

Supporting Information

Piperidine Alkaloids with Diverse Skeletons from

Anacyclus pyrethrum

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1. Inhibition Rates of 1–13 on the Menin–MLL1 Protein–Protein Interaction

Table S1. Percent Inhibition Rates of **1–13** on the Menin–MLL1 Protein–Protein Interaction^a

sample (20 μ M)	inhibition rate (%)	sample (20 μ M)	inhibition rate (%)
(+)- 1	21.78 $\pm$ 7.63	(-)- 5	27.06 $\pm$ 2.76
(-)- 1	19.66 $\pm$ 13.71	6	32.81 $\pm$ 10.17
(+)- 2	40.26 $\pm$ 24.02	7	27.89 $\pm$ 7.20
(-)- 2	11.45 $\pm$ 3.41	8	19.30 $\pm$ 1.70
(+)- 3	26.08 $\pm$ 3.33	9	23.33 $\pm$ 11.16
(-)- 3	29.93 $\pm$ 1.95	10	37.08 $\pm$ 0.83
(+)- 4	34.75 $\pm$ 12.66	11	30.29 $\pm$ 10.59
(-)- 4	41.86 $\pm$ 10.87	12	8.54 $\pm$ 6.62
(+)- 5	40.89 $\pm$ 8.36	13	34.09 $\pm$ 0.91

^a**MI-2-2** as the positive control with an IC₅₀ value of 0.19 $\pm$ 0.03 μ M

2. Chiral HPLC separations of the racemates 1–5

Racemic alkaloids **1–5** were separated by chiral HPLC columns of DAICEL CORPORATION Chiralpak IC, ID, IE and IF (5 μ m, 10 $\times$ 250 mm i.d.). The separation conditions and results were presented in table S1, and the separation chromatograms were also showed in figures S1 to S5.

Table S2. Chromatographic conditions and results of chiral HPLC separations

Racemates	$[\alpha]_D^{25}$ (c, MeOH)	Chiral column	Solvent <i>n</i> -hexane/EtOH	Flow rate (mL/min)	Enantiomers	Retention time (min)	Peak area ratio (A/A)
1	+1.2 (0.08)	ID	92:8	1.0	(+)- 1	16.3	(+) - 1 / (−) - 1 = 0.93
					(−)- 1	10.3	
2	−4.00 (0.10)	ID	94.5:5.5	1.0	(+)- 2	15.2	(+) - 2 / (−) - 2 = 0.96
					(−)- 2	11.5	
3	+2.2 (0.10)	IF	94:6	1.0	(+)- 3	17.3	(+) - 3 / (−) - 3 = 1.01
					(−)- 3	20.2	
4	+1.5 (0.20)	ID	92:8	1.0	(+)- 4	15.9	(+) - 4 / (−) - 4 = 1.03
					(−)- 4	19.5	
5	+0.05 (2.00)	ID	94.5:5.5	1.0	(−)- 5	11.5	(−) - 5 / (+) - 5 = 1.04
					(+)- 5	15.2	

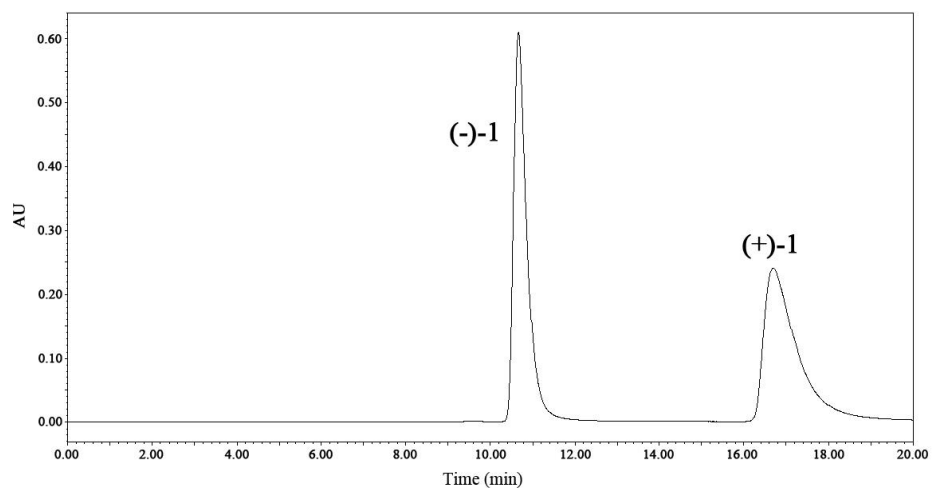


Figure S1. Chromatogram of chiral HPLC separation of compound **1**.

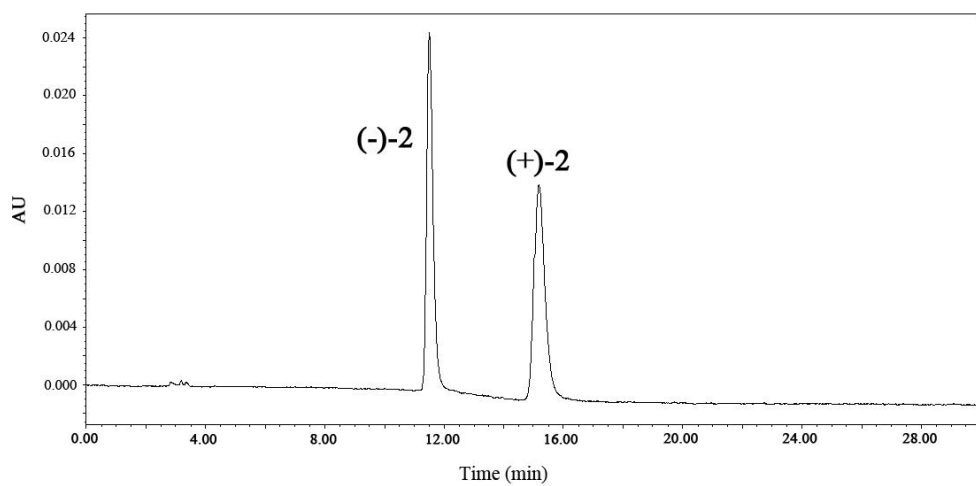


Figure S2. Chromatogram of chiral HPLC separation of compound **2**.

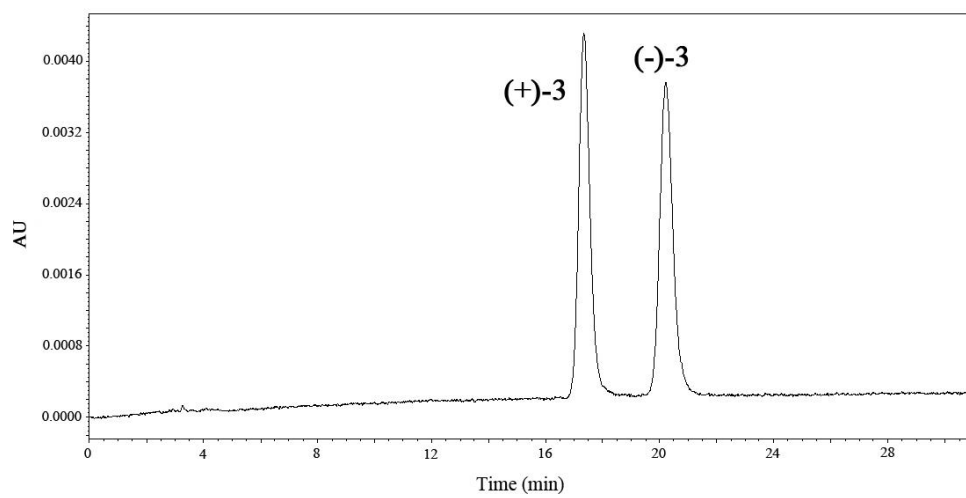


Figure S3. Chromatogram of chiral HPLC separation of compound **3**.

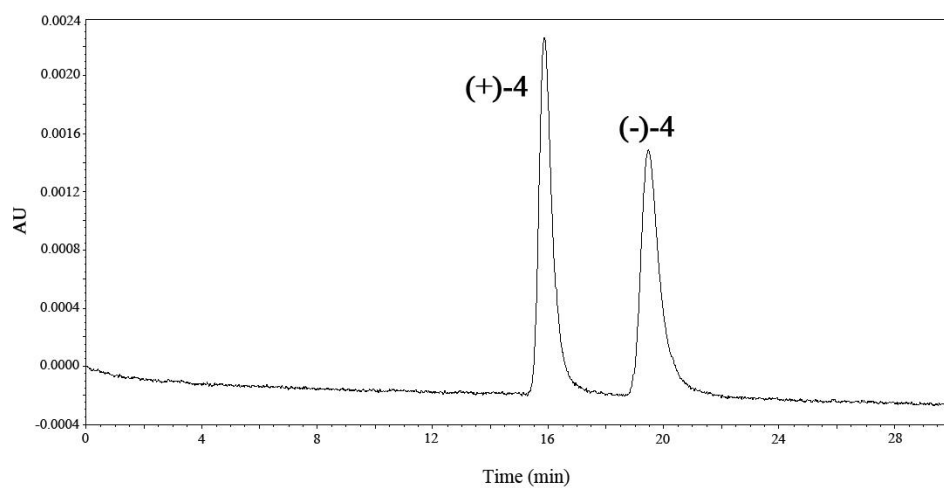


Figure S4. Chromatogram of chiral HPLC separation of compound 4.

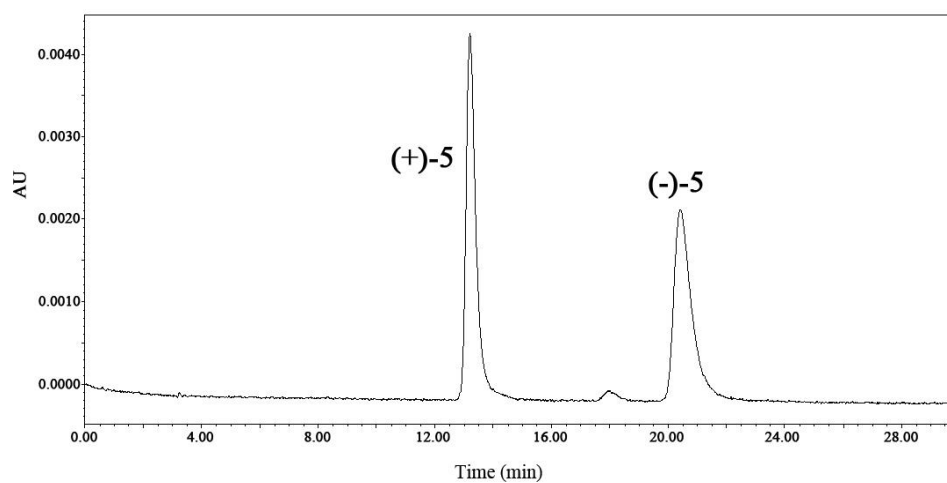


Figure S5. Chromatogram of chiral HPLC separation of compound 5.

3. Theoretical ECD calculations of the enantiomers (+)-1/(–)-1 to (+)-5/(–)-5

3.1 Geometrical optimization

The geometrical optimization of **1a** [(3a*S*,3b*S*)-**1**]/**1b** [(3a*R*,3b*R*)-**1**]/**1c** [(3a*S*,3b*R*)-**1**], **2a** [(8a*R*)-**2**]/**2b** [(8a*S*)-**2**], **3a** [(3a*S*)-**3**]/**3b** [(3a*R*)-**3**], **4a** [(3a*R*,4*R*,5*S*)-**4**]/**4b** [(3a*S*,4*S*,5*R*)-**4**], **5a** [(6*S*,7*R*)-**5**]/**5b** [(6*R*,7*S*)-**5**] (Figure S6-S10) were carried out by TmoleX 4.3 software.

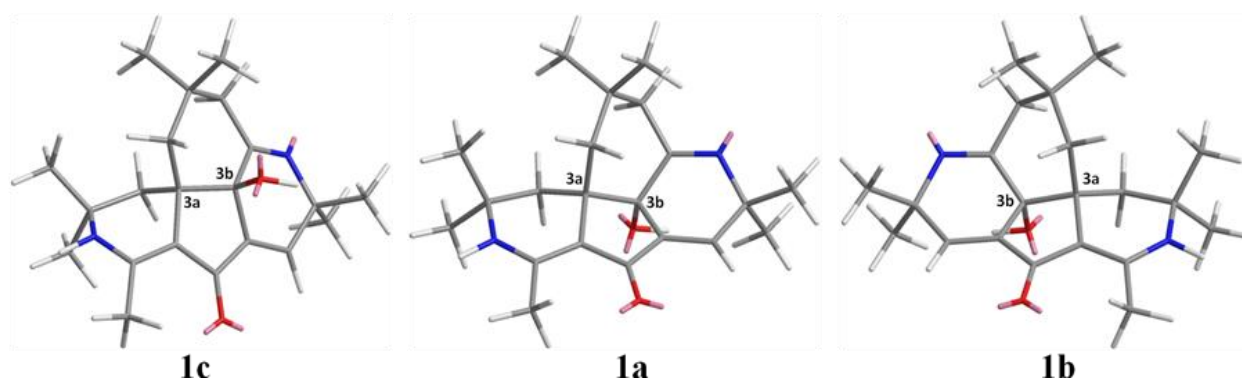


Figure S6. Geometrical optimized of **1a**, **1b** and **1c**.

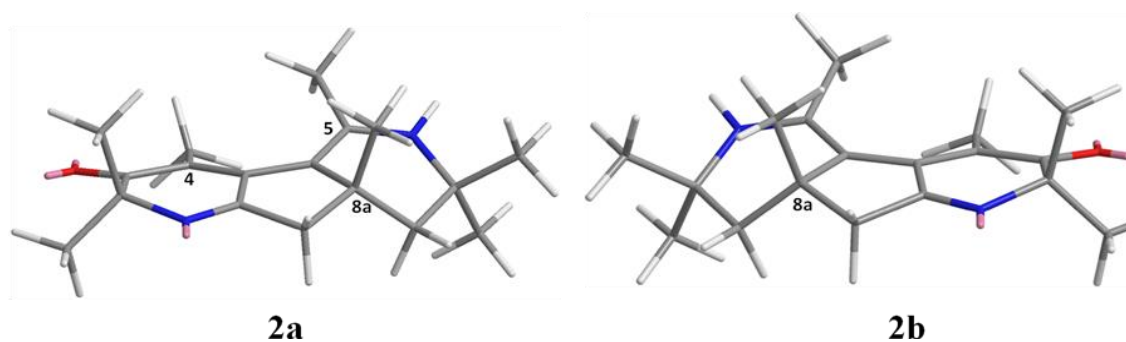


Figure S7. Geometrical optimized of **2a** and **2b**.

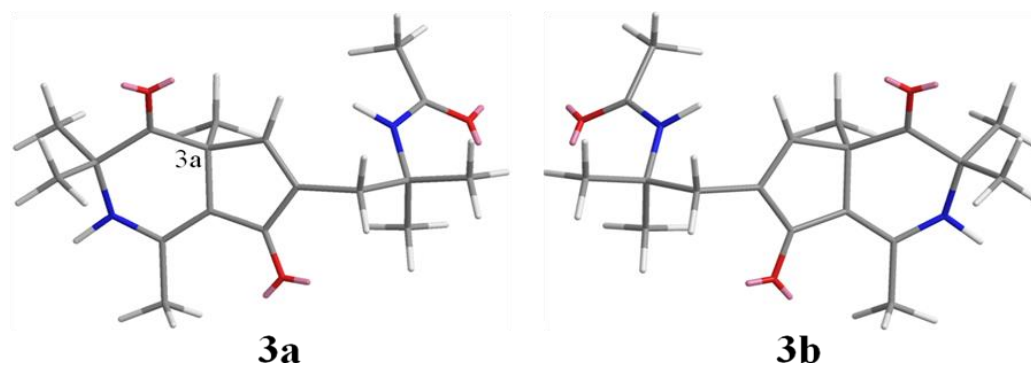


Figure S8. Geometrical optimized of **3a** and **3b**.

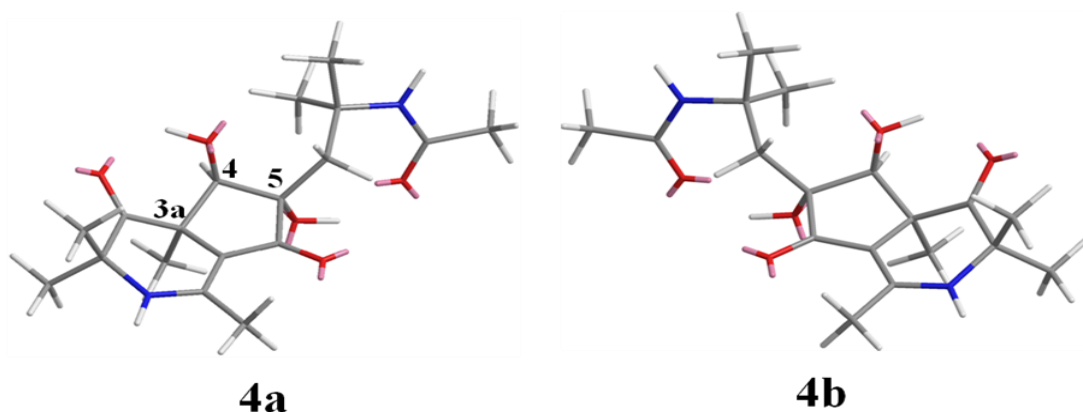


Figure S9. Geometrical optimized of **4a** and **4b**.



Figure S10. Geometrical optimized of **5a** and **5b**.

3.2 ECD calculation conditions

ECD calculation conditions of 1a, 1b and 1c: Atomic Attributes (Basis function set for all atoms: def-TZVP); Method (Level: DFT; Functional: b3-lyp; Gridsize: m3); COSMO setting of Solvation (Epsilon: infinity; Refractive index: 1.3); Excited states: Singlet; No. of excitations: 10; Graphics (Std. deviation: 15; Frequency shift: -10; Broadened by: Gaussian).

ECD calculation conditions of 2a and 2b: Atomic Attributes (Basis function set for all atoms: def-TZVP); Method (Level: DFT; Functional: pbe0; Gridsize: m3); COSMO setting of Solvation (Epsilon: infinity; Refractive index: 1.3); Excited states: Singlet; No. of excitations: 6; Graphics (Std. deviation: 17; Frequency shift: -5; Broadened by: Gaussian).

ECD calculation conditions of 3a and 3b: Atomic Attributes (Basis function set for all atoms: def-TZVP); Method (Level: DFT; Functional: pbe0; Gridsize: m3); COSMO setting of

Solvation (Epsilon: infinity; Refractive index: 1.3); Excited states: Singlet; No. of excitations: 15; Graphics (Std. deviation: 15; Frequency shift: +15; Broadened by: Gaussian).

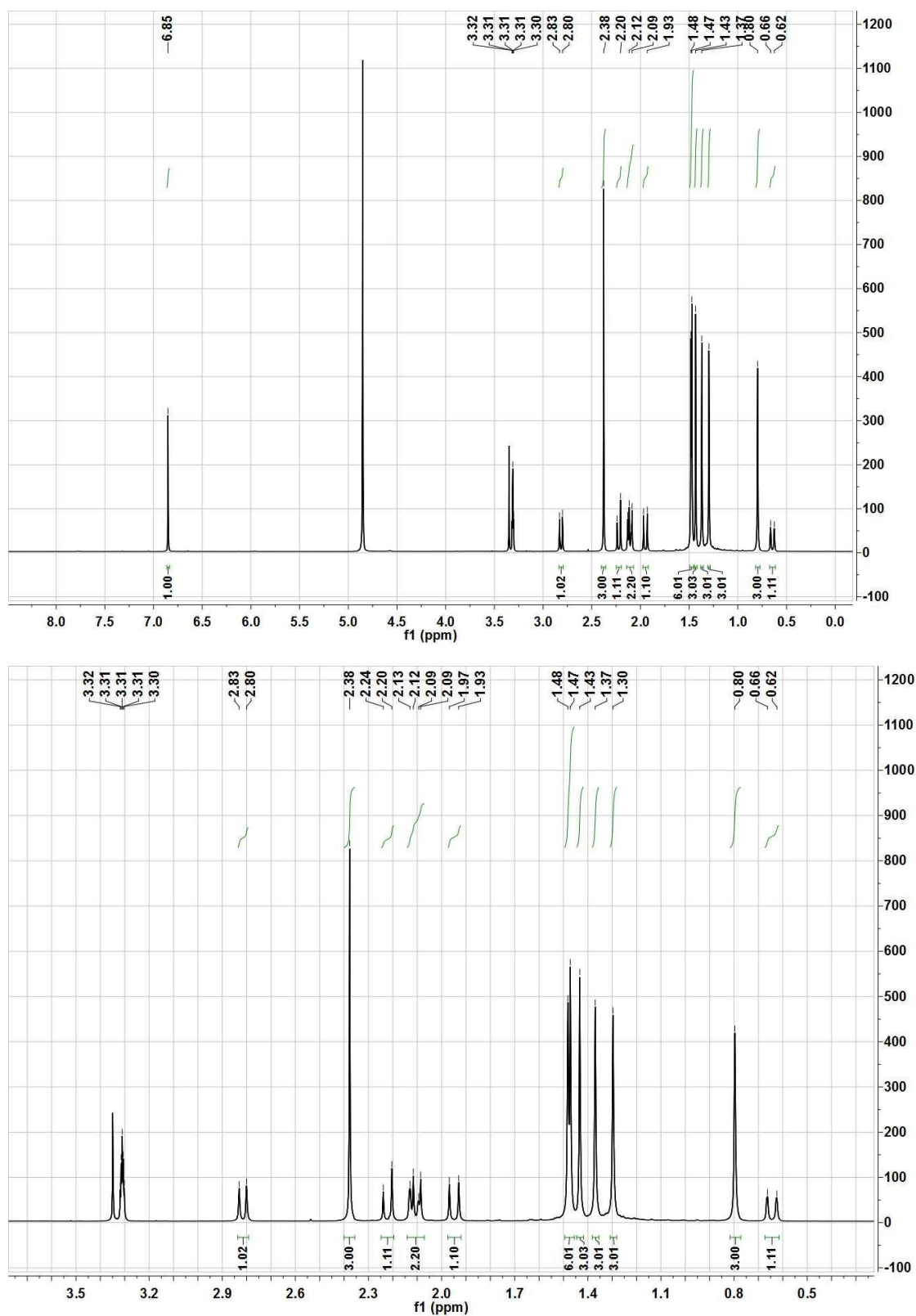
ECD calculation conditions of 4a and 4b: Atomic Attributes (Basis function set for all atoms: def-TZVP); Method (Level: DFT; Functional: pbe0; Gridsize: m3); COSMO setting of Solvation (Epsilon: infinity; Refractive index: 1.3); Excited states: Singlet; No. of excitations: 24; Graphics (Std. deviation: 15; Frequency shift: +10; Broadened by: Gaussian).

ECD calculation conditions of 5a and 5b: Atomic Attributes (Basis function set for all atoms: def-TZVP); Method (Level: DFT; Functional: b3-lyp; Gridsize: m3); COSMO setting of Solvation (Epsilon: infinity; Refractive index: 1.3); Excited states: Singlet; No. of excitations: 12; Graphics (Std. deviation: 16; Frequency shift: -25; Broadened by: Gaussian).

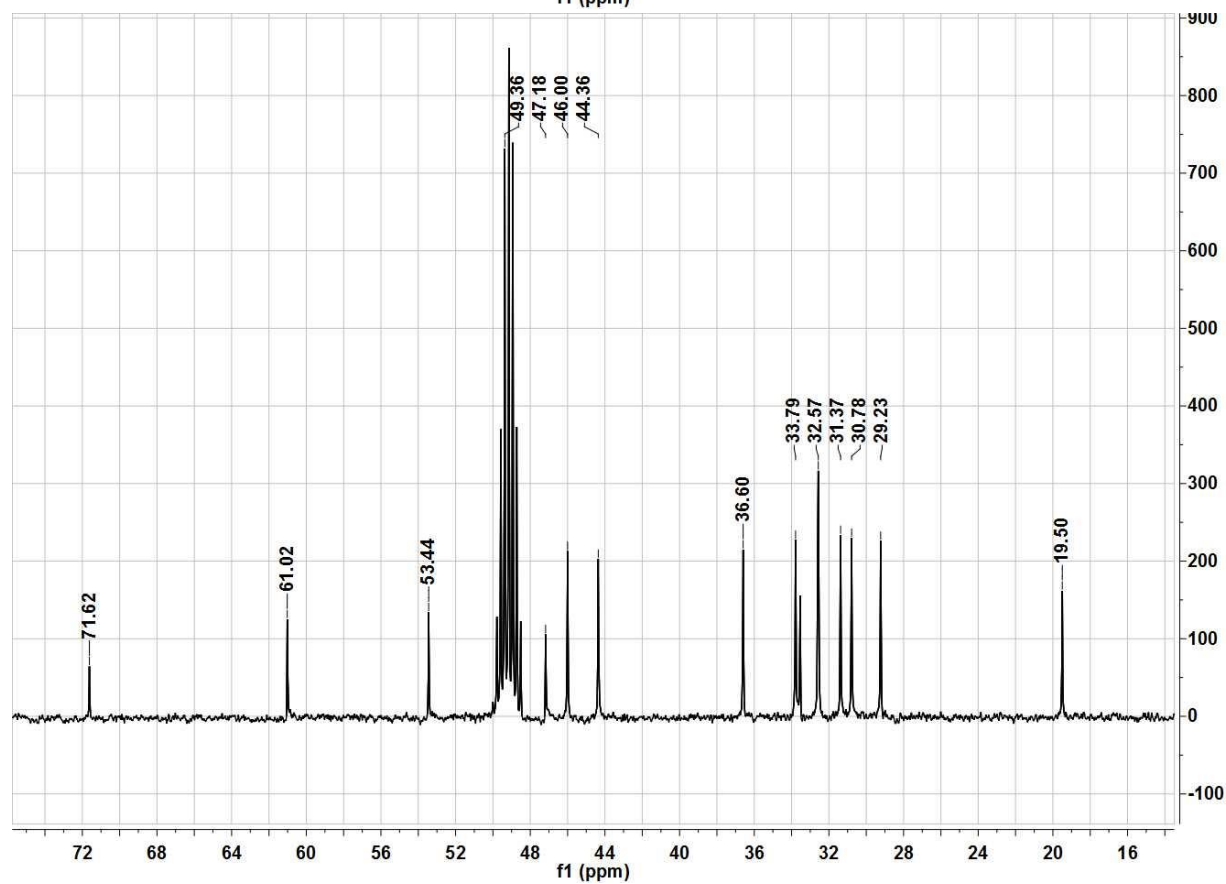
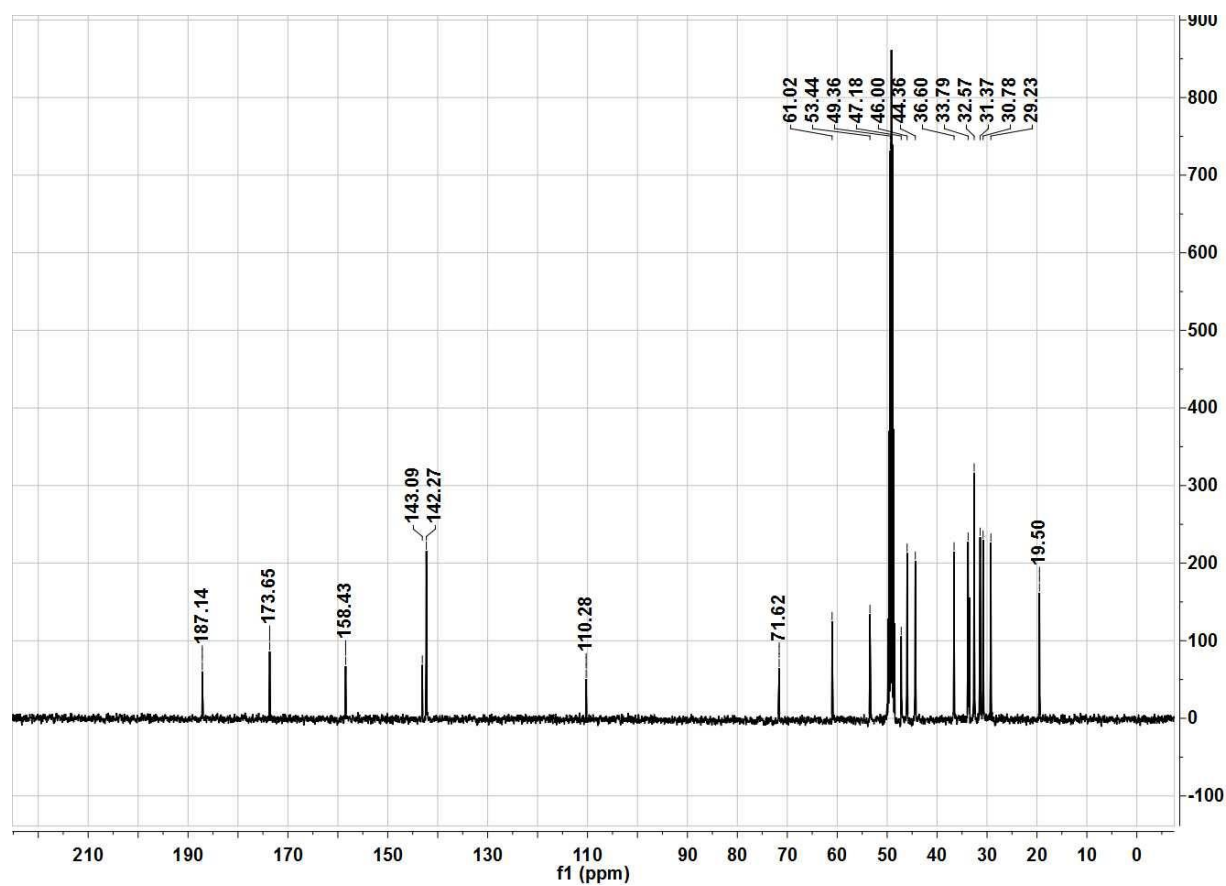
4. NMR, (+)HRESIMS and UV spectra

4.1 1D and 2D NMR of pyracyclumine A (1).

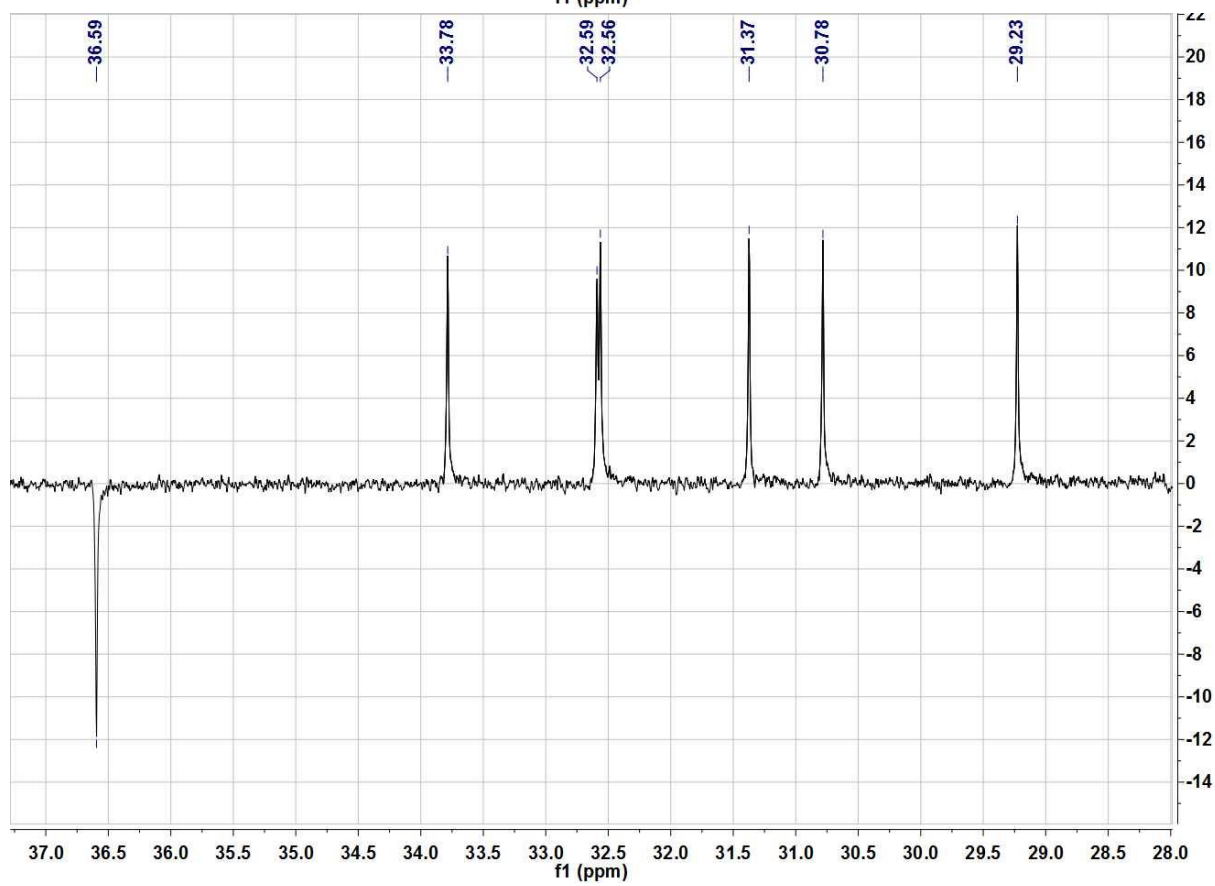
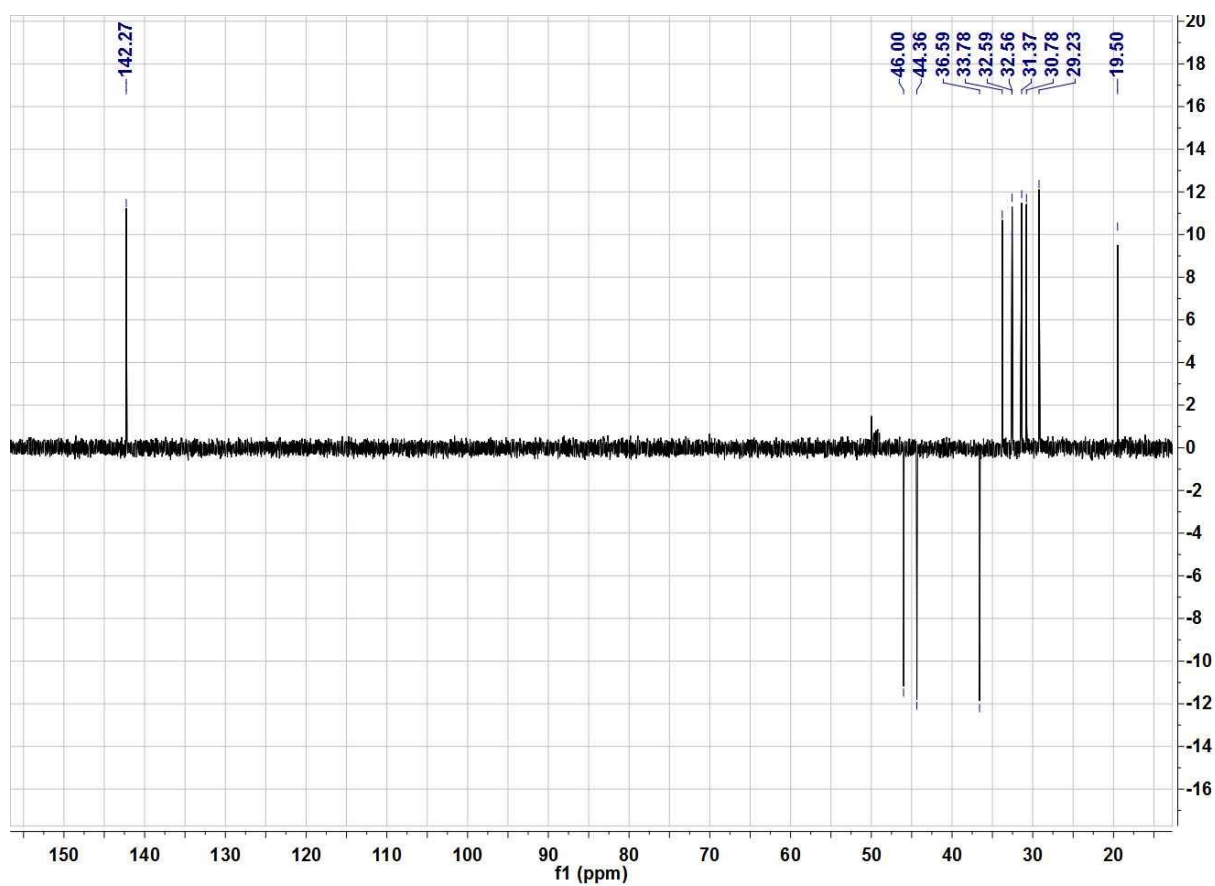
4.1.1 ^1H NMR (400 MHz, $\text{MeOH-}d_4$) spectra of **1**.



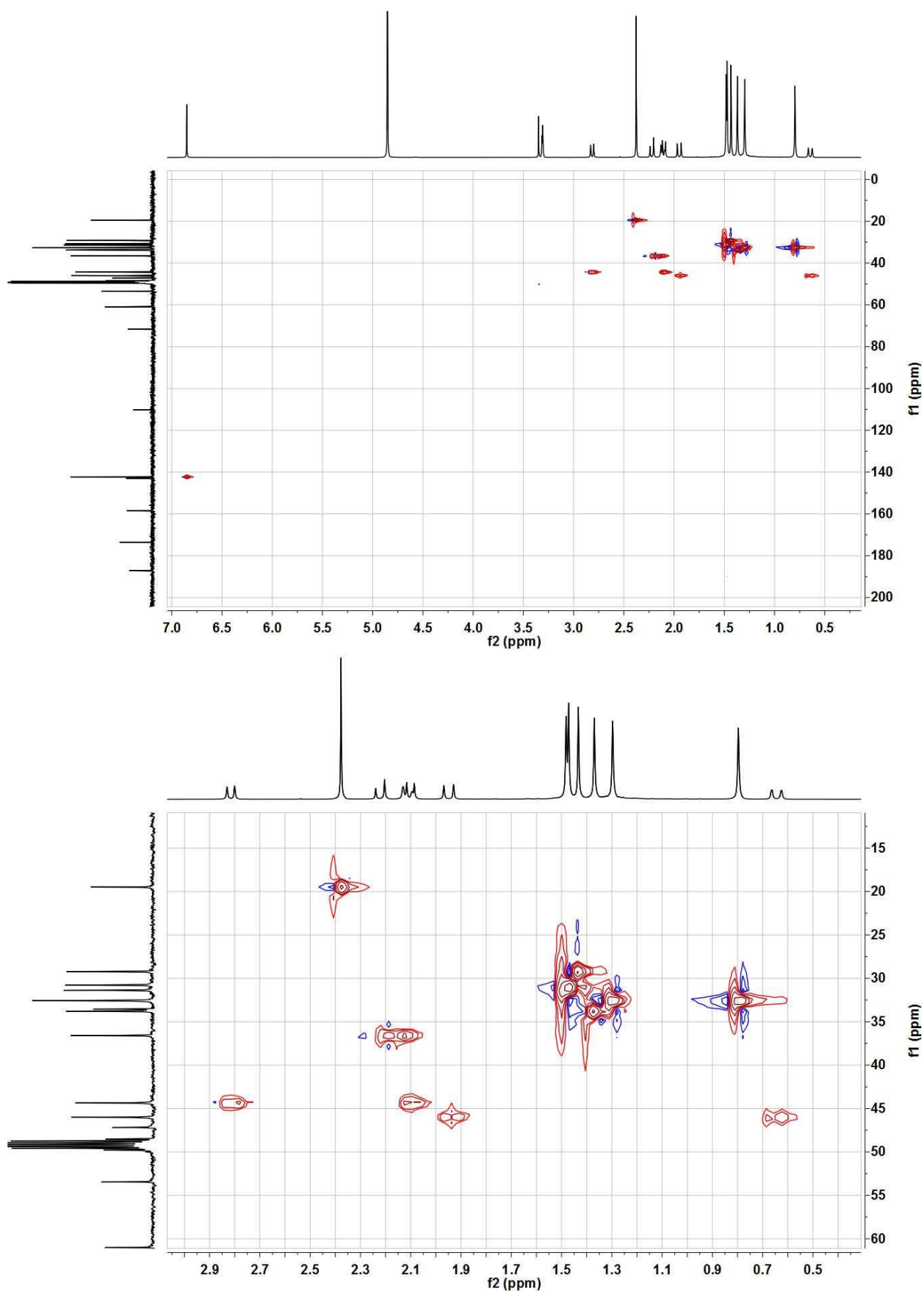
4.1.2 ^{13}C NMR (101 MHz, MeOH-d_4) spectra of **1**.



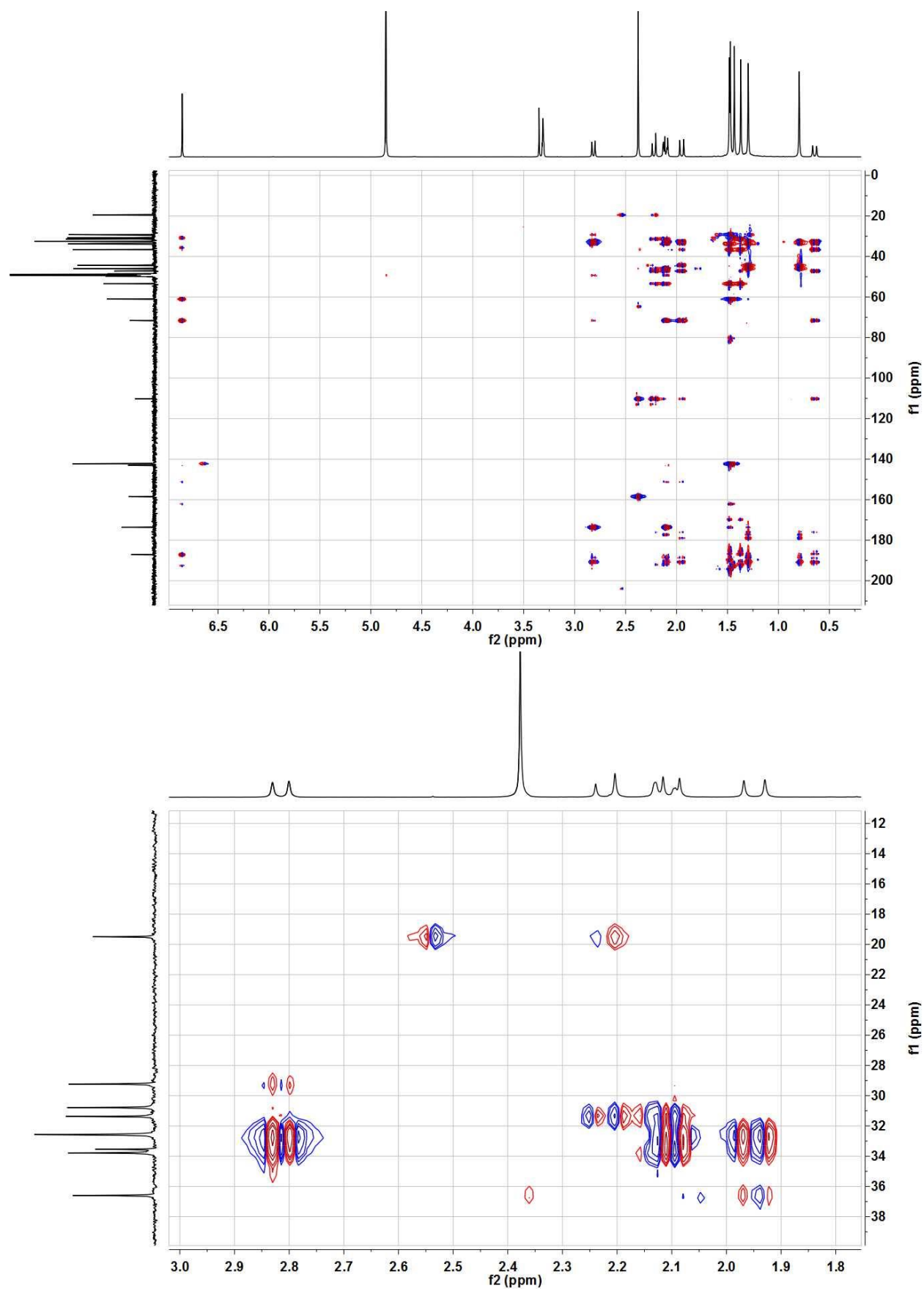
4.1.3 DEPT-135 spectra of **1**.

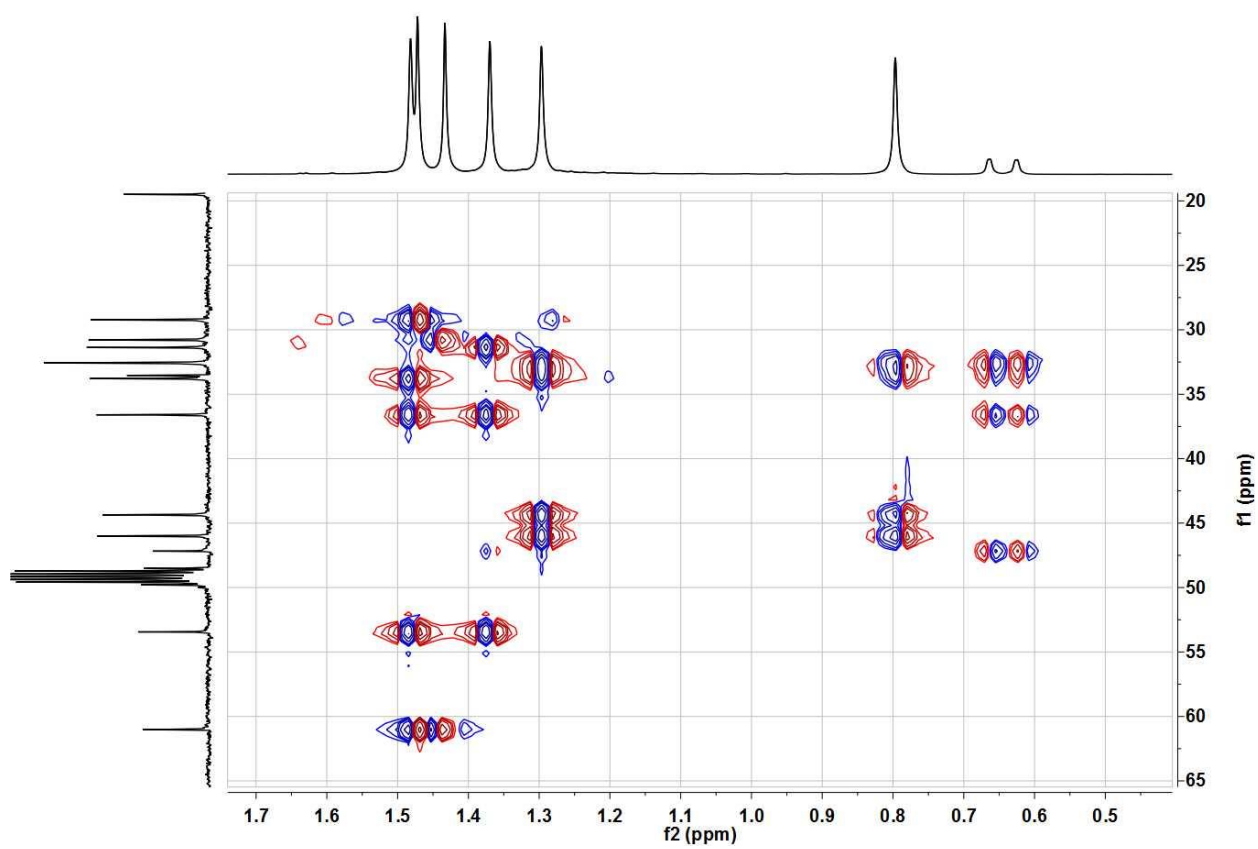
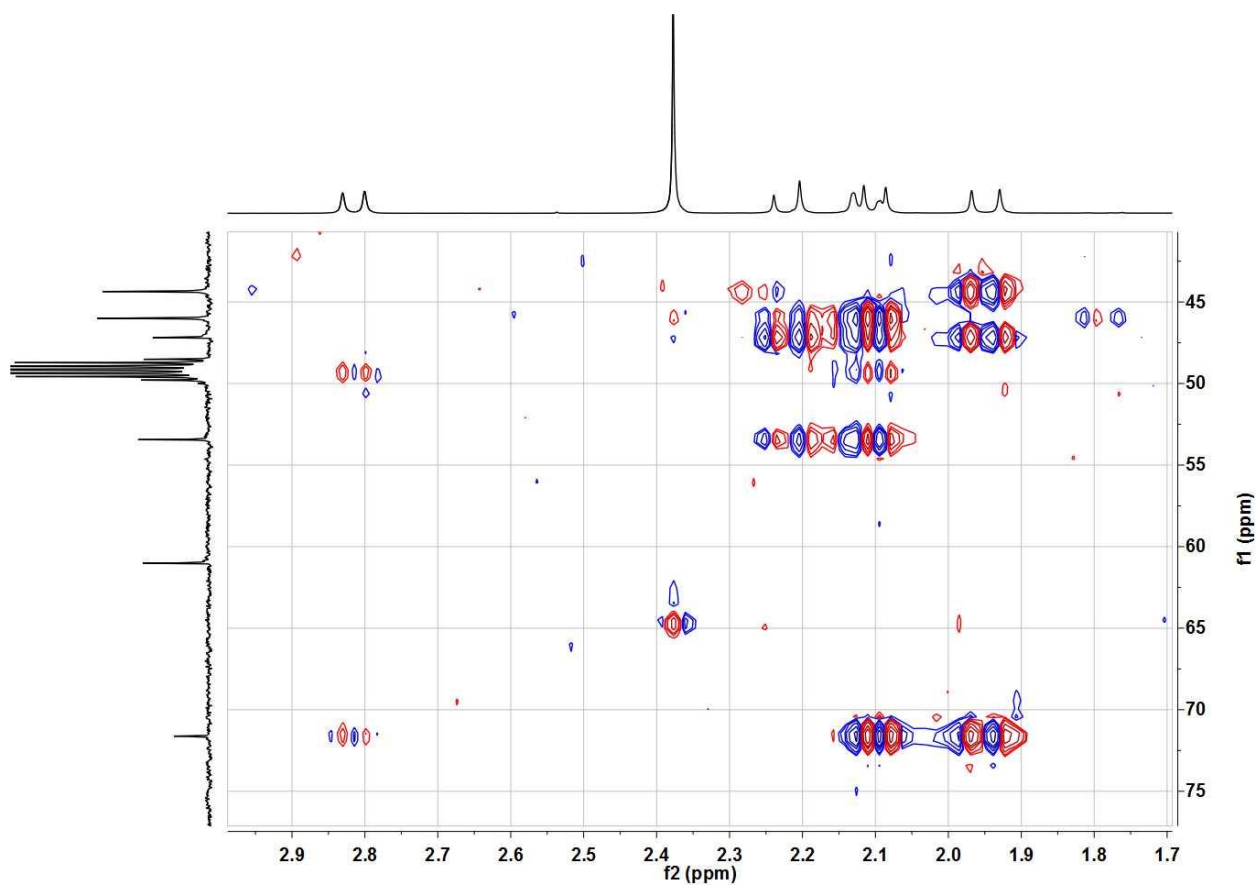


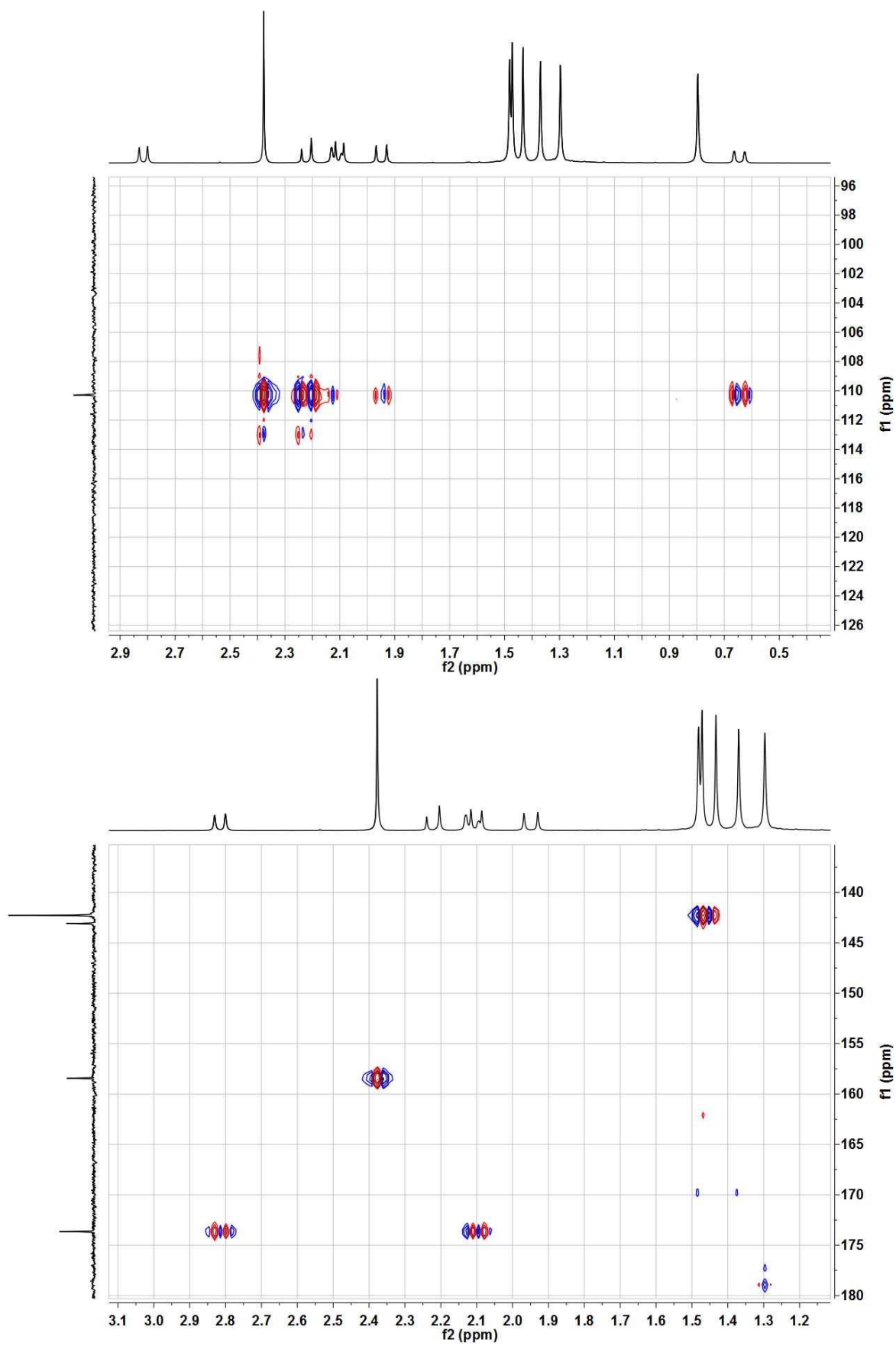
4.1.4 HSQC spectra of **1**.



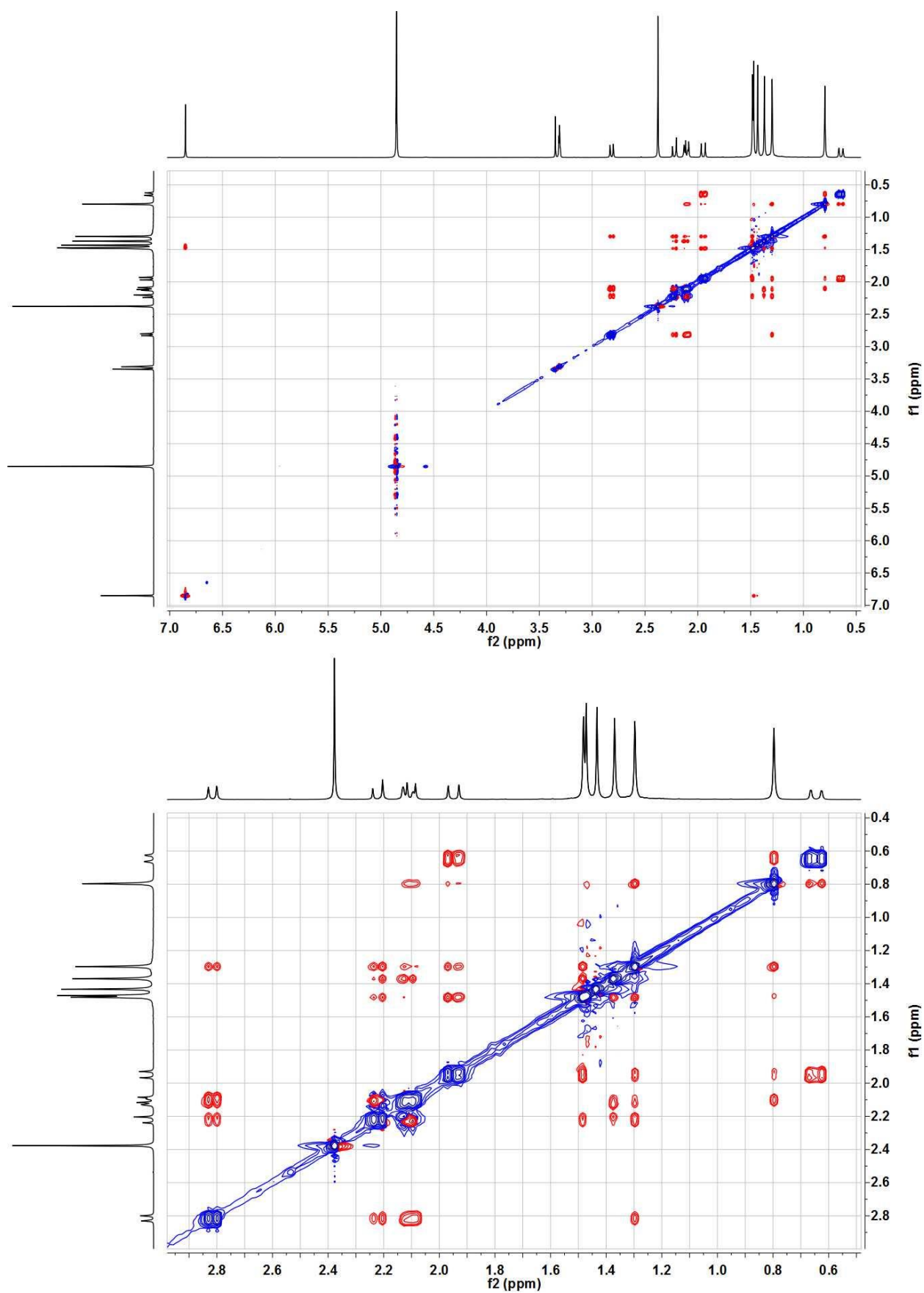
4.1.5 HMBC spectra of **1**.



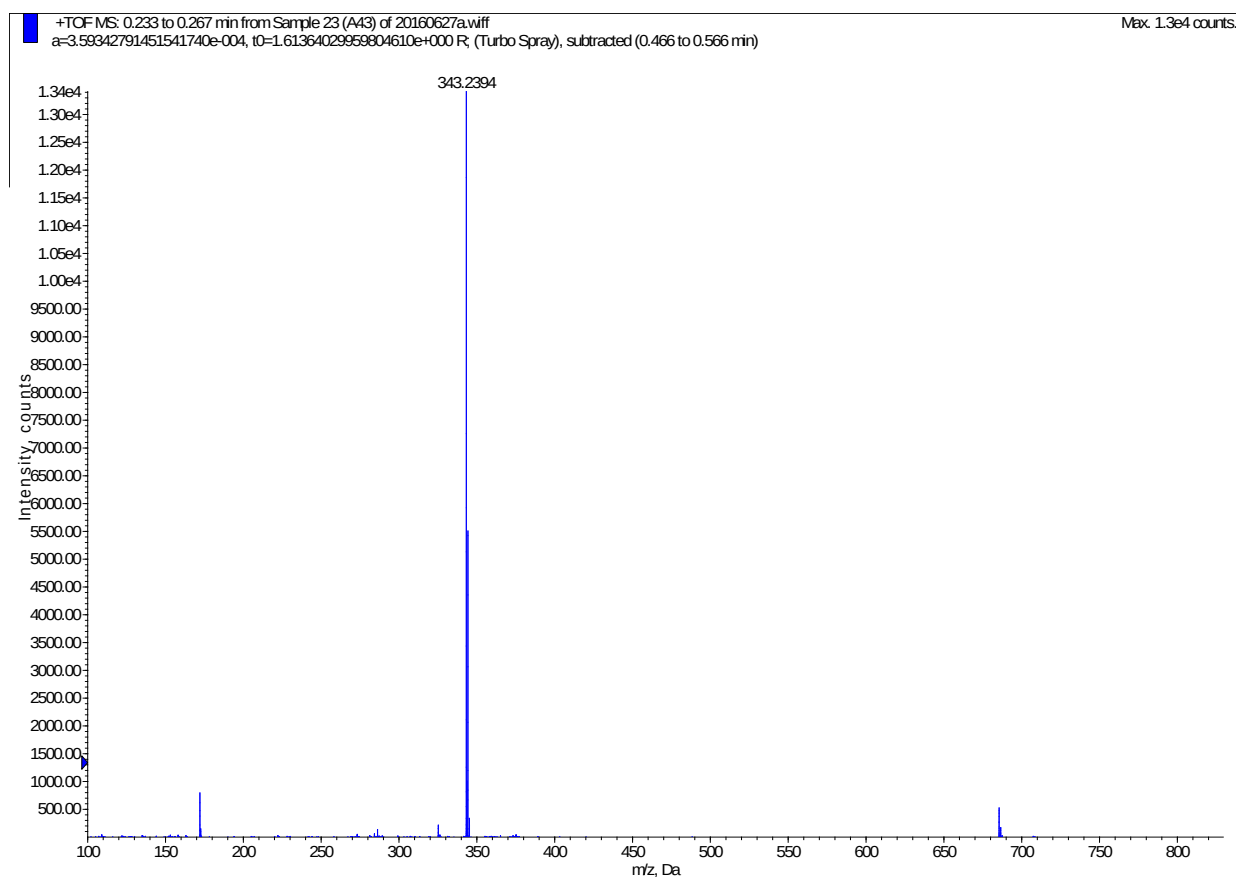




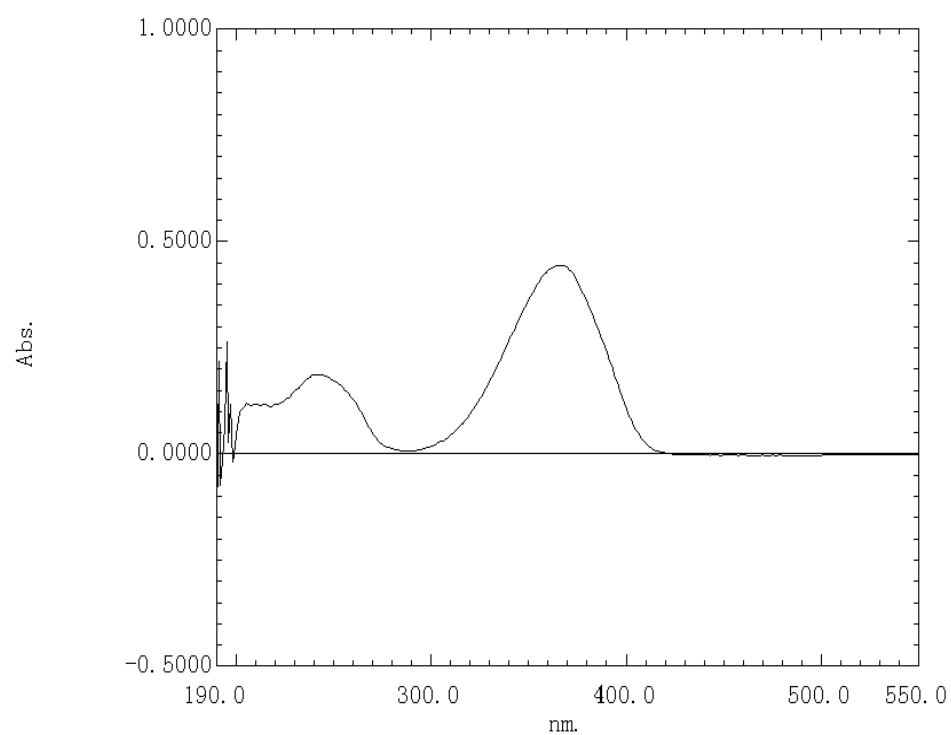
4.1.6 NOESY spectra of **1**.



4.1.7 (+)HRESIMS of **1**.

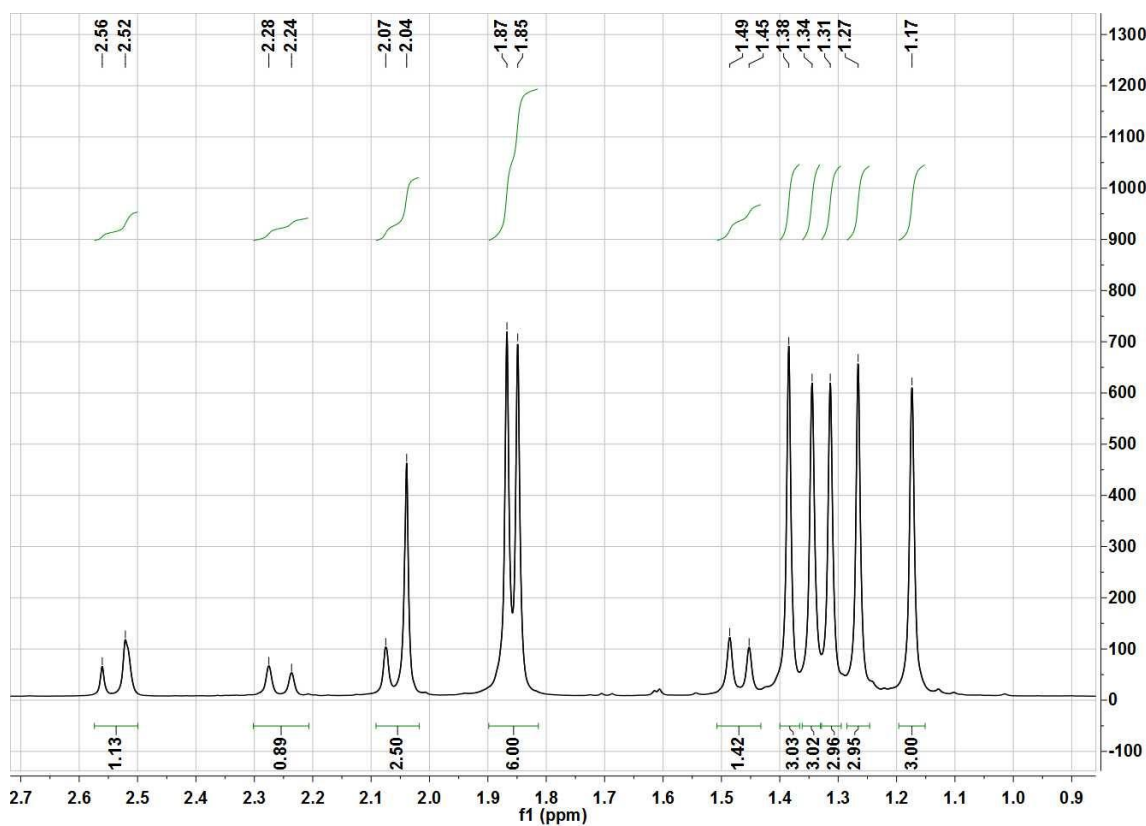
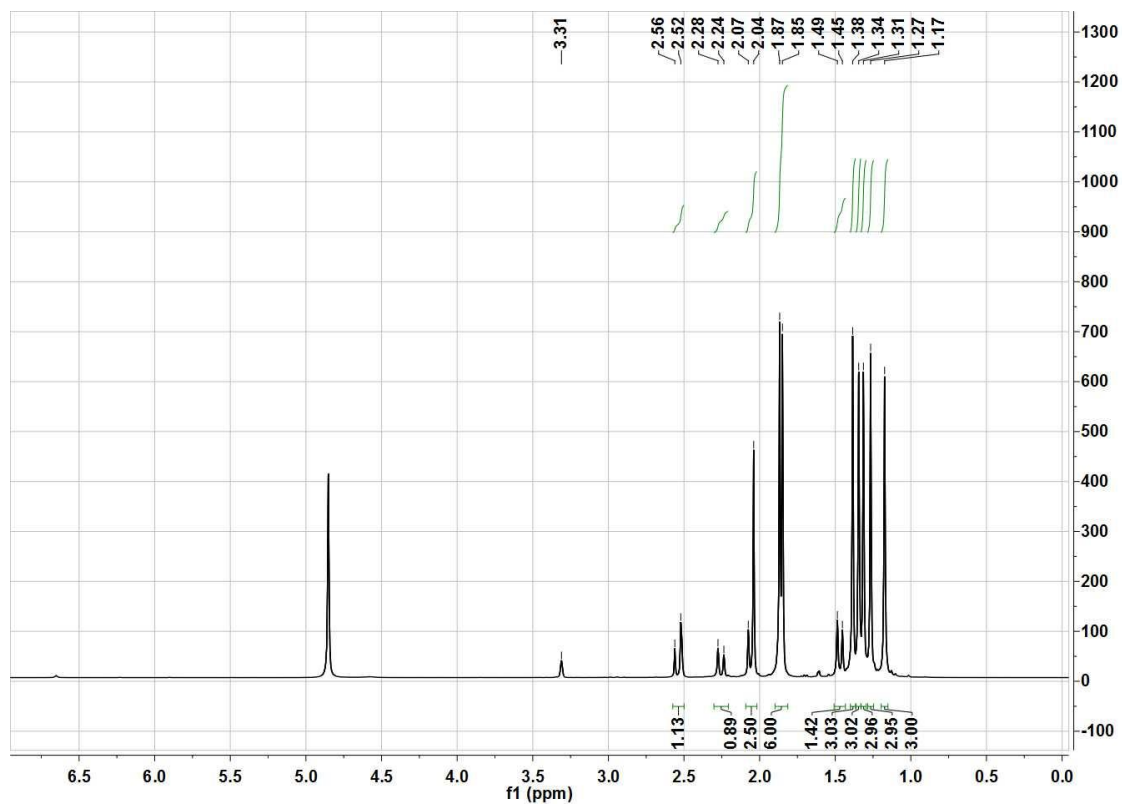


4.1.8 UV spectrum of **1**.

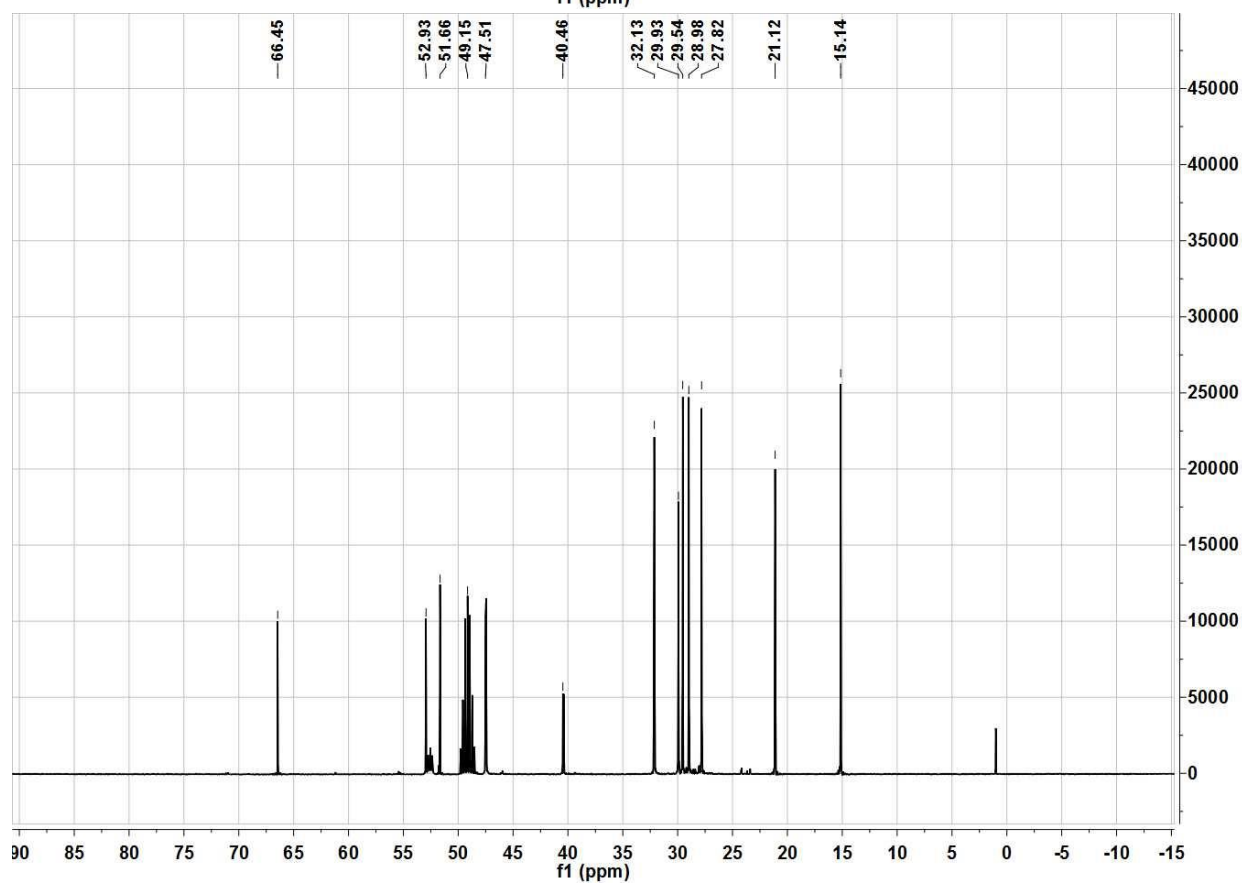
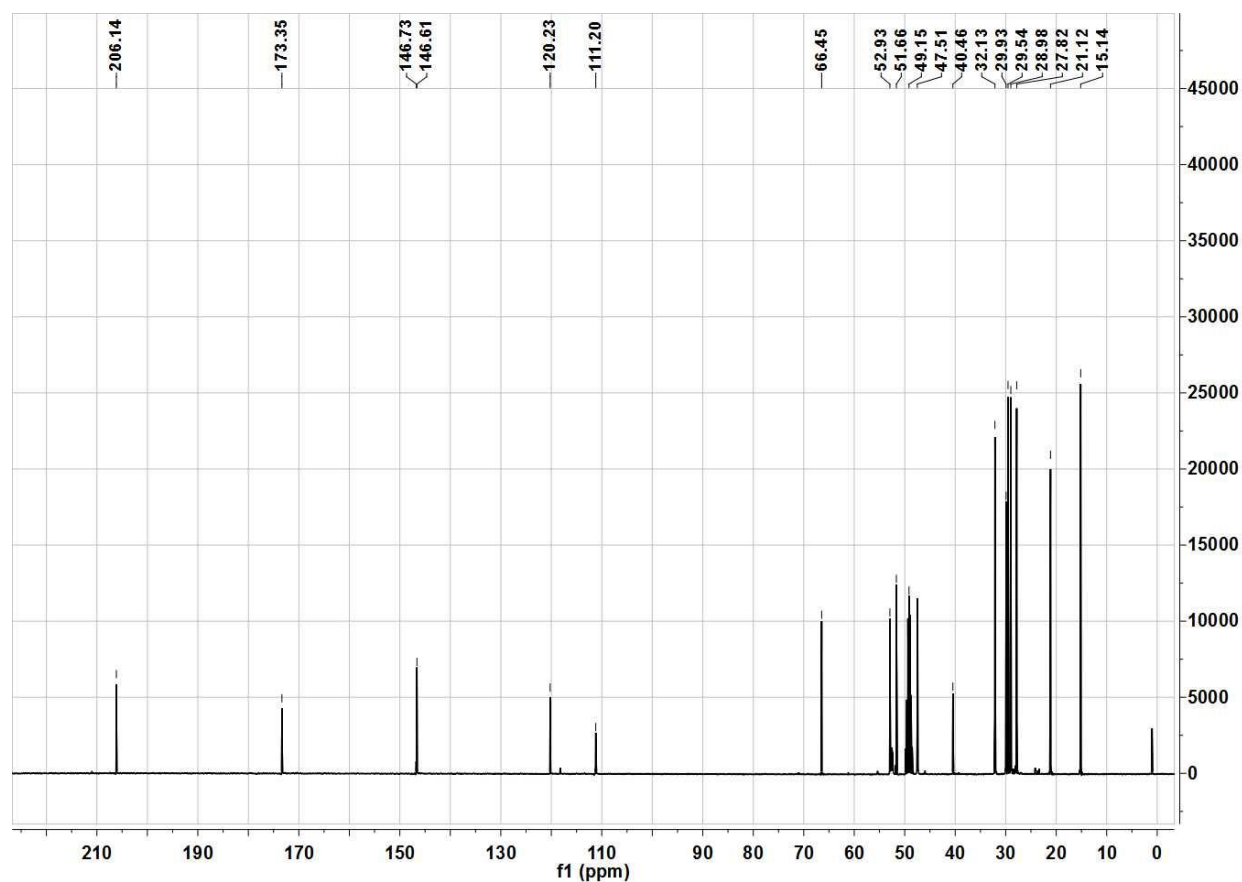


4.2 1D and 2D NMR of pyracyclumine B (2).

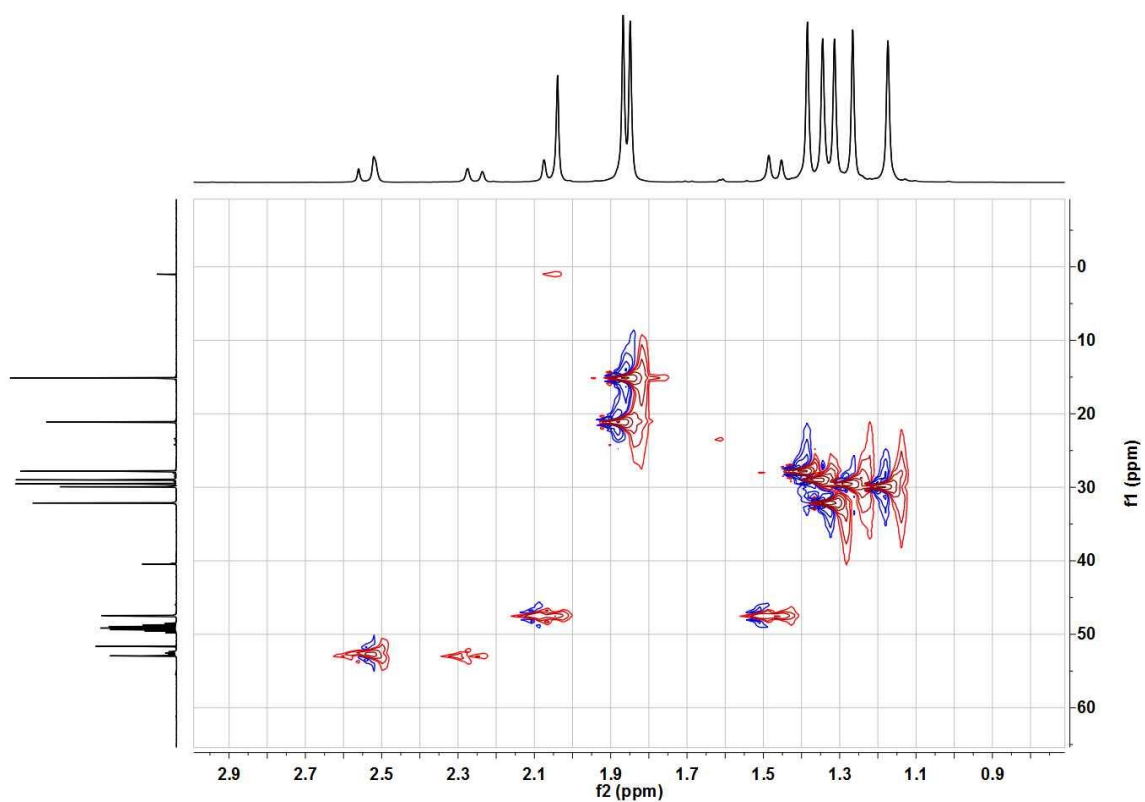
4.2.1 ^1H NMR (400 MHz, $\text{MeOH-}d_4$) spectra of 2.



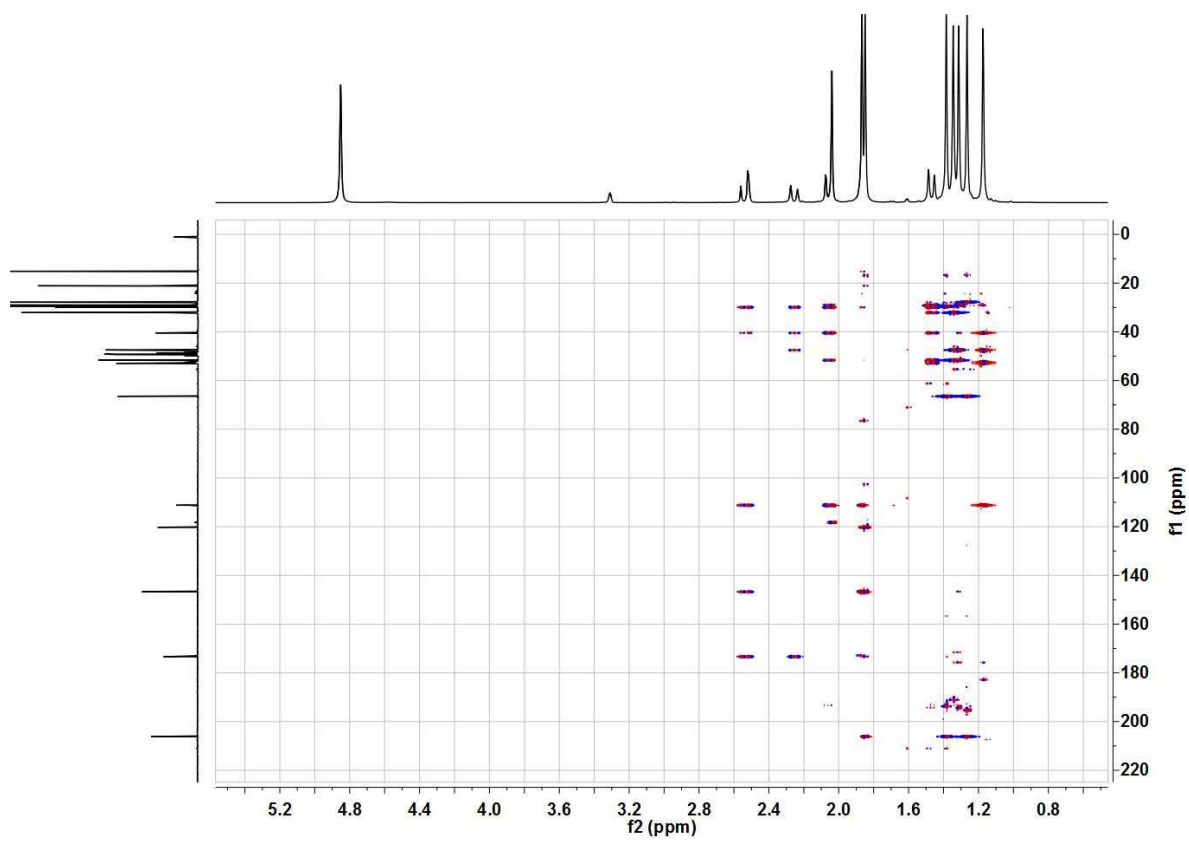
4.2.2 ^{13}C NMR (101 MHz, MeOH-d_4) spectra of 2.

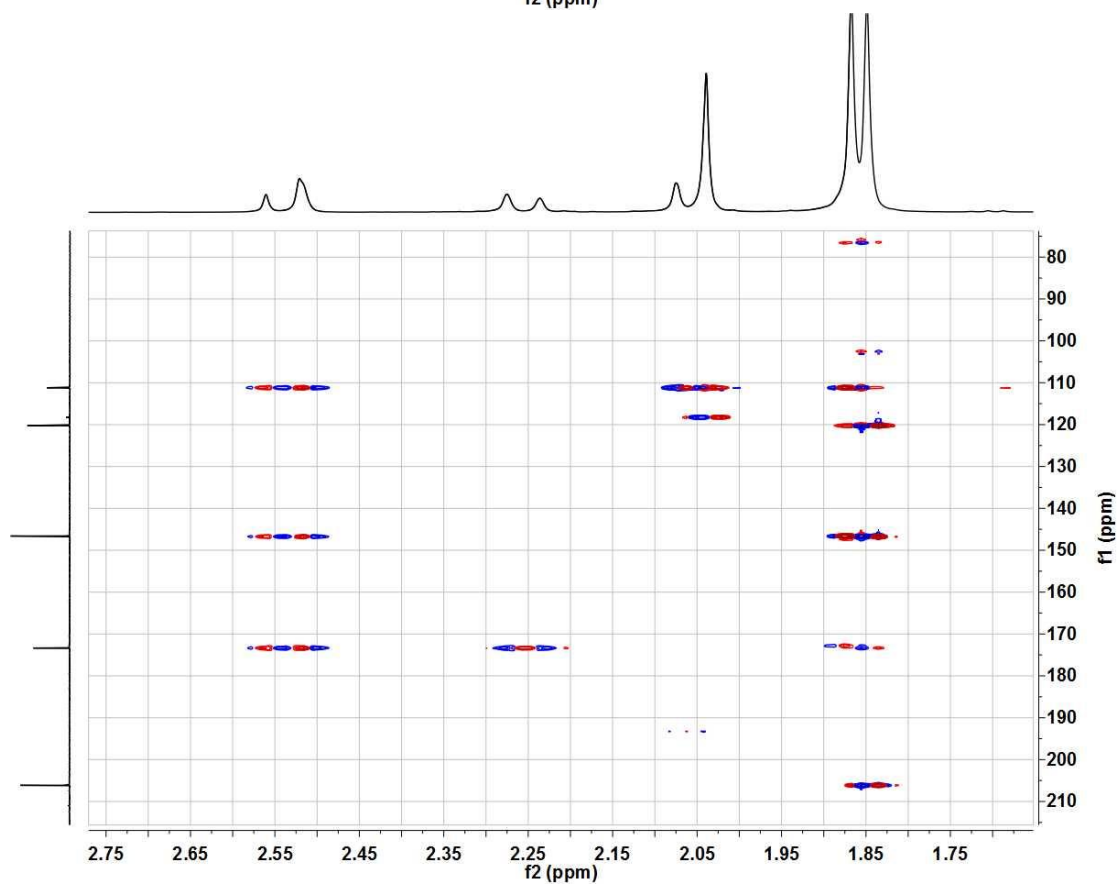
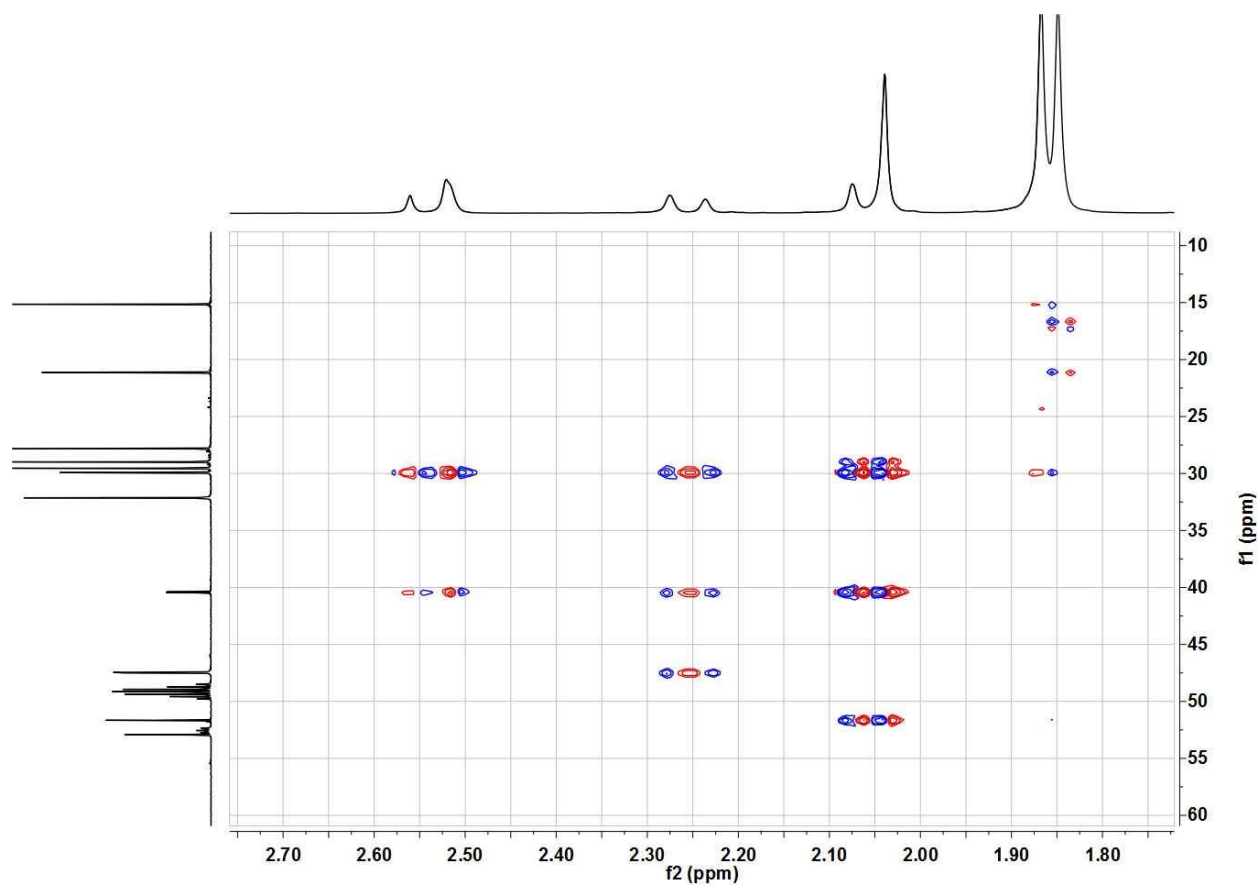


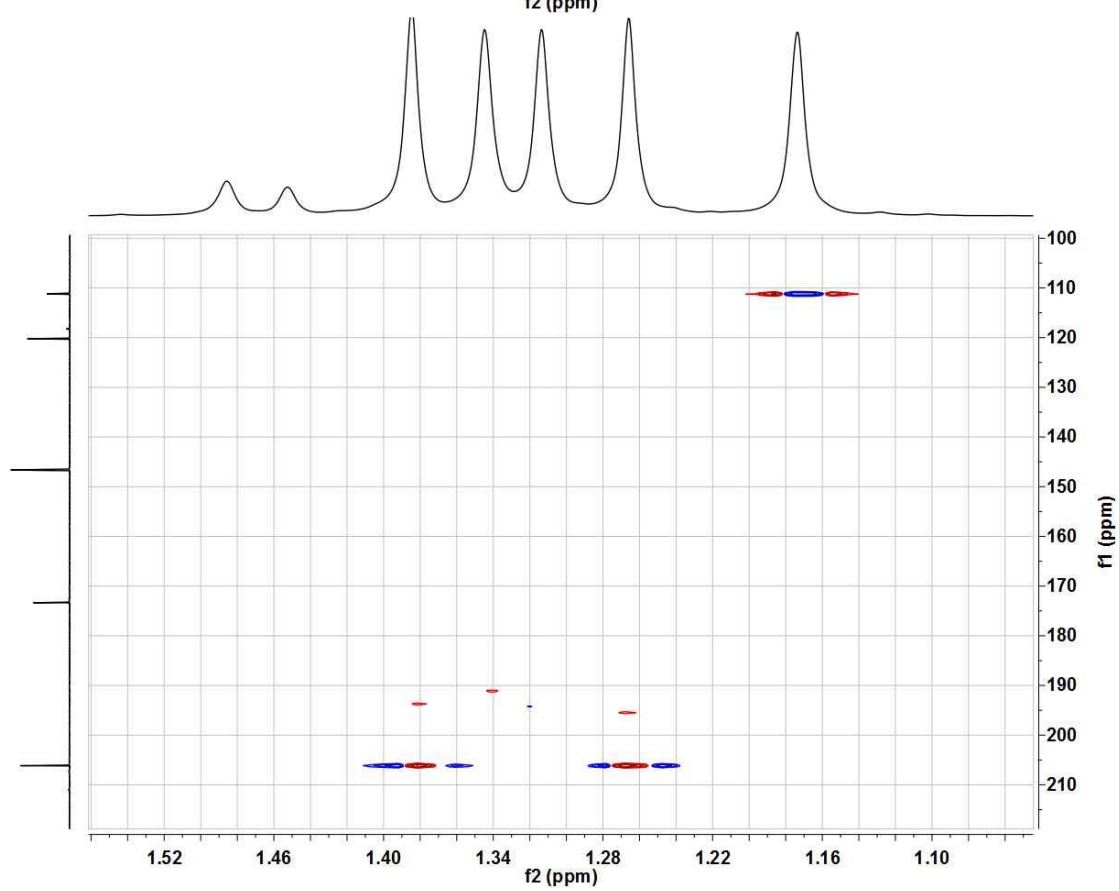
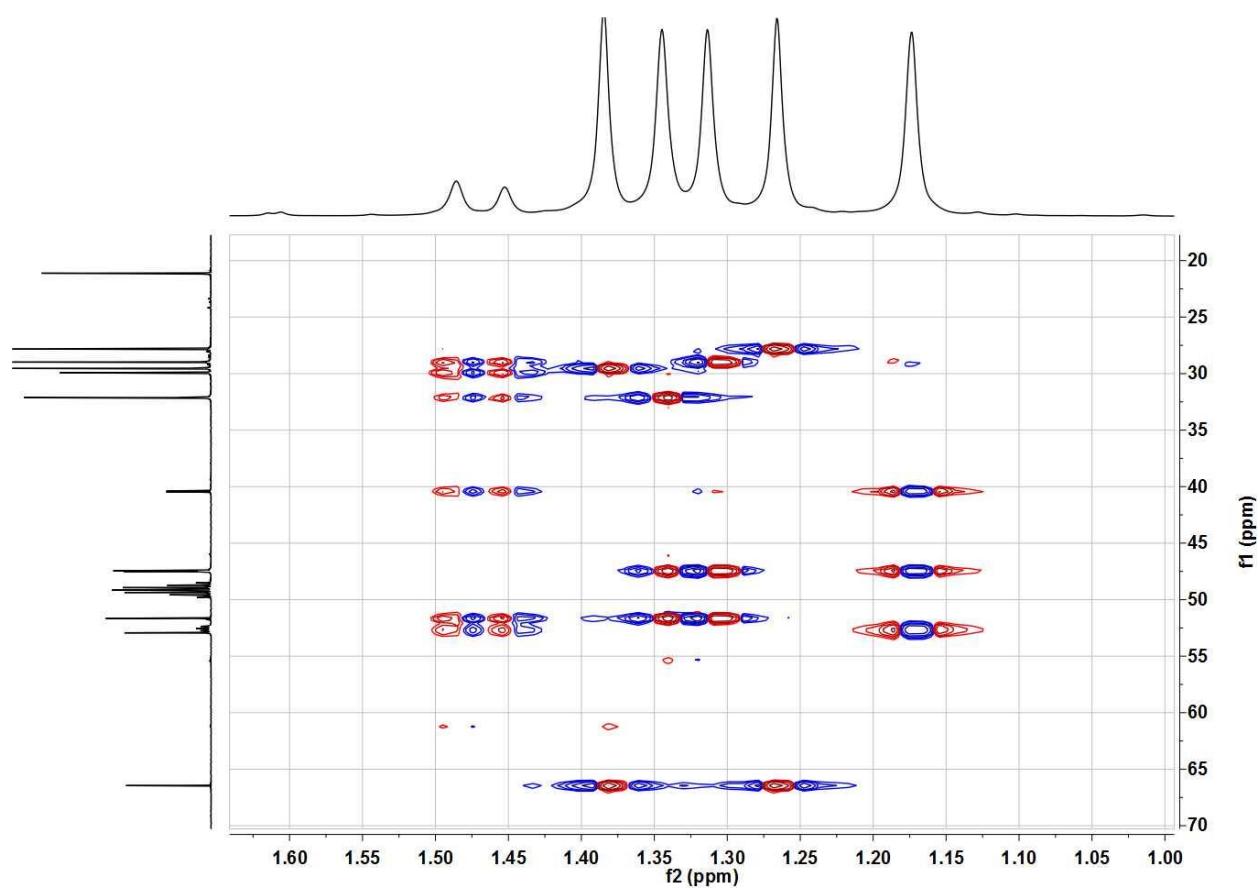
4.2.3 HSQC spectrum of 2.



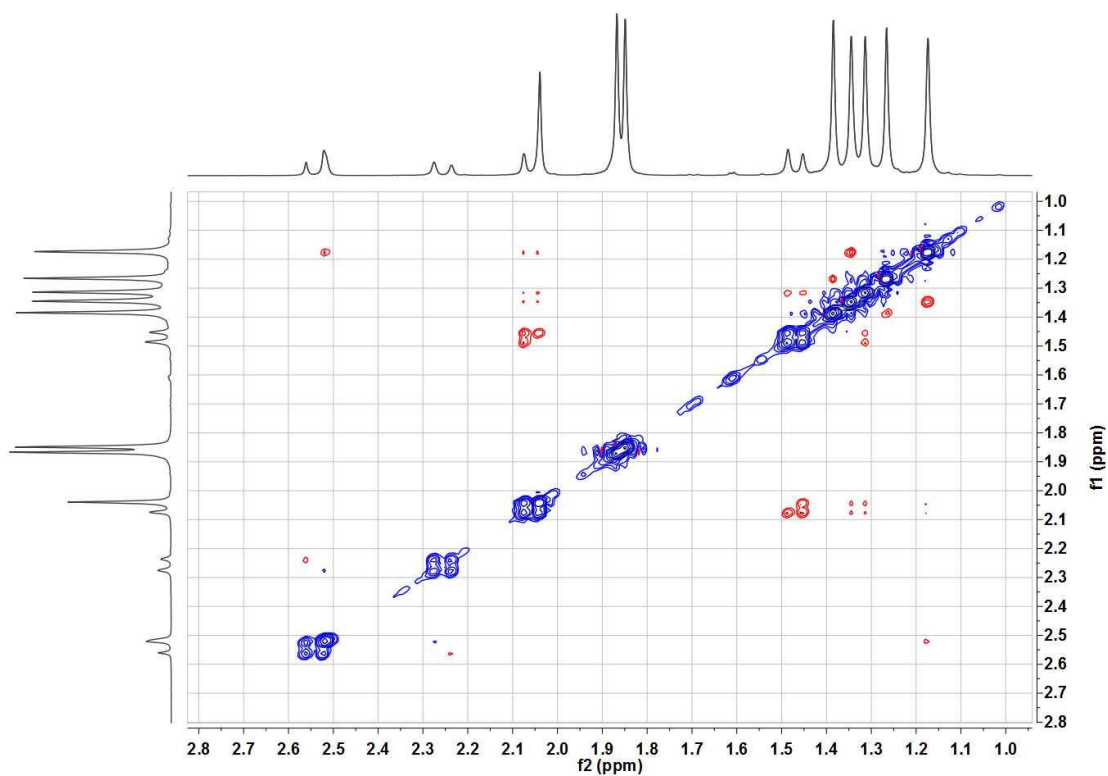
4.2.4 HMBC spectra of 2.



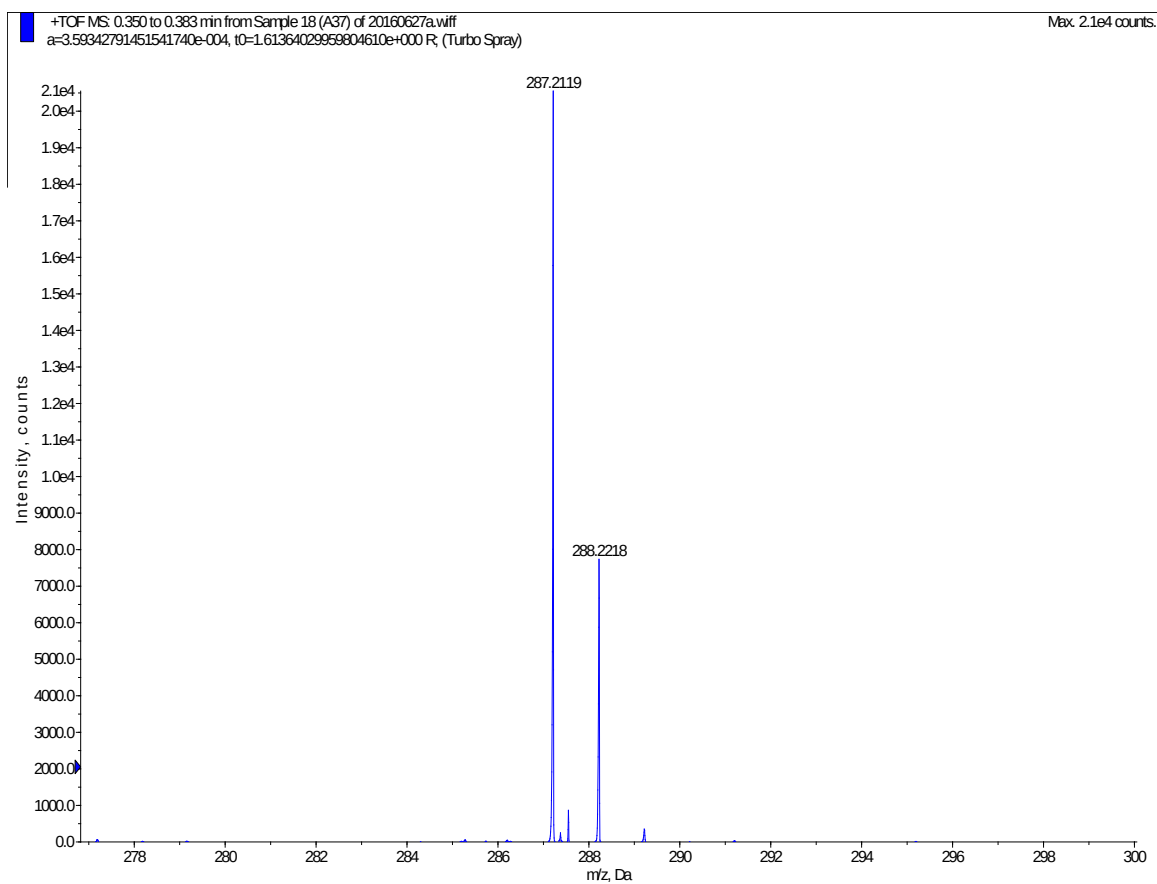




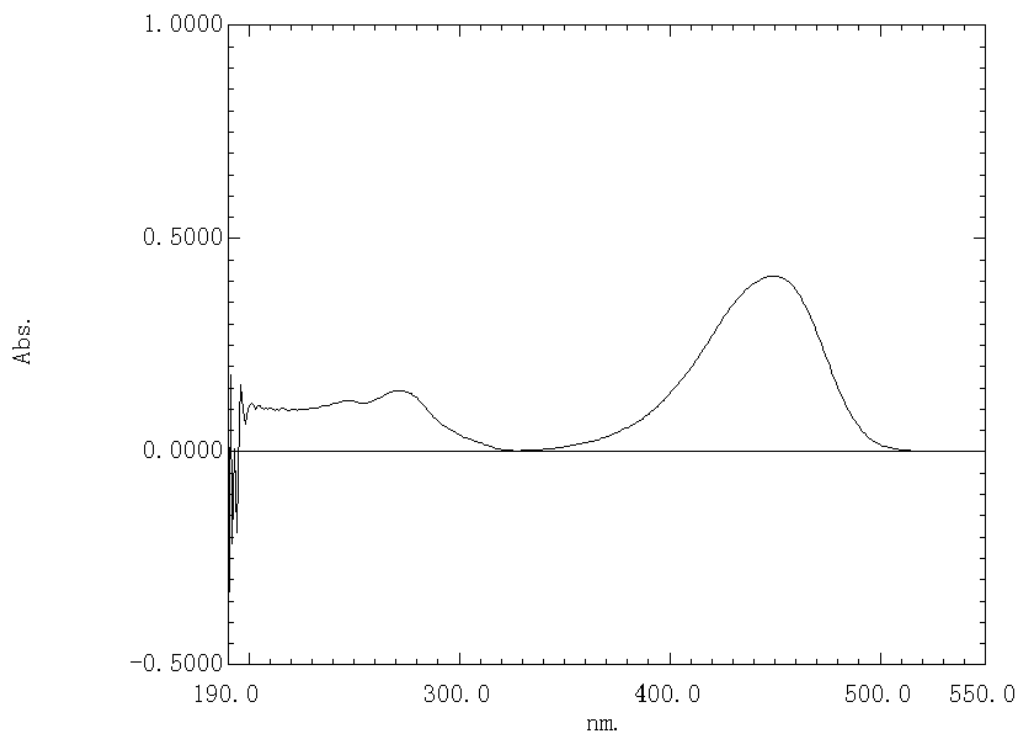
4.2.5 NOESY spectrum of 2.



4.2.6 (+)HRESIMS of 2.

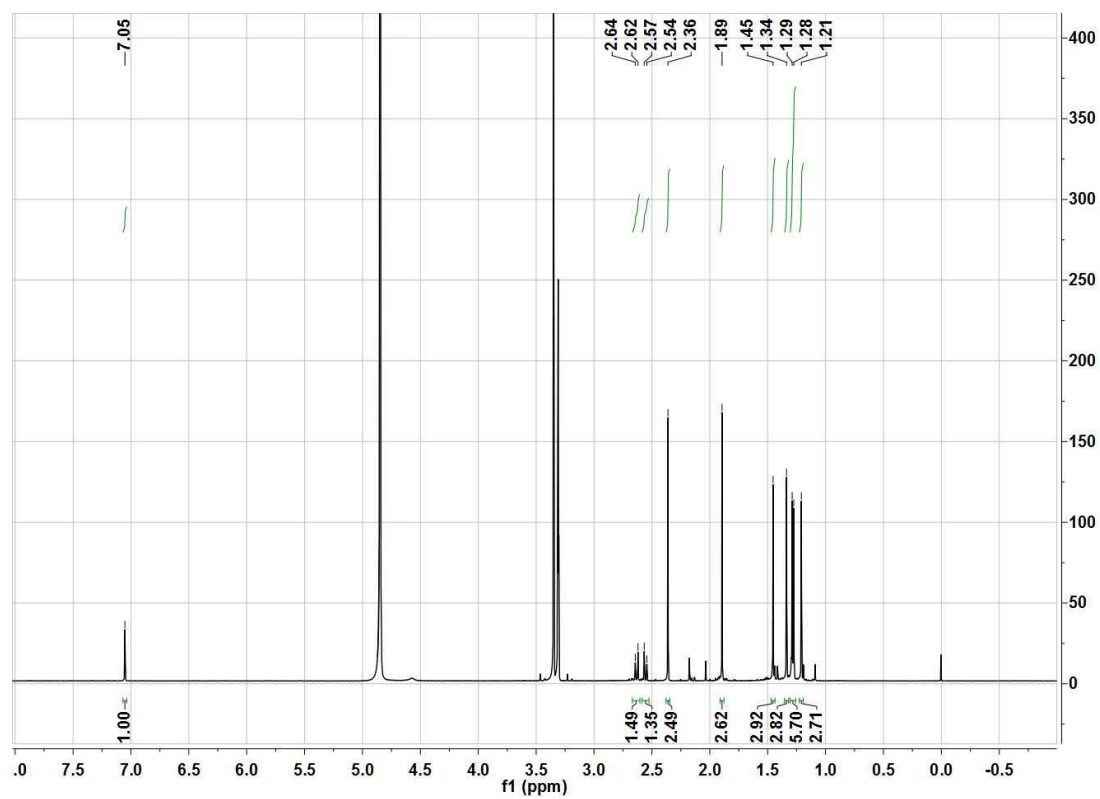


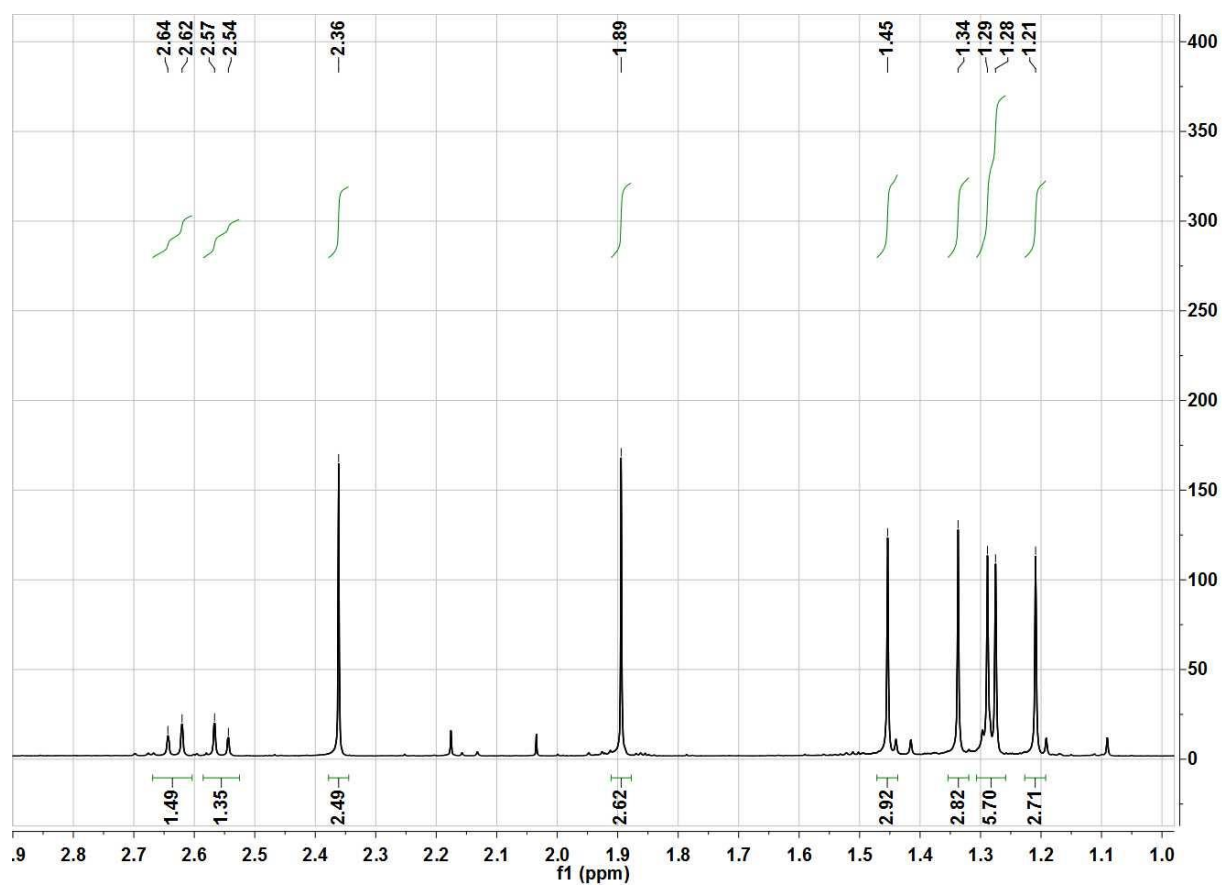
4.2.7 UV spectrum of **2**.



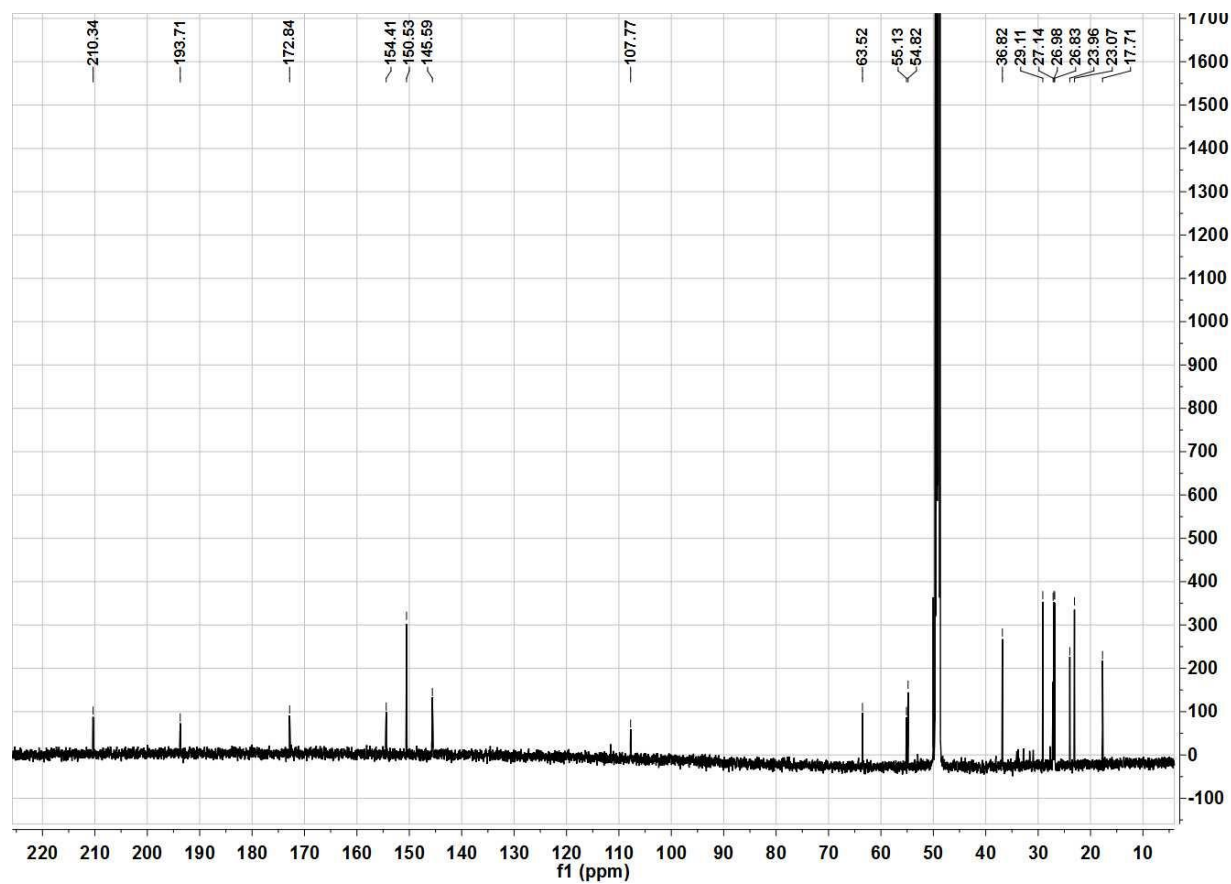
4.3 1D and 2D NMR of pyracyclumine C (**3**).

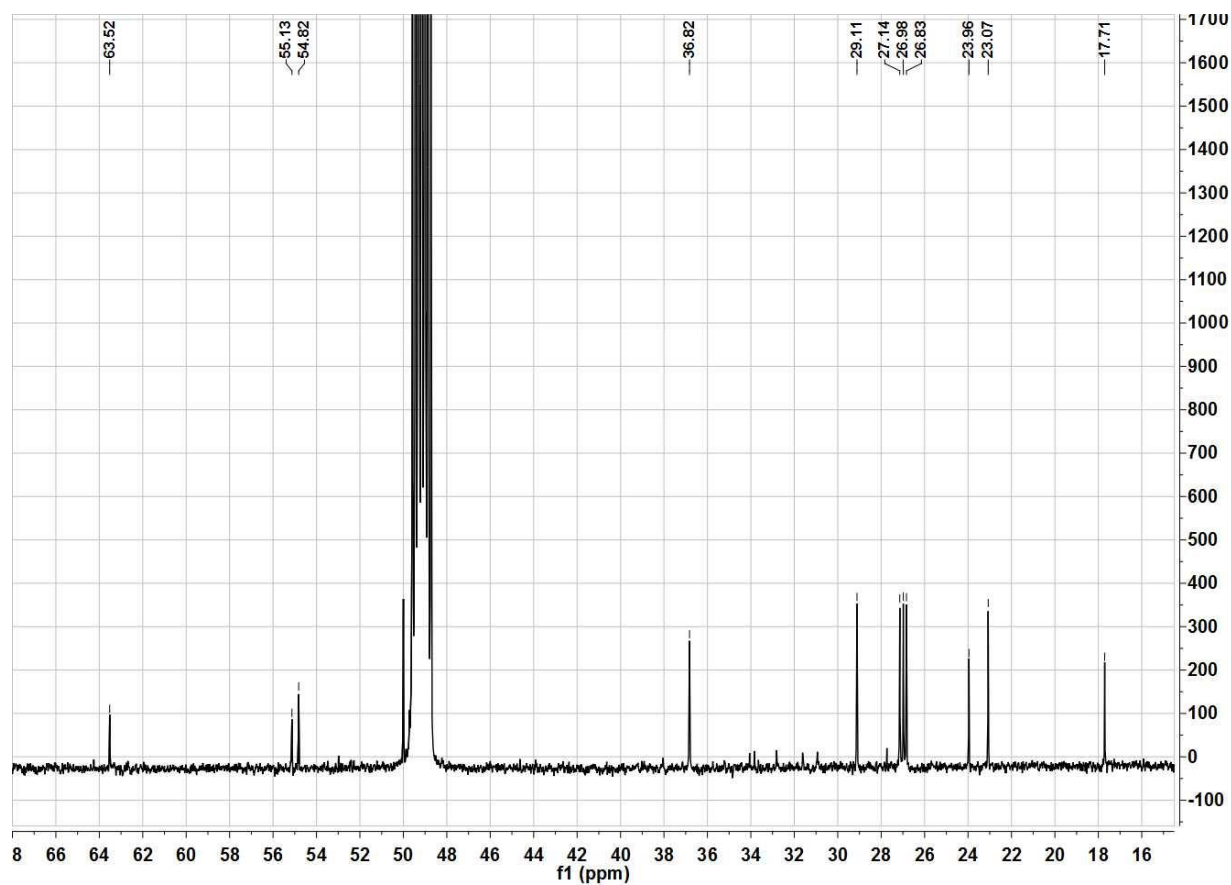
4.3.1 ^1H NMR (600 MHz, $\text{MeOH-}d_4$) spectra of **3**.



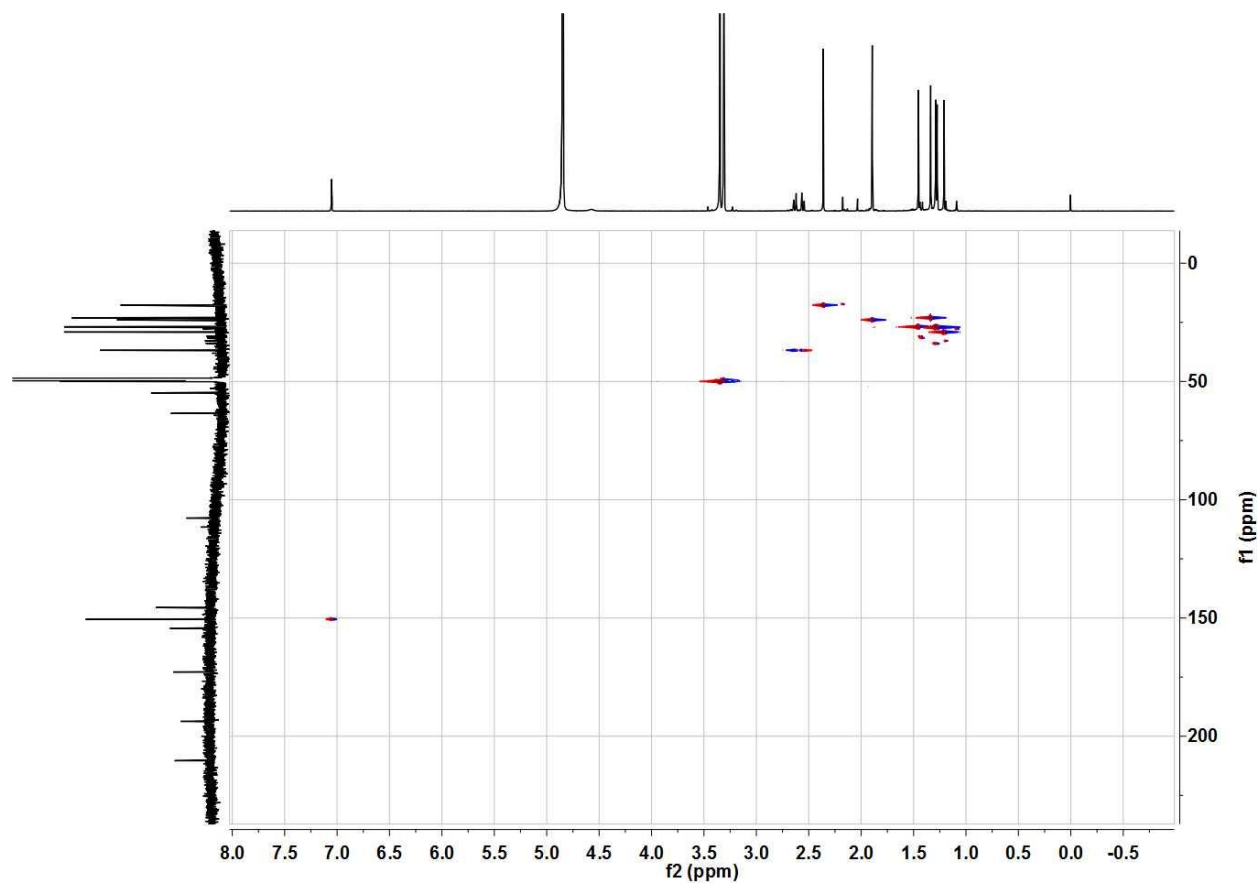


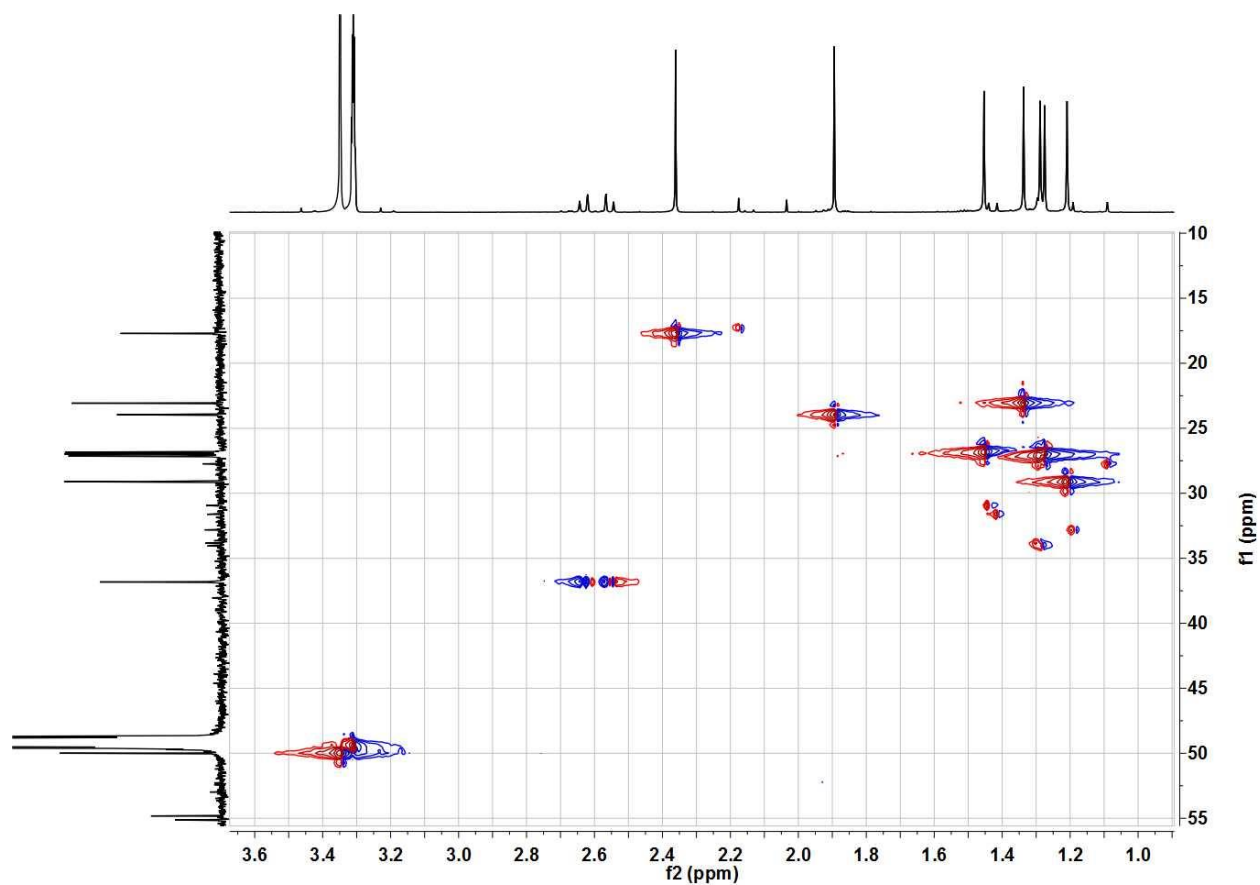
4.3.2 ¹³C NMR (150 MHz, MeOH-*d*₄) spectra of 3.



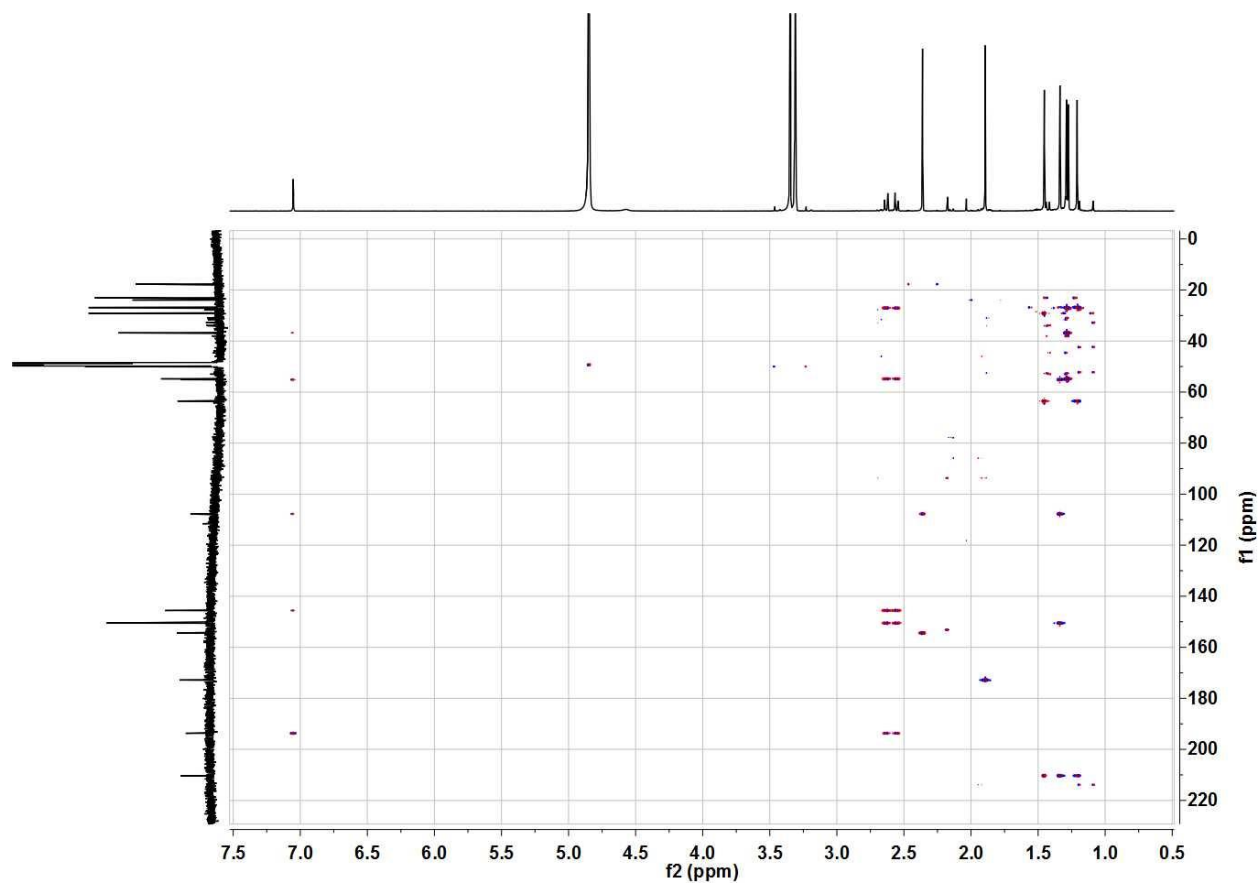


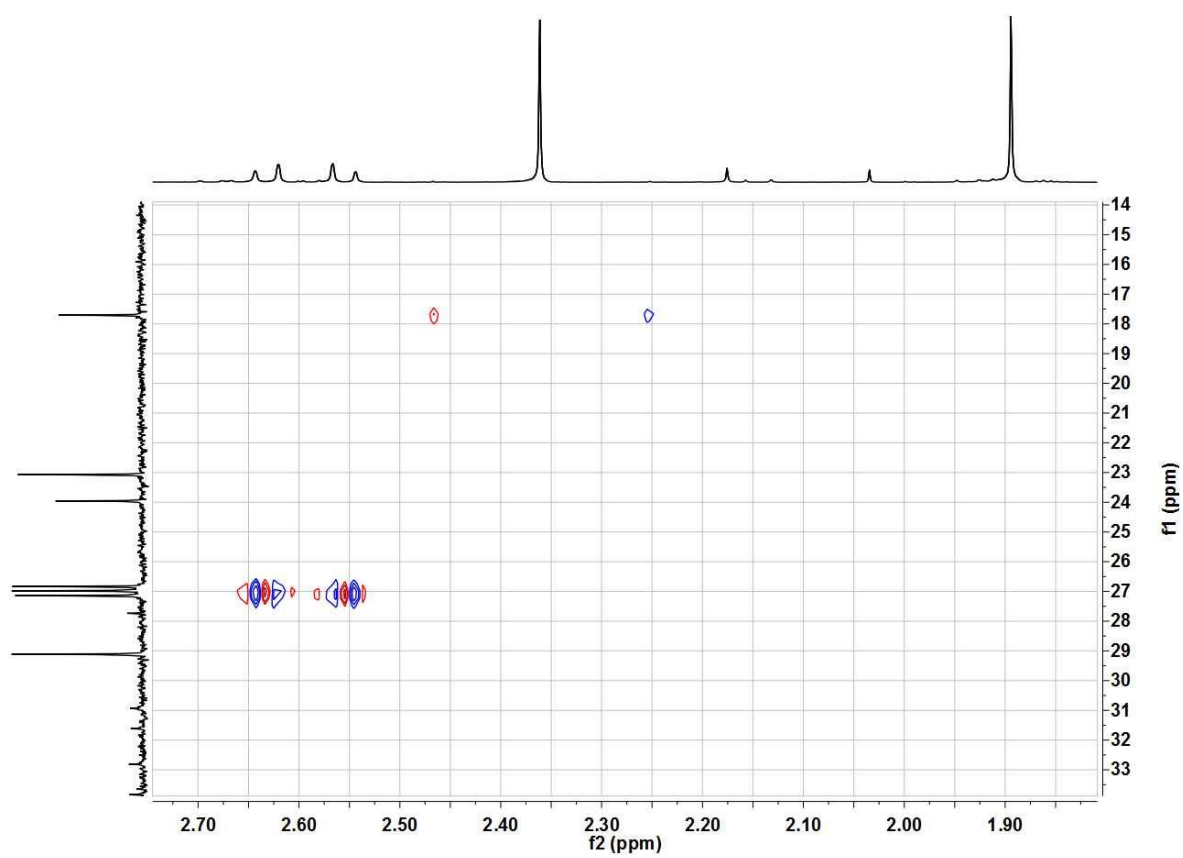
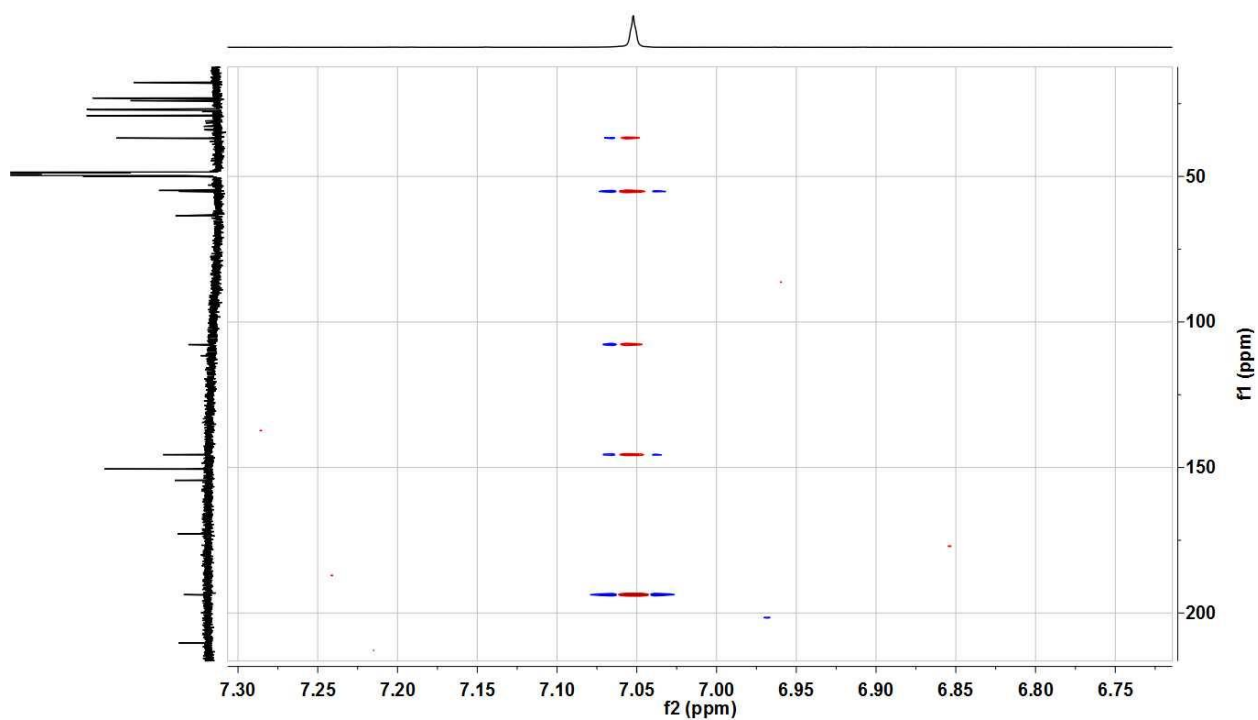
4.3.3 HSQC spectra of **3**.

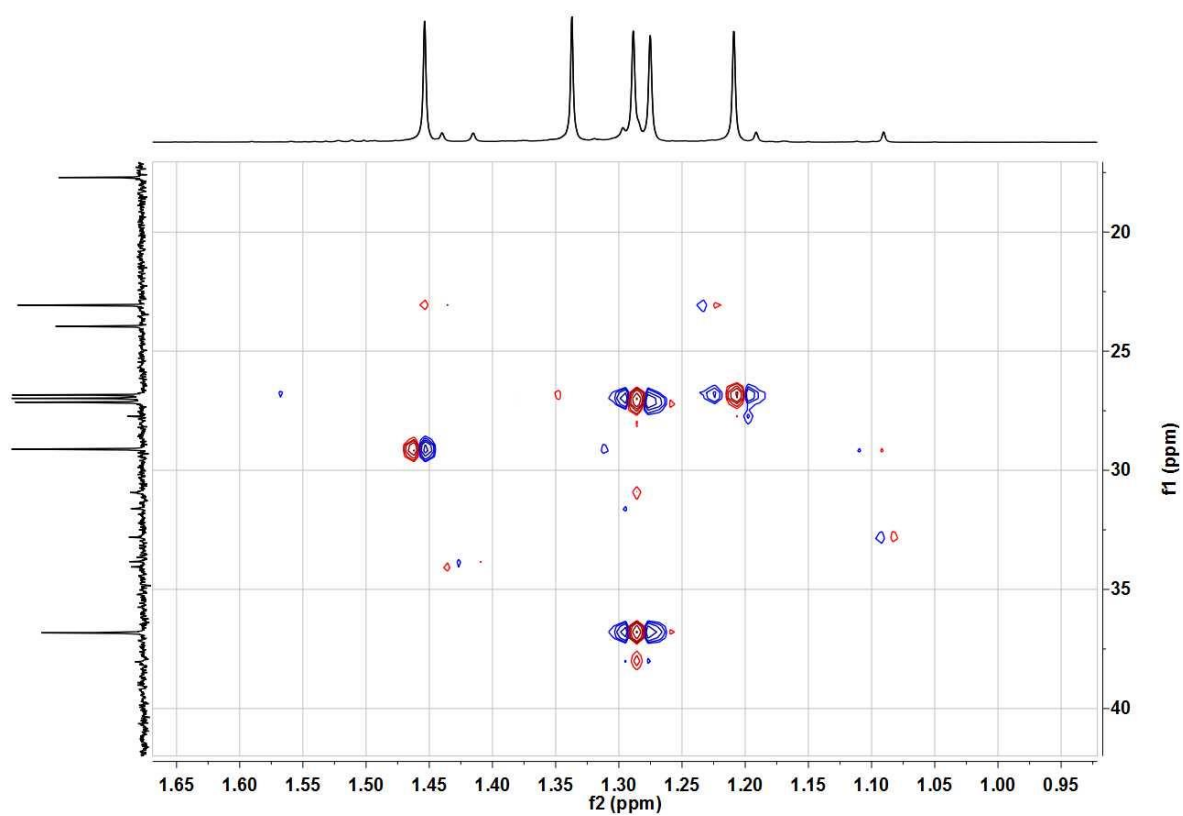
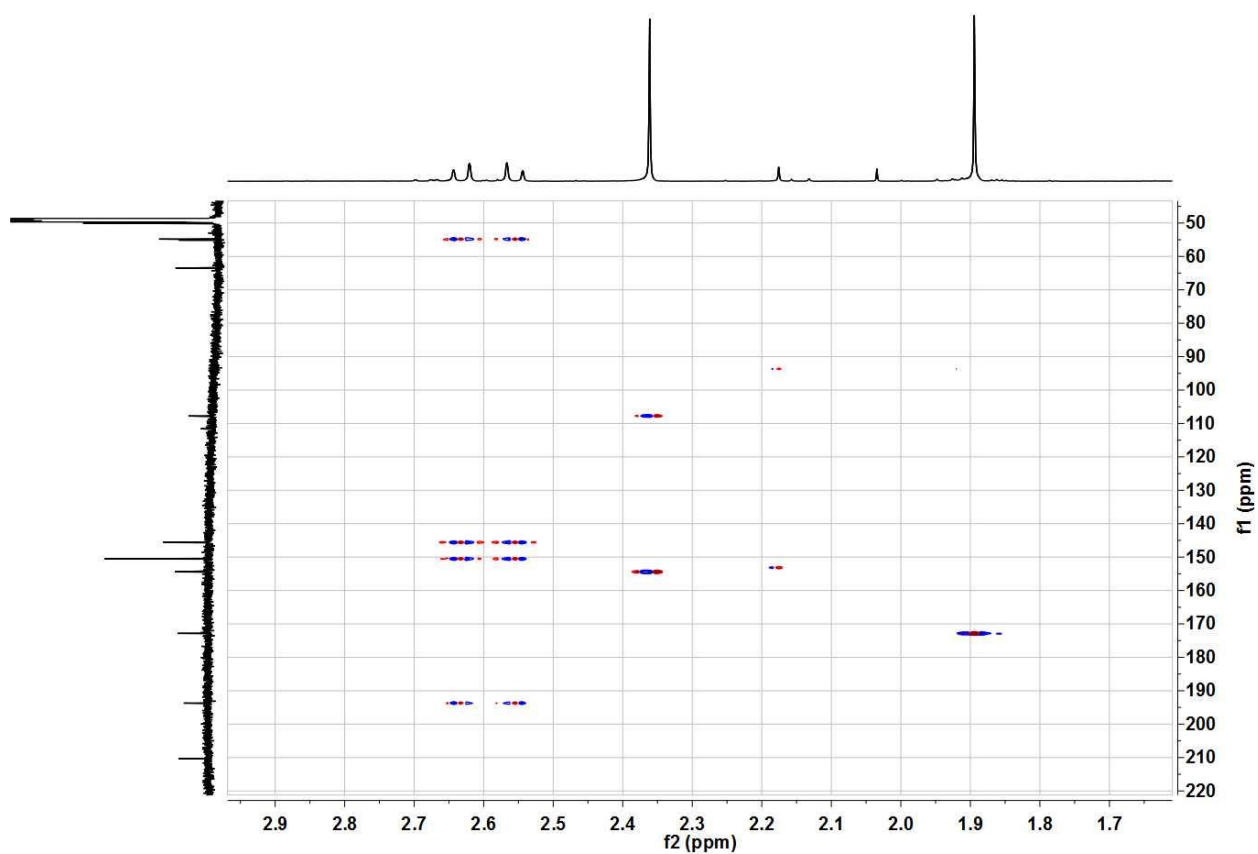


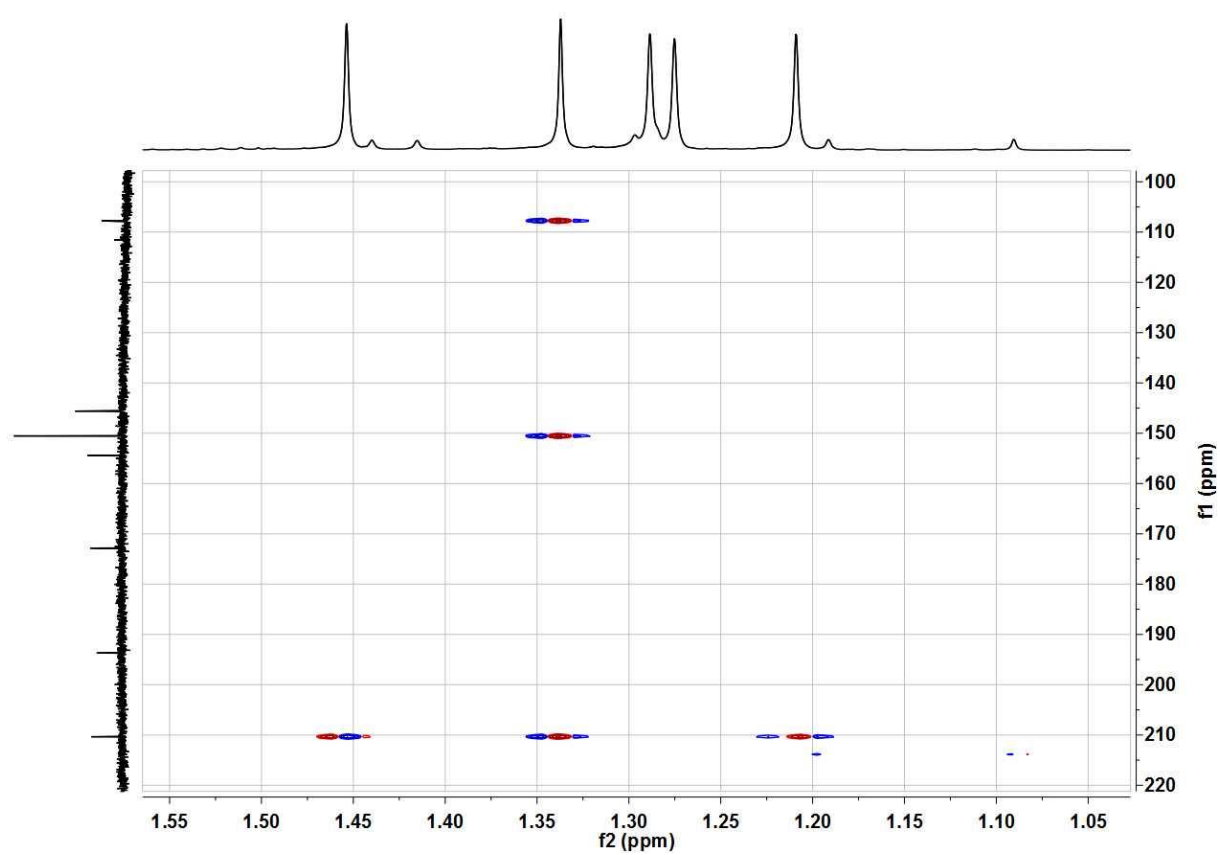
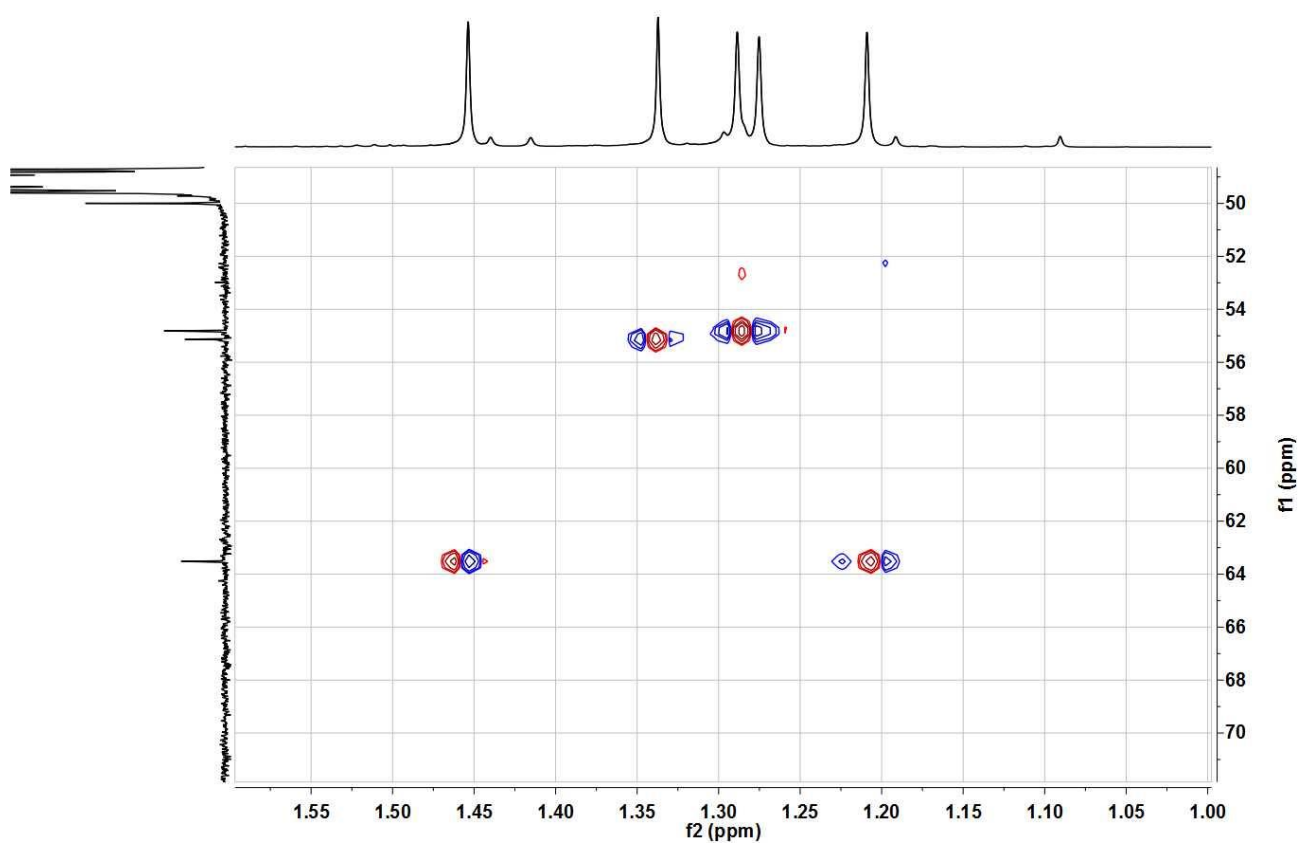


4.3.4 HMBC spectra of 3.

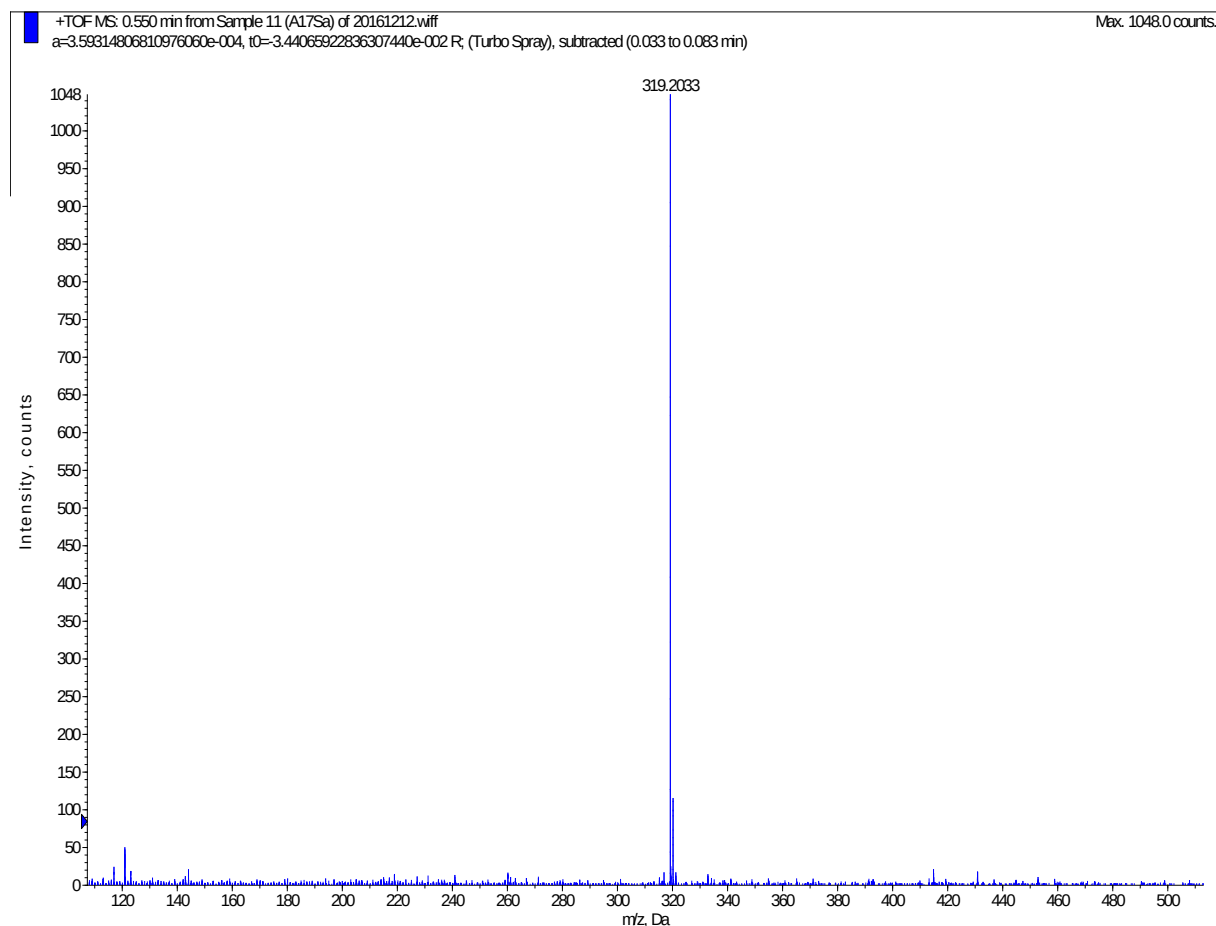




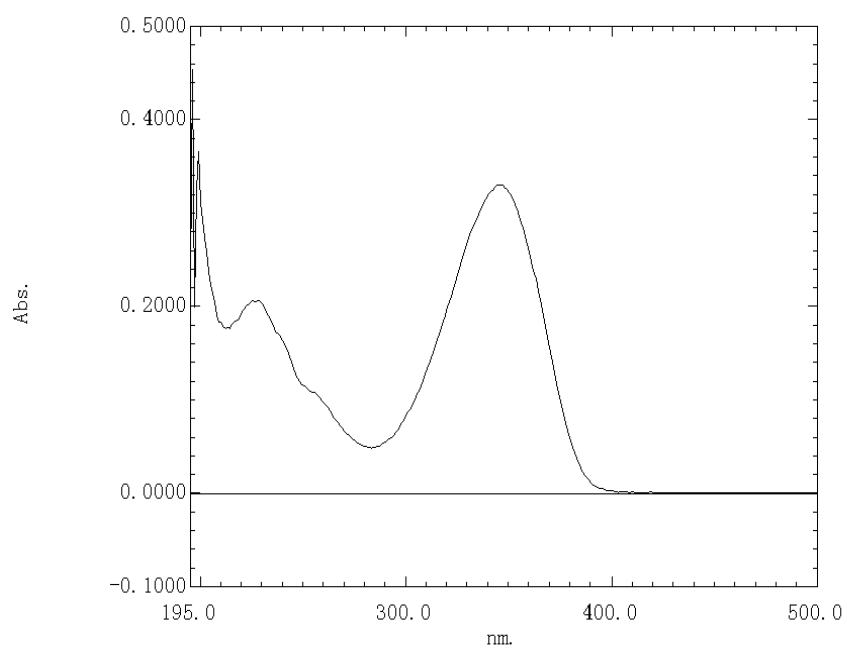




4.3.5 (+)HRESIMS of **3**.

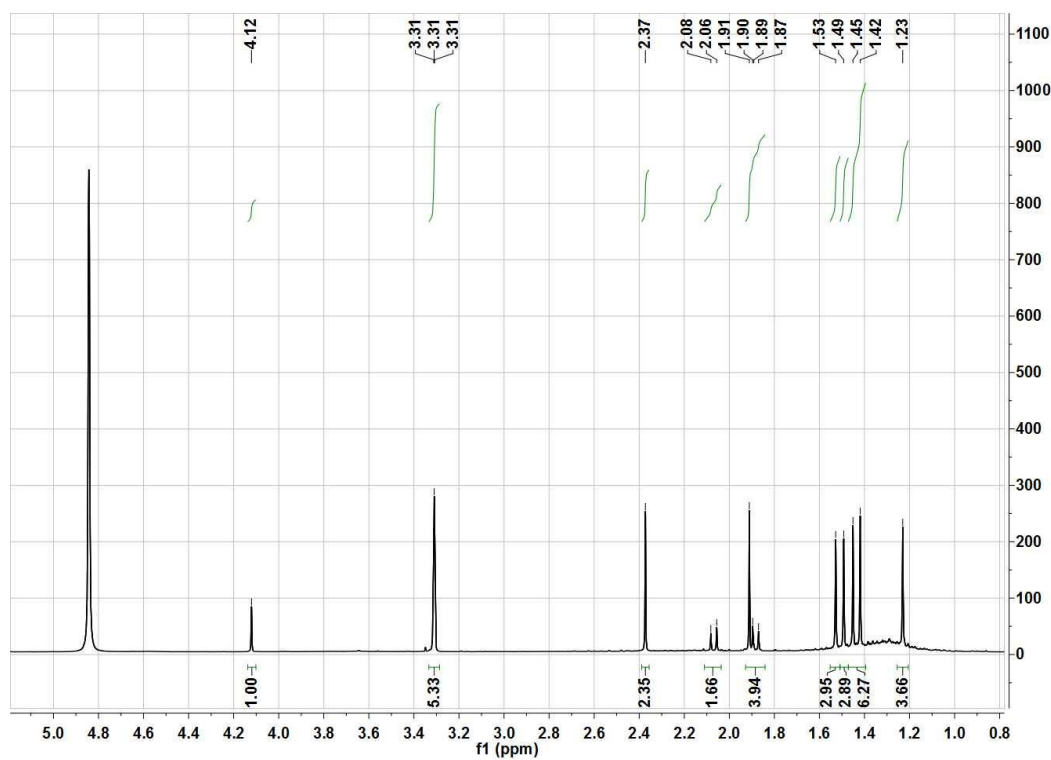


4.3.6 UV spectrum of **3**.

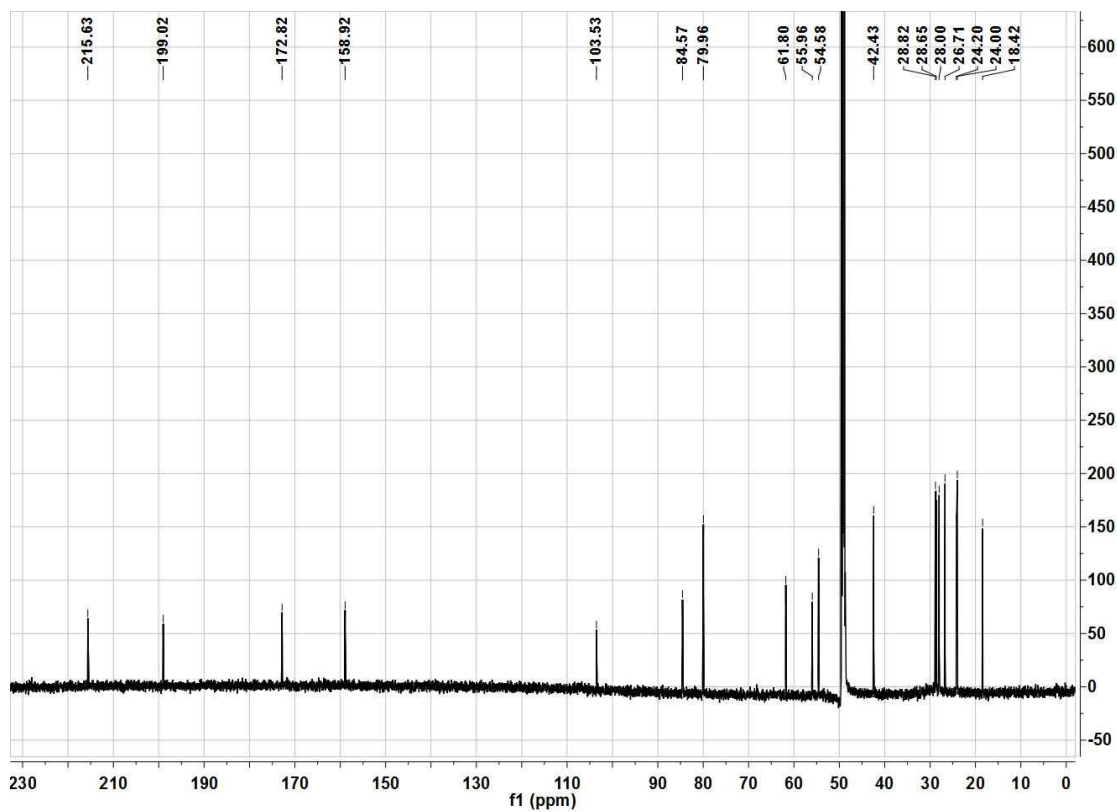


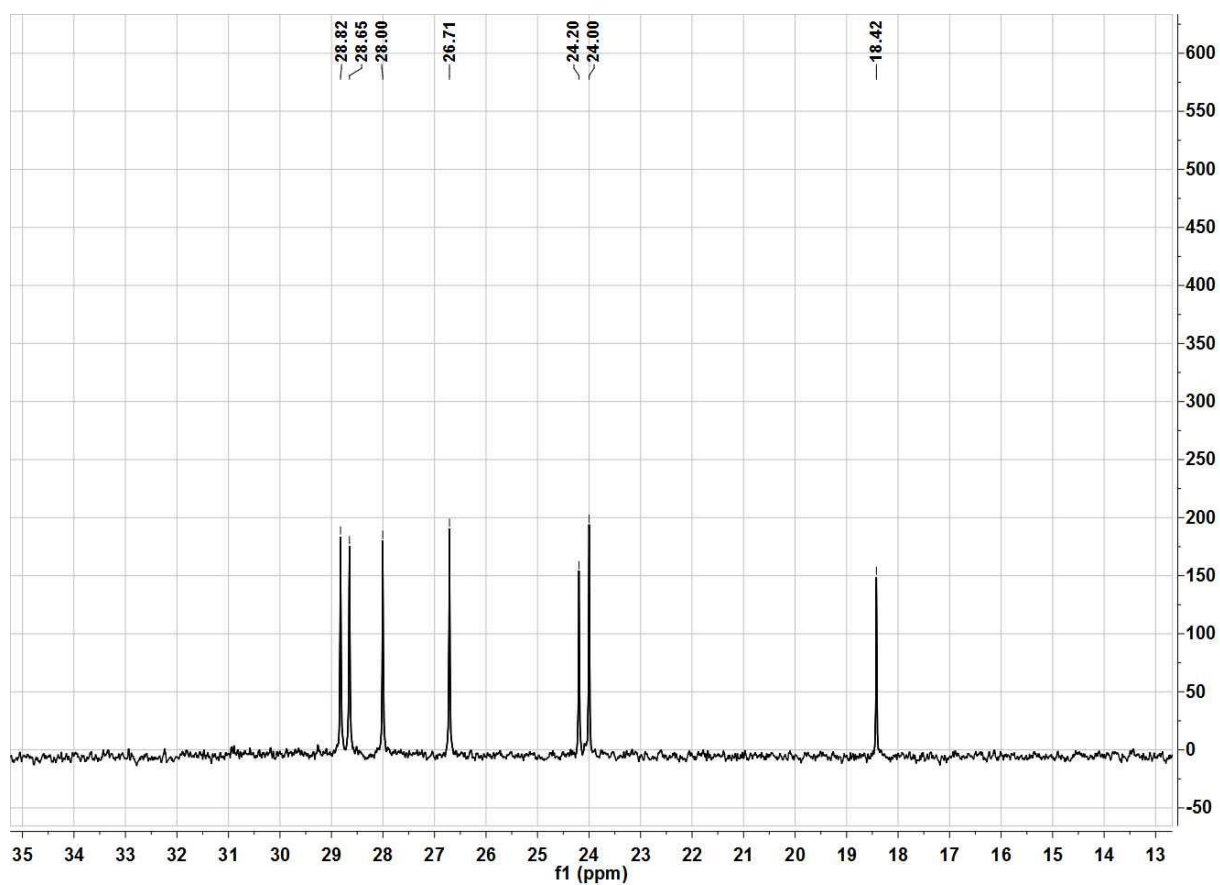
4.4 1D and 2D NMR of pyracyclumine D (4).

4.4.1 ^1H NMR (600 MHz, $\text{MeOH-}d_4$) spectrum of 4.

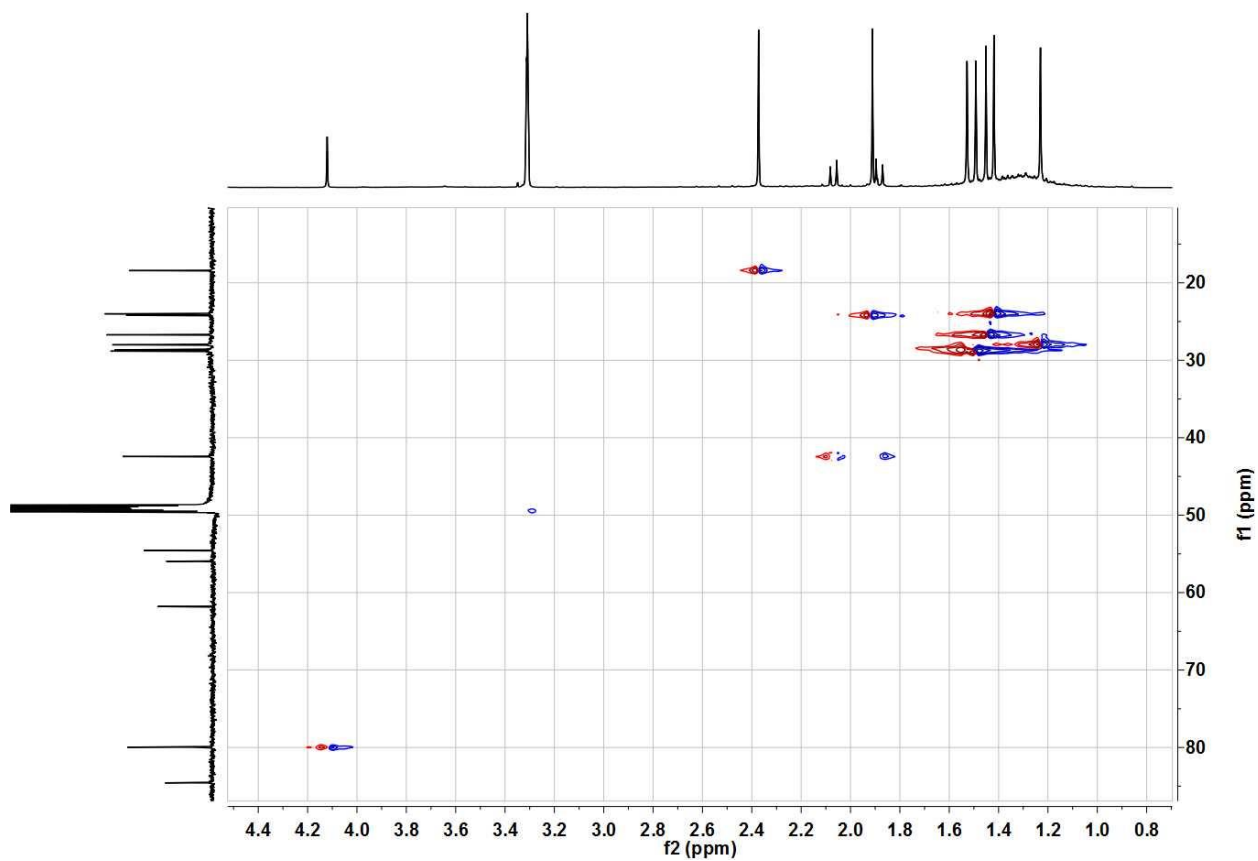


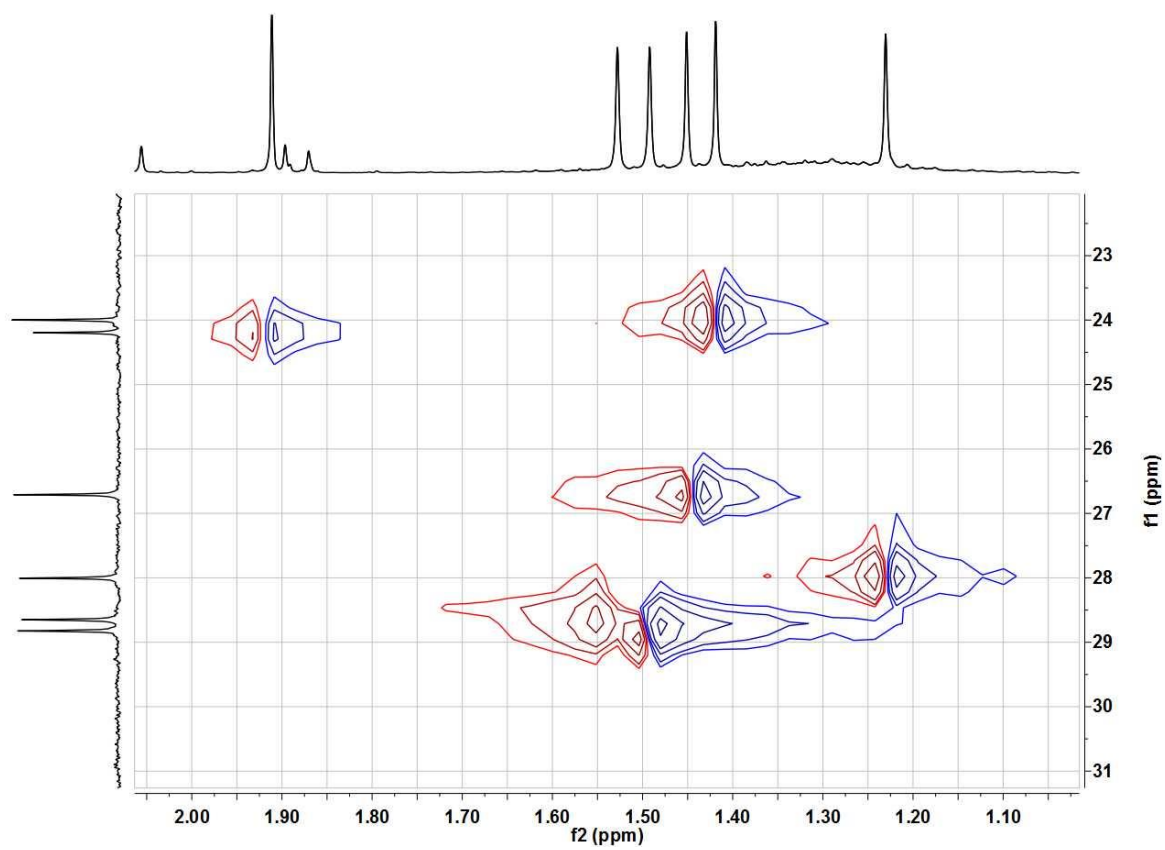
4.4.2 ^{13}C NMR (150 MHz, $\text{MeOH-}d_4$) spectra of 4.



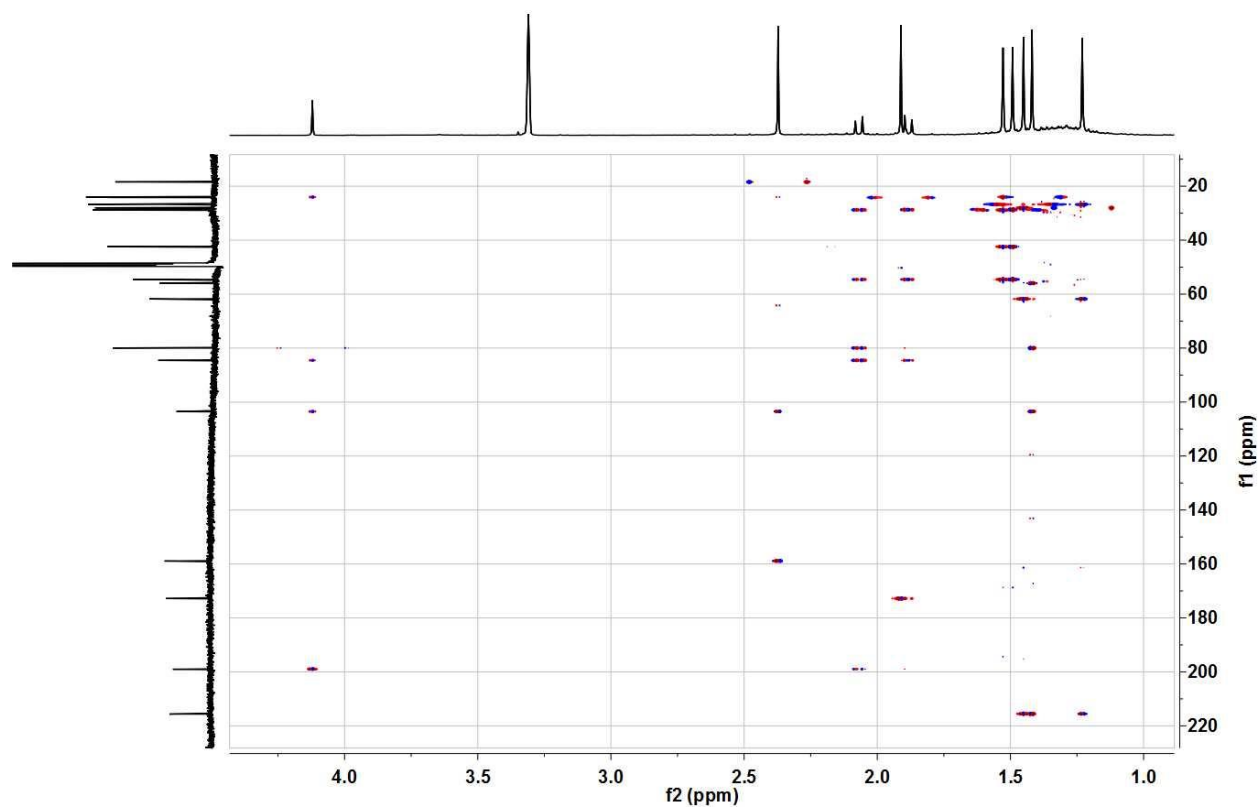


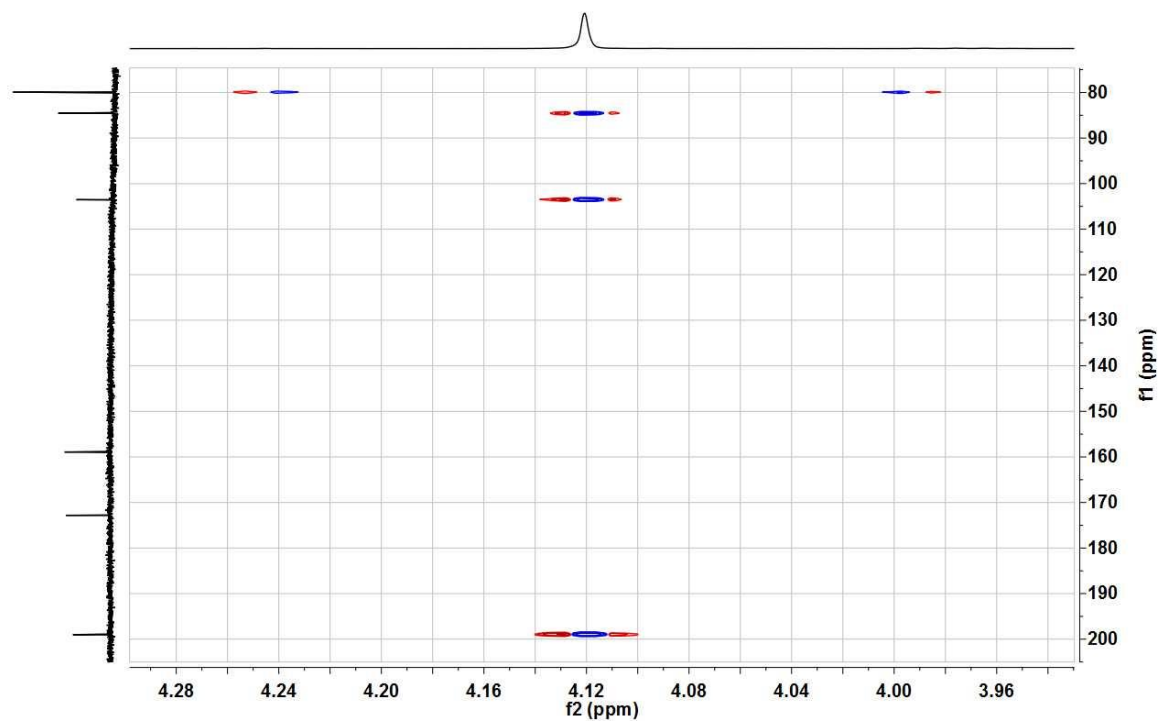
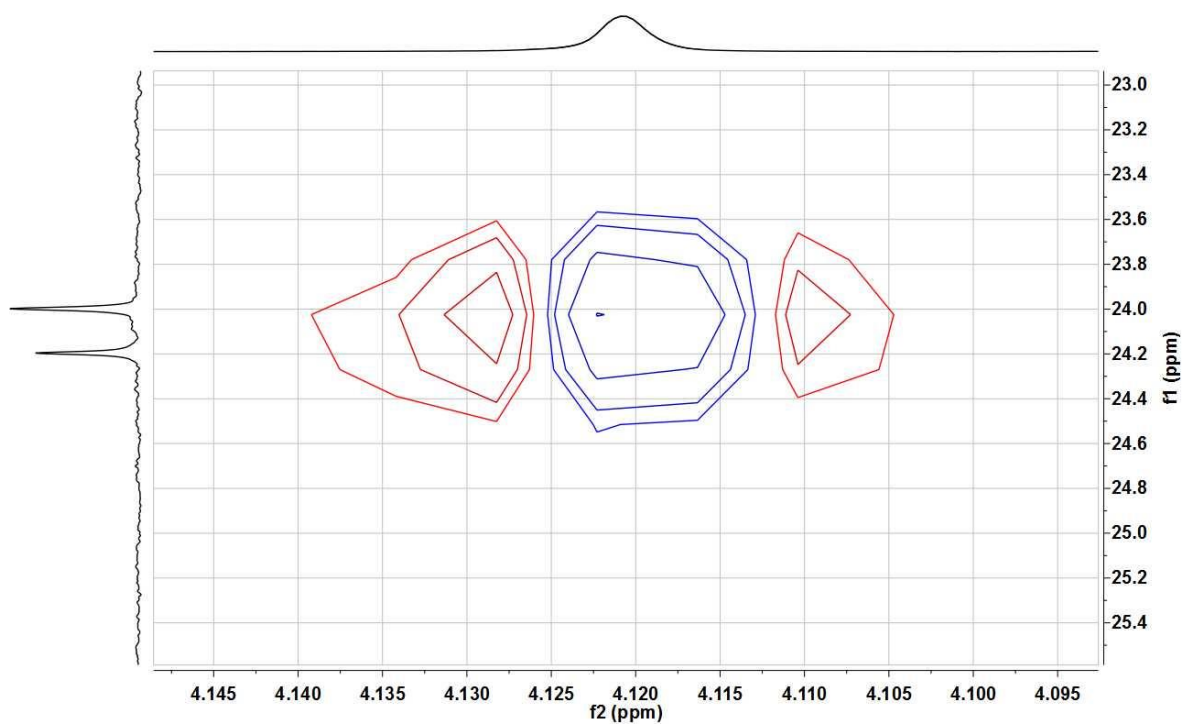
4.4.3 HSQC spectra of 4.

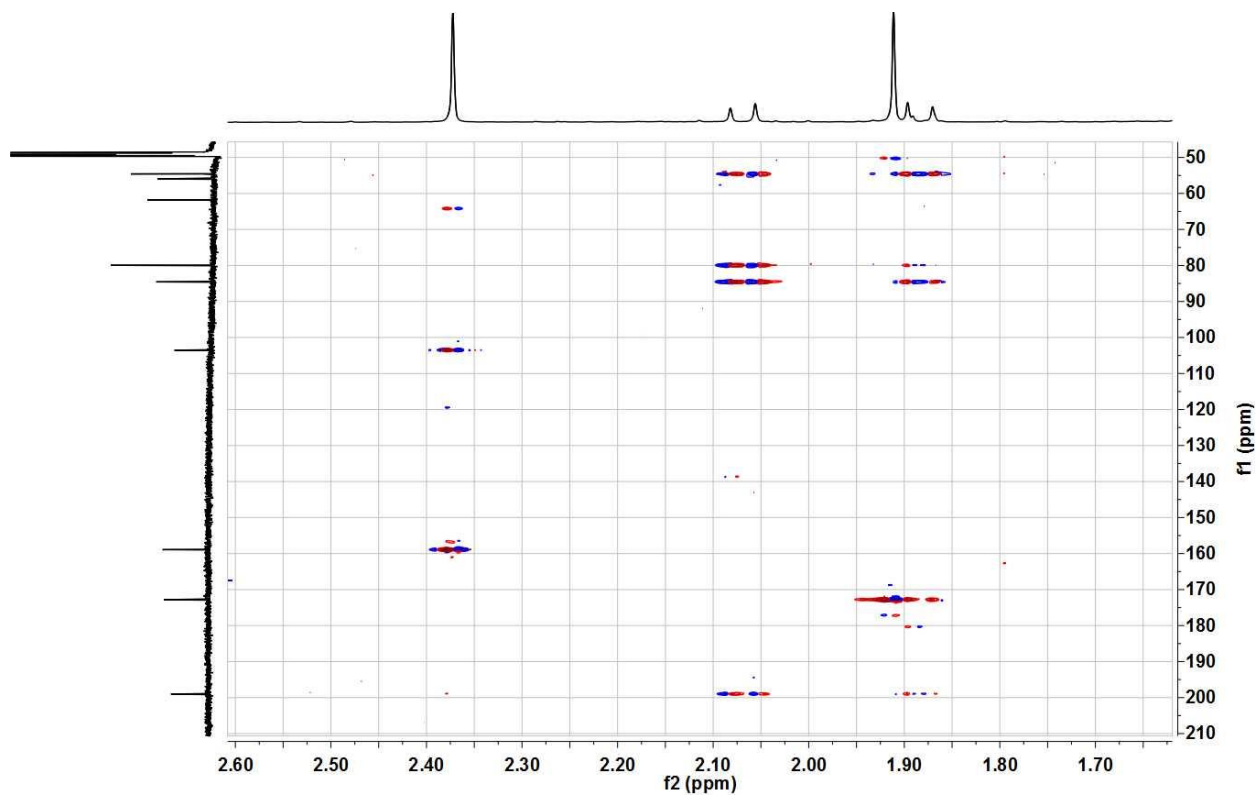
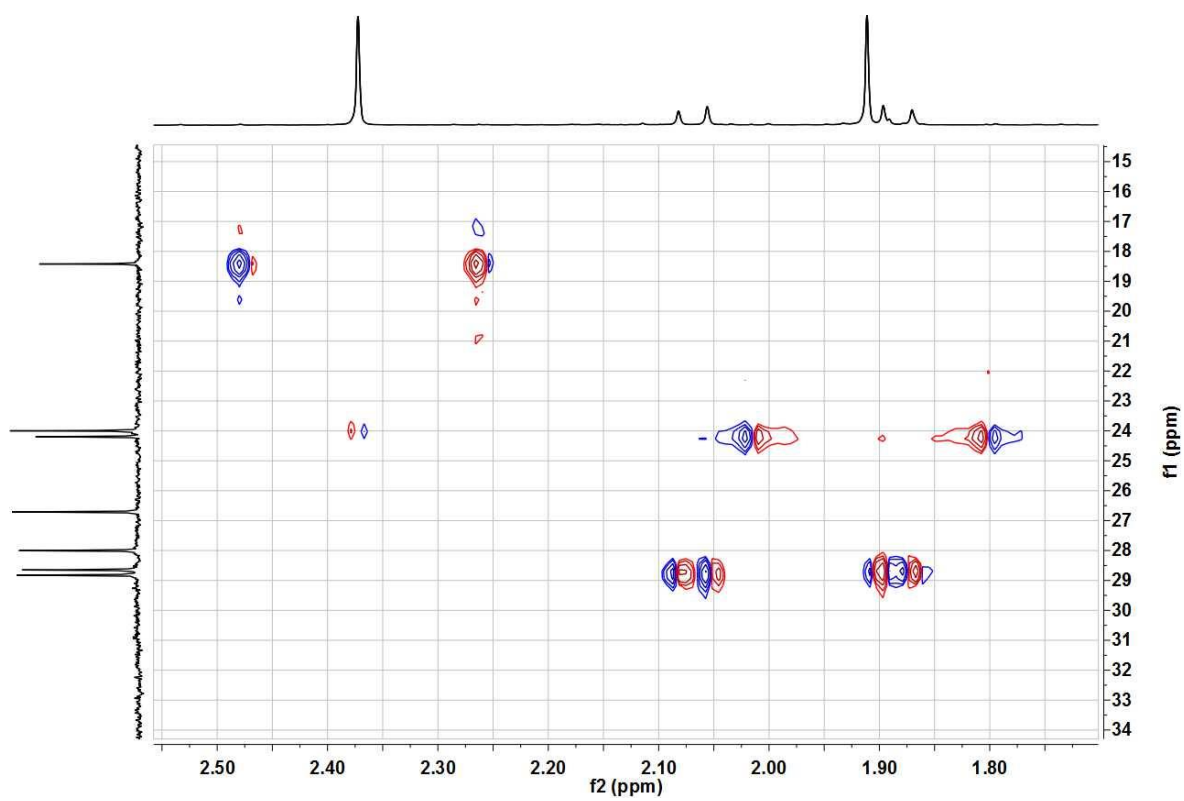


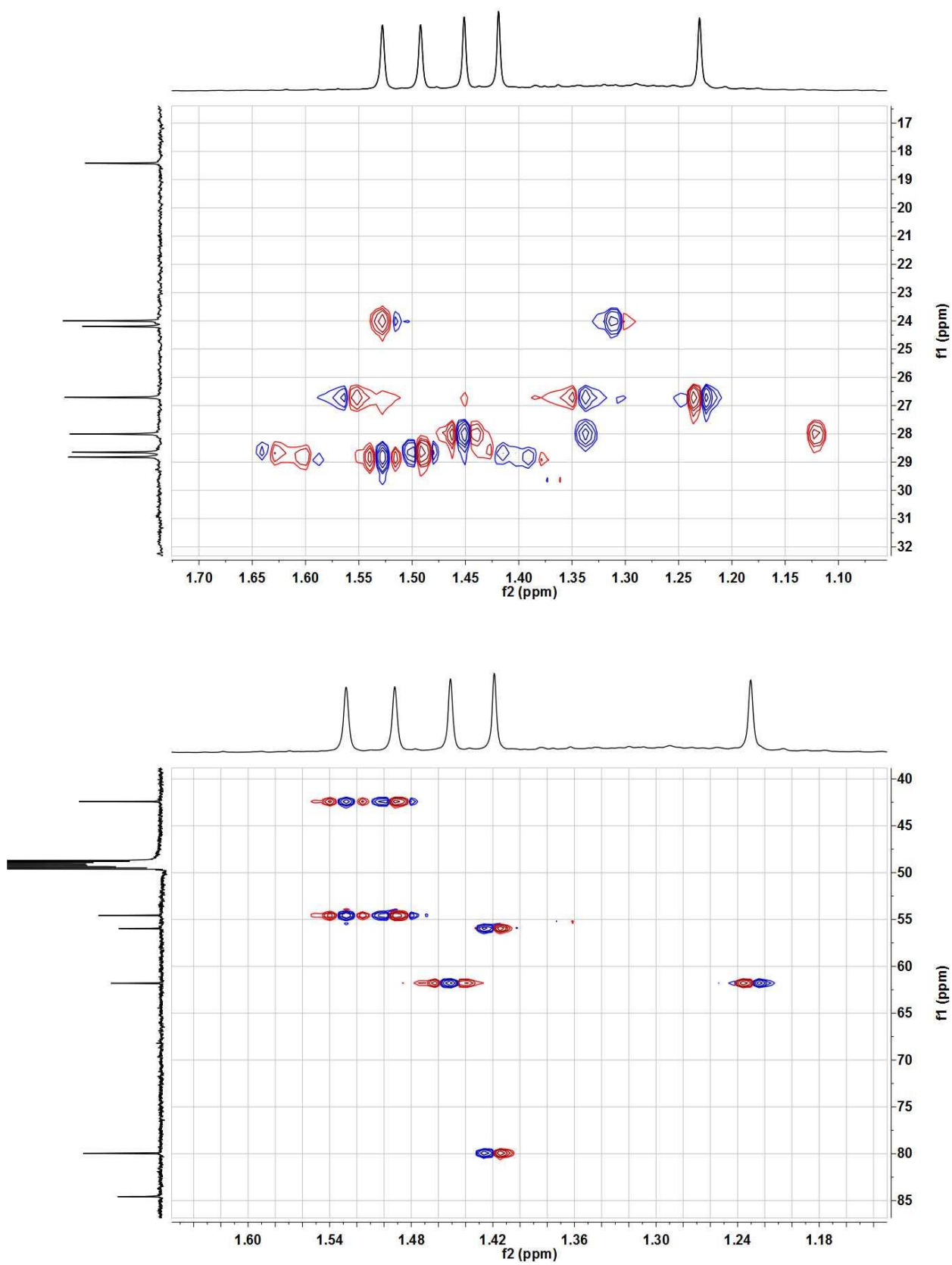


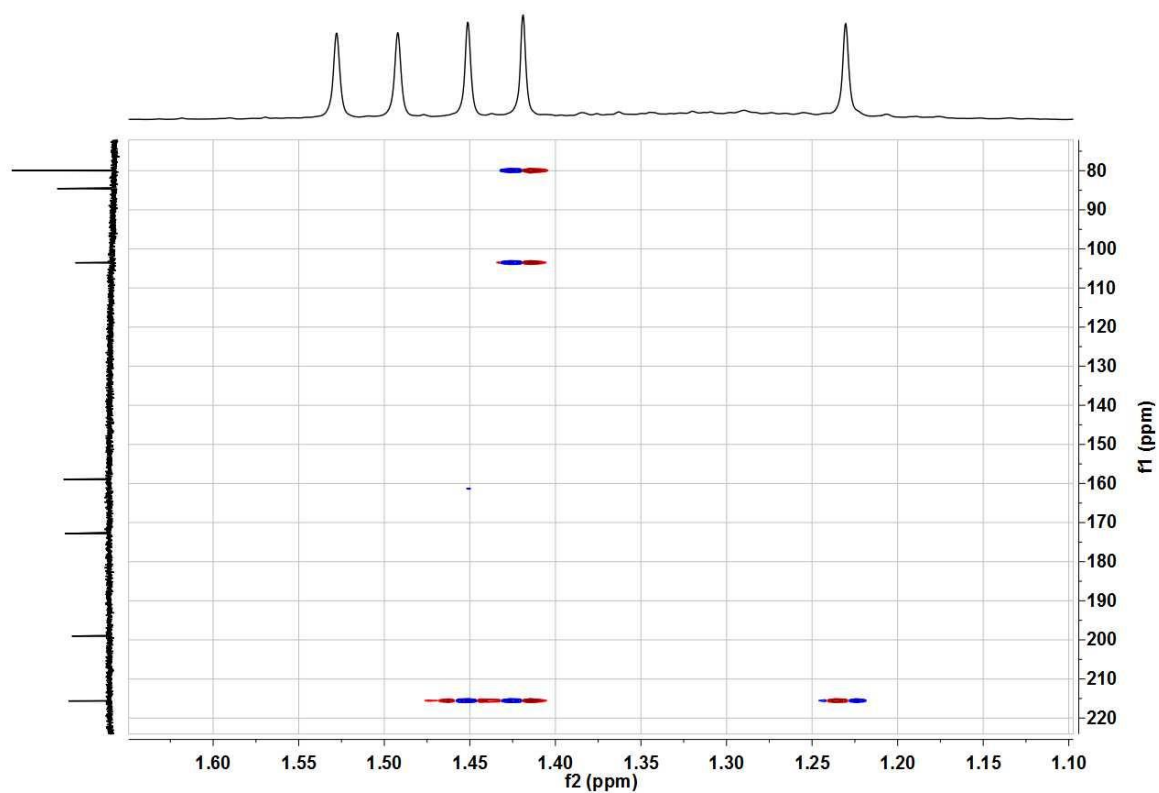
4.4.4 HMBC spectra of **4**.



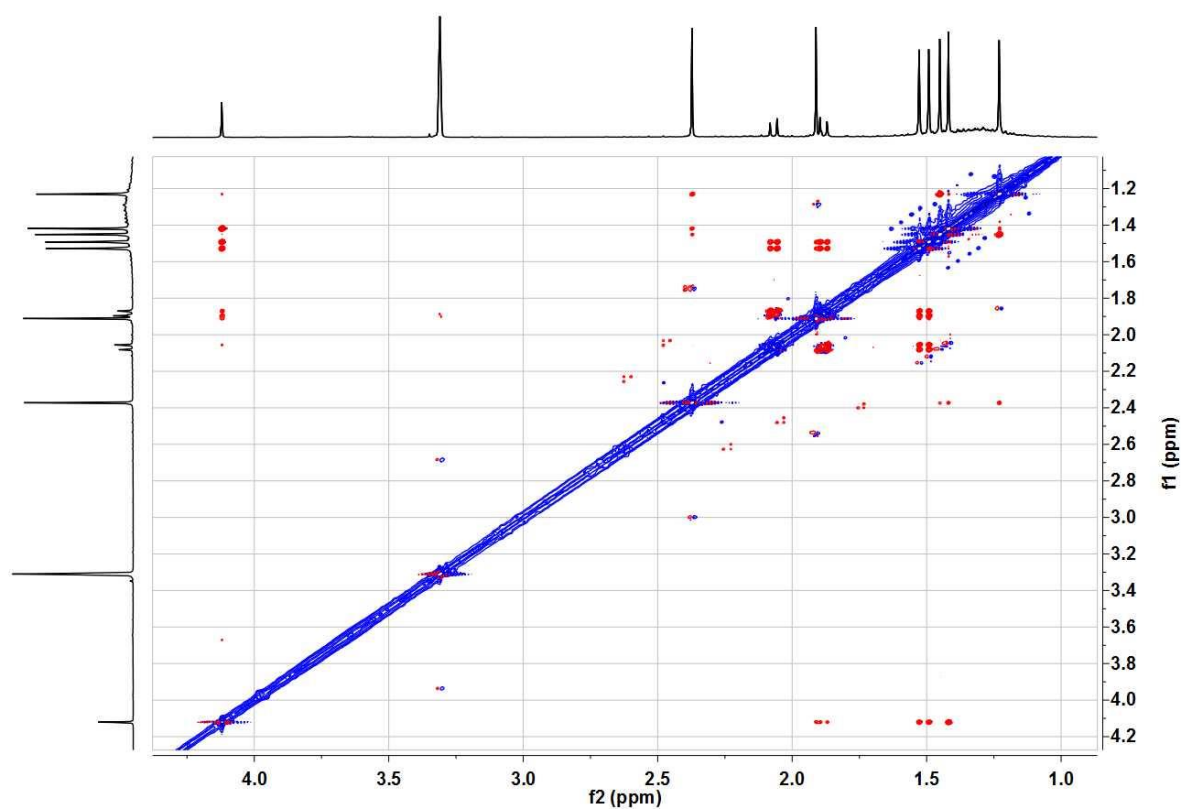


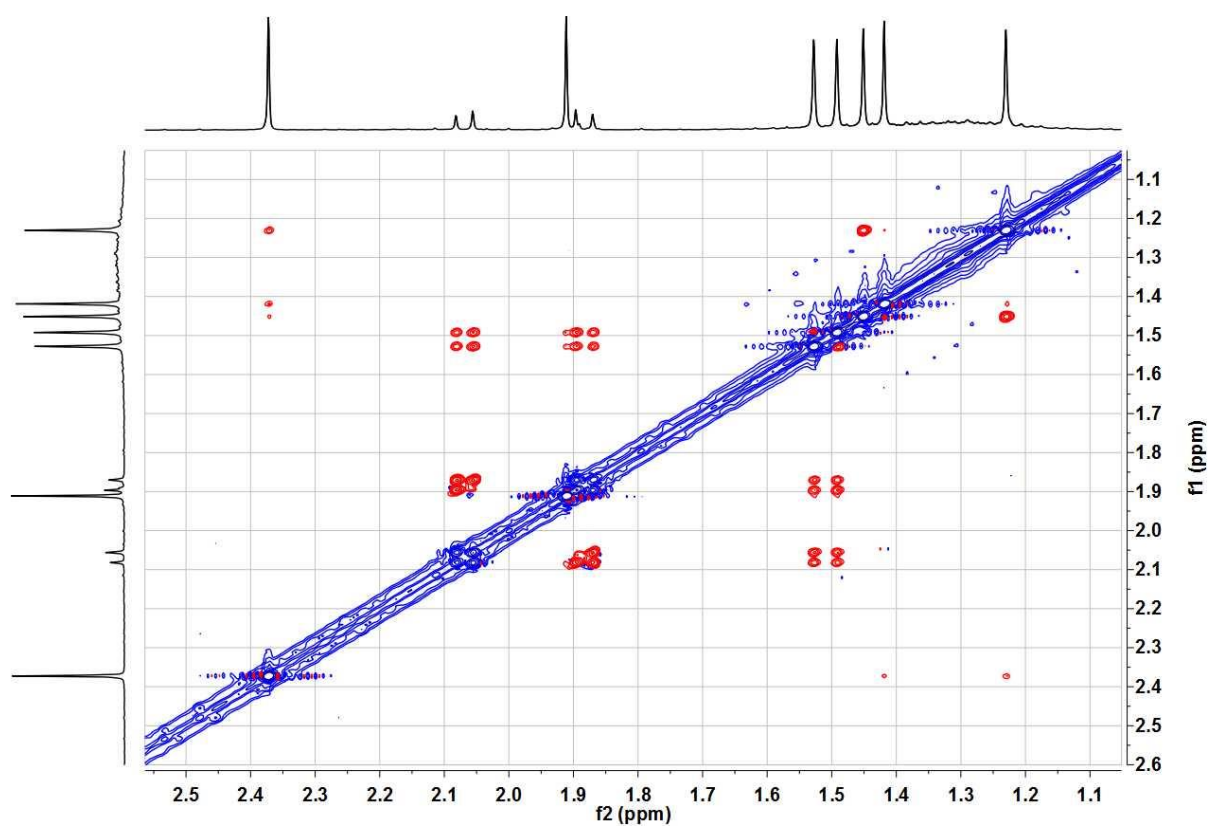
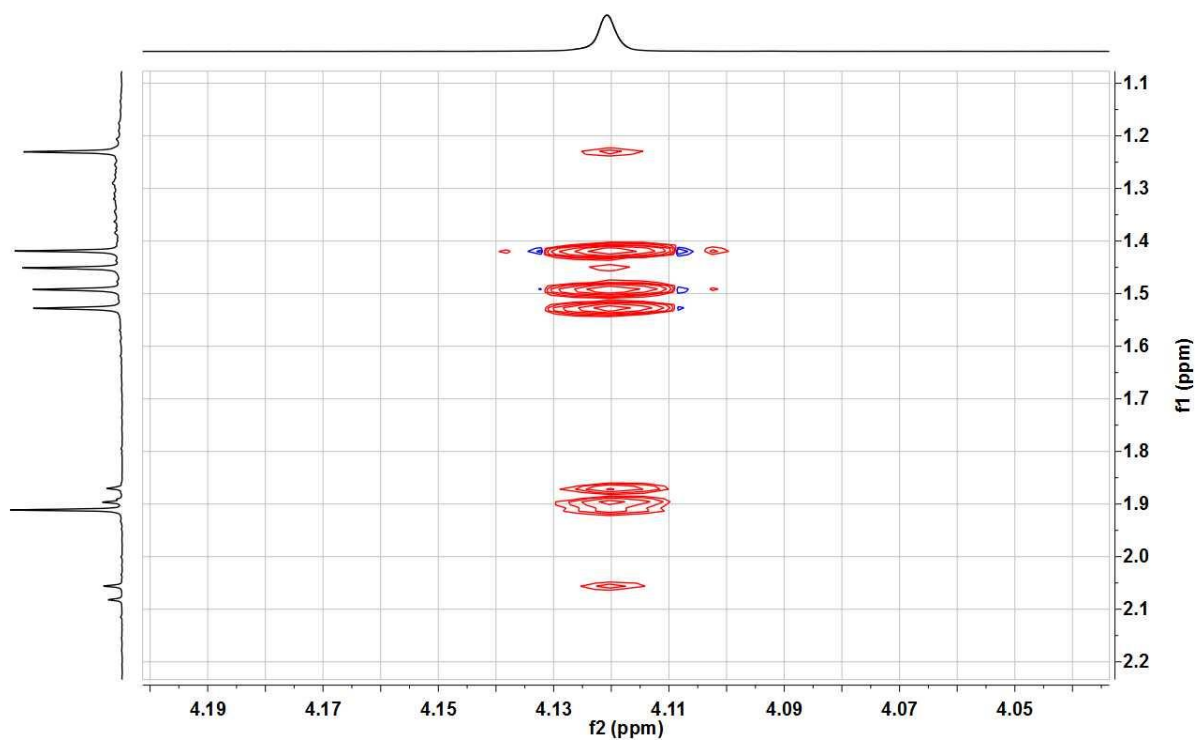




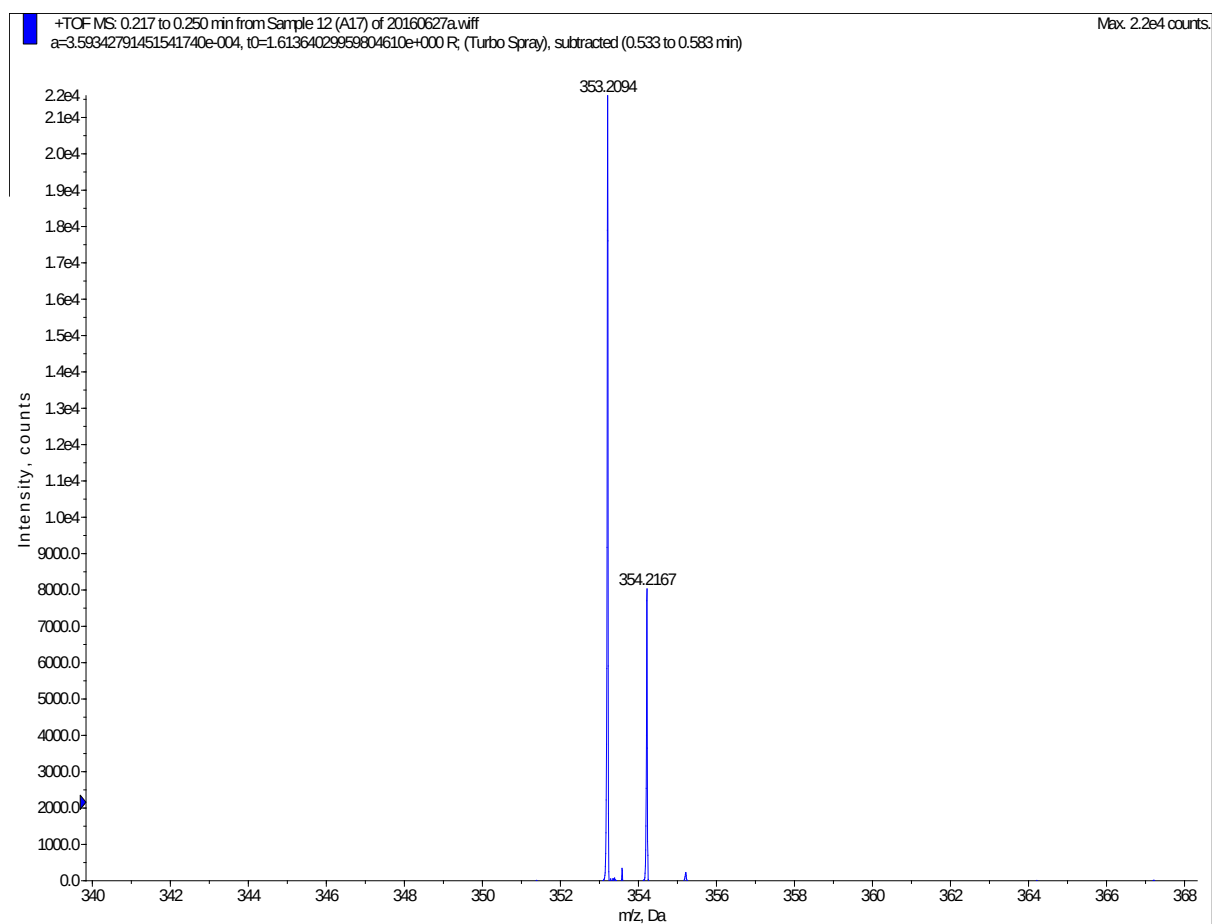


4.4.5 NOESY spectra of **4**.

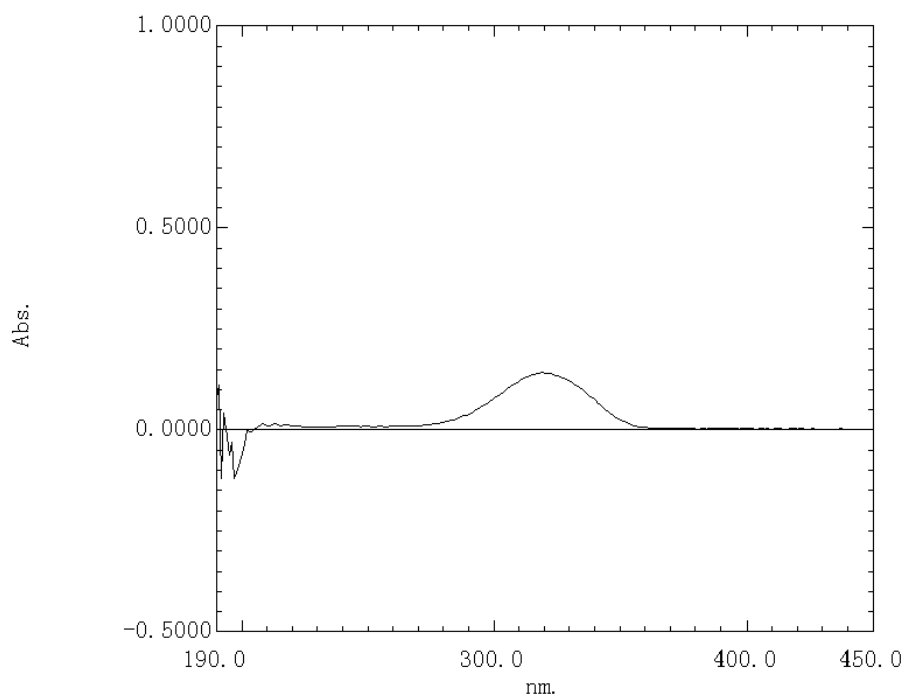




4.4.6 (+)HRESIMS of **4**.

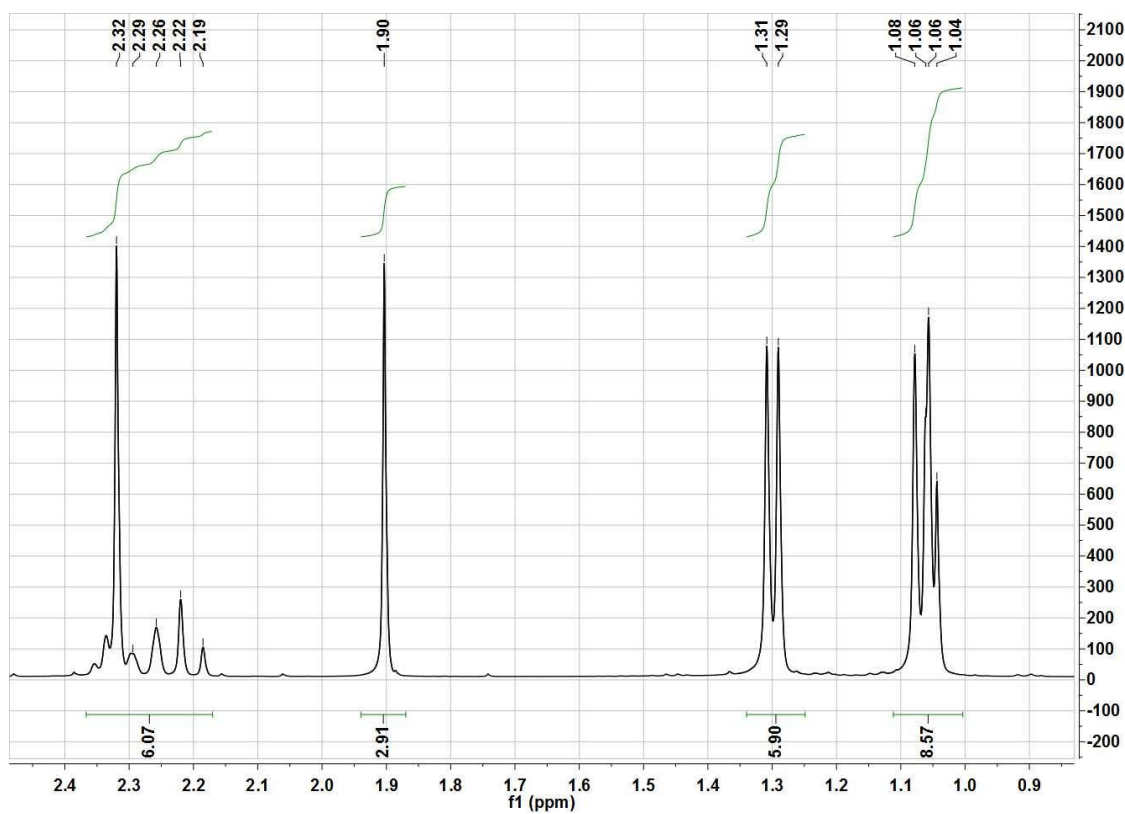
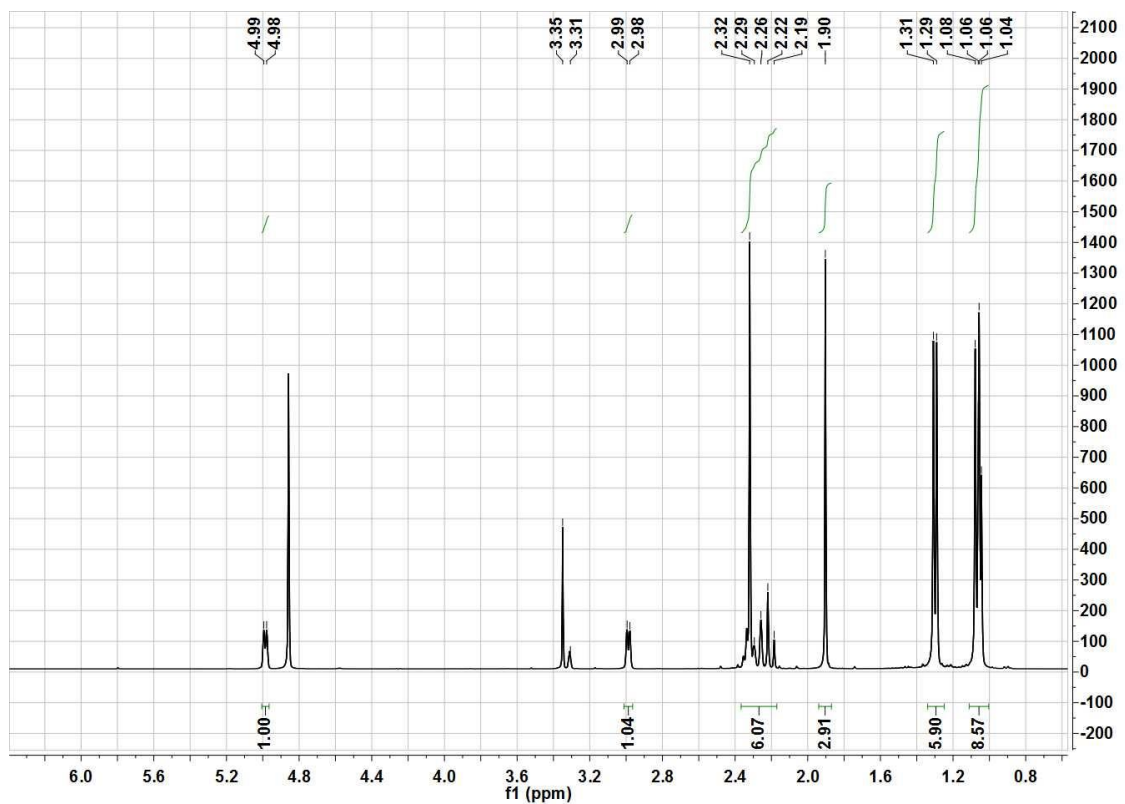


4.4.7 UV spectrum of **4**.

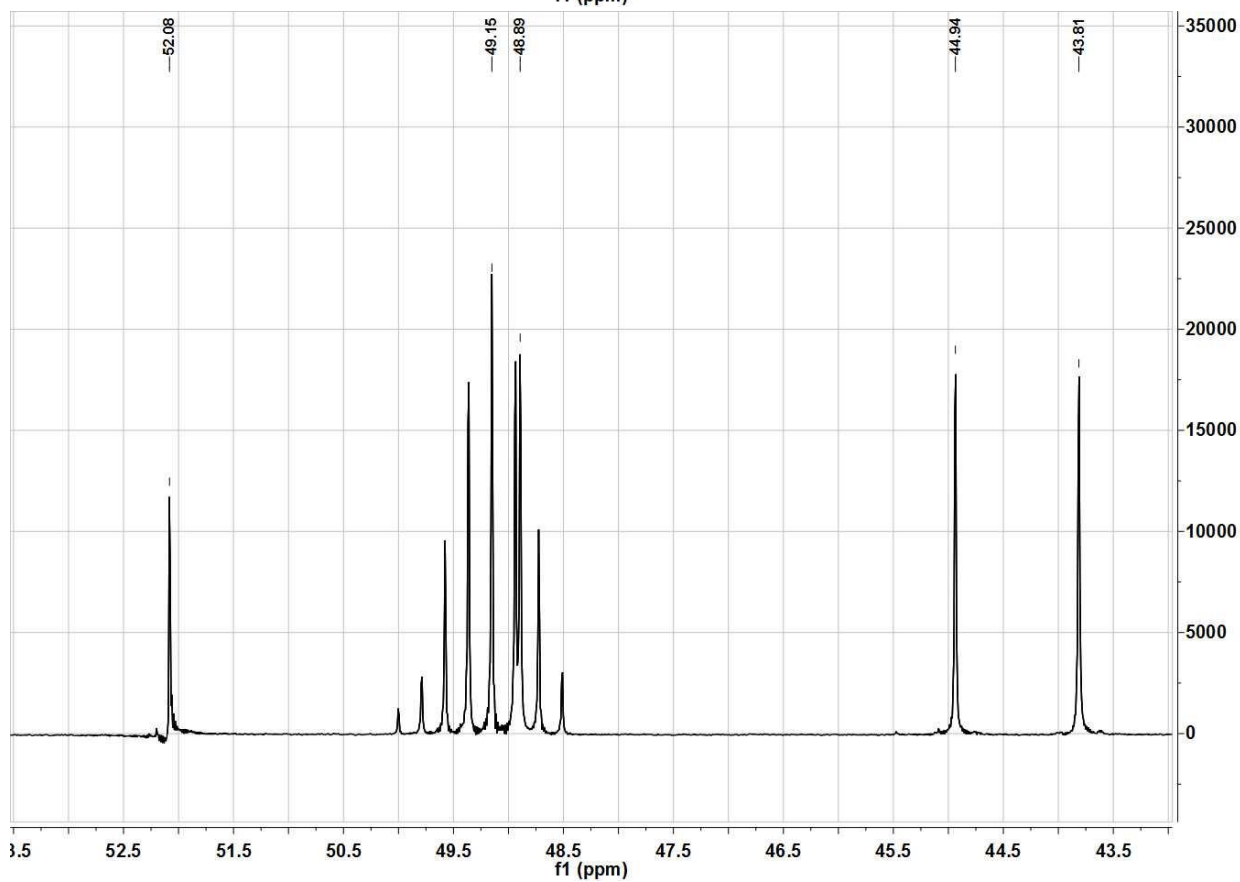
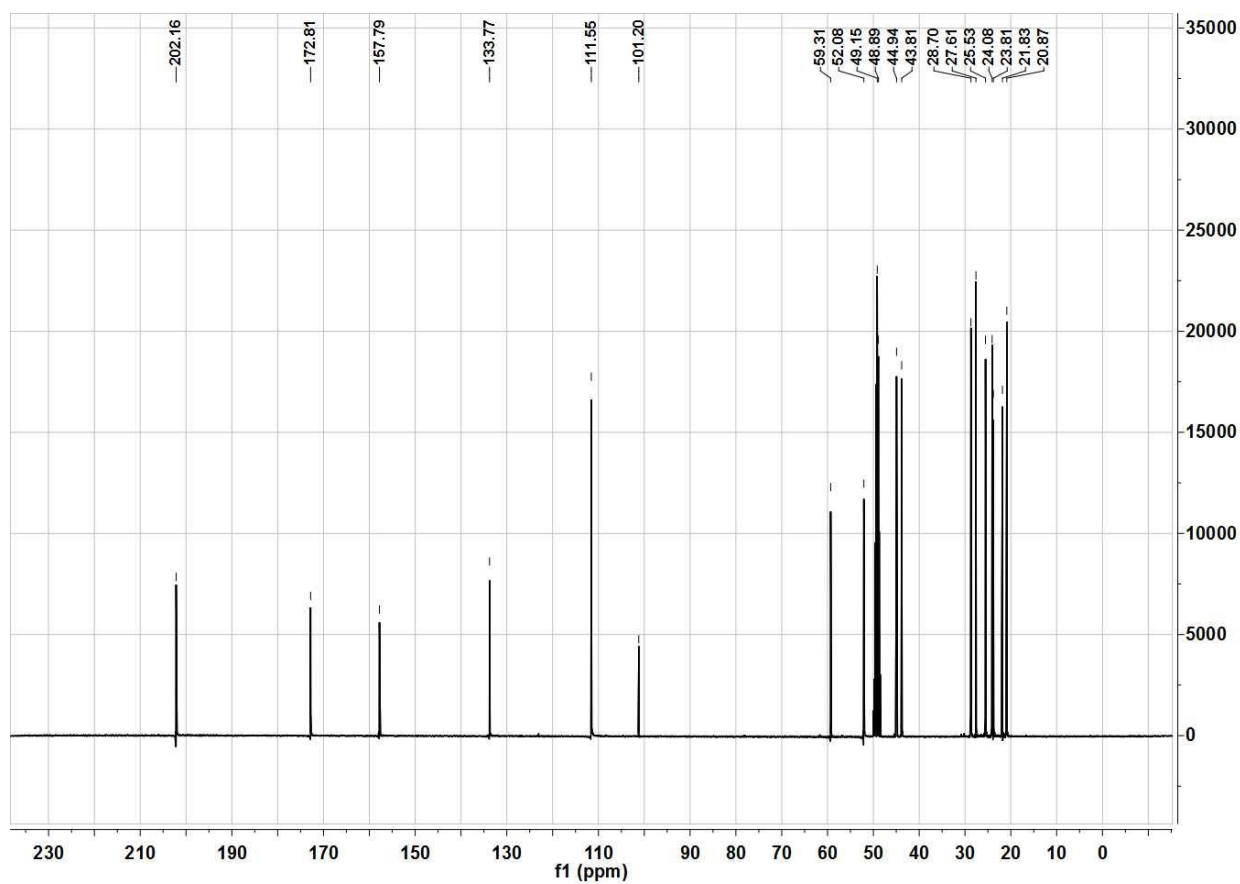


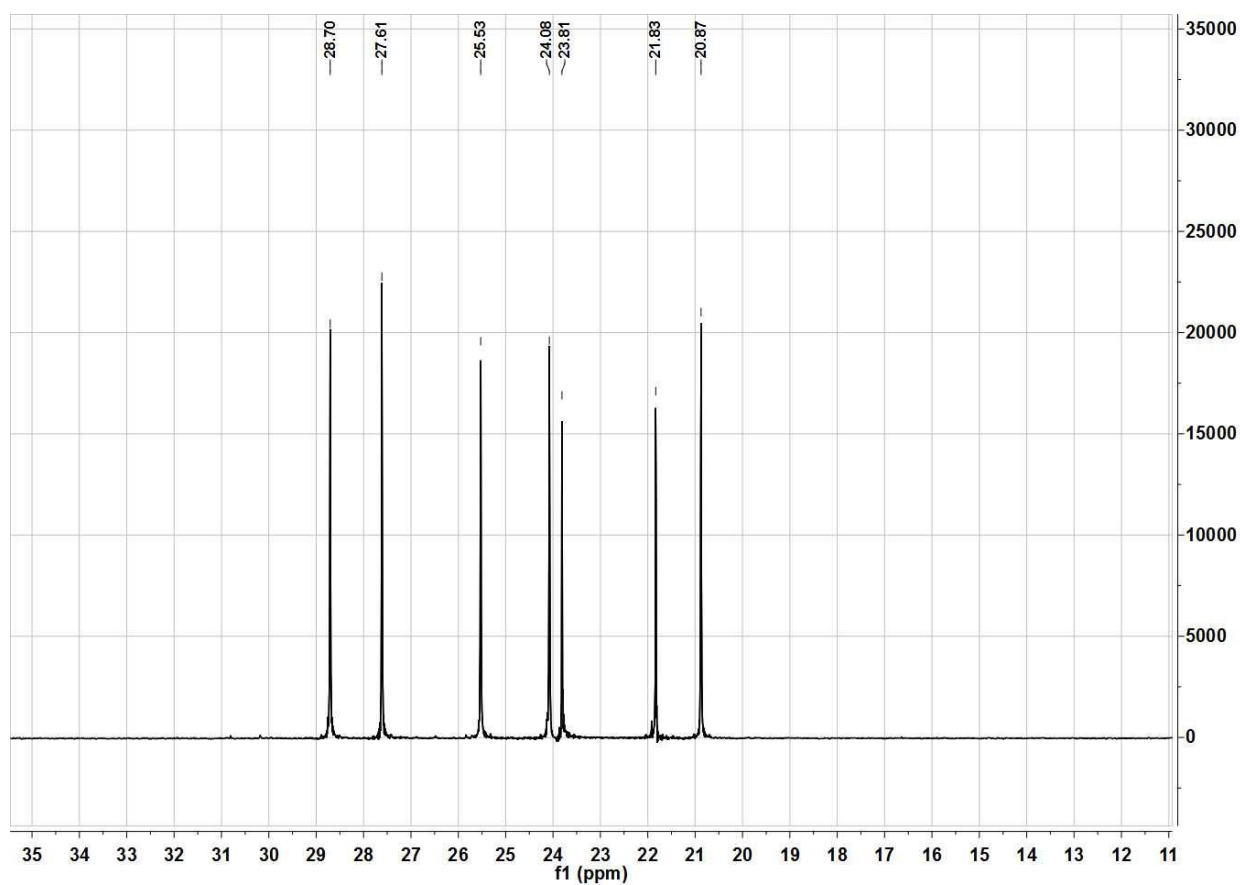
4.5 1D and 2D NMR of pyracyclumine E (5).

4.5.1 ^1H NMR (400 MHz, $\text{MeOH-}d_4$) spectra of 5.

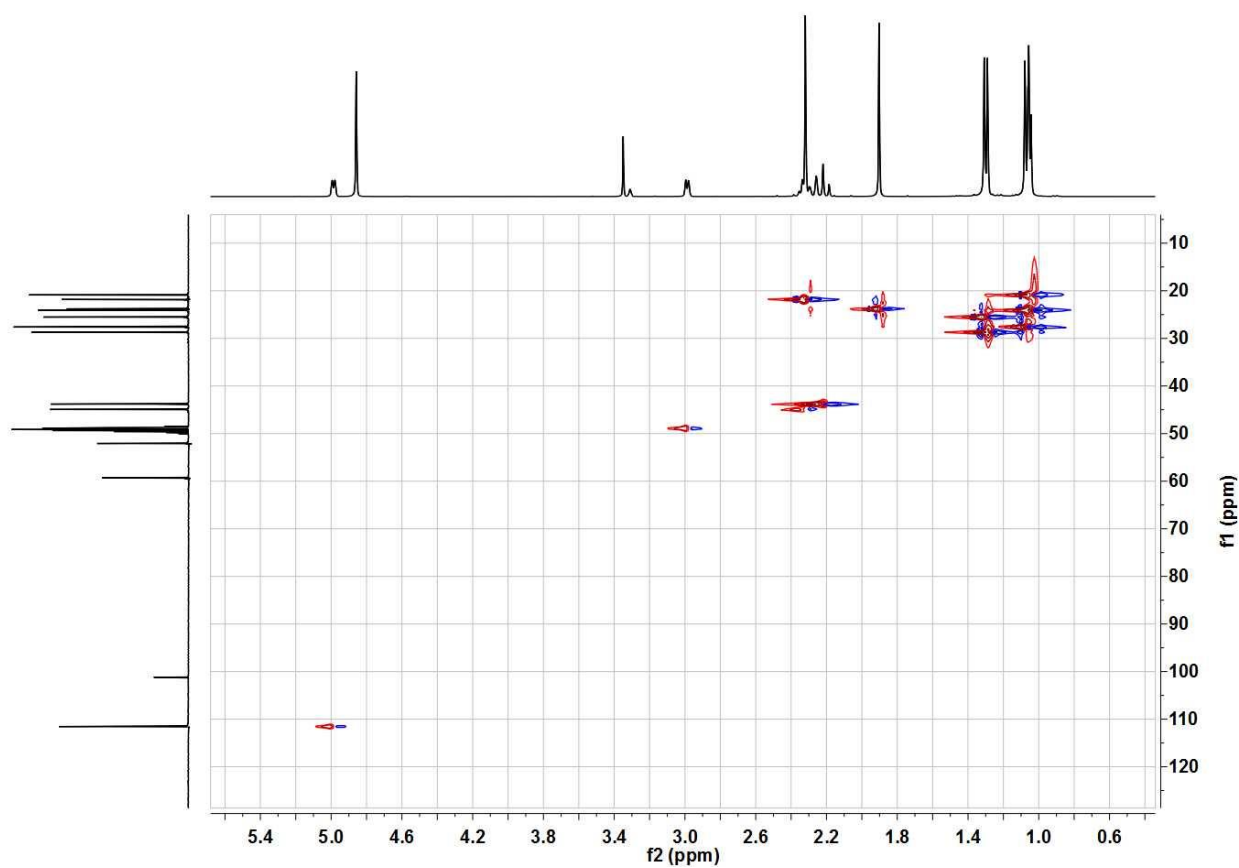


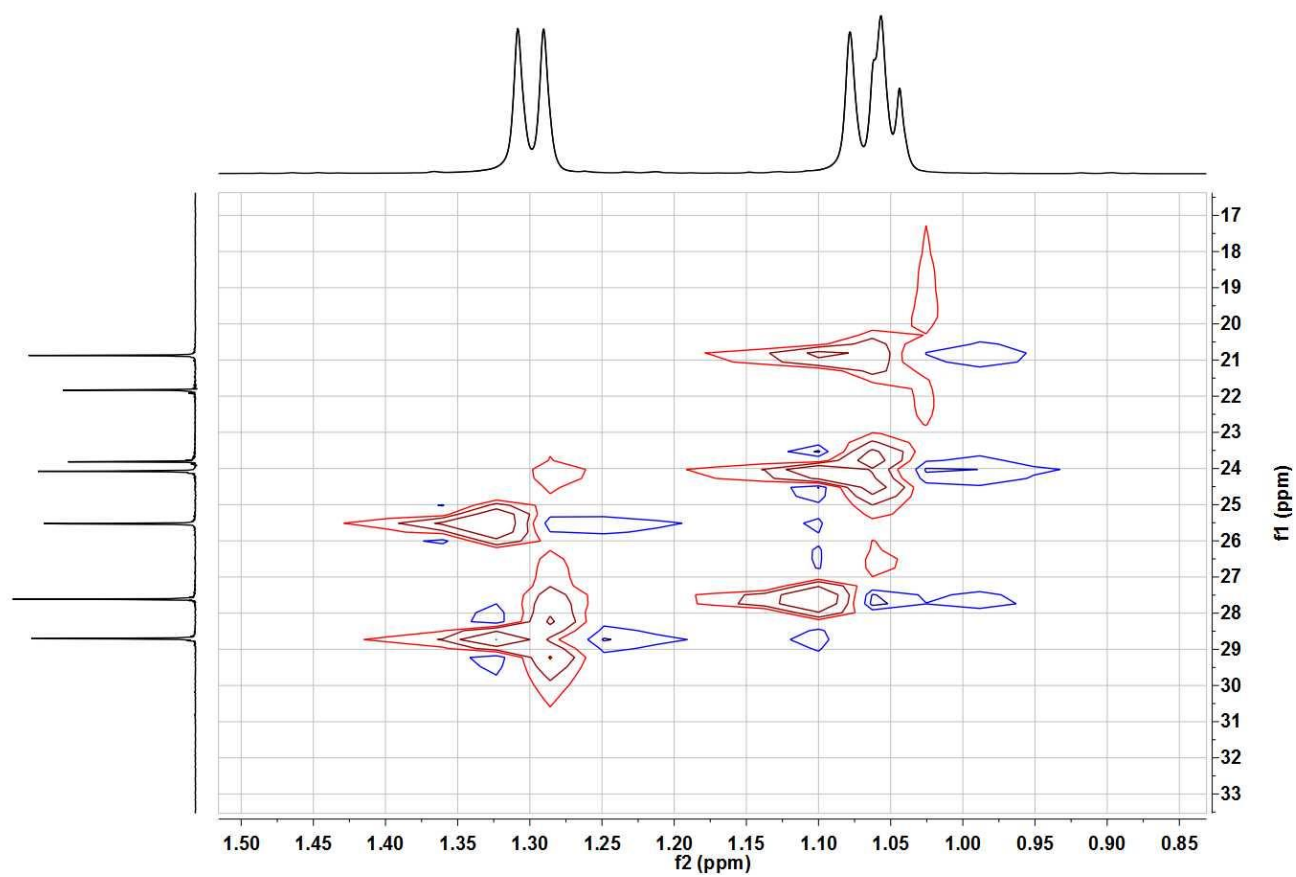
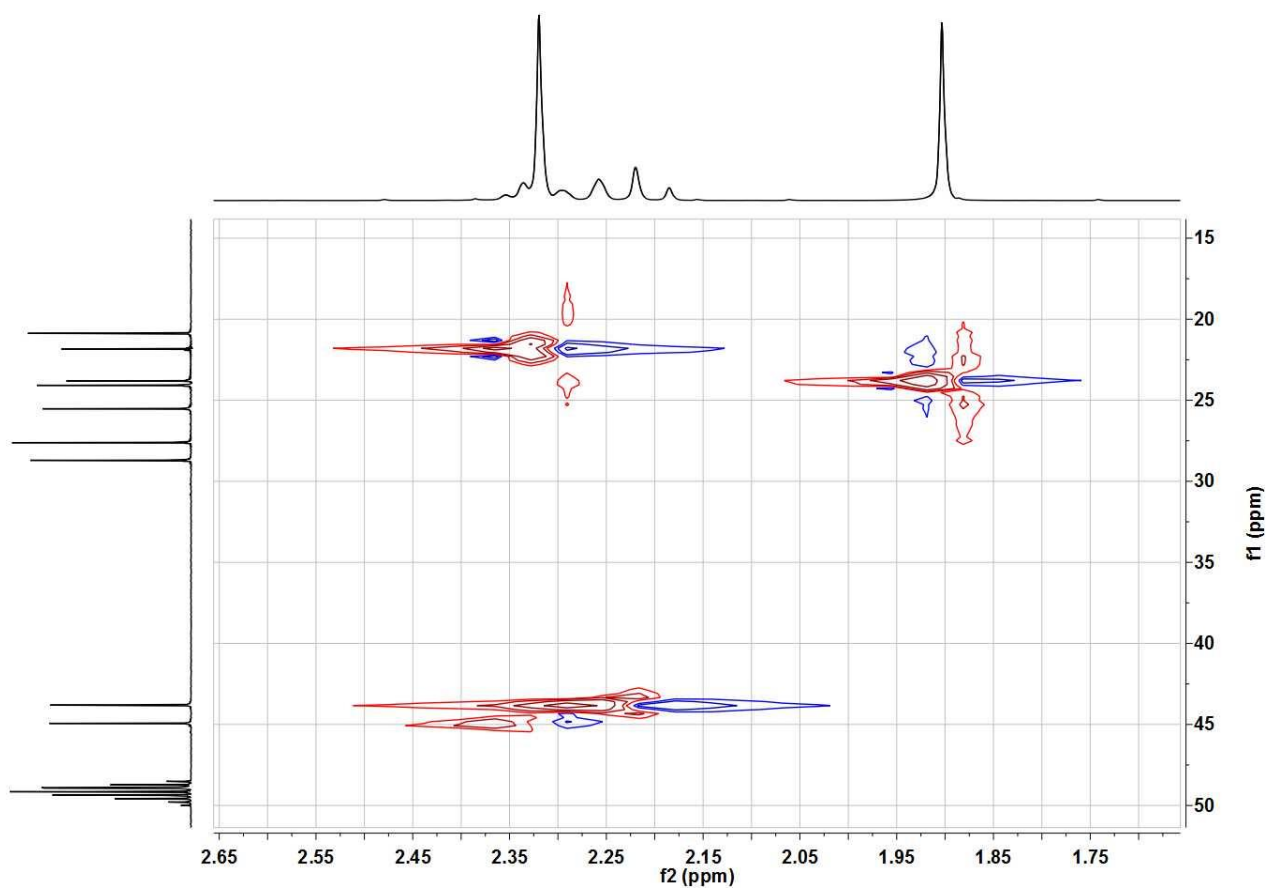
4.5.2 ^{13}C NMR (101 MHz, $\text{MeOH-}d_4$) spectra of 5.



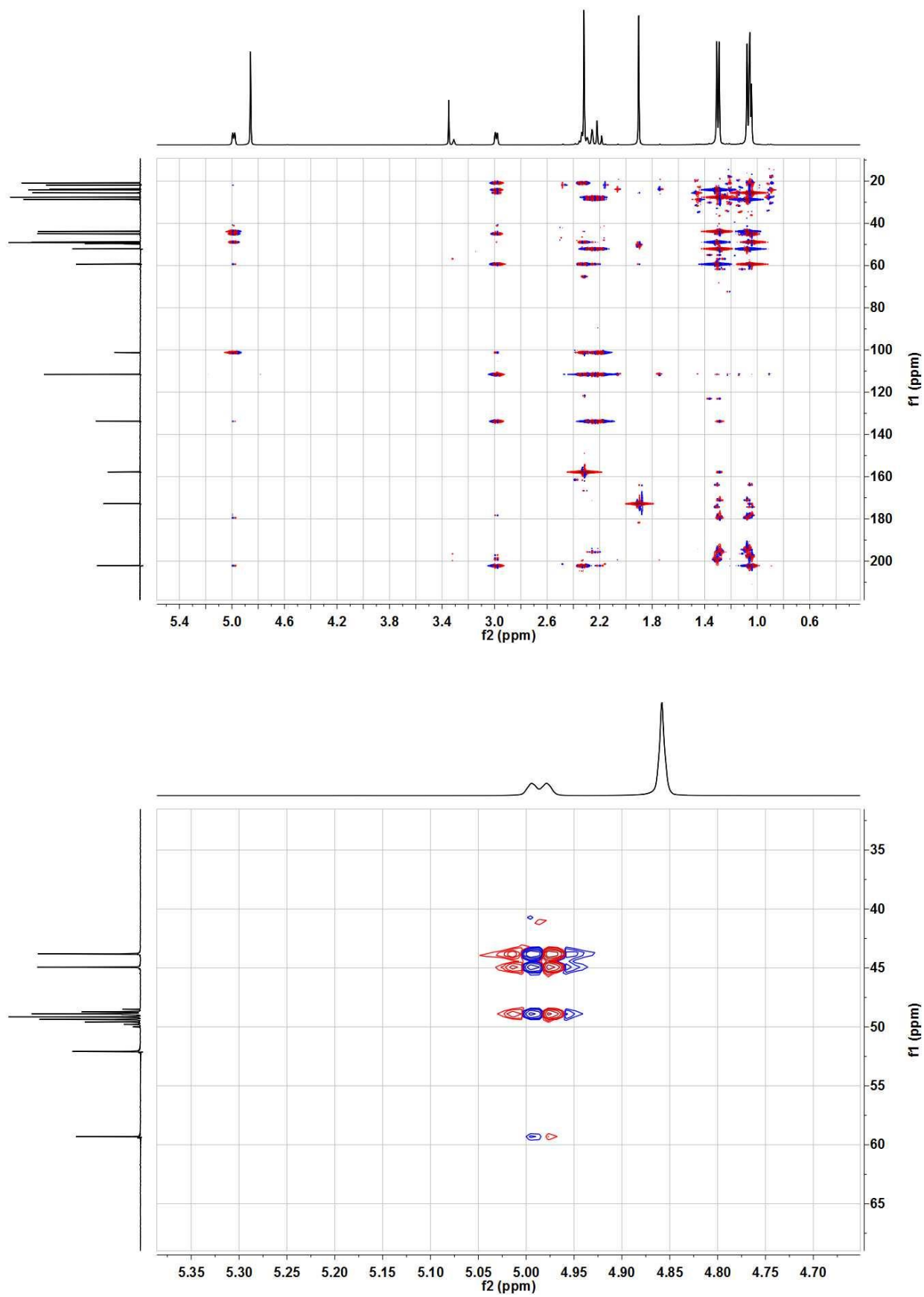


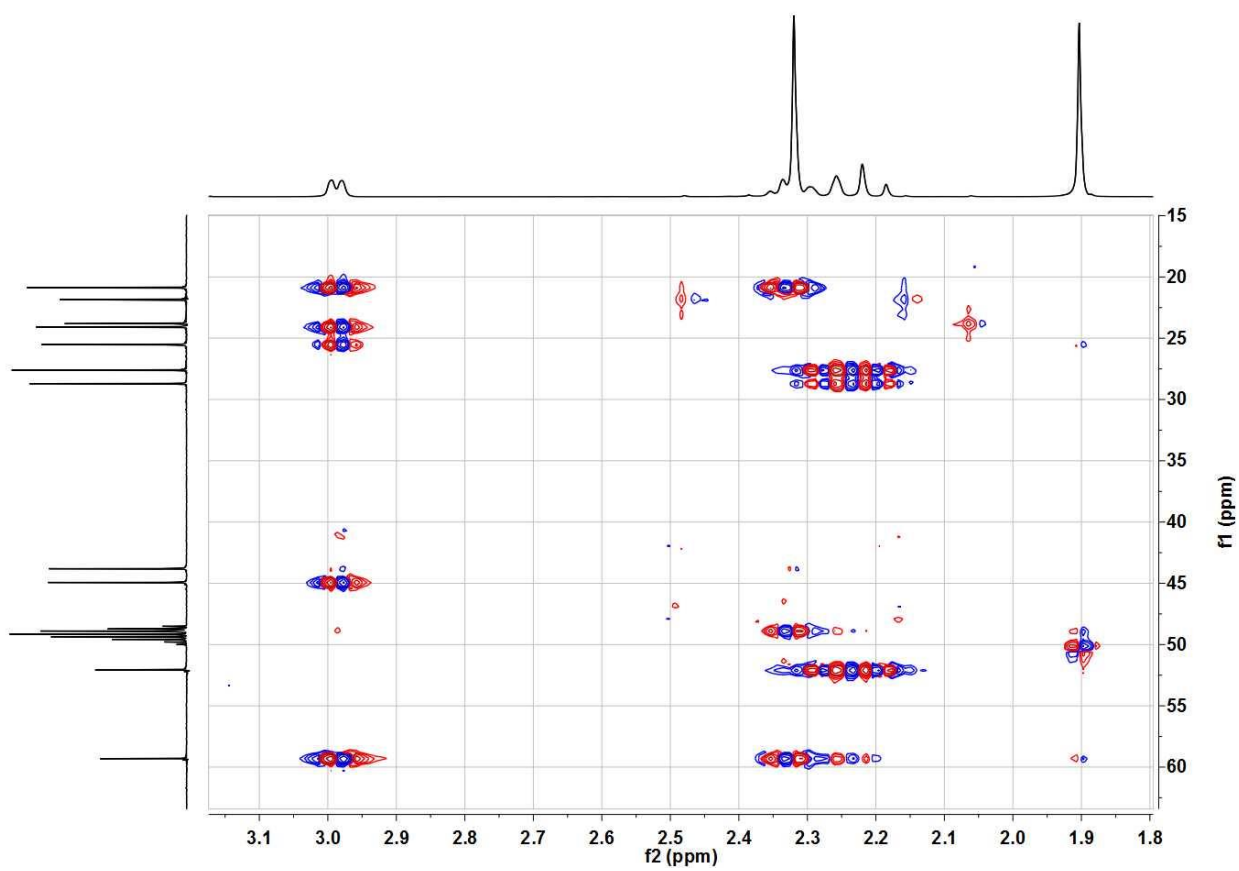
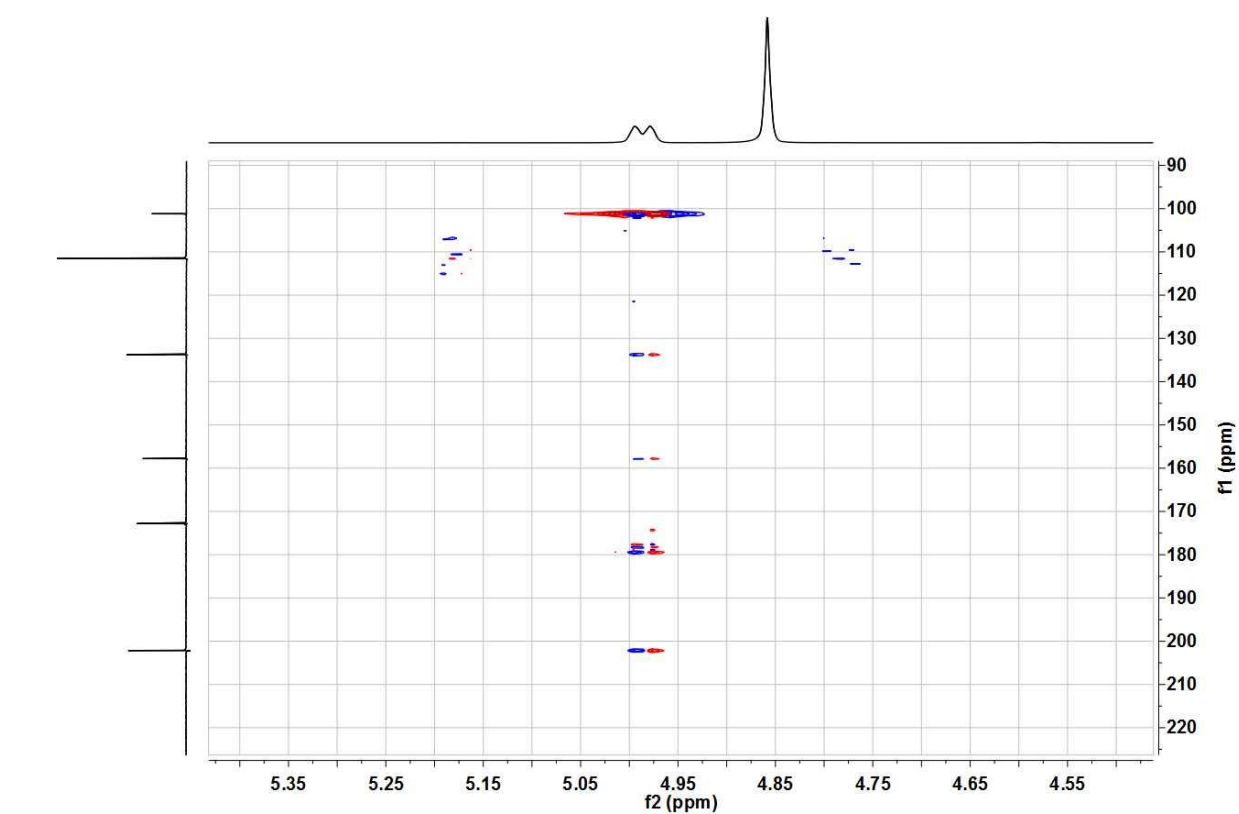
4.5.3 HSQC spectra of 5.

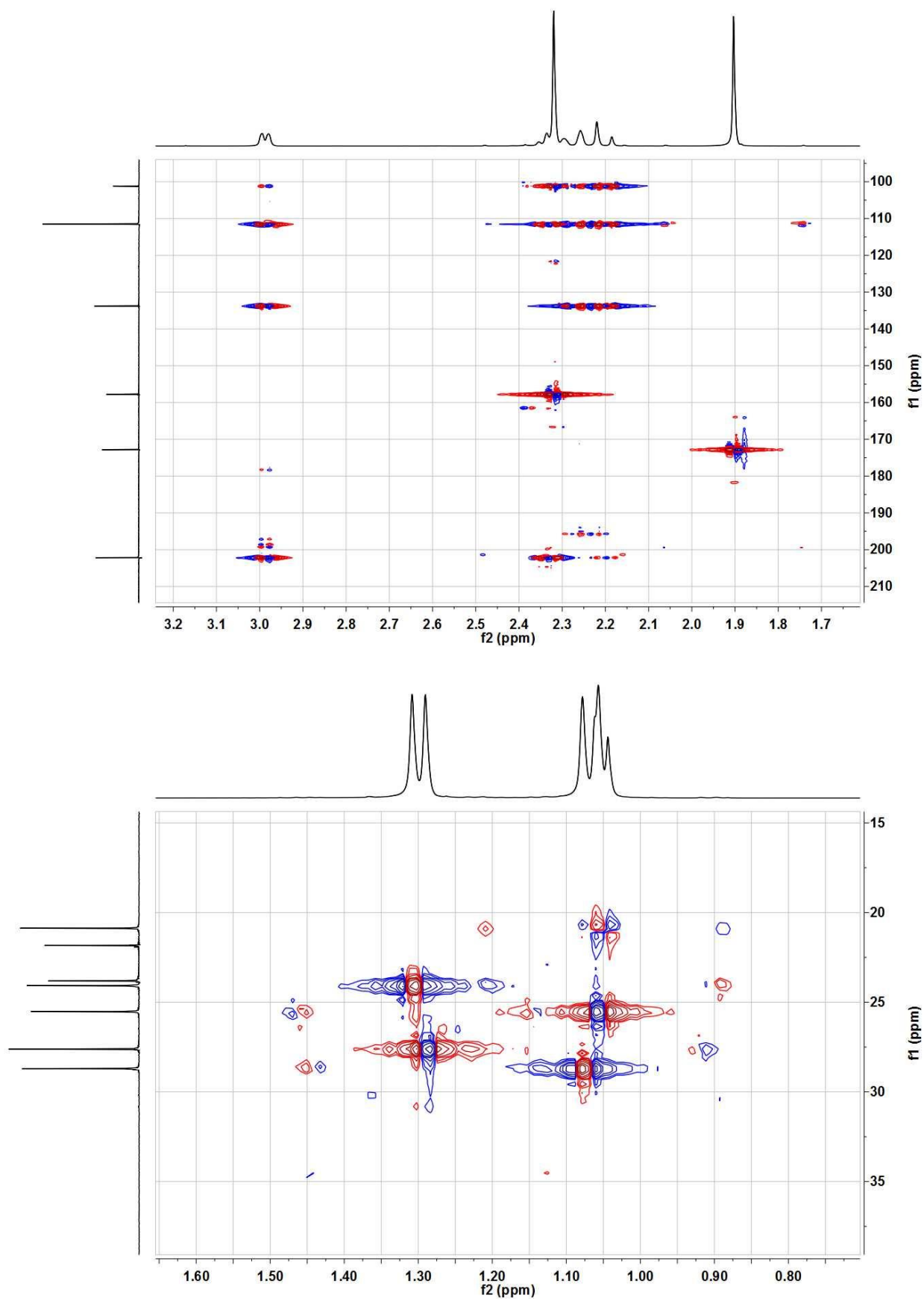


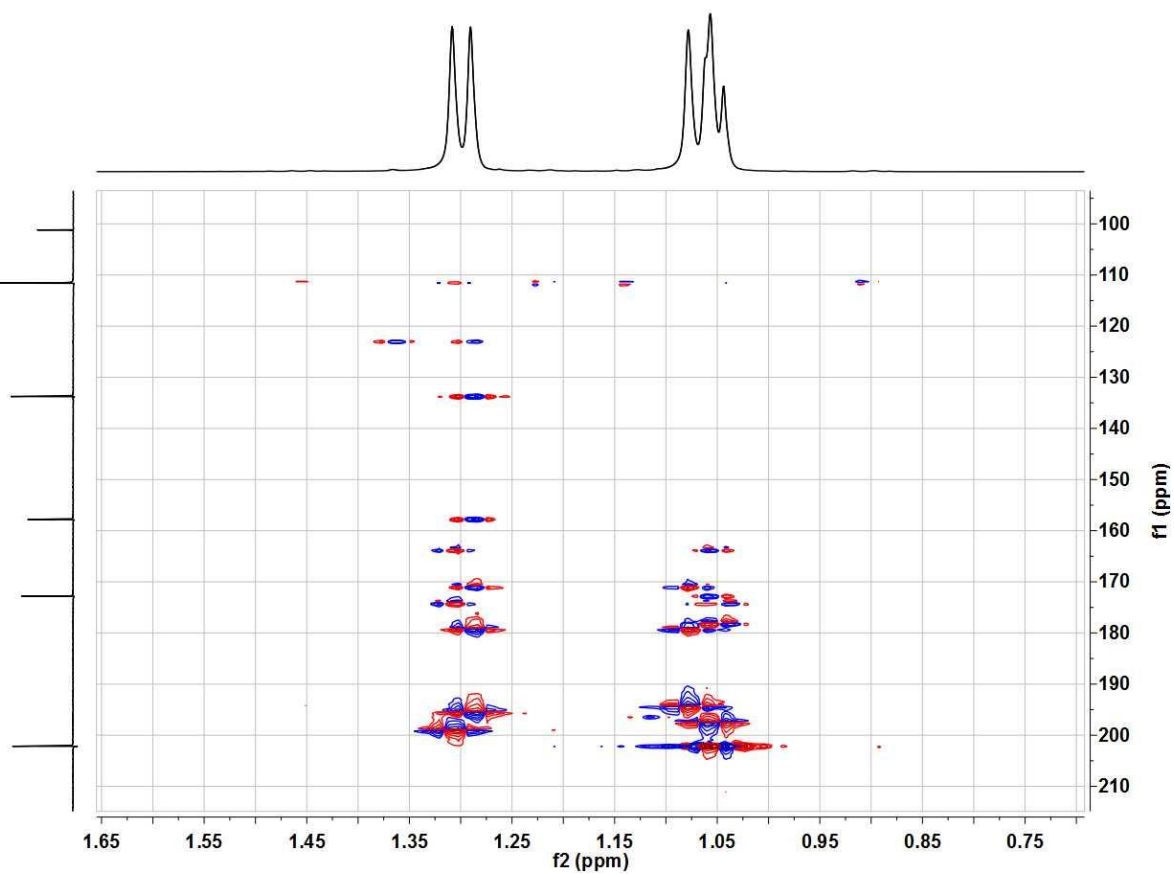
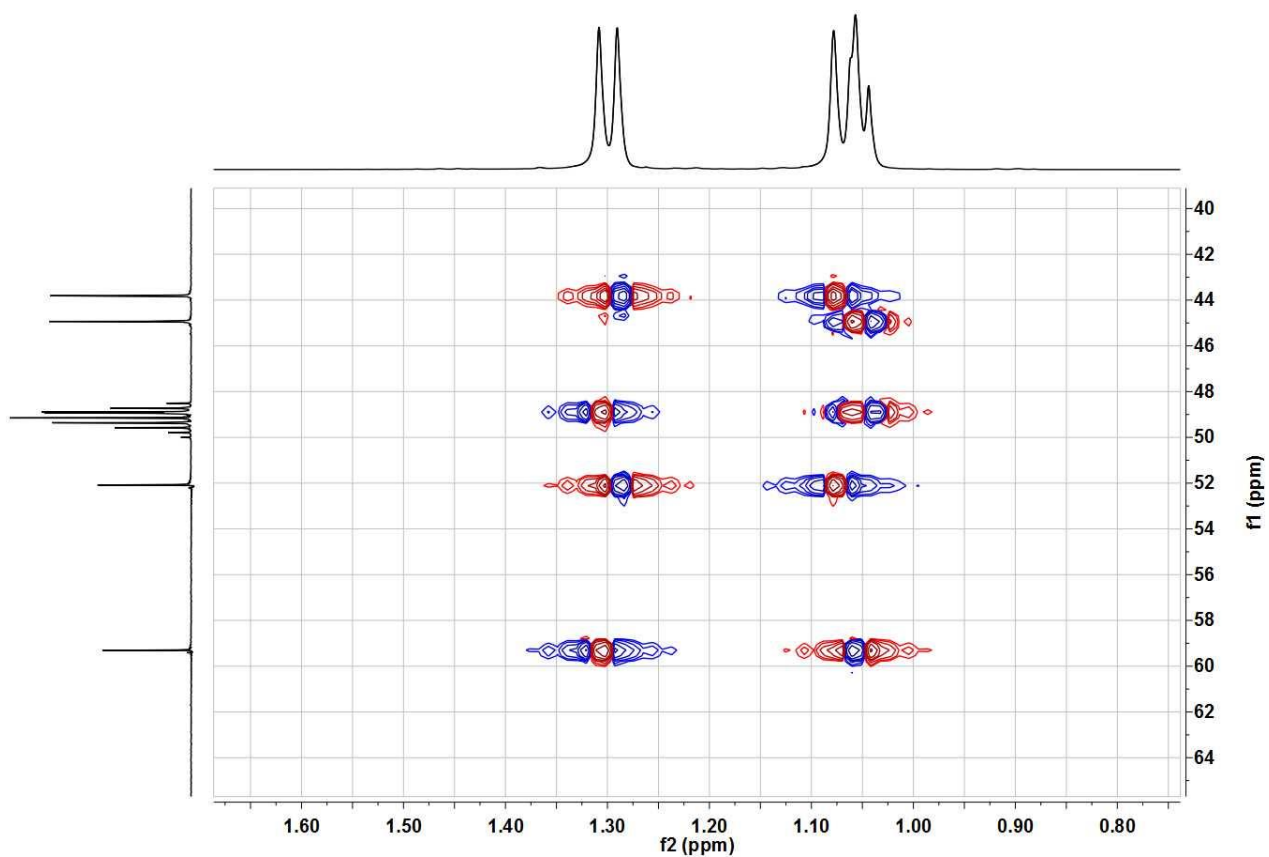


4.5.4 HMBC spectra of 5.

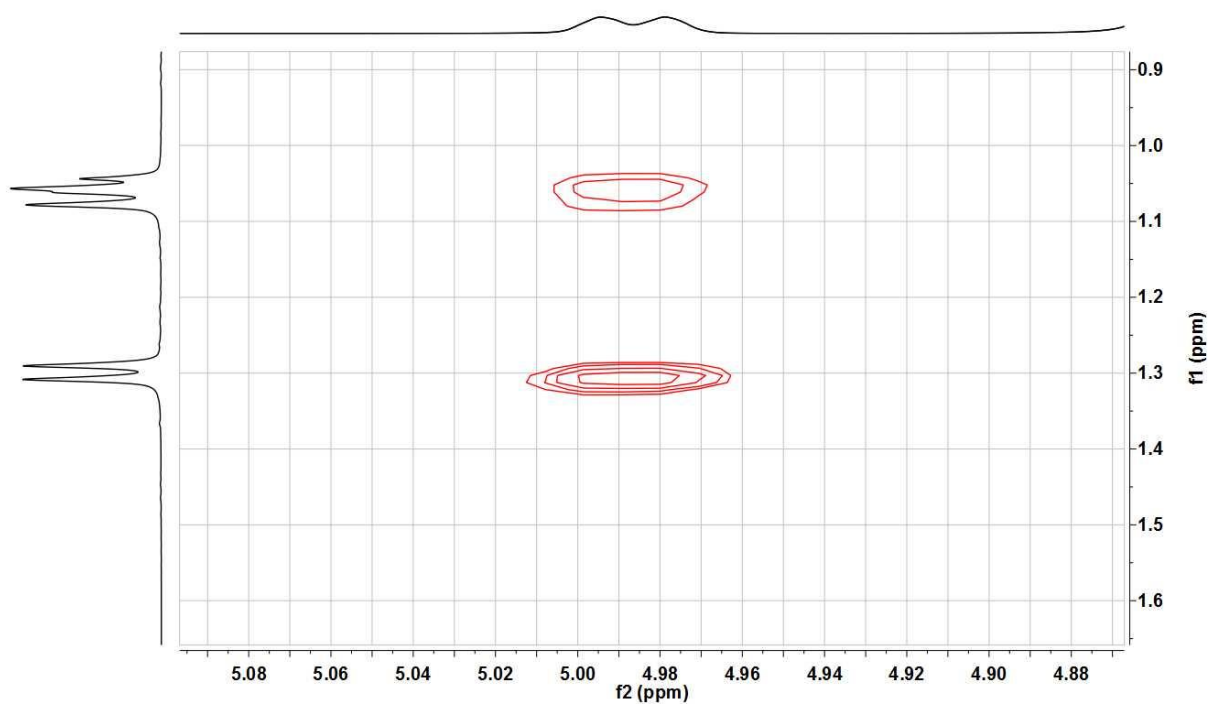
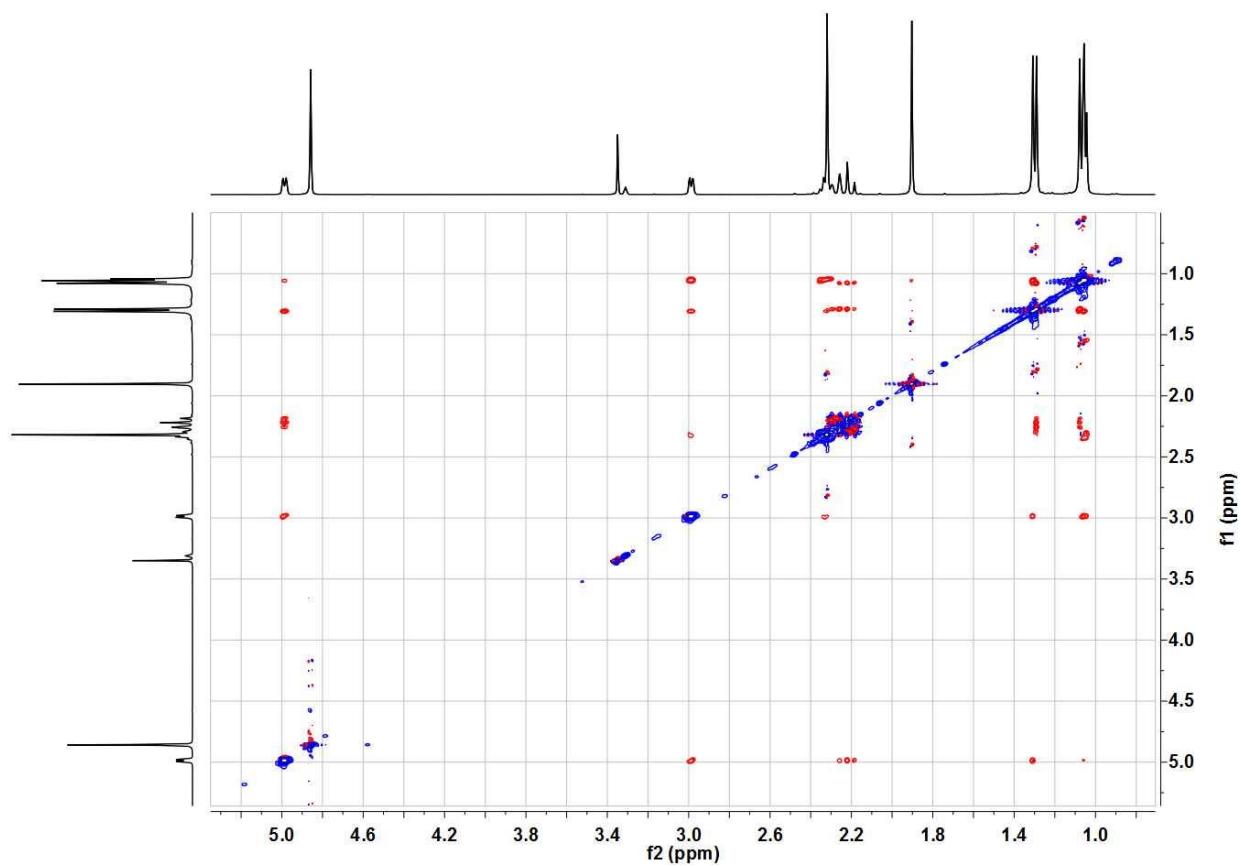


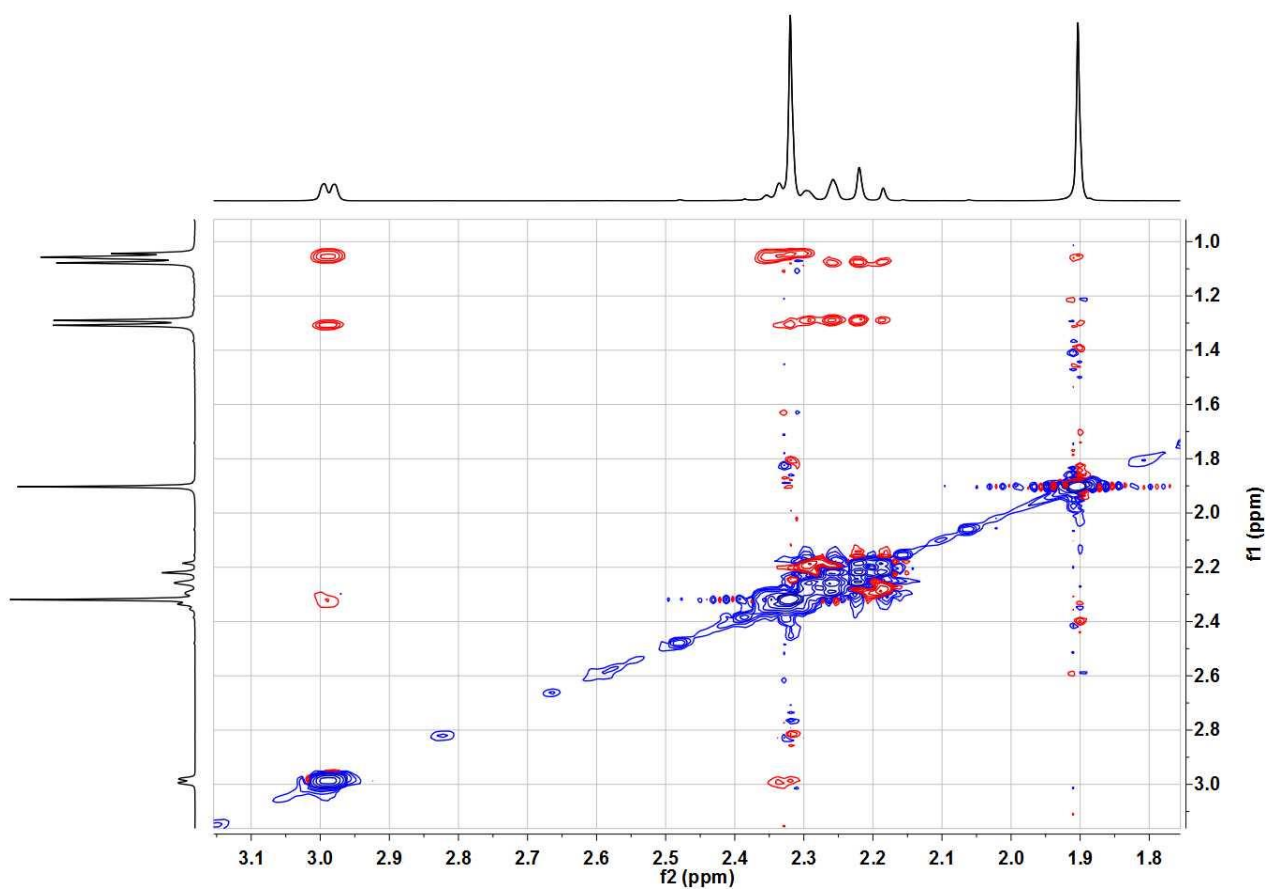
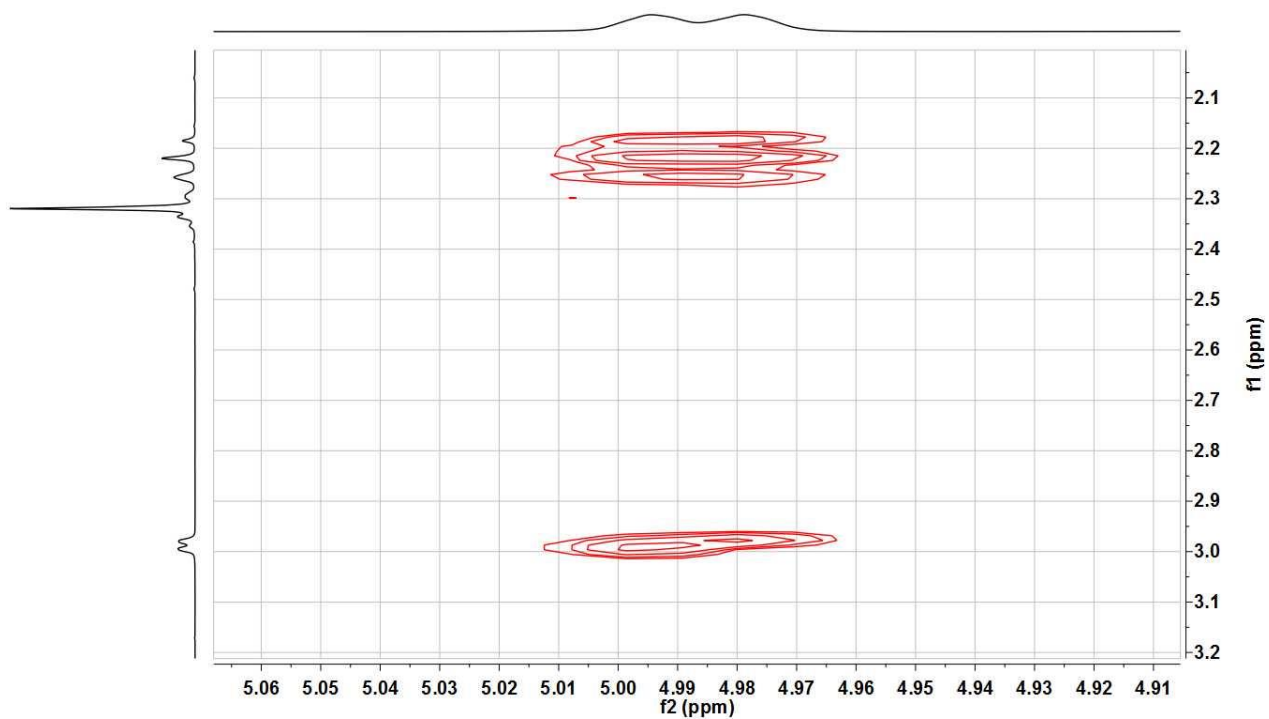




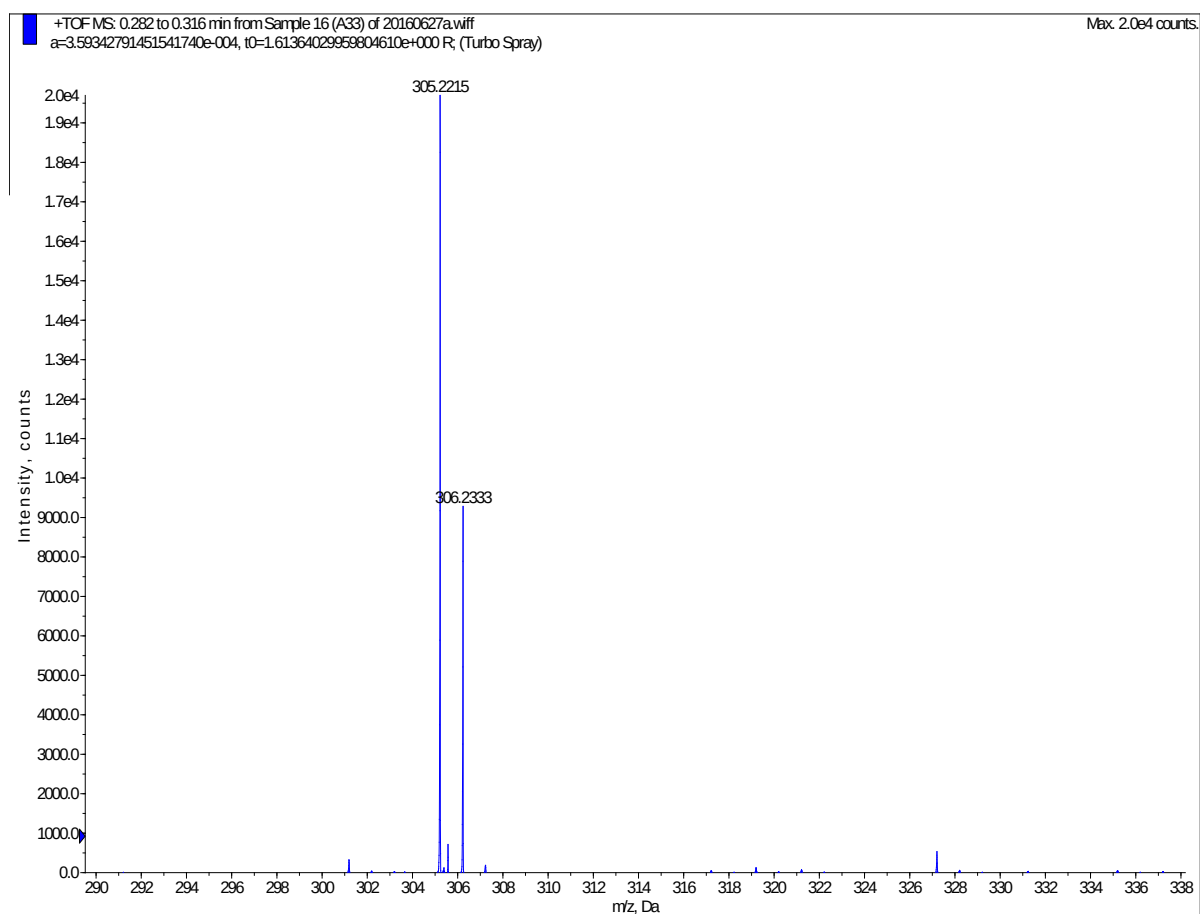


4.5.5 NOESY spectra of 5.

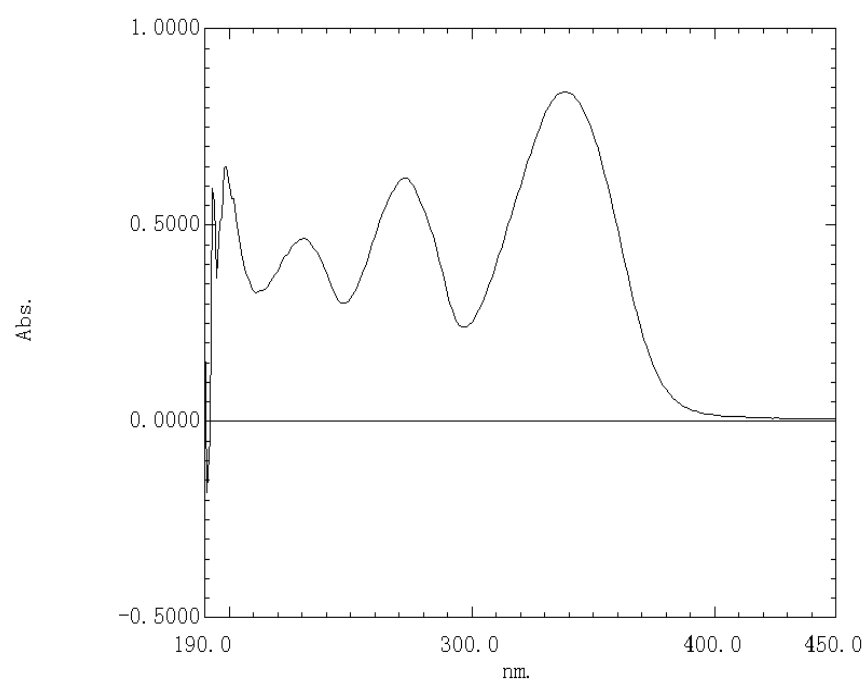




4.5.7 (+)HRESIMS of 5.

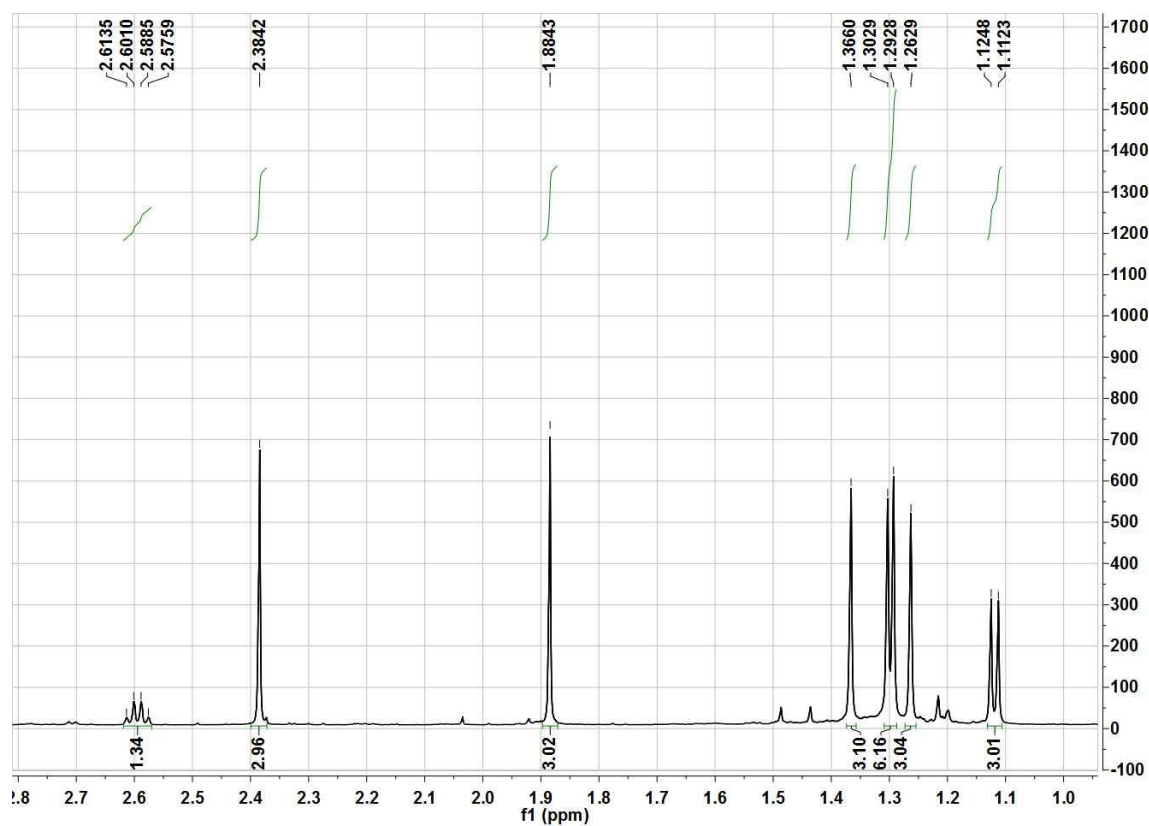
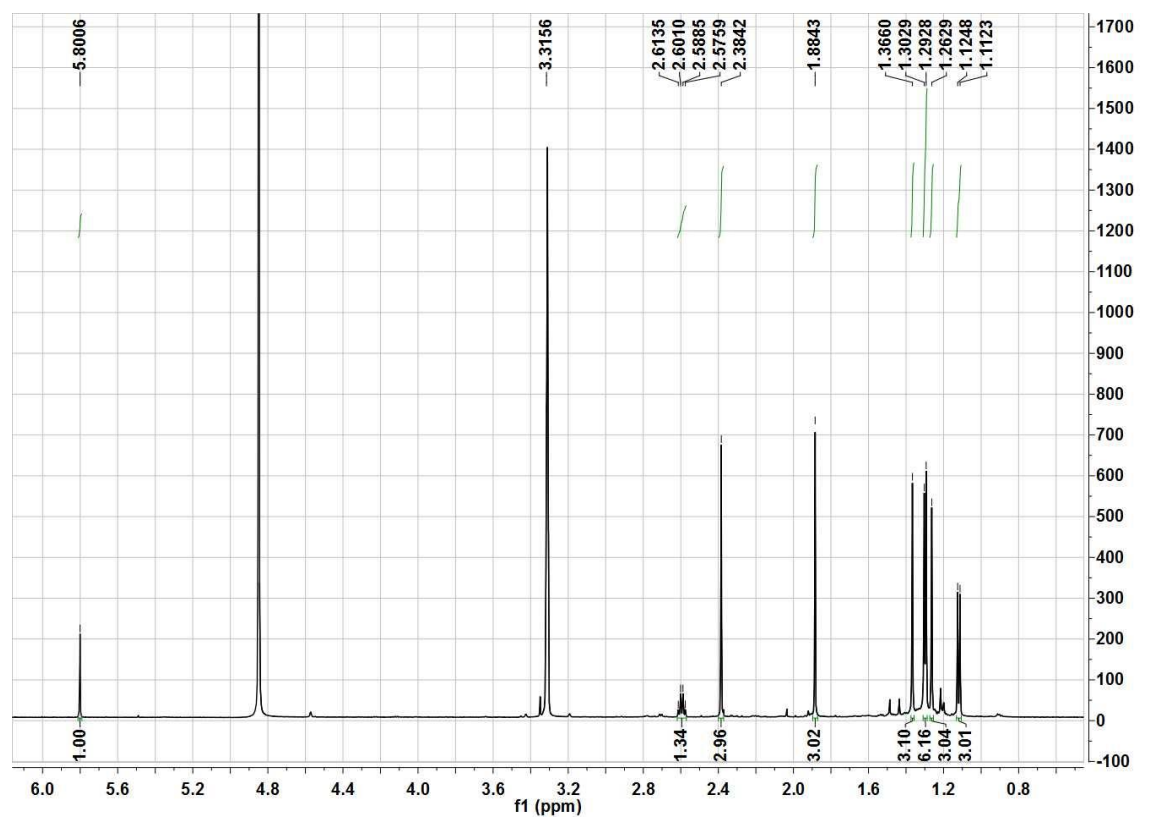


4.5.8 UV spectrum of 5.

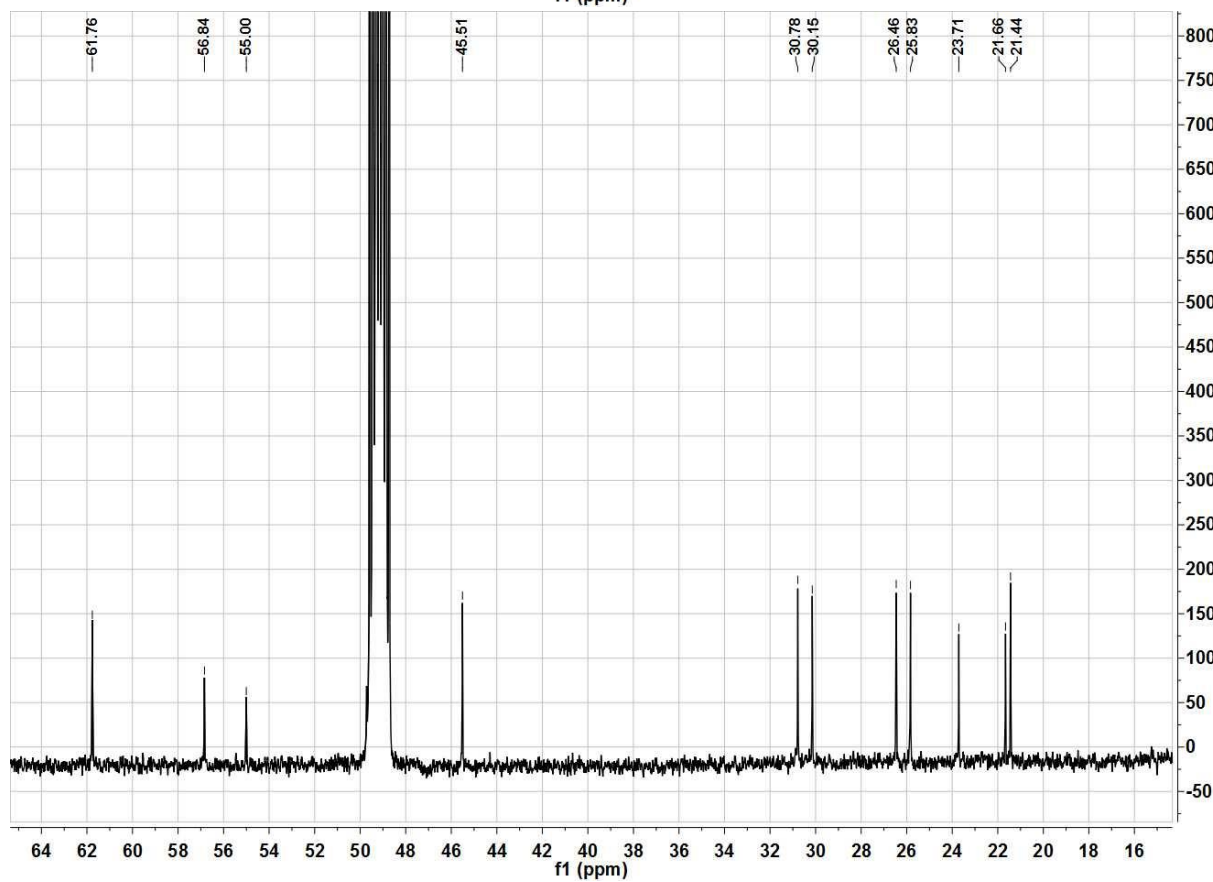
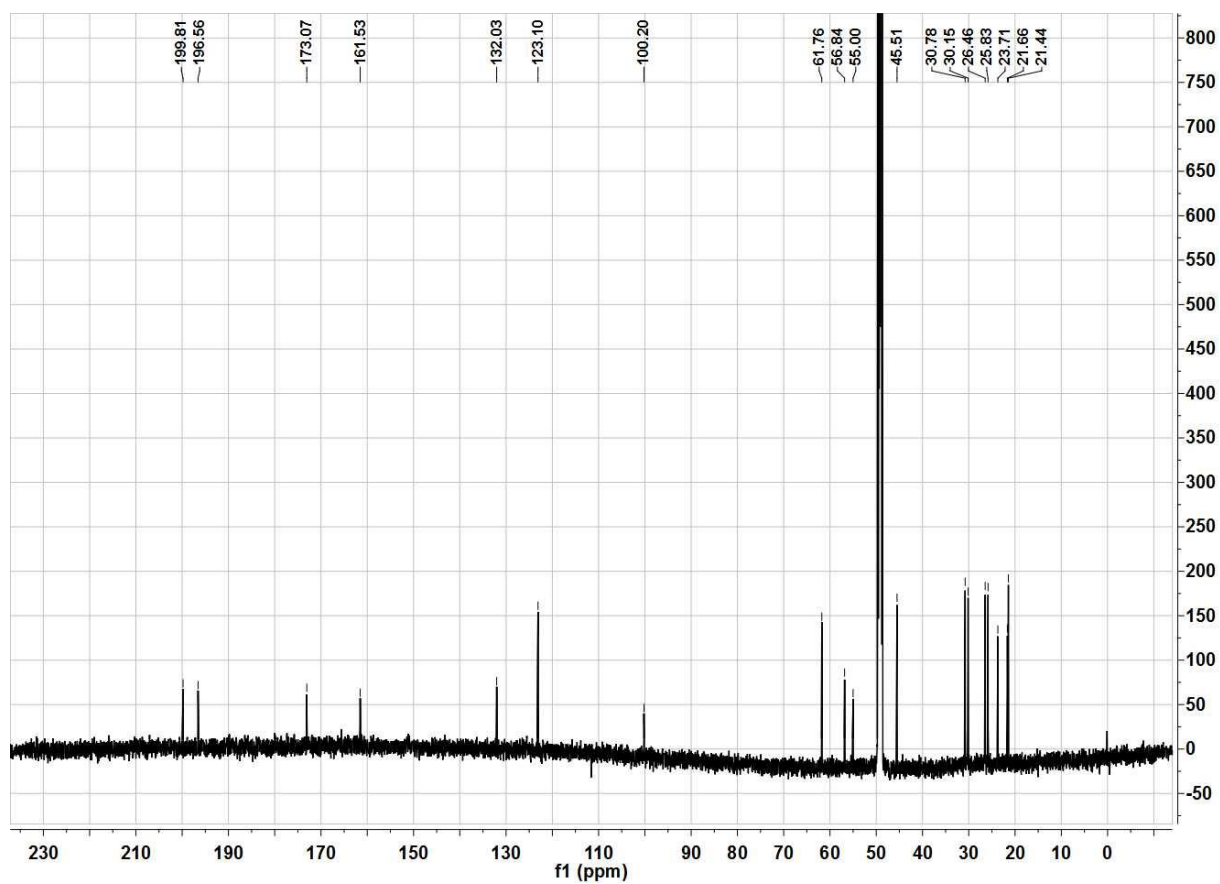


4.6 1D and 2D NMR of pyracyclumine F (6).

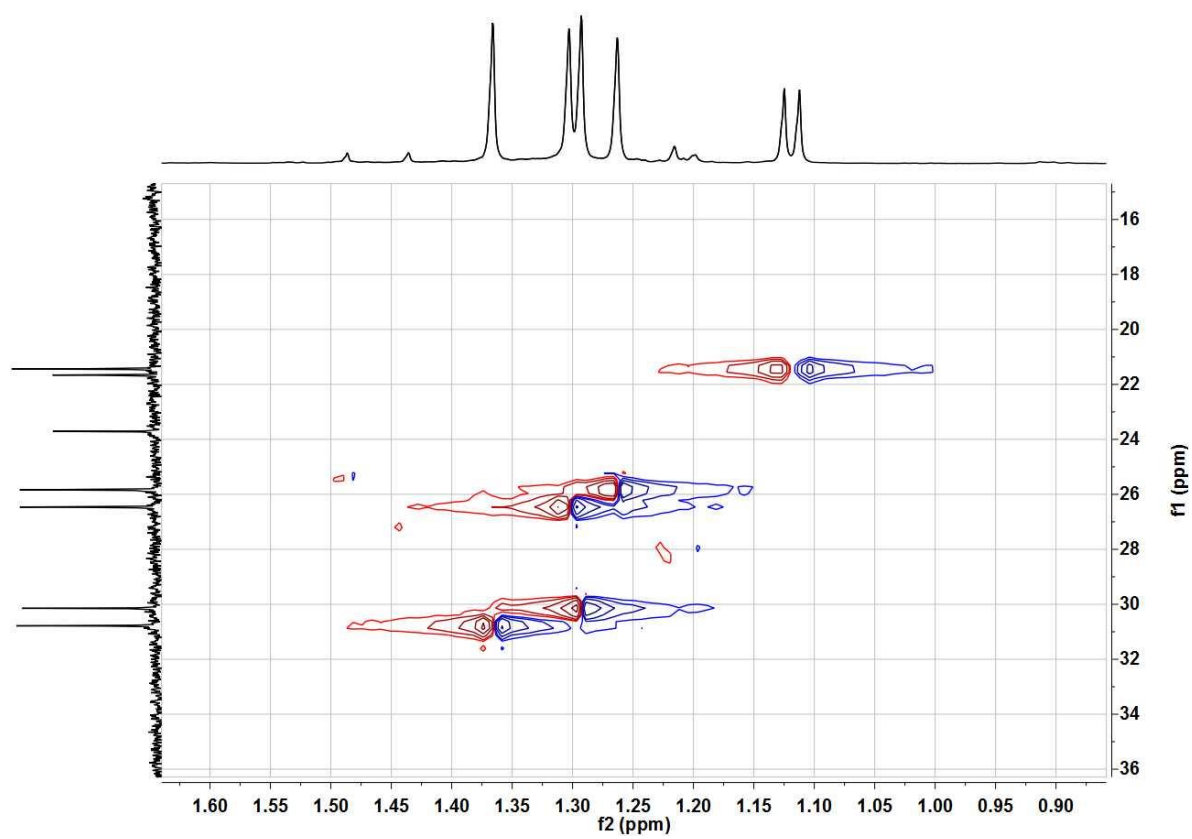
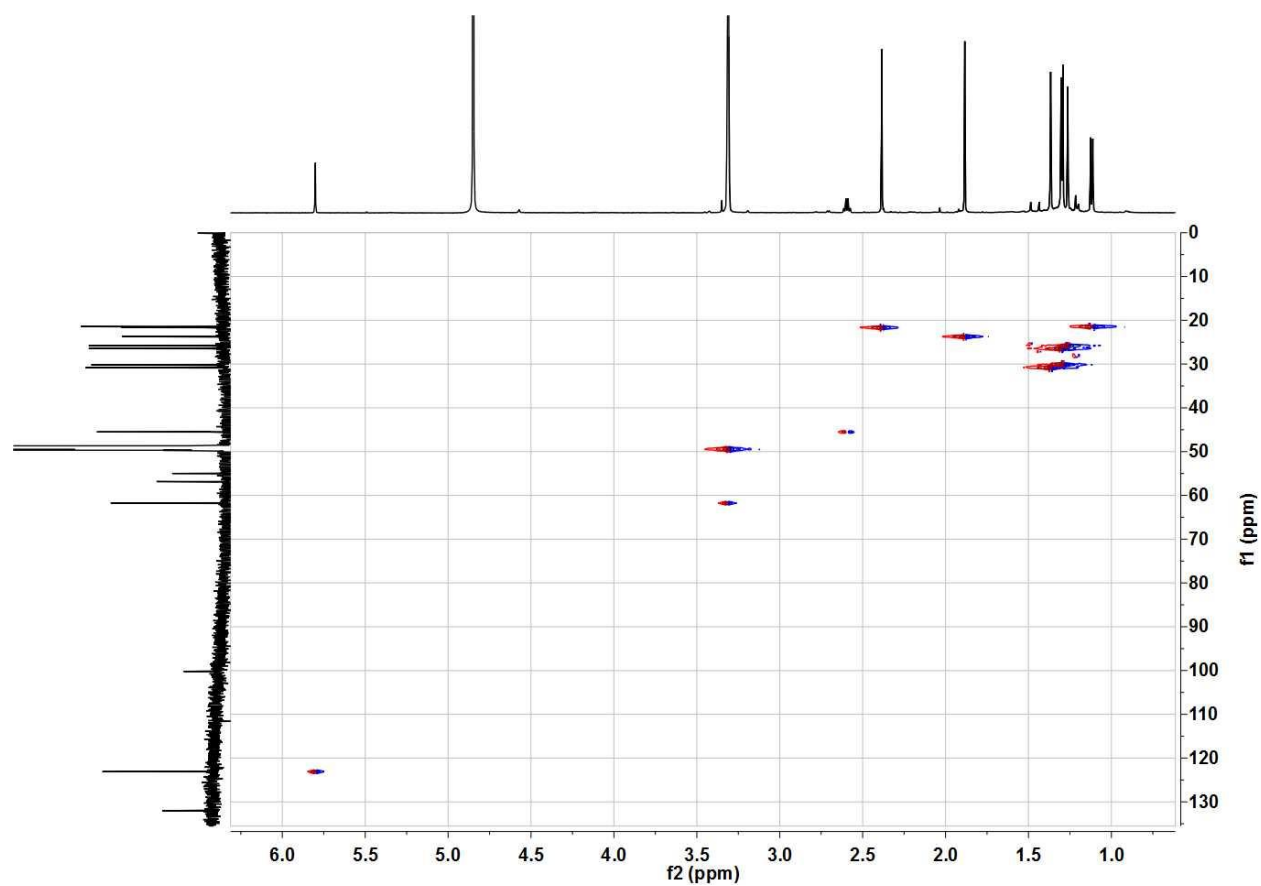
4.6.1 ^1H NMR (600 MHz, $\text{MeOH-}d_4$) spectra of 6.



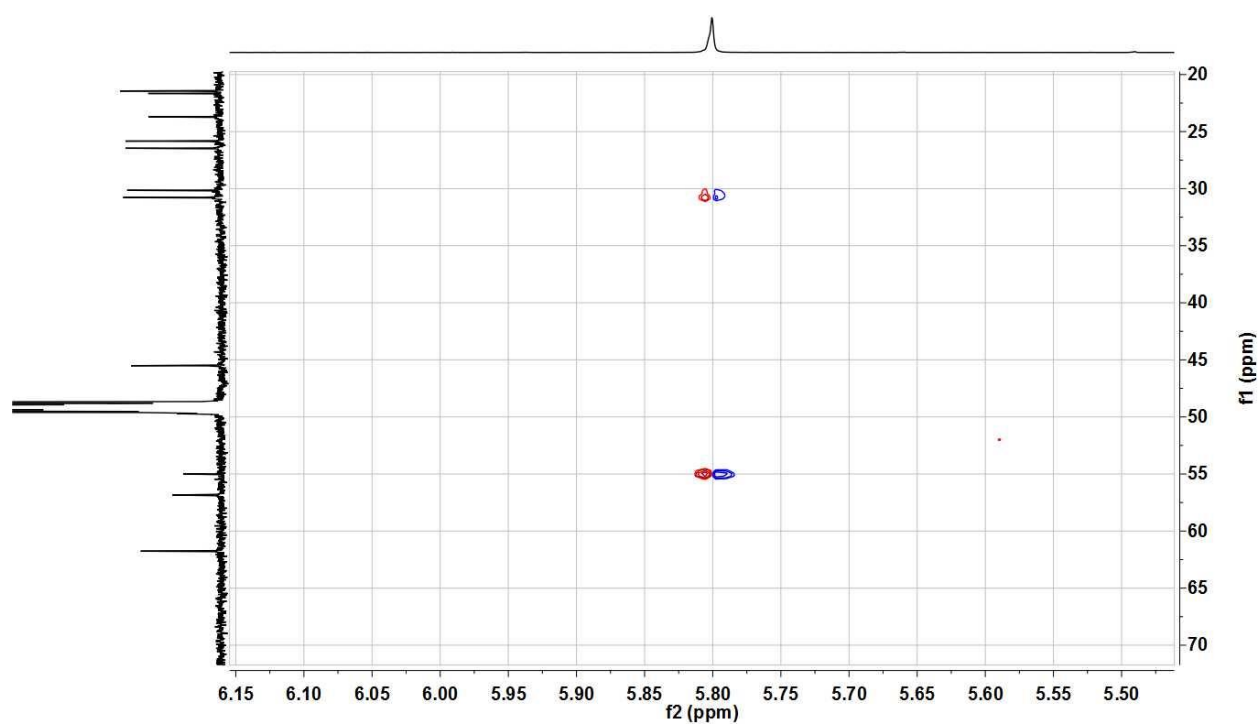
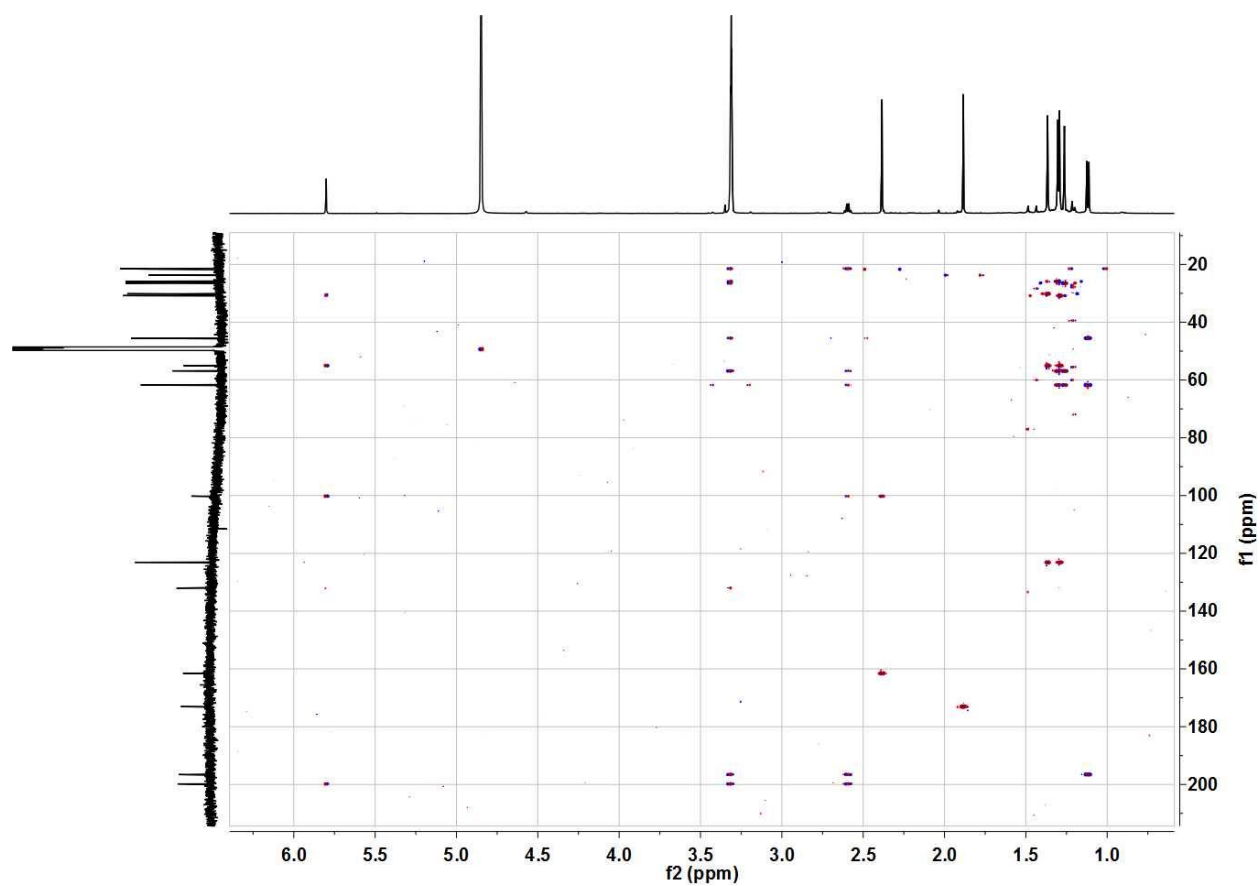
4.6.2 ^{13}C NMR (150 MHz, $\text{MeOH-}d_4$) spectra of **6**.

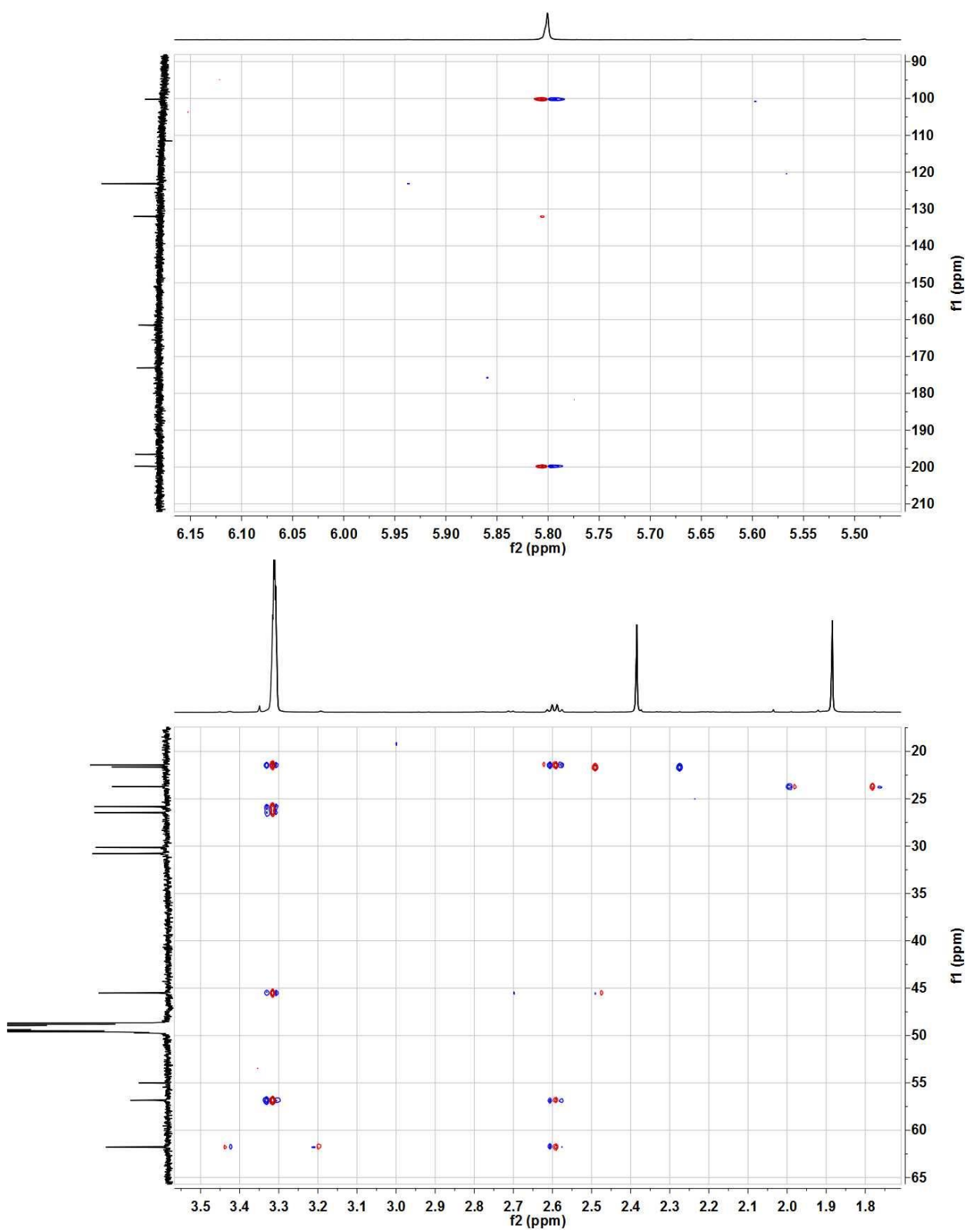


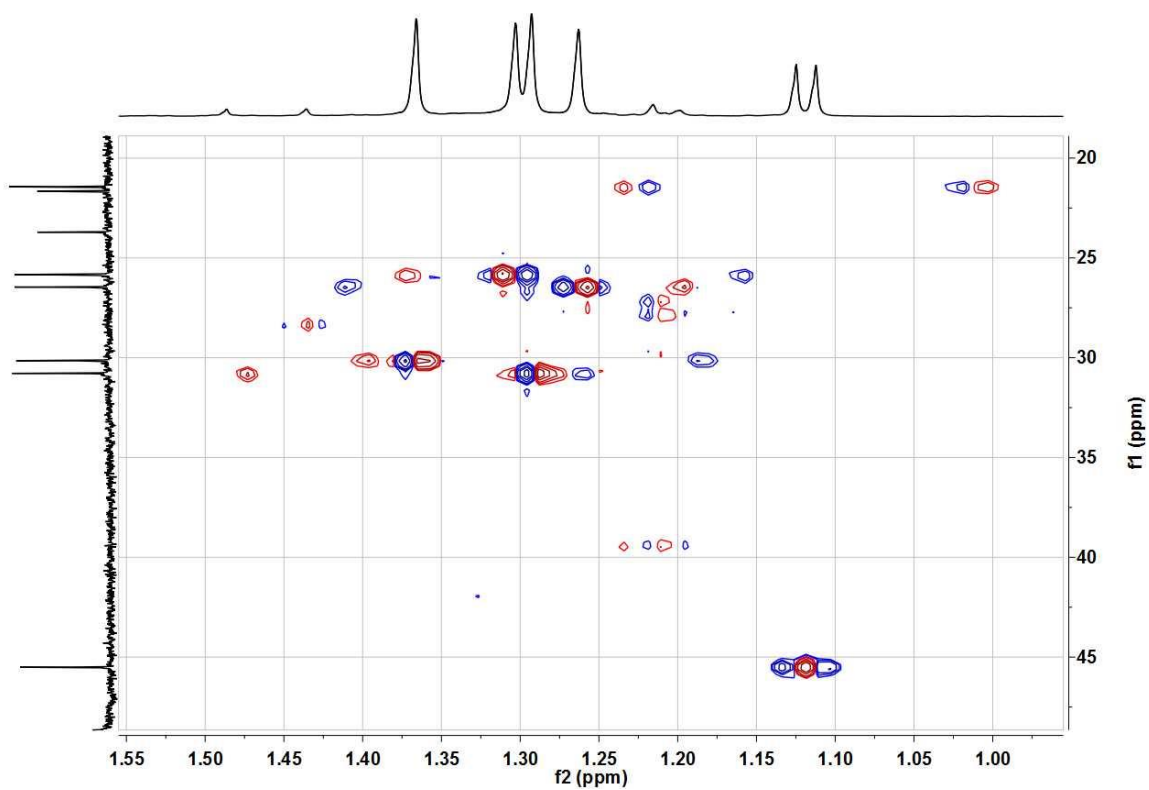
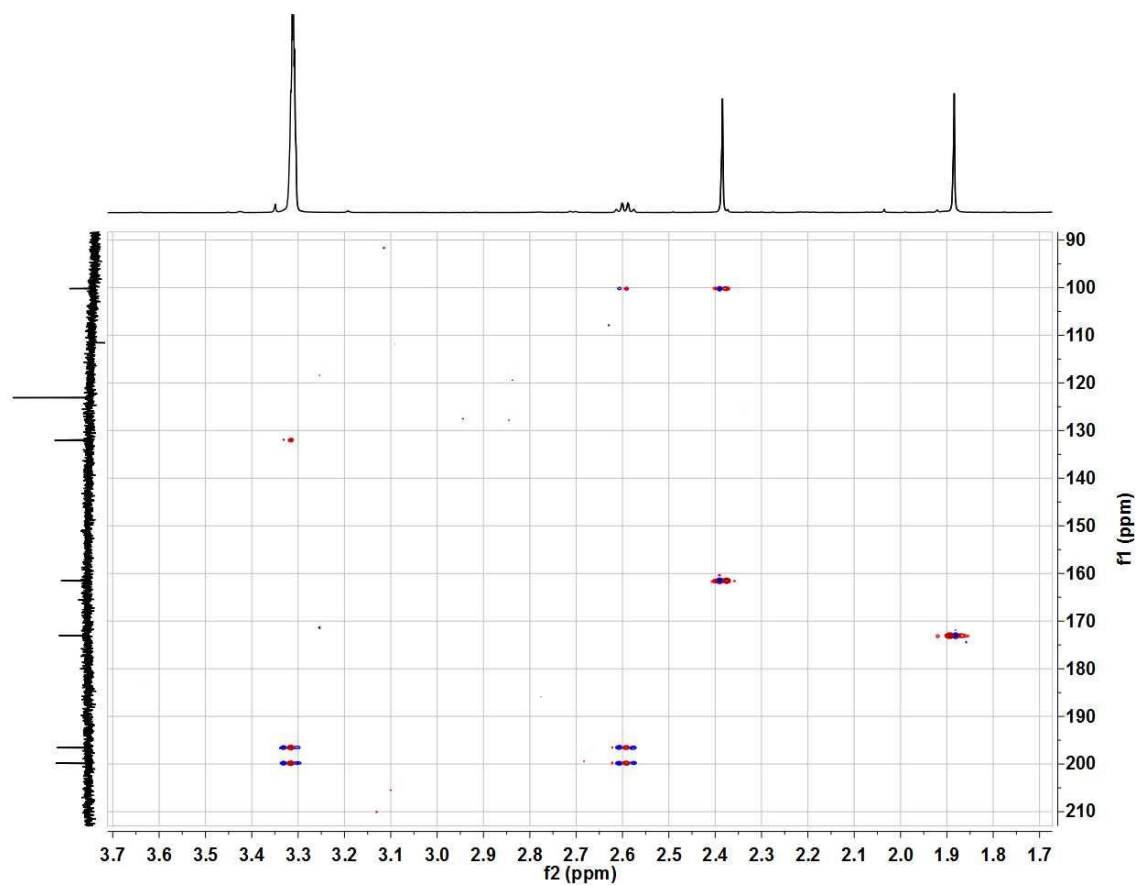
4.6.3 HSQC spectra of **6**.

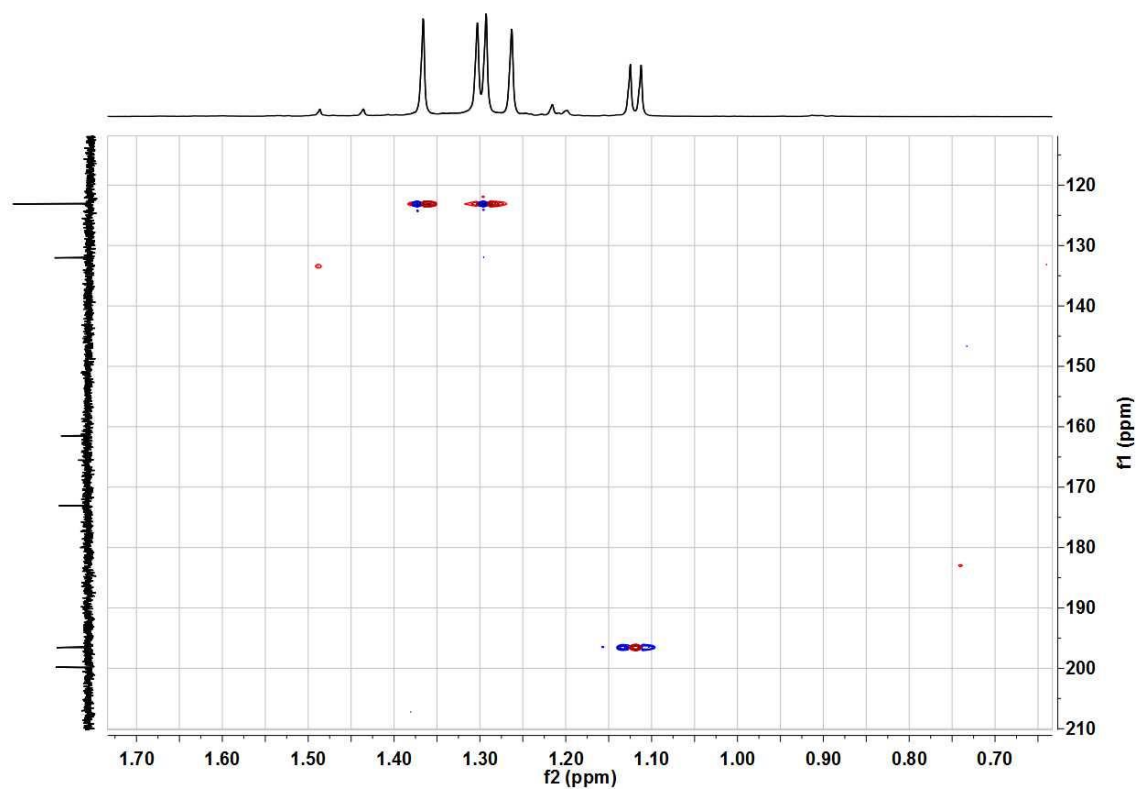
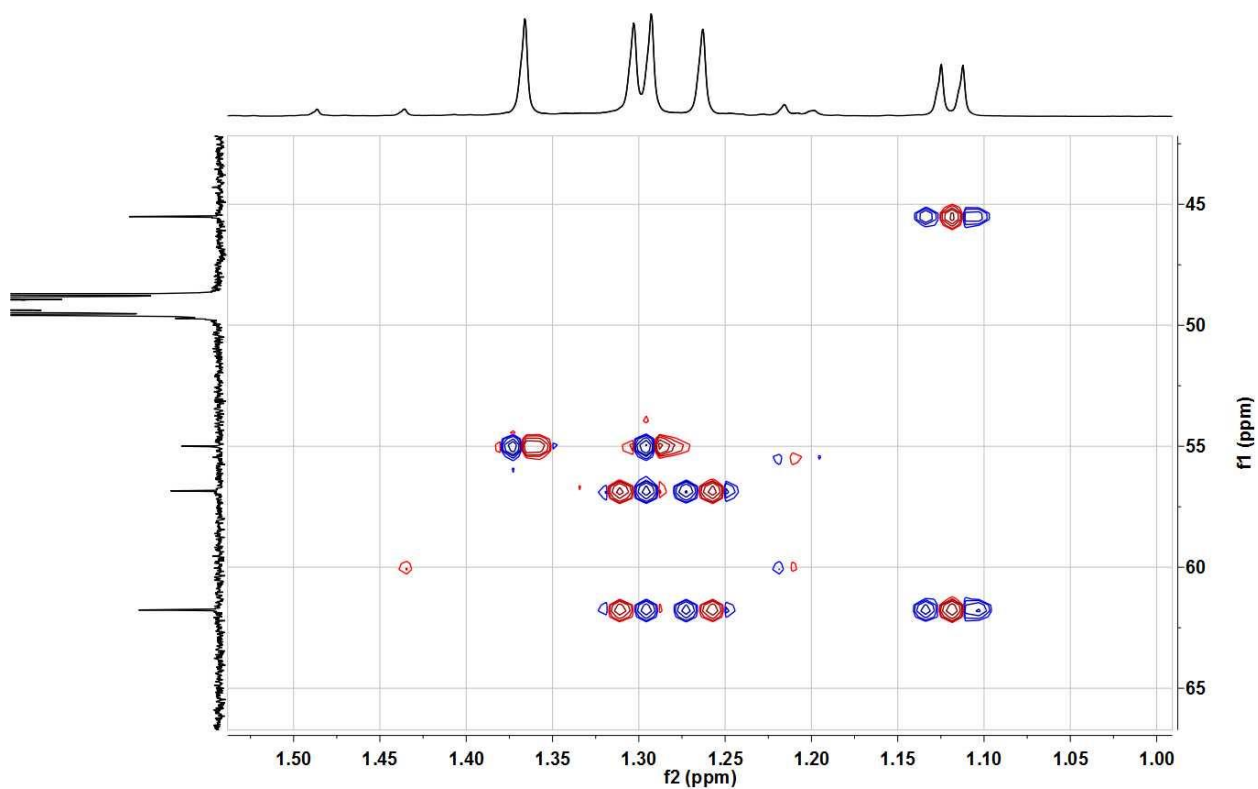


4.6.4 HMBC spectra of **6**.

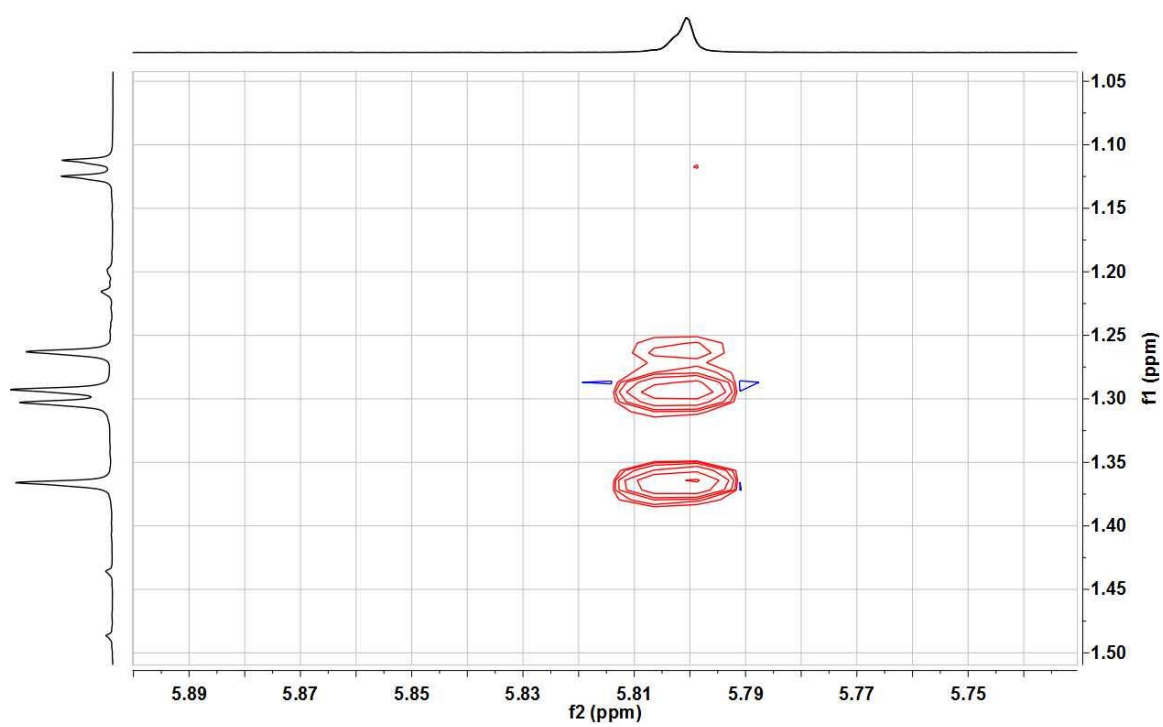
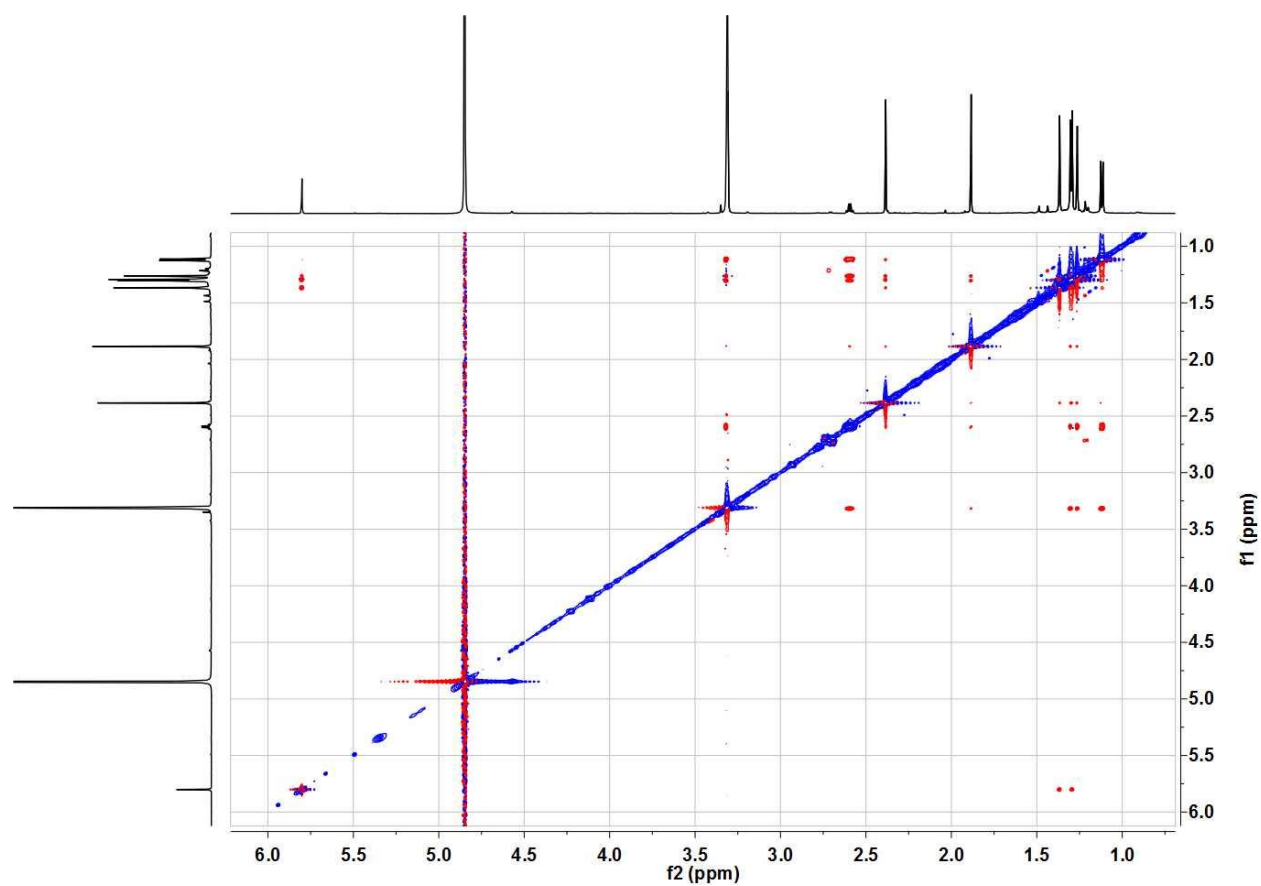


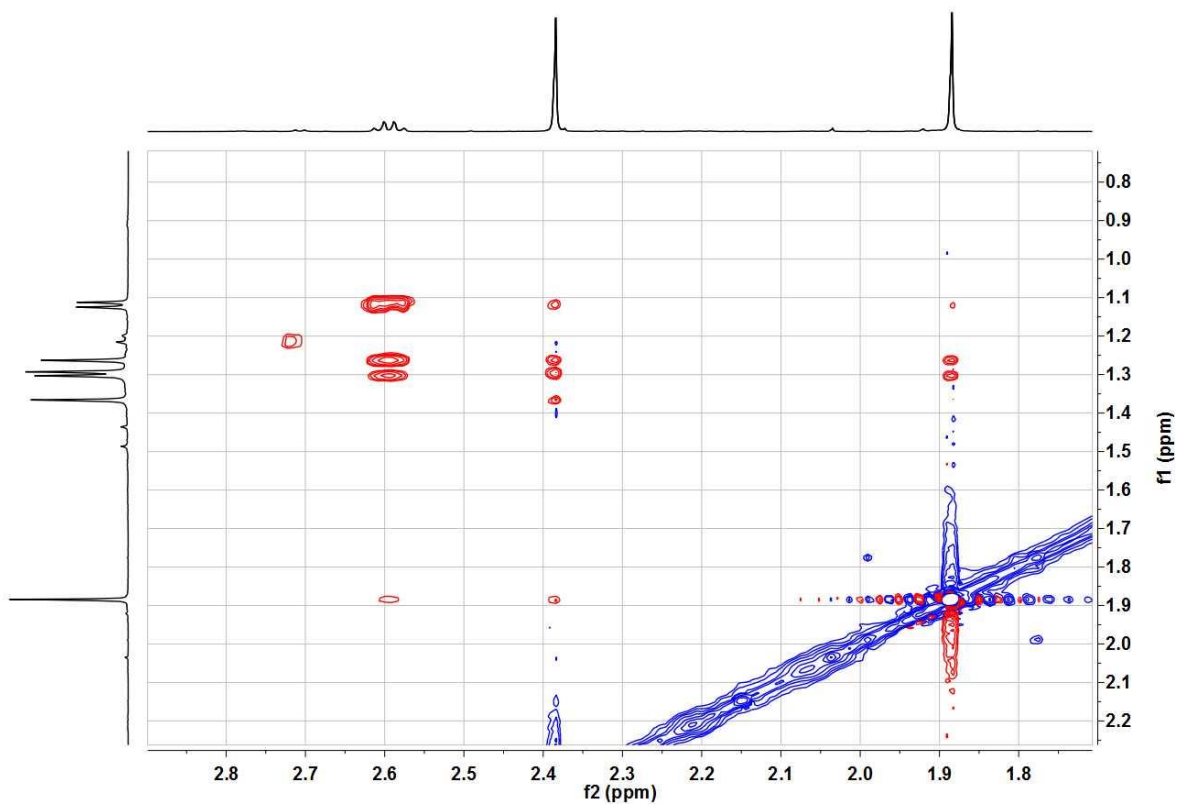
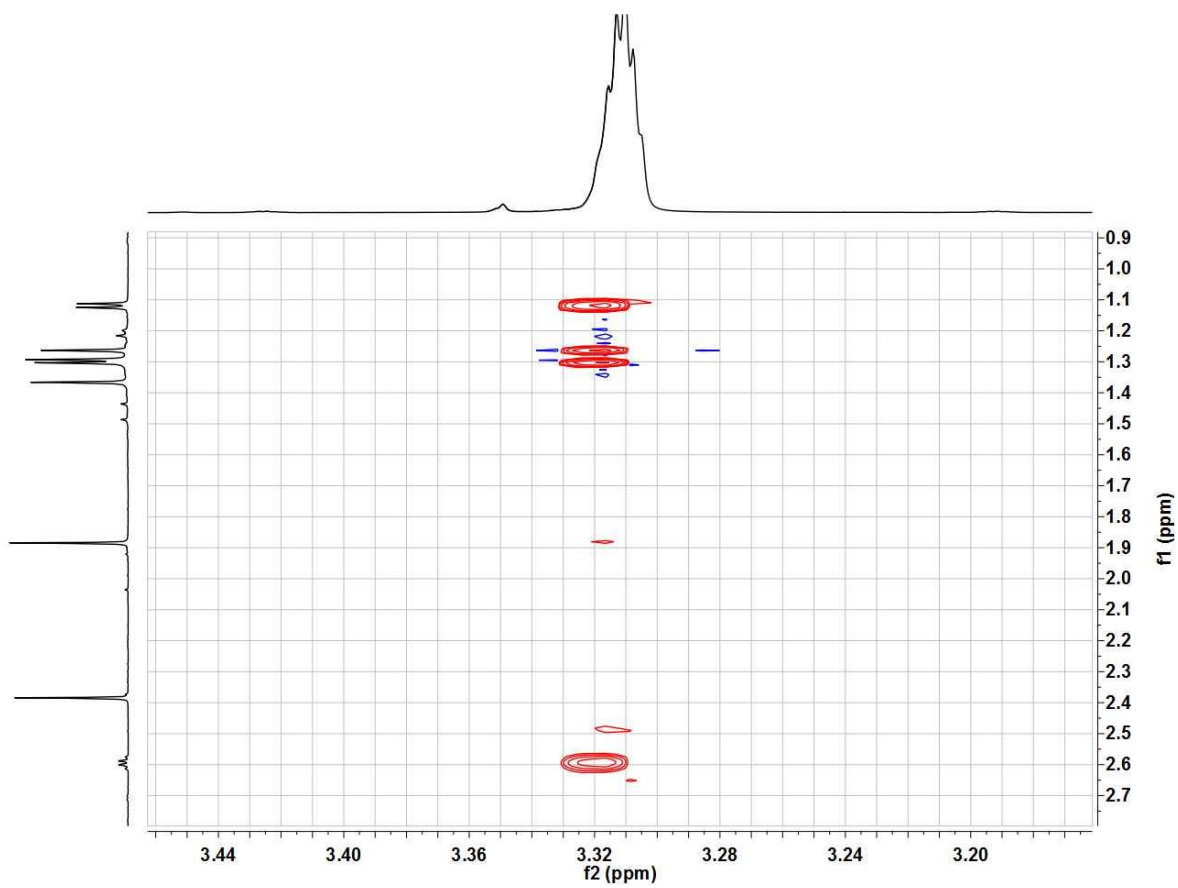




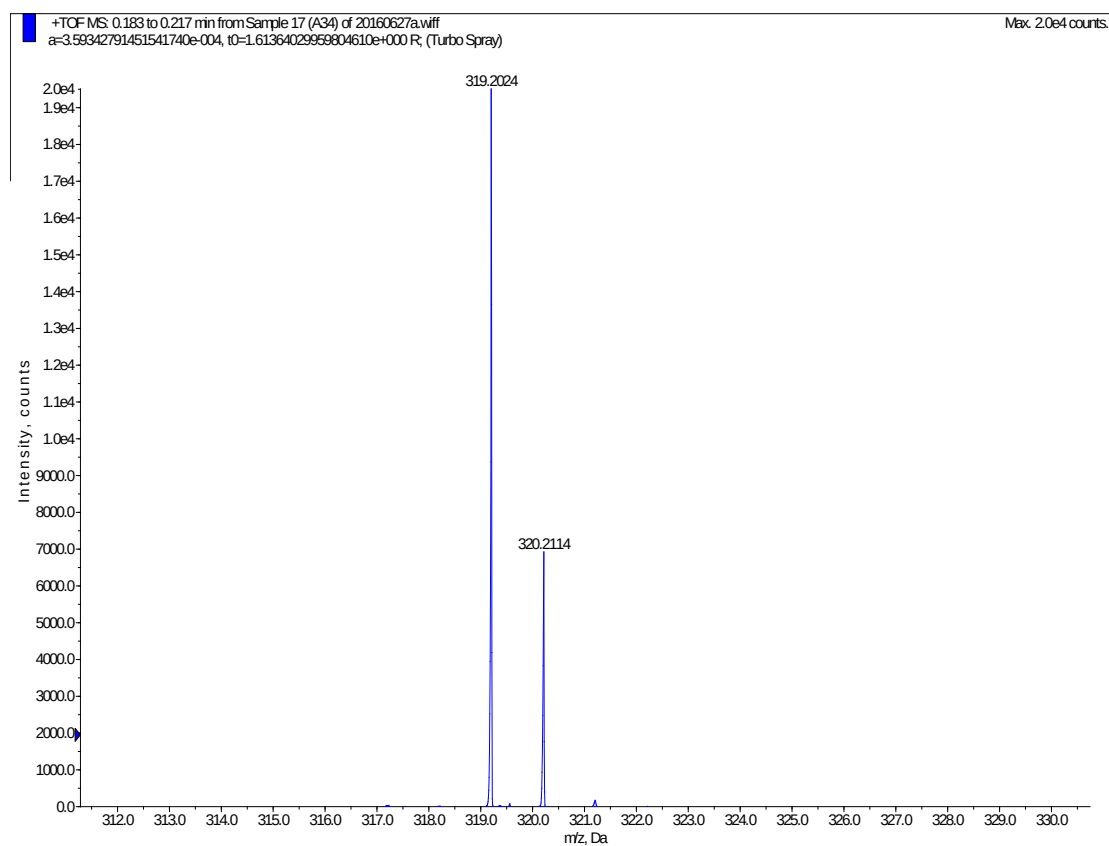


4.6.5 NOESY spectra of **6**.

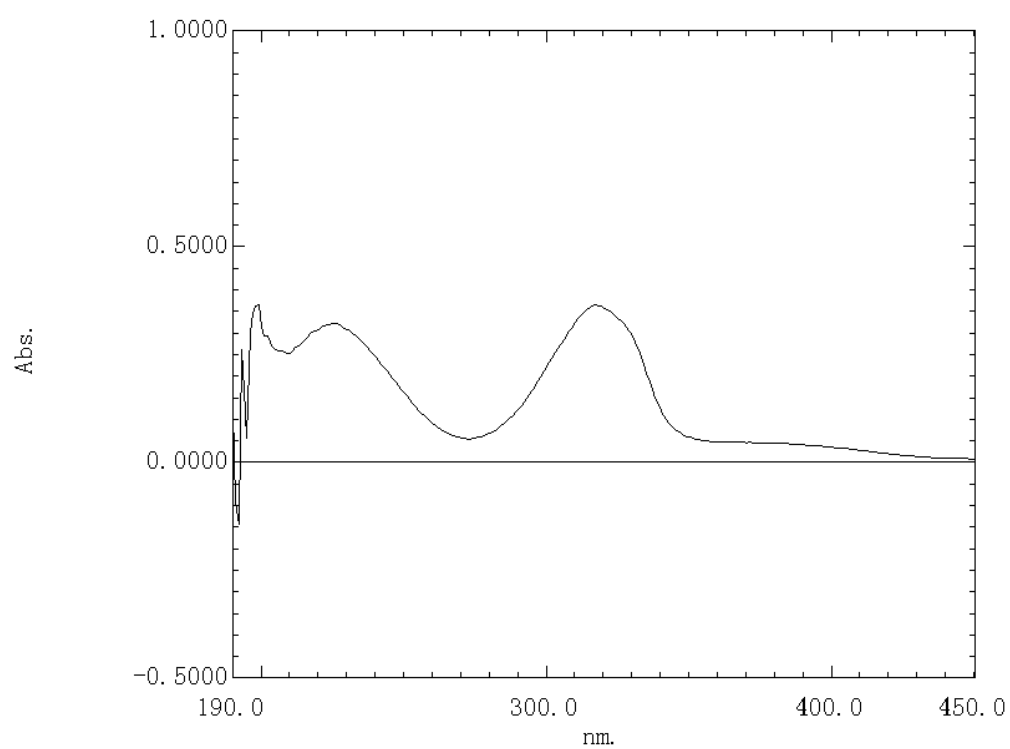




4.6.6 HR-ESI(+)MS of **6**.

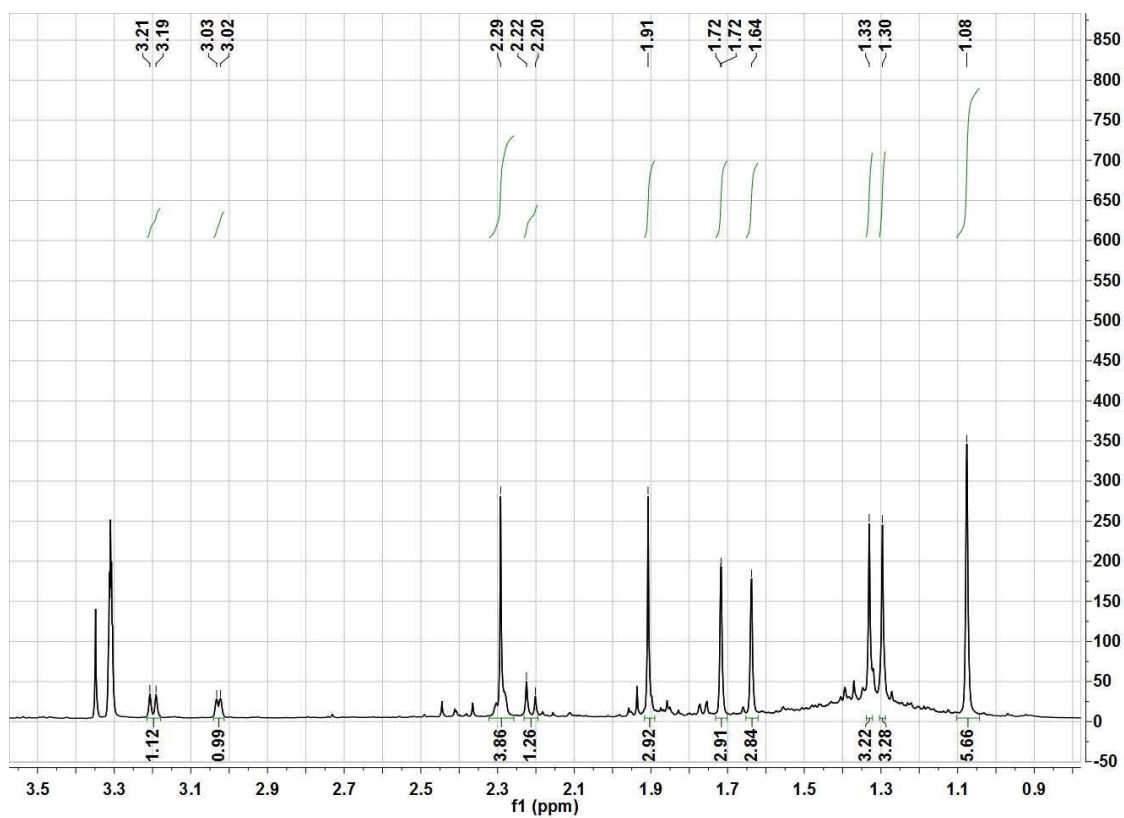
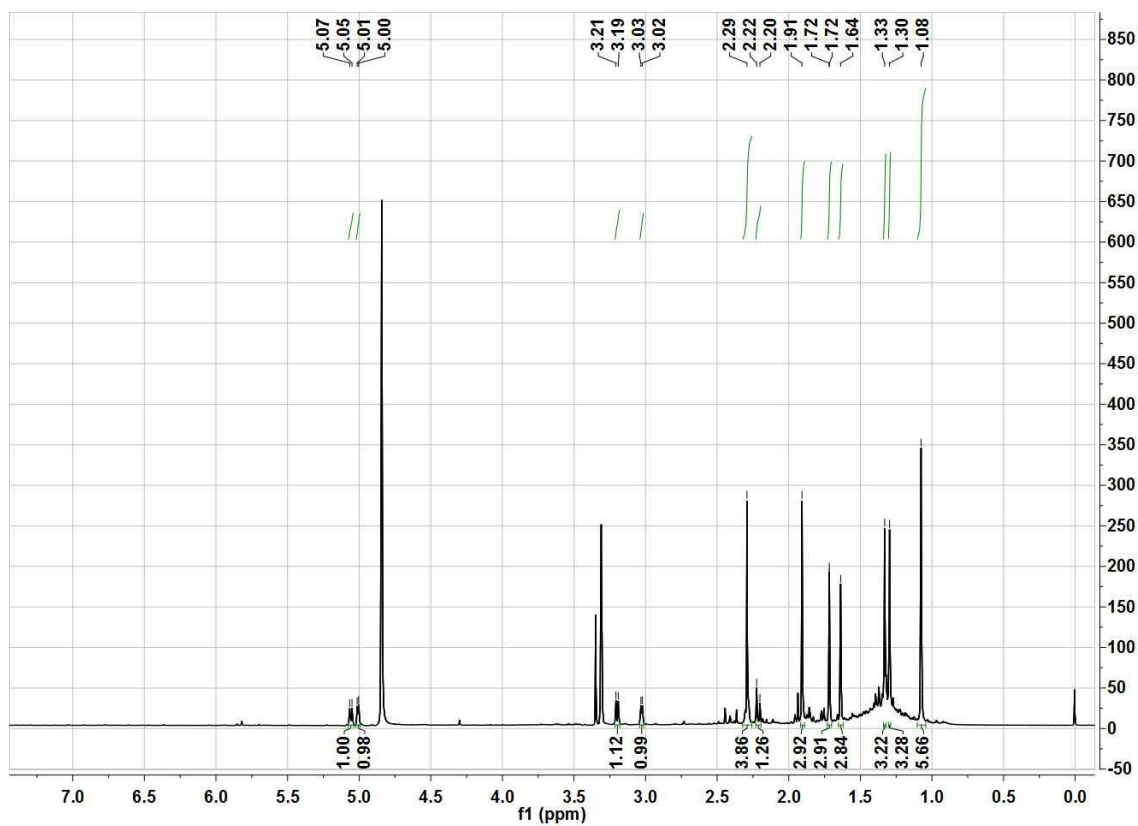


4.6.7 UV spectrum of **6**.

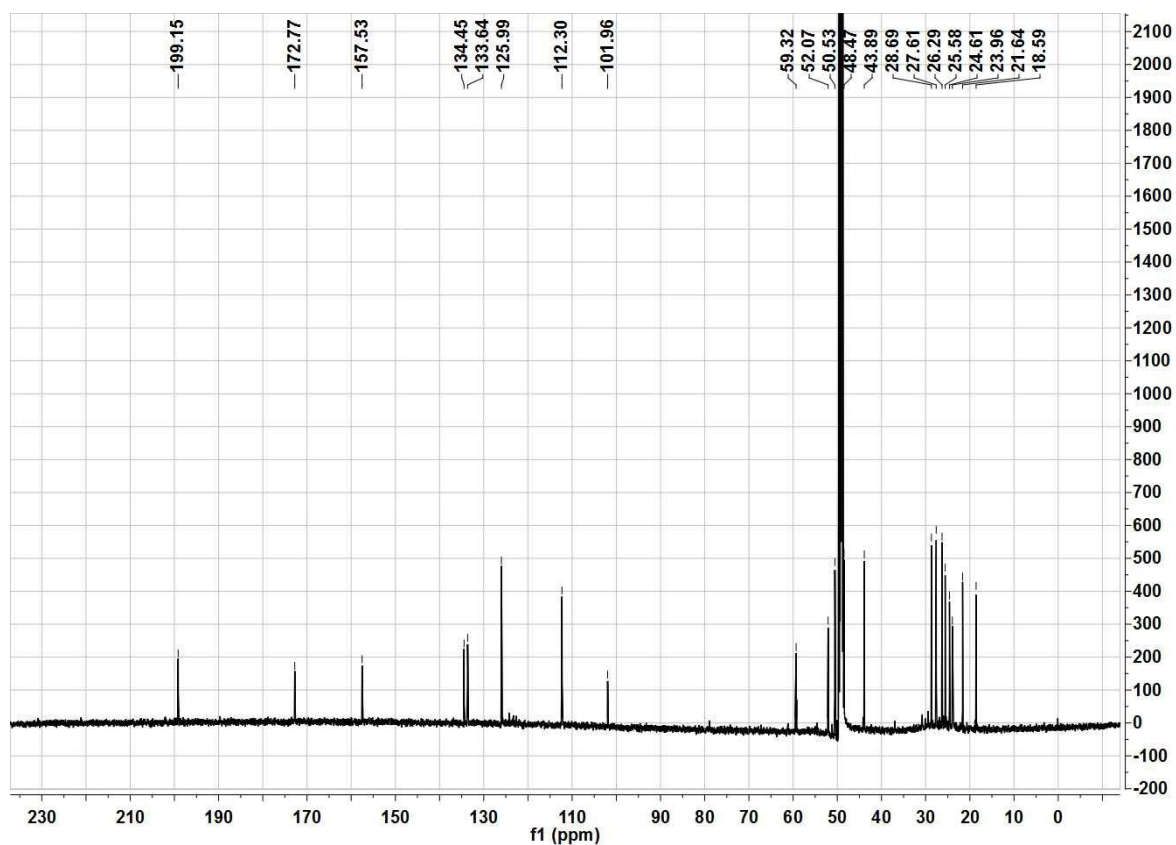


4.7 1D and 2D NMR of pyracyclumine G (7).

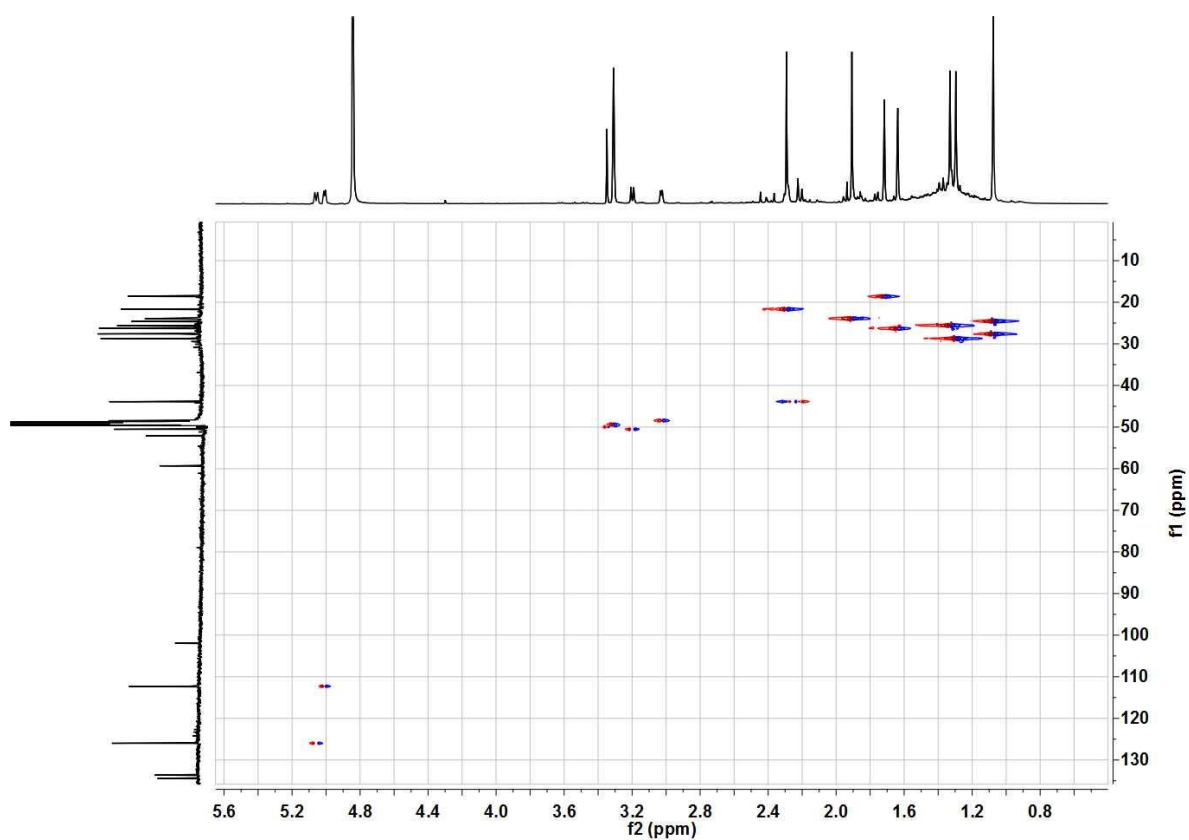
4.7.1 ^1H NMR (600 MHz, $\text{MeOH-}d_4$) spectra of 7.

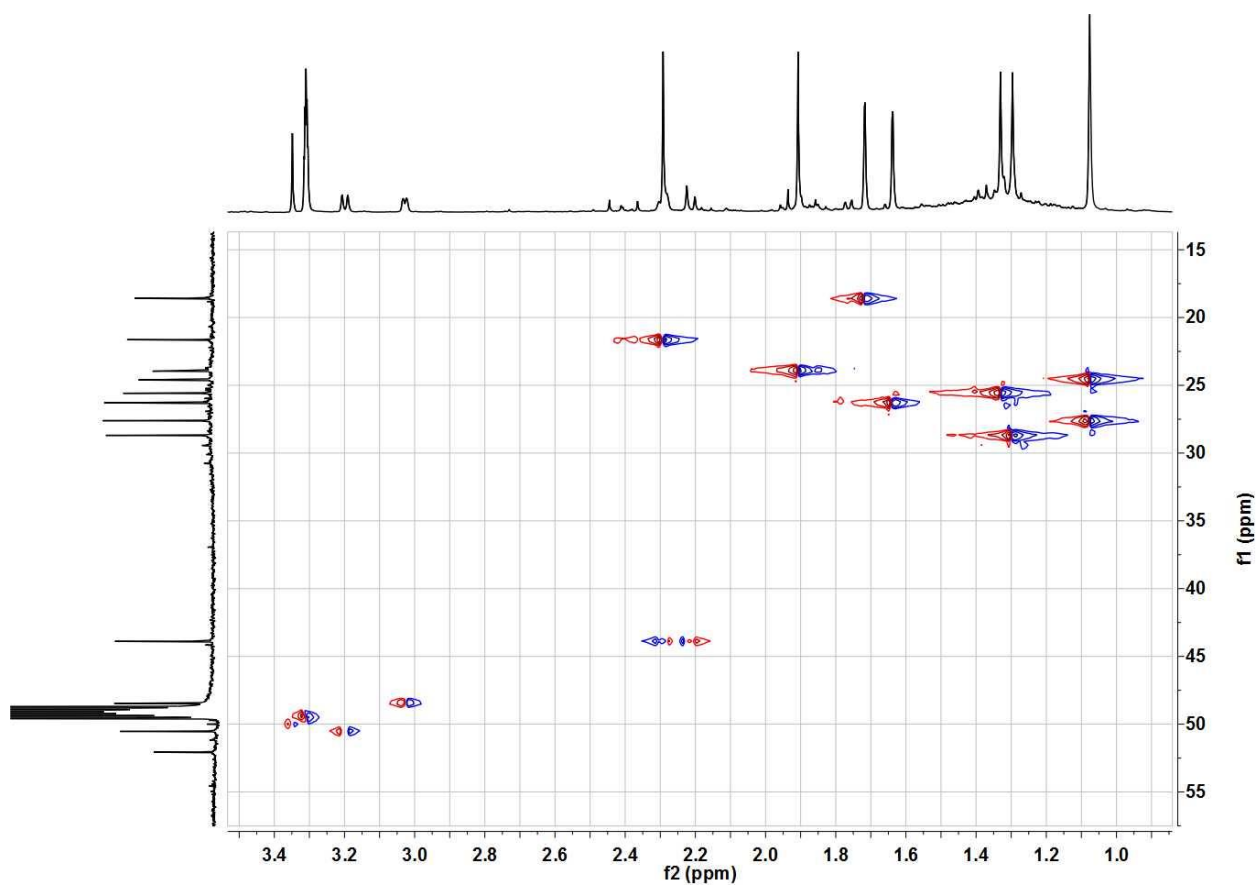


4.7.2 ^{13}C NMR (150 MHz, MeOH-d_4) spectrum of 7.

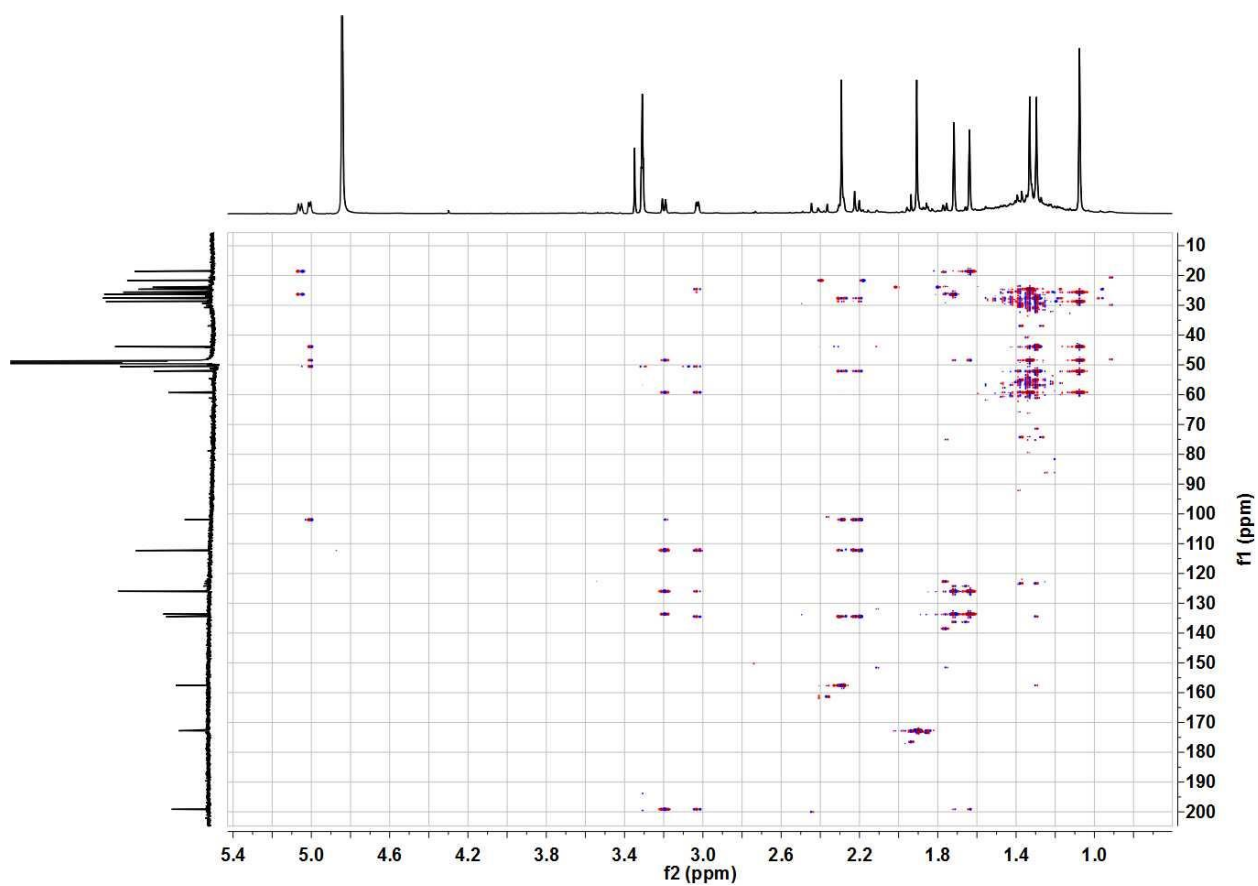


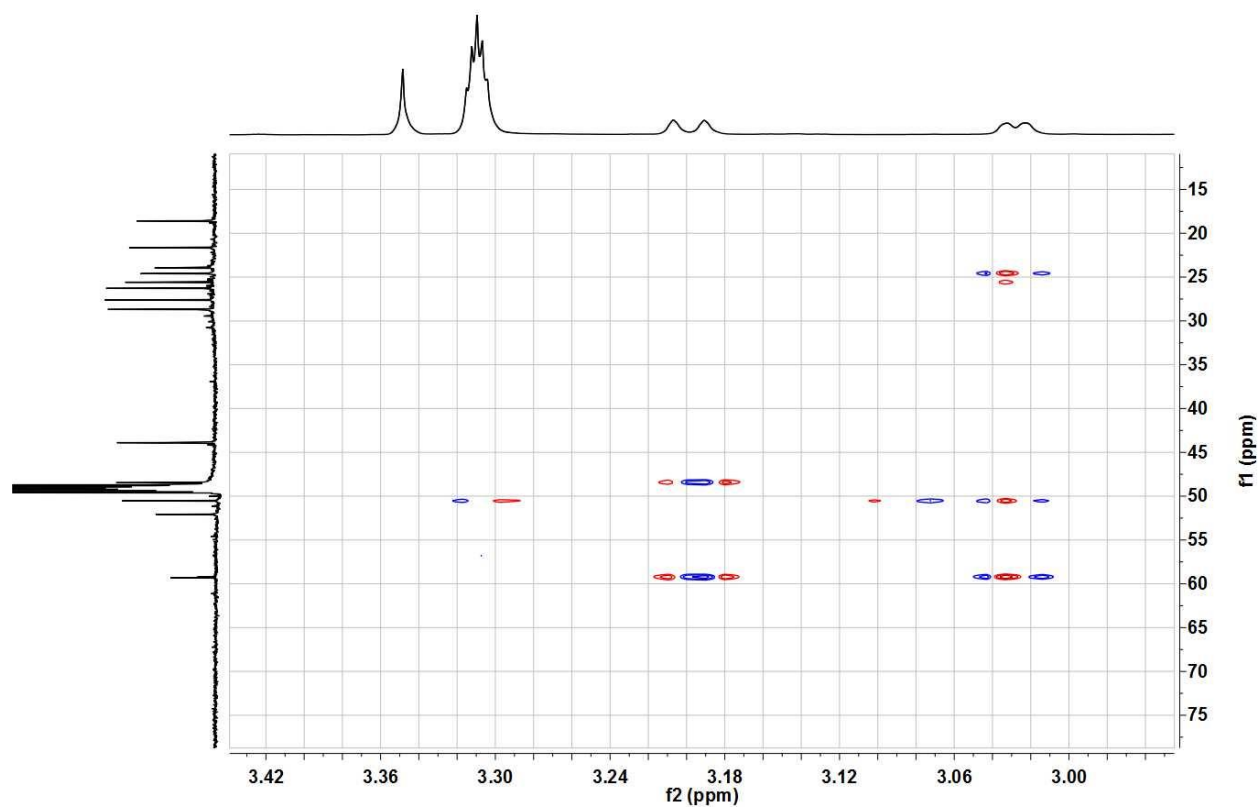
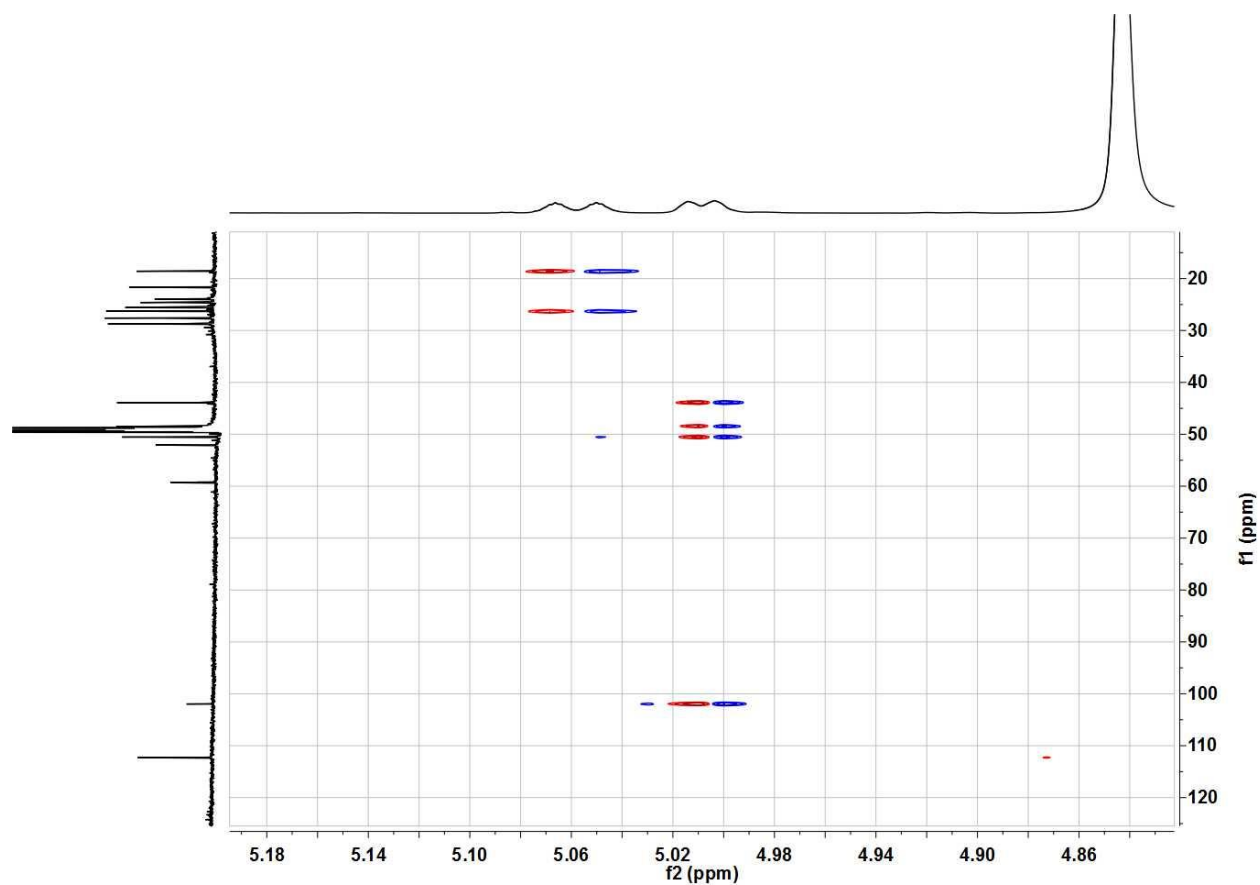
4.7.3 HSQC spectra of 7.

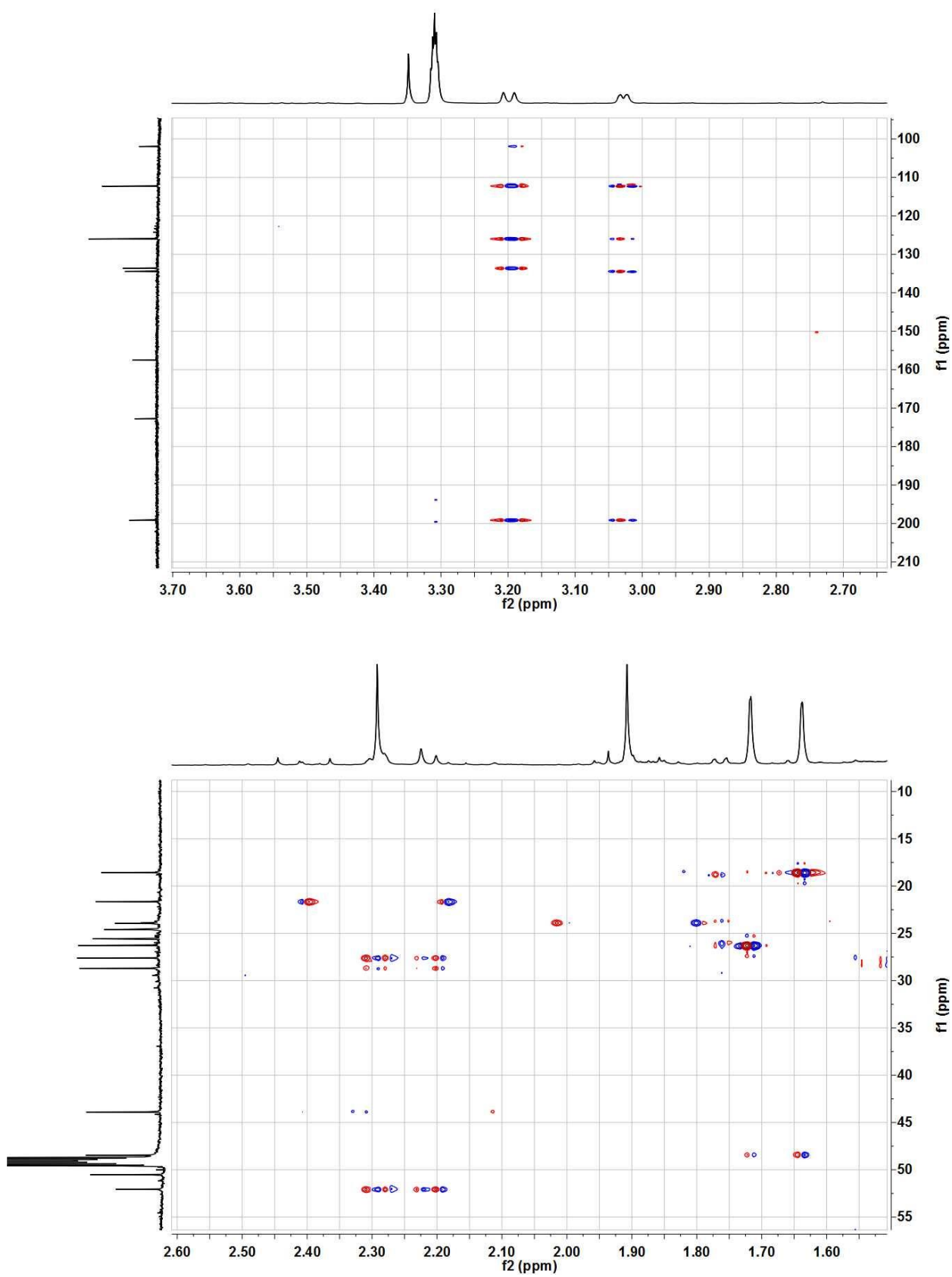


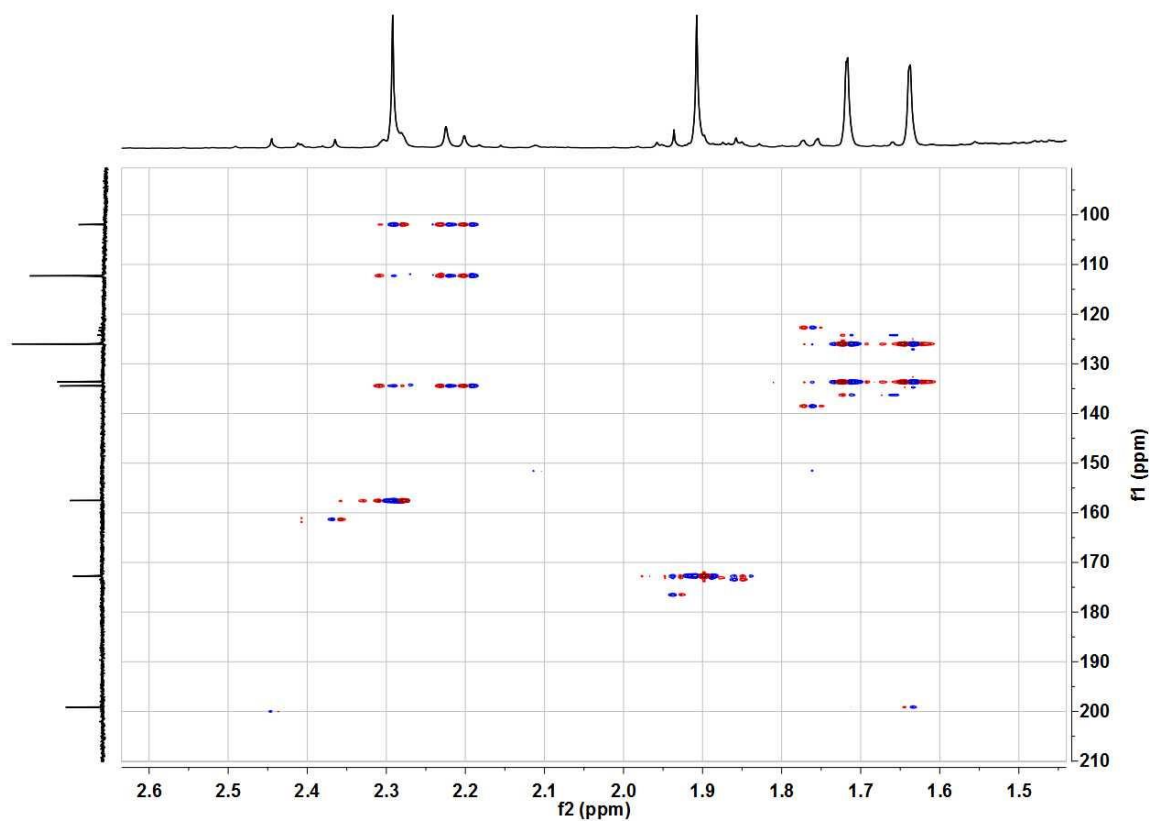
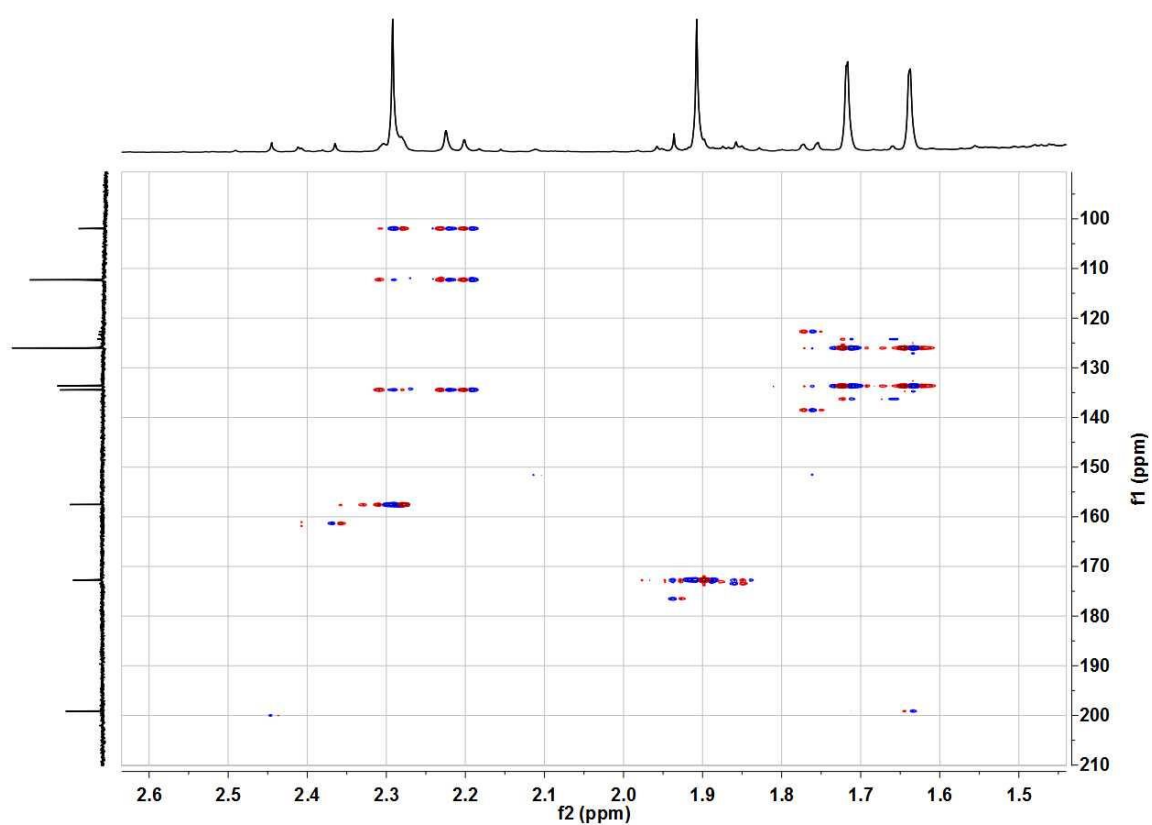


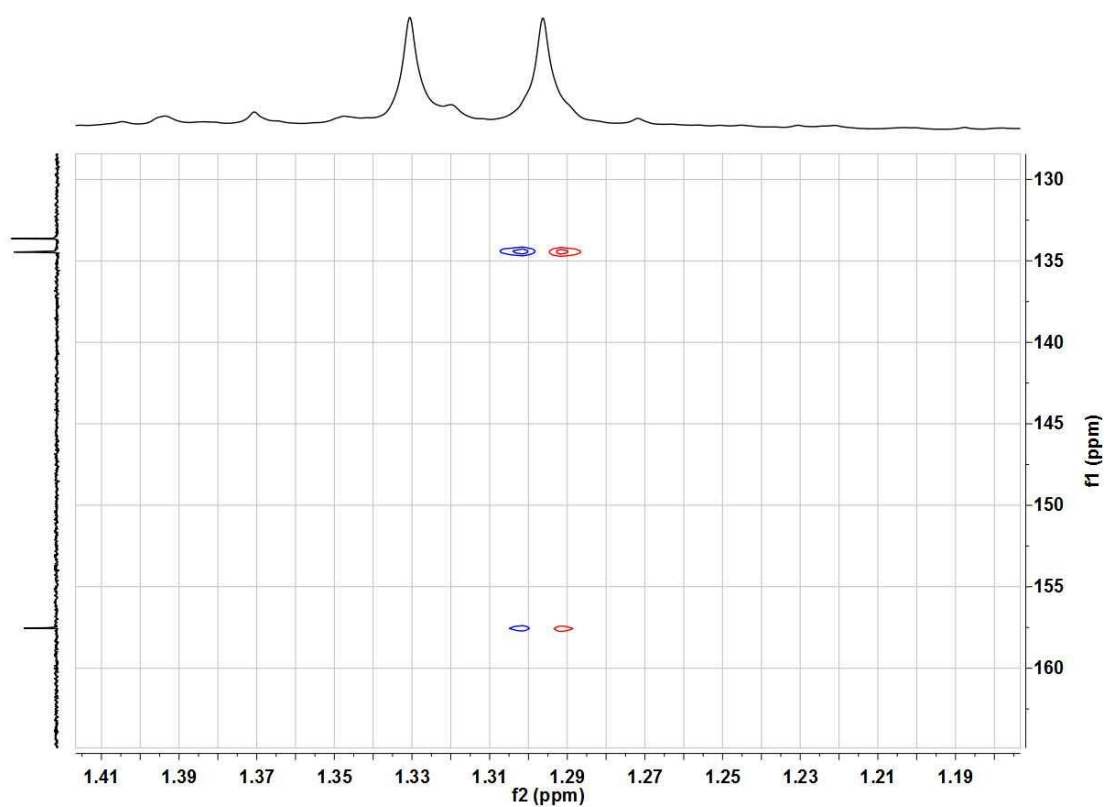
4.7.4 HMBC spectra of 7.



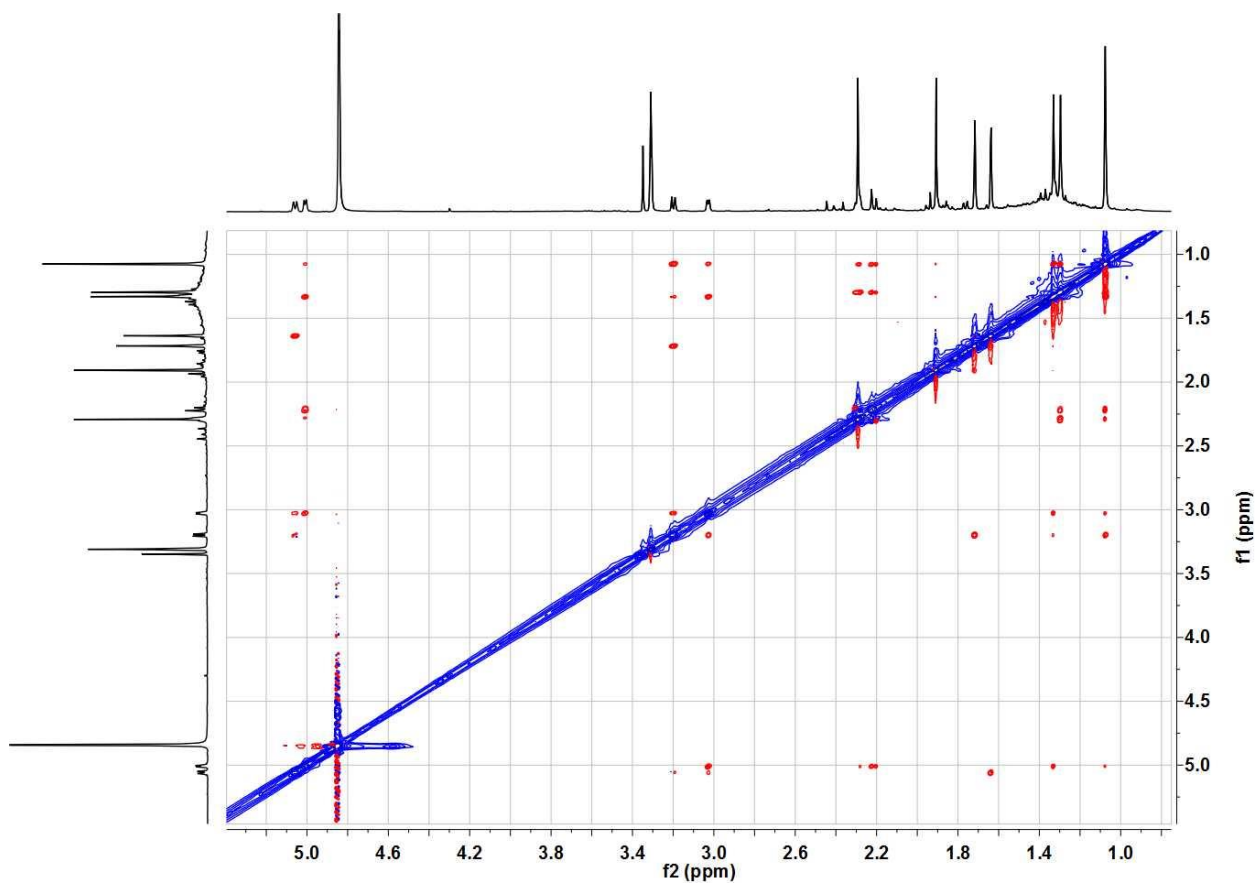


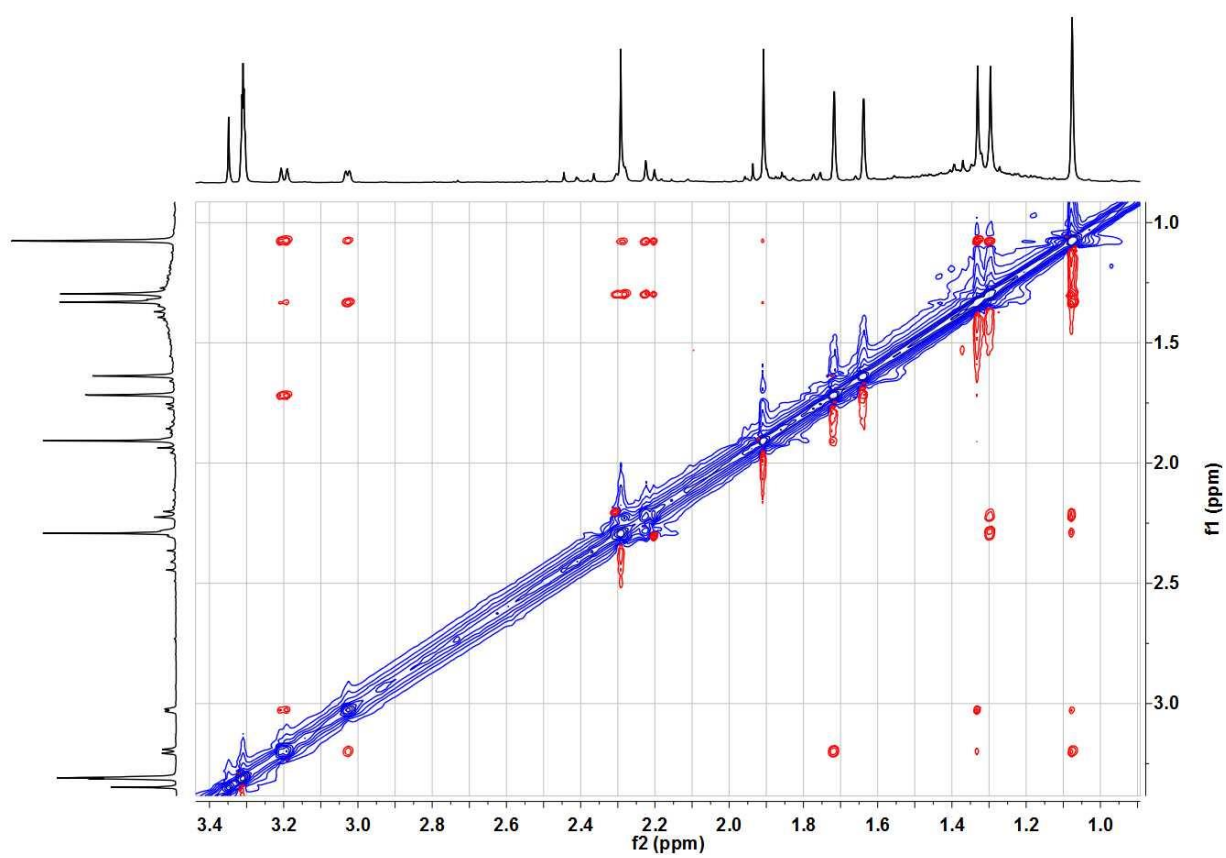
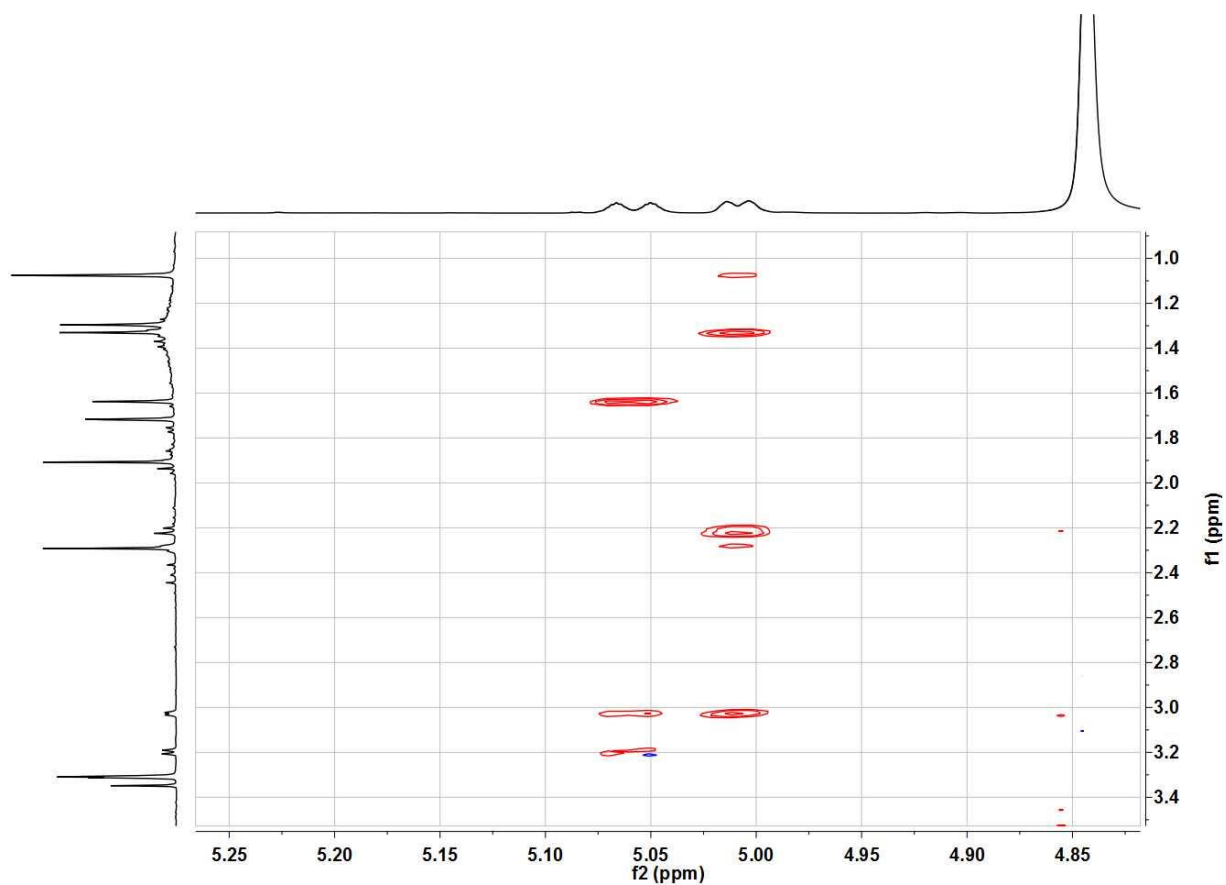




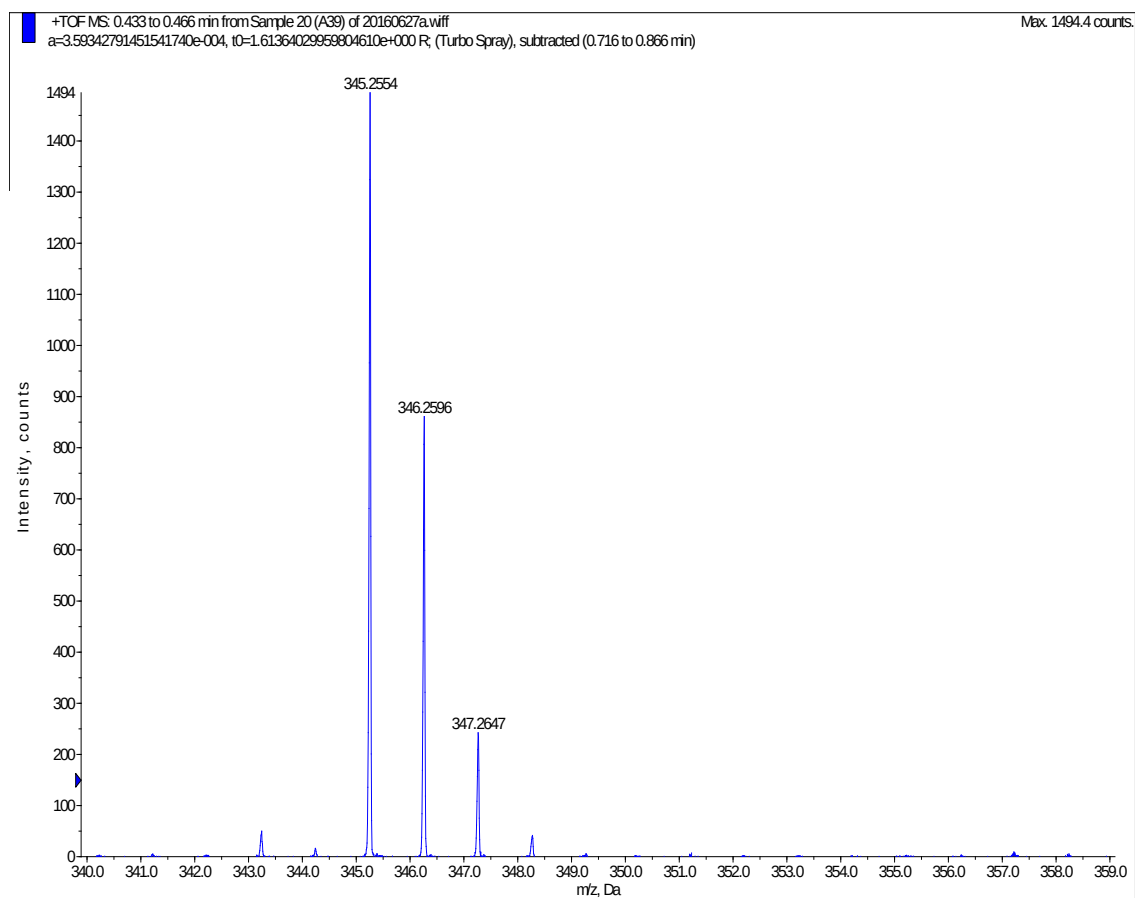


4.7.5 NOESY spectra of 7.

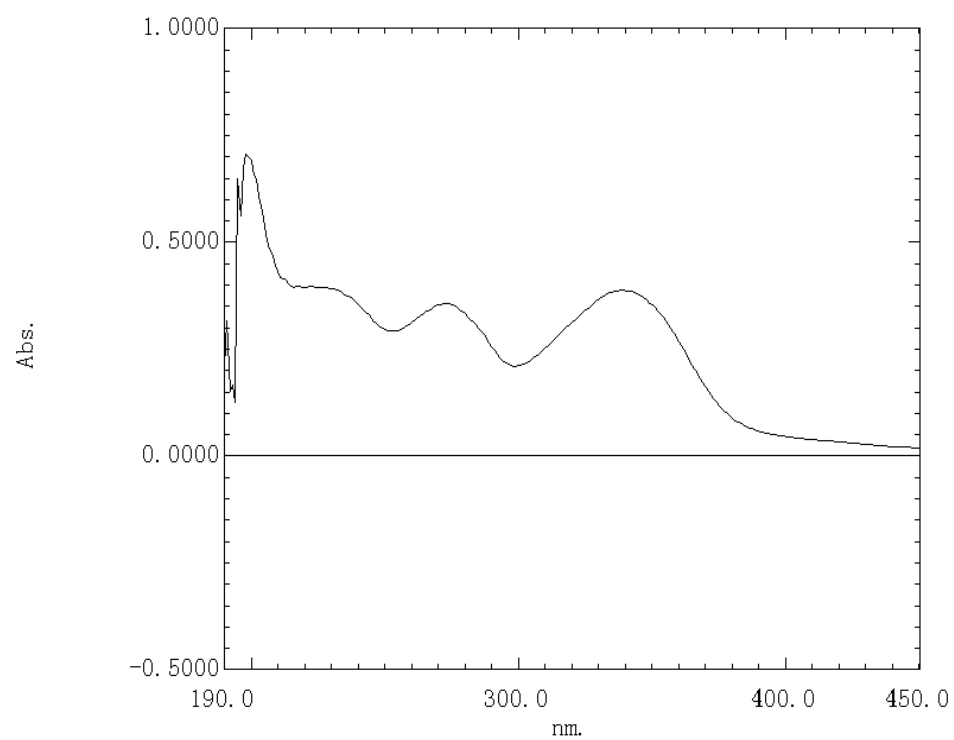




4.7.6 (+)HRESIMS of 7.

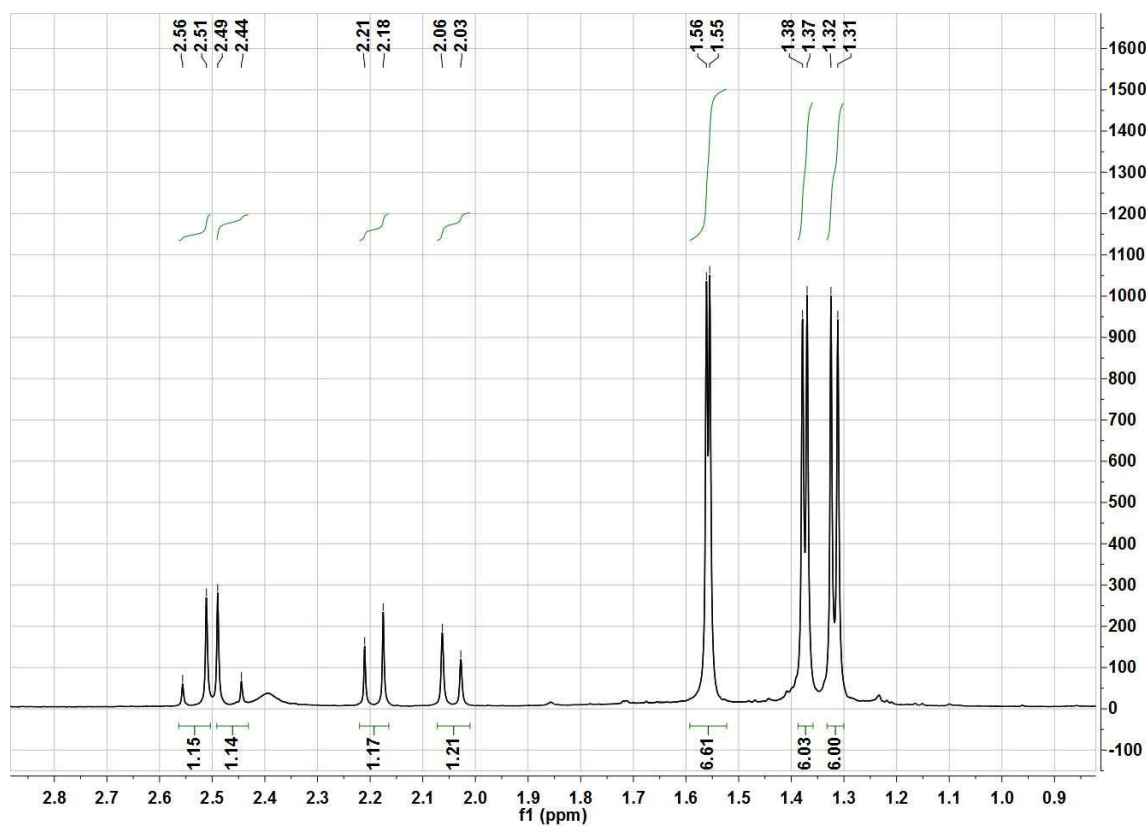
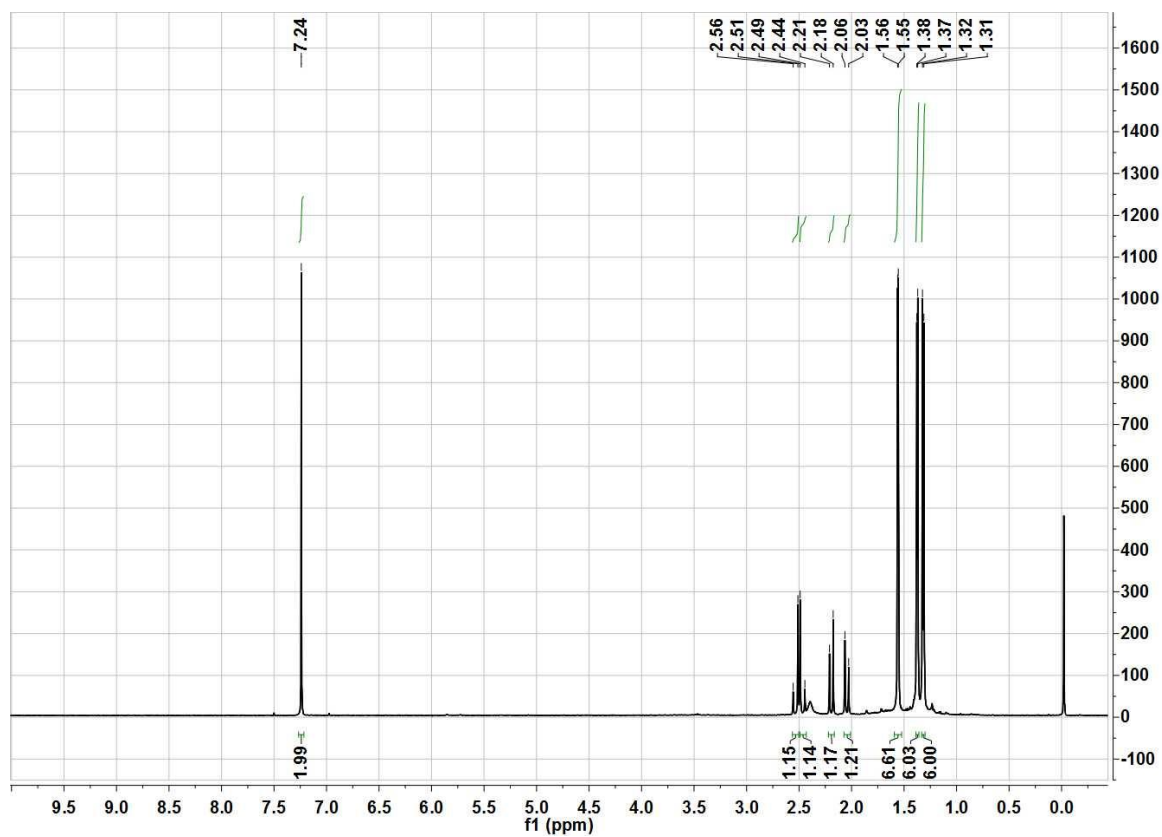


4.7.7 UV spectrum of 7.

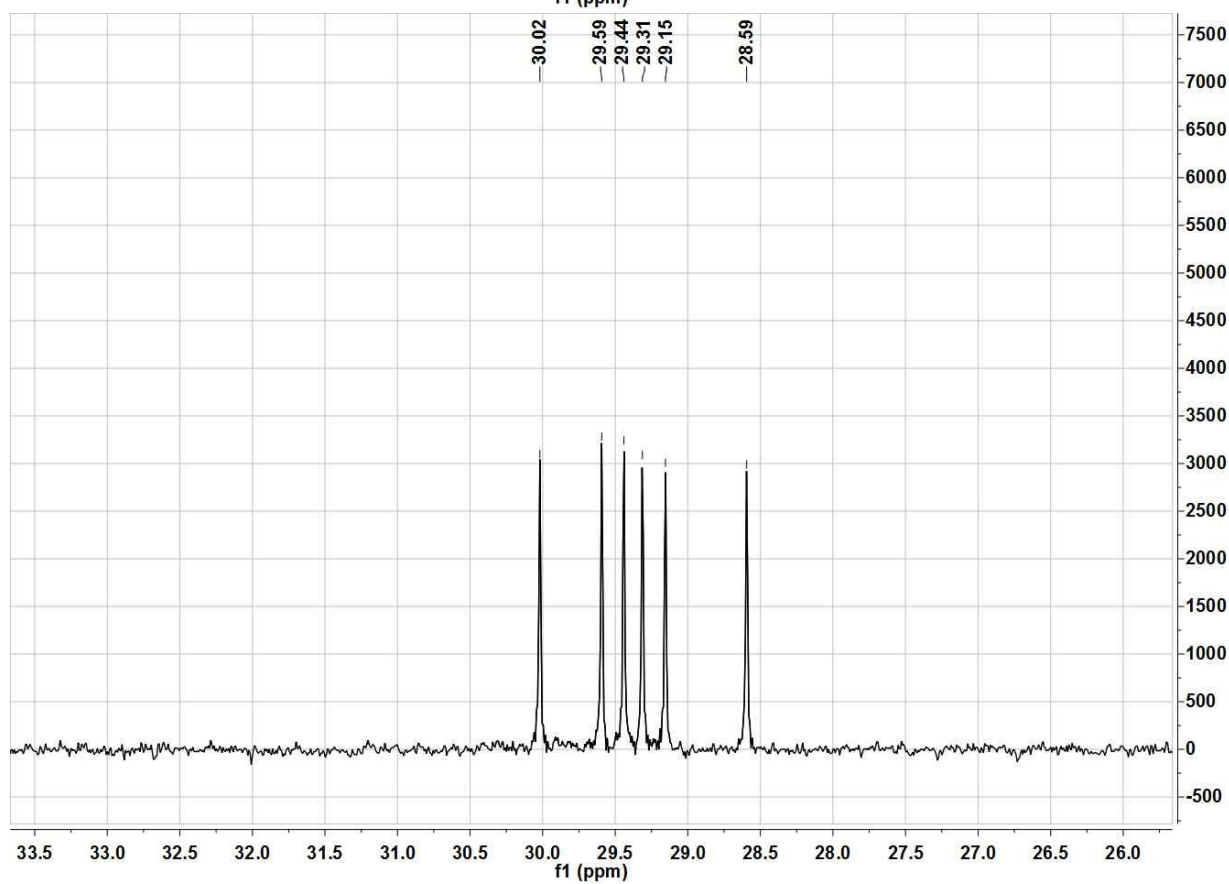
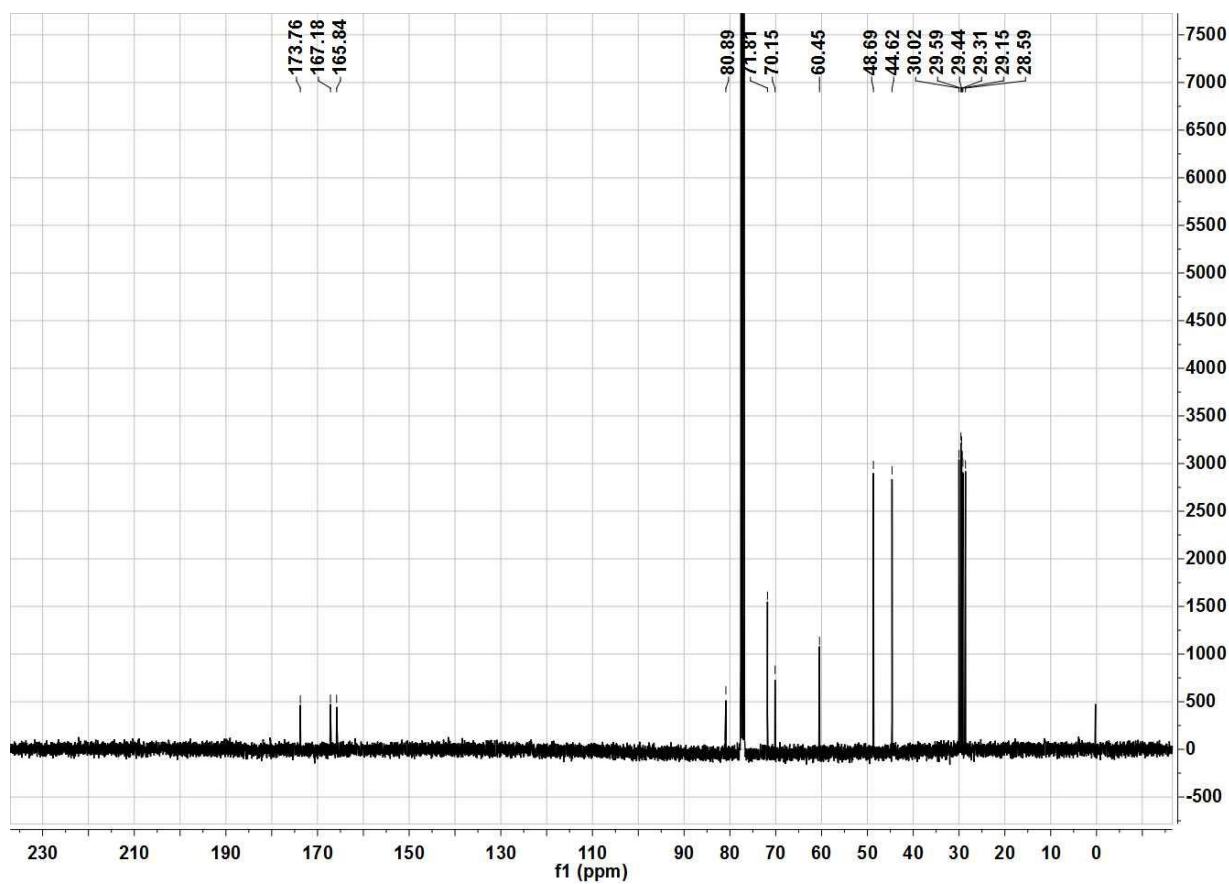


4.8 1D and 2D NMR of pyracyclumine H (8).

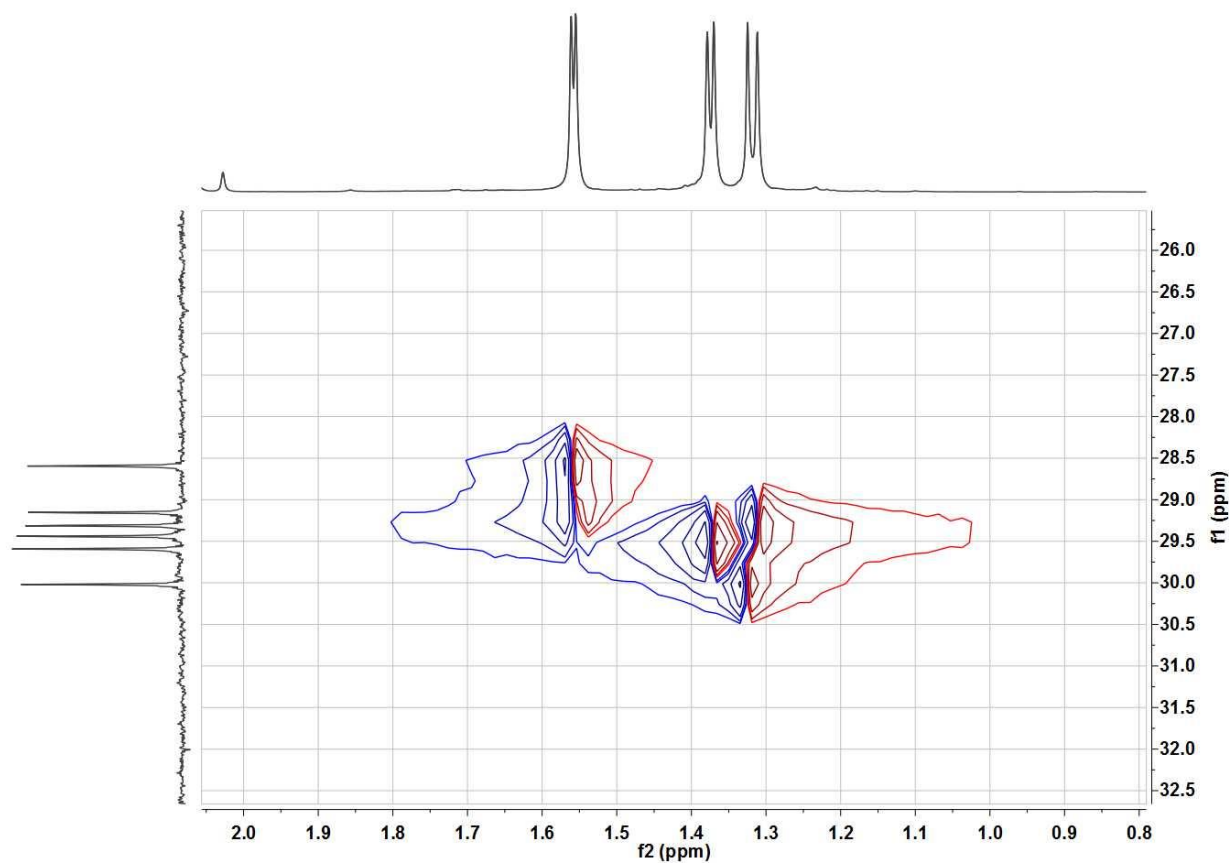
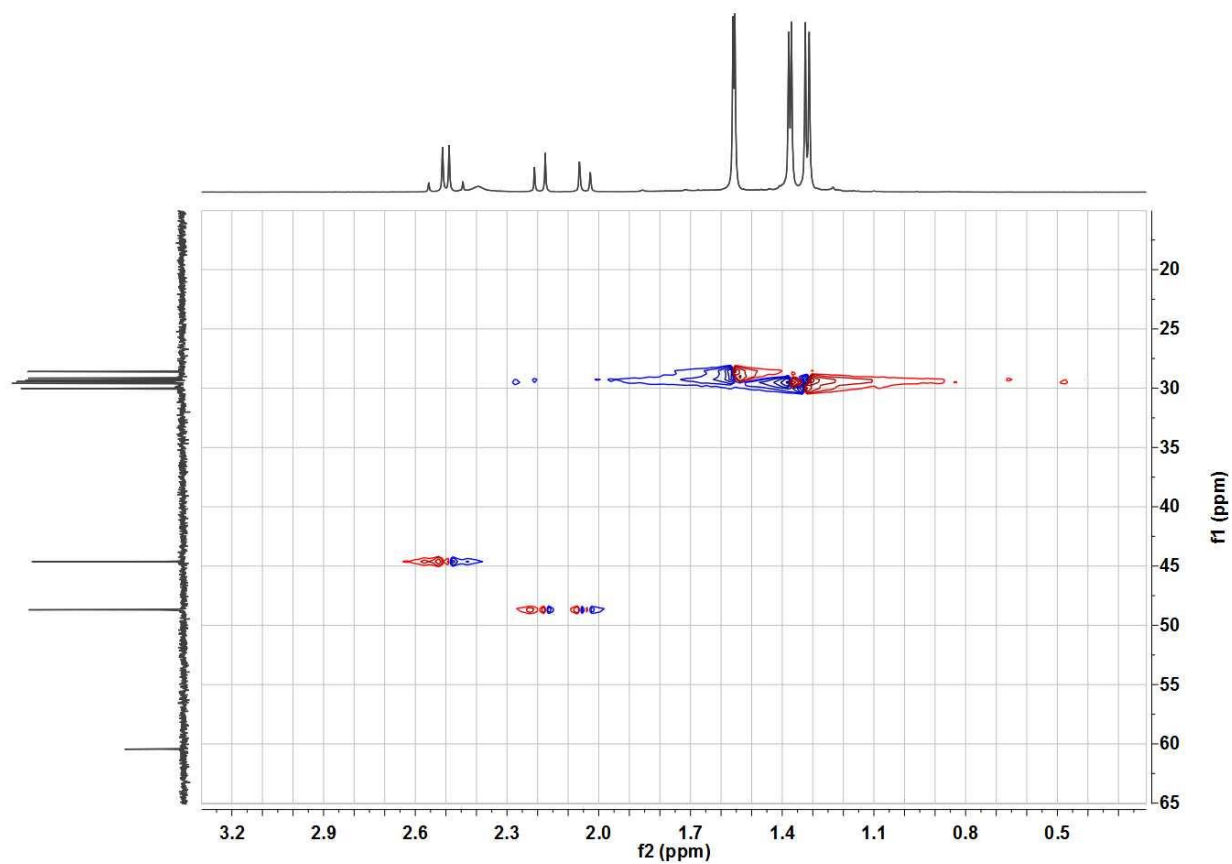
4.8.1 ^1H NMR (400 MHz, CDCl_3) spectra of **8**.



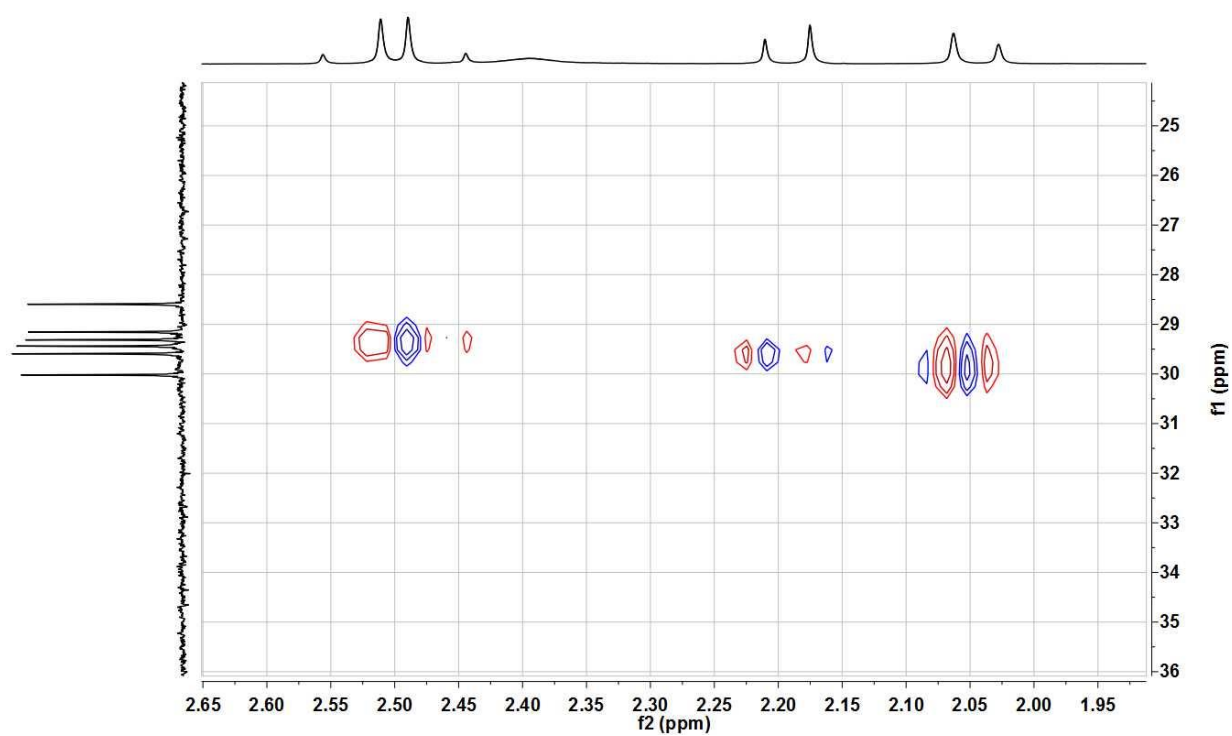
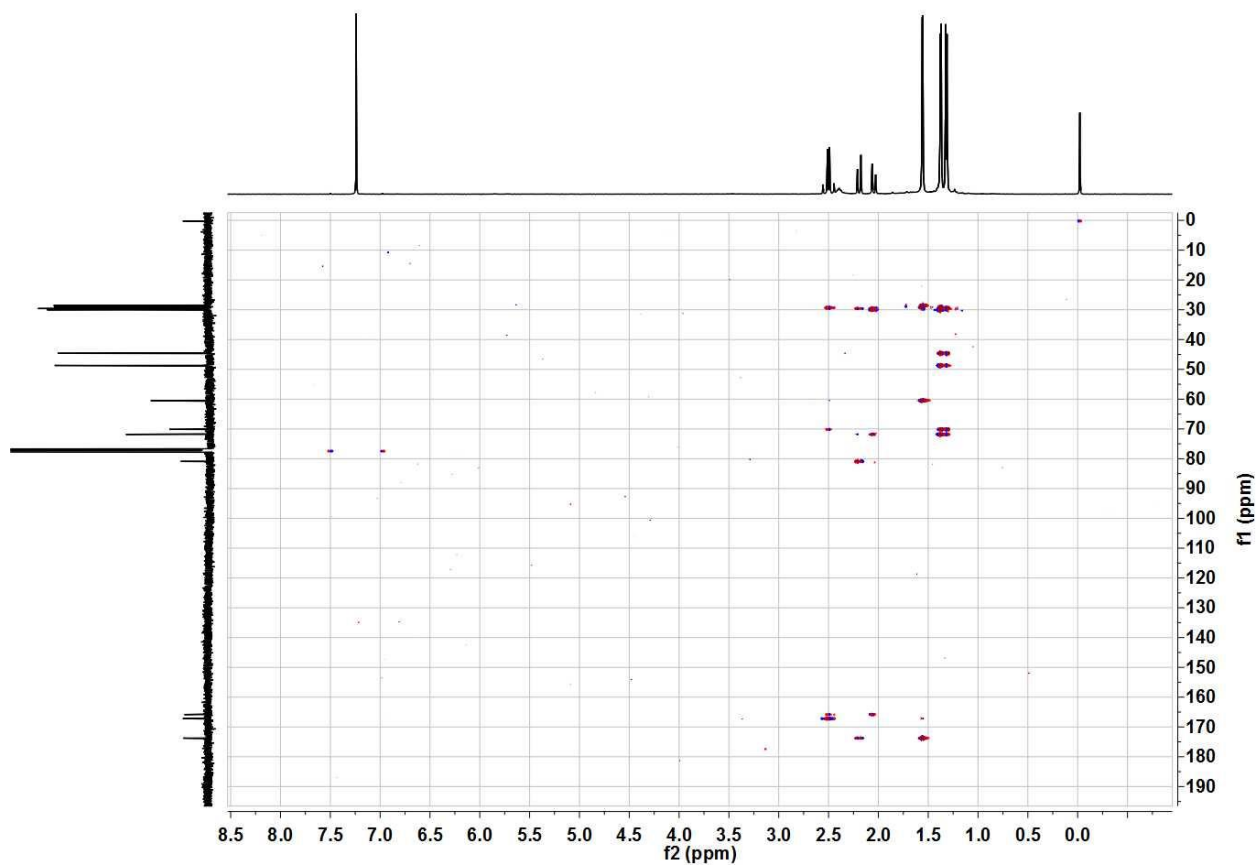
4.8.2 ^{13}C NMR (101 MHz, CDCl_3) spectra of **8**.

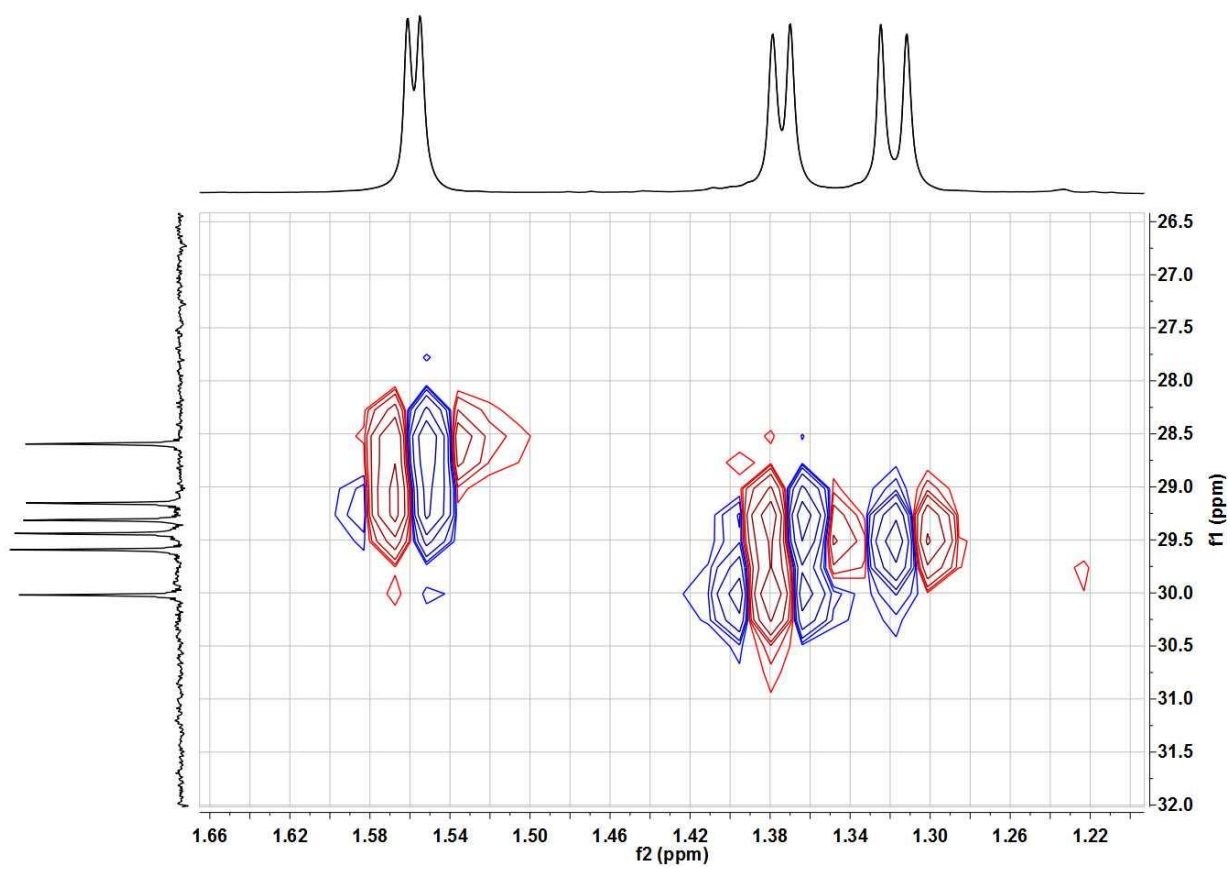
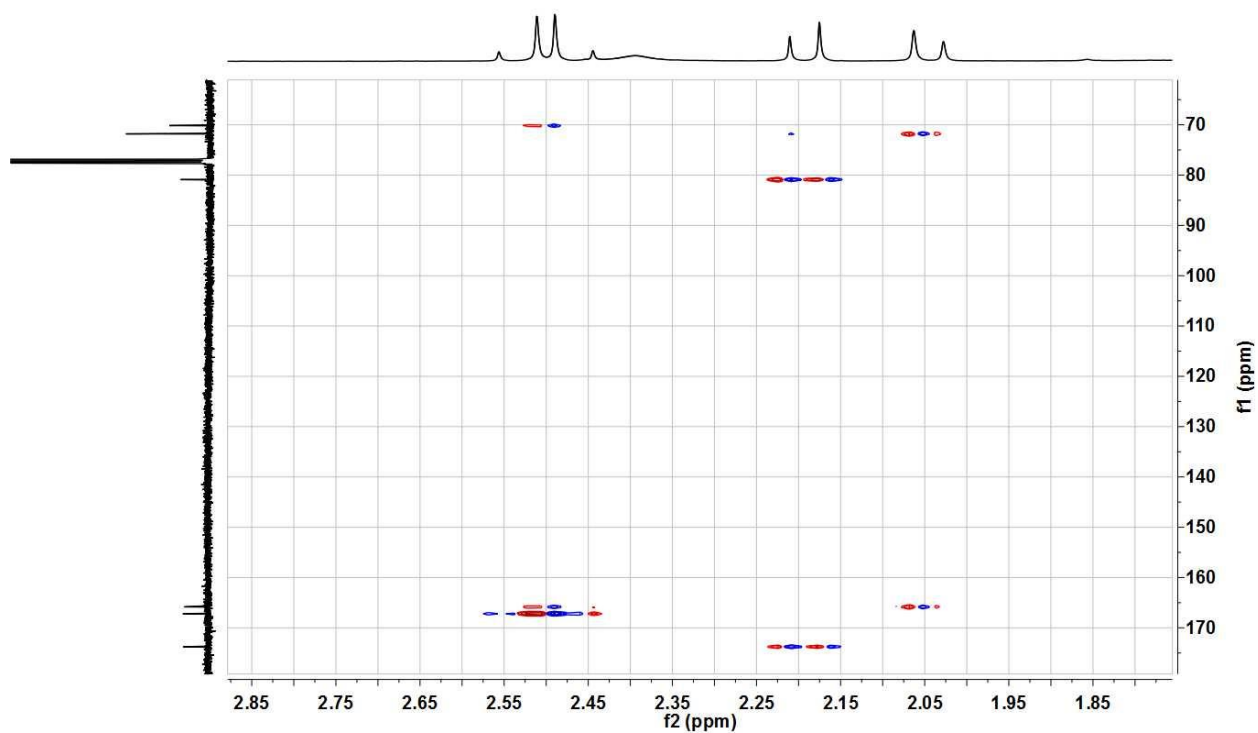


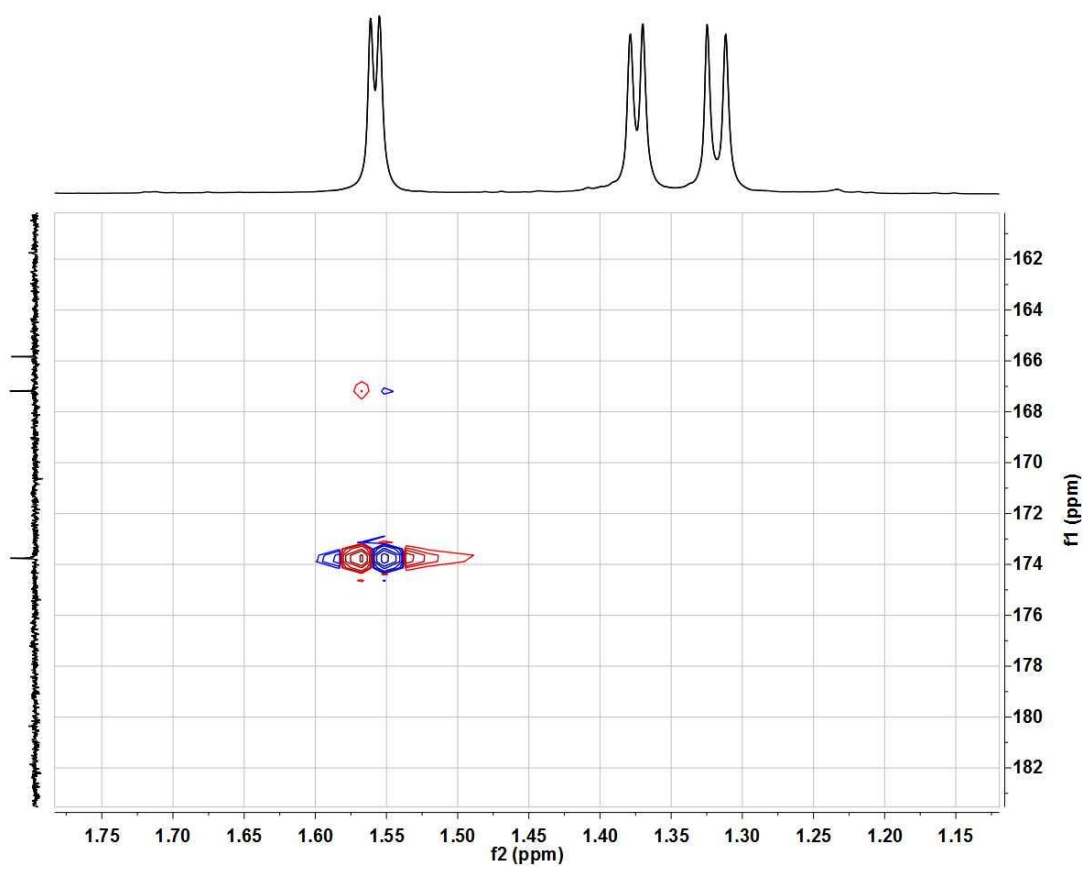
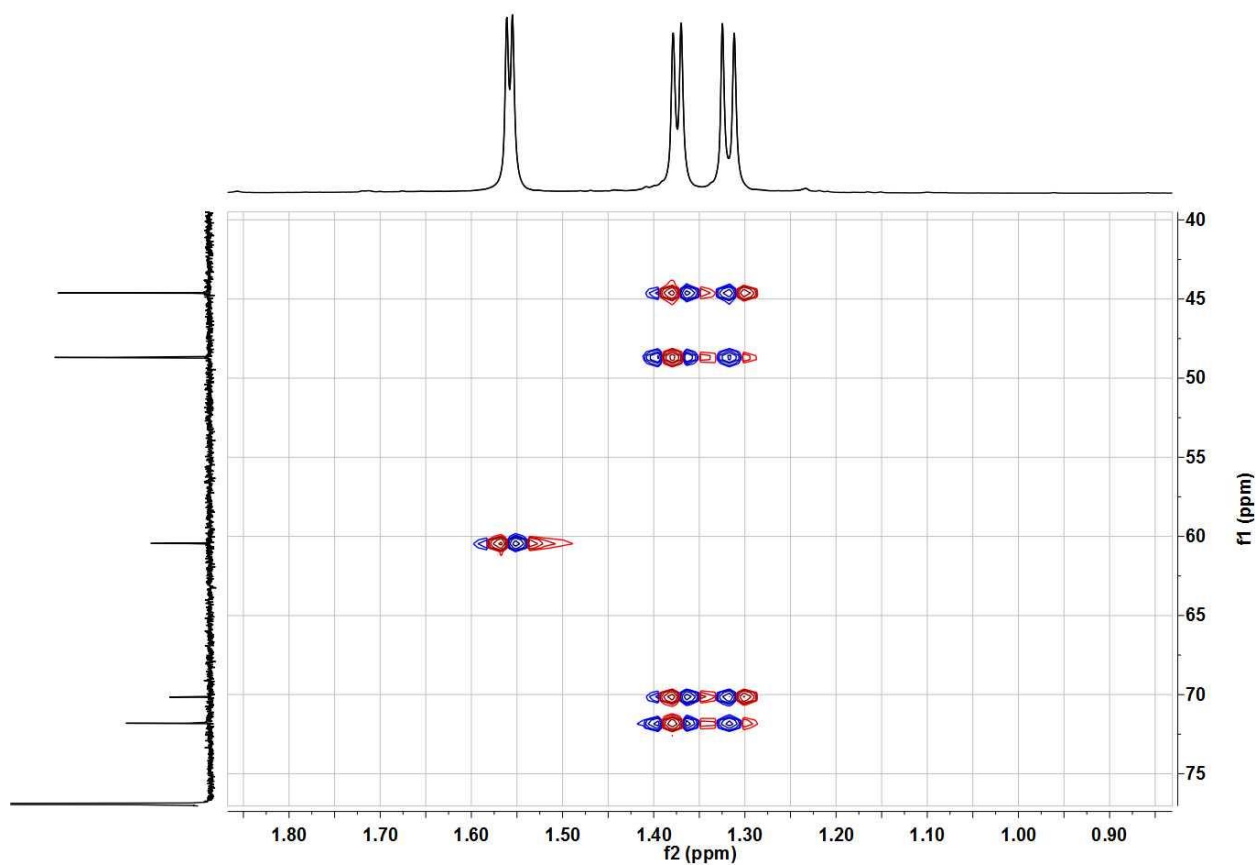
4.8.3 HSQC spectra of **8**.



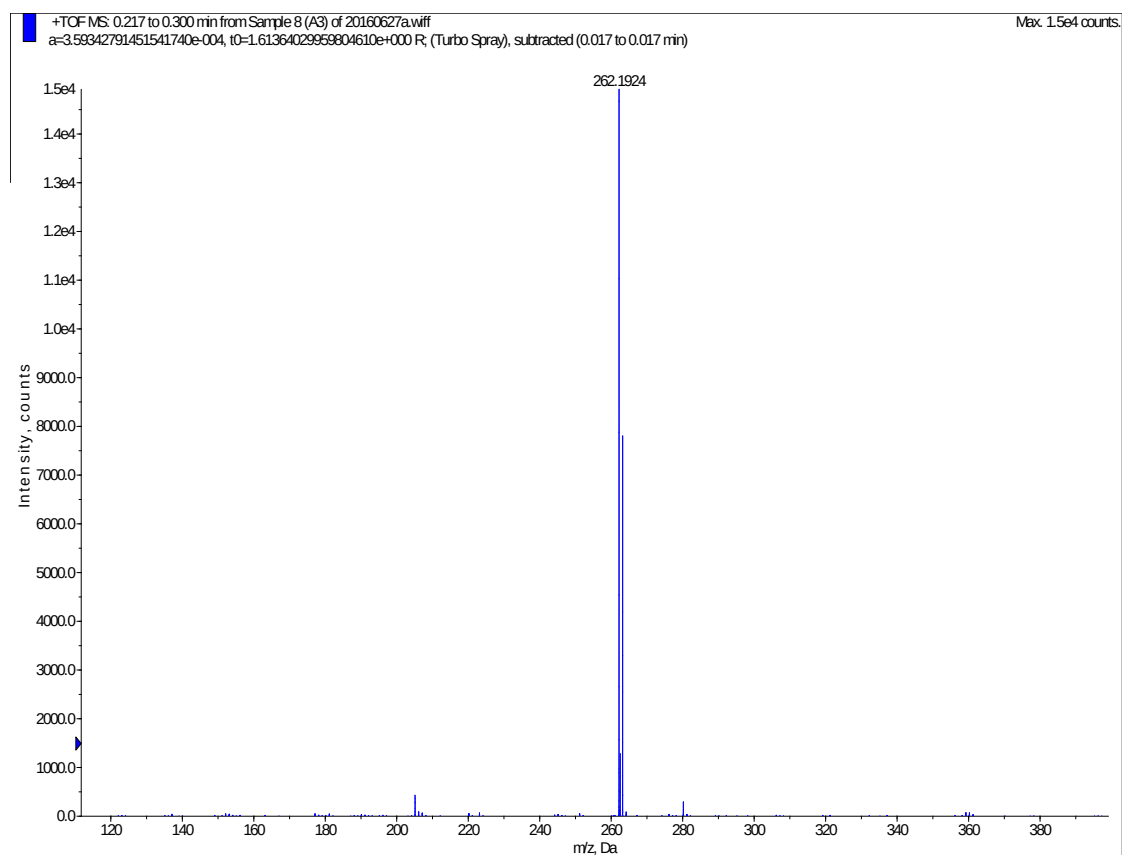
4.8.4 HMBC spectra of **8**.



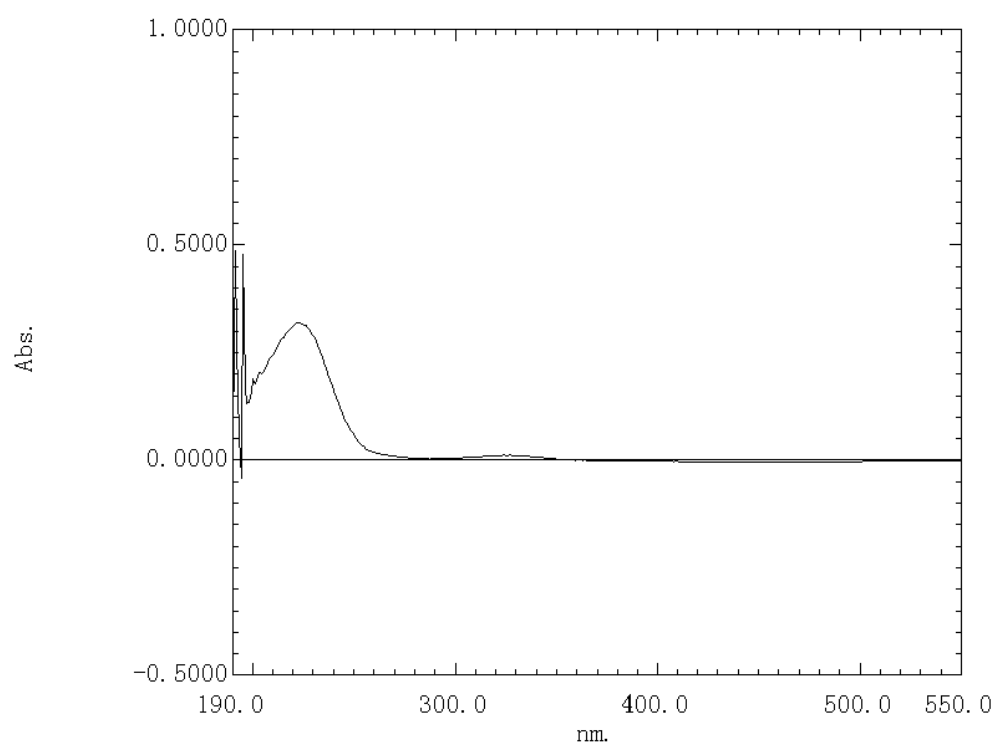




4.8.5 (+)HRESIMS of **8**.

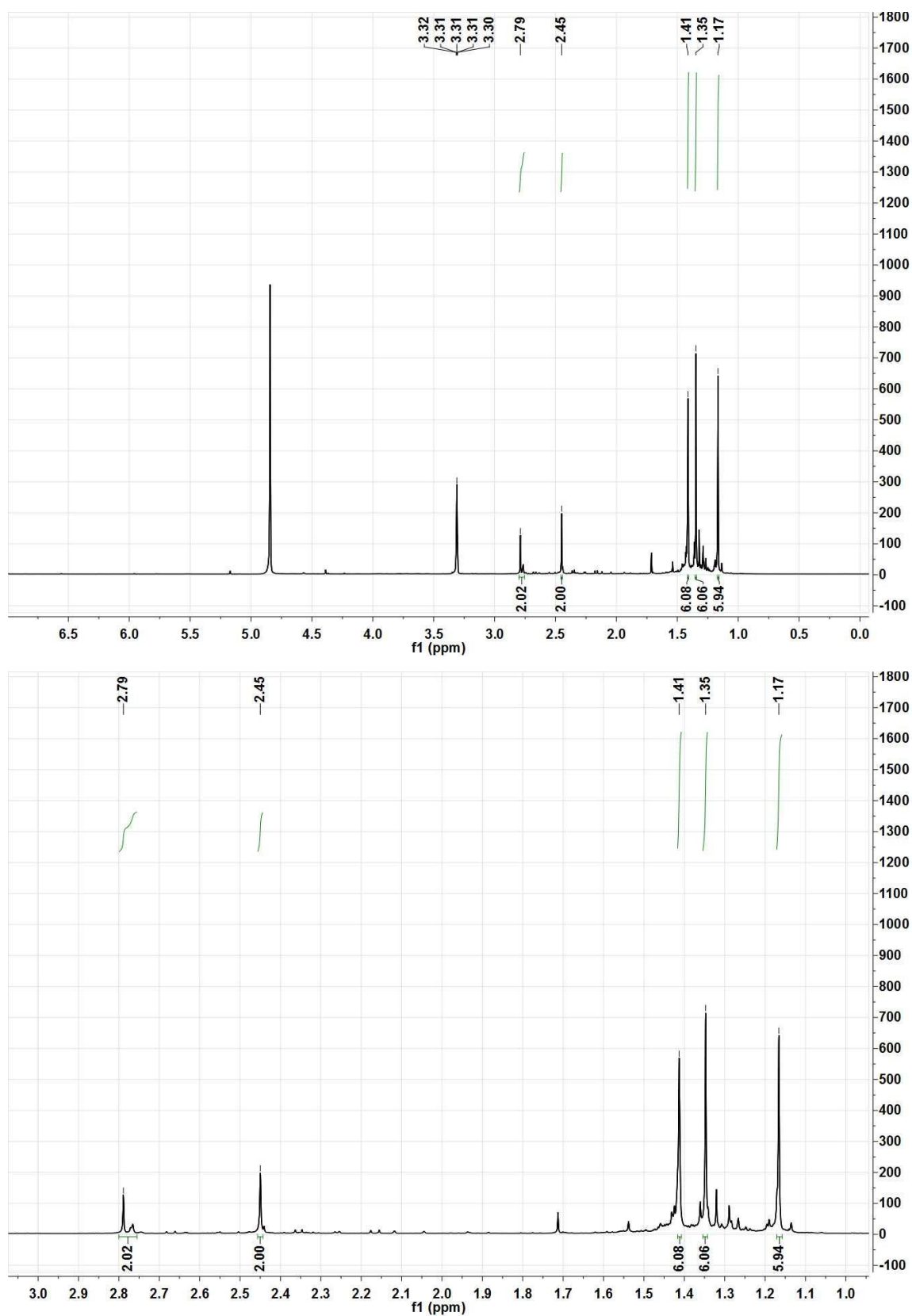


4.8.6 UV spectrum of **8**.

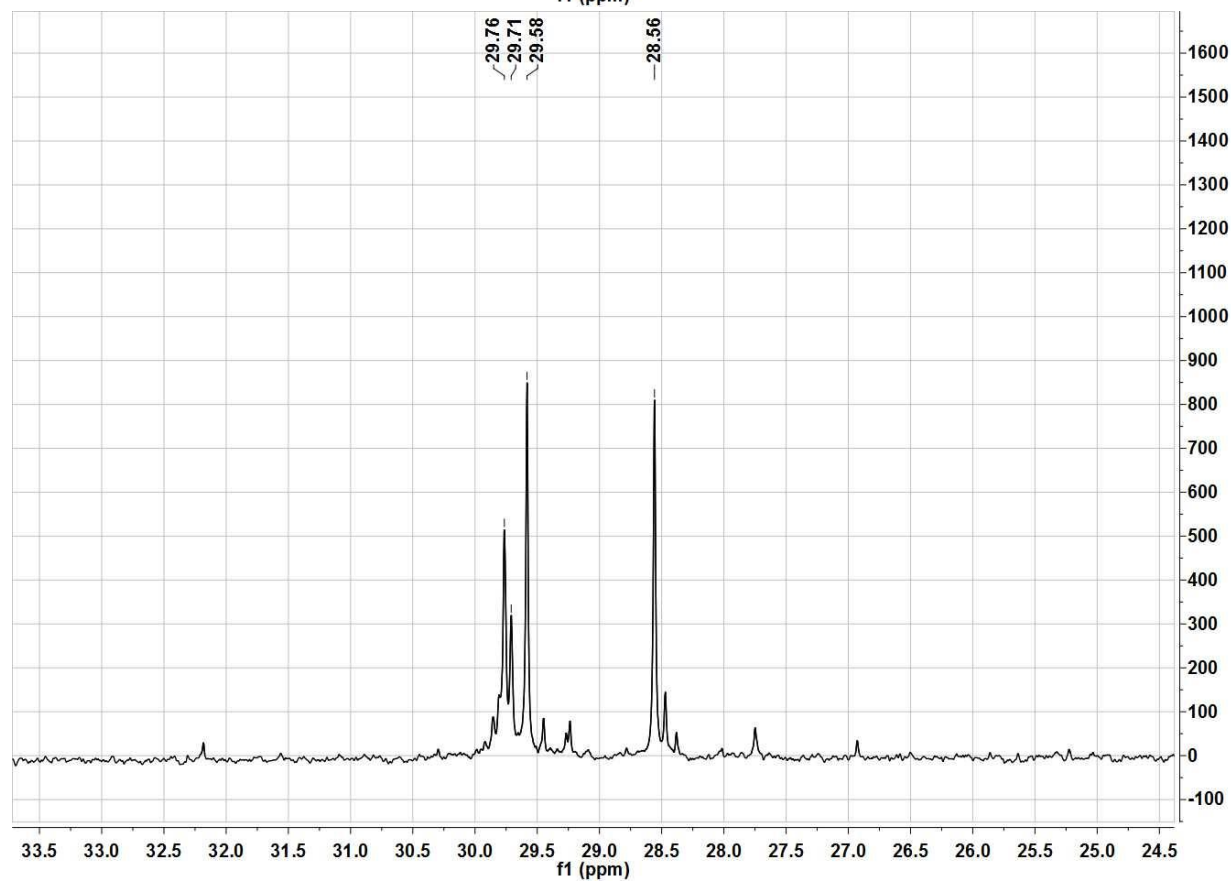
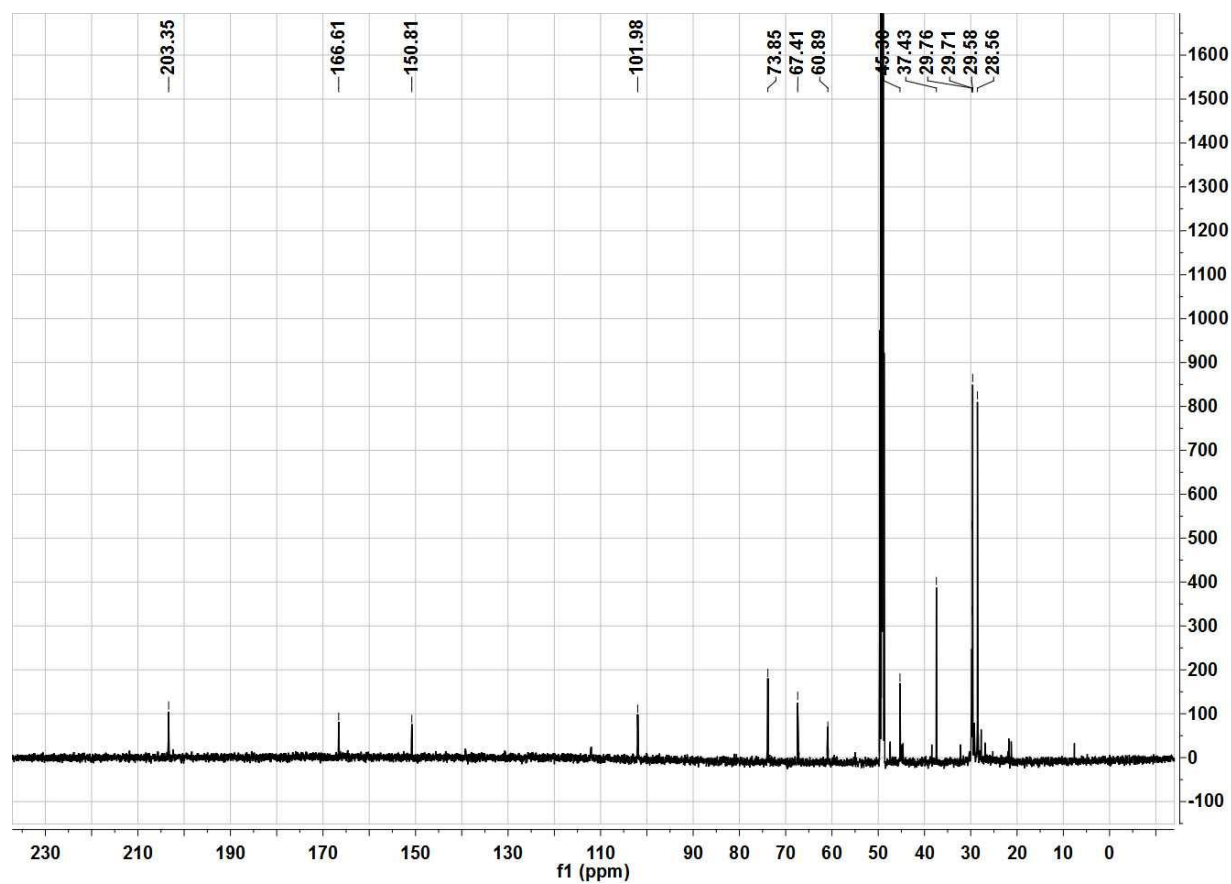


4.9 1D and 2D NMR of pyracyclumine I (9).

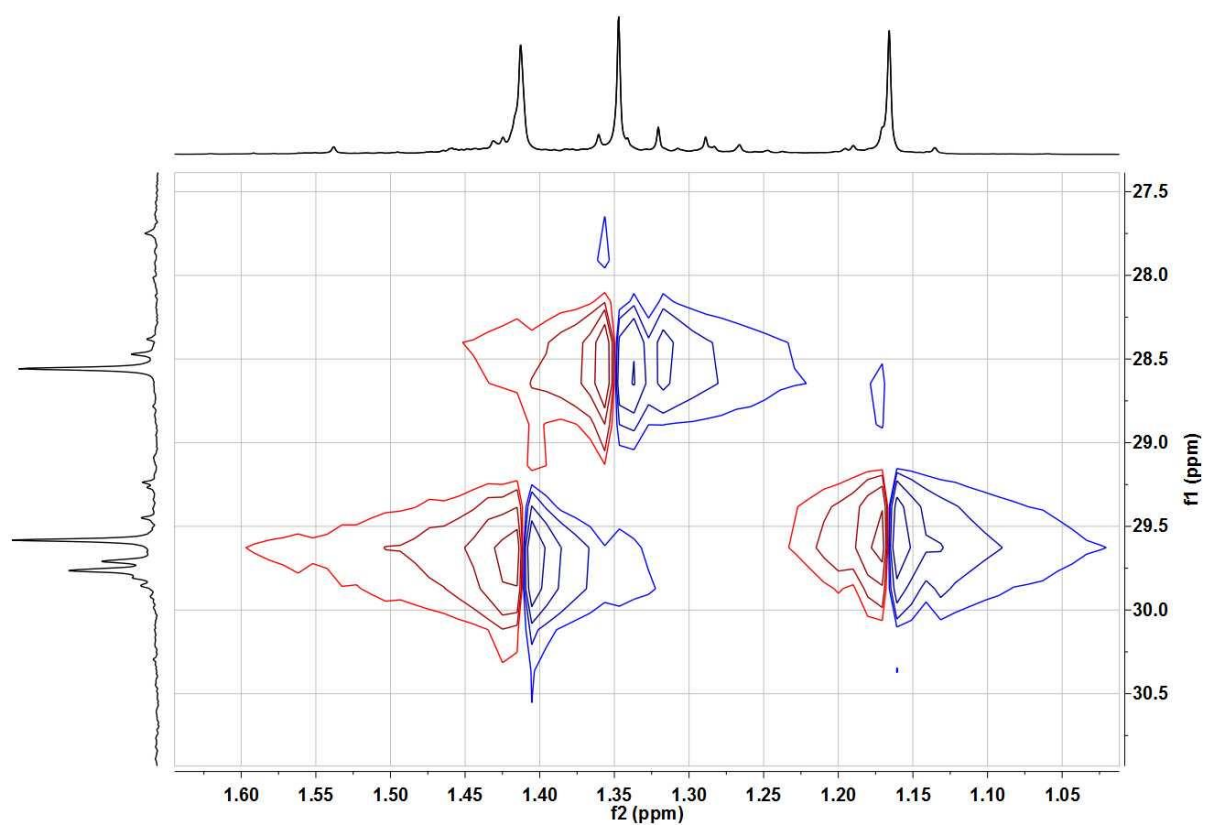
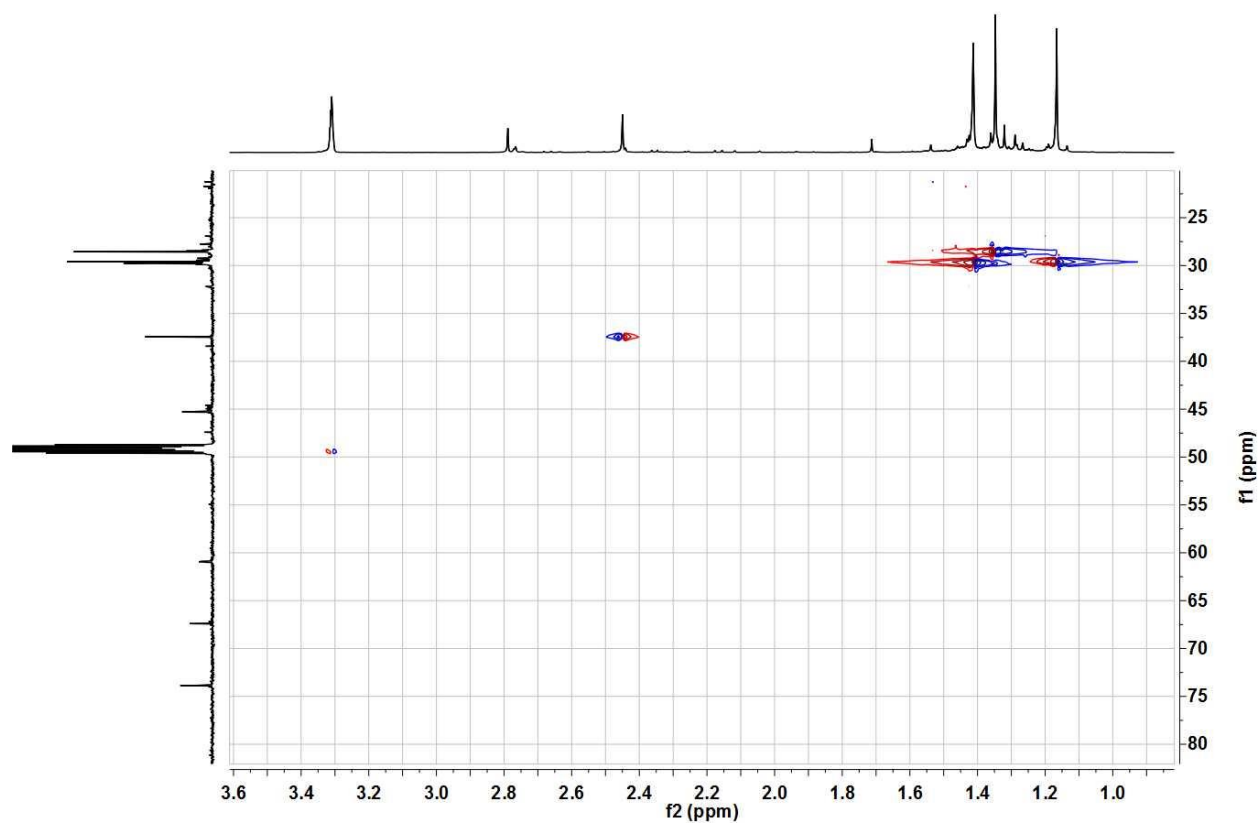
4.9.1 ^1H NMR (600 MHz, $\text{MeOH-}d_4$) spectra of 9.



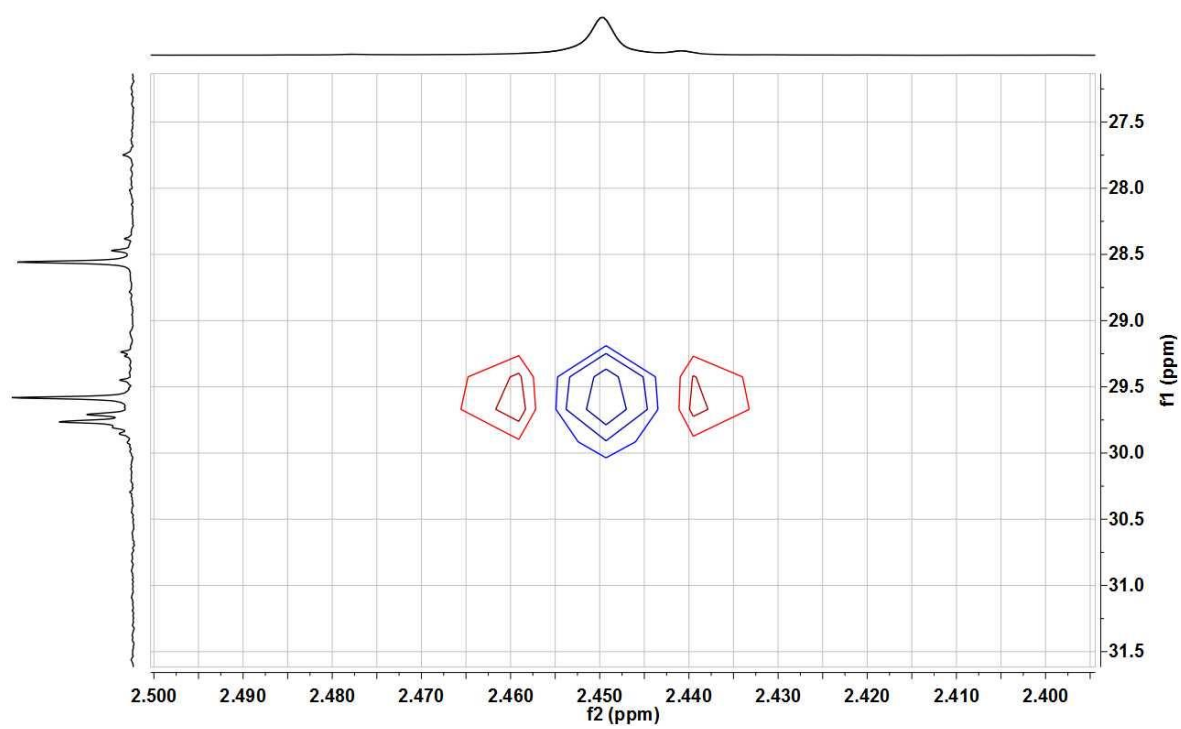
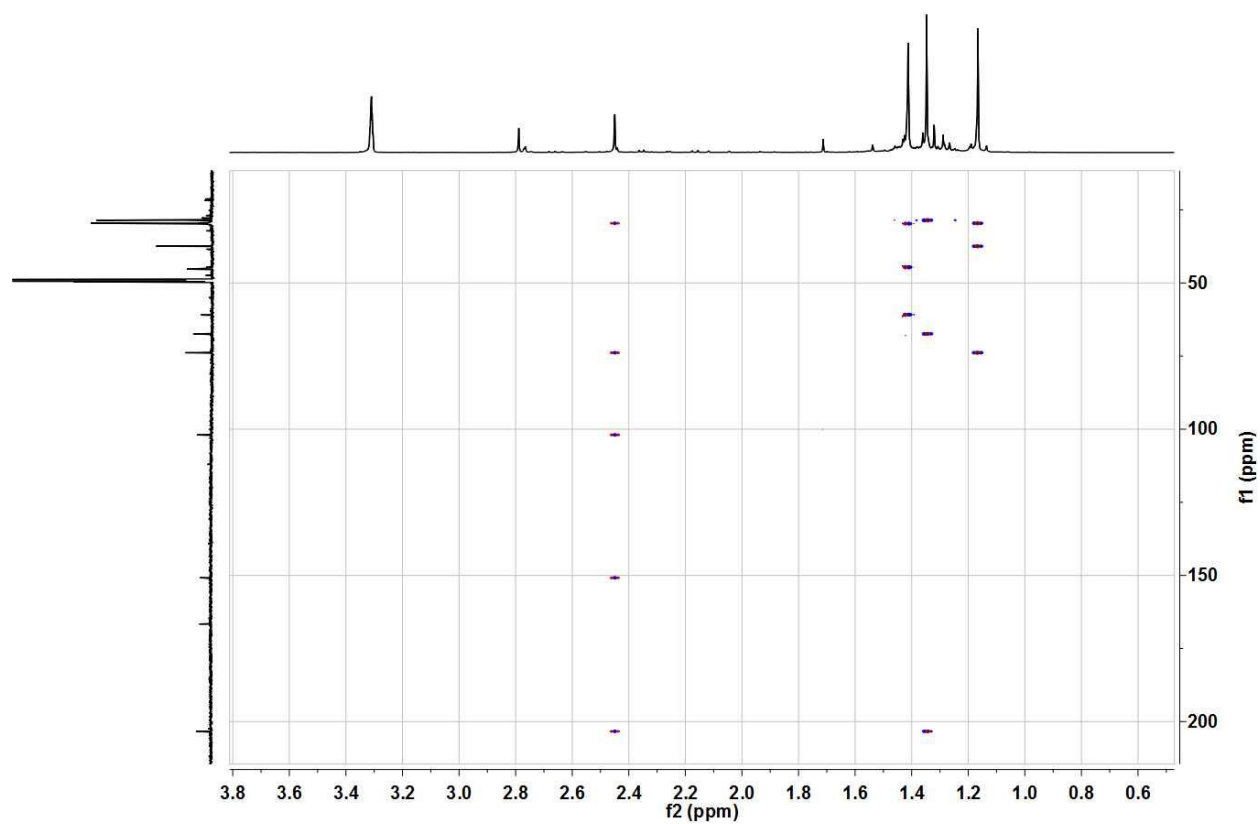
4.9.2 ^{13}C NMR (150 MHz, MeOH-d_4) spectra of **9**.

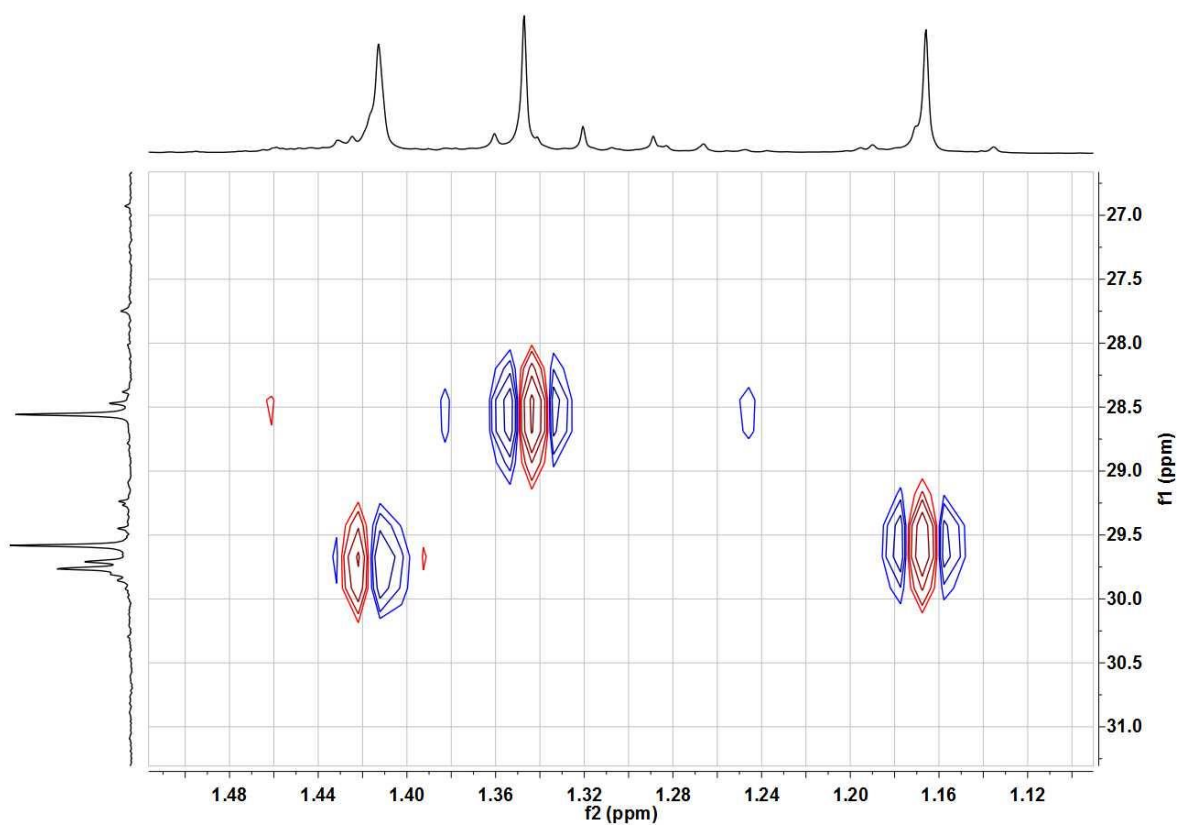
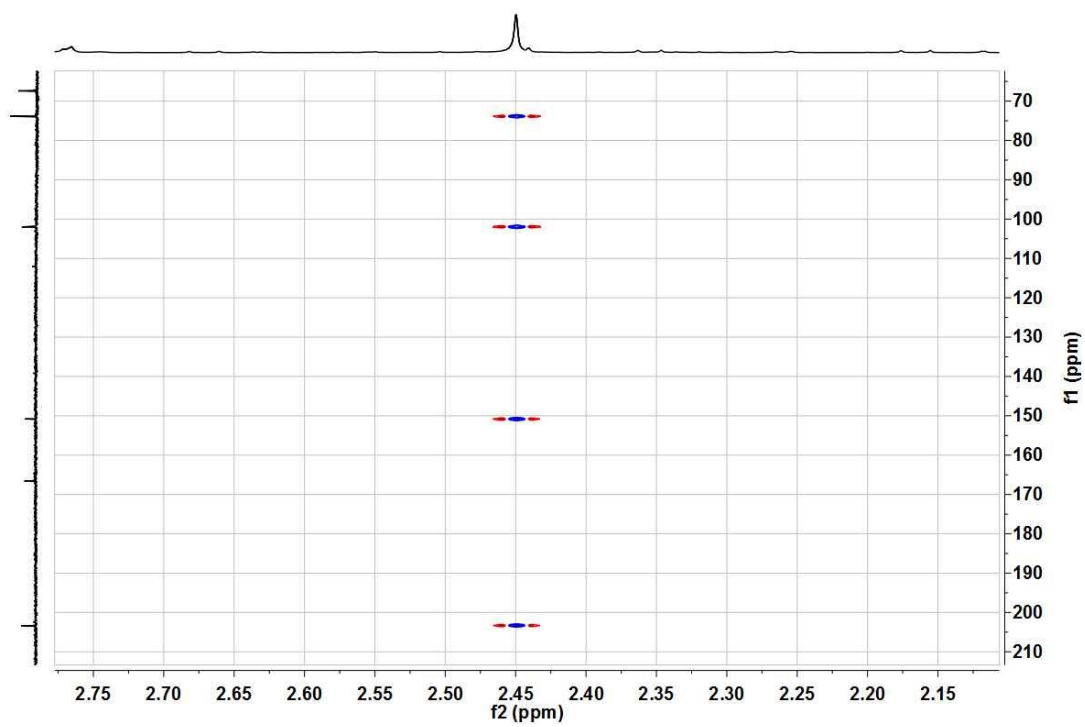


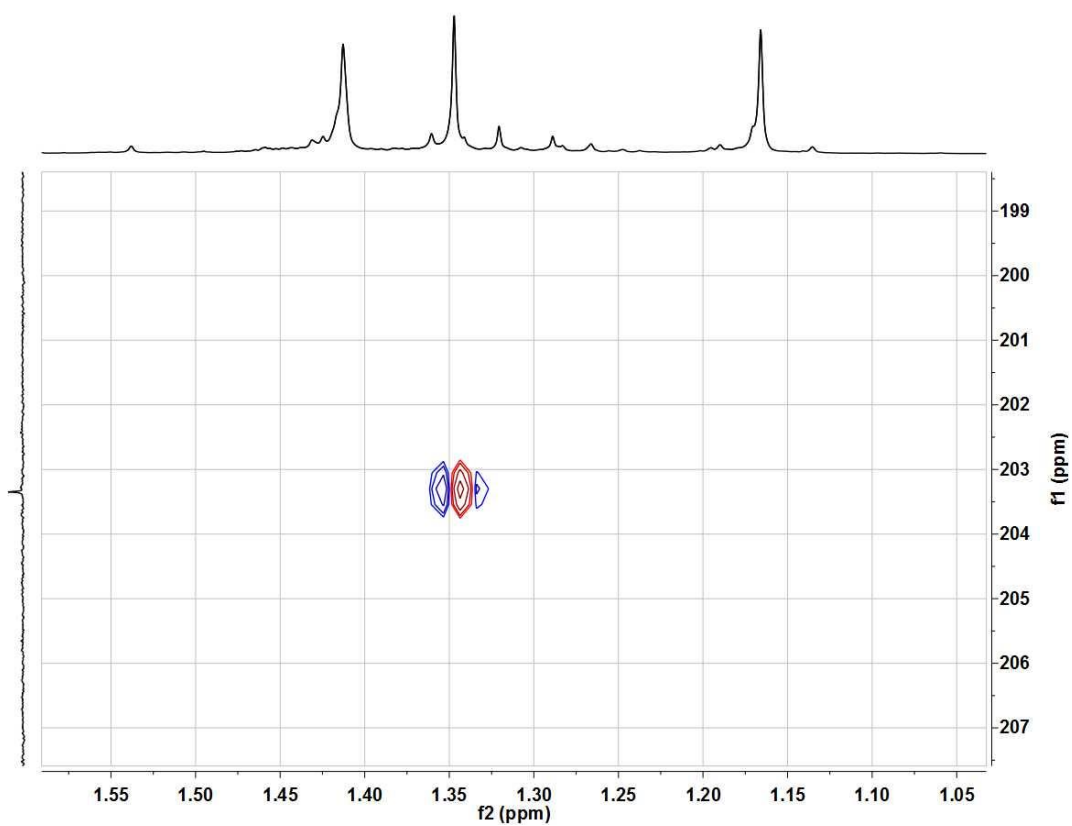
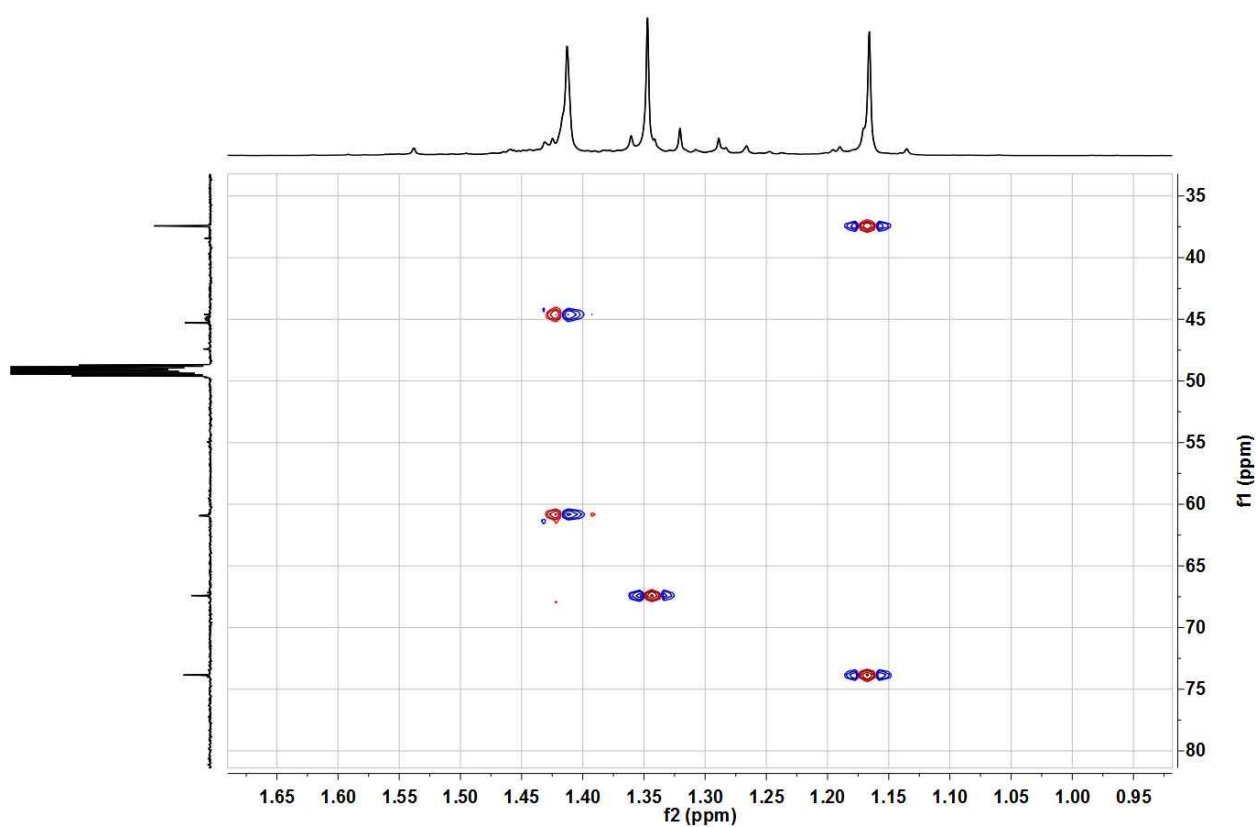
4.9.3 HSQC spectra of **9**.



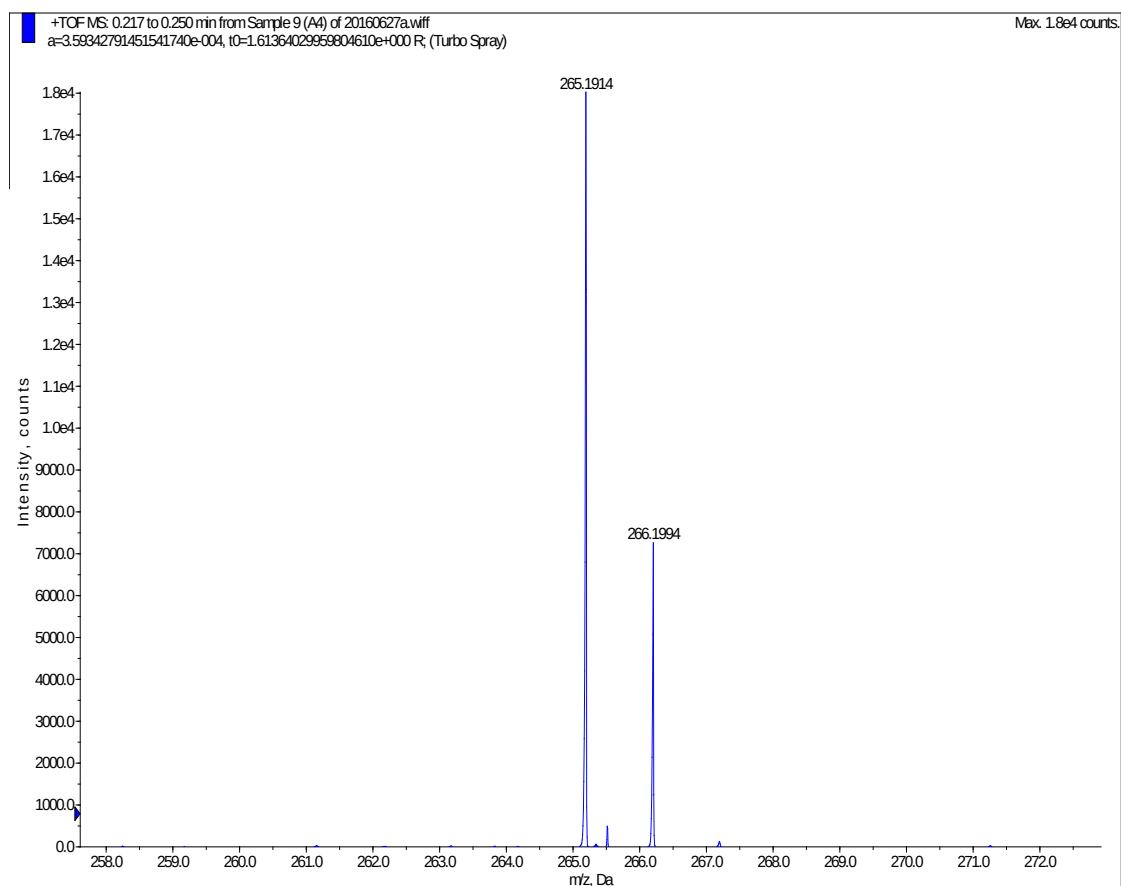
4.9.4 HMBC spectra of **9**.



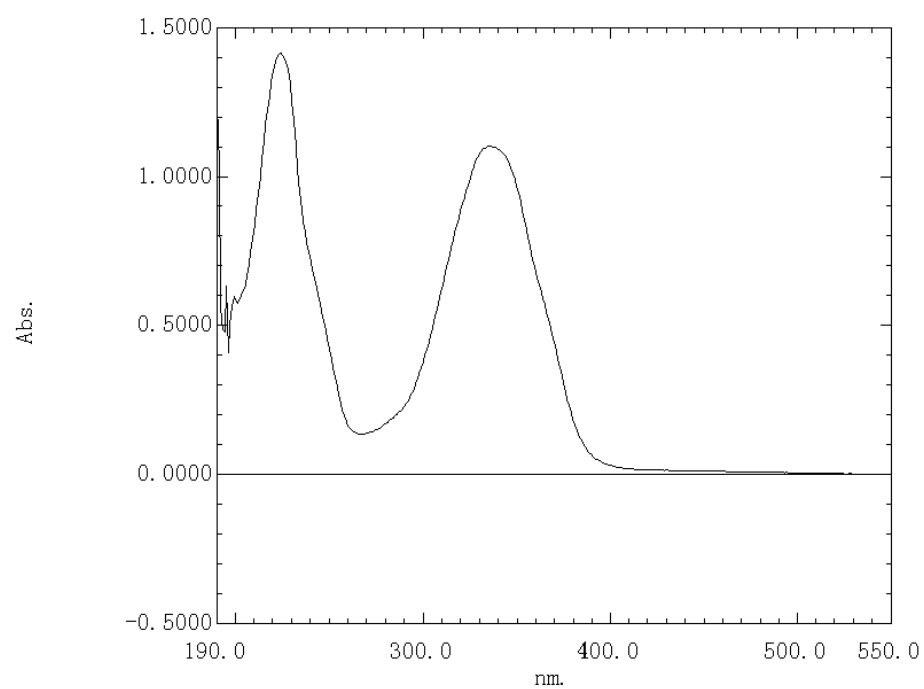




4.9.5 (+)HRESIMS of **9**.

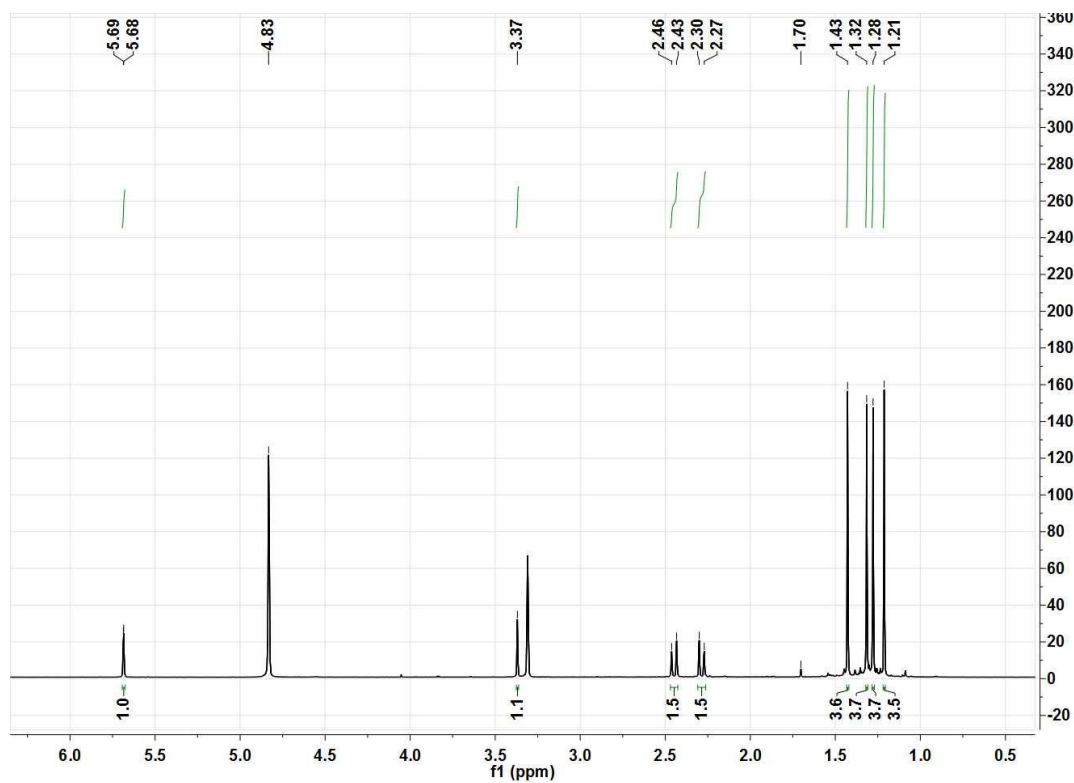


4.9.6 UV spectrum of **9**.

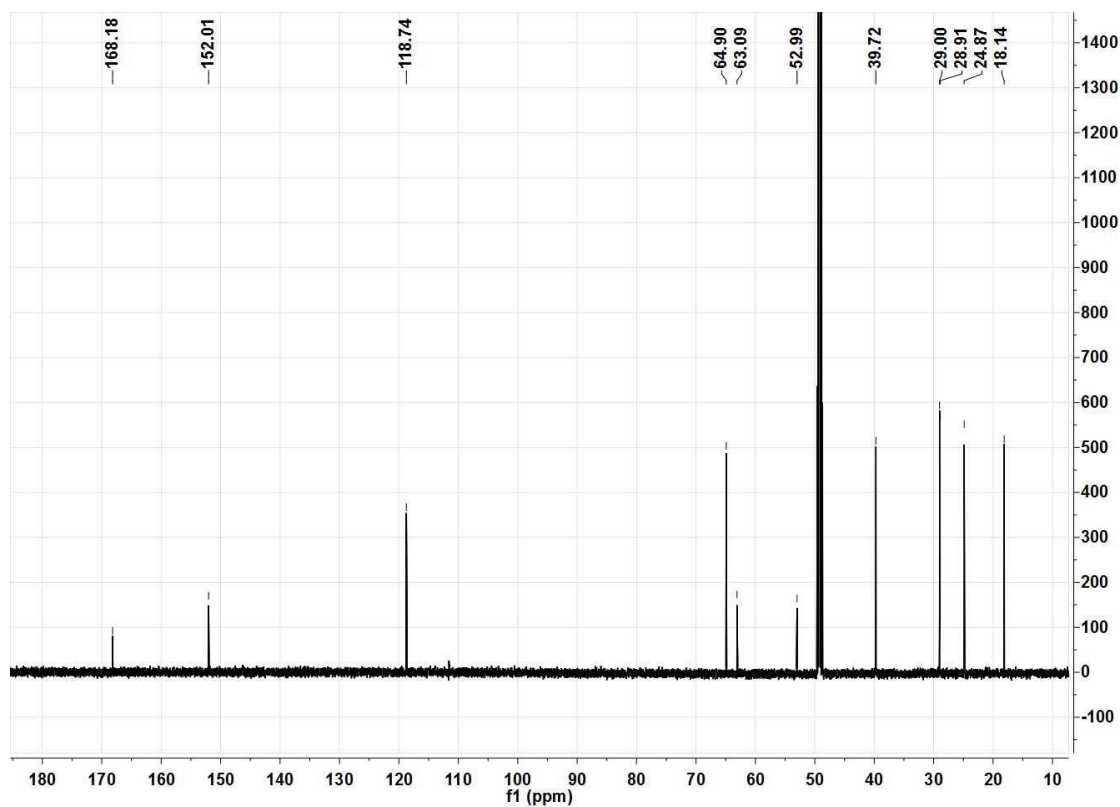


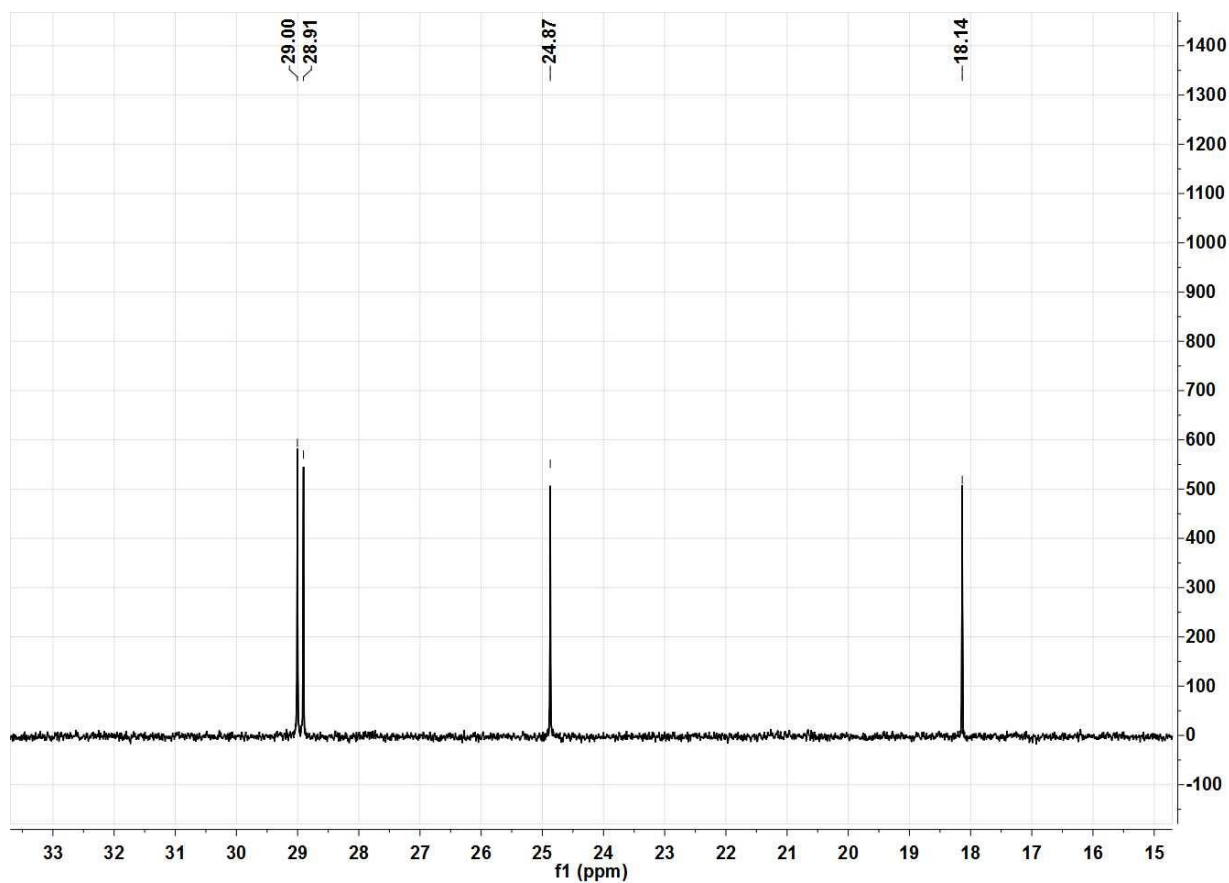
4.10 1D and 2D NMR of pyracyclumine J (10).

4.10.1 ^1H NMR (600 MHz, $\text{MeOH-}d_4$) spectrum of **10**.

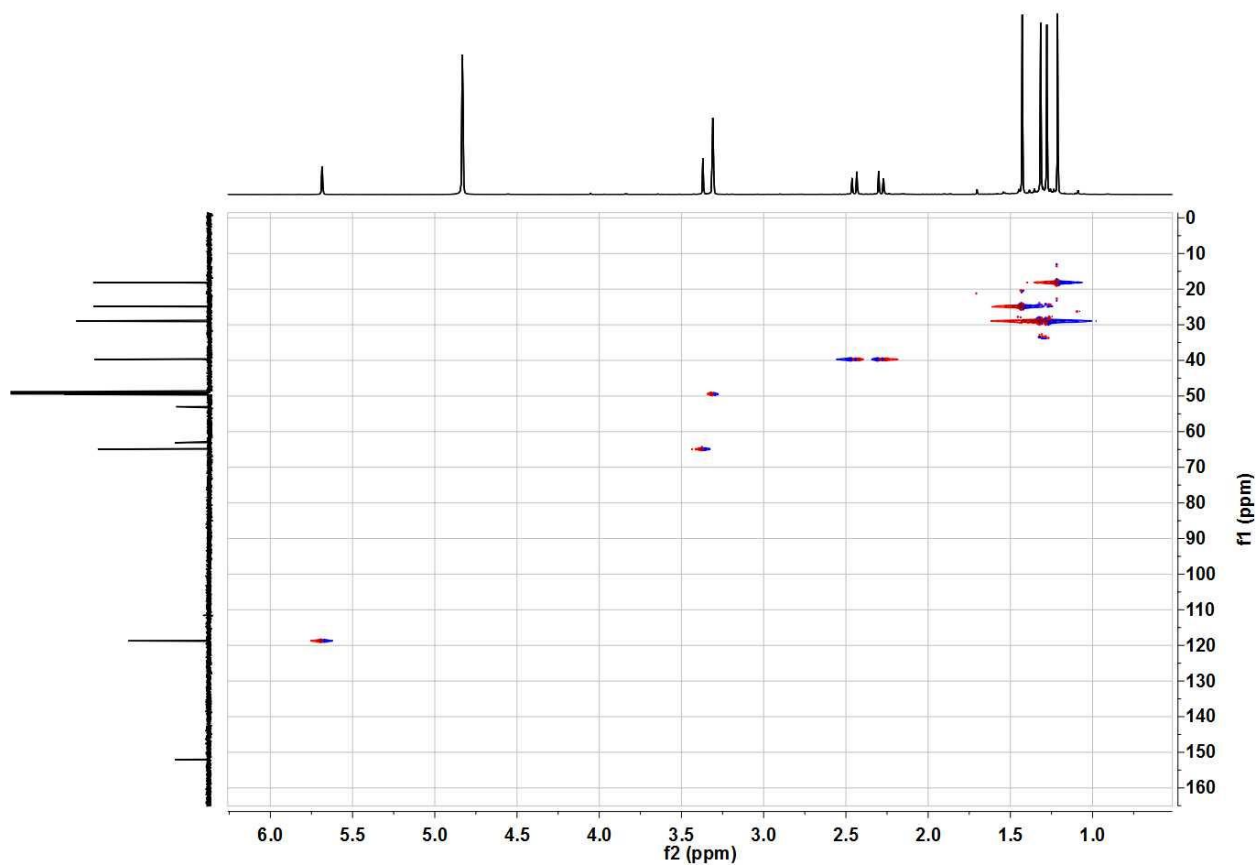


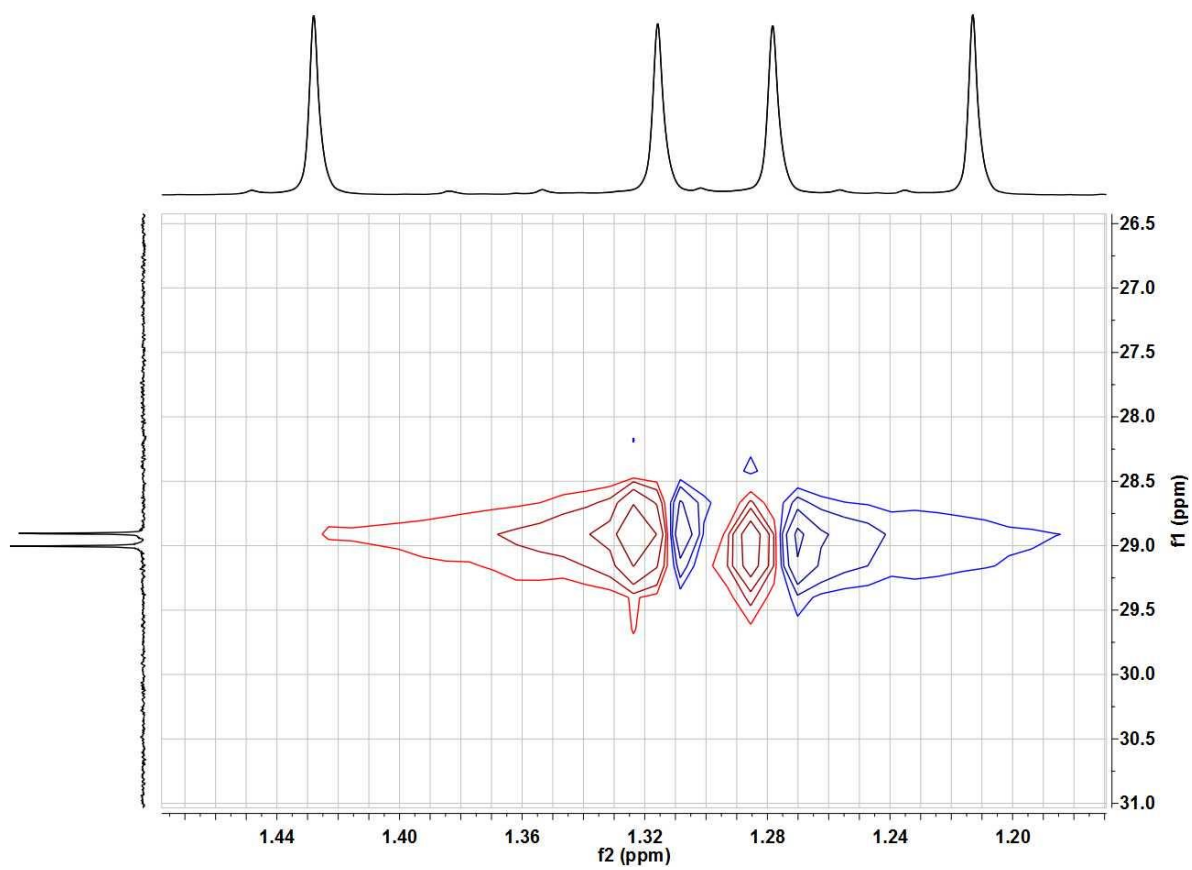
4.10.2 ^{13}C NMR (150 MHz, $\text{MeOH-}d_4$) spectra of **10**.



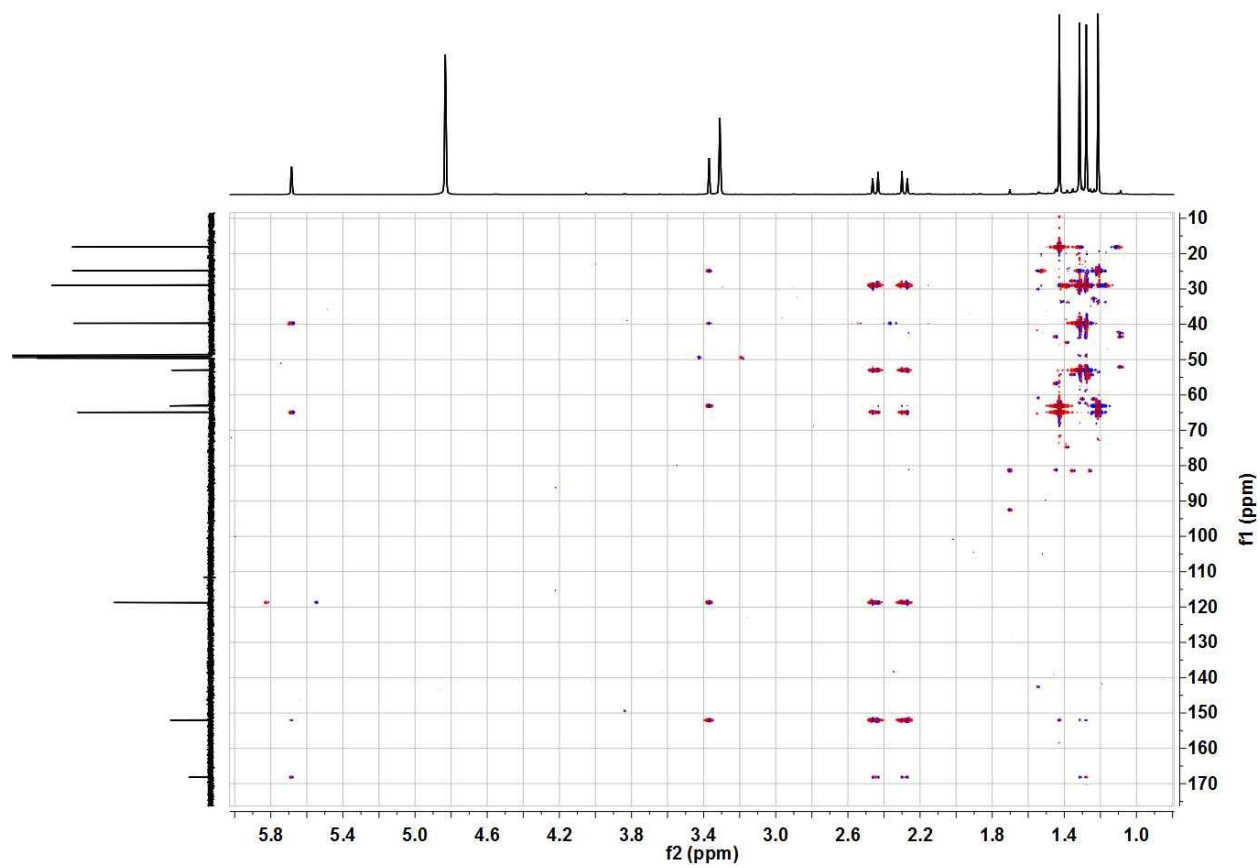


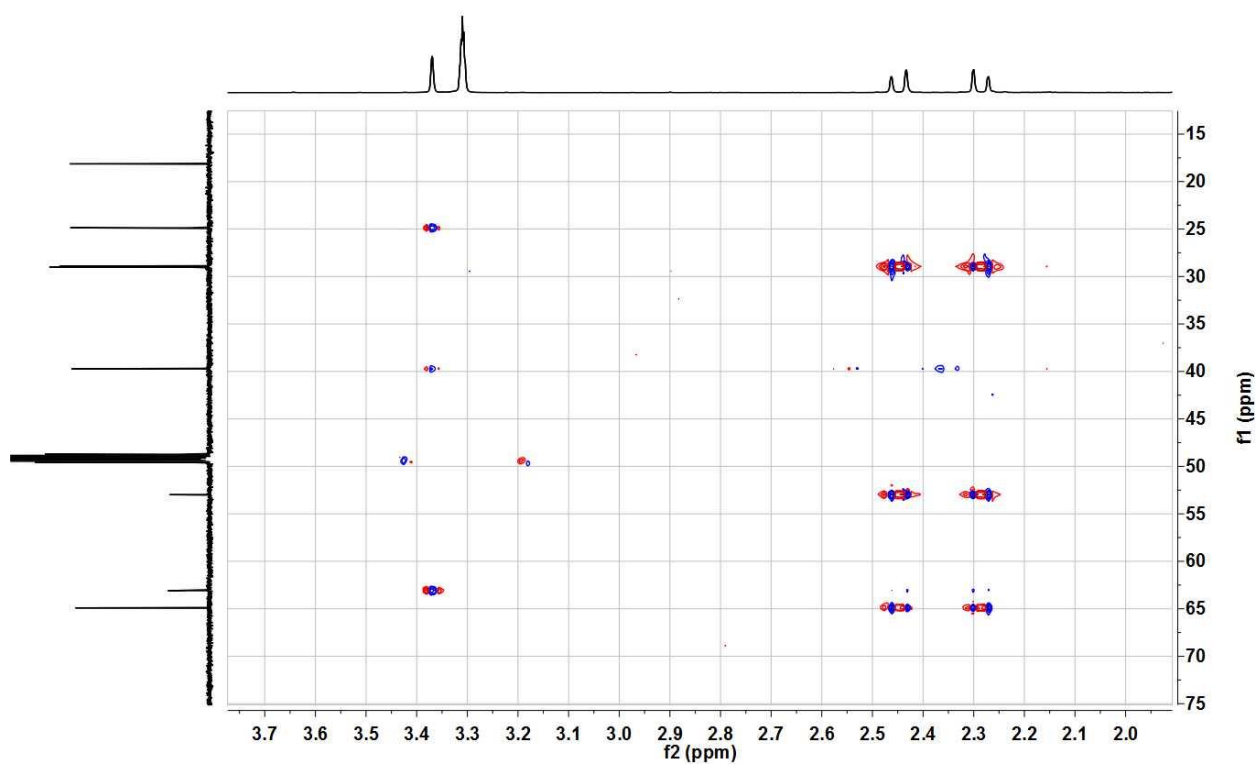
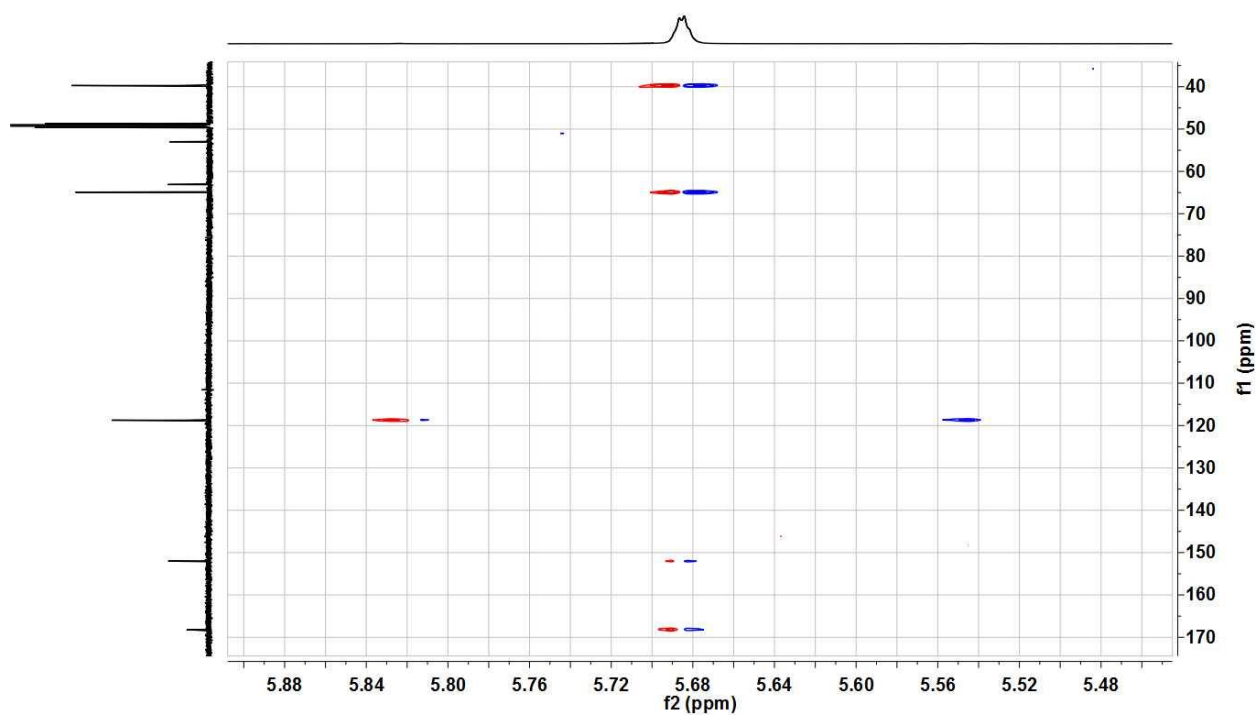
4.10.3 HSQC spectra of **10**.

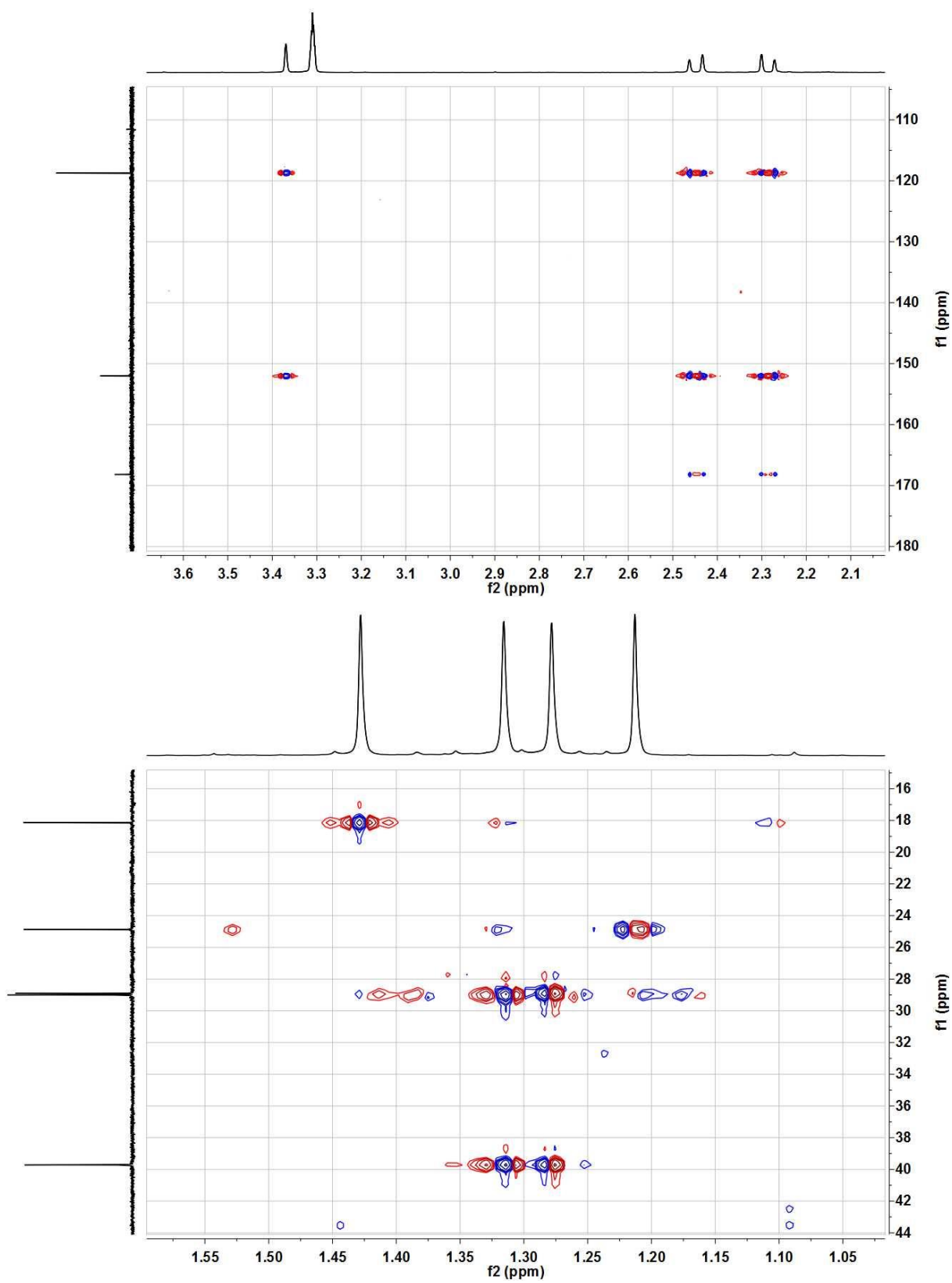


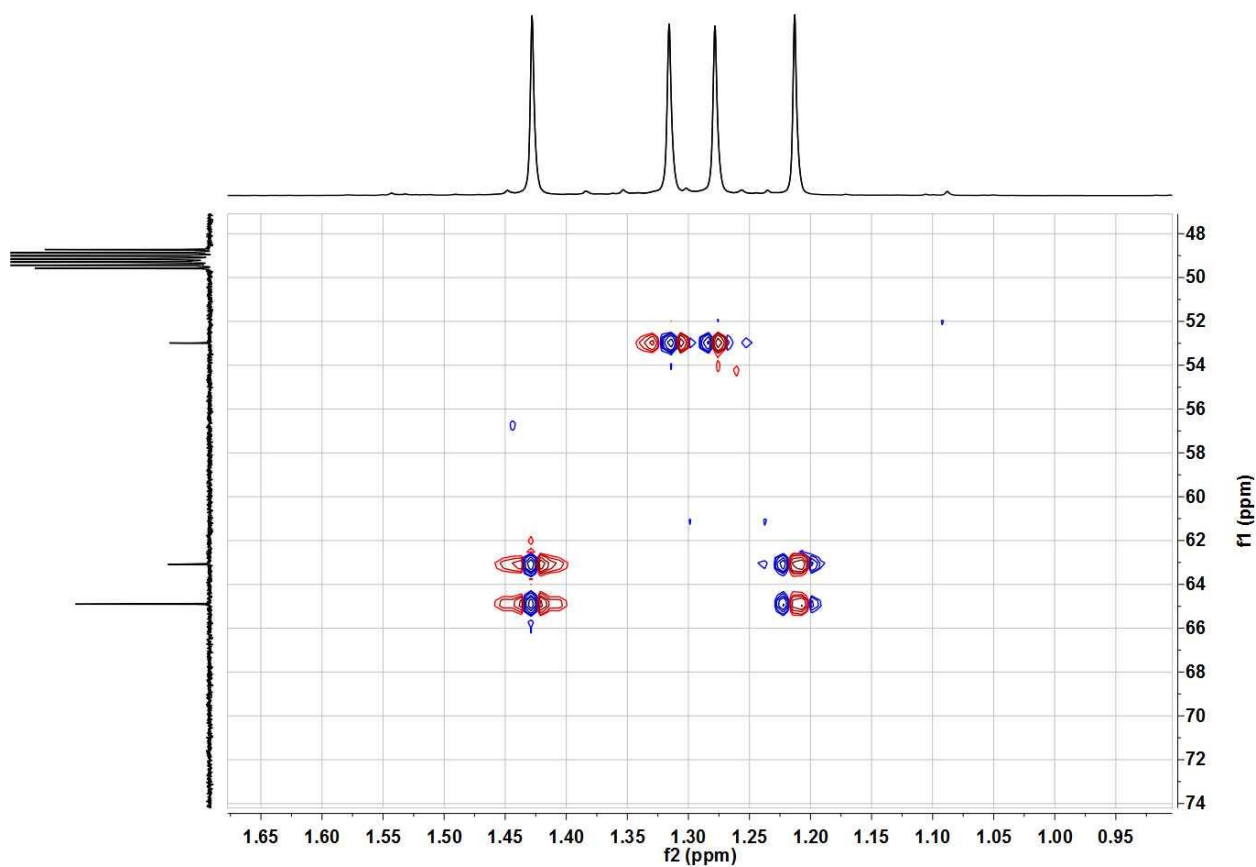


4.10.4 HMBC spectra of **10**.

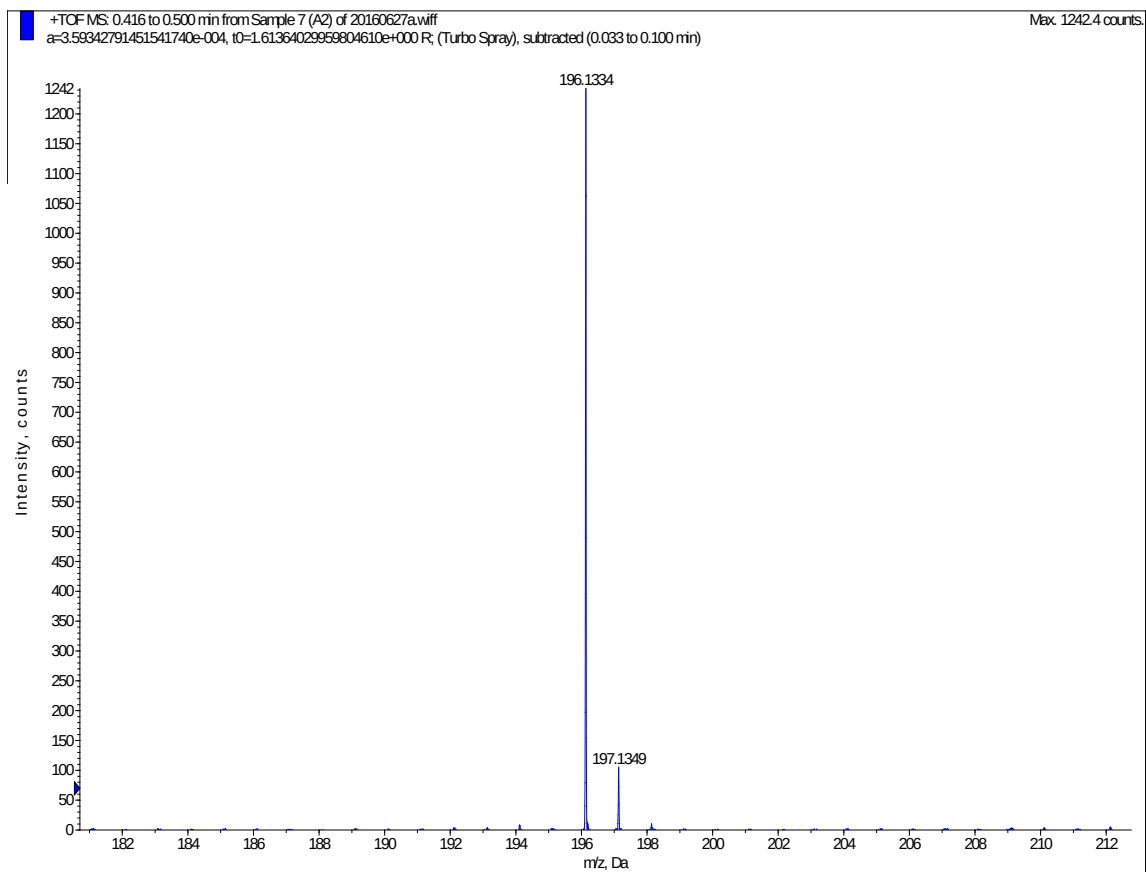




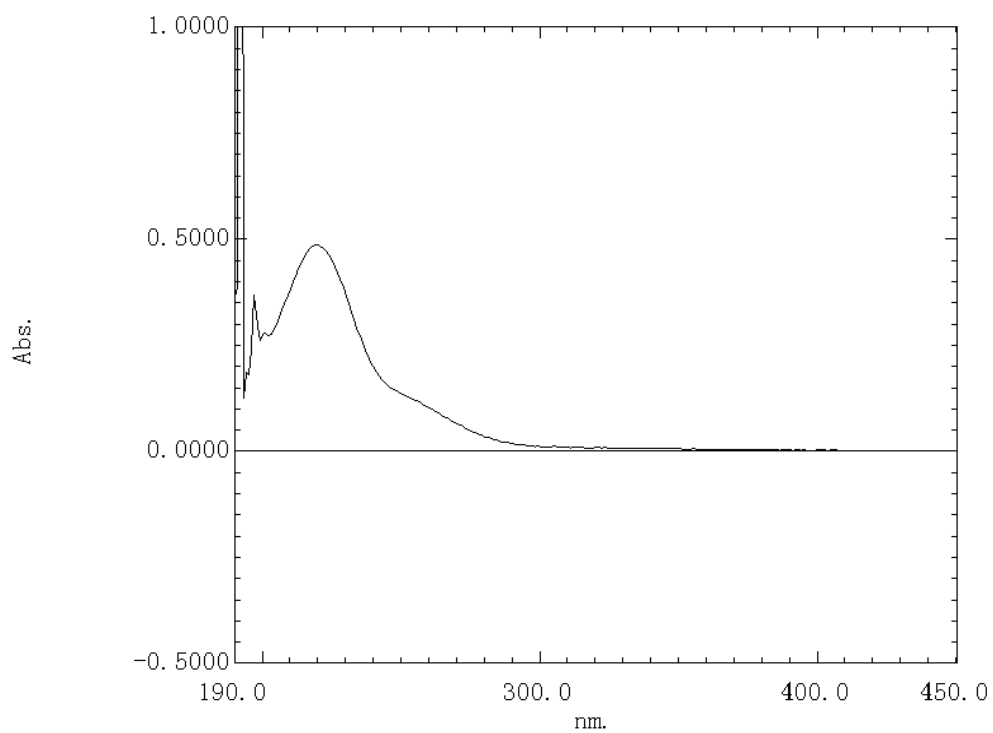




4.10.5 (+)HRESIMS of **10**.

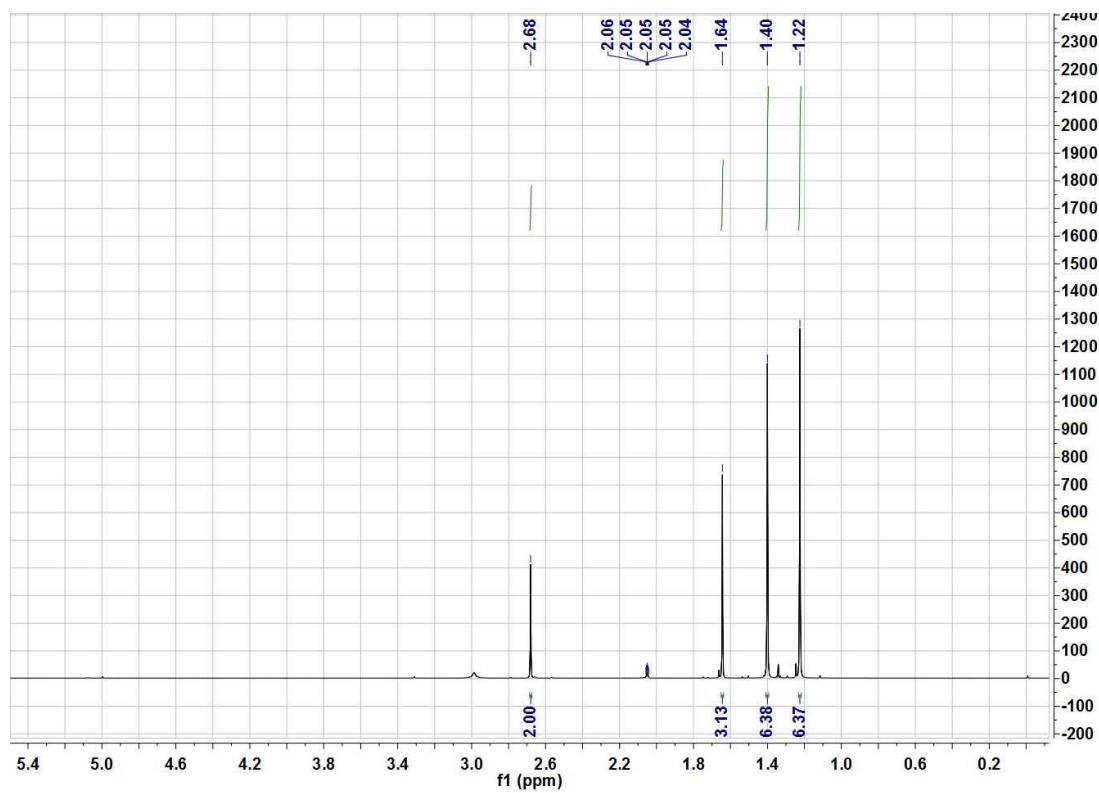


4.10.6 UV spectrum of **10**.

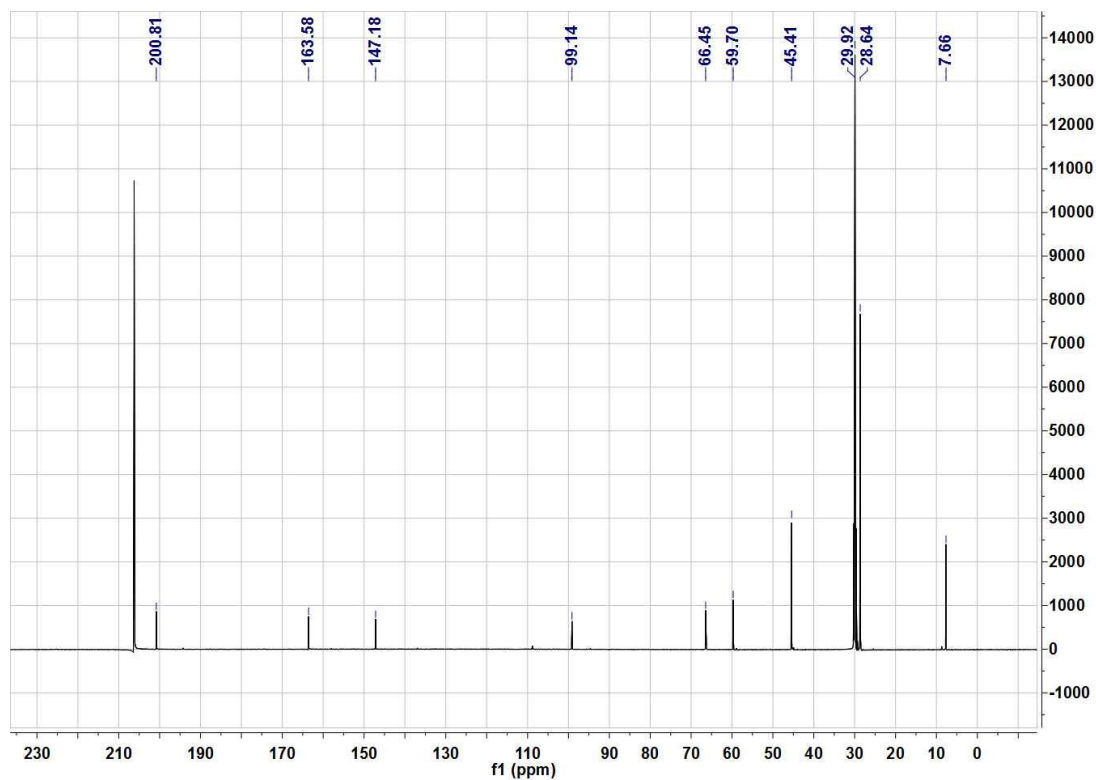


4.11 1D NMR of agrocybenine (**11**).

4.11.1 ^1H NMR (600 MHz, Acetone- d_6) spectrum of **11**.

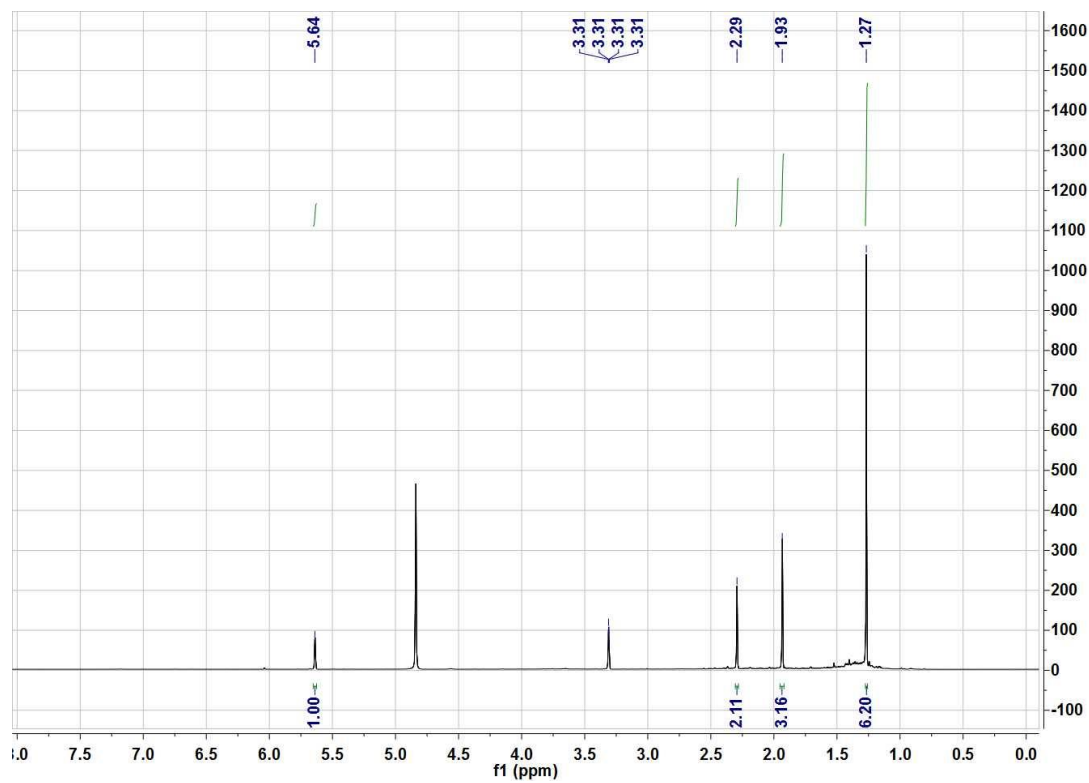


4.11.2 ^{13}C NMR (150 MHz, Acetone- d_6) spectrum of **11**.

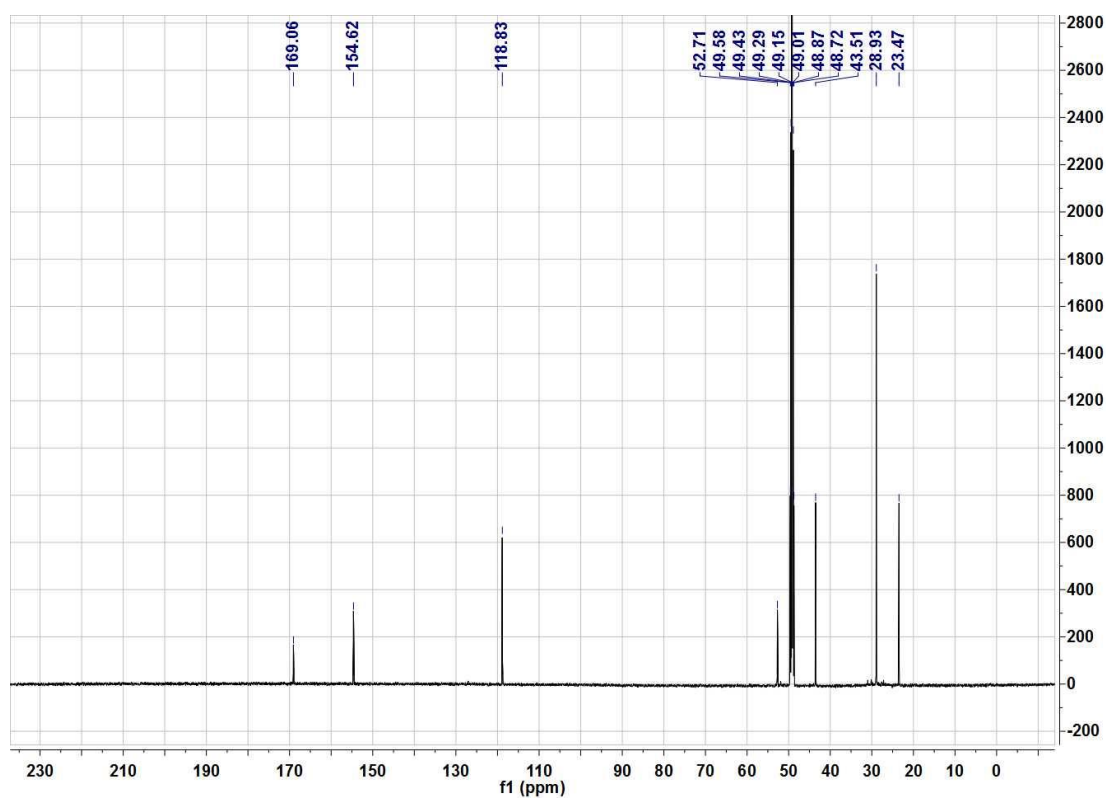


4.12 1D NMR of 4,6,6-trimethyl-5,6-dihydro-2(*1H*)-pyridone (**12**).

4.12.1 ^1H NMR (600 MHz, MeOH- d_4) spectrum of **12**.

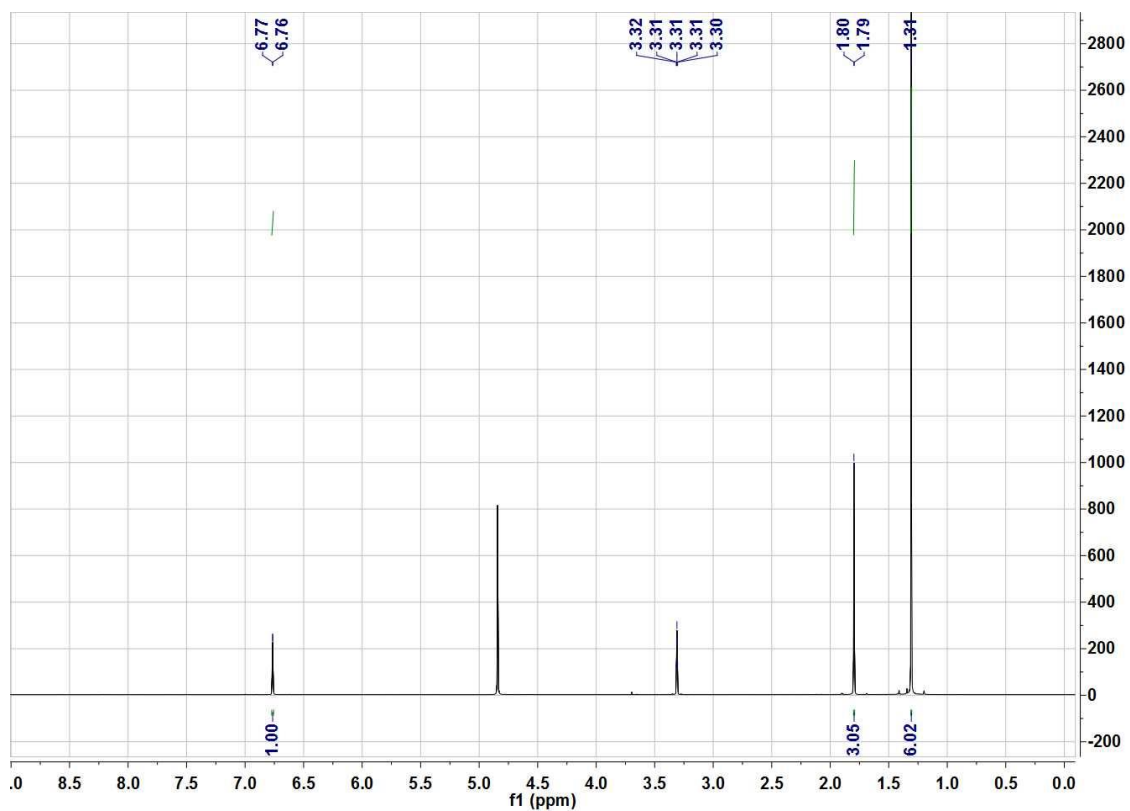


4.12.2 ^{13}C NMR (150 MHz, $\text{MeOH-}d_4$) spectrum of **12**.

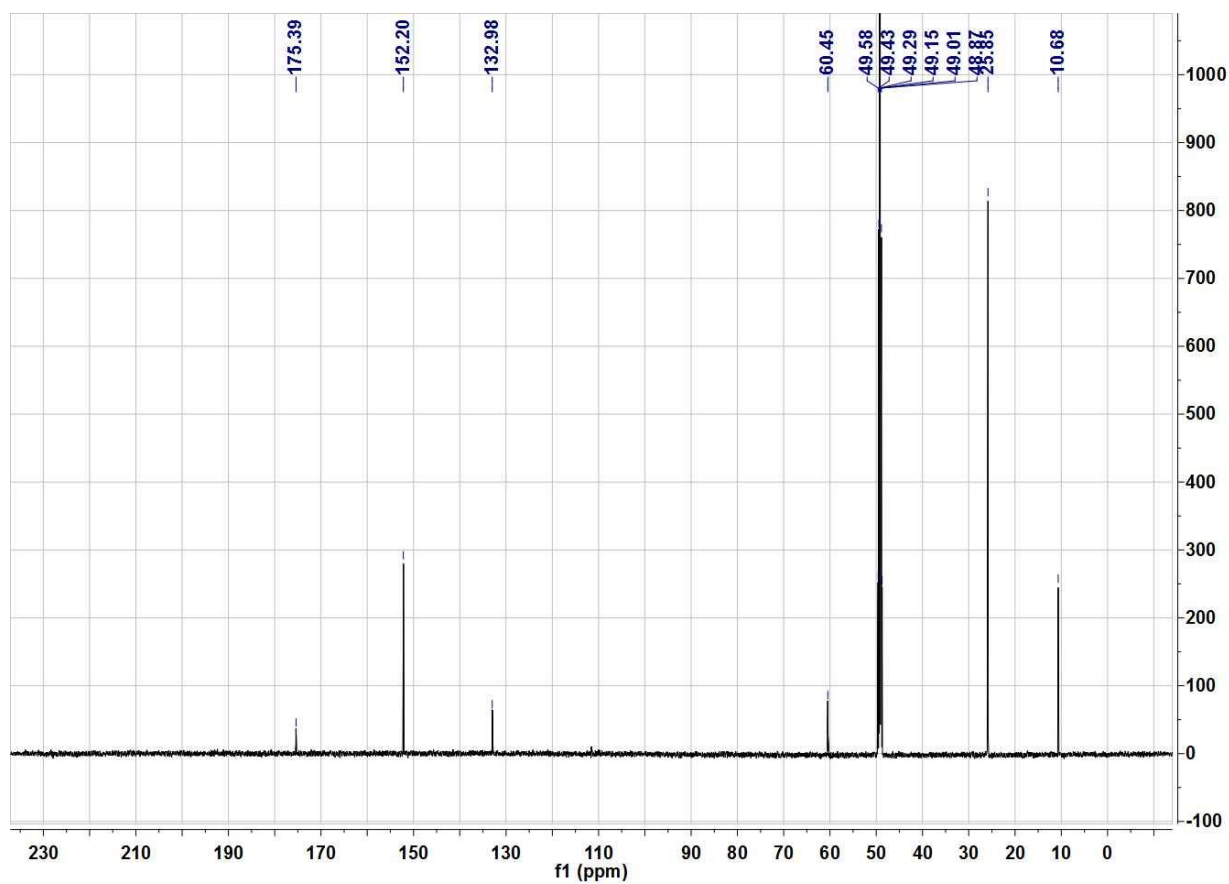


4.13 ^1H NMR of 3,5,5-trimethyl-1,5-dihydro-2H-pyrrol-2-one (**13**).

4.13.1 ^1H NMR (600 MHz, $\text{MeOH-}d_4$) spectrum of **13**.



4.13.2 ^{13}C NMR (150 MHz, $\text{MeOH-}d_4$) spectrum of **13**.



5. Experimental and Calculated ECD data

5.1 Experimental ECD data of (+)-1/(-)-1 and Calculated ECD data of 1a/1b/1c

Experimental ECD data				Calculated ECD data					
(+) -1		(-) -1		1a		1b		1c	
λ (nm)	$\Delta\epsilon$	λ (nm)	$\Delta\epsilon$	λ (nm)	$\Delta\epsilon$	λ (nm)	$\Delta\epsilon$	λ (nm)	$\Delta\epsilon$
400	0.943509	400	-0.97542	200	-2.65745	200	2.606081	200	-7.94877
399	1.05533	399	-1.08731	201.4286	-2.78241	201.4286	2.736846	201.4085	-8.68507
398	1.14731	398	-1.21493	202.8571	-2.88579	202.8571	2.848501	202.8169	-9.40595
397	1.23776	397	-1.33494	204.2857	-2.96326	204.2857	2.93692	204.2254	-10.0962
396	1.34676	396	-1.44546	205.7143	-3.01043	205.7143	2.997878	205.6338	-10.7399
395	1.43234	395	-1.5133	207.1429	-3.02296	207.1429	3.027095	207.0423	-11.3211
394	1.51414	394	-1.6014	208.5714	-2.99656	208.5714	3.020299	208.4507	-11.8242
393	1.56893	393	-1.66077	210	-2.92713	210	2.973297	209.8592	-12.2345
392	1.61465	392	-1.67502	211.4286	-2.81084	211.4286	2.88207	211.2676	-12.539
391	1.648	391	-1.69025	212.8571	-2.64425	212.8571	2.742897	212.6761	-12.7266
390	1.63326	390	-1.70129	214.2857	-2.42445	214.2857	2.552502	214.0845	-12.7887
389	1.60113	389	-1.7071	215.7143	-2.14926	215.7143	2.308244	215.493	-12.7197
388	1.61149	388	-1.67223	217.1429	-1.81743	217.1429	2.008323	216.9014	-12.5173
387	1.58323	387	-1.64315	218.5714	-1.42884	218.5714	1.652023	218.3099	-12.1822
386	1.51422	386	-1.59706	220	-0.98474	220	1.239965	219.7183	-11.7187
385	1.45437	385	-1.51571	221.4286	-0.48801	221.4286	0.774366	221.1268	-11.1344
384	1.403	384	-1.45944	222.8571	0.056613	222.8571	0.259286	222.5352	-10.4399
383	1.33044	383	-1.35608	224.2857	0.642379	224.2857	-0.29916	223.9437	-9.6484
382	1.25678	382	-1.27763	225.7143	1.260355	225.7143	-0.89266	225.3521	-8.77545
381	1.15379	381	-1.17658	227.1429	1.899374	227.1429	-1.51059	226.7606	-7.83832
380	1.04762	380	-1.08112	228.5714	2.546067	228.5714	-2.14007	228.169	-6.8555
379	0.964878	379	-0.9755	230	3.185006	230	-2.76609	229.5775	-5.84605
378	0.879127	378	-0.86792	231.4286	3.798977	231.4286	-3.37175	230.9859	-4.82909
377	0.808927	377	-0.72462	232.8571	4.369372	232.8571	-3.93869	232.3944	-3.82322
376	0.720368	376	-0.62917	234.2857	4.876719	234.2857	-4.44759	233.8028	-2.84601
375	0.662203	375	-0.54606	235.7143	5.301321	235.7143	-4.87883	235.2113	-1.91358
374	0.606527	374	-0.4511	237.1429	5.623982	237.1429	-5.21321	236.6197	-1.04021
373	0.533007	373	-0.37336	238.5714	5.826803	238.5714	-5.43277	238.0282	-0.23809
372	0.486661	372	-0.32898	240	5.893997	240	-5.52159	239.4366	0.482906
371	0.461161	371	-0.26063	241.4286	5.812684	241.4286	-5.46659	240.8451	1.115302
370	0.431014	370	-0.22773	242.8571	5.573616	242.8571	-5.25829	242.2535	1.654084
369	0.411405	369	-0.20218	244.2857	5.171798	244.2857	-4.8914	243.662	2.096643
368	0.39403	368	-0.20808	245.7143	4.606946	245.7143	-4.3653	245.0704	2.442676
367	0.408857	367	-0.1874	247.1429	3.883764	247.1429	-3.68428	246.4789	2.694031
366	0.441919	366	-0.16301	248.5714	3.011998	248.5714	-2.85766	247.8873	2.8545
365	0.451499	365	-0.15193	250	2.006279	250	-1.89956	249.2958	2.929589

364	0.485719	364	-0.17357	251.4286	0.885726	251.4286	-0.82855	250.7042	2.926253
363	0.522276	363	-0.1708	252.8571	-0.32665	252.8571	0.332973	252.1127	2.852617
362	0.541182	362	-0.19077	254.2857	-1.60471	254.2857	1.559535	253.5211	2.717694
361	0.546422	361	-0.25356	255.7143	-2.92015	255.7143	2.823514	254.9296	2.531094
360	0.546683	360	-0.31552	257.1429	-4.24348	257.1429	4.096145	256.338	2.302741
359	0.601228	359	-0.35336	258.5714	-5.54508	258.5714	5.34856	257.7465	2.042609
358	0.682173	358	-0.40309	260	-6.79627	260	6.552821	259.1549	1.760464
357	0.676646	357	-0.46418	261.4286	-7.9703	261.4286	7.682885	260.5634	1.465639
356	0.679971	356	-0.50211	262.8571	-9.0432	262.8571	8.715453	261.9718	1.166828
355	0.710516	355	-0.54001	264.2857	-9.99452	264.2857	9.630681	263.3803	0.871917
354	0.733245	354	-0.59879	265.7143	-10.8079	265.7143	10.41271	264.7887	0.587847
353	0.723539	353	-0.60993	267.1429	-11.4713	267.1429	11.05	266.1972	0.320512
352	0.710923	352	-0.64274	268.5714	-11.9774	268.5714	11.53548	267.6056	0.074693
351	0.680928	351	-0.61594	270	-12.3235	270	11.86654	269.0141	-0.14597
350	0.638189	350	-0.58036	271.4286	-12.5111	271.4286	12.04478	270.4225	-0.33896
349	0.597166	349	-0.51268	272.8571	-12.5457	272.8571	12.07567	271.831	-0.50288
348	0.517508	348	-0.43447	274.2857	-12.4366	274.2857	11.96812	273.2394	-0.63734
347	0.439931	347	-0.34435	275.7143	-12.1958	275.7143	11.73387	274.6479	-0.74288
346	0.329369	346	-0.25875	277.1429	-11.8378	277.1429	11.38692	276.0563	-0.82091
345	0.198708	345	-0.12672	278.5714	-11.3787	278.5714	10.94289	277.4648	-0.87351
344	0.03372	344	0.023828	280	-10.8359	280	10.4184	278.8732	-0.90337
343	-0.14295	343	0.193782	281.4286	-10.227	281.4286	9.830493	280.2817	-0.91363
342	-0.31169	342	0.378349	282.8571	-9.56958	282.8571	9.196076	281.6901	-0.90778
341	-0.50484	341	0.591959	284.2857	-8.88075	284.2857	8.531448	283.0986	-0.88955
340	-0.70713	340	0.773178	285.7143	-8.17644	285.7143	7.851902	284.507	-0.86282
339	-0.8858	339	0.98714	287.1429	-7.47126	287.1429	7.171393	285.9155	-0.83151
338	-1.07923	338	1.20153	288.5714	-6.77819	288.5714	6.502288	287.3239	-0.79957
337	-1.26512	337	1.43549	290	-6.10837	290	5.855199	288.7324	-0.77091
336	-1.44294	336	1.64979	291.4286	-5.47099	291.4286	5.23887	290.1408	-0.74938
335	-1.6226	335	1.84659	292.8571	-4.87329	292.8571	4.660145	291.5493	-0.73873
334	-1.79268	334	2.04006	294.2857	-4.32048	294.2857	4.123977	292.9577	-0.74264
333	-1.96336	333	2.21697	295.7143	-3.81588	295.7143	3.633492	294.3662	-0.76468
332	-2.13794	332	2.37658	297.1429	-3.36099	297.1429	3.190086	295.7746	-0.80832
331	-2.27513	331	2.52545	298.5714	-2.95561	298.5714	2.79356	297.1831	-0.8769
330	-2.38012	330	2.66595	300	-2.59802	300	2.442272	298.5915	-0.97356
329	-2.46252	329	2.78498	301.4286	-2.28514	301.4286	2.133312	300	-1.10126
328	-2.54254	328	2.85953	302.8571	-2.01274	302.8571	1.862689	301.4085	-1.26265
327	-2.61759	327	2.93874	304.2857	-1.77567	304.2857	1.625532	302.8169	-1.45999
326	-2.6511	326	2.98927	305.7143	-1.56802	305.7143	1.416297	304.2254	-1.69504
325	-2.66069	325	3.00919	307.1429	-1.38341	307.1429	1.228977	305.6338	-1.96891
324	-2.65483	324	3.00999	308.5714	-1.21518	308.5714	1.057322	307.0423	-2.28196
323	-2.63679	323	2.9986	310	-1.05664	310	0.895056	308.4507	-2.63362
322	-2.60613	322	2.9723	311.4286	-0.9013	311.4286	0.736095	309.8592	-3.02228

321	-2.55866	321	2.92915	312.8571	-0.74311	312.8571	0.574762	311.2676	-3.44518
320	-2.51033	320	2.86265	314.2857	-0.57666	314.2857	0.405986	312.6761	-3.8983
319	-2.42785	319	2.78735	315.7143	-0.39739	315.7143	0.225495	314.0845	-4.37637
318	-2.34218	318	2.69876	317.1429	-0.20179	317.1429	0.029979	315.493	-4.87285
317	-2.24822	317	2.60634	318.5714	0.012496	318.5714	-0.18277	316.9014	-5.38002
316	-2.15888	316	2.50841	320	0.246527	320	-0.41376	318.3099	-5.88911
315	-2.06766	315	2.40031	321.4286	0.500025	321.4286	-0.66273	319.7183	-6.3905
314	-1.96897	314	2.28338	322.8571	0.771364	322.8571	-0.92816	321.1268	-6.87402
313	-1.86318	313	2.16567	324.2857	1.057624	324.2857	-1.20731	322.5352	-7.32921
312	-1.7579	312	2.04413	325.7143	1.354704	325.7143	-1.49632	323.9437	-7.74572
311	-1.6459	311	1.91844	327.1429	1.657483	327.1429	-1.79033	325.3521	-8.11364
310	-1.53755	310	1.79139	328.5714	1.960044	328.5714	-2.08374	326.7606	-8.42392
309	-1.42857	309	1.67332	330	2.25593	330	-2.37041	328.169	-8.66873
308	-1.32009	308	1.54478	331.4286	2.538434	331.4286	-2.64392	329.5775	-8.84171
307	-1.20849	307	1.4193	332.8571	2.800899	332.8571	-2.89789	330.9859	-8.93835
306	-1.09614	306	1.2917	334.2857	3.037022	334.2857	-3.12626	332.3944	-8.95609
305	-0.98894	305	1.16671	335.7143	3.241141	335.7143	-3.32353	333.8028	-8.89447
304	-0.87953	304	1.04274	337.1429	3.408483	337.1429	-3.48504	335.2113	-8.75514
303	-0.76502	303	0.921307	338.5714	3.535374	338.5714	-3.60717	336.6197	-8.54177
302	-0.65064	302	0.795632	340	3.619384	340	-3.68747	338.0282	-8.25992
301	-0.53319	301	0.66565	341.4286	3.659413	341.4286	-3.72475	339.4366	-7.91676
300	-0.41168	300	0.52873	342.8571	3.655707	342.8571	-3.71915	340.8451	-7.52081
299	-0.28151	299	0.37755	344.2857	3.609813	344.2857	-3.67205	342.2535	-7.08154
298	-0.1385	298	0.220657	345.7143	3.524466	345.7143	-3.586	343.662	-6.60903
297	0.018459	297	0.050917	347.1429	3.403431	347.1429	-3.46456	345.0704	-6.11358
296	0.191117	296	-0.14147	348.5714	3.251303	348.5714	-3.31215	346.4789	-5.60535
295	0.388574	295	-0.35468	350	3.073277	350	-3.13379	347.8873	-5.09401
294	0.607202	294	-0.59398	351.4286	2.874915	351.4286	-2.93487	349.2958	-4.58846
293	0.857526	293	-0.85889	352.8571	2.661904	352.8571	-2.72098	350.7042	-4.09663
292	1.13678	292	-1.15893	354.2857	2.439834	354.2857	-2.49763	352.1127	-3.62525
291	1.44881	291	-1.49568	355.7143	2.214004	355.7143	-2.27007	353.5211	-3.17982
290	1.79663	290	-1.86964	357.1429	1.989253	357.1429	-2.04312	354.9296	-2.76453
289	2.18359	289	-2.28636	358.5714	1.769839	358.5714	-1.82108	356.338	-2.38229
288	2.61005	288	-2.74528	360	1.559348	360	-1.60757	357.7465	-2.0348
287	3.06959	287	-3.24671	361.4286	1.360656	361.4286	-1.40555	359.1549	-1.72269
286	3.56478	286	-3.7881	362.8571	1.175915	362.8571	-1.21725	360.5634	-1.4456
285	4.09851	285	-4.36581	364.2857	1.006584	364.2857	-1.04421	361.9718	-1.20239
284	4.65747	284	-4.98255	365.7143	0.853476	365.7143	-0.88735	363.3803	-0.99129
283	5.24455	283	-5.62831	367.1429	0.716834	367.1429	-0.74699	364.7887	-0.81005
282	5.84797	282	-6.30207	368.5714	0.596417	368.5714	-0.62296	366.1972	-0.65612
281	6.4628	281	-6.98321	370	0.491585	370	-0.51469	367.6056	-0.52677
280	7.08056	280	-7.66361	371.4286	0.401403	371.4286	-0.42129	369.0141	-0.41919
279	7.68384	279	-8.32844	372.8571	0.324718	372.8571	-0.34165	370.4225	-0.33064

278	8.2548	278	-8.96977	374.2857	0.260248	374.2857	-0.27451	371.831	-0.25851
277	8.78824	277	-9.55889	375.7143	0.206649	375.7143	-0.21853	373.2394	-0.20033
276	9.2508	276	-10.0827	377.1429	0.162576	377.1429	-0.17236	374.6479	-0.15388
275	9.64657	275	-10.5271	378.5714	0.126724	378.5714	-0.1347	376.0563	-0.11716
274	9.94612	274	-10.8674	380	0.097871	380	-0.10431	377.4648	-0.08842
273	10.1434	273	-11.0936	381.4286	0.074893	381.4286	-0.08003	378.8732	-0.06614
272	10.2209	272	-11.1868	382.8571	0.056785	382.8571	-0.06084	380.2817	-0.04904
271	10.1717	271	-11.1529	384.2857	0.042661	384.2857	-0.04583	381.6901	-0.03604
270	9.98707	270	-10.9648	385.7143	0.031757	385.7143	-0.03421	383.0986	-0.02625
269	9.65522	269	-10.6103	387.1429	0.023425	387.1429	-0.0253	384.507	-0.01896
268	9.17172	268	-10.0705	388.5714	0.017121	388.5714	-0.01855	385.9155	-0.01357
267	8.53625	267	-9.36741	390	0.012399	390	-0.01347	387.3239	-0.00963
266	7.75012	266	-8.50222	391.4286	0.008898	391.4286	-0.00969	388.7324	-0.00677
265	6.81329	265	-7.46905	392.8571	0.006328	392.8571	-0.00691	390.1408	-0.00472
264	5.7281	264	-6.27641	394.2857	0.004459	394.2857	-0.00488	391.5493	-0.00326
263	4.51065	263	-4.93038	395.7143	0.003113	395.7143	-0.00342	392.9577	-0.00223
262	3.17358	262	-3.4543	397.1429	0.002154	397.1429	-0.00237	394.3662	-0.00151
261	1.72633	261	-1.85939	398.5714	0.001477	398.5714	-0.00163	395.7746	-0.00102
260	0.200874	260	-0.17185	400	0	400	0	397.1831	-0.00068
259	-1.37917	259	1.56891					398.5915	-0.00045
258	-2.97548	258	3.33227					400	0
257	-4.56284	257	5.08559						
256	-6.11035	256	6.78925						
255	-7.58487	255	8.41697						
254	-8.9475	254	9.91442						
253	-10.1692	253	11.2588						
252	-11.221	252	12.4189						
251	-12.1006	251	13.3957						
250	-12.7813	250	14.144						
249	-13.2694	249	14.6809						
248	-13.5566	248	14.9836						
247	-13.6505	247	15.0734						
246	-13.5563	246	14.9533						
245	-13.2672	245	14.6273						
244	-12.8126	244	14.1181						
243	-12.2049	243	13.432						
242	-11.4656	242	12.5973						
241	-10.611	241	11.6326						
240	-9.67361	240	10.5875						
239	-8.67446	239	9.47851						
238	-7.63266	238	8.32799						
237	-6.57787	237	7.14518						
236	-5.53608	236	5.98001						

235	-4.52409	235	4.85494						
234	-3.56502	234	3.78515						
233	-2.67098	233	2.78966						
232	-1.84759	232	1.87188						
231	-1.10997	231	1.04214						
230	-0.44547	230	0.292018						
229	0.152154	229	-0.38704						
228	0.691898	228	-0.98673						
227	1.16473	227	-1.52212						
226	1.591	226	-2.00546						
225	1.98751	225	-2.44136						
224	2.36419	224	-2.86023						
223	2.71385	223	-3.25091						
222	3.04972	222	-3.61701						
221	3.35998	221	-3.9616						
220	3.66603	220	-4.29954						
219	3.94038	219	-4.59565						
218	4.19491	218	-4.89557						
217	4.41081	217	-5.15781						
216	4.6199	216	-5.38332						
215	4.79271	215	-5.58081						
214	4.96672	214	-5.73886						
213	5.07023	213	-5.86352						
212	5.16373	212	-5.95417						
211	5.24048	211	-6.02204						
210	5.26909	210	-6.03304						
209	5.30161	209	-6.03977						
208	5.28895	208	-5.99169						
207	5.21867	207	-5.88738						
206	5.08052	206	-5.70149						
205	4.86776	205	-5.44174						
204	4.60879	204	-5.10498						
203	4.30245	203	-4.71302						
202	3.97932	202	-4.29126						
201	3.66176	201	-3.84983						
200	3.36654	200	-3.42234						

5.2 Experimental ECD data of (+)-2/(-)-2 and Calculated ECD data of 2a/2b

Experimental ECD data				Calculated ECD data			
(+)-2		(-)-2		2a		2b	
λ (nm)	$\Delta\epsilon$	λ (nm)	$\Delta\epsilon$	λ (nm)	$\Delta\epsilon$	λ (nm)	$\Delta\epsilon$
500	0.07544	500	-0.09229	200	0.401705	200	-0.43545
499	0.169371	499	0.233337	202.2059	0.486947	202.2059	-0.52949

498	0.188608	498	0.166982	204.4118	0.579719	204.4118	-0.6327
497	0.233967	497	0.09633	206.6176	0.677639	206.6176	-0.74285
496	0.251467	496	0.082592	208.8235	0.777464	208.8235	-0.85688
495	0.237714	495	-0.03097	211.0294	0.875135	211.0294	-0.97087
494	0.261571	494	-0.05551	213.2353	0.965916	213.2353	-1.08024
493	0.227624	493	-0.0724	215.4412	1.044596	215.4412	-1.17992
492	0.241318	492	-0.10709	217.6471	1.105754	217.6471	-1.26464
491	0.271267	491	-0.10486	219.8529	1.14407	219.8529	-1.32916
490	0.32498	490	-0.08505	222.0588	1.154626	222.0588	-1.36862
489	0.349066	489	-0.1068	224.2647	1.133191	224.2647	-1.37877
488	0.359699	488	-0.13314	226.4706	1.076425	226.4706	-1.35611
487	0.384925	487	-0.13061	228.6765	0.982004	228.6765	-1.29802
486	0.427772	486	-0.12395	230.8824	0.848625	230.8824	-1.20269
485	0.456796	485	-0.15176	233.0882	0.675914	233.0882	-1.06899
484	0.48338	484	-0.1649	235.2941	0.464251	235.2941	-0.89629
483	0.51915	483	-0.18274	237.5	0.21455	237.5	-0.68424
482	0.546462	482	-0.21372	239.7059	-0.07194	239.7059	-0.43256
481	0.56681	481	-0.24135	241.9118	-0.3938	241.9118	-0.14101
480	0.588209	480	-0.26003	244.1176	-0.74943	244.1176	0.190594
479	0.598218	479	-0.28654	246.3235	-1.13698	246.3235	0.562119
478	0.608931	478	-0.29782	248.5294	-1.55404	248.5294	0.972724
477	0.63247	477	-0.29984	250.7353	-1.99731	250.7353	1.420319
476	0.632061	476	-0.29702	252.9412	-2.46209	252.9412	1.900985
475	0.624038	475	-0.28346	255.1471	-2.94188	255.1471	2.408431
474	0.615019	474	-0.27623	257.3529	-3.42807	257.3529	2.9336
473	0.599207	473	-0.26004	259.5588	-3.9098	259.5588	3.464543
472	0.587031	472	-0.23478	261.7647	-4.37413	261.7647	3.986618
471	0.555133	471	-0.21397	263.9706	-4.80651	263.9706	4.483061
470	0.533486	470	-0.17583	266.1765	-5.19157	266.1765	4.935909
469	0.498751	469	-0.13443	268.3824	-5.51412	268.3824	5.327205
468	0.468959	468	-0.07675	270.5882	-5.7603	270.5882	5.640355
467	0.425574	467	-0.03853	272.7941	-5.9188	272.7941	5.861509
466	0.373005	466	0.018661	275	-5.98188	275	5.980767
465	0.309485	465	0.069975	277.2059	-5.94614	277.2059	5.993099
464	0.244551	464	0.13092	279.4118	-5.81296	279.4118	5.898837
463	0.178509	463	0.198114	281.6176	-5.58849	281.6176	5.703693
462	0.100513	462	0.268441	283.8235	-5.28323	283.8235	5.418302
461	0.021472	461	0.339812	286.0294	-4.91118	286.0294	5.057338
460	-0.05225	460	0.413119	288.2353	-4.48885	288.2353	4.638333
459	-0.13804	459	0.496476	290.4412	-4.03395	290.4412	4.180313
458	-0.2202	458	0.592486	292.6471	-3.56418	292.6471	3.70242
457	-0.30375	457	0.681188	294.8529	-3.0961	294.8529	3.222657
456	-0.38947	456	0.777033	297.0588	-2.64418	297.0588	2.756856

455	-0.48072	455	0.871905	299.2647	-2.22017	299.2647	2.317954
454	-0.57818	454	0.955881	301.4706	-1.83274	301.4706	1.915606
453	-0.68031	453	1.0453	303.6765	-1.48746	303.6765	1.55611
452	-0.77684	452	1.13978	305.8824	-1.18695	305.8824	1.242615
451	-0.86123	451	1.23955	308.0882	-0.93133	308.0882	0.975538
450	-0.94771	450	1.33831	310.2941	-0.7187	310.2941	0.753107
449	-1.02225	449	1.43573	312.5	-0.54572	312.5	0.571972
448	-1.10303	448	1.51922	314.7059	-0.40817	314.7059	0.427806
447	-1.18729	447	1.60163	316.9118	-0.30145	316.9118	0.315859
446	-1.26827	446	1.6752	319.1176	-0.22107	319.1176	0.231427
445	-1.34179	445	1.75585	321.3235	-0.16296	321.3235	0.17024
444	-1.41819	444	1.83935	323.5294	-0.12377	323.5294	0.128758
443	-1.47856	443	1.91789	325.7353	-0.1011	325.7353	0.104403
442	-1.53125	442	1.97963	327.9412	-0.09368	327.9412	0.095731
441	-1.58494	441	2.03746	330.1471	-0.10144	330.1471	0.102576
440	-1.63305	440	2.08183	332.3529	-0.12574	332.3529	0.126173
439	-1.67863	439	2.1124	334.5588	-0.1694	334.5588	0.169262
438	-1.71261	438	2.13389	336.7647	-0.23681	336.7647	0.236178
437	-1.73665	437	2.15871	338.9706	-0.33398	338.9706	0.332895
436	-1.75094	436	2.16634	341.1765	-0.46854	341.1765	0.467007
435	-1.75761	435	2.17014	343.3824	-0.64957	343.3824	0.647598
434	-1.75373	434	2.13894	345.5882	-0.88737	345.5882	0.884969
433	-1.73537	433	2.11229	347.7941	-1.19297	347.7941	1.190165
432	-1.69924	432	2.08271	350	-1.57743	350	1.574287
431	-1.65232	431	2.0286	352.2059	-2.05098	352.2059	2.047573
430	-1.59808	430	1.96579	354.4118	-2.62183	354.4118	2.618265
429	-1.5333	429	1.8928	356.6176	-3.29492	356.6176	3.291325
428	-1.46038	428	1.80449	358.8235	-4.07061	358.8235	4.067084
427	-1.37403	427	1.6954	361.0294	-4.94342	361.0294	4.93998
426	-1.26671	426	1.57009	363.2353	-5.90098	363.2353	5.897523
425	-1.14681	425	1.42206	365.4412	-6.92346	365.4412	6.919676
424	-1.00623	424	1.2669	367.6471	-7.98354	367.6471	7.978814
423	-0.85717	423	1.09043	369.8529	-9.04705	369.8529	9.040367
422	-0.68741	422	0.905078	372.0588	-10.0743	372.0588	10.06423
421	-0.50777	421	0.701369	374.2647	-11.0224	374.2647	11.00691
420	-0.30025	420	0.489938	376.4706	-11.8476	376.4706	11.82424
419	-0.08958	419	0.255898	378.6765	-12.5088	378.6765	12.47453
418	0.138788	418	0.017267	380.8824	-12.9703	380.8824	12.92182
417	0.371907	417	-0.243	383.0882	-13.2051	383.0882	13.13886
416	0.613593	416	-0.51454	385.2941	-13.1973	385.2941	13.10961
415	0.864458	415	-0.80219	387.5	-12.9431	387.5	12.83079
414	1.12572	414	-1.08991	389.7059	-12.4522	389.7059	12.31247
413	1.38919	413	-1.38748	391.9118	-11.7465	391.9118	11.57748

412	1.66006	412	-1.68801	394.1176	-10.8588	394.1176	10.6597
411	1.9309	411	-1.99781	396.3235	-9.83011	396.3235	9.601505
410	2.20672	410	-2.30042	398.5294	-8.7068	398.5294	8.45052
409	2.48389	409	-2.61008	400.7353	-7.53678	400.7353	7.256062
408	2.76809	408	-2.91871	402.9412	-6.36636	402.9412	6.065688
407	3.04683	407	-3.22912	405.1471	-5.23726	405.1471	4.922125
406	3.32807	406	-3.5434	407.3529	-4.18427	407.3529	3.860873
405	3.60354	405	-3.85124	409.5588	-3.23375	409.5588	2.908643
404	3.87828	404	-4.16415	411.7647	-2.40302	411.7647	2.082697
403	4.149	403	-4.46097	413.9706	-1.70047	413.9706	1.391037
402	4.42483	402	-4.75875	416.1765	-1.12649	416.1765	0.833324
401	4.68897	401	-5.05106	418.3824	-0.67481	418.3824	0.402311
400	4.94111	400	-5.33387	420.5882	-0.33415	420.5882	0.085594
399	5.1879	399	-5.60696	422.7941	-0.08999	422.7941	-0.13255
398	5.41915	398	-5.8661	425	0.073819	425	-0.26943
397	5.63939	397	-6.11312	427.2059	0.173594	427.2059	-0.34242
396	5.85705	396	-6.3474	429.4118	0.224725	429.4118	-0.36782
395	6.05749	395	-6.56986	431.6176	0.240896	431.6176	-0.36003
394	6.24848	394	-6.78195	433.8235	0.233644	433.8235	-0.33107
393	6.43189	393	-6.9764	436.0294	0.212198	436.0294	-0.29048
392	6.59102	392	-7.16361	438.2353	0.183548	438.2353	-0.24534
391	6.73366	391	-7.32938	440.4412	0.152672	440.4412	-0.2006
390	6.85884	390	-7.48554	442.6471	0.122847	442.6471	-0.15938
389	6.9753	389	-7.6244	444.8529	0.096003	444.8529	-0.12337
388	7.0741	388	-7.74058	447.0588	0.073068	447.0588	-0.09322
387	7.162	387	-7.83401	449.2647	0.05427	449.2647	-0.06885
386	7.23434	386	-7.92043	451.4706	0.039393	451.4706	-0.04976
385	7.29111	385	-7.98604	453.6765	0.027977	453.6765	-0.03523
384	7.33156	384	-8.04679	455.8824	0.019458	455.8824	-0.02444
383	7.35963	383	-8.07453	458.0882	0.013262	458.0882	-0.01663
382	7.37031	382	-8.10218	460.2941	0.008863	460.2941	-0.0111
381	7.37007	381	-8.11114	462.5	0.00581	462.5	-0.00727
380	7.35813	380	-8.09896	464.7059	0.003738	464.7059	-0.00467
379	7.338	379	-8.08169	466.9118	0.002361	466.9118	-0.00295
378	7.29983	378	-8.05933	469.1176	0.001464	469.1176	-0.00183
377	7.25466	377	-8.02386	471.3235	0.000891	471.3235	-0.00111
376	7.20454	376	-7.96918	473.5294	0.000533	473.5294	-0.00067
375	7.14231	375	-7.90418	475.7353	0.000313	475.7353	-0.00039
374	7.07163	374	-7.82135	477.9412	0.000181	477.9412	-0.00023
373	6.98706	373	-7.7324	480.1471	0.000103	480.1471	-0.00013
372	6.89812	372	-7.62662	482.3529	5.72E-05	482.3529	-7.2E-05
371	6.79735	371	-7.514	484.5588	3.14E-05	484.5588	-3.9E-05
370	6.68651	370	-7.39103	486.7647	1.69E-05	486.7647	-2.1E-05

369	6.56609	369	-7.25165	488.9706	8.95E-06	488.9706	-1.1E-05
368	6.43278	368	-7.10629	491.1765	4.66E-06	491.1765	-5.9E-06
367	6.29005	367	-6.95534	493.3824	2.38E-06	493.3824	-3E-06
366	6.13556	366	-6.79541	495.5882	1.2E-06	495.5882	-1.5E-06
365	5.97511	365	-6.61663	497.7941	5.92E-07	497.7941	-7.5E-07
364	5.81137	364	-6.4377	500	0	500	0
363	5.64113	363	-6.24945				
362	5.47378	362	-6.05157				
361	5.29114	361	-5.85135				
360	5.11428	360	-5.6495				
359	4.93102	359	-5.45225				
358	4.74868	358	-5.25103				
357	4.56858	357	-5.04729				
356	4.3906	356	-4.84841				
355	4.20953	355	-4.65016				
354	4.03447	354	-4.45164				
353	3.85717	353	-4.25269				
352	3.68149	352	-4.06811				
351	3.51046	351	-3.87583				
350	3.34362	350	-3.68118				
349	3.18359	349	-3.49309				
348	3.02423	348	-3.30696				
347	2.86698	347	-3.12408				
346	2.71825	346	-2.94666				
345	2.5715	345	-2.77247				
344	2.42821	344	-2.58941				
343	2.29145	343	-2.41279				
342	2.15531	342	-2.24715				
341	2.0283	341	-2.08057				
340	1.9022	340	-1.92454				
339	1.78232	339	-1.76974				
338	1.66679	338	-1.62045				
337	1.55721	337	-1.4622				
336	1.44893	336	-1.31031				
335	1.34083	335	-1.16034				
334	1.23301	334	-1.02224				
333	1.13431	333	-0.87479				
332	1.03372	332	-0.73081				
331	0.937312	331	-0.58122				
330	0.841554	330	-0.43782				
329	0.750837	329	-0.29574				
328	0.65808	328	-0.15577				
327	0.566602	327	-0.01102				

326	0.478225	326	0.132427				
325	0.387218	325	0.279599				
324	0.29514	324	0.423531				
323	0.204782	323	0.57058				
322	0.112422	322	0.714944				
321	0.013035	321	0.861056				
320	-0.0825	320	1.01667				
319	-0.18179	319	1.17004				
318	-0.28652	318	1.32141				
317	-0.39019	317	1.47177				
316	-0.4977	316	1.62833				
315	-0.6074	315	1.7881				
314	-0.71688	314	1.93577				
313	-0.82652	313	2.08837				
312	-0.93696	312	2.23447				
311	-1.03862	311	2.36944				
310	-1.13438	310	2.48098				
309	-1.22219	309	2.57844				
308	-1.28943	308	2.66733				
307	-1.33494	307	2.73189				
306	-1.35881	306	2.7588				
305	-1.35224	305	2.74839				
304	-1.30593	304	2.70407				
303	-1.23081	303	2.61619				
302	-1.11126	302	2.48728				
301	-0.94798	301	2.314				
300	-0.74975	300	2.09388				
299	-0.51066	299	1.82103				
298	-0.23638	298	1.50604				
297	0.081449	297	1.1528				
296	0.436146	296	0.764893				
295	0.816775	295	0.33436				
294	1.22092	294	-0.12117				
293	1.64419	293	-0.60986				
292	2.08236	292	-1.11243				
291	2.53214	291	-1.62685				
290	2.98842	290	-2.14864				
289	3.4416	289	-2.67206				
288	3.89448	288	-3.18567				
287	4.3345	287	-3.68317				
286	4.75812	286	-4.16905				
285	5.15792	285	-4.63831				
284	5.53664	284	-5.09076				

283	5.89287	283	-5.50595				
282	6.21165	282	-5.89749				
281	6.50075	281	-6.25547				
280	6.75369	280	-6.57918				
279	6.96783	279	-6.85817				
278	7.13778	278	-7.0927				
277	7.26063	277	-7.27584				
276	7.34041	276	-7.40588				
275	7.3598	275	-7.48012				
274	7.32767	274	-7.50988				
273	7.24286	273	-7.47294				
272	7.09997	272	-7.3746				
271	6.89855	271	-7.21131				
270	6.64943	270	-6.98516				
269	6.34782	269	-6.70521				
268	5.98933	268	-6.36156				
267	5.58499	267	-5.97629				
266	5.14687	266	-5.53292				
265	4.6763	265	-5.05691				
264	4.17646	264	-4.56162				
263	3.65694	263	-4.03339				
262	3.12727	262	-3.50155				
261	2.59348	261	-2.96382				
260	2.0661	260	-2.43092				
259	1.55353	259	-1.90048				
258	1.07165	258	-1.39018				
257	0.617401	257	-0.91762				
256	0.190949	256	-0.48128				
255	-0.19255	255	-0.09326				
254	-0.5412	254	0.271881				
253	-0.84534	253	0.586644				
252	-1.10349	252	0.86038				
251	-1.31346	251	1.0938				
250	-1.48835	250	1.28594				
249	-1.62149	249	1.43321				
248	-1.71836	248	1.5425				
247	-1.7784	247	1.62179				
246	-1.81833	246	1.66473				
245	-1.83323	245	1.67984				
244	-1.8166	244	1.68489				
243	-1.78817	243	1.66149				
242	-1.73526	242	1.63873				
241	-1.67026	241	1.59682				

240	-1.59441	240	1.53277				
239	-1.51085	239	1.46783				
238	-1.40663	238	1.39902				
237	-1.30723	237	1.31814				
236	-1.19676	236	1.23823				
235	-1.08351	235	1.13789				
234	-0.96628	234	1.03315				
233	-0.84765	233	0.926087				
232	-0.72221	232	0.81723				
231	-0.59742	231	0.712112				
230	-0.47236	230	0.607779				
229	-0.34946	229	0.494383				
228	-0.23043	228	0.392157				
227	-0.1091	227	0.286646				
226	0.021298	226	0.168042				
225	0.157735	225	0.054102				
224	0.318565	224	-0.09252				
223	0.501247	223	-0.2297				
222	0.712834	222	-0.40753				
221	0.939842	221	-0.63057				
220	1.21283	220	-0.885				
219	1.35326	219	-1.00574				
218	1.49897	218	-1.1243				
217	1.64222	217	-1.25307				
216	1.80287	216	-1.39226				
215	1.98921	215	-1.56667				
214	2.21748	214	-1.79466				
213	2.48222	213	-2.08619				
212	2.8108	212	-2.41485				
211	3.20583	211	-2.80644				
210	3.64371	210	-3.27042				
209	4.12235	209	-3.79993				
208	4.63961	208	-4.35467				
207	5.20554	207	-4.93536				
206	5.77754	206	-5.53457				
205	6.36872	205	-6.19843				
204	6.99028	204	-6.82161				
203	7.59233	203	-7.44329				
202	8.14302	202	-8.07902				
201	8.65002	201	-8.6057				
200	8.96906	200	-9.02459				

5.3 Experimental ECD data of (+)-3/(-)-3 and Calculated ECD data of 3a/3b

Experimental ECD data				Calculated ECD data			
(+)-3		(-)-3		3a		3b	
λ (nm)	$\Delta\epsilon$	λ (nm)	$\Delta\epsilon$	λ (nm)	$\Delta\epsilon$	λ (nm)	$\Delta\epsilon$
400	-0.13385	400	0.174711	200	-1.71228	200	1.399537
399	-0.11687	399	0.166143	201.4184	-1.87316	201.4184	1.518003
398	-0.09879	398	0.148908	202.8369	-2.02469	202.8369	1.624937
397	-0.08036	397	0.121227	204.2553	-2.16182	204.2553	1.715895
396	-0.04814	396	0.094452	205.6738	-2.27961	205.6738	1.786643
395	-0.0078	395	0.064068	207.0922	-2.3735	207.0922	1.833469
394	0.035858	394	0.024501	208.5106	-2.43969	208.5106	1.853522
393	0.095233	393	-0.02473	209.9291	-2.47551	209.9291	1.845152
392	0.170827	392	-0.08311	211.3475	-2.47975	211.3475	1.808232
391	0.247441	391	-0.15635	212.766	-2.453	212.766	1.744434
390	0.330747	390	-0.24497	214.1844	-2.39786	214.1844	1.657429
389	0.430555	389	-0.34124	215.6028	-2.3191	215.6028	1.552981
388	0.548989	388	-0.44734	217.0213	-2.22364	217.0213	1.438926
387	0.672303	387	-0.57052	218.4397	-2.12049	218.4397	1.325
386	0.813751	386	-0.70478	219.8582	-2.02043	219.8582	1.22253
385	0.971859	385	-0.85326	221.2766	-1.93556	221.2766	1.143984
384	1.14453	384	-1.01446	222.695	-1.87885	222.695	1.102393
383	1.33922	383	-1.19761	224.1135	-1.86335	224.1135	1.110683
382	1.55836	382	-1.37984	225.5319	-1.9016	225.5319	1.180943
381	1.78178	381	-1.58651	226.9504	-2.00477	226.9504	1.323691
380	2.02597	380	-1.80431	228.3688	-2.18201	228.3688	1.547183
379	2.28634	379	-2.04121	229.7872	-2.43982	229.7872	1.856809
378	2.56544	378	-2.29036	231.2057	-2.78152	231.2057	2.254639
377	2.85094	377	-2.55837	232.6241	-3.20696	232.6241	2.739152
376	3.16543	376	-2.8357	234.0426	-3.71239	234.0426	3.305177
375	3.49159	375	-3.12668	235.461	-4.2906	235.461	3.944058
374	3.83302	374	-3.42393	236.8794	-4.9312	236.8794	4.64404
373	4.18486	373	-3.7422	238.2979	-5.6212	238.2979	5.390857
372	4.55372	372	-4.06647	239.7163	-6.34572	239.7163	6.16848
371	4.91613	371	-4.39676	241.1348	-7.08874	241.1348	6.959975
370	5.29216	370	-4.73486	242.5532	-7.83408	242.5532	7.748415
369	5.67333	369	-5.06845	243.9716	-8.56621	243.9716	8.517777
368	6.06625	368	-5.41564	245.3901	-9.27108	245.3901	9.253764
367	6.46039	367	-5.75689	246.8085	-9.93685	246.8085	9.944489
366	6.85055	366	-6.11173	248.227	-10.5543	248.227	10.58099
365	7.24206	365	-6.45838	249.6454	-11.1174	249.6454	11.15752
364	7.62616	364	-6.79464	251.0638	-11.6232	251.0638	11.67163
363	7.99375	363	-7.12657	252.4823	-12.0715	252.4823	12.12401

362	8.34817	362	-7.46346	253.9007	-12.4652	253.9007	12.51812
361	8.7077	361	-7.77175	255.3191	-12.8093	255.3191	12.8597
360	9.04115	360	-8.07587	256.7376	-13.1102	256.7376	13.15611
359	9.36806	359	-8.36078	258.156	-13.3756	258.156	13.41558
358	9.66437	358	-8.63297	259.5745	-13.613	259.5745	13.64651
357	9.94223	357	-8.89458	260.9929	-13.8299	260.9929	13.85675
356	10.2042	356	-9.13046	262.4113	-14.0323	262.4113	14.05293
355	10.4376	355	-9.34689	263.8298	-14.225	263.8298	14.24001
354	10.6462	354	-9.54473	265.2482	-14.4104	265.2482	14.42086
353	10.8265	353	-9.71259	266.6667	-14.5892	266.6667	14.59605
352	10.9832	352	-9.86139	268.0851	-14.7594	268.0851	14.76378
351	11.114	351	-9.99019	269.5035	-14.9172	269.5035	14.91997
350	11.2235	350	-10.0956	270.922	-15.0565	270.922	15.05846
349	11.3125	349	-10.1785	272.3404	-15.1697	272.3404	15.17136
348	11.3741	348	-10.2409	273.7589	-15.2477	273.7589	15.2494
347	11.4097	347	-10.2778	275.1773	-15.2807	275.1773	15.28241
346	11.4359	346	-10.2854	276.5957	-15.2582	276.5957	15.25979
345	11.4357	345	-10.2838	278.0142	-15.17	278.0142	15.17097
344	11.4143	344	-10.2721	279.4326	-15.0061	279.4326	15.00586
343	11.3874	343	-10.2409	280.8511	-14.7575	280.8511	14.75523
342	11.3277	342	-10.2035	282.2695	-14.4162	282.2695	14.4111
341	11.2557	341	-10.1503	283.6879	-13.976	283.6879	13.96702
340	11.1768	340	-10.0812	285.1064	-13.432	285.1064	13.4183
339	11.0868	339	-10.0057	286.5248	-12.7815	286.5248	12.76221
338	10.9876	338	-9.91869	287.9433	-12.0238	287.9433	11.99805
337	10.8721	337	-9.82441	289.3617	-11.1601	289.3617	11.12727
336	10.7574	336	-9.72247	290.7801	-10.1941	290.7801	10.15343
335	10.6326	335	-9.61585	292.1986	-9.13113	292.1986	9.08221
334	10.5076	334	-9.50337	293.617	-7.97884	293.617	7.921284
333	10.3835	333	-9.38772	295.0355	-6.74665	295.0355	6.680231
332	10.2569	332	-9.26865	296.4539	-5.44575	296.4539	5.37035
331	10.117	331	-9.15919	297.8723	-4.08884	297.8723	4.004461
330	9.99654	330	-9.04635	299.2908	-2.68989	299.2908	2.596662
329	9.87489	329	-8.9419	300.7092	-1.26389	300.7092	1.162048
328	9.76561	328	-8.83731	302.1277	0.173504	302.1277	-0.28359
327	9.65281	327	-8.73837	303.5461	1.606256	303.5461	-1.72412
326	9.55057	326	-8.64238	304.9645	3.018345	304.9645	-3.14339
325	9.44203	325	-8.55163	306.383	4.394105	306.383	-4.52559
324	9.34247	324	-8.45718	307.8014	5.718579	307.8014	-5.85564
323	9.24252	323	-8.37271	309.2199	6.977854	309.2199	-7.11949
322	9.15108	322	-8.28449	310.6383	8.15936	310.6383	-8.30442
321	9.05005	321	-8.20136	312.0567	9.25213	312.0567	-9.39934
320	8.96976	320	-8.11583	313.4752	10.247	313.4752	-10.395

319	8.89155	319	-8.03475	314.8936	11.13674	314.8936	-11.2839
318	8.8048	318	-7.96221	316.3121	11.91612	316.3121	-12.061
317	8.72136	317	-7.87852	317.7305	12.58191	317.7305	-12.7229
316	8.62748	316	-7.80054	319.1489	13.13282	319.1489	-13.2683
315	8.52989	315	-7.70906	320.5674	13.56932	320.5674	-13.6978
314	8.42287	314	-7.6155	321.9858	13.89352	321.9858	-14.0135
313	8.30684	313	-7.5156	323.4043	14.1089	323.4043	-14.2191
312	8.18449	312	-7.4076	324.8227	14.22008	324.8227	-14.3195
311	8.05154	311	-7.28004	326.2411	14.2326	326.2411	-14.3204
310	7.89651	310	-7.15165	327.6596	14.15266	327.6596	-14.2282
309	7.72833	309	-7.00035	329.078	13.98692	329.078	-14.05
308	7.53864	308	-6.8374	330.4965	13.74232	330.4965	-13.793
307	7.33524	307	-6.65912	331.9149	13.42594	331.9149	-13.4645
306	7.11419	306	-6.46135	333.3333	13.04491	333.3333	-13.0719
305	6.8648	305	-6.24356	334.7518	12.60633	334.7518	-12.6226
304	6.59611	304	-6.0048	336.1702	12.11726	336.1702	-12.124
303	6.30244	303	-5.74723	337.5887	11.58472	337.5887	-11.583
302	5.99156	302	-5.47042	339.0071	11.01567	339.0071	-11.0069
301	5.65316	301	-5.17225	340.4255	10.41706	340.4255	-10.4026
300	5.29968	300	-4.85102	341.844	9.795772	341.844	-9.77702
299	4.92599	299	-4.49561	343.2624	9.158688	343.2624	-9.13697
298	4.52604	298	-4.12542	344.6809	8.512599	344.6809	-8.48917
297	4.10325	297	-3.73697	346.0993	7.864173	346.0993	-7.84014
296	3.66587	296	-3.33029	347.5177	7.219882	347.5177	-7.1962
295	3.20051	295	-2.90546	348.9362	6.585909	348.9362	-6.56338
294	2.71113	294	-2.46948	350.3546	5.968043	350.3546	-5.94727
293	2.20253	293	-2.0122	351.773	5.37158	351.773	-5.353
292	1.67452	292	-1.53967	353.1915	4.801215	353.1915	-4.78509
291	1.13355	291	-1.03901	354.6099	4.260961	354.6099	-4.24742
290	0.569467	290	-0.53059	356.0284	3.754074	356.0284	-3.7431
289	-0.00586	289	0.001232	357.4468	3.283012	357.4468	-3.27449
288	-0.60472	288	0.54223	358.8652	2.849419	358.8652	-2.84316
287	-1.21269	287	1.09893	360.2837	2.454134	360.2837	-2.44988
286	-1.83626	286	1.6652	361.7021	2.097233	361.7021	-2.09471
285	-2.4754	285	2.24489	363.1206	1.77809	363.1206	-1.777
284	-3.114	284	2.83832	364.539	1.495464	364.539	-1.49552
283	-3.76694	283	3.44057	365.9574	1.247596	365.9574	-1.24852
282	-4.43462	282	4.0469	367.3759	1.032314	367.3759	-1.03385
281	-5.11128	281	4.66032	368.7943	0.847142	368.7943	-0.84909
280	-5.78191	280	5.27405	370.2128	0.689411	370.2128	-0.69158
279	-6.46308	279	5.89149	371.6312	0.556355	371.6312	-0.5586
278	-7.1388	278	6.50864	373.0496	0.445197	373.0496	-0.44741
277	-7.81405	277	7.12001	374.4681	0.35323	374.4681	-0.35533

276	-8.47815	276	7.72632	375.8865	0.277875	375.8865	-0.27981
275	-9.13004	275	8.31535	377.305	0.216726	377.305	-0.21846
274	-9.75646	274	8.88125	378.7234	0.167582	378.7234	-0.16911
273	-10.3629	273	9.42318	380.1418	0.128464	380.1418	-0.12978
272	-10.9293	272	9.94089	381.5603	0.097626	381.5603	-0.09873
271	-11.4657	271	10.4283	382.9787	0.073547	382.9787	-0.07447
270	-11.9592	270	10.8719	384.3972	0.054925	384.3972	-0.05568
269	-12.4168	269	11.282	385.8156	0.040661	385.8156	-0.04127
268	-12.8343	268	11.658	387.234	0.029838	387.234	-0.03032
267	-13.2	267	11.9993	388.6525	0.021704	388.6525	-0.02208
266	-13.527	266	12.2864	390.0709	0.01565	390.0709	-0.01594
265	-13.8032	265	12.5359	391.4894	0.011185	391.4894	-0.01141
264	-14.0279	264	12.732	392.9078	0.007924	392.9078	-0.00809
263	-14.2001	263	12.882	394.3262	0.005564	394.3262	-0.00569
262	-14.3087	262	12.981	395.7447	0.003872	395.7447	-0.00397
261	-14.3691	261	13.0317	397.1631	0.002671	397.1631	-0.00274
260	-14.3722	260	13.0384	398.5816	0.001827	398.5816	-0.00188
259	-14.3277	259	12.9962	400	0	400	0
258	-14.2255	258	12.9097				
257	-14.0838	257	12.7741				
256	-13.897	256	12.5993				
255	-13.6569	255	12.3896				
254	-13.3751	254	12.128				
253	-13.0475	253	11.8217				
252	-12.6701	252	11.4761				
251	-12.2444	251	11.0935				
250	-11.7806	250	10.6775				
249	-11.2886	249	10.2275				
248	-10.7638	248	9.74284				
247	-10.215	247	9.23027				
246	-9.64422	246	8.70391				
245	-9.0581	245	8.15058				
244	-8.45826	244	7.57974				
243	-7.84837	243	7.00889				
242	-7.23885	242	6.43933				
241	-6.63444	241	5.87276				
240	-6.05384	240	5.30653				
239	-5.48204	239	4.76809				
238	-4.94541	238	4.24262				
237	-4.44229	237	3.7451				
236	-3.96953	236	3.29117				
235	-3.54079	235	2.87245				
234	-3.15678	234	2.49935				

233	-2.84553	233	2.17042				
232	-2.588	232	1.8934				
231	-2.3953	231	1.65471				
230	-2.25952	230	1.47635				
229	-2.1915	229	1.35262				
228	-2.17803	228	1.28305				
227	-2.22925	227	1.27267				
226	-2.34023	226	1.31171				
225	-2.49626	225	1.38462				
224	-2.69559	224	1.49794				
223	-2.93718	223	1.66016				
222	-3.19769	222	1.85752				
221	-3.47635	221	2.04932				
220	-3.73513	220	2.24622				
219	-3.86522	219	2.33639				
218	-4.02591	218	2.44569				
217	-4.20387	217	2.58709				
216	-4.40321	216	2.76087				
215	-4.63423	215	2.96194				
214	-4.86884	214	3.17976				
213	-5.10117	213	3.39437				
212	-5.28938	212	3.56683				
211	-5.40988	211	3.70504				
210	-5.46237	210	3.79407				
209	-5.42638	209	3.80174				
208	-5.25571	208	3.71037				
207	-4.91477	207	3.4858				
206	-4.38748	206	3.12757				
205	-3.66333	205	2.57401				
204	-2.65882	204	1.84922				
203	-1.35135	203	0.920638				
202	0.22373	202	-0.24491				
201	2.04216	201	-1.65437				
200	4.1289	200	-3.31644				

5.4 Experimental ECD data of (+)-4/(-)-4 and Calculated ECD data of 4a/4b

Experimental ECD data				Calculated ECD data			
(+)-4		(-)-4		4a		4b	
λ (nm)	$\Delta\epsilon$	λ (nm)	$\Delta\epsilon$	λ (nm)	$\Delta\epsilon$	λ (nm)	$\Delta\epsilon$
400	-0.00688	400	0.011539	200	-3.06273	200	2.956206
399	-0.01319	399	0.010311	201.4706	-2.86054	201.4706	2.763752
398	-0.01669	398	0.013814	202.9412	-2.66119	202.9412	2.574477
397	-0.02489	397	0.018572	204.4118	-2.46713	204.4118	2.390681

396	-0.03092	396	0.024444	205.8824	-2.27992	205.8824	2.213752
395	-0.03954	395	0.029848	207.3529	-2.10015	207.3529	2.04416
394	-0.04817	394	0.036433	208.8235	-1.92755	208.8235	1.881508
393	-0.05433	393	0.043968	210.2941	-1.76103	210.2941	1.724631
392	-0.0648	392	0.058622	211.7647	-1.59888	211.7647	1.571742
391	-0.07628	391	0.068222	213.2353	-1.43894	213.2353	1.420616
390	-0.09454	390	0.086635	214.7059	-1.27879	214.7059	1.268797
389	-0.11206	389	0.104724	216.1765	-1.11601	216.1765	1.113824
388	-0.13452	388	0.126578	217.6471	-0.94839	217.6471	0.953453
387	-0.15743	387	0.149014	219.1176	-0.77415	219.1176	0.785875
386	-0.18107	386	0.178095	220.5882	-0.59215	220.5882	0.609907
385	-0.20836	385	0.208927	222.0588	-0.40204	222.0588	0.425154
384	-0.23777	384	0.238902	223.5294	-0.20437	223.5294	0.232123
383	-0.26373	383	0.268133	225	-0.00066	225	0.032291
382	-0.28641	382	0.299346	226.4706	0.206586	226.4706	-0.17189
381	-0.30828	381	0.324752	227.9412	0.413927	227.9412	-0.37702
380	-0.32801	380	0.341368	229.4118	0.61711	229.4118	-0.5789
379	-0.33783	379	0.354693	230.8824	0.81122	230.8824	-0.77262
378	-0.34504	378	0.352401	232.3529	0.990878	232.3529	-0.95284
377	-0.33624	377	0.339069	233.8235	1.150478	233.8235	-1.11393
376	-0.31696	376	0.315021	235.2941	1.284439	235.2941	-1.25028
375	-0.28549	375	0.273261	236.7647	1.38746	236.7647	-1.35655
374	-0.23284	374	0.214642	238.2353	1.454759	238.2353	-1.42789
373	-0.17057	373	0.134829	239.7059	1.482289	239.7059	-1.46015
372	-0.08634	372	0.041517	241.1765	1.466914	241.1765	-1.45009
371	0.012272	371	-0.07073	242.6471	1.406534	242.6471	-1.39548
370	0.130438	370	-0.20507	244.1176	1.300154	244.1176	-1.29519
369	0.271298	369	-0.35708	245.5882	1.147901	245.5882	-1.14922
368	0.429098	368	-0.53378	247.0588	0.950974	247.0588	-0.95862
367	0.605424	367	-0.72271	248.5294	0.711562	248.5294	-0.72543
366	0.794835	366	-0.93373	250	0.432712	250	-0.4526
365	1.00041	365	-1.16253	251.4706	0.118178	251.4706	-0.14375
364	1.22213	364	-1.40863	252.9412	-0.22774	252.9412	0.196909
363	1.45449	363	-1.67615	254.4118	-0.60034	254.4118	0.564758
362	1.70235	362	-1.95942	255.8824	-0.9947	255.8824	0.954914
361	1.9715	361	-2.25364	257.3529	-1.40574	257.3529	1.362333
360	2.2477	360	-2.56072	258.8235	-1.82831	258.8235	1.78189
359	2.53278	359	-2.88598	260.2941	-2.25728	260.2941	2.208422
358	2.82927	358	-3.21098	261.7647	-2.68746	261.7647	2.636739
357	3.13717	357	-3.55281	263.2353	-3.11369	263.2353	3.061606
356	3.45164	356	-3.89194	264.7059	-3.5307	264.7059	3.477721
355	3.76852	355	-4.2349	266.1765	-3.93318	266.1765	3.879676
354	4.08596	354	-4.57568	267.6471	-4.31567	267.6471	4.26194

353	4.4037	353	-4.91101	269.1176	-4.6726	269.1176	4.618868
352	4.70543	352	-5.23702	270.5882	-4.99836	270.5882	4.944734
351	5.00825	351	-5.54941	272.0588	-5.28729	272.0588	5.233815
350	5.2985	350	-5.85425	273.5294	-5.53389	273.5294	5.480515
349	5.56553	349	-6.13982	275	-5.73291	275	5.679516
348	5.82046	348	-6.41828	276.4706	-5.87959	276.4706	5.825975
347	6.05624	347	-6.67184	277.9412	-5.9698	277.9412	5.915712
346	6.27483	346	-6.89966	279.4118	-6.00028	279.4118	5.945416
345	6.46963	345	-7.10191	280.8824	-5.96878	280.8824	5.912811
344	6.63947	344	-7.28449	282.3529	-5.87422	282.3529	5.816791
343	6.78676	343	-7.43763	283.8235	-5.71675	283.8235	5.657493
342	6.91562	342	-7.56211	285.2941	-5.49776	285.2941	5.436315
341	7.01235	341	-7.66067	286.7647	-5.21983	286.7647	5.155849
340	7.08872	340	-7.72977	288.2353	-4.8866	288.2353	4.819753
339	7.13663	339	-7.76698	289.7059	-4.50258	289.7059	4.432563
338	7.1592	338	-7.77866	291.1765	-4.0729	291.1765	3.999459
337	7.15428	337	-7.75946	292.6471	-3.60308	292.6471	3.526002
336	7.12395	336	-7.71506	294.1176	-3.09875	294.1176	3.017873
335	7.07203	335	-7.63892	295.5882	-2.56541	295.5882	2.480628
334	6.98438	334	-7.53205	297.0588	-2.00822	297.0588	1.919497
333	6.87338	333	-7.39937	298.5294	-1.43186	298.5294	1.33924
332	6.73494	332	-7.2354	300	-0.84047	300	0.744078
331	6.56776	331	-7.0466	301.4706	-0.23763	301.4706	0.137699
330	6.37365	330	-6.82788	302.9412	0.373545	302.9412	-0.47666
329	6.15873	329	-6.58775	304.4118	0.990239	304.4118	-1.09606
328	5.92407	328	-6.31799	305.8824	1.609769	305.8824	-1.7177
327	5.66724	327	-6.02836	307.3529	2.229341	307.3529	-2.33861
326	5.39436	326	-5.71624	308.8235	2.845824	308.8235	-2.95554
325	5.10383	325	-5.37898	310.2941	3.455535	310.2941	-3.56466
324	4.7952	324	-5.02165	311.7647	4.054081	311.7647	-4.16144
323	4.47009	323	-4.64444	313.2353	4.636255	313.2353	-4.74057
322	4.12508	322	-4.25309	314.7059	5.196025	314.7059	-5.29596
321	3.76682	321	-3.85401	316.1765	5.726606	316.1765	-5.82076
320	3.39318	320	-3.43623	317.6471	6.220625	317.6471	-6.30762
319	3.0168	319	-3.01511	319.1176	6.670371	319.1176	-6.74889
318	2.62899	318	-2.58107	320.5882	7.068109	320.5882	-7.13694
317	2.23818	317	-2.14653	322.0588	7.406444	322.0588	-7.46454
316	1.84533	316	-1.7093	323.5294	7.678701	323.5294	-7.72522
315	1.45197	315	-1.27787	325	7.879308	325	-7.91366
314	1.06899	314	-0.84978	326.4706	8.004127	326.4706	-8.026
313	0.696244	313	-0.42886	327.9412	8.050741	327.9412	-8.06014
312	0.331985	312	-0.01794	329.4118	8.018642	329.4118	-8.01586
311	-0.02474	311	0.375351	330.8824	7.909337	330.8824	-7.89497

310	-0.36779	310	0.751833	332.3529	7.726338	332.3529	-7.70125
309	-0.69438	309	1.11497	333.8235	7.47505	333.8235	-7.44036
308	-1.00777	308	1.45581	335.2941	7.162566	335.2941	-7.11956
307	-1.30071	307	1.77719	336.7647	6.797376	336.7647	-6.7475
306	-1.57852	306	2.07908	338.2353	6.389014	338.2353	-6.33378
305	-1.83309	305	2.35609	339.7059	5.947666	339.7059	-5.88863
304	-2.0735	304	2.60516	341.1765	5.483768	341.1765	-5.42243
303	-2.29889	303	2.83753	342.6471	5.007609	342.6471	-4.94541
302	-2.49651	302	3.05209	344.1176	4.528973	344.1176	-4.46721
301	-2.67913	301	3.24058	345.5882	4.05682	345.5882	-3.99664
300	-2.84302	300	3.404	347.0588	3.599046	347.0588	-3.54142
299	-2.98366	299	3.55355	348.5294	3.162305	348.5294	-3.108
298	-3.11389	298	3.67504	350	2.751909	350	-2.70151
297	-3.22525	297	3.78542	351.4706	2.371798	351.4706	-2.32569
296	-3.32192	296	3.86675	352.9412	2.024575	352.9412	-1.98297
295	-3.39956	295	3.93127	354.4118	1.7116	354.4118	-1.67455
294	-3.45509	294	3.98014	355.8824	1.43312	355.8824	-1.40055
293	-3.49788	293	4.01285	357.3529	1.188433	357.3529	-1.16016
292	-3.52499	292	4.03729	358.8235	0.976064	358.8235	-0.95182
291	-3.53895	291	4.04703	360.2941	0.793951	360.2941	-0.7734
290	-3.54283	290	4.04494	361.7647	0.639618	361.7647	-0.62241
289	-3.53987	289	4.03217	363.2353	0.510339	363.2353	-0.49609
288	-3.52667	288	4.01831	364.7059	0.403282	364.7059	-0.39162
287	-3.50327	287	3.99716	366.1765	0.315624	366.1765	-0.30619
286	-3.47683	286	3.9765	367.6471	0.244649	367.6471	-0.2371
285	-3.45528	285	3.94521	369.1176	0.187815	369.1176	-0.18184
284	-3.42921	284	3.91093	370.5882	0.1428	370.5882	-0.13812
283	-3.40293	283	3.87839	372.0588	0.107532	372.0588	-0.10391
282	-3.37629	282	3.8452	373.5294	0.080198	373.5294	-0.07742
281	-3.3452	281	3.80921	375	0.059238	375	-0.05713
280	-3.31949	280	3.76786	376.4706	0.043336	376.4706	-0.04175
279	-3.29707	279	3.72871	377.9412	0.031399	377.9412	-0.03022
278	-3.26377	278	3.68918	379.4118	0.022531	379.4118	-0.02167
277	-3.22871	277	3.65833	380.8824	0.016013	380.8824	-0.01539
276	-3.19924	276	3.61674	382.3529	0.011271	382.3529	-0.01082
275	-3.16602	275	3.5728	383.8235	0.007858	383.8235	-0.00754
274	-3.12682	274	3.52219	385.2941	0.005425	385.2941	-0.0052
273	-3.08269	273	3.47582	386.7647	0.00371	386.7647	-0.00355
272	-3.03429	272	3.42184	388.2353	0.002513	388.2353	-0.0024
271	-2.98896	271	3.36516	389.7059	0.001685	389.7059	-0.00161
270	-2.93032	270	3.30512	391.1765	0.00112	391.1765	-0.00107
269	-2.87173	269	3.24104	392.6471	0.000737	392.6471	-0.0007
268	-2.8077	268	3.17239	394.1176	0.00048	394.1176	-0.00046

267	-2.7395	267	3.09657	395.5882	0.00031	395.5882	-0.0003
266	-2.66897	266	3.01215	397.0588	0.000198	397.0588	-0.00019
265	-2.58435	265	2.93198	398.5294	0.000125	398.5294	-0.00012
264	-2.49985	264	2.83491	392.9078	-1.9E-25	392.9078	1.86E-25
263	-2.40766	263	2.72901	394.3262	-2.8E-26	394.3262	2.7E-26
262	-2.30971	262	2.61883	395.7447	-3.9E-27	395.7447	3.8E-27
261	-2.20388	261	2.50313	397.1631	-5.3E-28	397.1631	5.17E-28
260	-2.0899	260	2.38063	398.5816	-7E-29	398.5816	6.83E-29
259	-1.96491	259	2.24834	400	0	400	0
258	-1.83788	258	2.11204				
257	-1.70468	257	1.96578				
256	-1.56432	256	1.8152				
255	-1.42564	255	1.65725				
254	-1.27923	254	1.49262				
253	-1.13771	253	1.32156				
252	-0.98923	252	1.1451				
251	-0.8401	251	0.96863				
250	-0.68625	250	0.786696				
249	-0.52594	249	0.597688				
248	-0.37099	248	0.410776				
247	-0.21395	247	0.222677				
246	-0.05591	246	0.033475				
245	0.102436	245	-0.15112				
244	0.260431	244	-0.34087				
243	0.417953	243	-0.5355				
242	0.569553	242	-0.72851				
241	0.718443	241	-0.92345				
240	0.863798	240	-1.11894				
239	1.00275	239	-1.30803				
238	1.13852	238	-1.50804				
237	1.25835	237	-1.69816				
236	1.3862	236	-1.87459				
235	1.50054	235	-2.05176				
234	1.60126	234	-2.2229				
233	1.6979	233	-2.3788				
232	1.78645	232	-2.52974				
231	1.87041	231	-2.65927				
230	1.92113	230	-2.75859				
229	1.97007	229	-2.84304				
228	2.00806	228	-2.91249				
227	2.03241	227	-2.96391				
226	2.03892	226	-3.00178				
225	2.03431	225	-3.02444				

224	2.01942	224	-3.02593				
223	1.98393	223	-3.01922				
222	1.93205	222	-2.9961				
221	1.8704	221	-2.94407				
220	1.78687	220	-2.88054				
219	1.69559	219	-2.78581				
218	1.58046	218	-2.68608				
217	1.45886	217	-2.55282				
216	1.32061	216	-2.39398				
215	1.16633	215	-2.21052				
214	0.992732	214	-1.99386				
213	0.801365	213	-1.75651				
212	0.594237	212	-1.489				
211	0.353391	211	-1.1764				
210	0.092087	210	-0.81938				
209	-0.19852	209	-0.43021				
208	-0.51336	208	0.0161				
207	-0.88216	207	0.517672				
206	-1.28302	206	1.08623				
205	-1.70972	205	1.70512				
204	-2.1949	204	2.42691				
203	-2.69141	203	3.21961				
202	-3.21781	202	4.06601				
201	-3.77118	201	4.94235				
200	-4.34963	200	5.828				

5.5 Experimental ECD data of (+)-5/(-)-5 and Calculated ECD data of 5a/5b

Experimental ECD data				Calculated ECD data			
(+)-5		(-)-5		5a		5b	
λ (nm)	$\Delta\epsilon$	λ (nm)	$\Delta\epsilon$	λ (nm)	$\Delta\epsilon$	λ (nm)	$\Delta\epsilon$
400	-0.13064	400	0.212066	200	-2.85934	200	3.189992
399	-0.13226	399	0.218169	201.4085	-2.53966	201.4085	2.737292
398	-0.13315	398	0.220544	202.8169	-2.2195	202.8169	2.28732
397	-0.12475	397	0.211136	204.2254	-1.90326	204.2254	1.848792
396	-0.12958	396	0.215704	205.6338	-1.59447	205.6338	1.429145
395	-0.13382	395	0.214258	207.0423	-1.29571	207.0423	1.034247
394	-0.13185	394	0.212485	208.4507	-1.00858	208.4507	0.668224
393	-0.1311	393	0.211429	209.8592	-0.73366	209.8592	0.333383
392	-0.13356	392	0.203766	211.2676	-0.47066	211.2676	0.030248
391	-0.1444	391	0.203837	212.6761	-0.21846	212.6761	-0.24229
390	-0.14459	390	0.201382	214.0845	0.024625	214.0845	-0.48677

389	-0.14998	389	0.206186	215.493	0.260732	215.493	-0.7068
388	-0.1631	388	0.217458	216.9014	0.492189	216.9014	-0.90678
387	-0.17608	387	0.227534	218.3099	0.721315	218.3099	-1.09146
386	-0.18931	386	0.241177	219.7183	0.950217	219.7183	-1.26562
385	-0.20147	385	0.2532	221.1268	1.180613	221.1268	-1.43371
384	-0.22599	384	0.264332	222.5352	1.413695	222.5352	-1.59955
383	-0.23902	383	0.283774	223.9437	1.650033	223.9437	-1.76612
382	-0.2464	382	0.291923	225.3521	1.889535	225.3521	-1.9354
381	-0.26822	381	0.30708	226.7606	2.13145	226.7606	-2.10836
380	-0.28558	380	0.322706	228.169	2.374429	228.169	-2.28493
379	-0.30589	379	0.348341	229.5775	2.616627	229.5775	-2.46413
378	-0.32506	378	0.382228	230.9859	2.855839	230.9859	-2.64426
377	-0.34793	377	0.403548	232.3944	3.089663	232.3944	-2.82309
376	-0.37646	376	0.424772	233.8028	3.315682	233.8028	-2.99814
375	-0.39777	375	0.454253	235.2113	3.531637	235.2113	-3.16693
374	-0.42233	374	0.469772	236.6197	3.735599	236.6197	-3.32726
373	-0.4511	373	0.488614	238.0282	3.926112	238.0282	-3.47741
372	-0.48276	372	0.514253	239.4366	4.102305	239.4366	-3.61636
371	-0.5203	371	0.533051	240.8451	4.26396	240.8451	-3.74388
370	-0.55906	370	0.558453	242.2535	4.411538	242.2535	-3.86063
369	-0.5996	369	0.583043	243.662	4.546154	243.662	-3.96812
368	-0.63724	368	0.602655	245.0704	4.669502	245.0704	-4.06862
367	-0.66963	367	0.619022	246.4789	4.783738	246.4789	-4.16502
366	-0.69217	366	0.655794	247.8873	4.891327	247.8873	-4.26063
365	-0.71404	365	0.672732	249.2958	4.994856	249.2958	-4.35888
364	-0.73216	364	0.699757	250.7042	5.096834	250.7042	-4.46307
363	-0.77122	363	0.727799	252.1127	5.199488	252.1127	-4.57606
362	-0.78974	362	0.745593	253.5211	5.304563	253.5211	-4.69997
361	-0.81651	361	0.773695	254.9296	5.413147	254.9296	-4.83593
360	-0.82125	360	0.79928	256.338	5.525529	256.338	-4.98388
359	-0.84723	359	0.822079	257.7465	5.641095	257.7465	-5.14237
358	-0.86328	358	0.83705	259.1549	5.758284	259.1549	-5.30855
357	-0.87275	357	0.838888	260.5634	5.874589	260.5634	-5.47818
356	-0.88213	356	0.859637	261.9718	5.98663	261.9718	-5.64567
355	-0.88312	355	0.870054	263.3803	6.090265	263.3803	-5.80436
354	-0.8802	354	0.872032	264.7887	6.180772	264.7887	-5.94673
353	-0.88172	353	0.876495	266.1972	6.253056	266.1972	-6.06479
352	-0.88741	352	0.873373	267.6056	6.301897	267.6056	-6.15045
351	-0.88703	351	0.883485	269.0141	6.322214	269.0141	-6.19592
350	-0.87337	350	0.877172	270.4225	6.309332	270.4225	-6.19418
349	-0.85031	349	0.880484	271.831	6.259237	271.831	-6.13937
348	-0.83424	348	0.873222	273.2394	6.168809	273.2394	-6.02713
347	-0.80854	347	0.853558	274.6479	6.036011	274.6479	-5.85491

346	-0.78769	346	0.835171	276.0563	5.860028	276.0563	-5.62219
345	-0.76979	345	0.81077	277.4648	5.641357	277.4648	-5.33055
344	-0.75246	344	0.781492	278.8732	5.381823	278.8732	-4.98367
343	-0.711	343	0.758549	280.2817	5.084539	280.2817	-4.58727
342	-0.67774	342	0.724416	281.6901	4.753799	281.6901	-4.14881
341	-0.65425	341	0.699905	283.0986	4.394926	283.0986	-3.67727
340	-0.62256	340	0.671172	284.507	4.014065	284.507	-3.1827
339	-0.59453	339	0.652932	285.9155	3.617948	285.9155	-2.67585
338	-0.56873	338	0.626342	287.3239	3.213634	287.3239	-2.16768
337	-0.53969	337	0.581375	288.7324	2.808247	288.7324	-1.66894
336	-0.51615	336	0.54728	290.1408	2.408714	290.1408	-1.1897
335	-0.49019	335	0.527864	291.5493	2.021533	291.5493	-0.73903
334	-0.4718	334	0.499158	292.9577	1.652558	292.9577	-0.32466
333	-0.45941	333	0.475341	294.3662	1.306834	294.3662	0.047257
332	-0.44537	332	0.464887	295.7746	0.988471	295.7746	0.372258
331	-0.43892	331	0.451591	297.1831	0.700566	297.1831	0.64765
330	-0.44054	330	0.451864	298.5915	0.44518	298.5915	0.872457
329	-0.44335	329	0.43784	300	0.223349	300	1.047318
328	-0.43663	328	0.441903	301.4085	0.035144	301.4085	1.17431
327	-0.43237	327	0.450272	302.8169	-0.12024	302.8169	1.256719
326	-0.44824	326	0.474697	304.2254	-0.24435	304.2254	1.29879
325	-0.45763	325	0.494896	305.6338	-0.33936	305.6338	1.305448
324	-0.48117	324	0.523296	307.0423	-0.40792	307.0423	1.282036
323	-0.5148	323	0.545368	308.4507	-0.453	308.4507	1.23405
322	-0.53118	322	0.576493	309.8592	-0.47775	309.8592	1.166917
321	-0.56903	321	0.615018	311.2676	-0.48537	311.2676	1.0858
320	-0.60574	320	0.65699	312.6761	-0.47901	312.6761	0.995439
319	-0.65917	319	0.695242	314.0845	-0.46166	314.0845	0.900046
318	-0.70814	318	0.738713	315.493	-0.43606	315.493	0.80323
317	-0.75824	317	0.783992	316.9014	-0.4047	316.9014	0.707971
316	-0.81271	316	0.832581	318.3099	-0.36972	318.3099	0.616615
315	-0.87111	315	0.873656	319.7183	-0.33296	319.7183	0.530909
314	-0.93531	314	0.914998	321.1268	-0.29589	321.1268	0.452052
313	-1.00536	313	0.971814	322.5352	-0.25971	322.5352	0.380756
312	-1.06711	312	1.023185	323.9437	-0.2253	323.9437	0.317326
311	-1.11736	311	1.080003	325.3521	-0.19327	325.3521	0.261732
310	-1.16478	310	1.125581	326.7606	-0.16402	326.7606	0.21369
309	-1.20284	309	1.173351	328.169	-0.13777	328.169	0.172725
308	-1.2494	308	1.196745	329.5775	-0.11457	329.5775	0.138238
307	-1.27041	307	1.21209	330.9859	-0.09435	330.9859	0.109562
306	-1.29256	306	1.2141	332.3944	-0.07696	332.3944	0.085998
305	-1.26647	305	1.196485	333.8028	-0.0622	333.8028	0.06686
304	-1.22068	304	1.15709	335.2113	-0.04981	335.2113	0.051489

303	-1.15058	303	1.096901	336.6197	-0.03953	336.6197	0.03928
302	-1.05329	302	1.017904	338.0282	-0.0311	338.0282	0.029687
301	-0.93313	301	0.90585	339.4366	-0.02425	339.4366	0.022229
300	-0.78129	300	0.777308	340.8451	-0.01874	340.8451	0.016492
299	-0.6018	299	0.625996	342.2535	-0.01437	342.2535	0.012123
298	-0.39497	298	0.449698	343.662	-0.01092	343.662	0.00883
297	-0.14973	297	0.247076	345.0704	-0.00823	345.0704	0.006373
296	0.092955	296	0.029819	346.4789	-0.00615	346.4789	0.004558
295	0.371393	295	-0.20334	347.8873	-0.00456	347.8873	0.003231
294	0.67351	294	-0.45588	349.2958	-0.00335	349.2958	0.002269
293	0.996105	293	-0.73197	350.7042	-0.00244	350.7042	0.00158
292	1.3385	292	-1.02086	352.1127	-0.00177	352.1127	0.00109
291	1.68629	291	-1.33298	353.5211	-0.00127	353.5211	0.000745
290	2.06042	290	-1.65313	354.9296	-0.0009	354.9296	0.000505
289	2.45689	289	-1.99801	356.338	-0.00064	356.338	0.000339
288	2.85879	288	-2.33939	357.7465	-0.00045	357.7465	0.000226
287	3.26633	287	-2.69358	359.1549	-0.00031	359.1549	0.000149
286	3.66287	286	-3.04515	360.5634	-0.00021	360.5634	9.73E-05
285	4.05943	285	-3.39693	361.9718	-0.00015	361.9718	6.3E-05
284	4.45523	284	-3.74978	363.3803	-9.9E-05	363.3803	4.05E-05
283	4.82414	283	-4.09291	364.7887	-6.7E-05	364.7887	2.58E-05
282	5.19154	282	-4.43021	366.1972	-4.4E-05	366.1972	1.63E-05
281	5.53304	281	-4.75821	367.6056	-2.9E-05	367.6056	1.02E-05
280	5.85076	280	-5.05676	369.0141	-1.9E-05	369.0141	6.3E-06
279	6.14631	279	-5.34285	370.4225	-1.3E-05	370.4225	3.87E-06
278	6.41182	278	-5.60773	371.831	-8.2E-06	371.831	2.36E-06
277	6.65512	277	-5.85857	373.2394	-5.2E-06	373.2394	1.42E-06
276	6.8679	276	-6.08349	374.6479	-3.3E-06	374.6479	8.51E-07
275	7.04292	275	-6.27291	376.0563	-2.1E-06	376.0563	5.05E-07
274	7.18325	274	-6.42838	377.4648	-1.3E-06	377.4648	2.97E-07
273	7.29694	273	-6.55473	378.8732	-8.2E-07	378.8732	1.73E-07
272	7.38448	272	-6.65052	380.2817	-5.1E-07	380.2817	9.98E-08
271	7.4388	271	-6.71869	381.6901	-3.1E-07	381.6901	5.71E-08
270	7.4619	270	-6.76591	383.0986	-1.9E-07	383.0986	3.24E-08
269	7.45624	269	-6.79332	384.507	-1.1E-07	384.507	1.82E-08
268	7.43191	268	-6.81019	385.9155	-6.8E-08	385.9155	1.02E-08
267	7.38728	267	-6.80156	387.3239	-4E-08	387.3239	5.61E-09
266	7.31476	266	-6.77307	388.7324	-2.4E-08	388.7324	3.07E-09
265	7.24068	265	-6.73008	390.1408	-1.4E-08	390.1408	1.67E-09
264	7.12581	264	-6.65804	391.5493	-8.1E-09	391.5493	8.98E-10
263	7.00225	263	-6.56702	392.9577	-4.7E-09	392.9577	4.79E-10
262	6.88423	262	-6.45874	394.3662	-2.7E-09	394.3662	2.53E-10
261	6.73805	261	-6.34648	395.7746	-1.5E-09	395.7746	1.33E-10

260	6.58236	260	-6.20909	397.1831	-8.5E-10	397.1831	6.89E-11
259	6.40327	259	-6.06224	398.5915	-4.7E-10	398.5915	3.55E-11
258	6.22724	258	-5.90732				
257	6.04056	257	-5.73845				
256	5.83825	256	-5.5577				
255	5.64584	255	-5.3683				
254	5.44247	254	-5.1742				
253	5.23953	253	-4.99306				
252	5.03608	252	-4.80001				
251	4.8306	251	-4.60685				
250	4.63969	250	-4.40675				
249	4.43862	249	-4.21614				
248	4.22559	248	-4.02639				
247	4.02668	247	-3.8442				
246	3.81746	246	-3.64824				
245	3.61253	245	-3.4759				
244	3.42584	244	-3.30765				
243	3.2299	243	-3.14516				
242	3.04717	242	-3.00326				
241	2.86796	241	-2.85558				
240	2.7001	240	-2.72108				
239	2.54558	239	-2.60781				
238	2.39214	238	-2.50578				
237	2.24808	237	-2.40917				
236	2.10598	236	-2.31575				
235	1.95318	235	-2.24996				
234	1.81088	234	-2.18095				
233	1.67483	233	-2.11742				
232	1.54384	232	-2.05622				
231	1.42045	231	-2.00784				
230	1.3104	230	-1.96537				
229	1.18606	229	-1.92583				
228	1.07054	228	-1.88709				
227	0.957758	227	-1.84741				
226	0.855105	226	-1.83295				
225	0.760625	225	-1.82478				
224	0.679825	224	-1.79435				
223	0.596719	223	-1.77119				
222	0.5125	222	-1.76171				
221	0.407641	221	-1.73824				
220	0.29505	220	-1.71346				
219	0.16772	219	-1.66616				
218	0.047391	218	-1.62071				

217	-0.08634	217	-1.48216				
216	-0.21678	216	-1.3669				
215	-0.39898	215	-1.21869				
214	-0.57941	214	-1.06073				
213	-0.7799	213	-0.87261				
212	-1.00355	212	-0.66358				
211	-1.2445	211	-0.42397				
210	-1.51484	210	-0.15881				
209	-1.7999	209	0.150417				
208	-2.10509	208	0.485479				
207	-2.44104	207	0.857669				
206	-2.82581	206	1.29041				
205	-3.29026	205	1.74746				
204	-3.77539	204	2.31723				
203	-4.28818	203	2.96454				
202	-4.9103	202	3.70225				
201	-5.52094	201	4.47221				
200	-6.11856	200	5.22312				