-0.412603	4.273788	-0.279318
25	1	0	-0.346999	5.322583	-0.009510
26	1	0	-0.658368	4.223146	-1.338260
27	1	0	-1.231996	3.839678	0.279887
28	6	0	2.067680	4.254695	-0.725813
29	1	0	1.939867	4.187097	-1.804388
30	1	0	2.105812	5.307458	-0.468979
31	1	0	3.030338	3.825869	-0.468820
32	6	0	2.154473	1.368866	0.009188
33	8	0	2.591160	1.379801	1.122508
34	7	0	2.765895	0.723717	-1.016496
35	1	0	2.524315	0.935423	-1.955991
36	7	0	3.997976	0.128305	-0.848508
37	6	0	4.008880	-1.217061	-0.412653
38	6	0	2.924211	-2.064100	-0.578032
39	6	0	5.186427	-1.713527	0.137227
40	6	0	3.021169	-3.391377	-0.188920
41	1	0	2.008407	-1.694554	-0.997420
42	6	0	5.270410	-3.037230	0.521474
43	1	0	6.033708	-1.061057	0.262496
44	6	0	4.187762	-3.888871	0.361221
45	1	0	2.169549	-4.036407	-0.316934
46	1	0	6.186280	-3.404092	0.950635
47	1	0	4.253891	-4.918399	0.663359
48	8	0	-1.479176	0.634043	2.557401
49	1	0	-0.186745	1.345196	1.372552
50	1	0	4.585376	0.706403	-0.285422

E(RHF) = -1159.59934424 h
Sum of electronic and thermal Free Energies = -1159.215612 h

HF/6-31+G(d.p). gas phase

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.414732	-1.807578	-1.810237
2	6	0	-5.419557	-1.778615	-0.435154
3	6	0	-4.395225	-1.149876	0.281194
4	6	0	-3.329689	-0.527200	-0.390541
5	6	0	-3.344523	-0.573174	-1.795044
6	6	0	-4.360770	-1.196029	-2.486486
7	1	0	-5.262160	-1.629184	2.213492
8	1	0	-6.205470	-2.293057	-2.352731
9	1	0	-6.221746	-2.246066	0.109775
10	6	0	-4.429379	-1.141159	1.735557
11	6	0	-2.273491	0.123736	0.404938
12	1	0	-2.556757	-0.123912	-2.369726
13	1	0	-4.334115	-1.208552	-3.562038
14	6	0	-2.337975	0.108785	1.865056
15	6	0	-3.485109	-0.564428	2.479681
16	1	0	-3.519083	-0.565475	3.553404
17	6	0	-1.222584	0.769400	-0.202221
18	1	0	-1.192328	0.808843	-1.275599
19	7	0	-0.204603	1.379980	0.384763
20	6	0	0.841978	2.079065	-0.331672
21	1	0	0.632312	1.980964	-1.393231
22	6	0	0.899539	3.577693	0.026521
23	1	0	1.102253	3.639490	1.091631
24	6	0	-0.437105	4.264685	-0.263504
25	1	0	-0.380949	5.314903	0.003833
26	1	0	-0.687624	4.209660	-1.321441
27	1	0	-1.249867	3.824112	0.300810
28	6	0	2.039909	4.275101	-0.723800
29	1	0	1.902287	4.209697	-1.801542
30	1	0	2.068824	5.327699	-0.463978
31	1	0	3.009846	3.856389	-0.477274
32	6	0	2.164154	1.382222	0.001437
33	8	0	2.630618	1.411854	1.103352
34	7	0	2.747080	0.714770	-1.027770
35	1	0	2.482589	0.912897	-1.964488
36	7	0	3.981378	0.116611	-0.883797
37	6	0	4.001009	-1.222043	-0.427518
38	6	0	2.917408	-2.075798	-0.573456
39	6	0	5.184643	-1.706126	0.123607
40	6	0	3.021058	-3.398900	-0.164544
41	1	0	1.996799	-1.716800	-0.991622
42	6	0	5.276371	-3.025561	0.526714
43	1	0	6.030165	-1.049269	0.236619
44	6	0	4.194425	-3.884933	0.385789
45	1	0	2.170639	-4.048116	-0.276897
46	1	0	6.195906	-3.382396	0.956064
47	1	0	4.266137	-4.909365	0.703134
48	8	0	-1.488268	0.635042	2.568419
49	1	0	-0.185048	1.355258	1.388198
50	1	0	4.589460	0.701990	-0.350833

E(RHF) = -1159.62860459 h
Sum of electronic and thermal Free Energies = -1159.245454 h

B3LYP/3-21G. gas phase

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.769477	-2.031896	-1.591150
2	6	0	-5.717931	-1.914822	-0.212742
3	6	0	-4.653948	-1.240961	0.422083
4	6	0	-3.605990	-0.665273	-0.355736
5	6	0	-3.686222	-0.801446	-1.761508
6	6	0	-4.741549	-1.468023	-2.365162
7	1	0	-5.424142	-1.577834	2.421954
8	1	0	-6.590644	-2.551610	-2.069621
9	1	0	-6.501237	-2.344003	0.403664
10	6	0	-4.610994	-1.127306	1.860485
11	6	0	-2.521000	0.023873	0.334170
12	1	0	-2.913240	-0.381799	-2.393730
13	1	0	-4.771599	-1.554182	-3.445529
14	6	0	-2.498525	0.124353	1.792008
15	6	0	-3.605898	-0.490967	2.504874
16	1	0	-3.576899	-0.410027	3.583691
17	6	0	-1.466014	0.613552	-0.363504
18	1	0	-1.434392	0.572889	-1.448500
19	7	0	-0.457920	1.250820	0.235509
20	6	0	0.676434	1.867397	-0.456514
21	1	0	0.627860	1.612935	-1.522197
22	6	0	0.662269	3.415456	-0.278995
23	1	0	0.766139	3.594991	0.798255
24	6	0	-0.665291	4.015943	-0.779597
25	1	0	-0.668482	5.099392	-0.618918
26	1	0	-0.787890	3.830688	-1.854755
27	1	0	-1.517764	3.585443	-0.248447
28	6	0	1.856127	4.055674	-1.021110
29	1	0	1.775933	3.871004	-2.100675
30	1	0	1.853662	5.139231	-0.865735
31	1	0	2.815632	3.664632	-0.668304
32	6	0	1.940862	1.301274	0.206616
33	8	0	2.078325	1.261239	1.436492
34	7	0	2.924974	0.903683	-0.663544
35	1	0	2.916265	1.150858	-1.647933
36	7	0	4.189938	0.513546	-0.133589
37	6	0	4.478936	-0.878401	-0.119470
38	6	0	3.736432	-1.810659	-0.853363
39	6	0	5.593360	-1.318803	0.613602
40	6	0	4.106732	-3.155881	-0.857788
41	1	0	2.865005	-1.482336	-1.402722
42	6	0	5.951592	-2.663454	0.609551
43	1	0	6.178698	-0.601351	1.178277
44	6	0	5.213262	-3.593135	-0.129262
45	1	0	3.517616	-3.864898	-1.428325
46	1	0	6.811722	-2.986011	1.184952
47	1	0	5.494950	-4.638877	-0.132316
48	8	0	-1.563523	0.719404	2.434048
49	1	0	-0.525682	1.224675	1.294959
50	1	0	4.332113	0.985718	0.764093

E(RB3LYP) = -1160.48473037 h
Sum of electronic and thermal Free Energies = -1160.128460 h

B3LYP/6-31G(d). gas phase

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.464530	-2.112269	-1.656316
2	6	0	-5.487957	-1.933639	-0.283557
3	6	0	-4.477620	-1.206367	0.376610
4	6	0	-3.402922	-0.635088	-0.365214
5	6	0	-3.404050	-0.838419	-1.763141
6	6	0	-4.408965	-1.556896	-2.394626
7	1	0	-5.355155	-1.486956	2.342657
8	1	0	-6.248834	-2.674953	-2.154227
9	1	0	-6.294485	-2.357497	0.310787
10	6	0	-4.520010	-1.036524	1.808731
11	6	0	-2.372746	0.115527	0.353894
12	1	0	-2.605525	-0.433906	-2.377707
13	1	0	-4.372031	-1.689680	-3.472881
14	6	0	-2.439350	0.264804	1.811586
15	6	0	-3.571129	-0.351415	2.490437
16	1	0	-3.608392	-0.229850	3.568563
17	6	0	-1.315122	0.721429	-0.319646
18	1	0	-1.247342	0.661032	-1.403651
19	7	0	-0.336450	1.412803	0.266696
20	6	0	0.763693	2.054848	-0.433434
21	1	0	0.626973	1.862398	-1.506931
22	6	0	0.795657	3.586713	-0.192137
23	1	0	0.946640	3.721502	0.886759
24	6	0	-0.529018	4.244627	-0.596696
25	1	0	-0.496451	5.319425	-0.387504
26	1	0	-0.721552	4.123337	-1.671270
27	1	0	-1.376285	3.822105	-0.049251
28	6	0	1.981365	4.230044	-0.927487
29	1	0	1.906157	4.081192	-2.013299
30	1	0	1.998162	5.309938	-0.747013
31	1	0	2.942954	3.827343	-0.591460
32	6	0	2.068271	1.406789	0.065465
33	8	0	2.425225	1.484868	1.230696
34	7	0	2.790039	0.729870	-0.886786
35	1	0	2.646933	0.946900	-1.865428
36	7	0	4.069272	0.253529	-0.579385
37	6	0	4.175314	-1.130825	-0.265205
38	6	0	3.235123	-2.071295	-0.697760
39	6	0	5.311066	-1.560565	0.435305
40	6	0	3.433684	-3.425983	-0.426807
41	1	0	2.348801	-1.742914	-1.229863
42	6	0	5.498416	-2.914387	0.700010
43	1	0	6.045214	-0.830536	0.769176
44	6	0	4.561867	-3.857873	0.270131
45	1	0	2.692232	-4.146526	-0.762138
46	1	0	6.380442	-3.231836	1.249919
47	1	0	4.709004	-4.913305	0.479508
48	8	0	-1.576927	0.897768	2.471465
49	1	0	-0.406598	1.436205	1.300120
50	1	0	4.456513	0.832647	0.163318

E(RB3LYP) = -1166.88779352
Sum of electronic and thermal Free Energies = -1166.534366

B3LYP/6-31+G(d). gas phase

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.363126	-2.135745	-1.686870
2	6	0	-5.426005	-1.923750	-0.318548
3	6	0	-4.435177	-1.176843	0.353219
4	6	0	-3.340529	-0.620020	-0.371332
5	6	0	-3.301135	-0.856793	-1.765138
6	6	0	-4.286659	-1.594312	-2.408725
7	1	0	-5.367481	-1.412478	2.301951
8	1	0	-6.131730	-2.712913	-2.193308
9	1	0	-6.248821	-2.336058	0.262022
10	6	0	-4.518682	-0.973306	1.779759
11	6	0	-2.331060	0.150485	0.359776
12	1	0	-2.487136	-0.465481	-2.367944
13	1	0	-4.218056	-1.752970	-3.482214
14	6	0	-2.440743	0.331767	1.809778
15	6	0	-3.589130	-0.269010	2.472891
16	1	0	-3.658746	-0.123466	3.546869
17	6	0	-1.257511	0.744858	-0.302409
18	1	0	-1.169209	0.659234	-1.383120
19	7	0	-0.289329	1.451914	0.282475
20	6	0	0.808538	2.093459	-0.426230
21	1	0	0.650740	1.913619	-1.499253
22	6	0	0.850572	3.622800	-0.173337
23	1	0	1.008138	3.754593	0.905273
24	6	0	-0.475285	4.286980	-0.568939
25	1	0	-0.436500	5.361475	-0.356414
26	1	0	-0.673662	4.170055	-1.643618
27	1	0	-1.323088	3.868407	-0.018233
28	6	0	2.032548	4.265994	-0.916252
29	1	0	1.944333	4.126300	-2.002859
30	1	0	2.055899	5.344823	-0.726877
31	1	0	2.996666	3.857059	-0.593958
32	6	0	2.117468	1.421502	0.033812
33	8	0	2.528848	1.512774	1.181426
34	7	0	2.773064	0.698487	-0.932823
35	1	0	2.575628	0.874107	-1.910600
36	7	0	4.035313	0.154534	-0.682096
37	6	0	4.082649	-1.213682	-0.289998
38	6	0	3.059334	-2.116488	-0.599838
39	6	0	5.237495	-1.673132	0.360934
40	6	0	3.194244	-3.464650	-0.255983
41	1	0	2.158158	-1.767383	-1.093109
42	6	0	5.361451	-3.019623	0.698991
43	1	0	6.035324	-0.973680	0.602432
44	6	0	4.341371	-3.926688	0.392006
45	1	0	2.388561	-4.154343	-0.494907
46	1	0	6.258901	-3.359562	1.209646
47	1	0	4.438675	-4.975091	0.659336
48	8	0	-1.592849	0.984249	2.475611
49	1	0	-0.374661	1.516074	1.311657
50	1	0	4.532962	0.754136	-0.027358

E(RB3LYP) = -1166.93192641 h
Sum of electronic and thermal Free Energies = -1166.579367 h

B3LYP/6-31G(d.p). gas phase

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.409848	-2.151292	-1.630877
2	6	0	-5.435585	-1.949910	-0.261759
3	6	0	-4.434476	-1.198370	0.385493
4	6	0	-3.367418	-0.627007	-0.367144
5	6	0	-3.366929	-0.852258	-1.761788
6	6	0	-4.362440	-1.594235	-2.379672
7	1	0	-5.307076	-1.452996	2.356652
8	1	0	-6.186397	-2.732007	-2.118659
9	1	0	-6.236190	-2.373489	0.339571
10	6	0	-4.478741	-1.002228	1.813743
11	6	0	-2.346572	0.146832	0.337740
12	1	0	-2.575770	-0.445272	-2.383194
13	1	0	-4.325658	-1.744052	-3.455042
14	6	0	-2.417237	0.325949	1.790071
15	6	0	-3.539316	-0.290856	2.481924
16	1	0	-3.578486	-0.148658	3.556867
17	6	0	-1.287462	0.745723	-0.341907
18	1	0	-1.207202	0.659199	-1.423314
19	7	0	-0.326911	1.457125	0.246545
20	6	0	0.784971	2.085037	-0.446857
21	1	0	0.653053	1.897315	-1.521738
22	6	0	0.835348	3.614895	-0.201749
23	1	0	0.991342	3.742675	0.876742
24	6	0	-0.482094	4.289752	-0.600080
25	1	0	-0.436952	5.362163	-0.387050
26	1	0	-0.678598	4.174971	-1.673560
27	1	0	-1.331854	3.874837	-0.052837
28	6	0	2.027230	4.244744	-0.937649
29	1	0	1.944542	4.105018	-2.023024
30	1	0	2.062276	5.321784	-0.749823
31	1	0	2.982752	3.824738	-0.609327
32	6	0	2.079610	1.420143	0.056230
33	8	0	2.448565	1.514021	1.216652
34	7	0	2.777824	0.708195	-0.886953
35	1	0	2.629145	0.903425	-1.868124
36	7	0	4.042400	0.198794	-0.574036
37	6	0	4.111341	-1.185493	-0.253978
38	6	0	3.137918	-2.100178	-0.667924
39	6	0	5.242924	-1.644946	0.434525
40	6	0	3.299332	-3.458218	-0.390343
41	1	0	2.255433	-1.749010	-1.190449
42	6	0	5.392297	-3.001677	0.706518
43	1	0	6.002781	-0.935705	0.753035
44	6	0	4.422505	-3.919212	0.295213
45	1	0	2.532938	-4.158028	-0.711112
46	1	0	6.270936	-3.342085	1.246765
47	1	0	4.540493	-4.976526	0.509873
48	8	0	-1.561257	0.985284	2.436314
49	1	0	-0.429218	1.493887	1.281711
50	1	0	4.443911	0.771396	0.165048

E(RB3LYP) = -1166.92838626 h
Sum of electronic and thermal Free Energies = -1166.576126 h

B3LYP/6-31+G(d.p). gas phase

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.342182	-2.147843	-1.669172
2	6	0	-5.399532	-1.929663	-0.301912
3	6	0	-4.410314	-1.172331	0.360785
4	6	0	-3.323600	-0.612298	-0.373081
5	6	0	-3.290288	-0.854417	-1.766205
6	6	0	-4.273928	-1.601990	-2.400091
7	1	0	-5.329297	-1.401748	2.315835
8	1	0	-6.108713	-2.732394	-2.168310
9	1	0	-6.215778	-2.344339	0.284581
10	6	0	-4.487379	-0.960416	1.786132
11	6	0	-2.315644	0.167441	0.347869
12	1	0	-2.483783	-0.458657	-2.374758
13	1	0	-4.211231	-1.764950	-3.472413
14	6	0	-2.420050	0.359230	1.795504
15	6	0	-3.559391	-0.244354	2.469580
16	1	0	-3.624278	-0.091880	3.542102
17	6	0	-1.243315	0.760396	-0.319313
18	1	0	-1.151197	0.664784	-1.398695
19	7	0	-0.285265	1.474943	0.270084
20	6	0	0.820042	2.110297	-0.431889
21	1	0	0.667553	1.936088	-1.506355
22	6	0	0.872260	3.637988	-0.173796
23	1	0	1.028097	3.762812	0.905171
24	6	0	-0.447465	4.313343	-0.569978
25	1	0	-0.401961	5.385114	-0.351630
26	1	0	-0.642211	4.203743	-1.644951
27	1	0	-1.299031	3.897860	-0.024980
28	6	0	2.061335	4.274733	-0.910360
29	1	0	1.973660	4.142260	-1.996780
30	1	0	2.093699	5.350955	-0.714763
31	1	0	3.019824	3.855715	-0.588361
32	6	0	2.122899	1.428266	0.030584
33	8	0	2.542602	1.529160	1.174412
34	7	0	2.763983	0.685825	-0.930416
35	1	0	2.558713	0.845779	-1.908013
36	7	0	4.016345	0.122741	-0.675434
37	6	0	4.044804	-1.245348	-0.285044
38	6	0	3.002340	-2.130854	-0.580917
39	6	0	5.199897	-1.723962	0.351808
40	6	0	3.118901	-3.480692	-0.237413
41	1	0	2.101528	-1.767449	-1.062445
42	6	0	5.304637	-3.071677	0.690122
43	1	0	6.011907	-1.038492	0.581768
44	6	0	4.265682	-3.961519	0.396722
45	1	0	2.299446	-4.156399	-0.465339
46	1	0	6.201717	-3.426366	1.189444
47	1	0	4.348438	-5.010333	0.663654
48	8	0	-1.571507	1.023908	2.451572
49	1	0	-0.392896	1.537613	1.301015
50	1	0	4.523330	0.715199	-0.022902

E(RB3LYP) = -1166.97172143 h
Sum of electronic and thermal Free Energies = -1166.620315 h

B3P86/6-31+G(d.p). gas phase

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.366523	-2.202998	-1.619726
2	6	0	-5.420940	-1.957170	-0.260857
3	6	0	-4.432192	-1.188767	0.381362
4	6	0	-3.350149	-0.647482	-0.364839
5	6	0	-3.319153	-0.916628	-1.748912
6	6	0	-4.302216	-1.674400	-2.362642
7	1	0	-5.345042	-1.374718	2.338422
8	1	0	-6.134193	-2.797069	-2.104974
9	1	0	-6.235775	-2.358415	0.336609
10	6	0	-4.504643	-0.946021	1.796305
11	6	0	-2.345720	0.141200	0.333767
12	1	0	-2.513018	-0.532957	-2.366033
13	1	0	-4.242685	-1.859717	-3.431200
14	6	0	-2.443261	0.367106	1.768974
15	6	0	-3.575412	-0.216090	2.459357
16	1	0	-3.636487	-0.038971	3.528076
17	6	0	-1.271864	0.716718	-0.342981
18	1	0	-1.172168	0.600506	-1.420745
19	7	0	-0.327331	1.434728	0.248099
20	6	0	0.775939	2.061908	-0.444318
21	1	0	0.650779	1.856946	-1.518136
22	6	0	0.802159	3.587485	-0.226902
23	1	0	0.934571	3.740209	0.851751
24	6	0	-0.511814	4.225434	-0.667645
25	1	0	-0.492055	5.302456	-0.476816
26	1	0	-0.678127	4.084267	-1.743095
27	1	0	-1.367889	3.807303	-0.132406
28	6	0	1.991481	4.212816	-0.954541
29	1	0	1.925111	4.048168	-2.037424
30	1	0	2.009999	5.293903	-0.790493
31	1	0	2.947749	3.813257	-0.603452
32	6	0	2.074036	1.423851	0.062223
33	8	0	2.453772	1.544178	1.215614
34	7	0	2.769835	0.705946	-0.869998
35	1	0	2.596734	0.865353	-1.853375
36	7	0	4.028588	0.210417	-0.565501
37	6	0	4.114156	-1.163430	-0.236920
38	6	0	3.109483	-2.074622	-0.565422
39	6	0	5.286867	-1.618831	0.376549
40	6	0	3.281321	-3.427988	-0.279002
41	1	0	2.192593	-1.725200	-1.026877
42	6	0	5.444957	-2.969789	0.660555
43	1	0	6.072496	-0.911092	0.628322
44	6	0	4.444863	-3.886038	0.332635
45	1	0	2.489250	-4.126281	-0.532802
46	1	0	6.357010	-3.308049	1.143221
47	1	0	4.570879	-4.940370	0.555962
48	8	0	-1.591107	1.045658	2.404154
49	1	0	-0.472299	1.505393	1.283786
50	1	0	4.455341	0.801176	0.143202

E(RB3P86) = -1170.42606021 h
Sum of electronic and thermal Free Energies = -1170.073320 h

B3PW91/6-31+G(d.p). gas phase

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.351677	-2.194161	-1.633196
2	6	0	-5.405454	-1.957444	-0.271303
3	6	0	-4.418680	-1.187998	0.375926
4	6	0	-3.338591	-0.635638	-0.367917
5	6	0	-3.308904	-0.895647	-1.755427
6	6	0	-4.289915	-1.654709	-2.374065
7	1	0	-5.330178	-1.391850	2.334617
8	1	0	-6.117635	-2.788909	-2.121806
9	1	0	-6.218405	-2.367012	0.324093
10	6	0	-4.491907	-0.955122	1.794511
11	6	0	-2.335342	0.154255	0.336646
12	1	0	-2.506200	-0.503796	-2.372641
13	1	0	-4.230570	-1.832003	-3.444674
14	6	0	-2.434653	0.371012	1.775978
15	6	0	-3.565778	-0.224489	2.462715
16	1	0	-3.628272	-0.055259	3.533261
17	6	0	-1.262498	0.736710	-0.338025
18	1	0	-1.163017	0.623392	-1.416202
19	7	0	-0.317061	1.458095	0.251460
20	6	0	0.790283	2.083314	-0.441418
21	1	0	0.659522	1.886129	-1.516006
22	6	0	0.828243	3.610622	-0.214946
23	1	0	0.966579	3.756990	0.864244
24	6	0	-0.485127	4.264038	-0.644793
25	1	0	-0.454258	5.339908	-0.445525
26	1	0	-0.659973	4.133204	-1.720603
27	1	0	-1.342474	3.850407	-0.107190
28	6	0	2.020590	4.235403	-0.944087
29	1	0	1.950339	4.079790	-2.028502
30	1	0	2.045416	5.315657	-0.771529
31	1	0	2.976548	3.828832	-0.598997
32	6	0	2.087235	1.427942	0.058315
33	8	0	2.474284	1.541816	1.210282
34	7	0	2.767699	0.699940	-0.880187
35	1	0	2.586557	0.857276	-1.862370
36	7	0	4.020479	0.179208	-0.588913
37	6	0	4.086182	-1.194019	-0.247137
38	6	0	3.067075	-2.094879	-0.566350
39	6	0	5.254616	-1.662580	0.368271
40	6	0	3.219889	-3.449362	-0.268393
41	1	0	2.153615	-1.737672	-1.029886
42	6	0	5.394122	-3.014721	0.662973
43	1	0	6.051800	-0.964751	0.613929
44	6	0	4.379130	-3.919948	0.344973
45	1	0	2.416564	-4.138375	-0.514889
46	1	0	6.302908	-3.362168	1.146759
47	1	0	4.490269	-4.974721	0.577140
48	8	0	-1.587255	1.049700	2.416441
49	1	0	-0.452393	1.527719	1.285061
50	1	0	4.476171	0.768907	0.101886

E(RB3PW91) = -1166.52060017 h
Sum of electronic and thermal Free Energies = -1166.168250 h

BHandHLYP/6-31+G(d.p). gas phase

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.447727	-1.869131	-1.749988
2	6	0	-5.450137	-1.797786	-0.376101
3	6	0	-4.418607	-1.155038	0.318768
4	6	0	-3.347957	-0.561086	-0.381942
5	6	0	-3.367010	-0.653302	-1.782925
6	6	0	-4.391018	-1.289478	-2.451228
7	1	0	-5.275324	-1.564244	2.261341
8	1	0	-6.245759	-2.366061	-2.275677
9	1	0	-6.255142	-2.241780	0.188556
10	6	0	-4.441057	-1.098904	1.758194
11	6	0	-2.293932	0.102486	0.379197
12	1	0	-2.571542	-0.228751	-2.371120
13	1	0	-4.368811	-1.338654	-3.527942
14	6	0	-2.340806	0.133819	1.832084
15	6	0	-3.476844	-0.502074	2.475845
16	1	0	-3.499725	-0.467180	3.551819
17	6	0	-1.243485	0.736051	-0.255229
18	1	0	-1.210118	0.759744	-1.333158
19	7	0	-0.237025	1.352541	0.341604
20	6	0	0.815167	2.052795	-0.358016
21	1	0	0.629845	1.936671	-1.426005
22	6	0	0.842512	3.552131	-0.019251
23	1	0	1.028799	3.623689	1.051025
24	6	0	-0.495002	4.209724	-0.336738
25	1	0	-0.466644	5.262615	-0.069853
26	1	0	-0.720637	4.147924	-1.401244
27	1	0	-1.312062	3.751331	0.210595
28	6	0	1.982575	4.250351	-0.755401
29	1	0	1.860935	4.171192	-1.835562
30	1	0	1.997436	5.307672	-0.507342
31	1	0	2.953453	3.841573	-0.489351
32	6	0	2.138653	1.389077	0.016060
33	8	0	2.581612	1.436681	1.138812
34	7	0	2.768137	0.734333	-0.995112
35	1	0	2.511303	0.908800	-1.946573
36	7	0	4.015118	0.172365	-0.809954
37	6	0	4.058657	-1.175184	-0.390069
38	6	0	2.992433	-2.045157	-0.572841
39	6	0	5.244624	-1.649397	0.164102
40	6	0	3.116247	-3.376188	-0.199203
41	1	0	2.068511	-1.685863	-0.990568
42	6	0	5.356749	-2.977591	0.533867
43	1	0	6.075807	-0.976061	0.304979
44	6	0	4.293510	-3.852854	0.353733
45	1	0	2.278506	-4.039919	-0.339083
46	1	0	6.278808	-3.328876	0.967726
47	1	0	4.381699	-4.886058	0.644810
48	8	0	-1.462498	0.683782	2.514724
49	1	0	-0.260883	1.325132	1.360664
50	1	0	4.579757	0.769135	-0.229594

E(RBHandHLYP) = -1166.26411028 h
Sum of electronic and thermal Free Energies = -1165.895329 h

CAMB3LYP/6-31+G(d.p). gas phase

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.460101	-1.884575	-1.729254
2	6	0	-5.450608	-1.807509	-0.351470
3	6	0	-4.413012	-1.153777	0.333721
4	6	0	-3.349653	-0.555842	-0.382638
5	6	0	-3.381234	-0.652400	-1.787590
6	6	0	-4.410498	-1.299300	-2.446053
7	1	0	-5.254598	-1.560236	2.294402
8	1	0	-6.265805	-2.391839	-2.248931
9	1	0	-6.253231	-2.256550	0.227052
10	6	0	-4.422204	-1.089534	1.776922
11	6	0	-2.288544	0.118002	0.365774
12	1	0	-2.588341	-0.219881	-2.387440
13	1	0	-4.398988	-1.352524	-3.530279
14	6	0	-2.323005	0.159617	1.819872
15	6	0	-3.450388	-0.479396	2.482763
16	1	0	-3.460690	-0.435984	3.566234
17	6	0	-1.237552	0.751142	-0.281687
18	1	0	-1.200802	0.769233	-1.367880
19	7	0	-0.234326	1.373799	0.324361
20	6	0	0.829877	2.073737	-0.368401
21	1	0	0.647193	1.964705	-1.445787
22	6	0	0.863144	3.573776	-0.018405
23	1	0	1.051033	3.635848	1.059643
24	6	0	-0.475025	4.240125	-0.333078
25	1	0	-0.443917	5.297775	-0.057595
26	1	0	-0.701027	4.185607	-1.405025
27	1	0	-1.299707	3.777596	0.213354
28	6	0	2.010714	4.271509	-0.751099
29	1	0	1.888279	4.198642	-1.838634
30	1	0	2.032170	5.334078	-0.495851
31	1	0	2.984943	3.852451	-0.484931
32	6	0	2.152156	1.398610	0.008700
33	8	0	2.605089	1.449731	1.137434
34	7	0	2.775506	0.726395	-1.004023
35	1	0	2.513826	0.891799	-1.965118
36	7	0	4.020606	0.146695	-0.811637
37	6	0	4.044062	-1.206859	-0.389540
38	6	0	2.959446	-2.061656	-0.569791
39	6	0	5.227453	-1.700246	0.164570
40	6	0	3.062685	-3.398356	-0.193690
41	1	0	2.034332	-1.683624	-0.988170
42	6	0	5.318716	-3.033853	0.537378
43	1	0	6.075076	-1.034811	0.302995
44	6	0	4.237298	-3.894492	0.359388
45	1	0	2.208151	-4.053236	-0.331900
46	1	0	6.242078	-3.402328	0.972987
47	1	0	4.309918	-4.935939	0.653369
48	8	0	-1.432681	0.724765	2.497581
49	1	0	-0.284711	1.340452	1.357955
50	1	0	4.590684	0.742232	-0.219820

E(RCAM-B3LYP) = -1166.35183354 h
Sum of electronic and thermal Free Energies = -1165.994215 h

M062X/6-31+G(d.p). gas phase

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.539563	0.058714	-1.515791
2	6	0	-5.185763	-0.760300	-0.459531
3	6	0	-3.947671	-0.613675	0.189273
4	6	0	-3.030831	0.377501	-0.236614
5	6	0	-3.424253	1.216823	-1.297915
6	6	0	-4.647566	1.057230	-1.928336
7	1	0	-4.338888	-2.217041	1.605290
8	1	0	-6.497541	-0.061469	-2.010305
9	1	0	-5.867287	-1.532488	-0.111681
10	6	0	-3.608762	-1.466568	1.308780
11	6	0	-1.741807	0.481117	0.448058
12	1	0	-2.779312	2.024112	-1.629820
13	1	0	-4.917896	1.721546	-2.743480
14	6	0	-1.450307	-0.351032	1.612329
15	6	0	-2.448620	-1.349219	1.987270
16	1	0	-2.205290	-1.977871	2.837785
17	6	0	-0.733864	1.303083	-0.035210
18	1	0	-0.878929	1.847339	-0.968238
19	7	0	0.456760	1.482540	0.532561
20	6	0	1.578821	2.127770	-0.131965
21	1	0	1.189469	2.606539	-1.043102
22	6	0	2.253210	3.185135	0.746253
23	1	0	2.702803	2.656037	1.595554
24	6	0	1.227280	4.197355	1.254508
25	1	0	1.719201	4.956706	1.868816
26	1	0	0.741317	4.712144	0.415865
27	1	0	0.449667	3.723100	1.858341
28	6	0	3.366208	3.880029	-0.039959
29	1	0	2.952131	4.407459	-0.908482
30	1	0	3.865440	4.621791	0.589305
31	1	0	4.121677	3.170200	-0.385209
32	6	0	2.551678	0.996193	-0.517960
33	8	0	3.521720	0.702268	0.148916
34	7	0	2.189750	0.303368	-1.644306
35	1	0	1.330375	0.518757	-2.129960
36	7	0	2.738416	-0.936449	-1.932888
37	6	0	2.467200	-1.978293	-1.004697
38	6	0	1.353441	-1.944449	-0.165388
39	6	0	3.315617	-3.088945	-0.985349
40	6	0	1.102938	-3.008900	0.697735
41	1	0	0.683692	-1.090917	-0.165472
42	6	0	3.050934	-4.150307	-0.127609
43	1	0	4.183267	-3.115397	-1.639690
44	6	0	1.944064	-4.117654	0.721681
45	1	0	0.246686	-2.949543	1.363023
46	1	0	3.719684	-5.005528	-0.117853
47	1	0	1.746839	-4.942727	1.397727
48	8	0	-0.384942	-0.255682	2.256825
49	1	0	0.600918	0.940103	1.398911
50	1	0	3.728969	-0.841409	-2.128197

E(M062X) = -1166.4616787 h
Sum of electronic and thermal Free Energies = -1166.102187 h

PBE1PBE/6-31+G(d.p). gas phase

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.400317	-2.052808	-1.667868
2	6	0	-5.425393	-1.873842	-0.297916
3	6	0	-4.411313	-1.156065	0.362259
4	6	0	-3.333921	-0.596752	-0.375134
5	6	0	-3.331945	-0.798542	-1.770884
6	6	0	-4.339474	-1.507332	-2.402813
7	1	0	-5.293226	-1.426002	2.325084
8	1	0	-6.187707	-2.608670	-2.167602
9	1	0	-6.236825	-2.290204	0.294672
10	6	0	-4.454250	-0.984690	1.789992
11	6	0	-2.303491	0.140181	0.343657
12	1	0	-2.529194	-0.401220	-2.384409
13	1	0	-4.301529	-1.641011	-3.480509
14	6	0	-2.368800	0.291889	1.790884
15	6	0	-3.500598	-0.307527	2.471702
16	1	0	-3.538909	-0.184781	3.549591
17	6	0	-1.239351	0.739982	-0.325635
18	1	0	-1.169899	0.683913	-1.410858
19	7	0	-0.268873	1.413227	0.274307
20	6	0	0.815555	2.072302	-0.415899
21	1	0	0.662103	1.918799	-1.494861
22	6	0	0.850246	3.584855	-0.128934
23	1	0	1.015172	3.688237	0.951641
24	6	0	-0.474434	4.242700	-0.500653
25	1	0	-0.445621	5.310692	-0.263313
26	1	0	-0.674340	4.149625	-1.575991
27	1	0	-1.315540	3.803025	0.042160
28	6	0	2.018153	4.241311	-0.862263
29	1	0	1.919080	4.125938	-1.949419
30	1	0	2.044056	5.314211	-0.649716
31	1	0	2.983748	3.824982	-0.557821
32	6	0	2.123360	1.409451	0.030424
33	8	0	2.539363	1.496756	1.172000
34	7	0	2.777435	0.706938	-0.940545
35	1	0	2.557046	0.862950	-1.913678
36	7	0	4.020568	0.156548	-0.692872
37	6	0	4.054472	-1.204015	-0.308989
38	6	0	2.988721	-2.073124	-0.545074
39	6	0	5.232371	-1.695585	0.264363
40	6	0	3.105599	-3.420132	-0.207055
41	1	0	2.066906	-1.695780	-0.975106
42	6	0	5.335955	-3.039752	0.599935
43	1	0	6.065831	-1.020876	0.445606
44	6	0	4.274457	-3.913968	0.364629
45	1	0	2.265686	-4.084982	-0.388517
46	1	0	6.254035	-3.405797	1.050966
47	1	0	4.357490	-4.963527	0.629023
48	8	0	-1.495999	0.919294	2.442796
49	1	0	-0.374559	1.435299	1.311735
50	1	0	4.531746	0.748561	-0.045637

E(RPBE1PBE) = -1165.61999355 h
Sum of electronic and thermal Free Energies = -1165.265102 h

PBEh1PBE/6-31+G(d.p). gas phase

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.404398	-2.056719	-1.670096
2	6	0	-5.433397	-1.875344	-0.300713
3	6	0	-4.420356	-1.158181	0.361131
4	6	0	-3.340132	-0.602015	-0.374017
5	6	0	-3.333993	-0.806332	-1.769051
6	6	0	-4.340594	-1.514469	-2.402762
7	1	0	-5.308191	-1.423264	2.321532
8	1	0	-6.190970	-2.612160	-2.171136
9	1	0	-6.247106	-2.289286	0.290135
10	6	0	-4.466988	-0.984332	1.788346
11	6	0	-2.310649	0.134707	0.346189
12	1	0	-2.528347	-0.411587	-2.380298
13	1	0	-4.299582	-1.650336	-3.479862
14	6	0	-2.379480	0.288346	1.792941
15	6	0	-3.514208	-0.307934	2.471454
16	1	0	-3.555015	-0.183269	3.548828
17	6	0	-1.245462	0.732467	-0.321956
18	1	0	-1.175603	0.674993	-1.406996
19	7	0	-0.274004	1.405519	0.276796
20	6	0	0.809318	2.064020	-0.415600
21	1	0	0.656511	1.905678	-1.493945
22	6	0	0.840637	3.577578	-0.134812
23	1	0	1.004022	3.685445	0.945467
24	6	0	-0.484861	4.230744	-0.510864
25	1	0	-0.459210	5.299671	-0.278189
26	1	0	-0.682912	4.132408	-1.585983
27	1	0	-1.325496	3.791174	0.032506
28	6	0	2.007998	4.233026	-0.869462
29	1	0	1.910252	4.112554	-1.956089
30	1	0	2.031970	5.306749	-0.661797
31	1	0	2.973915	3.819627	-0.562415
32	6	0	2.118437	1.407240	0.033458
33	8	0	2.529504	1.494317	1.176842
34	7	0	2.781174	0.712048	-0.936464
35	1	0	2.563914	0.869885	-1.909906
36	7	0	4.027451	0.171088	-0.684278
37	6	0	4.070101	-1.190569	-0.305322
38	6	0	3.011720	-2.066140	-0.548830
39	6	0	5.248869	-1.675381	0.271297
40	6	0	3.136647	-3.413225	-0.214833
41	1	0	2.089442	-1.693508	-0.981636
42	6	0	5.360555	-3.019657	0.602922
43	1	0	6.076414	-0.995221	0.458119
44	6	0	4.306405	-3.900424	0.360214
45	1	0	2.302522	-4.083404	-0.402056
46	1	0	6.279042	-3.380698	1.056636
47	1	0	4.395793	-4.950030	0.621489
48	8	0	-1.507432	0.914952	2.446177
49	1	0	-0.377444	1.430546	1.313370
50	1	0	4.530143	0.764847	-0.032104

E(RPBEh1PBE) = -1165.74215745 h
Sum of electronic and thermal Free Energies = -1165.387305 h

TPSSh/6-31+G(d.p). gas phase

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.344530	-2.328512	-1.588661
2	6	0	-5.418070	-2.045606	-0.233025
3	6	0	-4.449803	-1.234526	0.399181
4	6	0	-3.367941	-0.688205	-0.354826
5	6	0	-3.318912	-0.994374	-1.735749
6	6	0	-4.282196	-1.793909	-2.338998
7	1	0	-5.380180	-1.384703	2.355356
8	1	0	-6.094077	-2.953057	-2.064605
9	1	0	-6.229977	-2.448323	0.367927
10	6	0	-4.544059	-0.951647	1.809595
11	6	0	-2.384305	0.144085	0.333558
12	1	0	-2.517404	-0.606179	-2.356908
13	1	0	-4.209051	-2.005651	-3.402089
14	6	0	-2.508700	0.415401	1.764609
15	6	0	-3.636771	-0.175809	2.462131
16	1	0	-3.715586	0.031817	3.524387
17	6	0	-1.304082	0.710217	-0.351129
18	1	0	-1.179492	0.549545	-1.420126
19	7	0	-0.377776	1.473294	0.227521
20	6	0	0.746803	2.075532	-0.473099
21	1	0	0.641559	1.825395	-1.538978
22	6	0	0.767432	3.616472	-0.309691
23	1	0	0.876273	3.811187	0.764611
24	6	0	-0.544146	4.238521	-0.806211
25	1	0	-0.526381	5.322315	-0.653649
26	1	0	-0.684951	4.055606	-1.879404
27	1	0	-1.409833	3.836935	-0.272616
28	6	0	1.977847	4.218586	-1.040079
29	1	0	1.931020	4.013801	-2.117581
30	1	0	1.991319	5.305256	-0.912419
31	1	0	2.925839	3.829790	-0.654066
32	6	0	2.037012	1.453812	0.088585
33	8	0	2.391408	1.610382	1.253572
34	7	0	2.758180	0.697100	-0.802180
35	1	0	2.642156	0.862216	-1.795837
36	7	0	4.036491	0.251222	-0.435633
37	6	0	4.163135	-1.142561	-0.168398
38	6	0	3.233678	-2.082775	-0.629552
39	6	0	5.311333	-1.575741	0.514136
40	6	0	3.456326	-3.445537	-0.405940
41	1	0	2.337121	-1.751179	-1.142379
42	6	0	5.519457	-2.936644	0.734802
43	1	0	6.035655	-0.846137	0.867635
44	6	0	4.595733	-3.882601	0.273657
45	1	0	2.725313	-4.165745	-0.762165
46	1	0	6.407805	-3.258154	1.270704
47	1	0	4.761107	-4.941296	0.446442
48	8	0	-1.677340	1.139353	2.392033
49	1	0	-0.534269	1.585542	1.257158
50	1	0	4.343773	0.816754	0.356415

E(RTPSSh) = -1167.03408963 h
Sum of electronic and thermal Free Energies = -1166.683959 h

X3LYP/6-31+G(d.p). gas phase

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.349383	-2.113212	-1.677533
2	6	0	-5.400628	-1.907832	-0.308808
3	6	0	-4.405529	-1.162497	0.356846
4	6	0	-3.319497	-0.601567	-0.375079
5	6	0	-3.291922	-0.830668	-1.769680
6	6	0	-4.281250	-1.566559	-2.406680
7	1	0	-5.318279	-1.406037	2.312204
8	1	0	-6.120552	-2.688764	-2.179292
9	1	0	-6.216641	-2.323566	0.276755
10	6	0	-4.476101	-0.964081	1.784007
11	6	0	-2.305706	0.165998	0.349134
12	1	0	-2.485228	-0.433949	-2.376900
13	1	0	-4.223108	-1.719903	-3.480358
14	6	0	-2.402865	0.343475	1.797942
15	6	0	-3.542317	-0.260309	2.470500
16	1	0	-3.601854	-0.117854	3.544424
17	6	0	-1.235278	0.762227	-0.316215
18	1	0	-1.149523	0.678925	-1.396976
19	7	0	-0.272096	1.465822	0.275672
20	6	0	0.827991	2.108090	-0.425657
21	1	0	0.669823	1.944645	-1.500871
22	6	0	0.881147	3.631439	-0.152969
23	1	0	1.043227	3.745780	0.926061
24	6	0	-0.440106	4.308805	-0.535393
25	1	0	-0.394159	5.378485	-0.308369
26	1	0	-0.640502	4.208060	-1.609997
27	1	0	-1.288145	3.887939	0.010628
28	6	0	2.064860	4.274207	-0.890244
29	1	0	1.970068	4.151419	-1.977005
30	1	0	2.098910	5.348358	-0.685225
31	1	0	3.024855	3.851712	-0.578043
32	6	0	2.132172	1.423293	0.022923
33	8	0	2.560178	1.518572	1.163127
34	7	0	2.764657	0.685248	-0.945108
35	1	0	2.549092	0.843540	-1.920321
36	7	0	4.012768	0.112799	-0.700397
37	6	0	4.031566	-1.251238	-0.299243
38	6	0	2.973564	-2.125378	-0.568443
39	6	0	5.190760	-1.738131	0.321674
40	6	0	3.079164	-3.472719	-0.214632
41	1	0	2.069213	-1.754753	-1.037151
42	6	0	5.284413	-3.083104	0.670764
43	1	0	6.014872	-1.060860	0.530717
44	6	0	4.230057	-3.961934	0.403698
45	1	0	2.247656	-4.139834	-0.421799
46	1	0	6.185264	-3.444516	1.157662
47	1	0	4.304311	-5.008931	0.678880
48	8	0	-1.548780	0.996437	2.456283
49	1	0	-0.373401	1.518090	1.307386
50	1	0	4.534943	0.705035	-0.060340

E(RX3LYP) = -1166.43505324 h
Sum of electronic and thermal Free Energies = -1166.082714 h

ωB97XD/6-31+G(d.p). gas phase

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.581330	-0.763714	-1.687705
2	6	0	4.483439	-1.119037	-0.355159
3	6	0	3.240687	-1.422328	0.226618
4	6	0	2.057845	-1.361026	-0.547677
5	6	0	2.188050	-1.032022	-1.911542
6	6	0	3.419318	-0.730695	-2.468102
7	1	0	4.088298	-1.844650	2.184459
8	1	0	5.544781	-0.528428	-2.127160
9	1	0	5.375711	-1.166426	0.263847
10	6	0	3.158611	-1.798307	1.621724
11	6	0	0.775429	-1.611466	0.107547
12	1	0	1.318938	-1.022651	-2.561884
13	1	0	3.481605	-0.476504	-3.521738
14	6	0	0.723883	-2.022685	1.505953
15	6	0	1.990429	-2.092523	2.226900
16	1	0	1.936861	-2.377589	3.272067
17	6	0	-0.415099	-1.306160	-0.527924
18	1	0	-0.401047	-0.882347	-1.529661
19	7	0	-1.630601	-1.438710	0.001938
20	6	0	-2.780705	-0.718104	-0.525033
21	1	0	-2.757763	-0.804198	-1.621825
22	6	0	-4.097400	-1.302348	-0.005624
23	1	0	-4.092327	-1.171755	1.083418
24	6	0	-4.204667	-2.791728	-0.337911
25	1	0	-5.137130	-3.201042	0.061419
26	1	0	-4.207866	-2.949433	-1.423481
27	1	0	-3.376080	-3.365601	0.084415
28	6	0	-5.282475	-0.521329	-0.578653
29	1	0	-5.314462	-0.604482	-1.672266
30	1	0	-6.222343	-0.922972	-0.190136
31	1	0	-5.240498	0.538495	-0.310914
32	6	0	-2.592380	0.749329	-0.104850
33	8	0	-2.807943	1.143300	1.025973
34	7	0	-2.058200	1.553786	-1.073521
35	1	0	-2.063705	1.289450	-2.046016
36	7	0	-1.627034	2.842747	-0.787458
37	6	0	-0.346302	2.924981	-0.172985
38	6	0	0.686846	2.065740	-0.548125
39	6	0	-0.104462	3.919350	0.776048
40	6	0	1.944853	2.188002	0.034209
41	1	0	0.515721	1.296015	-1.291967
42	6	0	1.158938	4.044221	1.344798
43	1	0	-0.907827	4.583925	1.082550
44	6	0	2.189150	3.177868	0.982718
45	1	0	2.731541	1.499776	-0.261792
46	1	0	1.332050	4.814566	2.089868
47	1	0	3.168963	3.271090	1.438907
48	8	0	-0.350216	-2.280995	2.091307
49	1	0	-1.613160	-1.755553	0.983421
50	1	0	-2.336067	3.321002	-0.241830

E(RwB97XD) = -1166.58995740 h
Sum of electronic and thermal Free Energies = -1166.228962 h

BMK/3-21G. gas phase

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.107792	-1.311224	-1.711037
2	6	0	-5.906287	-1.643971	-0.378237
3	6	0	-4.727351	-1.256947	0.299508
4	6	0	-3.718376	-0.513139	-0.382094
5	6	0	-3.949940	-0.187960	-1.744082
6	6	0	-5.116592	-0.577076	-2.392764
7	1	0	-5.321053	-2.185071	2.180624
8	1	0	-7.014673	-1.612089	-2.223739
9	1	0	-6.656768	-2.210441	0.166205
10	6	0	-4.530441	-1.615448	1.698100
11	6	0	-2.507463	-0.128005	0.356910
12	1	0	-3.210463	0.373948	-2.303442
13	1	0	-5.263091	-0.311289	-3.434925
14	6	0	-2.326861	-0.499598	1.769105
15	6	0	-3.420503	-1.267482	2.384772
16	1	0	-3.278118	-1.538853	3.424452
17	6	0	-1.487368	0.606086	-0.247539
18	1	0	-1.579185	0.915830	-1.286403
19	7	0	-0.362184	0.975989	0.364913
20	6	0	0.691003	1.776350	-0.249176
21	1	0	0.616815	1.711084	-1.342625
22	6	0	0.591371	3.279136	0.195054
23	1	0	0.710670	3.284693	1.285862
24	6	0	-0.793532	3.867160	-0.187181
25	1	0	-0.858514	4.909059	0.146725
26	1	0	-0.922094	3.847909	-1.278300
27	1	0	-1.605902	3.301484	0.278450
28	6	0	1.724067	4.116769	-0.464383
29	1	0	1.611276	4.102421	-1.557603
30	1	0	1.658083	5.158027	-0.130945
31	1	0	2.715439	3.731716	-0.206060
32	6	0	2.021193	1.188625	0.276466
33	8	0	2.158347	0.849342	1.447596
34	7	0	3.031261	1.137769	-0.649055
35	1	0	2.950585	1.519672	-1.583867
36	7	0	4.323392	0.698045	-0.260258
37	6	0	4.589842	-0.690781	-0.323602
38	6	0	3.787028	-1.577816	-1.057202
39	6	0	5.736064	-1.184565	0.330177
40	6	0	4.127825	-2.932899	-1.135341
41	1	0	2.897338	-1.208406	-1.550200
42	6	0	6.065940	-2.538031	0.248881
43	1	0	6.365304	-0.504069	0.895578
44	6	0	5.265503	-3.424191	-0.486118
45	1	0	3.491609	-3.605572	-1.701372
46	1	0	6.949809	-2.900787	0.763511
47	1	0	5.523063	-4.475491	-0.545674
48	8	0	-1.300318	-0.188355	2.435757
49	1	0	-0.269587	0.651637	1.354464
50	1	0	4.633956	1.164099	0.591948

E(RBMK) = -1159.80354304 h
Sum of electronic and thermal Free Energies = -1159.443547 h

BMK/6-31G(d.p). gas phase

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.788879	-1.775786	-1.732269
2	6	0	-5.752091	-1.744776	-0.345073
3	6	0	-4.655841	-1.182595	0.344522
4	6	0	-3.559674	-0.627803	-0.377463
5	6	0	-3.616112	-0.685604	-1.791280
6	6	0	-4.705357	-1.241723	-2.453421
7	1	0	-5.493316	-1.606549	2.312767
8	1	0	-6.637405	-2.210909	-2.254697
9	1	0	-6.574487	-2.159237	0.236952
10	6	0	-4.634913	-1.174676	1.797239
11	6	0	-2.442840	-0.042641	0.377348
12	1	0	-2.794633	-0.302379	-2.391220
13	1	0	-4.711778	-1.266188	-3.541409
14	6	0	-2.430657	-0.075354	1.848998
15	6	0	-3.602869	-0.665968	2.510143
16	1	0	-3.588703	-0.668869	3.597424
17	6	0	-1.390398	0.600140	-0.271992
18	1	0	-1.401934	0.710408	-1.356735
19	7	0	-0.328661	1.132167	0.327629
20	6	0	0.700237	1.885906	-0.354360
21	1	0	0.565124	1.743828	-1.438011
22	6	0	0.630127	3.406103	-0.032475
23	1	0	0.770431	3.493965	1.054095
24	6	0	-0.742144	3.984635	-0.419919
25	1	0	-0.793189	5.046570	-0.151634
26	1	0	-0.906915	3.906036	-1.504653
27	1	0	-1.558505	3.464730	0.092933
28	6	0	1.768882	4.163652	-0.743403
29	1	0	1.698555	4.044294	-1.834698
30	1	0	1.704004	5.235681	-0.523937
31	1	0	2.758092	3.818444	-0.419690
32	6	0	2.062218	1.324250	0.101817
33	8	0	2.389839	1.322953	1.269871
34	7	0	2.866197	0.848769	-0.895534
35	1	0	2.692029	1.102935	-1.858398
36	7	0	4.189809	0.483145	-0.609736
37	6	0	4.419617	-0.891975	-0.343457
38	6	0	3.526148	-1.897054	-0.736036
39	6	0	5.632953	-1.241039	0.274041
40	6	0	3.849334	-3.239727	-0.506754
41	1	0	2.583181	-1.625816	-1.201156
42	6	0	5.942035	-2.582625	0.499373
43	1	0	6.328861	-0.457555	0.571017
44	6	0	5.053471	-3.593120	0.108662
45	1	0	3.145184	-4.012438	-0.809019
46	1	0	6.882082	-2.838744	0.983922
47	1	0	5.297423	-4.637798	0.285156
48	8	0	-1.495526	0.385123	2.525249
49	1	0	-0.313379	1.027367	1.353101
50	1	0	4.523868	1.065733	0.154958

E(RBMK) = -1166.18195791 h
Sum of electronic and thermal Free Energies = -1165.823789 h

BMK/6-31+G(d.p). gas phase

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.629948	-1.754294	-1.774142
2	6	0	-5.601160	-1.739897	-0.385202
3	6	0	-4.519293	-1.163003	0.318357
4	6	0	-3.430409	-0.576284	-0.390320
5	6	0	-3.478829	-0.615079	-1.806693
6	6	0	-4.552982	-1.186895	-2.483098
7	1	0	-5.358793	-1.629143	2.277719
8	1	0	-6.466427	-2.200486	-2.306981
9	1	0	-6.418499	-2.178449	0.186501
10	6	0	-4.507647	-1.172303	1.771486
11	6	0	-2.328407	0.021173	0.379294
12	1	0	-2.665241	-0.203907	-2.398915
13	1	0	-4.553255	-1.196846	-3.571508
14	6	0	-2.329590	-0.025015	1.849108
15	6	0	-3.490302	-0.647910	2.498010
16	1	0	-3.483696	-0.662929	3.585564
17	6	0	-1.278794	0.682937	-0.259256
18	1	0	-1.285470	0.793852	-1.343737
19	7	0	-0.228654	1.230848	0.346685
20	6	0	0.787628	2.008651	-0.333419
21	1	0	0.605362	1.923652	-1.416358
22	6	0	0.745115	3.508965	0.064893
23	1	0	0.928869	3.549726	1.147924
24	6	0	-0.637622	4.112289	-0.243946
25	1	0	-0.666815	5.164356	0.064962
26	1	0	-0.848544	4.074705	-1.323444
27	1	0	-1.437712	3.581342	0.284243
28	6	0	1.862449	4.287620	-0.658166
29	1	0	1.741615	4.224616	-1.750147
30	1	0	1.822381	5.347904	-0.381129
31	1	0	2.859504	3.913688	-0.394446
32	6	0	2.158091	1.394786	0.027305
33	8	0	2.598392	1.427009	1.158730
34	7	0	2.823496	0.807913	-1.011207
35	1	0	2.550634	0.976824	-1.969765
36	7	0	4.111649	0.286686	-0.838312
37	6	0	4.196872	-1.071939	-0.432049
38	6	0	3.132624	-1.972469	-0.578070
39	6	0	5.429459	-1.526025	0.070853
40	6	0	3.304986	-3.315990	-0.216413
41	1	0	2.172885	-1.628979	-0.952269
42	6	0	5.587665	-2.866405	0.430564
43	1	0	6.258931	-0.828002	0.177625
44	6	0	4.526863	-3.773325	0.288197
45	1	0	2.467494	-4.002336	-0.325759
46	1	0	6.545326	-3.201301	0.824202
47	1	0	4.650775	-4.815523	0.572697
48	8	0	-1.405676	0.451537	2.535128
49	1	0	-0.220217	1.134696	1.373309
50	1	0	4.633098	0.898516	-0.215080

E(RBMK) = -1166.21581585 h
Sum of electronic and thermal Free Energies = -1165.855581 h

BMK/6-31G(2df.2pd). gas phase

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.901802	-1.789948	-1.704538
2	6	0	-5.864756	-1.749579	-0.321027
3	6	0	-4.763830	-1.197919	0.362994
4	6	0	-3.662178	-0.664585	-0.360064
5	6	0	-3.720332	-0.730587	-1.770324
6	6	0	-4.814108	-1.275729	-2.426886
7	1	0	-5.605100	-1.592260	2.327274
8	1	0	-6.751794	-2.214701	-2.222763
9	1	0	-6.688875	-2.146640	0.261533
10	6	0	-4.744873	-1.175715	1.811864
11	6	0	-2.542012	-0.089580	0.389138
12	1	0	-2.900342	-0.360589	-2.371691
13	1	0	-4.822047	-1.305413	-3.509704
14	6	0	-2.535192	-0.097824	1.858921
15	6	0	-3.713040	-0.669762	2.519941
16	1	0	-3.701607	-0.660701	3.602759
17	6	0	-1.474503	0.516298	-0.262925
18	1	0	-1.470063	0.594962	-1.345917
19	7	0	-0.413056	1.044010	0.331539
20	6	0	0.635301	1.754640	-0.359809
21	1	0	0.570641	1.511783	-1.427587
22	6	0	0.520801	3.294413	-0.184021
23	1	0	0.583846	3.485393	0.892241
24	6	0	-0.830028	3.801703	-0.710902
25	1	0	-0.905047	4.882845	-0.574011
26	1	0	-0.930775	3.595525	-1.782324
27	1	0	-1.668641	3.336874	-0.190188
28	6	0	1.684465	4.013443	-0.887660
29	1	0	1.685345	3.794370	-1.961563
30	1	0	1.584144	5.095096	-0.776504
31	1	0	2.656322	3.728399	-0.478886
32	6	0	1.972019	1.265778	0.220150
33	8	0	2.182086	1.254725	1.409400
34	7	0	2.897803	0.869215	-0.700248
35	1	0	2.814743	1.185633	-1.653203
36	7	0	4.210534	0.616113	-0.280071
37	6	0	4.595892	-0.743248	-0.210225
38	6	0	3.947669	-1.743113	-0.941374
39	6	0	5.719220	-1.067513	0.563642
40	6	0	4.424759	-3.054544	-0.894166
41	1	0	3.075517	-1.499791	-1.531525
42	6	0	6.183270	-2.379094	0.604831
43	1	0	6.221871	-0.290450	1.128031
44	6	0	5.541039	-3.382975	-0.125811
45	1	0	3.912746	-3.821496	-1.462352
46	1	0	7.047801	-2.615733	1.212557
47	1	0	5.902641	-4.402167	-0.092842
48	8	0	-1.603549	0.361046	2.529037
49	1	0	-0.404986	0.969362	1.355609
50	1	0	4.351690	1.090806	0.604543

E(RBMK) = -1166.27470528 h
Sum of electronic and thermal Free Energies = -1165.916649 h

BMK/6-311G(d.p). gas phase

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.751207	-1.825939	-1.733420
2	6	0	-5.730295	-1.774052	-0.350049
3	6	0	-4.649256	-1.192316	0.342125
4	6	0	-3.552025	-0.639750	-0.373067
5	6	0	-3.593388	-0.718418	-1.784195
6	6	0	-4.667181	-1.293176	-2.448378
7	1	0	-5.503424	-1.594868	2.304233
8	1	0	-6.587583	-2.275556	-2.257888
9	1	0	-6.553904	-2.186630	0.226702
10	6	0	-4.645990	-1.161855	1.793299
11	6	0	-2.449713	-0.034082	0.385533
12	1	0	-2.773638	-0.335857	-2.381700
13	1	0	-4.662394	-1.332760	-3.533457
14	6	0	-2.459039	-0.036815	1.856593
15	6	0	-3.632560	-0.631236	2.508434
16	1	0	-3.631727	-0.616890	3.593531
17	6	0	-1.390589	0.593853	-0.260301
18	1	0	-1.386328	0.672818	-1.344816
19	7	0	-0.340425	1.147185	0.333800
20	6	0	0.692120	1.883218	-0.360552
21	1	0	0.560545	1.717409	-1.438175
22	6	0	0.624159	3.408255	-0.071689
23	1	0	0.773725	3.522746	1.008627
24	6	0	-0.751006	3.976434	-0.457646
25	1	0	-0.792976	5.046019	-0.230472
26	1	0	-0.936052	3.856481	-1.532952
27	1	0	-1.558441	3.483807	0.089839
28	6	0	1.753593	4.148396	-0.811336
29	1	0	1.673188	4.001896	-1.896248
30	1	0	1.689976	5.223260	-0.618328
31	1	0	2.744787	3.814640	-0.489559
32	6	0	2.050430	1.327292	0.109108
33	8	0	2.370325	1.336881	1.271974
34	7	0	2.856406	0.841550	-0.880250
35	1	0	2.683338	1.091898	-1.843045
36	7	0	4.178242	0.480969	-0.589766
37	6	0	4.420544	-0.890260	-0.325207
38	6	0	3.560868	-1.906183	-0.753148
39	6	0	5.617177	-1.225543	0.325237
40	6	0	3.900077	-3.242184	-0.525636
41	1	0	2.630539	-1.657063	-1.248764
42	6	0	5.943040	-2.559820	0.547797
43	1	0	6.287319	-0.435511	0.653281
44	6	0	5.087206	-3.580012	0.122257
45	1	0	3.221693	-4.022484	-0.856826
46	1	0	6.869170	-2.803220	1.059248
47	1	0	5.343032	-4.619412	0.297121
48	8	0	-1.545016	0.445983	2.534171
49	1	0	-0.327145	1.077493	1.358726
50	1	0	4.512474	1.066100	0.170723

E(RBMK) = -1166.41365523 h
Sum of electronic and thermal Free Energies = -1166.058135 h

BMK/6-311+G(d.p). gas phase

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.625154	-1.718539	-1.779645
2	6	0	-5.597290	-1.710533	-0.395067
3	6	0	-4.513364	-1.148050	0.309600
4	6	0	-3.422258	-0.568942	-0.393611
5	6	0	-3.469403	-0.604179	-1.806742
6	6	0	-4.545238	-1.161296	-2.483634
7	1	0	-5.355308	-1.616724	2.262210
8	1	0	-6.463108	-2.153700	-2.313831
9	1	0	-6.416936	-2.143442	0.172419
10	6	0	-4.501648	-1.165745	1.760503
11	6	0	-2.317501	0.015653	0.378093
12	1	0	-2.652819	-0.202285	-2.396061
13	1	0	-4.545094	-1.168893	-3.569440
14	6	0	-2.316643	-0.042581	1.846147
15	6	0	-3.483170	-0.658457	2.487253
16	1	0	-3.477120	-0.681109	3.572284
17	6	0	-1.270961	0.679908	-0.254077
18	1	0	-1.283898	0.806365	-1.334071
19	7	0	-0.216803	1.215340	0.349328
20	6	0	0.793759	2.002526	-0.325769
21	1	0	0.607037	1.932058	-1.405876
22	6	0	0.752465	3.494953	0.092301
23	1	0	0.937958	3.521478	1.172753
24	6	0	-0.628487	4.102197	-0.204663
25	1	0	-0.655558	5.148490	0.114319
26	1	0	-0.842929	4.076453	-1.280851
27	1	0	-1.425931	3.569125	0.319474
28	6	0	1.865360	4.282077	-0.622897
29	1	0	1.741041	4.233564	-1.712340
30	1	0	1.826874	5.336121	-0.332742
31	1	0	2.860842	3.905597	-0.368549
32	6	0	2.165411	1.385179	0.020622
33	8	0	2.610413	1.403461	1.142019
34	7	0	2.818843	0.811931	-1.031516
35	1	0	2.522399	0.975469	-1.982038
36	7	0	4.099896	0.273427	-0.885995
37	6	0	4.180723	-1.074282	-0.452195
38	6	0	3.111243	-1.966085	-0.568206
39	6	0	5.411068	-1.527574	0.045247
40	6	0	3.275926	-3.299580	-0.184087
41	1	0	2.153636	-1.621843	-0.939909
42	6	0	5.562697	-2.857995	0.425888
43	1	0	6.244746	-0.835798	0.131153
44	6	0	4.496234	-3.755538	0.313136
45	1	0	2.434601	-3.980285	-0.270763
46	1	0	6.519393	-3.193388	0.814185
47	1	0	4.615027	-4.790759	0.614407
48	8	0	-1.393492	0.416585	2.532457
49	1	0	-0.197172	1.109641	1.371924
50	1	0	4.660779	0.889915	-0.306371

E(RBMK) = -1166.42796844 h
Sum of electronic and thermal Free Energies = -1166.072010 h

BMK/6-311++G(d.p). gas phase

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.626979	-1.717452	-1.780360
2	6	0	-5.600978	-1.706644	-0.395745
3	6	0	-4.516466	-1.145700	0.309230
4	6	0	-3.422792	-0.571183	-0.393773
5	6	0	-3.467753	-0.609899	-1.806881
6	6	0	-4.544490	-1.164906	-2.484089
7	1	0	-5.361416	-1.609153	2.261800
8	1	0	-6.465495	-2.151312	-2.314753
9	1	0	-6.422545	-2.136226	0.171496
10	6	0	-4.505976	-1.161446	1.760183
11	6	0	-2.317539	0.012162	0.378081
12	1	0	-2.648729	-0.212337	-2.395760
13	1	0	-4.542890	-1.174921	-3.569881
14	6	0	-2.317619	-0.044826	1.846152
15	6	0	-3.486520	-0.656381	2.487125
16	1	0	-3.481407	-0.677948	3.572183
17	6	0	-1.270884	0.676264	-0.253991
18	1	0	-1.284392	0.803552	-1.333848
19	7	0	-0.216139	1.210819	0.349196
20	6	0	0.793004	1.999846	-0.325989
21	1	0	0.606361	1.928772	-1.406070
22	6	0	0.749367	3.492283	0.091808
23	1	0	0.937632	3.519412	1.171773
24	6	0	-0.633615	4.096579	-0.201677
25	1	0	-0.662022	5.142775	0.117477
26	1	0	-0.850692	4.070226	-1.277317
27	1	0	-1.428494	3.561689	0.324495
28	6	0	1.858885	4.281293	-0.626549
29	1	0	1.730890	4.232945	-1.715567
30	1	0	1.820002	5.335111	-0.335703
31	1	0	2.855675	3.905831	-0.375796
32	6	0	2.165615	1.384877	0.020679
33	8	0	2.609576	1.402630	1.142517
34	7	0	2.821029	0.814248	-1.031613
35	1	0	2.524252	0.977299	-1.982117
36	7	0	4.102697	0.277200	-0.886076
37	6	0	4.184681	-1.070471	-0.452115
38	6	0	3.115910	-1.963124	-0.568152
39	6	0	5.415230	-1.522693	0.045775
40	6	0	3.281397	-3.296320	-0.183330
41	1	0	2.158143	-1.619747	-0.940212
42	6	0	5.567730	-2.852847	0.427076
43	1	0	6.248415	-0.830297	0.131442
44	6	0	4.501902	-3.751161	0.314454
45	1	0	2.440604	-3.977696	-0.269859
46	1	0	6.524540	-3.187392	0.815812
47	1	0	4.621296	-4.786144	0.616334
48	8	0	-1.393598	0.412537	2.532537
49	1	0	-0.195999	1.104698	1.371689
50	1	0	4.662684	0.894149	-0.306057

E(RBMK) = -1166.42840901 h
Sum of electronic and thermal Free Energies = -1166.072634 h

BMK/6-311G(2df.2pd). gas phase

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.792475	-1.864067	-1.714066
2	6	0	-5.771172	-1.806786	-0.334247
3	6	0	-4.694723	-1.219220	0.353973
4	6	0	-3.601466	-0.667334	-0.361490
5	6	0	-3.644961	-0.748513	-1.769314
6	6	0	-4.713943	-1.328969	-2.429481
7	1	0	-5.547673	-1.613096	2.312981
8	1	0	-6.625340	-2.317642	-2.235847
9	1	0	-6.591394	-2.218821	0.243357
10	6	0	-4.694190	-1.178507	1.801569
11	6	0	-2.503938	-0.055813	0.393176
12	1	0	-2.832286	-0.359421	-2.367935
13	1	0	-4.710514	-1.369023	-3.512131
14	6	0	-2.522389	-0.037555	1.860338
15	6	0	-3.689965	-0.634957	2.513630
16	1	0	-3.694248	-0.612405	3.596294
17	6	0	-1.436546	0.550279	-0.253739
18	1	0	-1.416143	0.596371	-1.337348
19	7	0	-0.396094	1.114647	0.339015
20	6	0	0.648084	1.822847	-0.360402
21	1	0	0.562631	1.586494	-1.426902
22	6	0	0.547290	3.359632	-0.177025
23	1	0	0.647369	3.551556	0.895589
24	6	0	-0.815215	3.874867	-0.658333
25	1	0	-0.872422	4.957699	-0.532661
26	1	0	-0.958817	3.655813	-1.721666
27	1	0	-1.637229	3.426798	-0.099595
28	6	0	1.691529	4.067014	-0.918629
29	1	0	1.651988	3.850446	-1.991472
30	1	0	1.607627	5.148532	-0.799671
31	1	0	2.672667	3.769877	-0.543546
32	6	0	1.992868	1.320103	0.188689
33	8	0	2.253632	1.364566	1.364762
34	7	0	2.859599	0.839380	-0.745332
35	1	0	2.736774	1.095364	-1.712528
36	7	0	4.178436	0.550846	-0.378799
37	6	0	4.516874	-0.813546	-0.236864
38	6	0	3.762669	-1.838343	-0.807964
39	6	0	5.701095	-1.124411	0.441656
40	6	0	4.193538	-3.158951	-0.697510
41	1	0	2.841238	-1.606955	-1.323844
42	6	0	6.118540	-2.443915	0.547348
43	1	0	6.290976	-0.327106	0.879889
44	6	0	5.368893	-3.472478	-0.023648
45	1	0	3.596193	-3.946421	-1.140902
46	1	0	7.033400	-2.670104	1.081448
47	1	0	5.696737	-4.500558	0.058475
48	8	0	-1.617358	0.460405	2.536717
49	1	0	-0.402071	1.074372	1.364350
50	1	0	4.404376	1.086079	0.451643

E(RBMK) = -1166.49276710 h
Sum of electronic and thermal Free Energies = -1166.135004 h

BMK/D95. gas phase

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.691772	-1.605781	-1.826319
2	6	0	-5.624861	-1.695082	-0.431305
3	6	0	-4.514820	-1.165581	0.283717
4	6	0	-3.441636	-0.523857	-0.414969
5	6	0	-3.527120	-0.453697	-1.837802
6	6	0	-4.627388	-0.979761	-2.529062
7	1	0	-5.300000	-1.775185	2.236074
8	1	0	-6.541985	-2.012149	-2.368803
9	1	0	-6.426693	-2.176087	0.128506
10	6	0	-4.464127	-1.280730	1.739829
11	6	0	-2.311882	0.018797	0.365063
12	1	0	-2.728940	0.006172	-2.416995
13	1	0	-4.662920	-0.911850	-3.614694
14	6	0	-2.277339	-0.129060	1.831707
15	6	0	-3.417742	-0.800773	2.475503
16	1	0	-3.374078	-0.888243	3.558822
17	6	0	-1.262383	0.716849	-0.254439
18	1	0	-1.291621	0.893749	-1.330244
19	7	0	-0.190819	1.222030	0.378493
20	6	0	0.830188	2.033427	-0.278008
21	1	0	0.642458	2.015901	-1.364982
22	6	0	0.802830	3.517817	0.203795
23	1	0	1.010228	3.508506	1.283811
24	6	0	-0.592046	4.140702	-0.053543
25	1	0	-0.609645	5.180658	0.298058
26	1	0	-0.822997	4.144673	-1.131010
27	1	0	-1.381913	3.589066	0.471300
28	6	0	1.913285	4.328992	-0.514907
29	1	0	1.768297	4.305647	-1.606722
30	1	0	1.876841	5.377960	-0.193813
31	1	0	2.914193	3.941749	-0.282302
32	6	0	2.209771	1.407540	0.028898
33	8	0	2.694828	1.409237	1.169330
34	7	0	2.857690	0.868067	-1.061995
35	1	0	2.458802	0.913918	-1.990726
36	7	0	4.101635	0.234797	-0.955124
37	6	0	4.156589	-1.111080	-0.504690
38	6	0	2.998523	-1.911965	-0.387723
39	6	0	5.429757	-1.663076	-0.218518
40	6	0	3.120439	-3.258074	0.017552
41	1	0	2.017826	-1.488706	-0.590137
42	6	0	5.536907	-3.005783	0.188593
43	1	0	6.321750	-1.044627	-0.317369
44	6	0	4.383696	-3.815432	0.307160
45	1	0	2.222881	-3.865511	0.115055
46	1	0	6.518514	-3.418626	0.412853
47	1	0	4.468811	-4.852199	0.623509
48	8	0	-1.308882	0.313684	2.534755
49	1	0	-0.158246	1.060485	1.400008
50	1	0	4.838126	0.850720	-0.625688

E(RBMK) = -1165.94433625 h
Sum of electronic and thermal Free Energies = -1165.584142 h

BMK/D95V. gas phase

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.693639	-1.601563	-1.826503
2	6	0	-5.625055	-1.694875	-0.431923
3	6	0	-4.514293	-1.166999	0.283219
4	6	0	-3.442256	-0.522936	-0.414967
5	6	0	-3.529597	-0.448662	-1.837465
6	6	0	-4.630490	-0.973157	-2.528740
7	1	0	-5.296711	-1.782512	2.234844
8	1	0	-6.544353	-2.006694	-2.369160
9	1	0	-6.426035	-2.177796	0.127488
10	6	0	-4.461670	-1.286288	1.738916
11	6	0	-2.311706	0.017864	0.365149
12	1	0	-2.732341	0.013322	-2.416282
13	1	0	-4.667478	-0.902147	-3.614141
14	6	0	-2.275391	-0.134114	1.831093
15	6	0	-3.414549	-0.808028	2.474499
16	1	0	-3.369338	-0.898518	3.557540
17	6	0	-1.262957	0.717515	-0.253641
18	1	0	-1.293370	0.897058	-1.329014
19	7	0	-0.190849	1.221167	0.379421
20	6	0	0.829573	2.033798	-0.276469
21	1	0	0.641728	2.017425	-1.363451
22	6	0	0.801692	3.517640	0.206862
23	1	0	1.009053	3.507324	1.286853
24	6	0	-0.593454	4.140138	-0.050129
25	1	0	-0.611576	5.179729	0.302509
26	1	0	-0.824066	4.145069	-1.127669
27	1	0	-1.383175	3.587587	0.473949
28	6	0	1.911761	4.329993	-0.511169
29	1	0	1.766966	4.307037	-1.603023
30	1	0	1.874333	5.378772	-0.189571
31	1	0	2.912928	3.943440	-0.278539
32	6	0	2.209251	1.408241	0.029621
33	8	0	2.694568	1.409684	1.169929
34	7	0	2.857092	0.869217	-1.061318
35	1	0	2.457864	0.914798	-1.989941
36	7	0	4.101093	0.236281	-0.954637
37	6	0	4.156732	-1.109940	-0.505754
38	6	0	2.998938	-1.910820	-0.387316
39	6	0	5.430363	-1.662149	-0.222391
40	6	0	3.121636	-3.257171	0.016509
41	1	0	2.017860	-1.487268	-0.587273
42	6	0	5.538242	-3.005081	0.183338
43	1	0	6.322137	-1.043558	-0.322395
44	6	0	4.385318	-3.814717	0.303243
45	1	0	2.224294	-3.864727	0.115237
46	1	0	6.520215	-3.418183	0.405494
47	1	0	4.471001	-4.851758	0.618551
48	8	0	-1.306156	0.306983	2.534245
49	1	0	-0.157154	1.057243	1.400535
50	1	0	4.837886	0.852238	-0.626091

E(RBMK) = -1165.94443353 h
Sum of electronic and thermal Free Energies = -1165.584245 h

BMK/EPR-II. gas phase

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.776477	-1.801618	-1.733770
2	6	0	-5.737355	-1.771985	-0.340856
3	6	0	-4.642716	-1.191429	0.347625
4	6	0	-3.553592	-0.619157	-0.376461
5	6	0	-3.611376	-0.671400	-1.796510
6	6	0	-4.697622	-1.245492	-2.460045
7	1	0	-5.474266	-1.627908	2.321357
8	1	0	-6.617470	-2.247280	-2.255386
9	1	0	-6.551146	-2.198011	0.242048
10	6	0	-4.624466	-1.182977	1.805984
11	6	0	-2.439992	-0.019669	0.380649
12	1	0	-2.800715	-0.269606	-2.396490
13	1	0	-4.708623	-1.267036	-3.546154
14	6	0	-2.430991	-0.042376	1.856598
15	6	0	-3.597532	-0.652768	2.521717
16	1	0	-3.583960	-0.653201	3.607564
17	6	0	-1.380180	0.619116	-0.273012
18	1	0	-1.381631	0.708763	-1.358457
19	7	0	-0.323689	1.163237	0.330207
20	6	0	0.706753	1.911418	-0.354462
21	1	0	0.561894	1.781301	-1.436850
22	6	0	0.657874	3.431940	-0.016792
23	1	0	0.795692	3.512421	1.068380
24	6	0	-0.709785	4.032922	-0.411765
25	1	0	-0.746695	5.092257	-0.139172
26	1	0	-0.865171	3.959842	-1.496456
27	1	0	-1.535224	3.522182	0.092128
28	6	0	1.812746	4.177982	-0.726998
29	1	0	1.739331	4.060958	-1.816564
30	1	0	1.761092	5.247966	-0.503881
31	1	0	2.794028	3.816375	-0.402499
32	6	0	2.073582	1.331763	0.077898
33	8	0	2.436623	1.341255	1.237718
34	7	0	2.838888	0.814304	-0.935427
35	1	0	2.655819	1.090999	-1.889995
36	7	0	4.174109	0.447217	-0.677409
37	6	0	4.388915	-0.926667	-0.367298
38	6	0	3.500961	-1.941772	-0.768350
39	6	0	5.588117	-1.263899	0.295468
40	6	0	3.815911	-3.285629	-0.497865
41	1	0	2.574250	-1.687179	-1.270574
42	6	0	5.889123	-2.606660	0.560145
43	1	0	6.272728	-0.475358	0.599851
44	6	0	5.006169	-3.629089	0.163225
45	1	0	3.121488	-4.062921	-0.804130
46	1	0	6.811727	-2.853366	1.077642
47	1	0	5.241206	-4.667984	0.370754
48	8	0	-1.500929	0.435421	2.533367
49	1	0	-0.320113	1.079789	1.356620
50	1	0	4.516662	1.034955	0.079247

E(RBMK) = -1166.29230807 h
Sum of electronic and thermal Free Energies = -1165.936360 h

BMK/CC-pVTZ. gas phase

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.637853	-1.745933	-1.754838
2	6	0	-5.609818	-1.715548	-0.374109
3	6	0	-4.525325	-1.149420	0.319979
4	6	0	-3.433532	-0.589105	-0.390369
5	6	0	-3.480845	-0.647252	-1.799409
6	6	0	-4.557181	-1.207426	-2.465641
7	1	0	-5.368779	-1.579702	2.275257
8	1	0	-6.476014	-2.183253	-2.281031
9	1	0	-6.429361	-2.133284	0.199780
10	6	0	-4.514252	-1.142795	1.768328
11	6	0	-2.328292	0.001845	0.369912
12	1	0	-2.663638	-0.259628	-2.392609
13	1	0	-4.557123	-1.231474	-3.548308
14	6	0	-2.328420	-0.030765	1.836182
15	6	0	-3.496987	-0.629884	2.485216
16	1	0	-3.491802	-0.633952	3.567800
17	6	0	-1.283658	0.655014	-0.269764
18	1	0	-1.293752	0.767836	-1.348632
19	7	0	-0.234817	1.196581	0.329547
20	6	0	0.774305	1.978991	-0.344126
21	1	0	0.599724	1.898069	-1.422952
22	6	0	0.725102	3.472723	0.061293
23	1	0	0.916326	3.507293	1.137526
24	6	0	-0.658929	4.068914	-0.232653
25	1	0	-0.687707	5.116595	0.071310
26	1	0	-0.881216	4.026474	-1.303962
27	1	0	-1.446572	3.539901	0.304467
28	6	0	1.828086	4.259737	-0.664767
29	1	0	1.695390	4.204593	-1.750139
30	1	0	1.787759	5.312182	-0.380097
31	1	0	2.824101	3.888396	-0.416678
32	6	0	2.144168	1.376928	0.024897
33	8	0	2.565079	1.398820	1.154924
34	7	0	2.827291	0.817061	-1.009168
35	1	0	2.554804	0.983843	-1.963905
36	7	0	4.117204	0.312539	-0.829497
37	6	0	4.217763	-1.040523	-0.426160
38	6	0	3.175195	-1.951279	-0.588057
39	6	0	5.442753	-1.475955	0.091102
40	6	0	3.359667	-3.285061	-0.226692
41	1	0	2.221956	-1.620780	-0.975532
42	6	0	5.614143	-2.806515	0.449110
43	1	0	6.256156	-0.769269	0.209733
44	6	0	4.573515	-3.722287	0.292209
45	1	0	2.538073	-3.979850	-0.347771
46	1	0	6.565637	-3.127880	0.853543
47	1	0	4.707077	-4.757372	0.577026
48	8	0	-1.407441	0.435890	2.517501
49	1	0	-0.222493	1.098156	1.351678
50	1	0	4.624962	0.925743	-0.201939

E(RBMK) = -1166.52049573 h
Sum of electronic and thermal Free Energies = -1166.161034 h

e. Cartesian coordinates of 5b (I form)

BMK/6-31G(2df.2pd). gas phase

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.514062	-2.077685	-1.683965
2	6	0	-5.504270	-2.012009	-0.309778
3	6	0	-4.490855	-1.300881	0.382112
4	6	0	-3.452433	-0.640008	-0.343757
5	6	0	-3.498352	-0.722614	-1.763936
6	6	0	-4.496672	-1.420378	-2.410976
7	1	0	-5.286620	-1.744570	2.346223
8	1	0	-6.289612	-2.623060	-2.205867
9	1	0	-6.275288	-2.504045	0.272606
10	6	0	-4.494191	-1.235855	1.808319
11	6	0	-2.428697	0.071894	0.387635
12	1	0	-2.748399	-0.230429	-2.366815
13	1	0	-4.500409	-1.460171	-3.493450
14	6	0	-2.483860	0.111975	1.793976
15	6	0	-3.531774	-0.554551	2.494389
16	1	0	-3.522321	-0.499430	3.575104
17	6	0	-1.320076	0.728766	-0.294016
18	1	0	-1.256535	0.628649	-1.381337
19	7	0	-0.425616	1.398956	0.330719
20	6	0	0.662529	1.999677	-0.405325
21	1	0	0.587659	1.767633	-1.481730
22	6	0	0.674347	3.538620	-0.225743
23	1	0	0.788048	3.717667	0.847565
24	6	0	-0.649262	4.149049	-0.708267
25	1	0	-0.634890	5.234917	-0.588982
26	1	0	-0.811958	3.932779	-1.770305
27	1	0	-1.497234	3.755252	-0.146285
28	6	0	1.869731	4.159387	-0.967560
29	1	0	1.820161	3.943759	-2.040622
30	1	0	1.866328	5.245476	-0.851774
31	1	0	2.825049	3.789447	-0.587342
32	6	0	1.967878	1.413365	0.162180
33	8	0	2.289231	1.522692	1.320604
34	7	0	2.744877	0.761496	-0.757065
35	1	0	2.640071	0.994534	-1.731861
36	7	0	4.043446	0.382226	-0.387918
37	6	0	4.272011	-1.001693	-0.219381
38	6	0	3.460757	-1.974928	-0.811632
39	6	0	5.406910	-1.395165	0.505547
40	6	0	3.790194	-3.325561	-0.679226
41	1	0	2.578093	-1.679153	-1.360655
42	6	0	5.722256	-2.744634	0.632796
43	1	0	6.035645	-0.639209	0.962039
44	6	0	4.918296	-3.721587	0.038261
45	1	0	3.153775	-4.070349	-1.141547
46	1	0	6.598959	-3.032726	1.199689
47	1	0	5.168982	-4.769850	0.134196
48	8	0	-1.593822	0.742003	2.534769
49	1	0	-0.917677	1.146757	1.936193
50	1	0	4.293521	0.908706	0.441905

E(RBMK) = -1166.27705895 h
Sum of electronic and thermal Free Energies = -1165.915746 h

f. Cartesian coordinates of transition state

BMK/6-31G(2df.2pd). gas phase

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.522128	-2.309300	-1.468668
2	6	0	-5.521641	-2.030176	-0.116818
3	6	0	-4.506271	-1.236210	0.463609
4	6	0	-3.459677	-0.709107	-0.346797
5	6	0	-3.486431	-1.012069	-1.731514
6	6	0	-4.490841	-1.790613	-2.276297
7	1	0	-5.324535	-1.364515	2.466771
8	1	0	-6.302939	-2.917859	-1.906102
9	1	0	-6.305529	-2.418697	0.524119
10	6	0	-4.515706	-0.950063	1.873517
11	6	0	-2.435879	0.099074	0.284101
12	1	0	-2.713058	-0.633708	-2.387439
13	1	0	-4.482221	-2.004647	-3.338262
14	6	0	-2.474834	0.366644	1.694618
15	6	0	-3.559271	-0.190789	2.468836
16	1	0	-3.566767	0.024815	3.529657
17	6	0	-1.344975	0.666296	-0.430608
18	1	0	-1.240048	0.513855	-1.505049
19	7	0	-0.450169	1.382778	0.185311
20	6	0	0.679047	1.977174	-0.486051
21	1	0	0.638962	1.726462	-1.556759
22	6	0	0.686866	3.518811	-0.330729
23	1	0	0.749571	3.717655	0.743661
24	6	0	-0.609584	4.124686	-0.887525
25	1	0	-0.599604	5.211483	-0.778280
26	1	0	-0.716332	3.898176	-1.954275
27	1	0	-1.486471	3.738500	-0.365871
28	6	0	1.919936	4.122998	-1.023154
29	1	0	1.920636	3.889035	-2.093527
30	1	0	1.914085	5.210731	-0.926391
31	1	0	2.854251	3.757631	-0.590265
32	6	0	1.956498	1.390324	0.142423
33	8	0	2.208152	1.492064	1.318274
34	7	0	2.784955	0.752200	-0.738670
35	1	0	2.729003	0.986255	-1.717204
36	7	0	4.062050	0.368006	-0.306656
37	6	0	4.278928	-1.018212	-0.135795
38	6	0	3.491090	-1.985471	-0.767673
39	6	0	5.380071	-1.418615	0.635450
40	6	0	3.809791	-3.337928	-0.627600
41	1	0	2.634055	-1.684983	-1.353384
42	6	0	5.685048	-2.769804	0.769620
43	1	0	5.991907	-0.667161	1.121374
44	6	0	4.904184	-3.741085	0.136329
45	1	0	3.190609	-4.078279	-1.119503
46	1	0	6.535703	-3.063456	1.372136
47	1	0	5.146836	-4.790697	0.238068
48	8	0	-1.585060	1.076901	2.267875
49	1	0	-0.790090	1.387486	1.355448
50	1	0	4.274060	0.889925	0.536339

E(RBMK) = -1166.26825395 h
Sum of electronic and thermal Free Energies = -1165.912966 h
Imaginary frequency: -1462.9318 cm^{-1}

3. UV-visible spectroscopy

The chain of instabilities or the conjugation. within a molecule. causes the delocalization of the electrons π. This delocalisation facilitates the movement of the electrons along the links. This is accompanied by an approximation of energy levels between HOMO (Highest Occupied Molecular Orbital) and LUMO (Lowest Unoccupied Molecular Orbital). The energy difference between the conduction band or HOMO and that of valence (LUMO) defines the forbidden band or more simply "gap". Its corresponding energy (E_{og} for optical gap energy) is usually given in electron volt (eV).

The optical gap energy of the compounds **5a-e** was determined using the following relationship:

$$E_{og} = \frac{h \times c}{\lambda_{gap}}$$

With the following paramaters:

h= 6.626 070 040.10^{-34} J·s: refers to the Planck constant.

c = 299 792 458 m.s^{-1}: refers to the celerity of light in a vacuum.

λ_{gap}:(in m) denotes the wavelength at the UV-visible absorption threshold determined by the extrapolation of the tangent of the linear parts of the spectrum.

This equation can be simplified by replacing h and c by their numerical values:

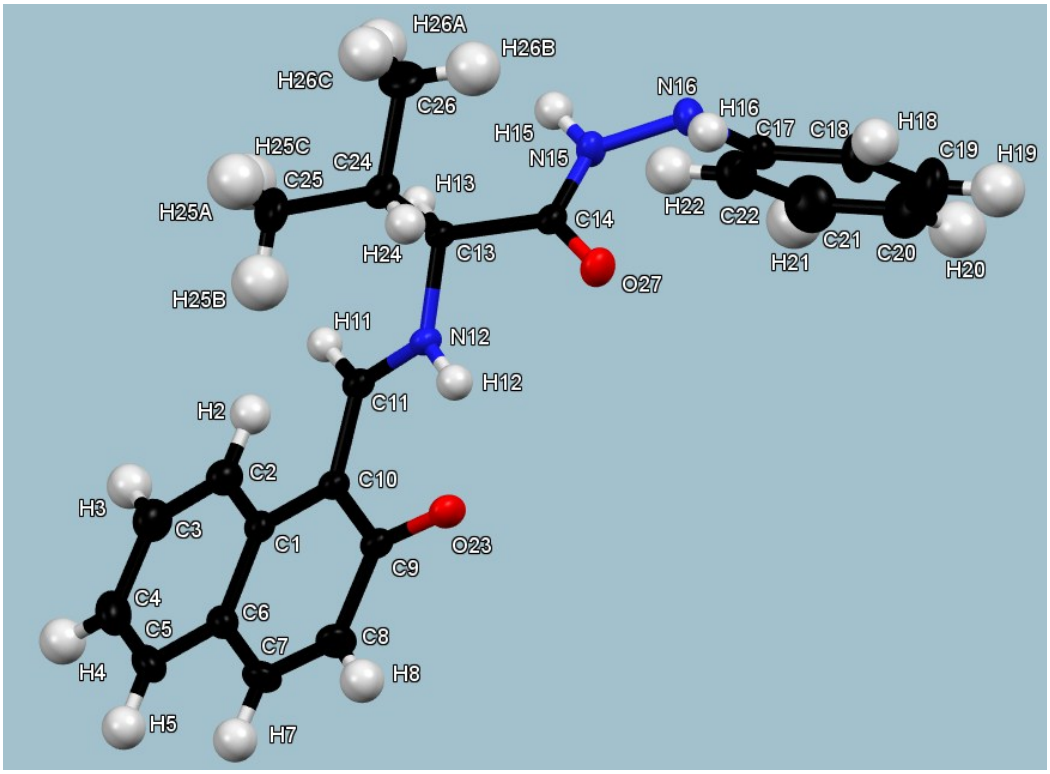
$$E_{og}(eV) = \frac{1240}{\lambda_{gap}(nm)}$$

As an example. the case of the compound **5b** gives: λ_{gap} = 449.27 nm. Applying this formula. E_{og}= 2.76 eV is obtained.

4. Crystallographic data

a. Crystallisation

A monocrystal of the compound **5b** was obtained by cold crystallization in a mixture methanol / diethyl ether 1:3. in a hemolysis tube left in the open air. which made it possible to carry out X-ray diffraction experiments. The ORTEP plate of this compound is presented below. We have found that (*S*)-**5b** assumes a stable form with intramolecular hydrogen bonds.



ORTEP of the compound **5b**.

Crystal of **5b**.

b. Main structure information (Table S3)

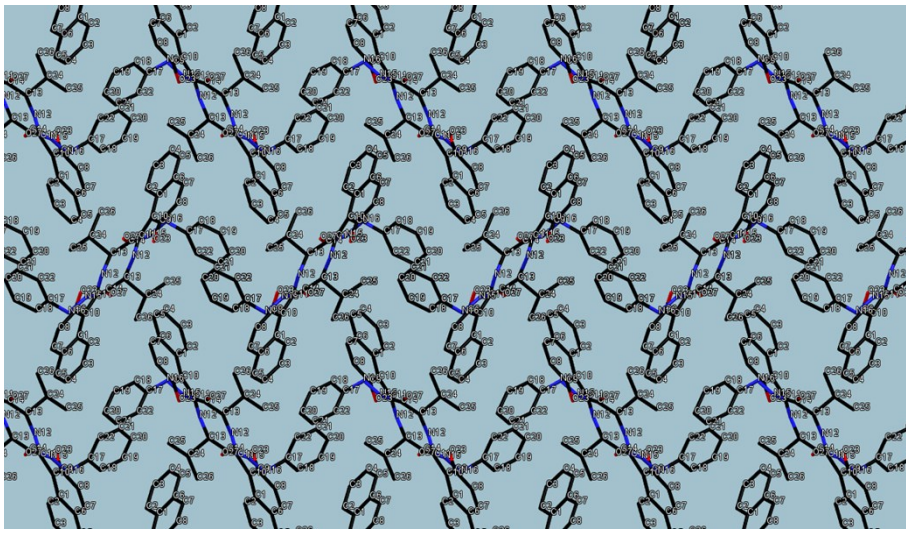
Formula	$C_{22}H_{23}N_3O_2$
Molecular weight	361.43
Compound name	(*E*)-1-(((3-methyl-1-oxo-1-(2-phenylhydrazinyl)butan-2-yl)iminio)methyl)naphthalen-2-olate
Space group	P 2_1 2_1 2_1
Space group (name Hall)	P 2_{ac} 2_{ab}
Cell setting	Orthorhombic
Cell lengths	**a** 10.3964(5) **b** 10.8708(5) **c** 17.5190(7)
Cell angles	α 90 β 90 γ 90
Cell volume	1979.95
Z	4
F (000)	768
Dx ($g.cm^{-3}$)	1.213
Mo *Kα* radiation, *λ*	0.71073 Å
θ	2.7–30.1°
μ	0.08 mm^{-1}
h. k .l max	14. 15. 24
Temperature (K)	200

c. Cartesian coordinates

ATOM	1 O23	0	2.009	0.696	10.176	1.00 0.00	O2
ATOM	2 O27	0	2.736	3.078	7.210	1.00 0.00	O2
ATOM	3 N12	0	4.120	1.842	9.258	1.00 0.00	N1
ATOM	4 N15	0	4.504	4.485	7.058	1.00 0.00	N1
ATOM	5 N16	0	3.817	5.404	6.244	1.00 0.00	N1
ATOM	6 C1	0	4.720	0.529	12.664	1.00 0.00	C1
ATOM	7 C2	0	5.954	1.107	13.017	1.00 0.00	C2
ATOM	8 C3	0	6.583	0.759	14.201	1.00 0.00	C3
ATOM	9 C4	0	6.012	-0.166	15.072	1.00 0.00	C4
ATOM	10 C5	0	4.789	-0.709	14.766	1.00 0.00	C5
ATOM	11 C6	0	4.122	-0.371	13.572	1.00 0.00	C6
ATOM	12 C7	0	2.824	-0.902	13.283	1.00 0.00	C7
ATOM	13 C8	0	2.129	-0.540	12.182	1.00 0.00	C8
ATOM	14 C9	0	2.690	0.367	11.209	1.00 0.00	C9
ATOM	15 C10	0	4.022	0.839	11.429	1.00 0.00	C1
ATOM	16 C11	0	4.688	1.514	10.391	1.00 0.00	C1
ATOM	17 C13	0	4.843	2.335	8.095	1.00 0.00	C1
ATOM	18 C14	0	3.920	3.348	7.421	1.00 0.00	C1
ATOM	19 C17	0	3.321	6.561	6.907	1.00 0.00	C1
ATOM	20 C18	0	2.233	7.216	6.345	1.00 0.00	C1
ATOM	21 C19	0	1.761	8.381	6.920	1.00 0.00	C1
ATOM	22 C20	0	2.364	8.899	8.048	1.00 0.00	C2
ATOM	23 C21	0	3.436	8.249	8.600	1.00 0.00	C2
ATOM	24 C22	0	3.933	7.079	8.033	1.00 0.00	C2
ATOM	25 C24	0	5.175	1.173	7.129	1.00 0.00	C2
ATOM	26 C25	0	6.043	0.129	7.826	1.00 0.00	C2
ATOM	27 C26	0	5.868	1.697	5.871	1.00 0.00	C2
ATOM	28 H2	0	6.359	1.743	12.439	1.00 0.00	H2
ATOM	29 H3	0	7.417	1.157	14.422	1.00 0.00	H3
ATOM	30 H4	0	6.464	-0.419	15.868	1.00 0.00	H4
ATOM	31 H5	0	4.387	-1.322	15.368	1.00 0.00	H5
ATOM	32 H7	0	2.439	-1.528	13.884	1.00 0.00	H7
ATOM	33 H8	0	1.256	-0.889	12.044	1.00 0.00	H8
ATOM	34 H11	0	5.600	1.745	10.520	1.00 0.00	H1
ATOM	35 H12	0	3.265	1.601	9.204	1.00 0.00	H1
ATOM	36 H13	0	5.686	2.787	8.386	1.00 0.00	H1
ATOM	37 H15	0	5.365	4.575	7.107	1.00 0.00	H1
ATOM	38 H16	0	3.161	5.023	5.824	1.00 0.00	H1
ATOM	39 H18	0	1.813	6.865	5.568	1.00 0.00	H1
ATOM	40 H19	0	1.018	8.829	6.536	1.00 0.00	H1
ATOM	41 H20	0	2.037	9.700	8.440	1.00 0.00	H2
ATOM	42 H21	0	3.847	8.602	9.381	1.00 0.00	H2
ATOM	43 H22	0	4.685	6.642	8.416	1.00 0.00	H2
ATOM	44 H24	0	4.318	0.736	6.856	1.00 0.00	H2
ATOM	45 H25A	0	6.260	-0.588	7.196	1.00 0.00	H2
ATOM	46 H25B	0	5.555	-0.244	8.589	1.00 0.00	H2
ATOM	47 H25C	0	6.870	0.550	8.141	1.00 0.00	H2
ATOM	48 H26A	0	6.712	2.128	6.119	1.00 0.00	H2
ATOM	49 H26B	0	5.287	2.350	5.427	1.00 0.00	H2
ATOM	50 H26C	0	6.048	0.951	5.262	1.00 0.00	H2

d. Supramolecular structure (View down crystallographic a axis)

Figure including atom labels



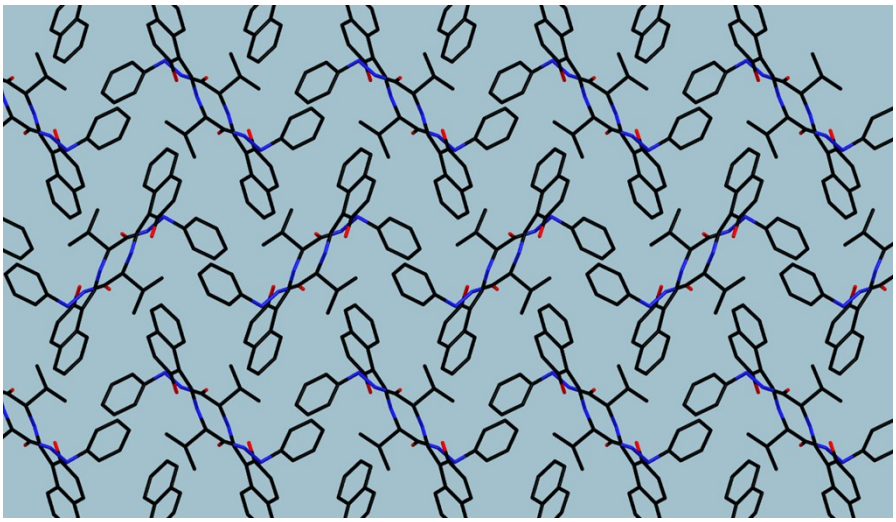
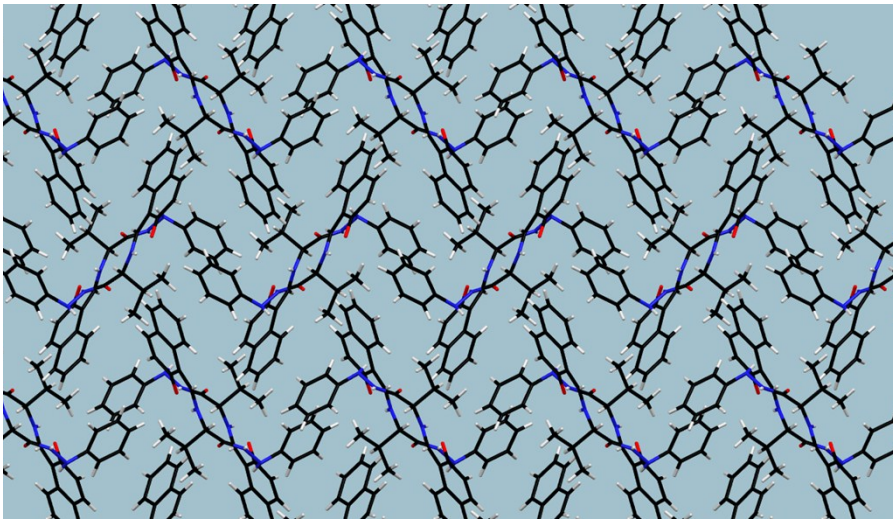


Figure including H atoms



5. Comparison between calculations and X-ray data (Table S4)

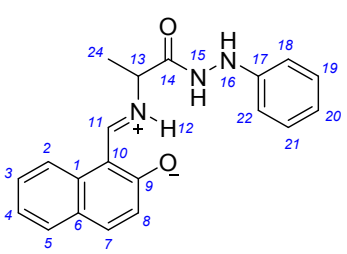
Investigation of calculation methods and basis sets for the selected geometrical parameters of **5b** in the gas phase.

			Distances					Angles			Dihedral angles				
			C(9)O(23)$^-$	C(11)N(12)	C(14)O(27)	O(23)N(12)	N(12)O(27)	C(10)C(11)N(12)	C(11)N(12)C(13)	O(23)N(12)O(27)	O(23)C(9)C(10)C(11)	C(9)C(10)C(11)N(12)	N(12)C(13)C(14)O(27)		
Entry	X-Ray values		**1.279**	**1.307**	**1.232**	**2.571**	**2.764**	**123.6**	**124.1**	**93.04**	**-9.9**	**5.8**	**-47.7**		
	X-Ray uncertaintly		0.002	0.002	0.002	0.002	0.002	0.2	0.2	0.05	0.2	0.2	0.2		
	Method	Basis set												Σ x-x_{ref}	MAD
1	HF	3-21G	1.24217	1.32648	1.21241	2.58543	**2.80096**	126.42061	124.57007	97.35925	-0.24071	0.90972	-52.30778	26.8946	2.067
2	HF	6-31G(d)	1.21900	1.32630	1.19583	2.64209	2.89549	127.47533	124.37650	104.14081	-1.28736	1.87023	-64.07889	44.4920	2.210
3	HF	6-31+G(d)	1.22188	1.32460	1.19683	2.64446	2.91820	127.60459	124.12116	105.64133	-0.75827	1.64122	-66.10013	48.6653	2.365
4	HF	6-31G(d.p)	1.21946	1.32561	1.19595	2.63606	2.90423	127.32102	124.25839	104.36729	-1.29333	1.83664	-65.20239	45.5986	2.239
5	HF	6-31+G(d.p)	1.22216	1.32425	1.19695	2.64028	2.92504	127.47553	123.97438	105.73267	-0.77925	1.62907	-66.97695	49.6019	2.385
6	B3LYP	3-21G	**1.28083**	1.33461	**1.23818**	2.51760	2.80624	123.25787	125.02065	**91.37241**	-0.12809	0.07742	**-47.91277**	**18.7689**	2.070
7	B3LYP	6-31G(d)	1.25692	1.33401	1.22118	2.58168	2.92598	124.75506	124.92368	100.19868	0.95680	1.28068	-62.89043	39.9365	2.397
8	B3LYP	6-31+G(d)	1.26015	1.33394	1.22253	2.59378	2.95871	125.20661	124.57711	103.03188	-1.11542	1.55874	-65.68787	43.3621	2.242
9	B3LYP	6-31G(d.p)	1.25899	1.33230	1.22128	2.55760	2.94068	124.19158	124.86621	100.17326	-0.48410	0.83096	-64.42113	39.8432	2.359
10	B3LYP	6-31+G(d.p)	1.26184	1.33260	1.22257	2.57230	2.96944	124.67618	124.52416	102.77493	-0.80562	1.25493	-68.82211	46.2558	2.377
11	B3P86	6-31+G(d.p)	1.26097	1.32554	1.22024	2.52924	2.94662	123.79294	124.41703	101.38566	-0.68570	1.21506	-65.22318	40.4508	2.303
12	B3PW91	6-31+G(d.p)	1.26051	1.32731	1.22057	2.54309	2.95262	124.05729	124.52831	101.55373	-0.53195	1.05533	-65.60852	41.6873	2.357
13	BHandHLYP	6-31+G(d.p)	1.24092	**1.32259**	1.20791	2.58292	2.93042	125.82722	124.17086	103.58604	-1.41370	1.85170	-66.44316	44.2780	2.189
14	BMK	6-31+G(d.p)	1.24553	1.33048	1.21451	2.60423	2.94790	125.49019	**124.10995**	102.81858	**-3.13584**	**3.41549**	-66.18654	39.6055	1.740
15	M062X	6-31+G(d.p)	1.24879	1.33122	1.21330	2.58901	3.18590	125.52331	123.69193	103.21062	6.99471	-5.55403	-97.69831	91.2621	5.057
16	PBE1PBE	6-31+G(d.p)	1.25714	1.32477	1.21814	2.54011	2.94941	124.11823	124.43147	101.86745	-1.15022	1.56987	-66.53419	41.7610	2.231
17	PBEh1PBE	6-31+G(d.p)	1.25691	1.32485	1.21815	2.54327	2.94578	124.21045	124.39339	101.93189	-1.22418	1.64016	-66.08189	41.2766	2.201
18	X3LYP	6-31+G(d.p)	1.26065	1.33158	1.22161	**2.57008**	2.96852	124.69236	124.48677	102.91721	-0.93947	1.36202	-67.14444	44.4581	2.312
19	CAM-B3LYP	6-31+G(d.p)	1.25354	1.32720	1.21729	2.56519	2.95451	125.00461	124.27026	102.84524	-1.12597	1.56015	-67.37626	44.3269	2.266
20	TPSSh	6-31+G(d.p)	1.26843	1.33235	1.22772	2.54666	2.95634	**123.79189**	124.41077	100.89960	0.04190	0.52367	-64.58505	40.7224	2.467
21	ωB97XD	6-31+G(d.p)	1.25022	1.33258	1.21673	2.59120	3.01688	125.47030	121.82958	101.38132	9.84347	-4.71185	-76.70157	72.0816	4.692
22	BMK	3-21G	1.26970	1.33340	**1.22698**	**2.55425**	**2.74615**	**124.34649**	124.62676	**89.79634**	-0.30243	0.77437	-41.38556	25.5299	2.058
23	BMK	6-31G(d.p)	1.24251	1.33037	1.21313	2.59792	2.88348	125.24688	124.30667	99.55878	-3.61713	3.73630	-58.97413	28.2182	**1.427**
24	BMK	6-31G(2df.2pd)	1.23595	1.32610	1.20771	2.59089	2.81797	125.30467	124.24648	96.80268	-2.87538	2.97796	**-51.61641**	**19.5372**	**1.429**
25	BMK	6-311G(d.p)	1.23598	1.32739	1.20610	2.60468	2.87477	125.66363	124.21656	100.26254	-2.91802	3.27433	-58.30060	29.7447	1.582
26	BMK	6-311G(2df.2pd)	1.23472	**1.32379**	1.20546	2.59796	2.85231	125.59797	**124.13211**	98.89063	-1.91852	2.32903	-55.83540	27.6714	1.766
27	BMK	6-311+G(d.p)	1.23857	1.32742	1.20660	2.60551	2.94226	125.68514	124.16587	103.16864	-3.61000	3.81147	-66.26406	39.4213	1.639
28	BMK	6-311++G(d.p)	1.23860	1.32743	1.20662	2.60589	2.94123	125.69588	124.14555	103.18462	-3.78186	3.92747	-66.16964	39.0447	1.600
29	BMK	D95	1.27601	1.34315	1.23930	2.59319	2.99790	125.11681	123.71228	102.56420	-2.48920	2.77104	-67.82499	42.2960	1.940
30	BMK	D95V	**1.27609**	1.34070	1.23929	2.59286	2.99768	125.11679	123.70078	102.53603	-2.46544	2.74712	-67.86255	42.3615	1.945
31	BMK	EPR-II	1.24552	1.33271	1.21535	2.60183	2.91111	125.11959	124.18934	100.49560	-2.78276	3.11576	-60.76117	32.1810	1.673
32	BMK	CC-pVTZ	1.23700	1.32383	1.20607	2.59631	2.92602	125.45585	124.34936	102.39898	**-3.83794**	**3.93153**	-65.17341	37.1402	1.554

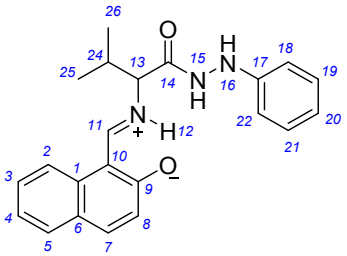
a) MAD is defined here as the sum of absolute relative gap on the eleven selected values: Σ |($value_{calcd}$ - $value_{X\text{-}ray}$) / $value_{X\text{-}ray}$|; b) the most accurate calculated values vis-à-vis of the each selected X-ray data are bolded; c) all atom numbers follow the labels of the crystallographic data.

6. Spectrum section

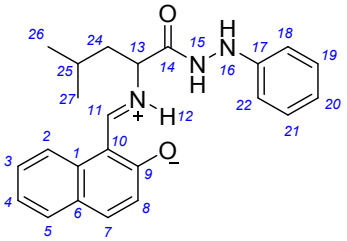
a. Labels of 5a-e for spectrum section and characterization



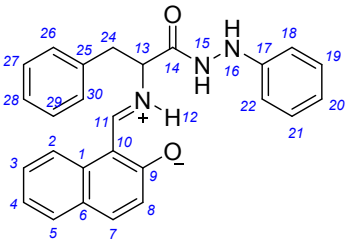
5a



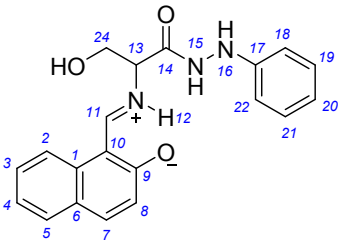
5b



5c



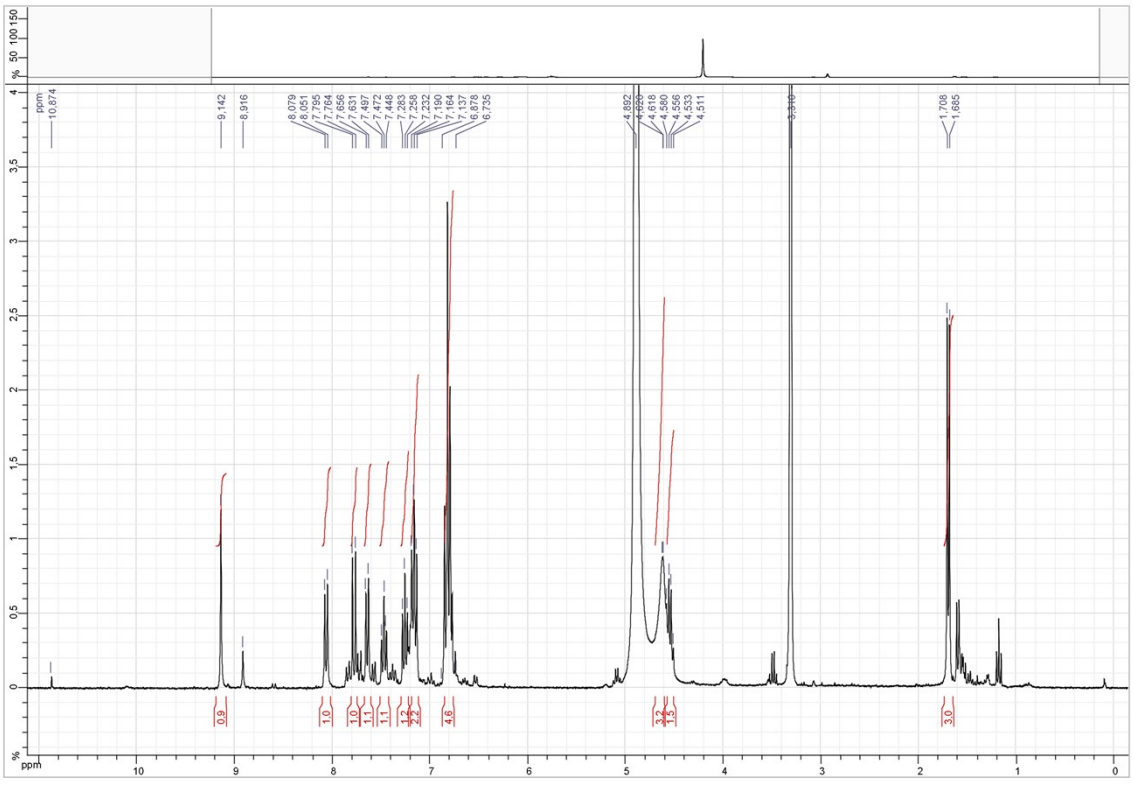
5d



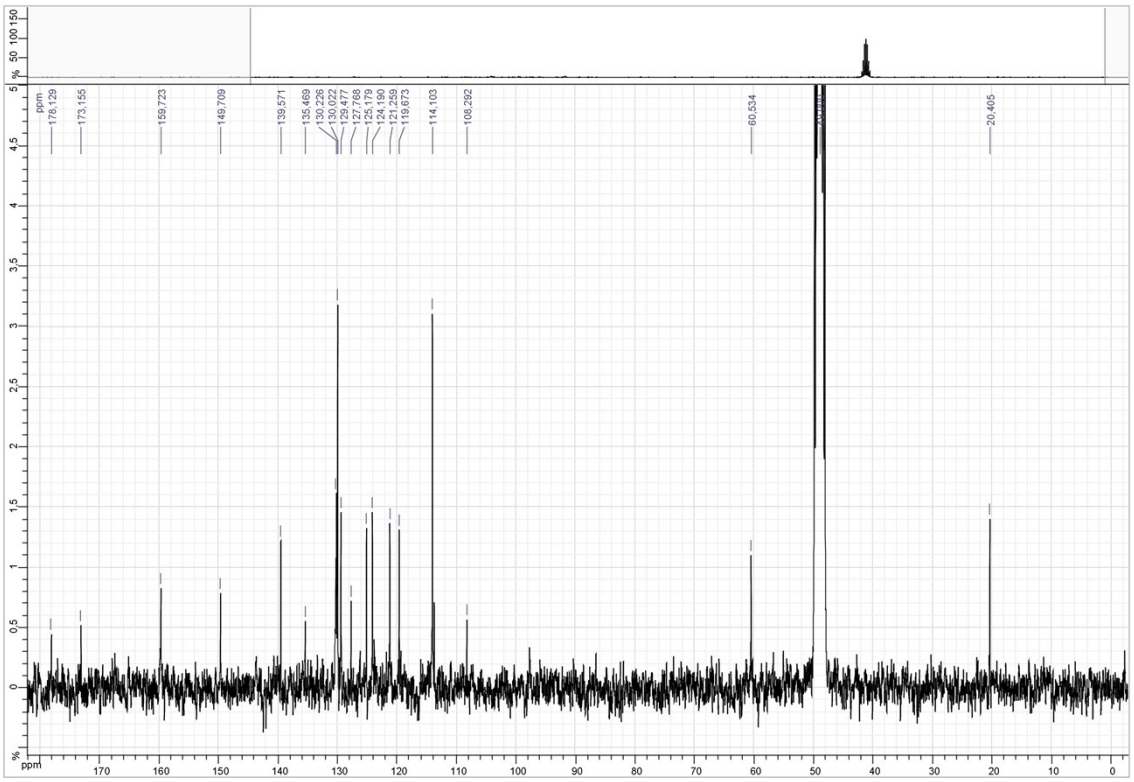
5e

b. NMR spectra of 5a

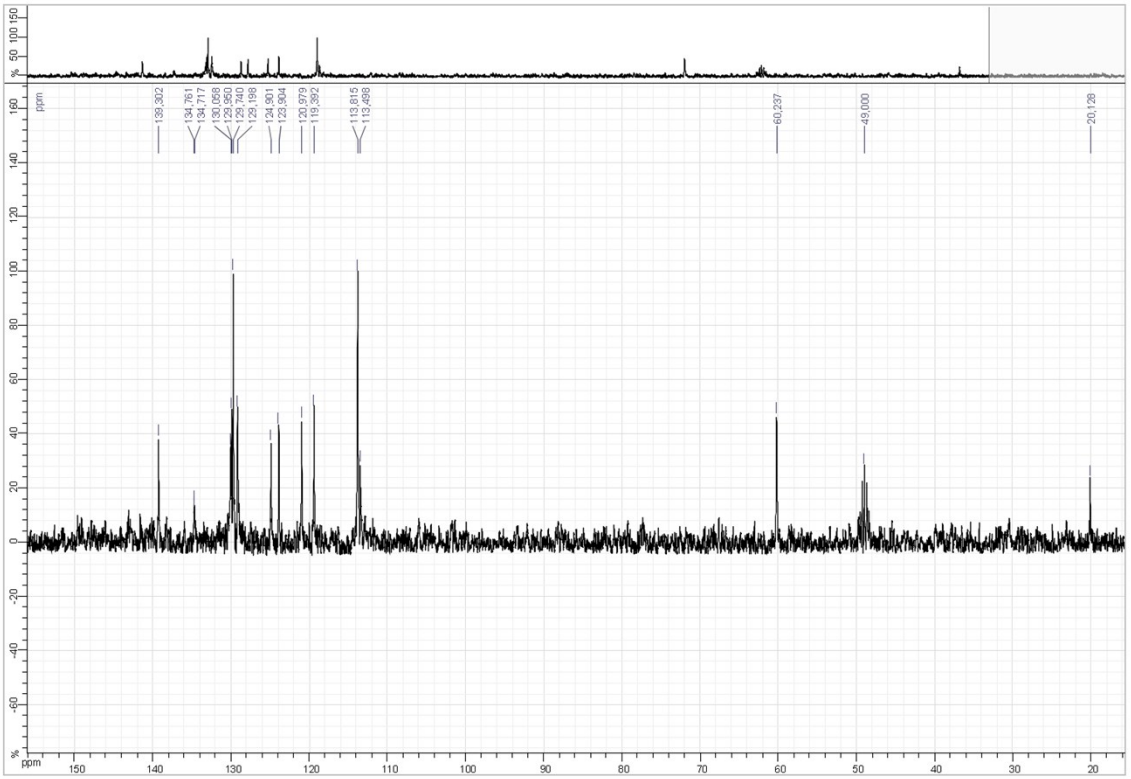
^{1}H NMR spectrum of **5a** in CD_3OD at 300 MHz



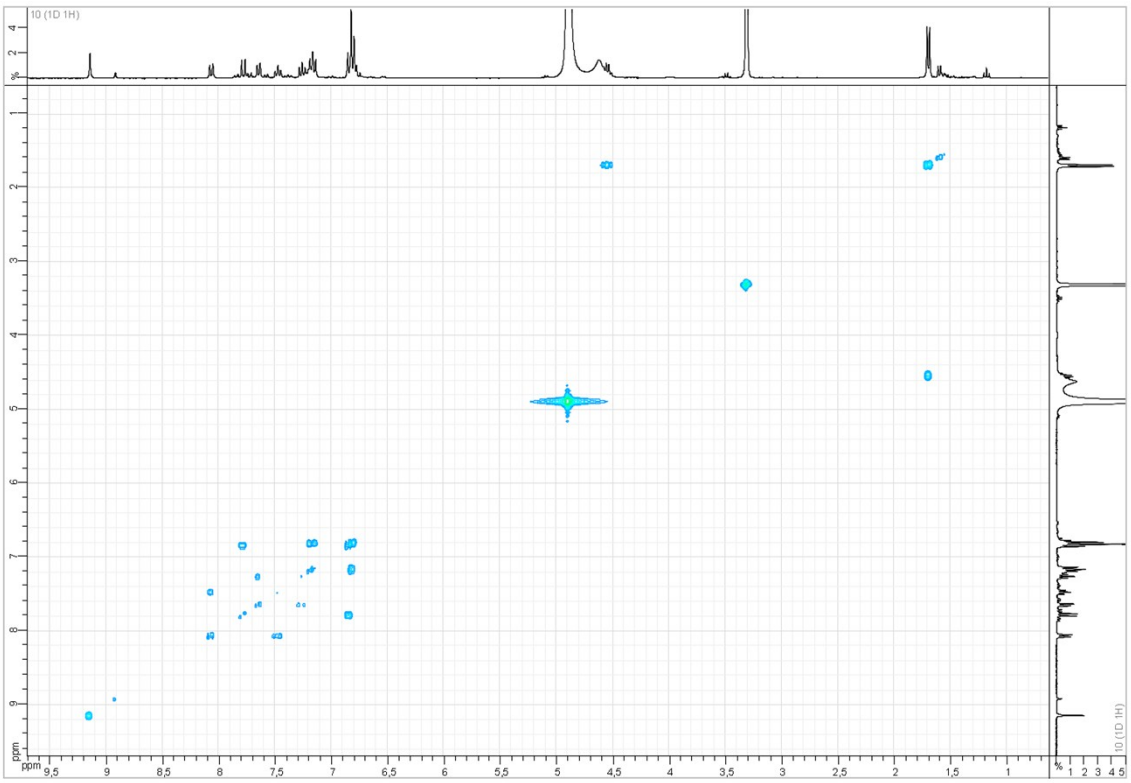
^{13}C NMR spectrum of **5a** in CD_3OD at 75 MHz



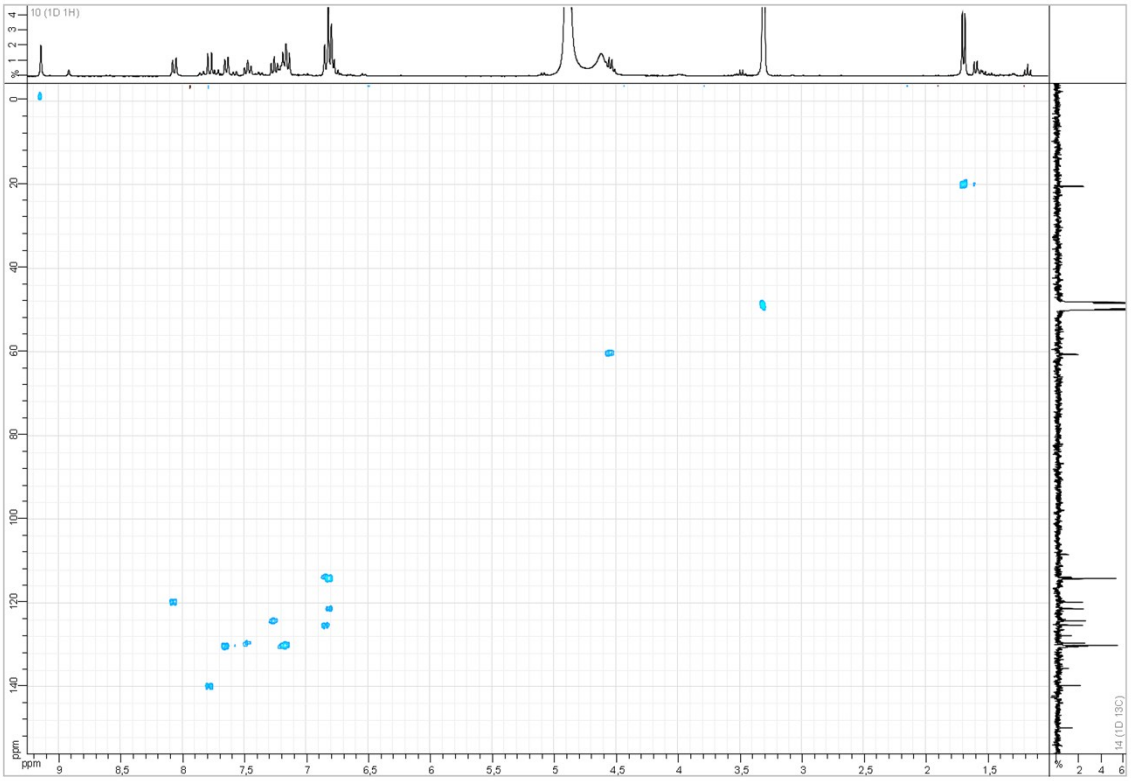
^{13}C (Dept135) NMR spectrum of **5a** in CD_3OD at 75 MHz



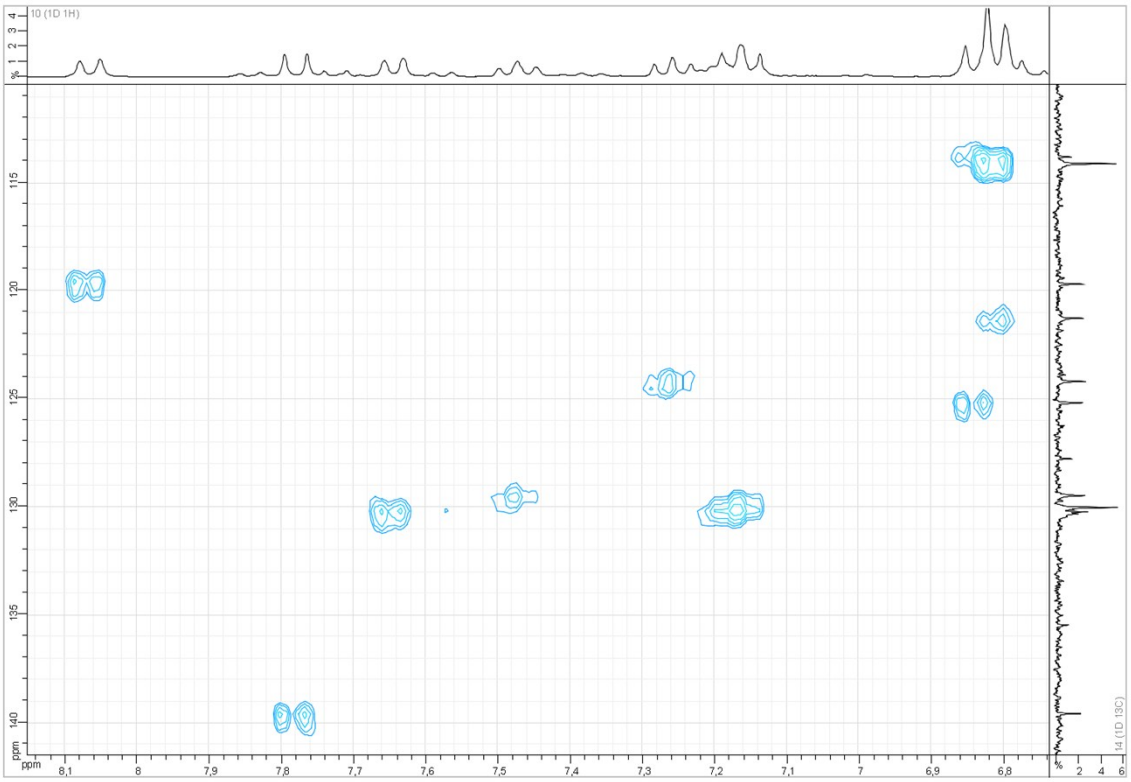
Cosy NMR spectrum of **5a** in CD_3OD



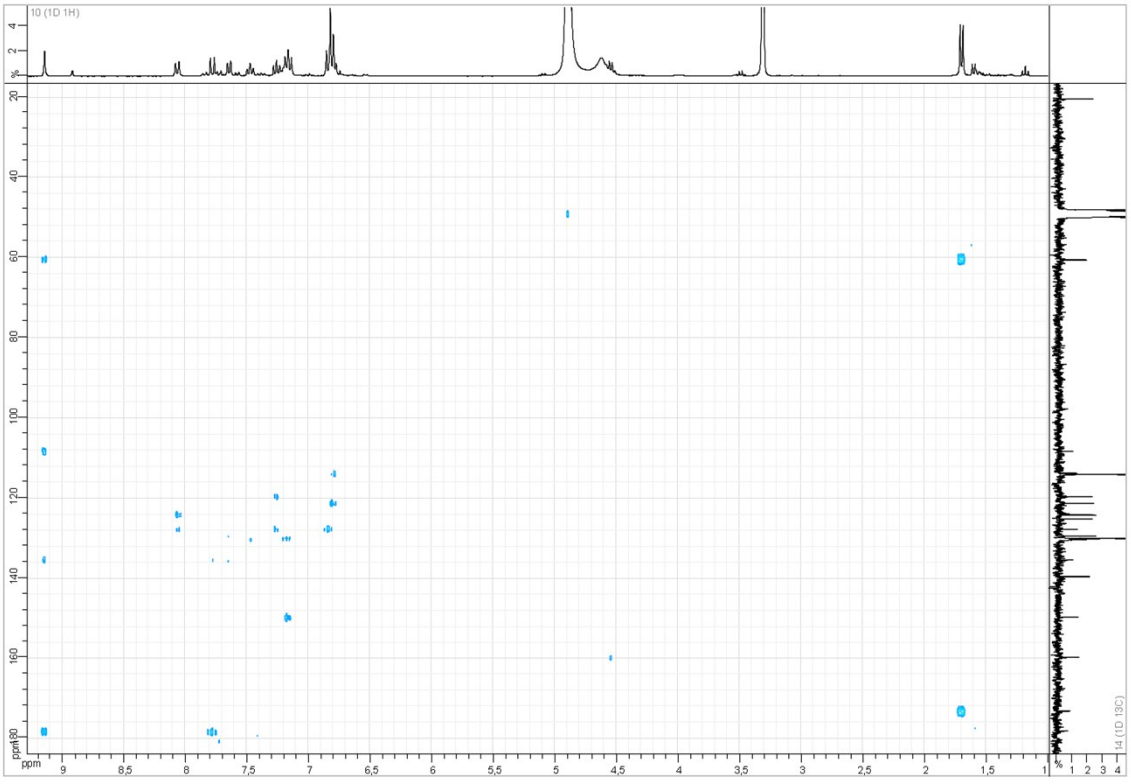
HSQC NMR spectrum of **5a** in CD_3OD



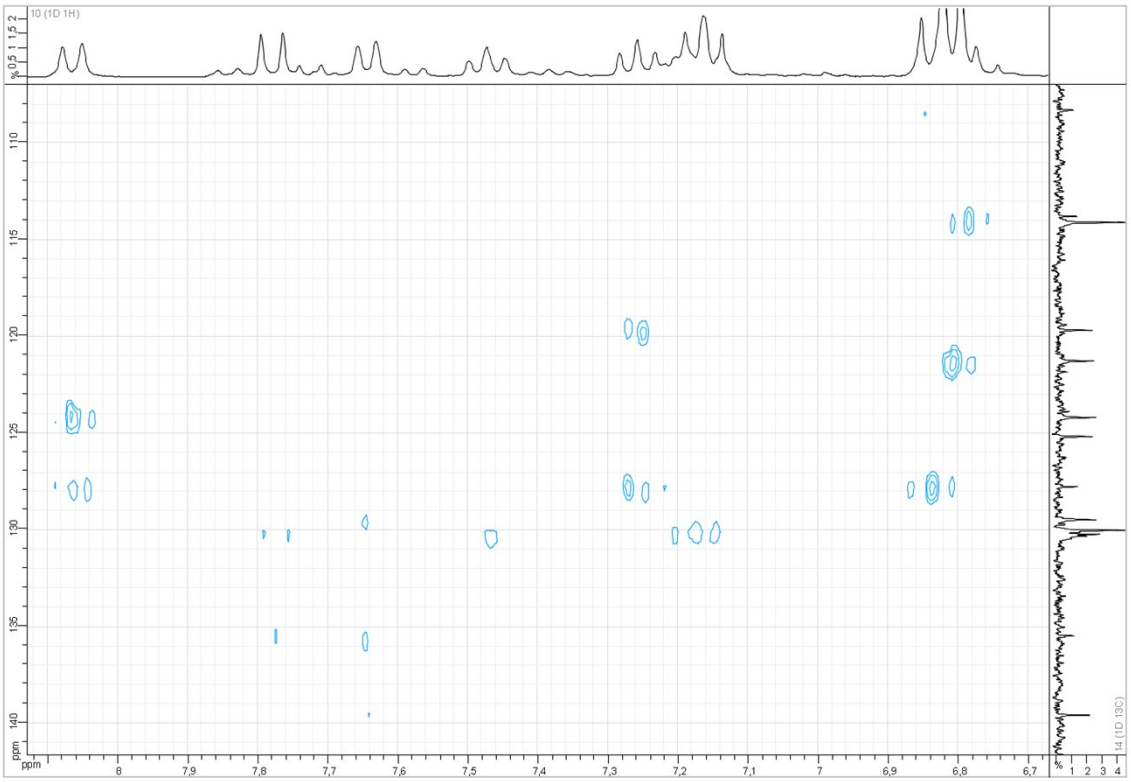
HSQC NMR spectrum of **5a** in CD_3OD (zoom)



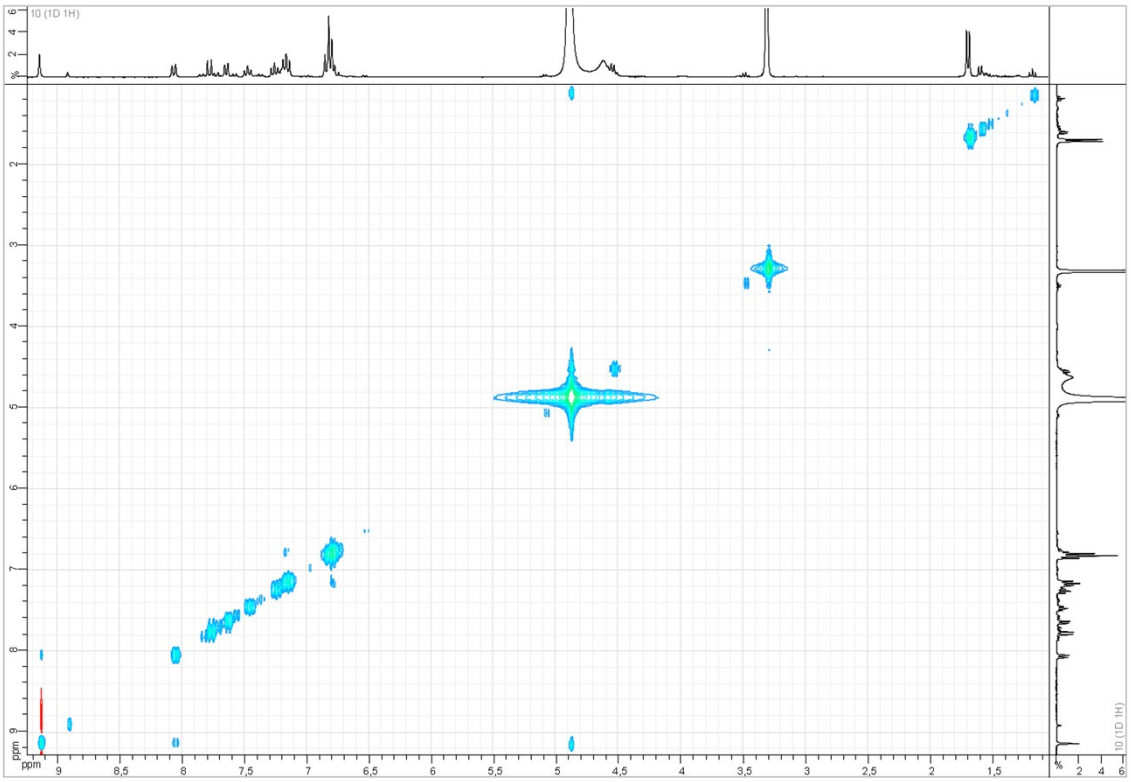
HMBC NMR spectrum of **5a** in CD_3OD



HMBC NMR spectrum of **5a** in CD_3OD (zoom)



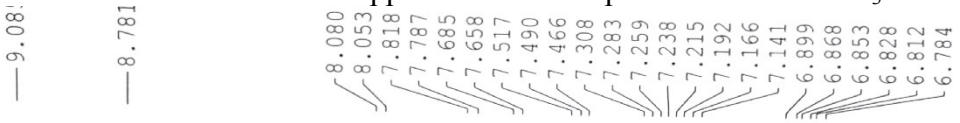
Noesy NMR spectrum of **5a** in CD_3OD

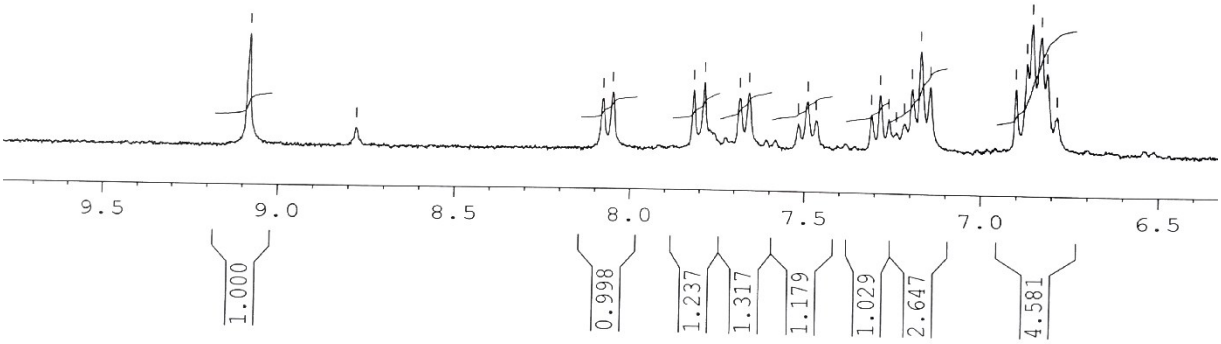


c. NMR spectra of 5b

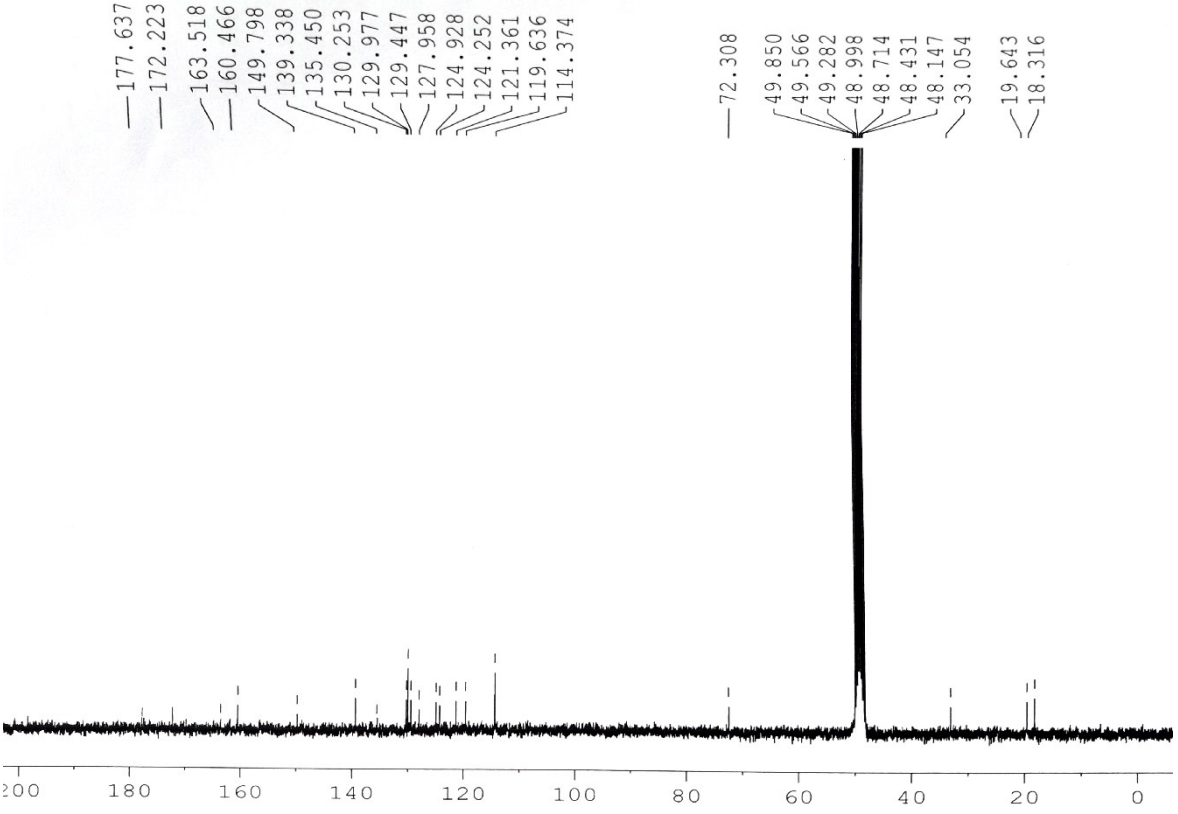
^{1}H NMR spectrum of **5b** in CD_3OD at 300 MHz

Magnification of the zone between 6.5 and 9.5 ppm of ^{1}H NMR spectrum of **5b** in CD_3OD

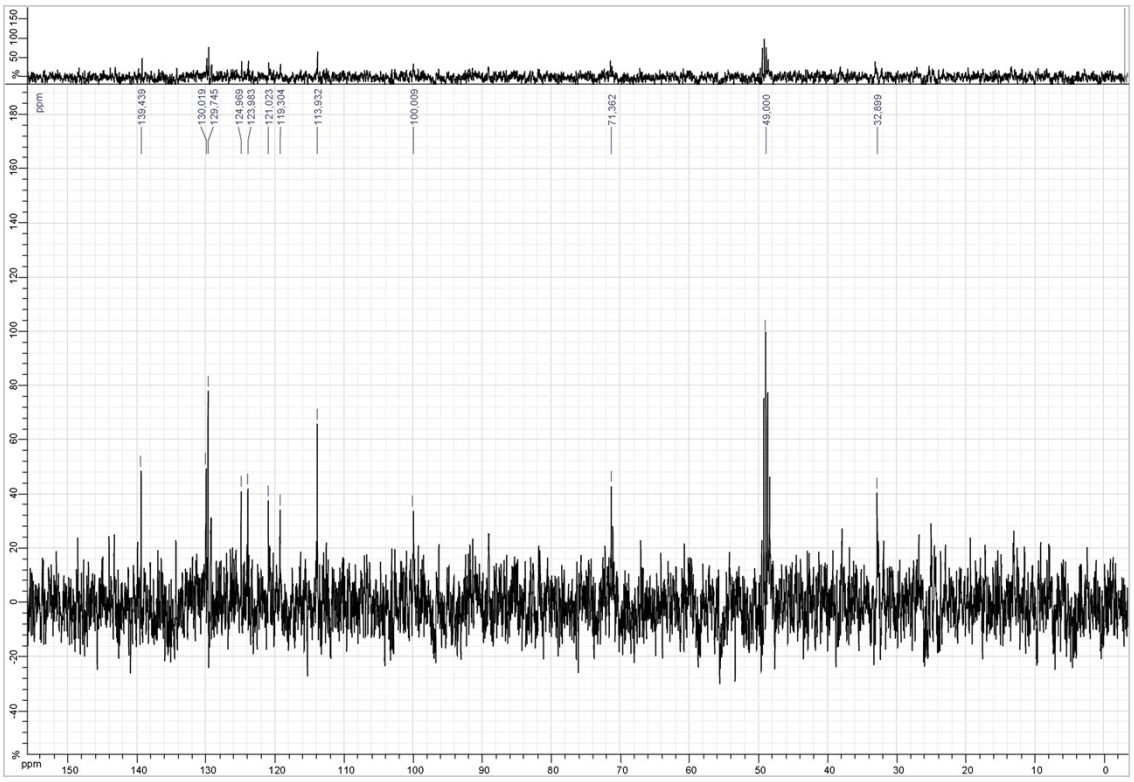




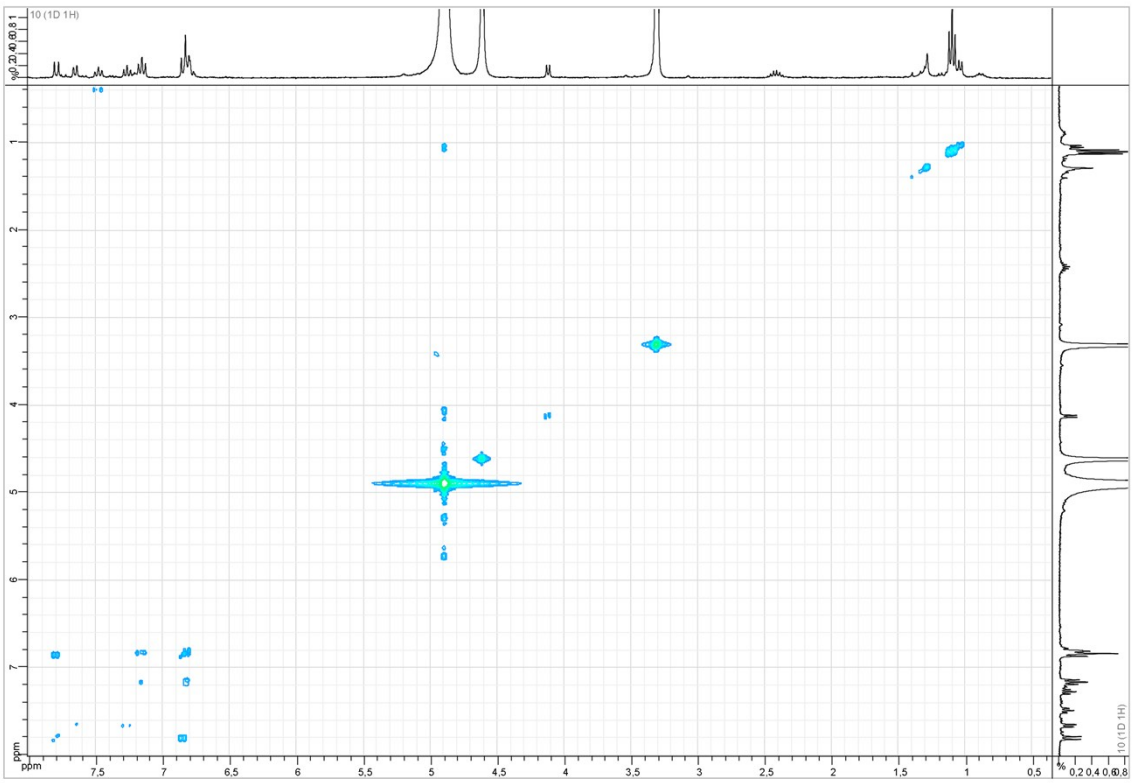
^{13}C NMR spectrum of **5b** in CD_3OD at 75 MHz



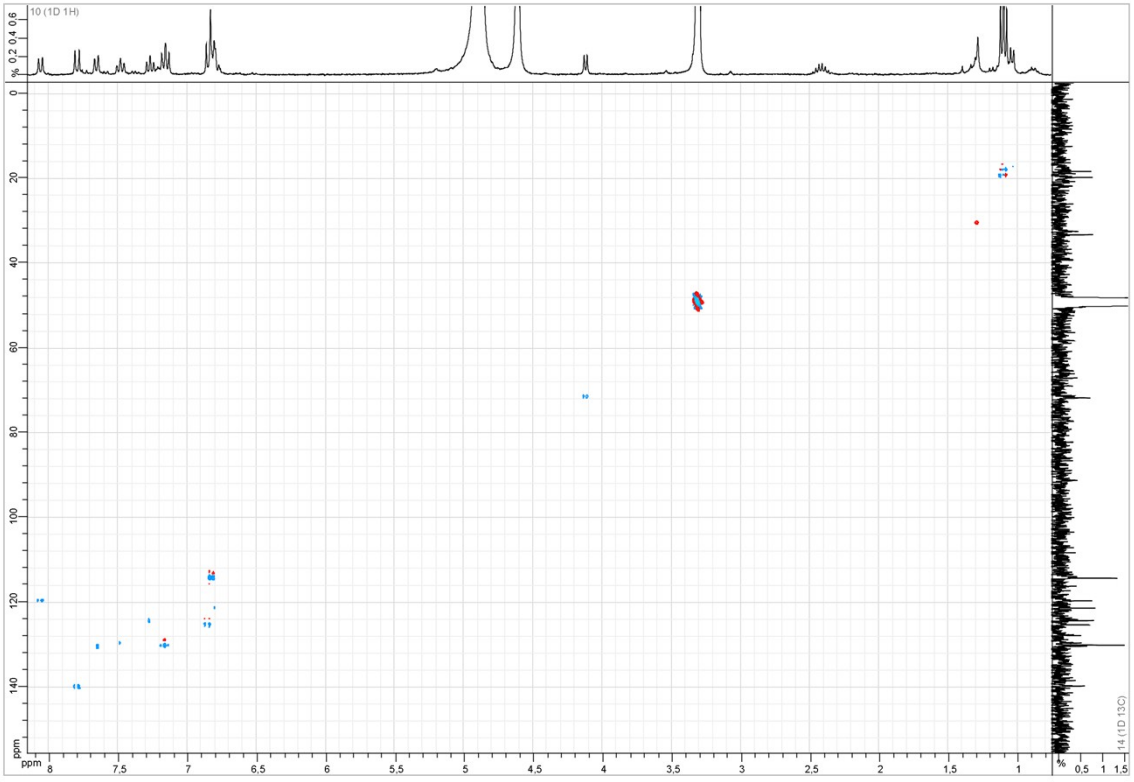
^{13}C (Dept135) NMR spectrum of **5a** in CD_3OD at 75 MHz



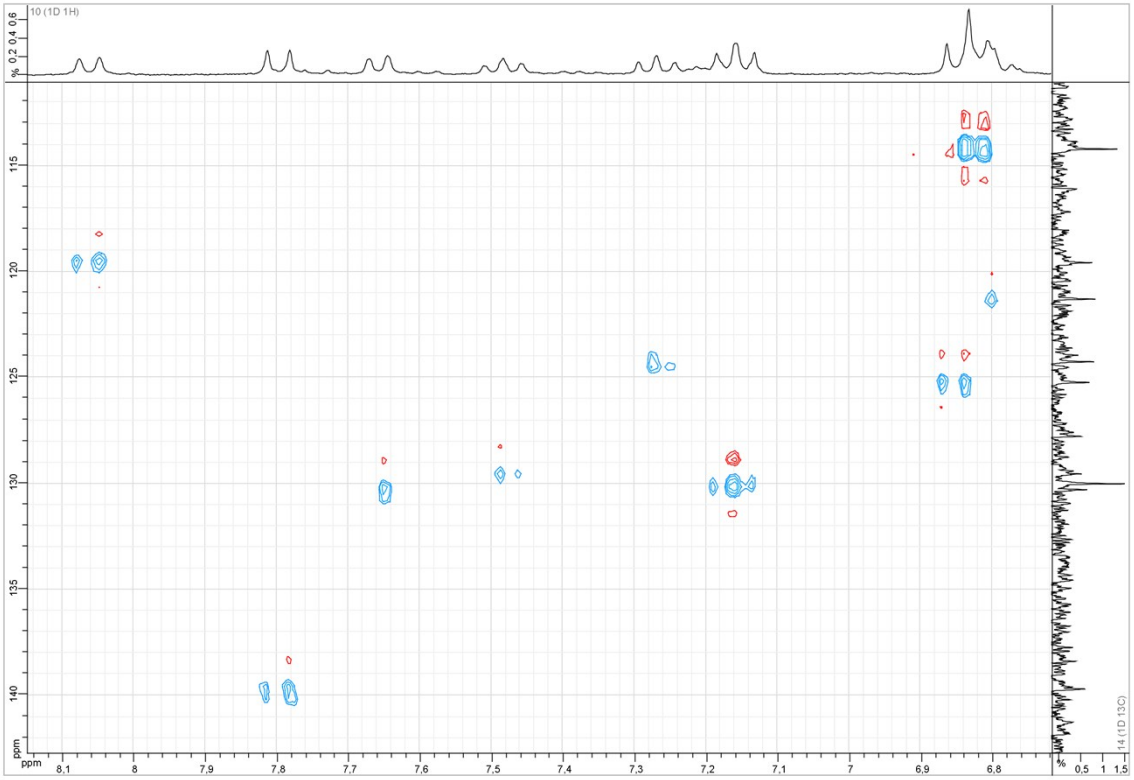
Cosy NMR spectrum of **5b** in CD_3OD



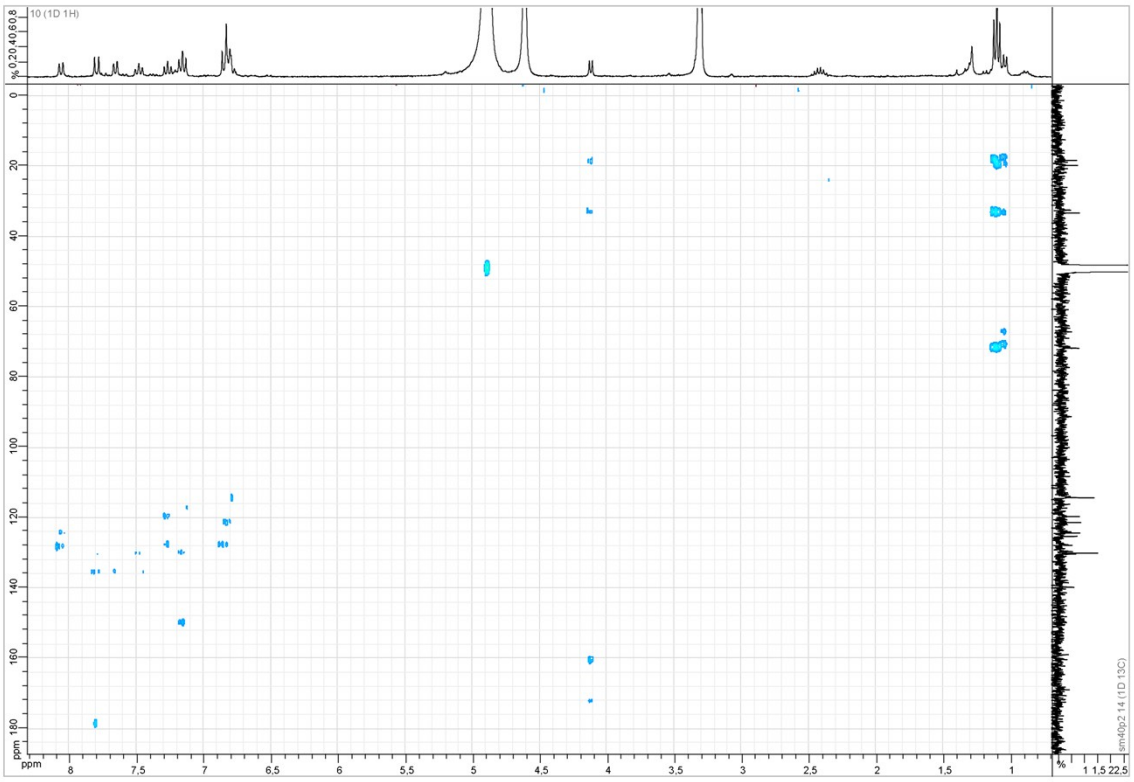
HSQC NMR spectrum of **5b** in CD_3OD



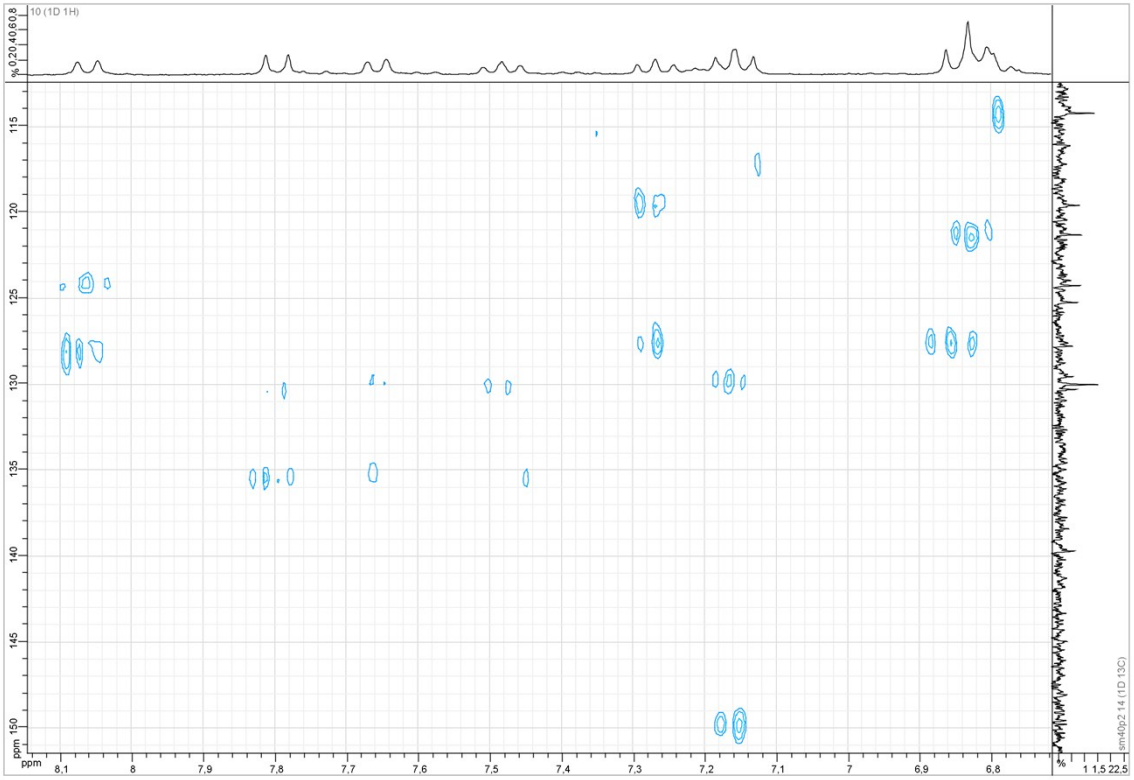
HSQC NMR spectrum of **5b** in CD_3OD (zoom)



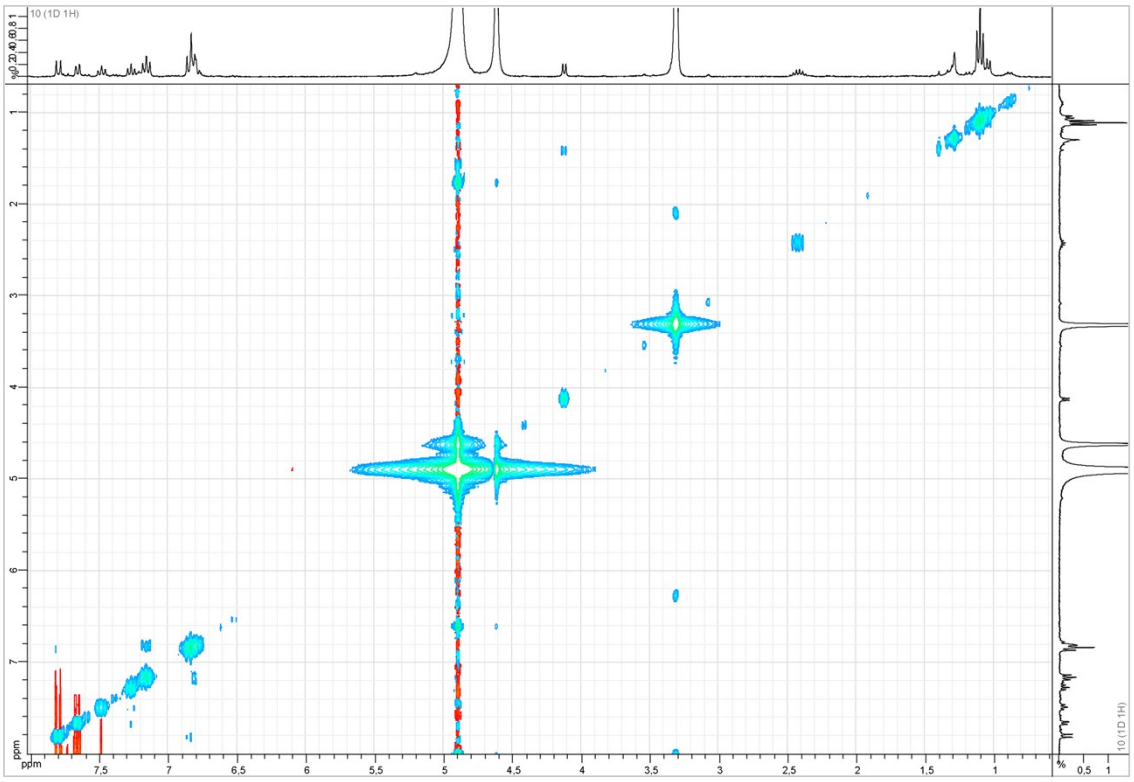
HMBC NMR spectrum of **5b** in CD_3OD



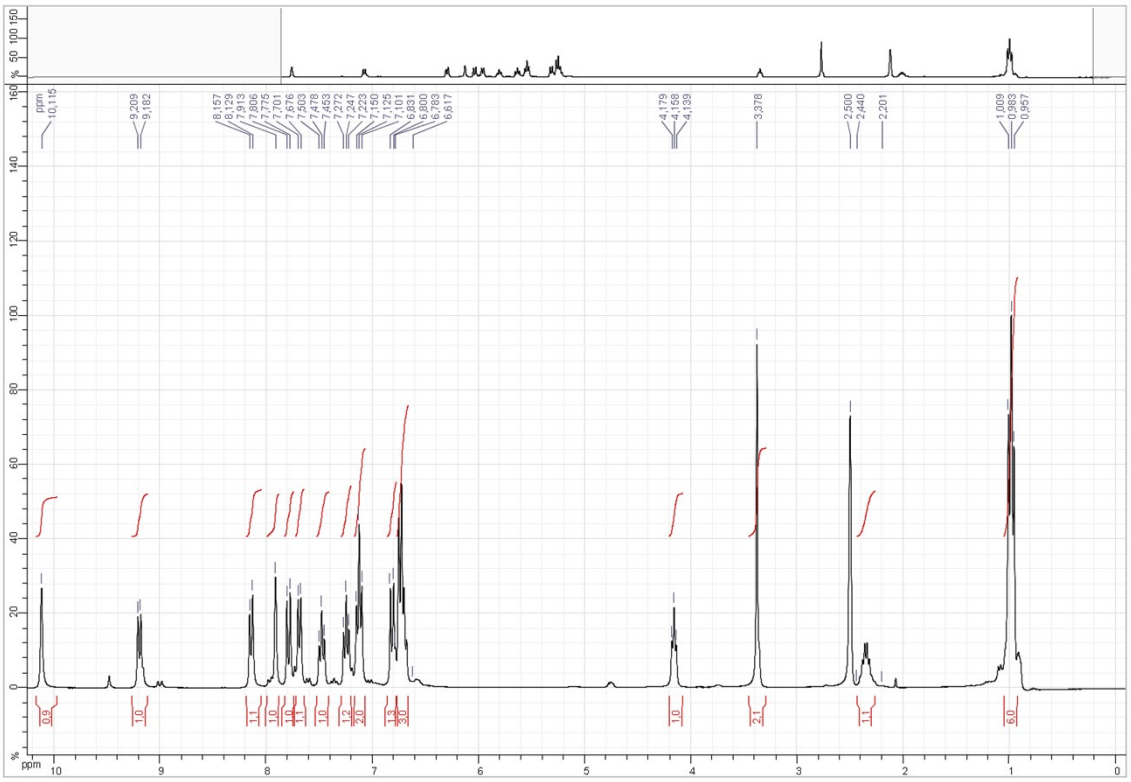
HMBC NMR spectrum of **5b** in CD_3OD (zoom)



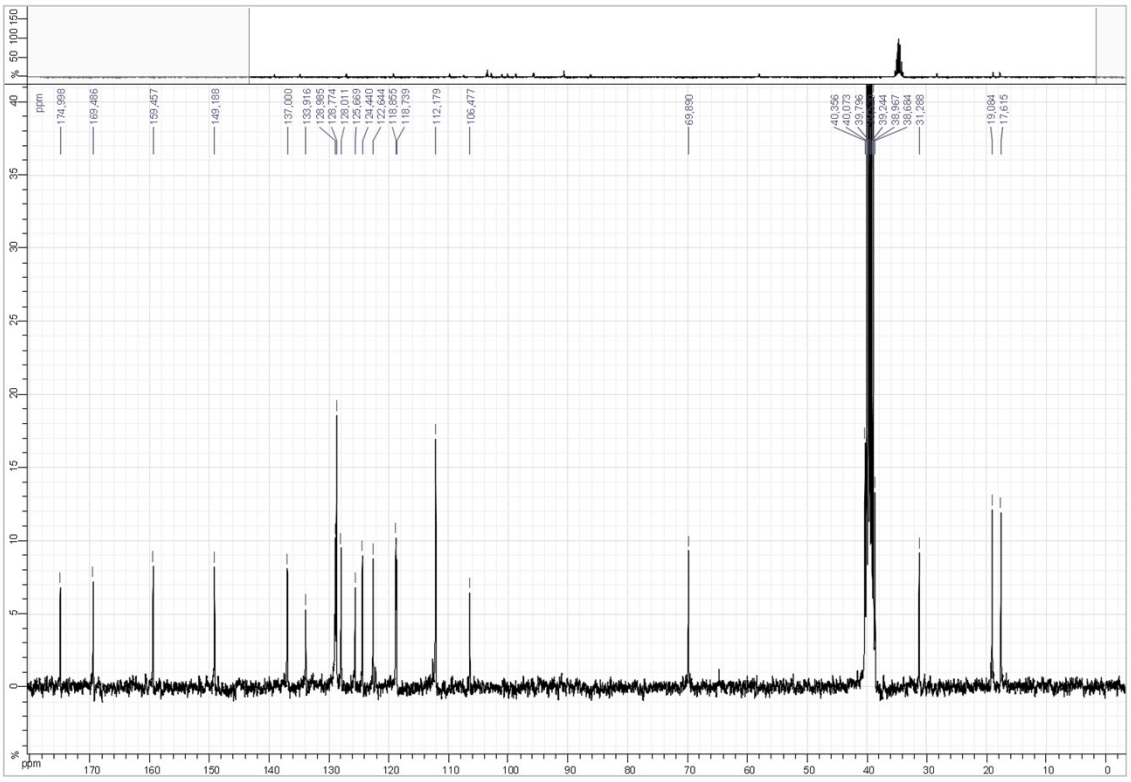
Noesy NMR spectrum of **5b** in CD_3OD



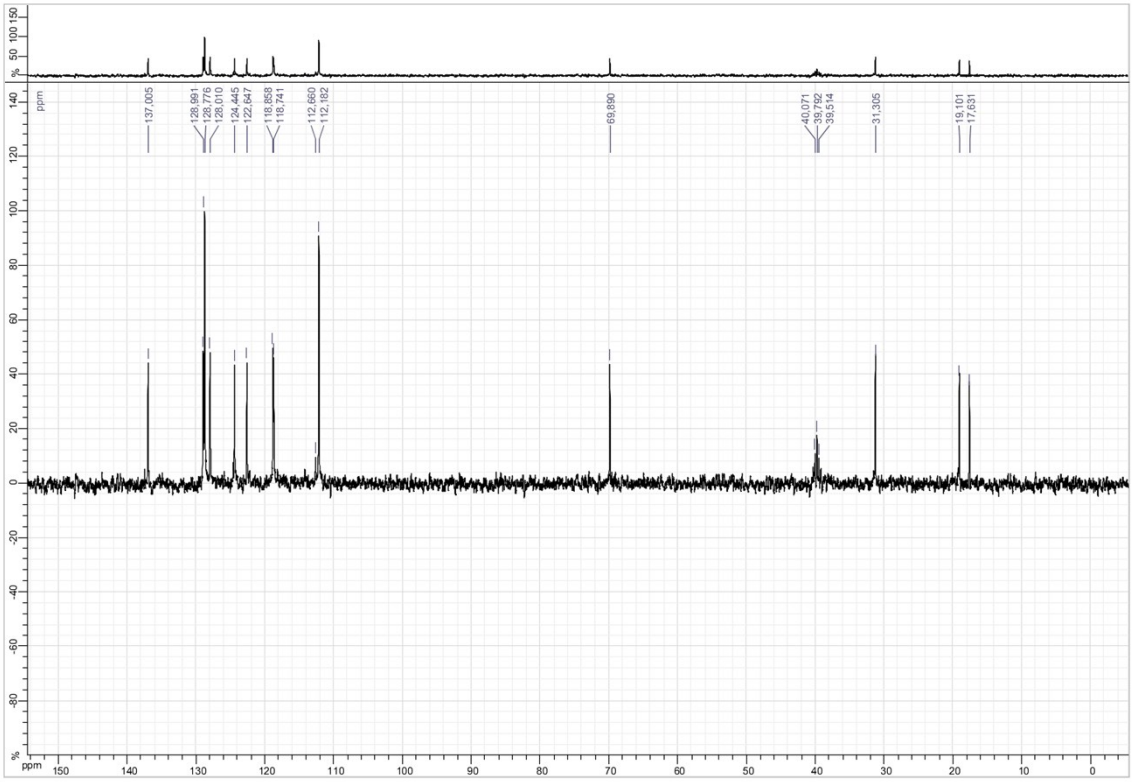
^{1}H NMR spectrum of **5b** in DMSO-d_6 at 300 MHz



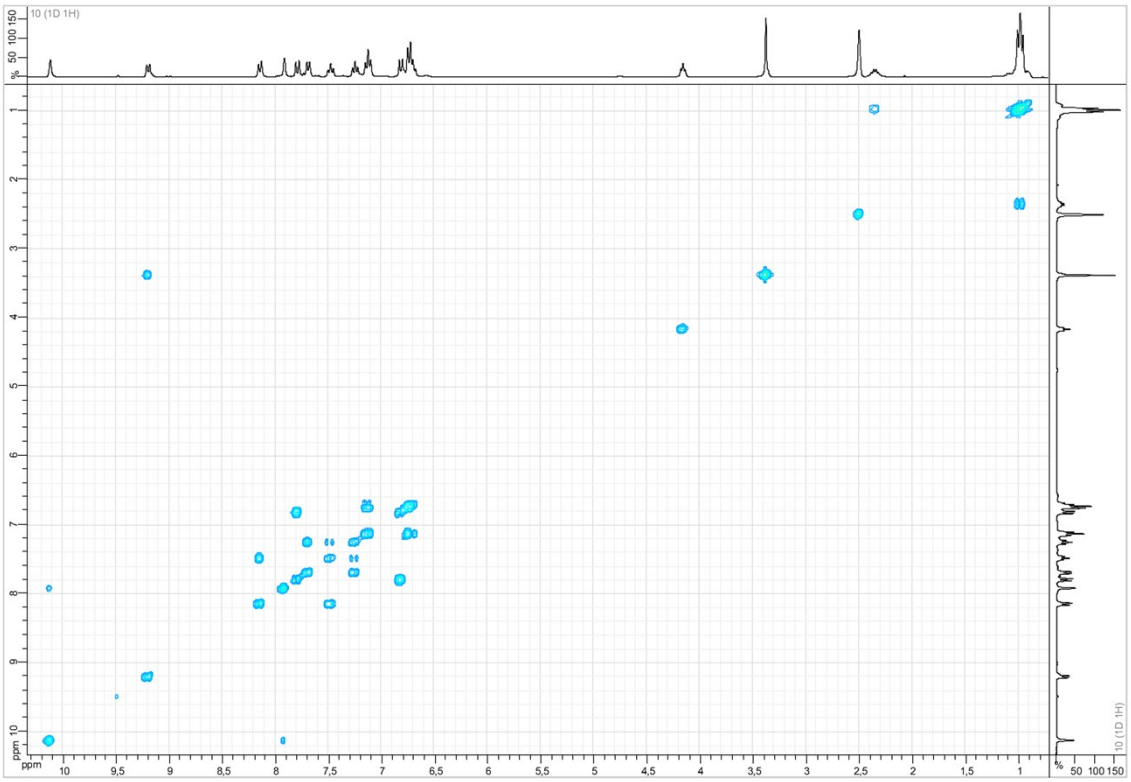
^{13}C NMR spectrum of **5b** in DMSO-d_6 at 75 MHz



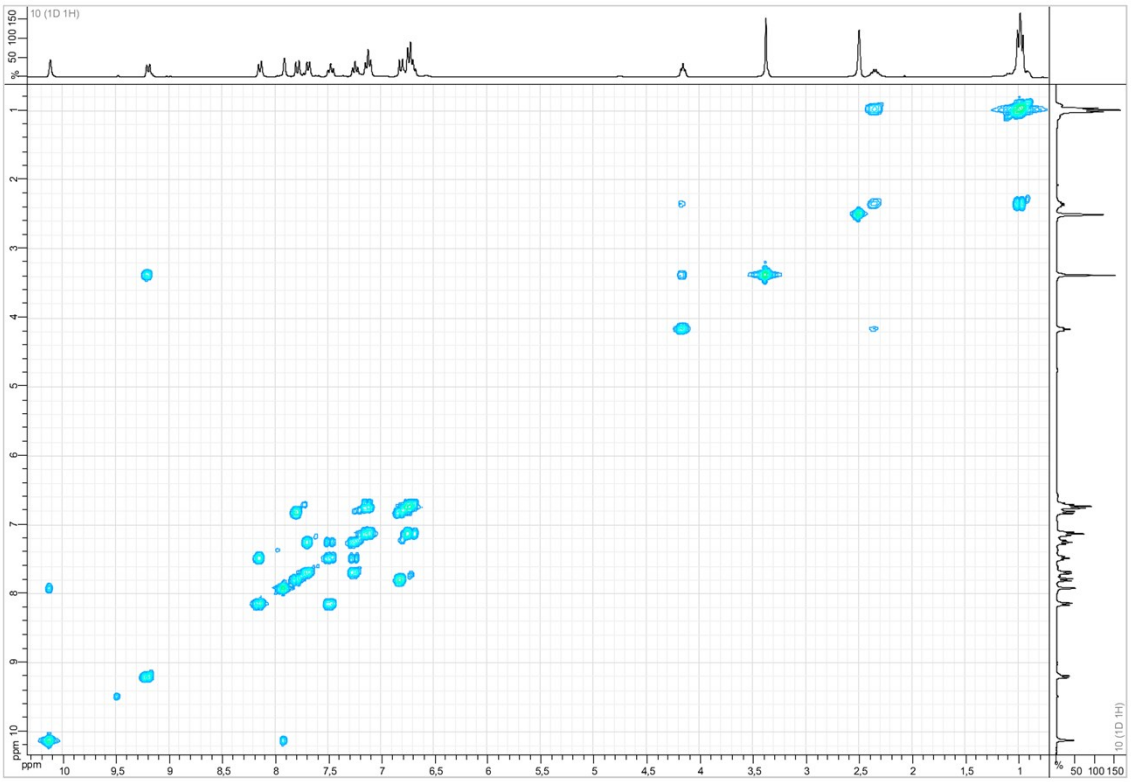
^{13}C (Dept135) NMR spectrum of **5b** in DMSO-d_6 at 75 MHz



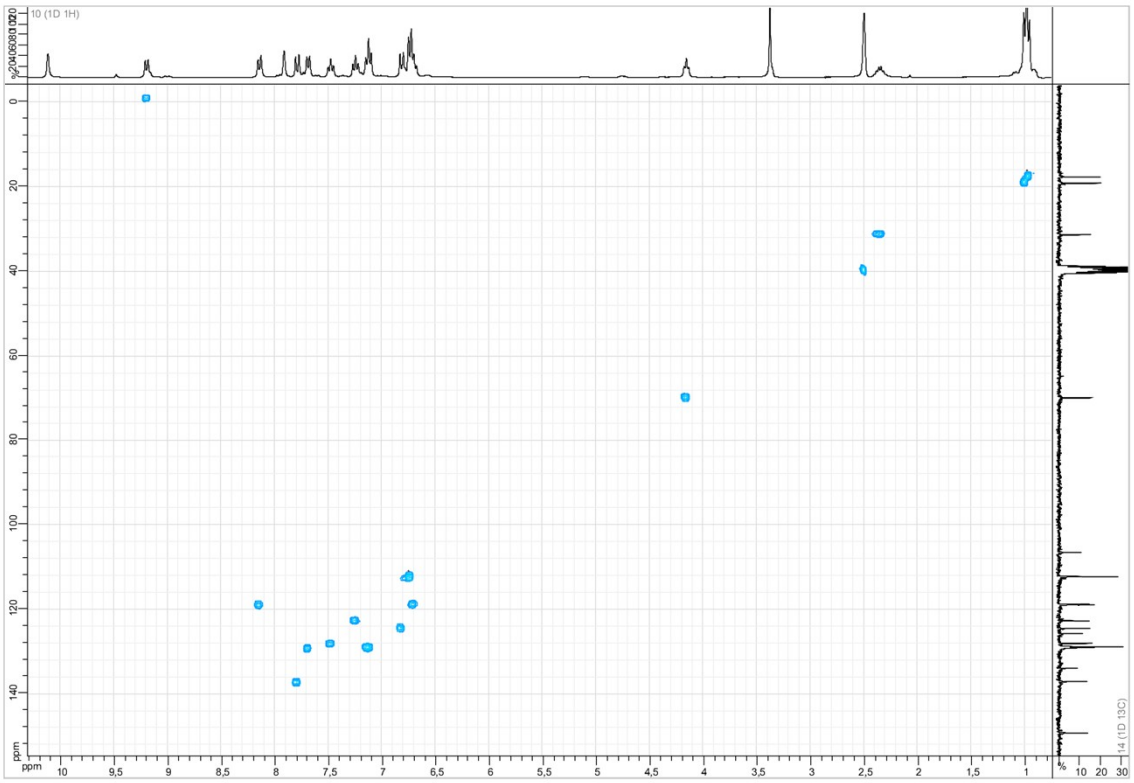
Cosy NMR spectrum of **5b** in DMSO-d_6



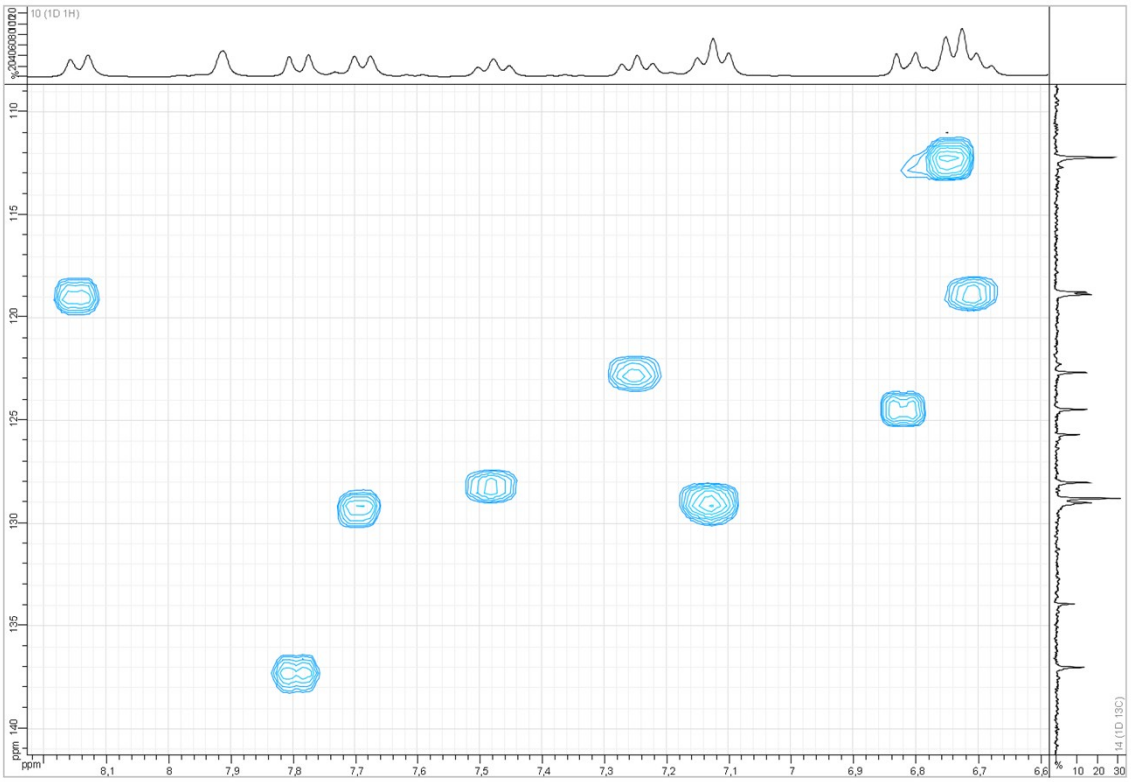
Cosy NMR spectrum of **5b** in DMSO-d_6 (deep cut)



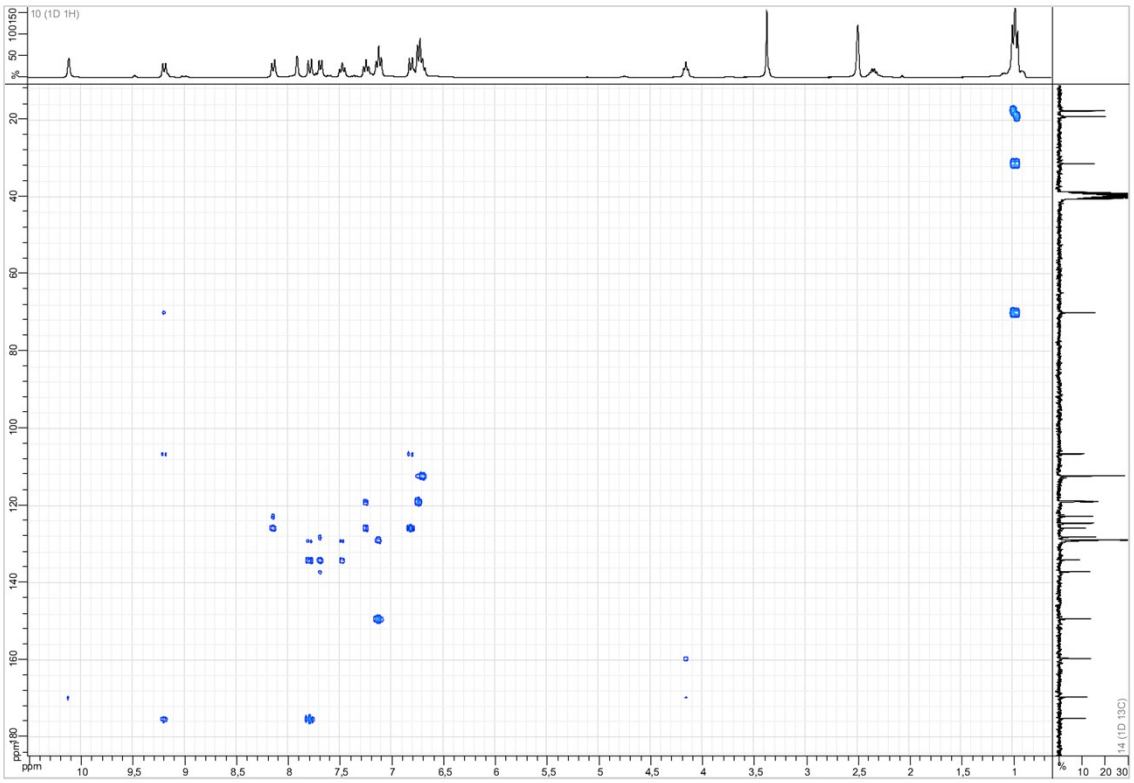
HSQC NMR spectrum of **5b** in DMSO-d_6



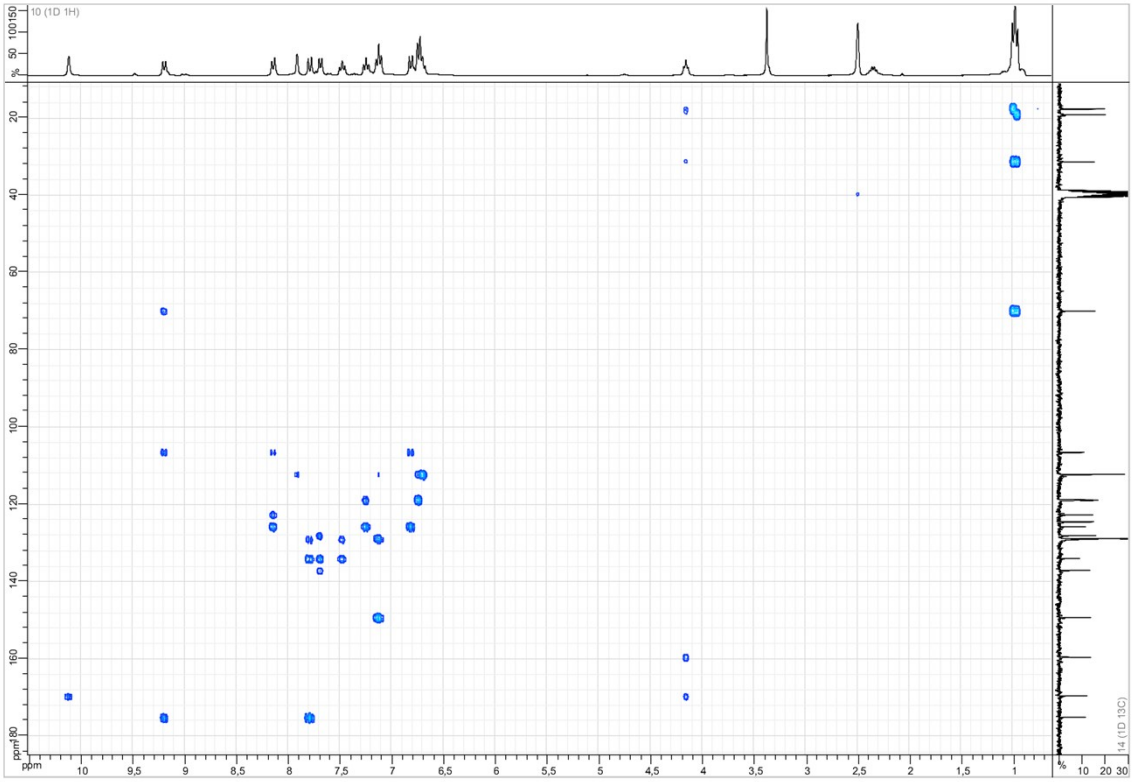
HSQC NMR spectrum of **5b** in DMSO-d_6 (zoom)



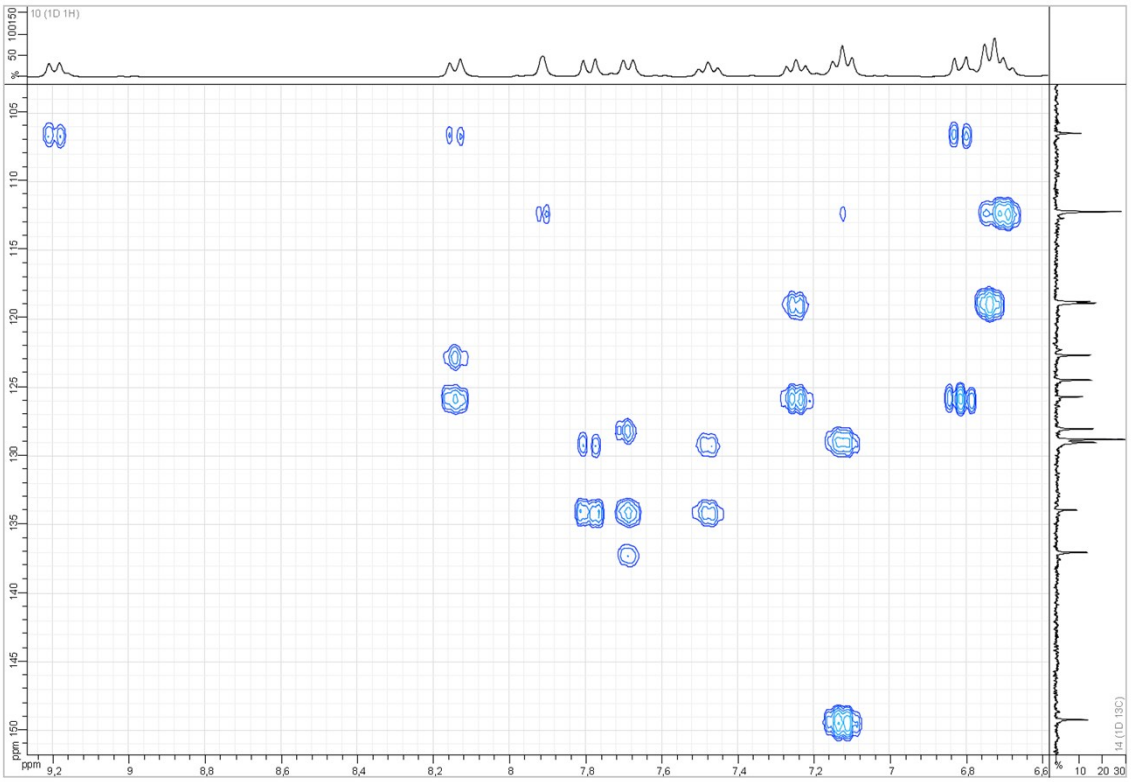
HMBC NMR spectrum of **5b** in DMSO-d_6



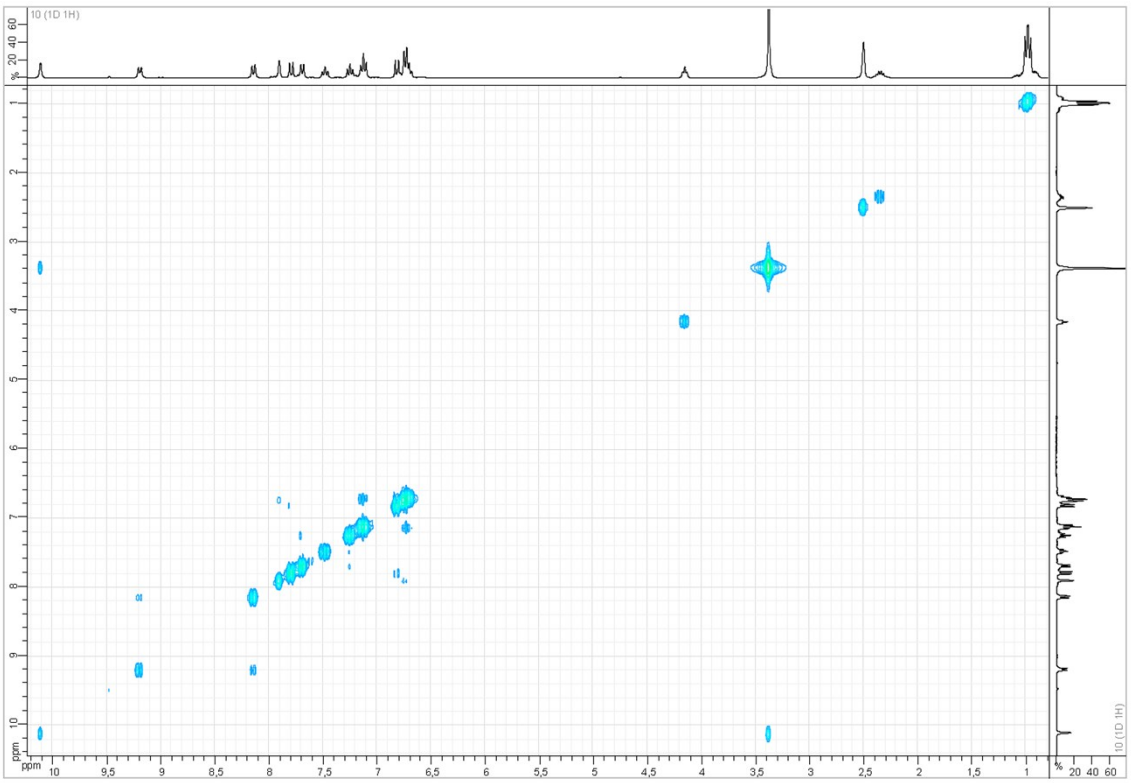
HMBC NMR spectrum of **5b** in DMSO-d_6 (deep cut)



HMBC NMR spectrum of **5b** in DMSO-d_6 (deep cut. zoom)

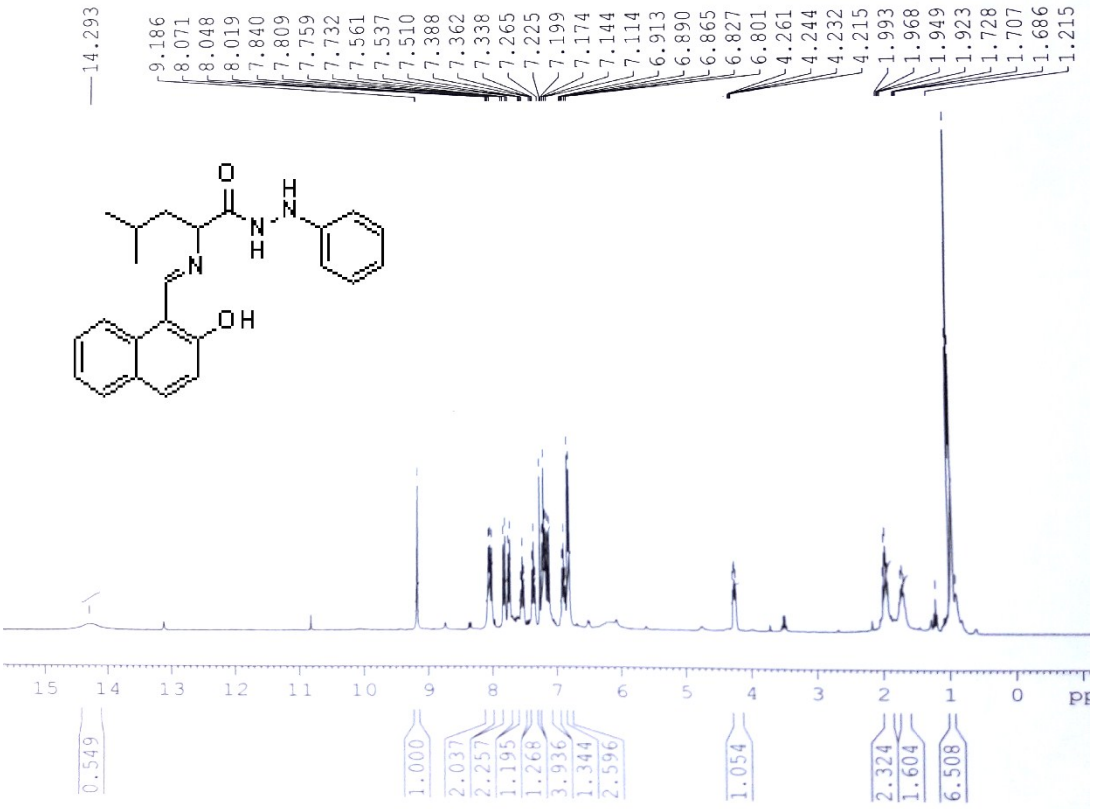


Noesy NMR spectrum of **5b** in DMSO-d_6

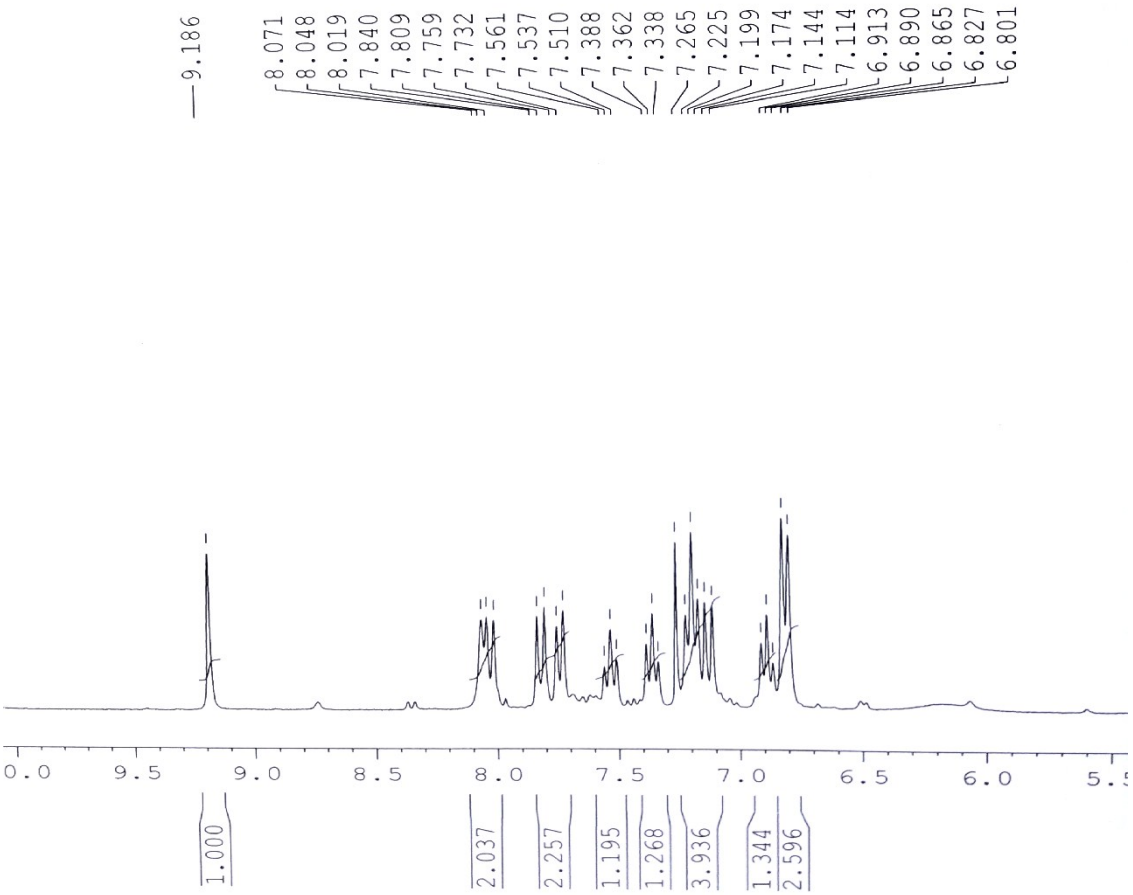


d. NMR spectra of 5c

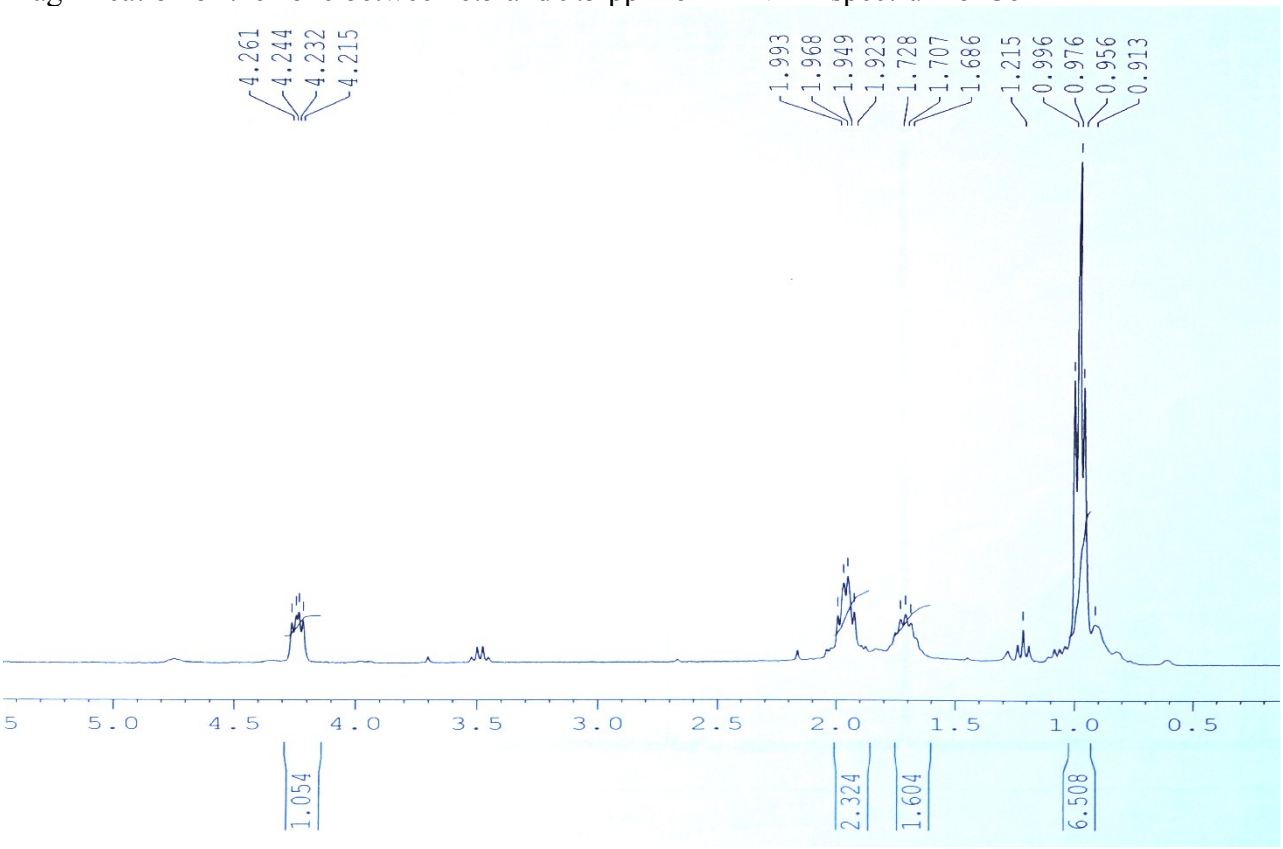
^{1}H NMR spectrum of **5c** in $CDCl_3$ at 300 MHz



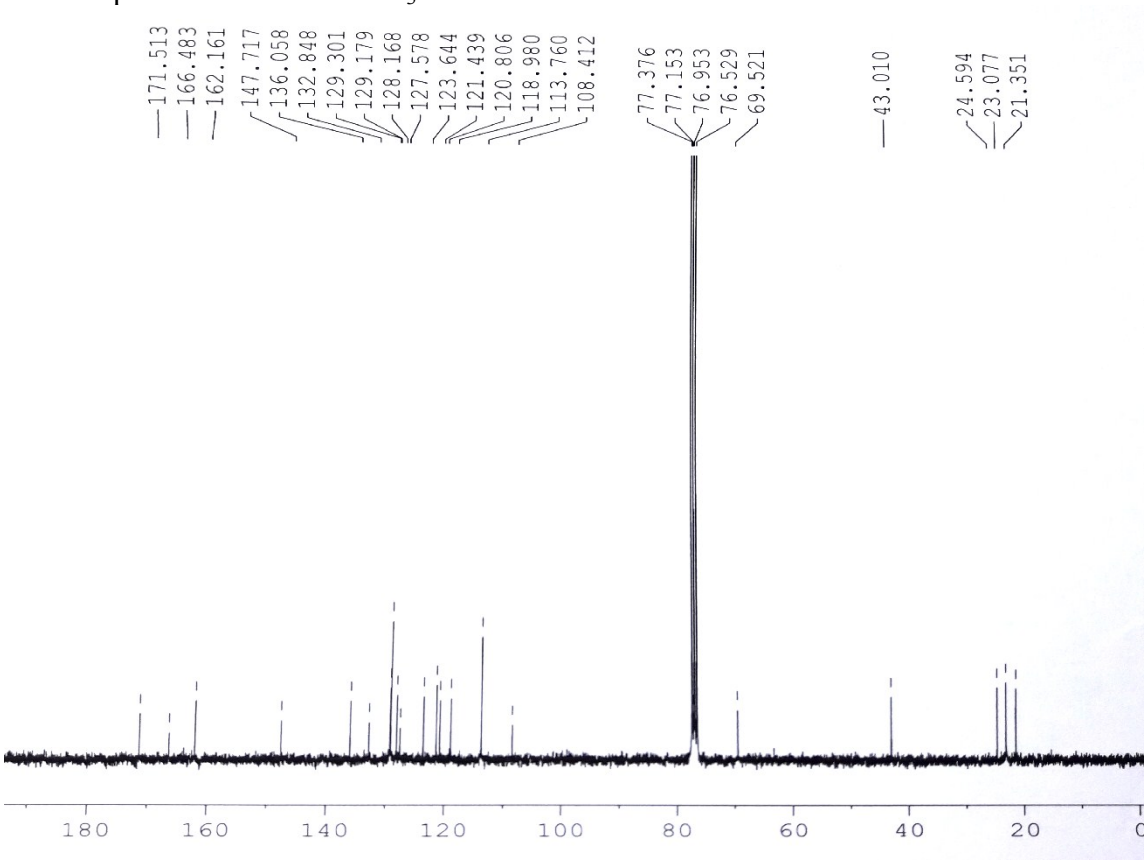
Magnification of the zone between 0.5 and 4.5 ppm of ^{1}H NMR spectrum of **5c**



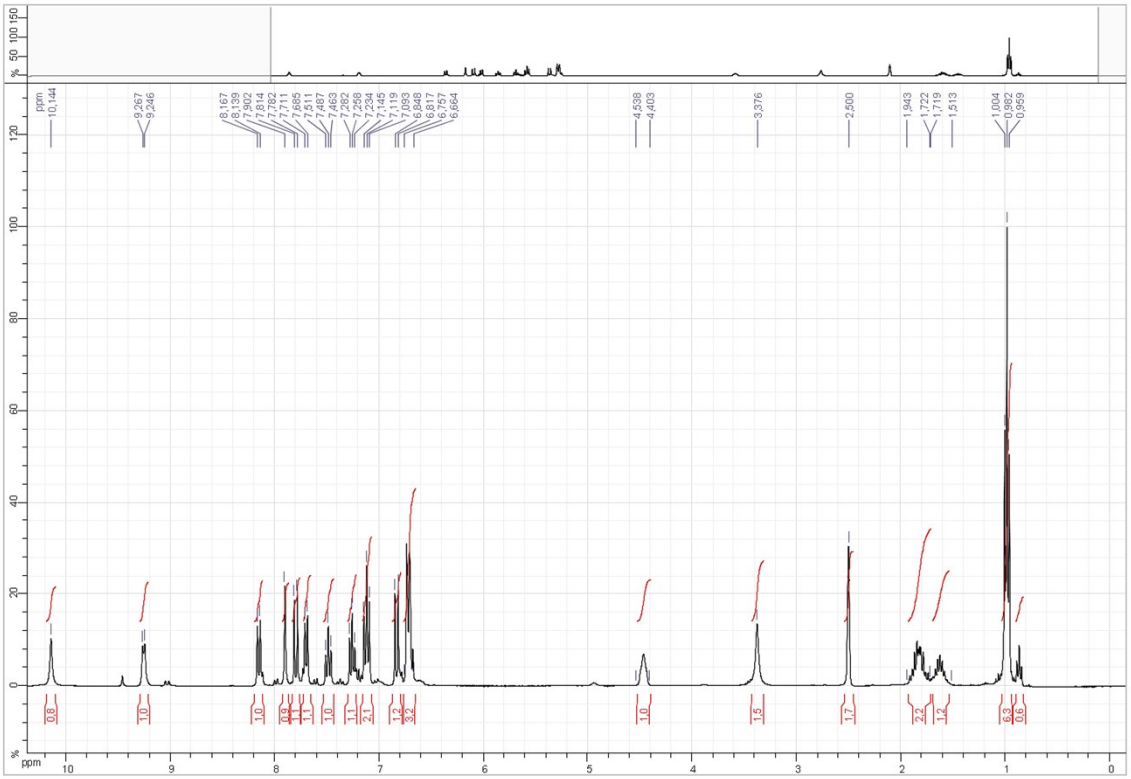
Magnification of the zone between 6.5 and 9.5 ppm of ^{1}H NMR spectrum of **5c**



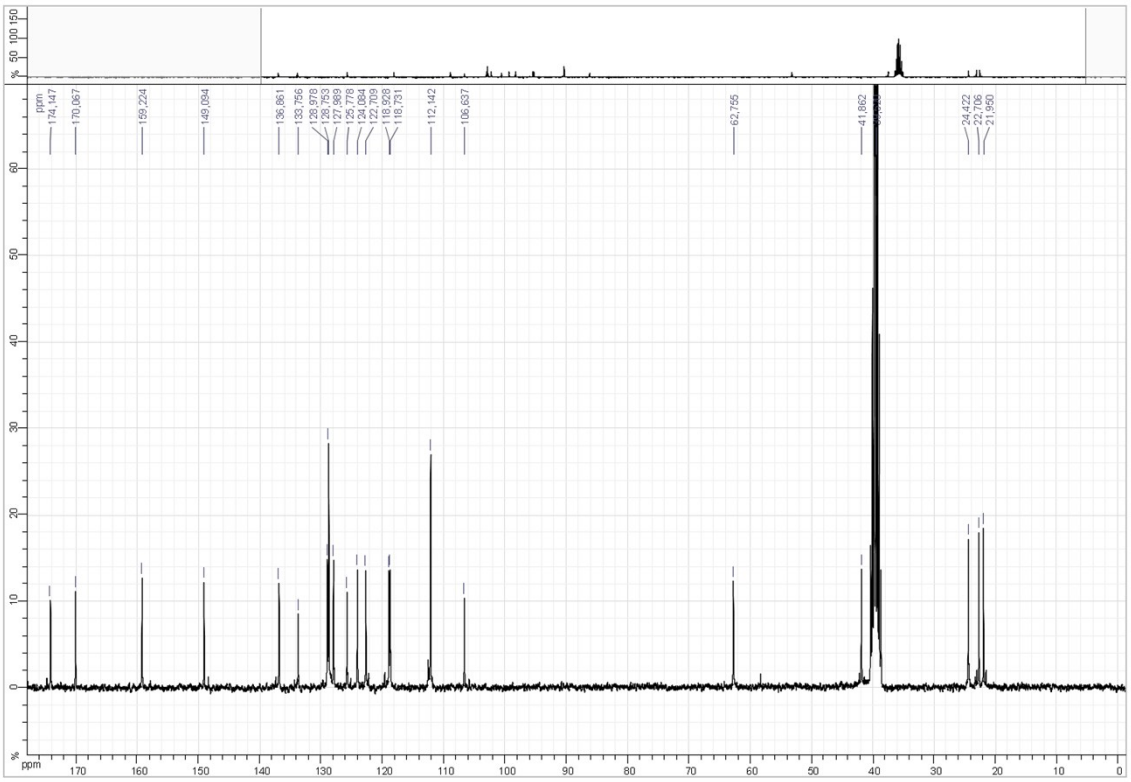
^{13}C NMR spectrum of **5c** in $CDCl_3$ at 75 MHz



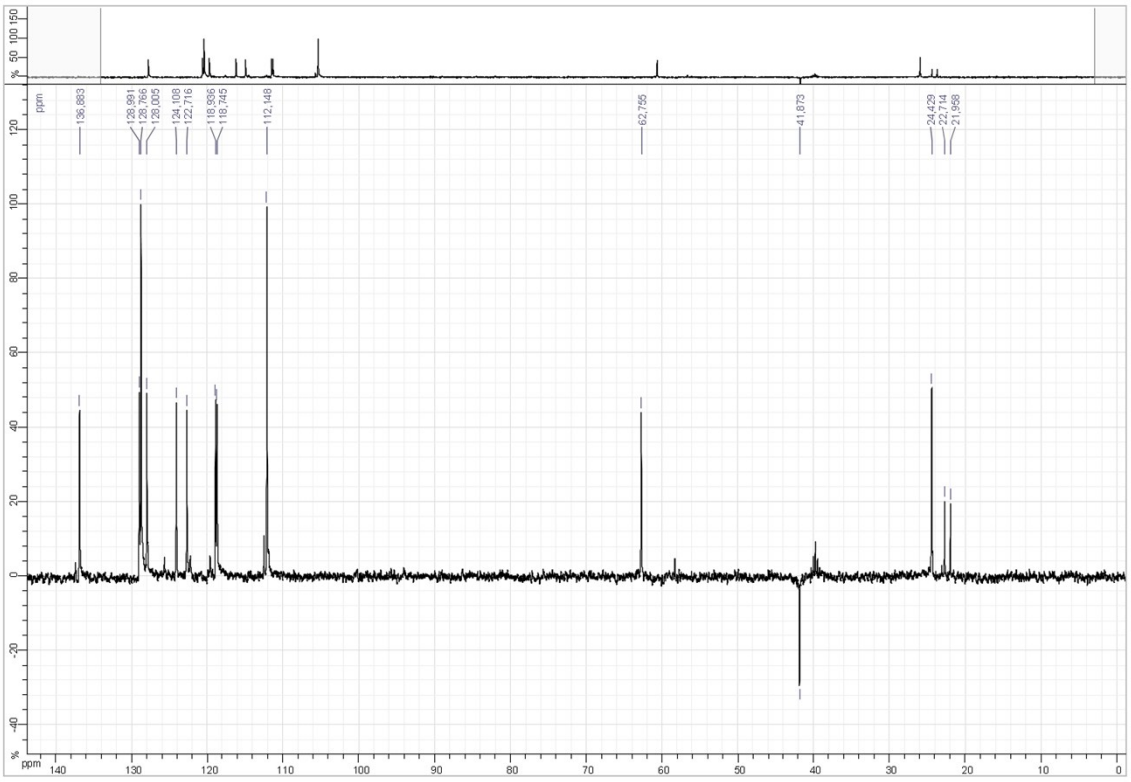
^{1}H NMR spectrum of **5c** in DMSO-d_6 at 300 MHz



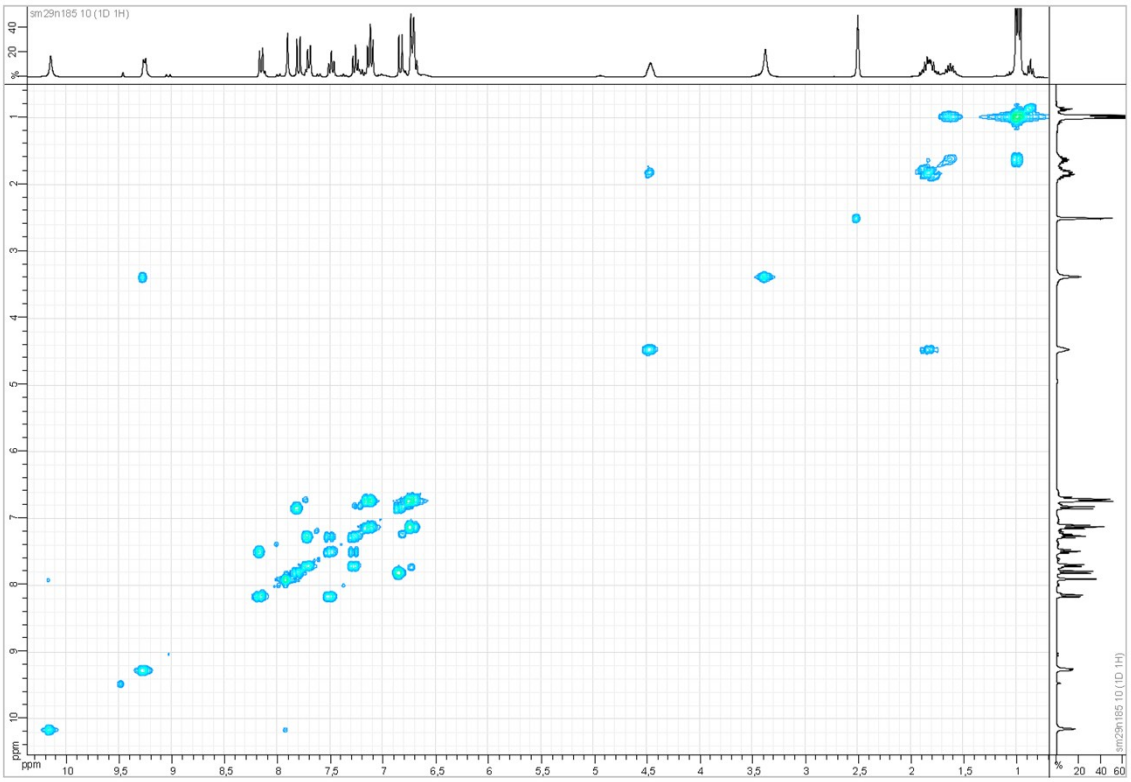
^{13}C NMR spectrum of **5c** in DMSO-d_6 at 75 MHz



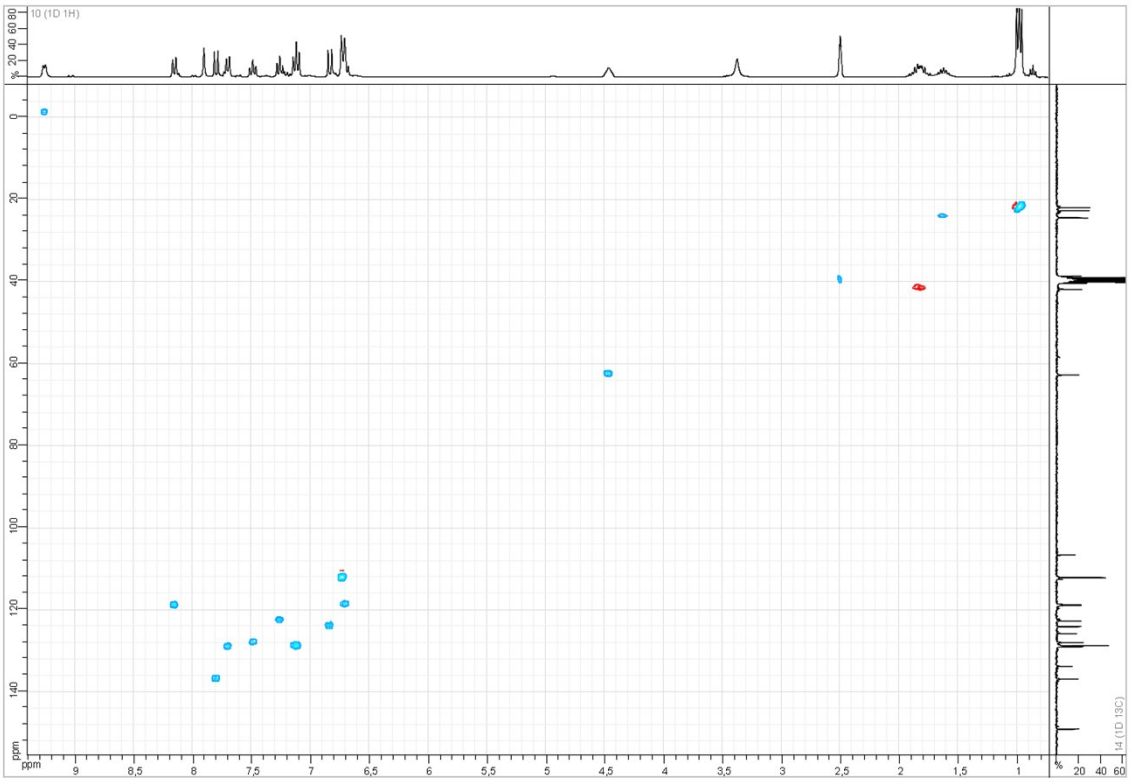
^{13}C (Dept135) NMR spectrum of **5c** in DMSO-d_6 at 75 MHz



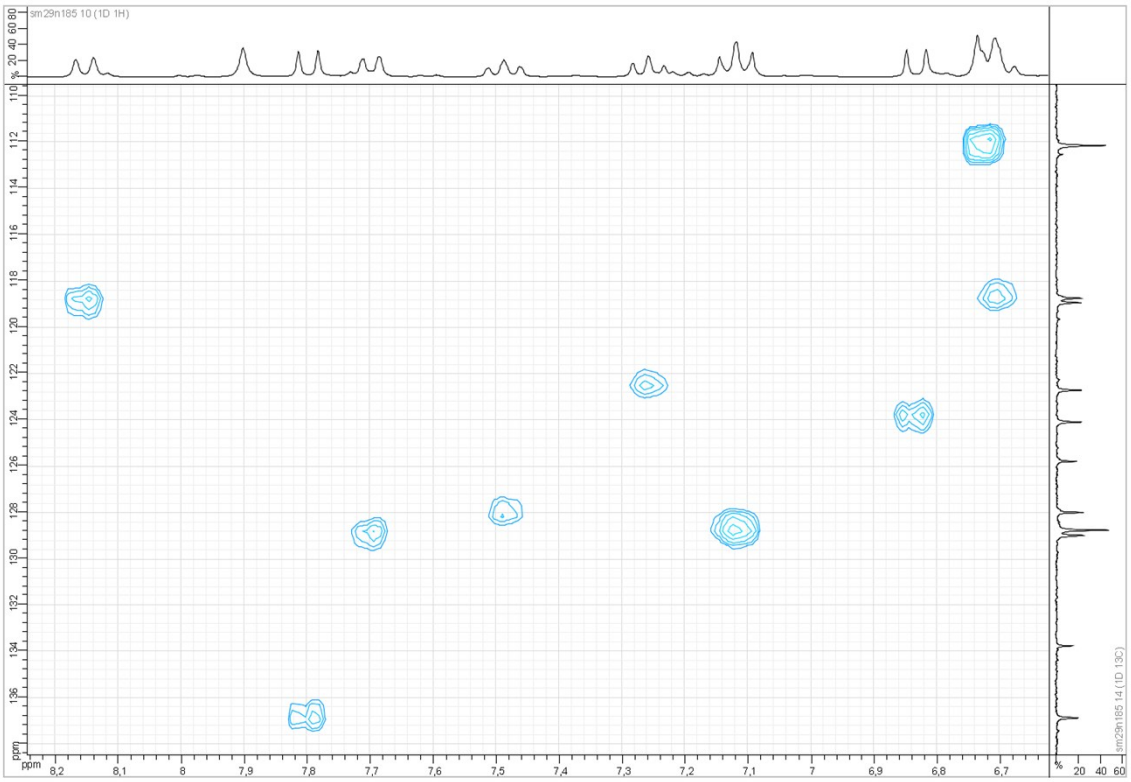
Cosy NMR spectrum of **5c** in DMSO-d_6



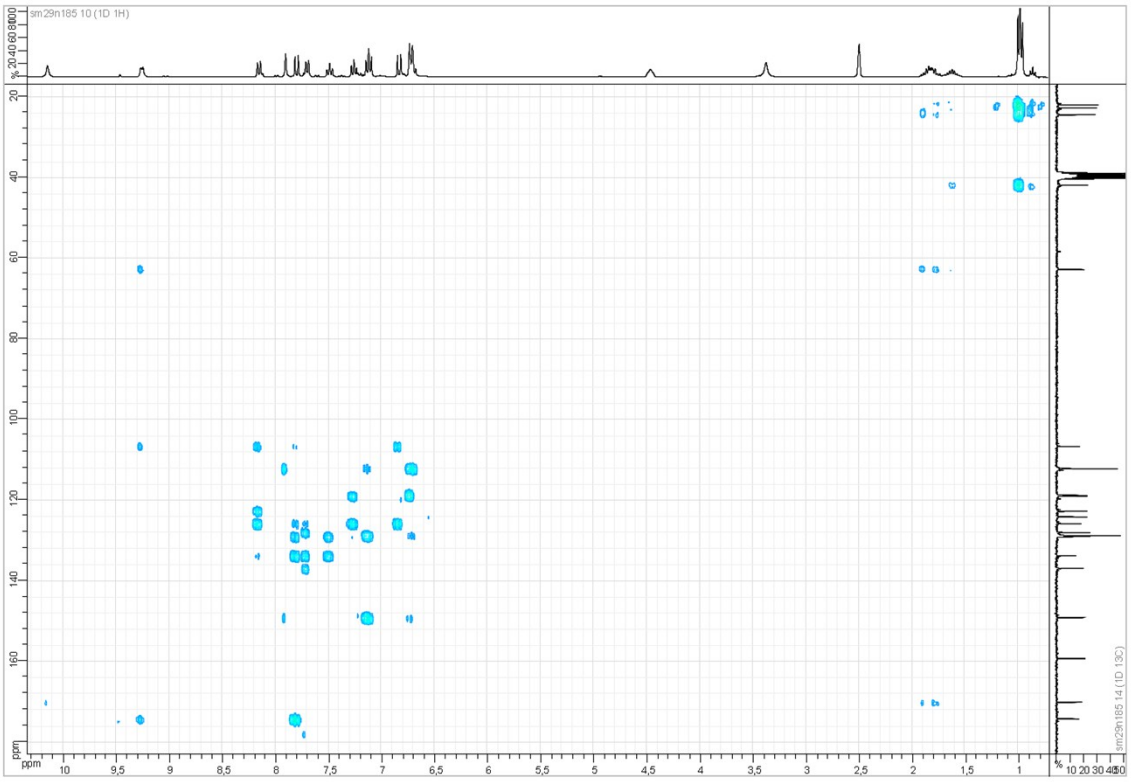
HSQC NMR spectrum of **5c** in DMSO-d_6



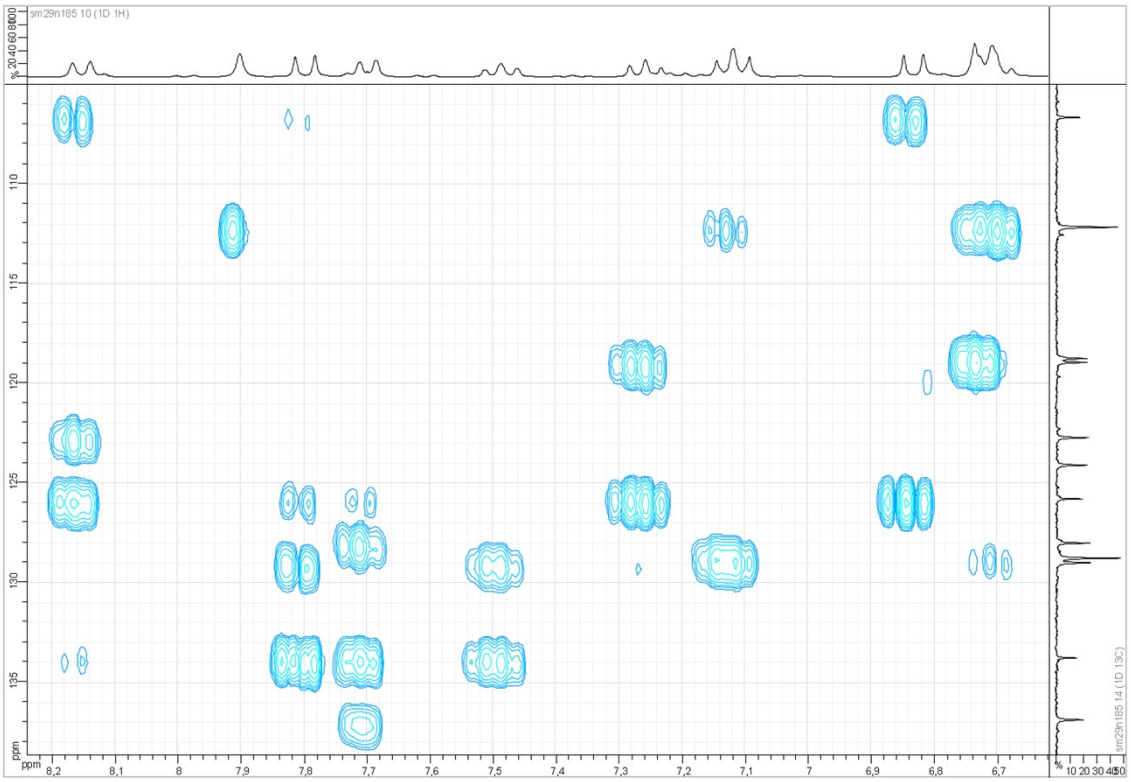
HSQC NMR spectrum of **5c** in DMSO-d_6 (zoom)



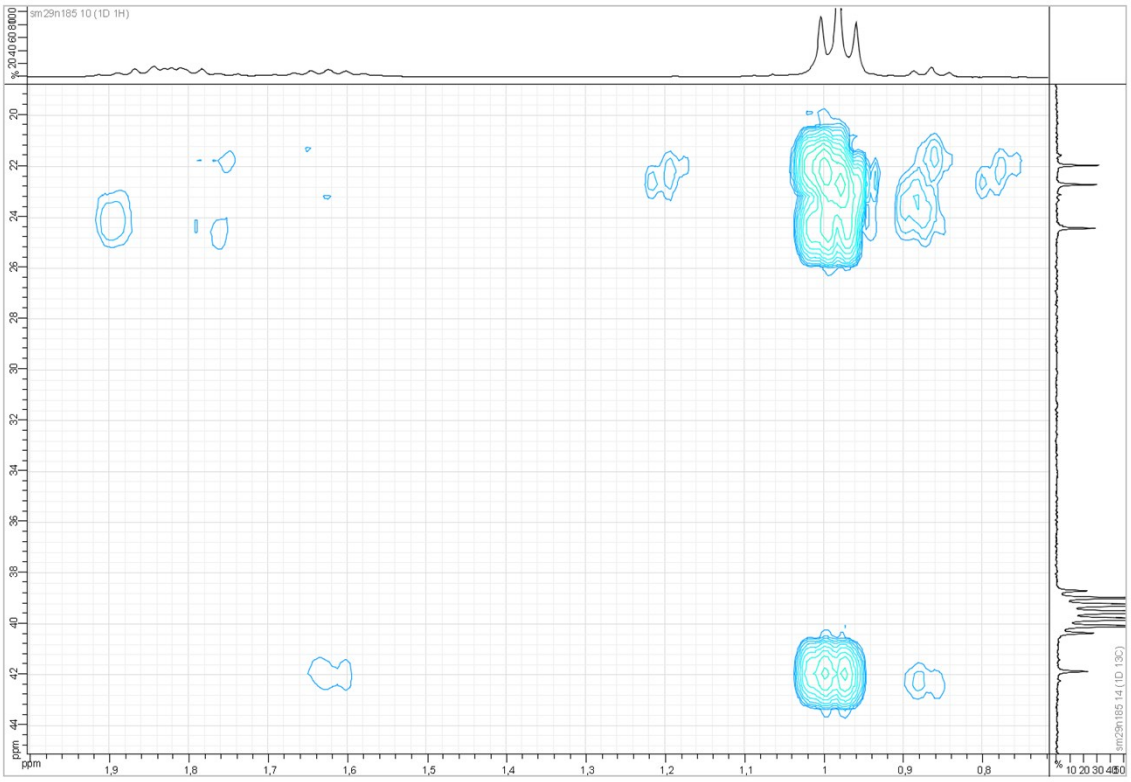
HMBC NMR spectrum of **5c** in DMSO-d_6



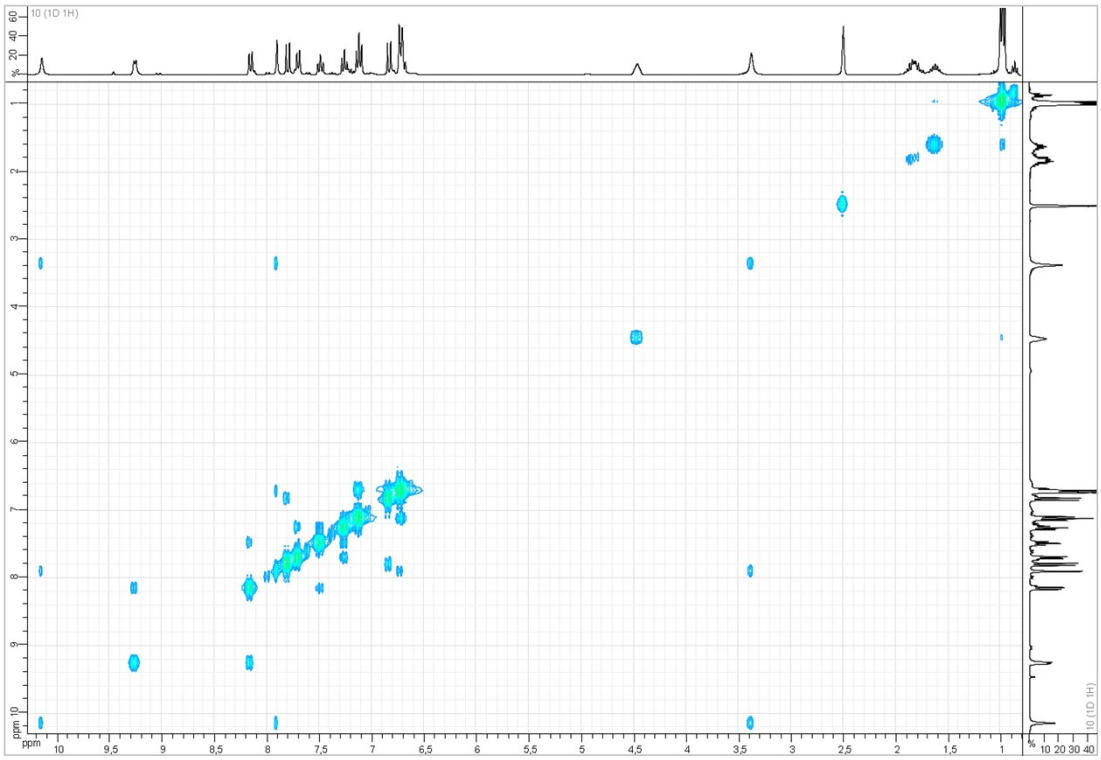
HMBC NMR spectrum of **5c** in DMSO-d_6 (1st zoom)



HMBC NMR spectrum of **5c** in DMSO-d_6 (2nd zoom)

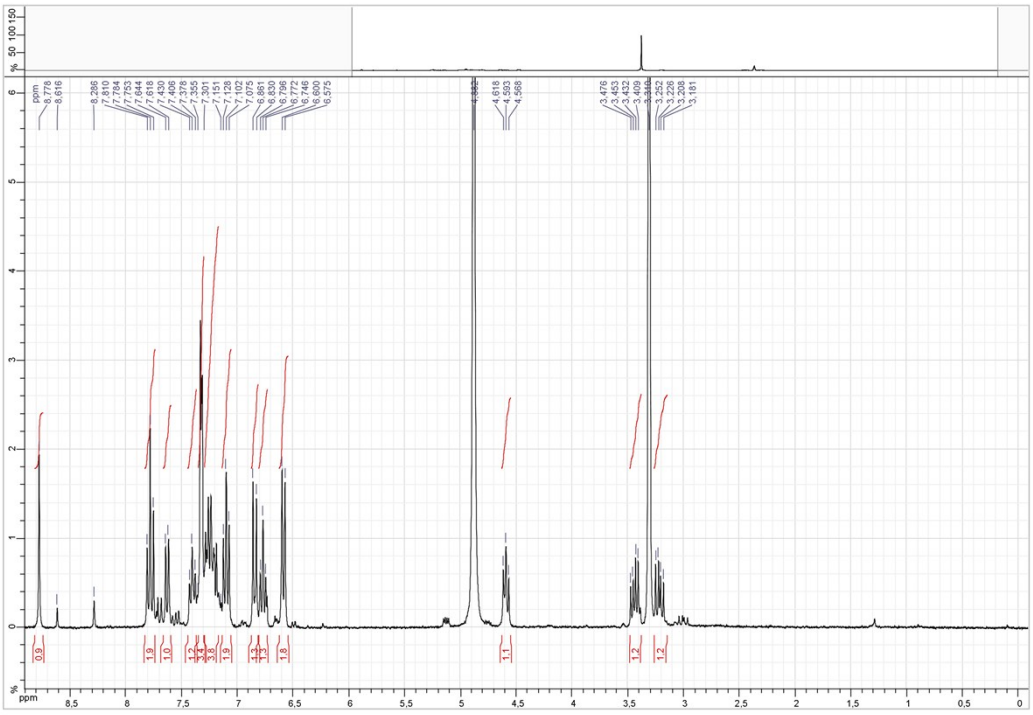


Noesy NMR spectrum of **5c** in DMSO-d_6

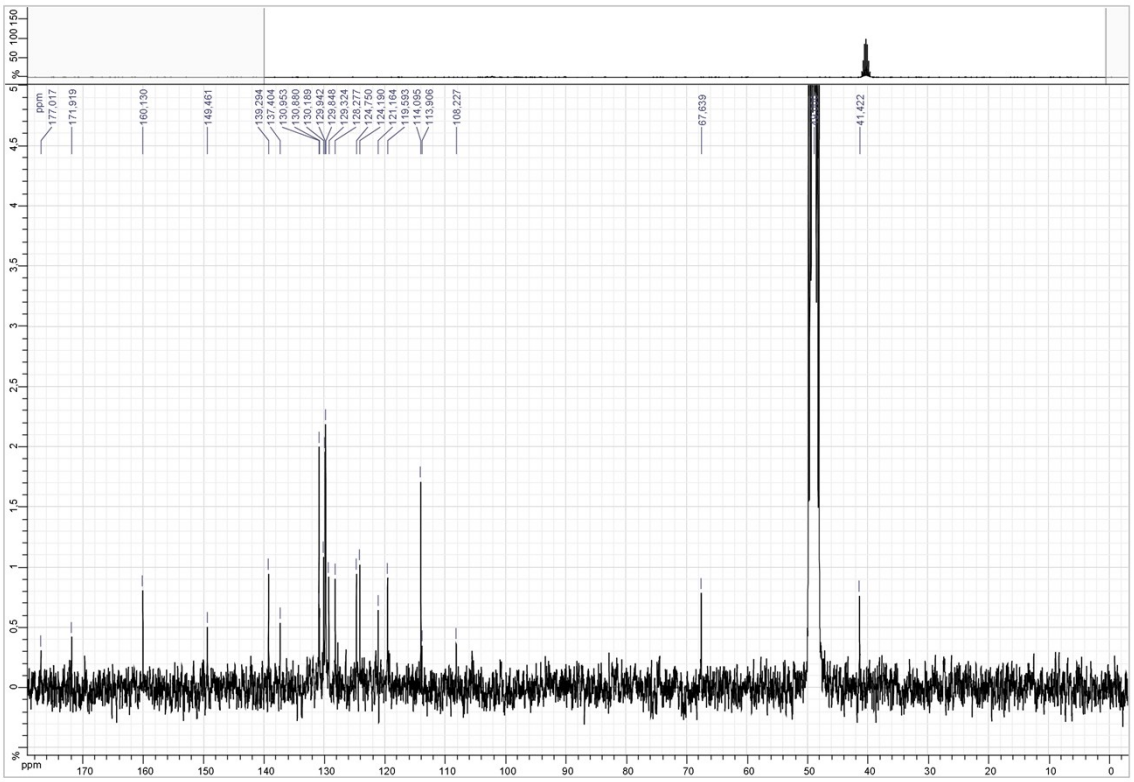


e. NMR spectra of 5d

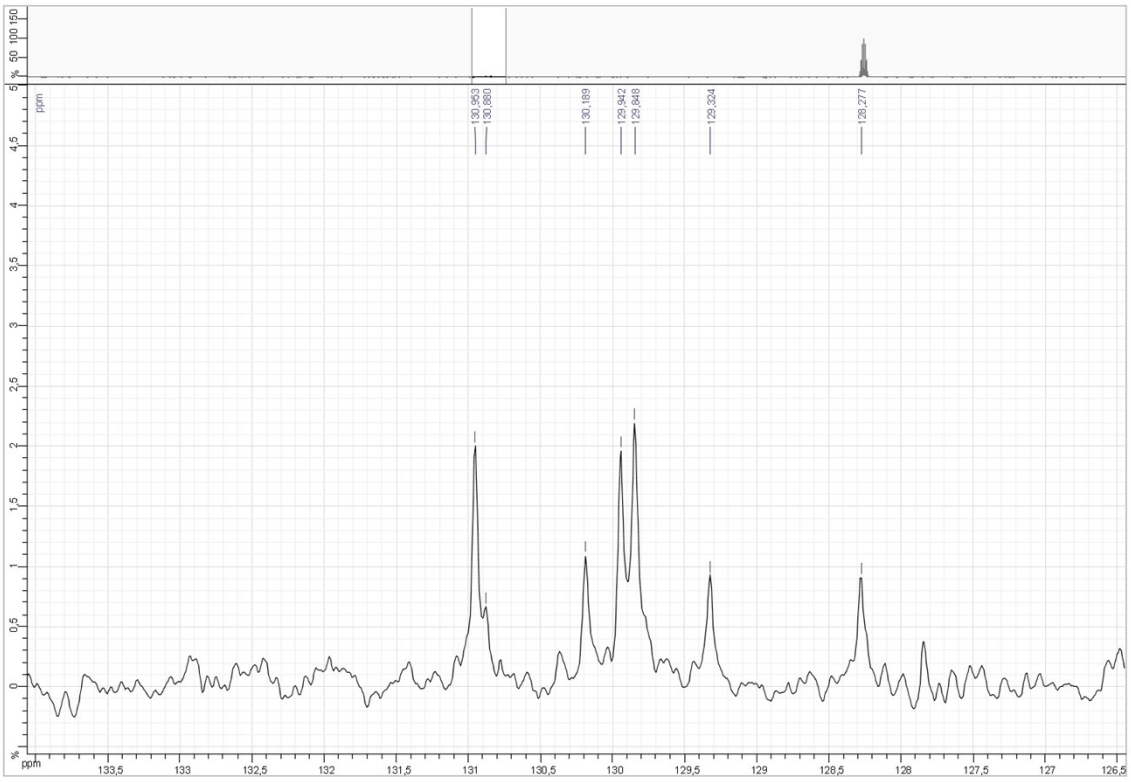
^{1}H NMR spectrum of **5d** in CD_3OD at 300 MHz



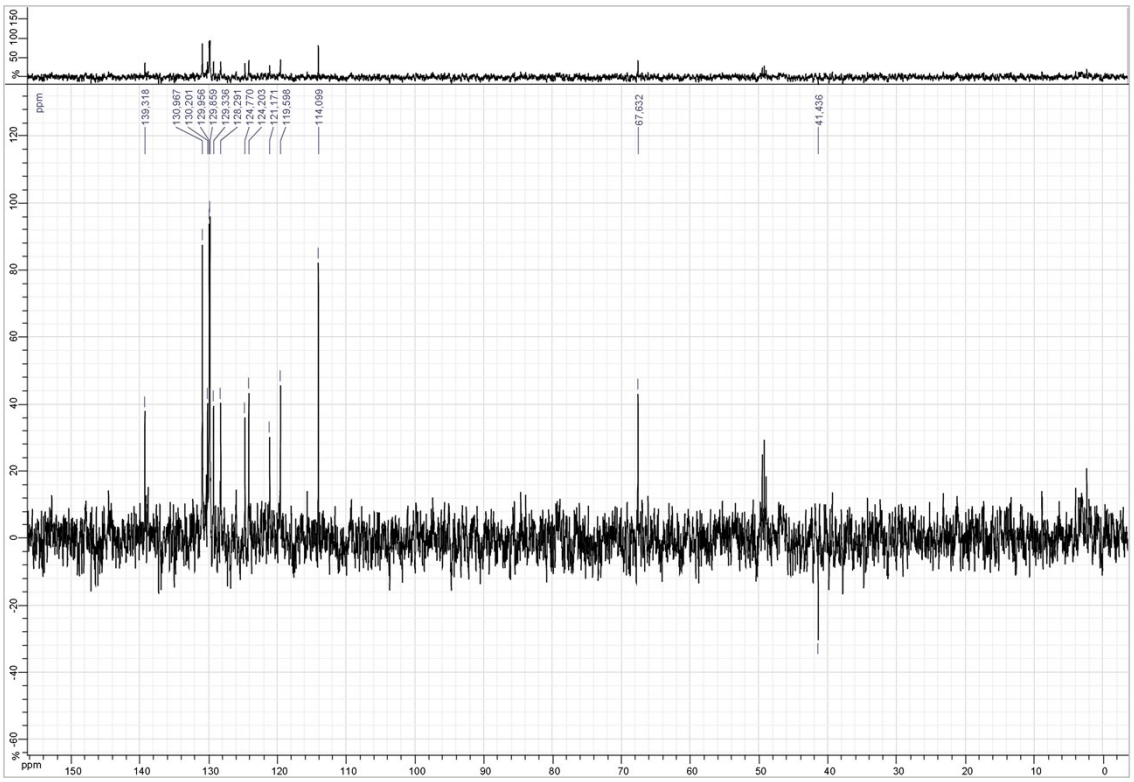
^{13}C NMR spectrum of **5d** in CD_3OD at 75 MHz



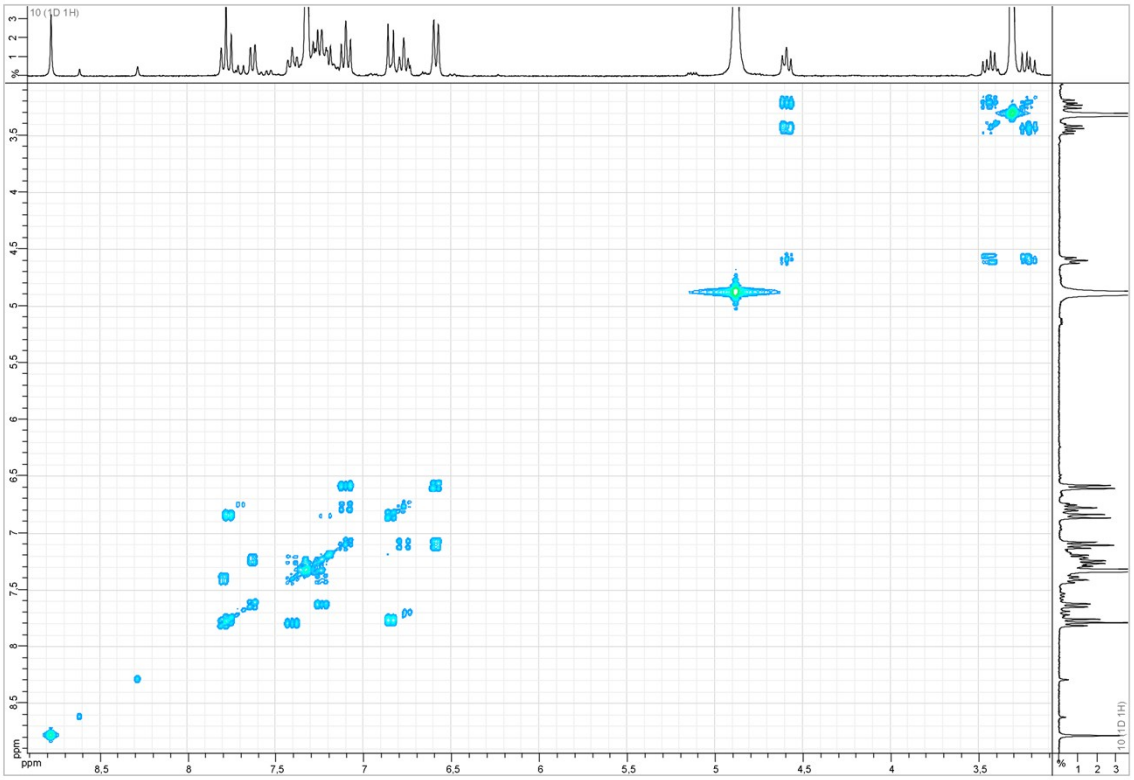
^{13}C NMR spectrum of **5d** in CD_3OD at 75 MHz (zoom)



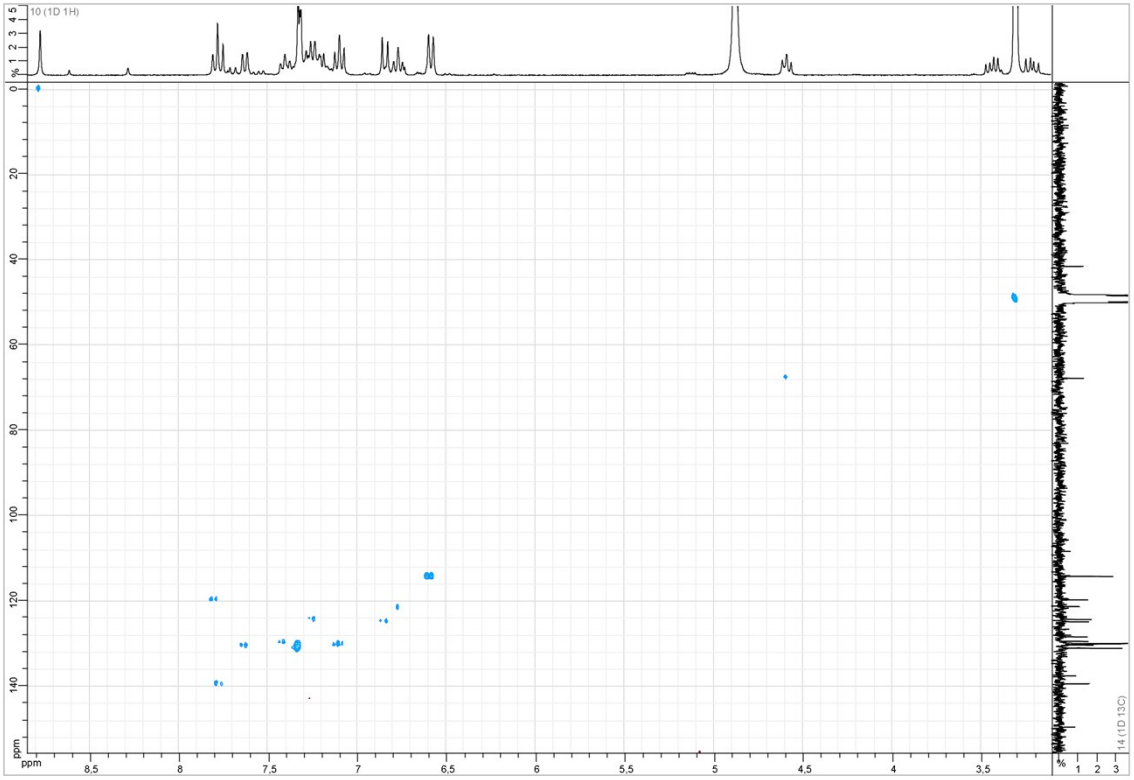
^{13}C (Dept135) NMR spectrum of **5d** in CD_3OD at 75 MHz



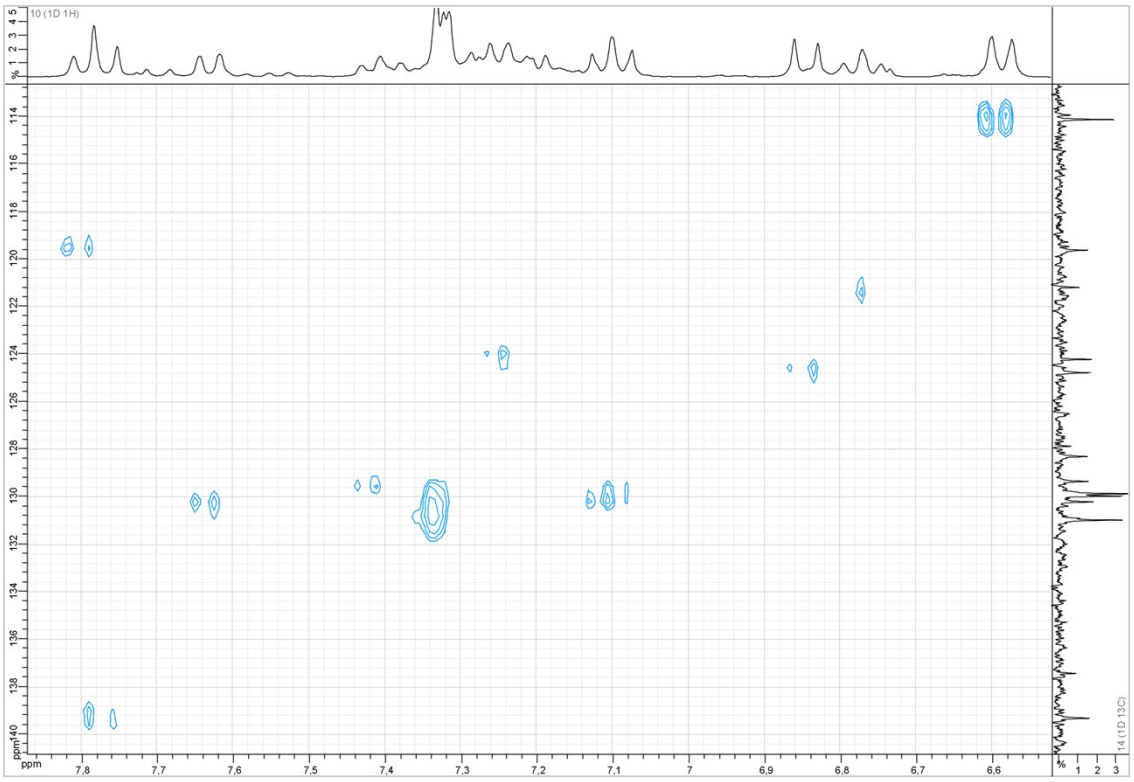
Cosy NMR spectrum of **5d** in CD_3OD



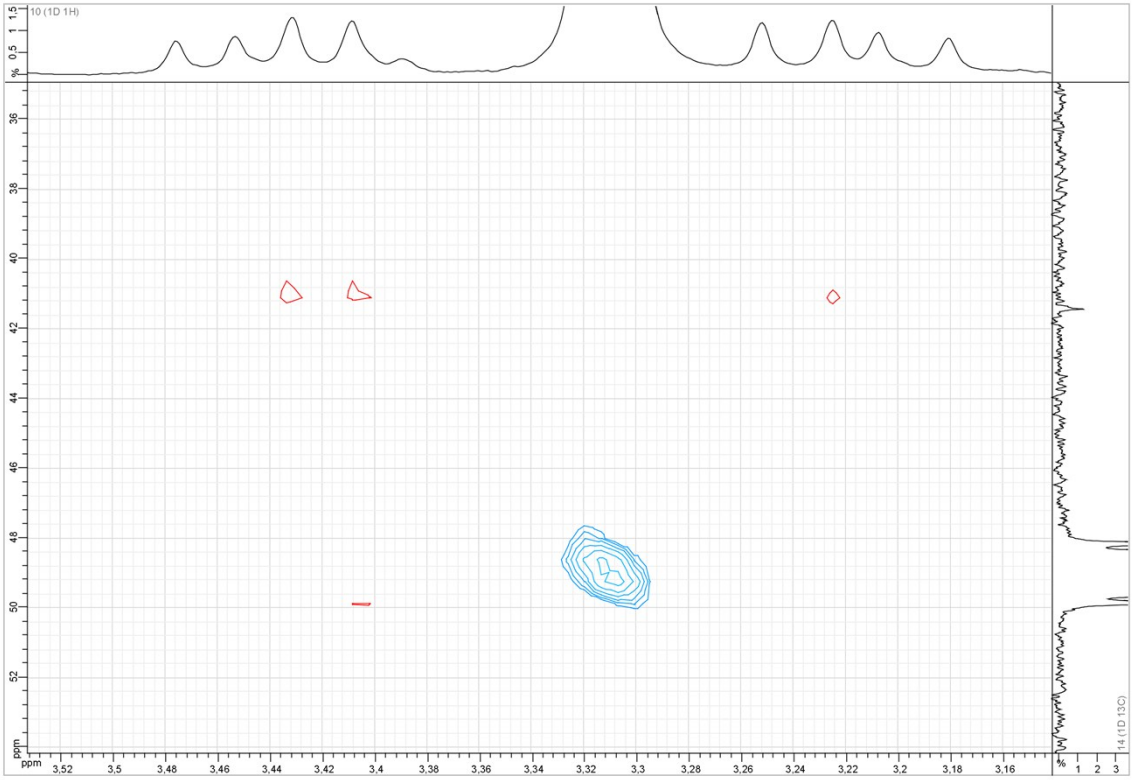
HSQC NMR spectrum of **5d** in CD_3OD



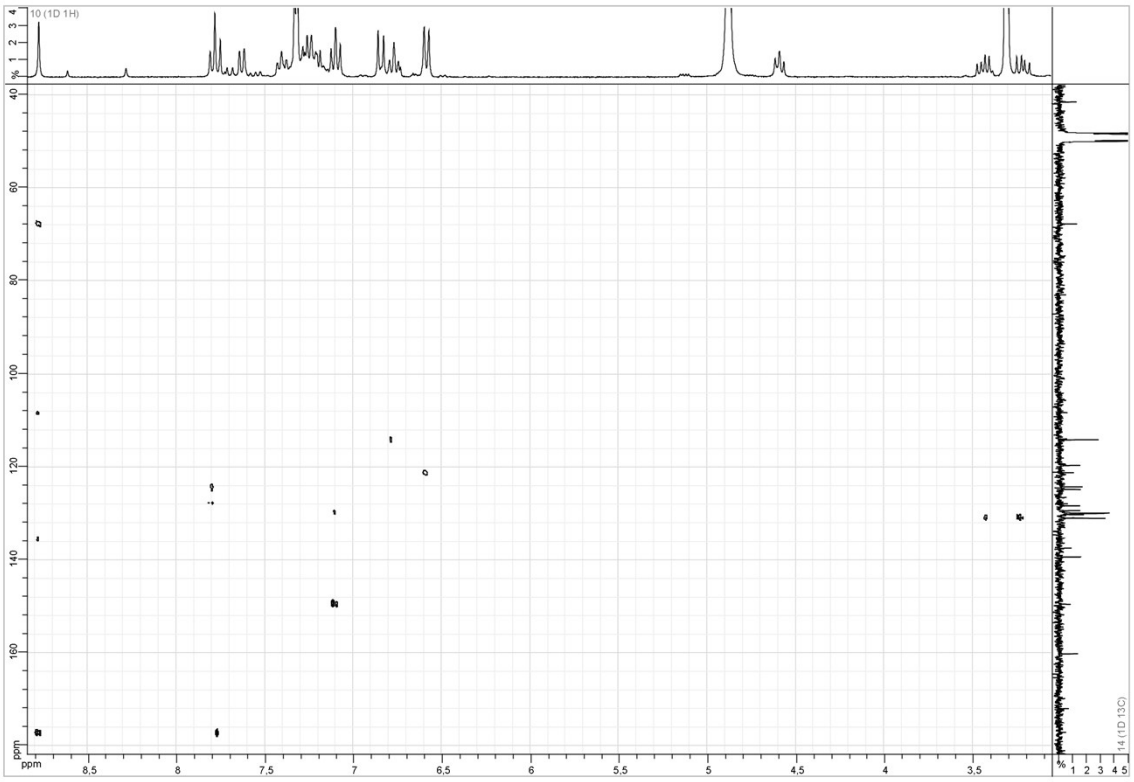
HSQC NMR spectrum of **5d** in CD_3OD (zoom 1)



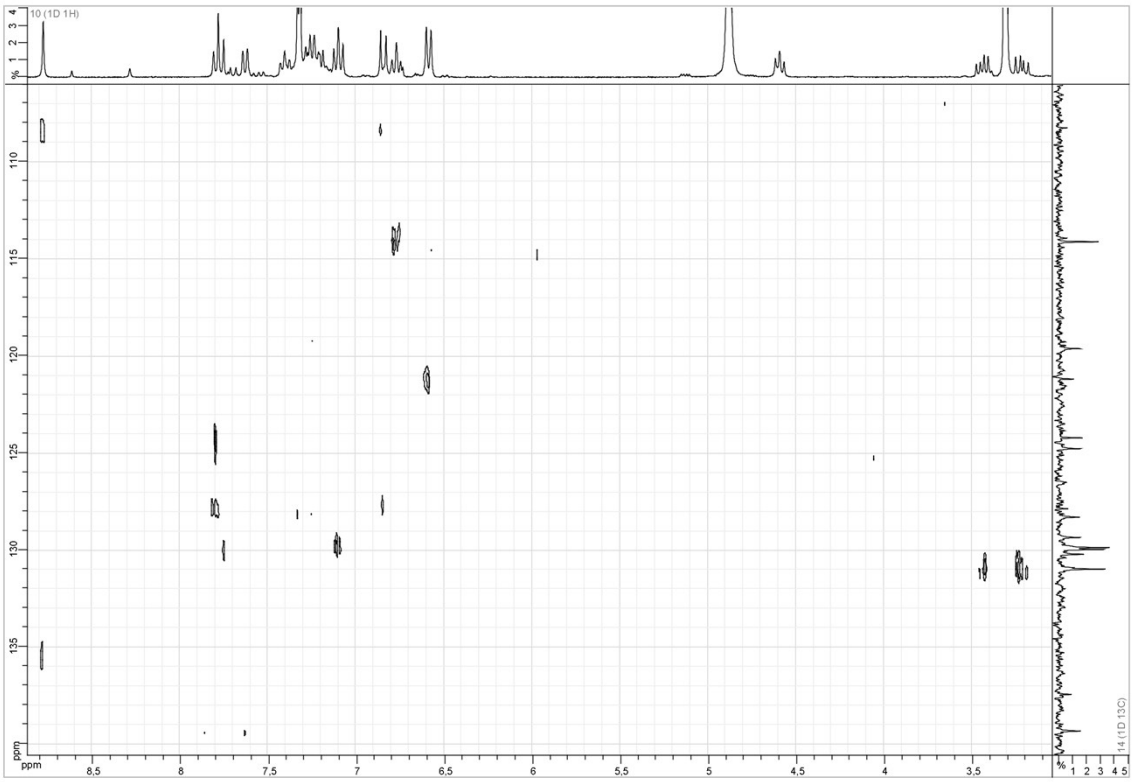
HSQC NMR spectrum of **5d** in CD_3OD (zoom 2)



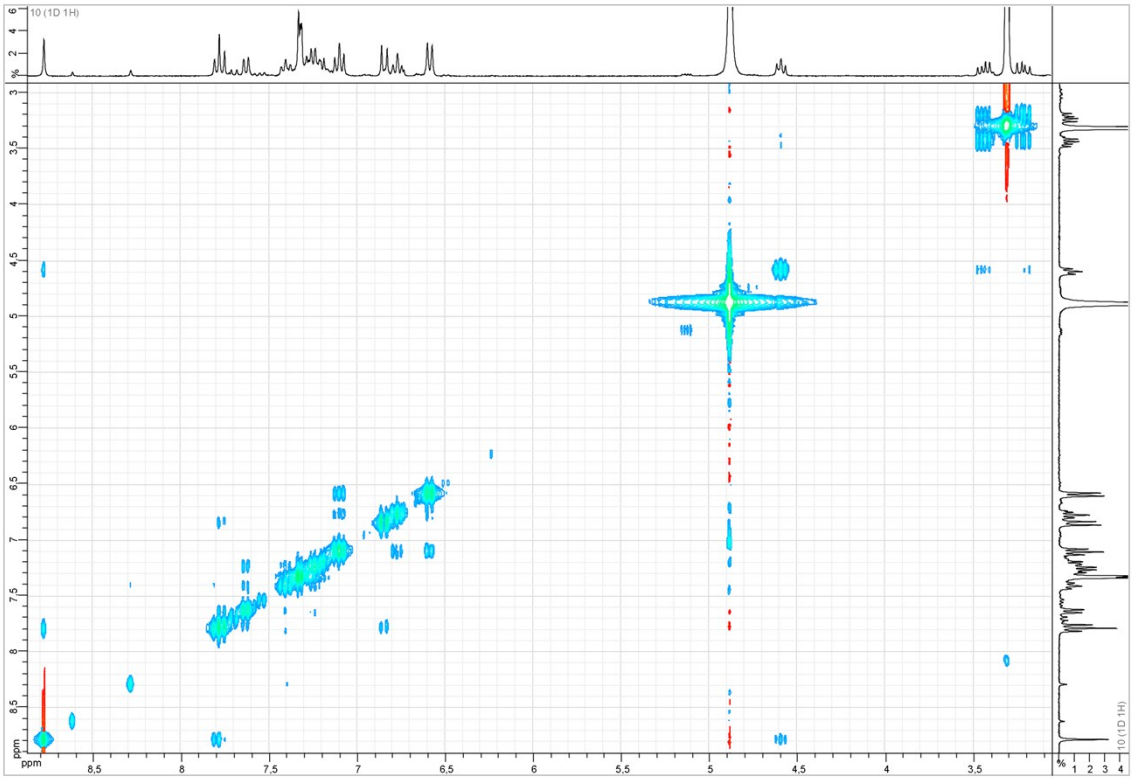
HMBC NMR spectrum of **5d** in CD_3OD



HMBC NMR spectrum of **5d** in CD_3OD (zoom)

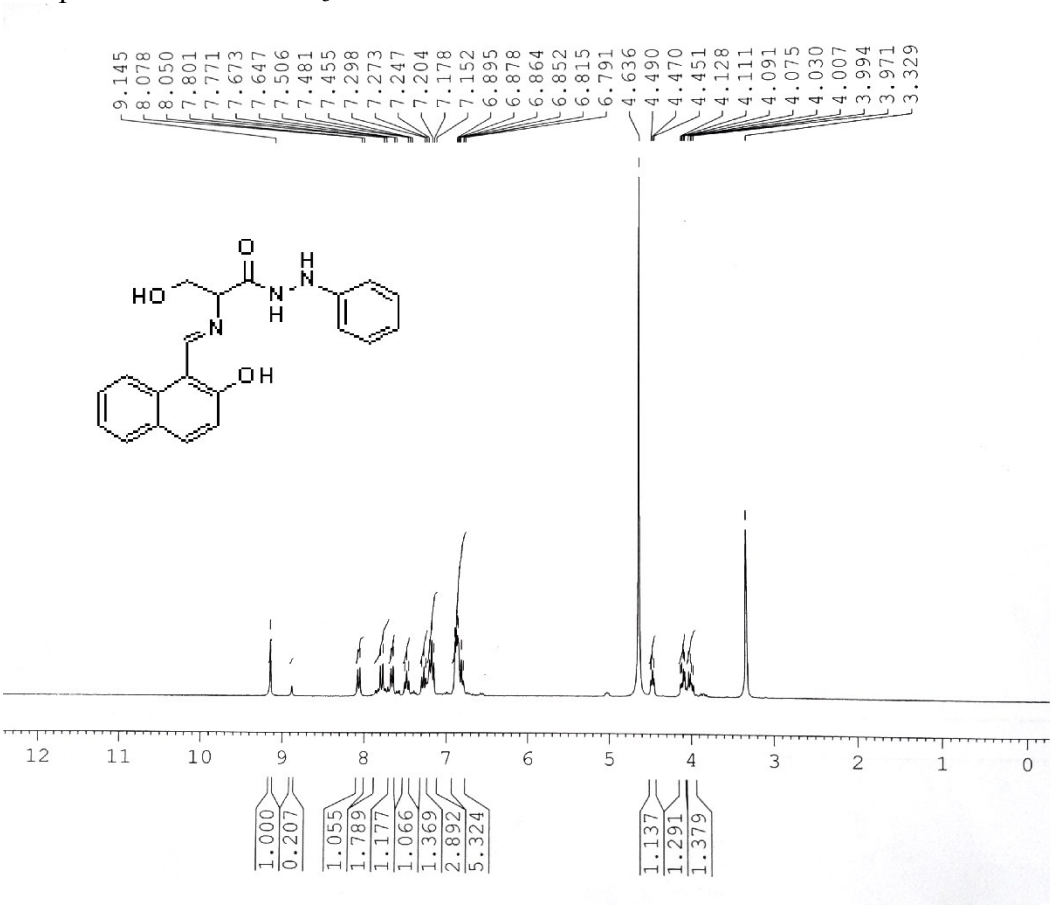


Noesy NMR spectrum of **5d** in CD_3OD

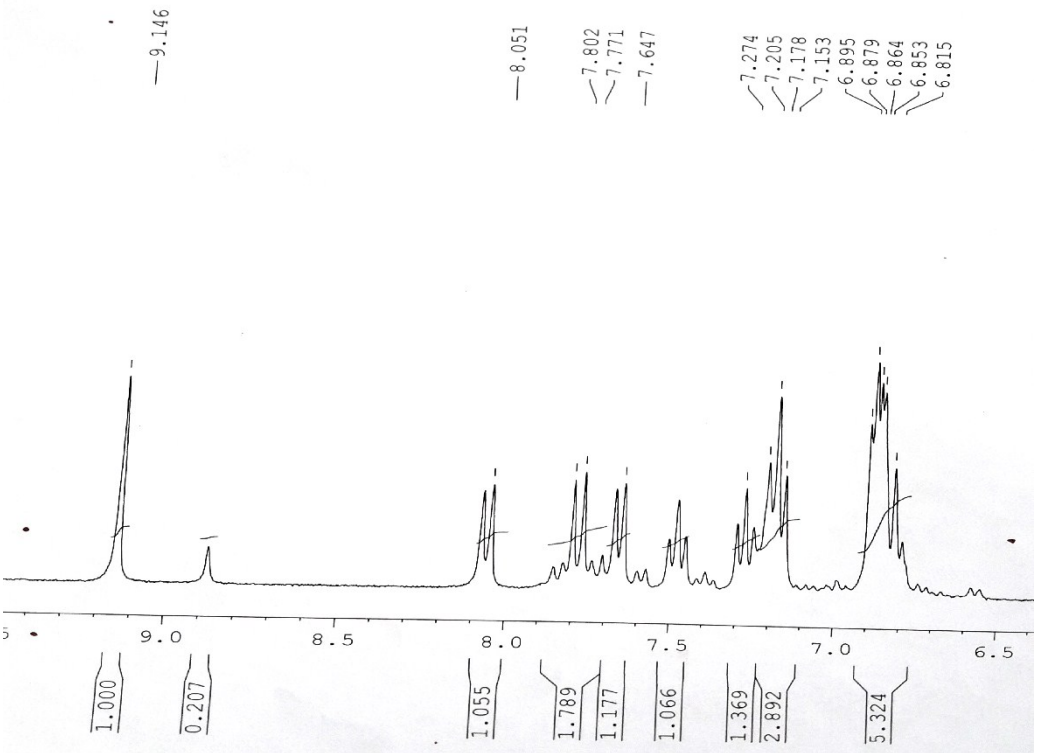


f. NMR spectra of 5e

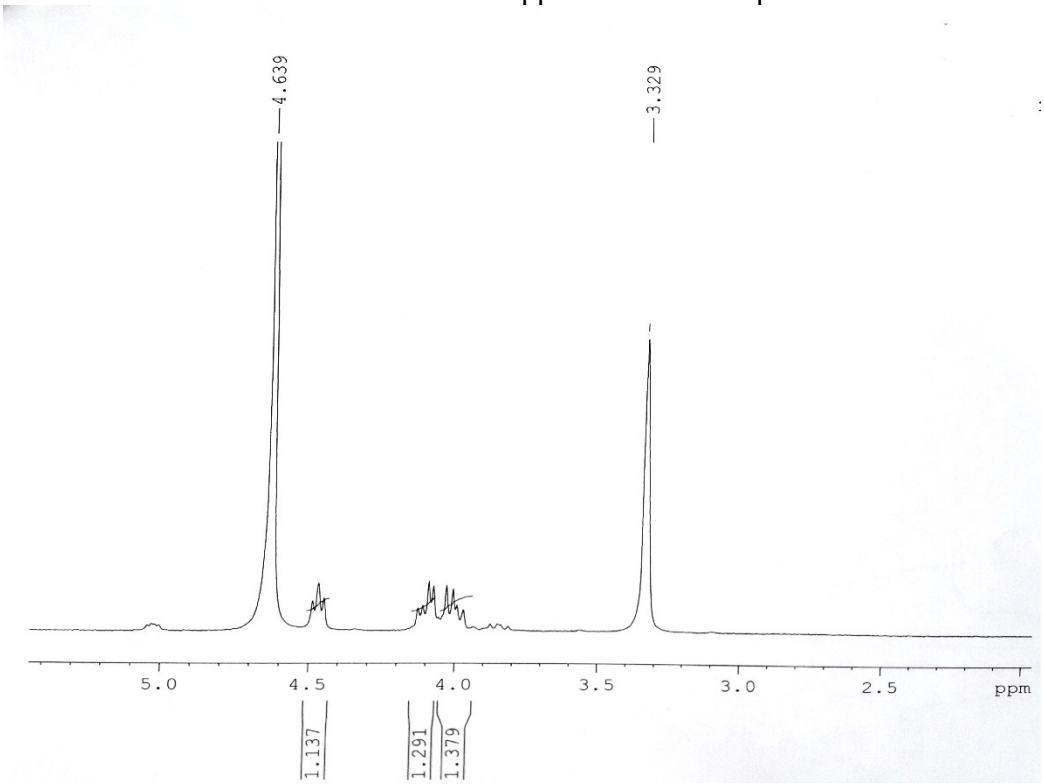
^{1}H NMR spectrum of **5e** in CD_3OD at 300 MHz



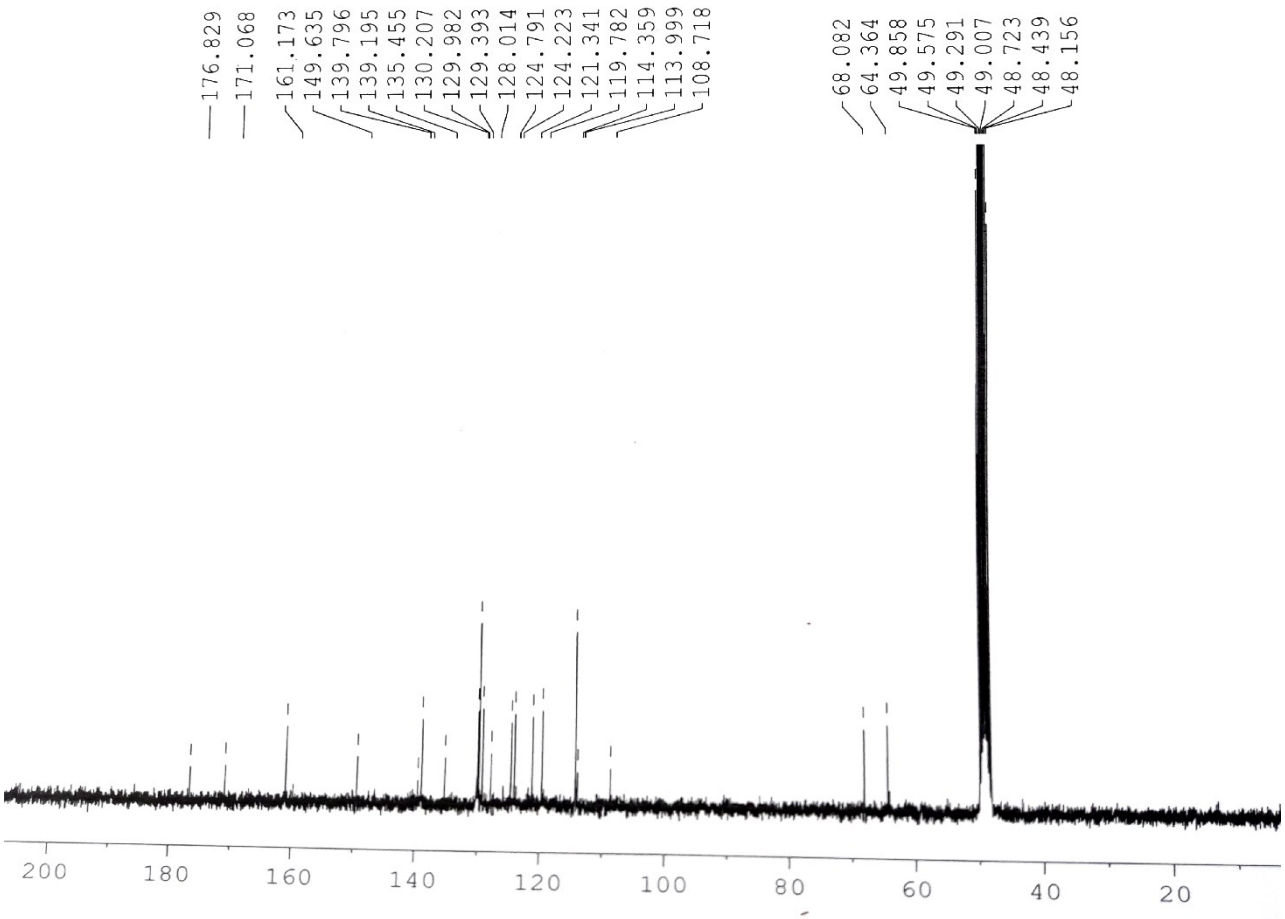
Magnification of the zone between 6.5 and 9.5 ppm of ^{1}H NMR spectrum of **5e**



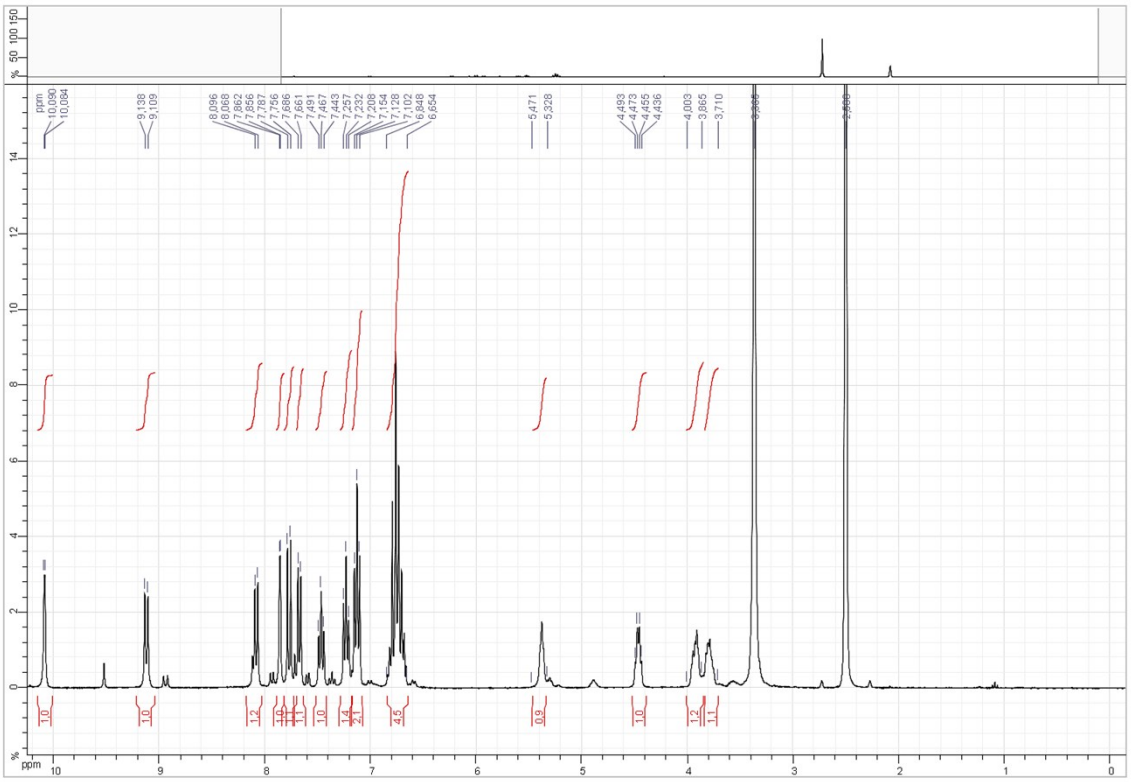
Magnification of the zone between 2.5 and 5.0 ppm of ^{1}H NMR spectrum of **5e**



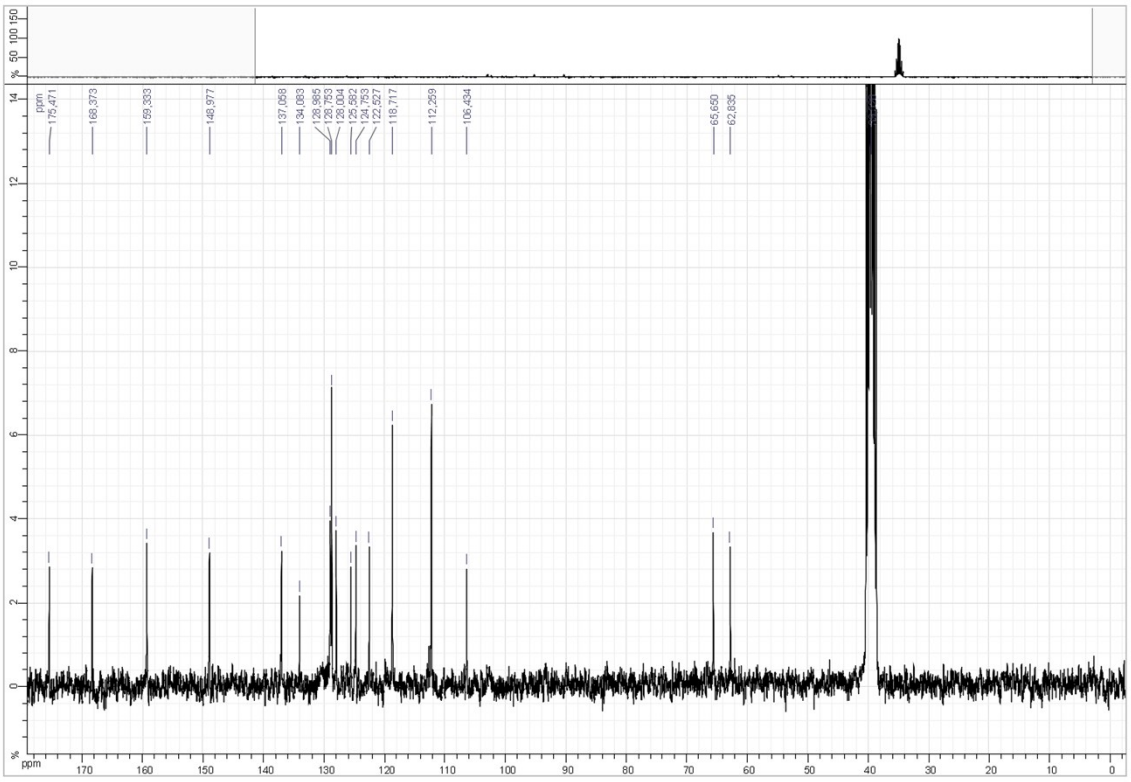
^{13}C NMR spectrum of **5e** in CD_3OD at 75 MHz



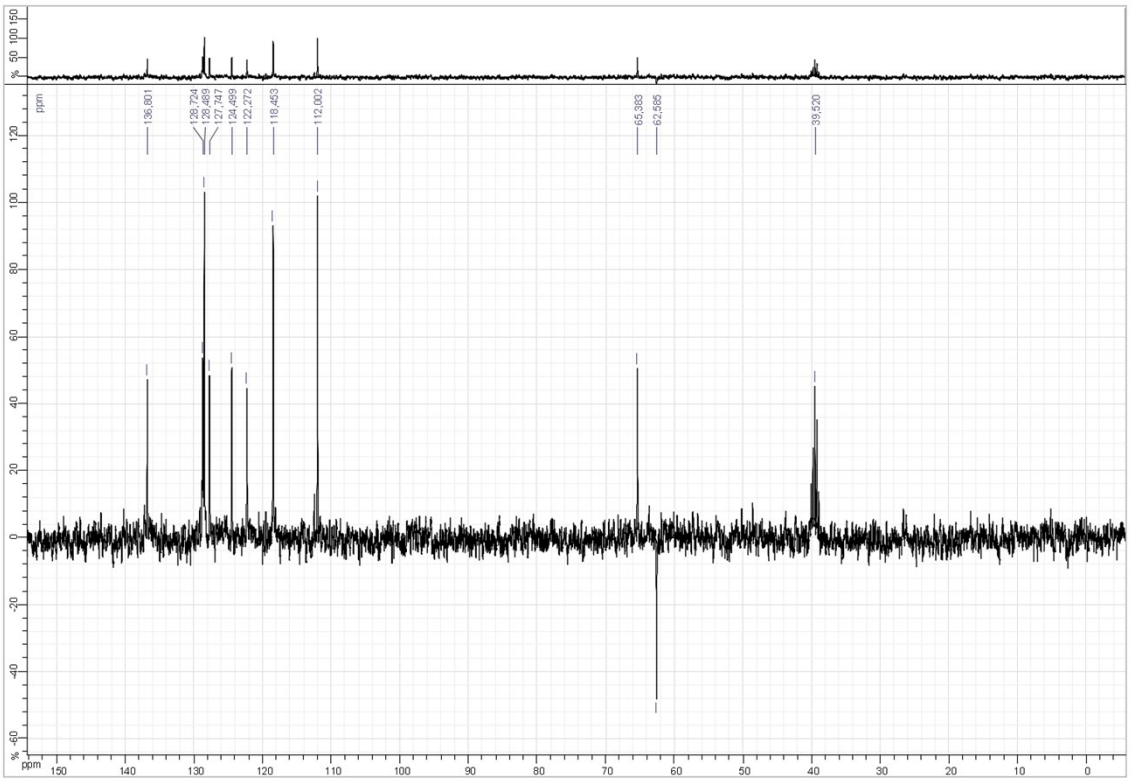
^{1}H NMR spectrum of **5e** in DMSO-d_6 at 300 MHz



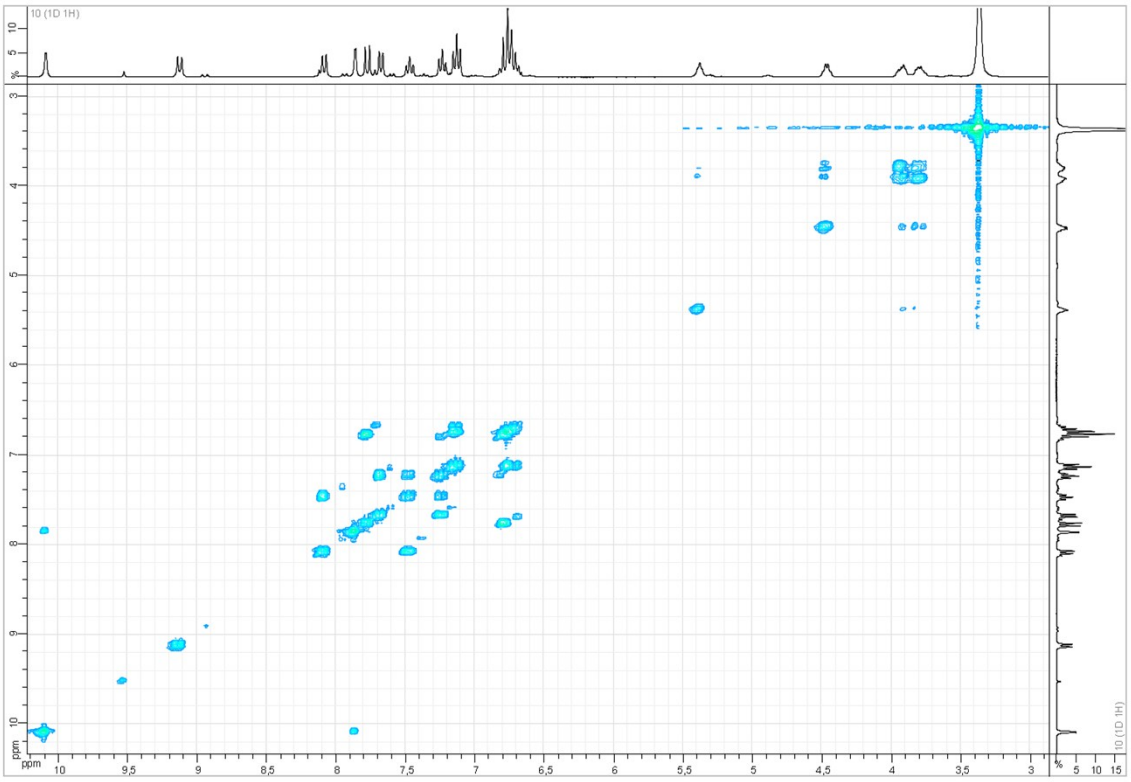
^{13}C NMR spectrum of **5e** in DMSO-d_6 at 75 MHz



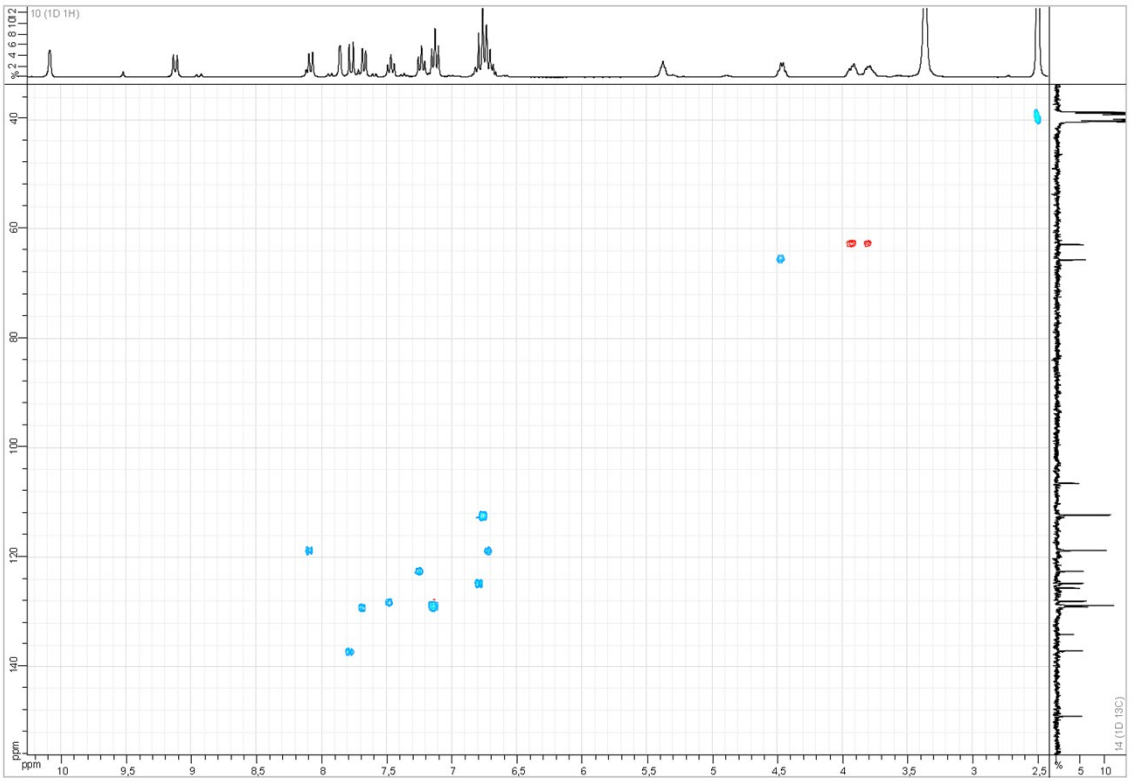
^{13}C (Dept135) NMR spectrum of **5e** in DMSO-d_6 at 75 MHz



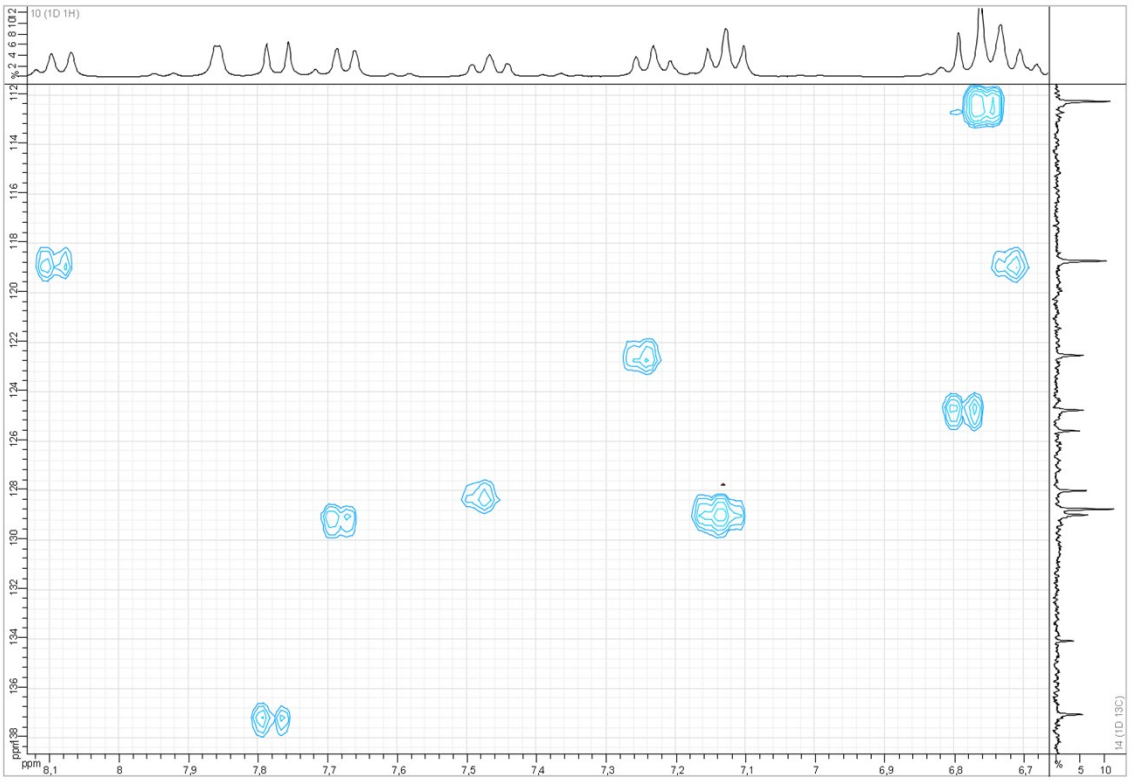
Cosy NMR spectrum of **5e** in DMSO-d_6



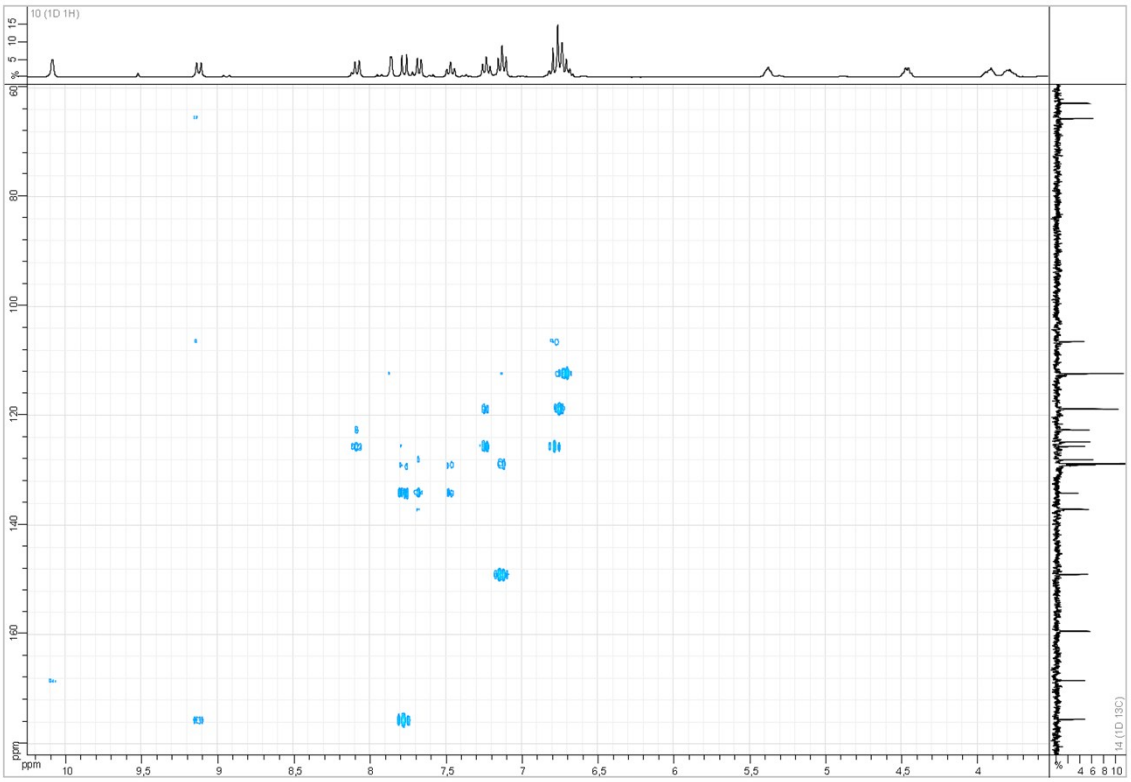
HSQC NMR spectrum of **5e** in DMSO-d_6



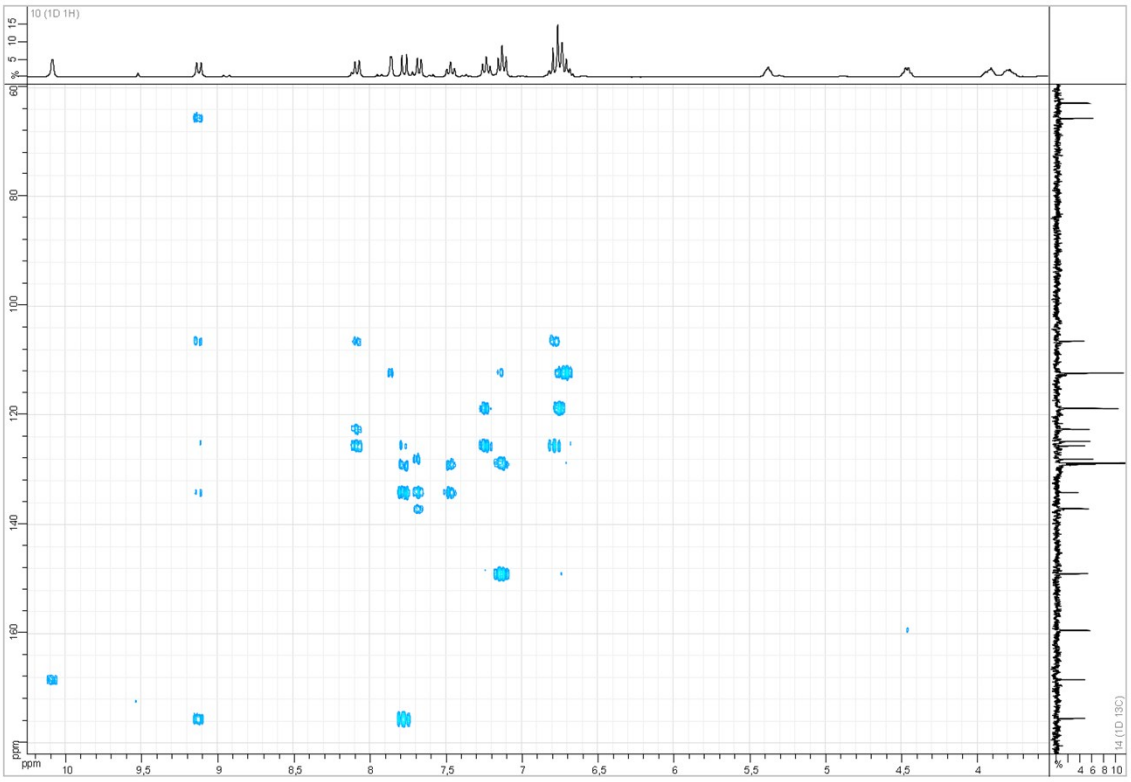
HSQC NMR spectrum of **5e** in DMSO-d_6 (zoom)



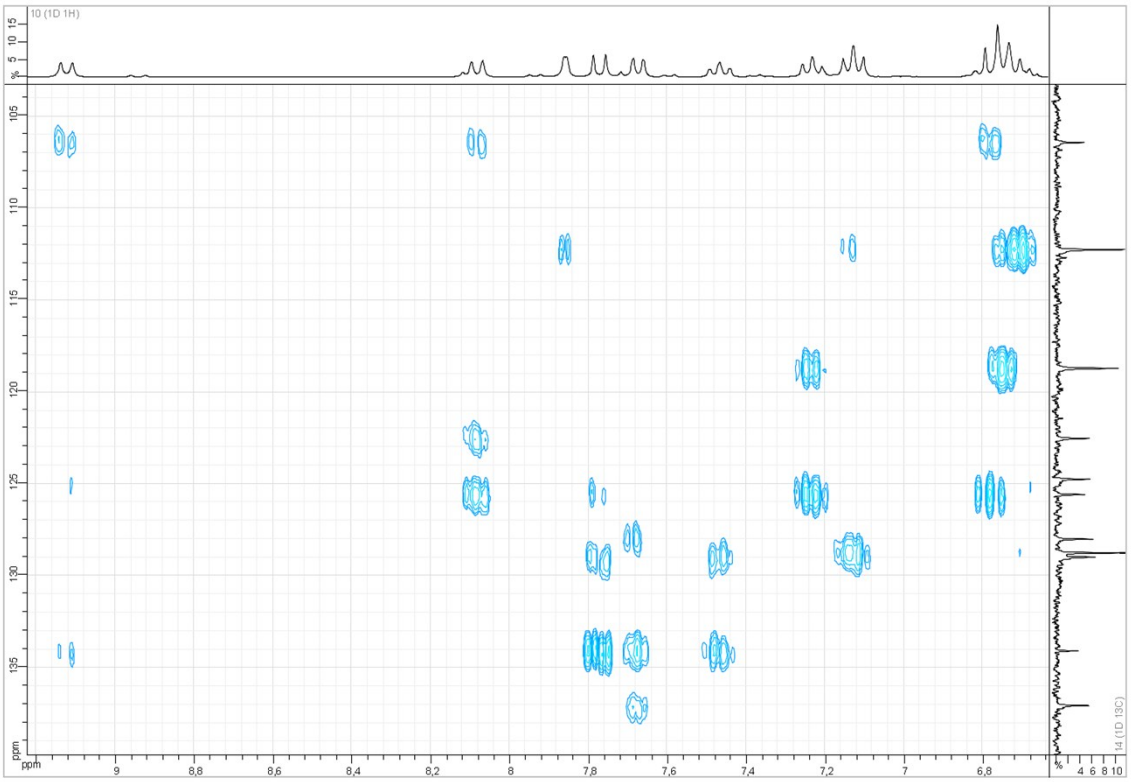
HMBC NMR spectrum of **5e** in DMSO-d_6



HMBC NMR spectrum of **5e** in DMSO-d_6 (deep cut)



HMBC NMR spectrum of **5e** in DMSO-d_6 (deep cut. zoom)



Noesy NMR spectrum of **5e** in DMSO-d_6