

Fusarins G-L with inhibition of NO from marine-derived fungus *Fusarium solani* 7227

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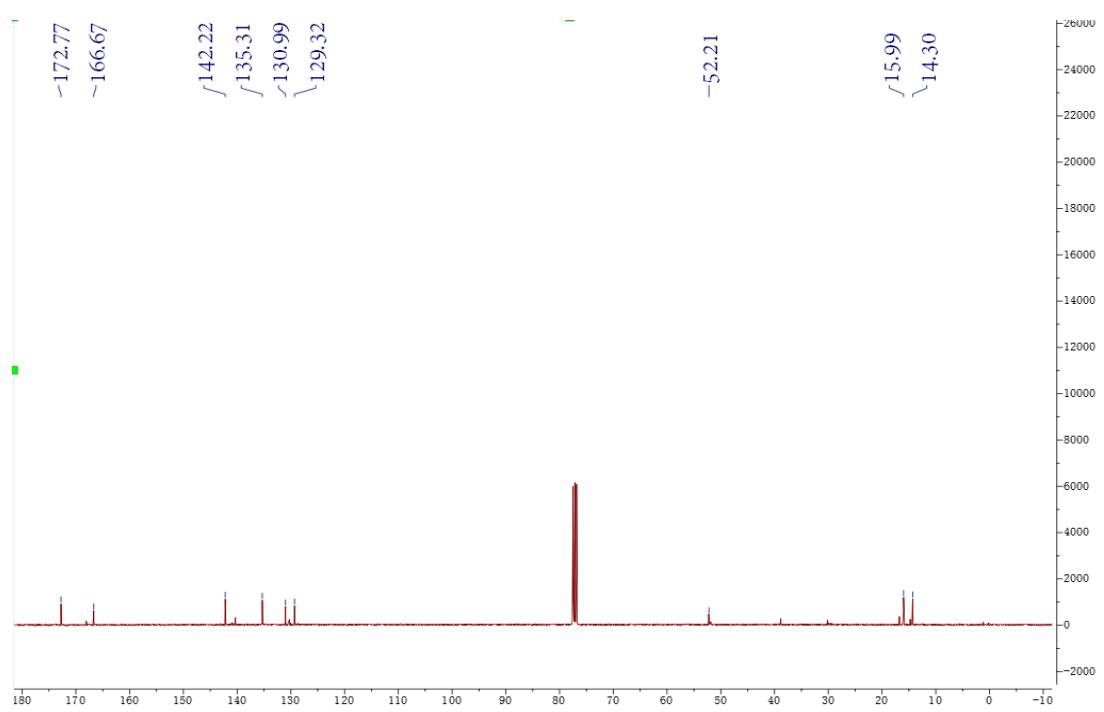
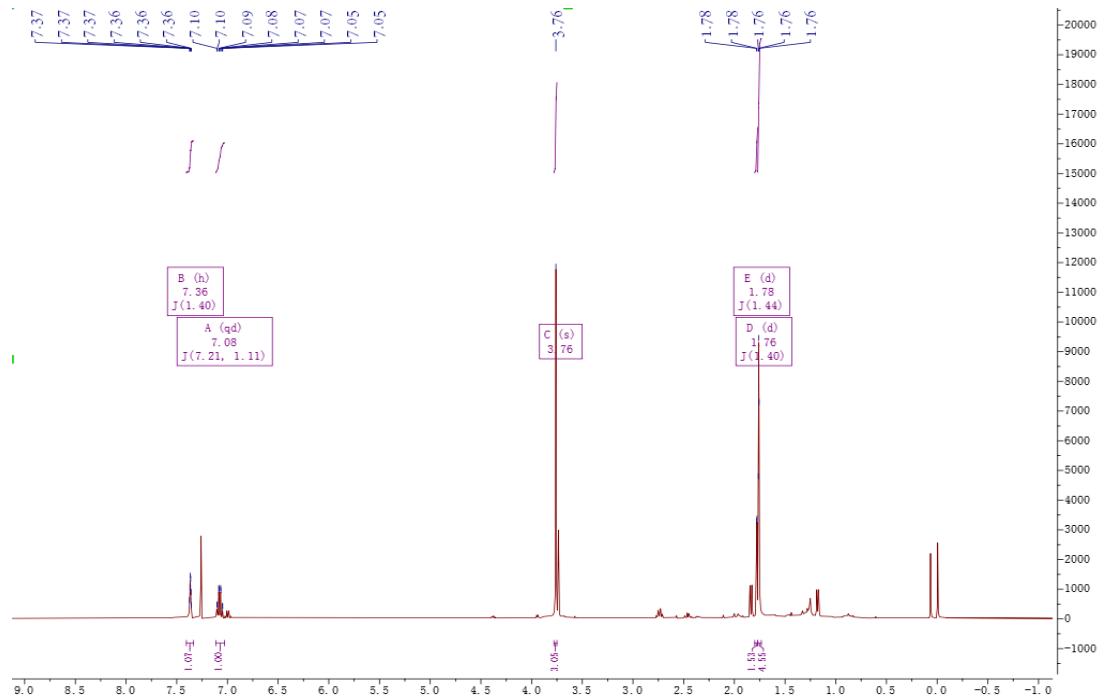


Figure S 1. ^1H NMR spectrum of **1** in CDCl_3 .

Figure S 2. ^{13}C NMR spectrum of **1** in CDCl_3 .

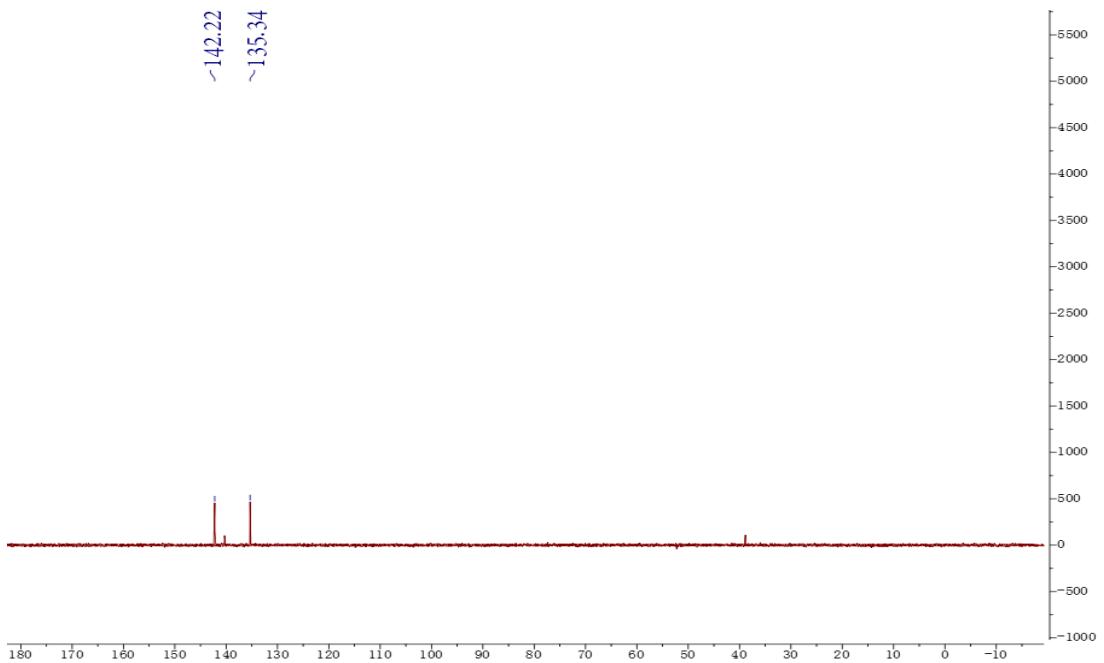


Figure S 3. DEPT-90 spectrum of 1 in CDCl_3 .

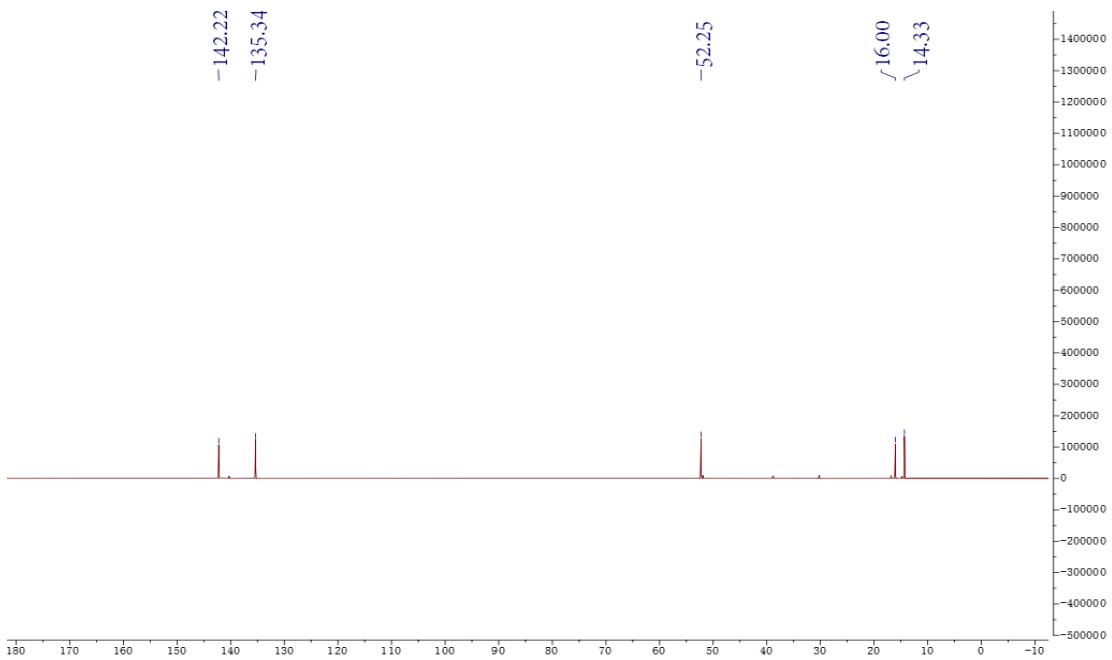


Figure S 4. DEPT-135 spectrum of 1 in CDCl_3 .

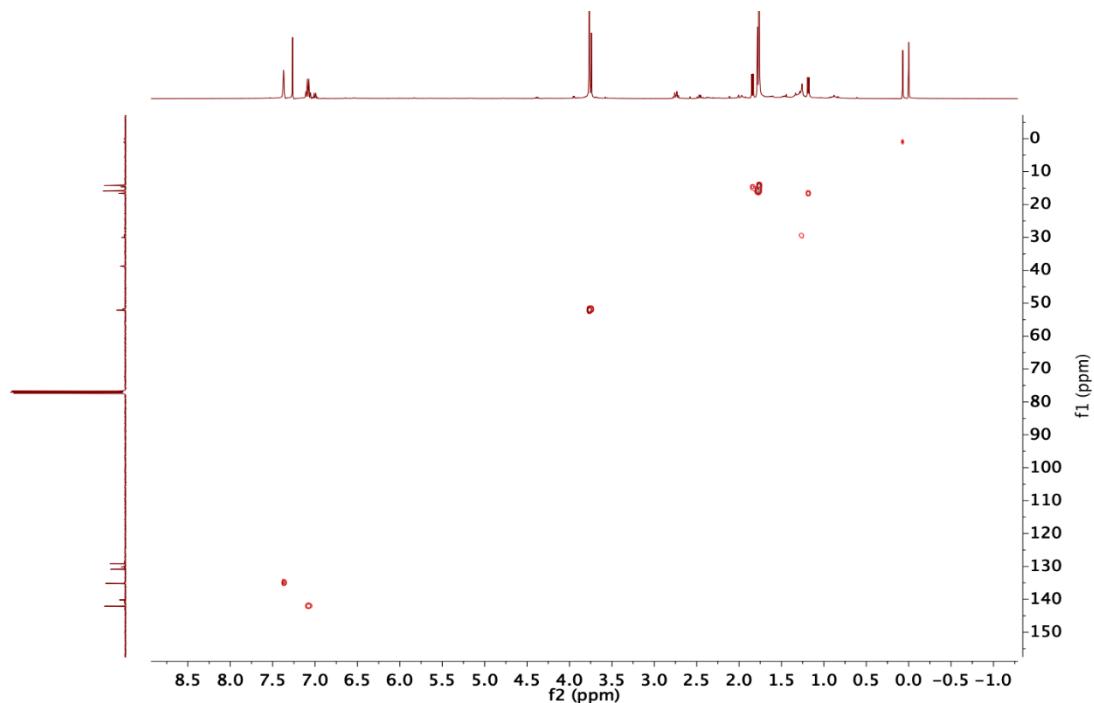


Figure S 5. HSQC spectrum of **1** in CDCl_3 .

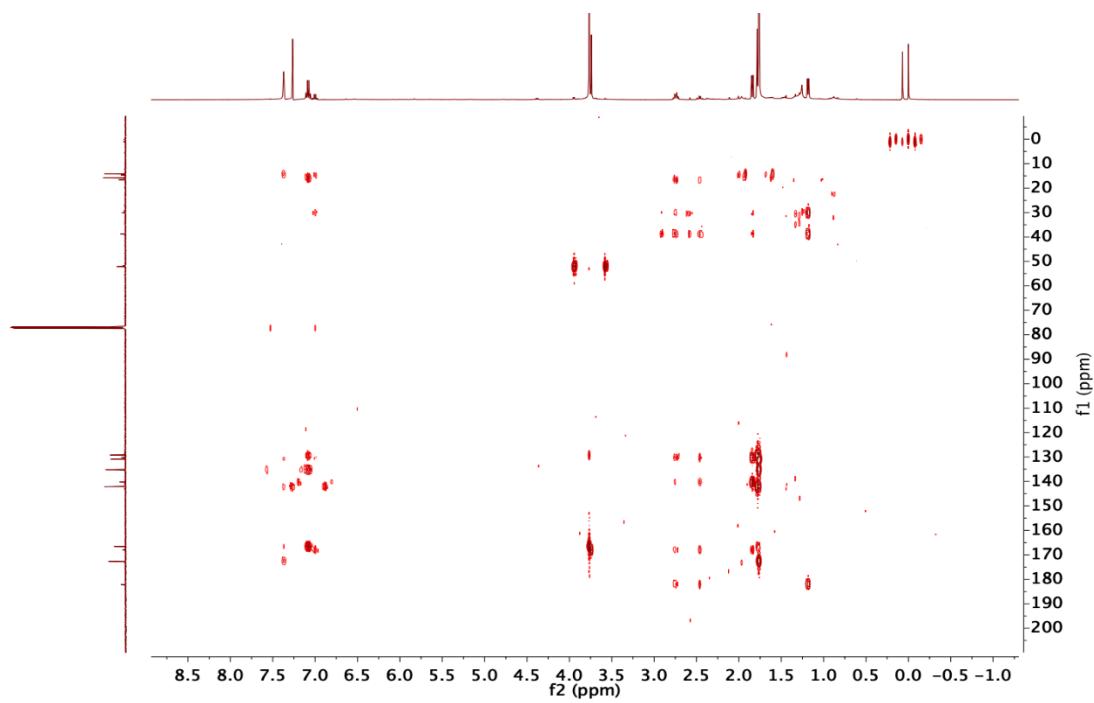


Figure S 6. HMBC spectrum of **1** in CDCl_3 .

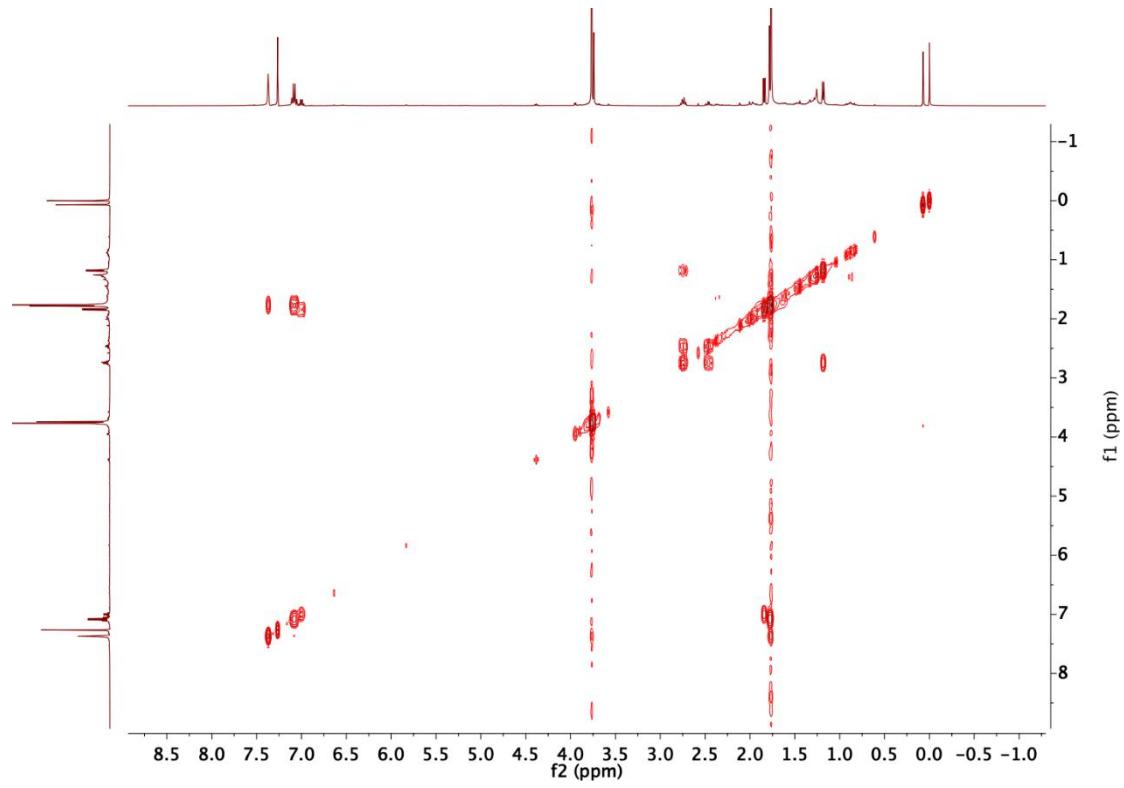


Figure S 7. ^1H - ^1H COSY spectrum of **1** in CDCl_3 .

Analysis Info

Analysis Name	D:\Data\2020\05\Liu lan\2005A0279\2005A0279_7227-15_neg_1uL_RA3_01_3541.d	Acquisition Date	5/22/2020 11:32:29 AM
Method	Tune_neg_low_LCMS.m	Operator	Demo User
Sample Name	2005A0279_7227-15_neg_1uL	Instrument	timTOF
Comment			1844426.00062

Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	0.6 Bar
Focus	Not active	Set Capillary	3500 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Waste

-MS, 0.08-0.09min

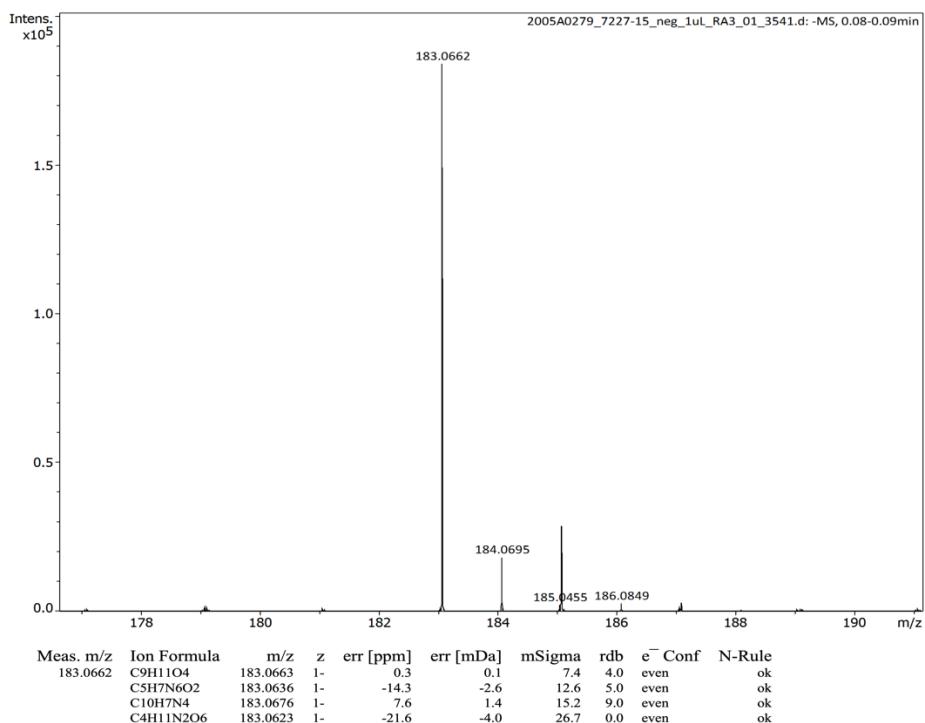


Figure S 8. HR-ESIMS spectrum of 1.

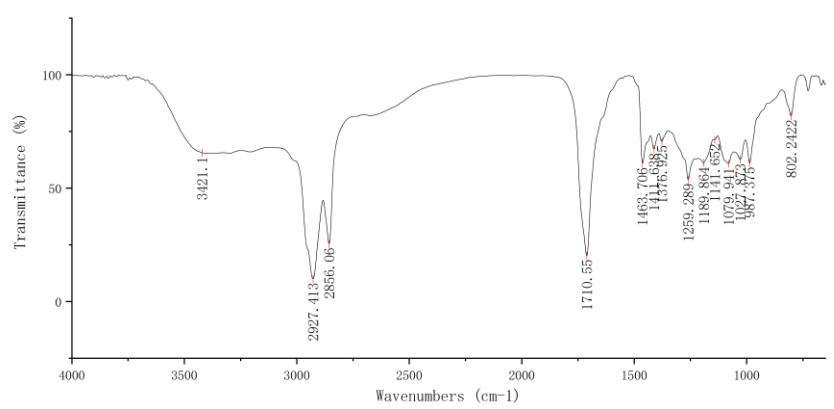


Figure S 9. IR spectrum of 1.

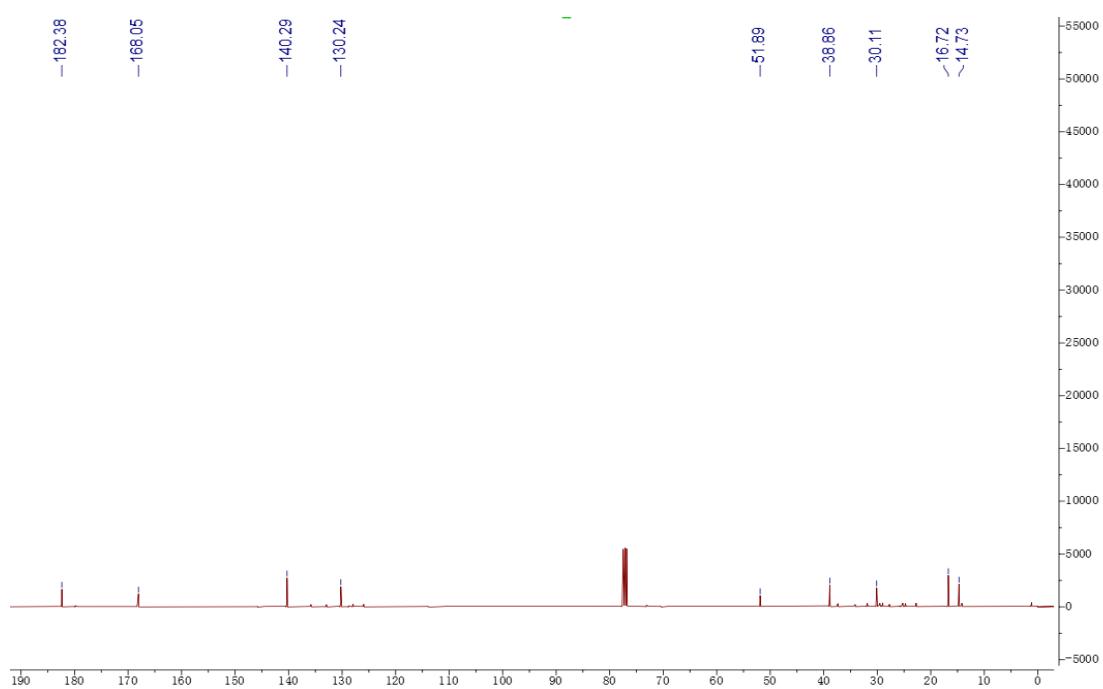
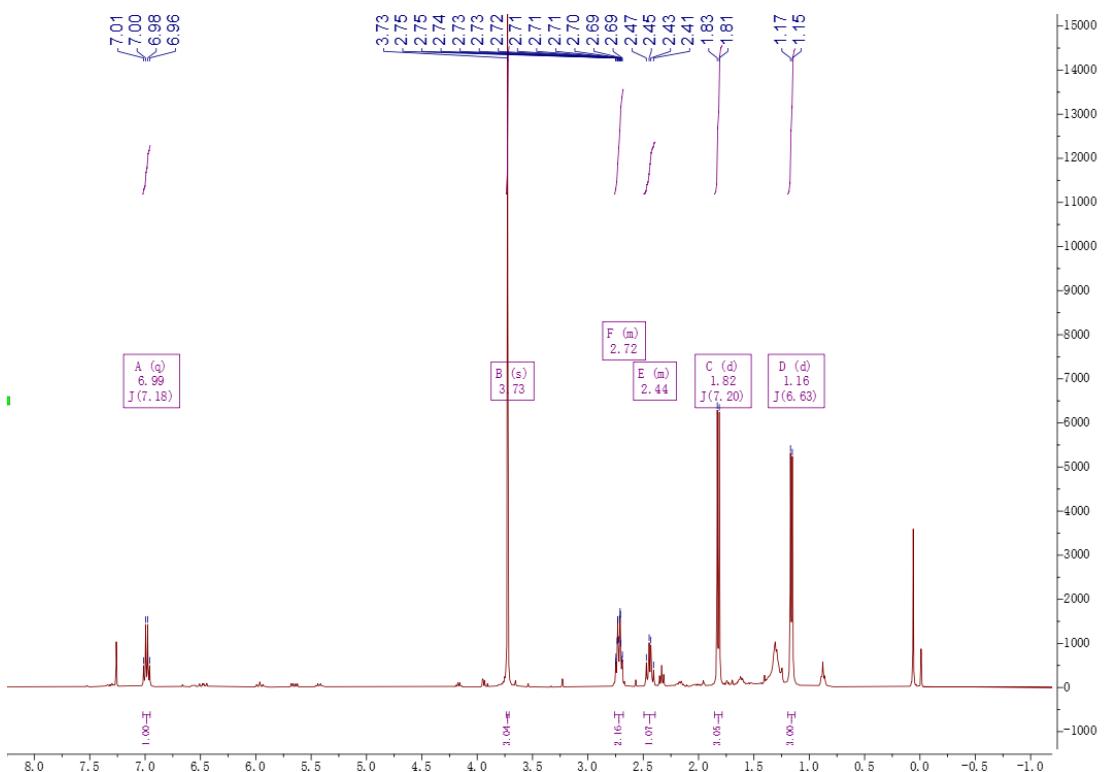


Figure S 11. ^{13}C NMR spectrum of 2 in CDCl_3 .

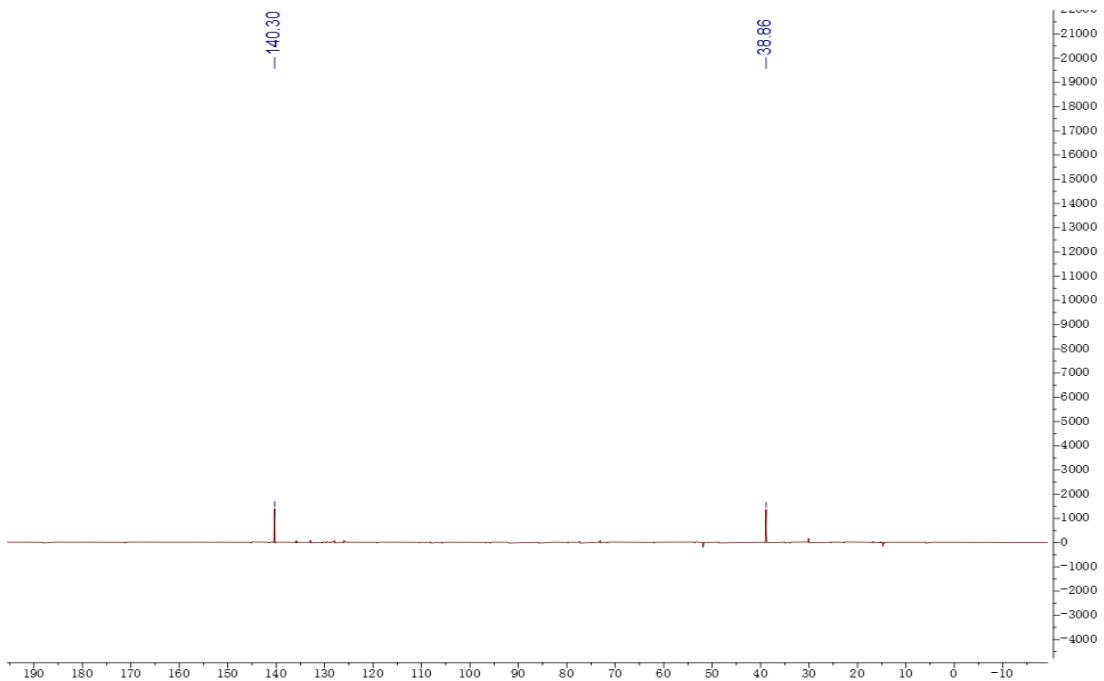


Figure S 12. DEPT-90 spectrum of **2** in CDCl_3 .

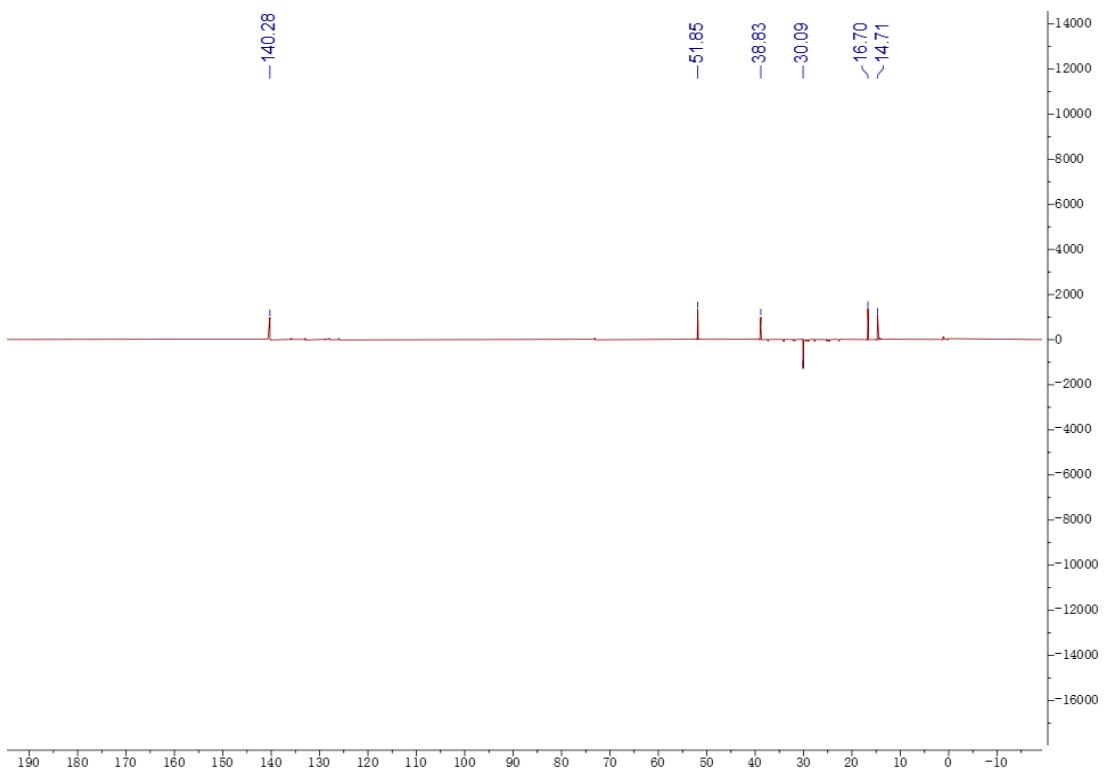


Figure S 13. DEPT-135 spectrum of **2** in CDCl_3 .

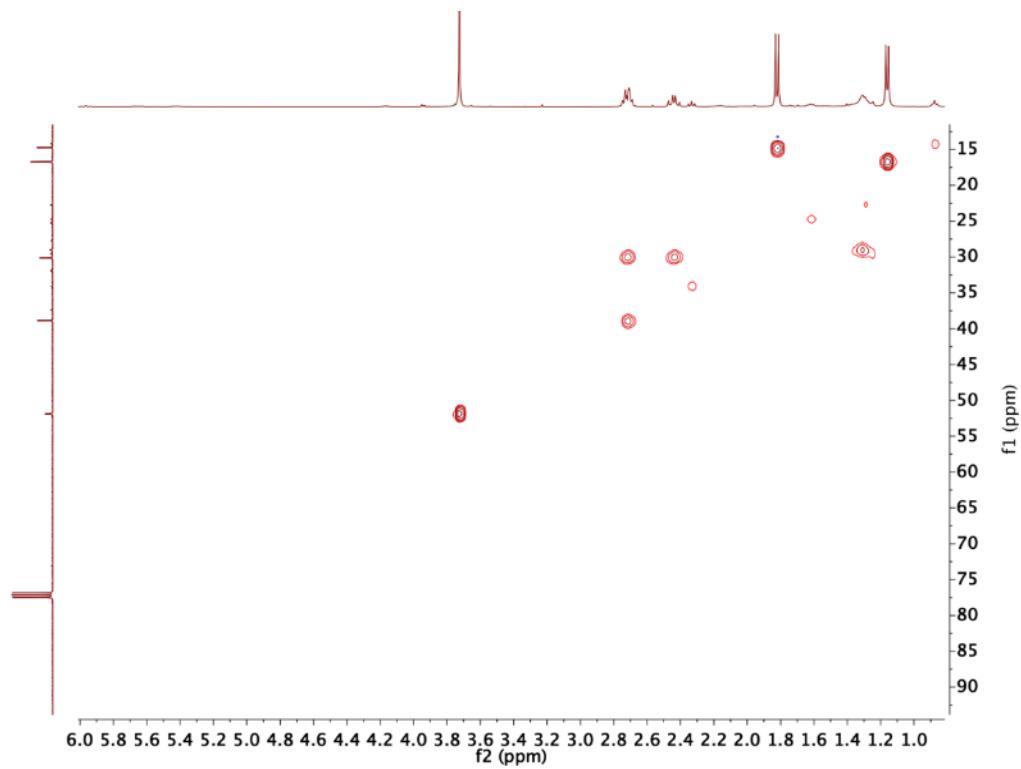


Figure S 14. HSQC spectrum of **2** in CDCl_3 .

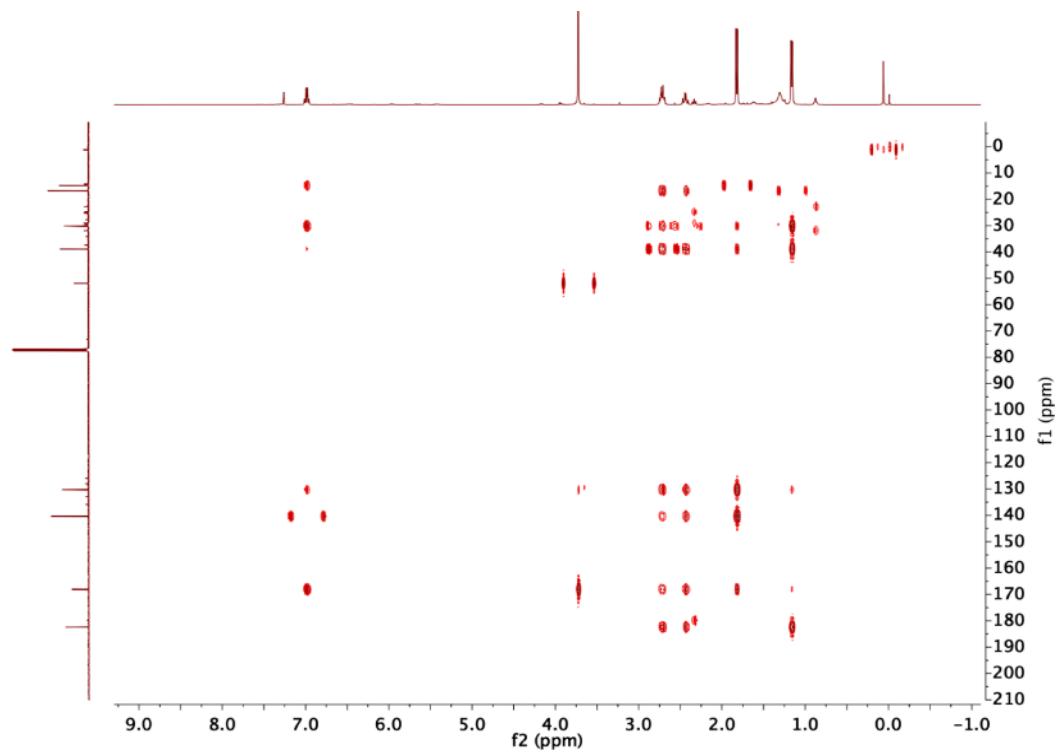


Figure S 15. HMBC spectrum of **2** in CDCl_3 .

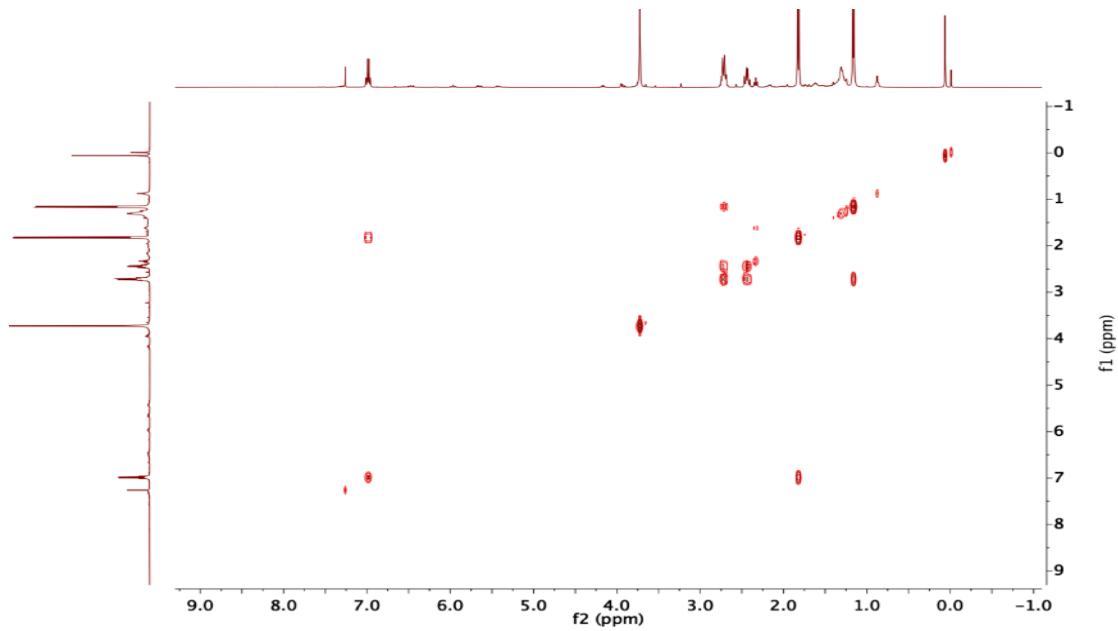


Figure S 16. ^1H - ^1H COSY spectrum of **2** in CDCl_3 .

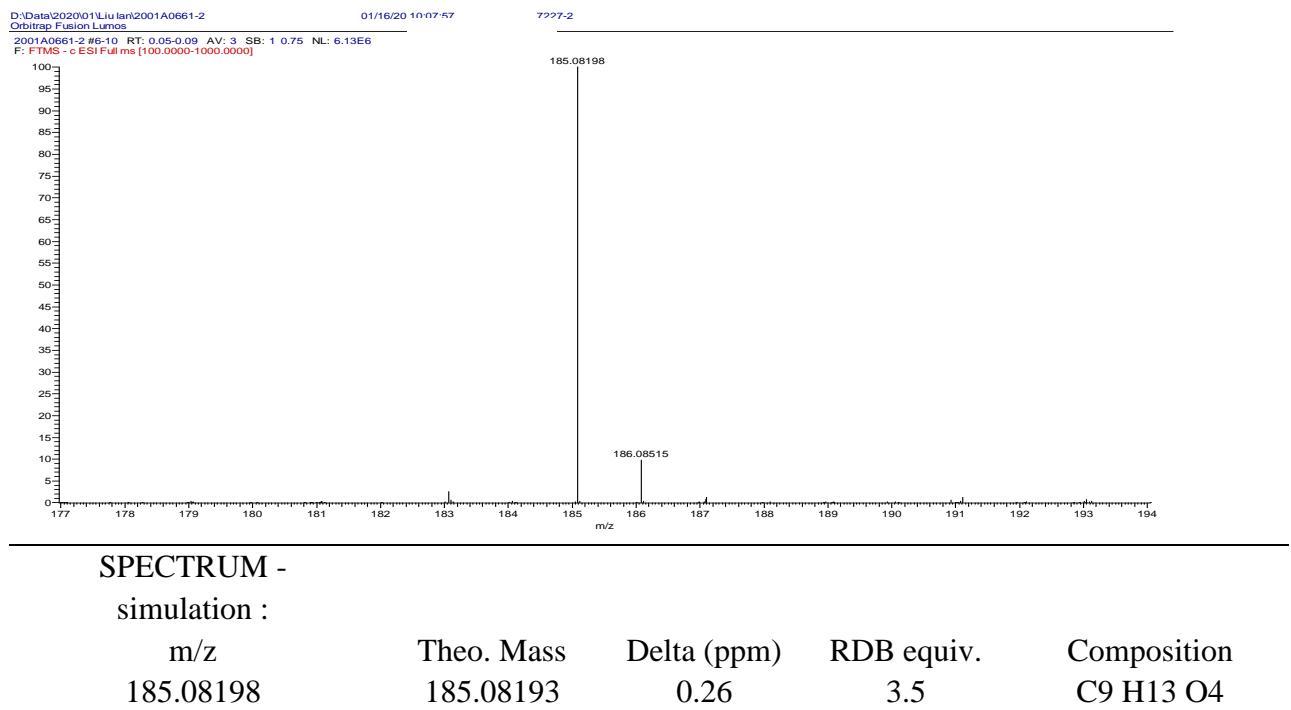


Figure S 17. HR-ESIMS spectrum of **2**.

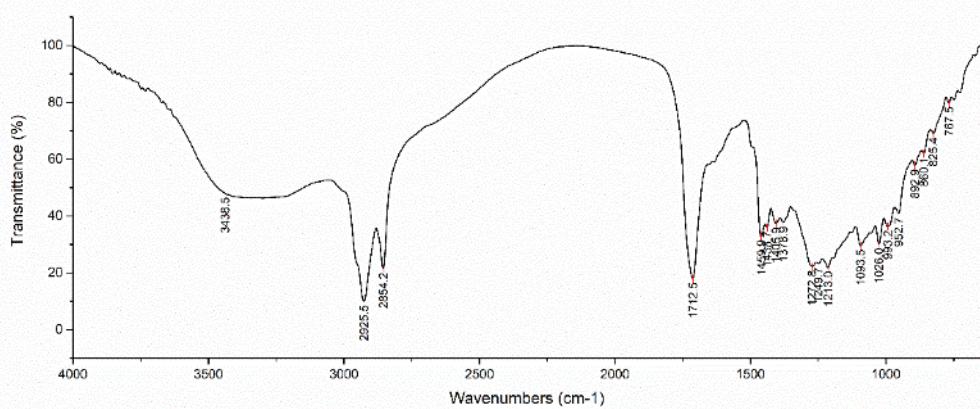


Figure S 18. IR spectrum of 2.

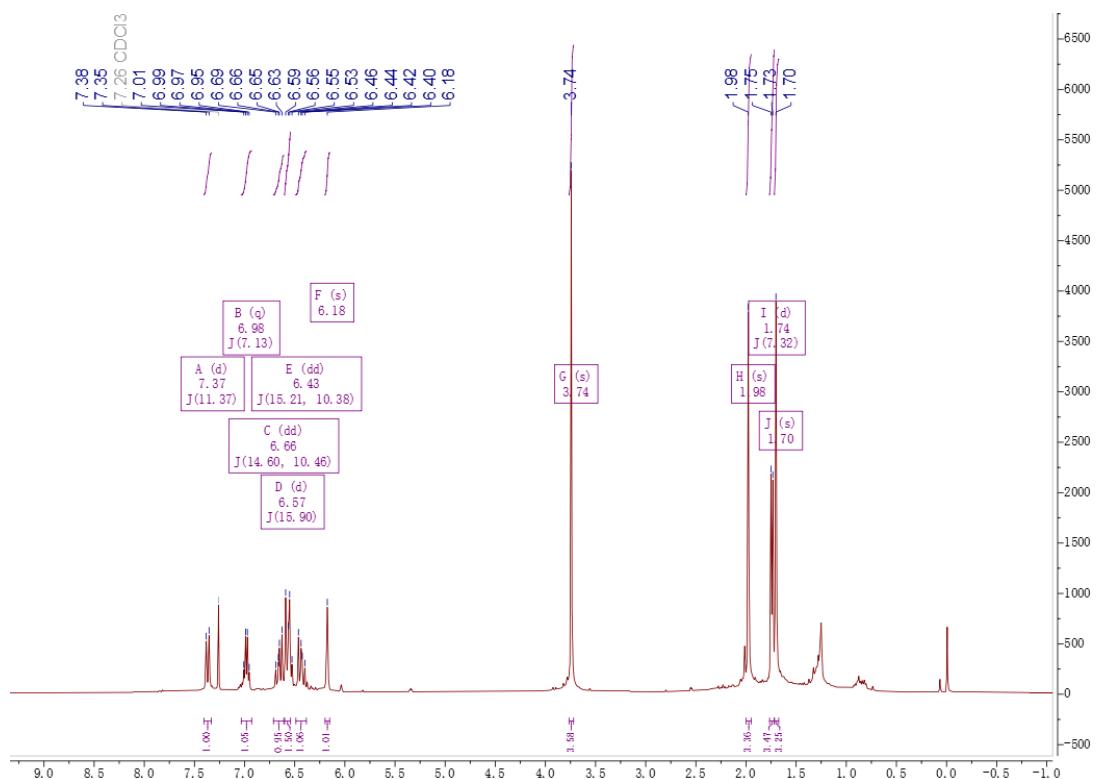


Figure S 19. ^1H NMR spectrum of **3** in CDCl_3 .

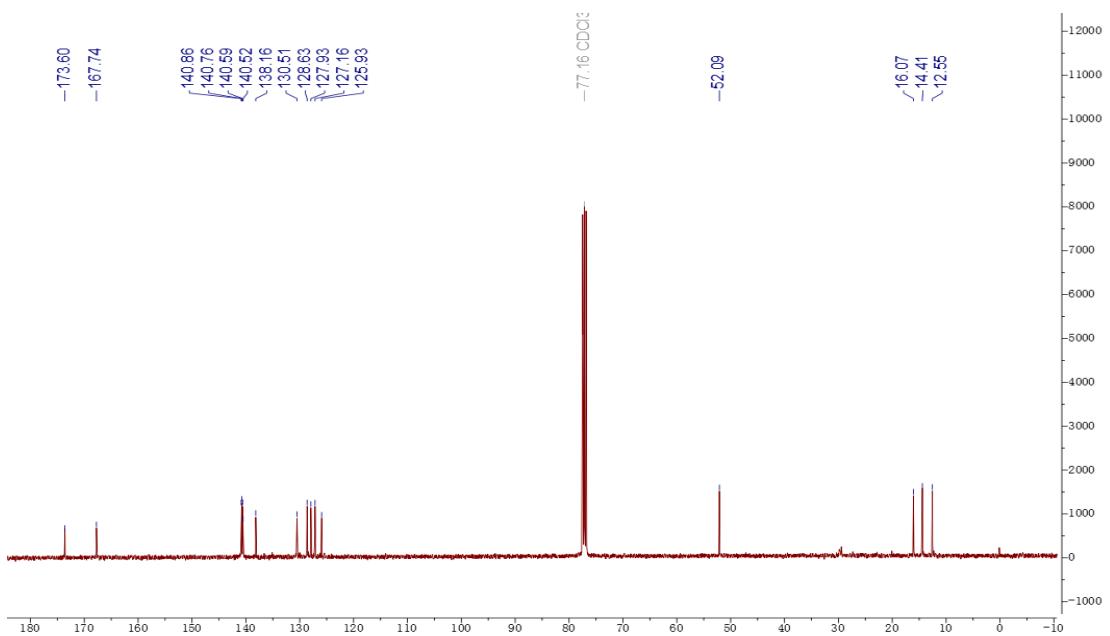


Figure S 20. ¹³C NMR spectrum of 3 in CDCl₃.

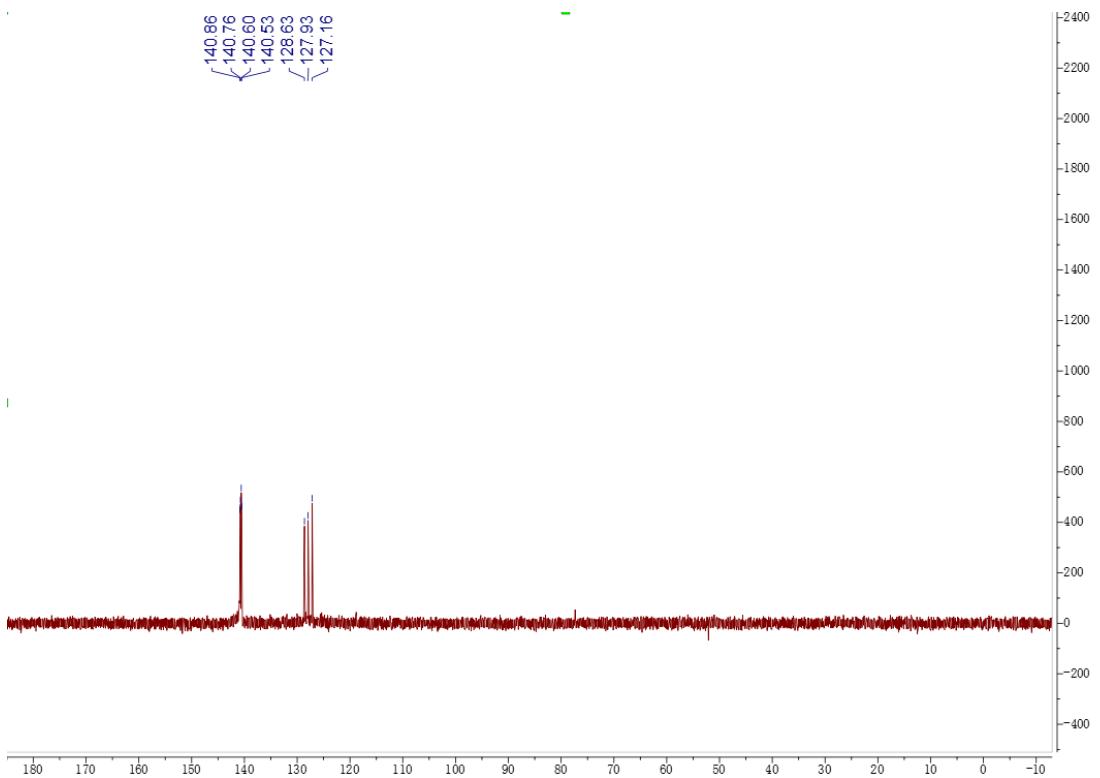


Figure S 21. DEPT-90 spectrum of 3 in CDCl₃.

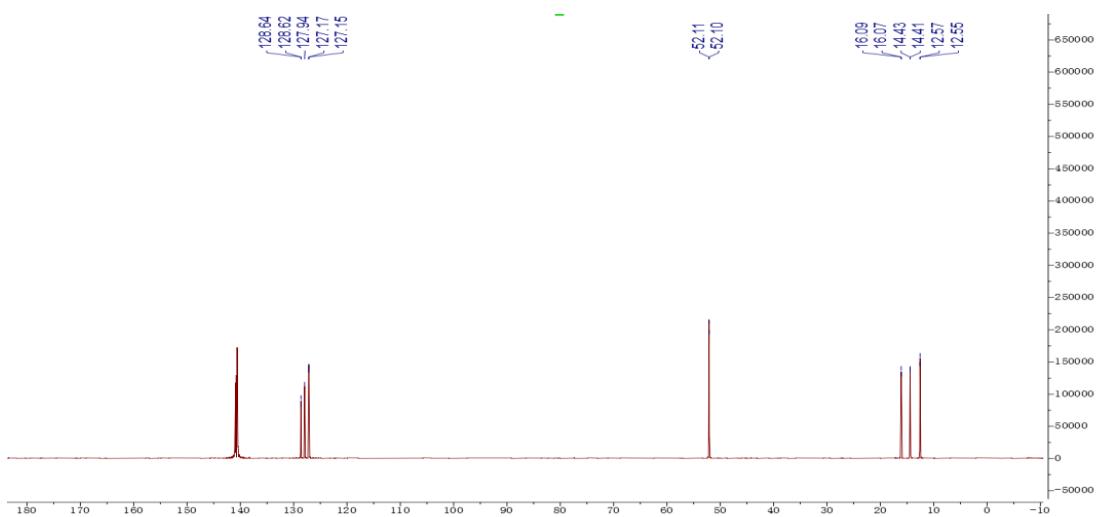


Figure S 22. DEPT-135 spectrum of 3 in CDCl_3 .

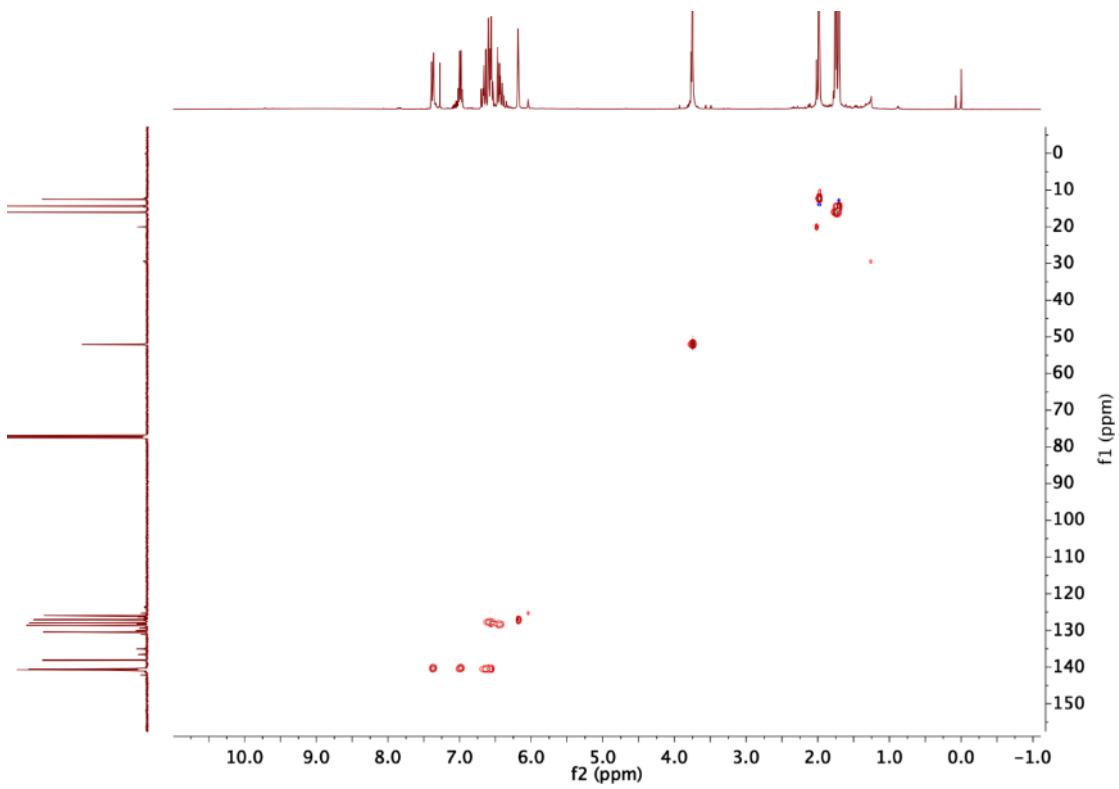


Figure S 23. HSQC spectrum of 3 in CDCl_3 .

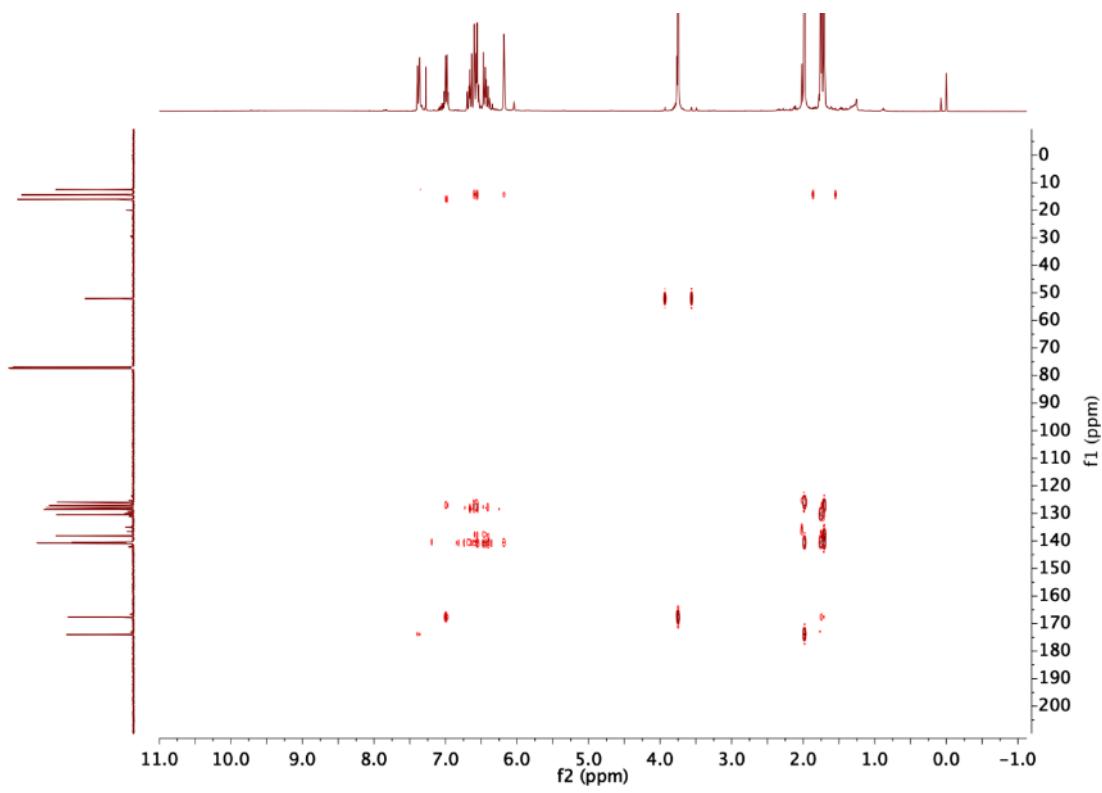


Figure S 24. HMBC spectrum of 3 in CDCl_3 .

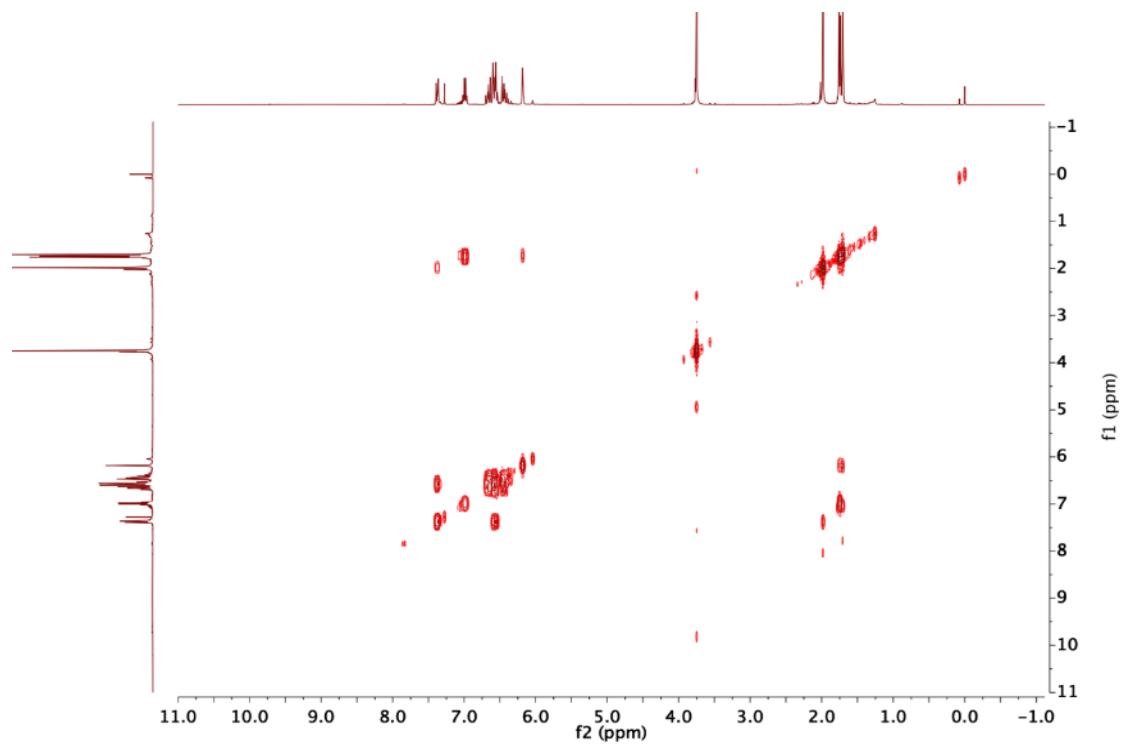
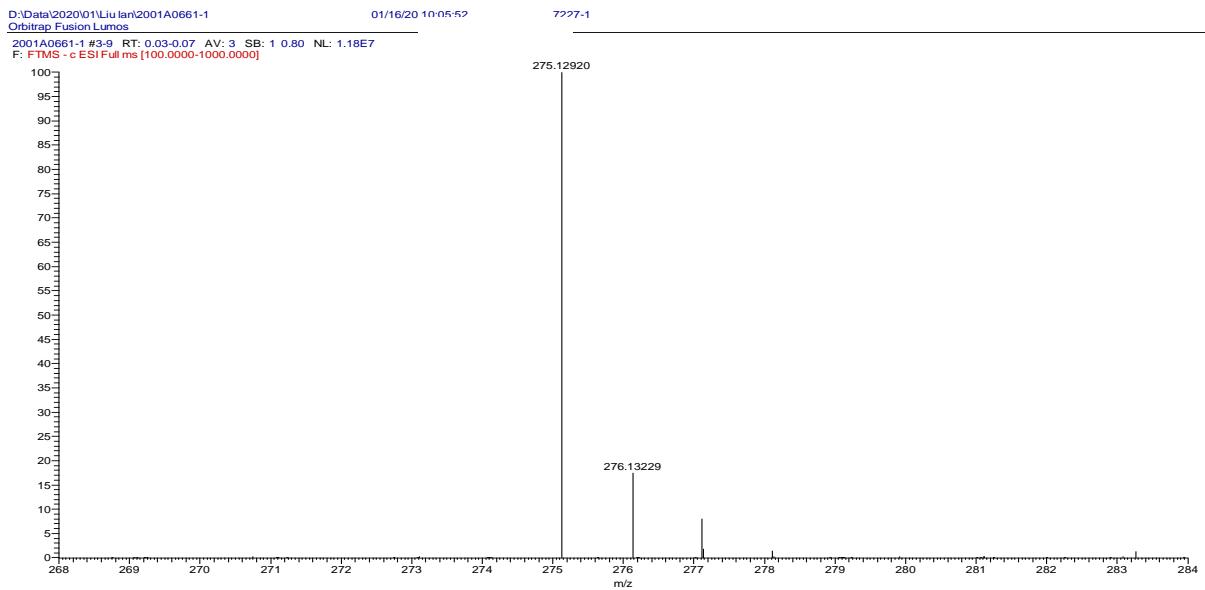


Figure S 25. ^1H - ^1H COSY spectrum of 3 in CDCl_3 .



SPECTRUM - simulation :

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
275.12920	275.12888	1.15	7.5	C16 H19 O4

Figure S 26. HR-ESIMS spectrum of 3.

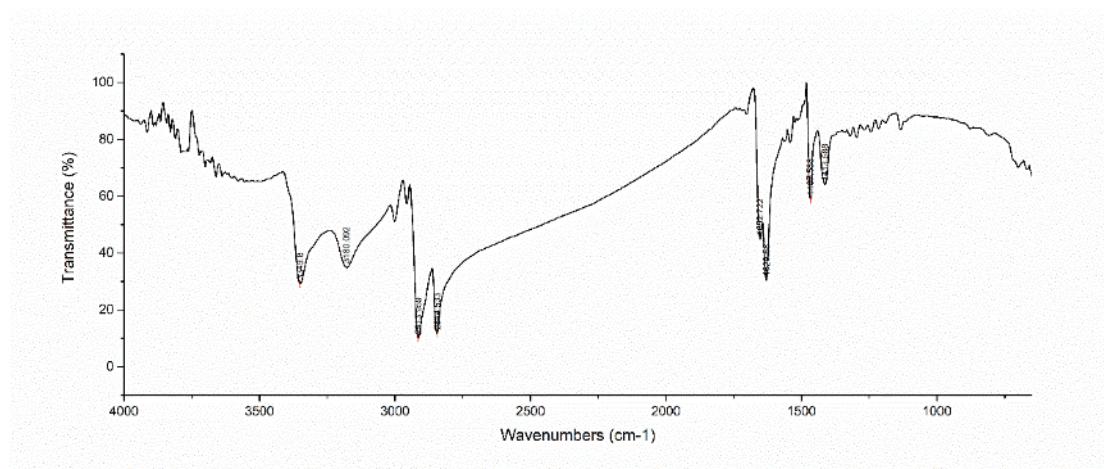


Figure S 27. IR spectrum of 3.

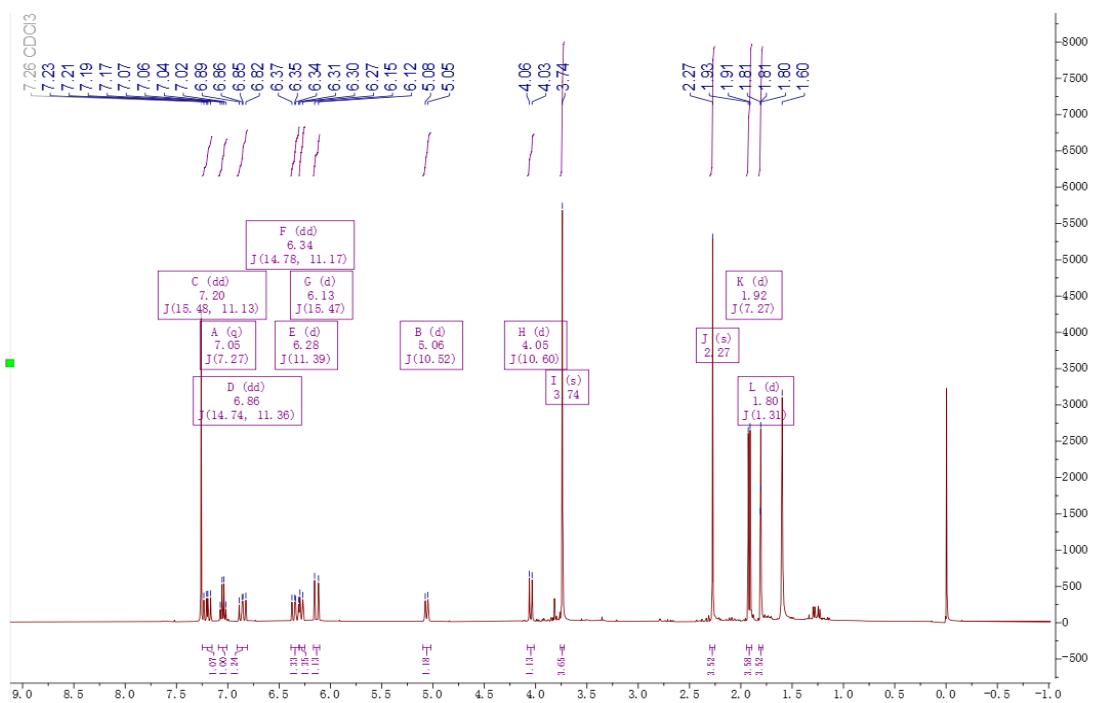


Figure S 28. ^1H NMR spectrum of **4** in CDCl_3 .

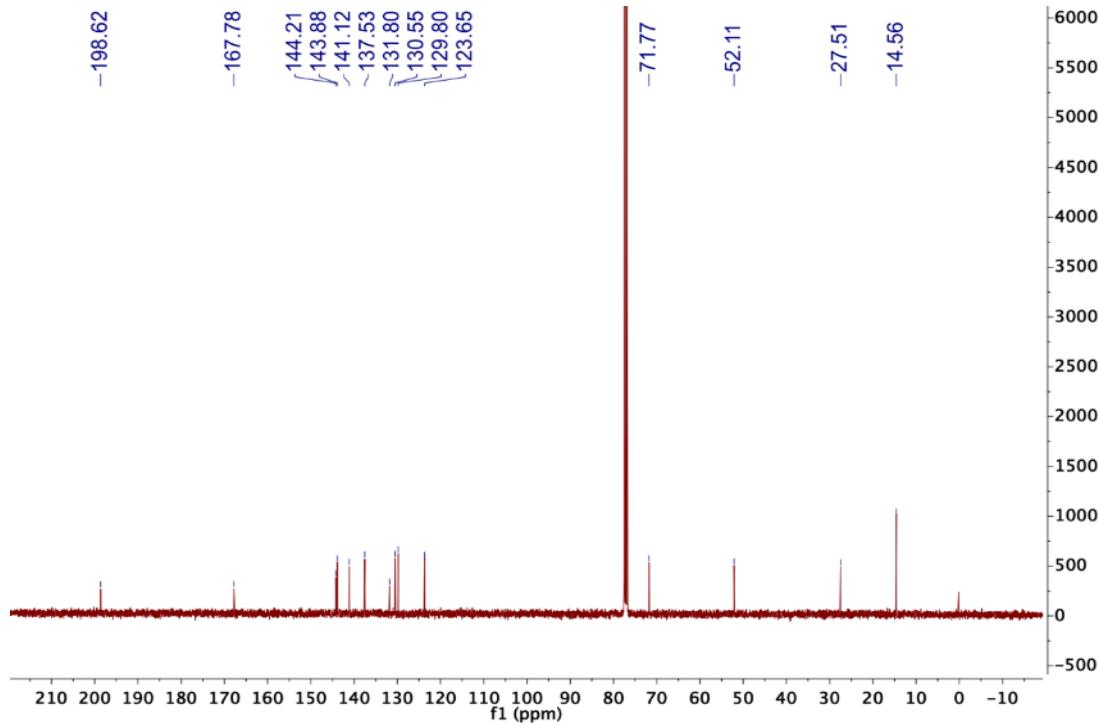


Figure S 29. ^{13}C NMR spectrum of 4 in CDCl_3 .

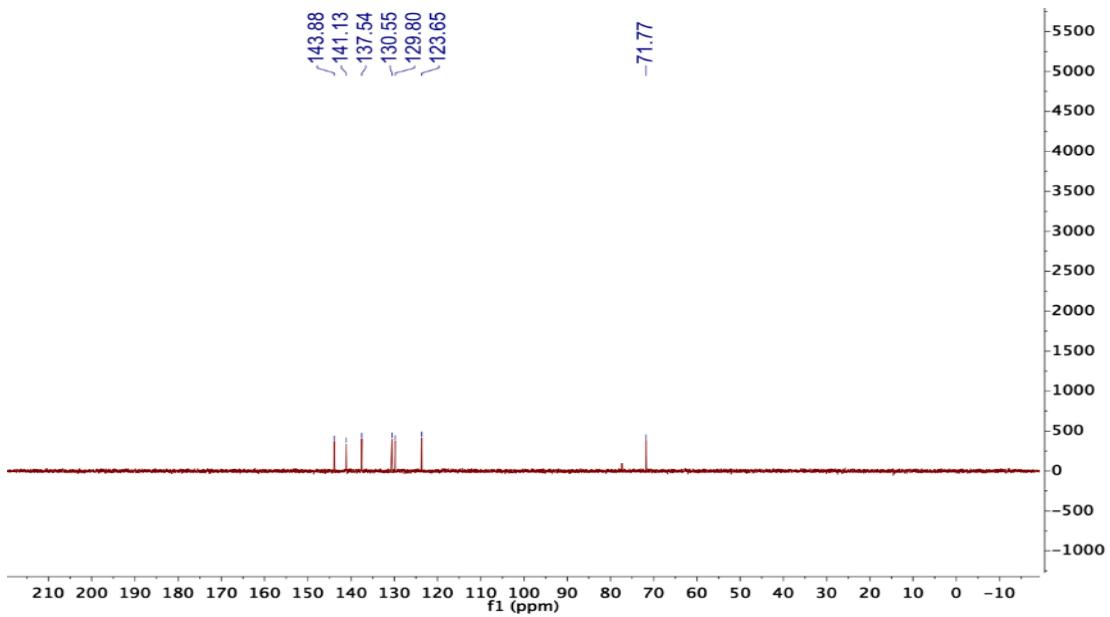


Figure S 30. DEPT-90 spectrum of 4 in CDCl_3 .

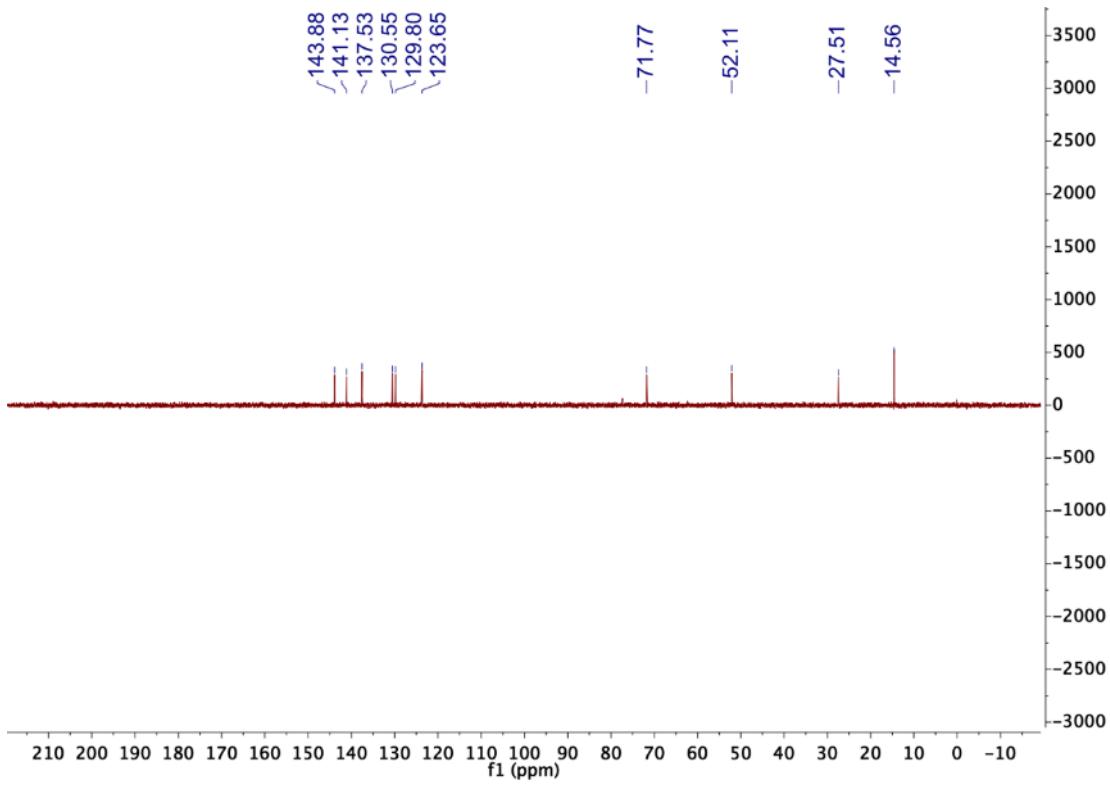


Figure S 31. DEPT-135 spectrum of 4 in CDCl_3 .

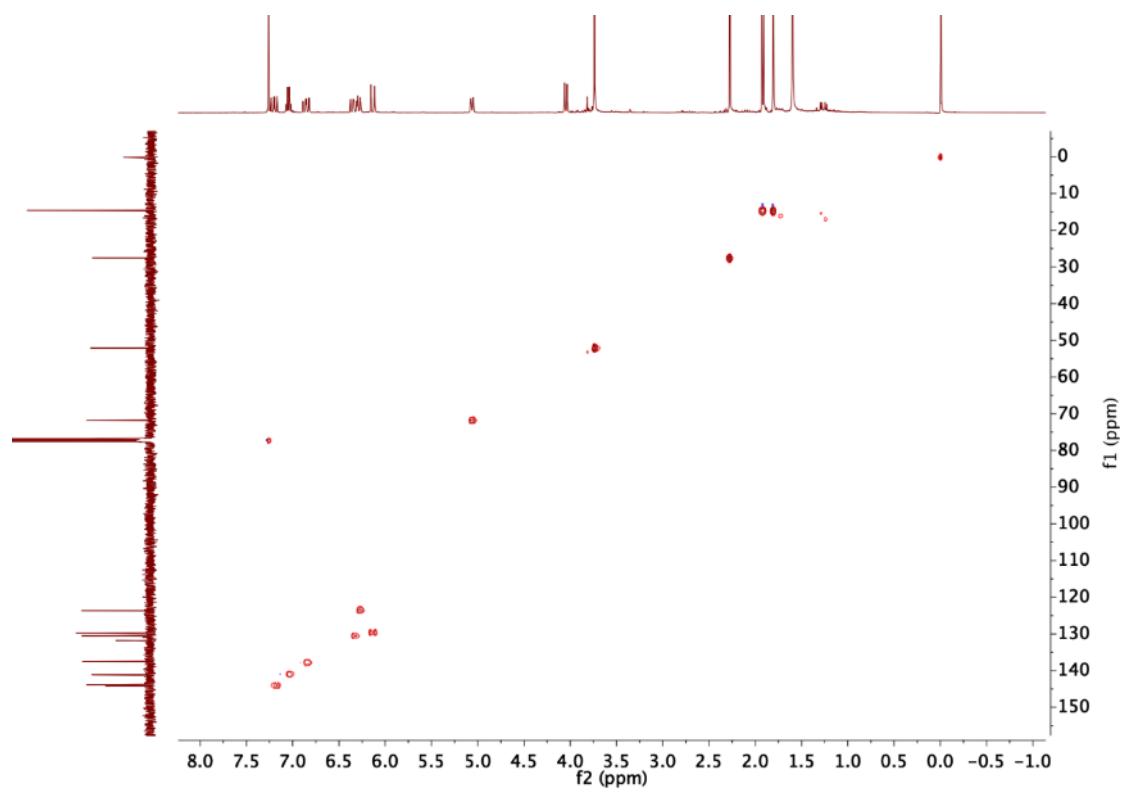


Figure S 32. HSQC spectrum of 4 in CDCl_3 .

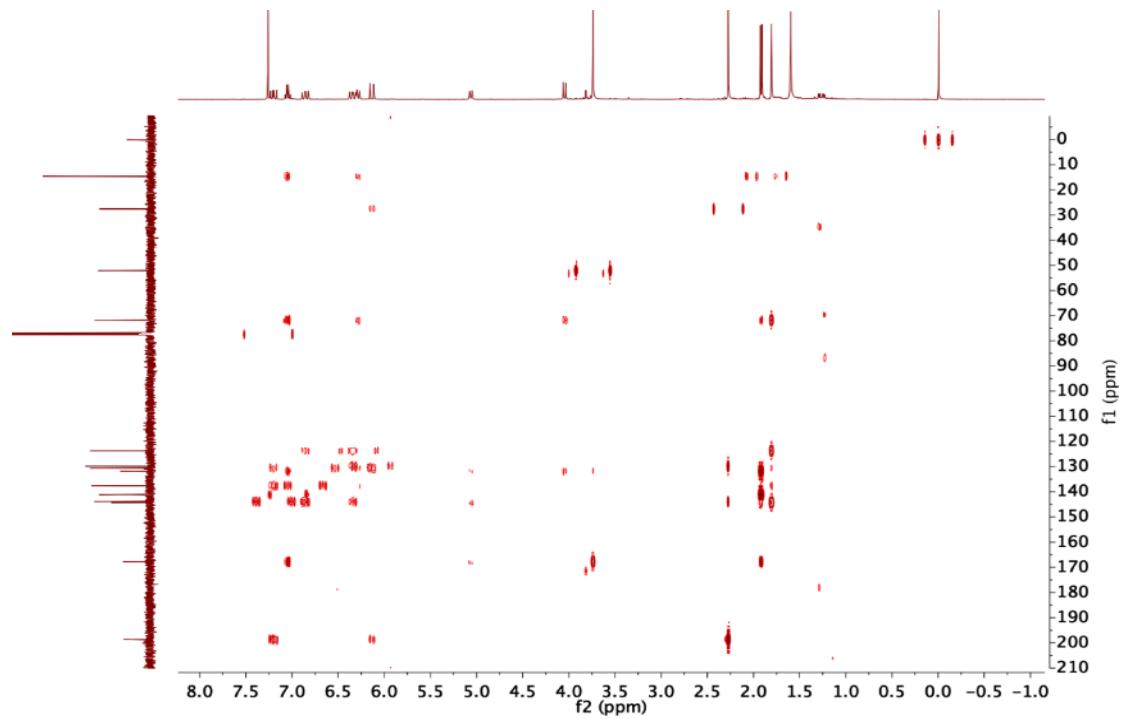


Figure S 33. HMBC spectrum of 4 in CDCl_3 .

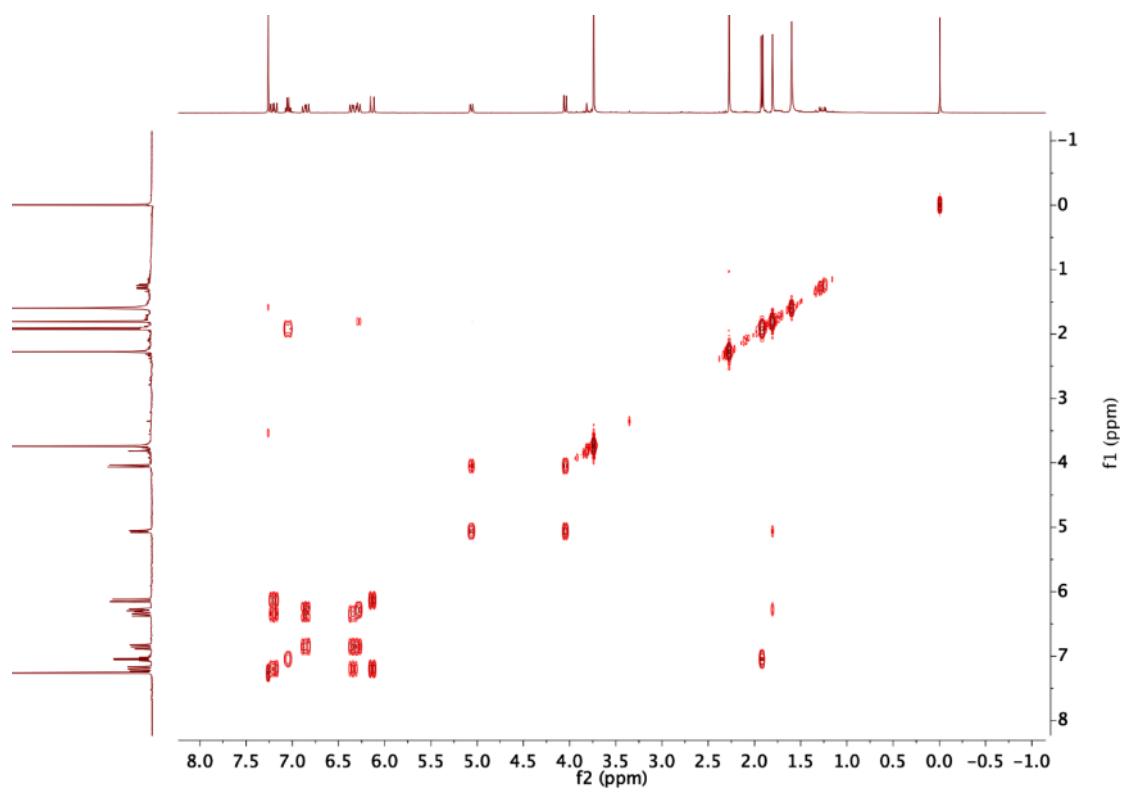


Figure S 34. ^1H - ^1H COSY spectrum of **4** in CDCl_3 .

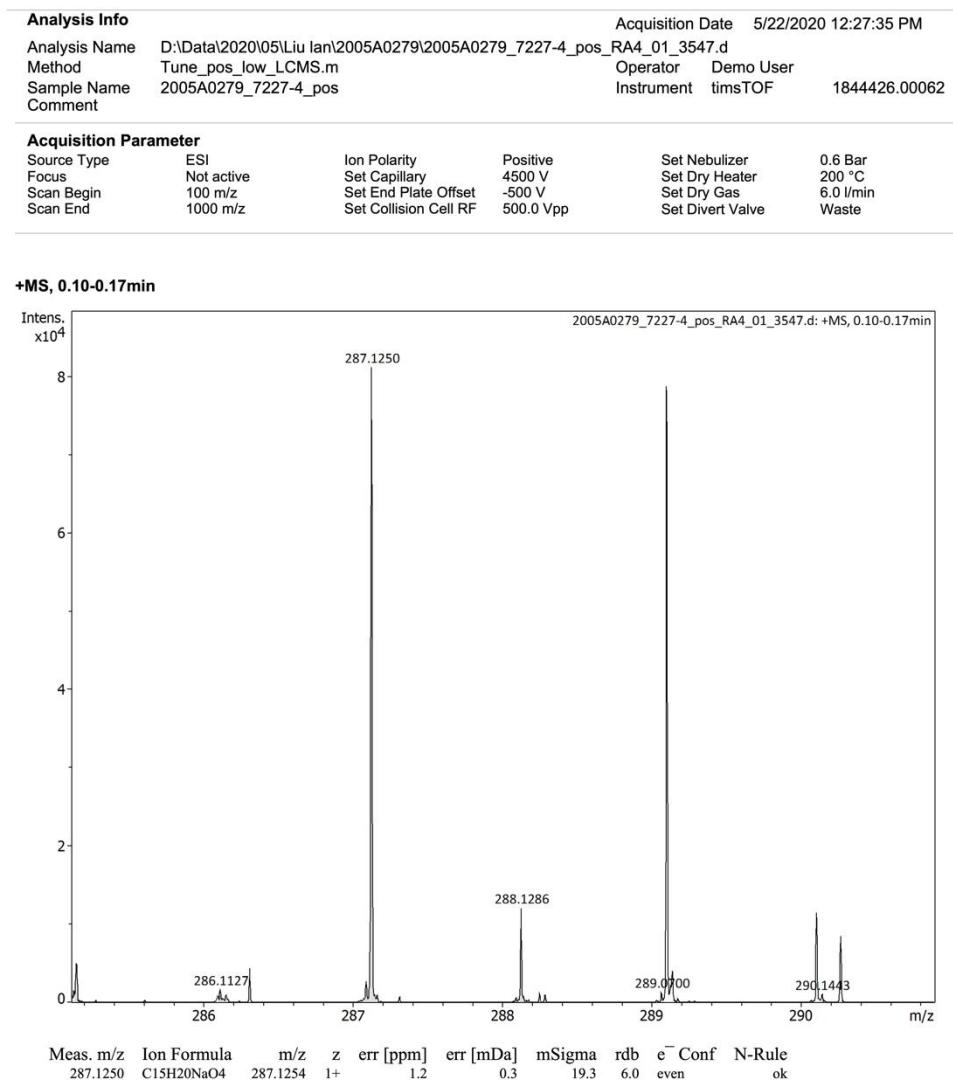


Figure S 35. HR-ESIMS spectrum of 4.

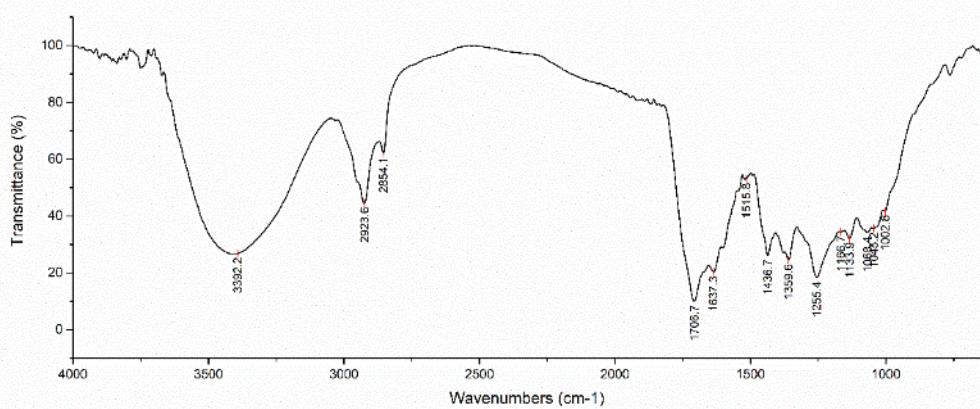


Figure S 36. IR spectrum of 4.

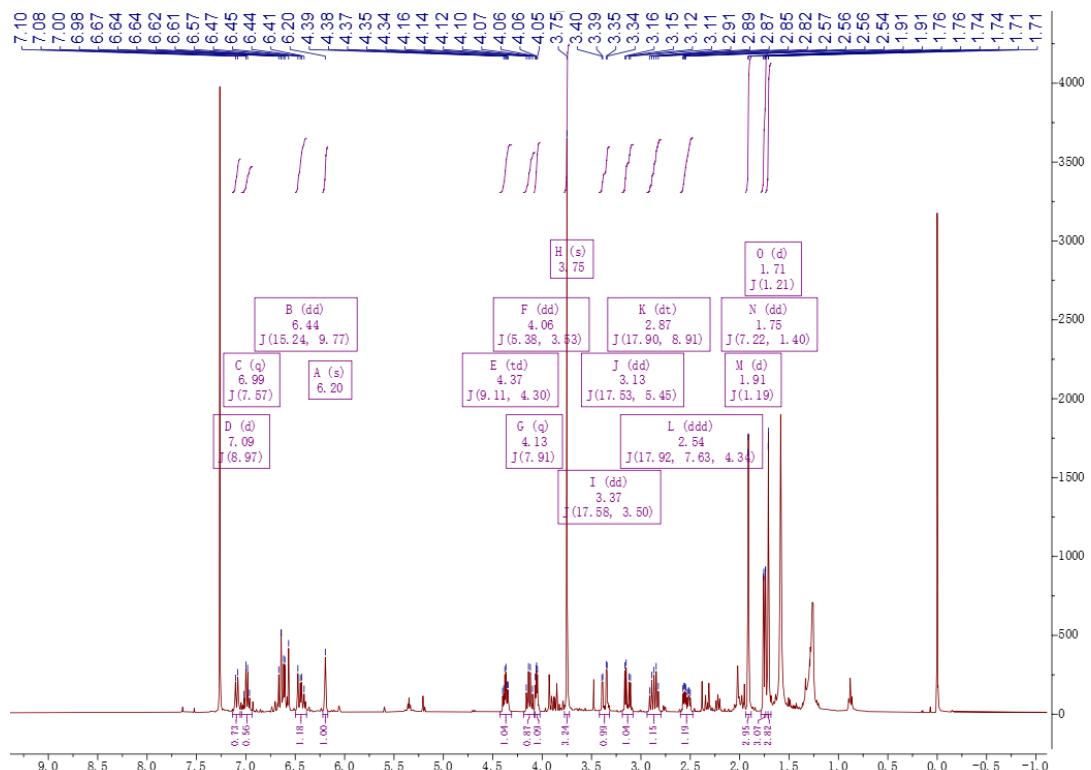


Figure S 37. ^1H NMR spectrum of 5 in CDCl_3 .

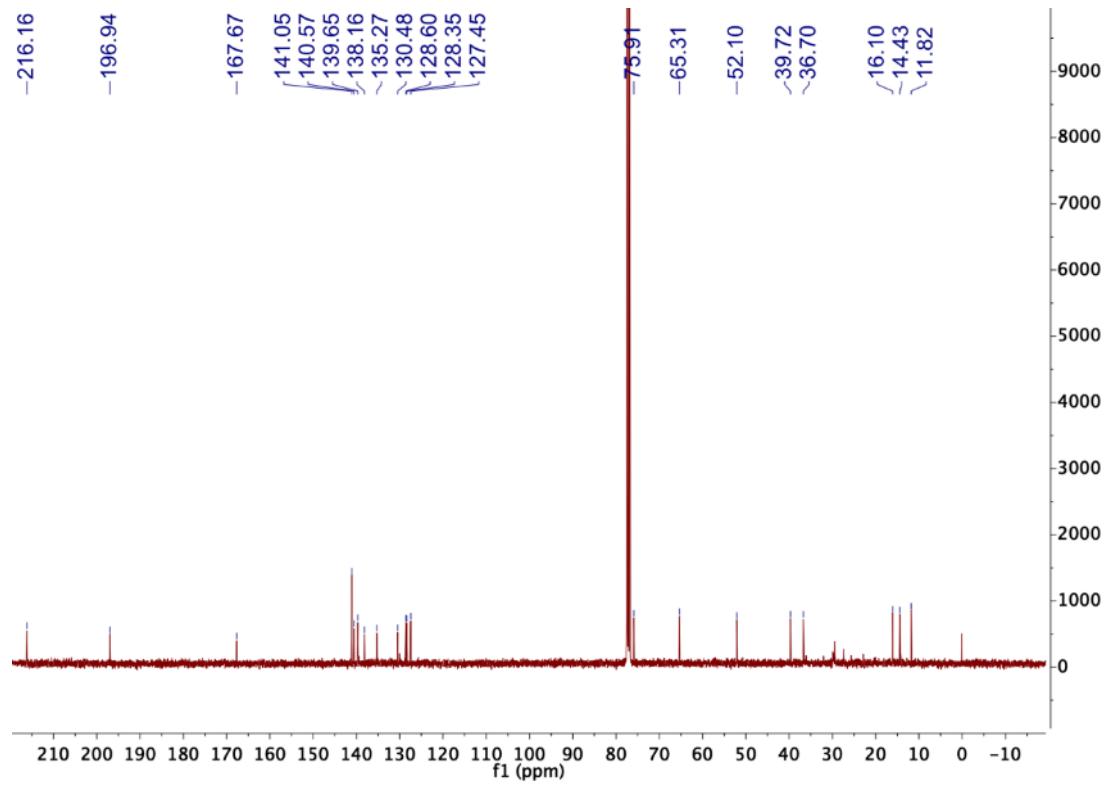


Figure S 38. ^{13}C NMR spectrum of **5** in CDCl_3 .

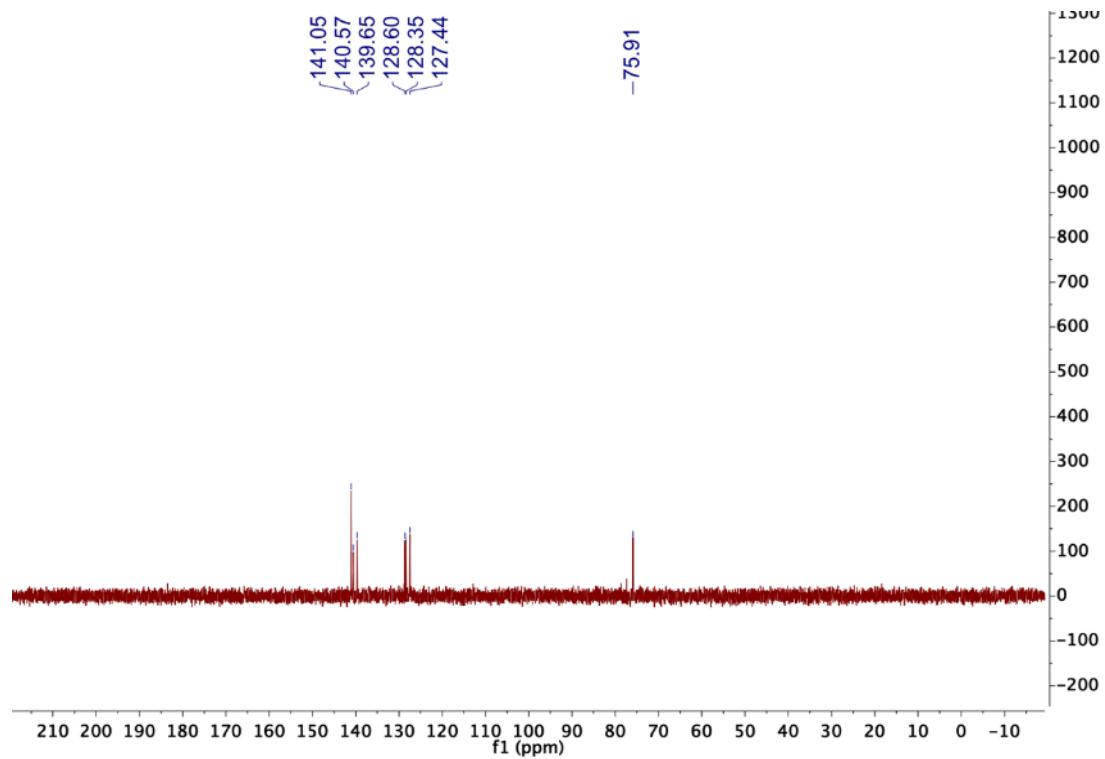


Figure S 39. DEPT-90 spectrum of **5** in CDCl_3 .

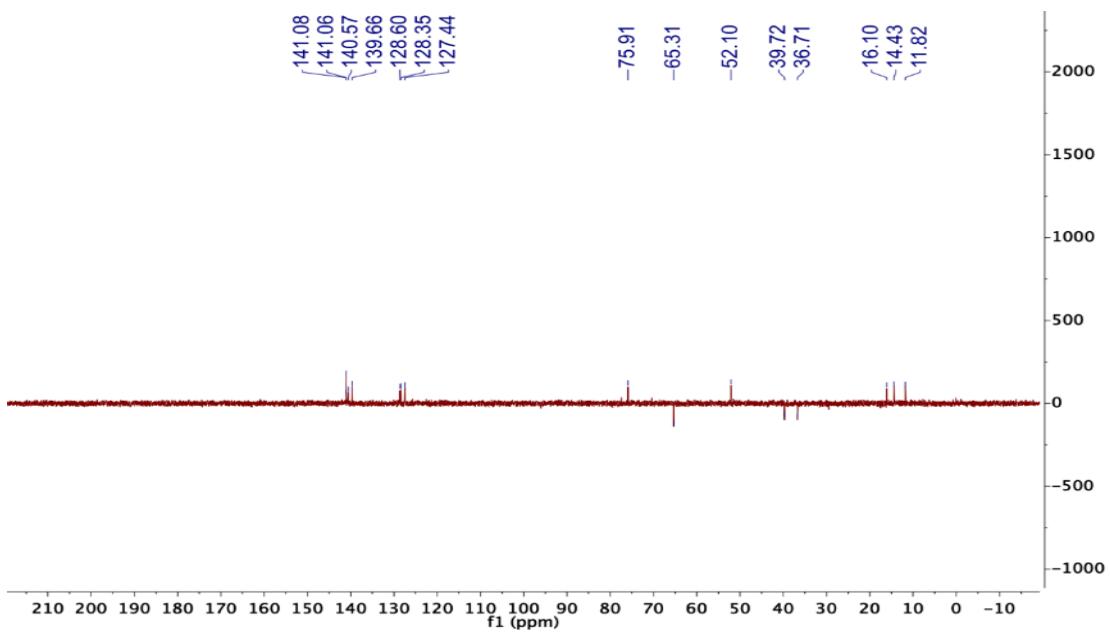


Figure S 40. DEPT-135 spectrum of **5** in CDCl_3 .

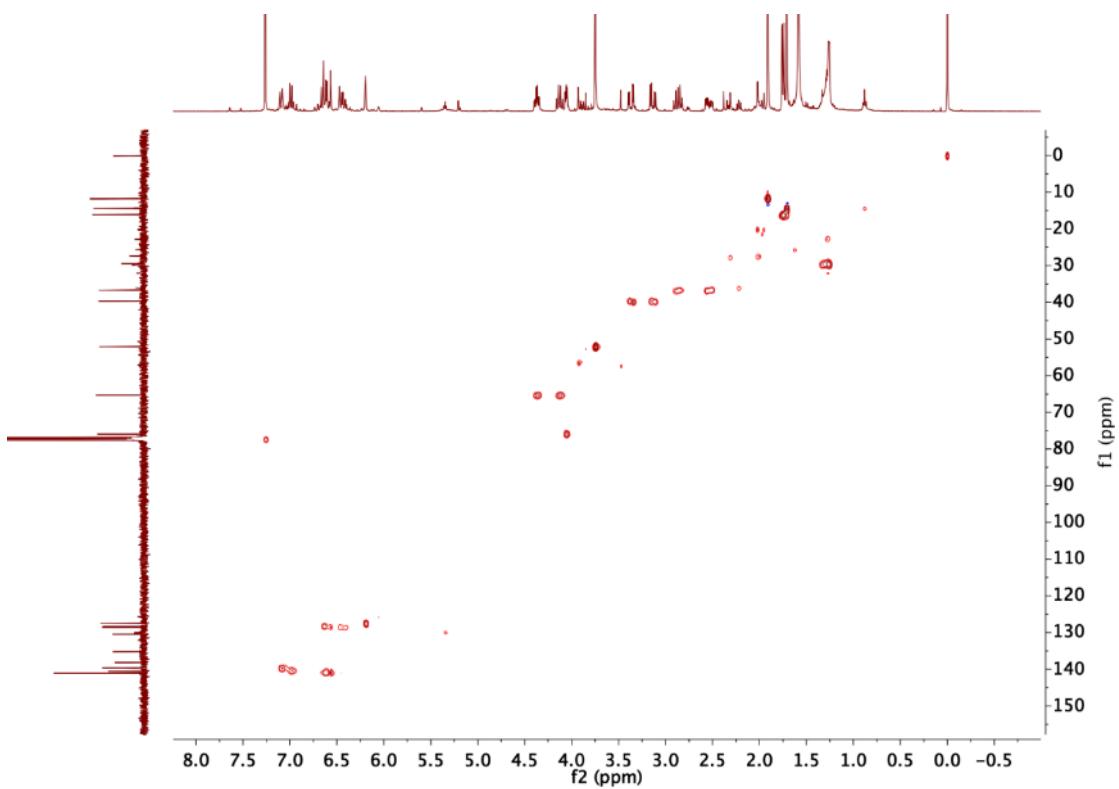


Figure S 41. HSQC spectrum of **5** in CDCl_3 .

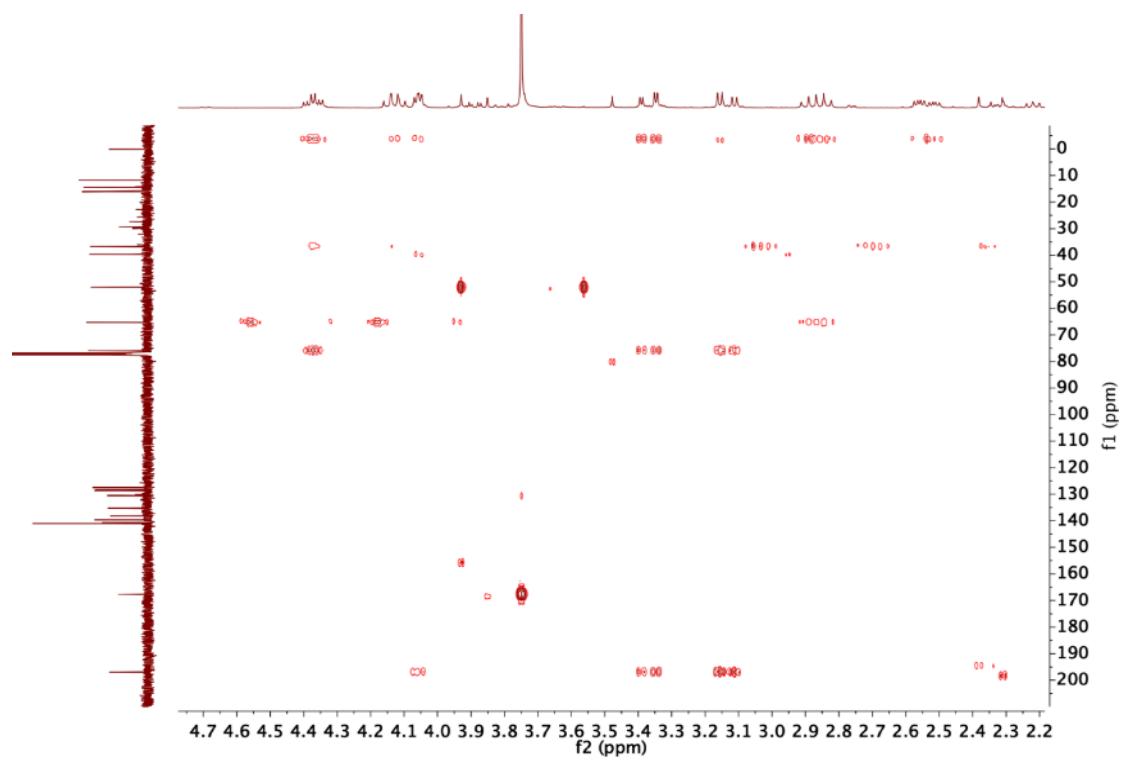


Figure S 42. HMBC spectrum of 5 in CDCl_3 .

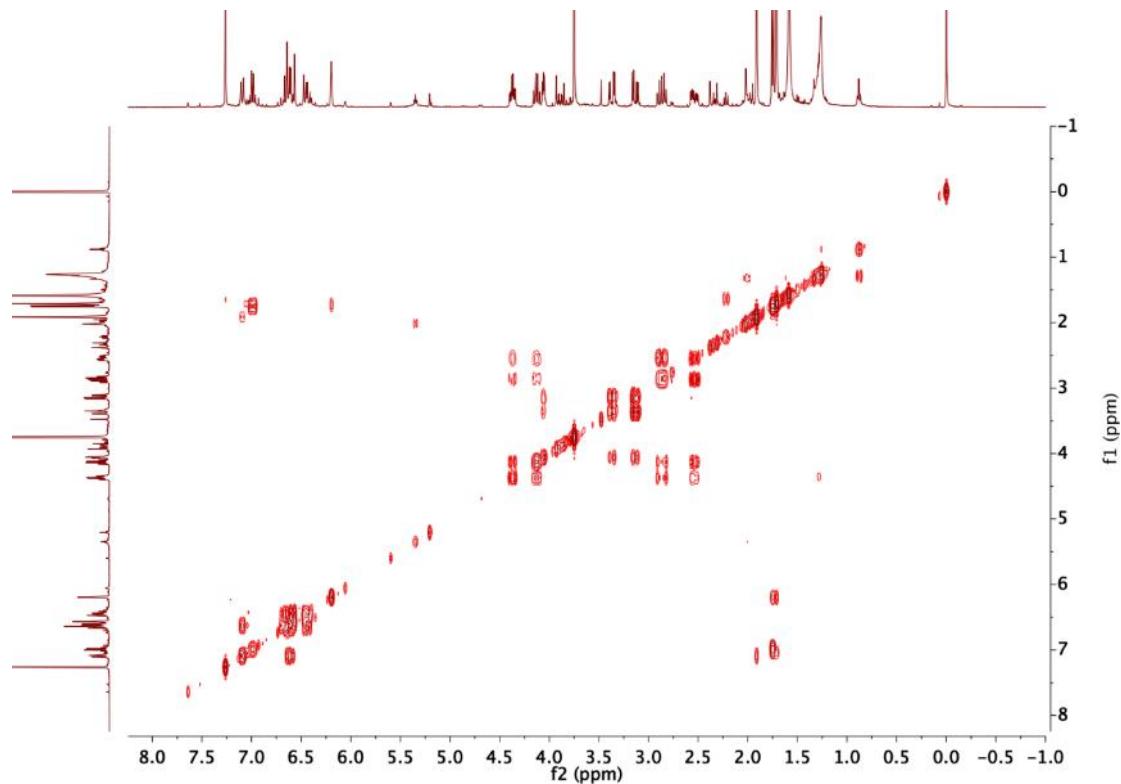
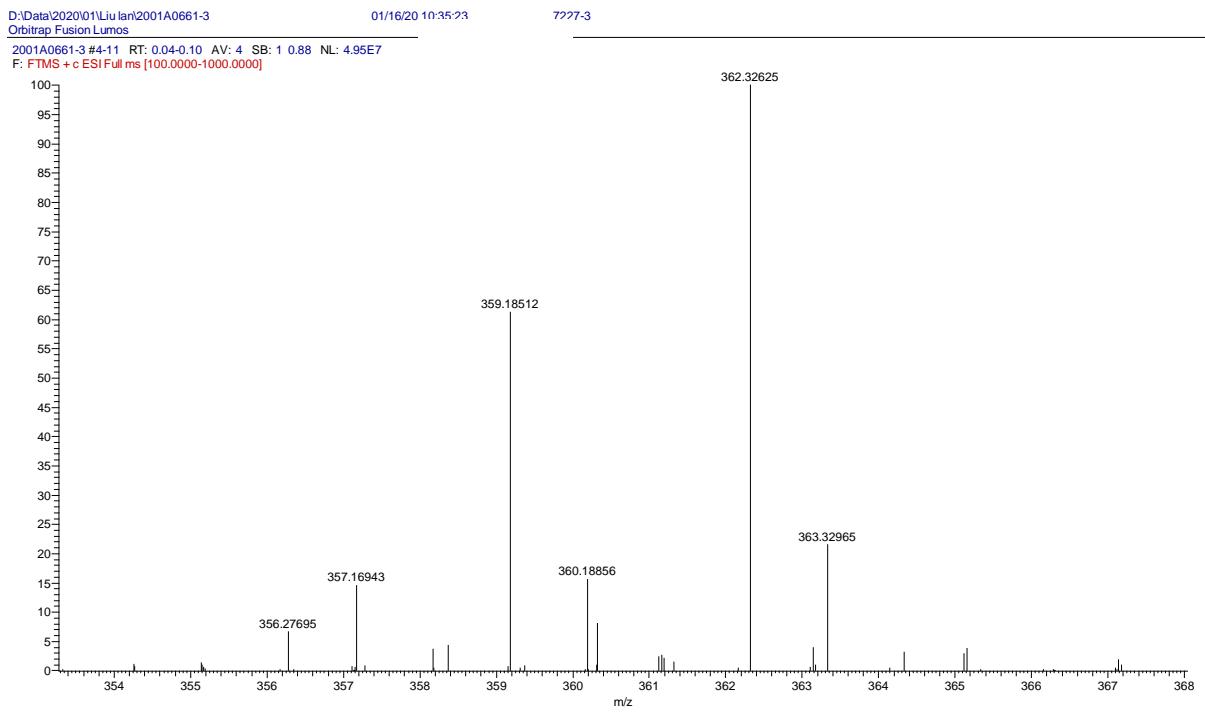


Figure S 43. ^1H - ^1H COSY spectrum of 5 in CDCl_3 .



SPECTRUM - simulation :

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
359.18512	359.1853	-0.50	8.5	C21 H27 O5

Figure S 44. HR-ESIMS spectrum of 5.

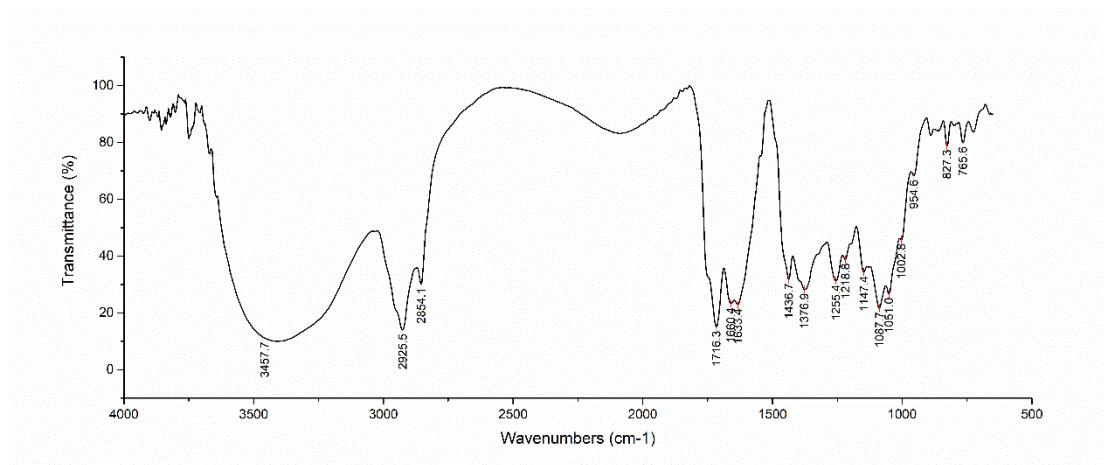


Figure S 45. IR spectrum of 5.

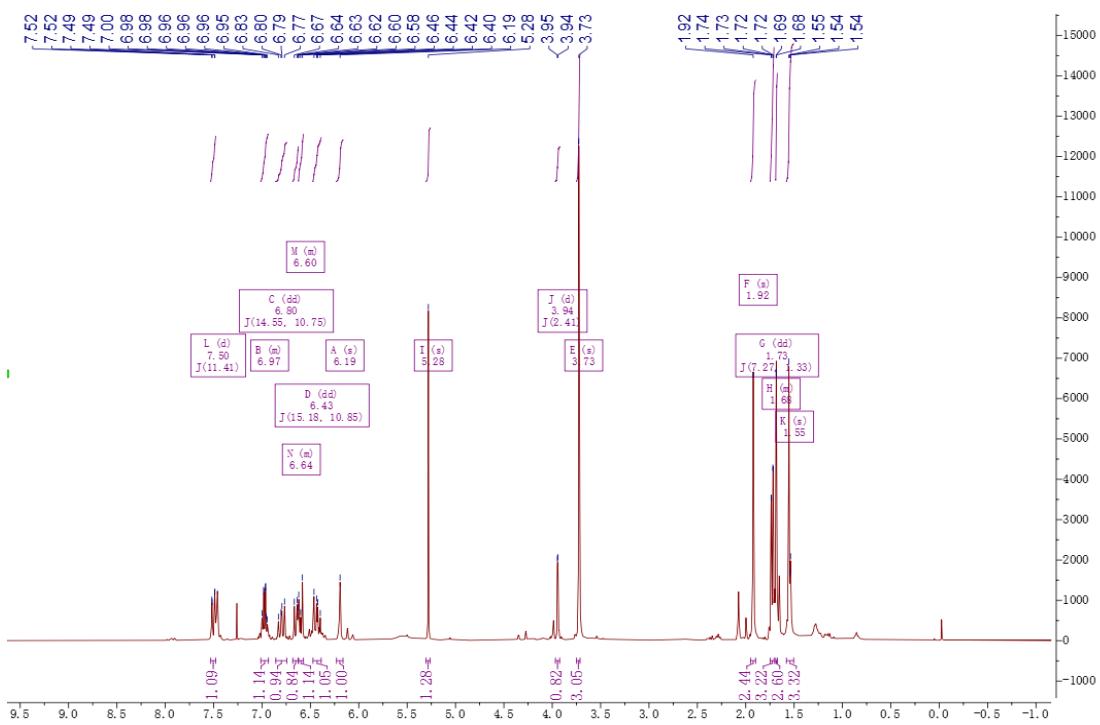


Figure S 46. ^1H NMR spectrum of **6** in CDCl_3 .

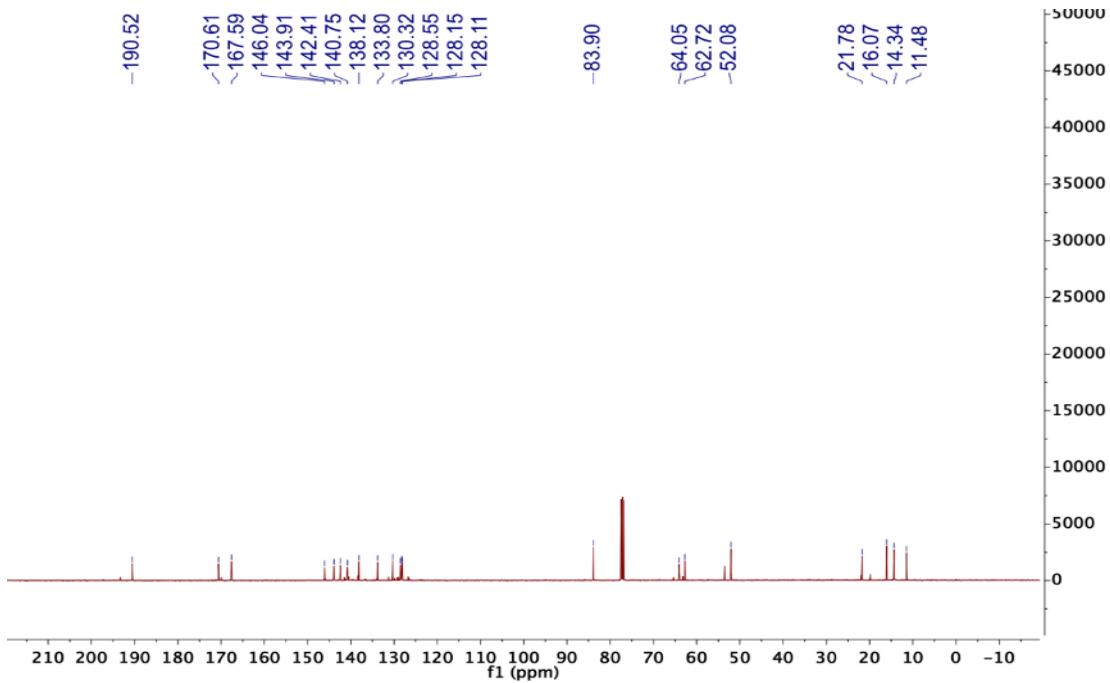


Figure S 47. ^{13}C NMR spectrum of **6** in CDCl_3 .

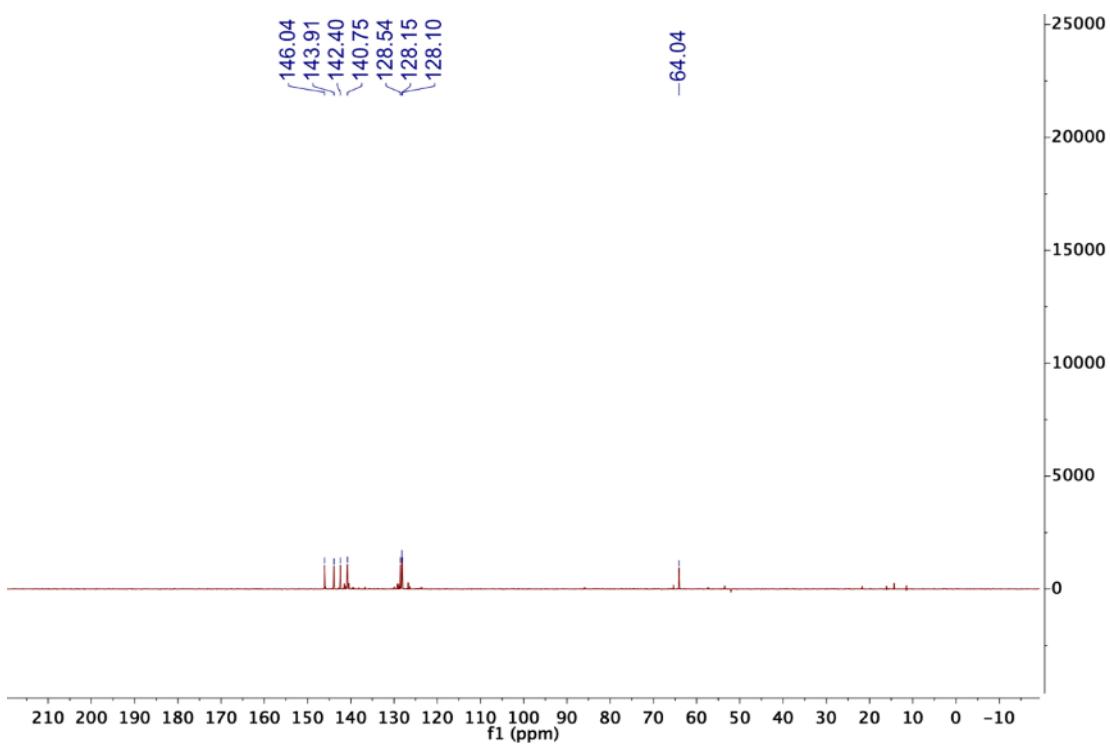


Figure S 48. DEPT-90 spectrum of 6 in CDCl₃.

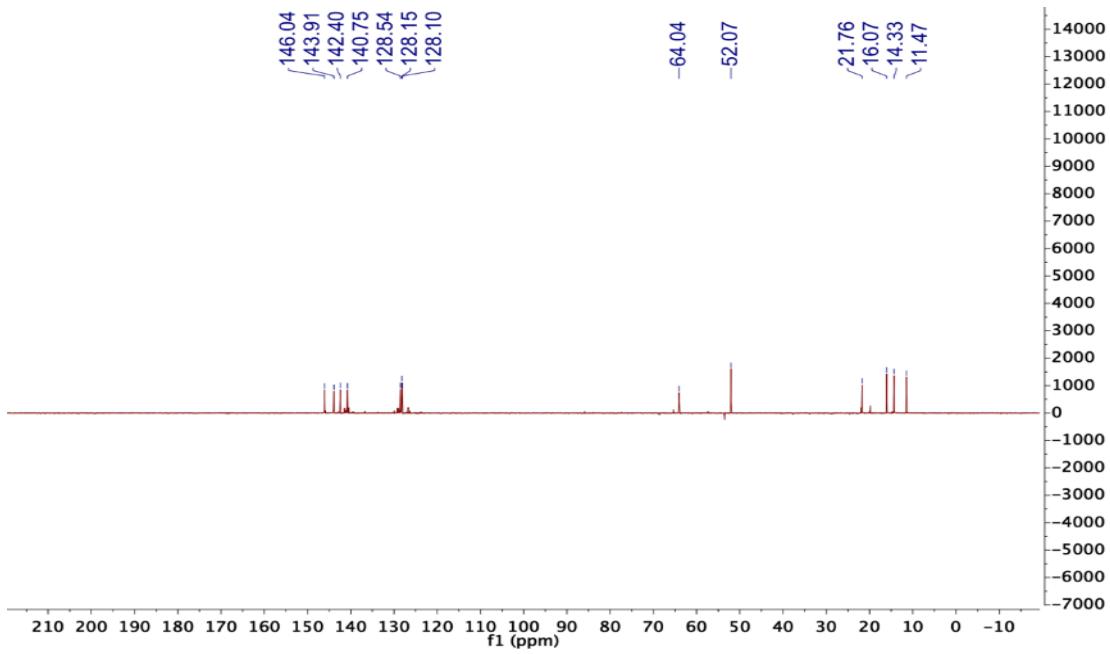


Figure S 49. DEPT-135 spectrum of 6 in CDCl₃.

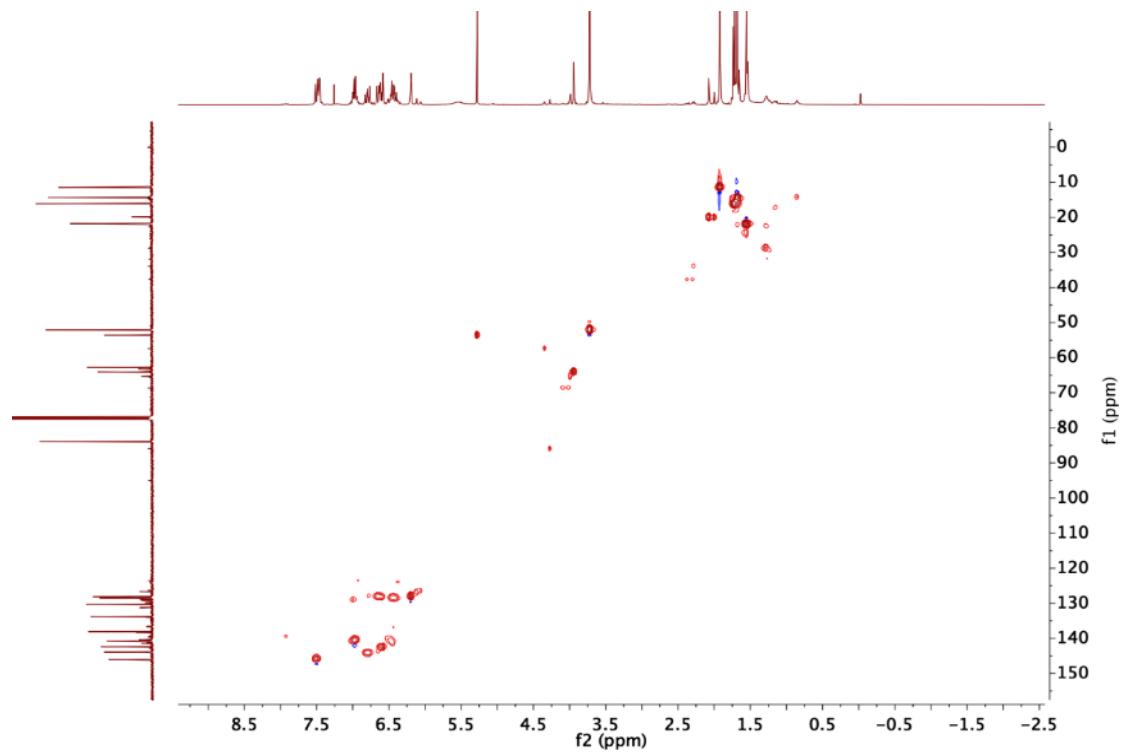


Figure S 50. HSQC spectrum of 6 in CDCl_3 .

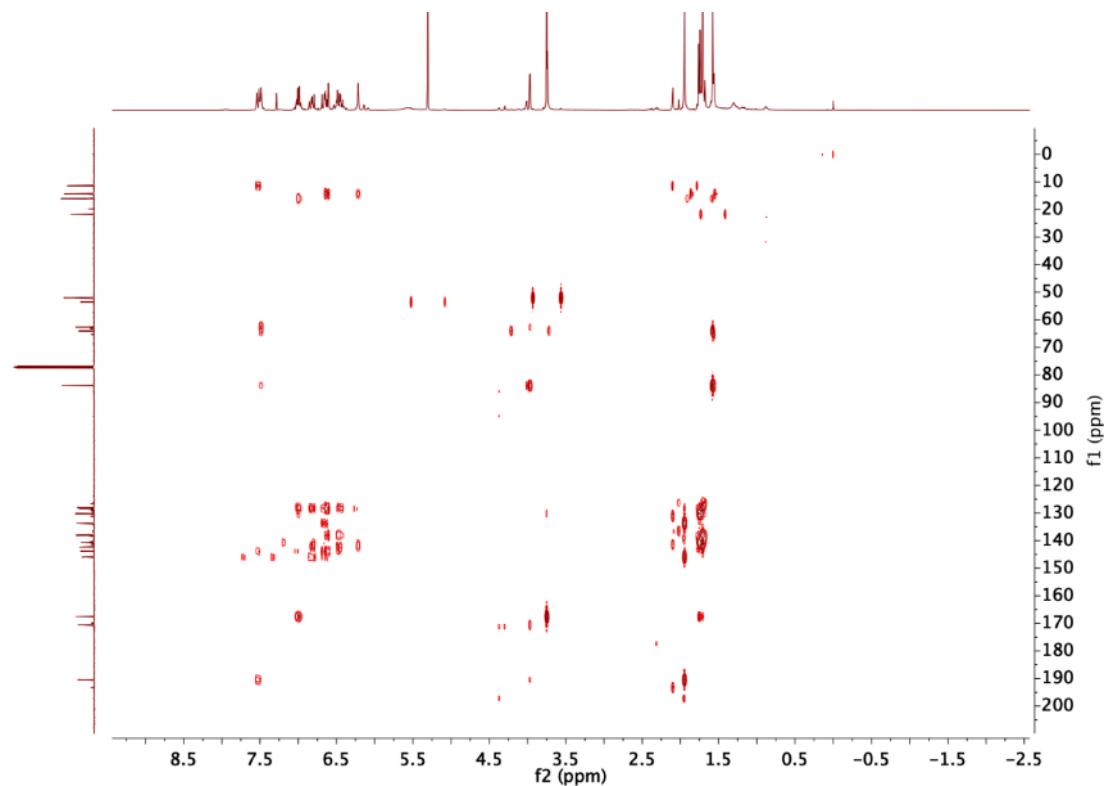


Figure S 51. HMBC spectrum of 6 in CDCl_3 .

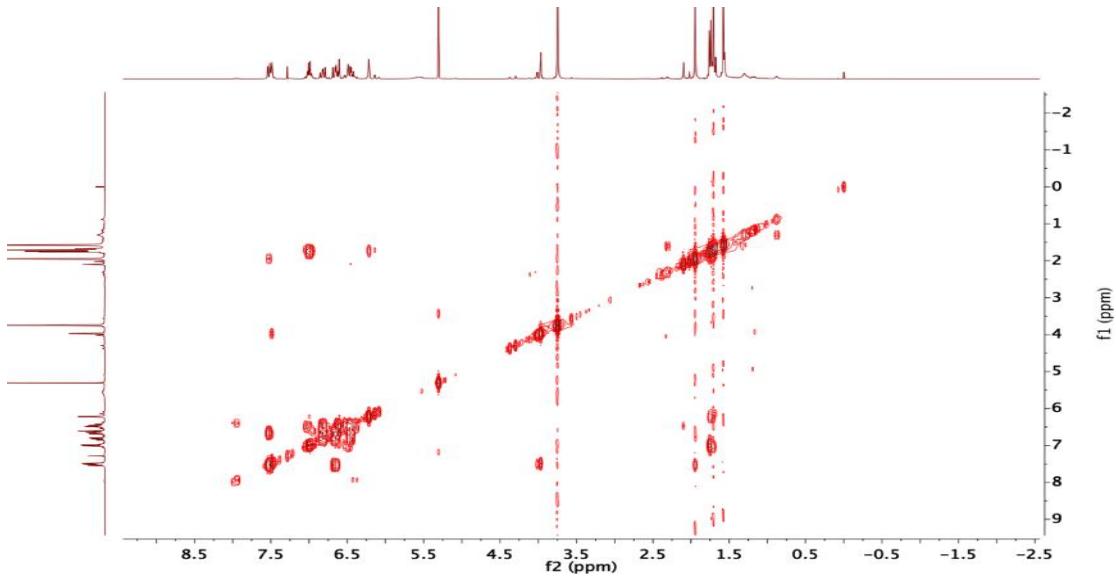
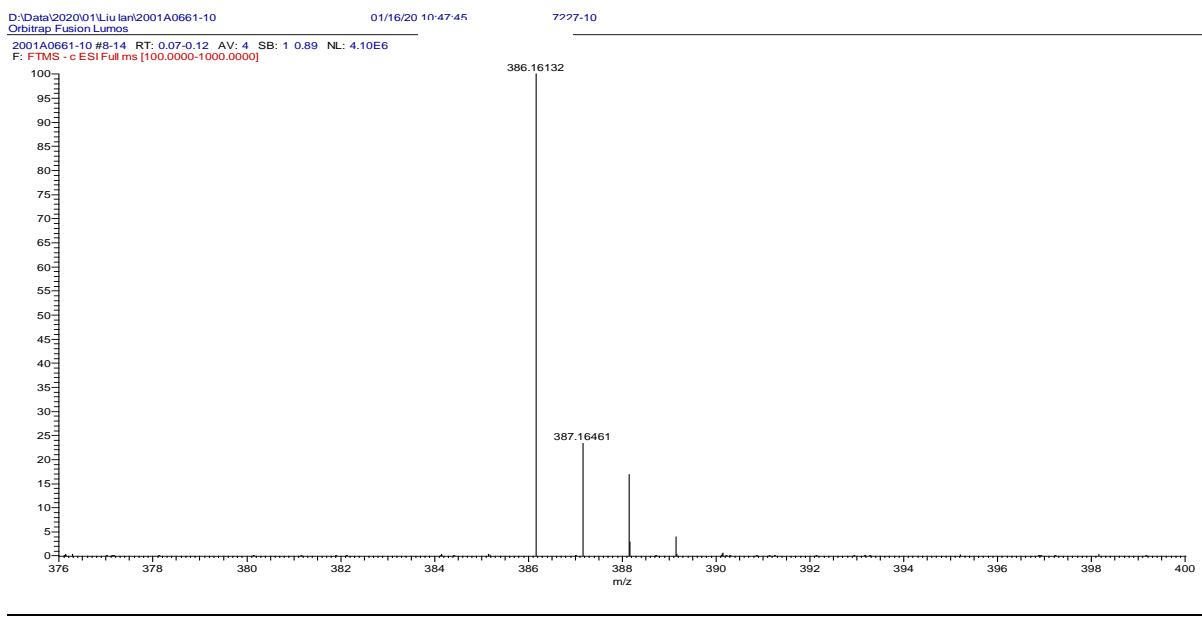


Figure S 52. ^1H - ^1H COSY spectrum of **6** in CDCl_3 .



SPECTRUM -
simulation :

m/z	Theo. Mass	Delta (ppm)	RDB	equiv.	Composition
386.16132	386.16091	1.06	10.5		C21 H24 O6 N

Figure S 53. HR-ESIMS spectrum of **6**.

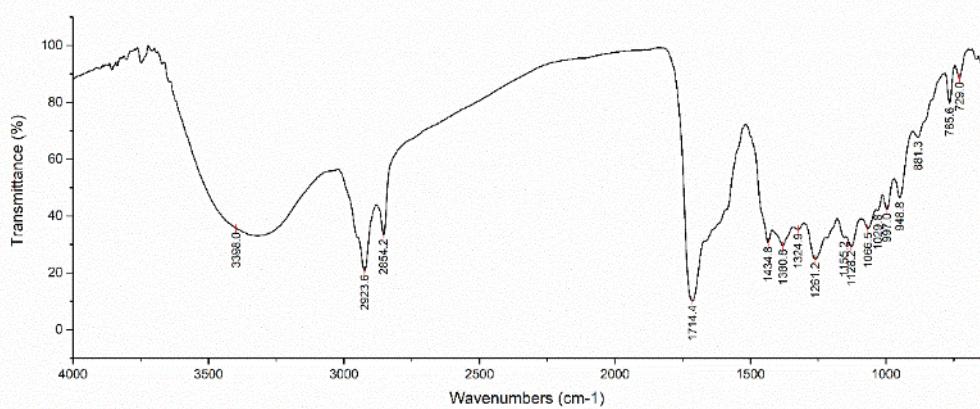


Figure S 54. IR spectrum of 6.

Table S1. Energy Analysis for the Conformers of (5*S*)-2.

Compound	E(Hartree)	E(kcal/mol)	rel.E(kcal/mol)	Qi	Boltzmann dist
2-a	-652.338	-409348	0	1	0.750132
2-b	-652.335	-409346	2.170371	0.025589	0.019195
2-c	-652.334	-409345	2.87516	0.007782	0.005838
2-d	-652.337	-409348	0.713406	0.299727	0.224835

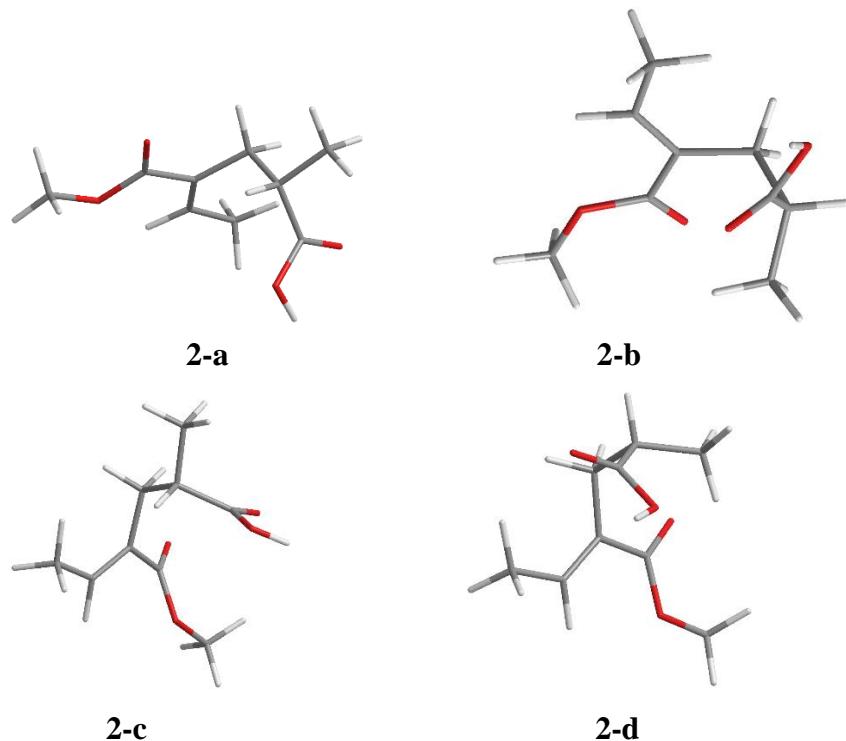
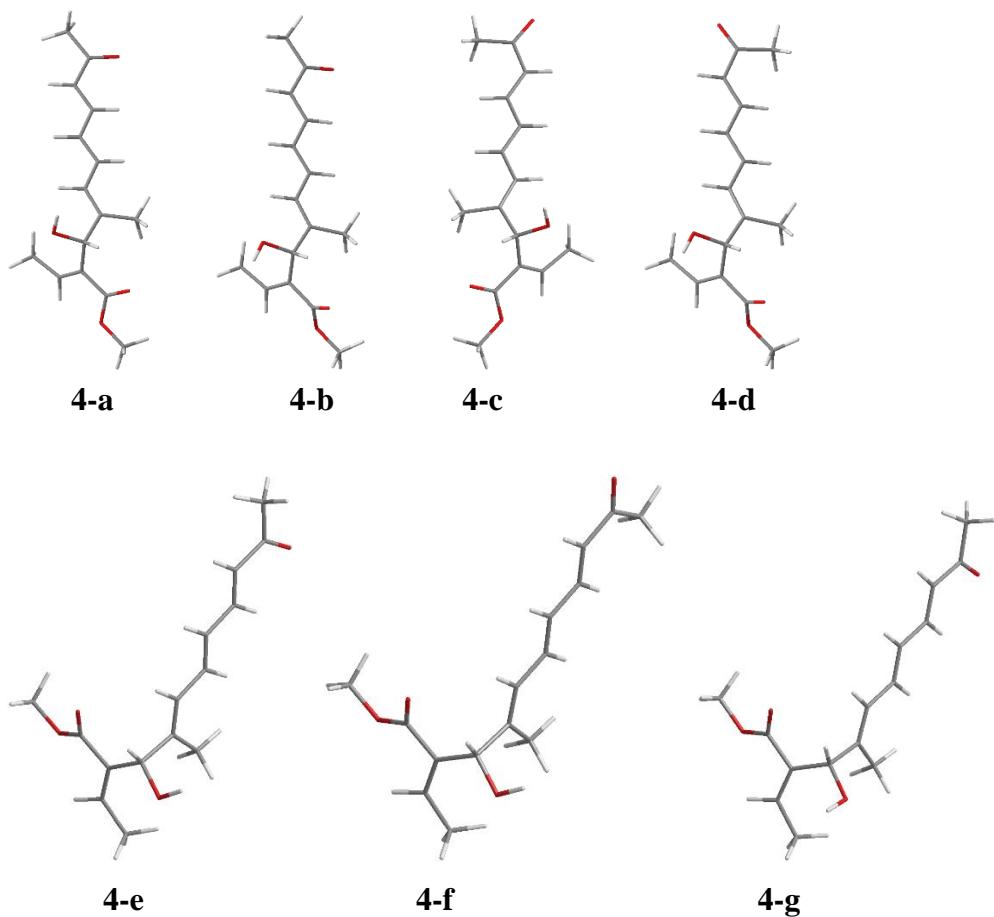


Figure S 55. The optimized low energy conformers of 2.

Table S2. Energy Analysis for the Conformers of (4S)-4.

	E(Hartree)	E(kcal/mol)	rel.E(kcal/mol)	Qi	Boltzmann dist
4-a	-884.534	-555053	0	1	0.072528
4-b	-884.534	-555053	-0.13286	1.251554	0.090773
4-c	-884.533	-555053	0.339281	0.563822	0.040893
4-d	-884.533	-555053	0.193439	0.721298	0.052314
4-e	-884.534	-555054	-0.40674	1.987644	0.14416
4-f	-884.534	-555054	-0.52816	2.440049	0.176972
4-g	-884.535	-555054	-0.57549	2.643116	0.1917
4-h	-884.535	-555054	-0.68504	3.180275	0.230659



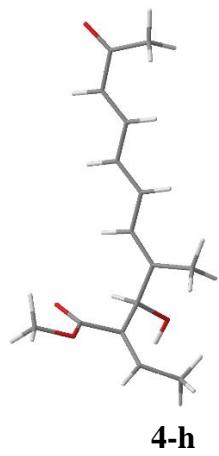
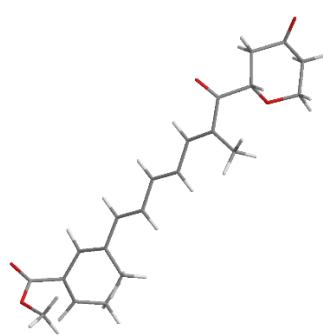


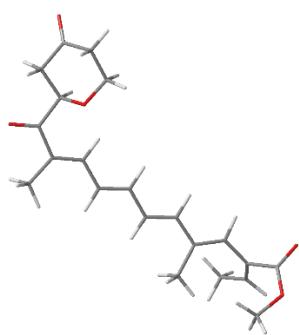
Figure S 56. The optimized low energy conformers of 4.

Table S3. Energy Analysis for the Conformers of (13S)-5.

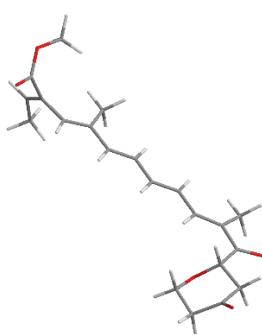
	E(Hartree)	E(kcal/mol)	rel.E(kcal/mol)	Qi	Boltzmann dist
5-a	-1192	-747992	0	1	0.066811
5-b	-1192	-747992	0.43718	0.477897	0.031929
5-c	-1192	-747991	1.224158	0.126502	0.008452
5-d	-1192	-747991	1.62048	0.064774	0.004328
5-e	-1192	-747992	0.256187	0.648769	0.043345
5-f	-1192	-747992	0.271373	0.632342	0.042247
5-g	-1192	-747993	-1.05911	5.981959	0.399658
5-h	-1192	-747993	-1.03904	5.782611	0.386339
5-i	-1192	-747991	0.814131	0.25284	0.016892



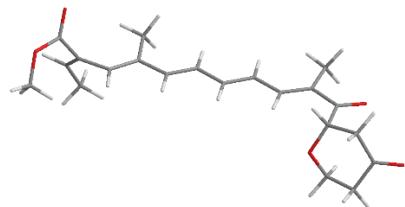
5-a



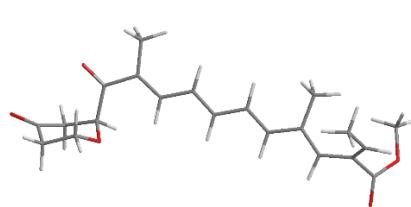
5-b



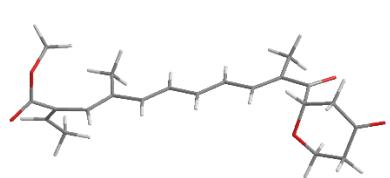
5-c



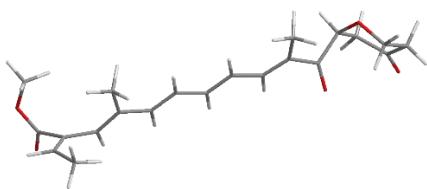
5-d



5-e



5-f



5-g

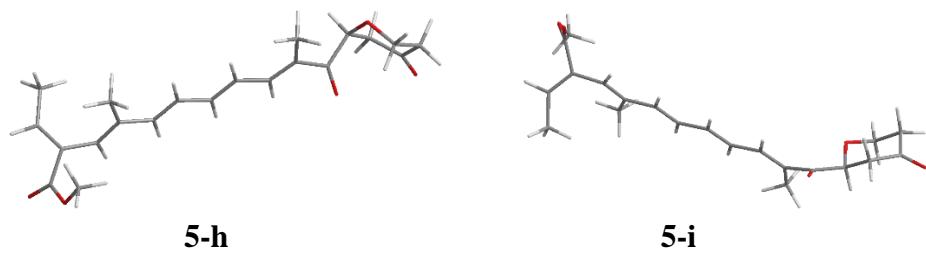
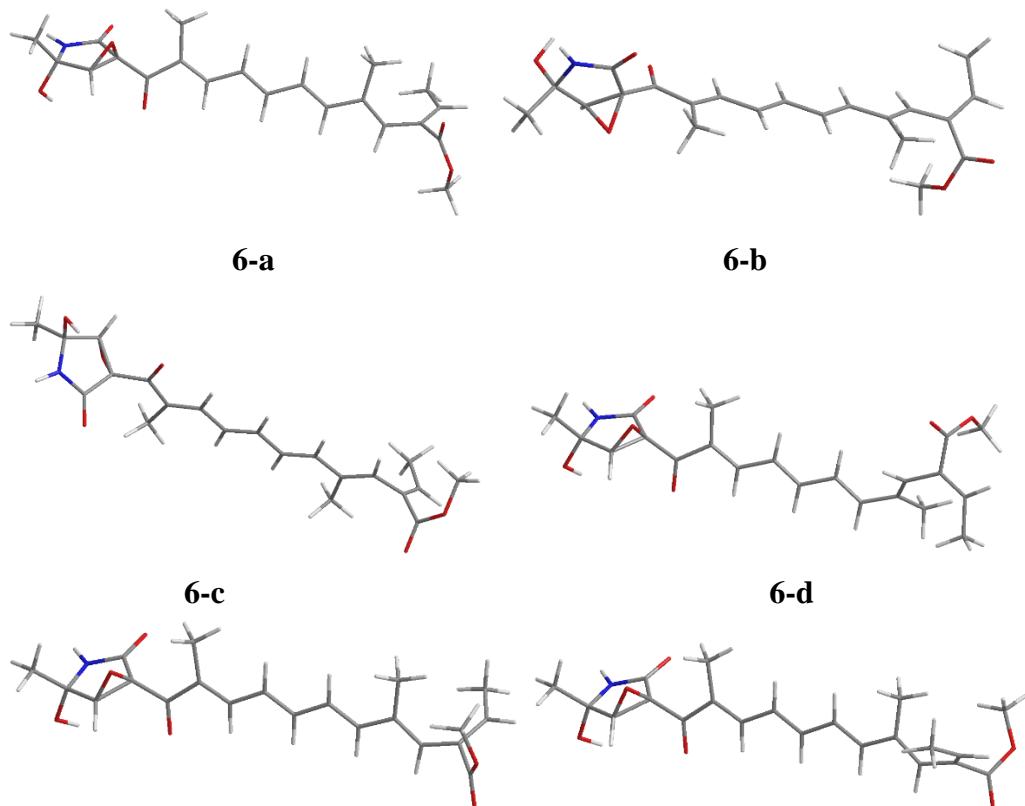


Figure S 57. The optimized low energy conformers of 5.

Table S4. Energy Analysis for the Conformers of (13*R*, 14*R*,15*S*)-6.

Compound	E(Hartree)	E(kcal/mol)	rel.E(kcal/mol)	Qi	Boltzmann dist
6-a	-1321.34	-829153	0	1	0.781632
6-b	-1321.34	-829152	1.327032	0.106326	0.083108
6-c	-1321.33	-829148	4.882758	0.000262	0.000205
6-d	-1321.33	-829146	6.788994	1.05E-05	8.19E-06
6-e	-1321.33	-829148	5.636861	7.34E-05	5.73E-05
6-f	-1321.34	-829150	2.943804	0.00693	0.005417
6-g	-1321.33	-829147	5.748432	6.08E-05	4.75E-05
6-h	-1321.34	-829152	1.0643	0.165711	0.129525



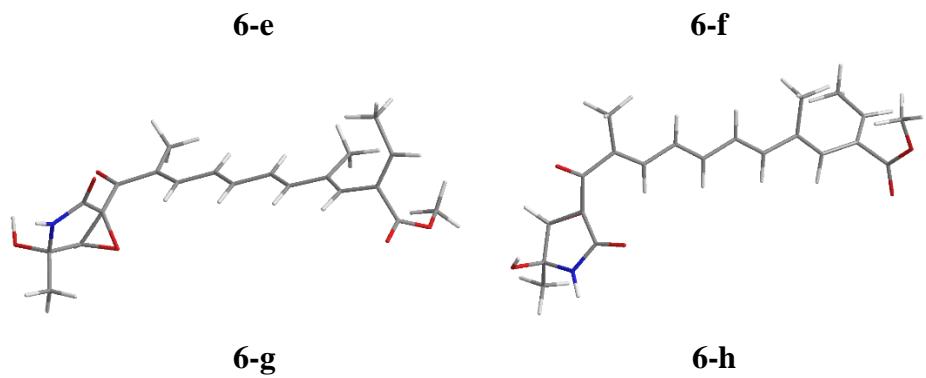
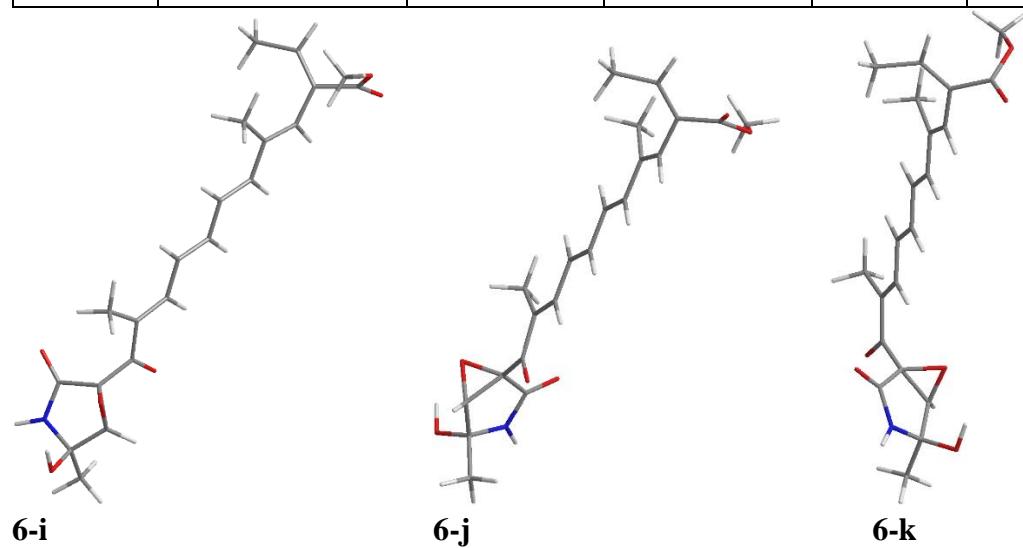
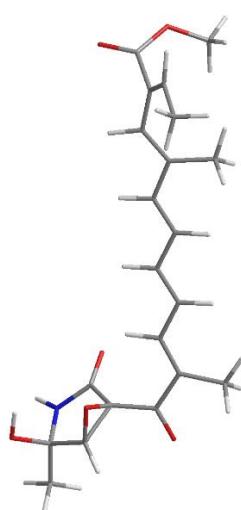


Figure S 58. The optimized low energy conformers of (13*R*, 14*R*,15*S*)-6.

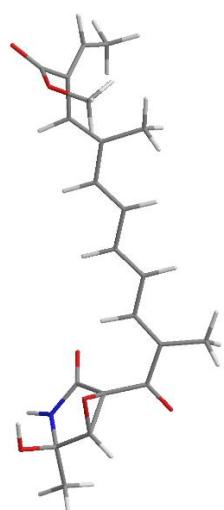
Table S5. Energy Analysis for the Conformers of (13*R*, 14*R*,15*R*)-6.

Compund	E(Hartree)	E(kcal/mol)	rel.E(kcal/mol)	Qi	Boltzmann dist
6-i	– 1320.7589508500	– 828788.7479	0	1	0.015356
6-j	– 1320.7587168500	– 828788.6011	0.146837216	0.780363	0.011983
6-k	– 1320.7618523300	– 828790.5686	-1.820706174	21.65029	0.33246
6-l	– 1320.7618578700	– 828790.5721	-1.824182577	21.77778	0.334417
6-m	– 1320.7617734100	– 828790.5191	-1.771183127	19.91312	0.305784





6-l



6-m

Figure S 59. The optimized low energy conformers of (13*R*, 14*R*,15*R*)-6.