

Chiral arylideneaminoimidazolidin-4-ones: green synthesis and isomerization mechanism in solution

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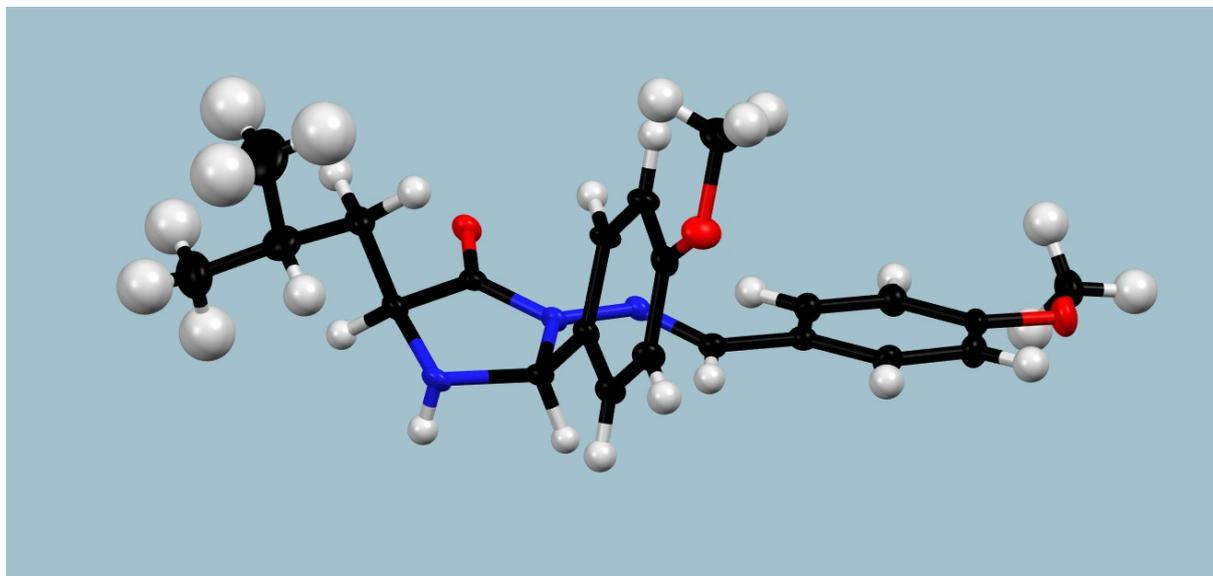
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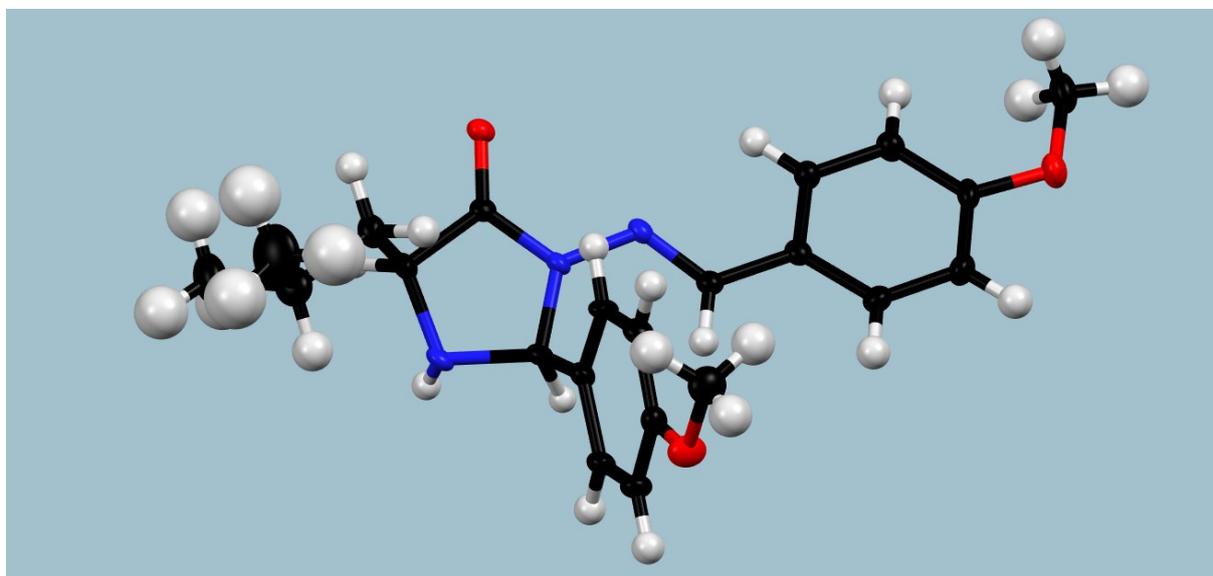
1. Crystallographic data

a. Crystallization

The 5-isobutyl-3-(4-methoxybenzylideneamino)-2-(4-methoxyphenyl)imidazolidin-4-one **5f** crystallized after filtration of ethanol as a single diastereoisomer with the (1*R*, 2*S*, 5*S*) (*E*) configuration. The ORTEP plate of this compound is presented below.

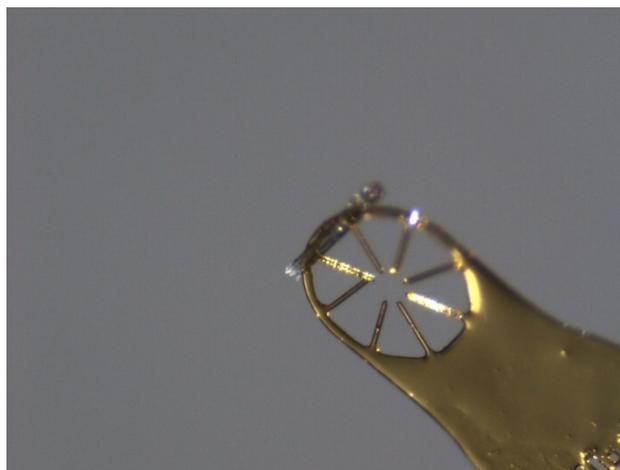


ORTEP of the compound **5f** at 30 % probability level (view 1).



ORTEP of the compound **5f** at 30 % probability level (view 2).

b. Photographs of crystals **5f**



c. Main structure information of **5f**

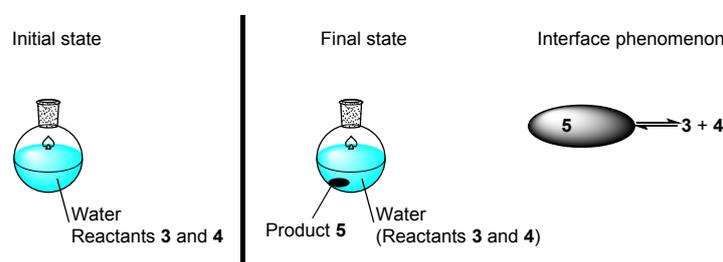
Formula	C ₂₂ H ₂₇ N ₃ O ₃
Molecular weight	381.46
Compound name	(2 <i>S</i> ,3 <i>E</i> ,5 <i>S</i>)-5-isobutyl-3-(4-methoxybenzylideneamino)-2-(4-methoxyphenyl)imidazolidin-4-one
Space group	<i>P</i> 2 ₁
Space group (name Hall)	P 2 _y b
Cell setting	Monoclinic
Cell lengths	a 13.957(2) b 5.4550(9) (6) c 14.7103(19)
Cell angles	α 90 β 107.844(9) γ 90
Cell volume	1066.1(3)
<i>Z</i>	2
F (000)	408
D _x (g.cm ⁻³)	1.188
Mo <i>K</i> α radiation, λ	0.71073 Å
θ	2.4-25.0°
μ	0.08 mm ⁻¹
h. k .l max	16, 6, 17
Temperature (K)	200

2. Water sensitivity of the products **5a-m**

The products **5a-m** were prepared in water from **3** and **4**, however subsequent analyses showed the very water-sensitive character of **5**. This unexpected result needs to be clarify.

Three non-refutable observations can be made:

- The reactants **3** and **4** are soluble in water therefore a single phase is observed, as specified in the article.
- The products **5** are not soluble in water.
- The products **5** are stable in the solid state at room temperature.



The efficient collision between the molecules **3** and **4** leads to the formation of the molecule **5** by the well-known condensation mechanism. This process is reversible in water according to a molecular point of view since a single molecule **5** is surrounded by water molecules. However, as time goes by, the hydrophobic property of **5** suggests that the collisions of molecules of **5** each other give birth to aggregates. These ones are not soluble and the internal molecules **5** are protected from the hydrolysis, especially if the reactivity center (iminic carbon) is not correctly oriented vis-a-vis of water molecules. The addition of aggregates affords **5** as the sole solid product. It could be explained also the “procedure time” of 11 h which could be divided in a short microscopic “time reaction” and a longer macroscopic “aggregation time”.

This phenomenon explains that the isolation by simple filtration induces in this case a high purity of the products **5** since no reactants are inside the solid and they can only be formed at the interface, merging immediately with the liquid phase. After isolation, if the products **5** are dissolved in a non-aqueous solvent, each molecules **5** can easily interact with the residual water.

The both phenomena (interface and solubility) are so important that clarify why a solid aggregate of **5** can be much more stable in water (2 phases) compared to a solution of **5** in an organic solvent (1 phase). To conclude, the water sensitivity of **5** is depending on its physical state.

3. Calculations

a. Energies conversions

Gibbs energy is defined as the sum of the electronic and thermal free energies and it is given in hartrees.

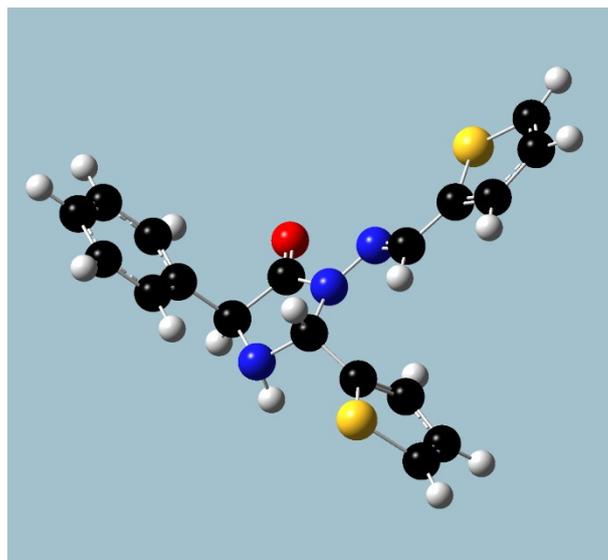
Conversion factor from hartree to $\text{kJ}\cdot\text{mol}^{-1}$: 2625.499640

according to : $1 \text{ hartree} = (4.35974434 \cdot 10^{-18} \text{ J} * 6.02214129 \cdot 10^{23} \text{ mol}^{-1}) / 10^3$ with the fundamental constant values taken from the *National Institute of Standards and Technology* (NIST – USA).

b. Species (1*R*_N,2*R*_C,5*S*_C)-(E) out – **5b**

BMK/6-31++G(df,pd) in benzene CPCM-UFF

Center Number	Atomic Number	Atomic Type	Coordinates (Å)		
			X	Y	Z
1	6	0	-0.577627	1.133109	-0.021739
2	6	0	-2.477455	0.295639	1.121562
3	1	0	-2.995952	0.554333	2.049681
4	6	0	-1.262714	-0.593562	1.454354
5	8	0	-1.243959	-1.582383	2.149151
6	7	0	-0.196528	-0.055328	0.759210
7	7	0	-1.896514	1.495000	0.512103
8	1	0	-1.771563	2.211800	1.218174
9	6	0	-3.441675	-0.459800	0.195991
10	6	0	-4.001468	-1.675523	0.627786
11	6	0	-3.785555	0.048539	-1.063926
12	6	0	-4.892786	-2.371865	-0.194822
13	1	0	-3.725848	-2.075330	1.599618
14	6	0	-4.677451	-0.653543	-1.888154
15	1	0	-3.365429	0.995810	-1.385496
16	6	0	-5.233257	-1.863360	-1.456967
17	1	0	-5.319446	-3.310431	0.147355
18	1	0	-4.937981	-0.251452	-2.863312
19	1	0	-5.926539	-2.404076	-2.094916
20	7	0	0.933237	-0.819491	0.604241
21	6	0	1.801367	-0.487785	-0.278080
22	6	0	3.001690	-1.296201	-0.461936
23	6	0	4.012778	-1.056475	-1.367022
24	16	0	3.321771	-2.741436	0.484958
25	6	0	5.059531	-2.033464	-1.312128
26	1	0	4.004951	-0.209176	-2.044551
27	6	0	4.826626	-2.997904	-0.366204
28	1	0	5.938433	-2.014648	-1.945713
29	1	0	5.445132	-3.848769	-0.111933
30	1	0	1.709349	0.386834	-0.924544
31	6	0	0.400005	2.275509	0.141627
32	6	0	1.224639	2.538491	1.204614
33	16	0	0.527629	3.518863	-1.088493
34	6	0	1.976317	3.752772	1.043661
35	1	0	1.306288	1.881044	2.063744
36	6	0	1.709205	4.390889	-0.137372
37	1	0	2.683833	4.123899	1.776218
38	1	0	2.124158	5.315742	-0.515345
39	1	0	-0.662500	0.850579	-1.081976



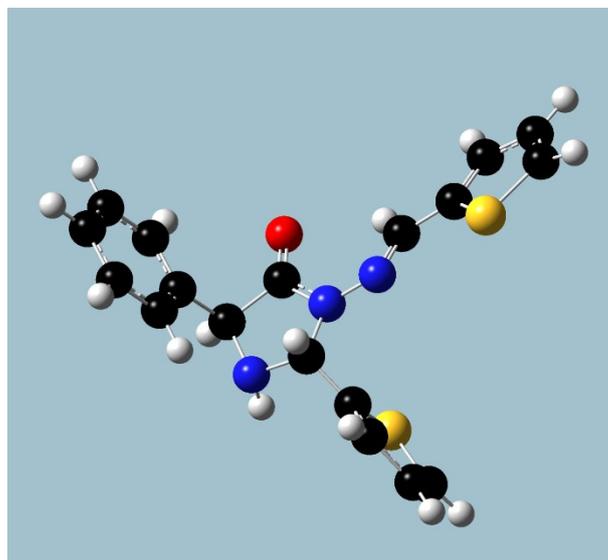
Gibbs energy= -1729.747165 h (T= 298.15K, P= 1 atm)

c. Species ($1R_N, 2R_C, 5S_C$)-(E) in **5b**

BMK/6-31++G(df,pd) in benzene CPCM-UFF

Center Number	Atomic Number	Atomic Type	Coordinates (Å)		
			X	Y	Z
1	6	0	0.726514	1.258663	0.262727
2	6	0	2.408836	0.264331	-1.055343
3	1	0	2.844758	0.463515	-2.039072
4	6	0	1.089117	-0.518772	-1.245907
5	8	0	0.923520	-1.534583	-1.892959
6	7	0	0.143866	0.144032	-0.503887
7	7	0	2.000305	1.513287	-0.409900
8	1	0	1.881692	2.245629	-1.101088
9	6	0	3.392158	-0.570788	-0.225173
10	6	0	3.863081	-1.791345	-0.740509
11	6	0	3.833059	-0.140175	1.033857
12	6	0	4.759407	-2.570687	-0.001574
13	1	0	3.520936	-2.130616	-1.713950
14	6	0	4.730477	-0.924114	1.773880
15	1	0	3.488852	0.813232	1.420582
16	6	0	5.195210	-2.139928	1.260192
17	1	0	5.116428	-3.512039	-0.409501
18	1	0	5.064934	-0.580385	2.748712
19	1	0	5.893091	-2.744691	1.832179
20	7	0	-1.053018	-0.360609	-0.027033
21	6	0	-1.687719	-1.221643	-0.736179
22	6	0	-2.939723	-1.783182	-0.243536
23	6	0	-3.736717	-2.689835	-0.908075
24	16	0	-3.625857	-1.359781	1.319844
25	6	0	-4.910603	-3.053533	-0.173041
26	1	0	-3.485458	-3.079251	-1.889041
27	6	0	-4.986929	-2.419104	1.040180
28	1	0	-5.658434	-3.750622	-0.532675
29	1	0	-5.760069	-2.506151	1.792570
30	1	0	-1.342253	-1.565246	-1.709141
31	6	0	-0.163108	2.470662	0.309601
32	6	0	-0.460908	3.236375	1.404246
33	16	0	-0.917863	3.117555	-1.143676
34	6	0	-1.295132	4.365561	1.095873
35	1	0	-0.098907	3.001921	2.399661
36	6	0	-1.619316	4.435765	-0.231148
37	1	0	-1.637419	5.082402	1.833333
38	1	0	-2.237813	5.164990	-0.737613
39	1	0	0.896739	0.923105	1.295345

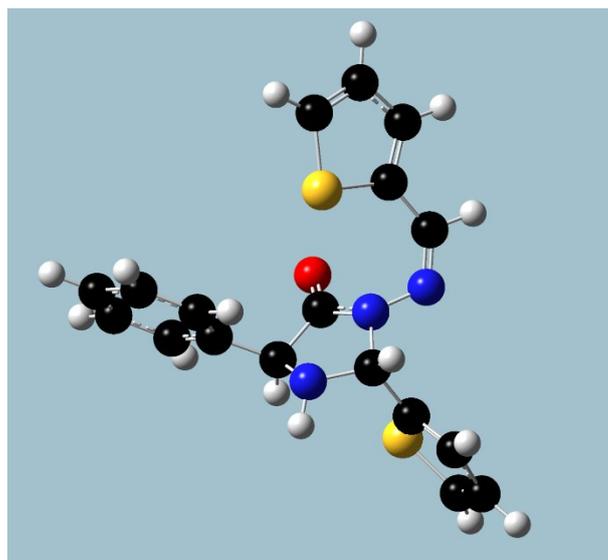
Gibbs energy= -1729.748995 h (T= 298.15K, P= 1 atm)



d. Species (1R_N,2R_C,5S_C)-(Z) – 5b

BMK/6-31++G(df,pd) benzene CPCM-UFF

Center Number	Atomic Number	Atomic Type	Coordinates (Å)		
			X	Y	Z
1	6	0	-1.529593	0.079008	-1.063880
2	6	0	-0.289720	-1.561126	0.133975
3	1	0	-0.974055	-2.070864	0.832245
4	6	0	-0.043264	-0.164043	0.737528
5	8	0	0.535956	0.097429	1.767741
6	7	0	-0.629892	0.739221	-0.119976
7	7	0	-0.901479	-1.243343	-1.154542
8	1	0	-1.559101	-1.949110	-1.464549
9	6	0	0.993276	-2.375182	0.029575
10	6	0	1.371512	-3.204727	1.095670
11	6	0	1.822828	-2.278383	-1.097728
12	6	0	2.568212	-3.929674	1.038866
13	1	0	0.730211	-3.283579	1.969960
14	6	0	3.017840	-3.006250	-1.156387
15	1	0	1.516581	-1.641793	-1.921835
16	6	0	3.394328	-3.832681	-0.088637
17	1	0	2.850422	-4.570492	1.869354
18	1	0	3.652619	-2.928425	-2.034670
19	1	0	4.319468	-4.399982	-0.136841
20	7	0	-0.982790	2.034803	0.289817
21	6	0	-0.019487	2.857010	0.496050
22	1	0	-0.354788	3.822345	0.877450
23	6	0	1.420771	2.792969	0.256457
24	6	0	2.270593	3.824407	0.614188
25	16	0	2.299465	1.550335	-0.626099
26	6	0	3.620961	3.624314	0.198740
27	1	0	1.925212	4.697658	1.157705
28	6	0	3.784058	2.446865	-0.488216
29	1	0	4.427841	4.319475	0.397859
30	1	0	4.691455	2.044976	-0.920572
31	6	0	-2.984756	0.086472	-0.629219
32	6	0	-4.060626	0.449045	-1.396141
33	16	0	-3.502186	-0.459488	0.962510
34	6	0	-5.320931	0.291644	-0.721224
35	1	0	-3.958996	0.819399	-2.411092
36	6	0	-5.182569	-0.188205	0.551966
37	1	0	-6.279249	0.533160	-1.166736
38	1	0	-5.951724	-0.395854	1.284050
39	1	0	-1.481473	0.586556	-2.033398



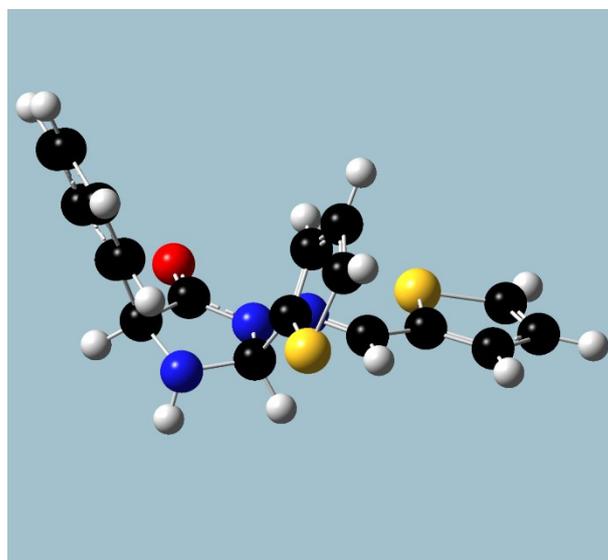
Gibbs energy= -1729.740789 h (T= 298.15K, P= 1 atm)

e. Species ($1R_N, 2S_C, 5S_C$)-(E) out -5b

BMK/6-31++G(df,pd) in benzene CPCM-UFF

Center Number	Atomic Number	Atomic Type	Coordinates (Å)		
			X	Y	Z
1	6	0	0.301295	0.462569	-1.408099
2	6	0	1.896670	-1.286105	-1.374474
3	1	0	-0.358194	0.882281	-2.177314
4	1	0	2.201691	-2.027646	-2.120433
5	6	0	0.580917	-1.789974	-0.741129
6	8	0	0.362943	-2.881610	-0.267650
7	7	0	-0.308062	-0.741737	-0.834257
8	7	0	1.526624	-0.031282	-2.043441
9	1	0	1.339010	-0.214708	-3.022336
10	6	0	3.021144	-1.150692	-0.339035
11	6	0	3.368004	-2.264230	0.446571
12	6	0	3.739586	0.044499	-0.196123
13	6	0	4.416414	-2.177729	1.369848
14	1	0	2.806929	-3.188341	0.340041
15	6	0	4.791027	0.127140	0.727582
16	1	0	3.473328	0.900353	-0.806977
17	6	0	5.132898	-0.980998	1.512182
18	1	0	4.673157	-3.043129	1.974138
19	1	0	5.342611	1.057575	0.830240
20	1	0	5.950228	-0.914406	2.224718
21	7	0	-1.596168	-0.889628	-0.392859
22	6	0	-2.383828	0.121070	-0.430137
23	6	0	0.572232	1.503989	-0.333640
24	6	0	0.483158	1.374091	1.025963
25	16	0	1.123692	3.110917	-0.783533
26	6	0	0.863423	2.567360	1.733663
27	1	0	0.161145	0.458800	1.510984
28	6	0	1.230354	3.586140	0.898898
29	1	0	0.860612	2.650616	2.814414
30	1	0	1.558637	4.585010	1.154008
31	6	0	-3.771413	-0.011403	-0.003210
32	6	0	-4.711949	0.996092	0.028306
33	16	0	-4.450917	-1.535670	0.545921
34	6	0	-5.991264	0.554752	0.497728
35	1	0	-4.491097	2.014290	-0.274209
36	6	0	-6.002091	-0.779652	0.813075
37	1	0	-6.856220	1.200318	0.595117
38	1	0	-6.826746	-1.371434	1.188688
39	1	0	-2.079236	1.116365	-0.762009

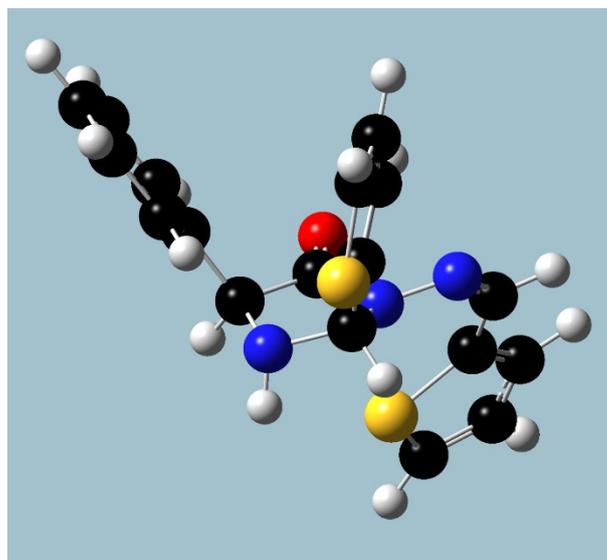
Gibbs energy= -1729.748494 h (T= 298.15K, P= 1 atm)



f. Species (1R_N,2S_C,5S_C)-(Z) – 5b

BMK/6-31++G(df,pd) in benzene CPCM-UFF

Center Number	Atomic Number	Atomic Type	Coordinates (Å)		
			X	Y	Z
1	6	0	0.234064	1.213408	-0.890881
2	6	0	0.403443	-1.143145	-0.950440
3	1	0	-0.218297	1.995462	-1.507455
4	1	0	-0.134791	-1.886739	-1.549772
5	6	0	-0.557887	-0.709832	0.182072
6	8	0	-1.054396	-1.404108	1.042507
7	7	0	-0.781105	0.636008	-0.001968
8	7	0	0.611742	0.077805	-1.739947
9	1	0	0.012658	0.062080	-2.557169
10	6	0	1.677711	-1.801072	-0.412093
11	6	0	1.563174	-2.979072	0.347197
12	6	0	2.949769	-1.281819	-0.688786
13	6	0	2.708015	-3.622764	0.829683
14	1	0	0.578037	-3.378565	0.569668
15	6	0	4.095683	-1.931637	-0.208365
16	1	0	3.038257	-0.374891	-1.277439
17	6	0	3.979681	-3.101802	0.551463
18	1	0	2.606576	-4.529370	1.419623
19	1	0	5.076653	-1.521657	-0.431737
20	1	0	4.868818	-3.604604	0.921335
21	7	0	-1.339797	1.441020	1.003631
22	6	0	-2.586762	1.260190	1.247901
23	1	0	-2.955881	1.861767	2.079354
24	6	0	-3.623796	0.465922	0.591657
25	6	0	-4.915929	0.388403	1.076541
26	16	0	-3.495760	-0.381170	-0.946560
27	6	0	-5.802372	-0.351631	0.236673
28	1	0	-5.212948	0.854663	2.010274
29	6	0	-5.179545	-0.820071	-0.892712
30	1	0	-6.848082	-0.523444	0.462611
31	1	0	-5.605215	-1.402083	-1.700098
32	6	0	1.420713	1.776467	-0.126545
33	6	0	1.757342	1.625467	1.190673
34	16	0	2.640106	2.705084	-0.988947
35	6	0	3.007859	2.250498	1.531205
36	1	0	1.131796	1.100455	1.903123
37	6	0	3.600067	2.871731	0.466563
38	1	0	3.433484	2.236266	2.528148
39	1	0	4.531284	3.421603	0.434733



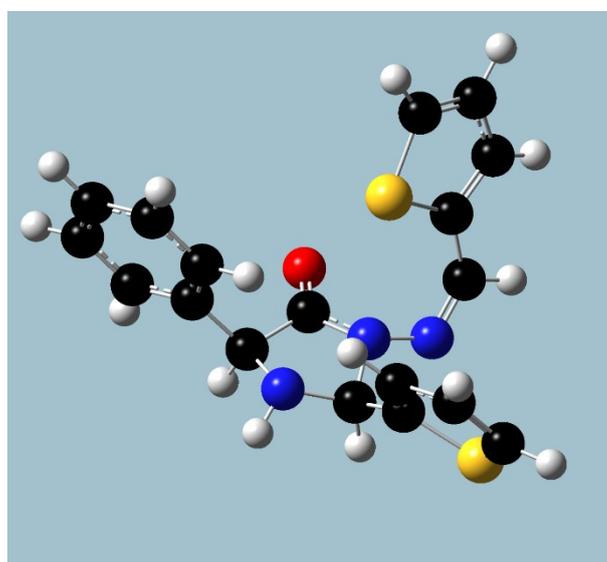
Gibbs energy= -1729.738151 h (T= 298.15K, P= 1 atm)

g. Species (1R_N,2S_C,5S_C)-(Z) – 5b

BMK/6-31++G(df,pd) in benzene CPCM-UFF

Center Number	Atomic Number	Atomic Type	Coordinates (Å)		
			X	Y	Z
1	6	0	-0.907713	1.582029	-0.902267
2	6	0	1.445577	1.394446	-1.109547
3	1	0	-1.238978	2.070465	-1.835997
4	1	0	1.729433	1.896080	-2.049938
5	6	0	0.773104	0.075434	-1.540348
6	8	0	1.300632	-0.870497	-2.081710
7	7	0	-0.557929	0.193792	-1.218320
8	7	0	0.368730	2.072784	-0.392818
9	1	0	0.430916	3.083387	-0.428821
10	6	0	2.697123	1.168127	-0.274423
11	6	0	3.958449	1.186118	-0.886454
12	6	0	2.601218	0.899375	1.100012
13	6	0	5.114749	0.938605	-0.134595
14	1	0	4.035951	1.394543	-1.950806
15	6	0	3.755526	0.654807	1.852305
16	1	0	1.621641	0.894143	1.568035
17	6	0	5.015571	0.673769	1.237013
18	1	0	6.087326	0.957131	-0.618120
19	1	0	3.673621	0.449390	2.916091
20	1	0	5.910705	0.487274	1.823359
21	7	0	-1.540825	-0.546907	-1.900100
22	6	0	-1.648577	-1.779185	-1.560751
23	1	0	-2.377589	-2.332585	-2.153881
24	6	0	-1.030315	-2.560418	-0.493280
25	6	0	-1.275754	-3.910713	-0.322207
26	16	0	-0.010825	-1.948459	0.804498
27	6	0	-0.648537	-4.463658	0.834425
28	1	0	-1.890672	-4.479252	-1.012165
29	6	0	0.060116	-3.523555	1.540987
30	1	0	-0.721173	-5.504686	1.125703
31	1	0	0.629661	-3.661128	2.451322
32	6	0	-2.000241	1.692338	0.137831
33	6	0	-1.869278	1.683858	1.502288
34	16	0	-3.685946	1.828543	-0.334738
35	6	0	-3.125686	1.785947	2.190109
36	1	0	-0.904488	1.613950	1.990236
37	6	0	-4.193045	1.873194	1.336162
38	1	0	-3.222133	1.796682	3.269909
39	1	0	-5.244498	1.956440	1.577700

Gibbs energy= -1729.738317 h (T= 298.15K, P= 1 atm)

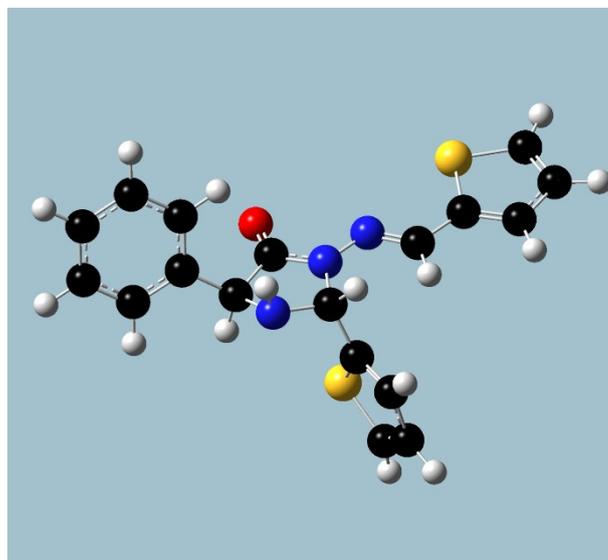


h. Species (1S_N,2R_C,5S_C)-(E) out – **5b**

BMK/6-31++G(df,pd) in benzene CPCM-UFF

Center Number	Atomic Number	Atomic Type	Coordinates (Å)		
			X	Y	Z
1	6	0	-0.341607	0.849012	-0.953564
2	6	0	-2.280689	0.210721	0.250755
3	1	0	-2.419865	0.972664	1.029942
4	6	0	-1.101790	-0.681115	0.695676
5	8	0	-1.105290	-1.542080	1.544115
6	7	0	-0.021030	-0.269288	-0.055239
7	7	0	-1.807583	0.859195	-0.989235
8	1	0	-2.122147	0.311046	-1.784586
9	6	0	-3.581815	-0.542327	0.051785
10	6	0	-4.793320	0.023360	0.474076
11	6	0	-3.593525	-1.791507	-0.591747
12	6	0	-6.004008	-0.646817	0.253778
13	1	0	-4.788676	0.988100	0.974925
14	6	0	-4.801094	-2.462261	-0.811838
15	1	0	-2.658484	-2.251217	-0.903652
16	6	0	-6.009514	-1.890314	-0.389590
17	1	0	-6.936508	-0.199929	0.586032
18	1	0	-4.798113	-3.431638	-1.301856
19	1	0	-6.946197	-2.414428	-0.556583
20	7	0	1.206067	-0.846951	0.136506
21	6	0	2.215282	-0.385325	-0.505210
22	6	0	0.248567	2.165847	-0.480124
23	6	0	0.724038	3.182107	-1.266531
24	16	0	0.325081	2.592991	1.221266
25	6	0	1.152145	4.328438	-0.512768
26	1	0	0.762580	3.121663	-2.349476
27	6	0	0.997163	4.161705	0.836802
28	1	0	1.560172	5.227191	-0.961141
29	1	0	1.242335	4.847535	1.636875
30	1	0	0.045462	0.648600	-1.959300
31	6	0	3.529158	-0.997804	-0.349279
32	6	0	4.694661	-0.587820	-0.960232
33	16	0	3.805756	-2.397510	0.676561
34	6	0	5.825611	-1.393912	-0.610699
35	1	0	4.737732	0.262771	-1.632329
36	6	0	5.501126	-2.402925	0.258702
37	1	0	6.828014	-1.226233	-0.986986
38	1	0	6.152840	-3.153935	0.685922
39	1	0	2.165251	0.471684	-1.180112

Gibbs energy= -1729.745735 h (T= 298.15K, P= 1 atm)

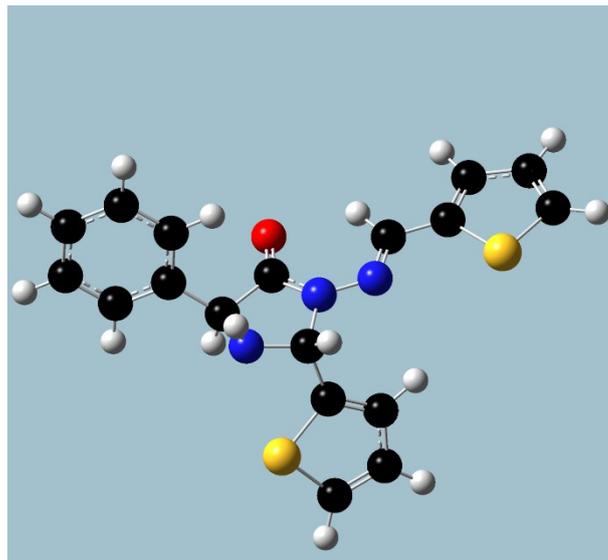


i. Species (1S_N,2R_C,5S_C)-(E) in – 5b

BMK/6-31++G(df,pd) in benzene CPCM-UFF

Center Number	Atomic Number	Atomic Type	Coordinates (Å)		
			X	Y	Z
1	6	0	-0.429304	0.997436	-0.996691
2	6	0	-2.141945	0.002638	0.276684
3	1	0	-2.316425	0.679800	1.123832
4	6	0	-0.813013	-0.731784	0.560353
5	8	0	-0.627713	-1.632616	1.358002
6	7	0	0.119323	-0.148392	-0.253128
7	7	0	-1.873472	0.798689	-0.938752
8	1	0	-2.179819	0.276730	-1.753635
9	6	0	-3.335686	-0.918760	0.117428
10	6	0	-4.565159	-0.583508	0.701765
11	6	0	-3.236778	-2.090965	-0.651589
12	6	0	-5.686010	-1.403516	0.516056
13	1	0	-4.645888	0.319672	1.300937
14	6	0	-4.354406	-2.911188	-0.837631
15	1	0	-2.283041	-2.372119	-1.092796
16	6	0	-5.582632	-2.567476	-0.255271
17	1	0	-6.633949	-1.132685	0.971962
18	1	0	-4.265700	-3.816817	-1.430636
19	1	0	-6.450062	-3.205192	-0.398534
20	7	0	1.478156	-0.354490	-0.343109
21	6	0	2.041345	-1.263276	0.370599
22	6	0	-0.021028	2.325143	-0.369482
23	6	0	1.234810	2.775859	-0.050095
24	16	0	-1.241419	3.534400	-0.004090
25	6	0	1.232346	4.101766	0.504832
26	1	0	2.127171	2.179634	-0.201921
27	6	0	-0.025367	4.637007	0.591776
28	1	0	2.128961	4.623278	0.820557
29	1	0	-0.317727	5.609270	0.966245
30	1	0	-0.072709	0.949639	-2.029591
31	6	0	3.478944	-1.474197	0.254217
32	6	0	4.225770	-2.376172	0.980869
33	16	0	4.491738	-0.565879	-0.862477
34	6	0	5.620330	-2.347028	0.653855
35	1	0	3.787133	-3.031847	1.725609
36	6	0	5.912799	-1.425297	-0.317654
37	1	0	6.364711	-2.980780	1.121604
38	1	0	6.876729	-1.192387	-0.751165
39	1	0	1.499059	-1.892354	1.073386

Gibbs energy= -1729.746925 h (T= 298.15K, P= 1 atm)

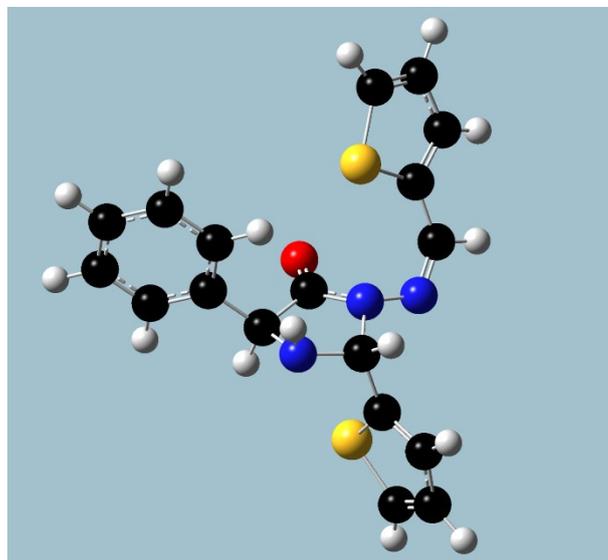


j. Species (1S_N,2R_C,5S_C)-(Z) – 5b

BMK/6-31++G(df,pd) in benzene CPCM-UFF

Center Number	Atomic Number	Atomic Type	Coordinates (Å)		
			X	Y	Z
1	6	0	-1.498427	0.045756	-1.086432
2	6	0	-0.307111	-1.575478	0.149929
3	1	0	-1.009638	-2.039452	0.854959
4	6	0	-0.001405	-0.168178	0.713860
5	8	0	0.585390	0.104068	1.737323
6	7	0	-0.570965	0.732594	-0.164882
7	7	0	-0.978715	-1.321899	-1.132445
8	1	0	-0.316755	-1.407934	-1.896206
9	6	0	0.920365	-2.463463	0.047847
10	6	0	1.022366	-3.604966	0.855151
11	6	0	1.970391	-2.153201	-0.833572
12	6	0	2.153547	-4.428461	0.784576
13	1	0	0.214337	-3.850273	1.539180
14	6	0	3.098348	-2.977405	-0.910000
15	1	0	1.916109	-1.262531	-1.455149
16	6	0	3.192879	-4.117732	-0.099943
17	1	0	2.219227	-5.309575	1.416113
18	1	0	3.903960	-2.726927	-1.594215
19	1	0	4.069558	-4.756010	-0.159113
20	7	0	-0.938059	2.021750	0.249354
21	6	0	0.002547	2.862753	0.478909
22	1	0	-0.362948	3.819448	0.854662
23	6	0	1.449048	2.838428	0.269501
24	6	0	2.262342	3.896541	0.632045
25	16	0	2.381339	1.611110	-0.577723
26	6	0	3.626441	3.730484	0.246303
27	1	0	1.881792	4.765727	1.158390
28	6	0	3.838441	2.551138	-0.422329
29	1	0	4.408378	4.451245	0.453777
30	1	0	4.765834	2.170163	-0.830152
31	6	0	-2.947472	0.124755	-0.647902
32	6	0	-4.004549	0.533878	-1.415497
33	16	0	-3.484731	-0.358763	0.955073
34	6	0	-5.268489	0.457507	-0.733072
35	1	0	-3.889037	0.879621	-2.437484
36	6	0	-5.149206	-0.004324	0.548442
37	1	0	-6.214898	0.739334	-1.180286
38	1	0	-5.924423	-0.159132	1.287044
39	1	0	-1.436497	0.500883	-2.078781

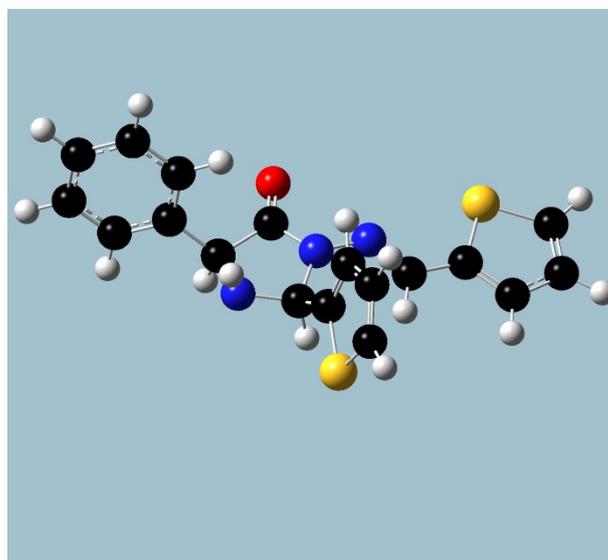
Gibbs energy = -1729.739811 h (T= 298.15K, P= 1 atm)



k. Species (1S_N,2S_C,5S_C)-(E) out – 5b

BMK/6-31++G(df,pd) in benzene CPCM-UFF

Center Number	Atomic Number	Atomic Type	Coordinates (Å)		
			X	Y	Z
1	6	0	0.346712	0.822857	-0.917945
2	6	0	2.240196	-0.599029	-1.010626
3	1	0	-0.084516	0.866059	-1.929506
4	1	0	2.298847	-0.952299	-2.049614
5	6	0	1.071473	-1.368359	-0.366094
6	8	0	1.055726	-2.527705	-0.026463
7	7	0	0.011490	-0.481188	-0.316584
8	7	0	1.811575	0.811536	-0.999739
9	1	0	2.183835	1.264352	-0.169370
10	6	0	3.582764	-0.807377	-0.338395
11	6	0	4.737393	-0.980583	-1.114577
12	6	0	3.691476	-0.788106	1.062079
13	6	0	5.988654	-1.127630	-0.501419
14	1	0	4.658113	-0.997916	-2.198505
15	6	0	4.939826	-0.935434	1.676304
16	1	0	2.799538	-0.674081	1.674131
17	6	0	6.091598	-1.104171	0.894695
18	1	0	6.876161	-1.261503	-1.112968
19	1	0	5.011518	-0.926373	2.760018
20	1	0	7.060362	-1.220754	1.371893
21	7	0	-1.247708	-0.988700	-0.108211
22	6	0	-2.271981	-0.267102	-0.377667
23	6	0	-0.140299	1.990837	-0.090278
24	6	0	-0.309413	2.052443	1.268605
25	16	0	-0.510210	3.528252	-0.849888
26	6	0	-0.740414	3.346007	1.721921
27	1	0	-0.150787	1.199108	1.919513
28	6	0	-0.892905	4.243511	0.699536
29	1	0	-0.932221	3.588048	2.760938
30	1	0	-1.202963	5.278723	0.749090
31	6	0	-3.614906	-0.795882	-0.164736
32	6	0	-4.799390	-0.136228	-0.413092
33	16	0	-3.905465	-2.413130	0.459702
34	6	0	-5.956375	-0.923277	-0.105591
35	1	0	-4.836697	0.877215	-0.798714
36	6	0	-5.632730	-2.166975	0.371735
37	1	0	-6.975384	-0.577112	-0.233769
38	1	0	-6.300796	-2.960670	0.680159
39	1	0	-2.217592	0.752355	-0.763613



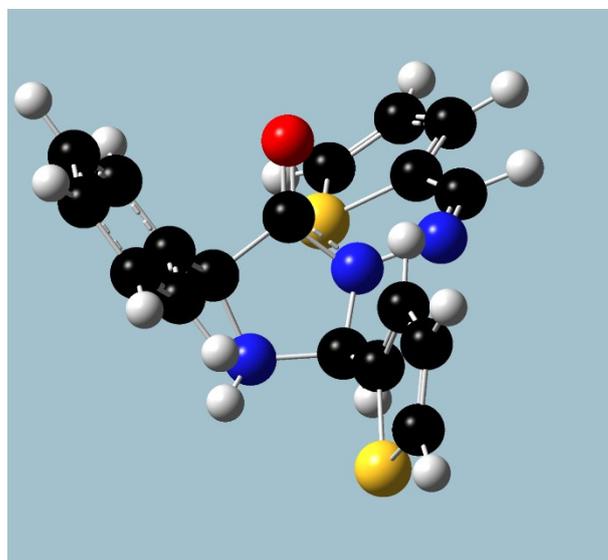
Gibbs energy= -1729.742994 h (T= 298.15K, P= 1 atm)

I. Species (1S_N,2S_C,5S_C)-(Z) – **5b**

BMK/6-31++G(df,pd) in benzene CPCM-UFF

Center Number	Atomic Number	Atomic Type	Coordinates (Å)		
			X	Y	Z
1	6	0	0.226331	1.229055	-0.872930
2	6	0	0.400333	-1.161001	-0.923312
3	1	0	-0.268871	1.985993	-1.490496
4	1	0	-0.178706	-1.895334	-1.499029
5	6	0	-0.521690	-0.705768	0.225483
6	8	0	-1.002233	-1.397028	1.096809
7	7	0	-0.741244	0.636227	0.038507
8	7	0	0.564262	0.062310	-1.705506
9	1	0	1.469306	0.150573	-2.150186
10	6	0	1.649595	-1.878306	-0.402774
11	6	0	1.499582	-3.204054	0.042374
12	6	0	2.921565	-1.288887	-0.364245
13	6	0	2.595790	-3.923126	0.527692
14	1	0	0.516595	-3.666633	0.012967
15	6	0	4.023893	-2.013959	0.112411
16	1	0	3.068580	-0.265474	-0.695488
17	6	0	3.865855	-3.329625	0.561072
18	1	0	2.461203	-4.945176	0.870280
19	1	0	5.003532	-1.545020	0.131081
20	1	0	4.721176	-3.888776	0.929063
21	7	0	-1.309219	1.454753	1.030740
22	6	0	-2.560159	1.278343	1.258306
23	1	0	-2.938027	1.886273	2.081215
24	6	0	-3.589246	0.480603	0.595757
25	6	0	-4.888588	0.413647	1.064429
26	16	0	-3.441683	-0.384432	-0.930144
27	6	0	-5.764877	-0.333183	0.221188
28	1	0	-5.196929	0.892954	1.987839
29	6	0	-5.126109	-0.817343	-0.893235
30	1	0	-6.814648	-0.498374	0.432792
31	1	0	-5.542585	-1.406870	-1.700045
32	6	0	1.404329	1.860161	-0.142775
33	6	0	1.811211	1.711124	1.155261
34	16	0	2.538486	2.859985	-1.048182
35	6	0	3.046297	2.389539	1.443960
36	1	0	1.247350	1.147914	1.889811
37	6	0	3.562812	3.045623	0.361240
38	1	0	3.517600	2.387028	2.420357
39	1	0	4.465307	3.638197	0.292986

Gibbs energy= -1729.736119 h (T= 298.15K, P= 1 atm)

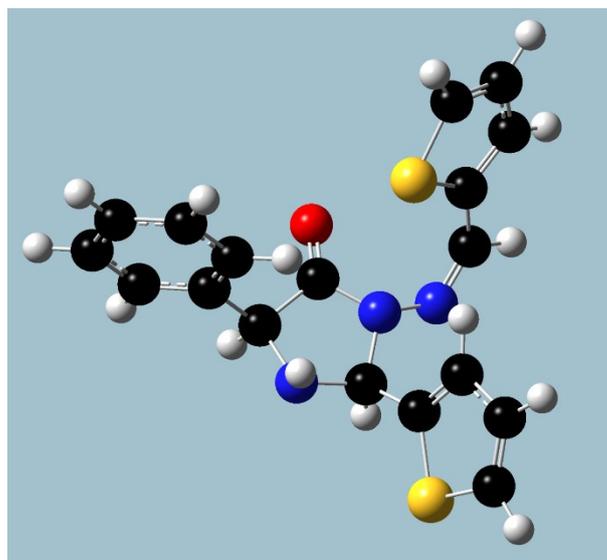


m. Species (1S_N,2S_C,5S_C)-(Z) – 5b

BMK/6-31++G(df,pd) in benzene CPCM-UFF

Center Number	Atomic Number	Atomic Type	Coordinates (Å)		
			X	Y	Z
1	6	0	0.891123	-1.476486	-0.998129
2	6	0	-1.438100	-1.217006	-1.161333
3	1	0	1.182440	-1.874993	-1.980696
4	1	0	-1.732636	-1.617872	-2.140919
5	6	0	-0.744182	0.131163	-1.458842
6	8	0	-1.246938	1.131830	-1.917398
7	7	0	0.595247	-0.040484	-1.156469
8	7	0	-0.382988	-2.058120	-0.577973
9	1	0	-0.439731	-2.033895	0.436120
10	6	0	-2.672193	-1.090455	-0.287360
11	6	0	-3.924866	-1.493723	-0.769234
12	6	0	-2.572515	-0.571354	1.015260
13	6	0	-5.064924	-1.384962	0.038317
14	1	0	-4.008054	-1.892117	-1.776929
15	6	0	-3.708291	-0.465817	1.824297
16	1	0	-1.607795	-0.242536	1.396509
17	6	0	-4.958432	-0.873761	1.336961
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19	1	0	-3.620134	-0.065652	2.830240
20	1	0	-5.840446	-0.790797	1.965181
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26	16	0	0.073488	2.290052	0.797820
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33	6	0	2.411875	-0.889800	1.015908
34	16	0	2.873761	-3.232132	0.015288
35	6	0	3.458506	-1.467329	1.814430
36	1	0	2.000945	0.101197	1.177232
37	6	0	3.811535	-2.722607	1.399728
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Gibbs energy= -1729,74359 h (T= 298.15K, P= 1 atm)



n. Species (1R_N,2R_C,5S_C)-(E) out – 5f

BMK/6-31++G(df,pd) benzene CPCM-UFF

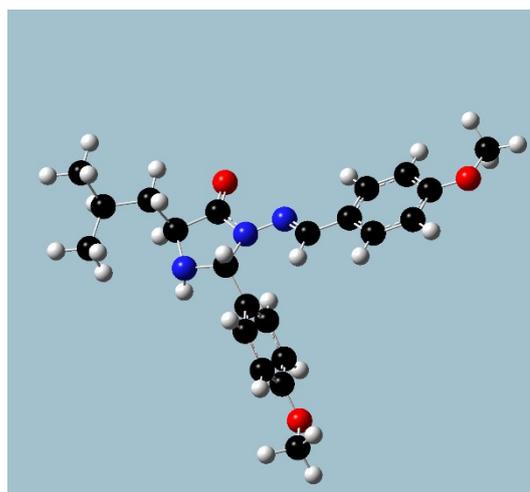
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4	6	0	-1.738123	-1.867006	1.148428
5	8	0	-1.410676	-2.846373	1.783007
6	7	0	-0.895860	-0.924014	0.598405
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8	1	0	-3.236901	0.576483	0.890092
9	7	0	0.453549	-1.190543	0.571057
10	6	0	1.209705	-0.519893	-0.215529
11	1	0	0.835144	0.266885	-0.873147
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13	6	0	-5.272835	-2.551239	-0.334701
14	1	0	-5.640465	-2.783868	0.675261
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17	1	0	-5.300769	-4.654707	-0.957855
18	1	0	-6.802622	-3.773030	-1.306627
19	1	0	-5.360014	-3.493035	-2.299052
20	6	0	-5.901104	-1.217792	-0.783467
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22	1	0	-5.538351	-0.942521	-1.781646
23	1	0	-6.992600	-1.308799	-0.828777
24	1	0	-3.319082	-2.286385	-1.257177
25	6	0	2.660335	-0.779578	-0.272148
26	6	0	3.446859	-0.057332	-1.192619
27	6	0	3.292084	-1.722317	0.556851
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33	1	0	5.429011	0.280268	-1.995996
34	1	0	5.128487	-2.677759	1.129621
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36	1	0	8.506225	-2.237762	-0.092457
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45	1	0	-1.588668	2.067097	-2.054001
46	6	0	-0.416021	3.298024	1.431337
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P= 1 atm)



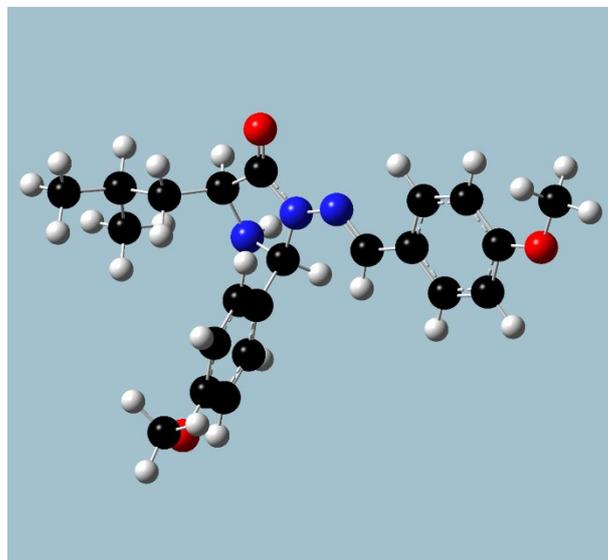
o. Species (1R_N,2S_C,5S_C)-(E) out – 5f

BMK/6-31++G(df,pd) benzene CPCM-UFF

Center Number	Atomic Number	Atomic Type	Coordinates (Å)		
			X	Y	Z
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5	6	0	-1.125819	-2.406728	-0.308273
6	8	0	-0.766492	-3.143435	-1.202094
7	7	0	-0.351130	-1.492215	0.366248
8	7	0	-2.369931	-1.455096	1.488690
9	1	0	-2.259012	-2.058225	2.297008
10	7	0	0.984741	-1.375873	0.077401
11	6	0	1.673287	-0.471421	0.668379
12	1	0	1.239146	0.241256	1.374527
13	6	0	-3.534895	-1.728657	-0.757707
14	6	0	-5.006115	-2.137219	-0.519956
15	1	0	-5.047527	-3.236136	-0.533802
16	1	0	-3.229304	-2.096117	-1.745439
17	6	0	-5.883189	-1.608175	-1.671735
18	1	0	-5.522252	-1.962112	-2.644196
19	1	0	-6.922897	-1.933551	-1.553158
20	1	0	-5.872408	-0.510885	-1.683890
21	6	0	-5.551949	-1.648796	0.835577
22	1	0	-4.976959	-2.049586	1.675373
23	1	0	-5.501549	-0.554510	0.892514
24	1	0	-6.598564	-1.951742	0.955540
25	1	0	-3.451587	-0.634170	-0.769232
26	6	0	-1.382281	0.740828	0.818575
27	6	0	-1.959150	1.665920	1.709976
28	6	0	-1.083332	1.162089	-0.478580
29	6	0	-2.237360	2.969155	1.312223
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34	1	0	-2.688000	3.684078	1.993693
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37	6	0	3.844794	0.667901	1.083569
38	6	0	3.808034	-1.191371	-0.465762
39	6	0	5.213379	0.821494	0.880045
40	1	0	3.329674	1.336333	1.769499
41	6	0	5.181046	-1.049417	-0.680787
42	1	0	3.257431	-1.969967	-0.984547
43	6	0	5.892293	-0.038051	-0.004401
44	1	0	5.777701	1.594274	1.392240
45	1	0	5.682703	-1.721910	-1.366460
46	6	0	7.958477	-0.658098	-1.002486
47	1	0	8.990241	-0.307295	-0.952514
48	1	0	7.911756	-1.704615	-0.675131
49	1	0	7.597995	-0.584977	-2.036491
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51	1	0	-2.536577	4.568391	-2.354312
52	1	0	-2.304028	6.180273	-1.619226
53	1	0	-0.905167	5.089928	-1.834968

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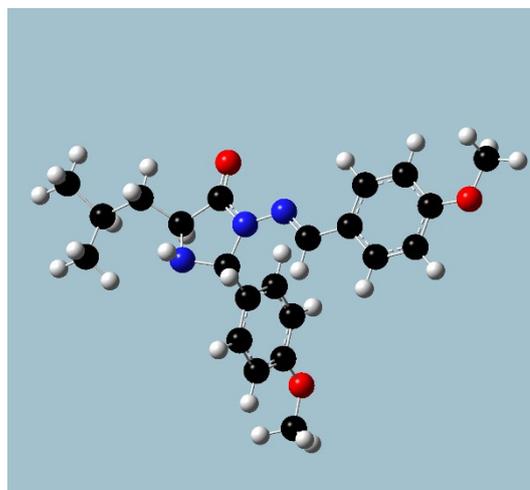


p. Species (1S_N,2R_C,5S_C)-(E) out – 5f

BMK/6-31++G(df,pd) benzene CPCM-UFF

Center Number	Atomic Number	Atomic Type	Coordinates (Å)		
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5	8	0	-1.122790	-2.765983	1.494555
6	7	0	-0.558092	-1.188733	-0.104590
7	7	0	-2.635079	-0.760784	-1.014831
8	7	0	0.798989	-1.296672	0.069386
9	6	0	1.565212	-0.483713	-0.558104
10	1	0	1.183316	0.310417	-1.204477
11	6	0	-3.821569	-2.666802	0.179810
12	6	0	-5.319658	-2.289171	0.206497
13	1	0	-5.481925	-1.640469	1.078770
14	1	0	-3.598979	-3.303702	1.044300
15	6	0	-6.169192	-3.563205	0.387841
16	1	0	-5.896664	-4.098985	1.304068
17	1	0	-7.235471	-3.315934	0.437541
18	1	0	-6.020583	-4.243156	-0.460928
19	6	0	-5.766073	-1.527298	-1.057285
20	1	0	-5.201741	-0.600190	-1.190166
21	1	0	-5.611022	-2.152112	-1.947117
22	1	0	-6.832987	-1.282840	-1.002138
23	1	0	-3.606922	-3.267200	-0.717668
24	6	0	3.030883	-0.561651	-0.426759
25	6	0	3.826655	0.387727	-1.100079
26	6	0	3.669504	-1.543290	0.350347
27	6	0	5.214292	0.363104	-0.998111
28	1	0	3.350284	1.154709	-1.706130
29	6	0	5.061841	-1.581354	0.462107
30	1	0	3.066520	-2.281032	0.870736
31	6	0	5.842902	-0.621962	-0.212936
32	1	0	5.831244	1.094094	-1.511178
33	1	0	5.524450	-2.350252	1.069395
34	6	0	7.883073	-1.521427	0.613336
35	1	0	8.942204	-1.278469	0.516049
36	1	0	7.590414	-1.459047	1.669206
37	1	0	7.705748	-2.540792	0.247412
38	8	0	7.188694	-0.571328	-0.165284
39	1	0	-0.842378	-0.229314	-1.962920
40	6	0	-1.238760	1.202421	-0.396624
41	6	0	-1.649195	2.255263	-1.222920
42	6	0	-0.839462	1.497233	0.917571
43	6	0	-1.675731	3.578611	-0.764665
44	1	0	-1.966394	2.044452	-2.241734
45	6	0	-0.858859	2.808678	1.392531
46	1	0	-0.501441	0.701836	1.576184
47	6	0	-1.278283	3.858205	0.555477
48	1	0	-2.001856	4.368996	-1.430341
49	1	0	-0.547434	3.042478	2.405834
50	8	0	-1.263115	5.094543	1.097197
51	6	0	-1.668581	6.188317	0.305073
52	1	0	-1.572157	7.073634	0.935212
53	1	0	-1.026861	6.298127	-0.578730
54	1	0	-2.712629	6.081149	-0.016672
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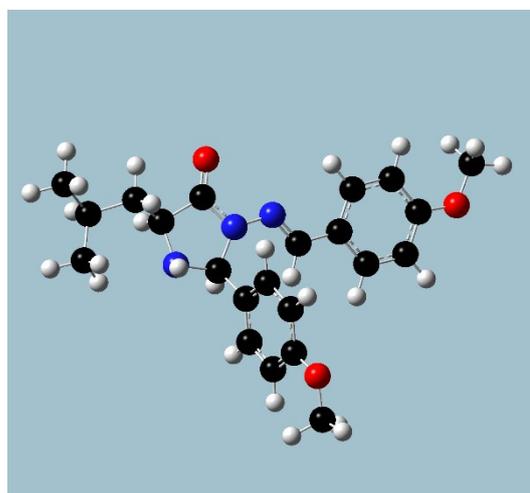


q. Species (1S_N,2S_C,5S_C)-(E) out – 5f

BMK/6-31++G(df,pd) benzene CPCM-UFF

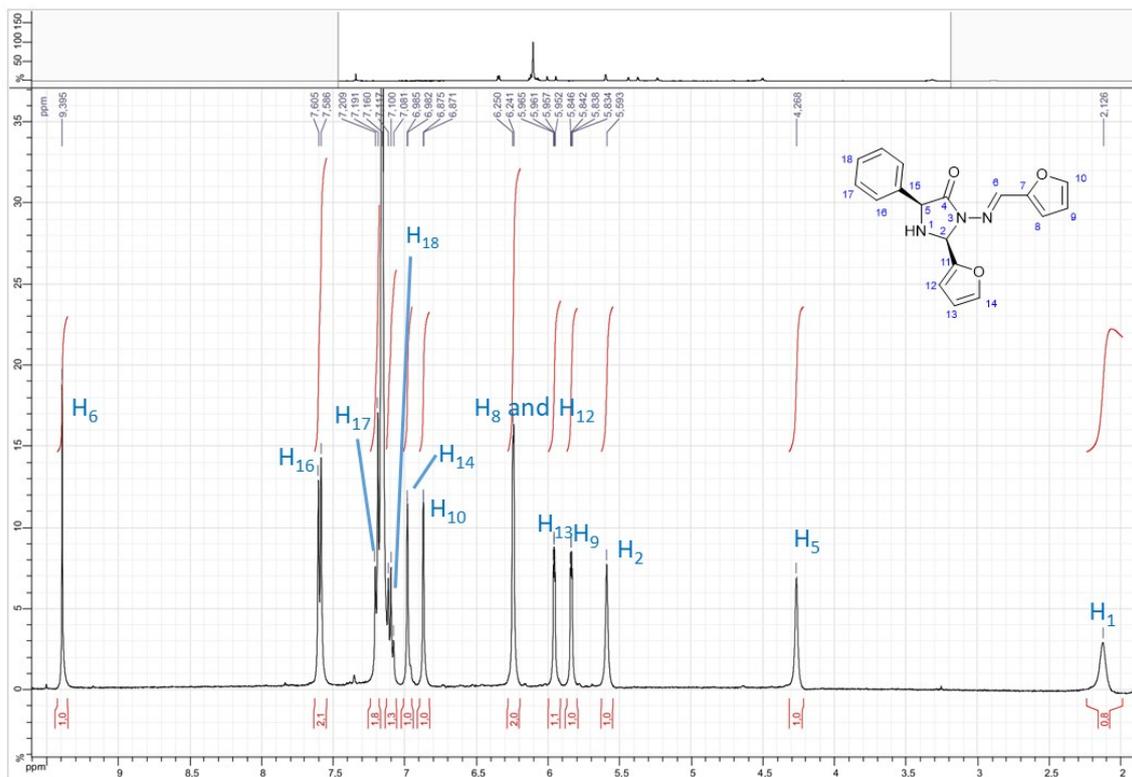
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4	6	0	1.598919	-2.227984	0.109891
5	8	0	1.305684	-3.278273	0.639257
6	7	0	0.756912	-1.164704	-0.132538
7	7	0	2.847138	-0.409502	-0.782095
8	7	0	-0.596812	-1.350533	0.028461
9	6	0	-1.411940	-0.514405	-0.497719
10	1	0	-1.086083	0.354407	-1.072514
11	6	0	4.119809	-2.220023	0.467530
12	6	0	5.528269	-2.246049	-0.167283
13	1	0	5.479927	-2.890273	-1.056569
14	1	0	3.883604	-3.219745	0.851350
15	6	0	6.526404	-2.870735	0.828304
16	1	0	6.218452	-3.880349	1.122195
17	1	0	7.529522	-2.929388	0.391451
18	1	0	6.591483	-2.257368	1.736309
19	6	0	6.015128	-0.849544	-0.603035
20	1	0	5.360530	-0.408261	-1.359946
21	1	0	6.043932	-0.173122	0.261957
22	1	0	7.029976	-0.907999	-1.012613
23	1	0	4.116336	-1.538641	1.332244
24	6	0	-2.868981	-0.685809	-0.348136
25	6	0	-3.733266	0.241584	-0.964504
26	6	0	-3.432593	-1.742752	0.386890
27	6	0	-5.115319	0.119462	-0.852722
28	1	0	-3.316024	1.066516	-1.537059
29	6	0	-4.817945	-1.878242	0.509389
30	1	0	-2.774931	-2.462060	0.865254
31	6	0	-5.668862	-0.942985	-0.113348
32	1	0	-5.784648	0.830754	-1.326197
33	1	0	-5.219958	-2.704089	1.084289
34	6	0	-7.633678	-2.022517	0.676806
35	1	0	-8.708644	-1.857691	0.589793
36	1	0	-7.379095	-3.006876	0.263750
37	1	0	-7.343669	-1.988137	1.734749
38	8	0	-7.014755	-0.986701	-0.054739
39	1	0	3.233418	0.130559	-0.012622
40	6	0	1.132622	1.309621	-0.383312
41	6	0	1.050739	2.379217	-1.278140
42	6	0	1.012956	1.567171	0.995194
43	6	0	0.856457	3.694056	-0.827460
44	1	0	1.137616	2.194741	-2.346575
45	6	0	0.817212	2.863759	1.460585
46	1	0	1.058310	0.742313	1.702007
47	6	0	0.739892	3.938451	0.551101
48	1	0	0.797509	4.501791	-1.547162
49	1	0	0.716693	3.072505	2.521277
50	8	0	0.548683	5.158299	1.093025
51	6	0	0.438951	6.273695	0.236671
52	1	0	-0.418377	6.168833	-0.440790
53	1	0	0.288165	7.140426	0.881678
54	1	0	1.353260	6.413565	-0.354180
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Gibbs energy= -1243.419867 h (T= 298.15K,
P= 1 atm)

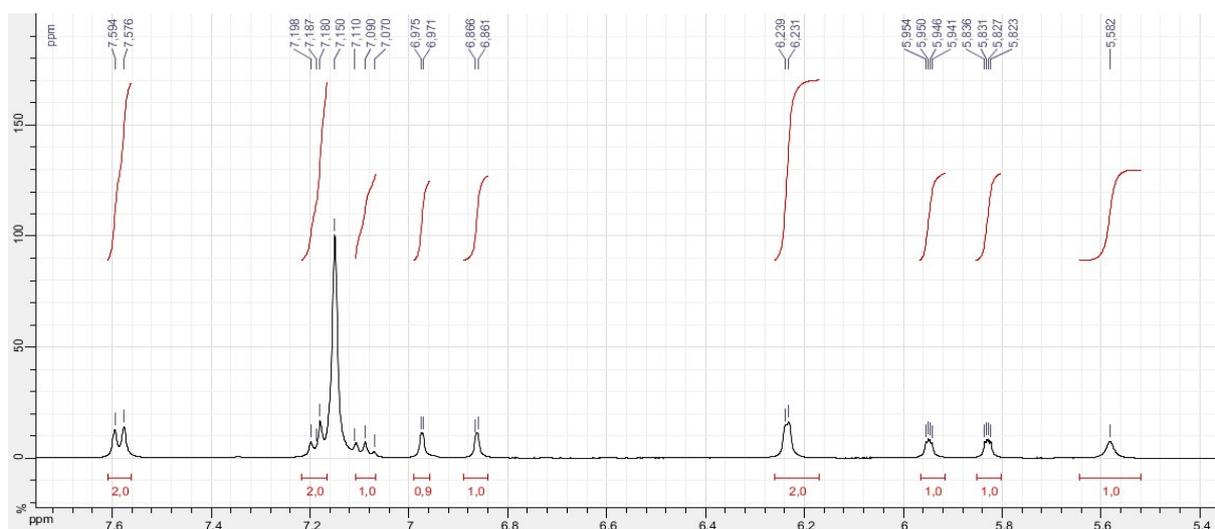


4. Spectrum section for compounds characterization

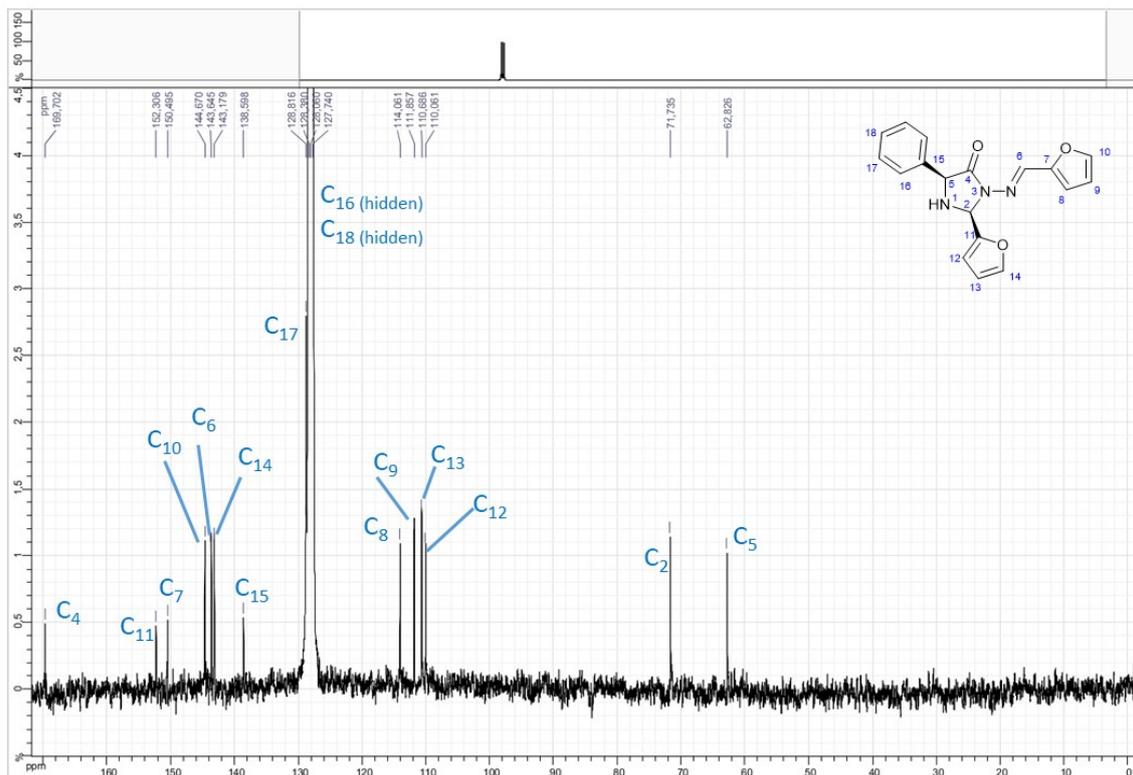
a. NMR spectra of **5a**



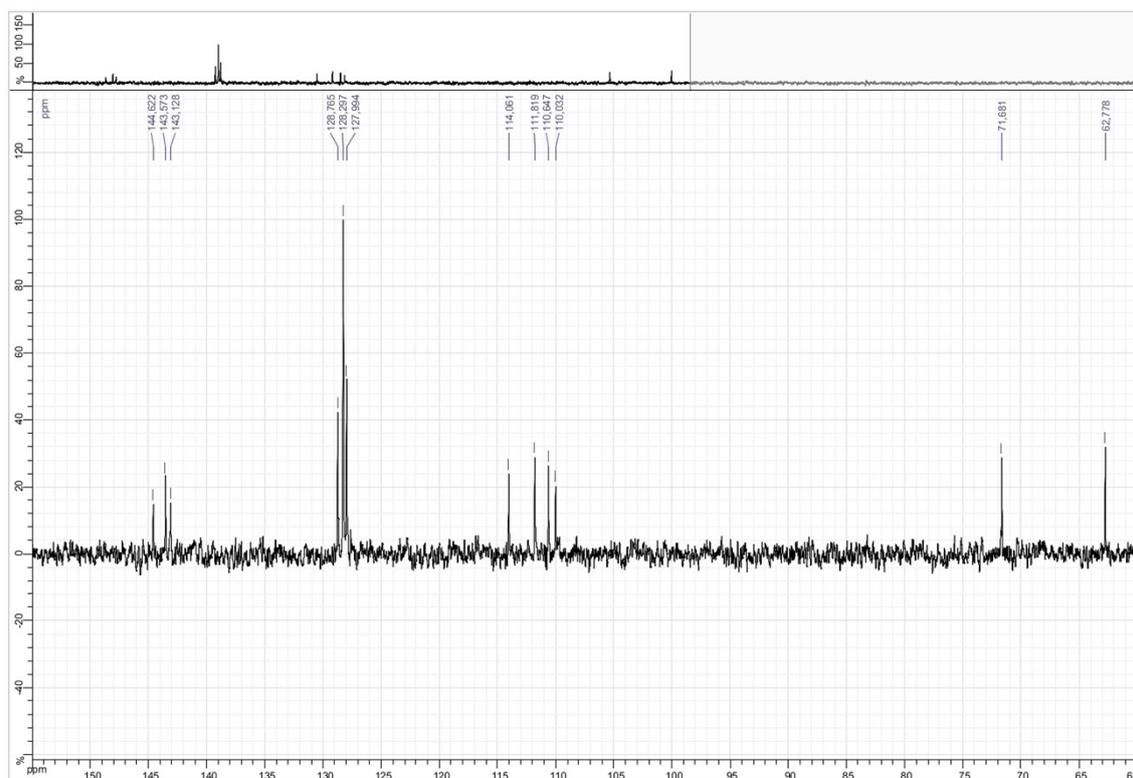
¹H NMR spectrum of compound **5a** in C₆D₆-d₆ at 400 MHz



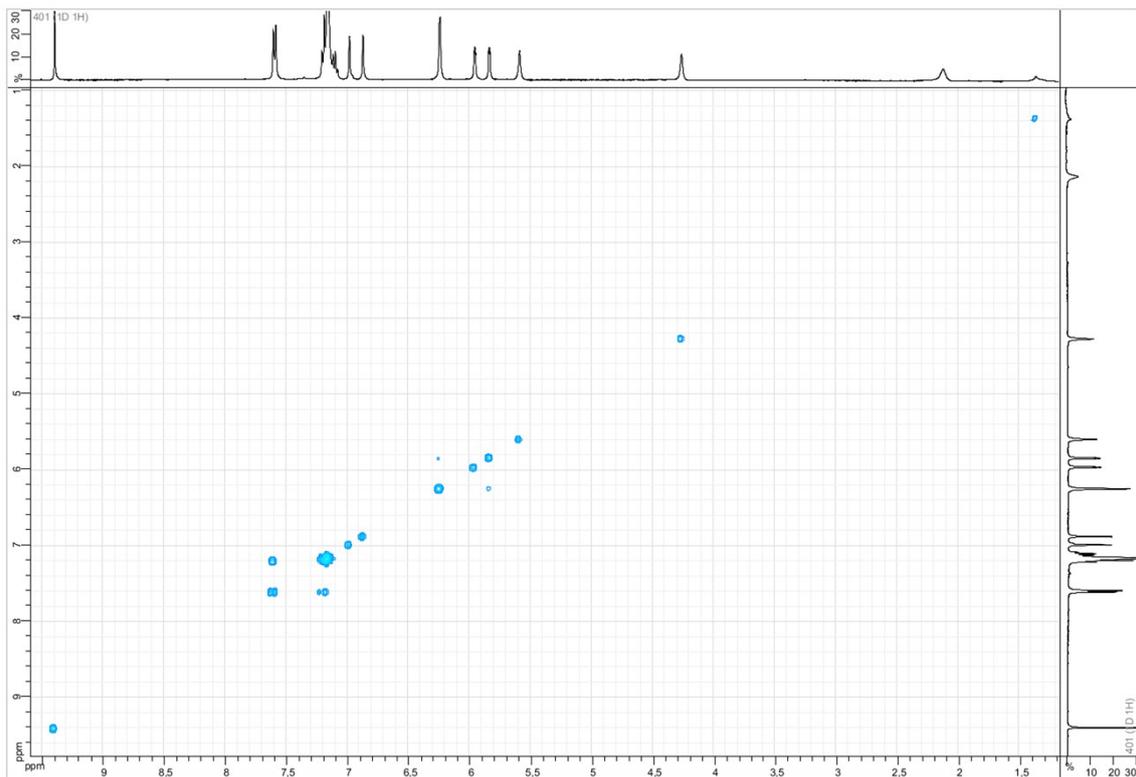
¹H NMR spectrum of compound **5a** in C₆D₆-d₆ at 400 MHz



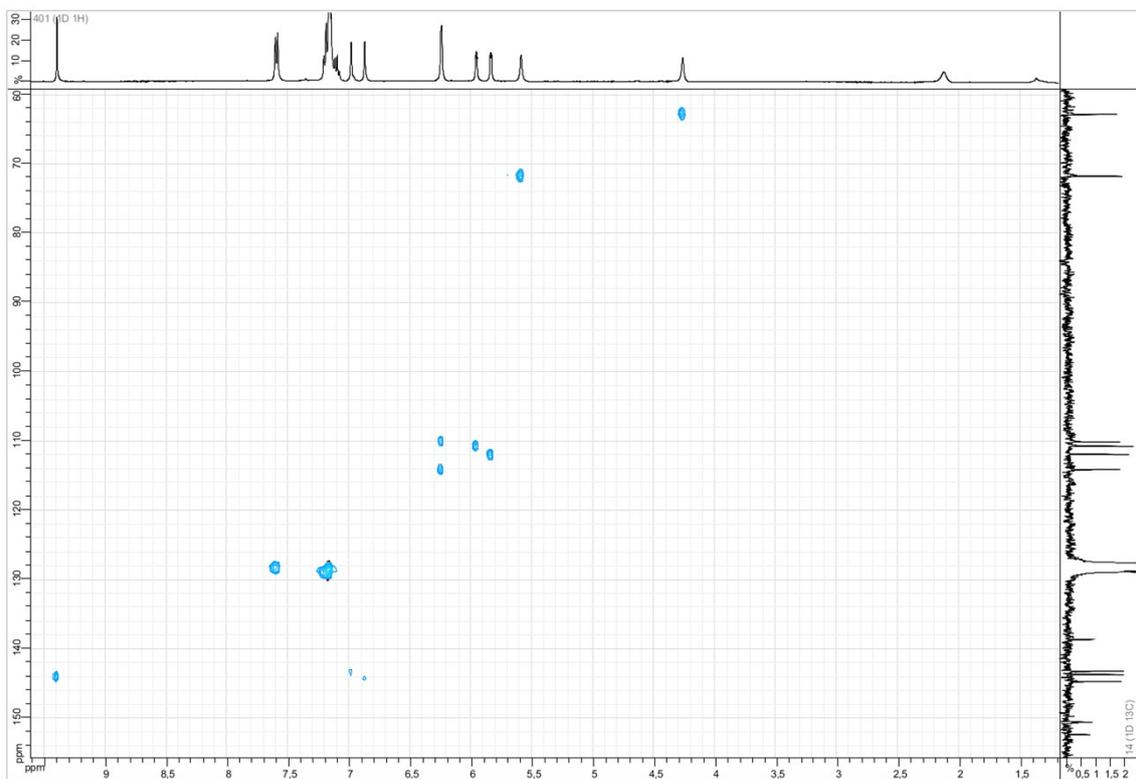
^{13}C NMR spectrum of compound **5a** in C_6D_6-d_6 at 75 MHz



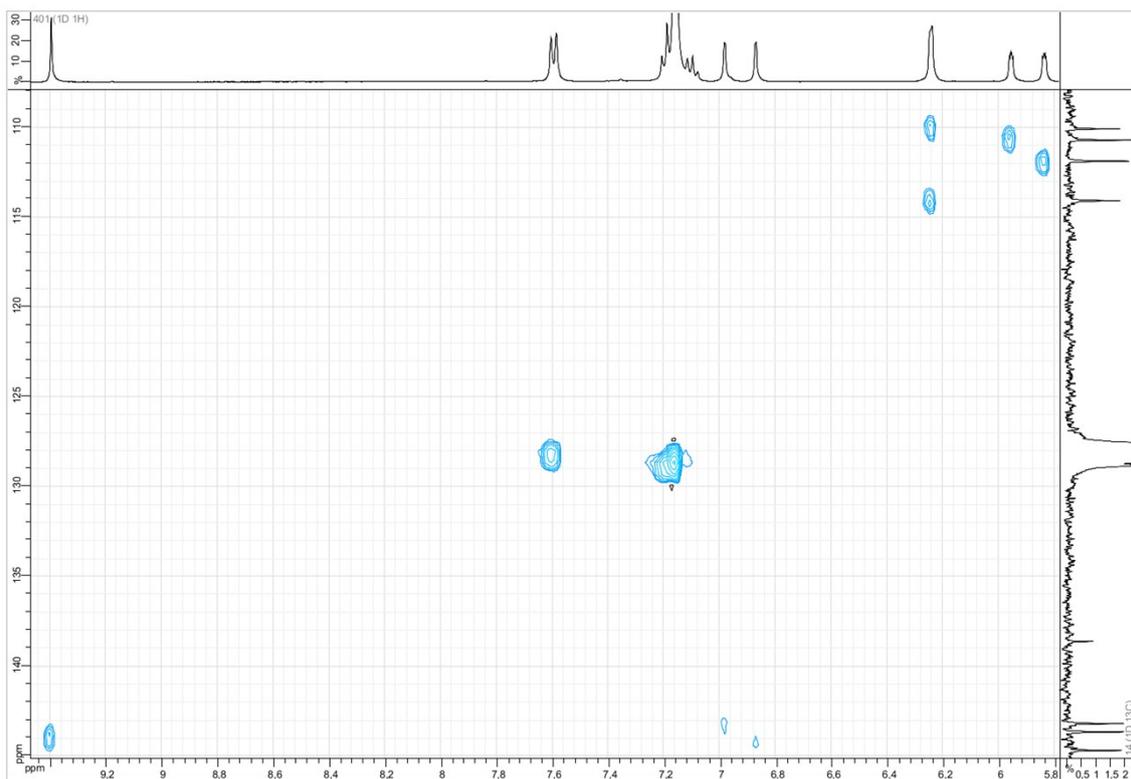
DEPT 135 NMR spectrum of compound **5a** in C_6D_6-d_6 at 75 MHz



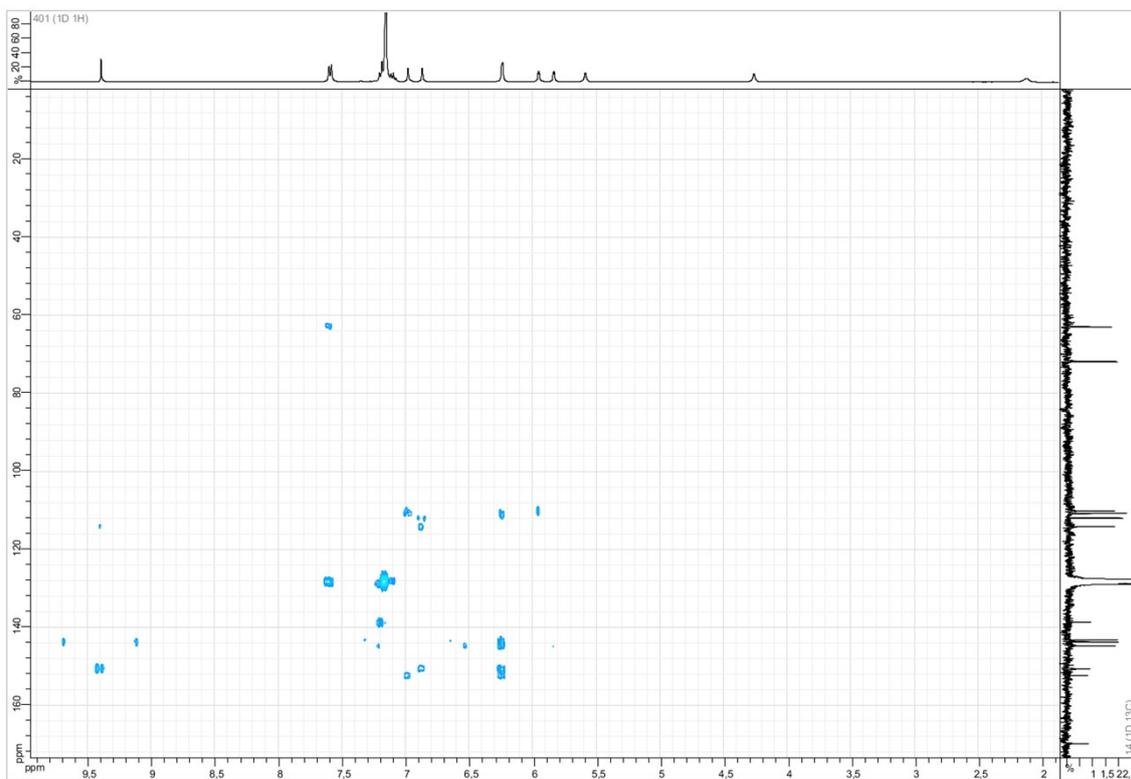
COSY NMR spectrum of compound **5a** in $C_6D_6-d_6$



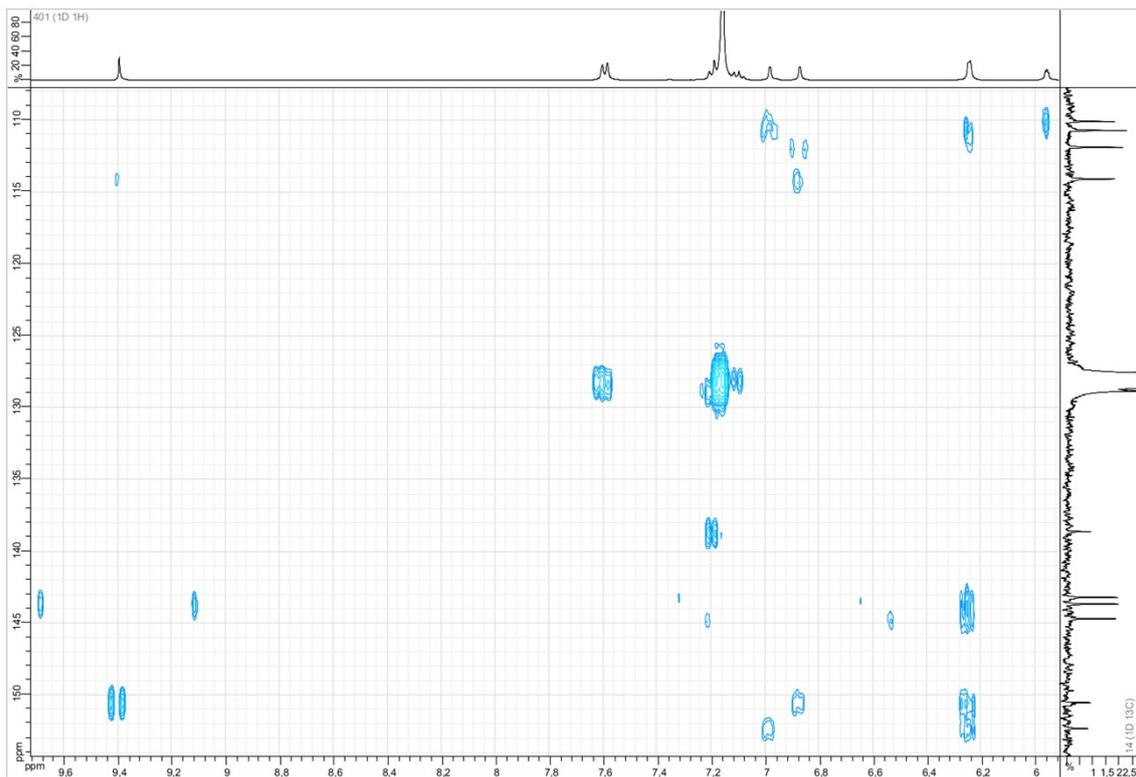
HSQC NMR spectrum of compound **5a** in $C_6D_6-d_6$



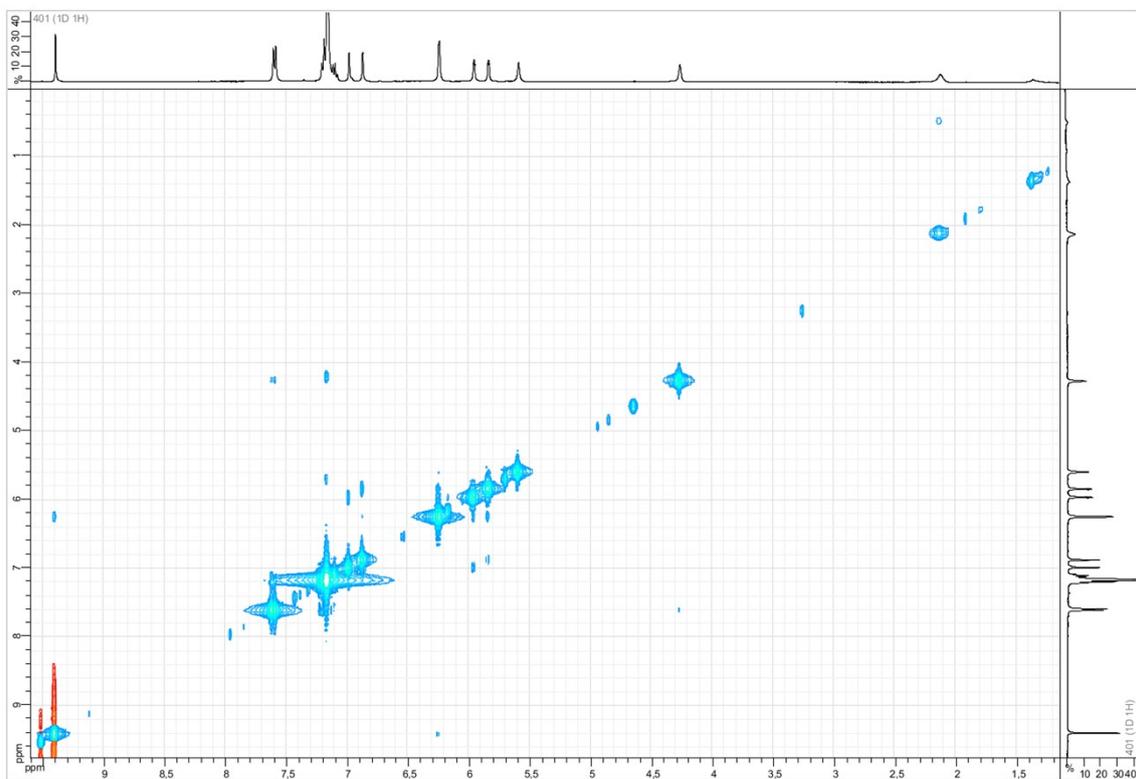
HSQC NMR spectrum of compound **5a** in $C_6D_6-d_6$ (zoom)



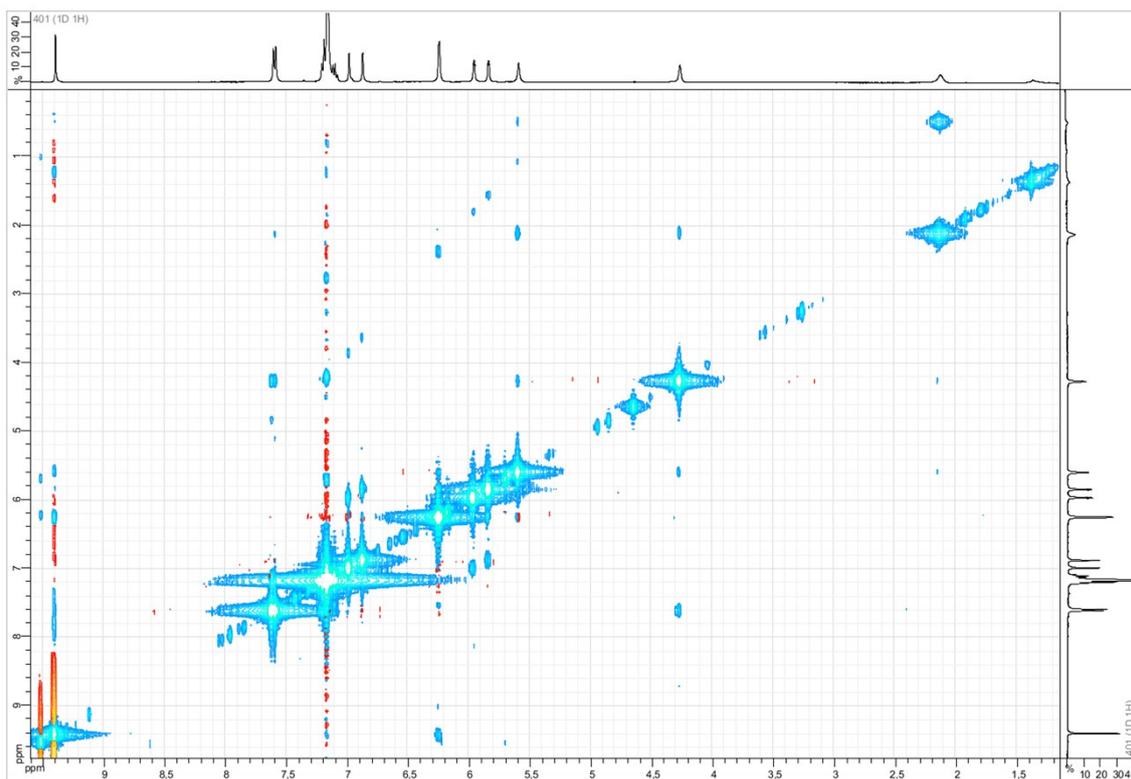
1H - ^{13}C HMBC NMR spectrum of compound **5a** in $C_6D_6-d_6$



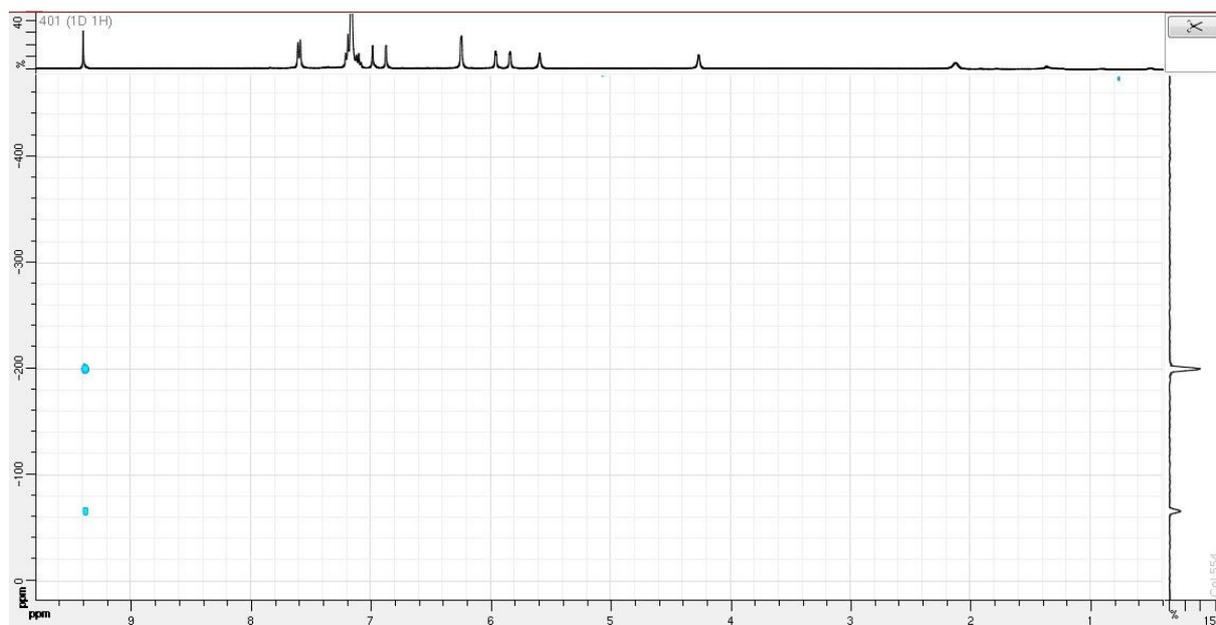
^1H - ^{13}C HMBC NMR spectrum of compound **5a** in C_6D_6 - d_6 (zoom)



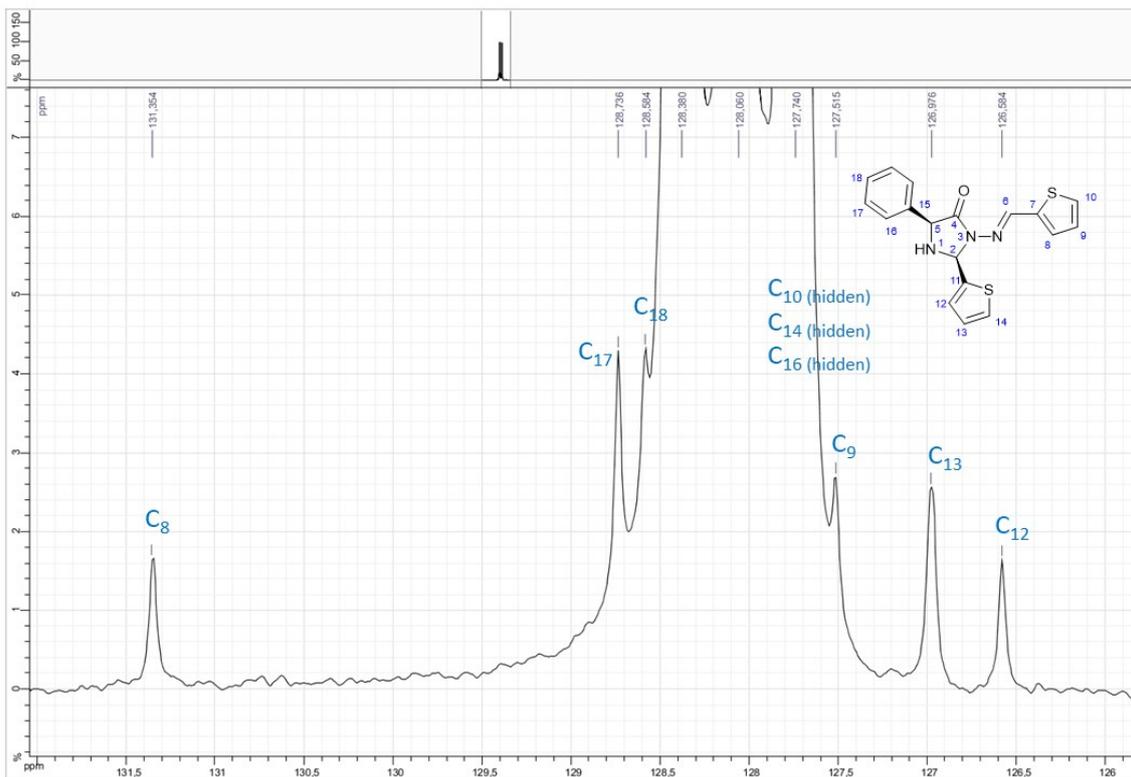
NOESY NMR spectrum of compound **5a** in C_6D_6 - d_6



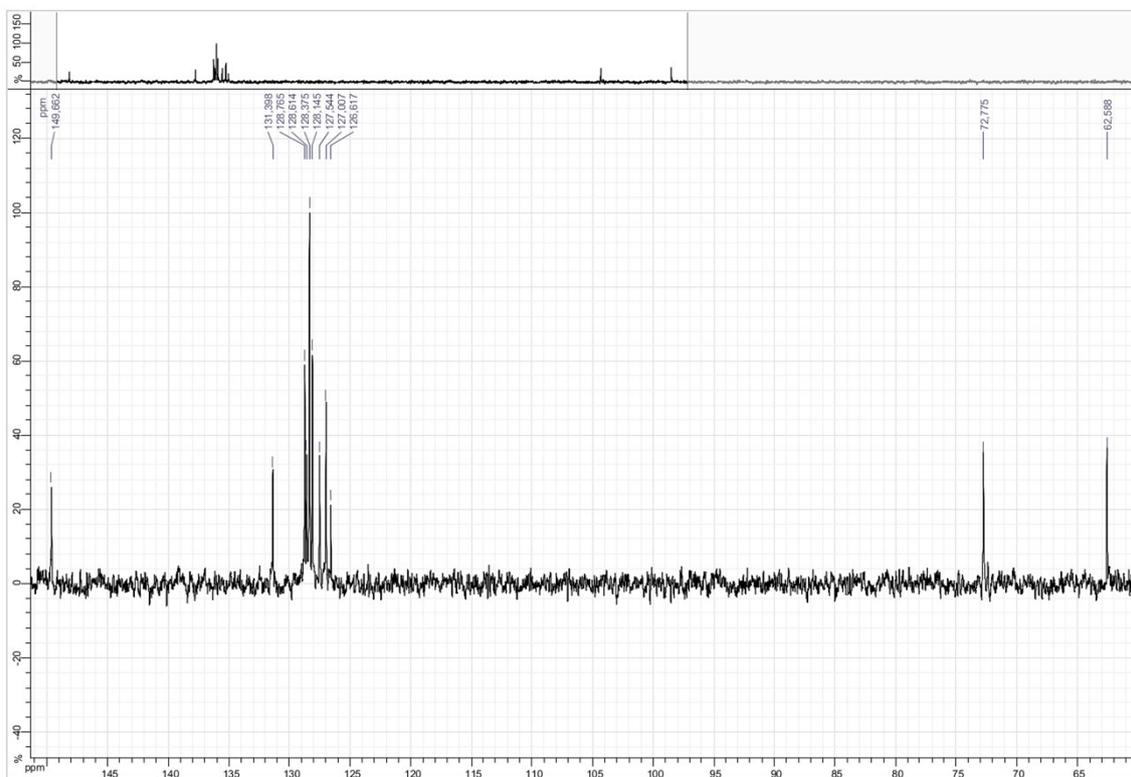
NOESY NMR spectrum of compound **5a** in $C_6D_6-d_6$ (deep cut)



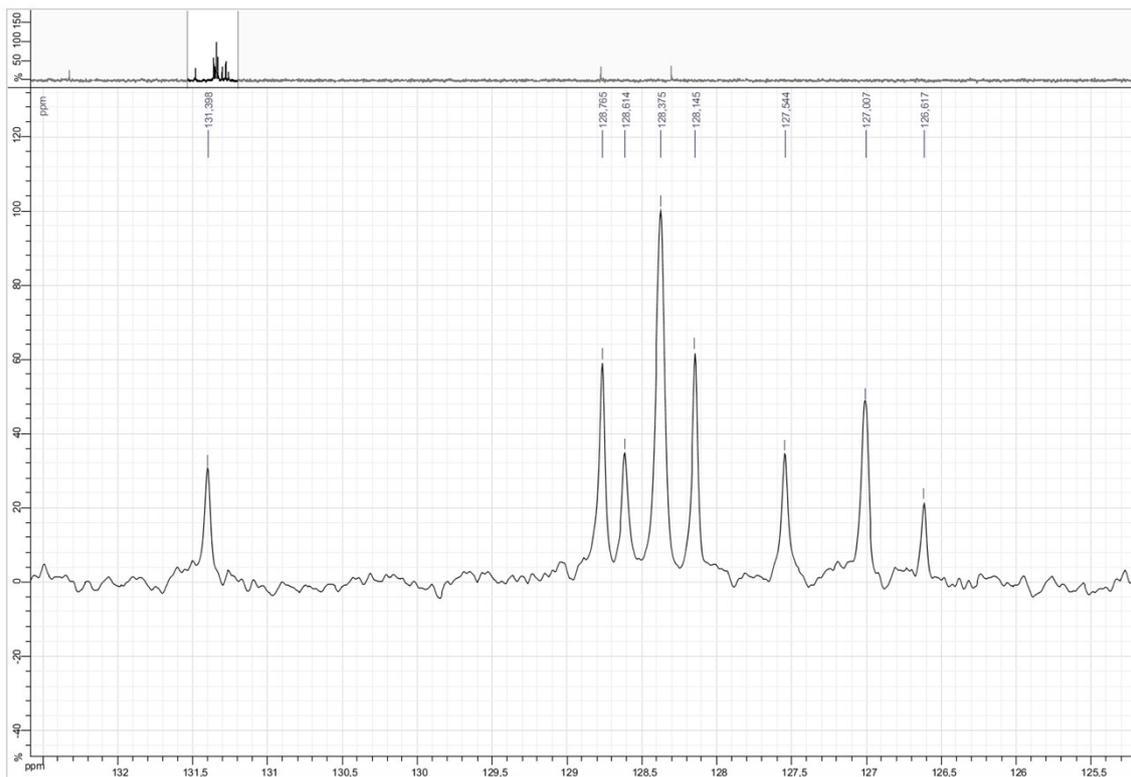
1H - ^{15}N HMBC NMR spectrum of compound **5a** in $C_6D_6-d_6$



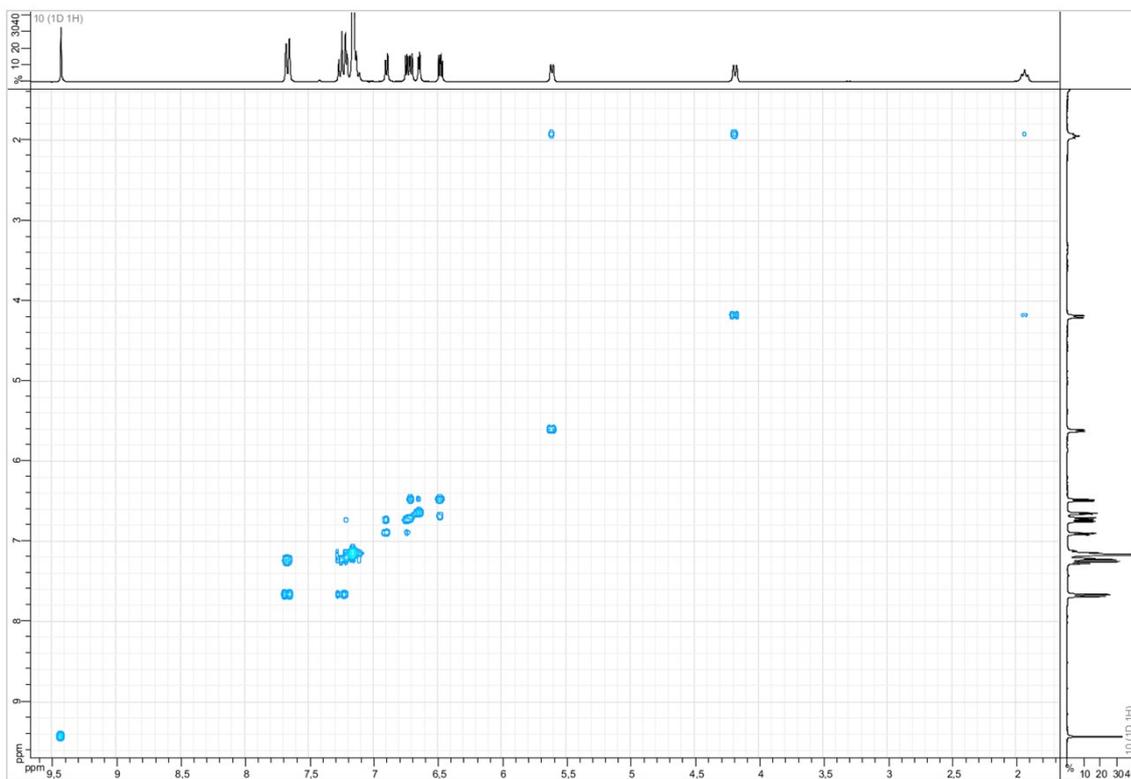
^{13}C NMR spectrum of compound **5b** in C_6D_6-d_6 at 75 MHz (zoom)



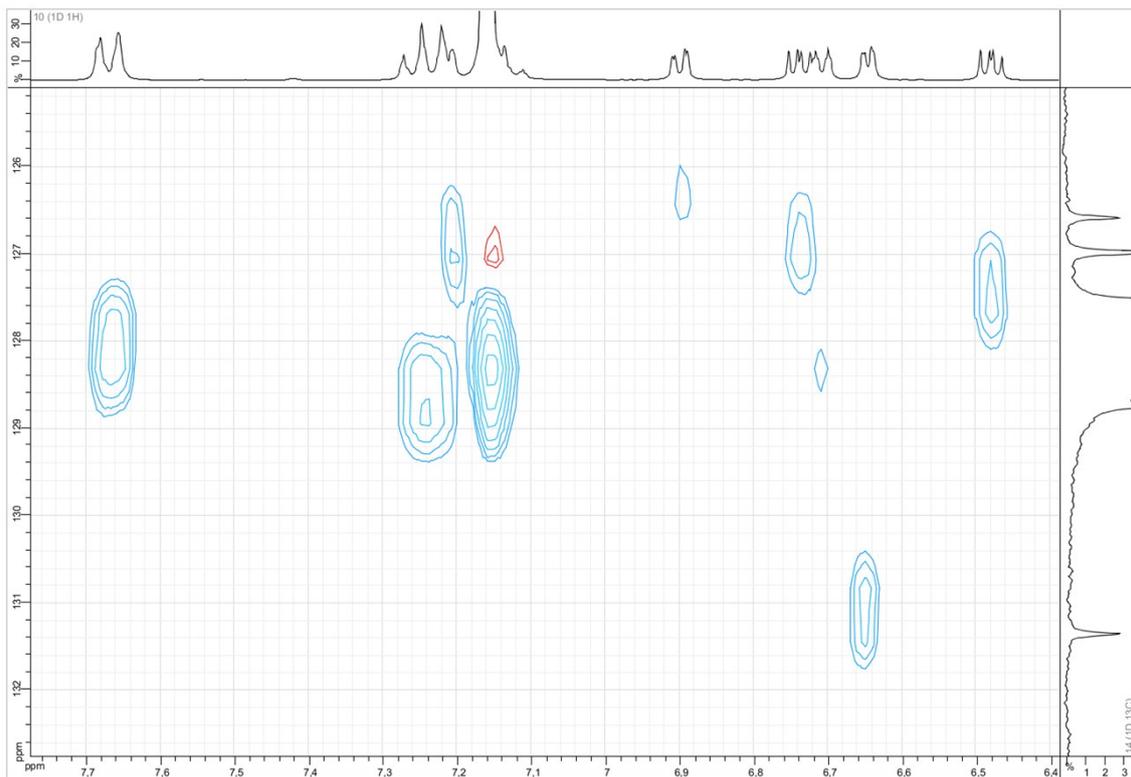
DEPT 135 NMR spectrum of compound **5b** in C_6D_6-d_6 at 75 MHz



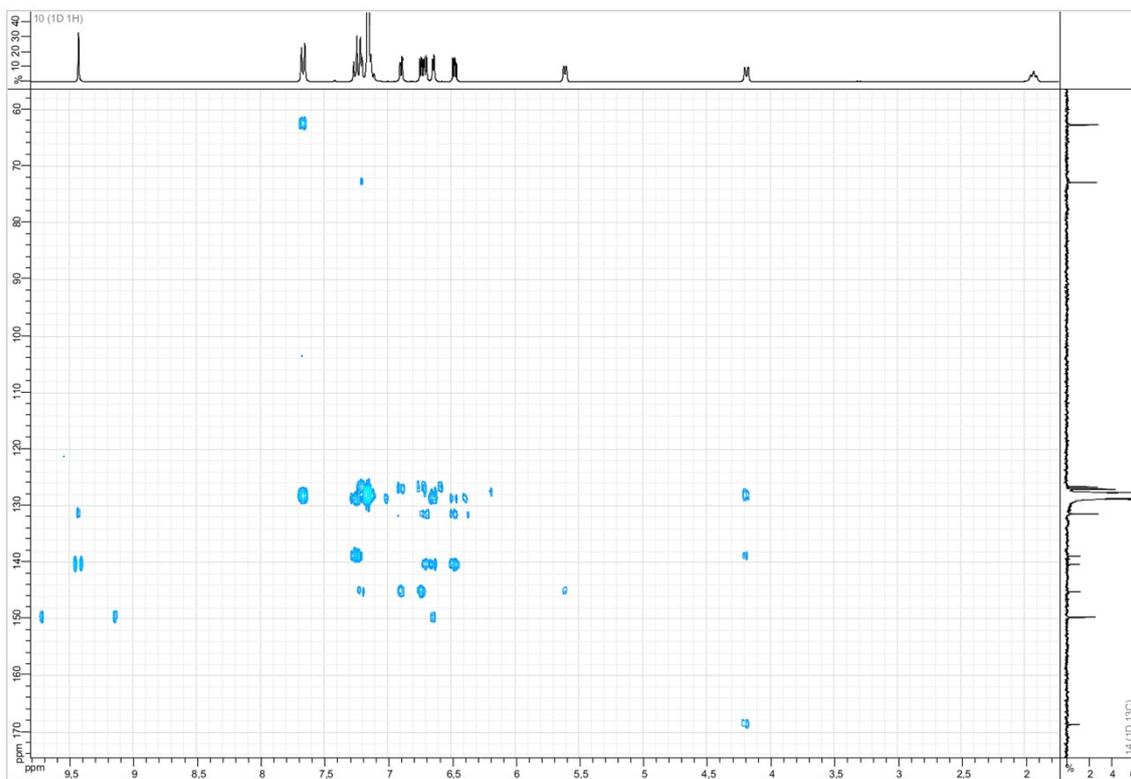
DEPT 135 NMR spectrum of compound **5b** in $C_6D_6-d_6$ at 75 MHz (zoom)



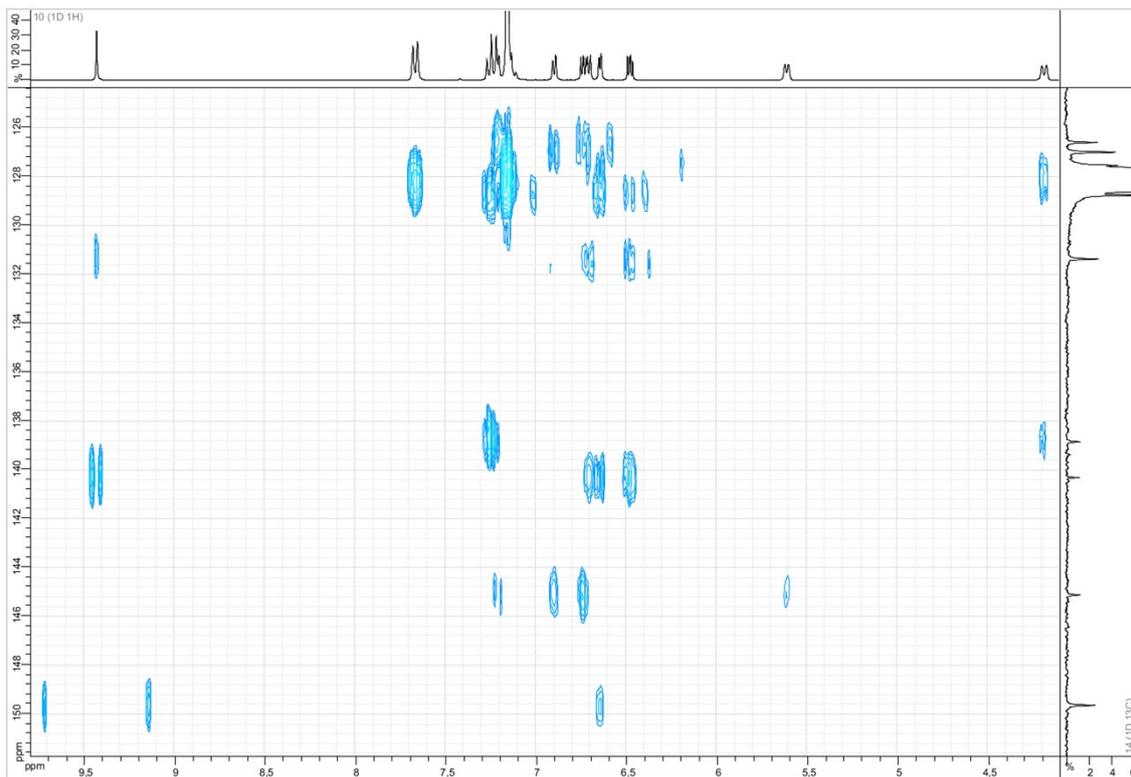
COSY NMR spectrum of compound **5b** in $C_6D_6-d_6$



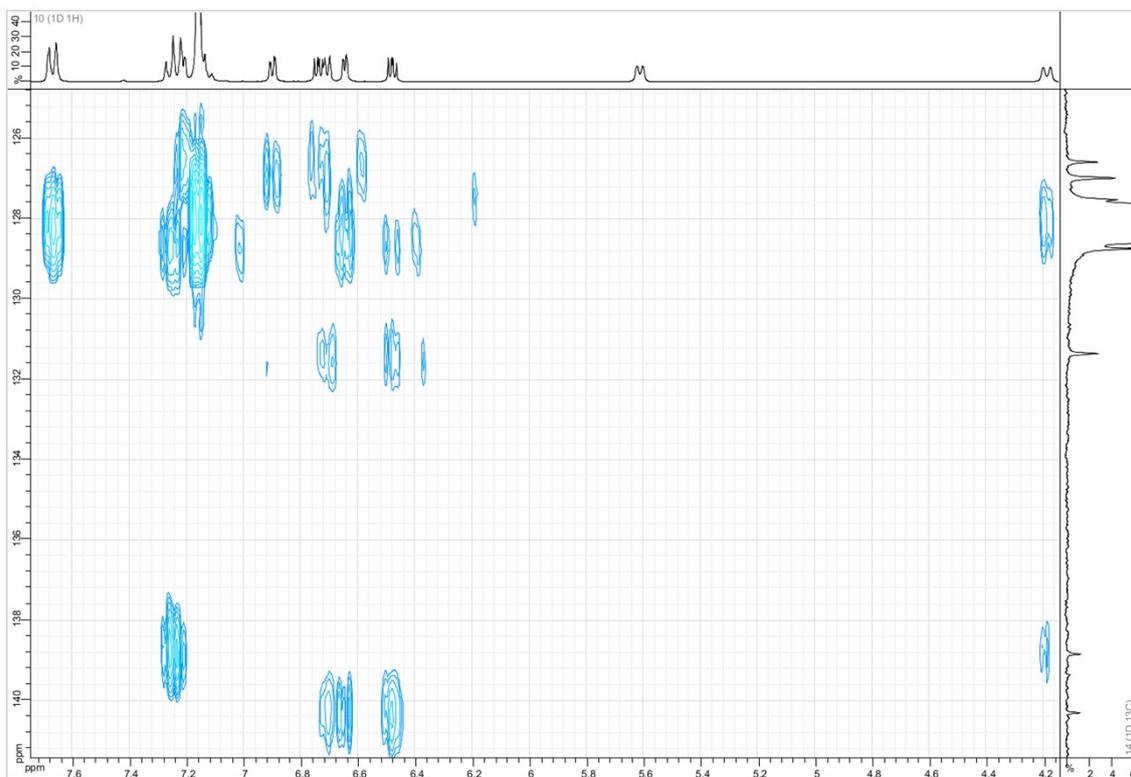
HSQC NMR spectrum of compound **5b** in $C_6D_6-d_6$ (zoom)



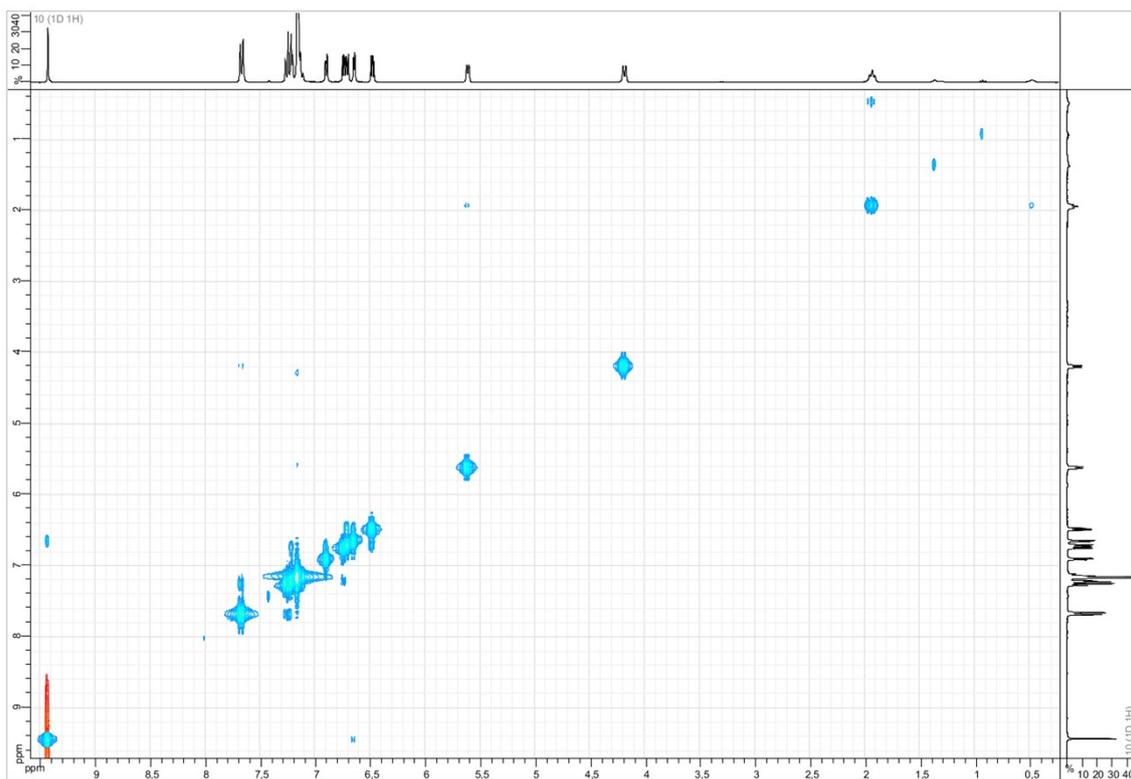
1H - ^{13}C HMBC NMR spectrum of compound **5b** in $C_6D_6-d_6$



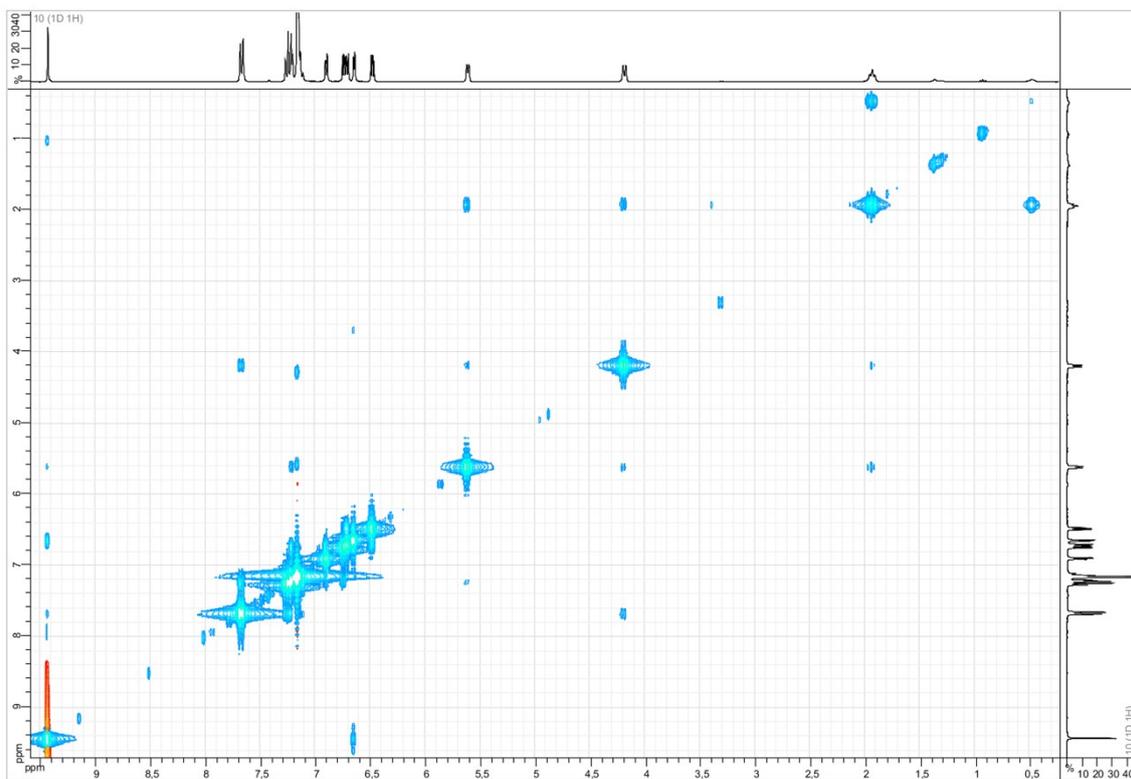
^1H - ^{13}C HMBC NMR spectrum of compound **5b** in C_6D_6 - d_6 (zoom 1)



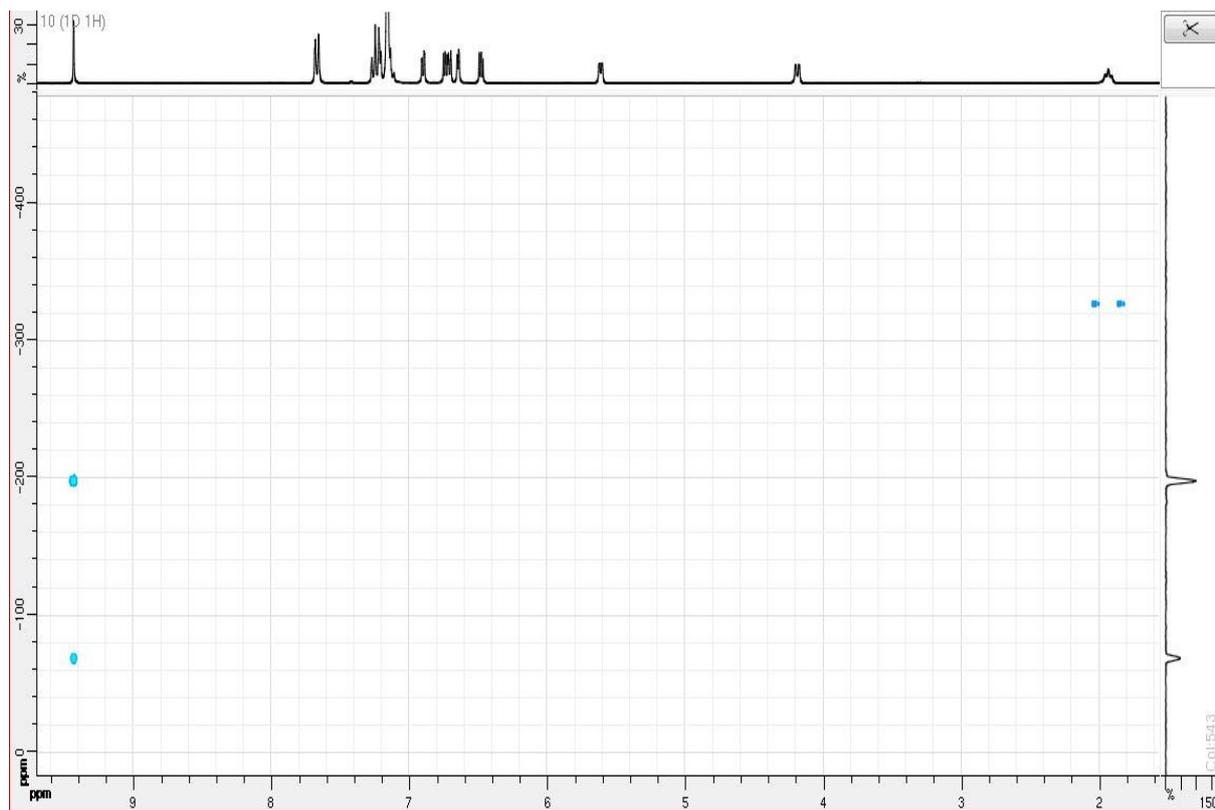
^1H - ^{13}C HMBC NMR spectrum of compound **5b** in C_6D_6 - d_6 (zoom 2)



NOESY NMR spectrum of compound **5b** in $C_6D_6-d_6$

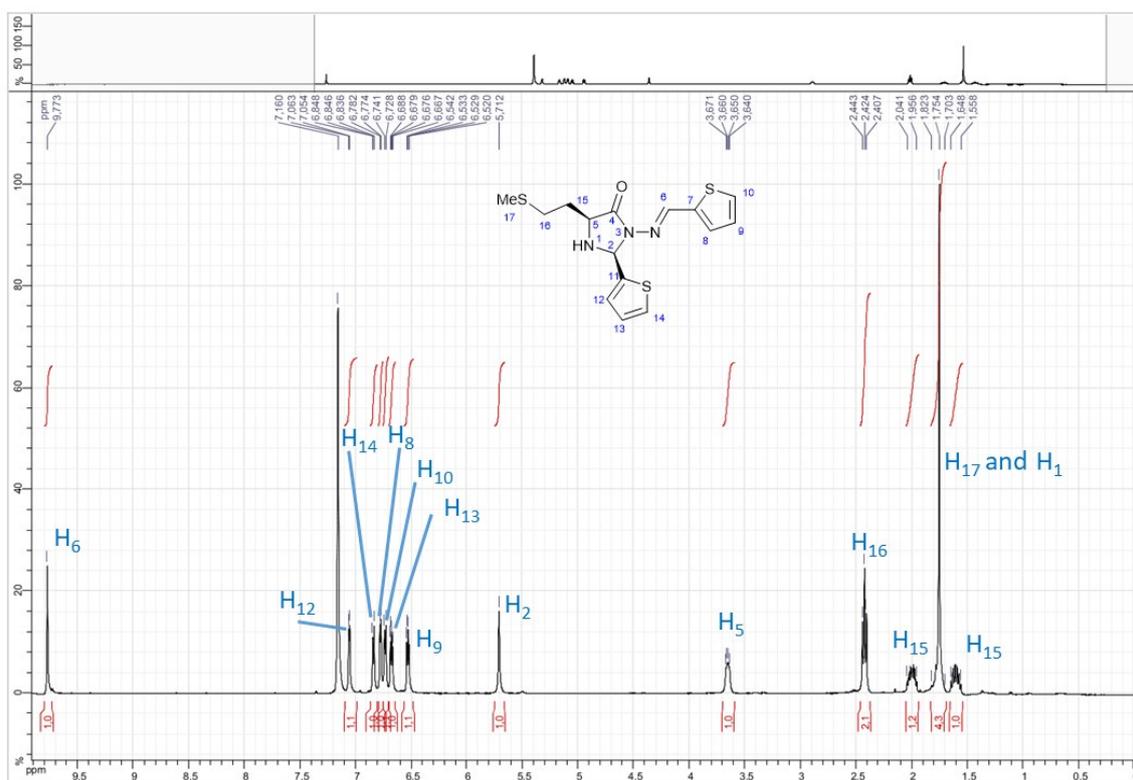


NOESY NMR spectrum of compound **5b** in $C_6D_6-d_6$ (deep cut)

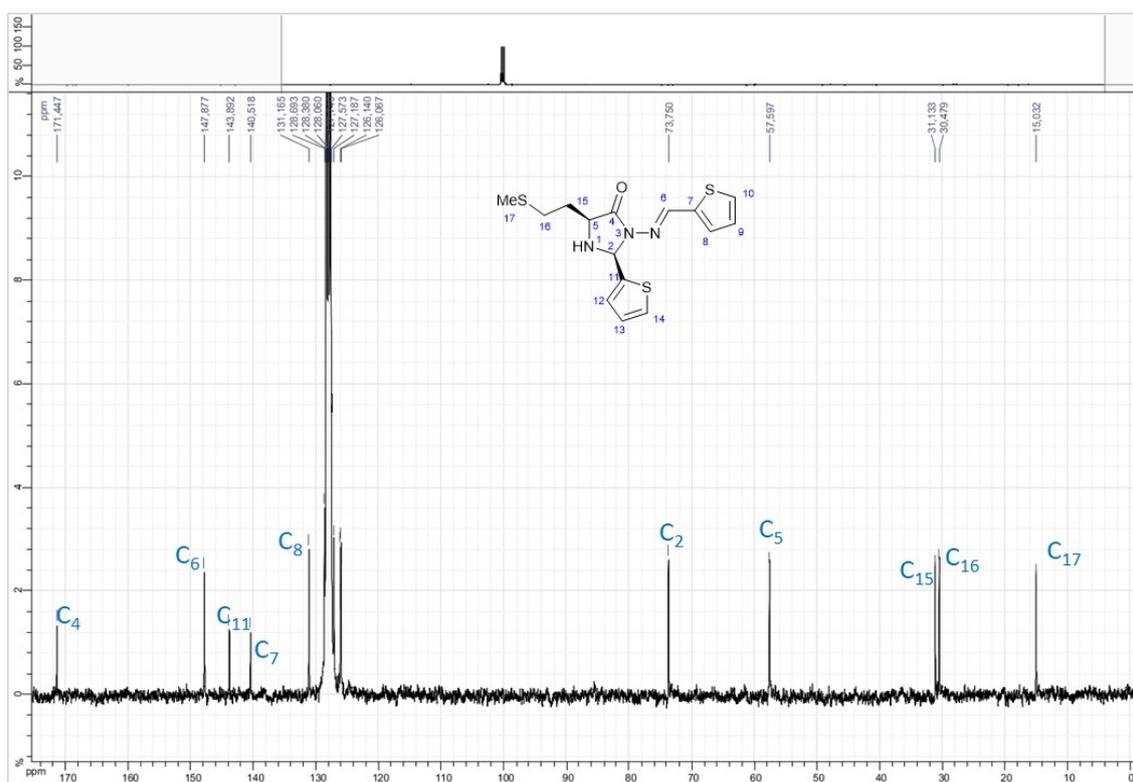


HMBC NMR ^1H - ^{15}N spectrum of compound **5b** in C_6D_6 - d_6

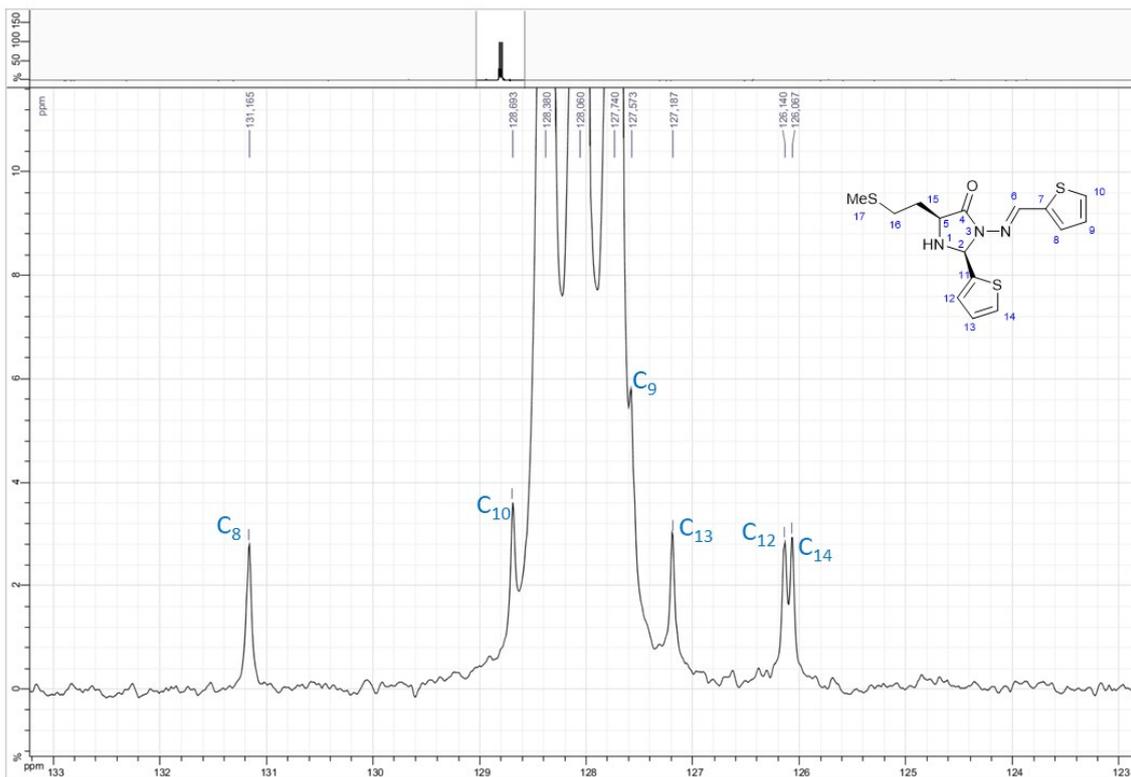
c. NMR spectra of **5c**



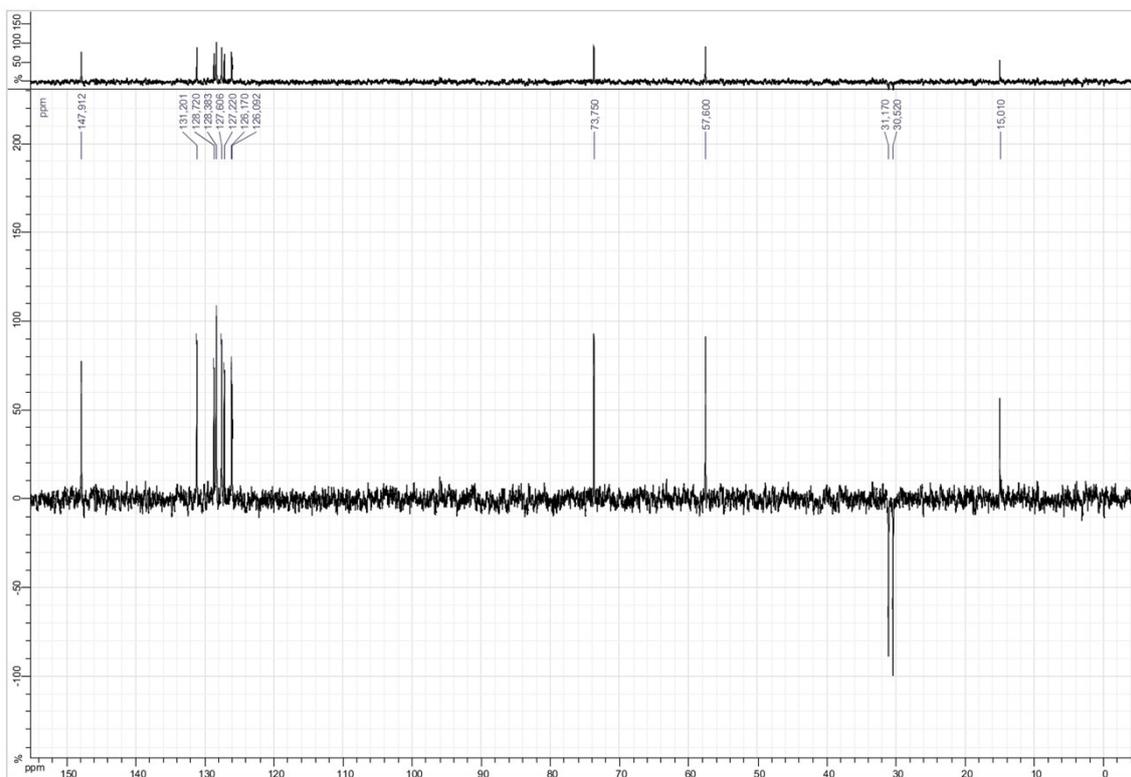
¹H NMR spectrum of compound **5c** in C₆D₆-d₆ at 400 MHz



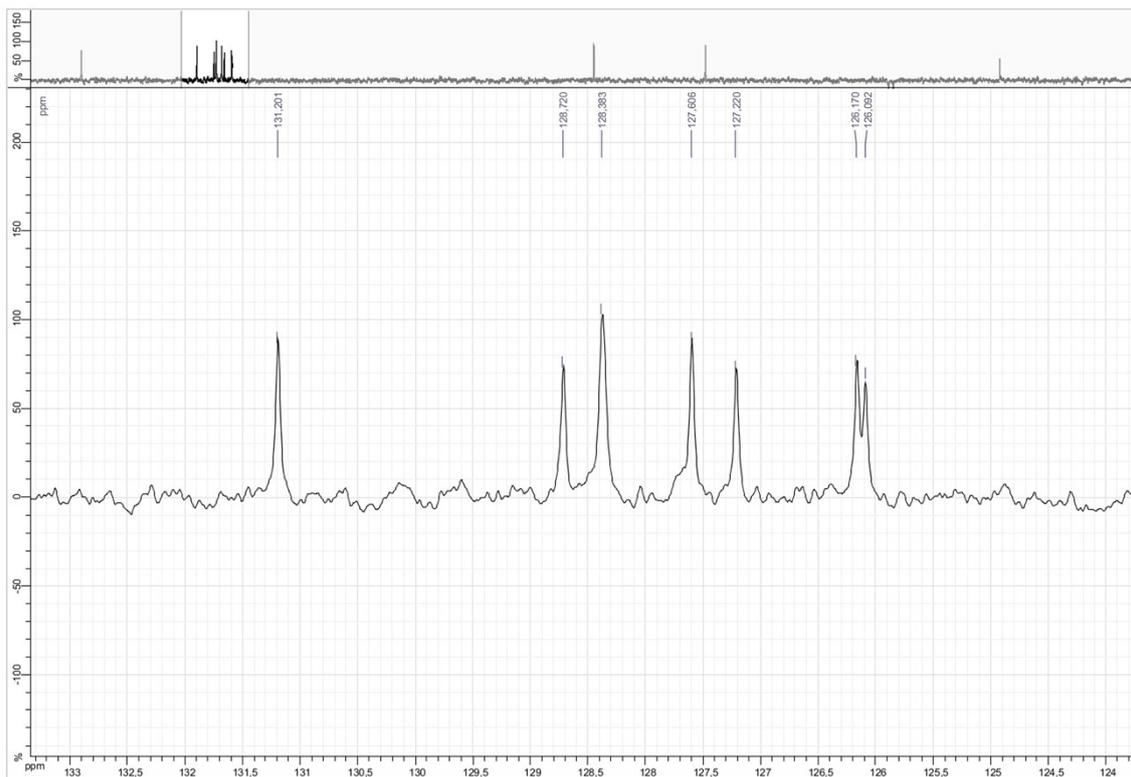
¹³C NMR spectrum of compound **5c** in C₆D₆-d₆ at 75 MHz



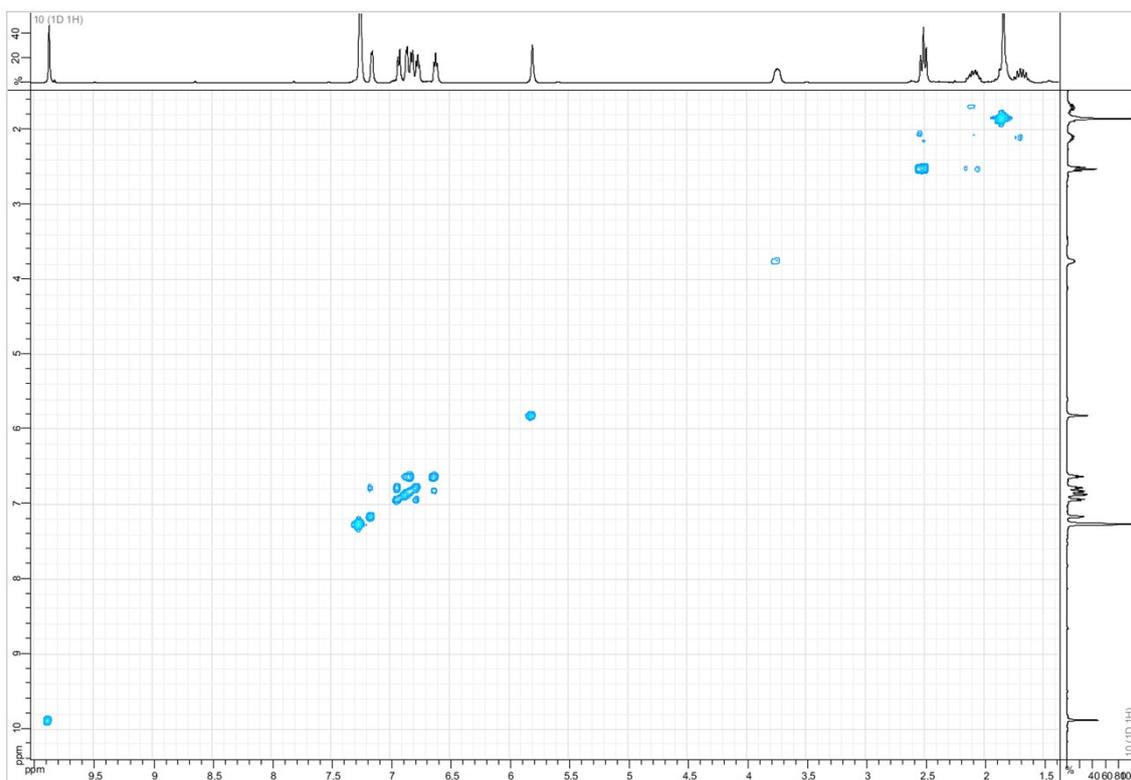
^{13}C NMR spectrum of compound **5c** in C_6D_6-d_6 at 75 MHz (zoom)



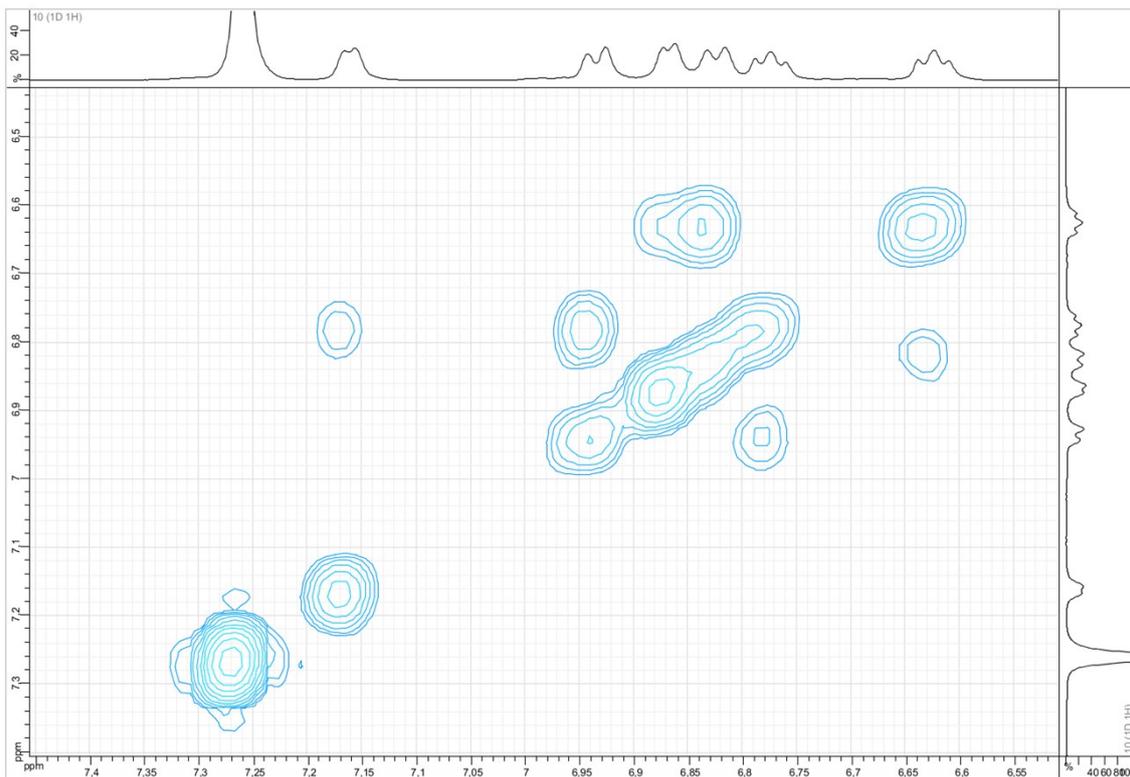
DEPT 135 NMR spectrum of compound **5c** in C_6D_6-d_6 at 75 MHz



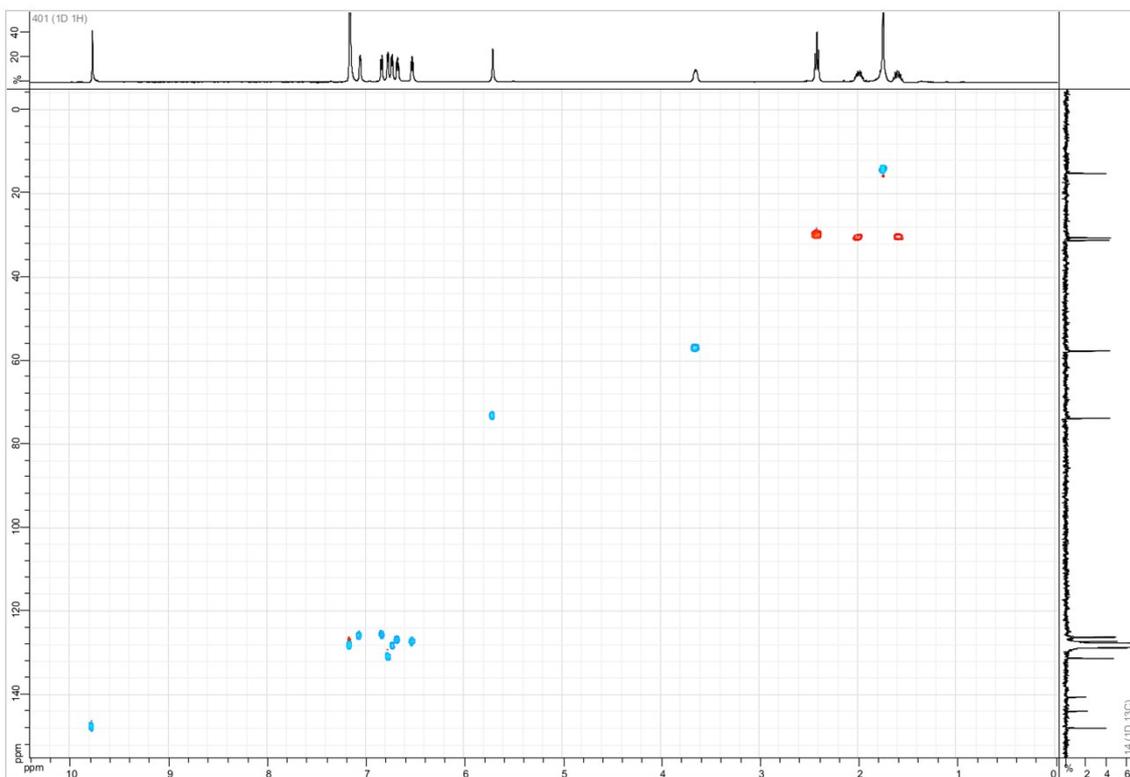
DEPT 135 NMR spectrum of compound **5c** in $C_6D_6-d_6$ at 75 MHz (zoom)



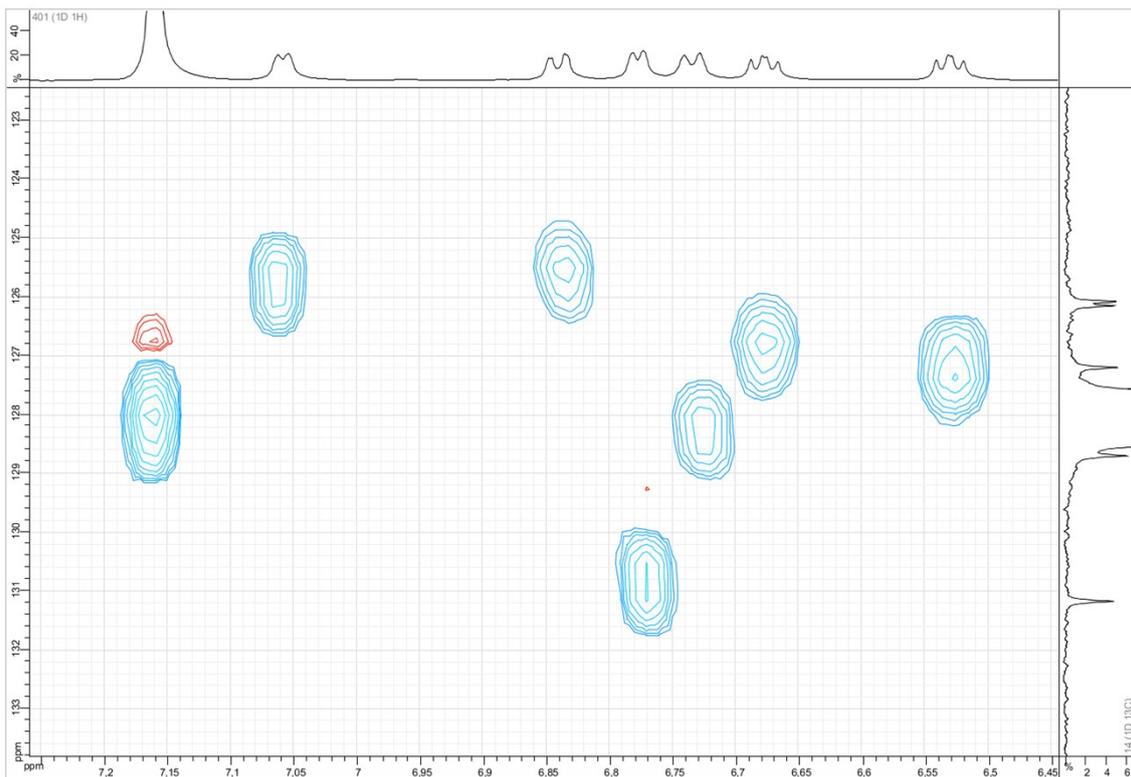
COSY NMR spectrum of compound **5c** in $C_6D_6-d_6$



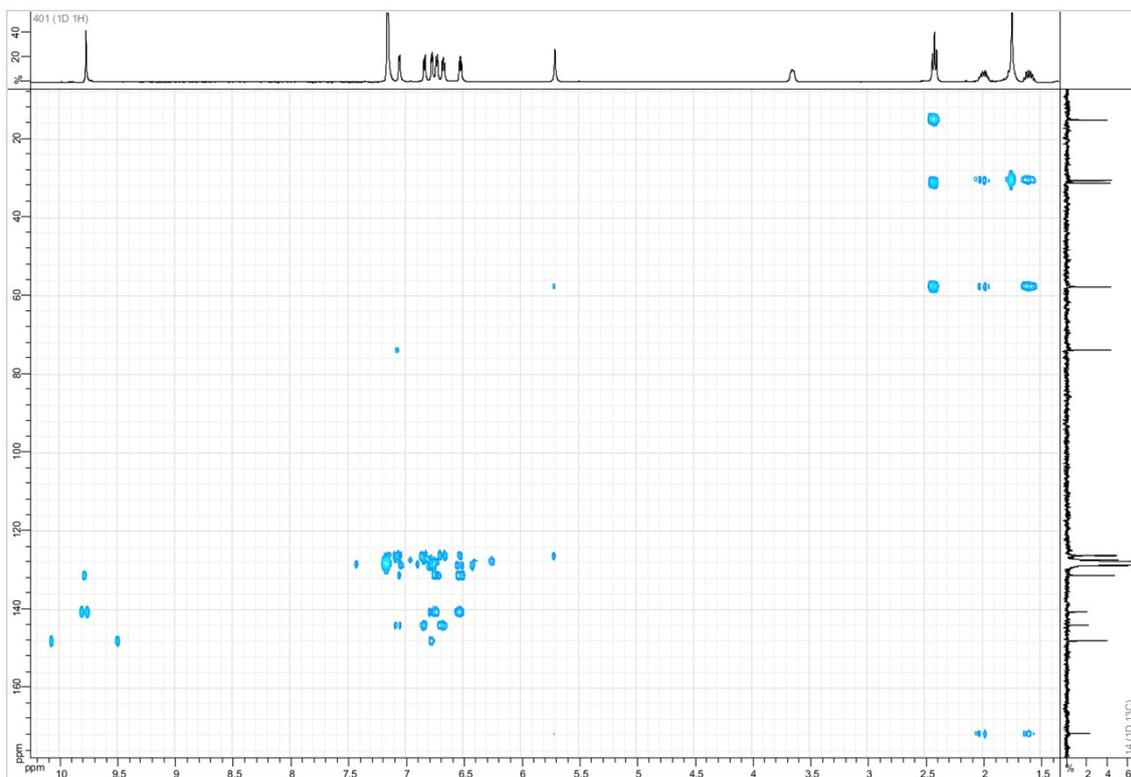
COSY NMR spectrum of compound **5c** in $C_6D_6-d_6$ (zoom)



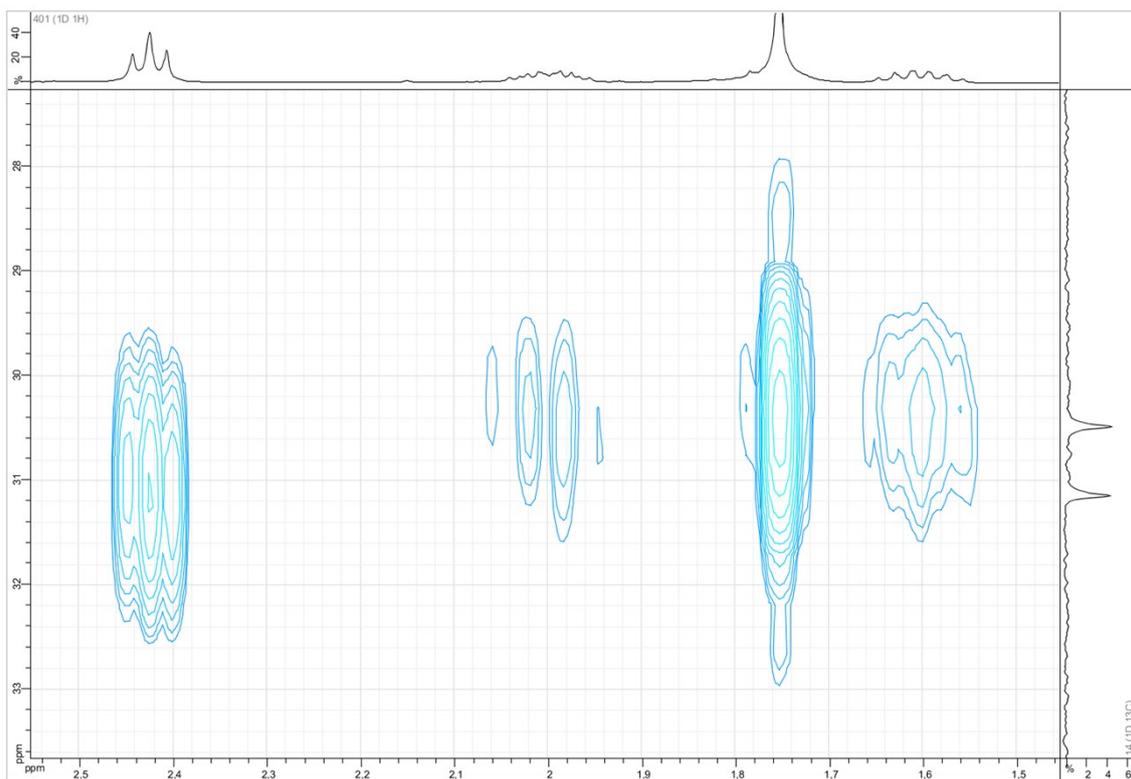
HSQC NMR spectrum of compound **5c** in $C_6D_6-d_6$



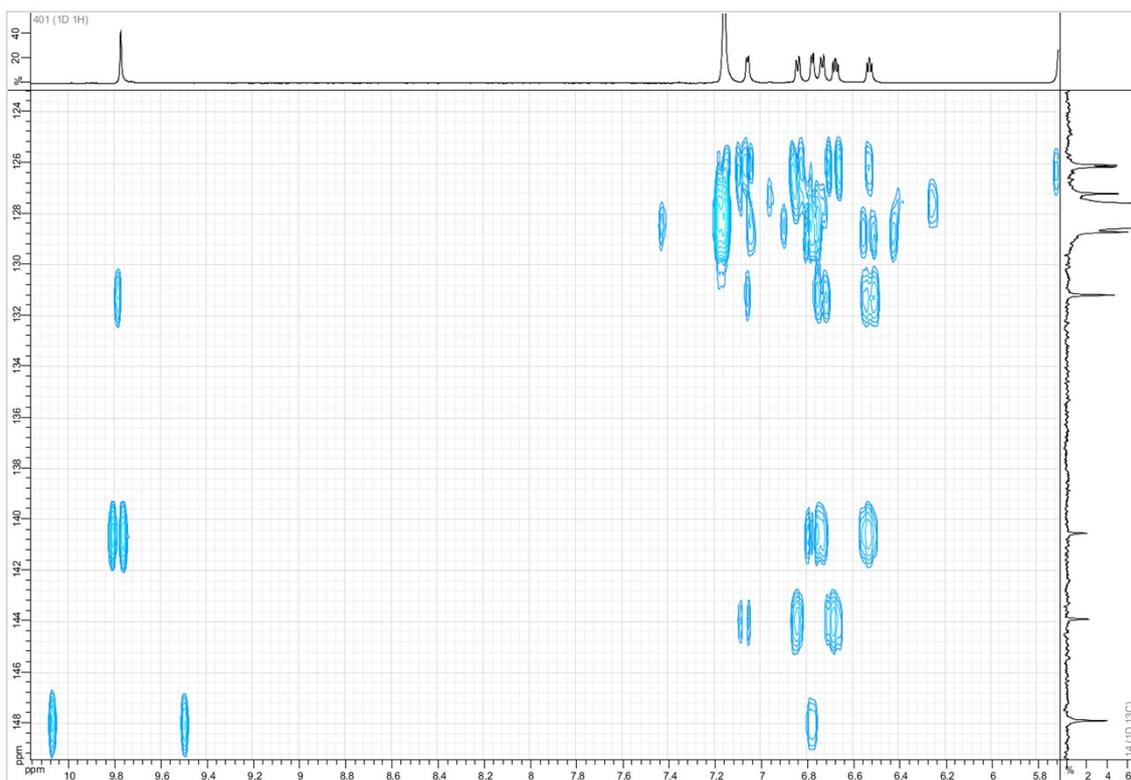
HSQC NMR spectrum of compound **5c** in $C_6D_6-d_6$ (zoom)



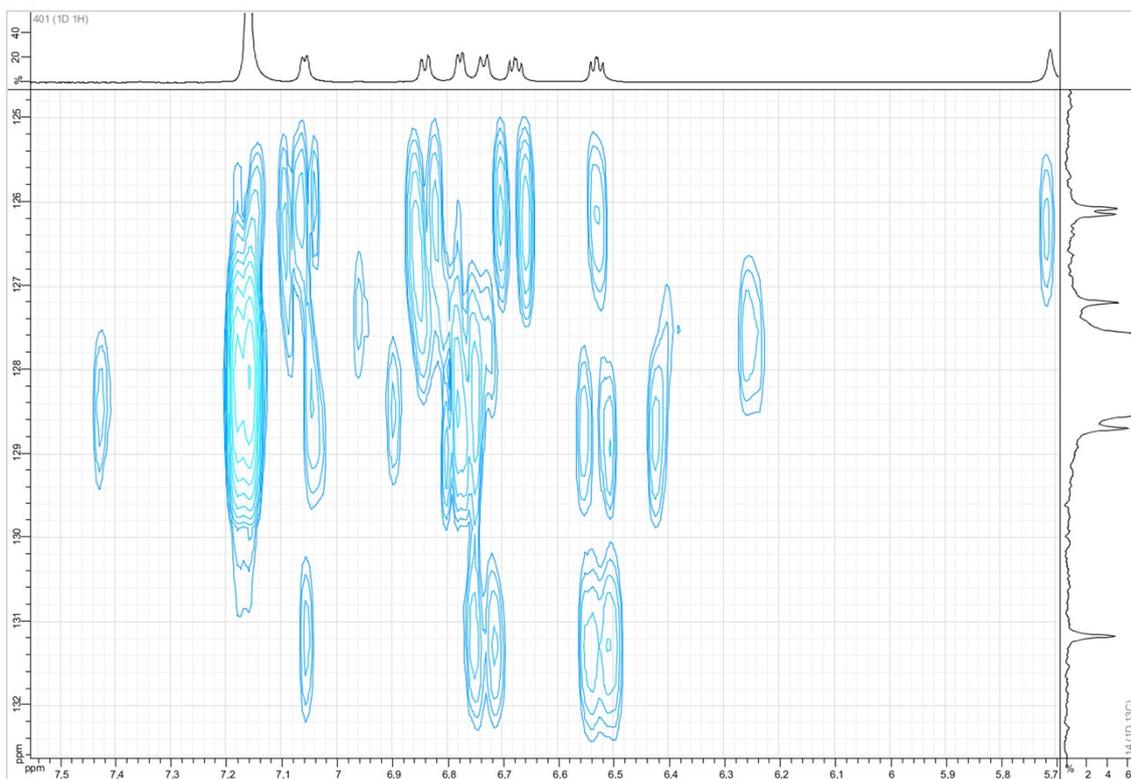
1H - ^{13}C HMBC NMR spectrum of compound **5c** in $C_6D_6-d_6$



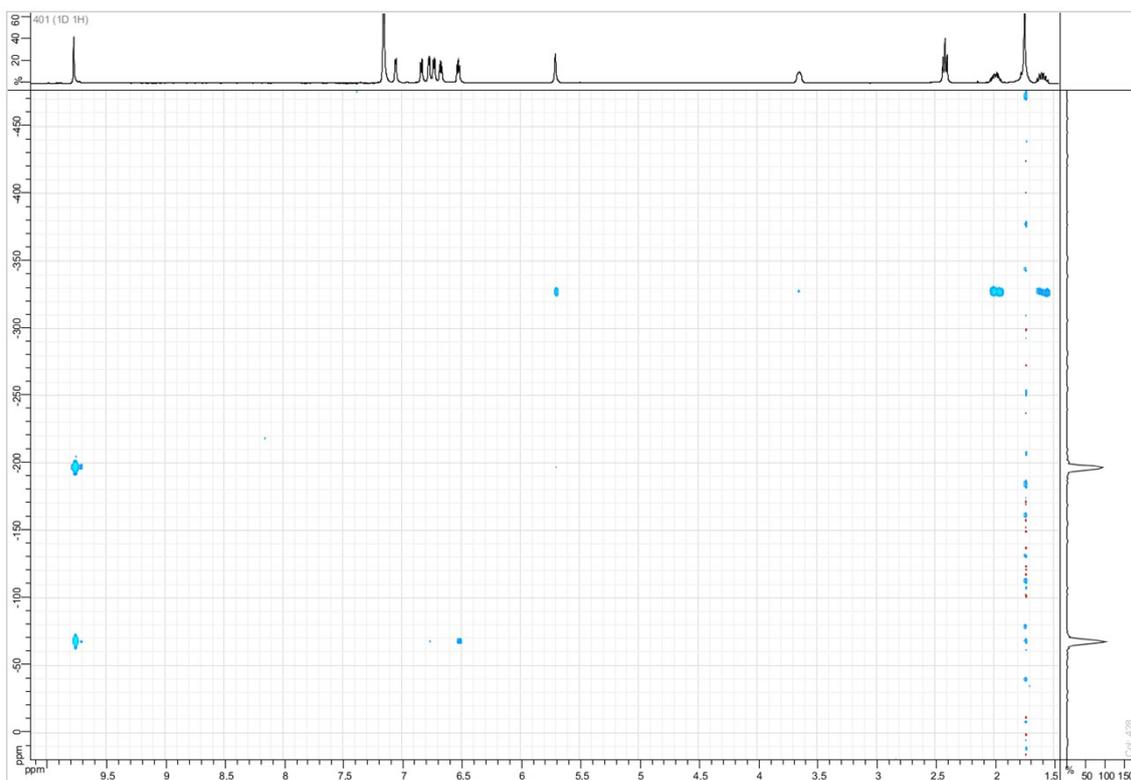
^1H - ^{13}C HMBC NMR spectrum of compound **5c** in C_6D_6 - d_6 (zoom 1)



^1H - ^{13}C HMBC NMR spectrum of compound **5c** in C_6D_6 - d_6 (zoom 2)

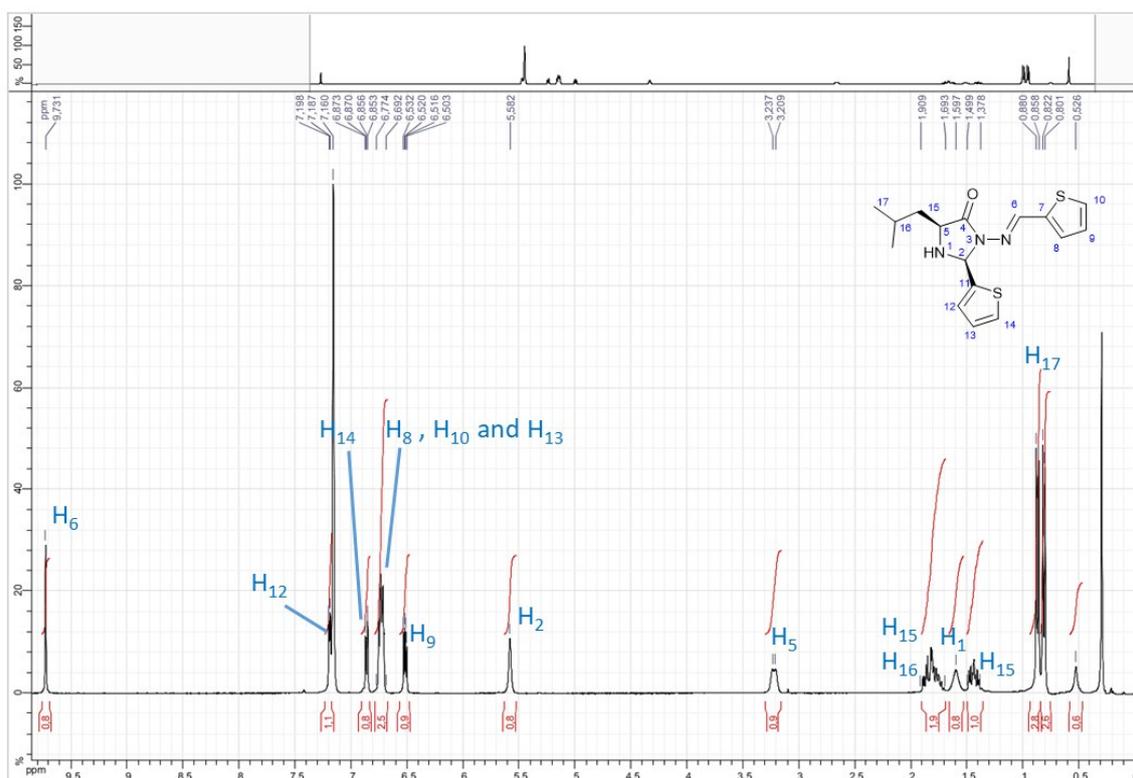


^1H - ^{13}C HMBC NMR spectrum of compound **5c** in C_6D_6 - d_6 (zoom 3)

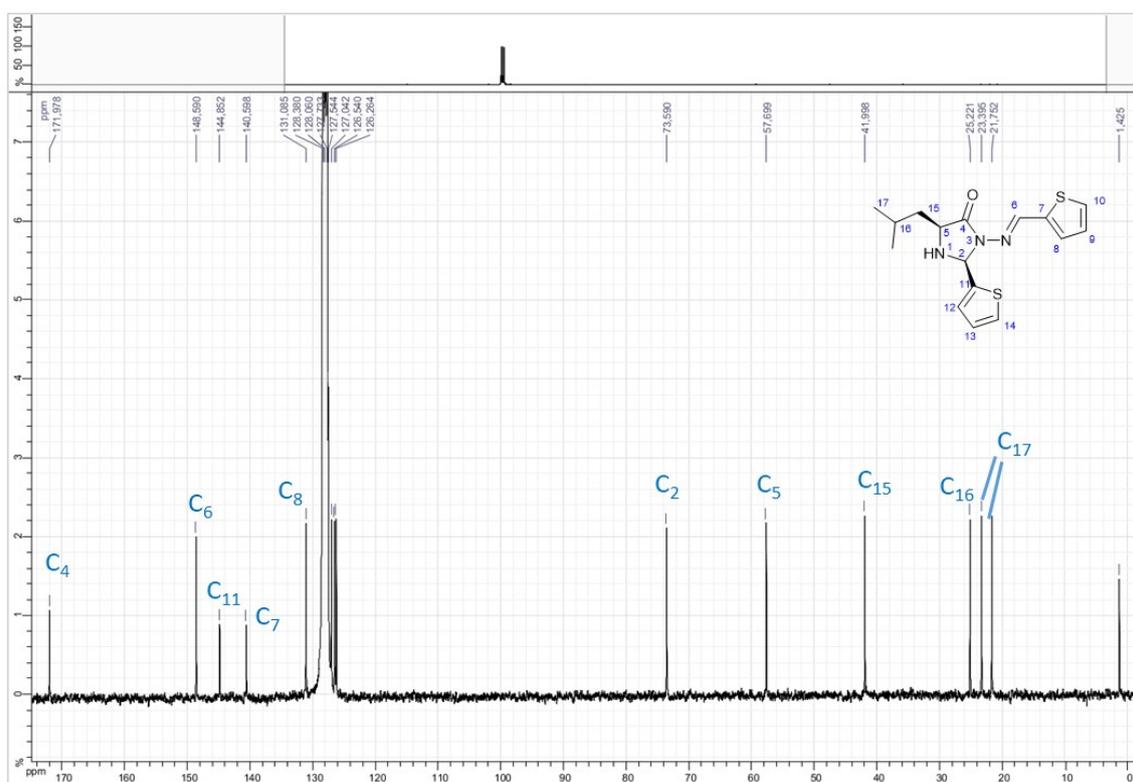


^1H - ^{15}N HMBC NMR spectrum of compound **5c** in C_6D_6 - d_6

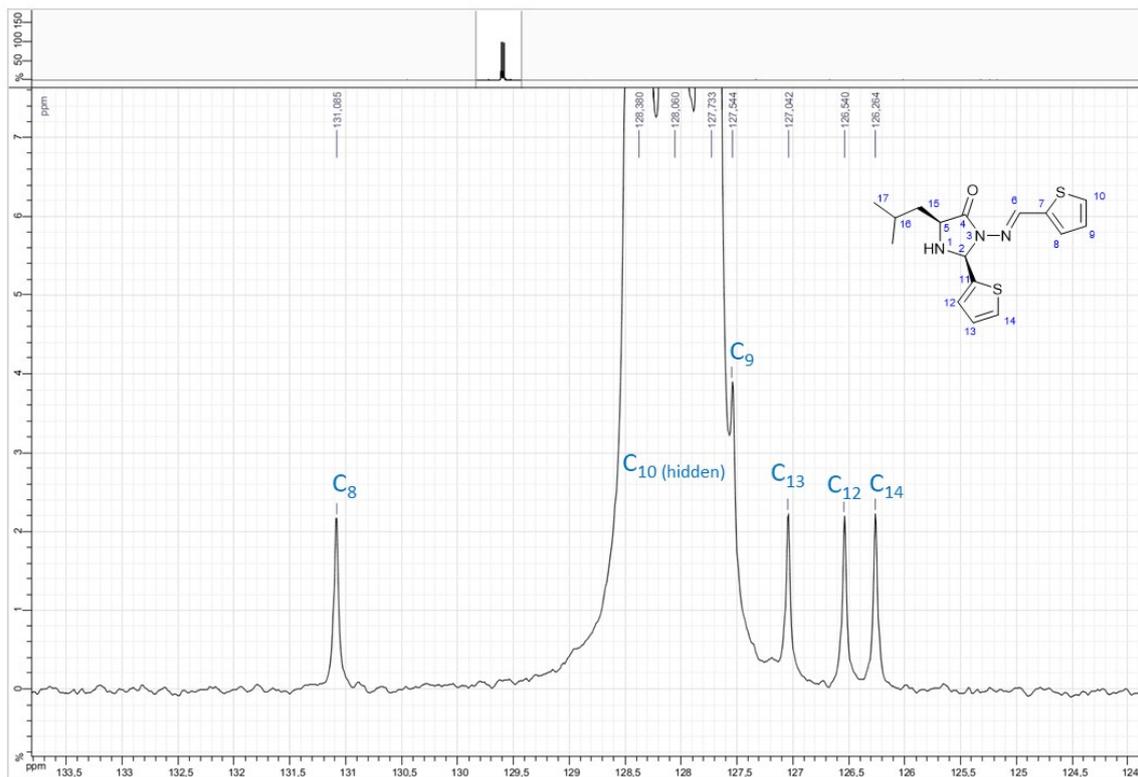
d. NMR spectra of **5d**



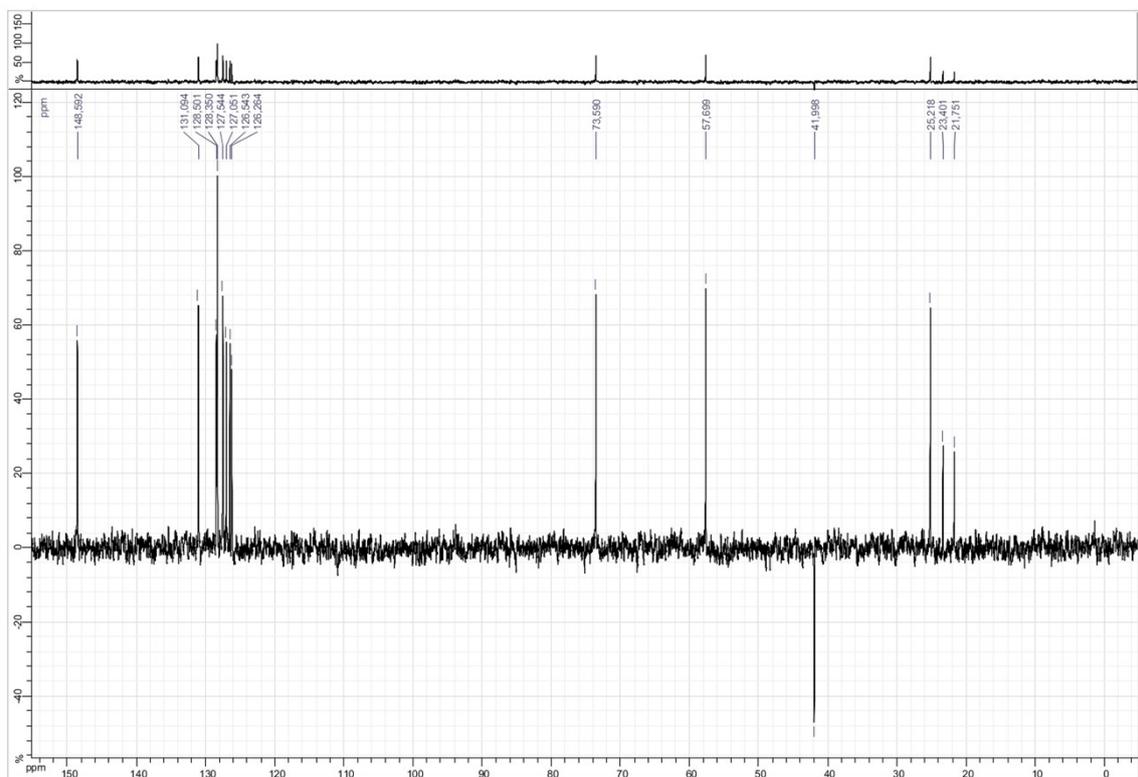
¹H NMR spectrum of compound **5d** in C₆D₆-d₆ at 300 MHz



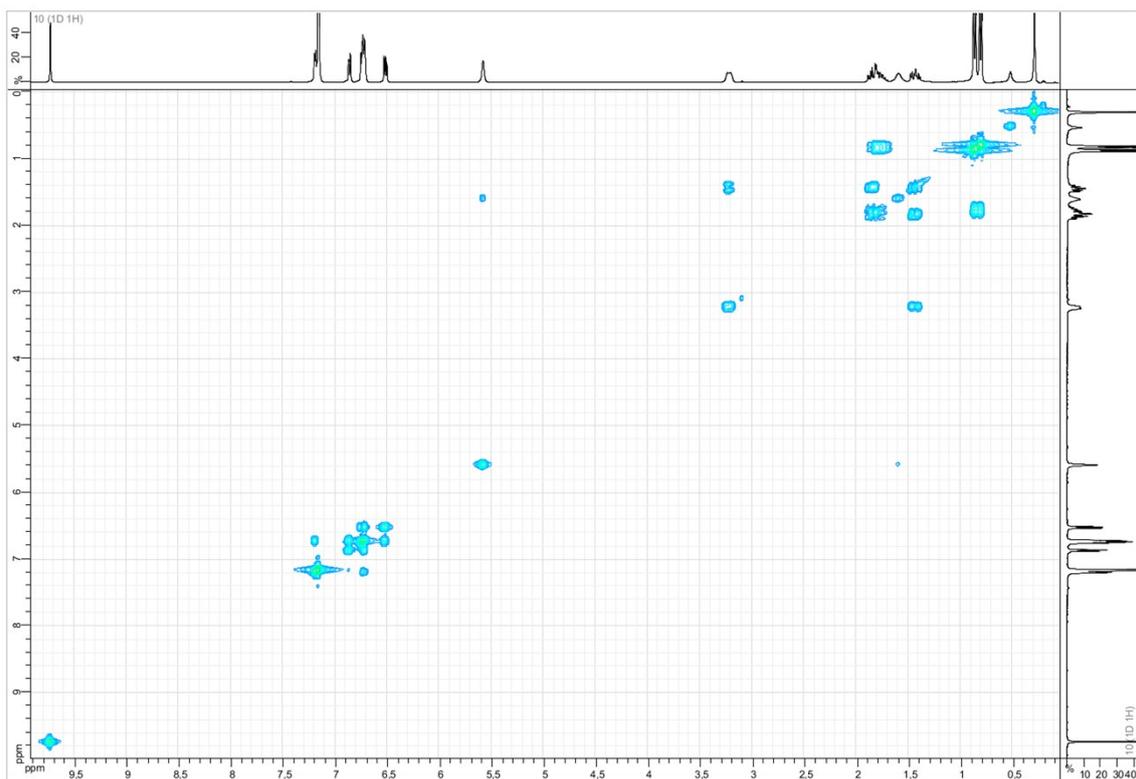
¹³C NMR spectrum of compound **5d** in C₆D₆-d₆ at 75 MHz



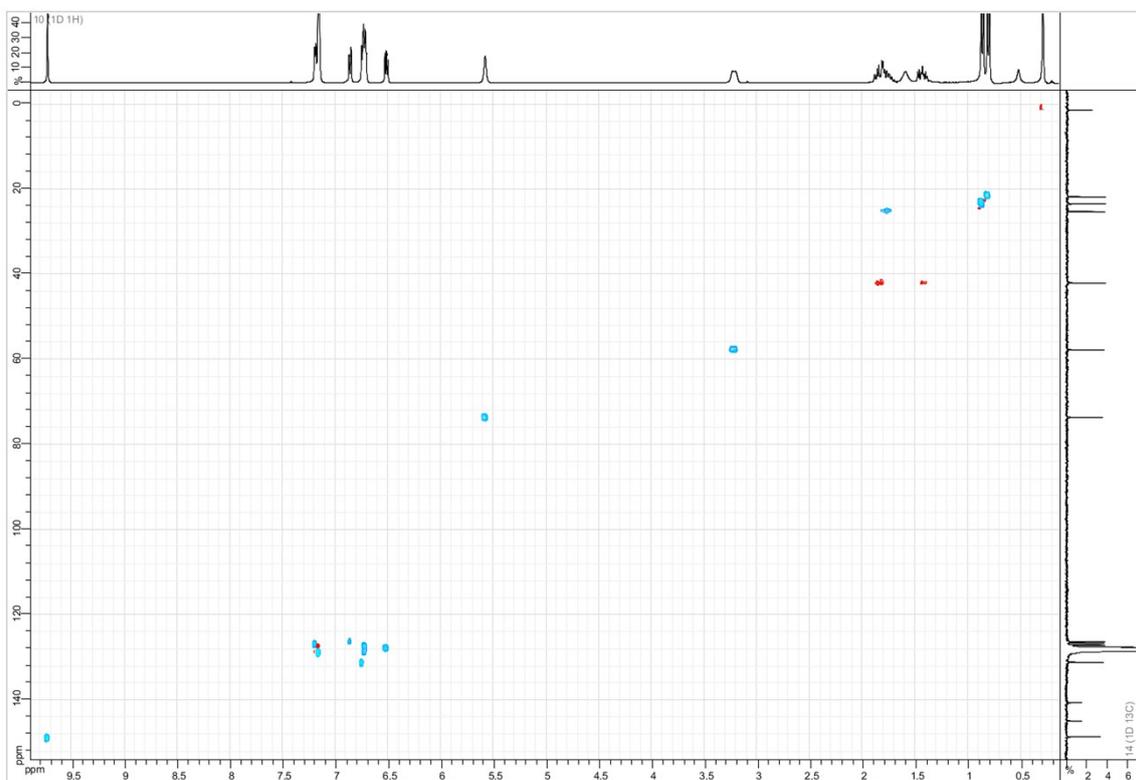
^{13}C NMR spectrum of compound **5d** in C_6D_6-d_6 at 75 MHz (zoom)



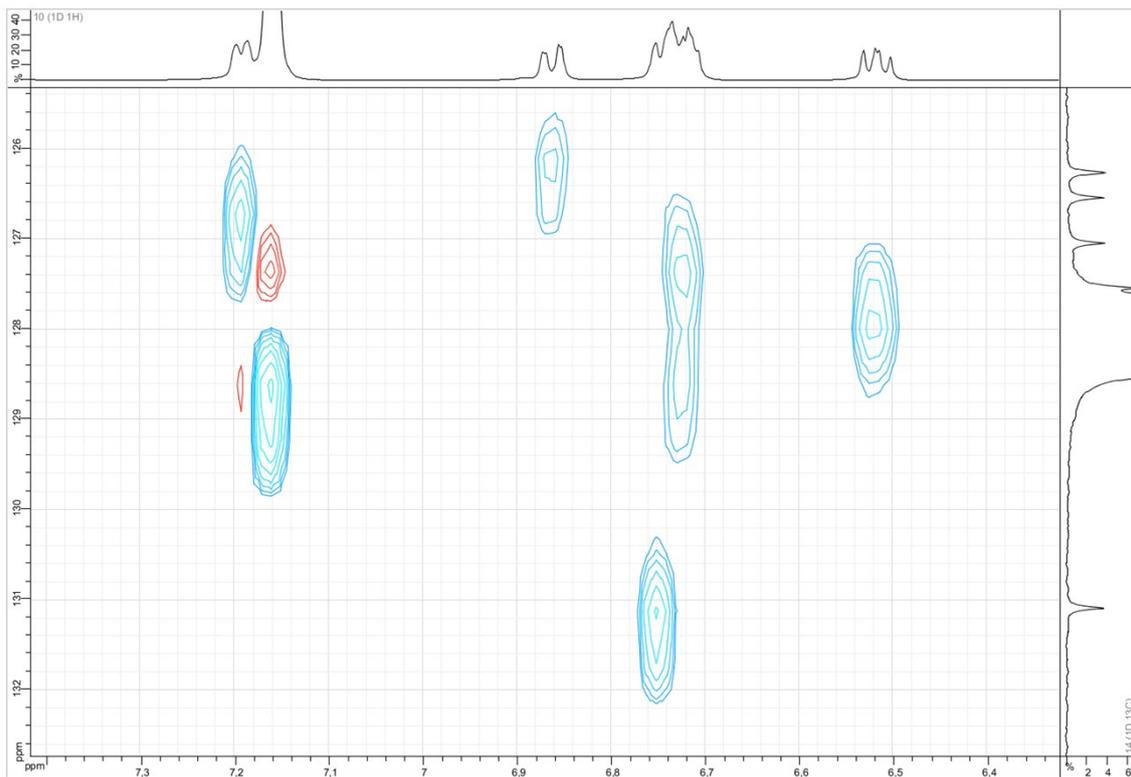
Dept ^{135}C NMR spectrum of compound **5d** in C_6D_6-d_6 at 75 MHz



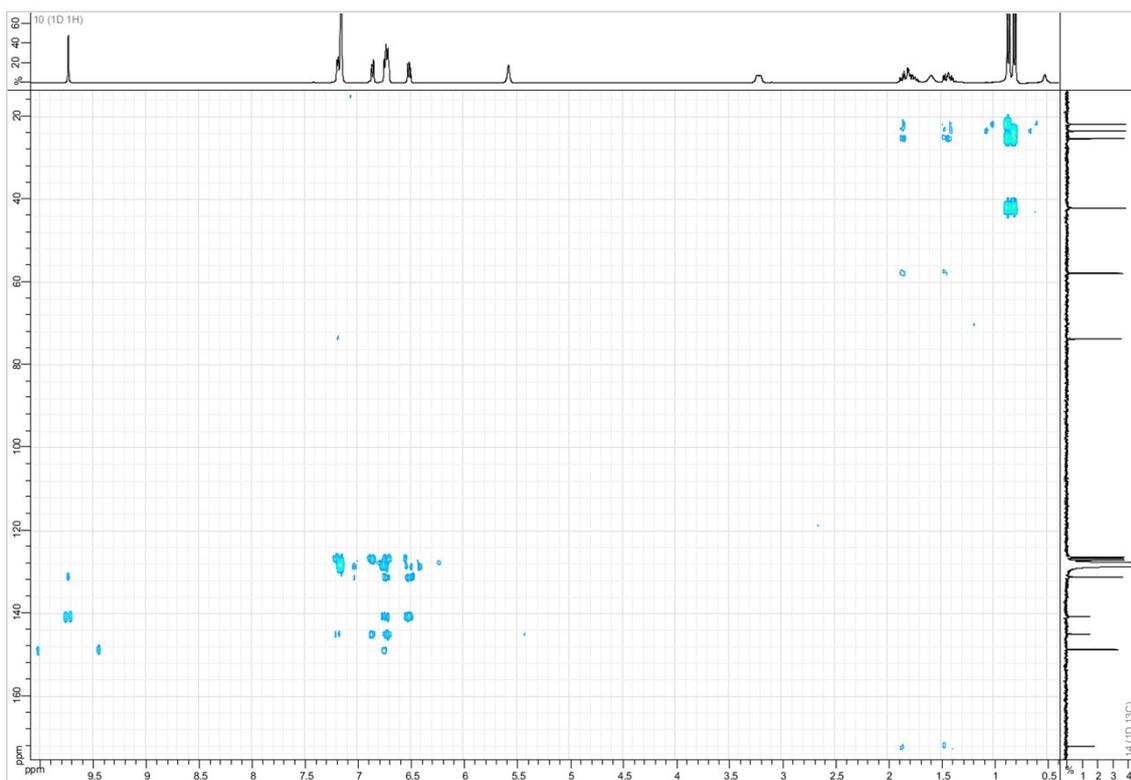
COSY NMR spectrum of compound **5d** in $C_6D_6-d_6$



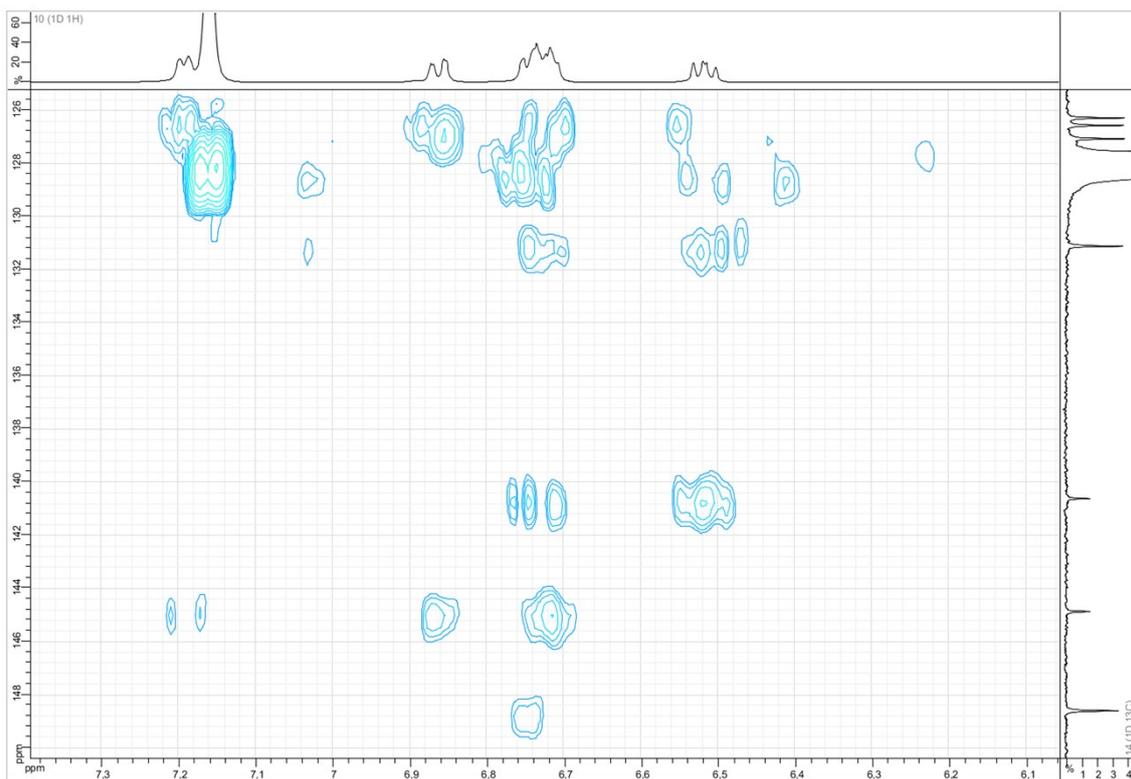
HSQC NMR spectrum of compound **5d** in $C_6D_6-d_6$



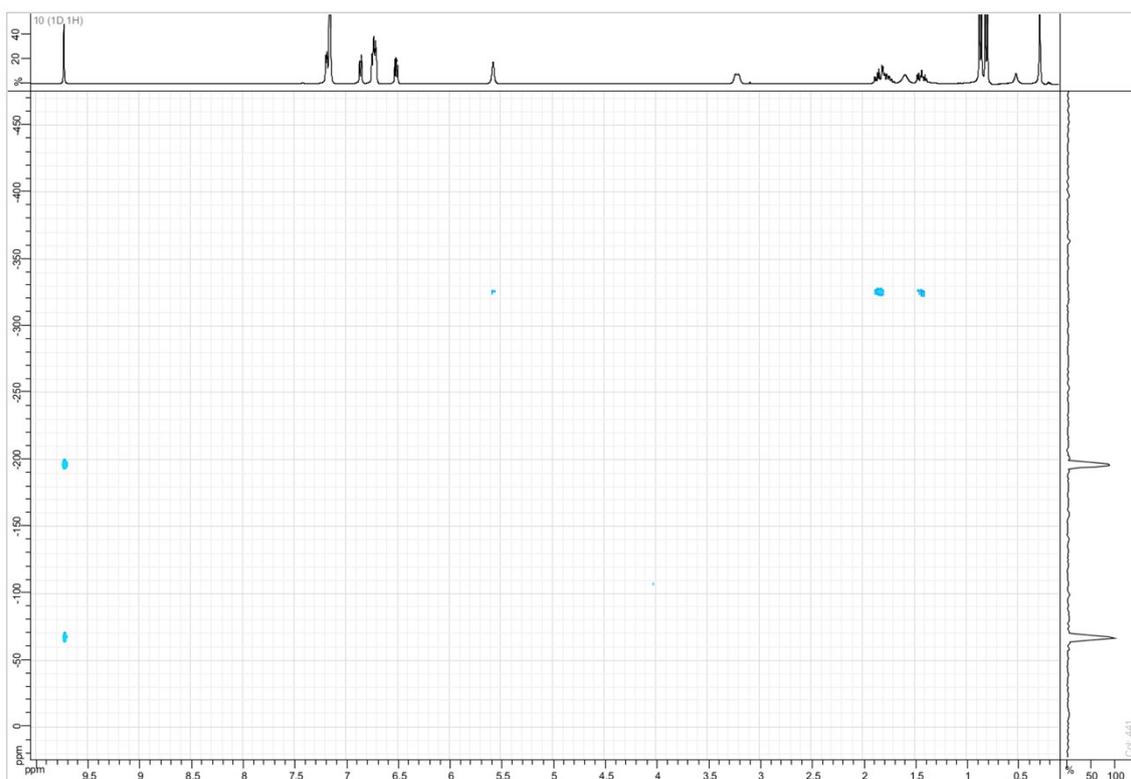
HSQC NMR spectrum of compound **5d** in $C_6D_6-d_6$ (zoom)



1H - ^{13}C HMBC NMR spectrum of compound **5d** in $C_6D_6-d_6$

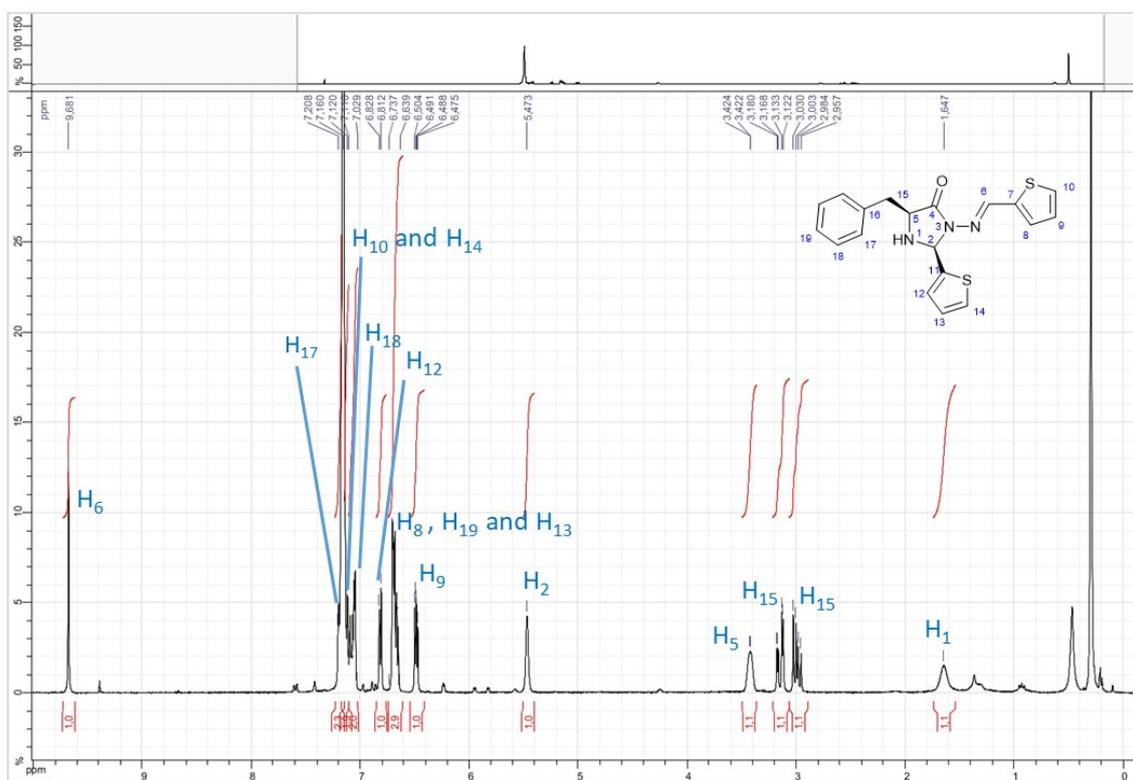


^1H - ^{13}C HMBC NMR spectrum of compound **5d** in C_6D_6 - d_6 (zoom)

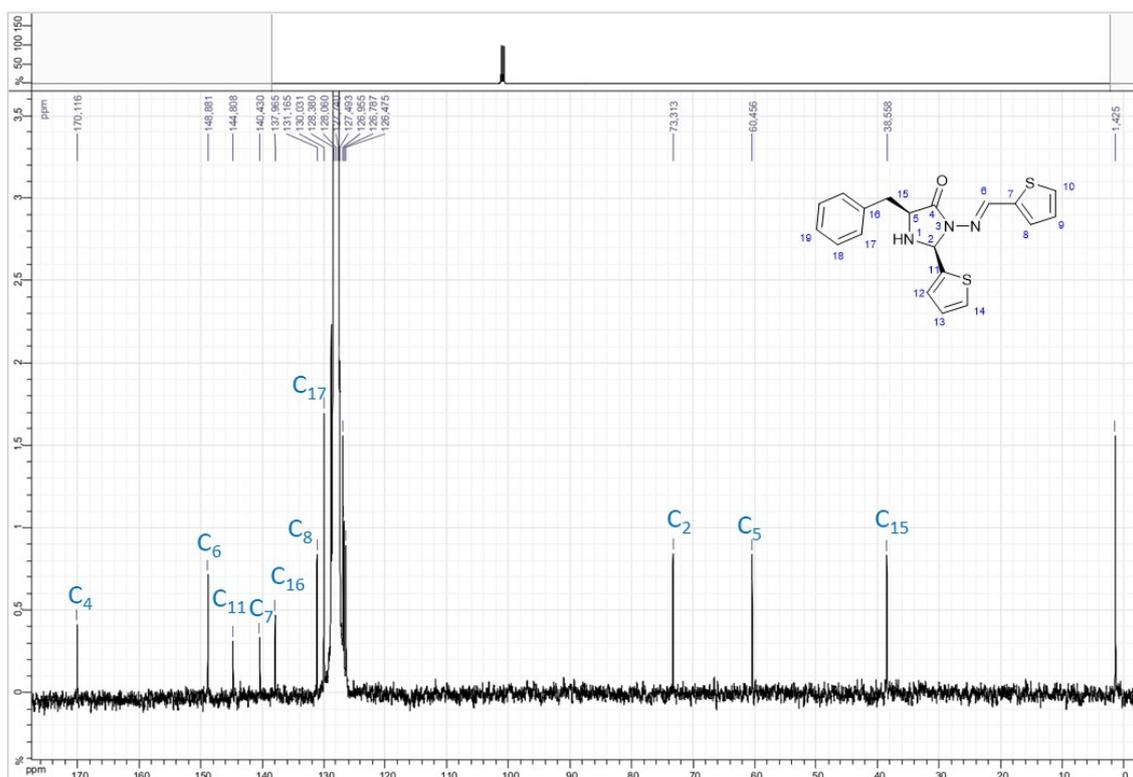


^1H - ^{15}N HMBC NMR spectrum of compound **5d** in C_6D_6 - d_6

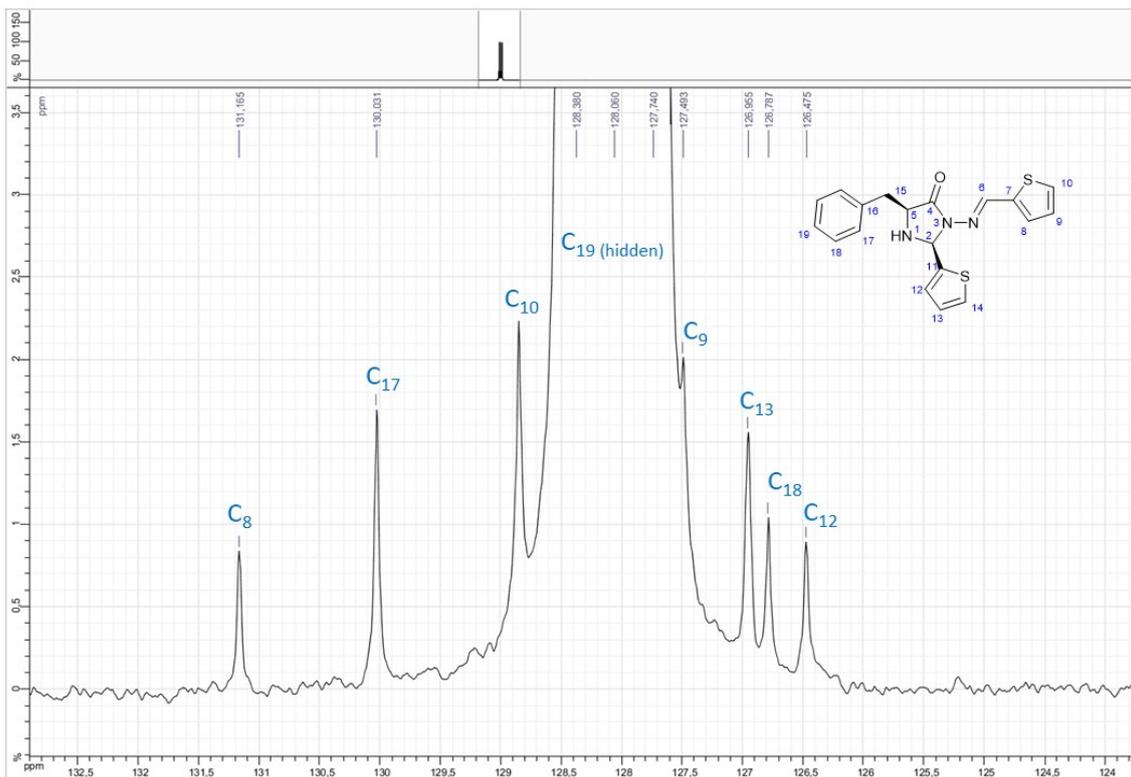
e. NMR spectra of **5e**



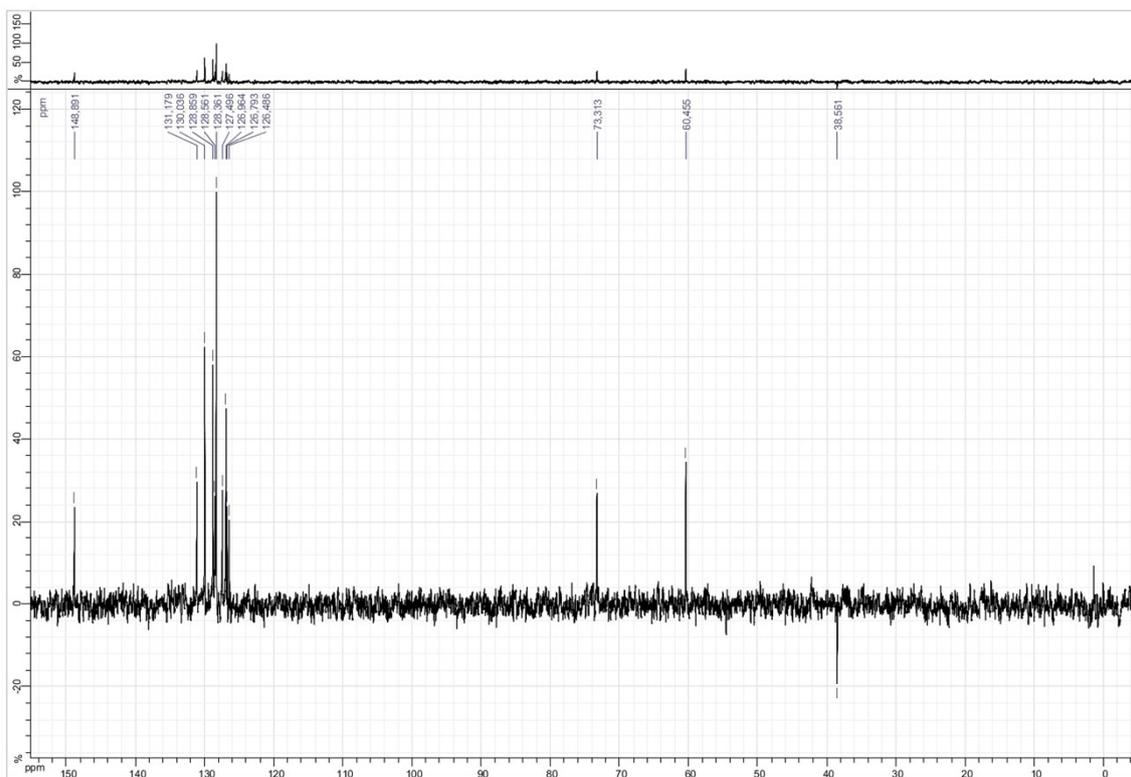
¹H NMR spectrum of compound **5e** in C₆D₆-d₆ at 300 MHz



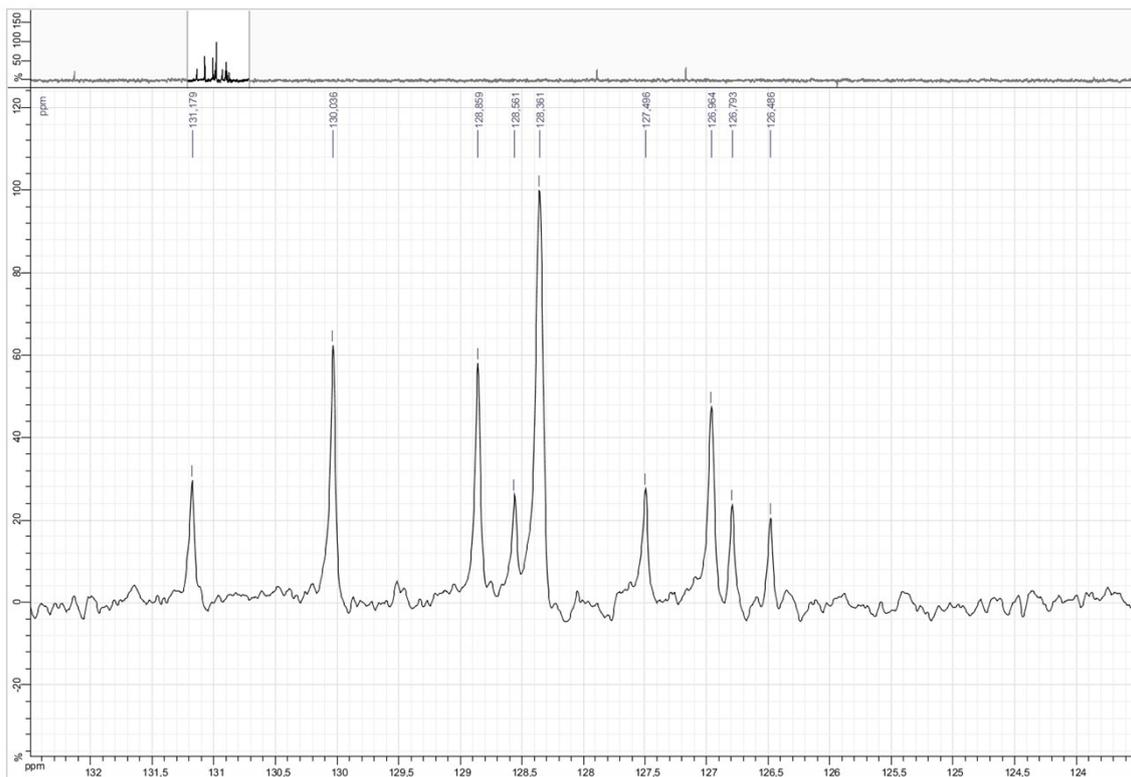
¹³C NMR spectrum of compound **5e** in C₆D₆-d₆ at 75 MHz



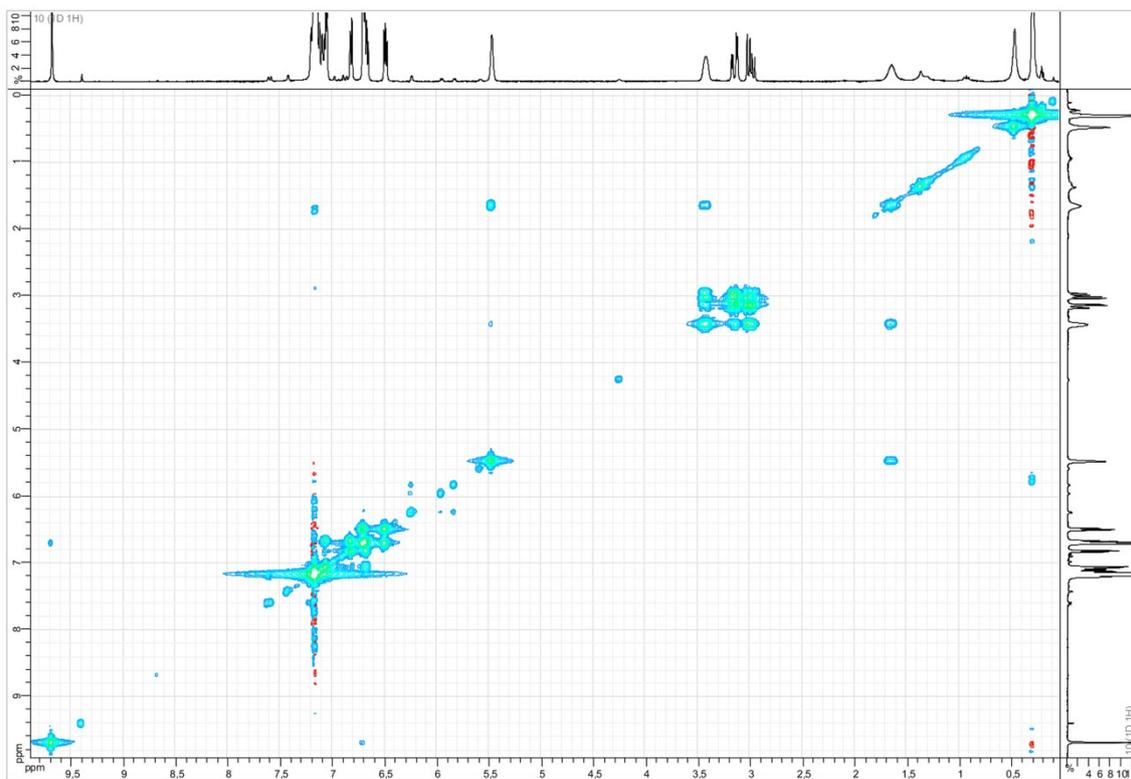
^{13}C NMR spectrum of compound **5e** in C_6D_6-d_6 at 75 MHz (zoom)



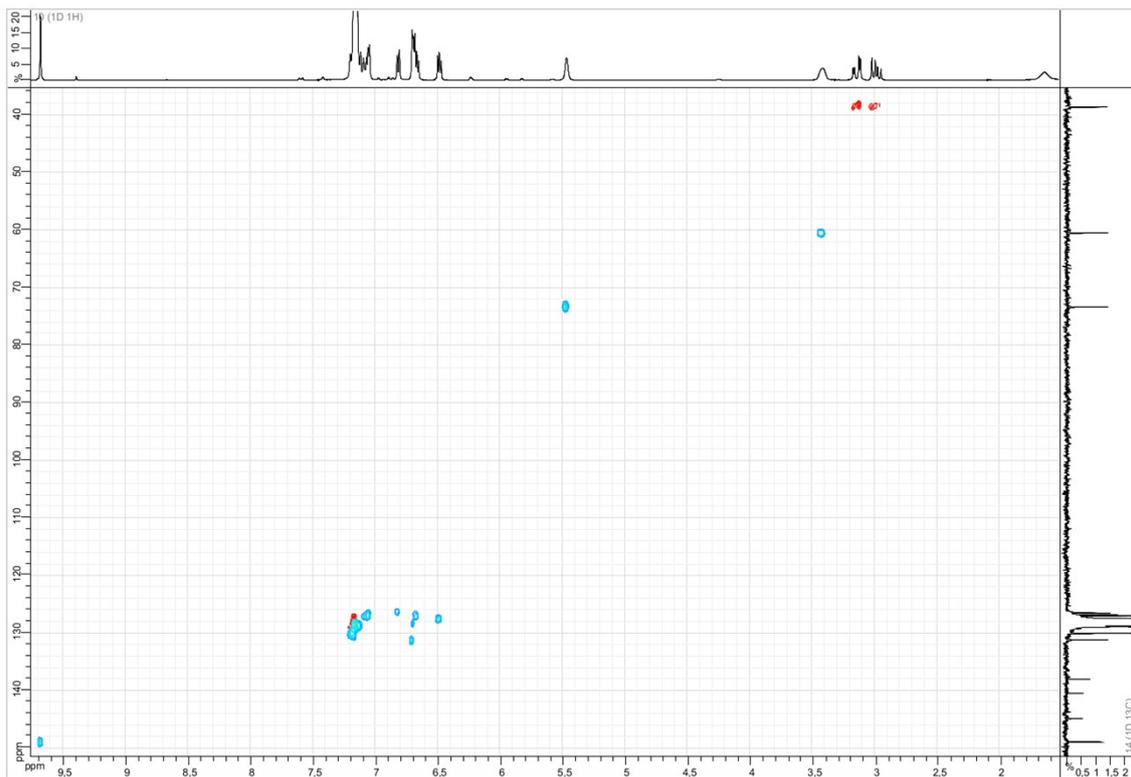
DEPT 135 NMR spectrum of compound **5e** in C_6D_6-d_6 at 75 MHz



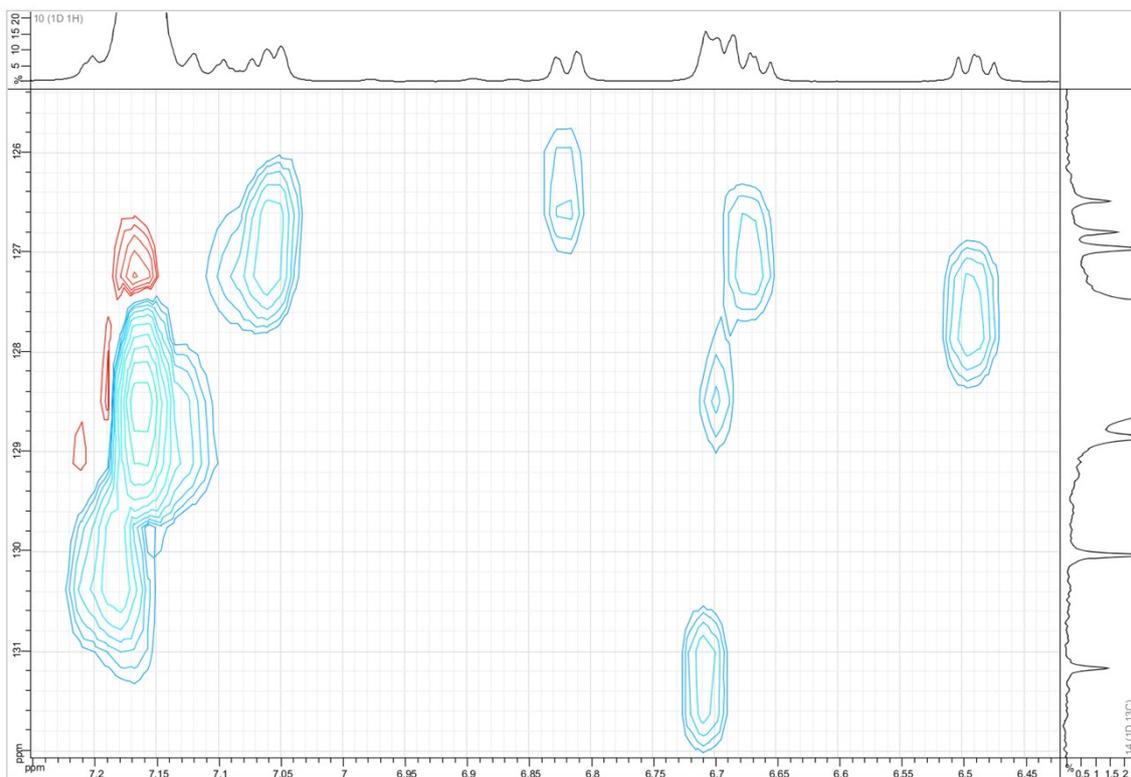
DEPT 135 NMR spectrum of compound **5e** in $C_6D_6-d_6$ at 75 MHz (zoom)



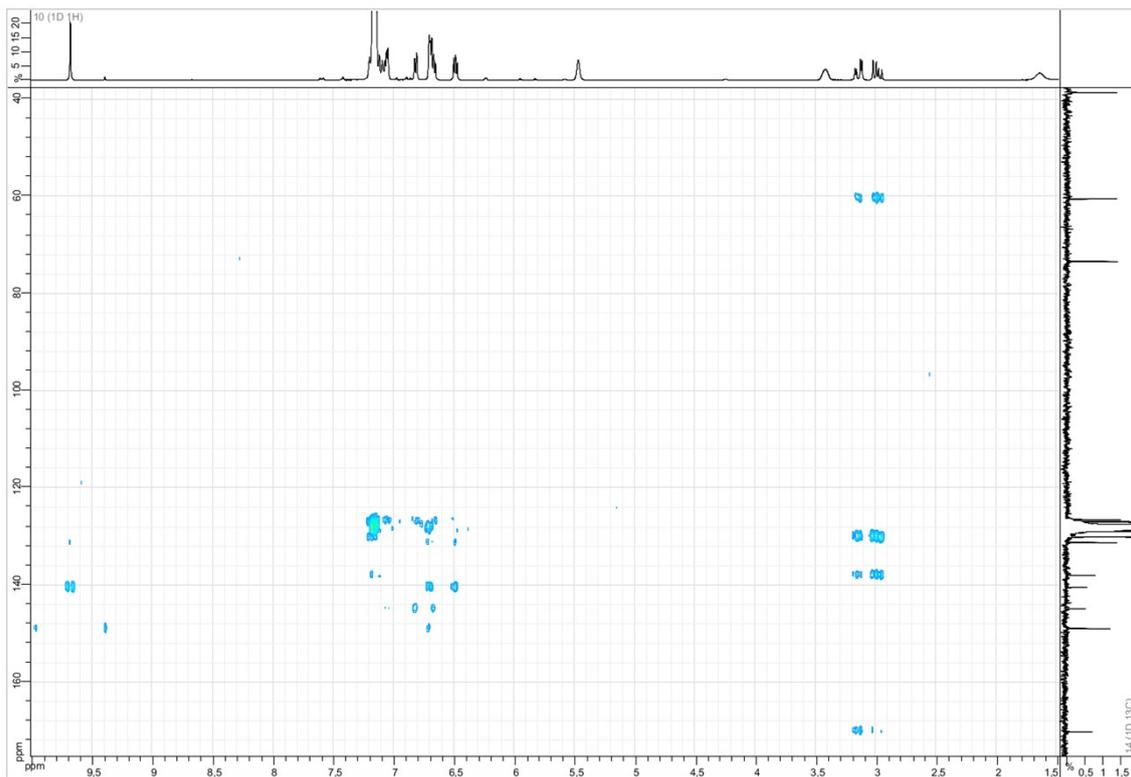
COSY NMR spectrum of compound **5e** in $C_6D_6-d_6$



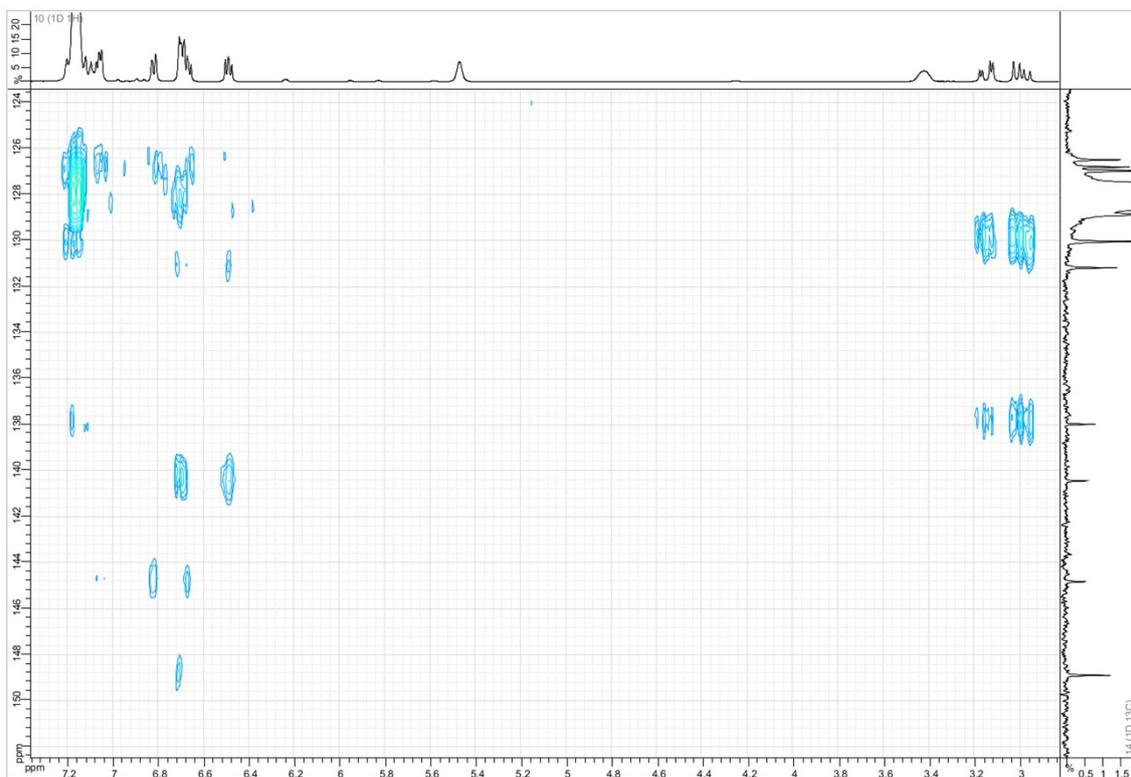
HSQC NMR spectrum of compound **5e** in $C_6D_6-d_6$



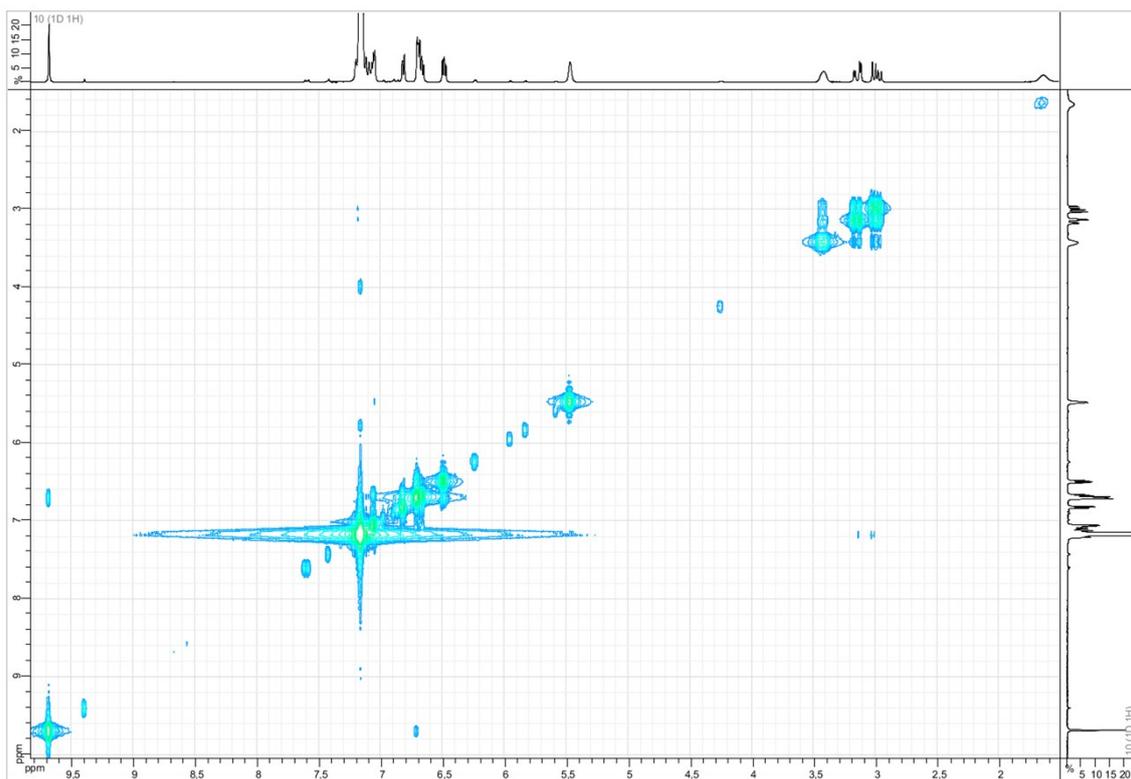
HSQC NMR spectrum of compound **5e** in $C_6D_6-d_6$ (zoom)



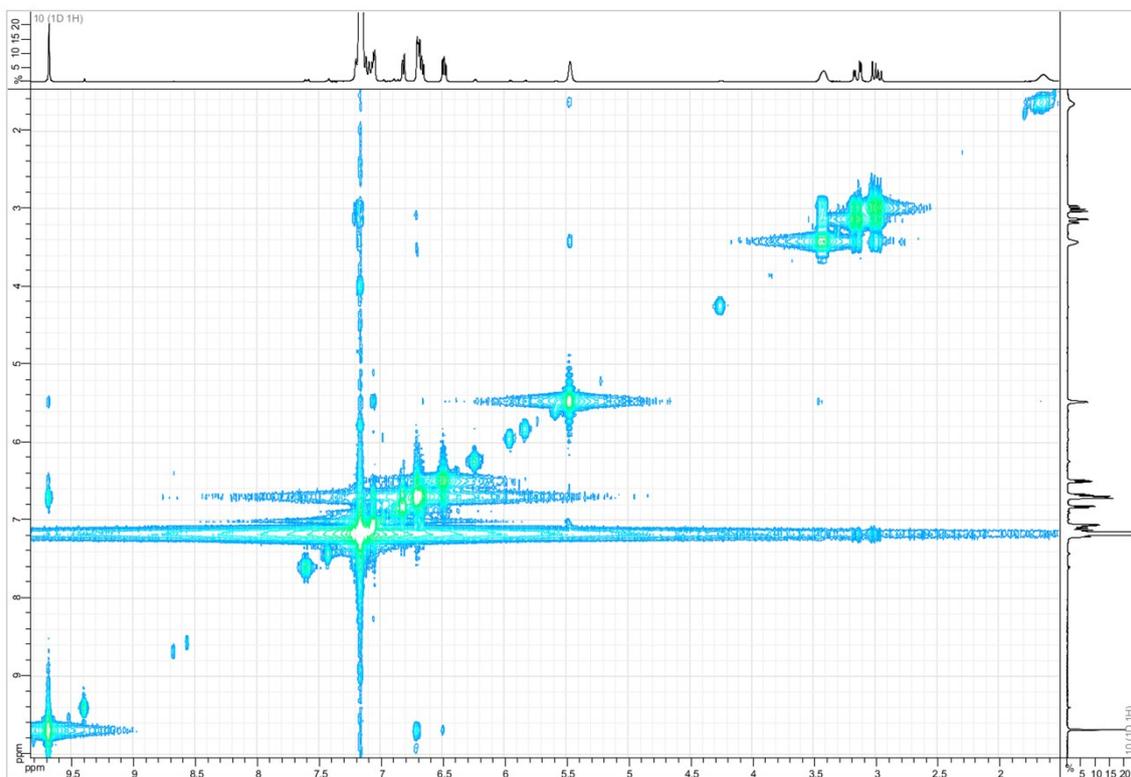
^1H - ^{13}C HMBC NMR spectrum of compound **5e** in C_6D_6 - d_6



^1H - ^{13}C HMBC NMR spectrum of compound **5e** in C_6D_6 - d_6 (zoom)

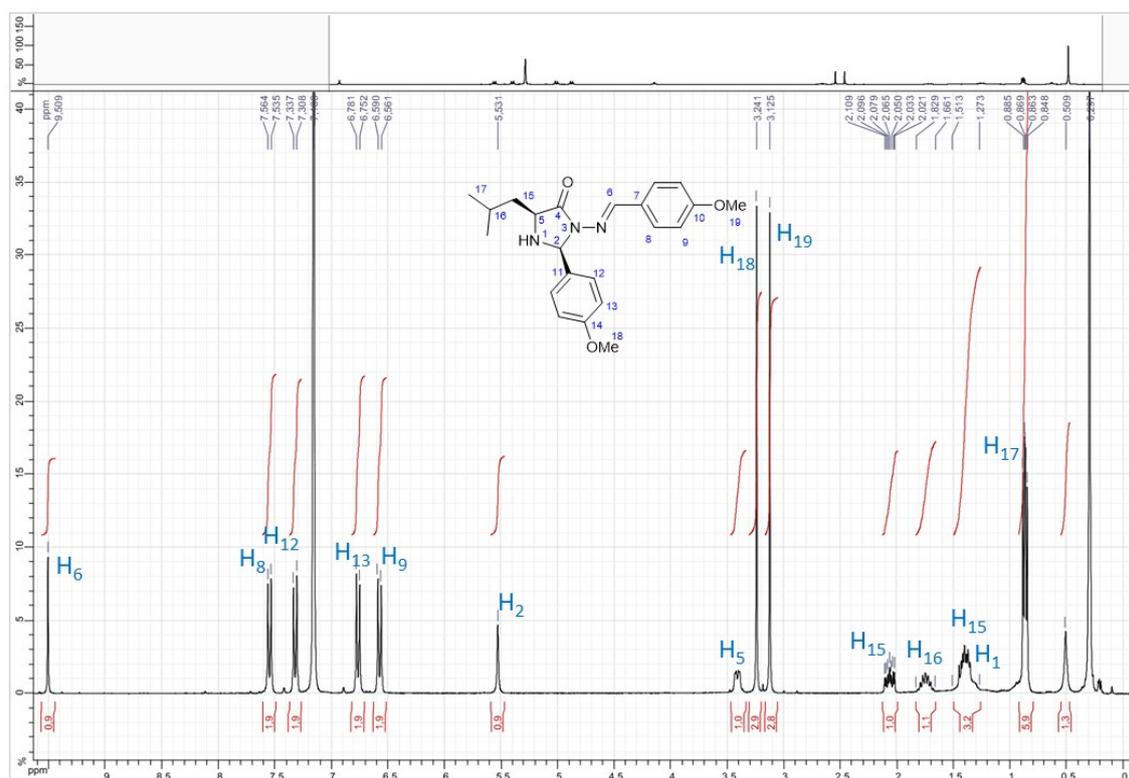


NOESY NMR spectrum of compound **5e** in $C_6D_6-d_6$

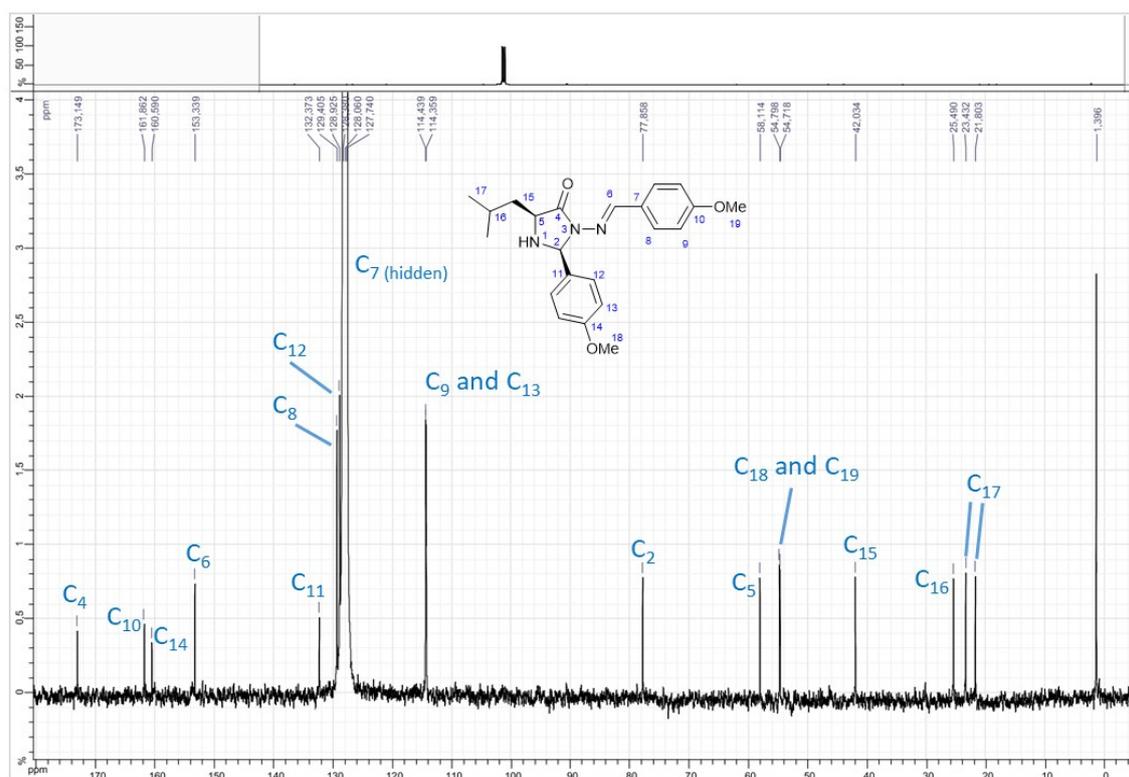


NOESY NMR spectrum of compound **5e** in $C_6D_6-d_6$ (deep cut)

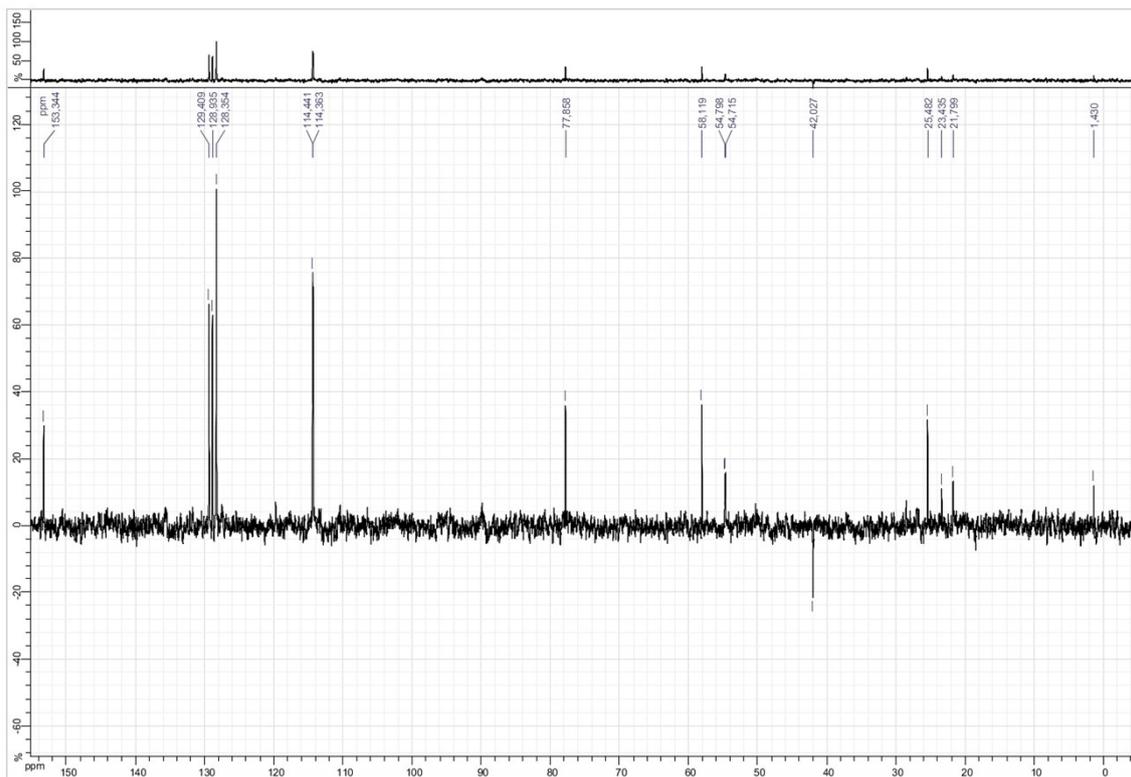
f. NMR spectra of **5f**



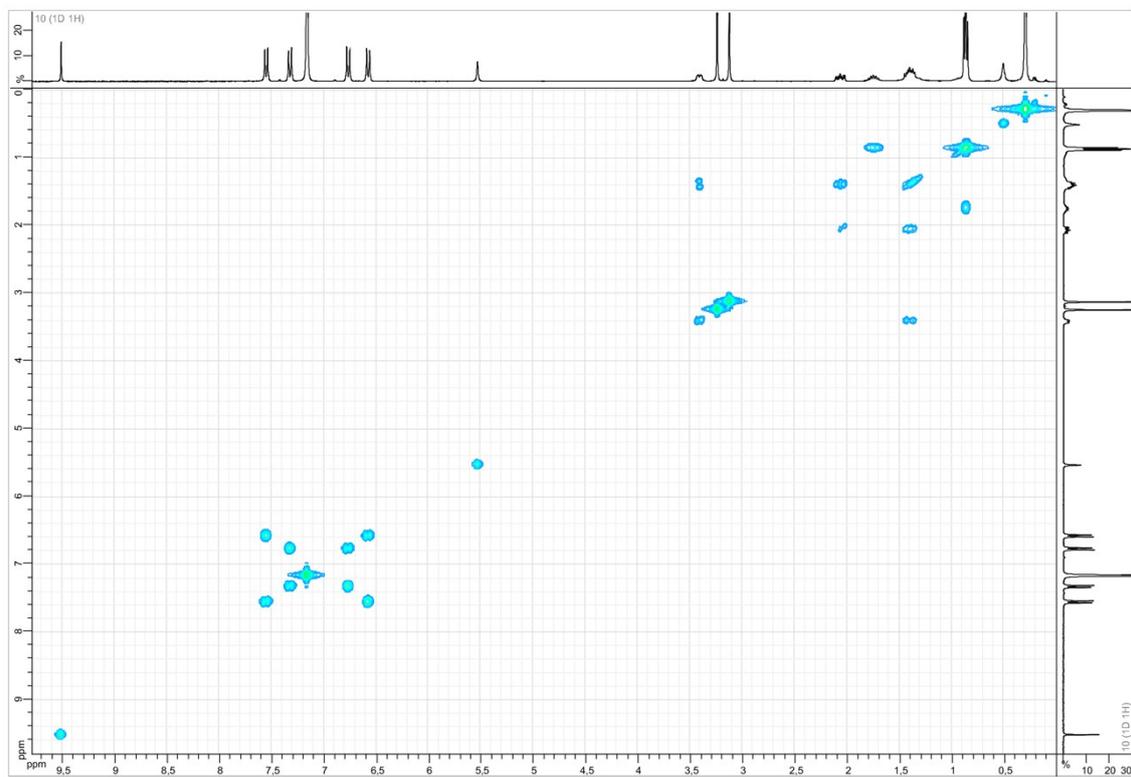
¹H NMR spectrum of compound **5f** in C₆D₆-d₆ at 300 MHz



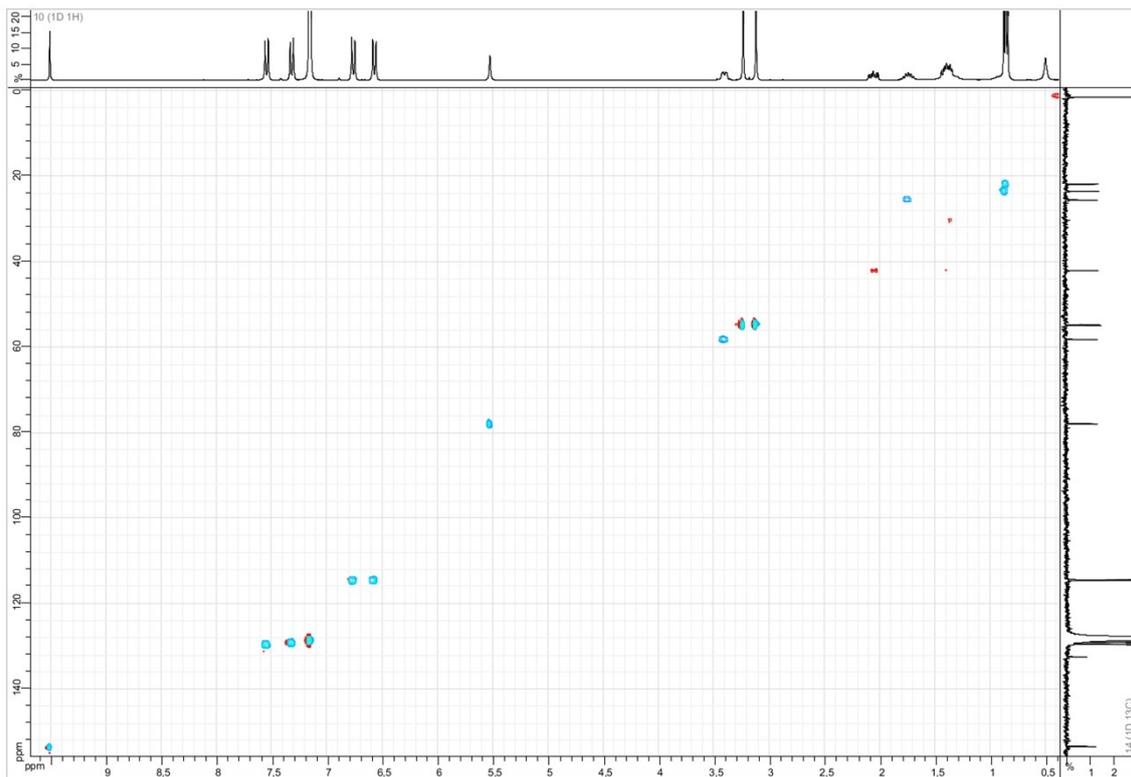
¹³C NMR spectrum of compound **5f** in C₆D₆-d₆ at 75 MHz



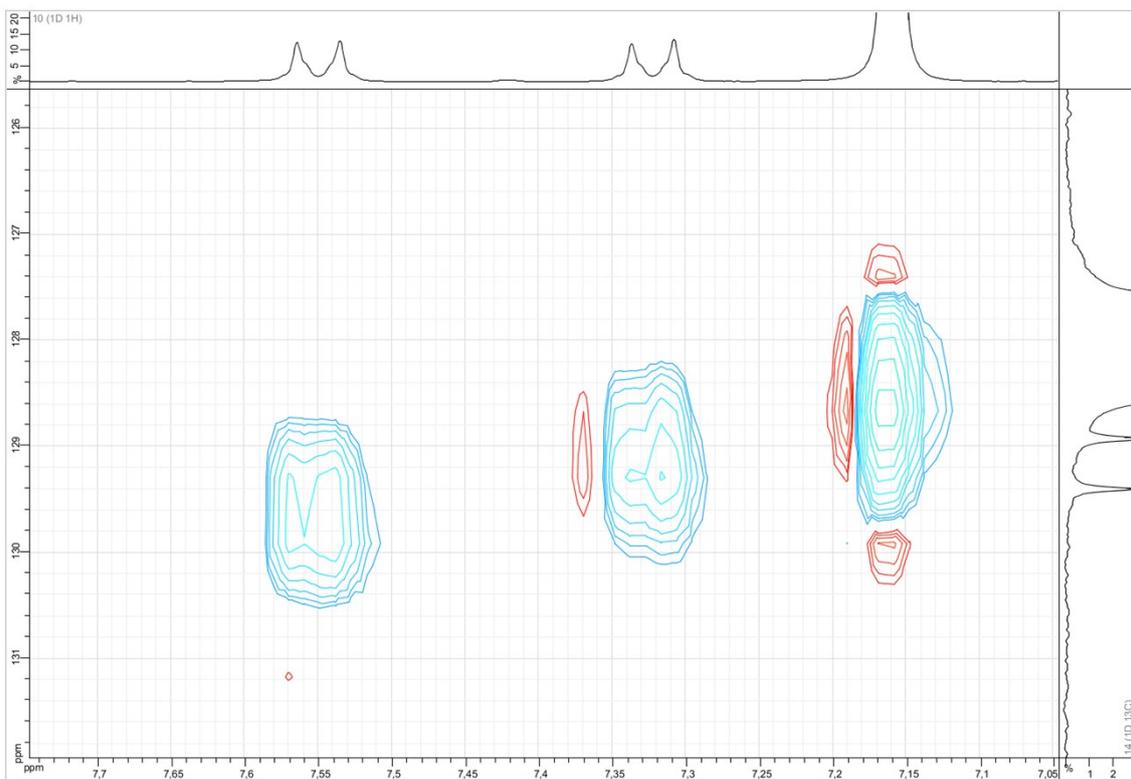
DEPT 135 NMR spectrum of compound **5f** in $C_6D_6-d_6$ at 75 MHz



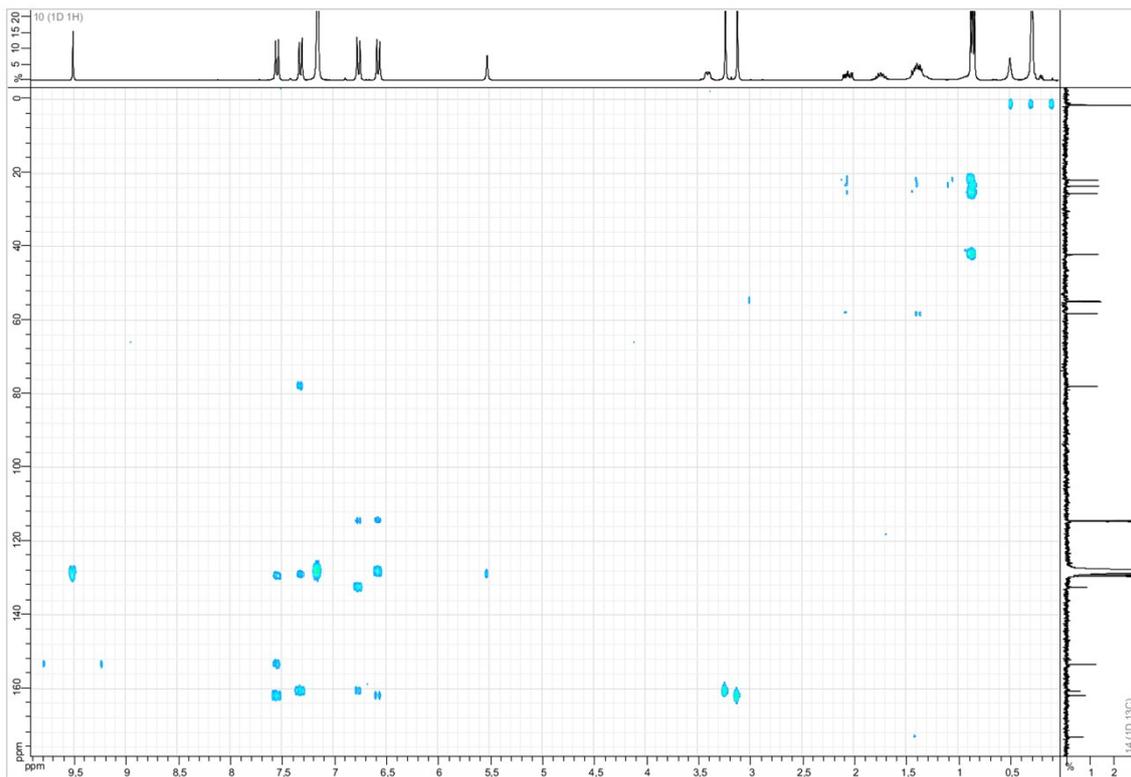
COSY NMR spectrum of compound **5f** in $C_6D_6-d_6$



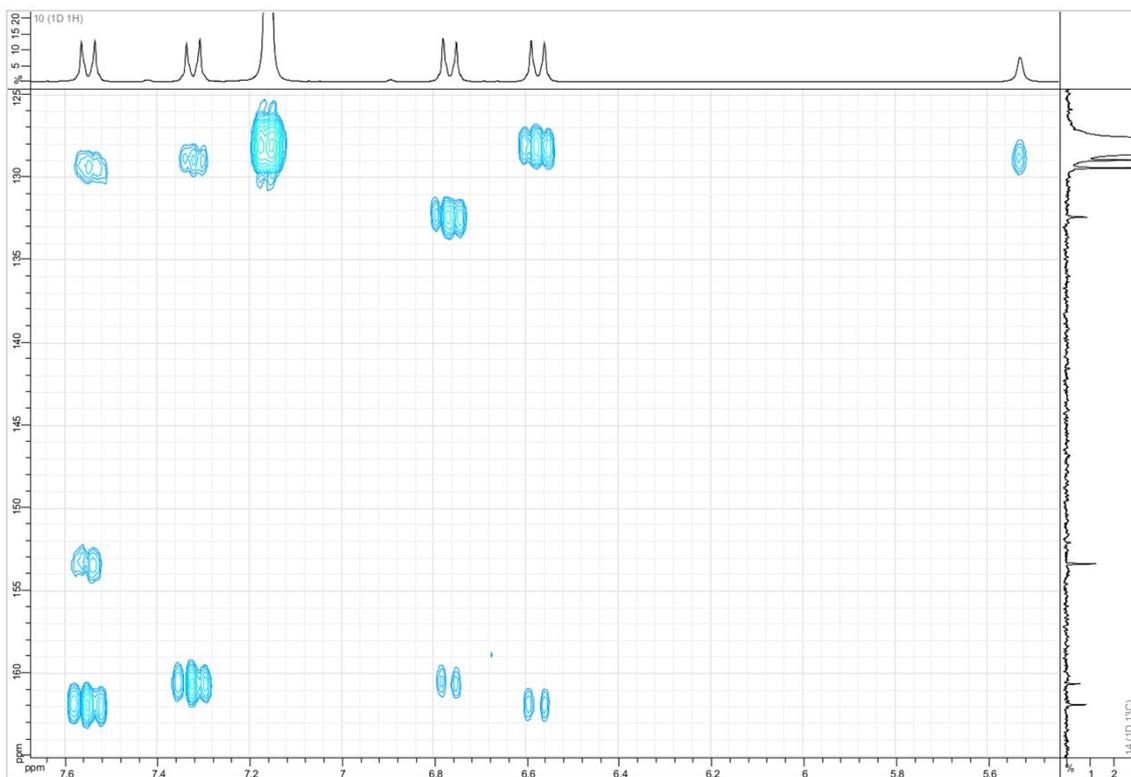
HSQC NMR spectrum of compound **5f** in $C_6D_6-d_6$



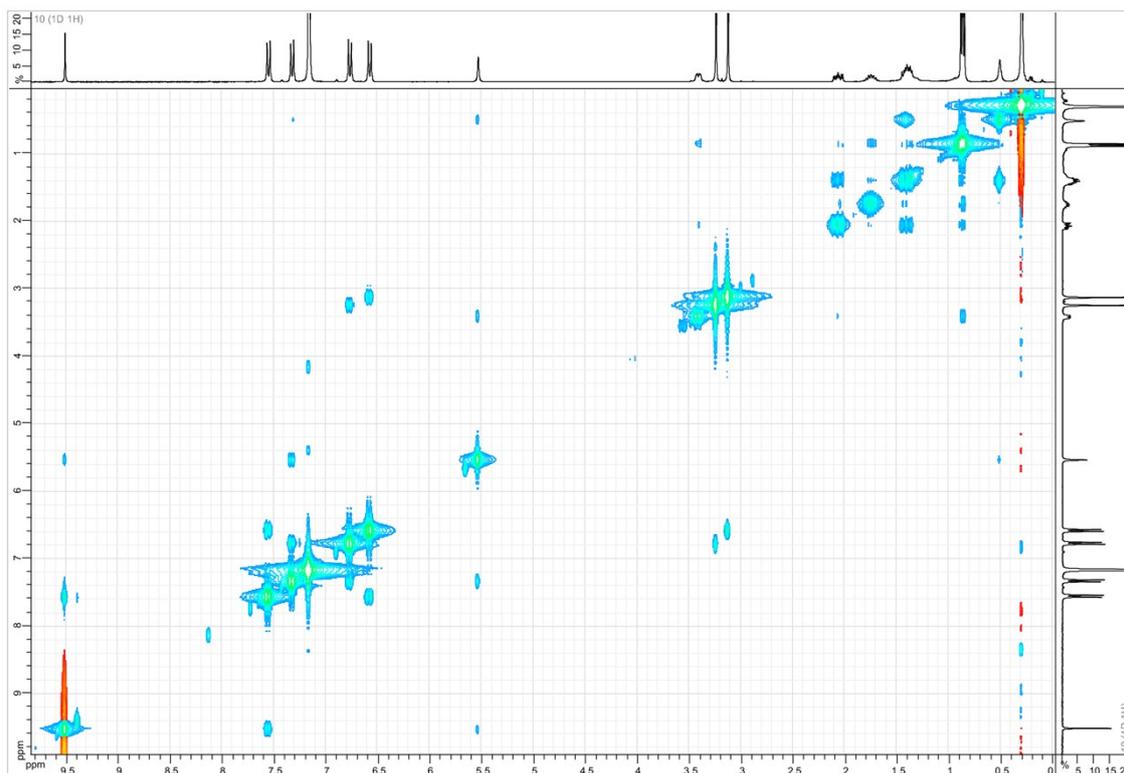
HSQC NMR spectrum of compound **5f** in $C_6D_6-d_6$ (zoom)



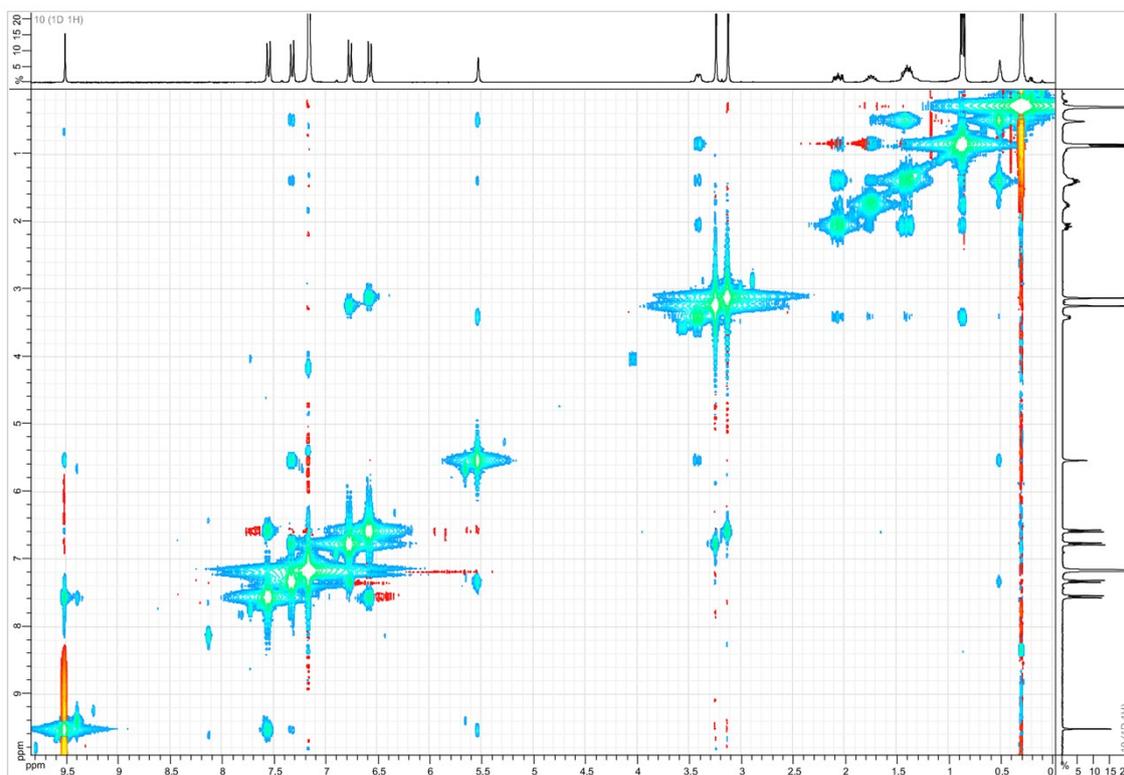
^1H - ^{13}C HMBC spectrum of compound **5f** in C_6D_6-d_6



^1H - ^{13}C HMBC spectrum of compound **5f** in C_6D_6-d_6 (zoom)

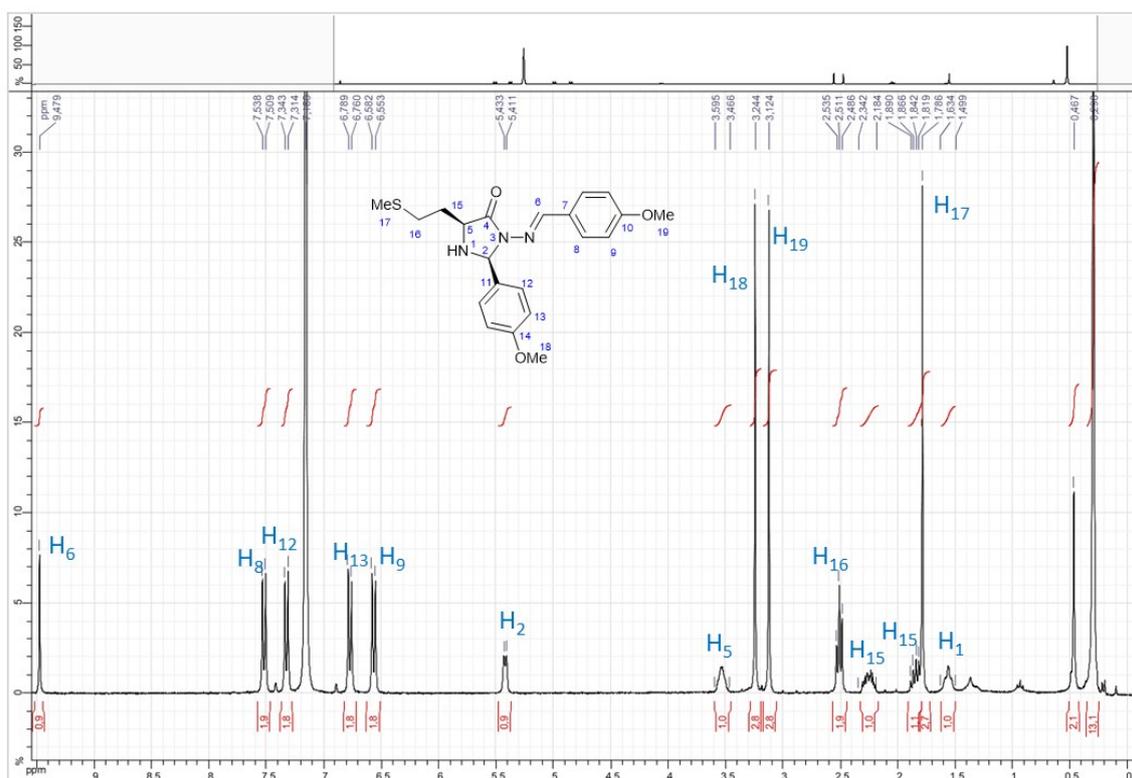


NOESY NMR spectrum of compound **5f** in $C_6D_6-d_6$

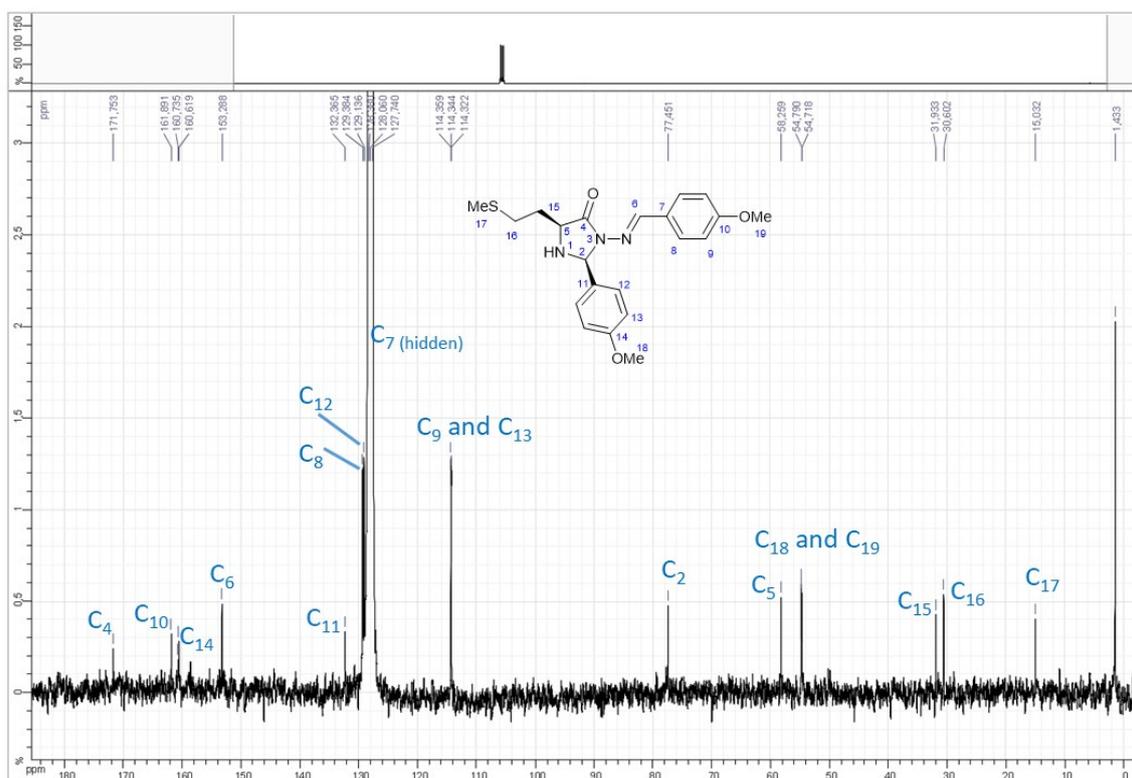


NOESY NMR spectrum of compound **5f** in $C_6D_6-d_6$ (deep cut)

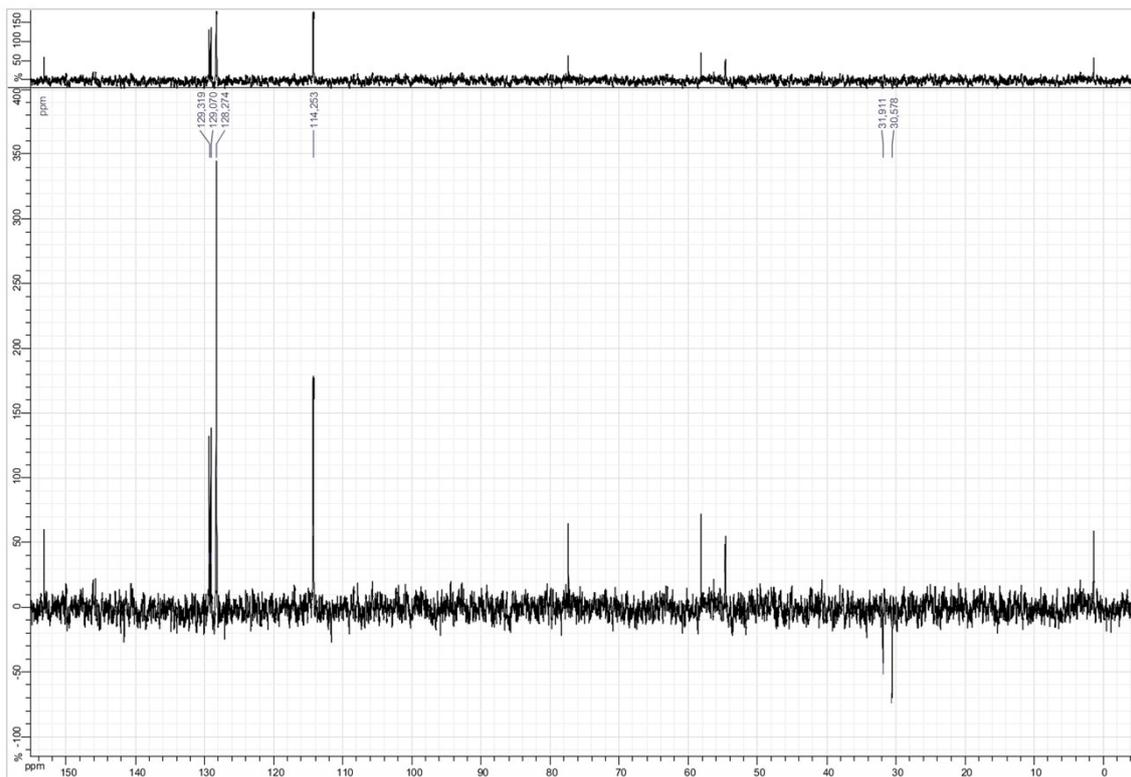
g. NMR spectra of **5g**



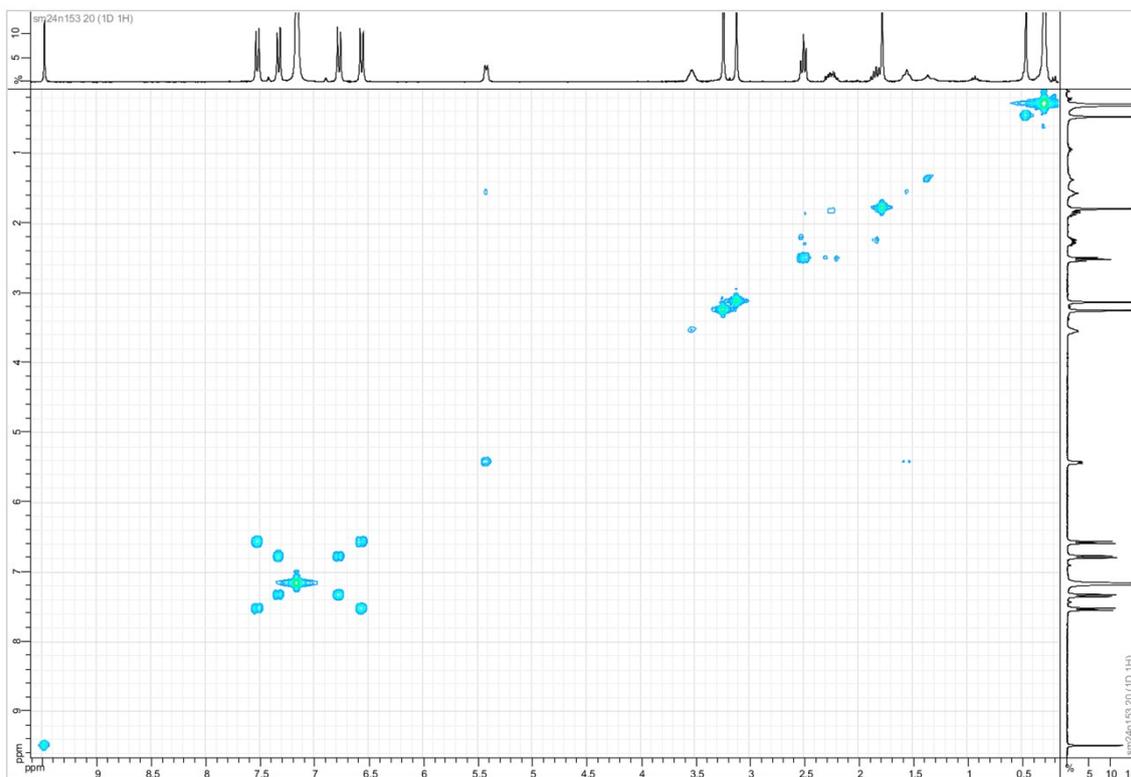
¹H NMR spectrum of compound **5g** in C₆D₆-d₆ at 300 MHz



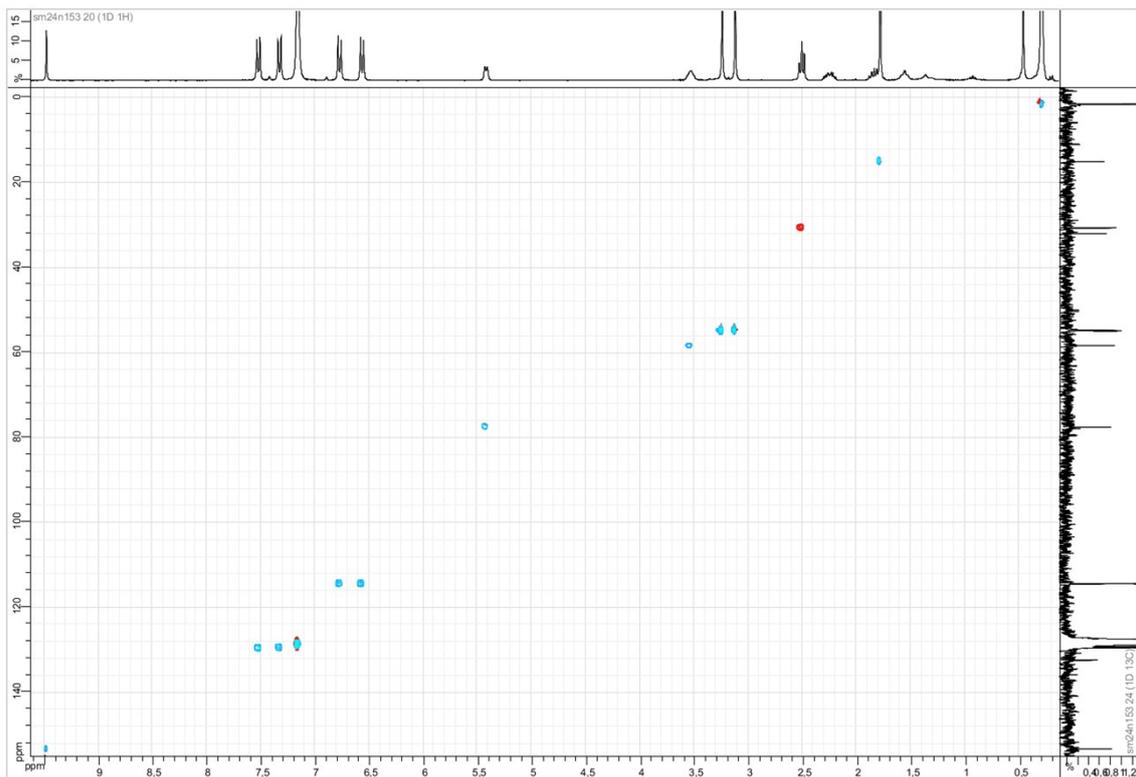
¹³C NMR spectrum of compound **5g** in C₆D₆-d₆ at 75 MHz



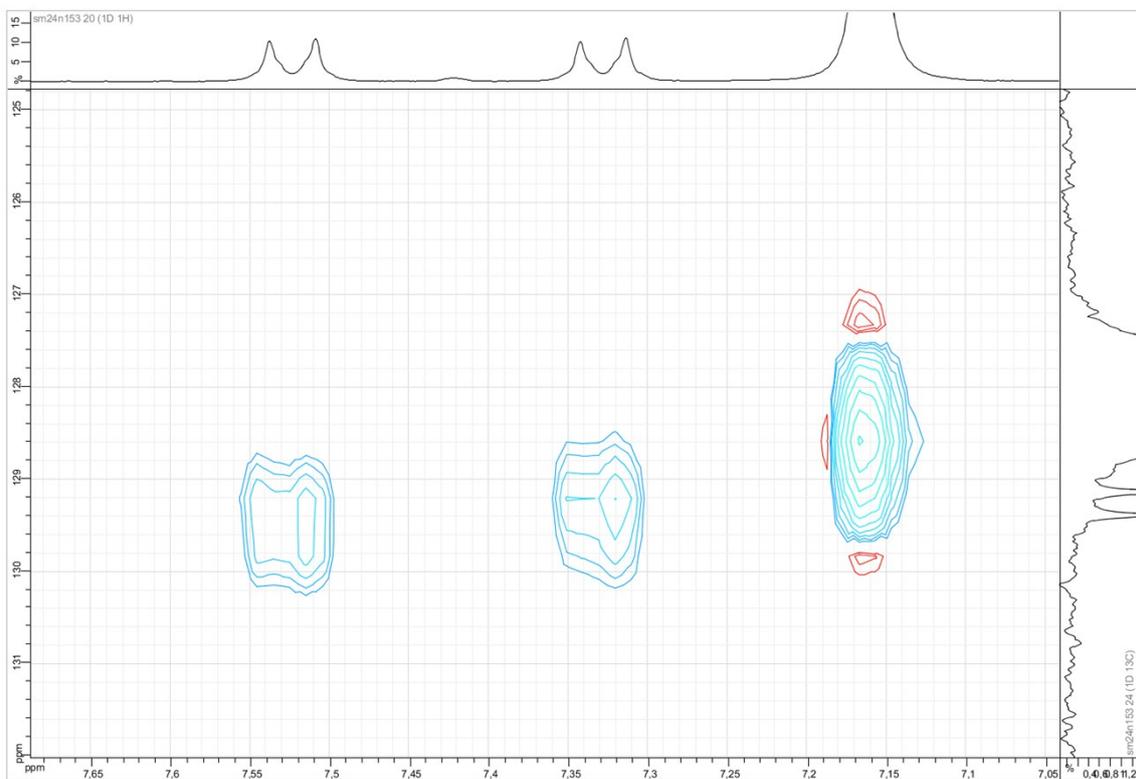
DEPT 135 NMR spectrum of compound **5g** in $C_6D_6-d_6$ at 75 MHz



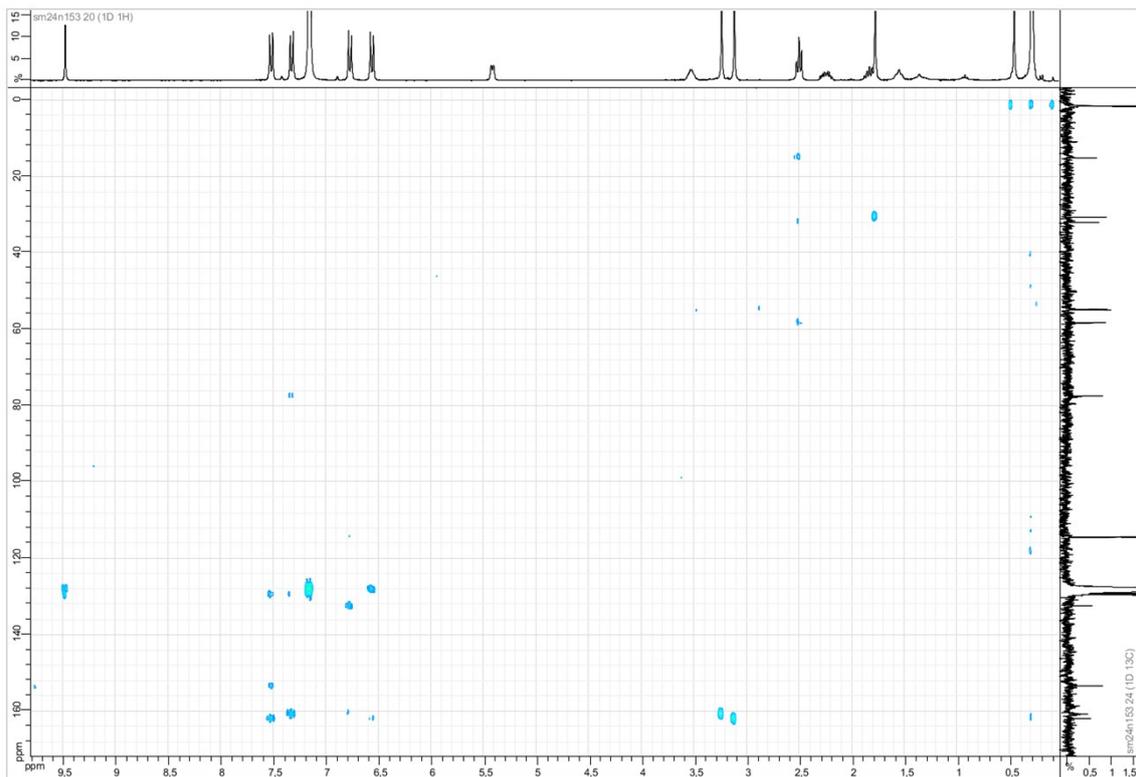
COSY NMR spectrum of compound **5g** in $C_6D_6-d_6$



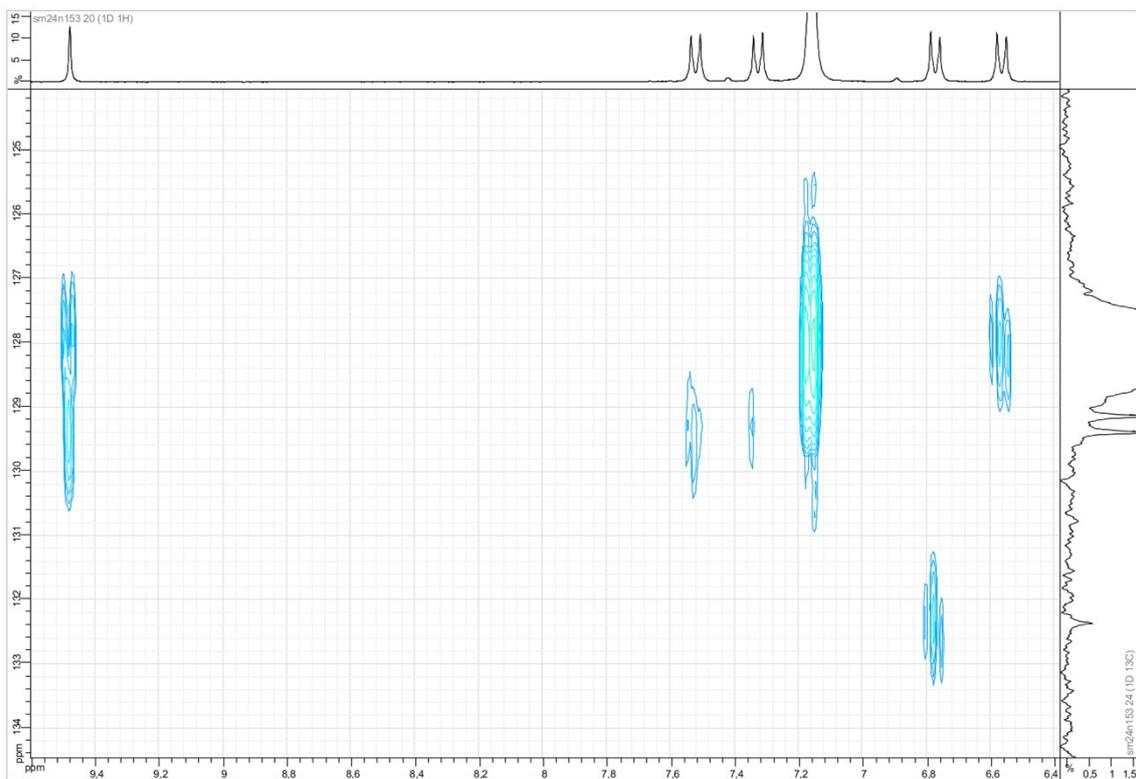
HSQC NMR spectrum of compound **5g** in $C_6D_6-d_6$



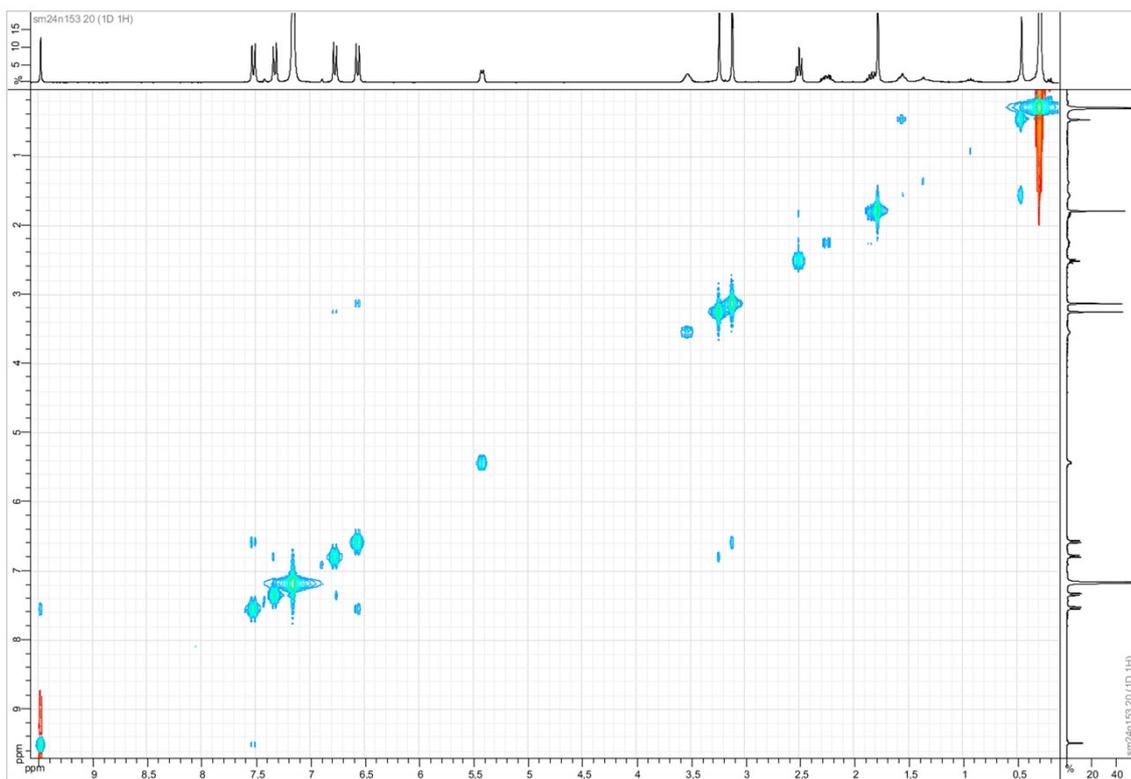
HSQC NMR spectrum of compound **5g** in $C_6D_6-d_6$ (zoom)



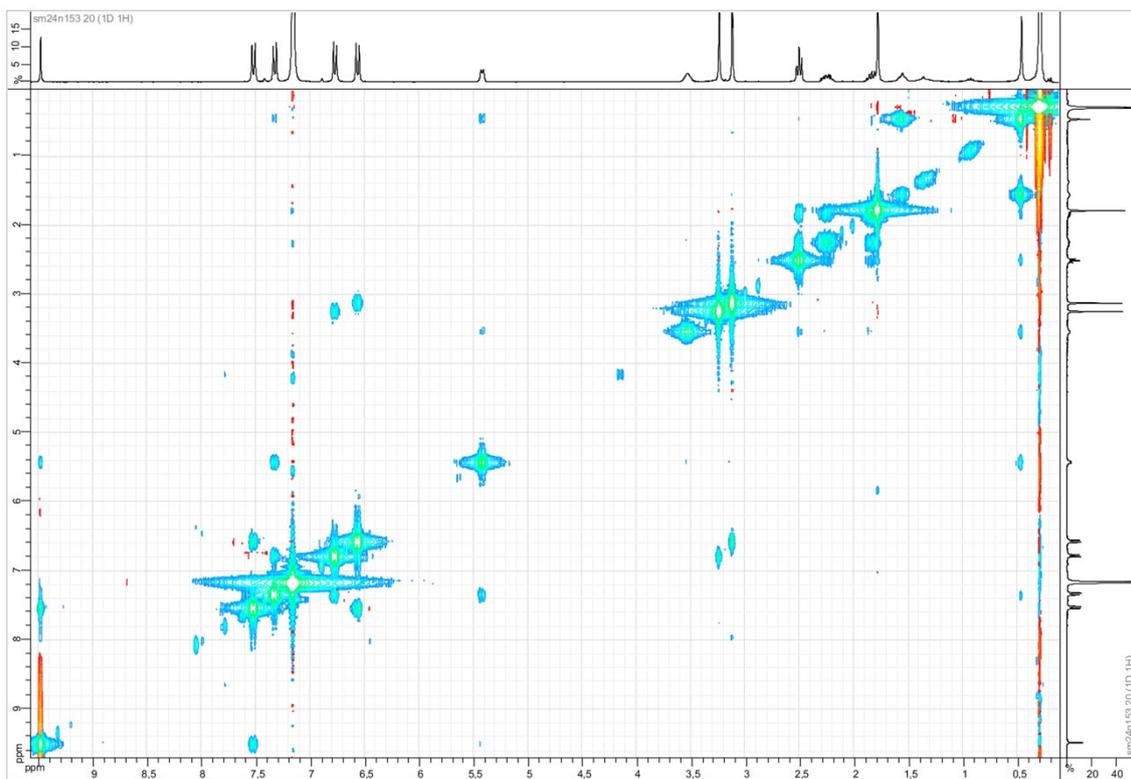
^1H - ^{13}C HMBC NMR spectrum of compound **5g** in C_6D_6 - d_6



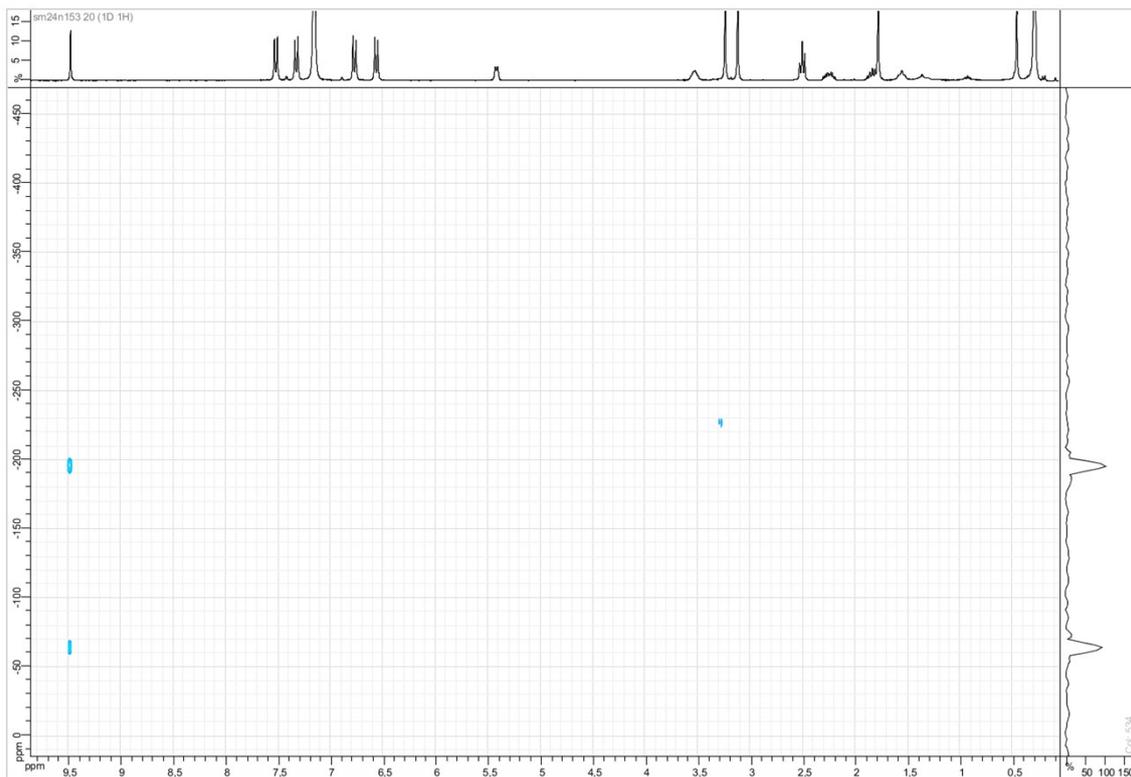
^1H - ^{13}C HMBC NMR spectrum of compound **5g** in C_6D_6 - d_6 (zoom)



NOESY NMR spectrum of compound **5g** in $C_6D_6-d_6$

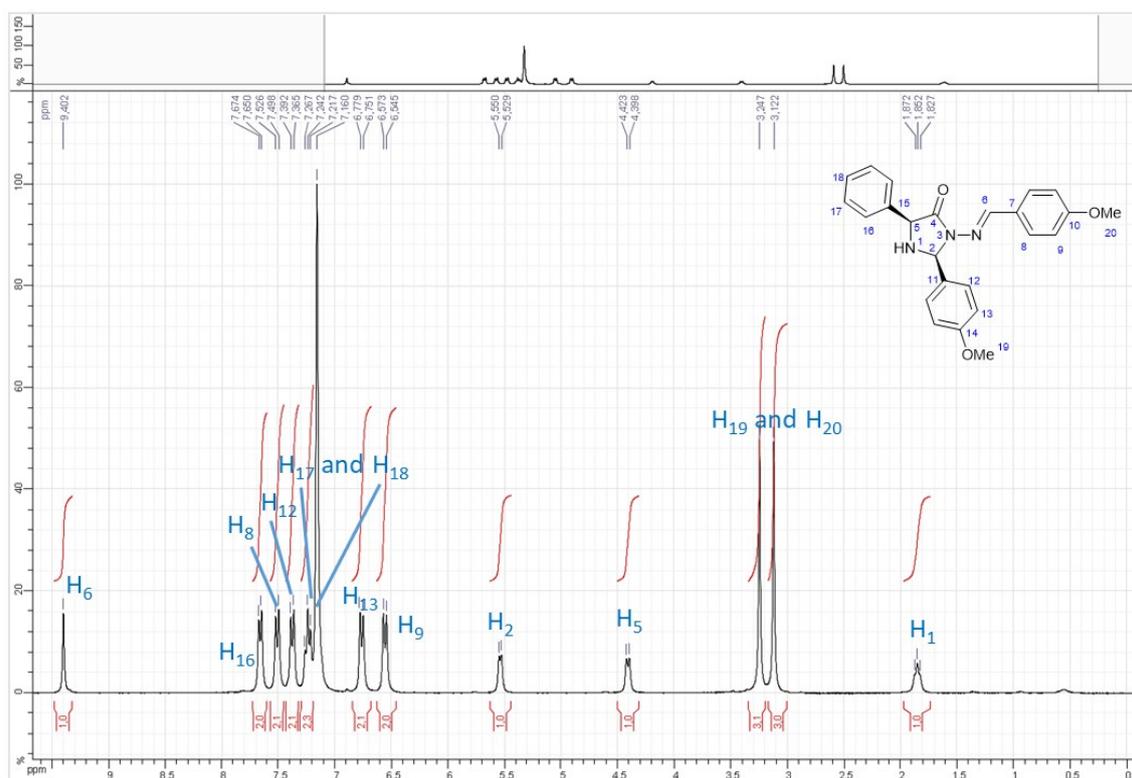


NOESY NMR spectrum of compound **5g** in $C_6D_6-d_6$ (deep cut)

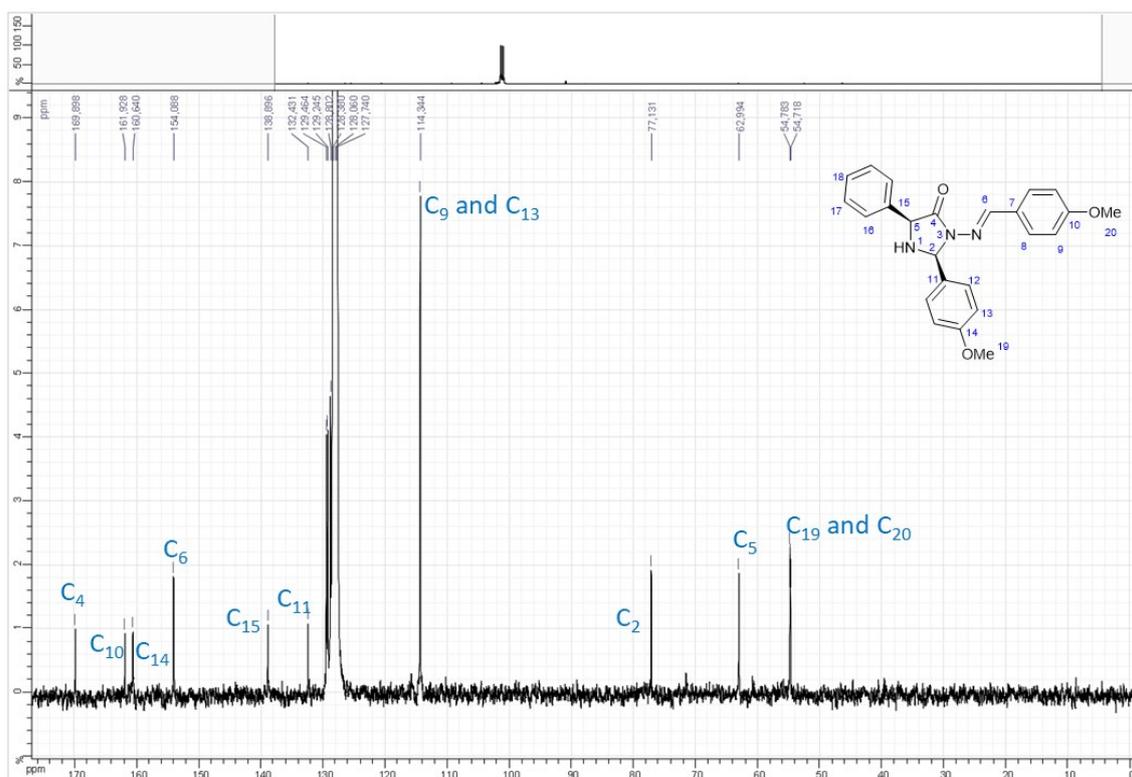


^1H - ^{15}N HMBC NMR spectrum of compound **5g** in C_6D_6 - d_6

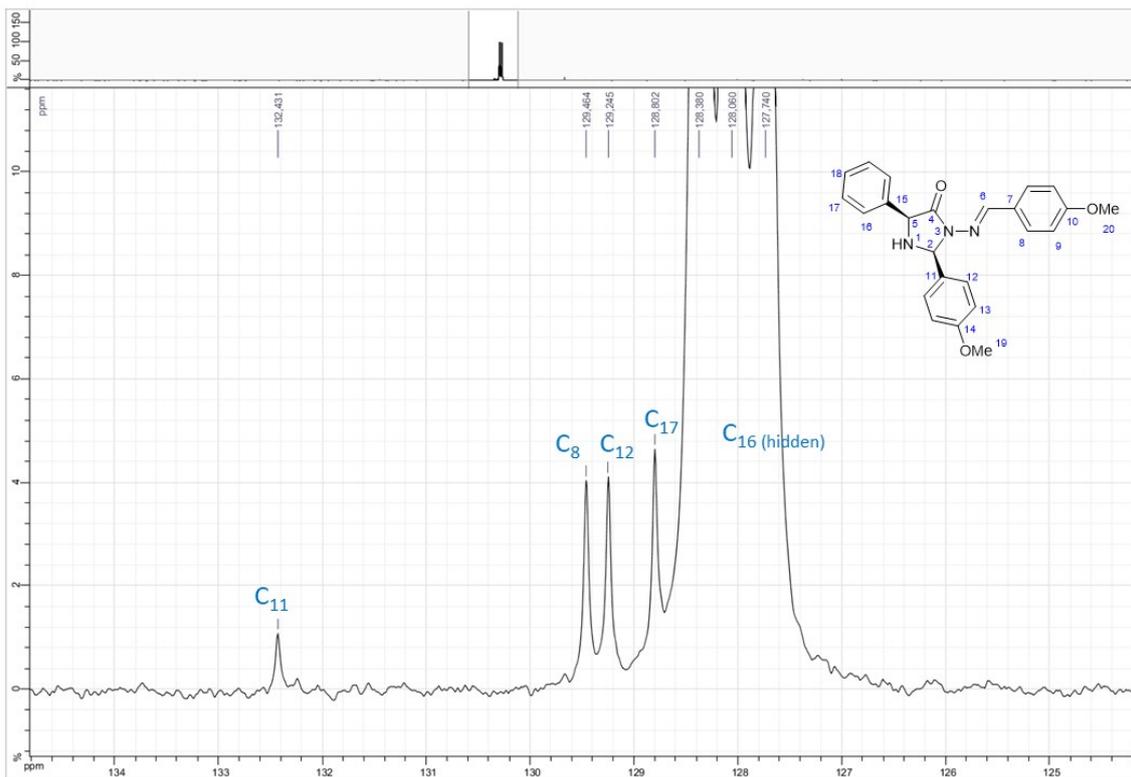
h. NMR spectra of **5h**



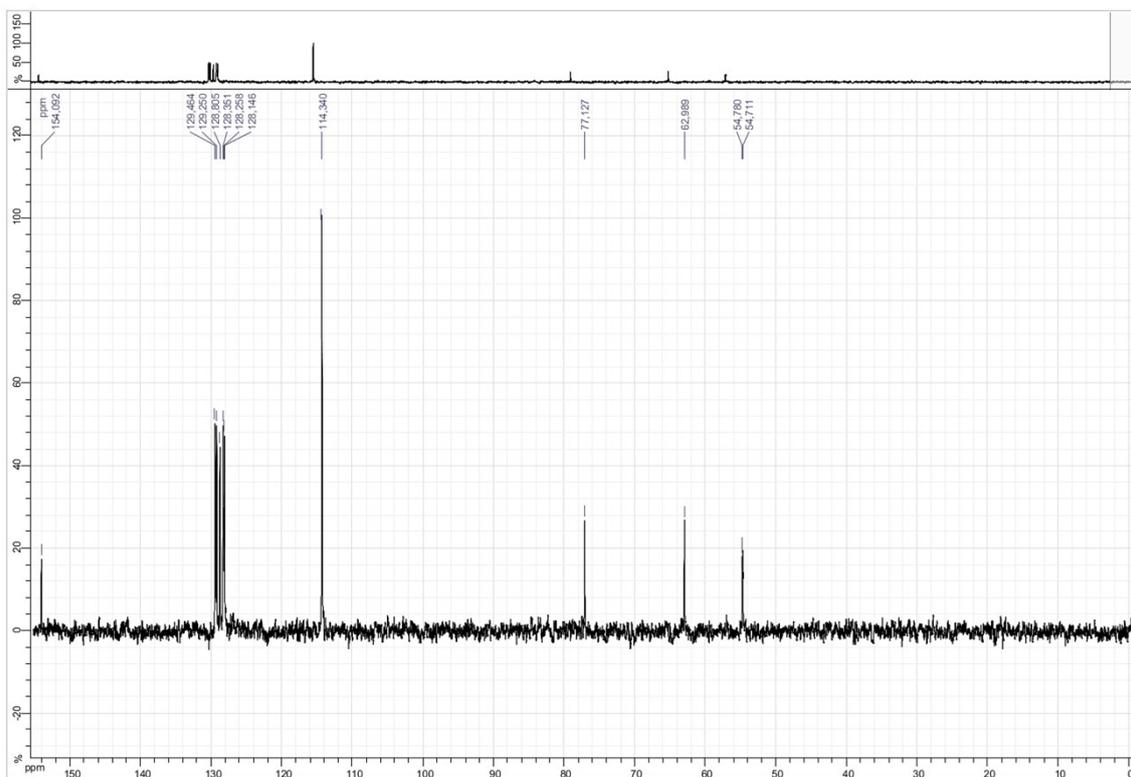
¹H NMR spectrum of compound **5h** in C₆D₆-d₆ at 300 MHz



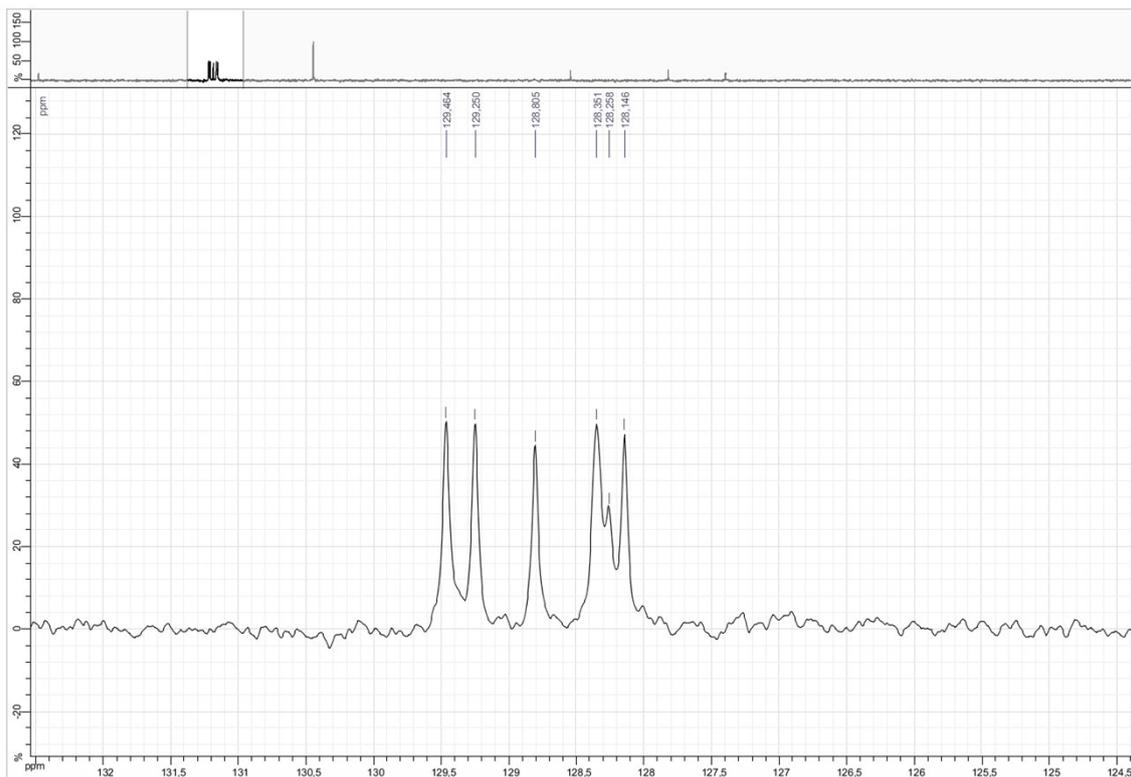
¹³C NMR spectrum of compound **5h** in C₆D₆-d₆ at 75 MHz



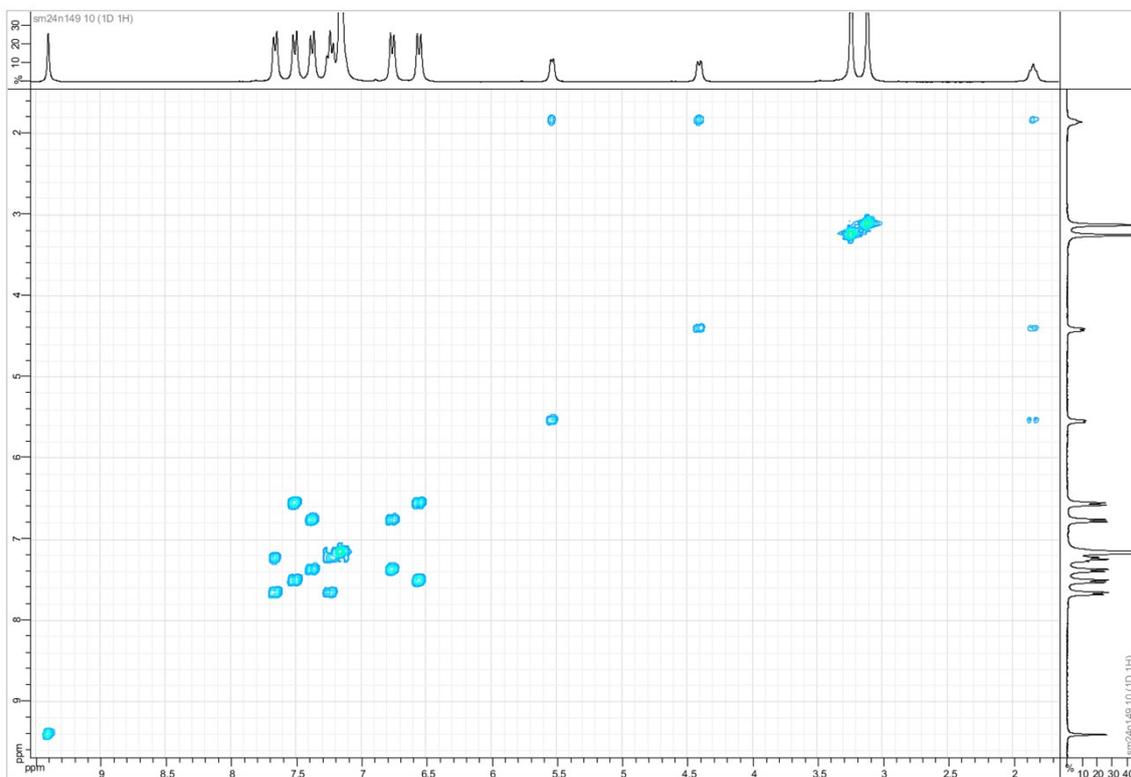
^{13}C NMR spectrum of compound **5h** in C_6D_6-d_6 at 75 MHz (zoom)



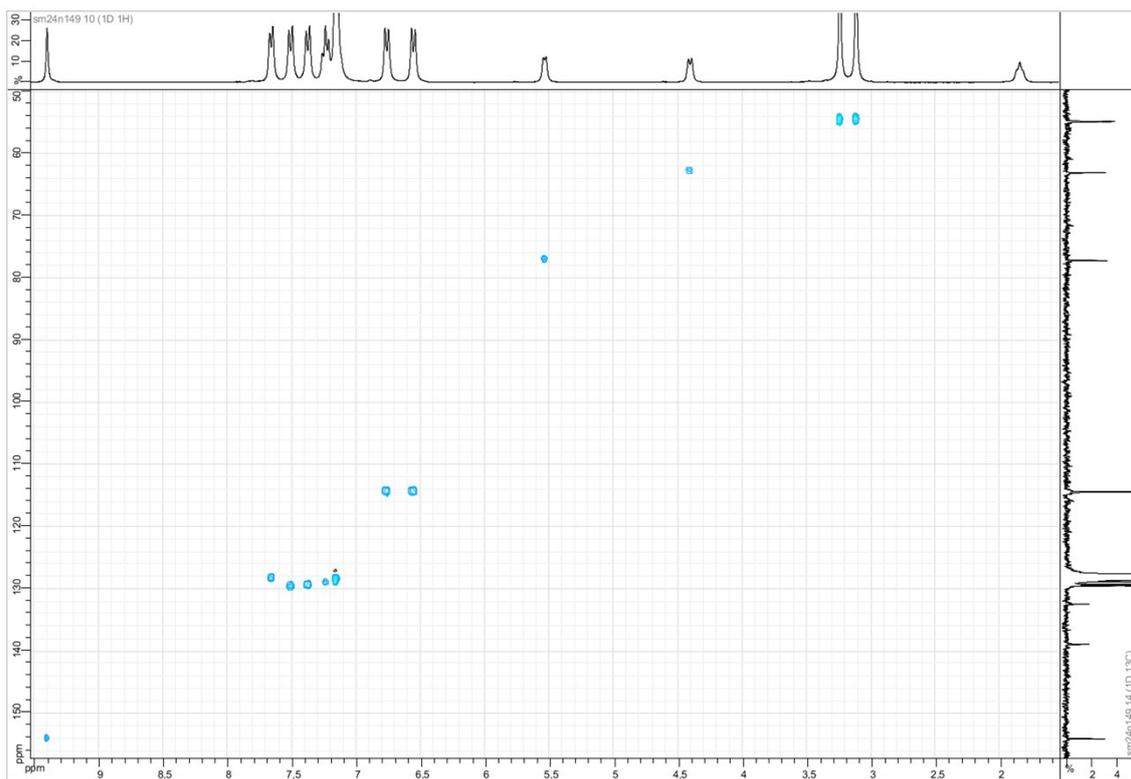
DEPT 135 NMR spectrum of compound **5h** in C_6D_6-d_6 at 75 MHz



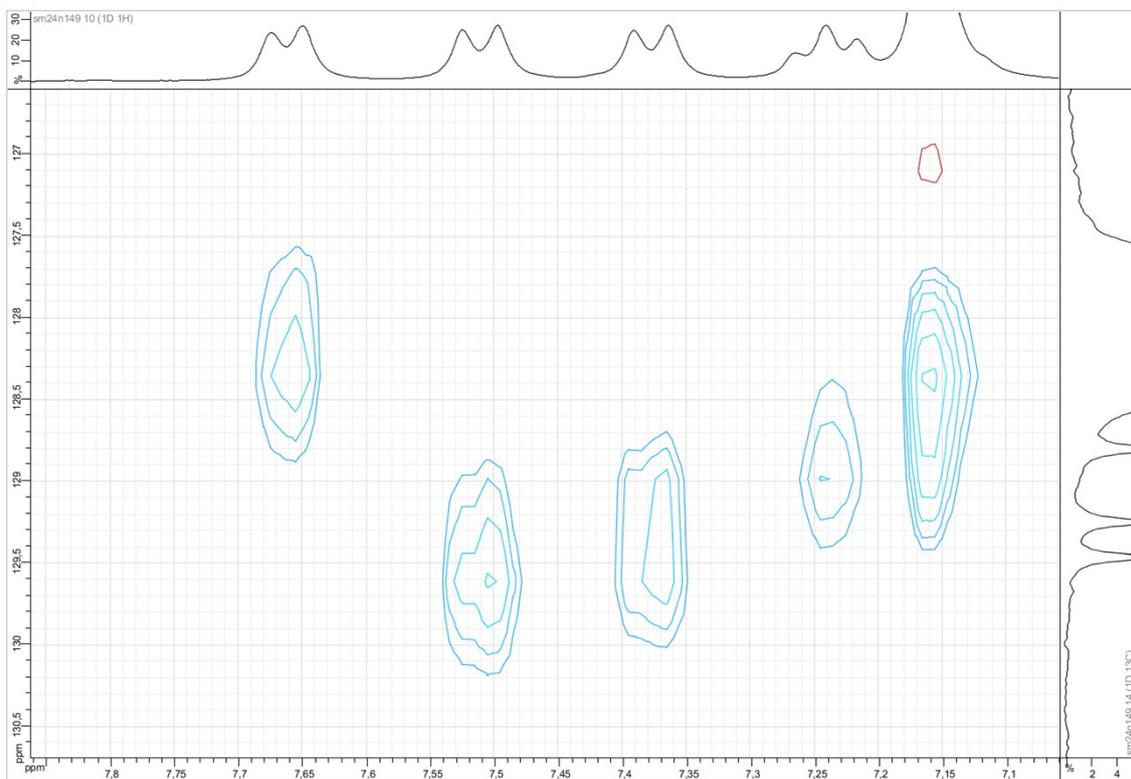
DEPT 135 NMR spectrum of compound **5h** in $C_6D_6-d_6$ at 75 MHz (zoom)



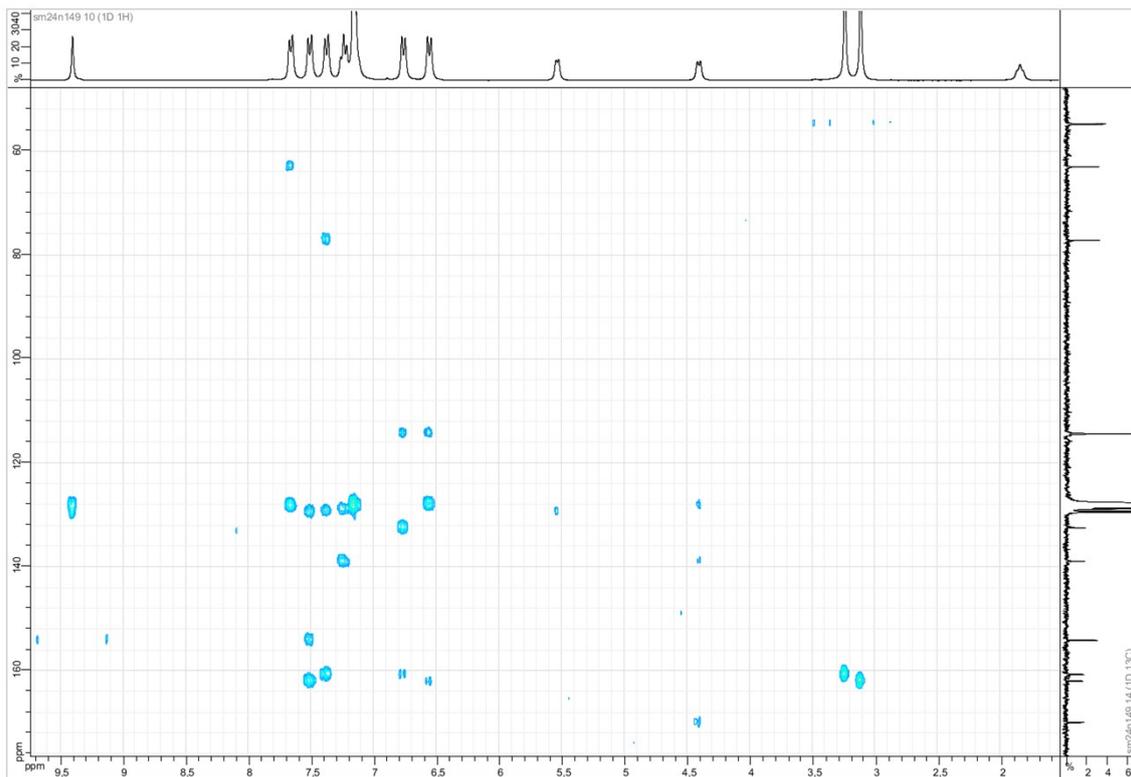
COSY NMR spectrum of compound **5h** in $C_6D_6-d_6$



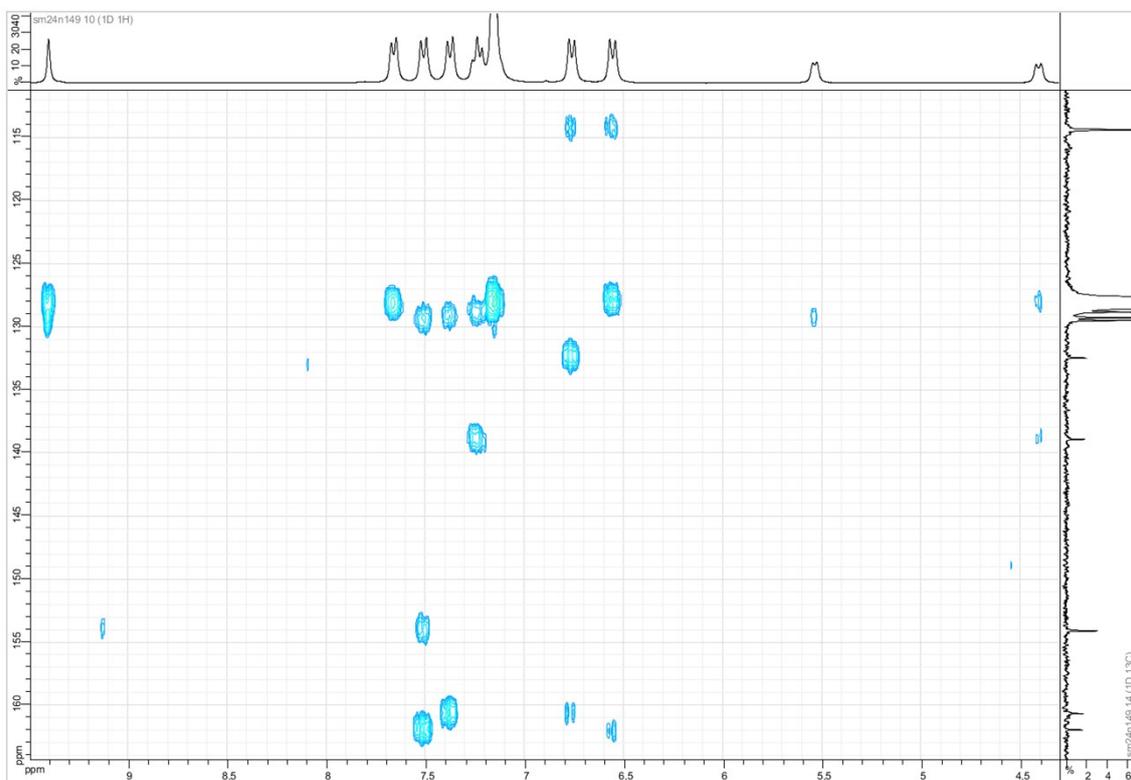
HSQC NMR spectrum of compound **5h** in $C_6D_6-d_6$



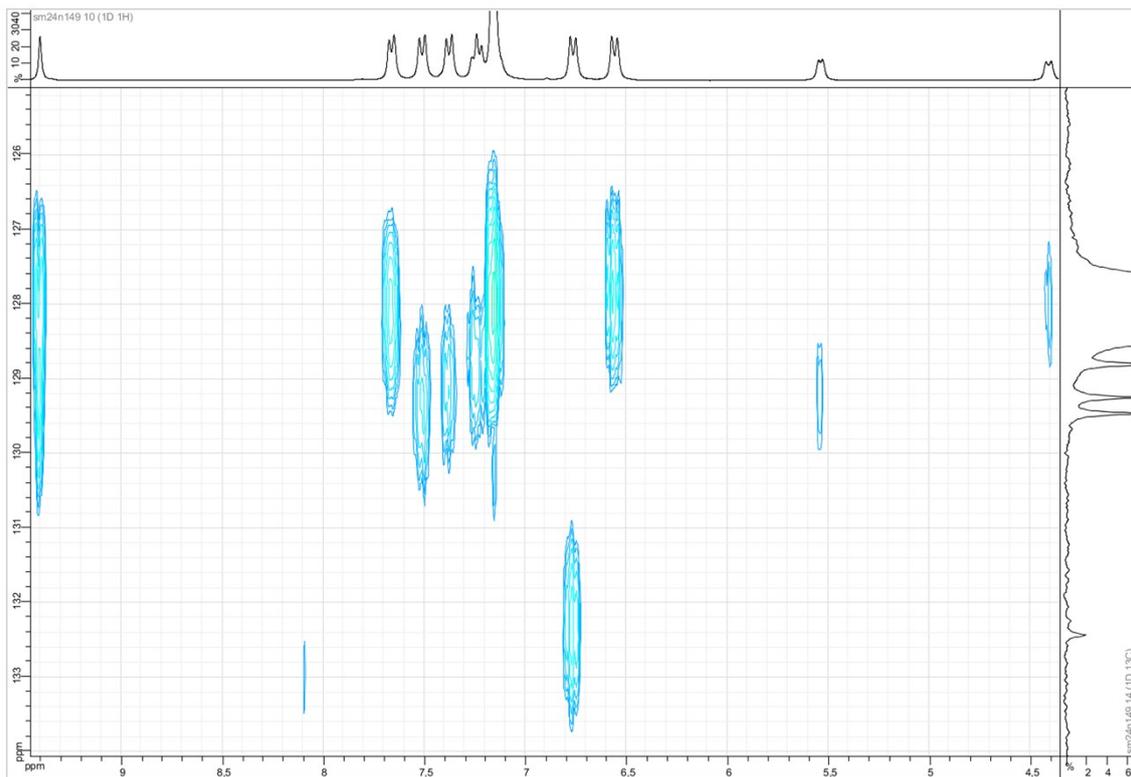
HSQC NMR spectrum of compound **5h** in $C_6D_6-d_6$ (zoom)



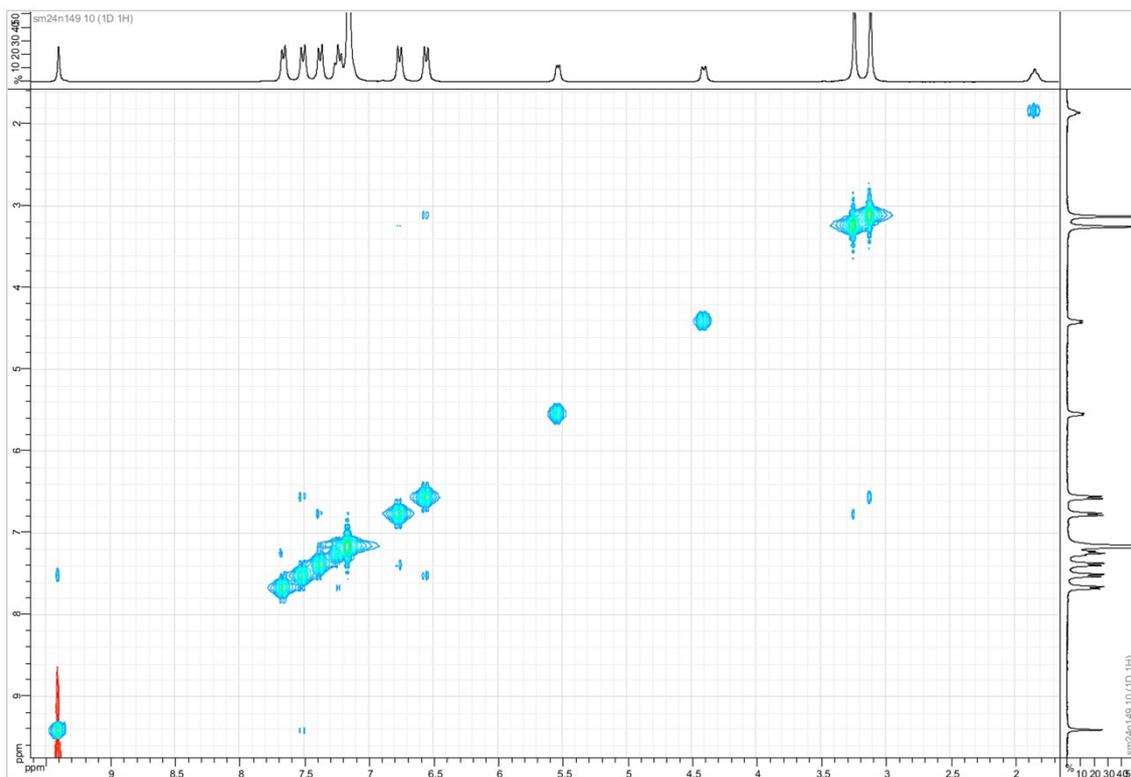
^1H - ^{13}C HMBC NMR spectrum of compound **5h** in C_6D_6 - d_6



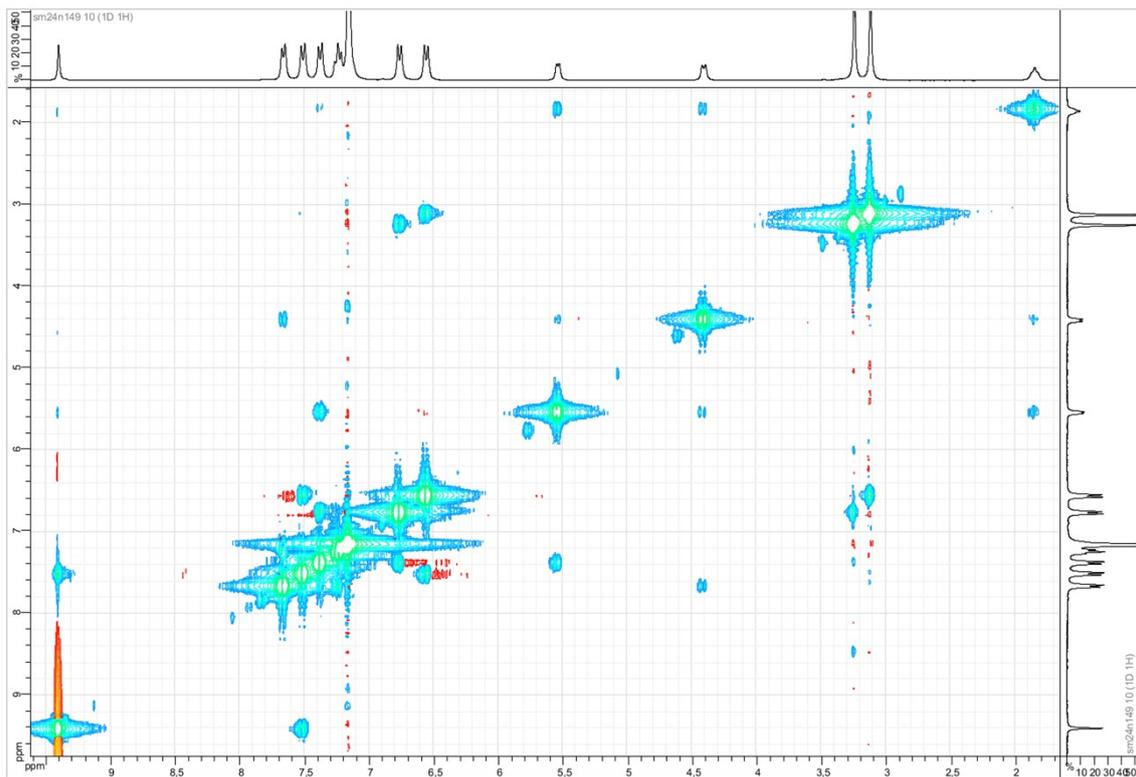
^1H - ^{13}C HMBC NMR spectrum of compound **5h** in C_6D_6 - d_6 (zoom 1)



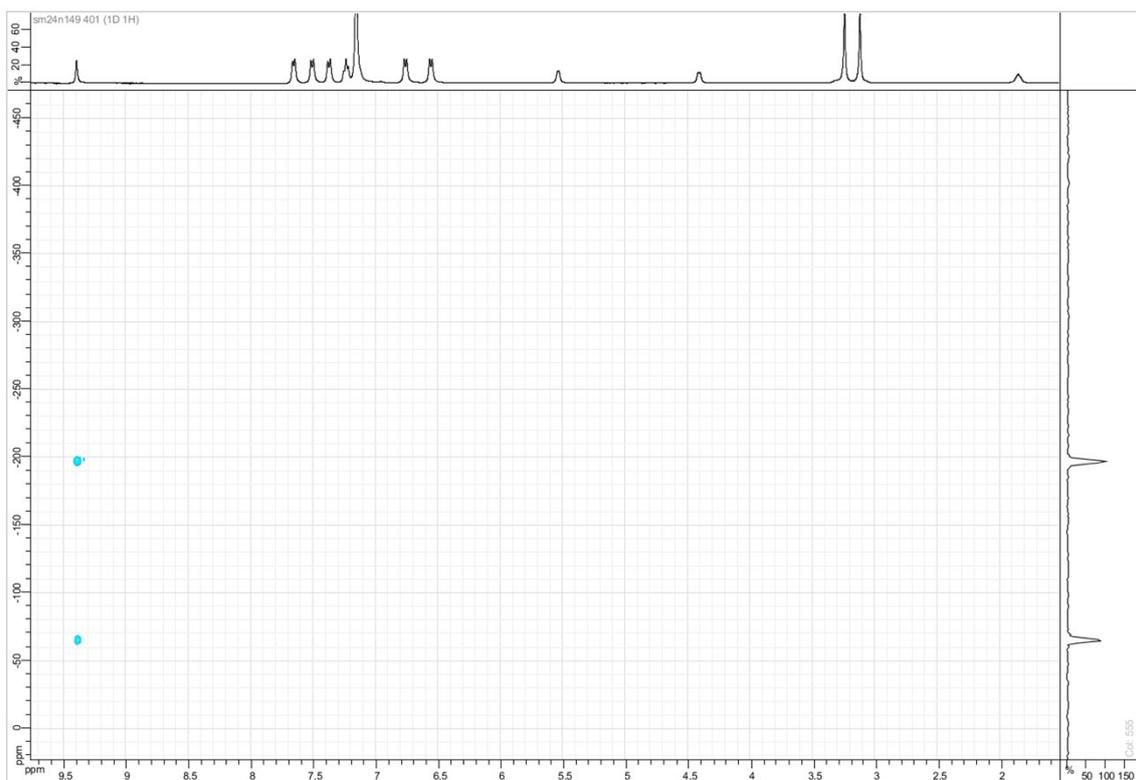
^1H - ^{13}C HMBC NMR spectrum of compound **5h** in C_6D_6 - d_6 (zoom 2)



NOESY NMR spectrum of compound **5h** in C_6D_6 - d_6

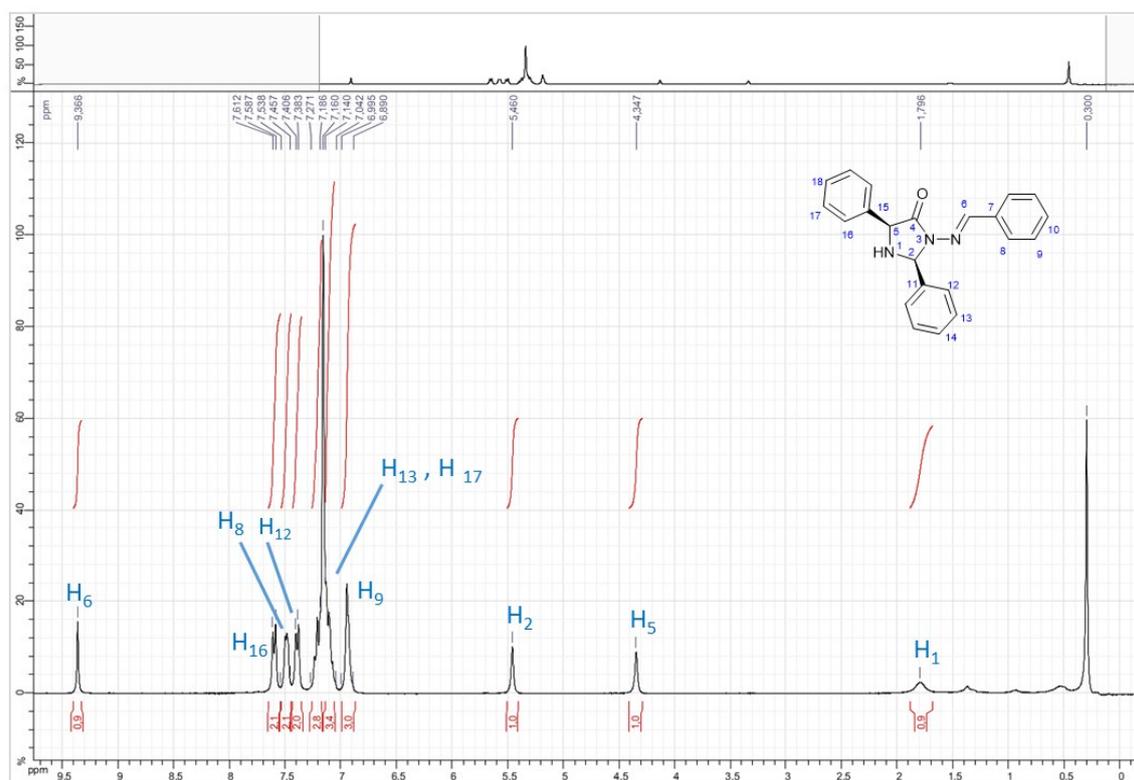


NOESY NMR spectrum of compound **5h** in $C_6D_6-d_6$ (deep cut)

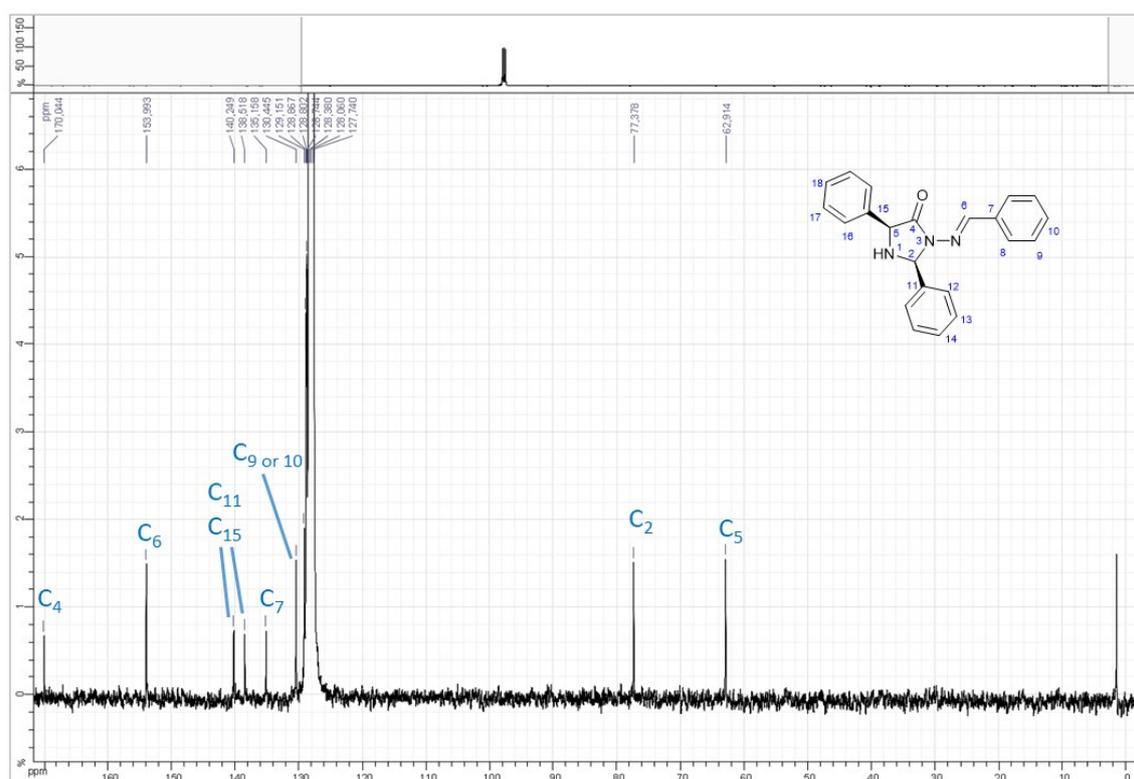


1H - ^{15}N HMBC NMR spectrum of compound **5h** in $C_6D_6-d_6$

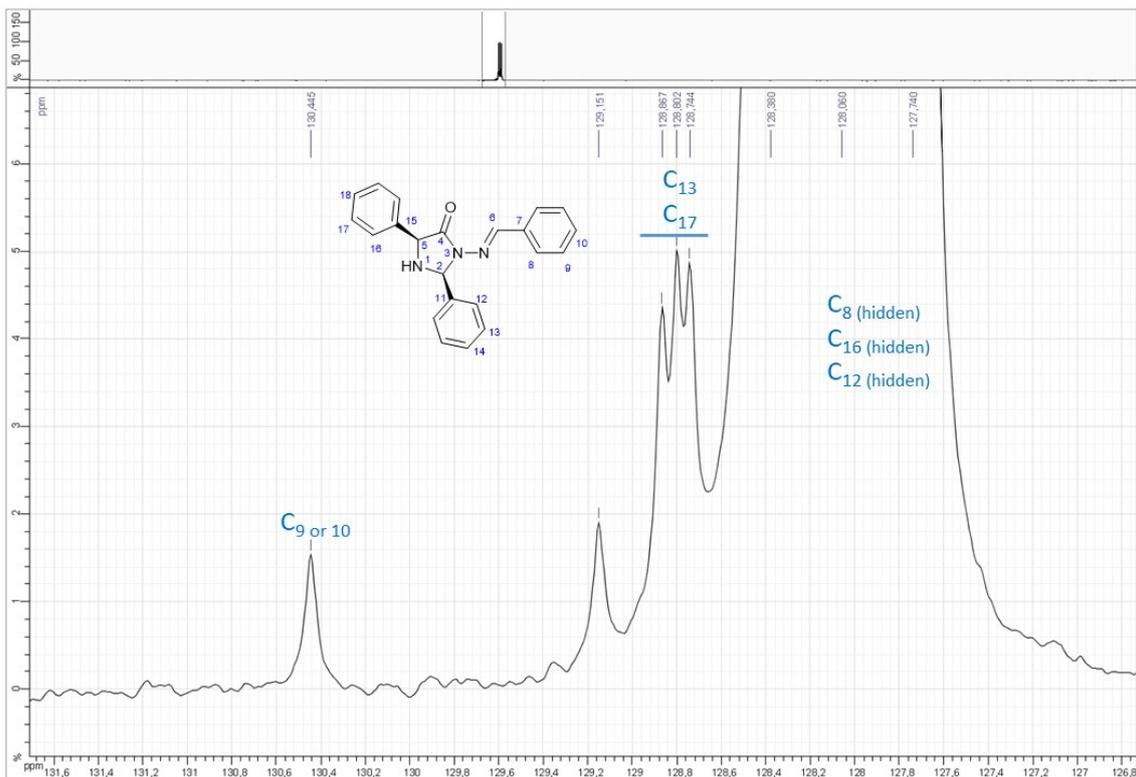
j. NMR spectra of **5i**



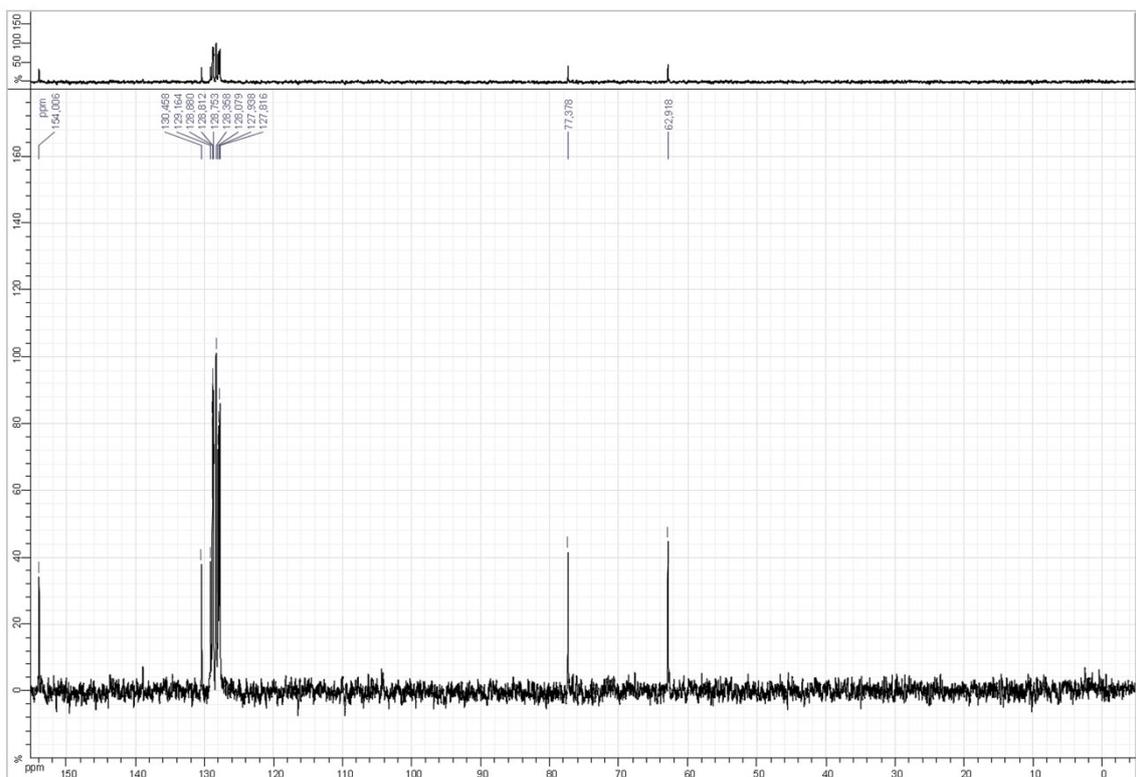
¹H NMR spectrum of compound **5i** in C₆D₆-d₆ at 300 MHz



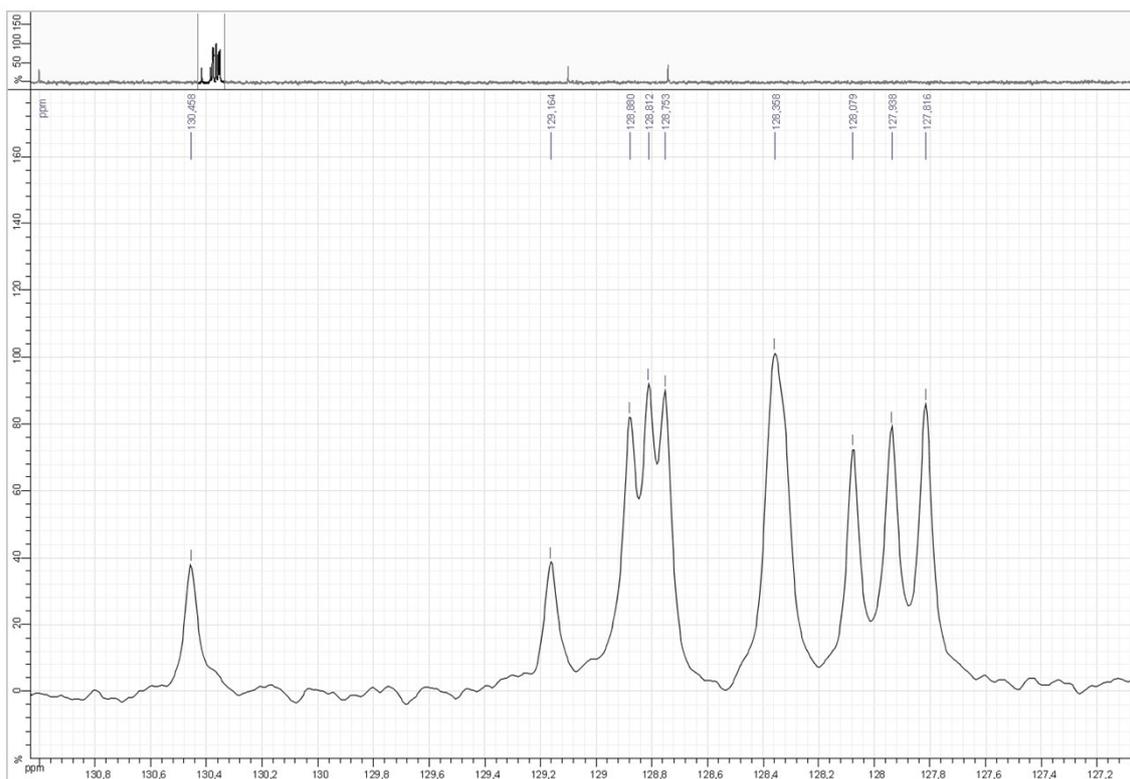
¹³C NMR spectrum of compound **5i** in C₆D₆-d₆ at 75 MHz



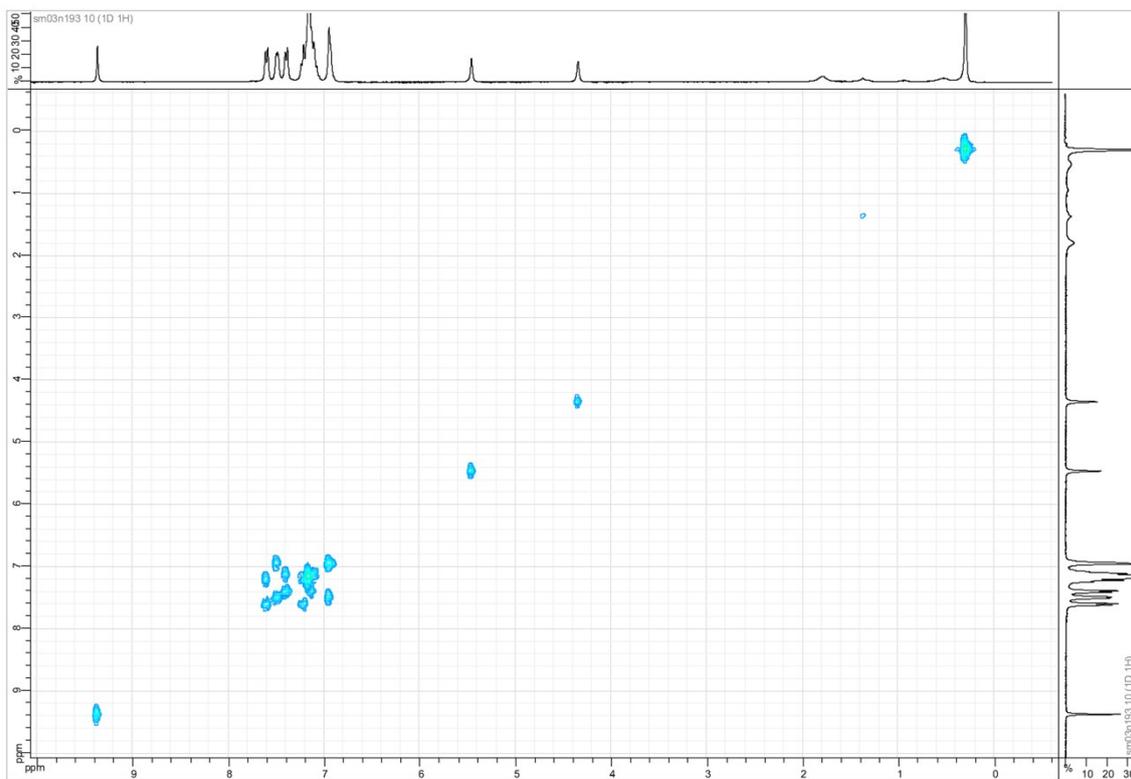
¹³C NMR spectrum of compound **5i** in C₆D₆-d₆ at 75 MHz (zoom)



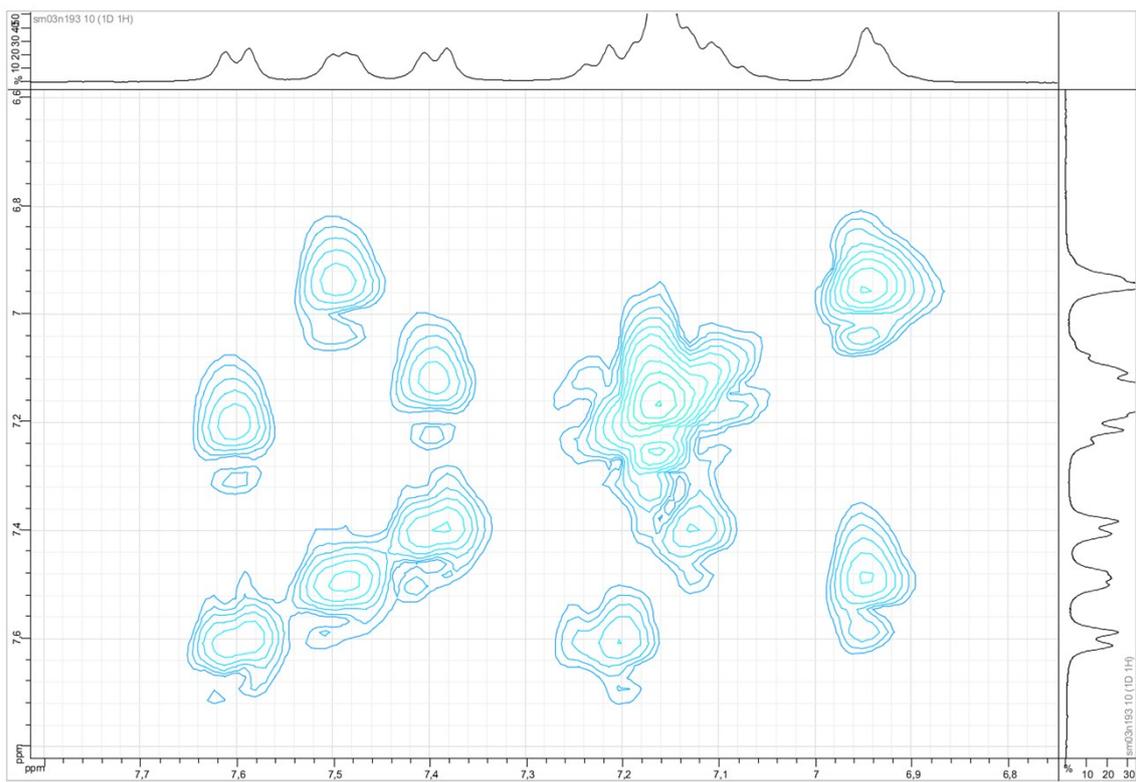
DEPT 135 NMR spectrum of compound **5i** in C₆D₆-d₆ at 75 MHz



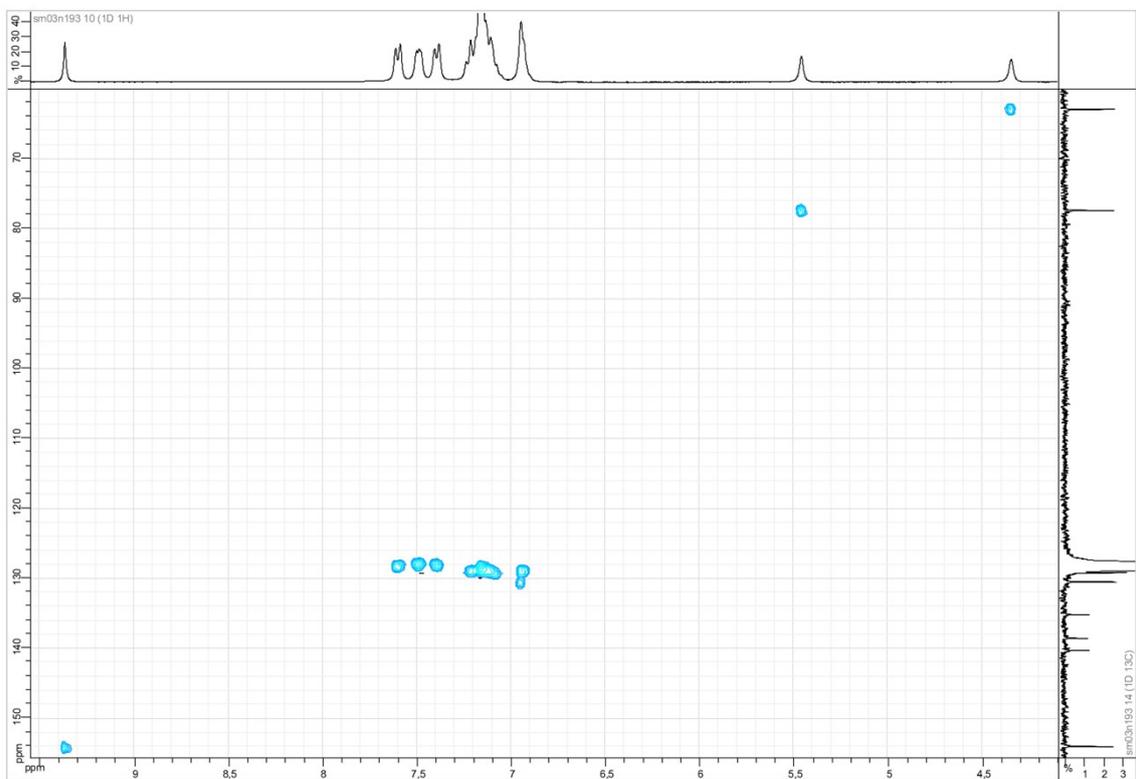
DEPT 135 NMR spectrum of compound **5i** in $C_6D_6-d_6$ at 75 MHz (zoom)



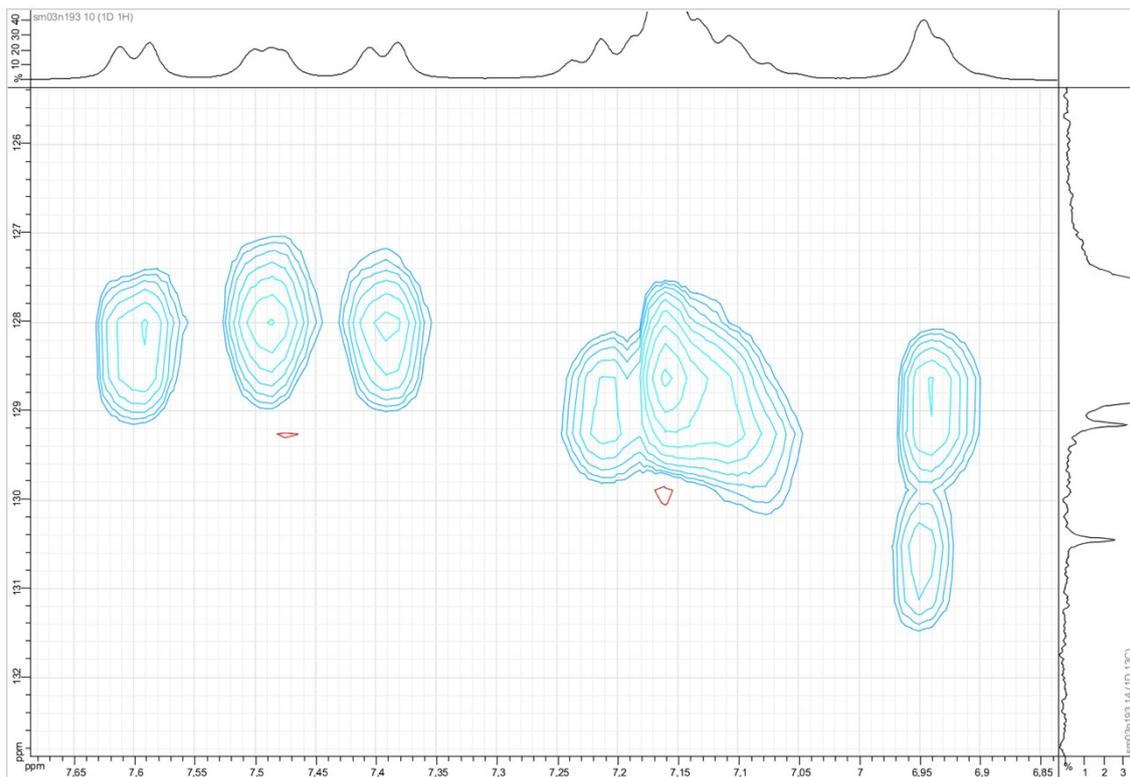
COSY NMR spectrum of compound **5i** in $C_6D_6-d_6$



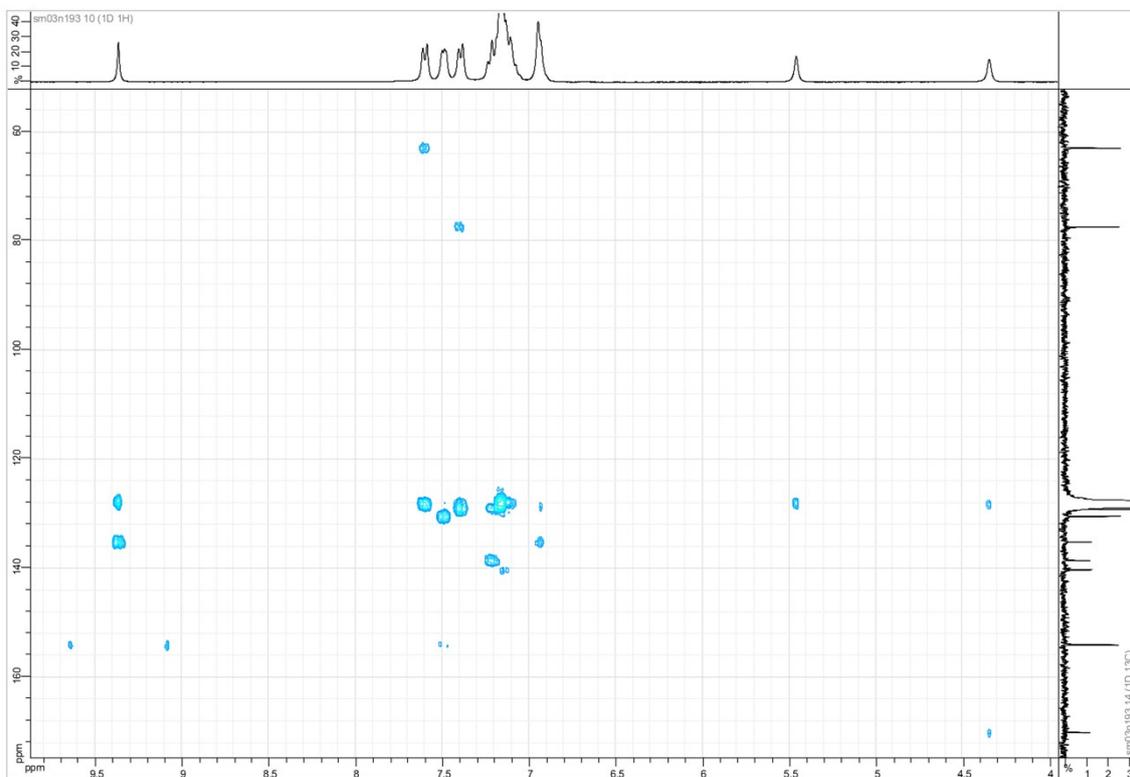
COSY NMR spectrum of compound **5i** in $C_6D_6-d_6$ (zoom)



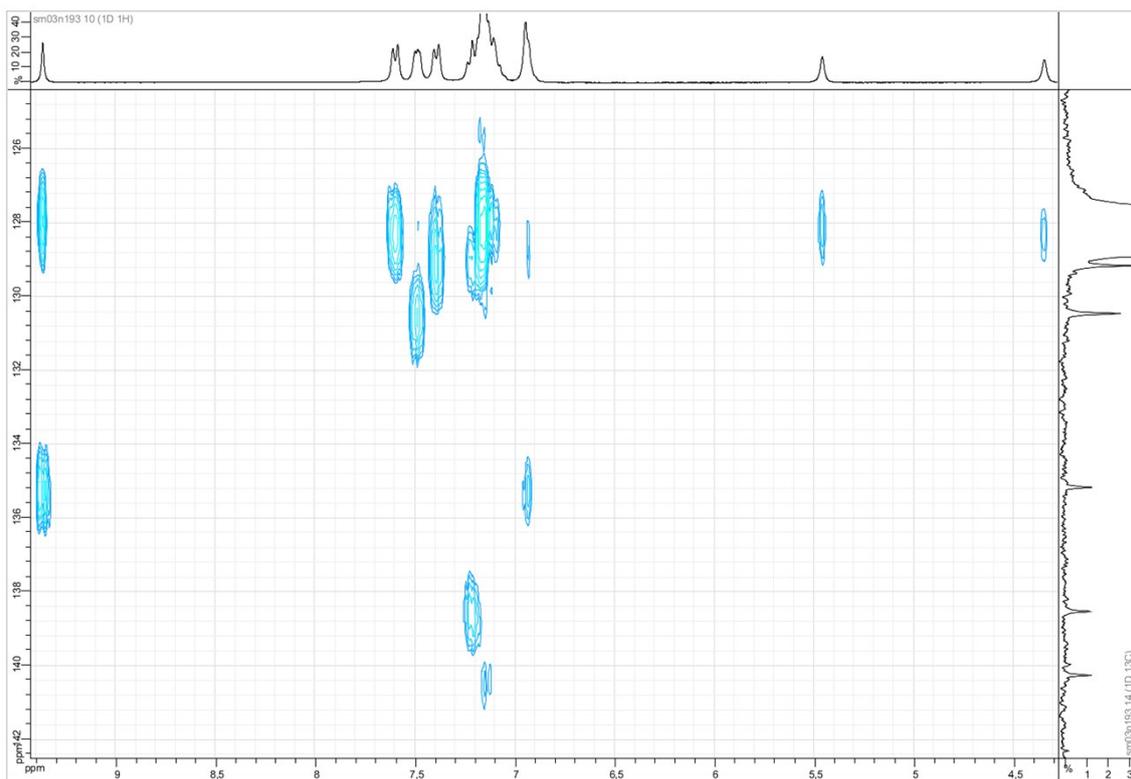
HSQC NMR spectrum of compound **5i** in $C_6D_6-d_6$



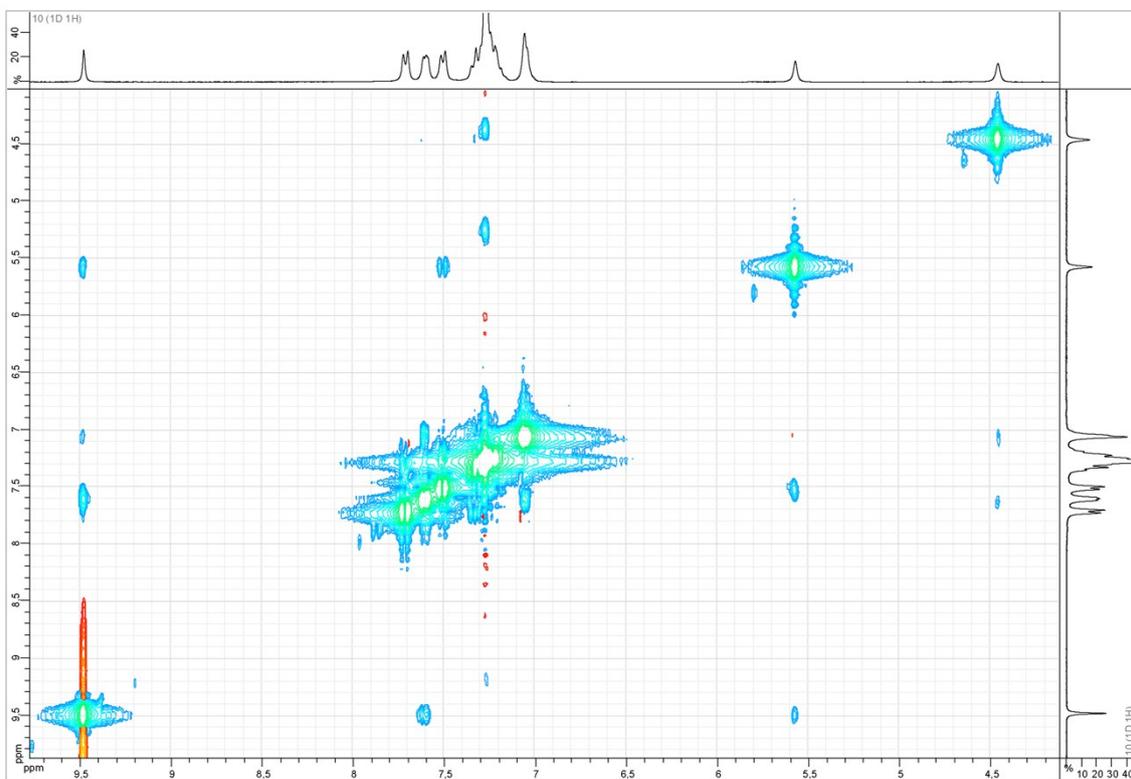
HSQC NMR spectrum of compound **5i** in $C_6D_6-d_6$ (zoom)



1H - ^{13}C HMBC NMR spectrum of compound **5i** in $C_6D_6-d_6$

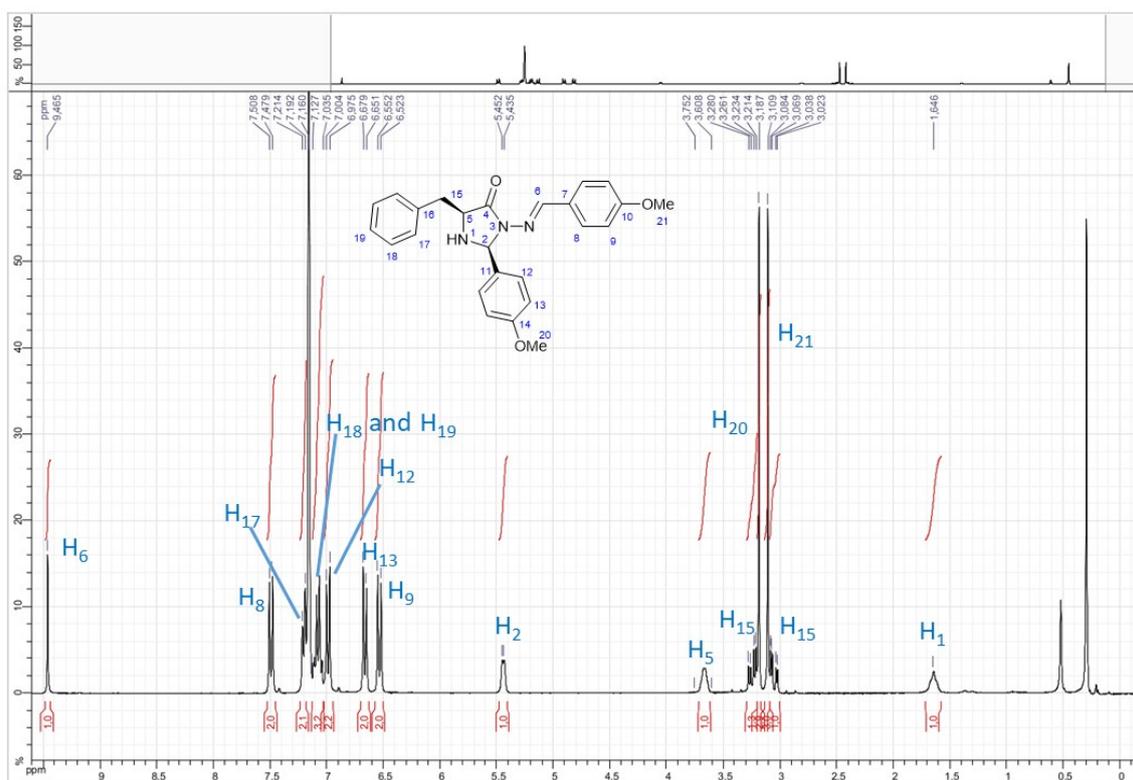


^1H - ^{13}C HMBC NMR spectrum of compound **5i** in C_6D_6-d_6 (zoom)

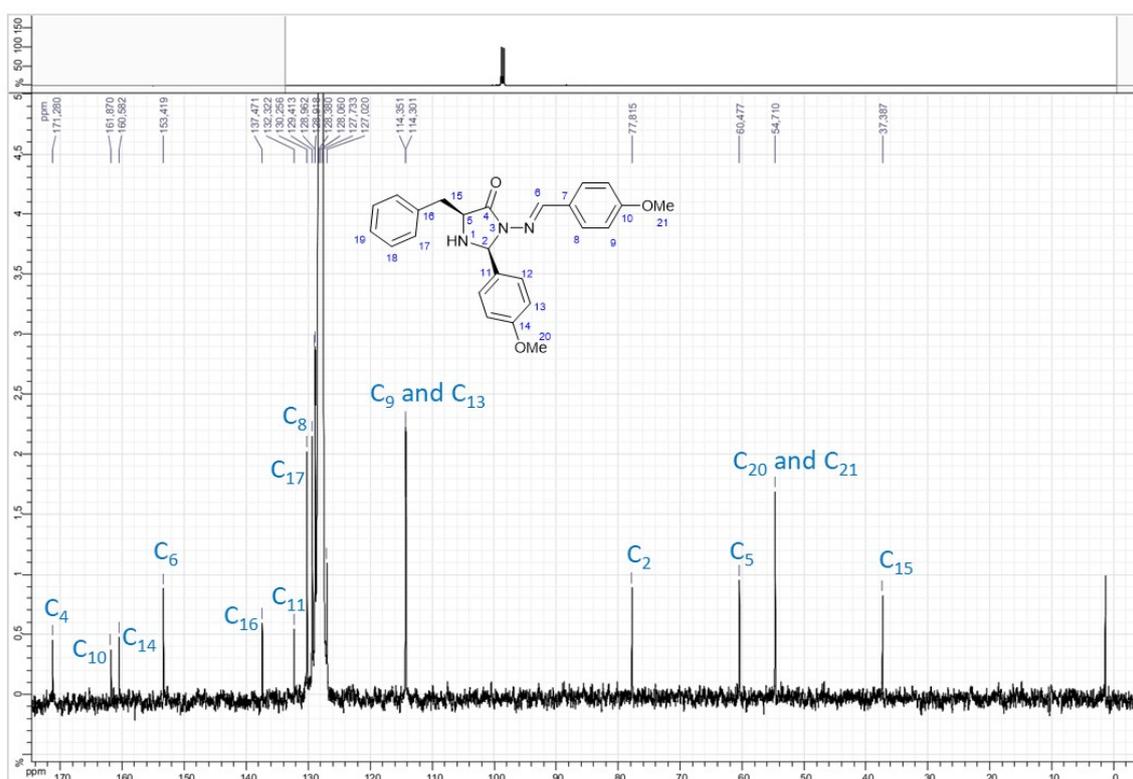


NOESY NMR spectrum of compound **5i** in C_6D_6-d_6

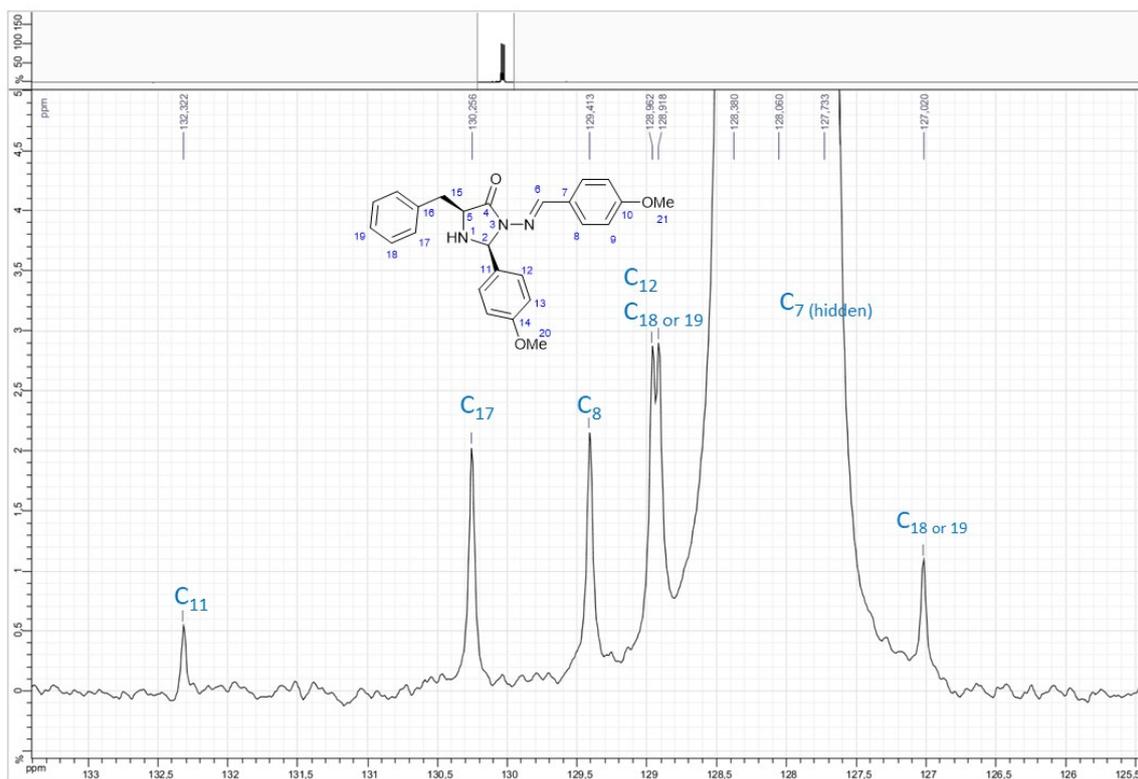
i. NMR spectra of **5j**



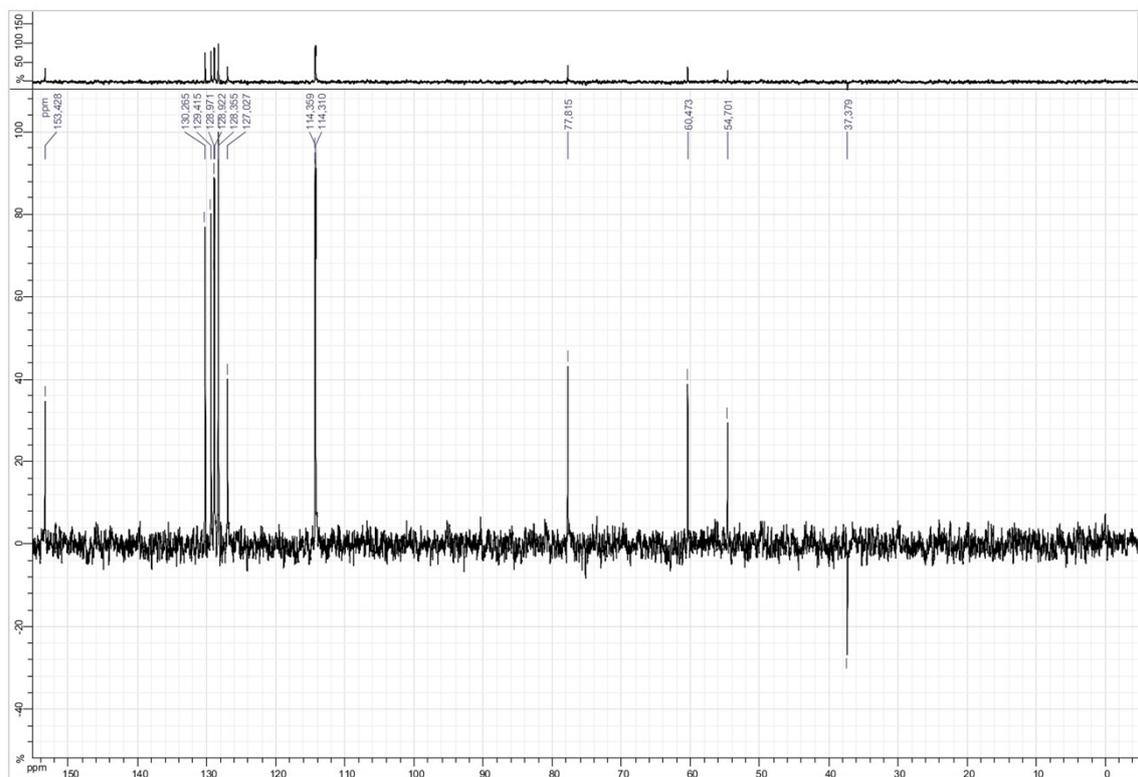
¹H NMR spectrum of compound **5j** in C₆D₆-d₆ at 400 MHz



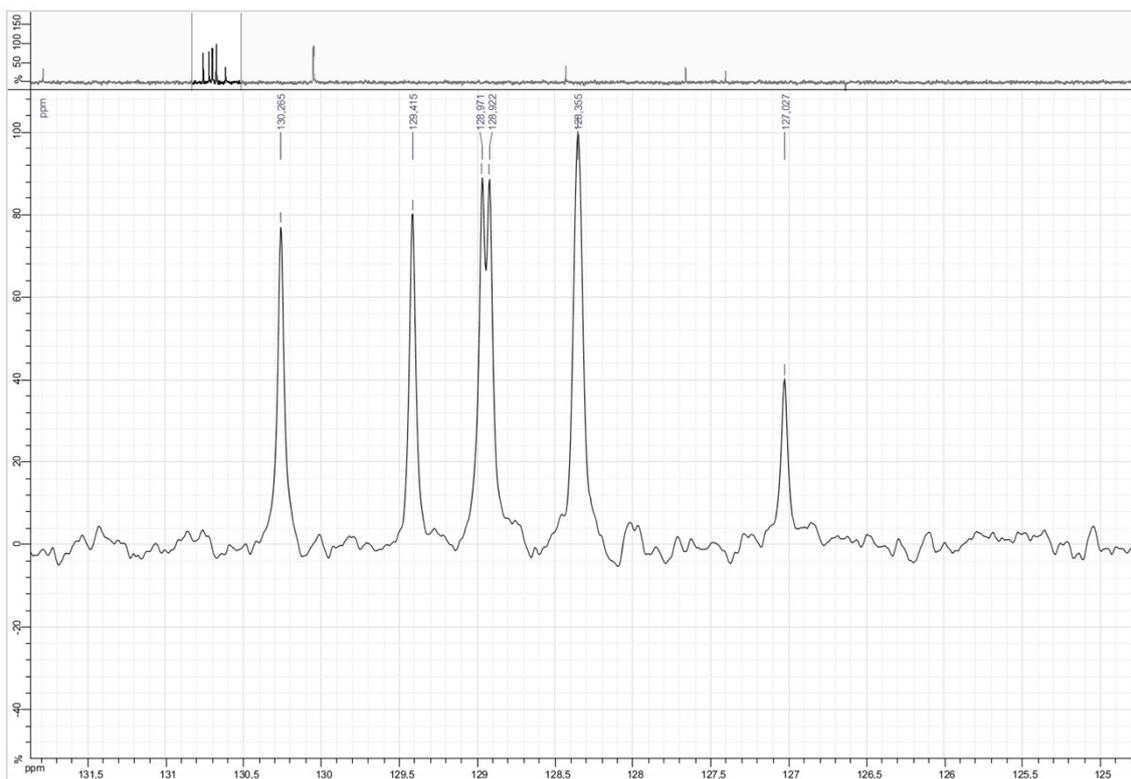
¹³C NMR spectrum of compound **5j** in C₆D₆-d₆ at 75 MHz



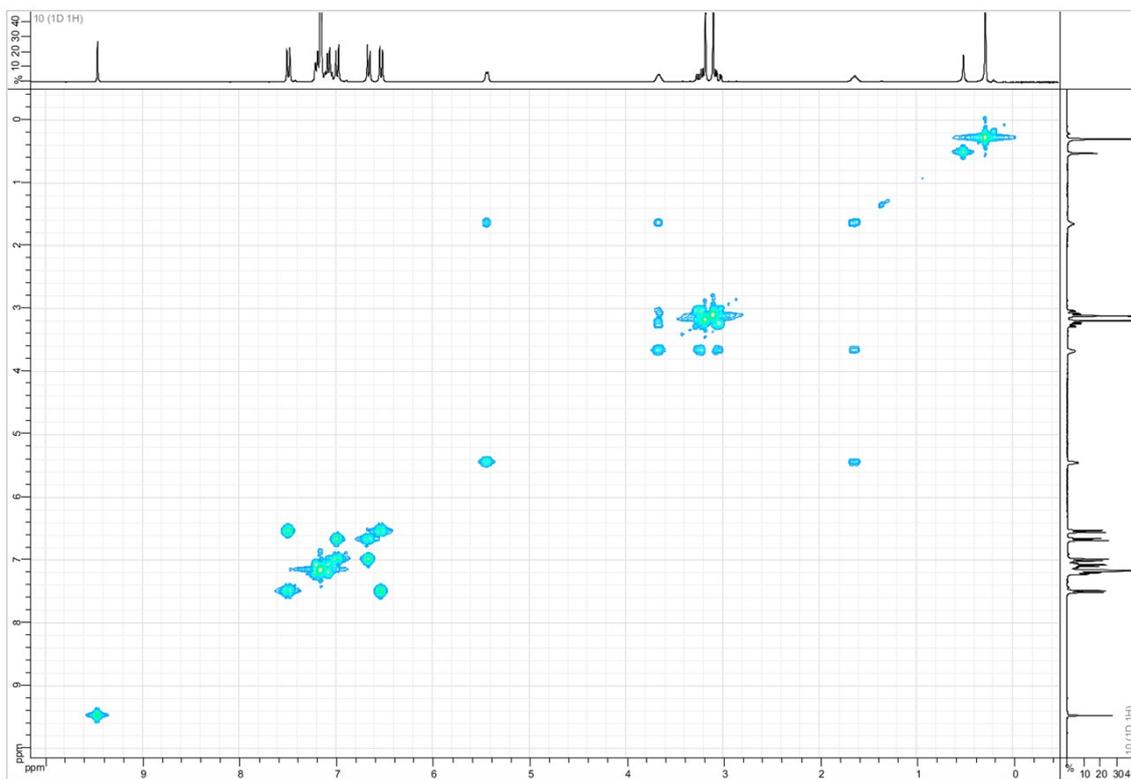
^{13}C NMR spectrum of compound **5j** in C_6D_6-d_6 at 75 MHz (zoom)



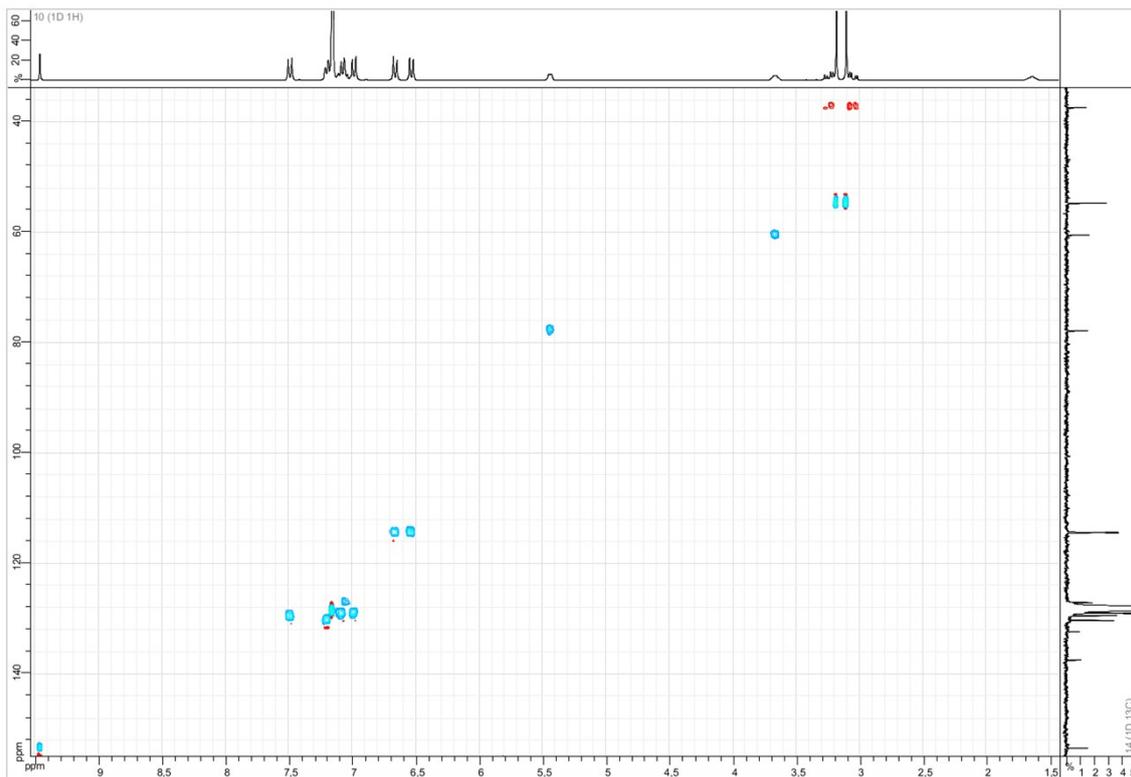
DEPT 135 NMR spectrum of compound **5j** in C_6D_6-d_6 at 75 MHz



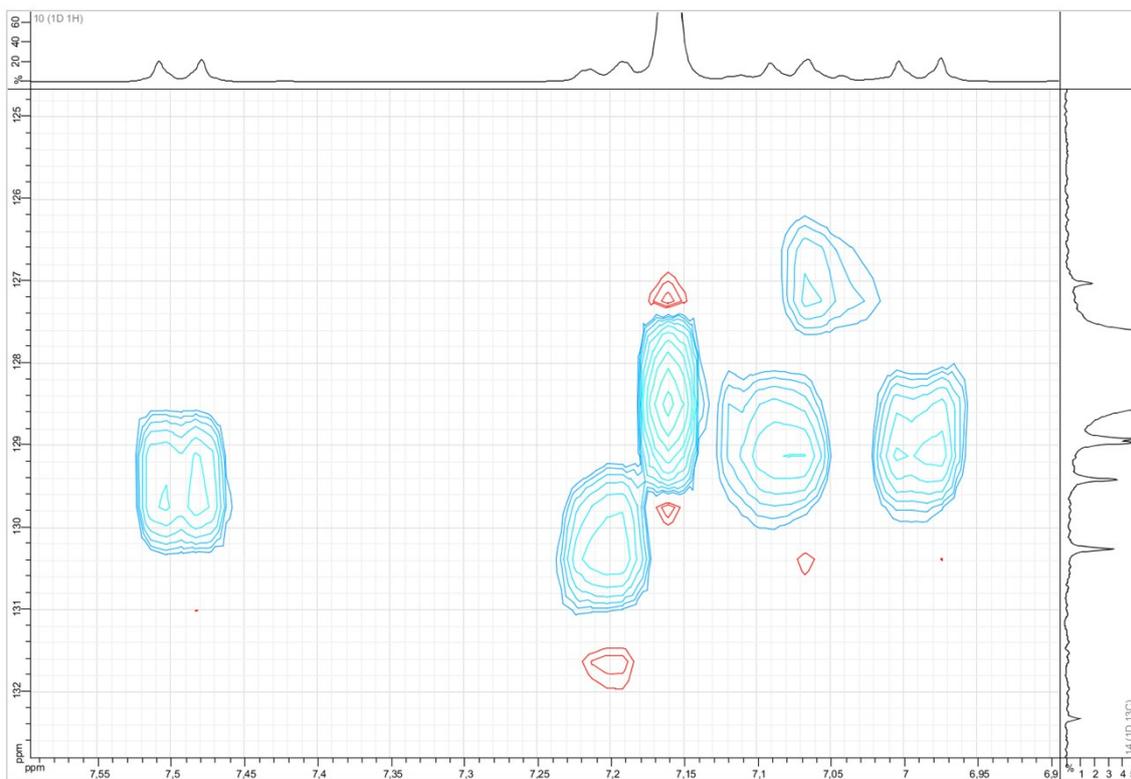
DEPT 135 NMR spectrum of compound **5j** in $C_6D_6-d_6$ at 75 MHz (zoom)



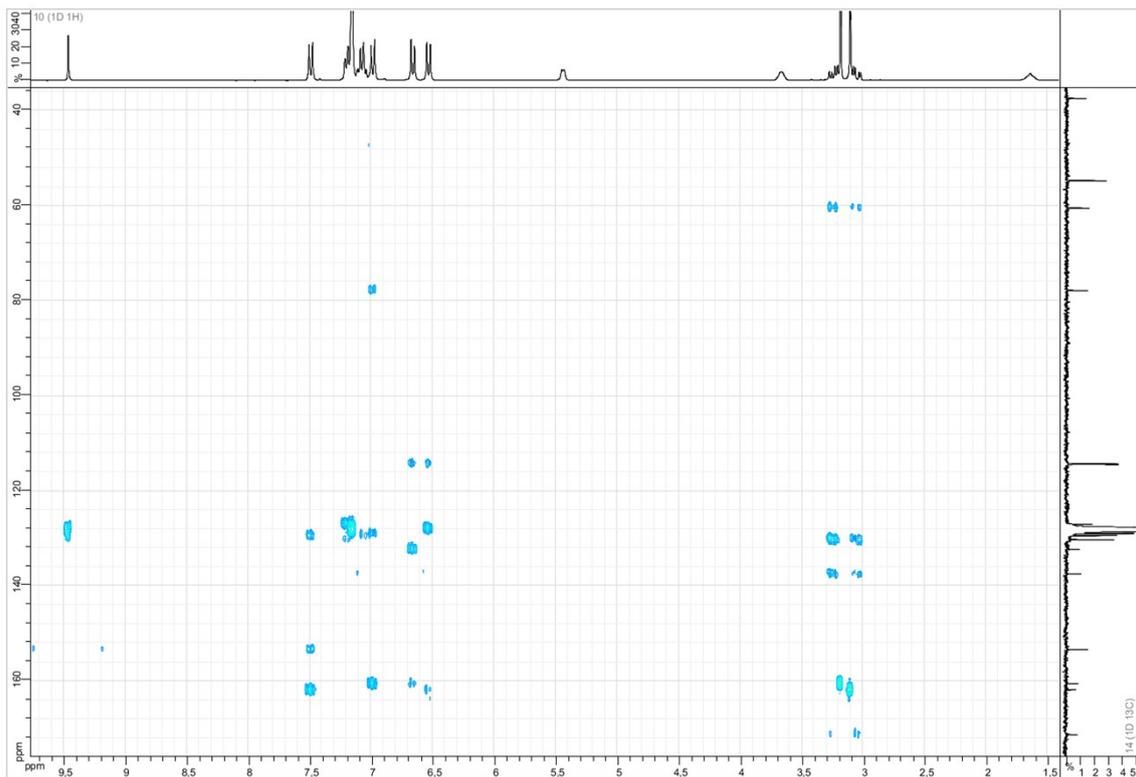
COSY NMR spectrum of compound **5j** in $C_6D_6-d_6$



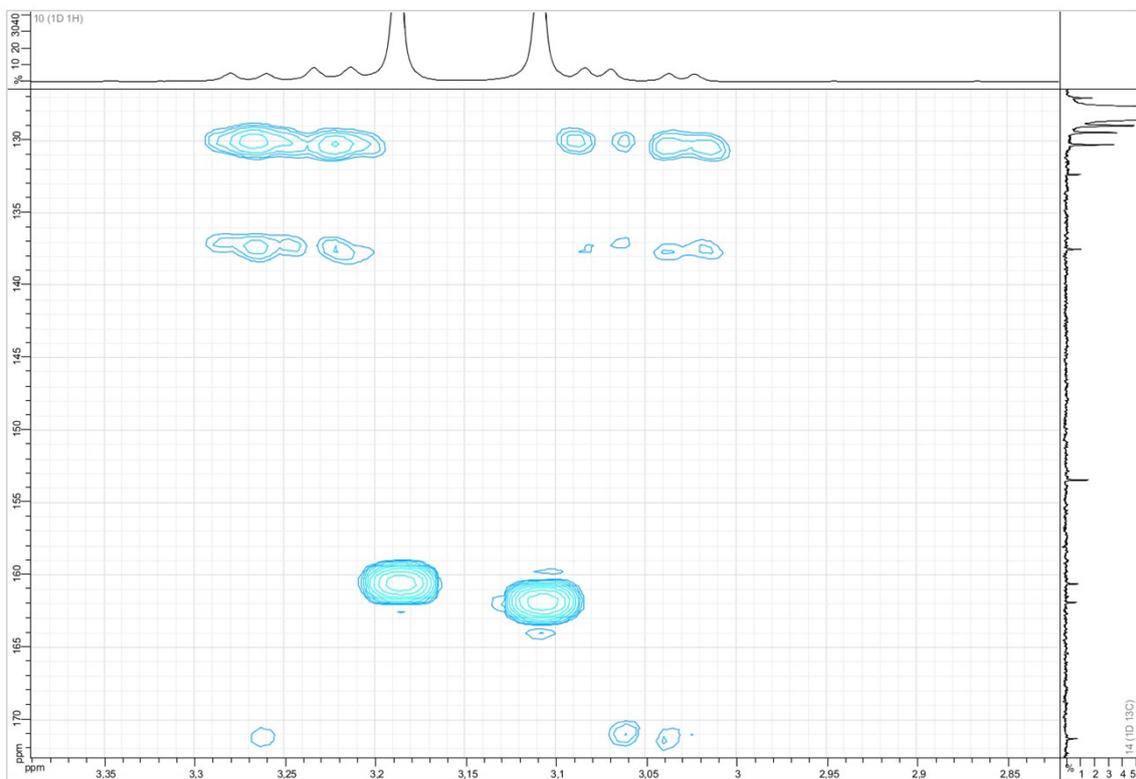
HSQC NMR spectrum of compound **5j** in $C_6D_6-d_6$



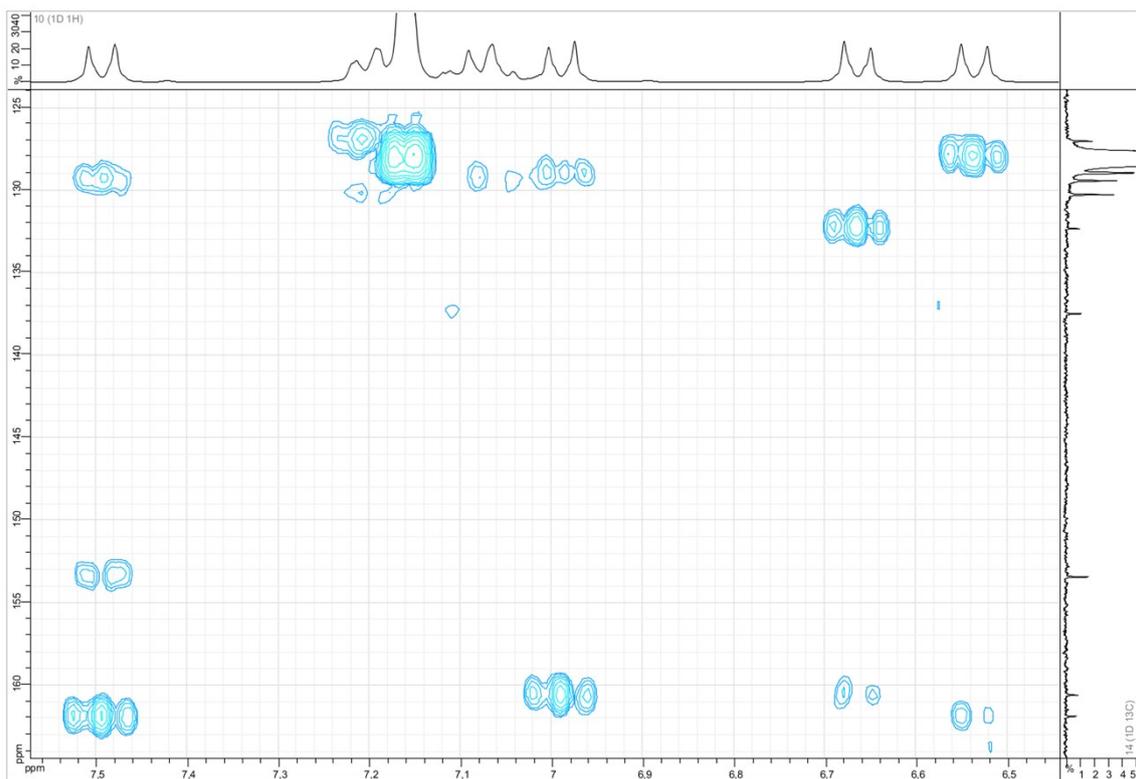
HSQC NMR spectrum of compound **5j** in $C_6D_6-d_6$ (zoom)



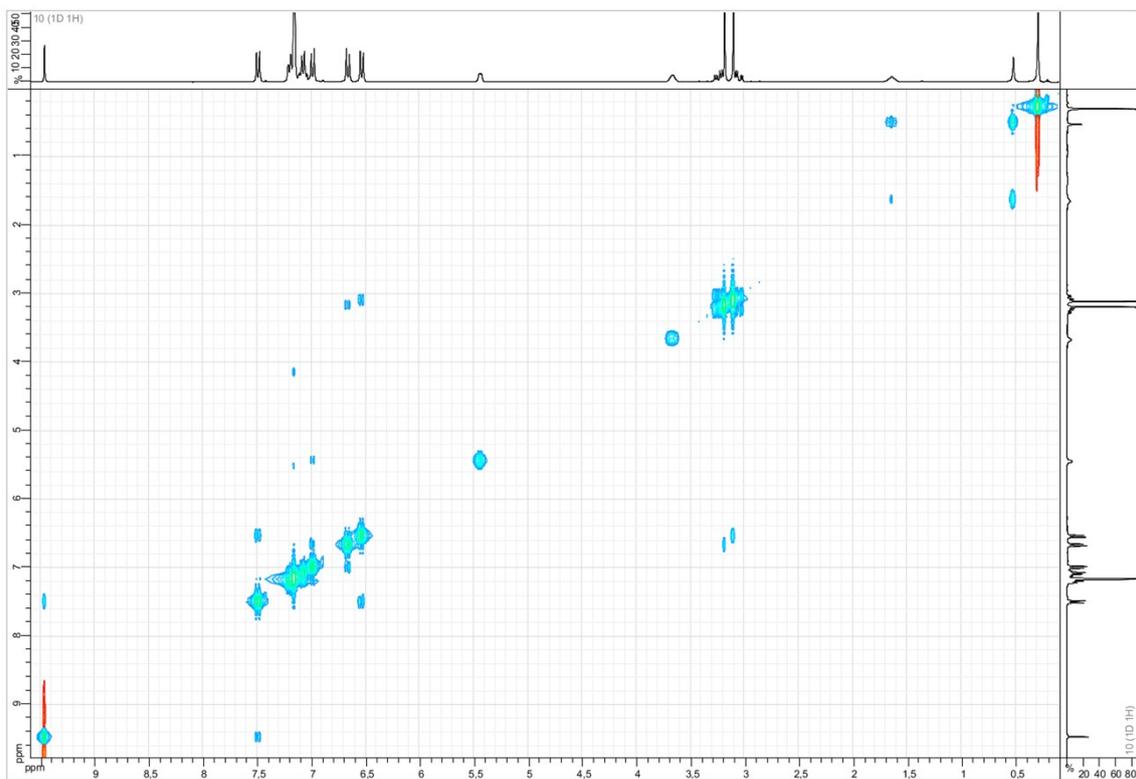
^1H - ^{13}C HMBC NMR spectrum of compound **5j** in C_6D_6-d_6



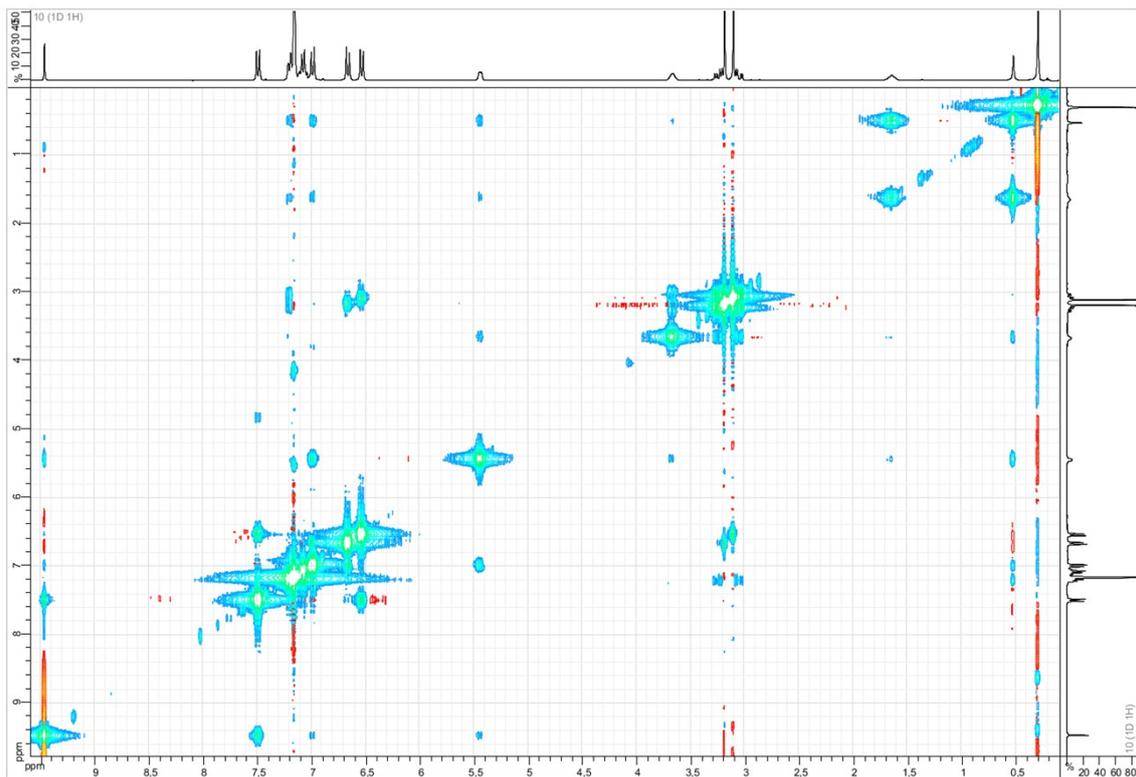
^1H - ^{13}C HMBC NMR spectrum of compound **5j** in C_6D_6-d_6 (zoom 1)



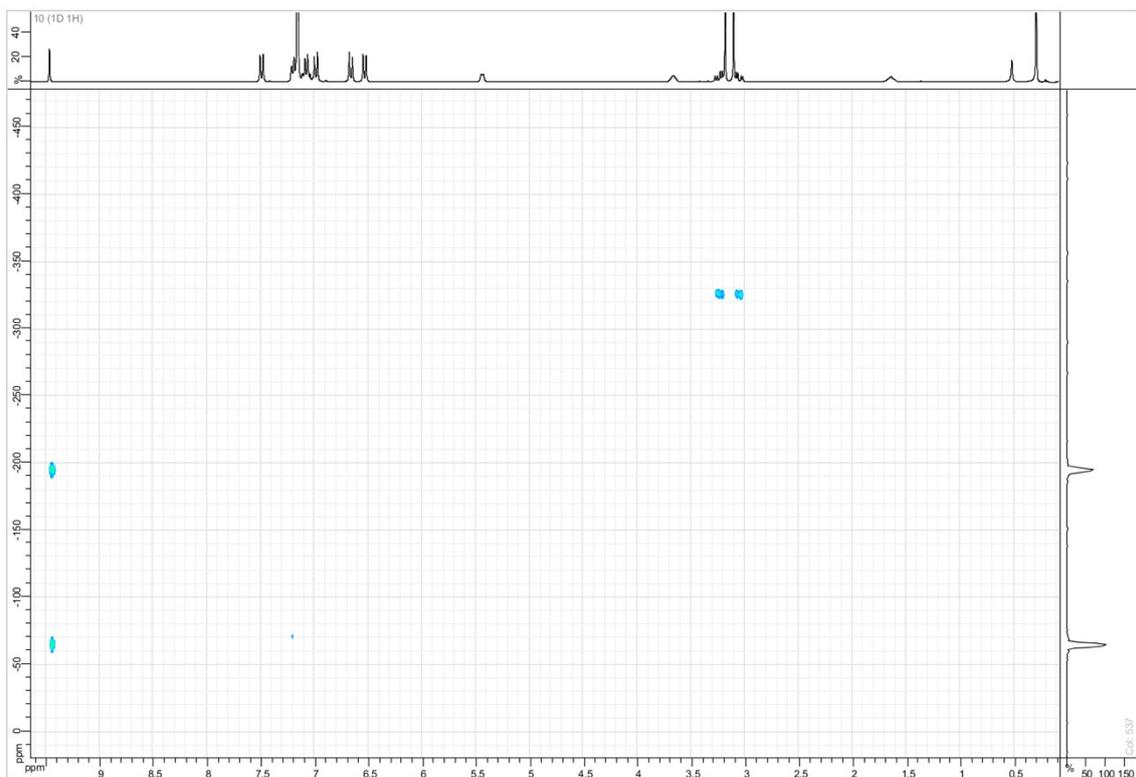
^1H - ^{13}C HMBC NMR spectrum of compound **5j** in C_6D_6 - d_6 (zoom 2)



NOESY NMR spectrum of compound **5j** in C_6D_6 - d_6

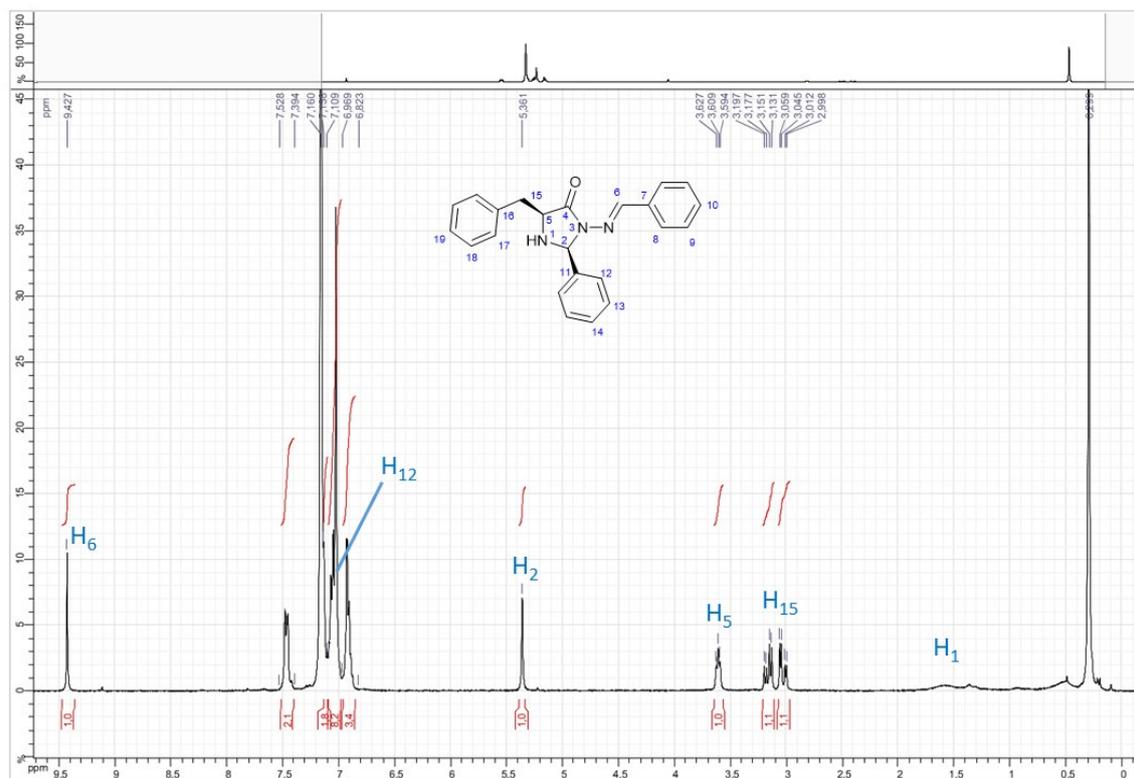


NOESY NMR spectrum of compound **5j** in $C_6D_6-d_6$ (deep cut)

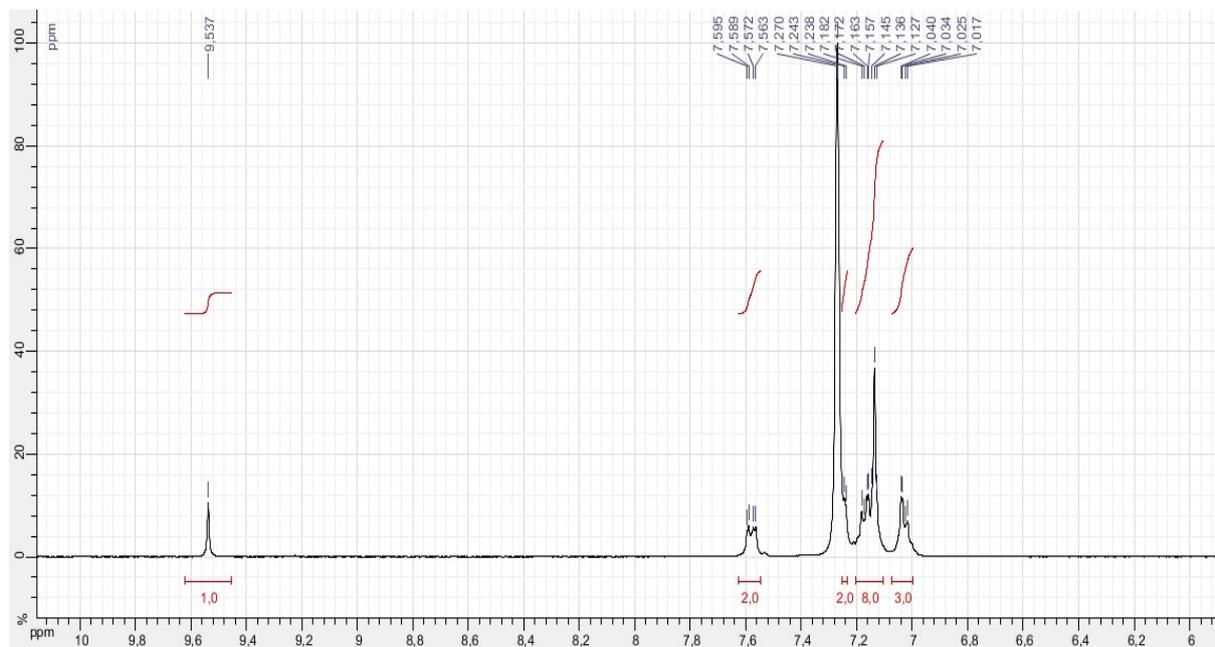


1H - ^{15}N HMBC NMR spectrum of compound **5j** in $C_6D_6-d_6$

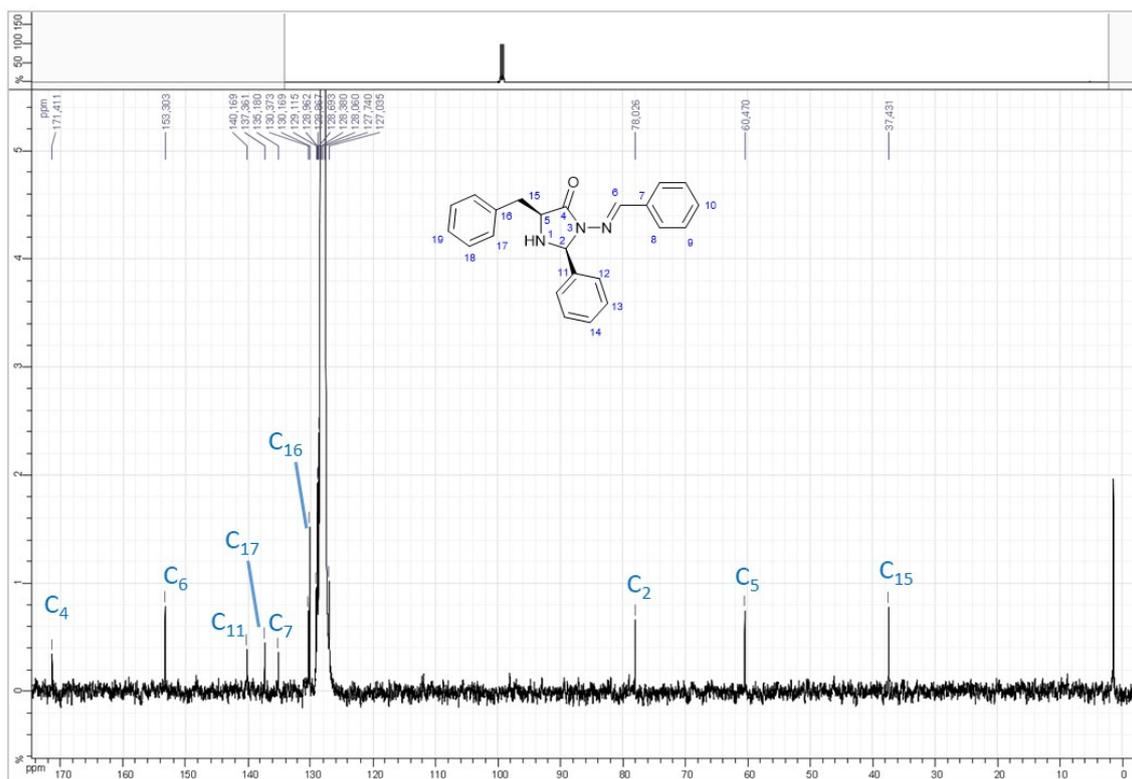
k. NMR spectra of **5k**



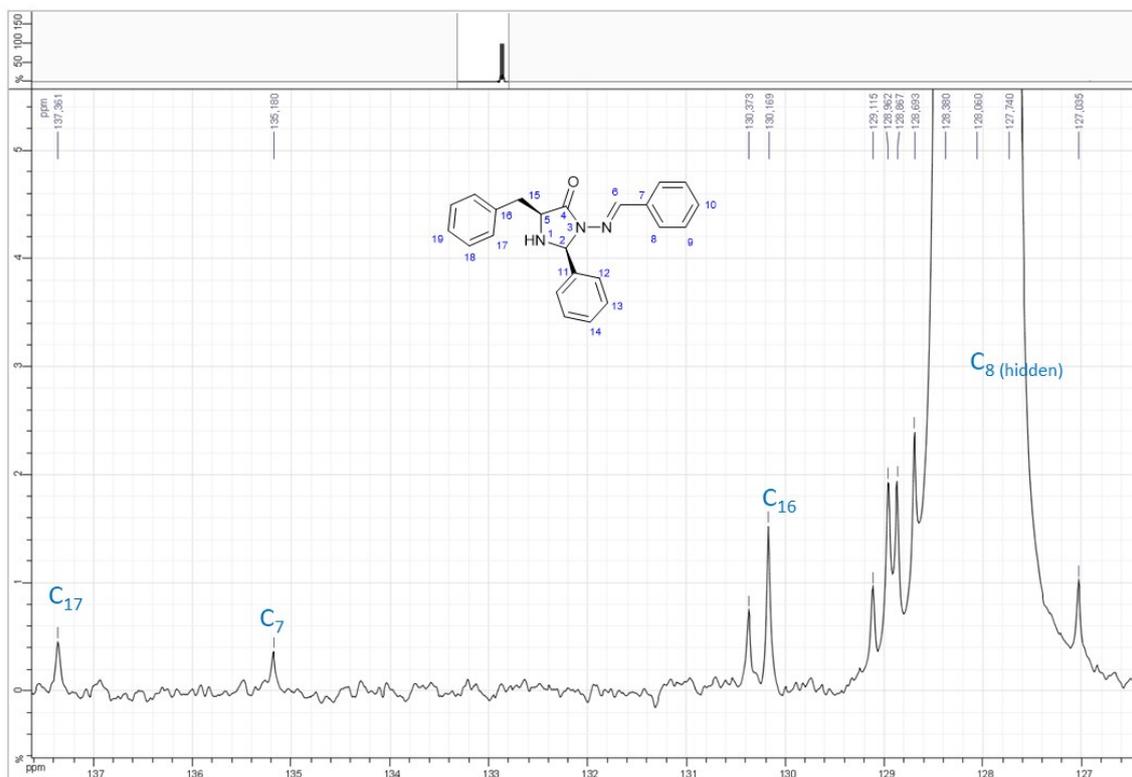
¹H NMR spectrum of compound **5k** in $C_6D_6-d_6$ at 300 MHz



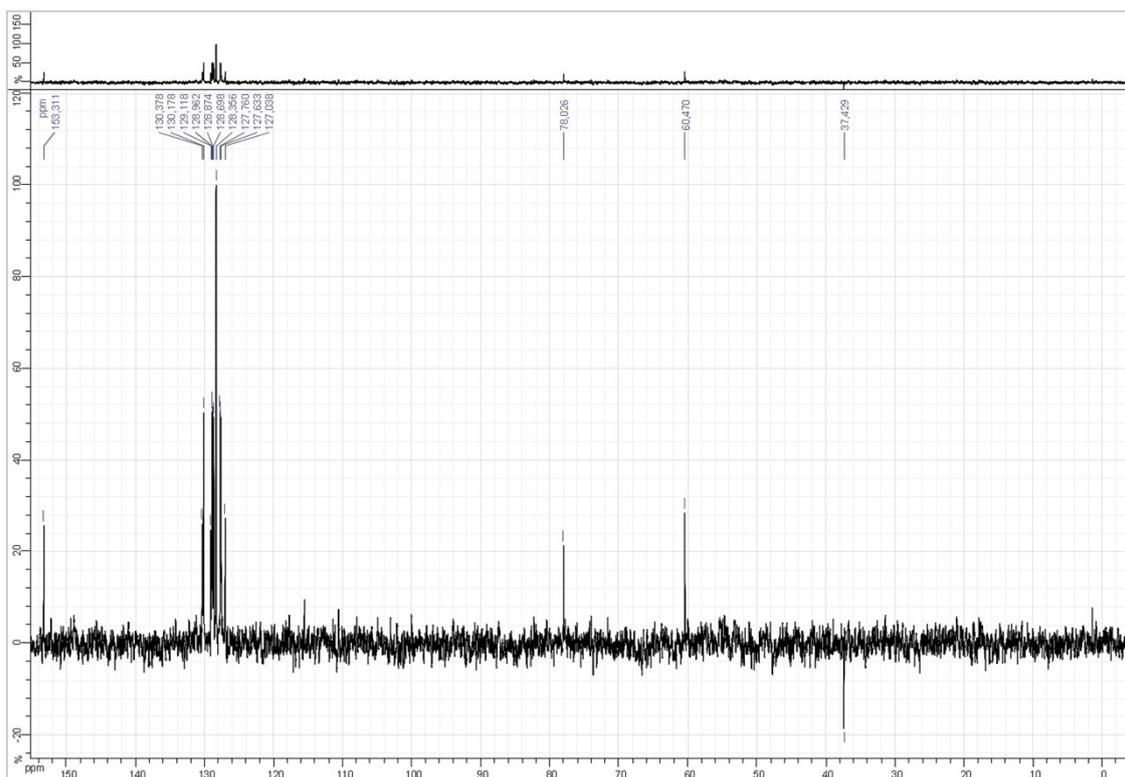
¹H NMR spectrum of compound **5k** in $C_6D_6-d_6$ at 300 MHz (zoom)



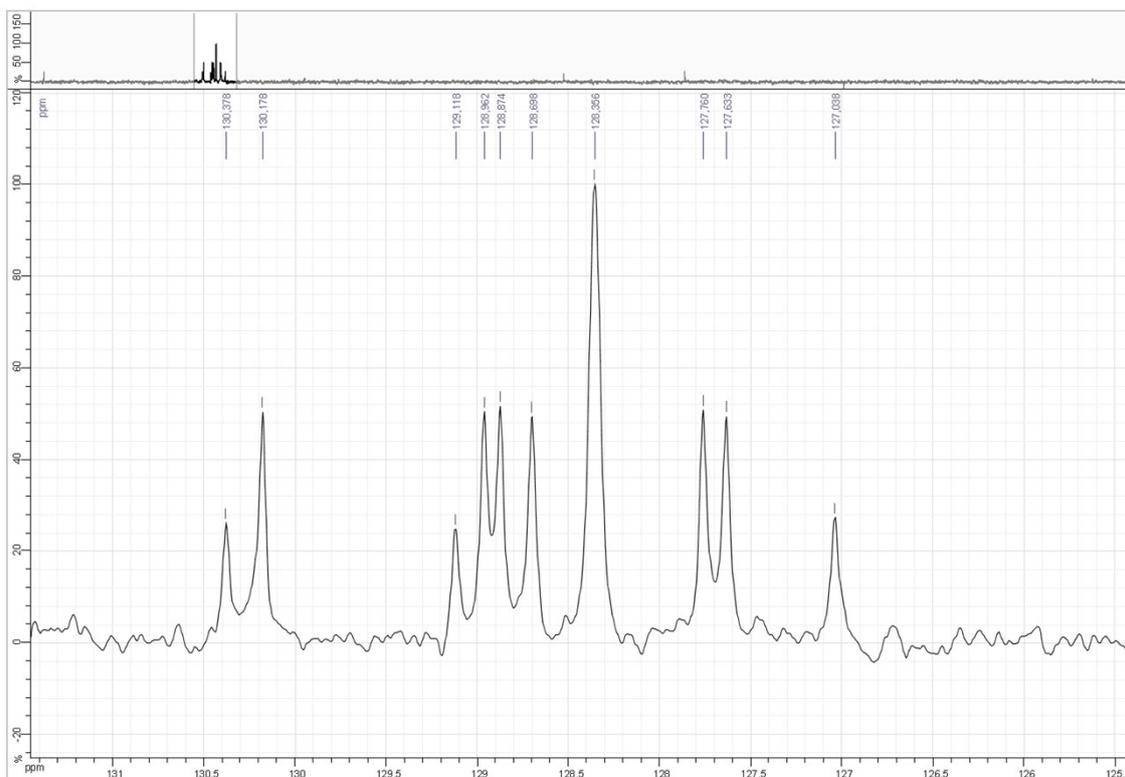
¹³C NMR spectrum of compound **5k** in C₆D₆-d₆ at 75 MHz



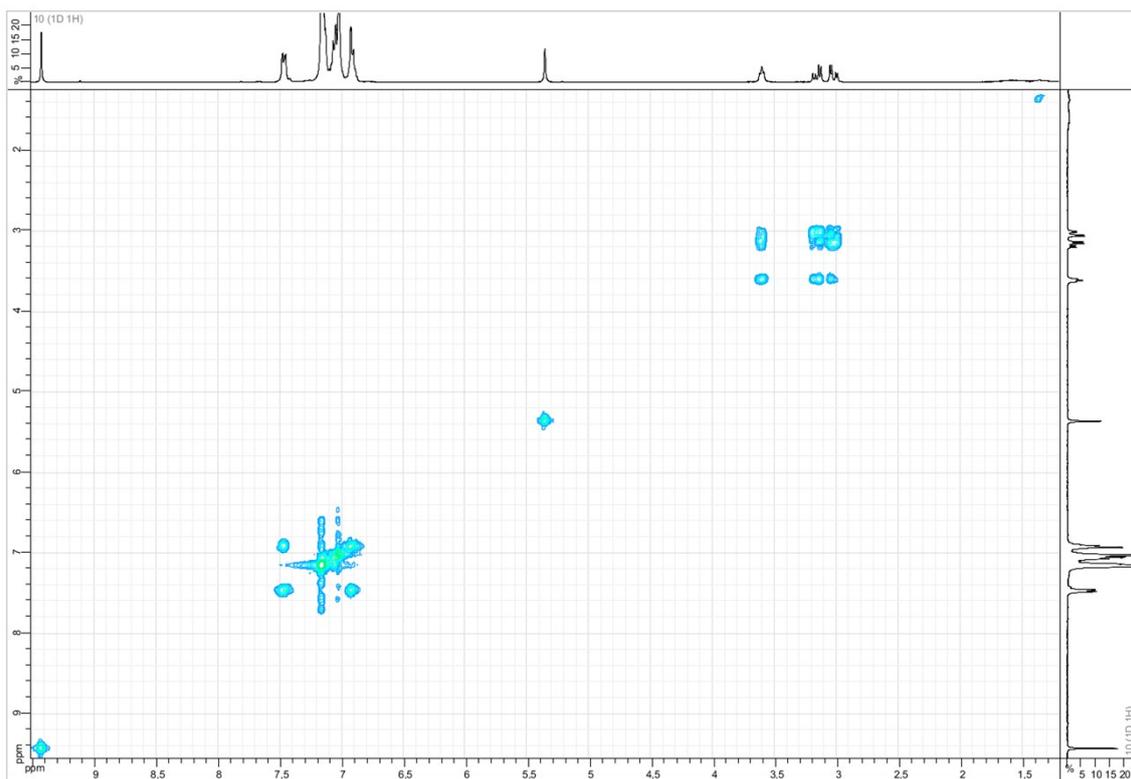
¹³C NMR spectrum of compound **5k** in C₆D₆-d₆ at 75 MHz (zoom)



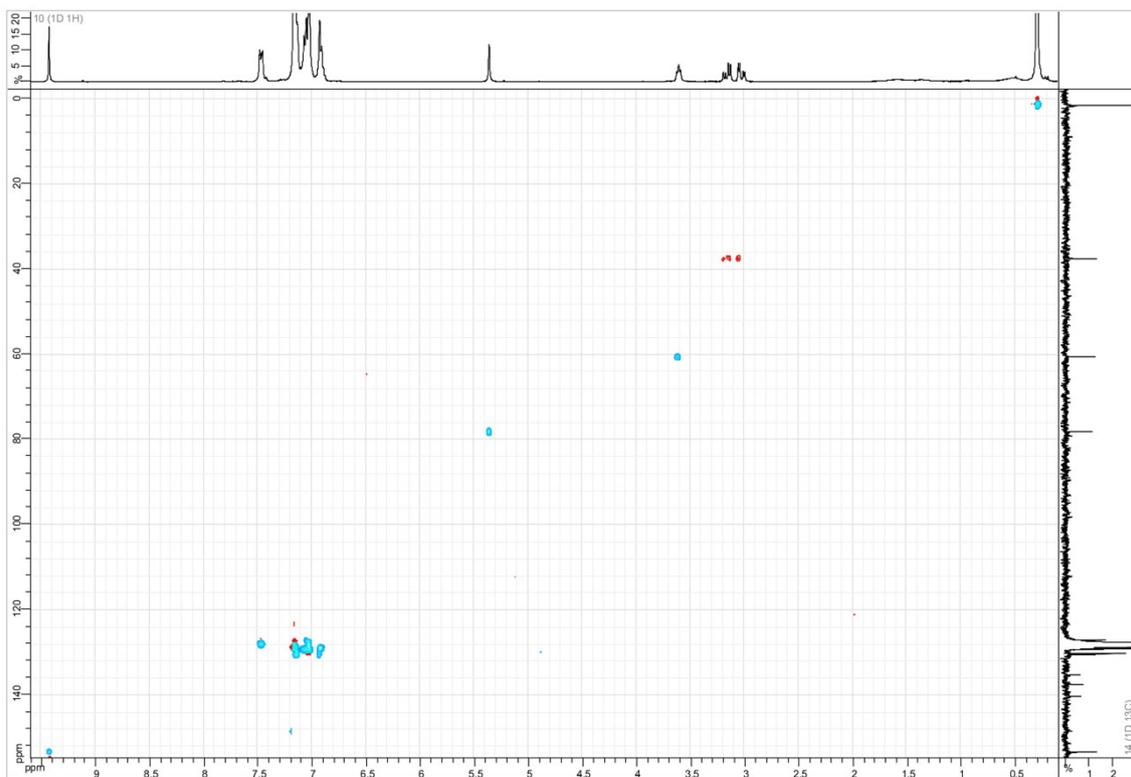
DEPT 135 NMR spectrum of compound **5k** in $C_6D_6-d_6$ at 75 MHz



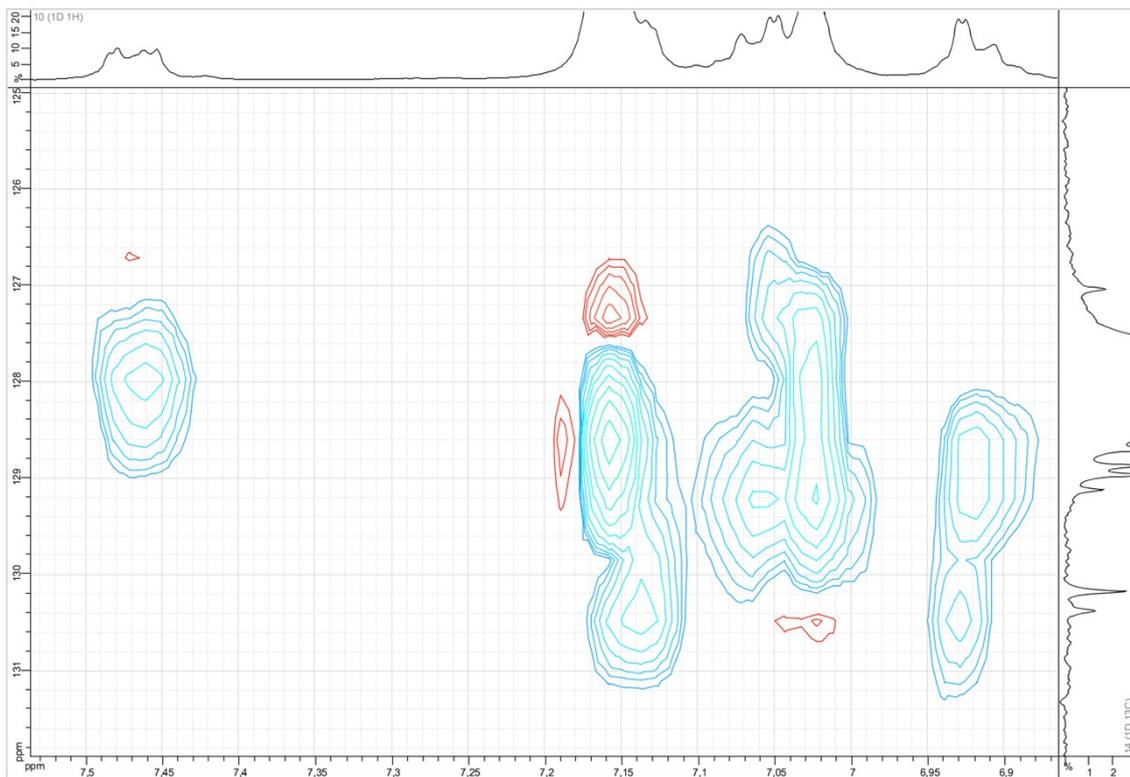
DEPT 135 NMR spectrum of compound **5k** in $C_6D_6-d_6$ at 75 MHz (zoom)



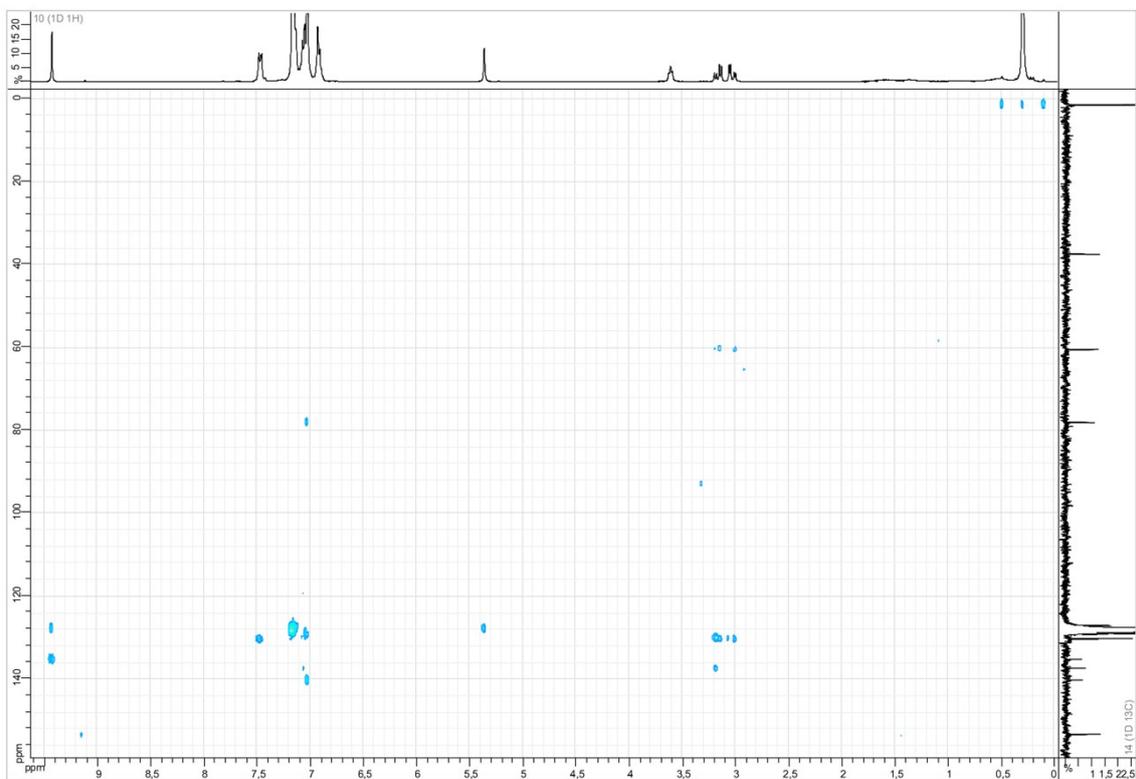
COSY NMR spectrum of compound **5k** in $C_6D_6-d_6$



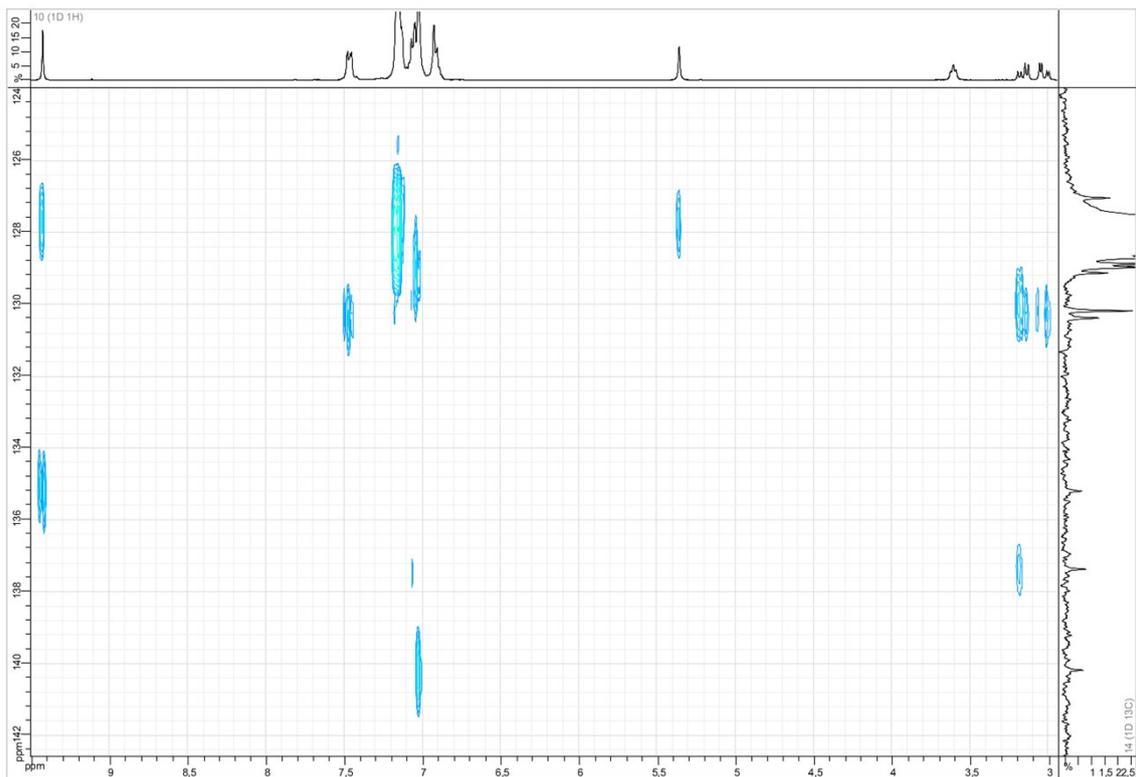
HSQC NMR spectrum of compound **5k** in $C_6D_6-d_6$



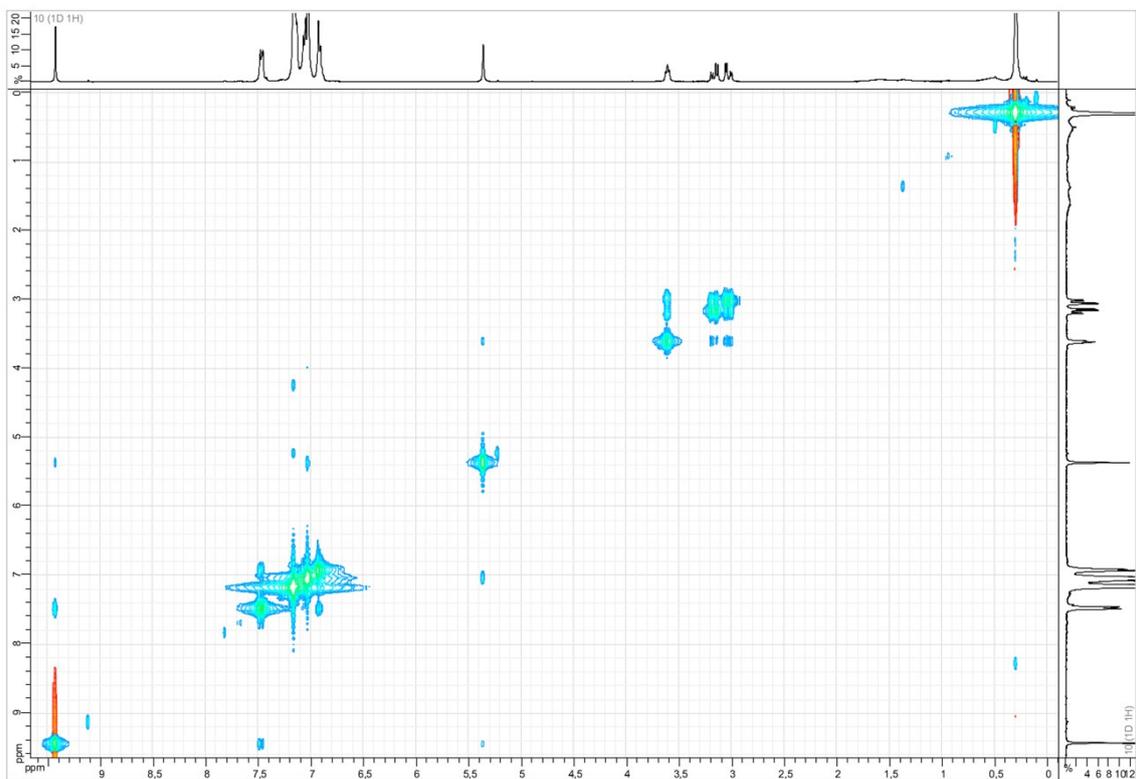
HSQC NMR spectrum of compound **5k** in $C_6D_6-d_6$ (zoom)



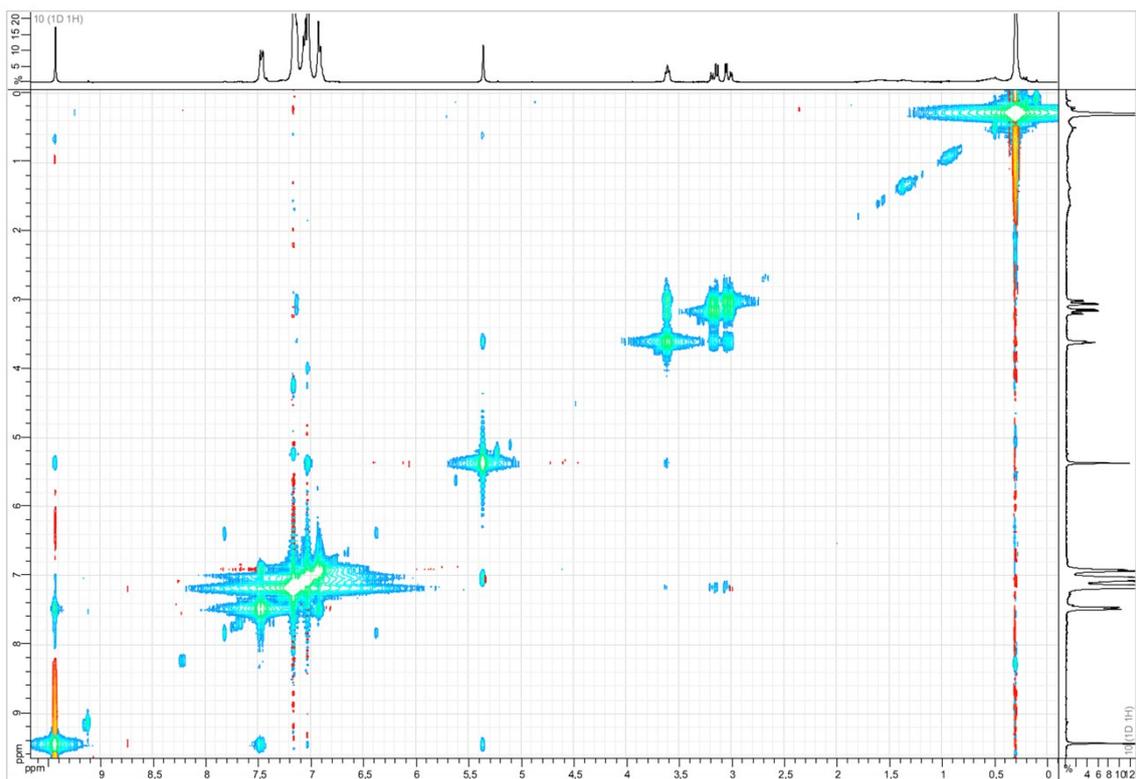
1H - ^{13}C HMBC NMR spectrum of compound **5k** in $C_6D_6-d_6$



^1H - ^{13}C HMBC NMR spectrum of compound **5k** in C_6D_6 - d_6 (zoom)

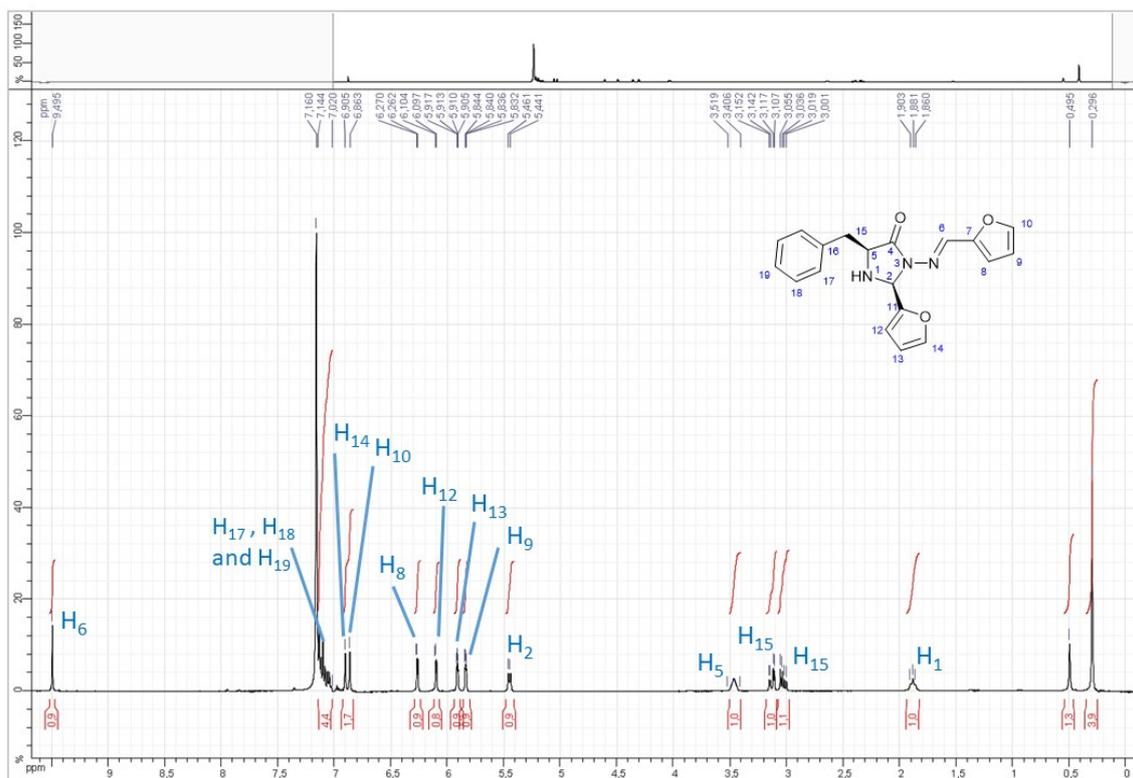


NOESY NMR spectrum of compound **5k** in C_6D_6 - d_6

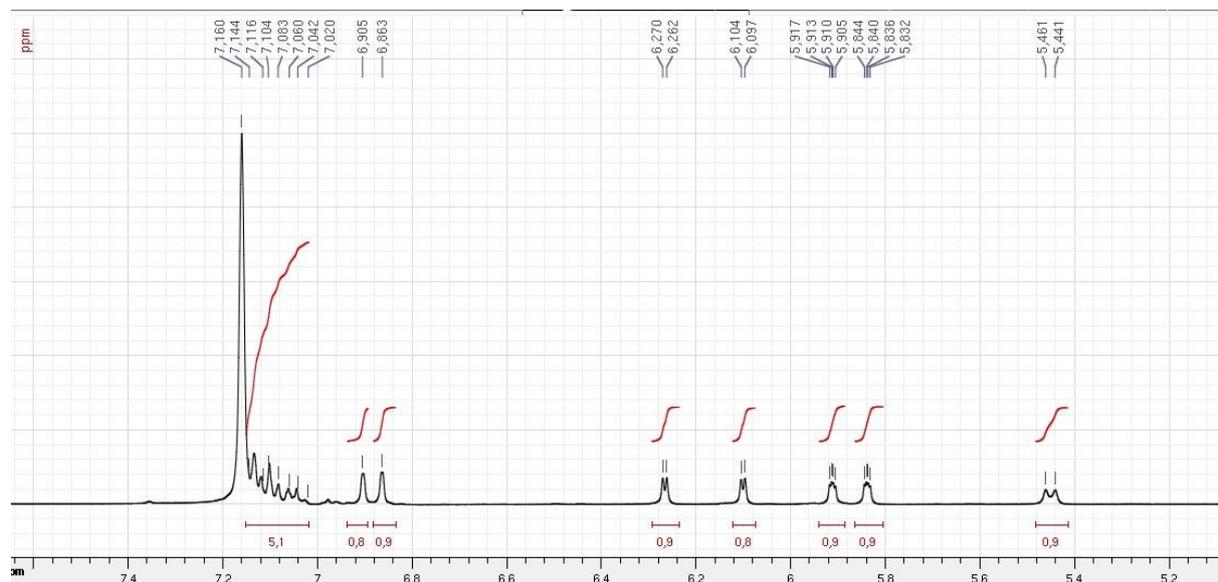


NOESY NMR spectrum of compound **5k** in $C_6D_6-d_6$ (deep cut)

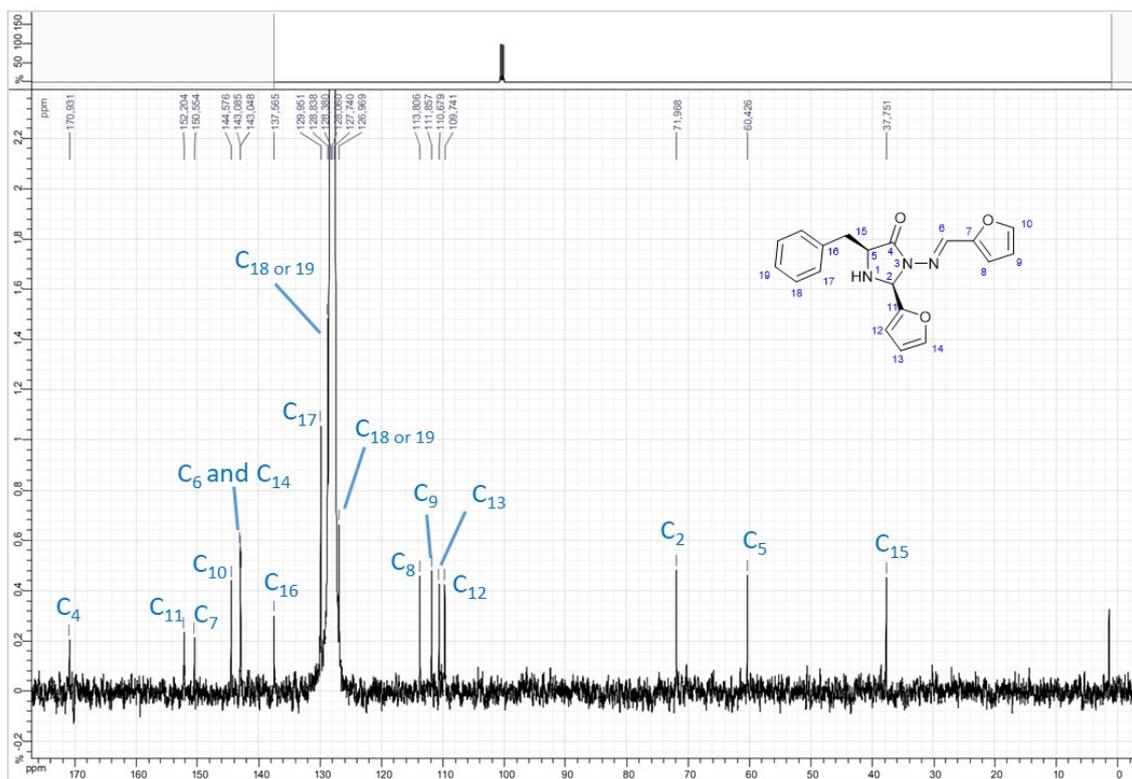
1. NMR spectra of **51**



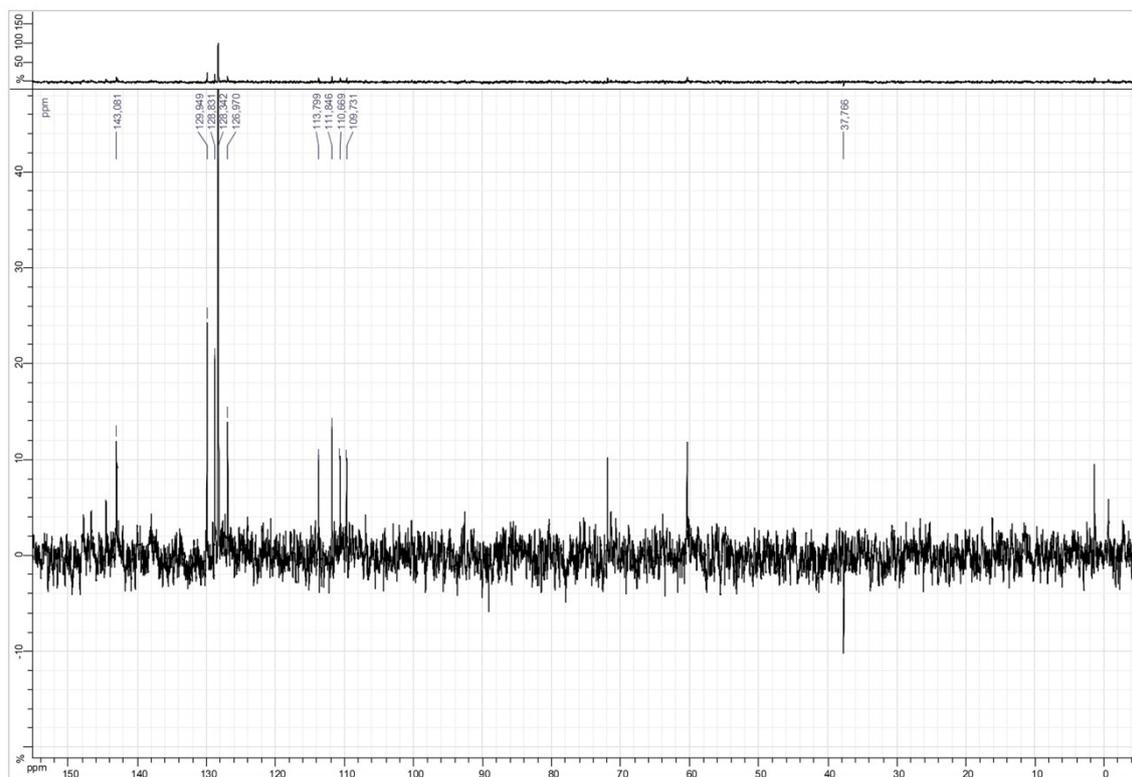
¹H NMR spectrum of compound **51** in C₆D₆-d₆ at 400 MHz



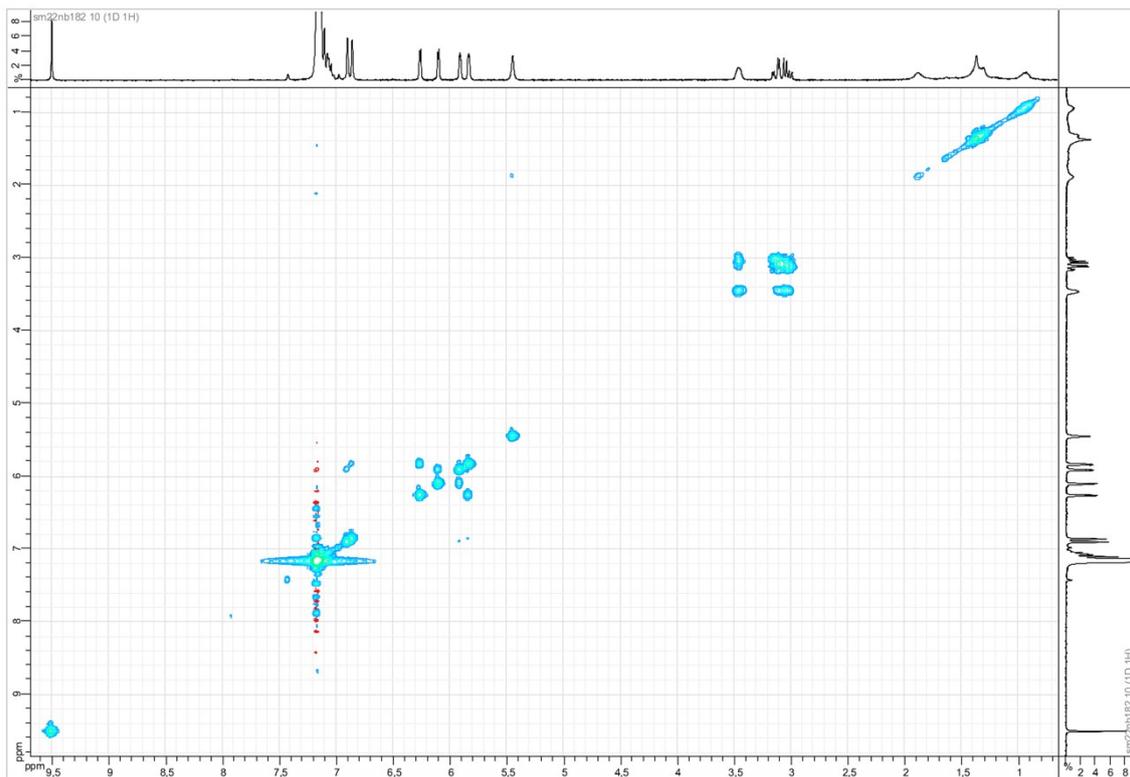
¹H NMR spectrum of compound **51** in C₆D₆-d₆ at 400 MHz



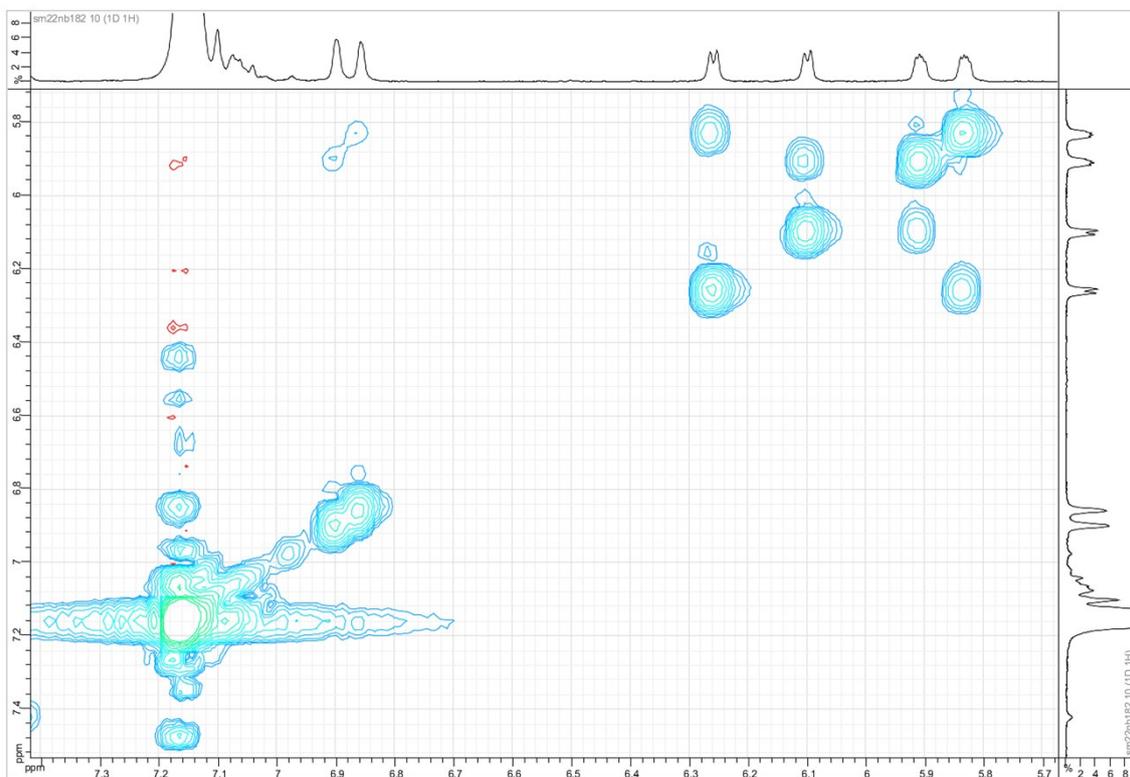
¹³C NMR spectrum of compound **5I** in C₆D₆-d₆ at 75 MHz



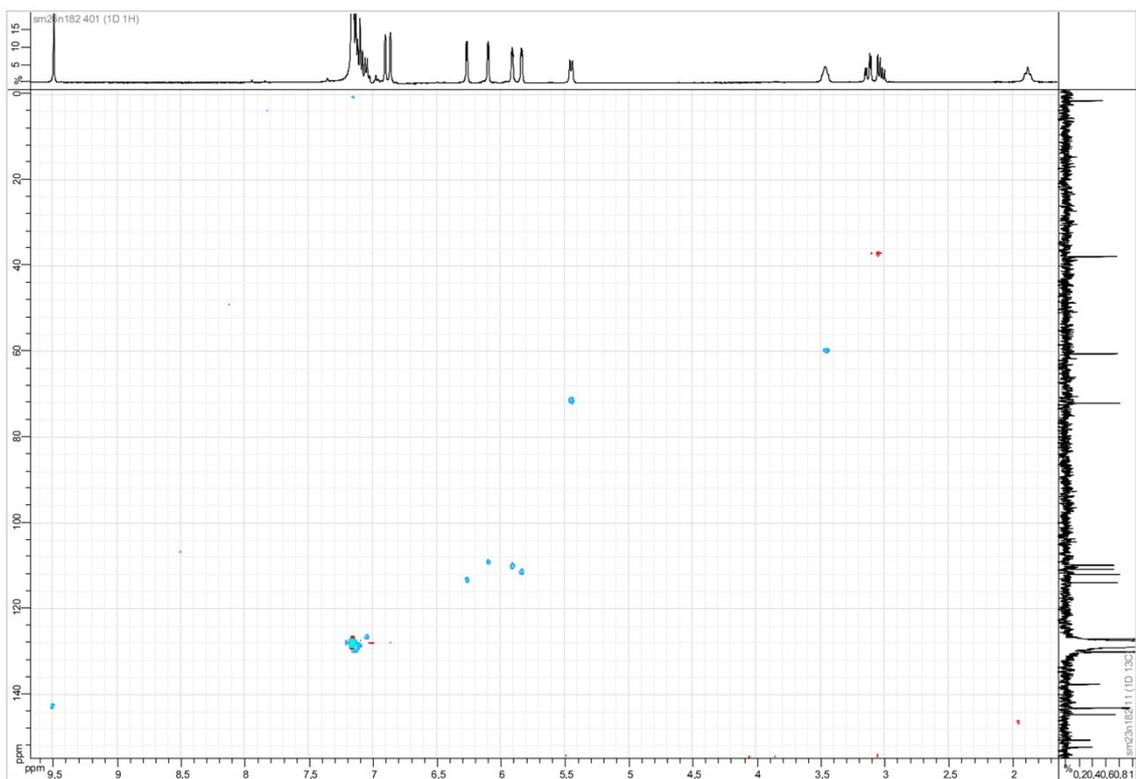
DEPT 135 NMR spectrum of compound **5I** in C₆D₆-d₆ at 75 MHz



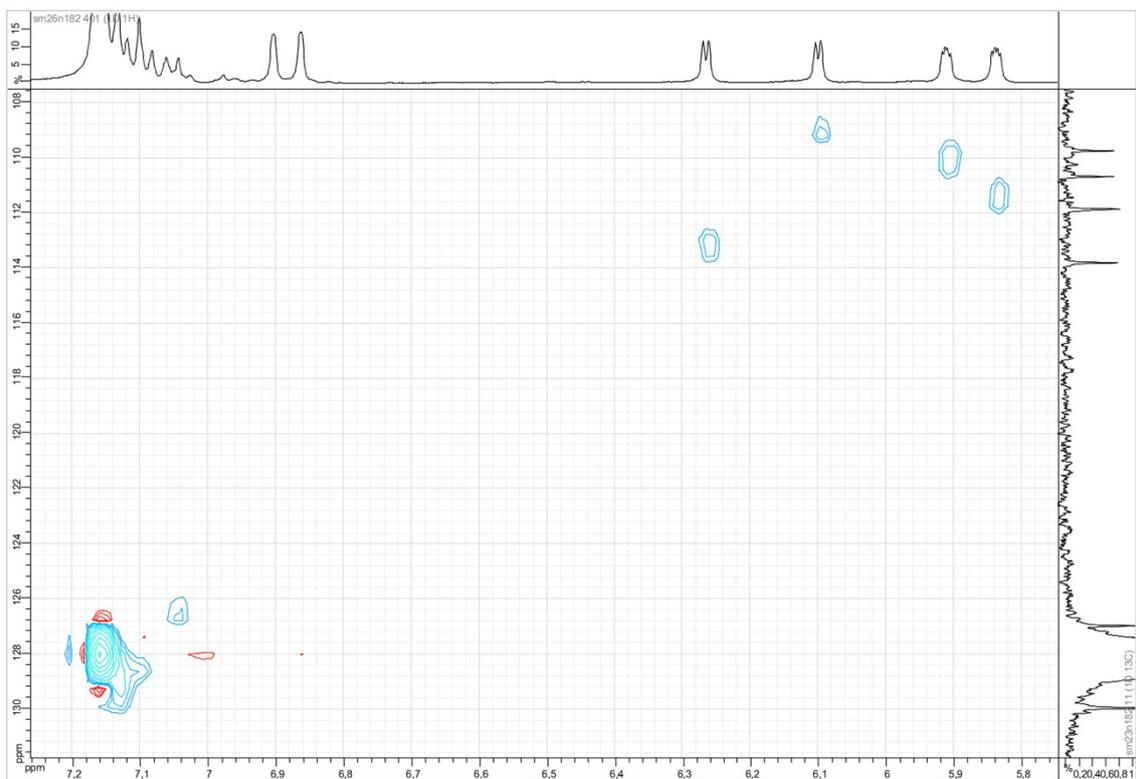
COSY NMR spectrum of compound **5I** in $C_6D_6-d_6$



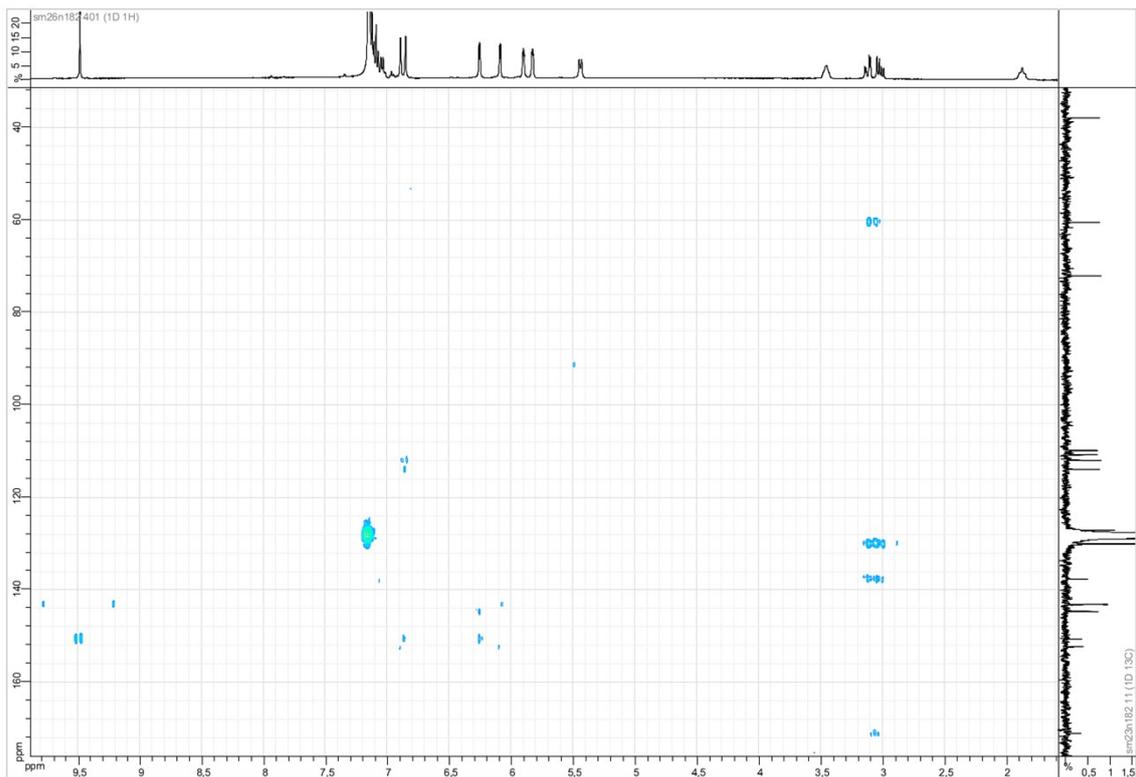
COSY NMR spectrum of compound **5I** in $C_6D_6-d_6$ (deep cut and zoom)



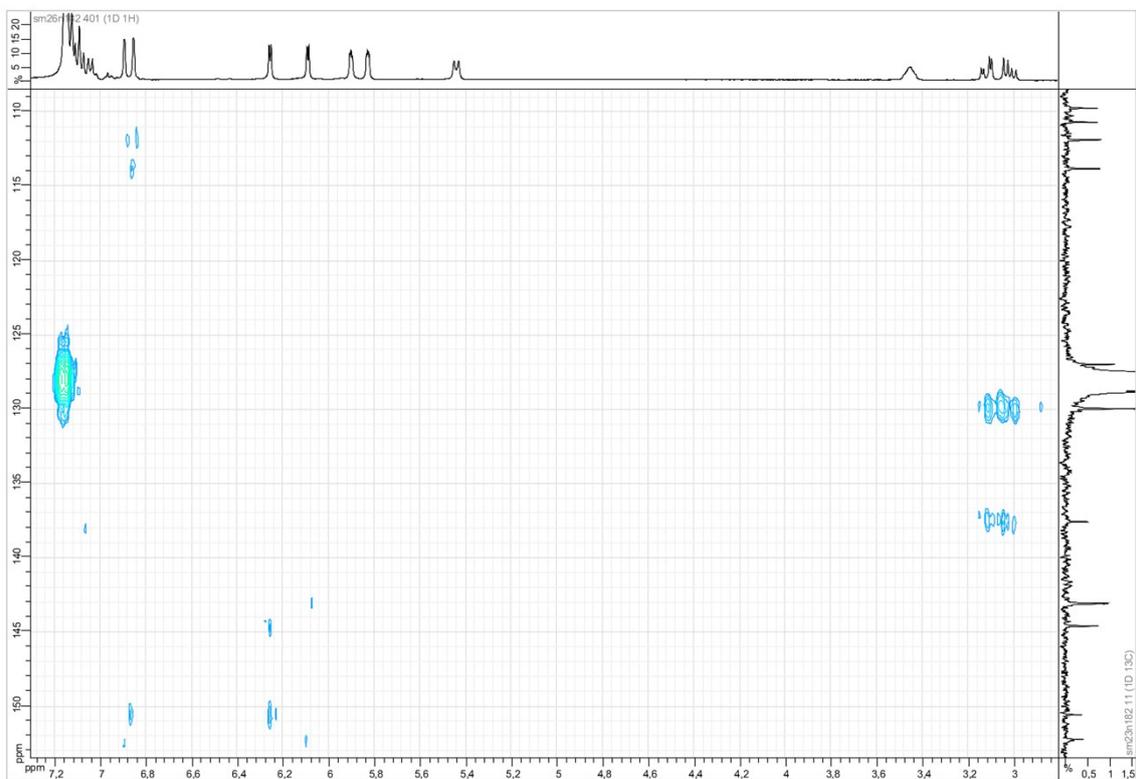
HSQC NMR spectrum of compound **5I** in $C_6D_6-d_6$



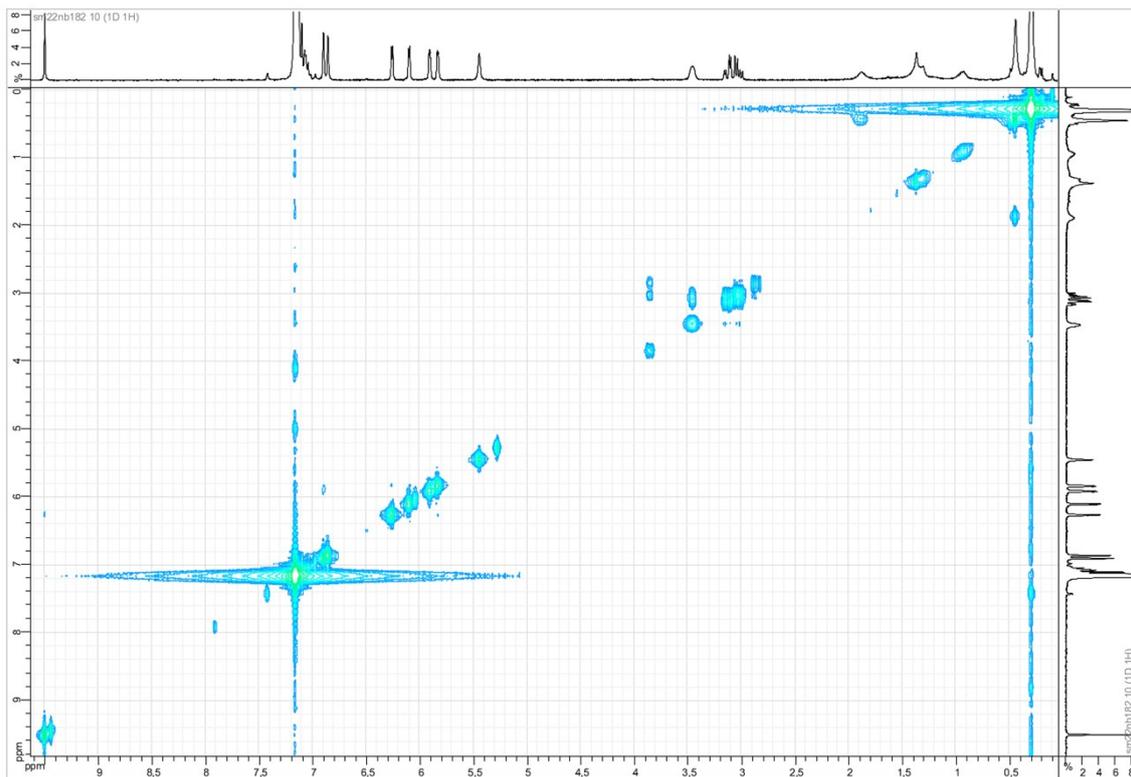
HSQC NMR spectrum of compound **5I** in $C_6D_6-d_6$ (zoom)



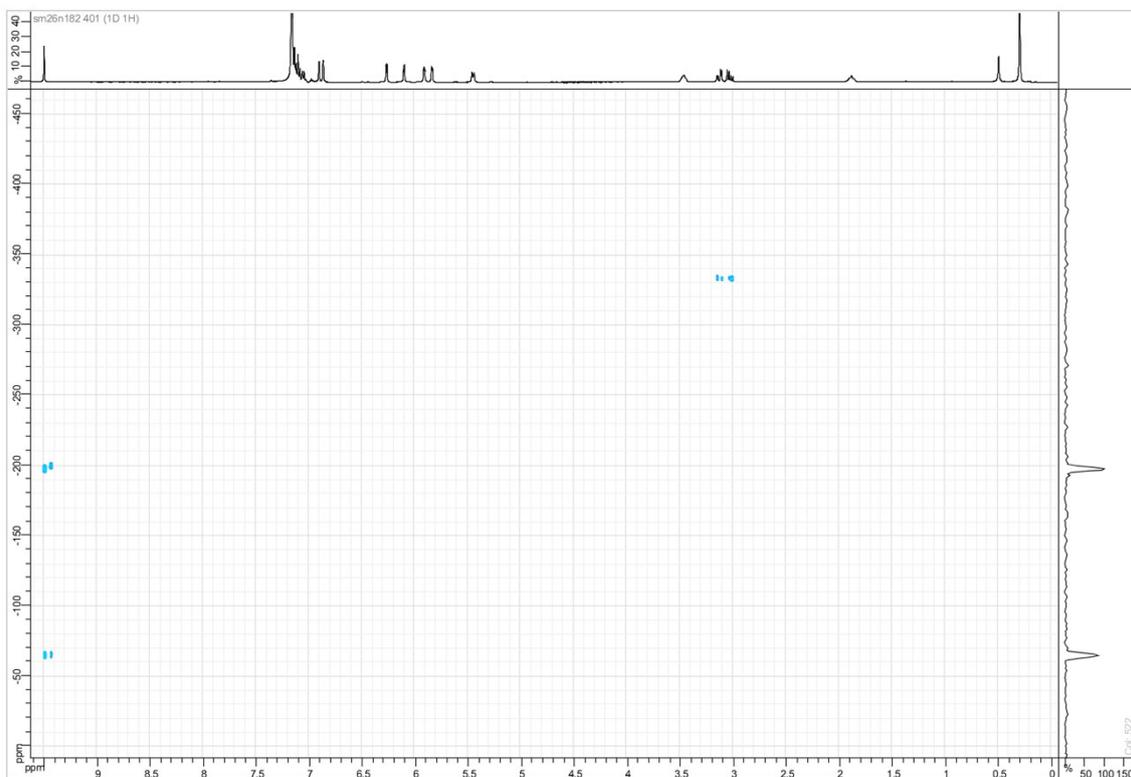
^1H - ^{13}C HMBC NMR spectrum of compound **5I** in C_6D_6 - d_6



^1H - ^{13}C HMBC NMR spectrum of compound **5I** in C_6D_6 - d_6 (zoom)

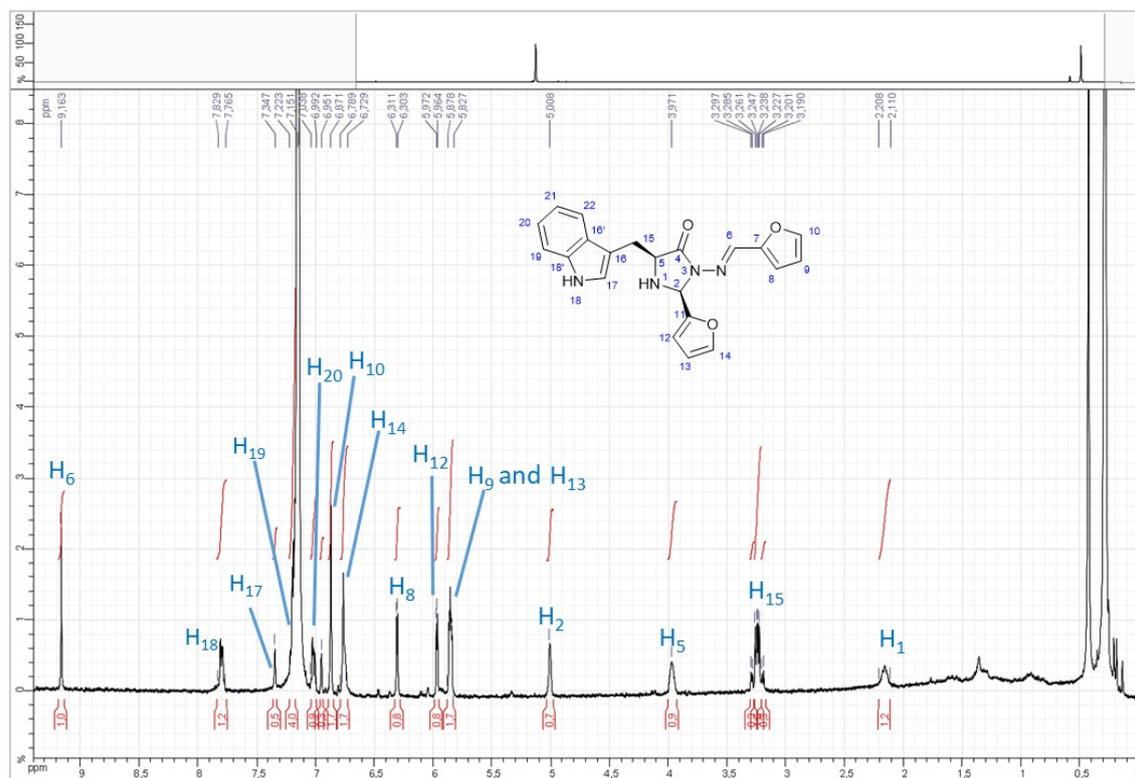


NOESY NMR spectrum of compound **5I** in $C_6D_6-d_6$

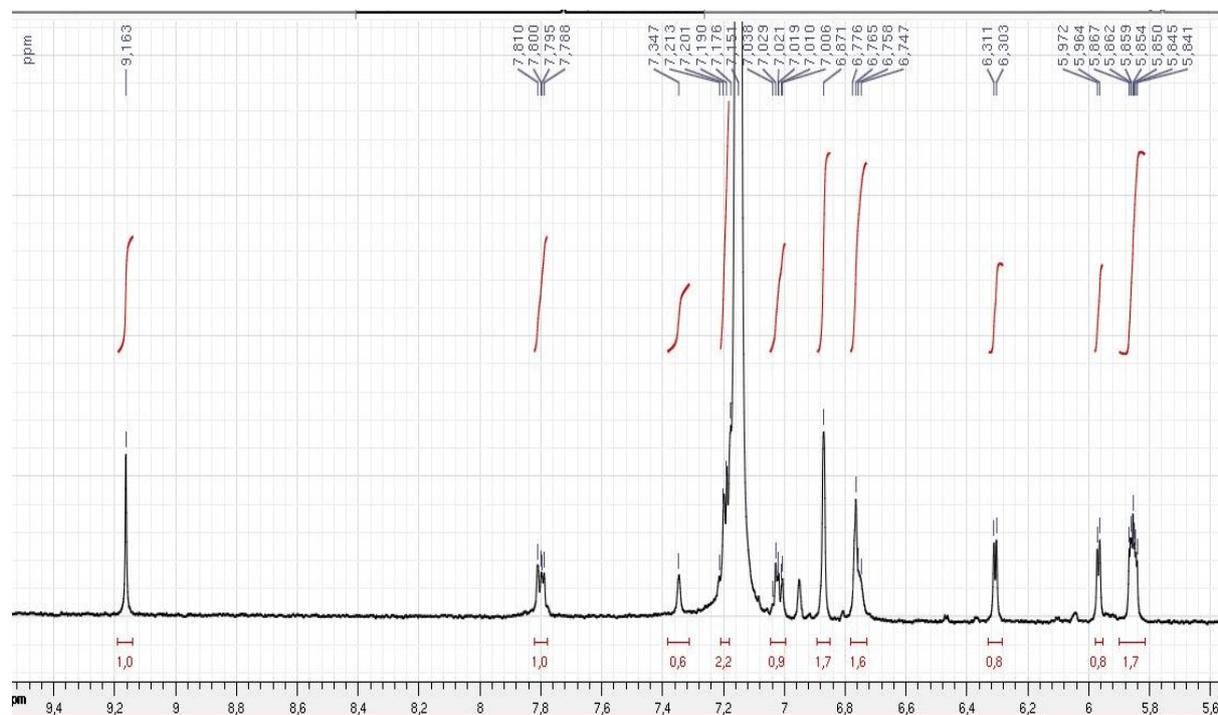


1H - ^{15}N HMBC NMR spectrum of compound **5I** in $C_6D_6-d_6$

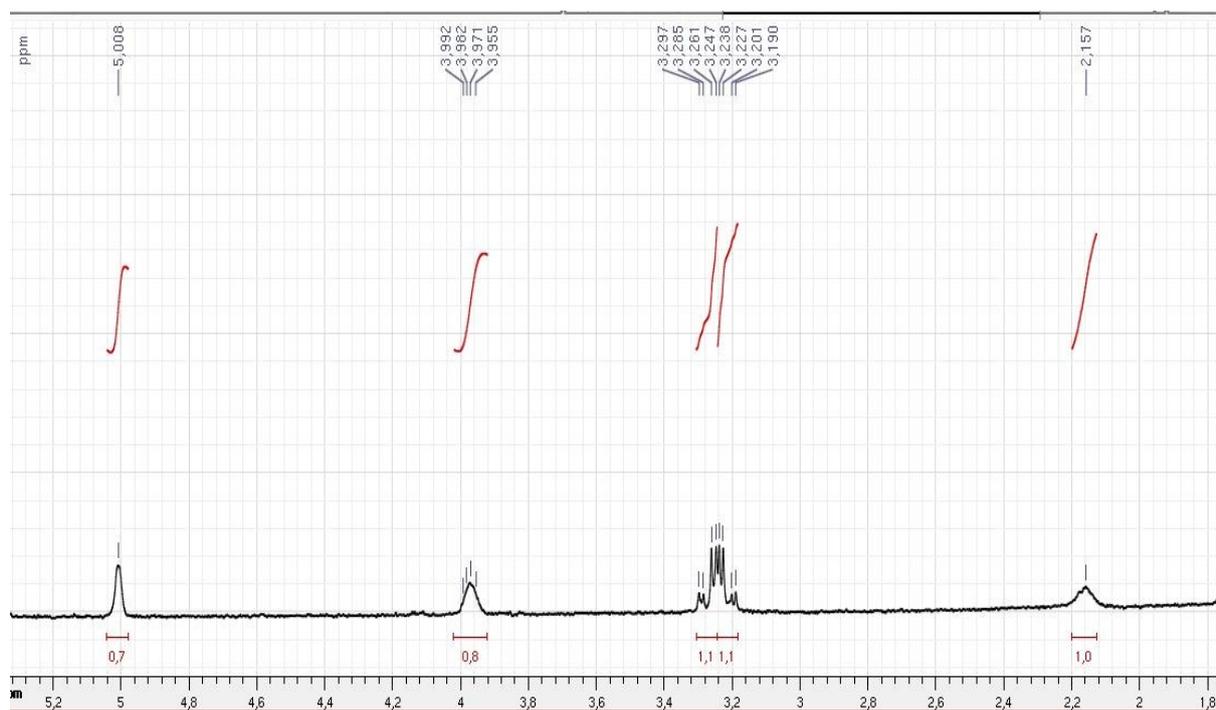
m. NMR spectra of **5m**



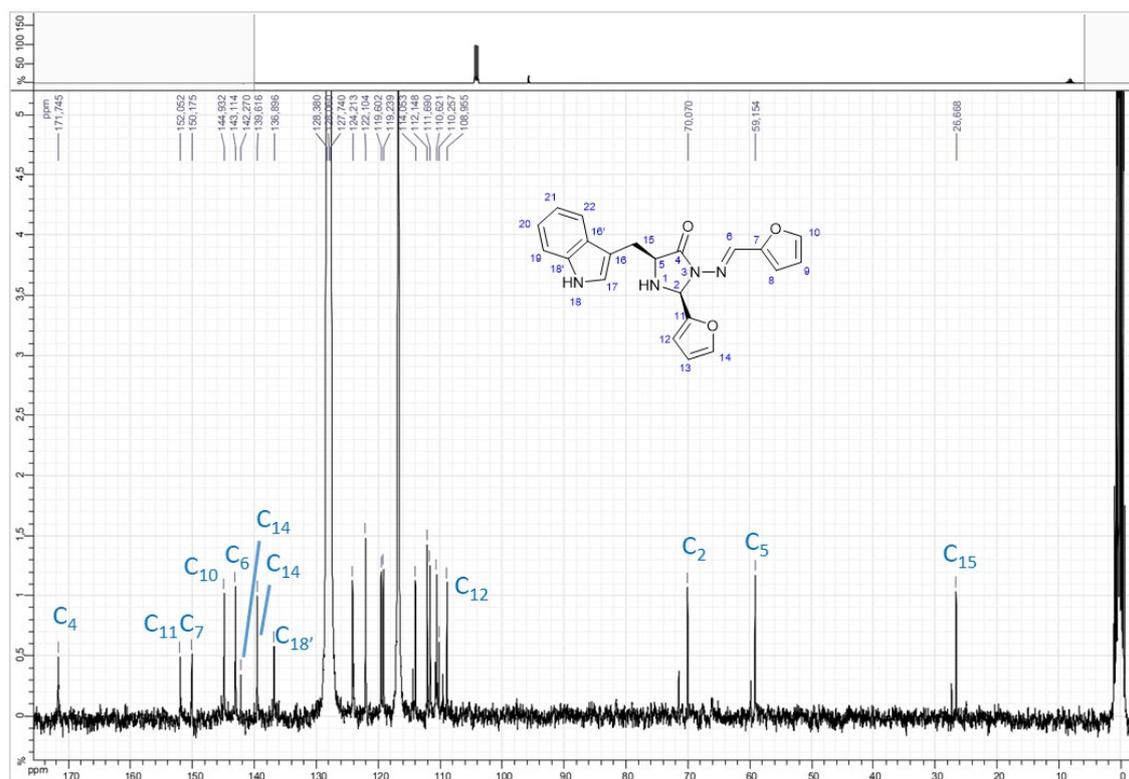
¹H NMR spectrum of compound **5m** in C₆D₆-d₆ at 300 MHz



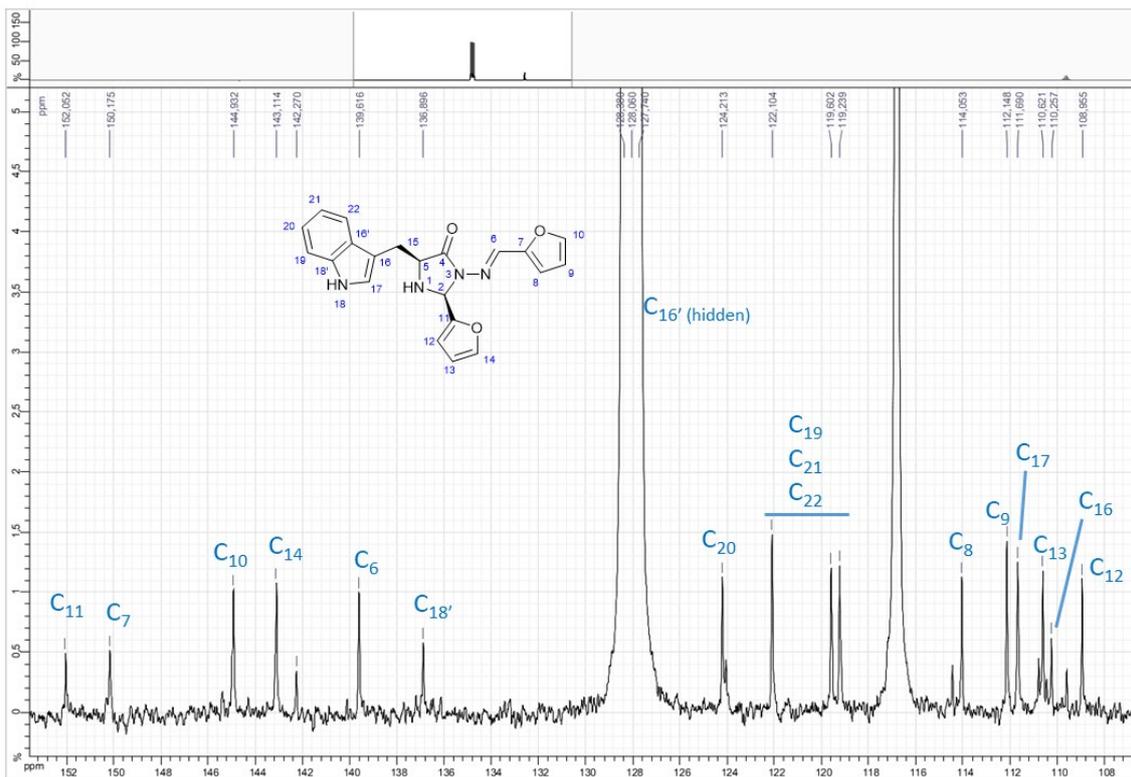
¹H NMR spectrum of compound **5m** in C₆D₆-d₆ at 300 MHz (zoom 1)



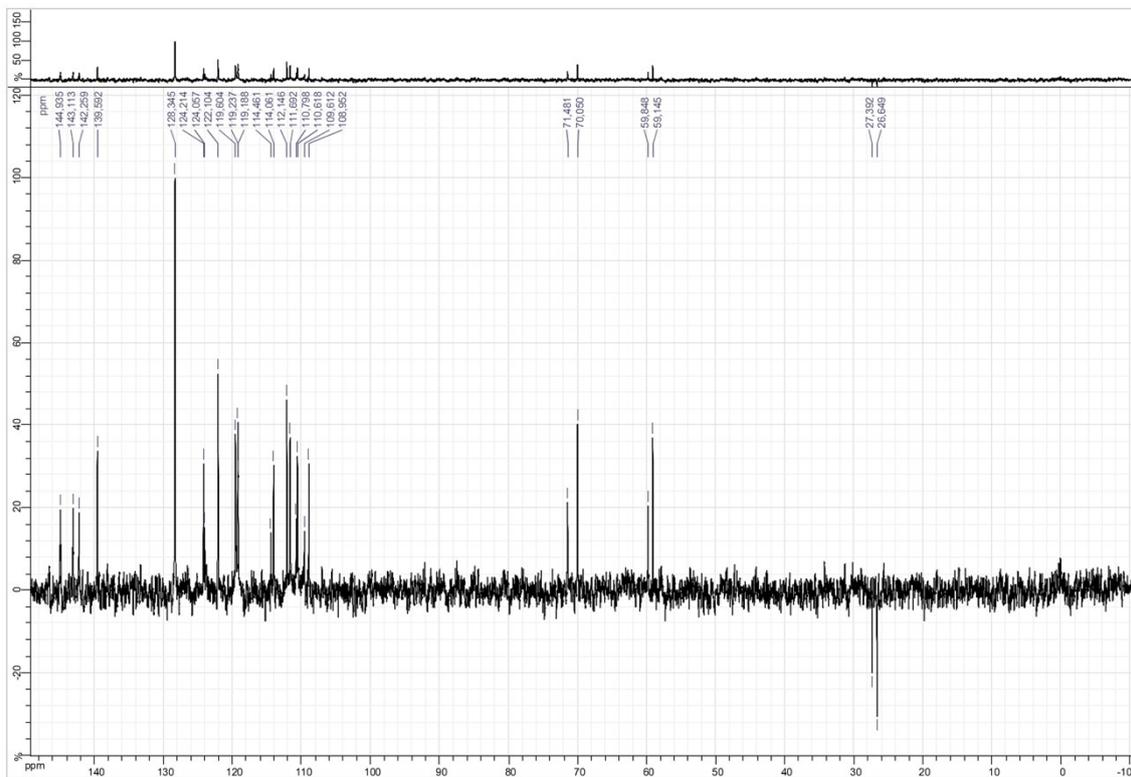
¹H NMR spectrum of compound **5m** in C₆D₆-d₆ at 300 MHz (zoom 2)



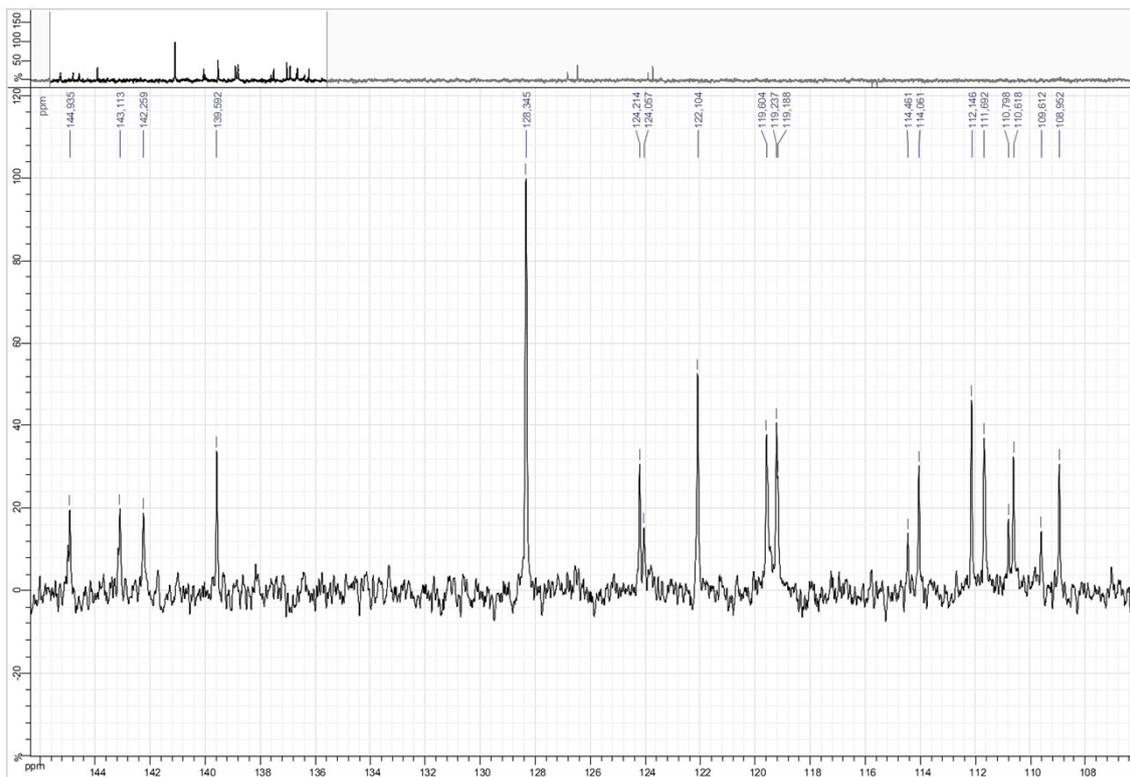
¹³C NMR spectrum of compound **5m** in C₆D₆-d₆ at 75 MHz



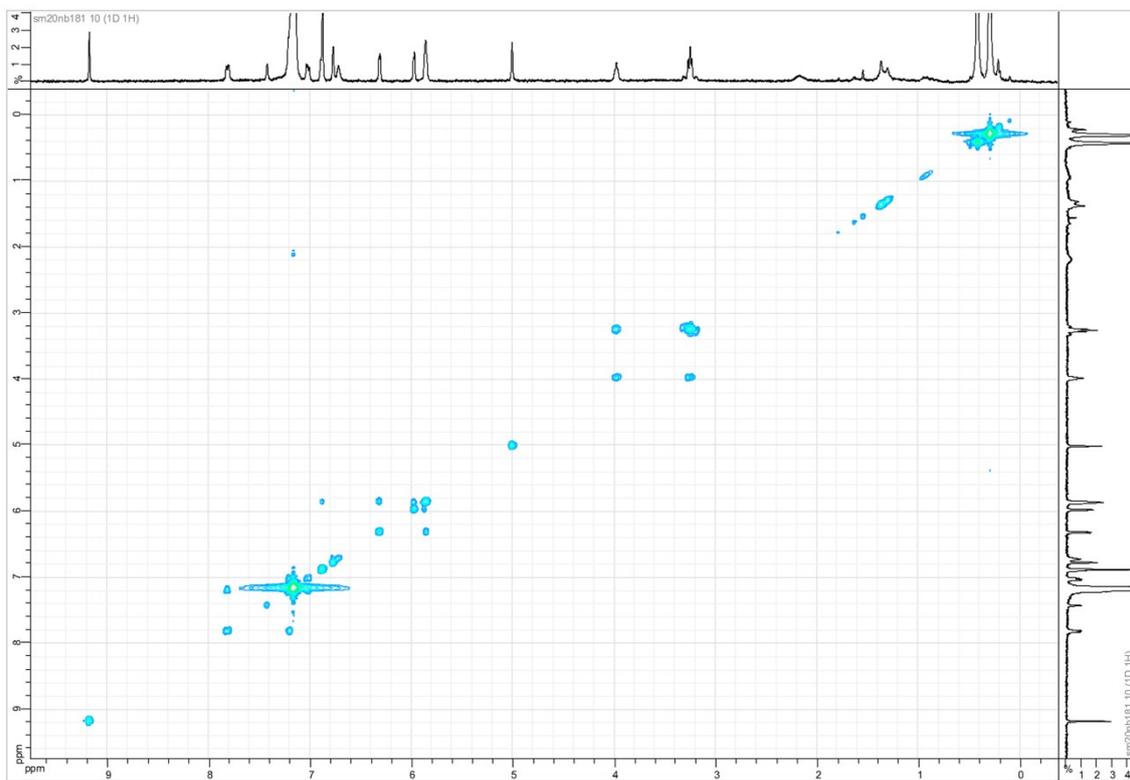
^{13}C NMR spectrum of compound **5m** in C_6D_6-d_6 at 75 MHz (zoom)



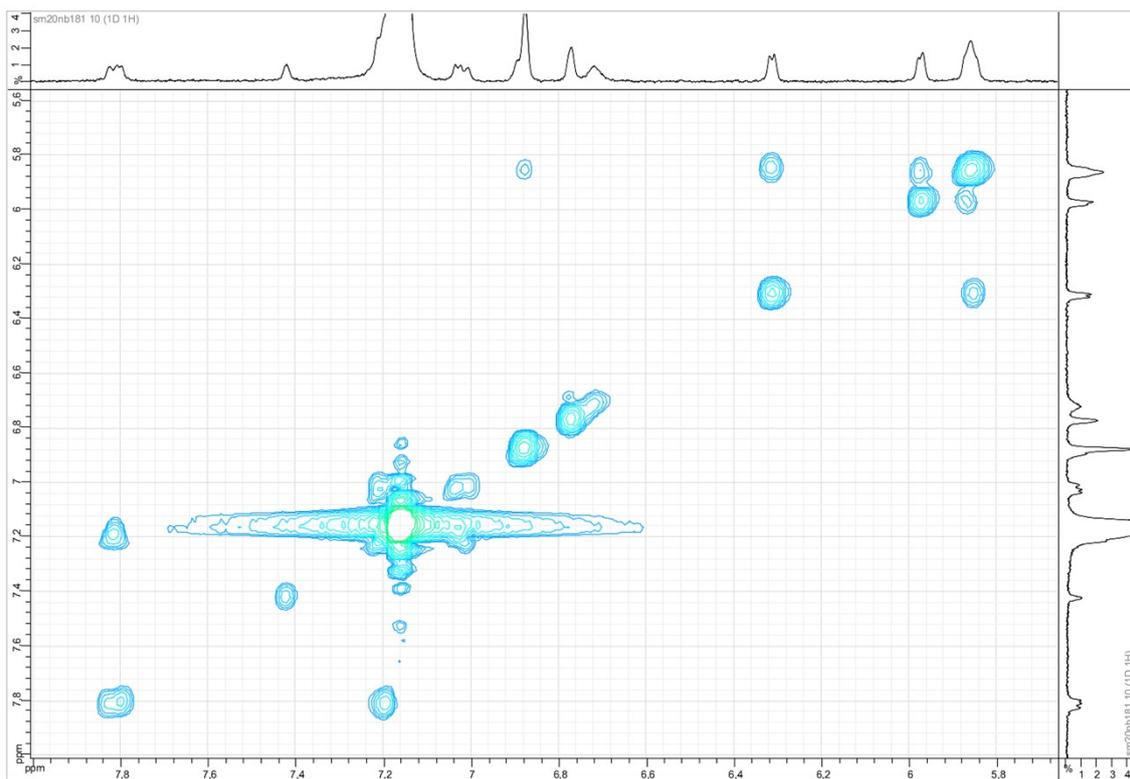
Dept ^{135}C NMR spectrum of compound **5m** in C_6D_6-d_6 & some drops $\text{MeCN}-d_3$ at 75 MHz



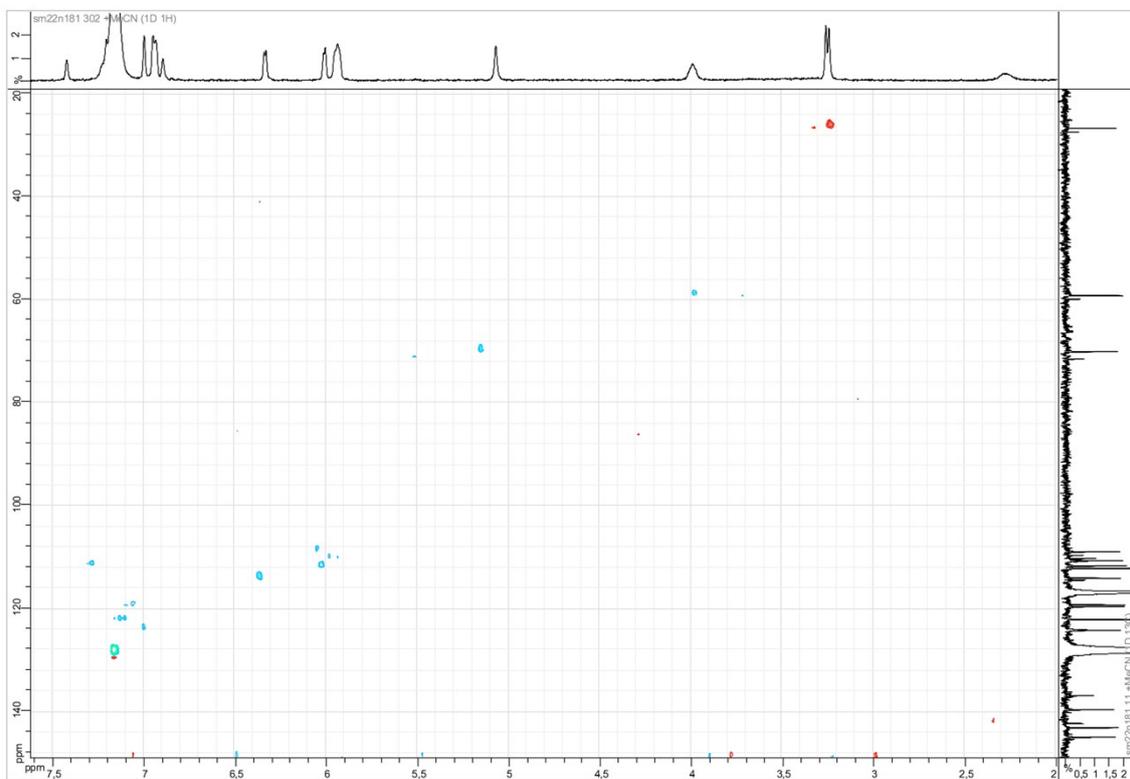
Dept 135 NMR spectrum of compound **5m** in C₆D₆-d₆ & some drops MeCN-d₃ at 75 MHz
(zoom)



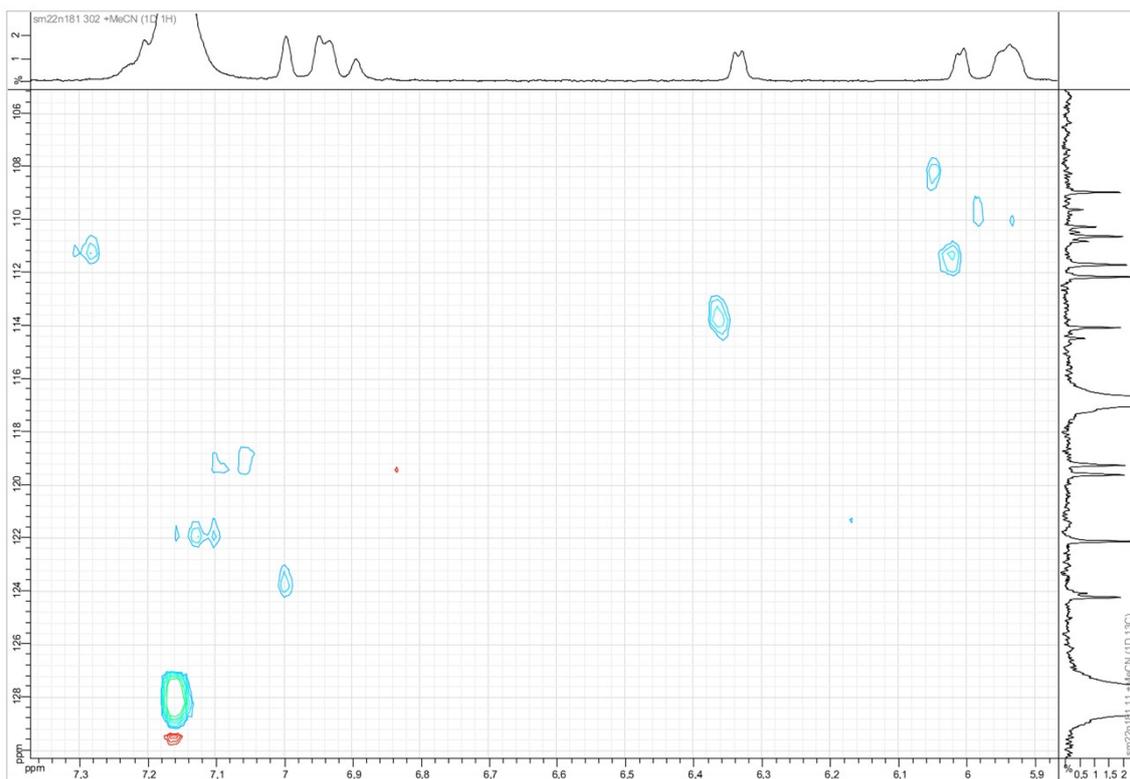
COSY NMR spectrum of compound **5m** in C₆D₆-d₆



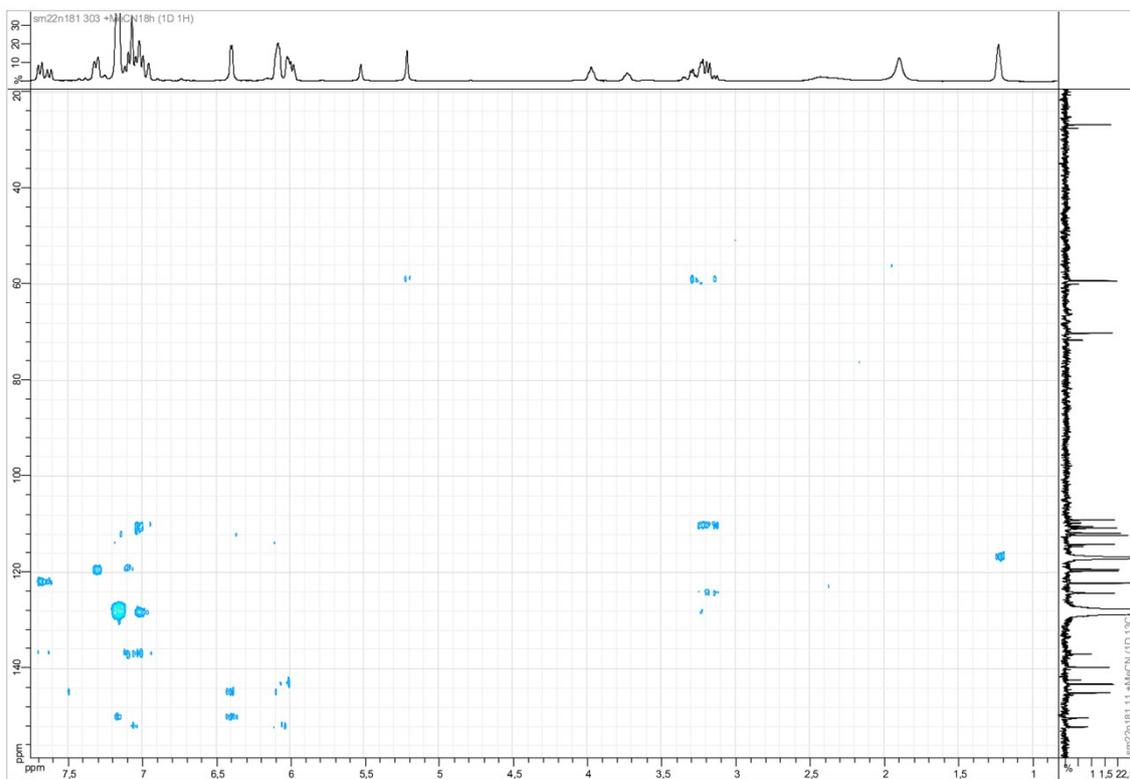
COSY NMR spectrum of compound **5m** in $C_6D_6-d_6$ (zoom)



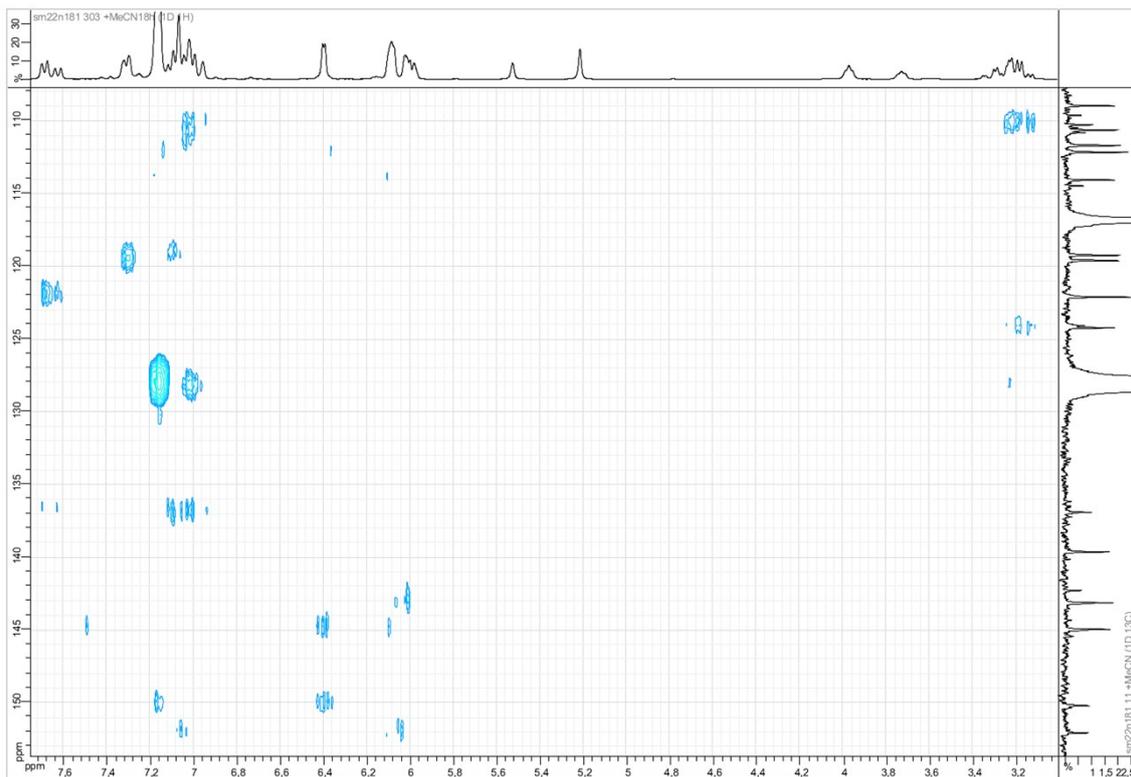
HSQC NMR spectrum of compound **5m** in $C_6D_6-d_6$ & some drops $MeCN-d_3$



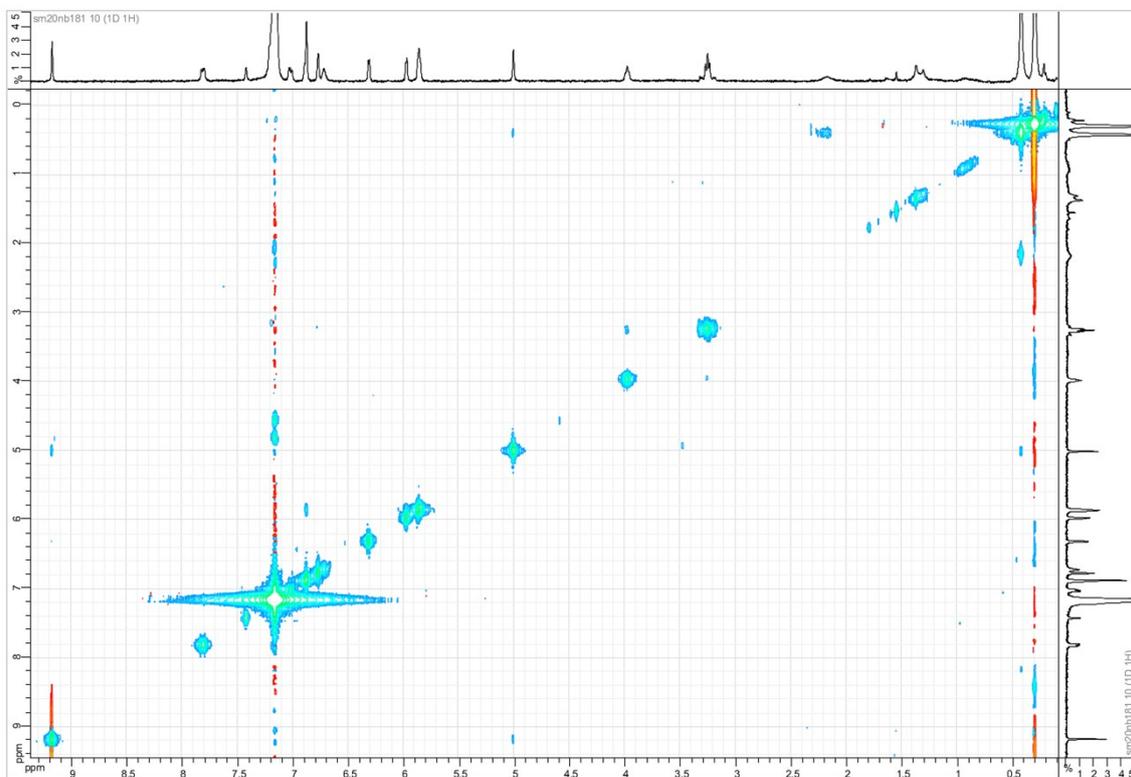
HSQC NMR spectrum of compound **5m** in $C_6D_6-d_6$ & some drops $MeCN-d_3$ (zoom)



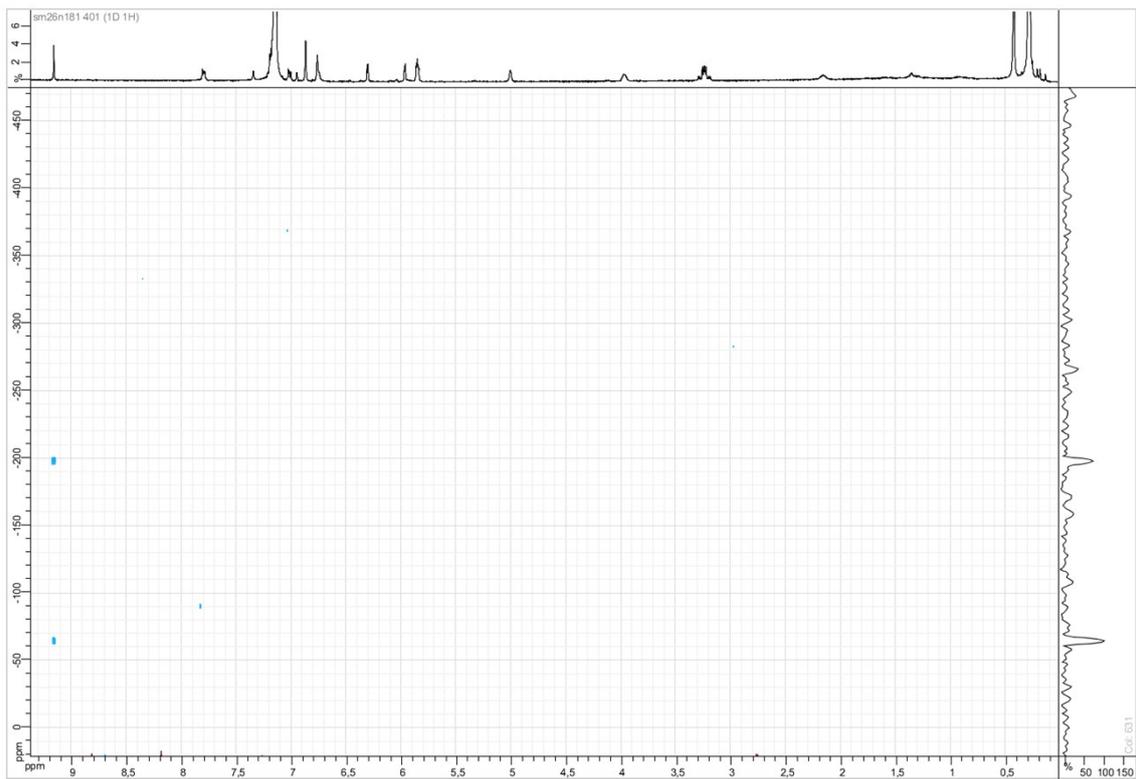
1H - ^{13}C HMBC NMR spectrum of compound **5m** in $C_6D_6-d_6$ & some drops $MeCN-d_3$



^1H - ^{13}C HMBC NMR spectrum of compound **5m** in C_6D_6 - d_6 & some drops MeCN - d_3 (zoom)



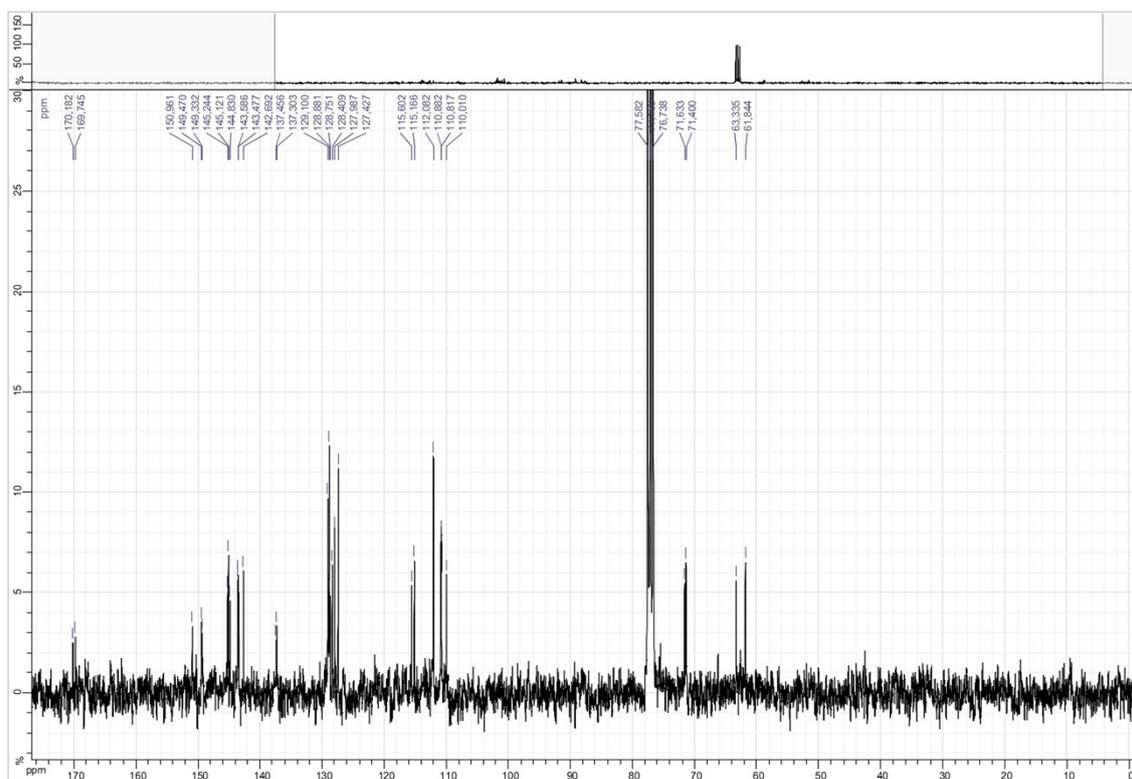
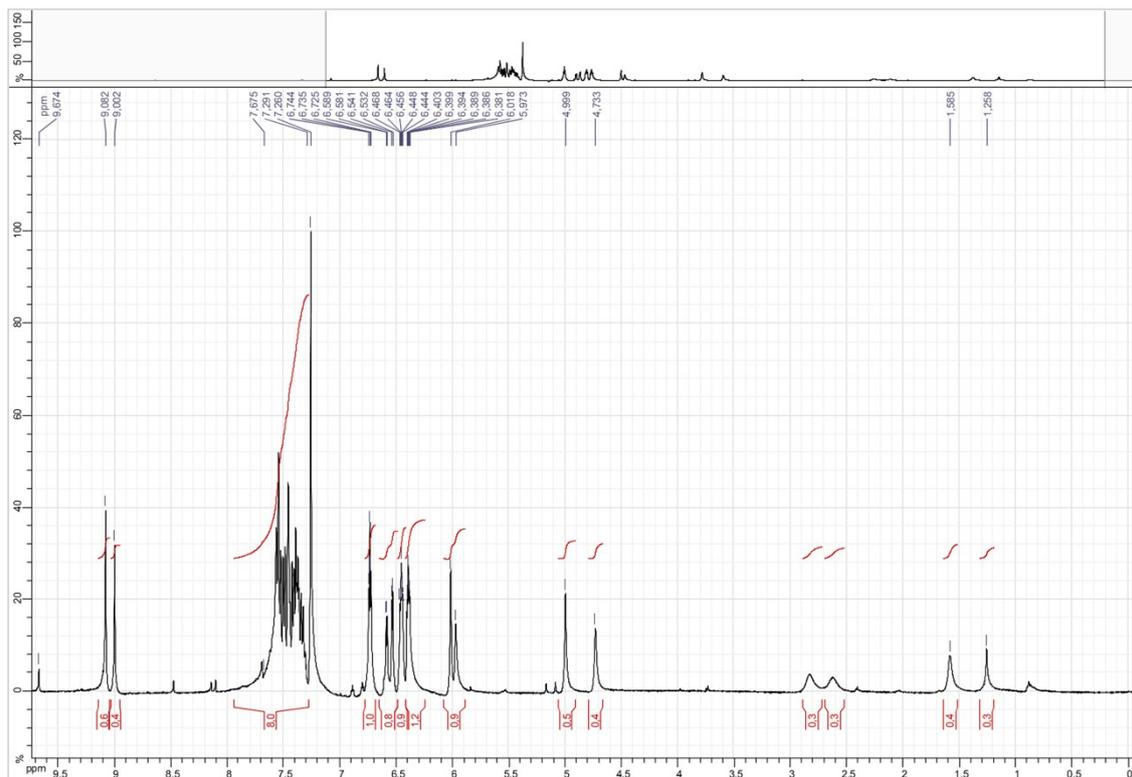
NOESY NMR spectrum of compound **5m** in C_6D_6 - d_6

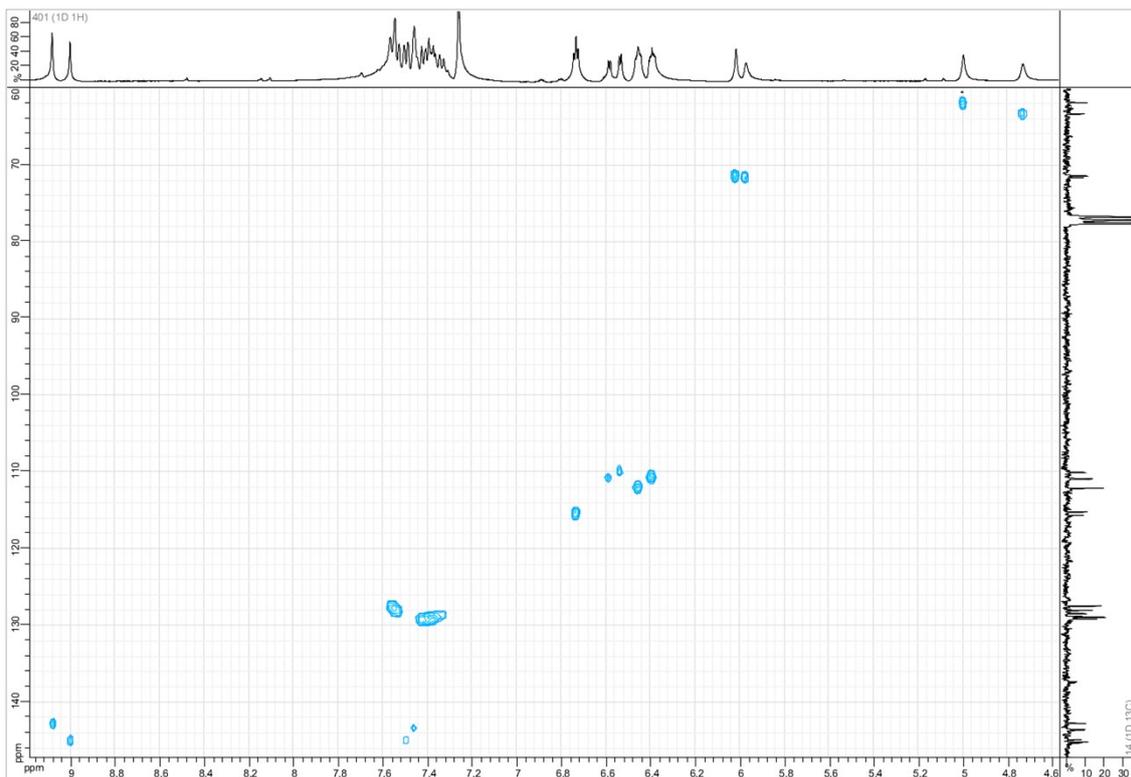


^1H - ^{15}N HMBC NMR spectrum of compound **5m** in C_6D_6 - d_6 & some drops MeCN - d_3

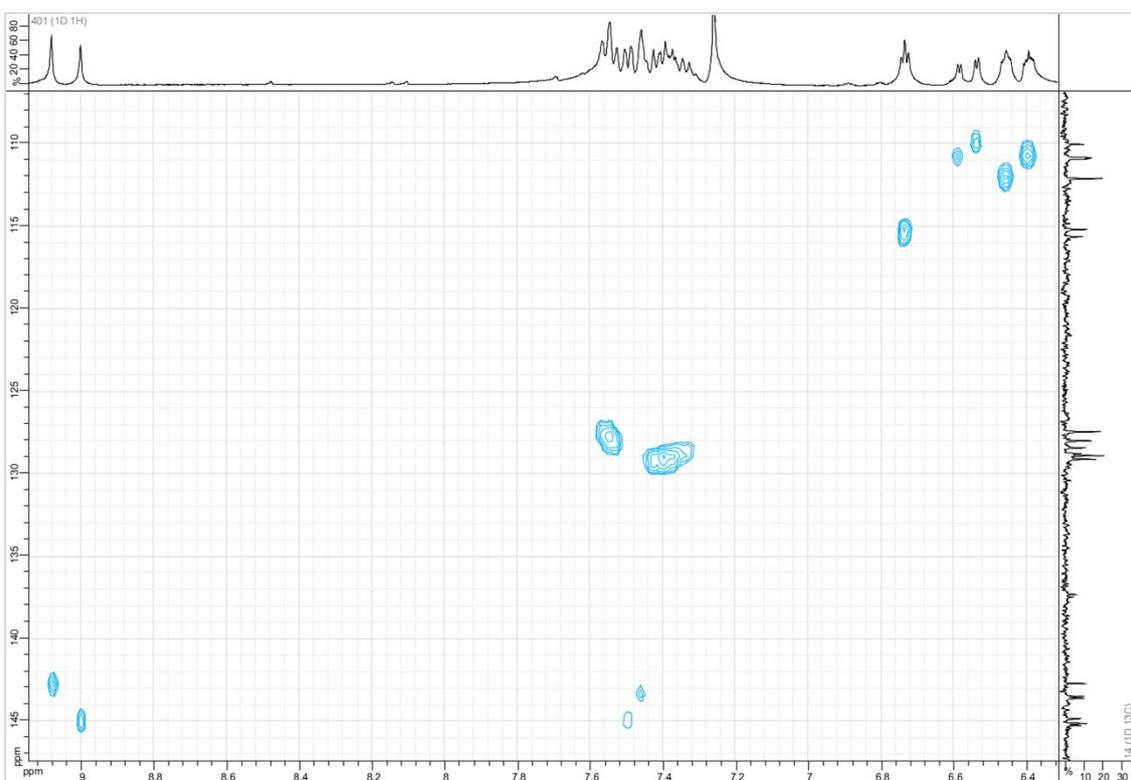
5. Spectrum section for kinetic behaviors

a. NMR spectra of **5a**

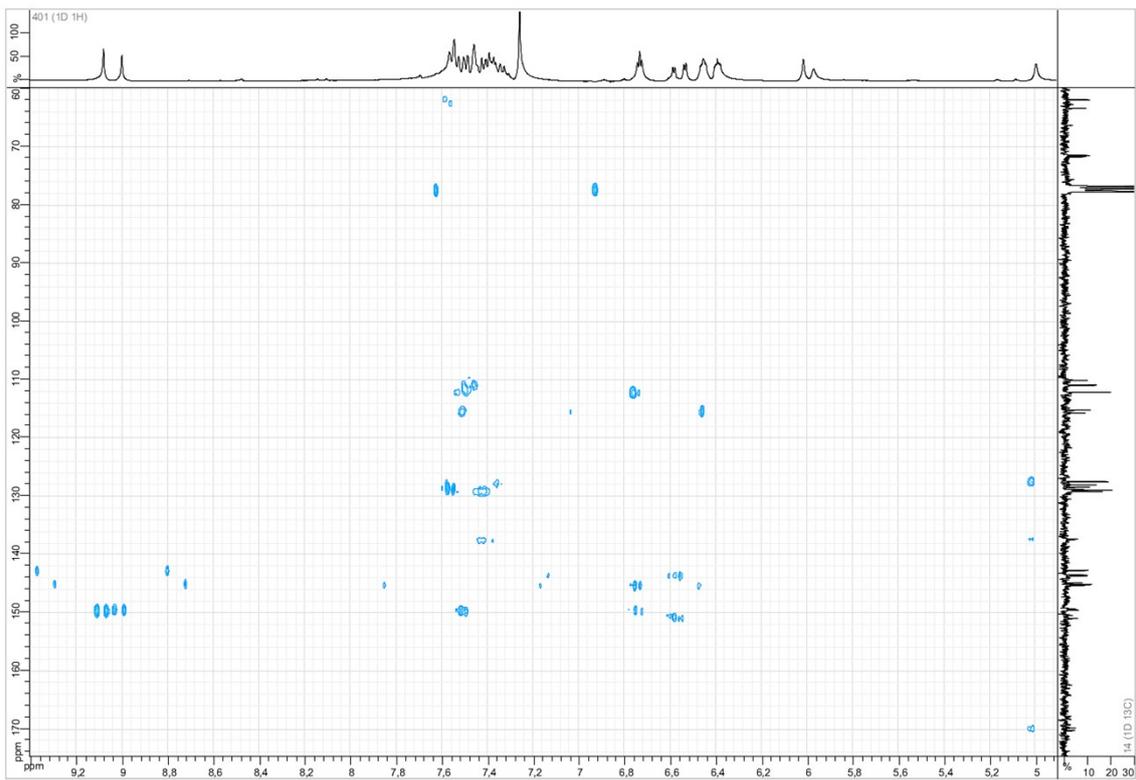




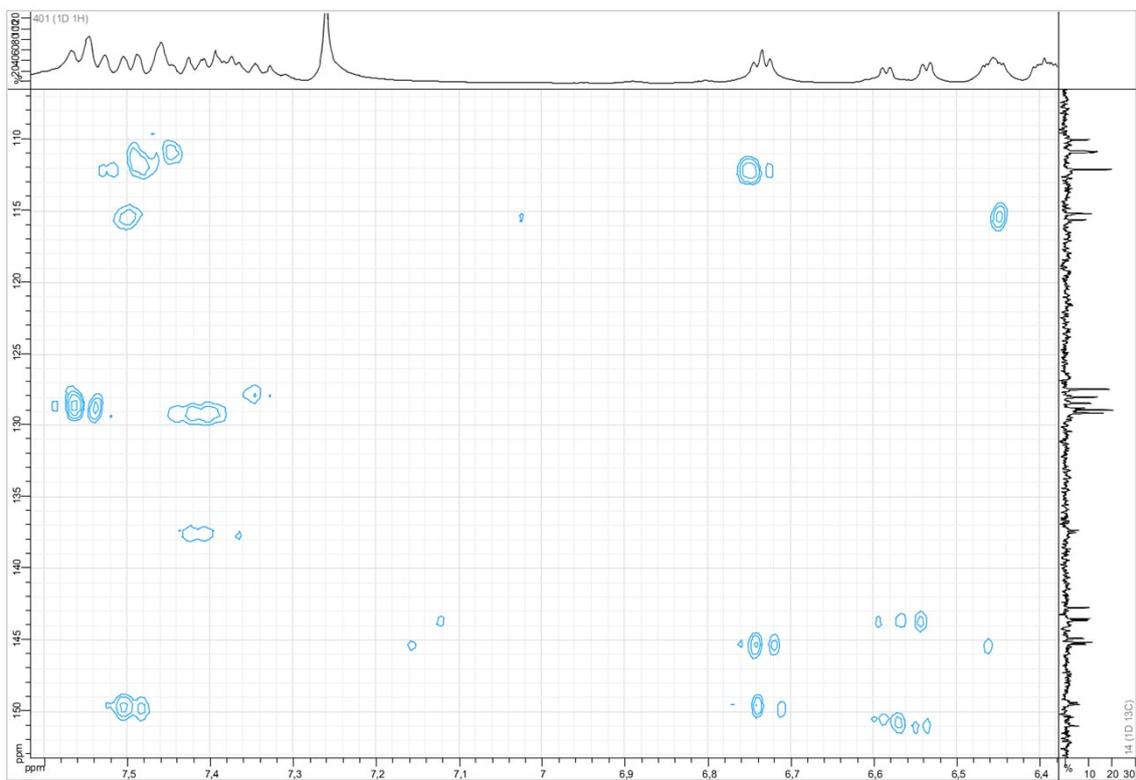
HSQC NMR spectrum in CDCl₃



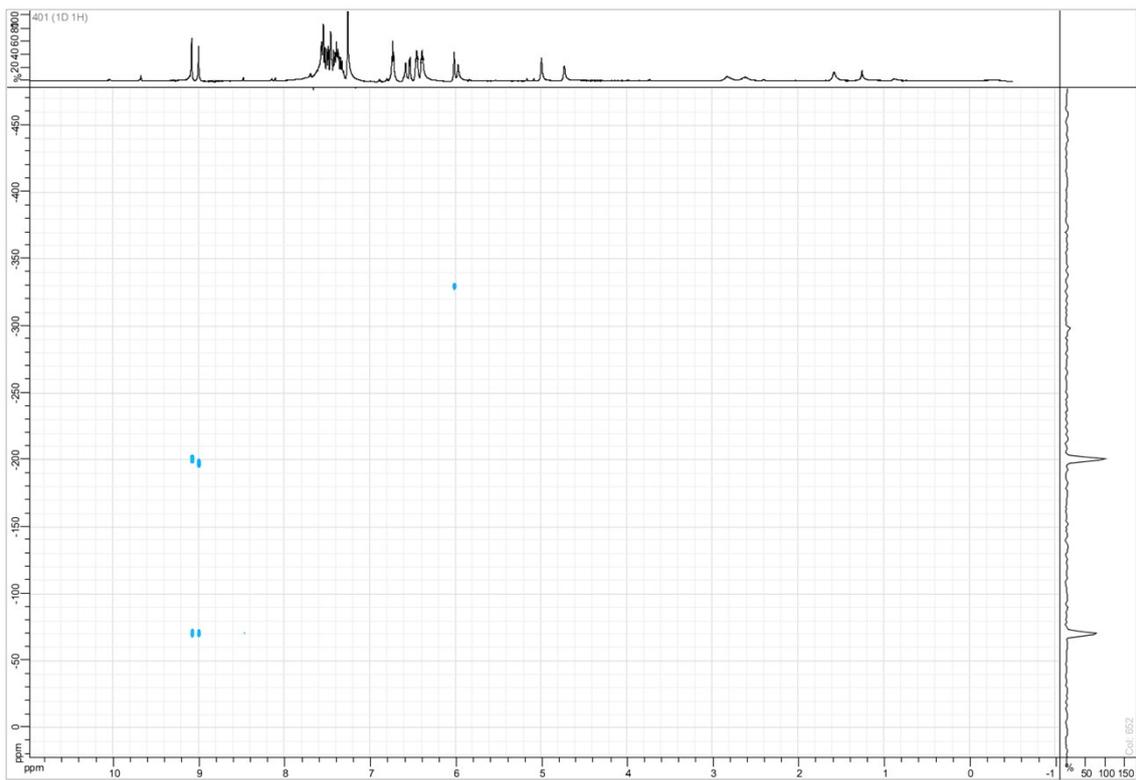
HSQC NMR spectrum in CDCl₃ (zoom)



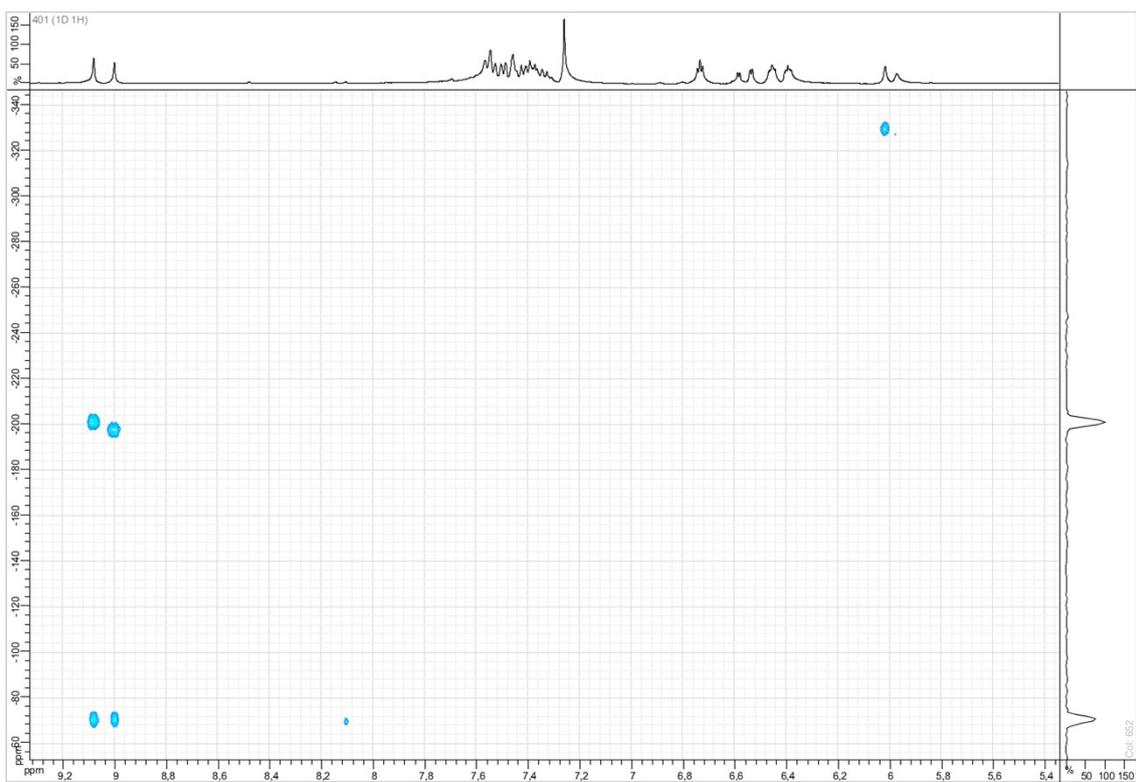
$^1\text{H} - ^{13}\text{C}$ HMBC NMR spectrum in CDCl_3



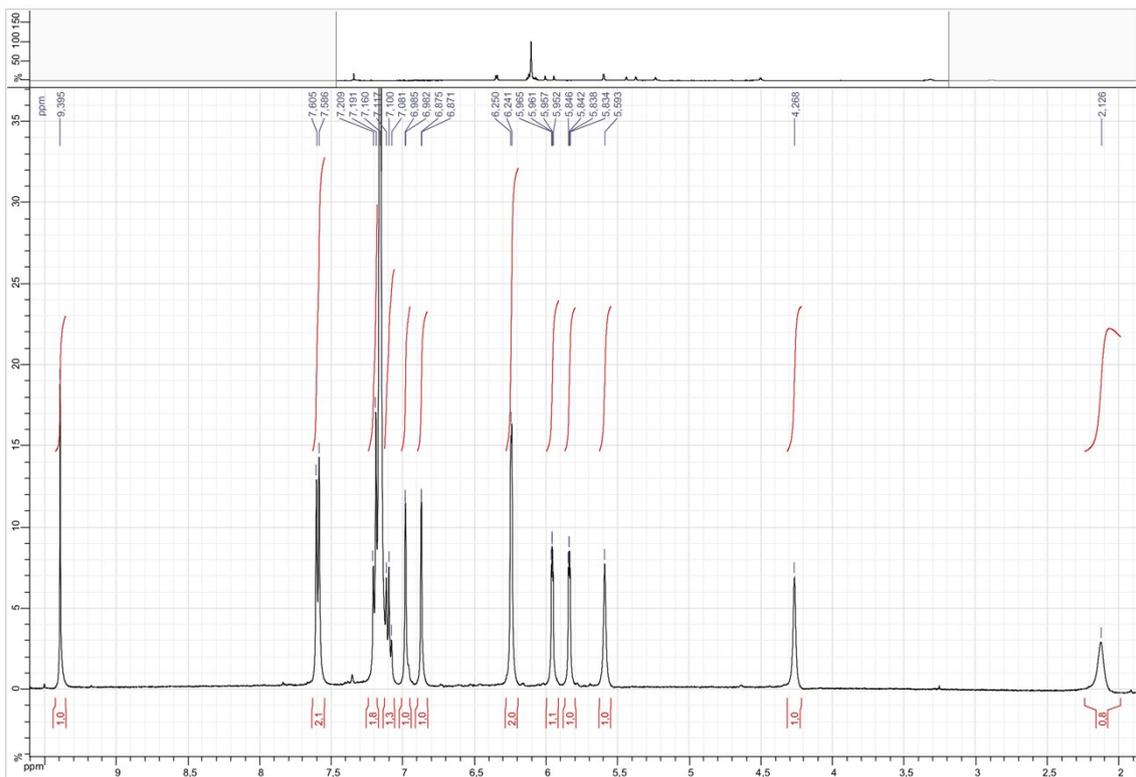
$^1\text{H} - ^{13}\text{C}$ HMBC NMR spectrum in CDCl_3 (zoom)



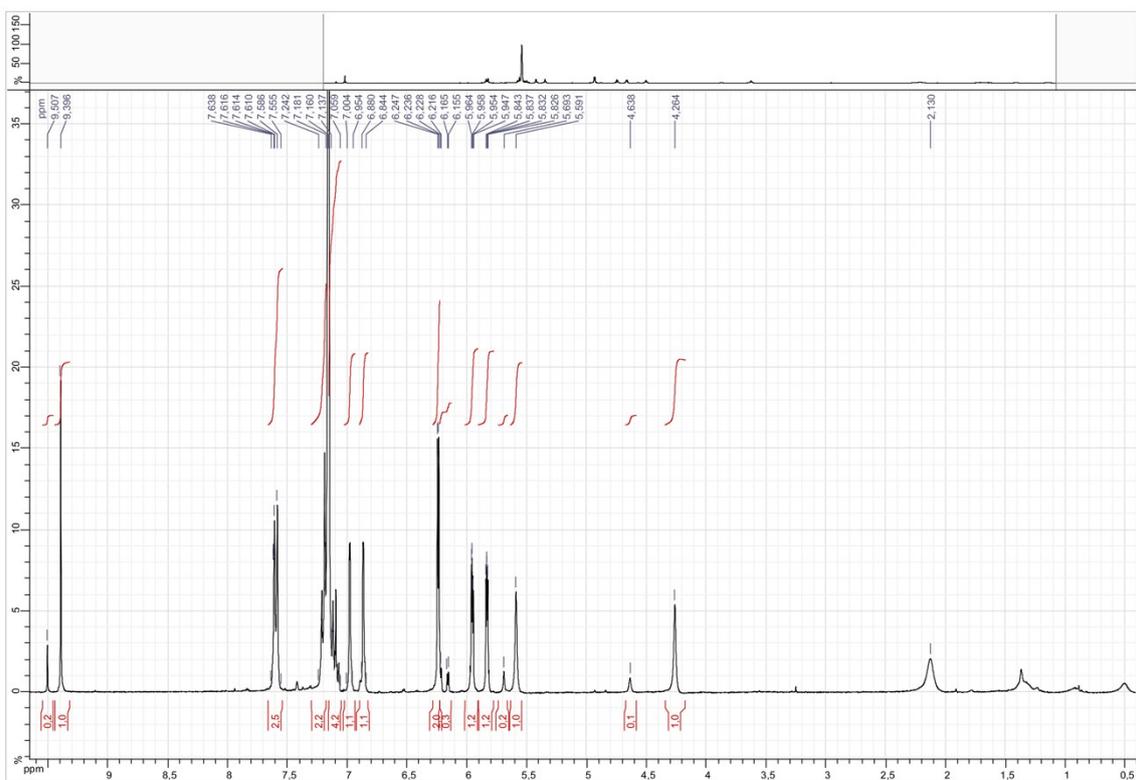
$^1\text{H} - ^{15}\text{N}$ HMBC NMR spectrum in CDCl_3



$^1\text{H} - ^{13}\text{C}$ HMBC NMR spectrum in CDCl_3 (zoom)

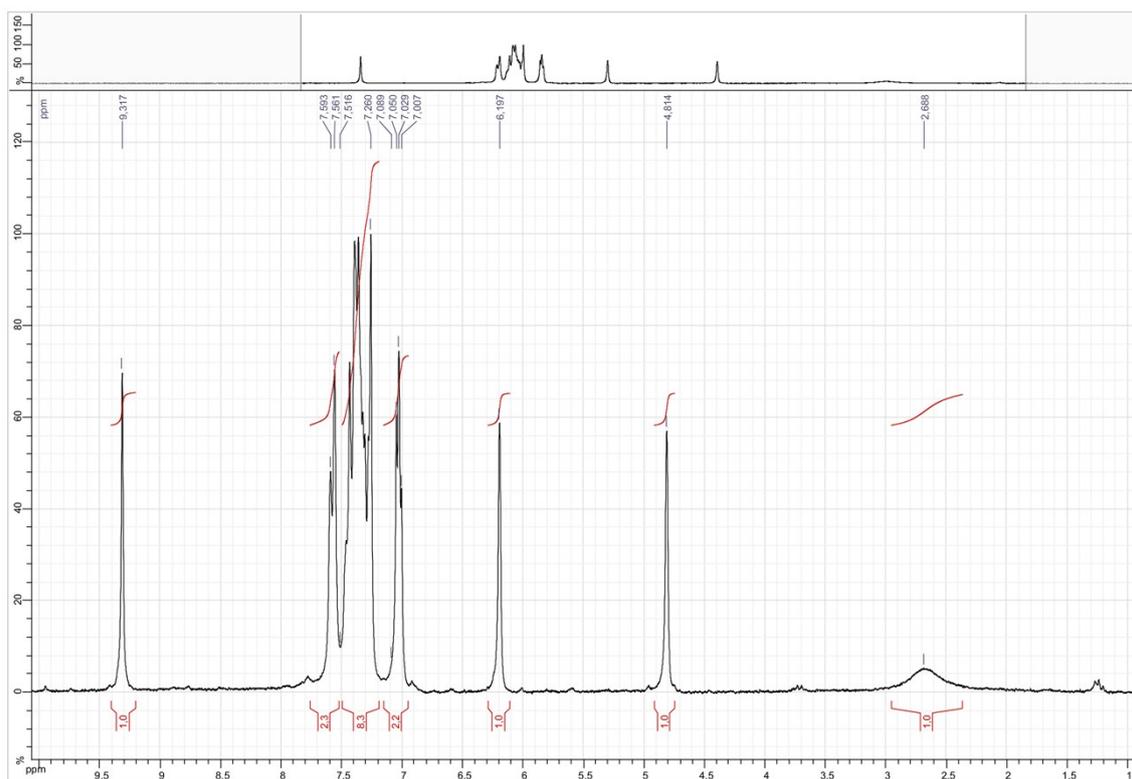


^1H NMR spectrum in C_6D_6 (400 MHz) immediately

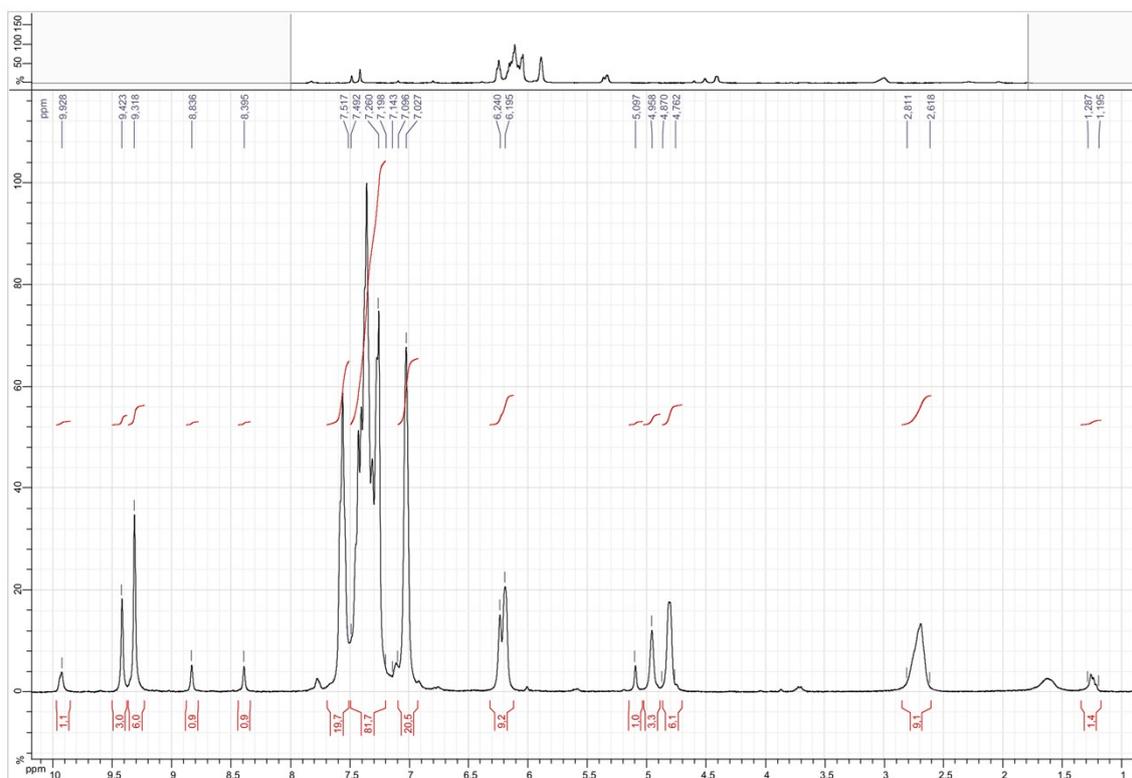


^1H NMR spectrum in C_6D_6 (400 MHz) after 24 h

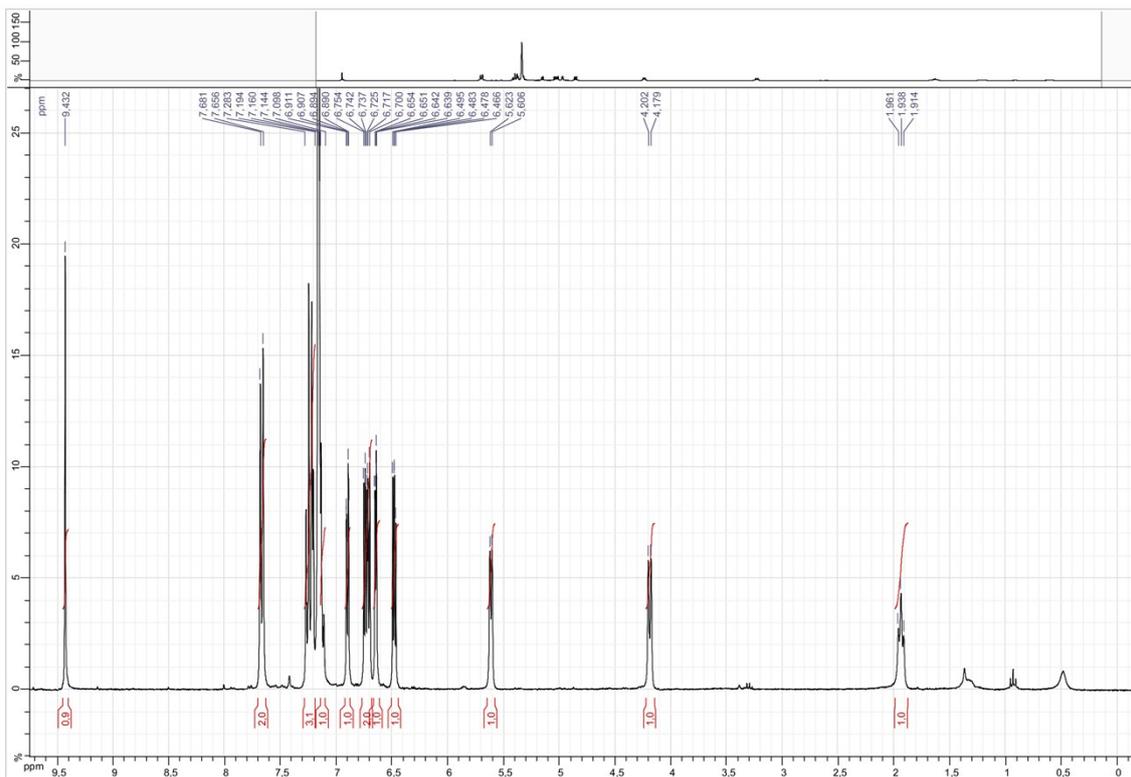
b. NMR spectra of **5b**



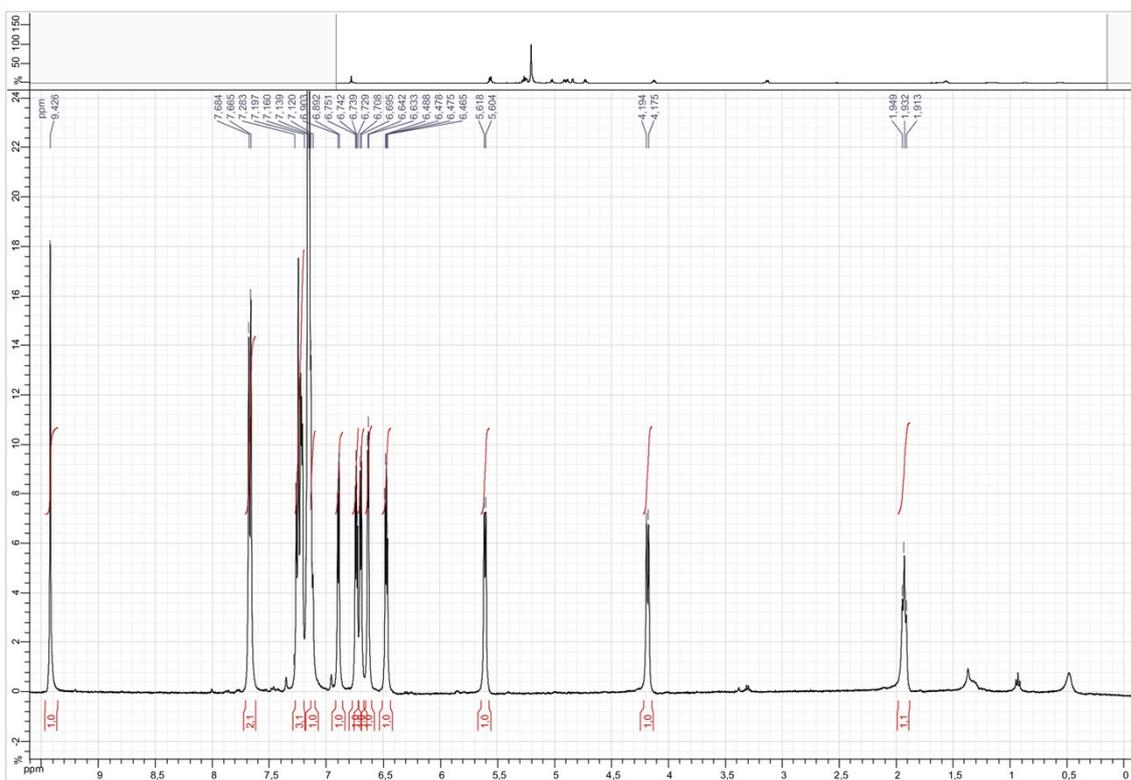
¹H NMR spectrum in CDCl₃ (200 MHz) immediately



¹H NMR spectrum in CDCl₃ (200 MHz) after 48 h

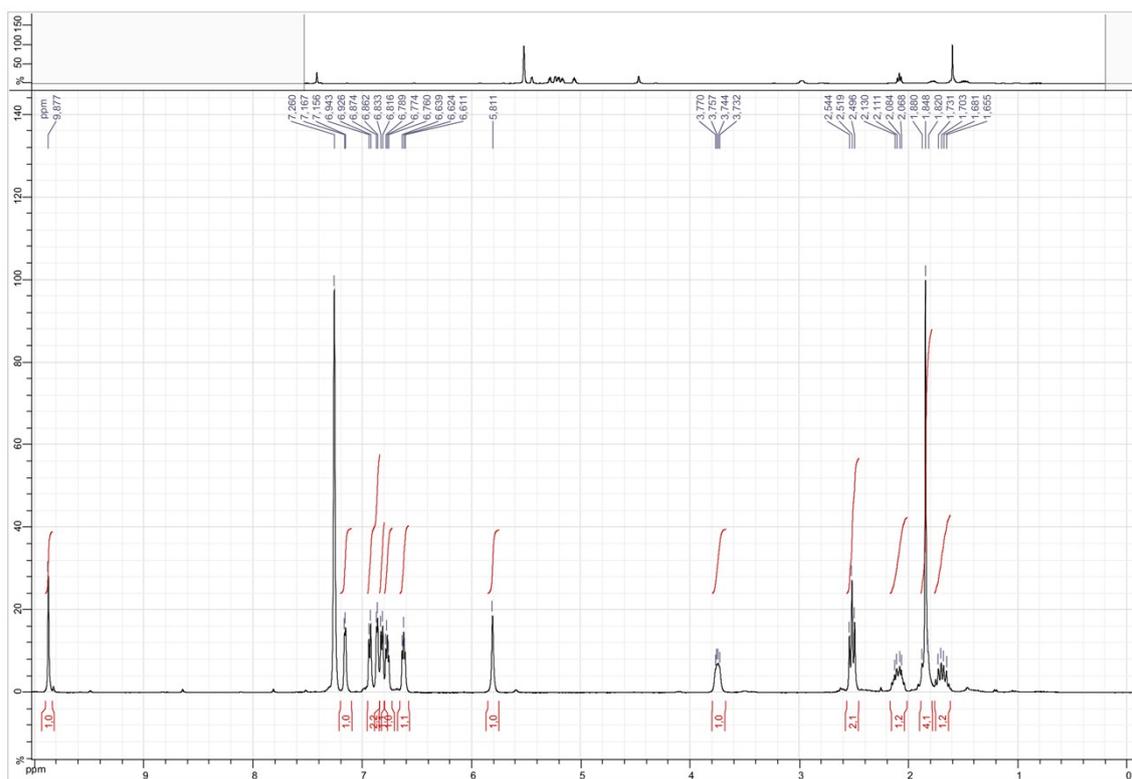


^1H NMR spectrum in C_6D_6 (300 MHz) immediately

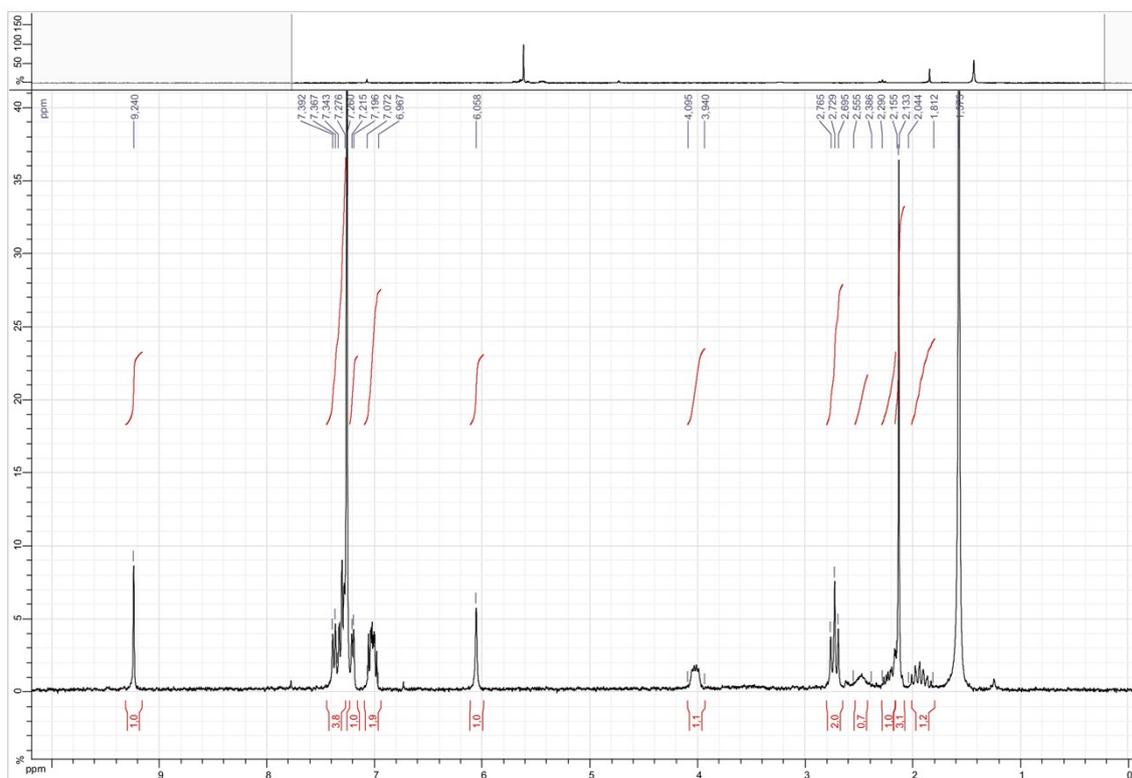


^1H NMR spectrum in C_6D_6 (300 MHz) after 48 h

c. NMR spectra of **5c**

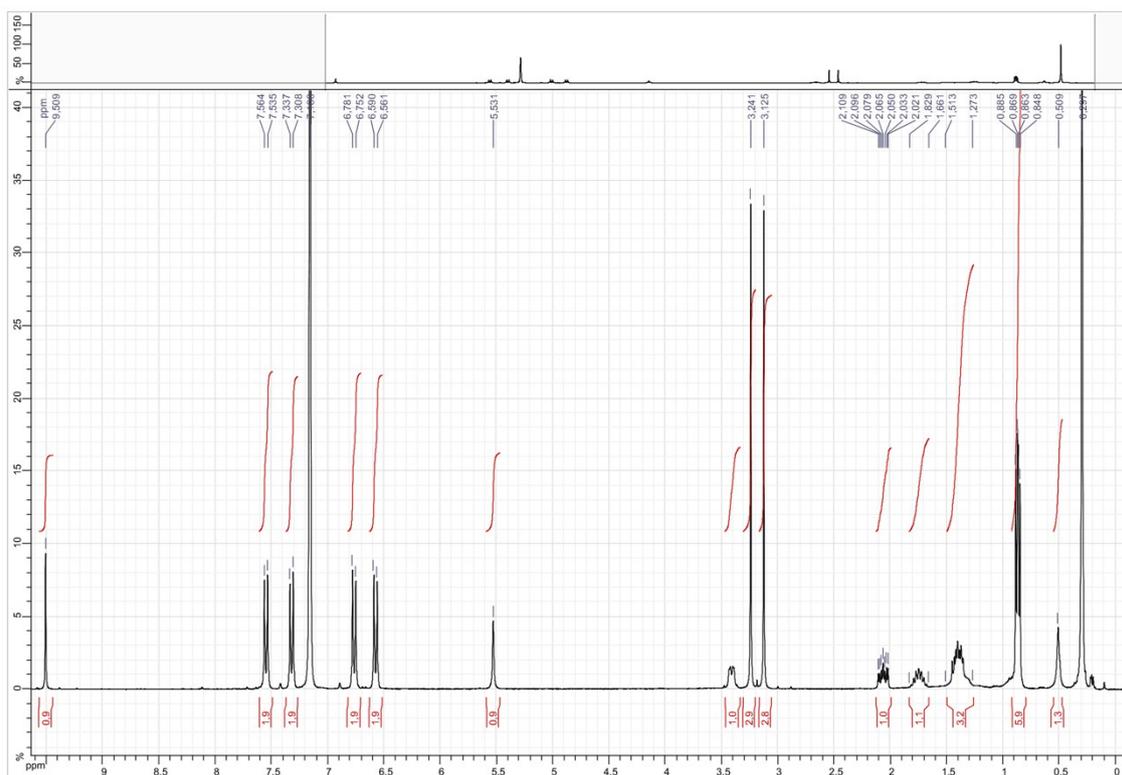


¹H NMR spectrum in CDCl₃ (200 MHz) immediately

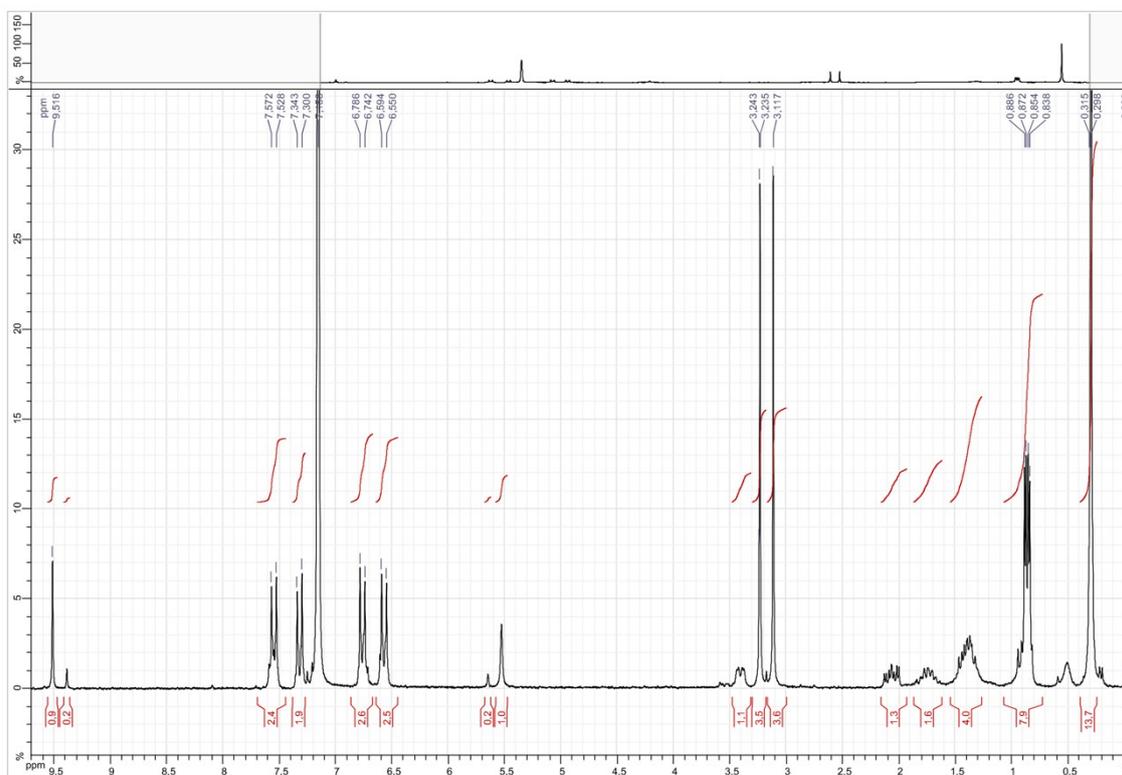


¹H NMR spectrum in CDCl₃ (200 MHz) after 5 min

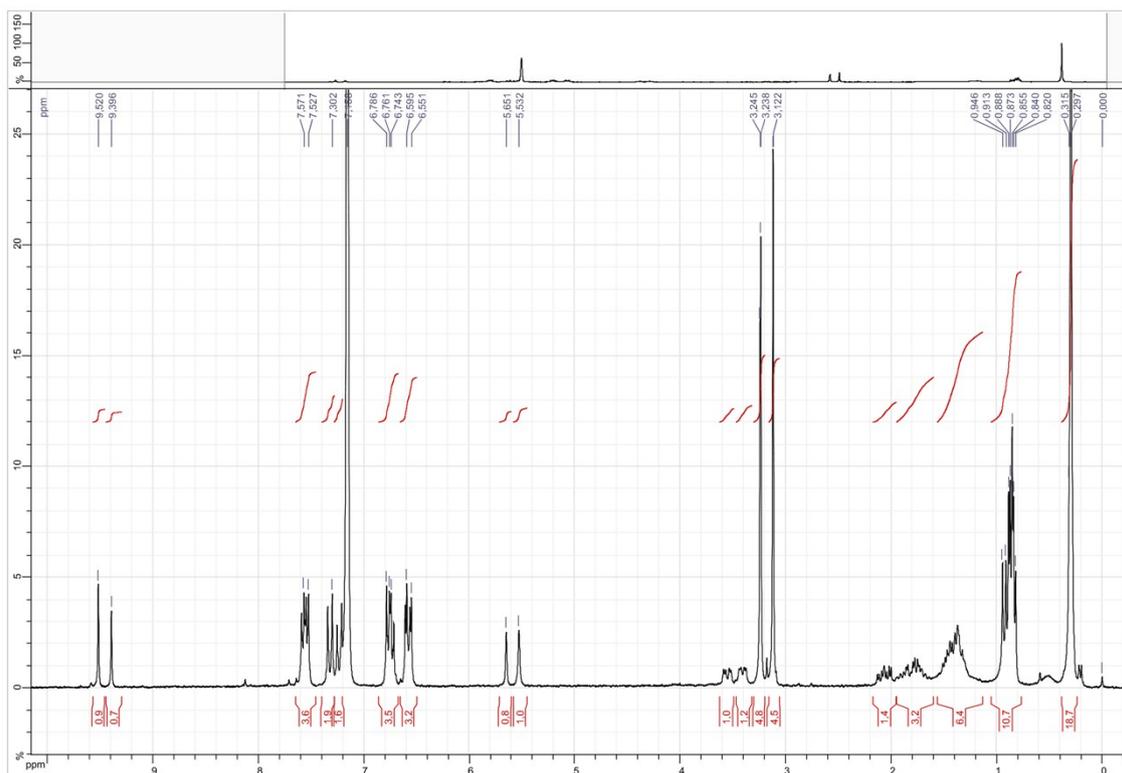
d. NMR spectra of **5f**



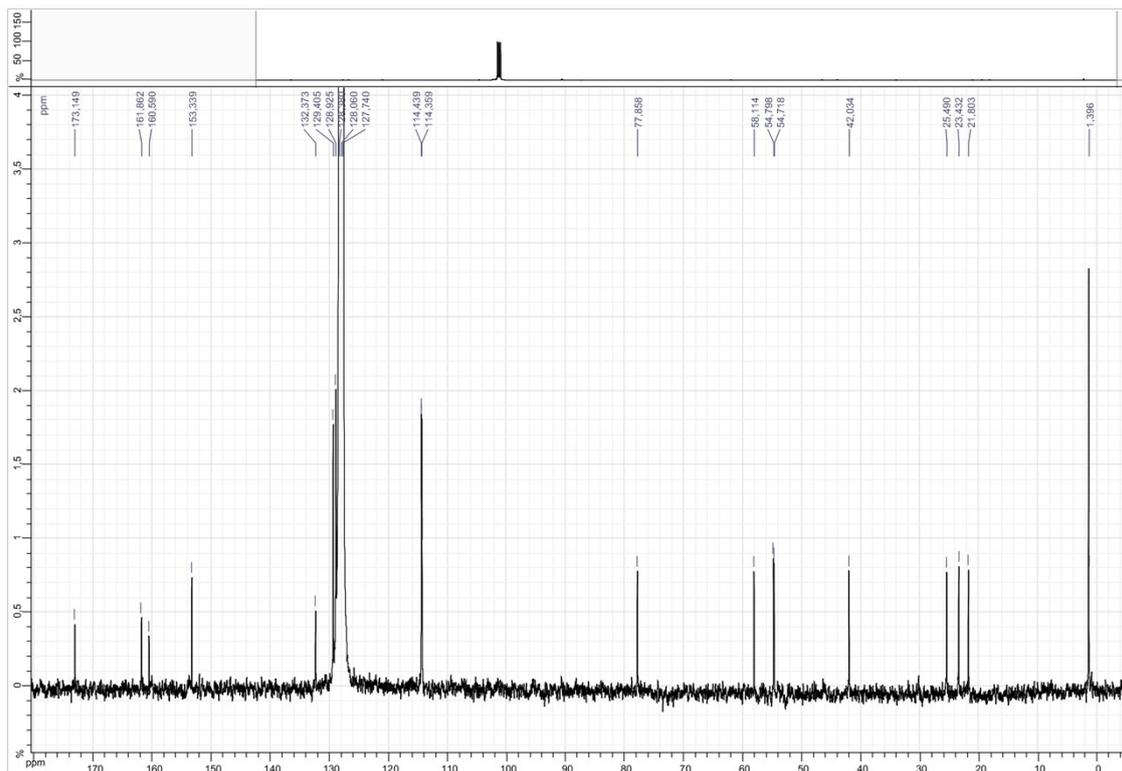
¹H NMR spectrum in C₆D₆ (400 MHz) immediately



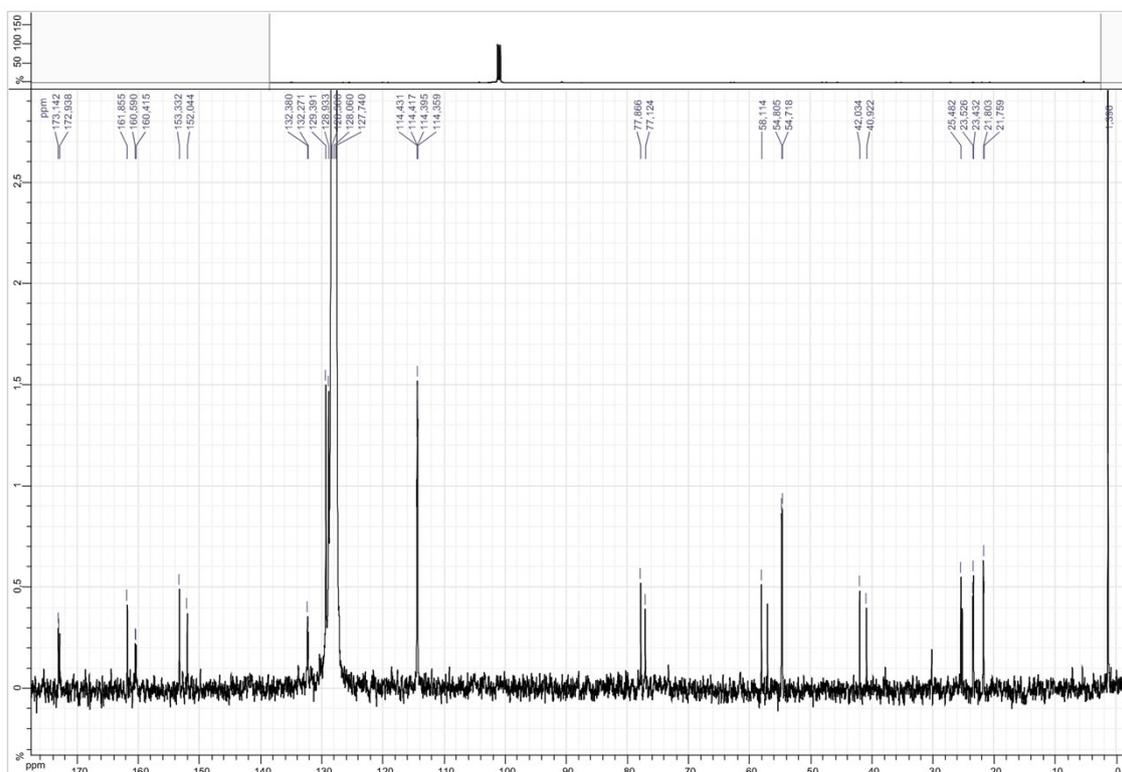
¹H NMR spectrum in C₆D₆ (200 MHz) after 3 months at 4°C



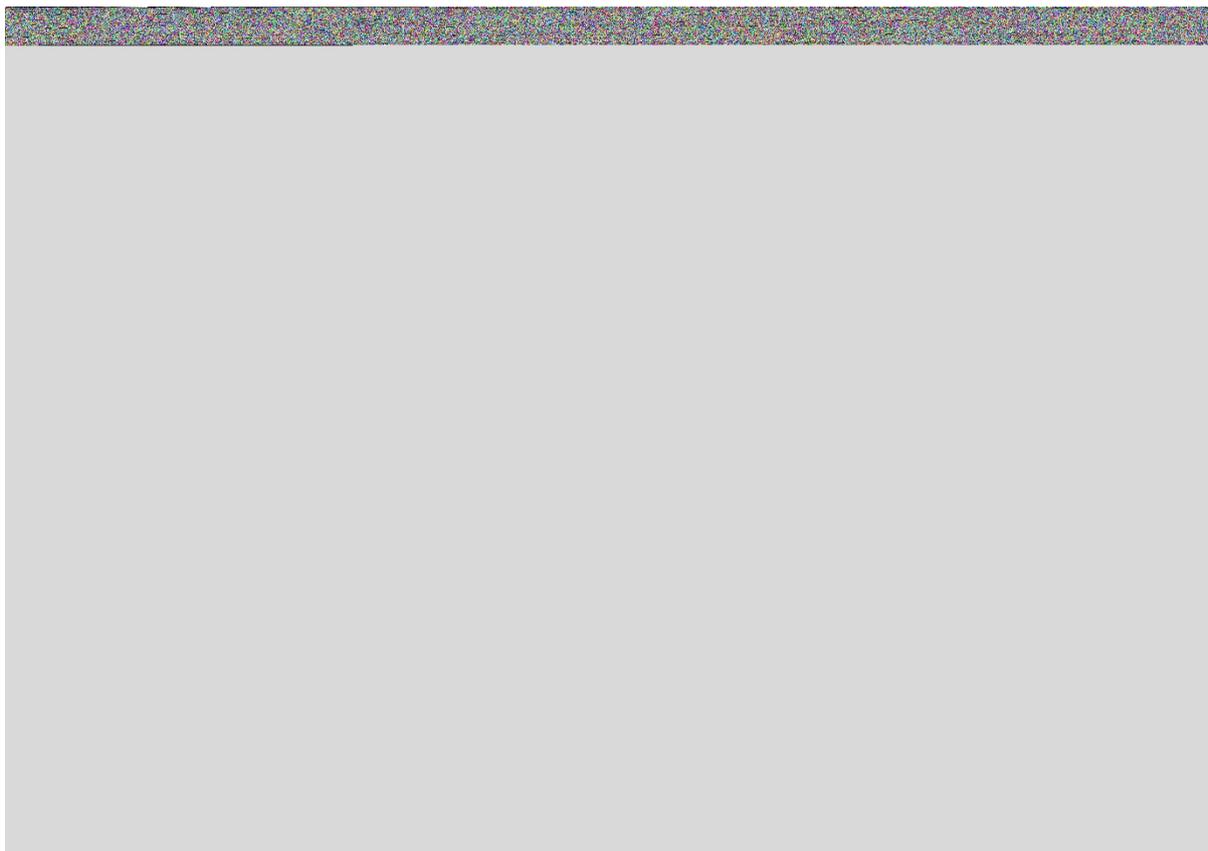
^1H NMR spectrum in C_6D_6 (200 MHz) after 2 days at 40°C



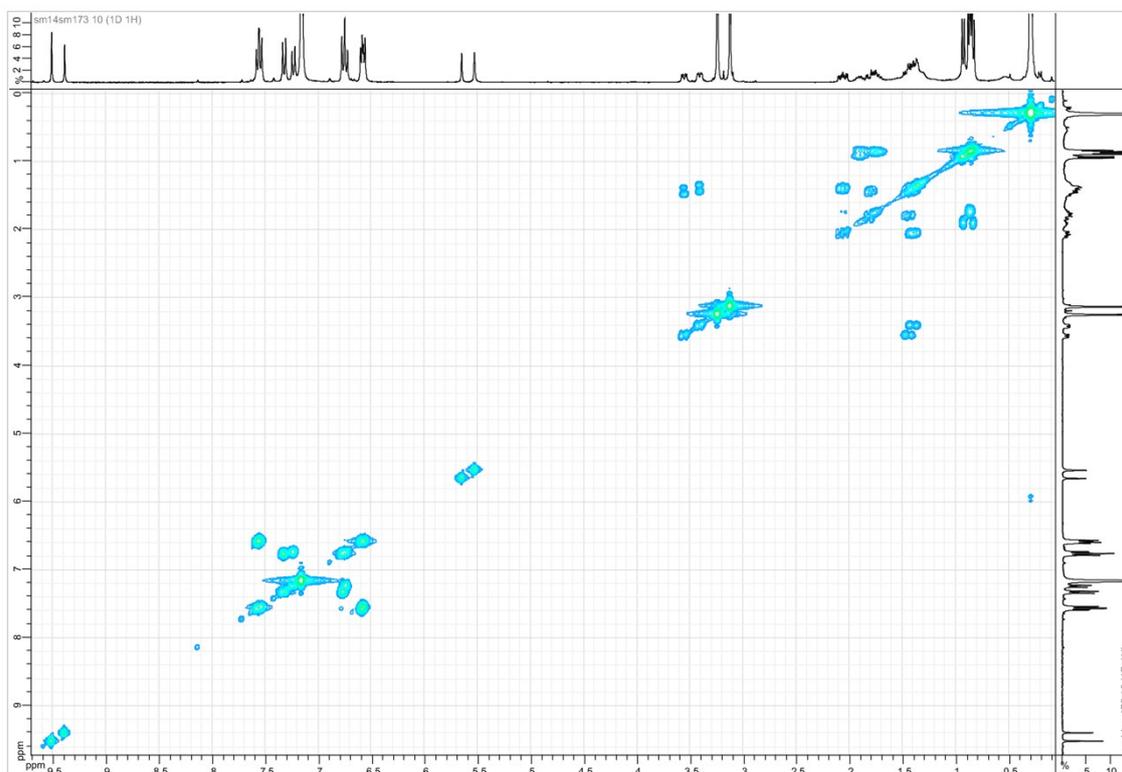
¹³C NMR spectrum in C₆D₆ (75 MHz) immediately



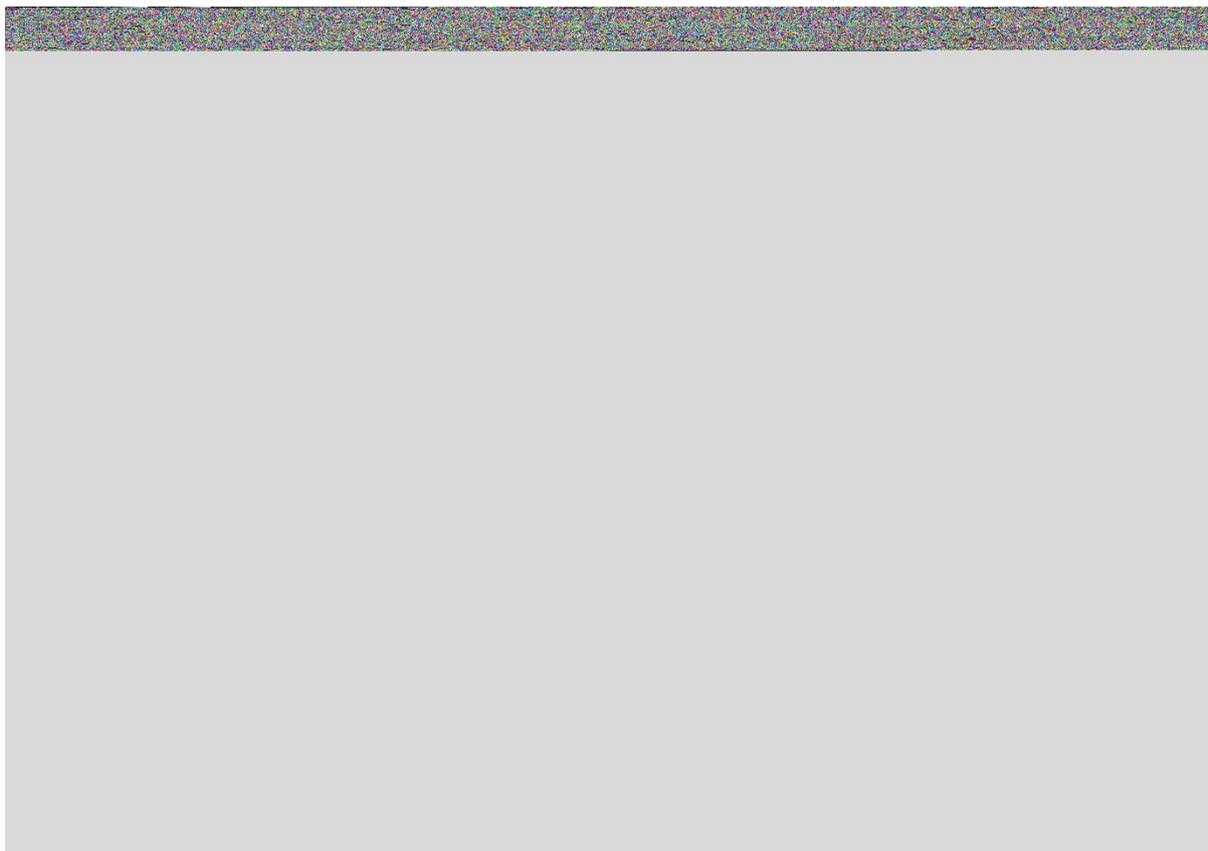
¹³C NMR spectrum in C₆D₆ (75 MHz) after 2 days at 40 °C



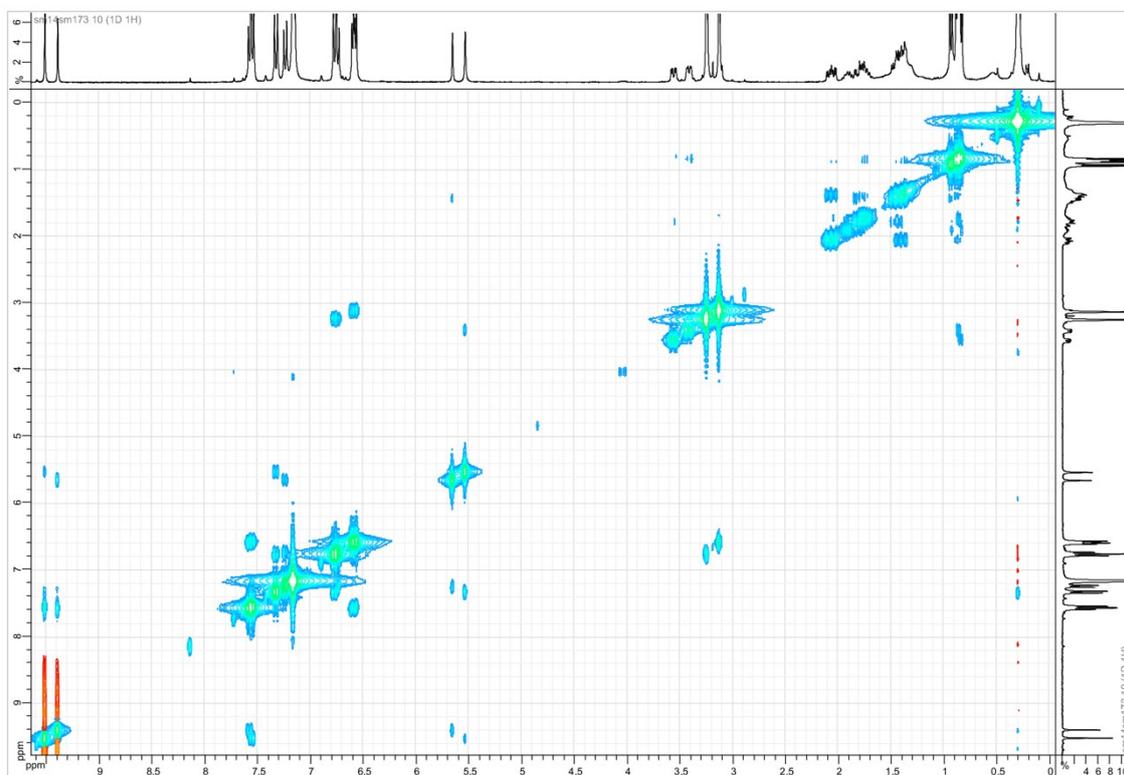
COSY NMR spectrum in C_6D_6 immediately



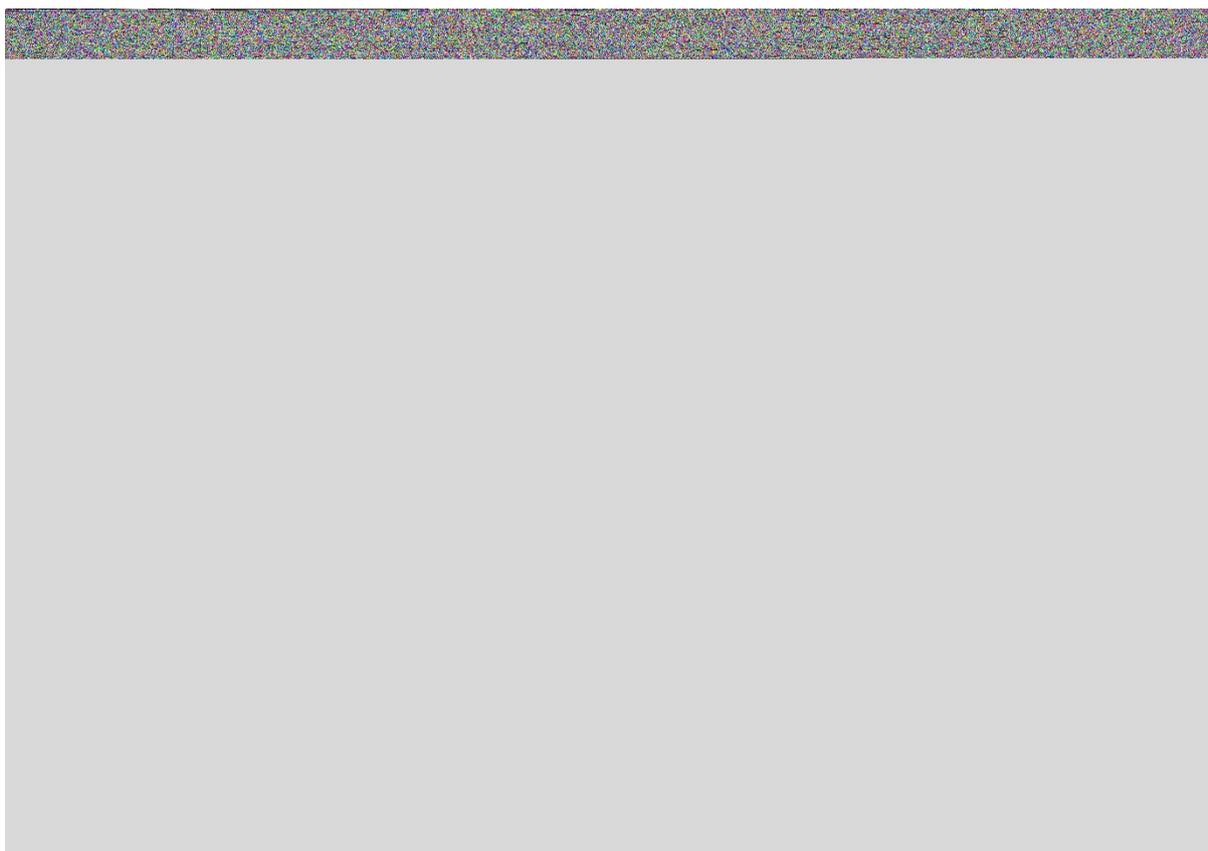
COSY NMR spectrum in C_6D_6 after 2 days at 40 °C



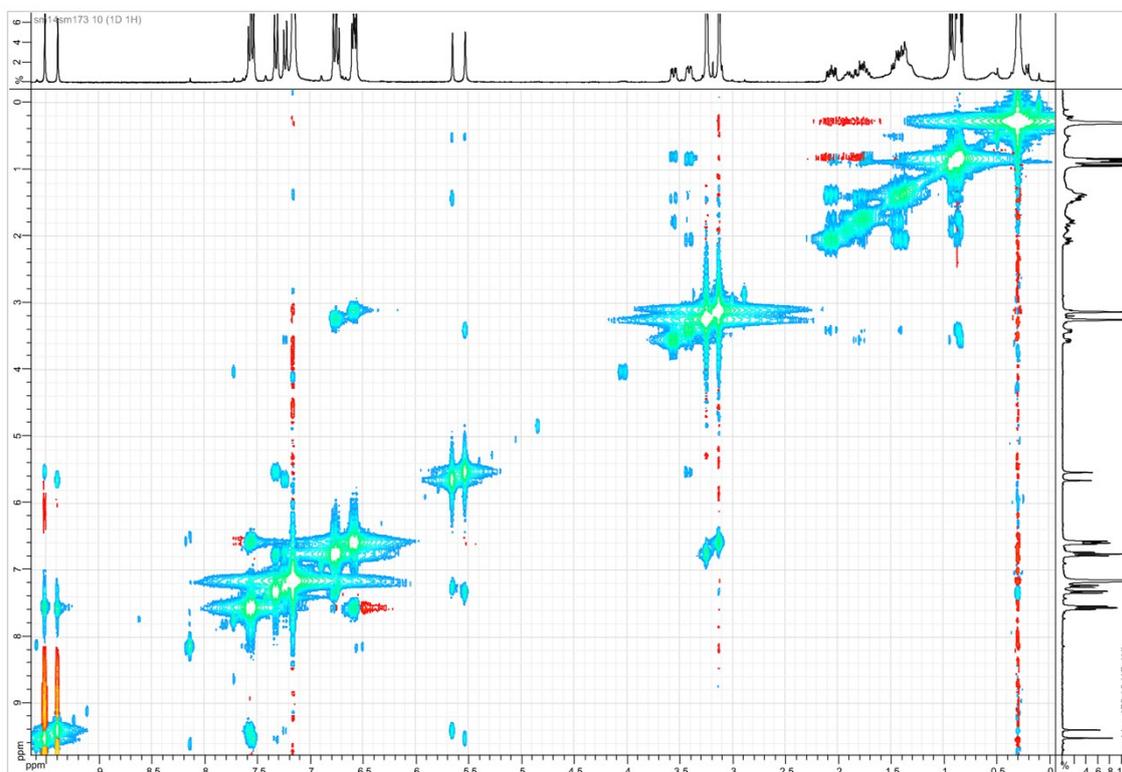
NOESY NMR spectrum in C_6D_6 immediately



NOESY NMR spectrum in C_6D_6 after 2 days at 40 °C

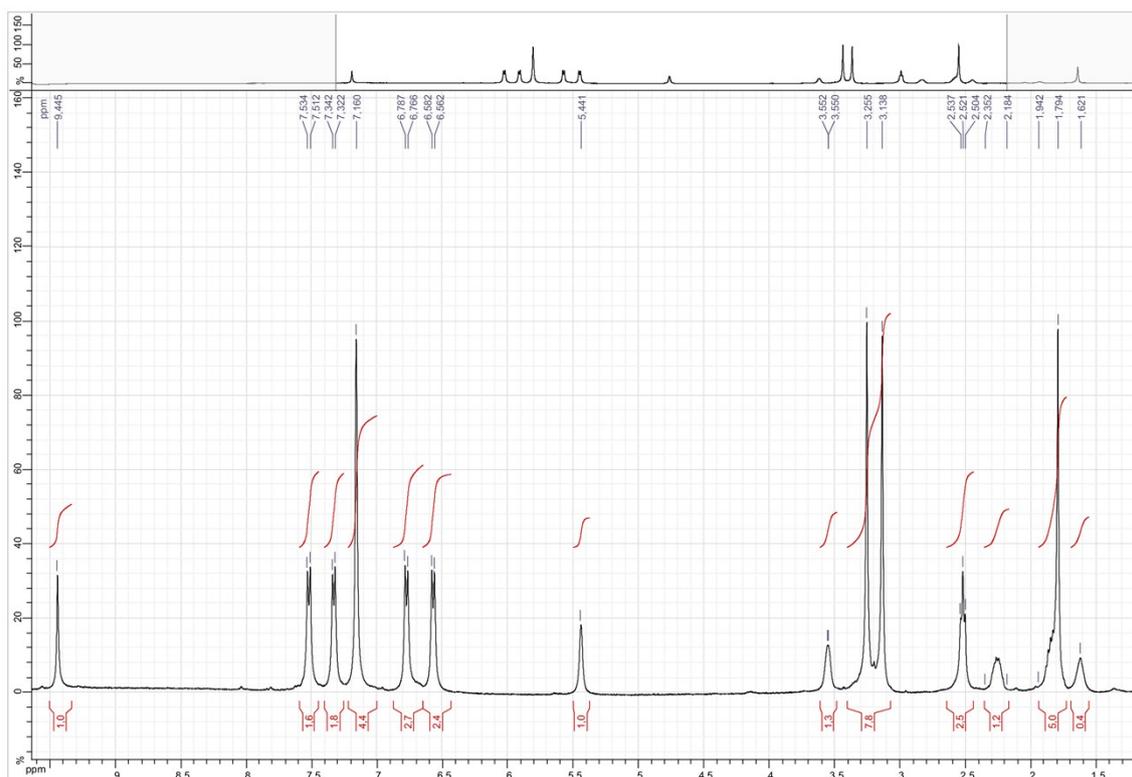


NOESY NMR spectrum in C_6D_6 immediately (deep cut)

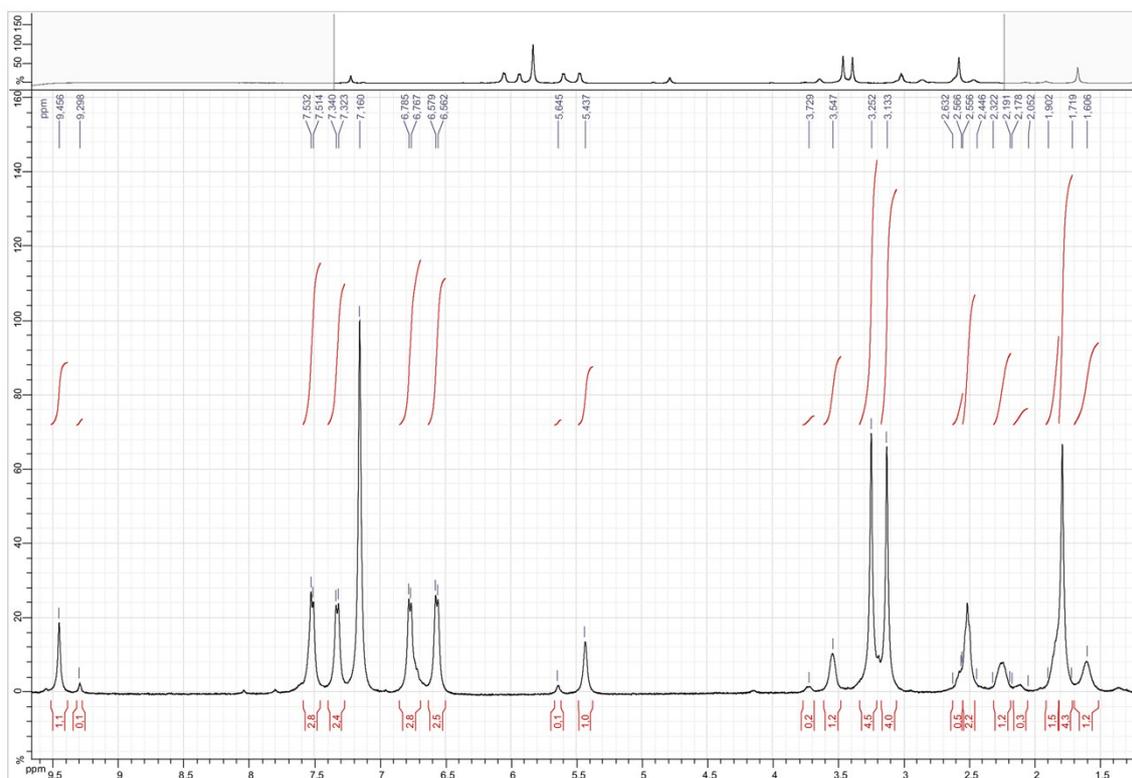


NOESY NMR spectrum in C_6D_6 after 2 days at 40 °C (deep cut)

e. NMR spectra of **5g**

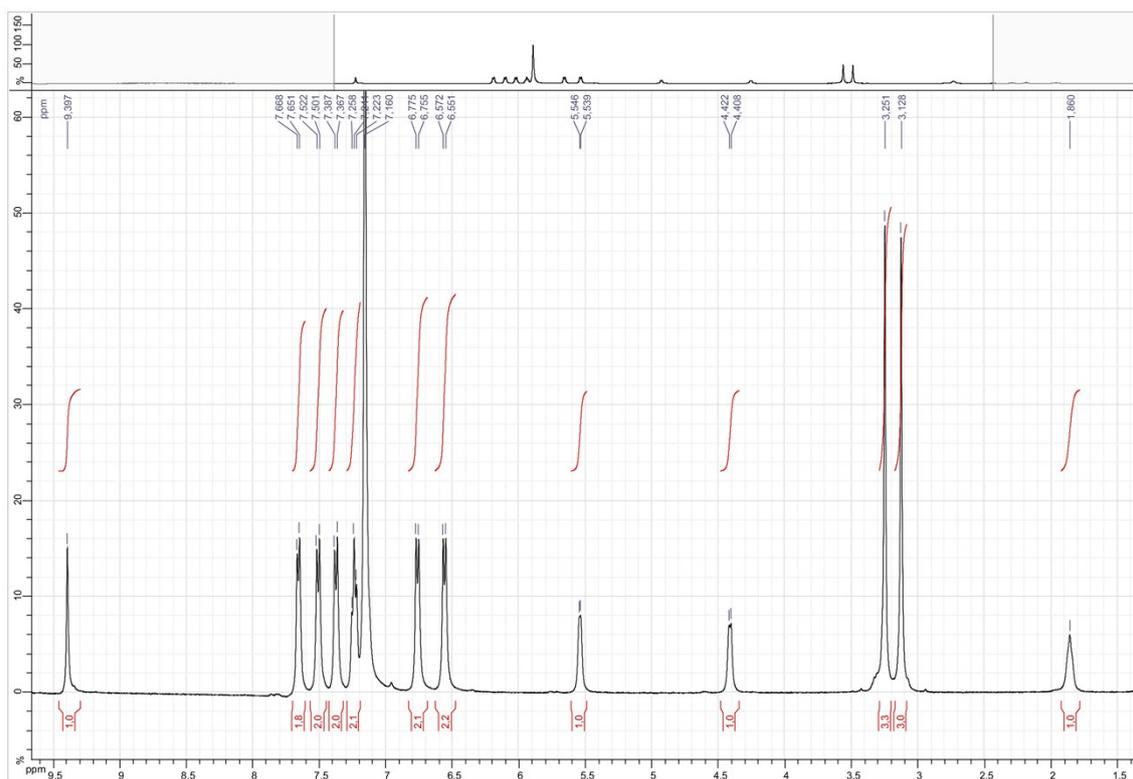


¹H NMR spectrum in C₆D₆ (400 MHz) immediately

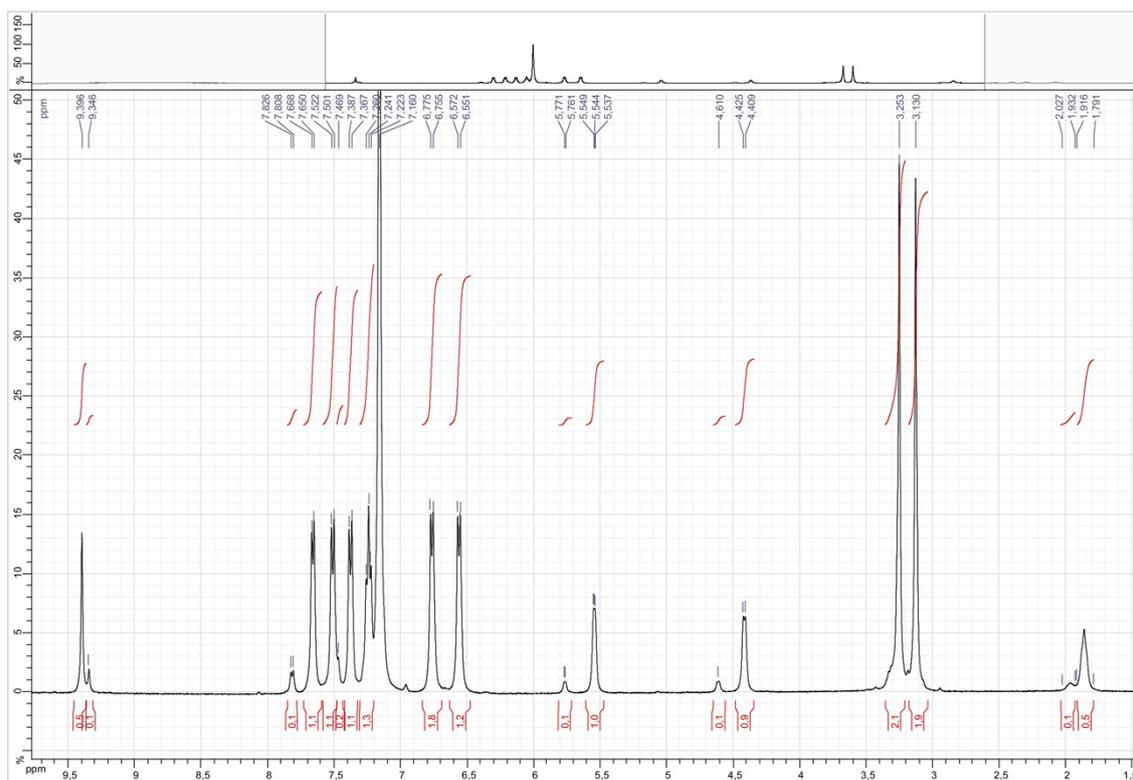


¹H NMR spectrum in C₆D₆ (400 MHz) after 60 h

f. NMR spectra of **5h**

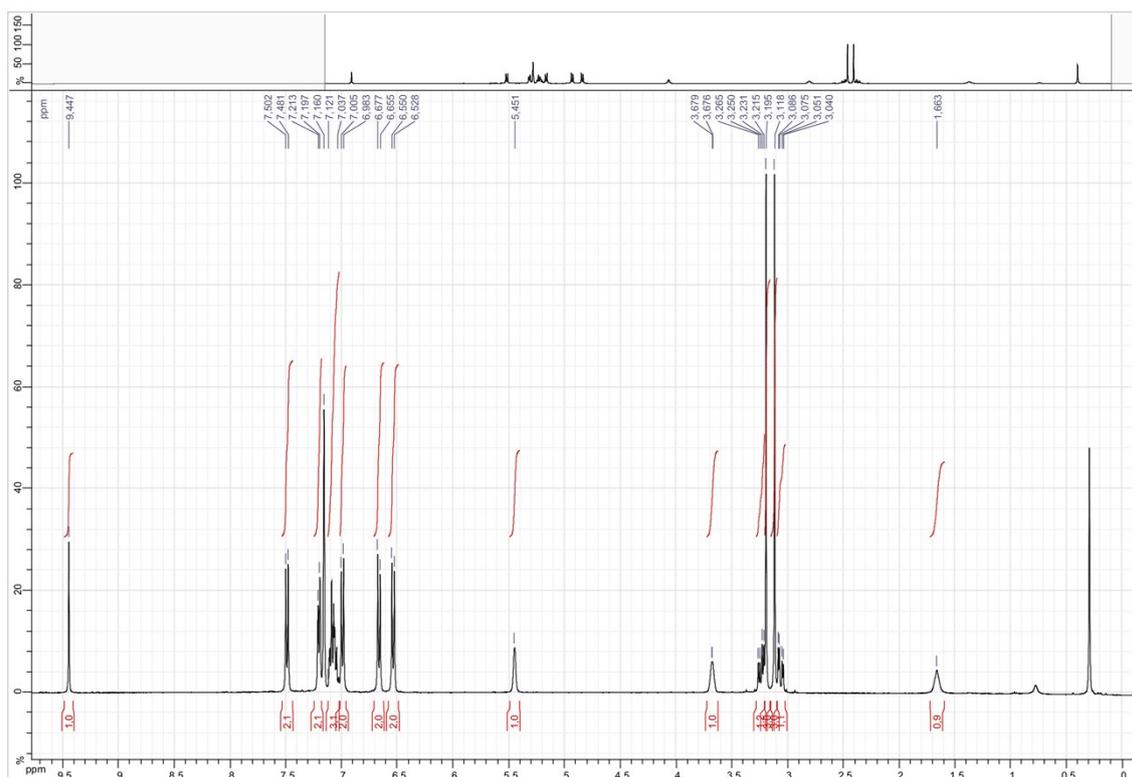


¹H NMR spectrum in C₆D₆ (400 MHz) immediately

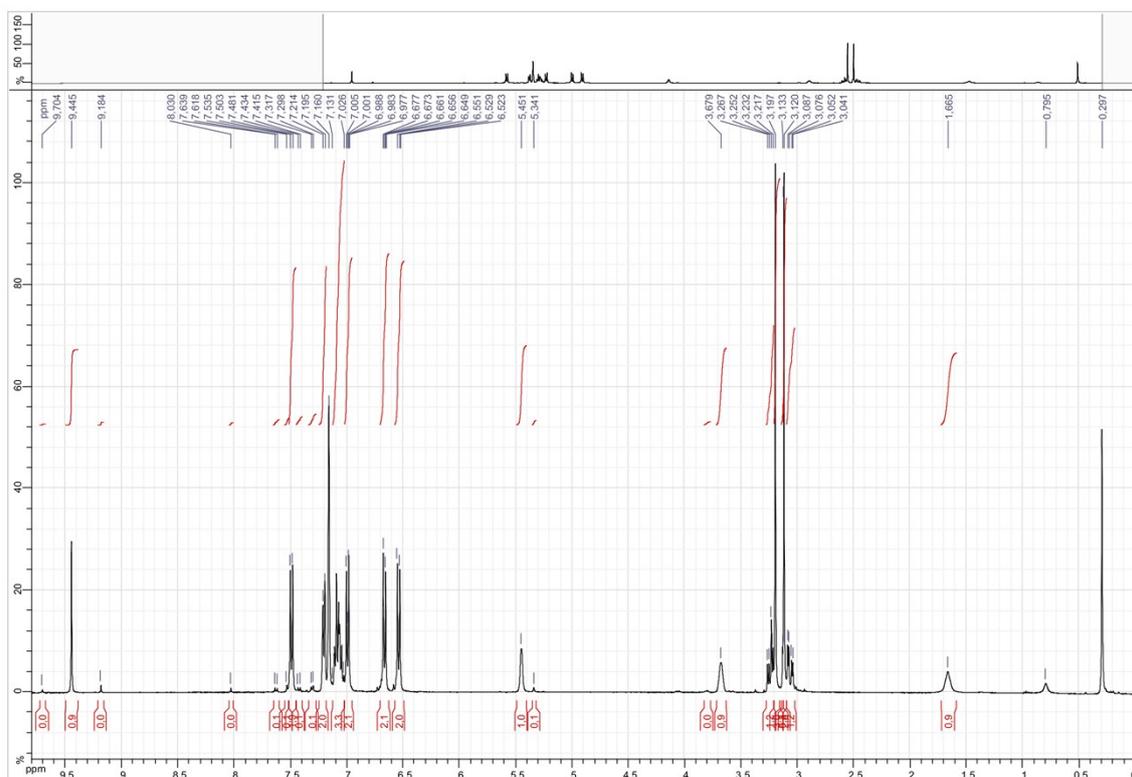


¹H NMR spectrum in C₆D₆ (400 MHz) after 60 h

g. NMR spectra of **5j**

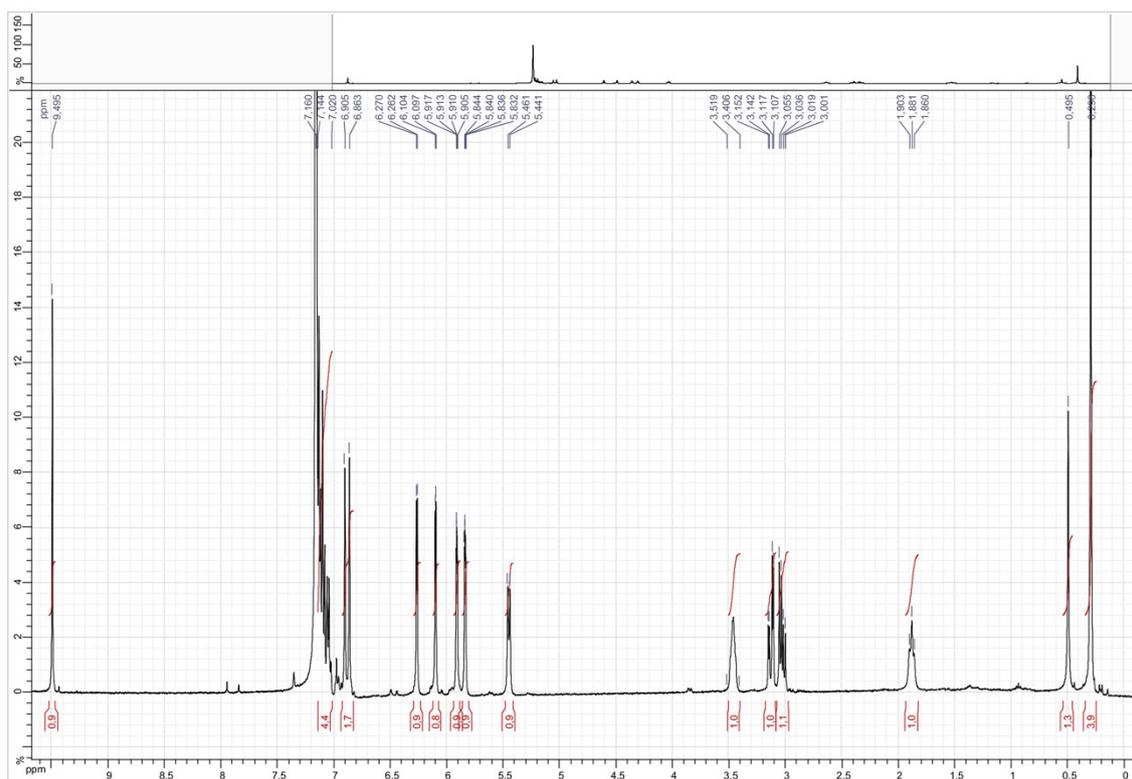


¹H NMR spectrum in C₆D₆ (400 MHz) immediately

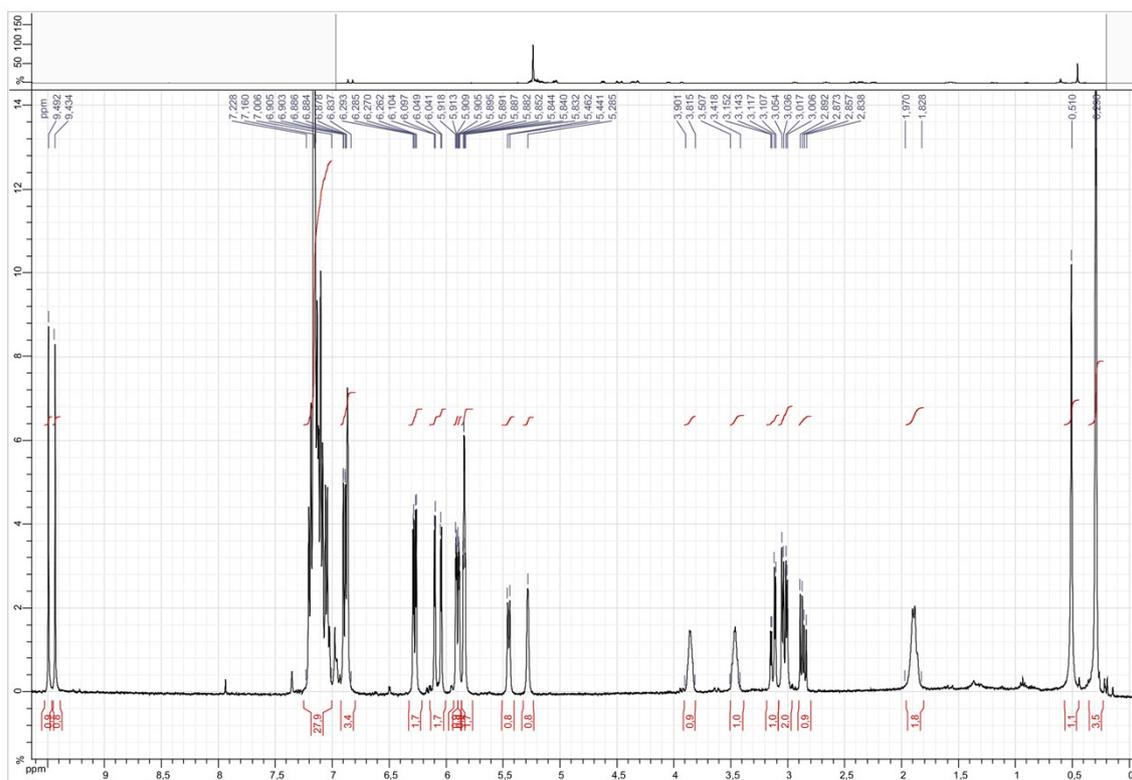


¹H NMR spectrum in C₆D₆ (400 MHz) after 18 h

h. NMR spectra of **51**

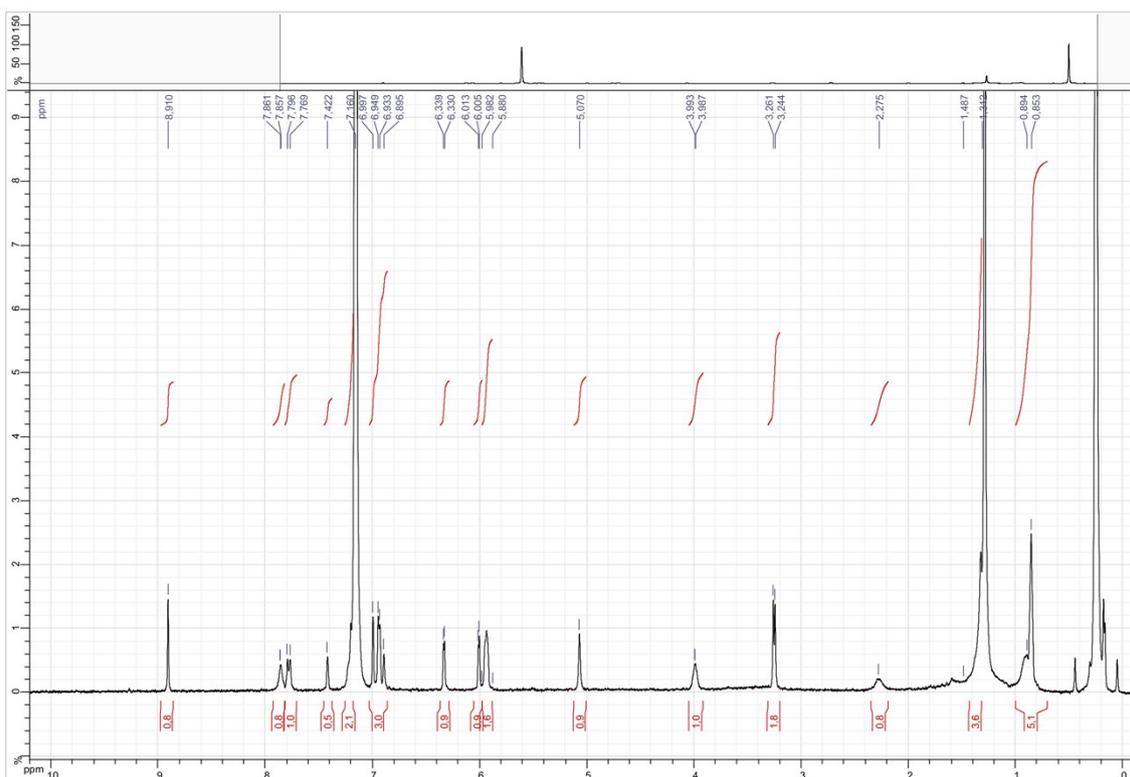


¹H NMR spectrum in C₆D₆ (400 MHz) immediately

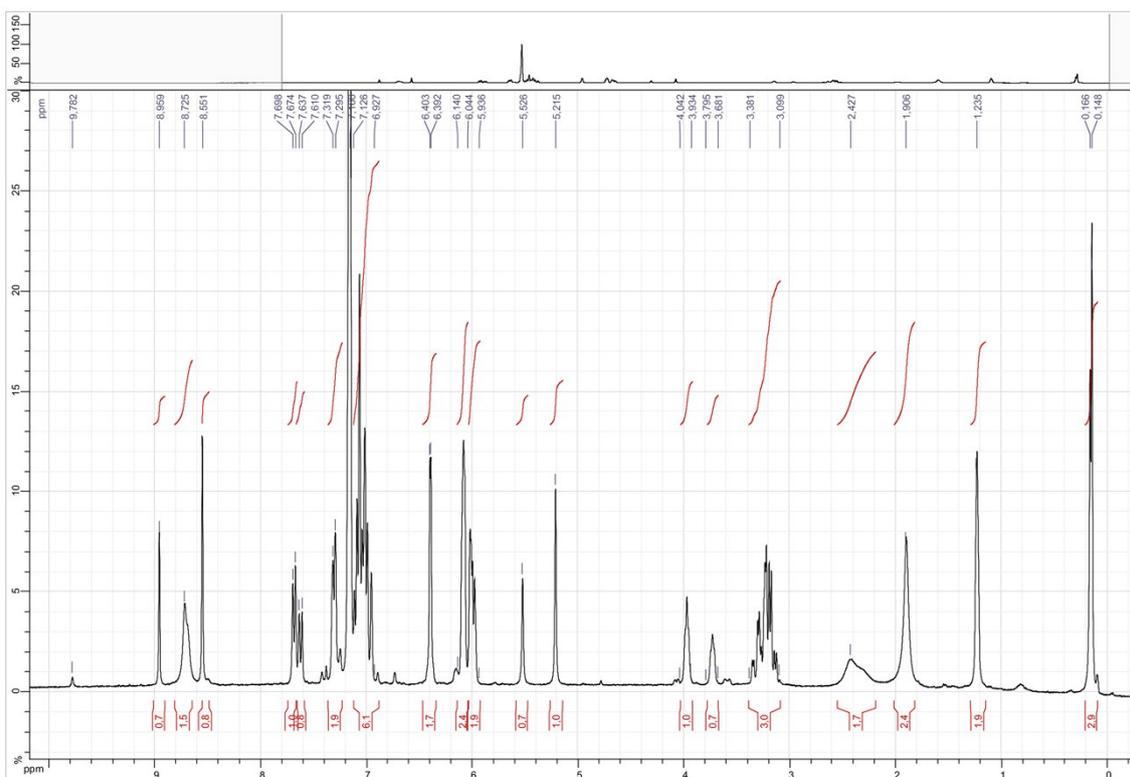


¹H NMR spectrum in C₆D₆ (400 MHz) after 6 h

i. NMR spectra of **5m**



¹H NMR spectrum in C₆D₆ + 3 drops of CD₃CN (300 MHz) immediately



¹H NMR spectrum in C₆D₆ + 3 drops of CD₃CN (300 MHz) after 18 h