Supporting Information

Further Verticillene Diterpenoids, Eudesmane Sesquiterpe-noids, and Hydroperoxysteroids from a Taiwanese Soft Coral *Cespitularia* sp.

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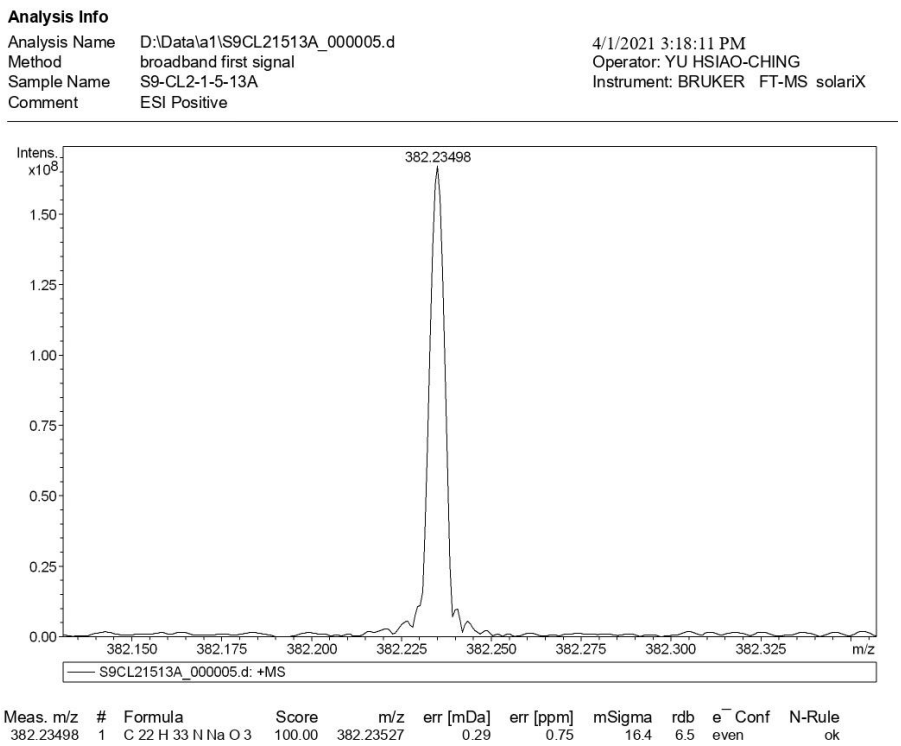

Figure S1. HRESIMS of compound **1**

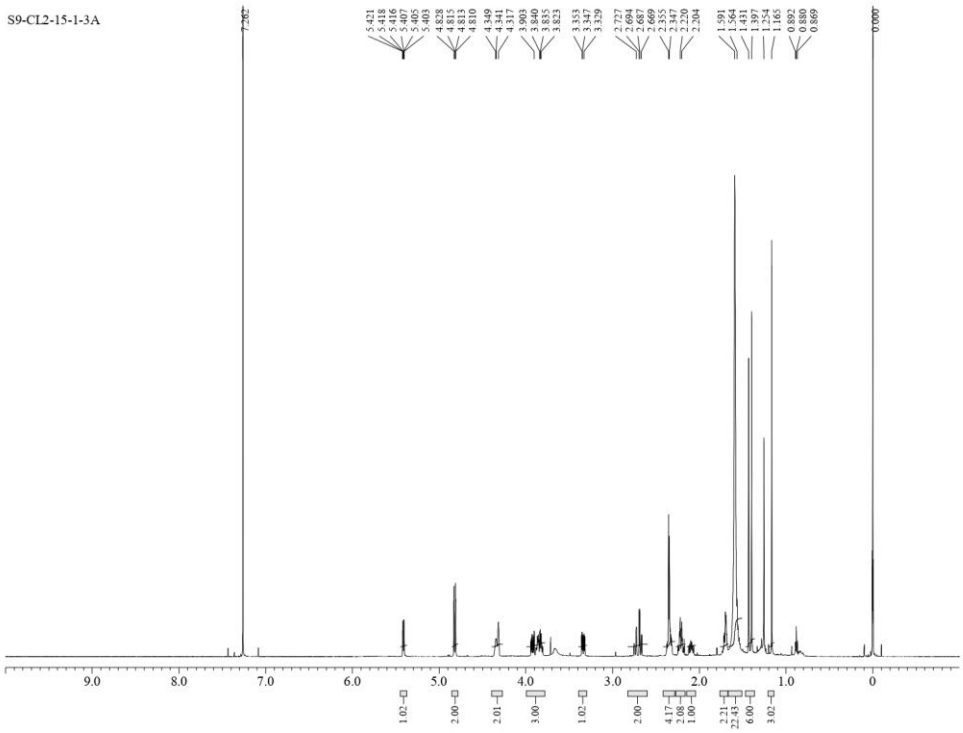

Figure S2. ^{1}H NMR spectrum (600MHz) of compound **1** in $CDCl_3$

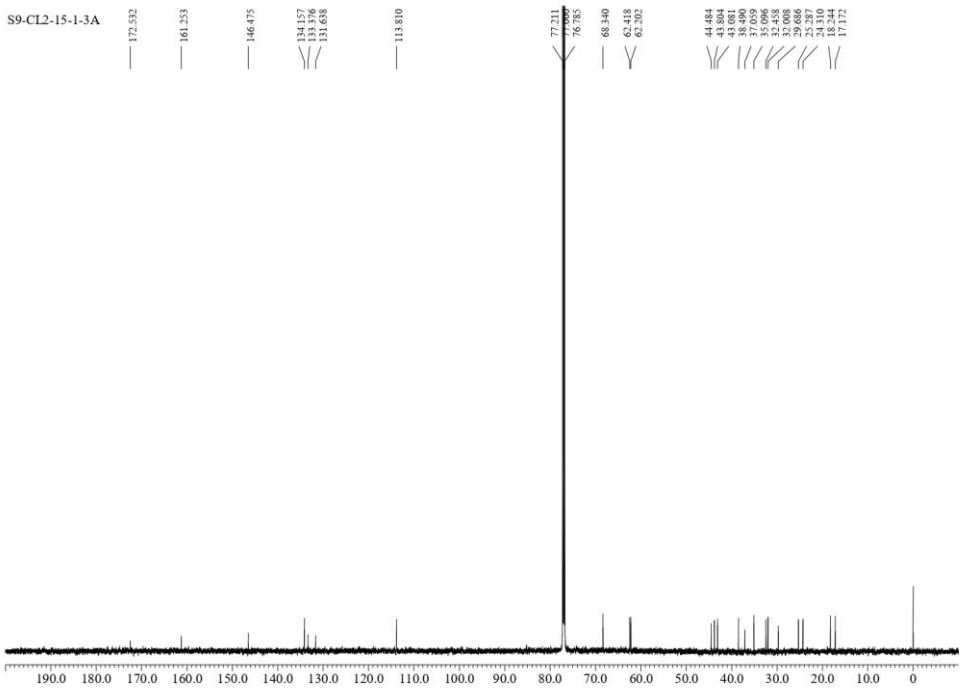

Figure S3. ^{13}C NMR spectrum (150 MHz) of compound **1** in $CDCl_3$

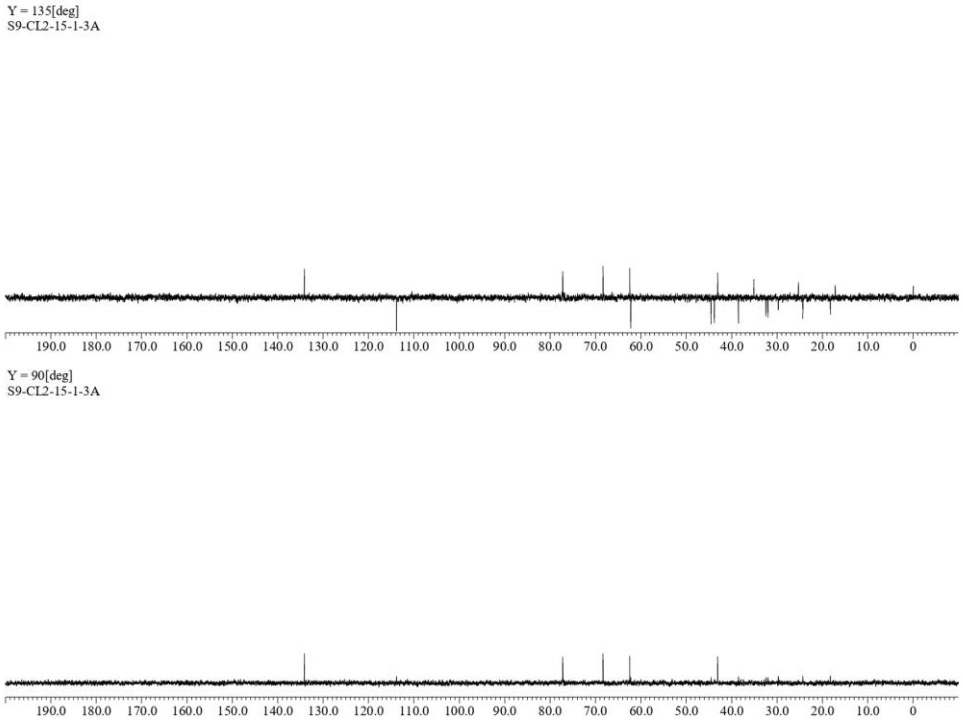

Figure S4. DEPT spectrum (150 MHz) of compound **1** in $CDCl_3$

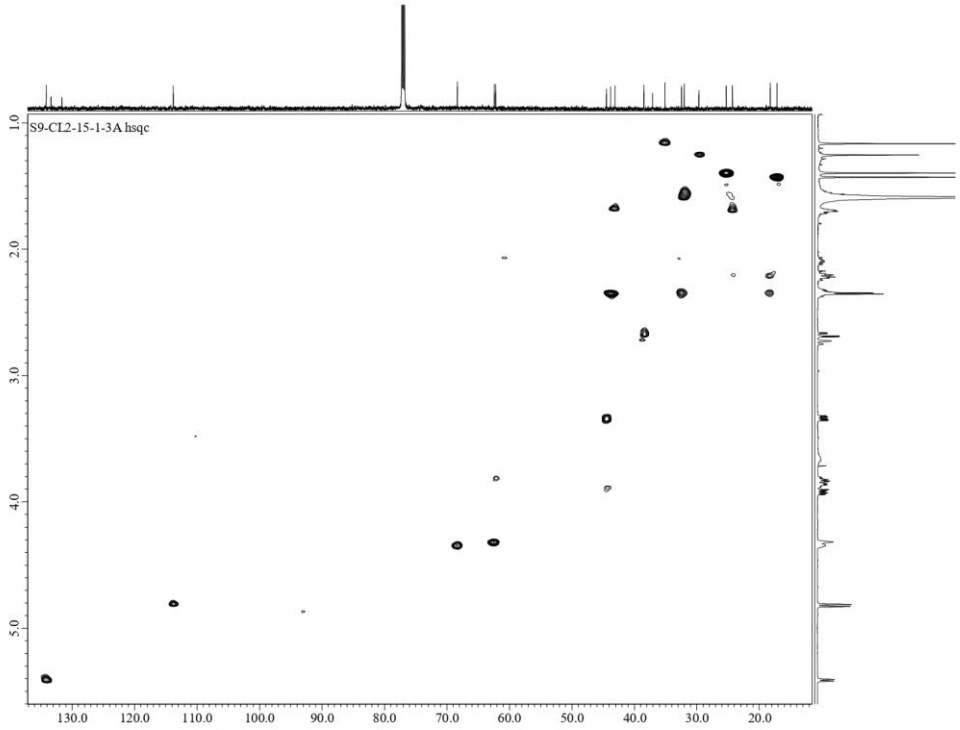

Figure S5. HSQC spectrum of compound **1** in $CDCl_3$

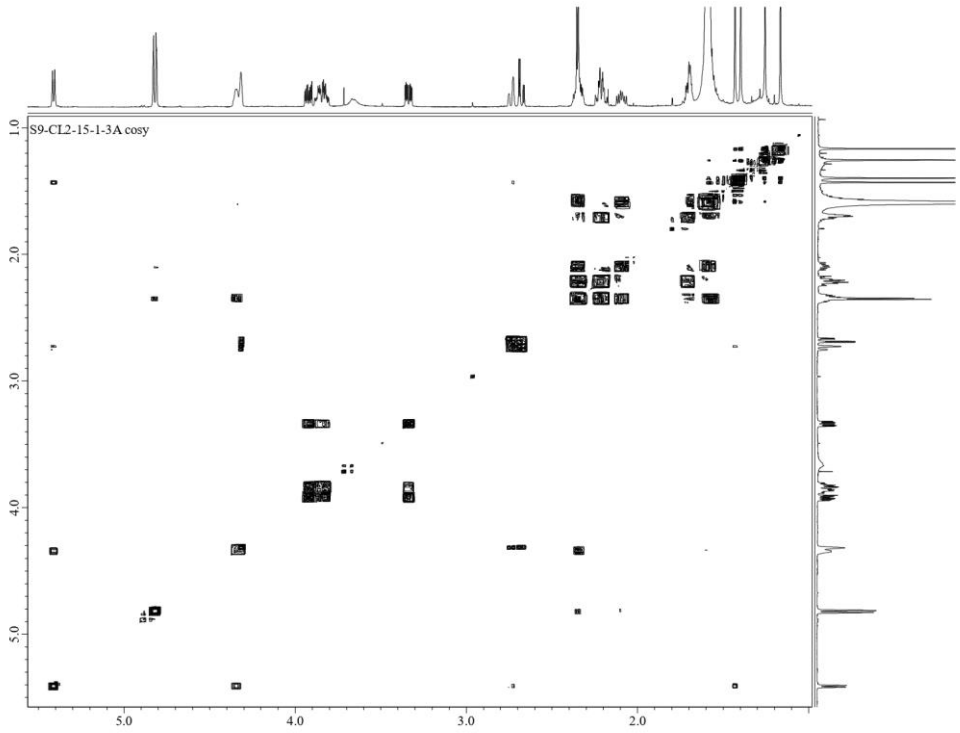

Figure S6. ^1H-^1H COSY spectrum of compound **1** in $CDCl_3$

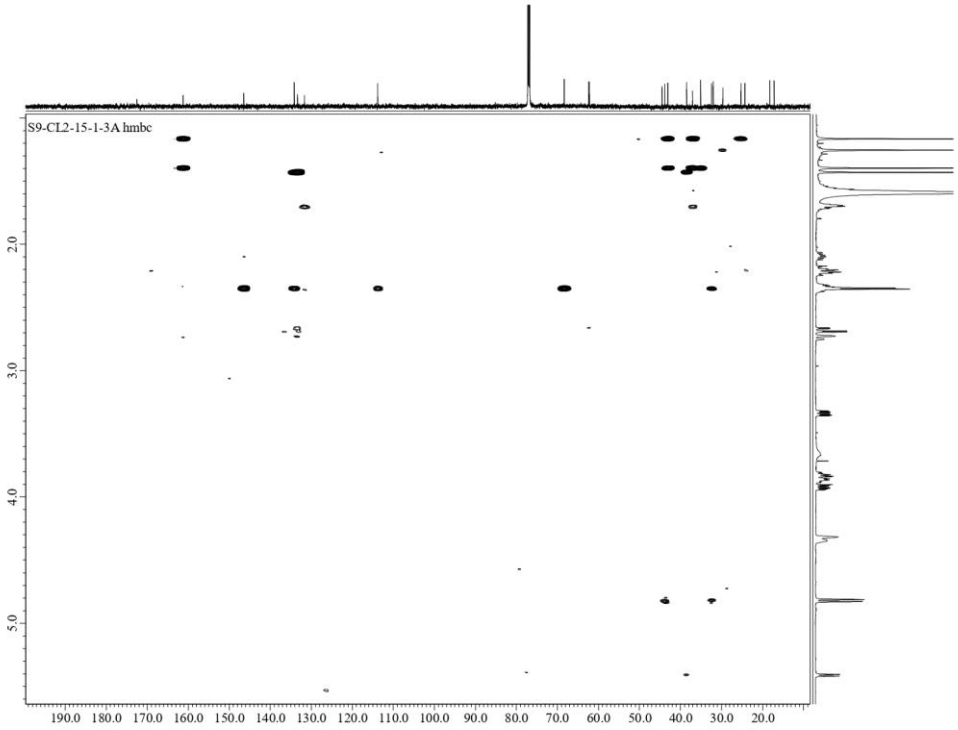

Figure S7. HMBC spectrum of compound **1** in $CDCl_3$

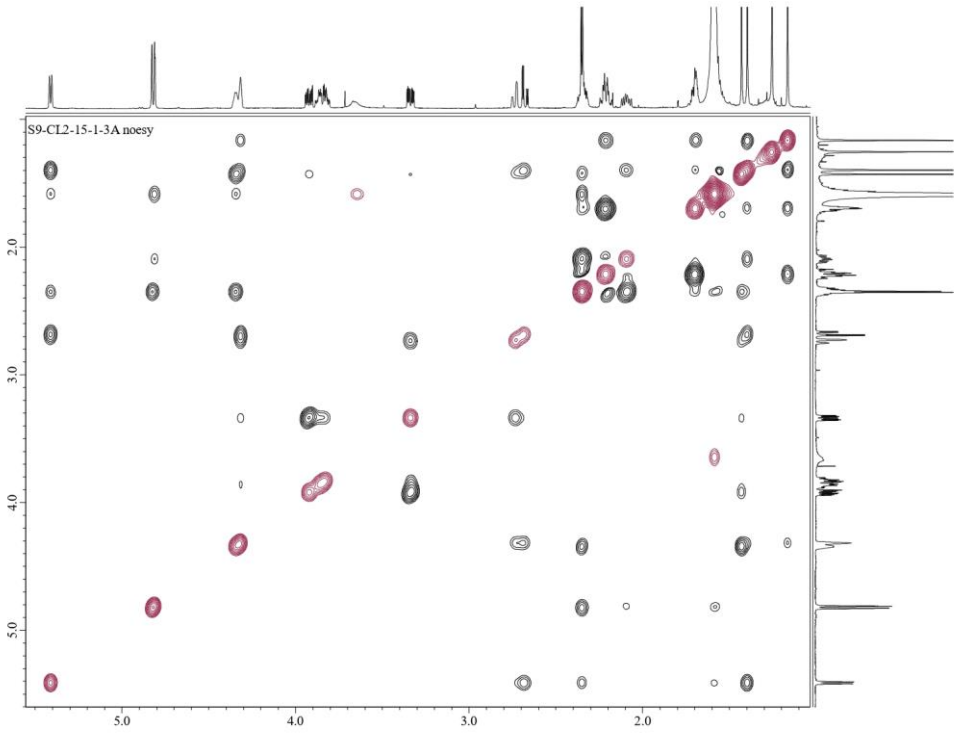

Figure S8. NOESY spectrum of compound **1** in $CDCl_3$

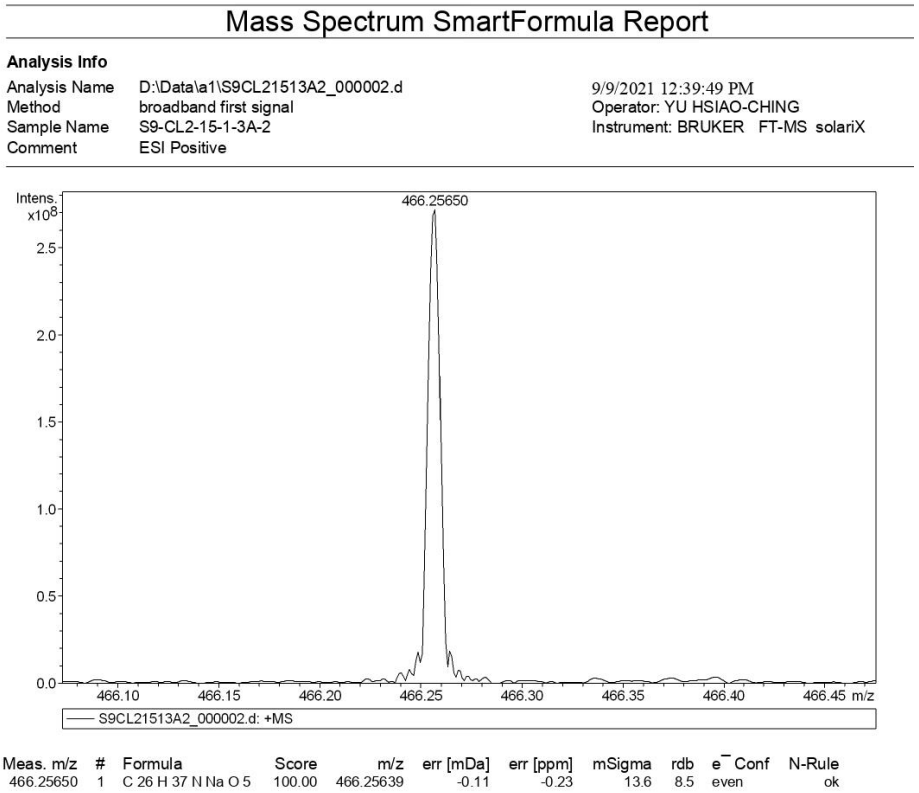

Figure S9. HRESIMS of compound **1a**

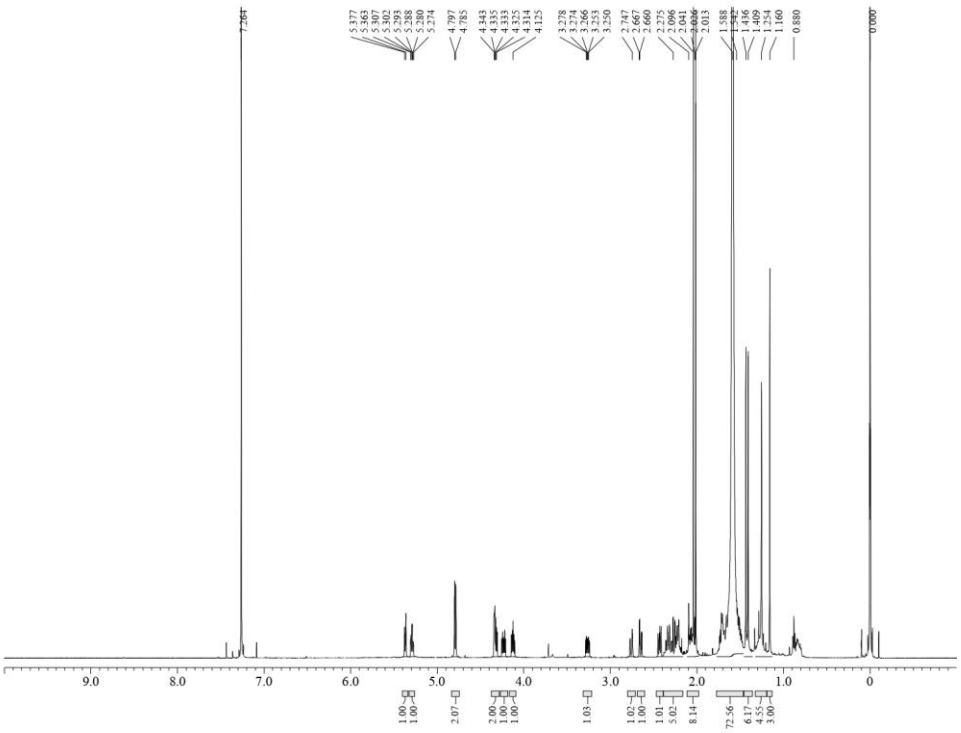

Figure S10. ^{1}H NMR spectrum (600MHz) of compound **1a** in $CDCl_3$

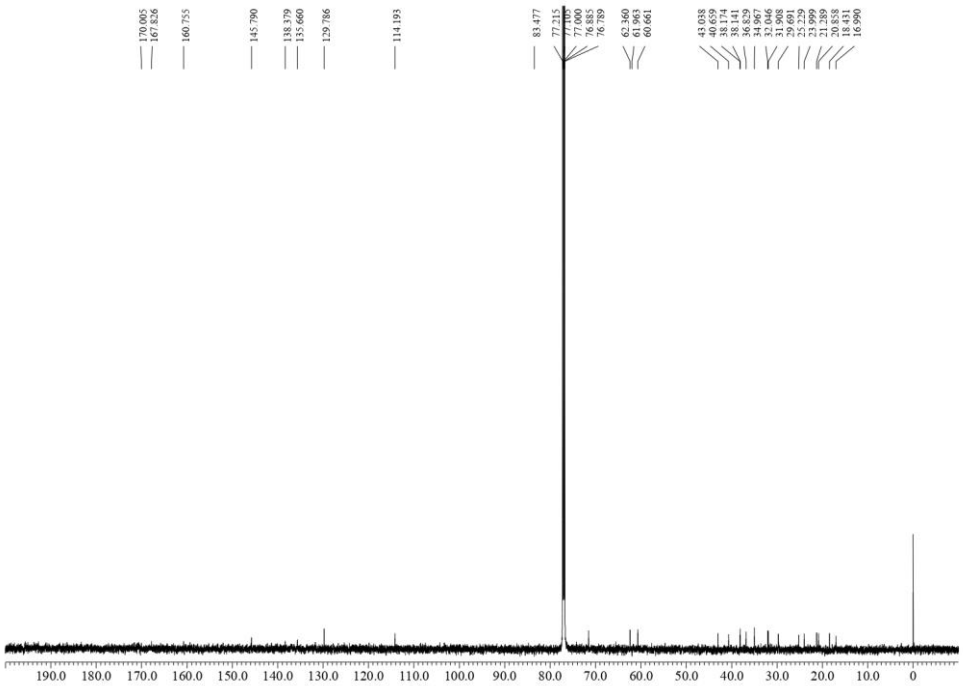

Figure S11. ^{13}C NMR spectrum (150 MHz) of compound **1a** in $CDCl_3$

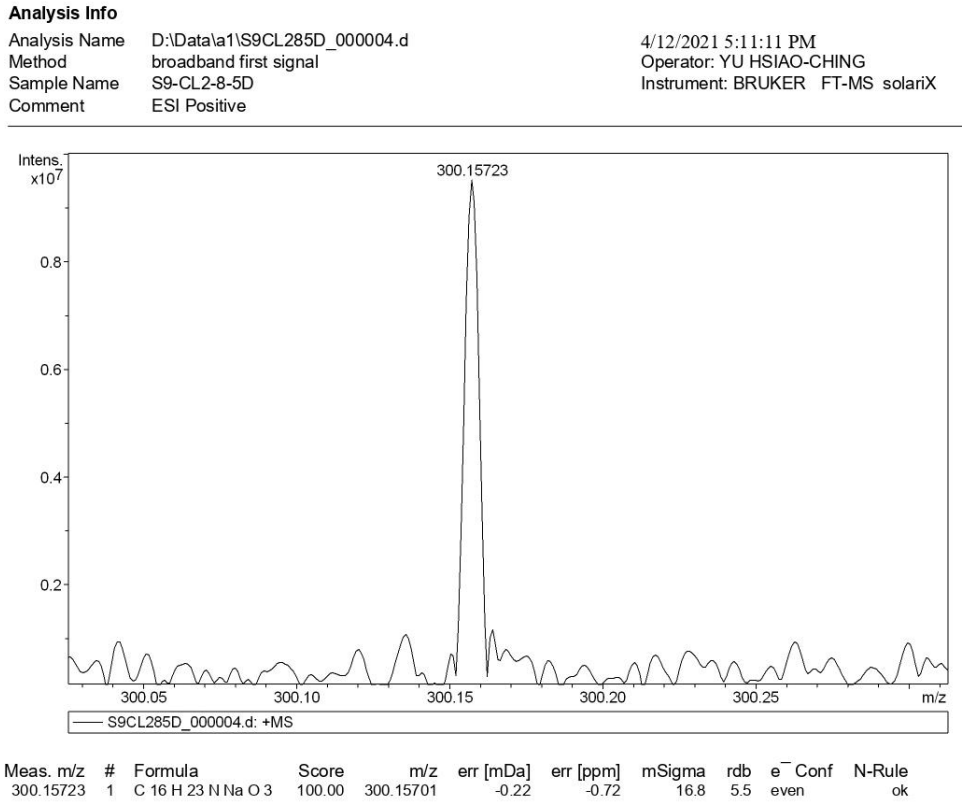

Figure S12. HRESIMS of compound **2**

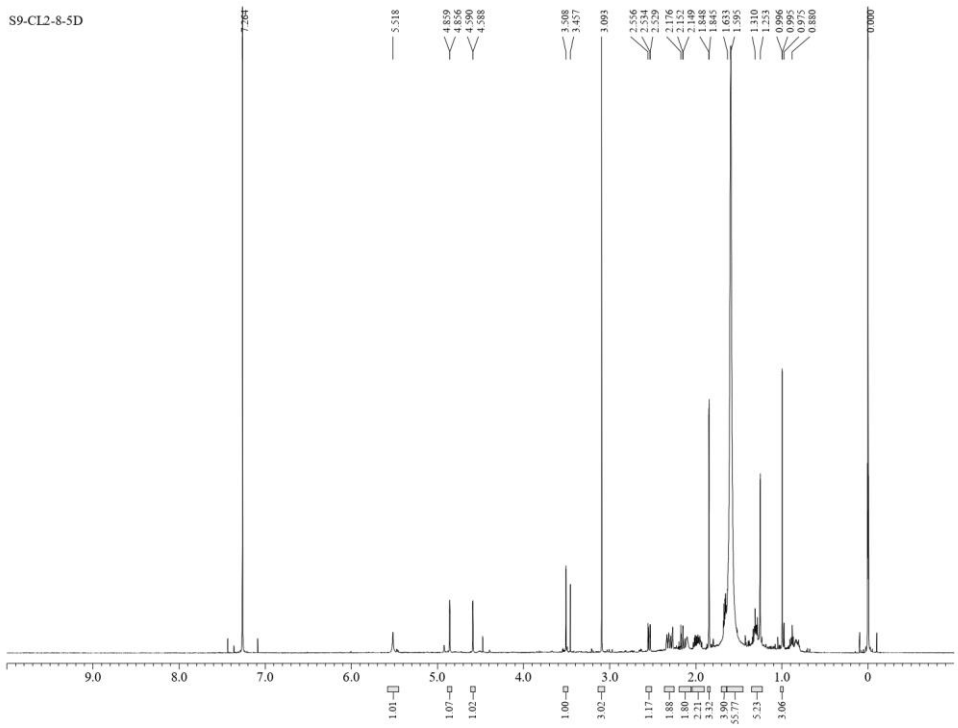

Figure S13. ^{1}H NMR spectrum (600MHz) of compound **2** in $CDCl_3$

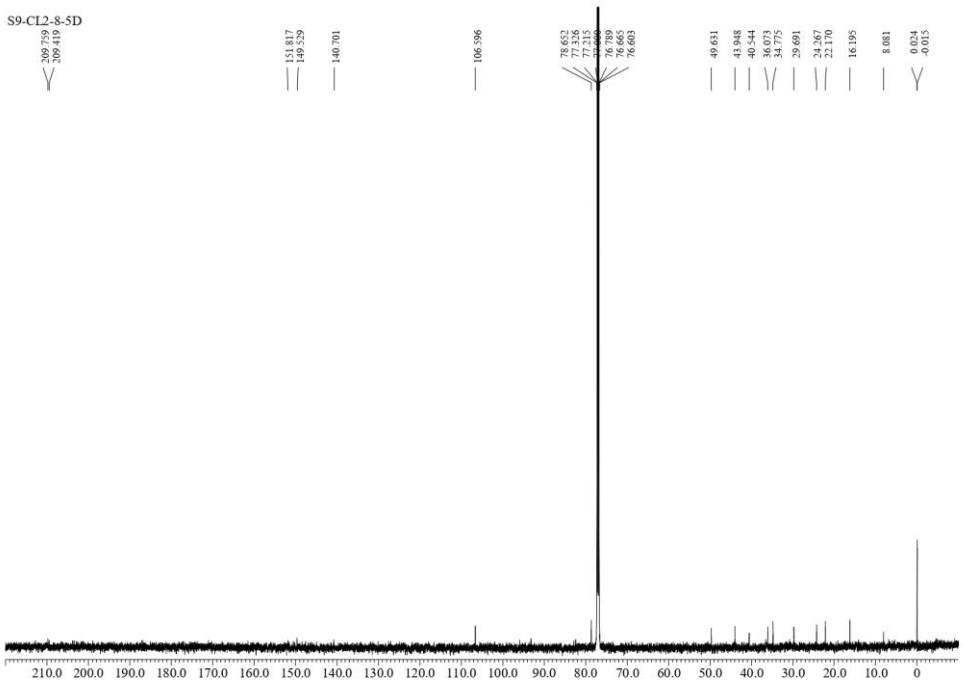

Figure S14. ^{13}C NMR spectrum (150 MHz) of compound **2** in $CDCl_3$

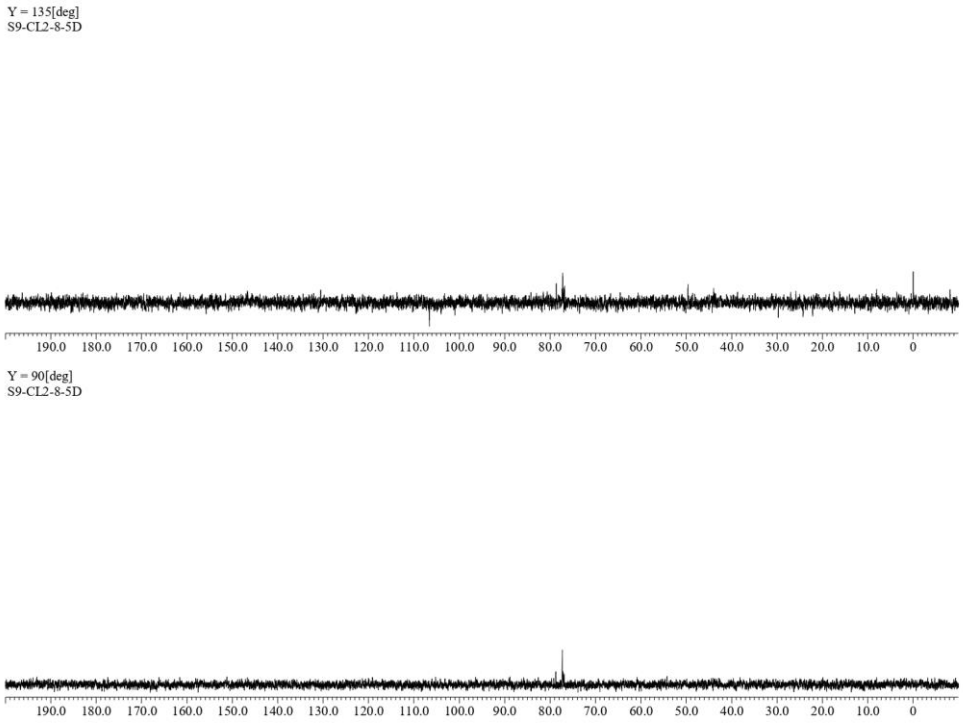

Figure S15. DEPT spectrum (150 MHz) of compound **2** in $CDCl_3$

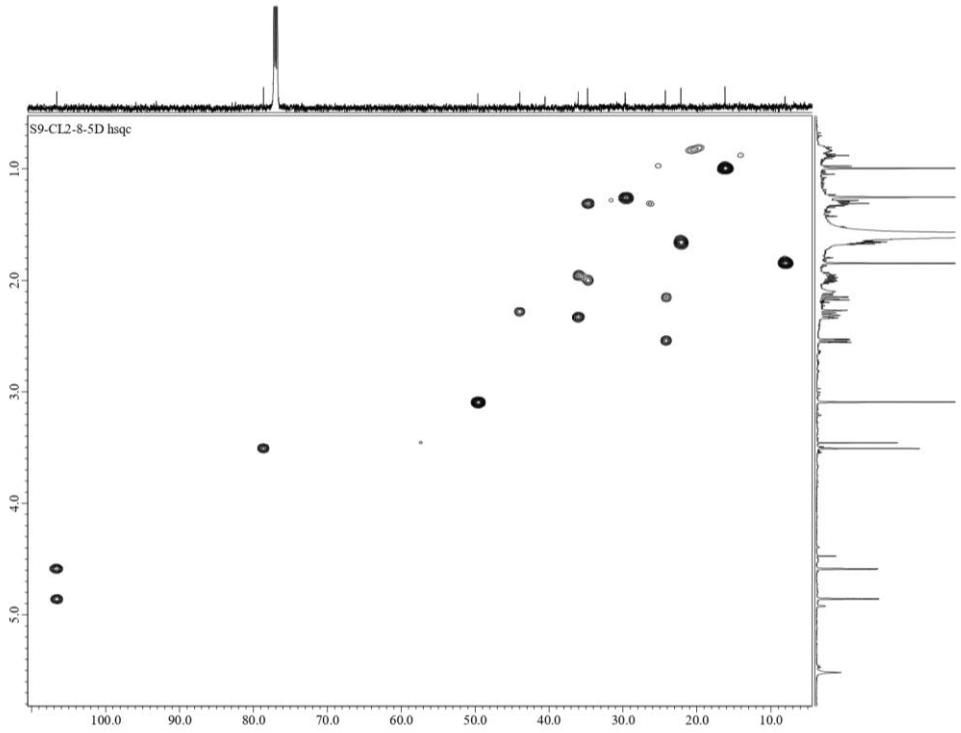

Figure S16. HSQC spectrum of compound **2** in $CDCl_3$

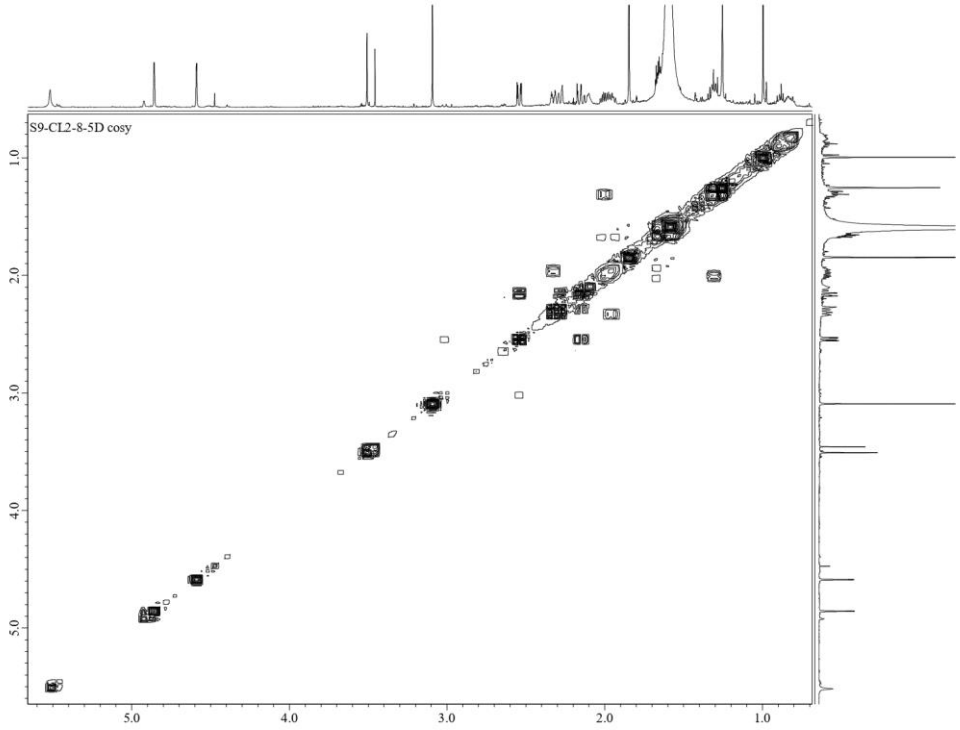

Figure S17. ^{1}H-^{1}H COSY spectrum of compound **2** in $CDCl_3$

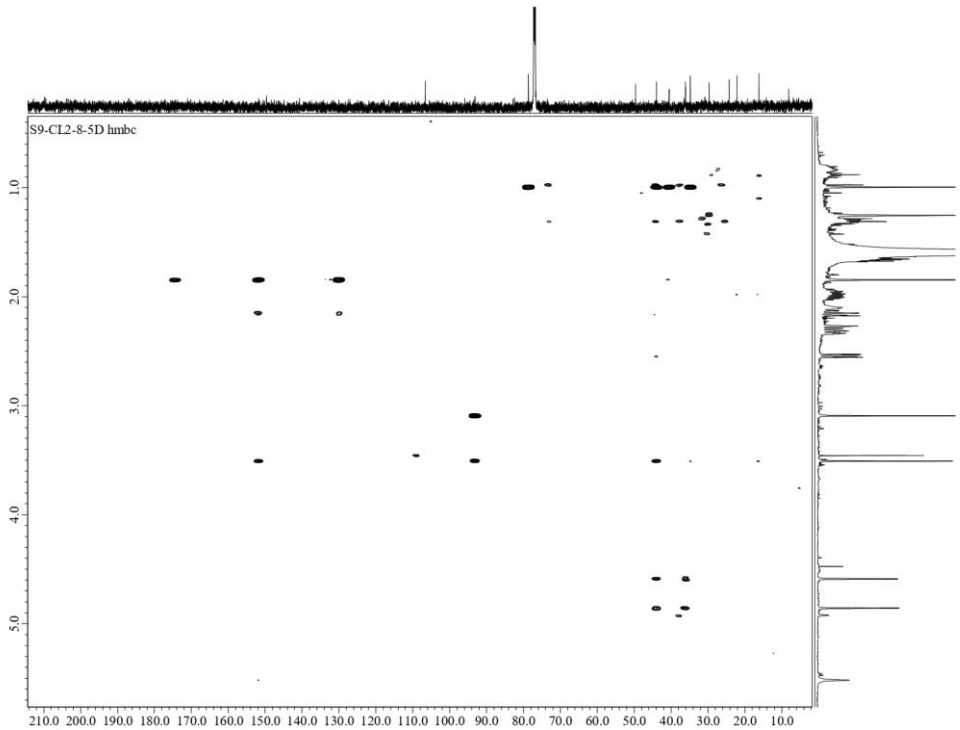

Figure S18. HMBC spectrum of compound **2** in $CDCl_3$

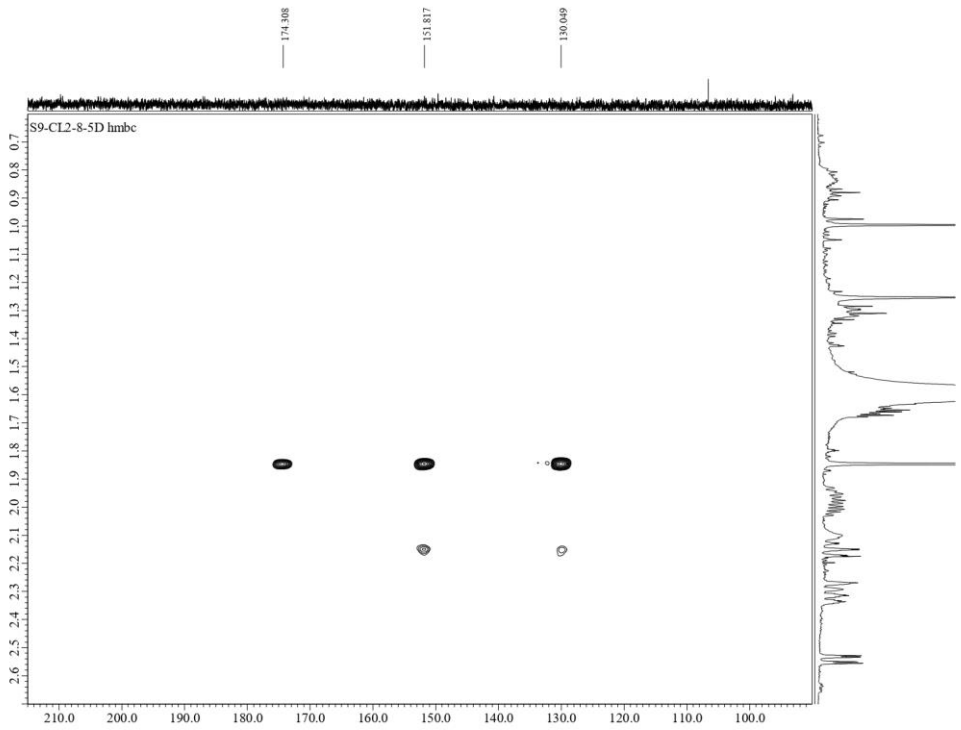

Figure S19. The amplificatory HMBC spectrum of compound **2** in $CDCl_3$

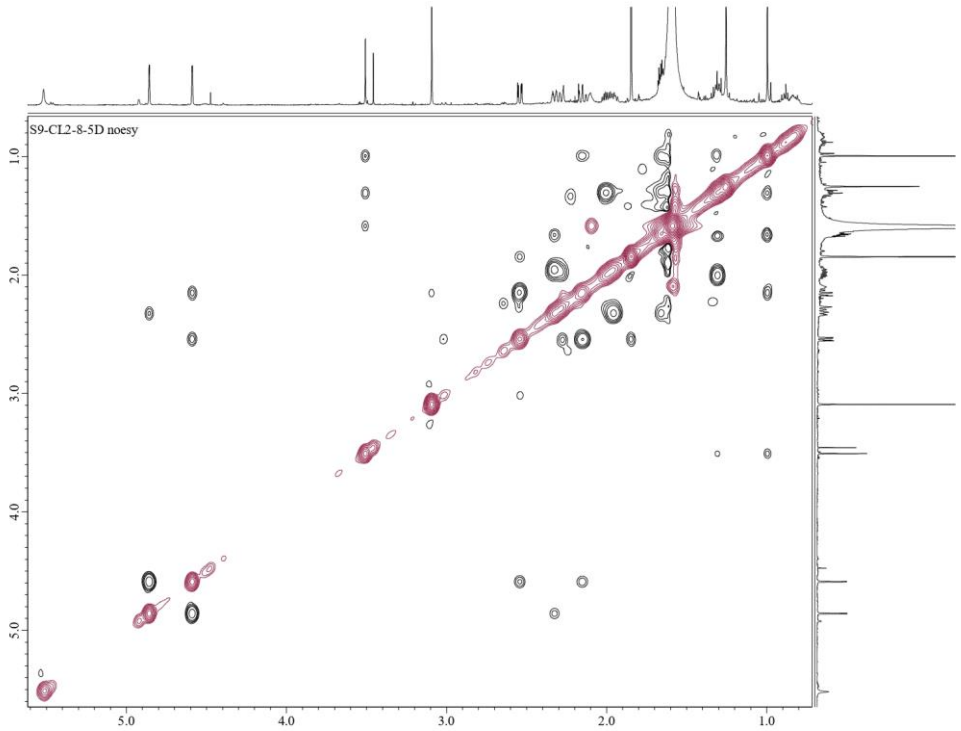

Figure S20. NOESY spectrum of compound **2** in $CDCl_3$

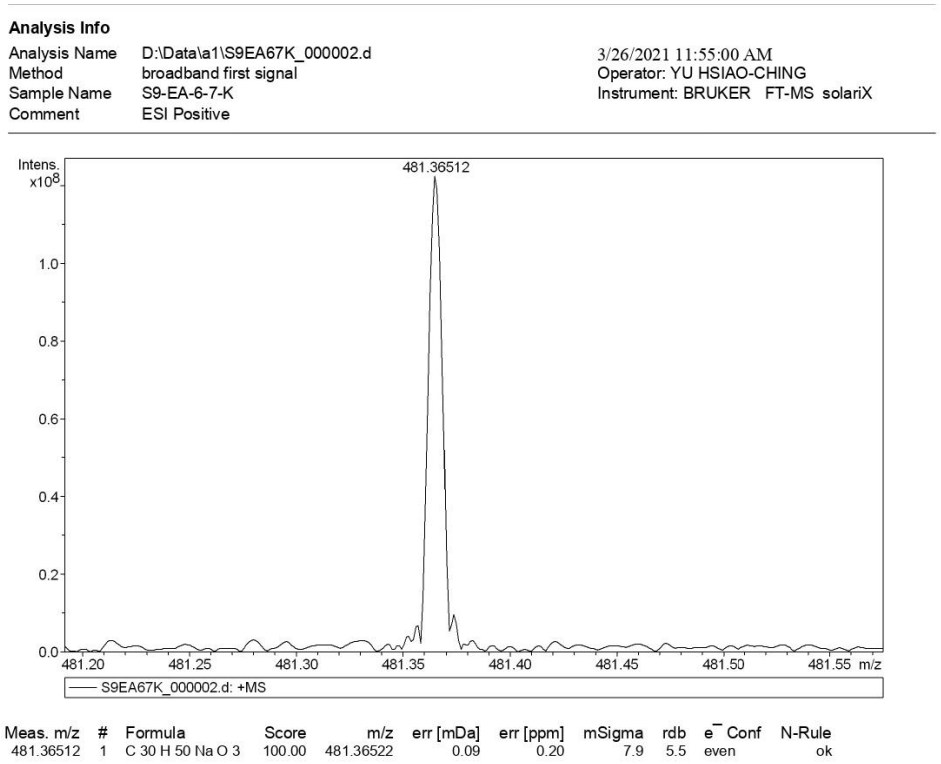

Figure S21. HRESIMS of compound **3**

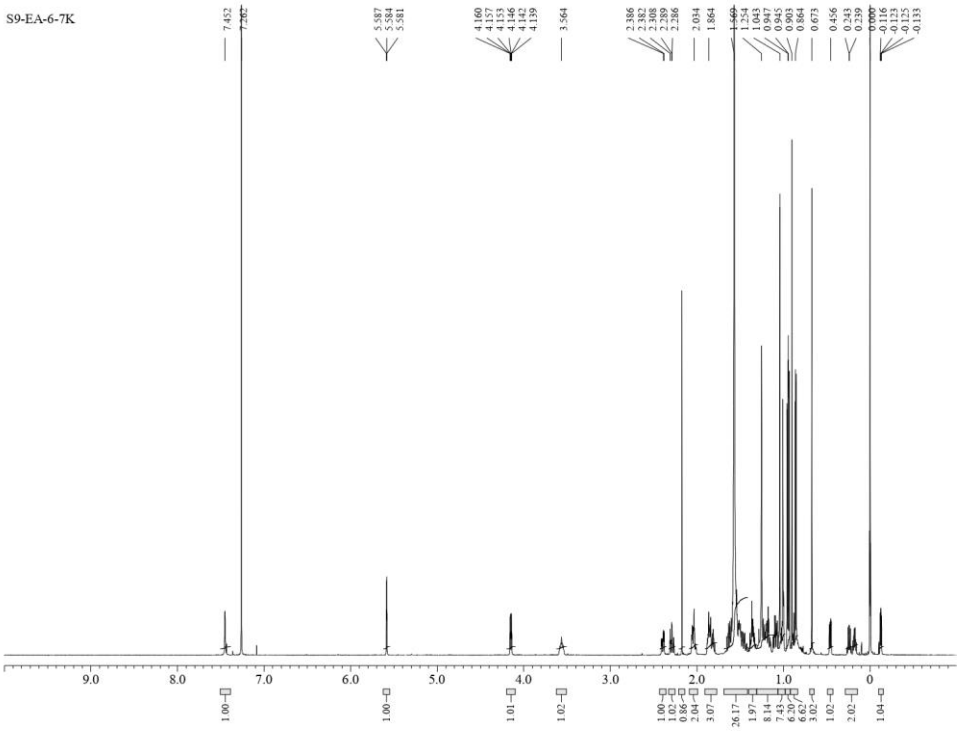

Figure S22. ^{1}H NMR spectrum (600MHz) of compound **3** in $CDCl_3$

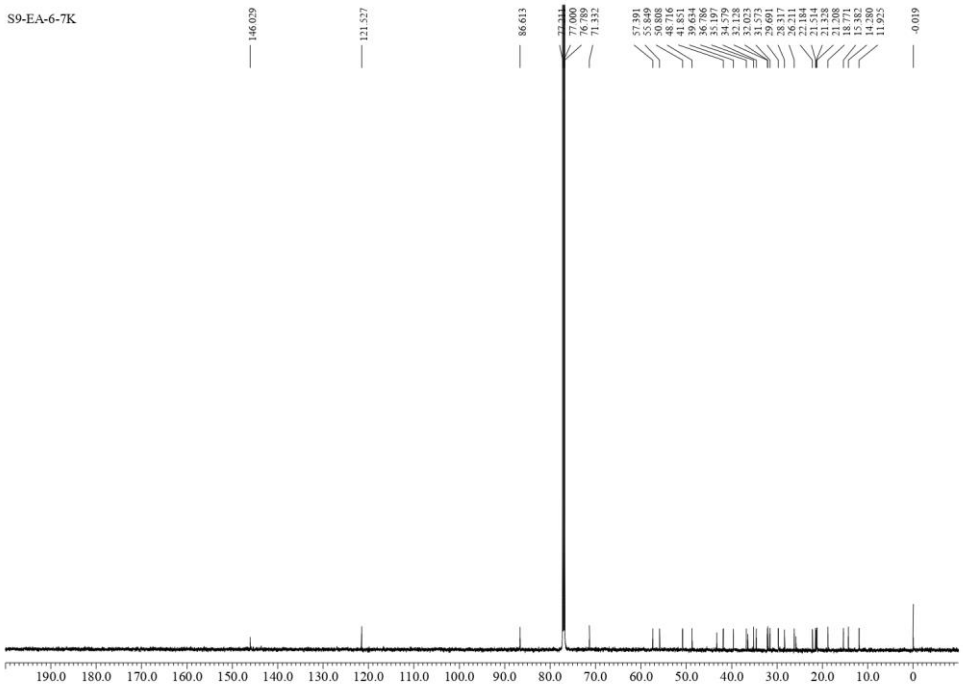

Figure S23. ^{13}C NMR spectrum (150 MHz) of compound **3** in $CDCl_3$

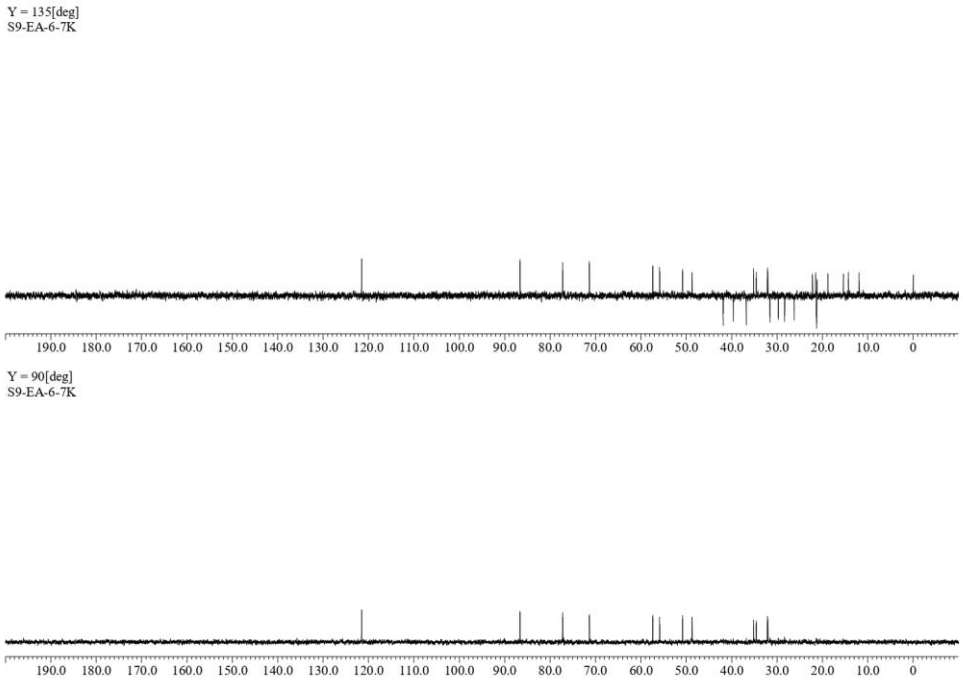

Figure S24. DEPT spectrum (150 MHz) of compound **3** in $CDCl_3$

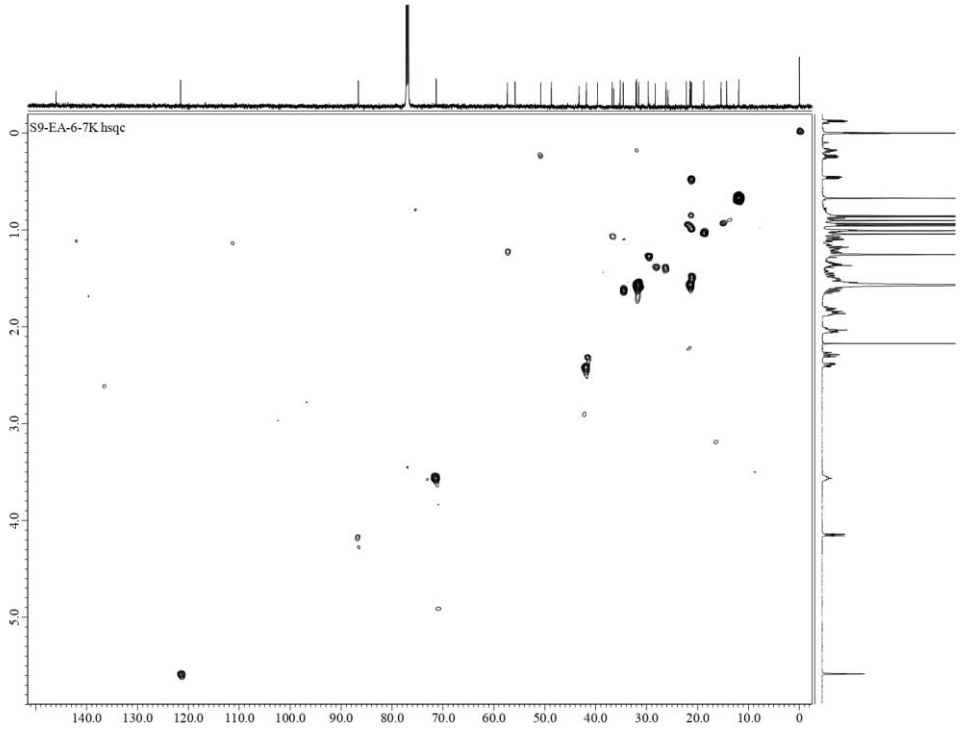

Figure S25. HSQC spectrum of compound **3** in $CDCl_3$

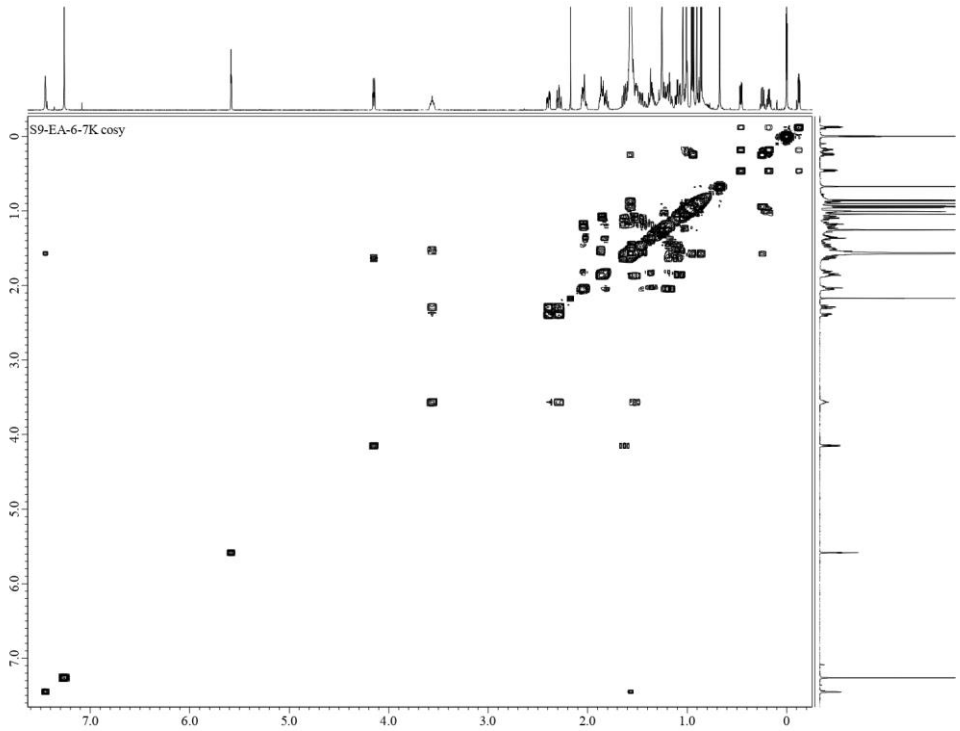

Figure S26. ^{1}H-^{1}H COSY spectrum of compound **3** in $CDCl_3$

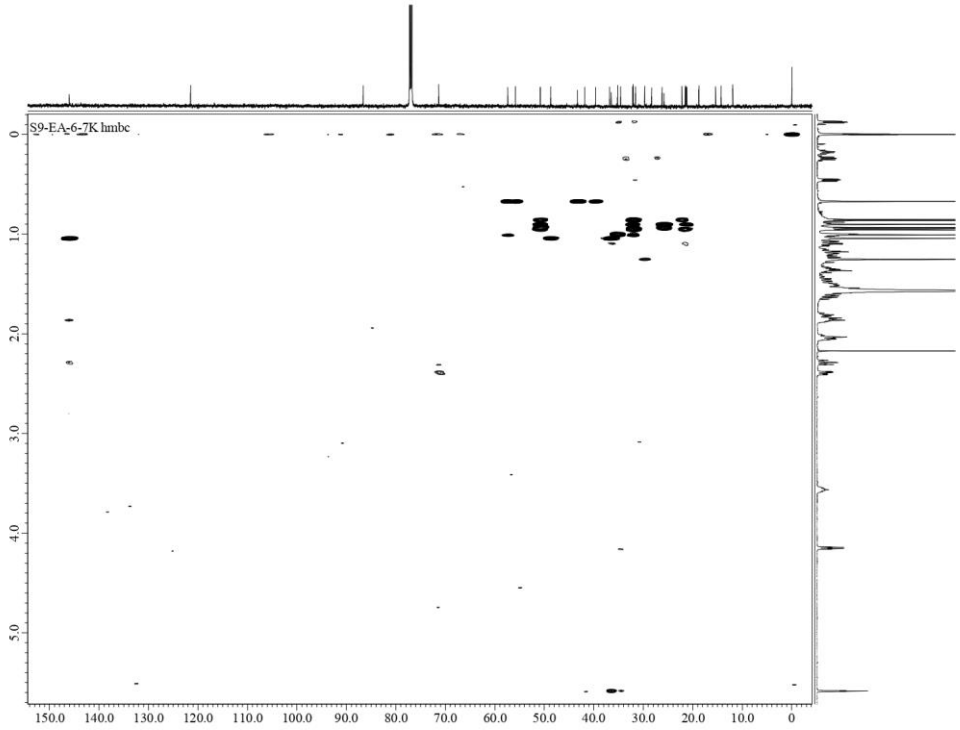

Figure S27. HMBC spectrum of compound **3** in $CDCl_3$

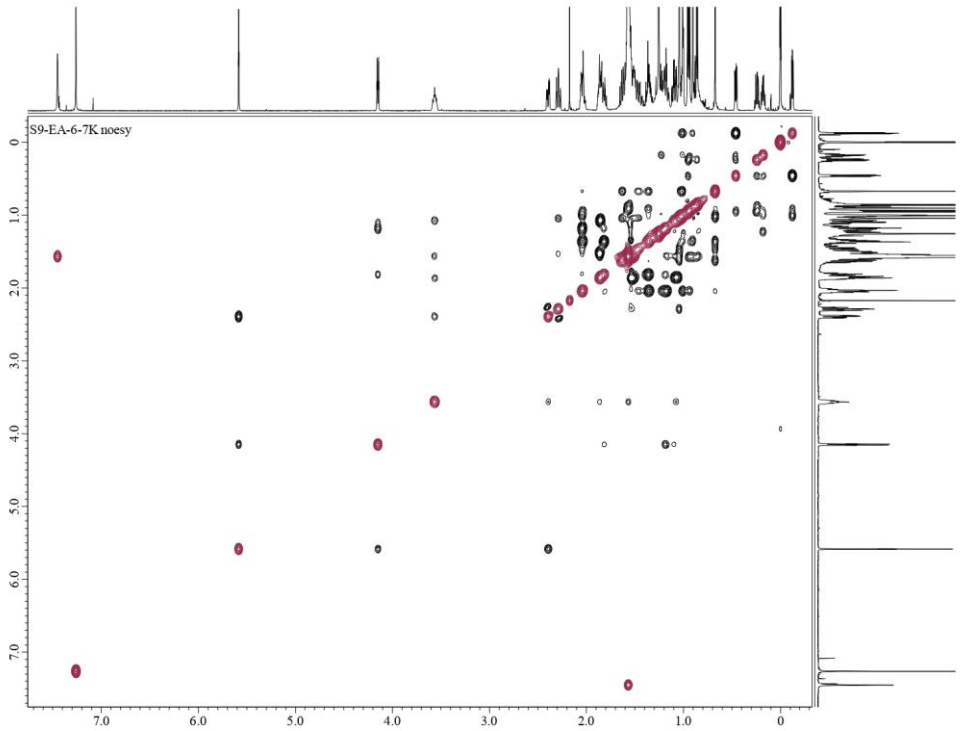

Figure S28. NOESY spectrum of compound **3** in $CDCl_3$

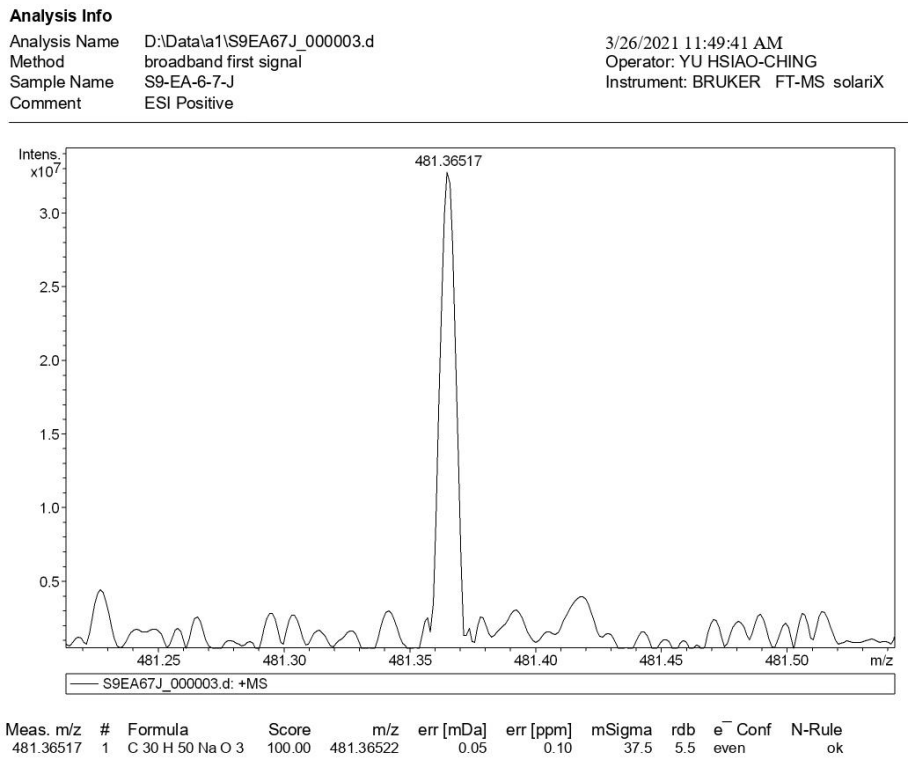

Figure S29. HRESIMS of compound **4**

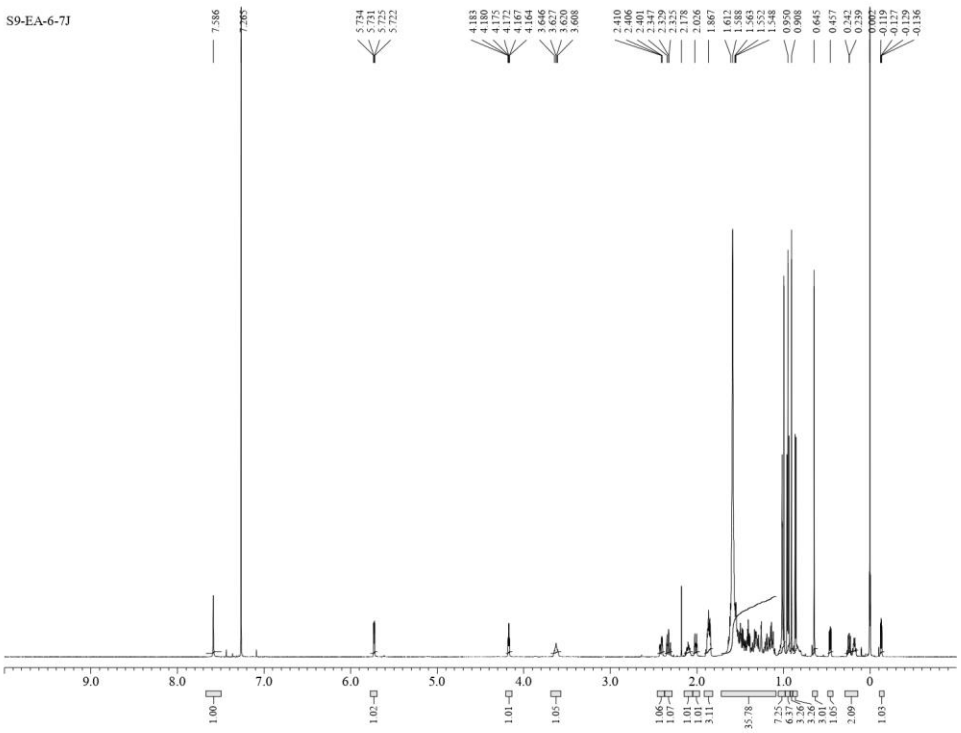

Figure S30. ^{1}H NMR spectrum (600MHz) of compound **4** in $CDCl_3$

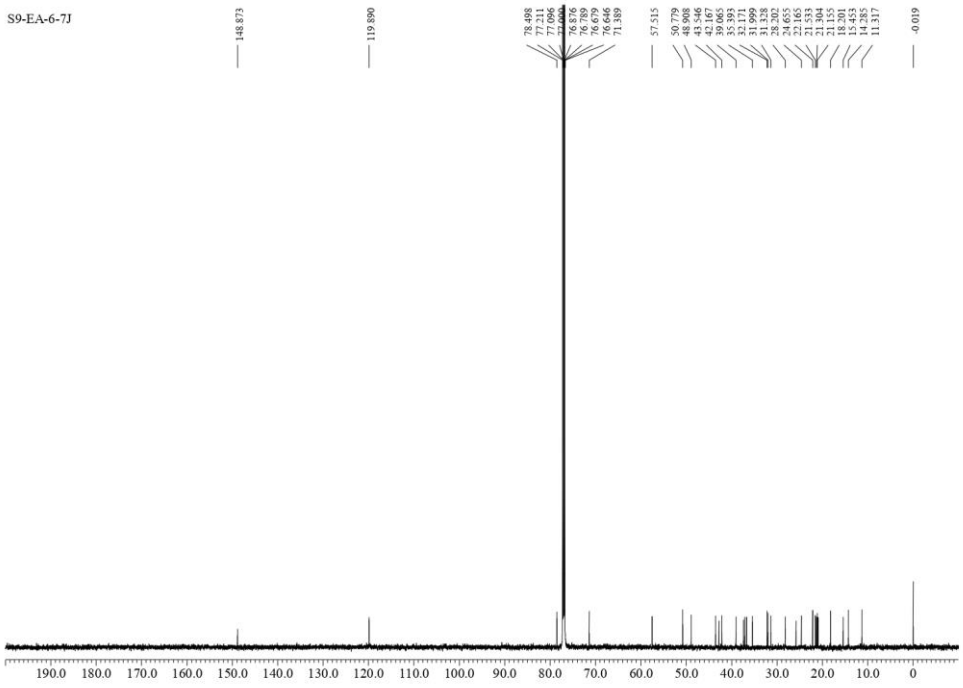

Figure S31. ^{13}C NMR spectrum (150 MHz) of compound **4** in $CDCl_3$

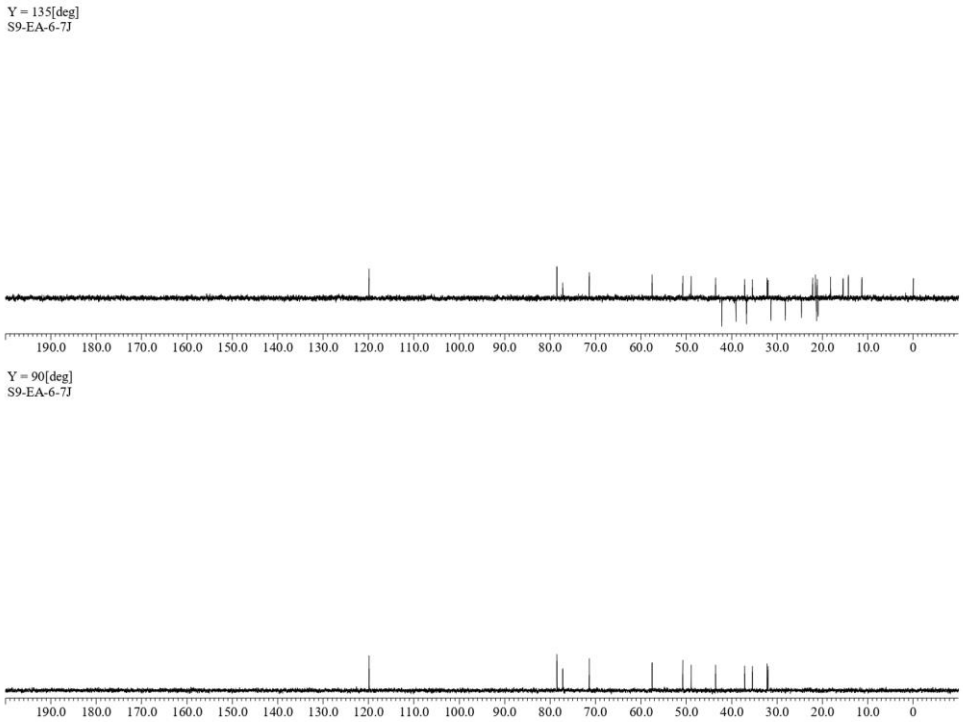

Figure S32. DEPT spectrum (150 MHz) of compound **4** in $CDCl_3$

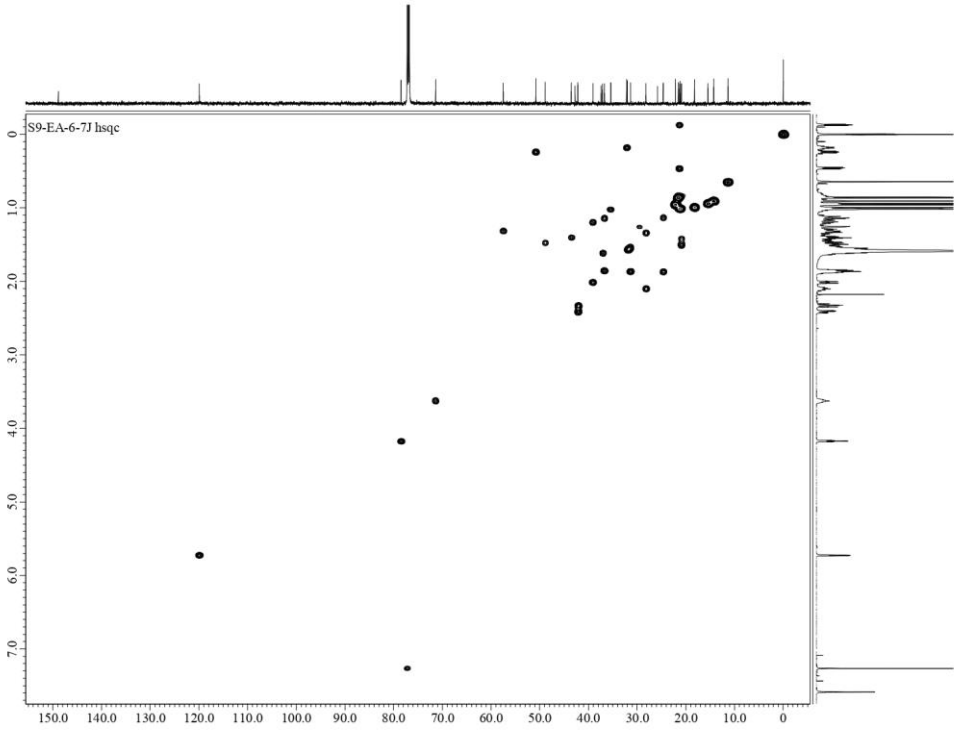

Figure S33. HSQC spectrum of compound **4** in $CDCl_3$

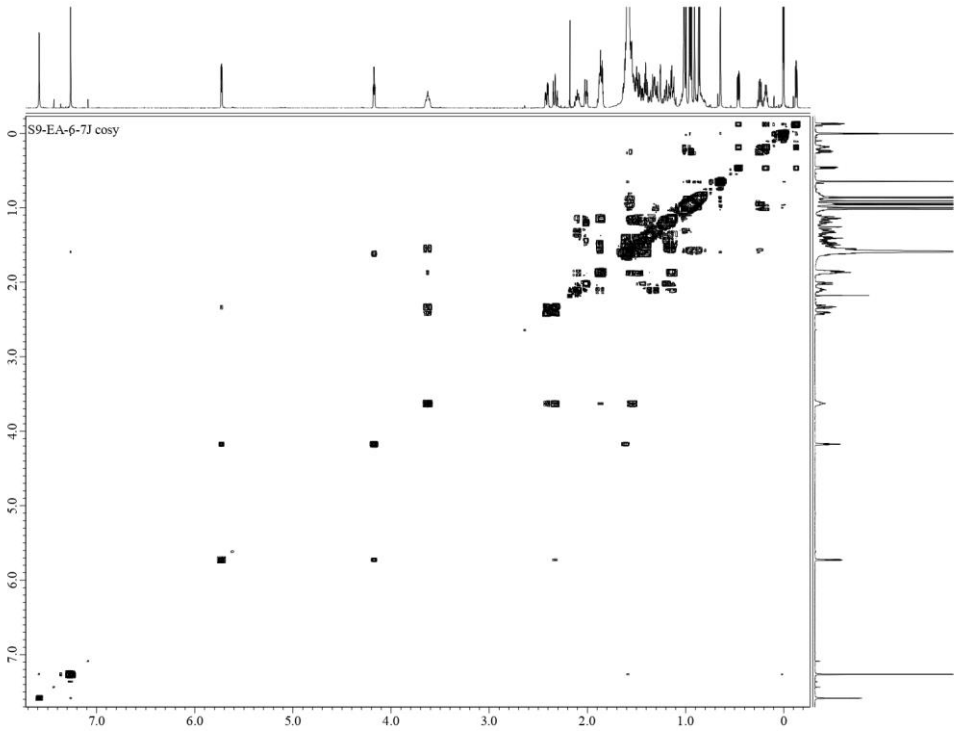

Figure S34. ^{1}H-^{1}H COSY spectrum of compound **4** in $CDCl_3$

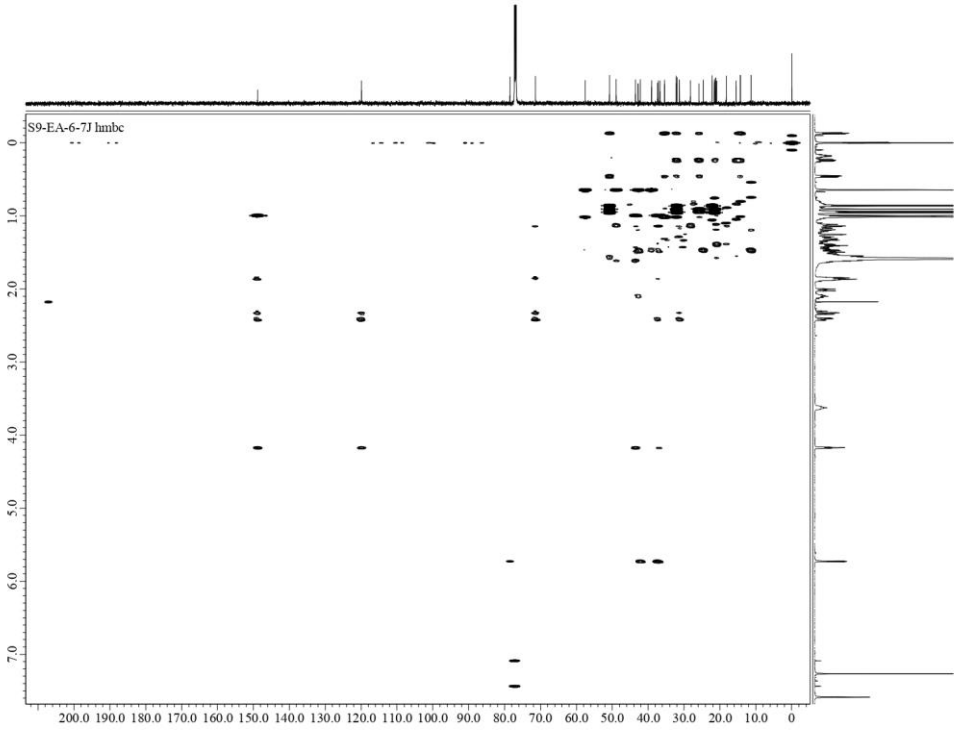

Figure S35. HMBC spectrum of compound **4** in $CDCl_3$

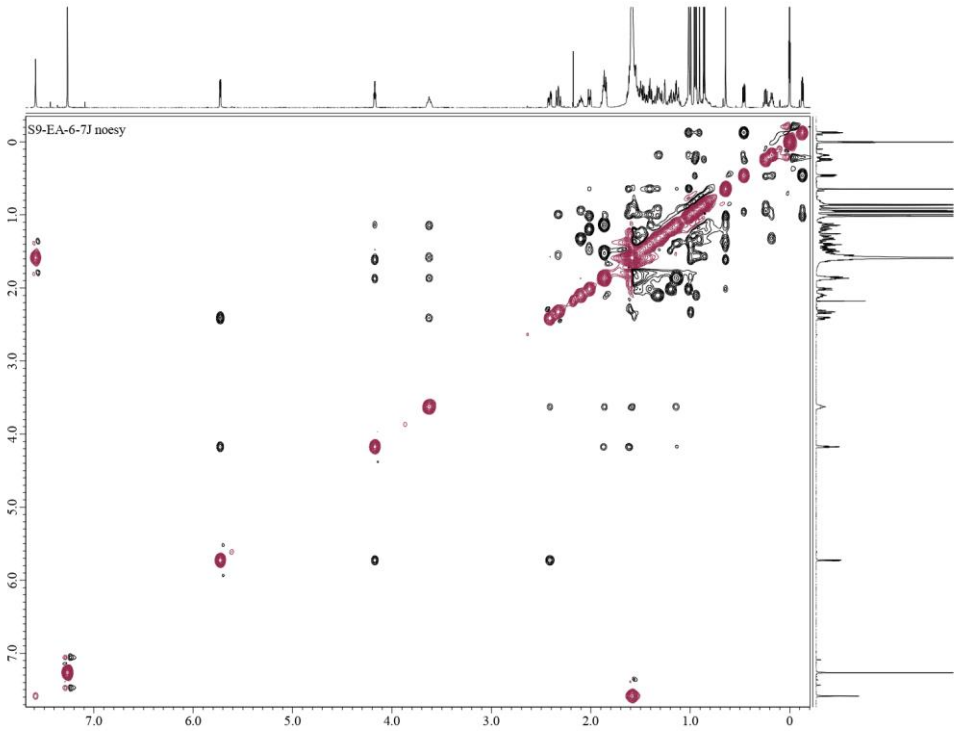

Figure S36. NOESY spectrum of compound **4** in $CDCl_3$

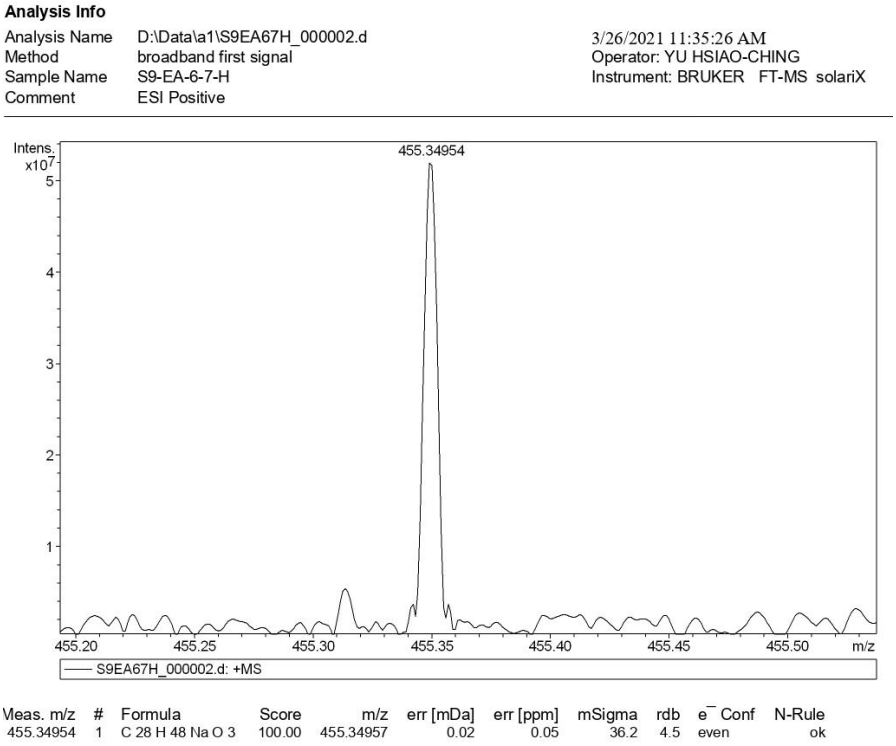

Figure S37. HRESIMS of compound **5**

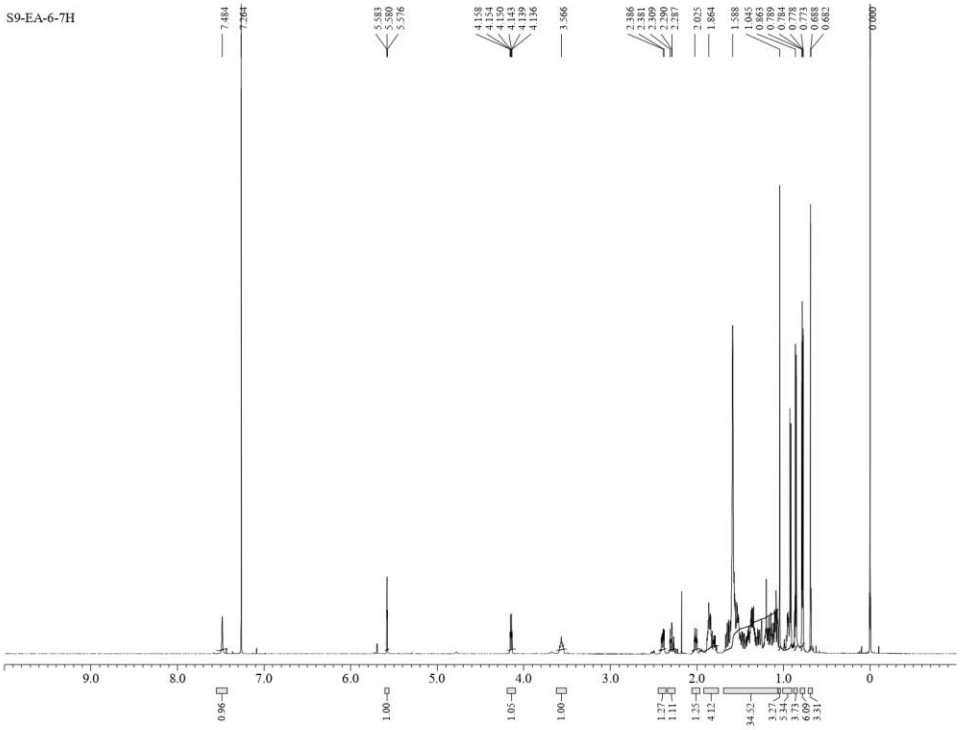

Figure S38. ^{1}H NMR spectrum (600MHz) of compound **5** in $CDCl_3$

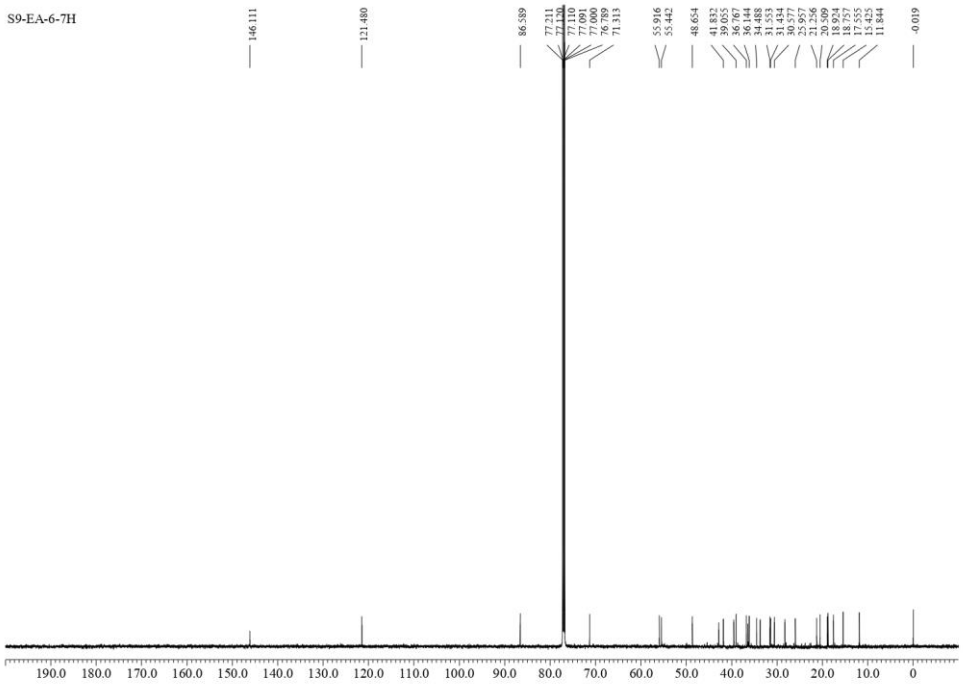

Figure S39. ^{13}C NMR spectrum (150 MHz) of compound **5** in $CDCl_3$

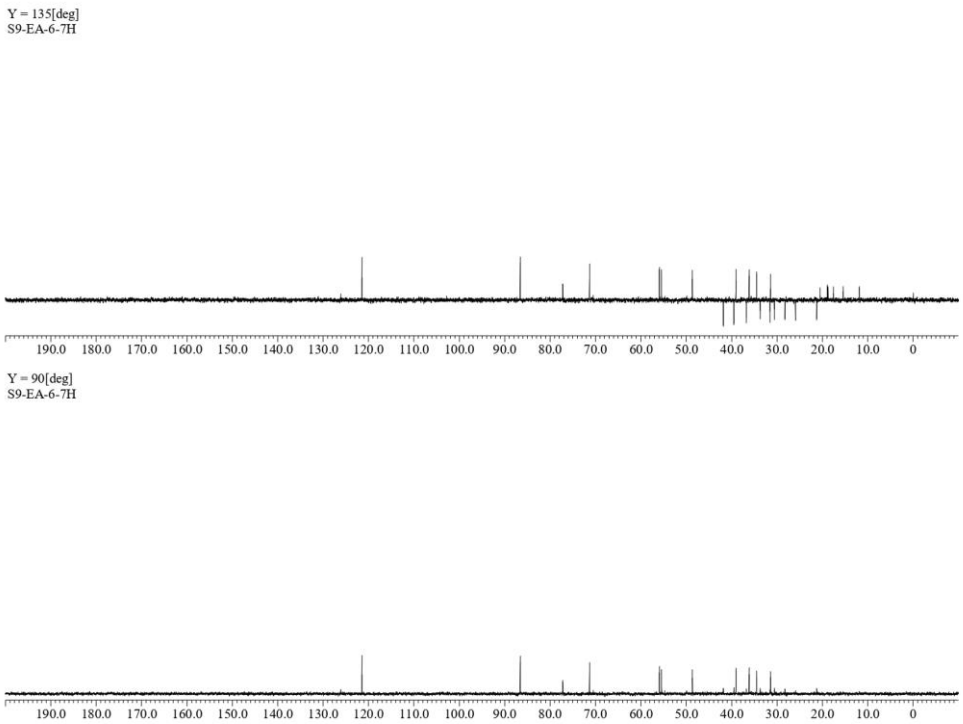

Figure S40. DEPT spectrum (150 MHz) of compound **5** in $CDCl_3$

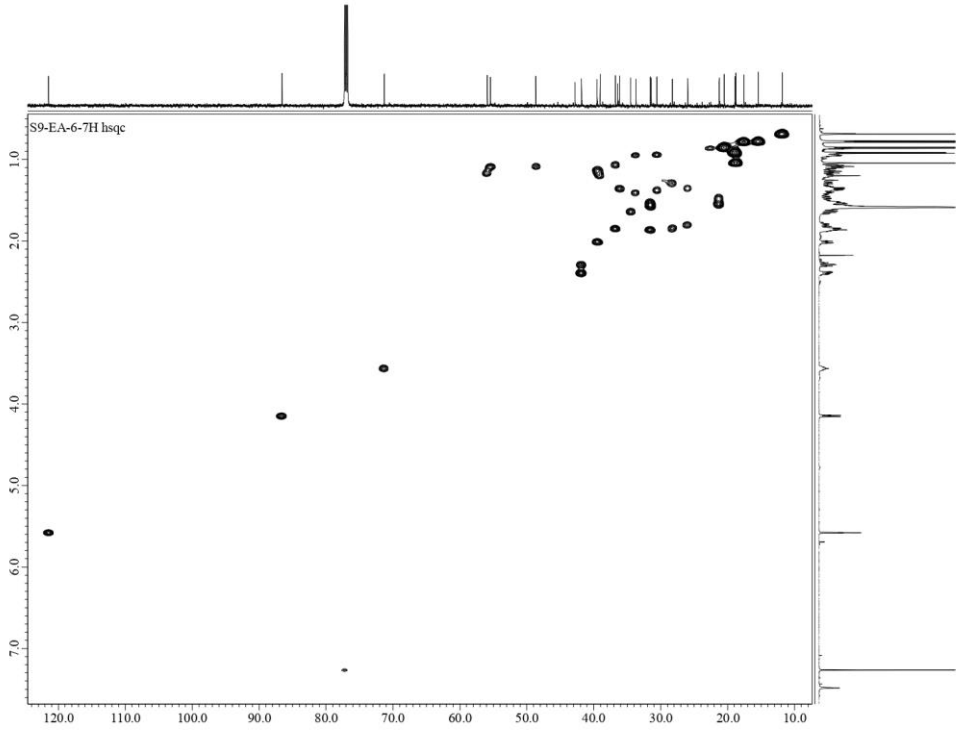

Figure S41. HSQC spectrum of compound **5** in $CDCl_3$

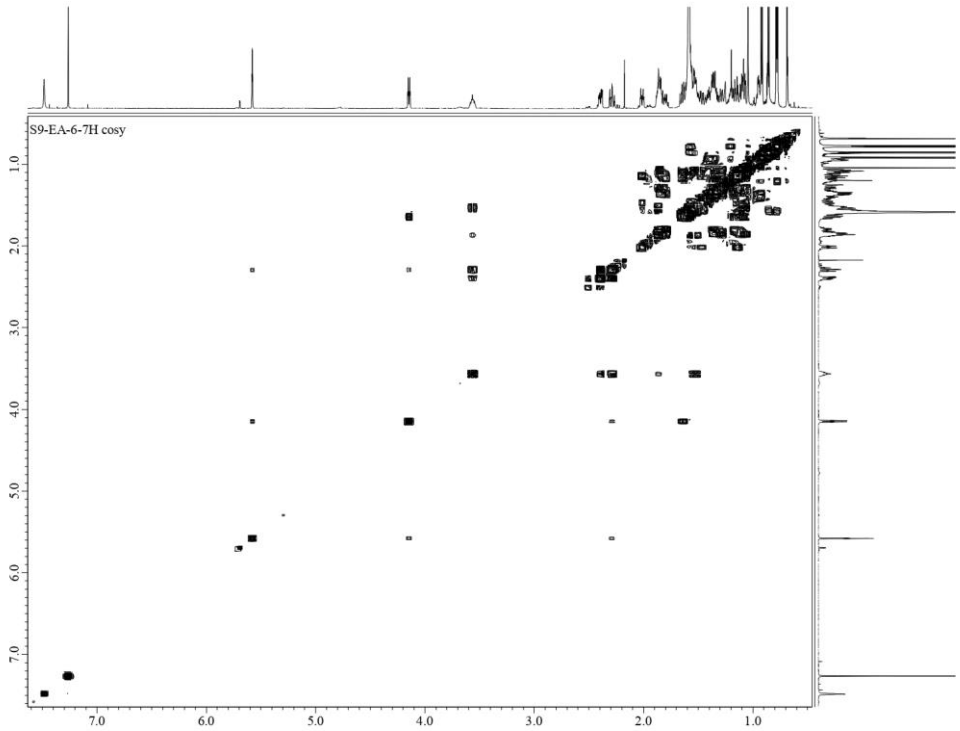

Figure S42. ^{1}H-^{1}H COSY spectrum of compound **5** in $CDCl_3$

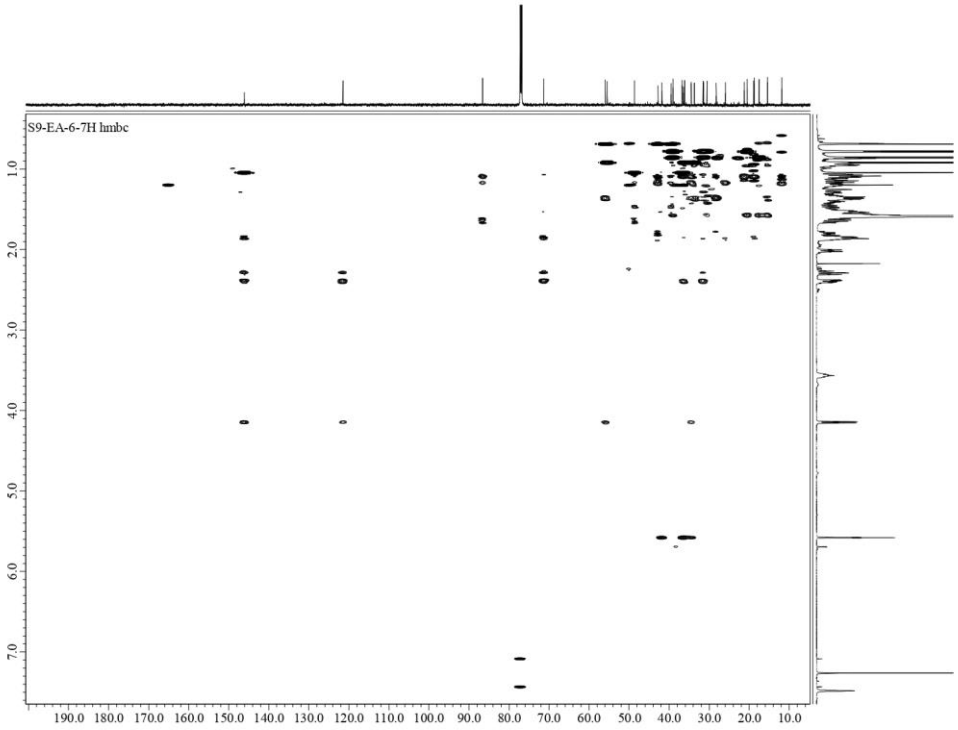

Figure S43. HMBC spectrum of compound **5** in $CDCl_3$

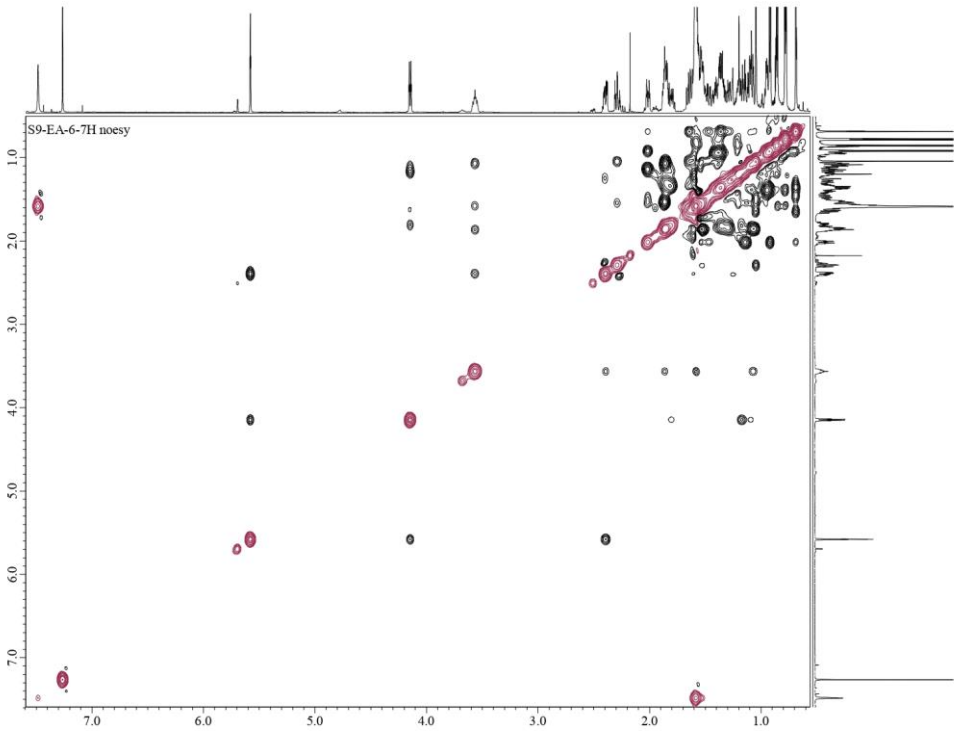

Figure S44. NOESY spectrum of compound **5** in $CDCl_3$

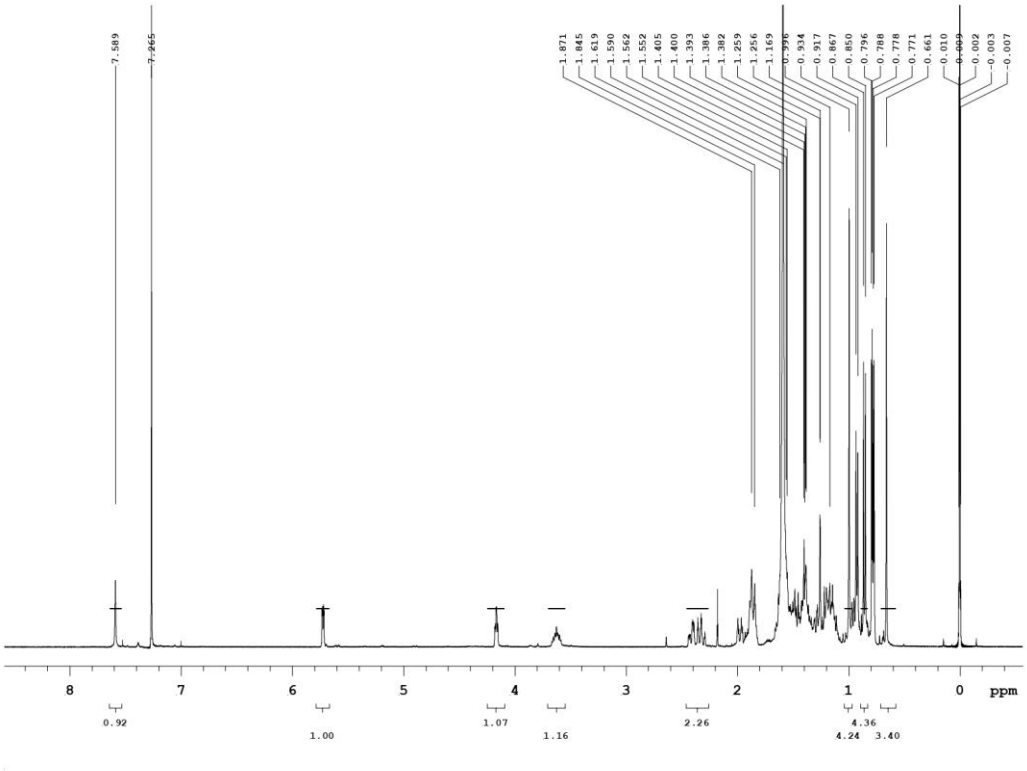

Figure S45. ^{1}H NMR spectrum (400MHz) of compound **6** in $CDCl_3$

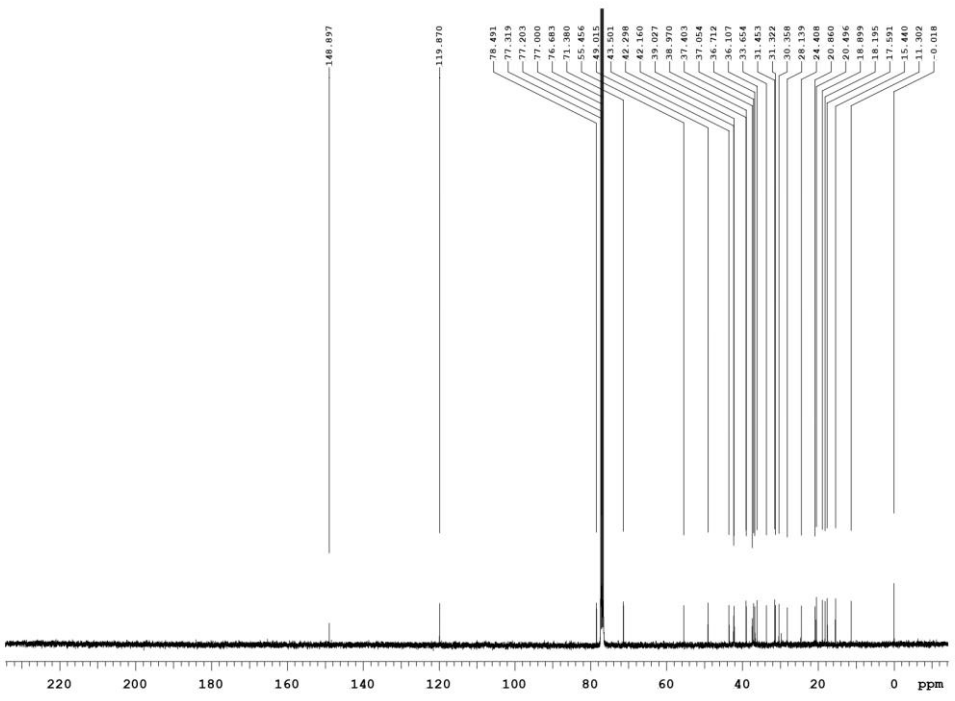

Figure S46. ^{13}C NMR spectrum (100 MHz) of compound **6** in $CDCl_3$

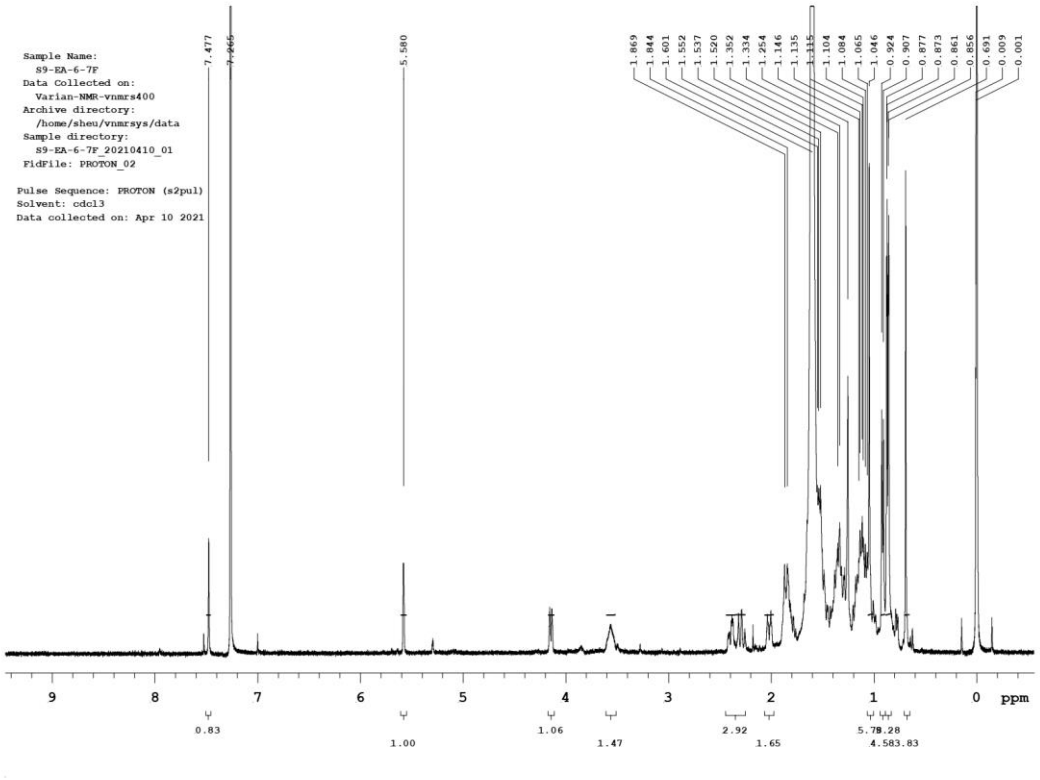

Figure S47. ^{1}H NMR spectrum (400MHz) of compound **7** in $CDCl_3$

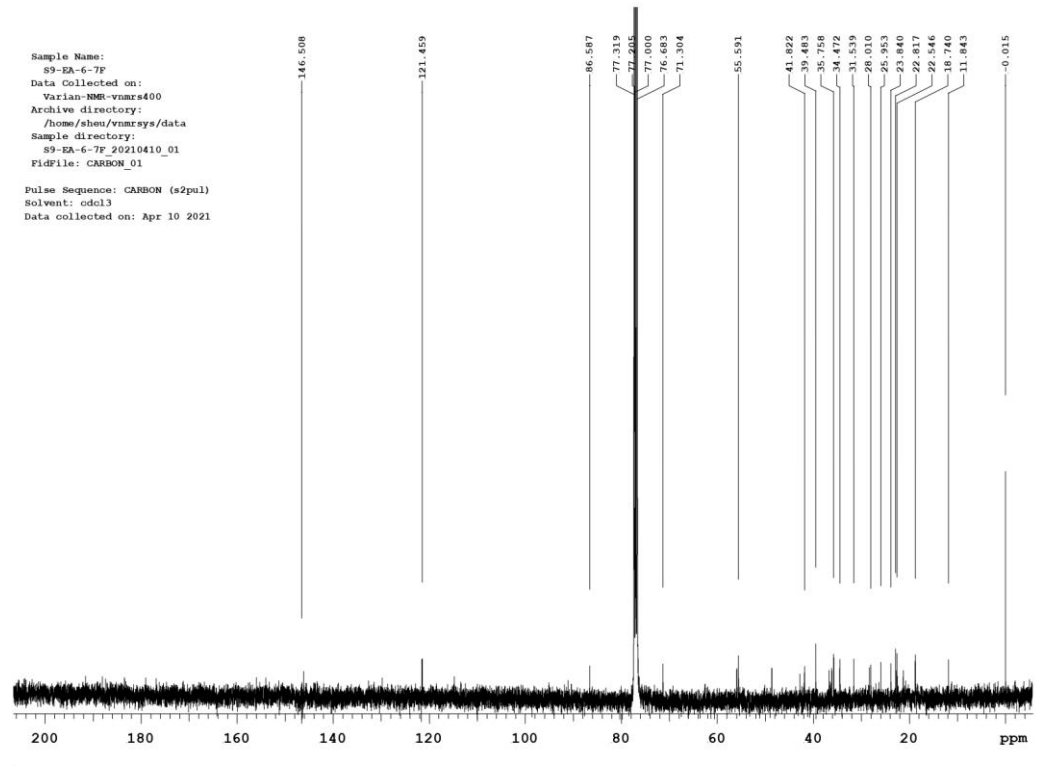

Figure S48. ^{13}C NMR spectrum (100 MHz) of compound **7** in $CDCl_3$

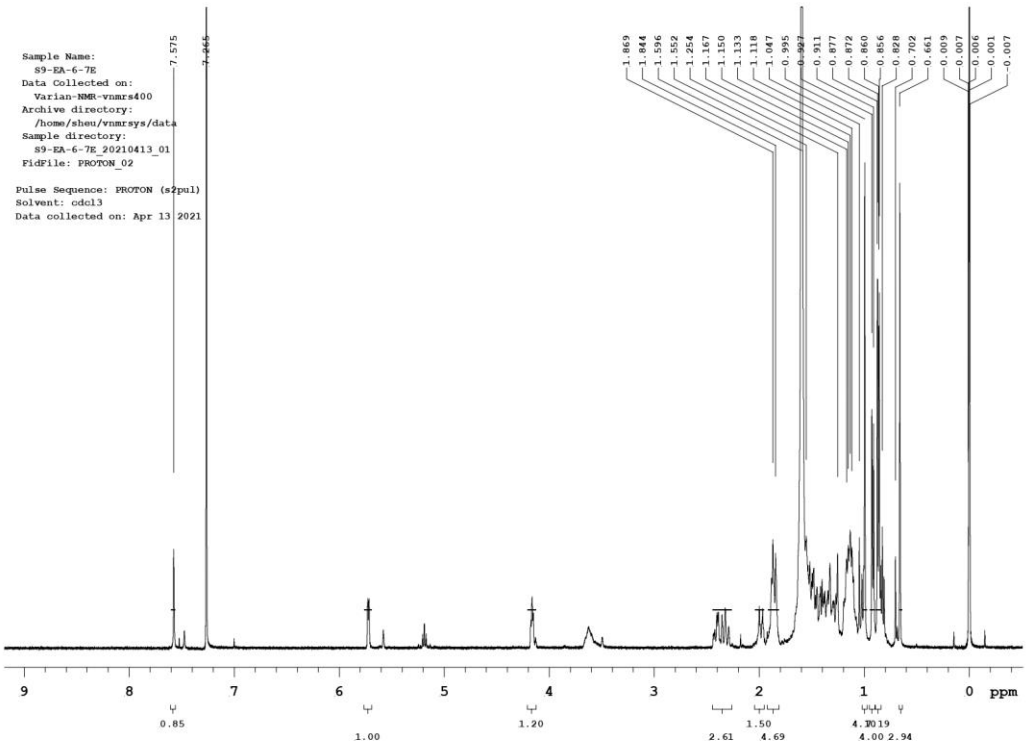

Figure S49. ^{1}H NMR spectrum (400MHz) of compound **8** in $CDCl_3$

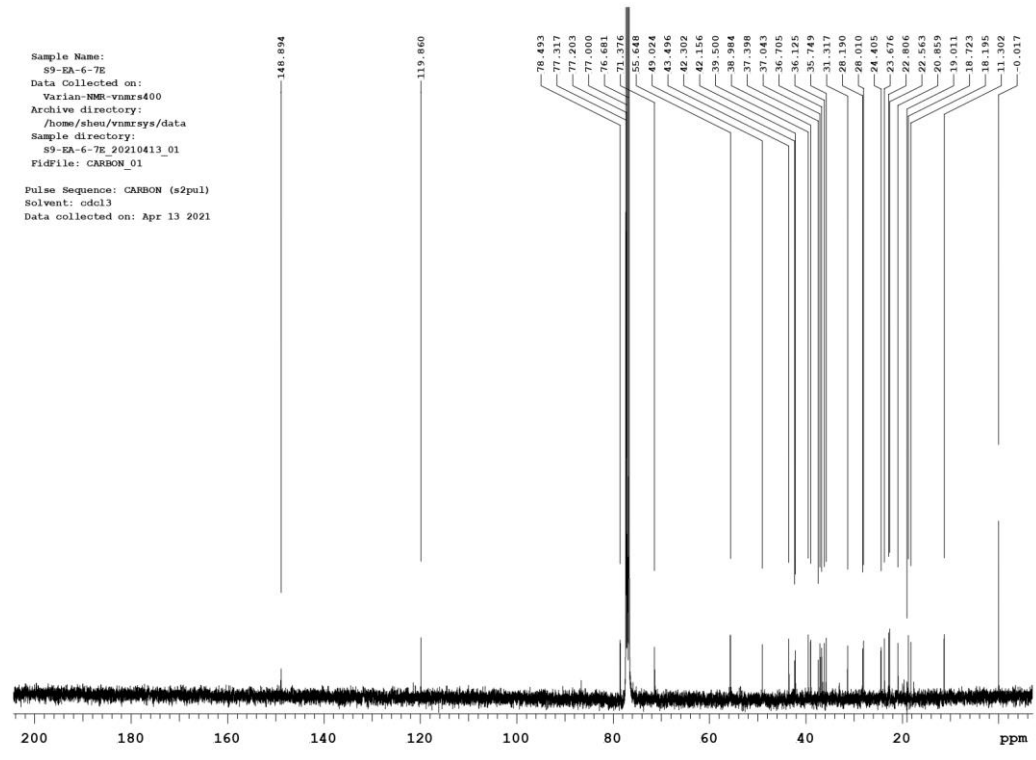

Figure S50. ^{13}C NMR spectrum (100 MHz) of compound **8** in $CDCl_3$

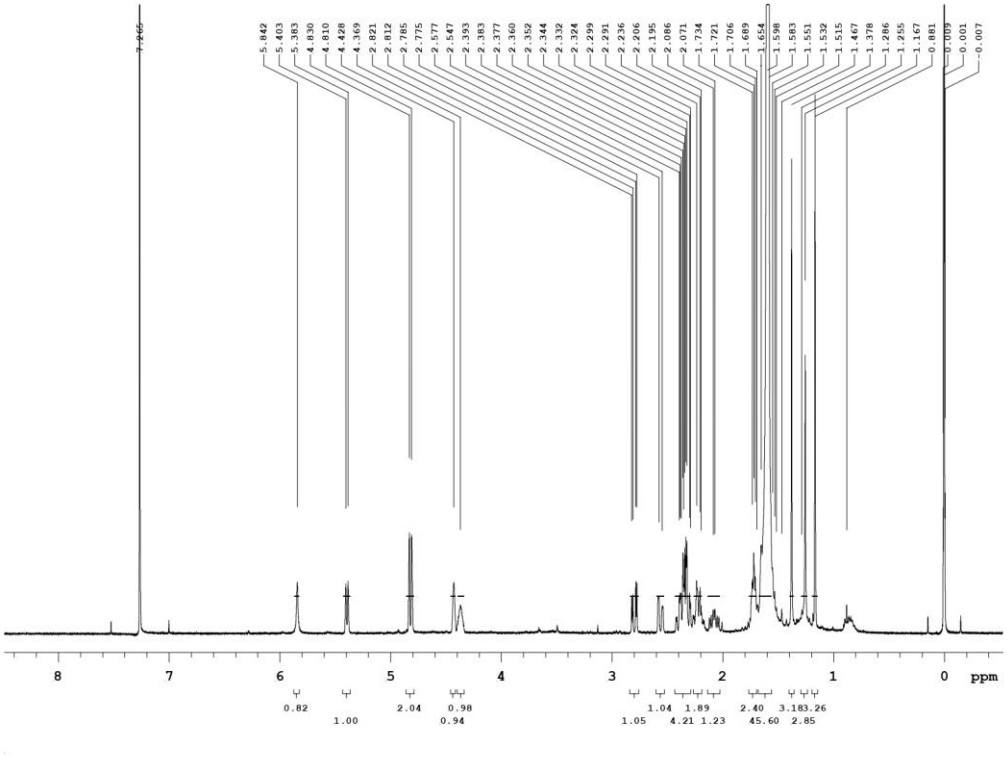

Figure S51. ^{1}H NMR spectrum (400MHz) of compound **9** in $CDCl_3$

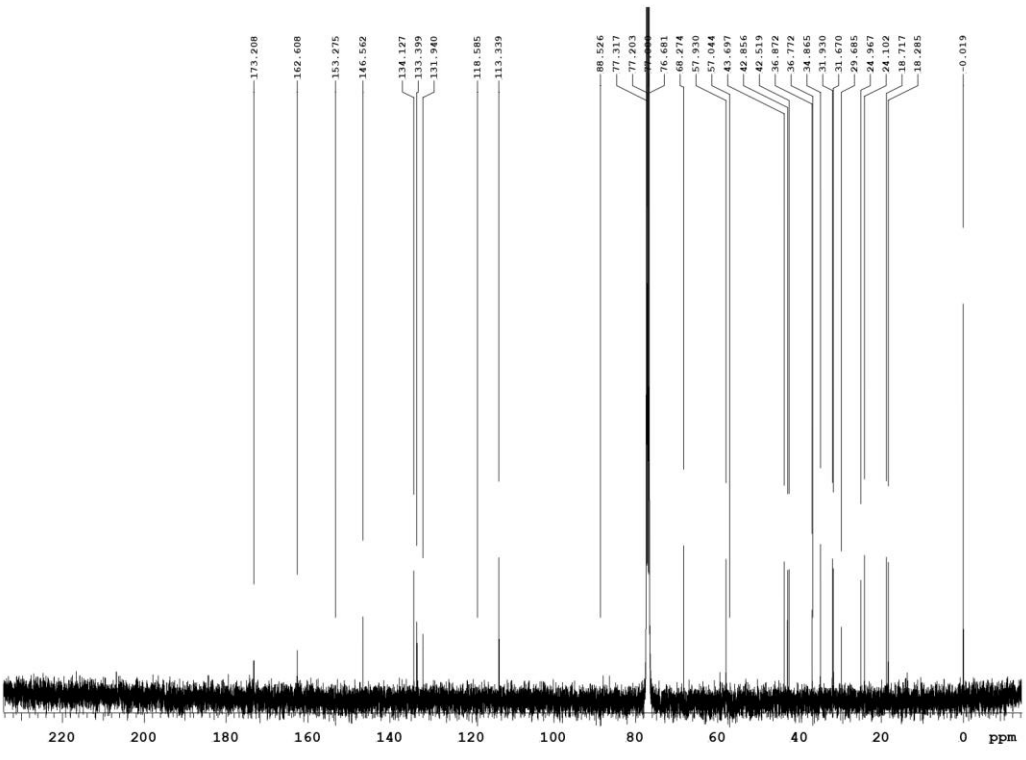

Figure S52. ^{13}C NMR spectrum (100 MHz) of compound **9** in $CDCl_3$

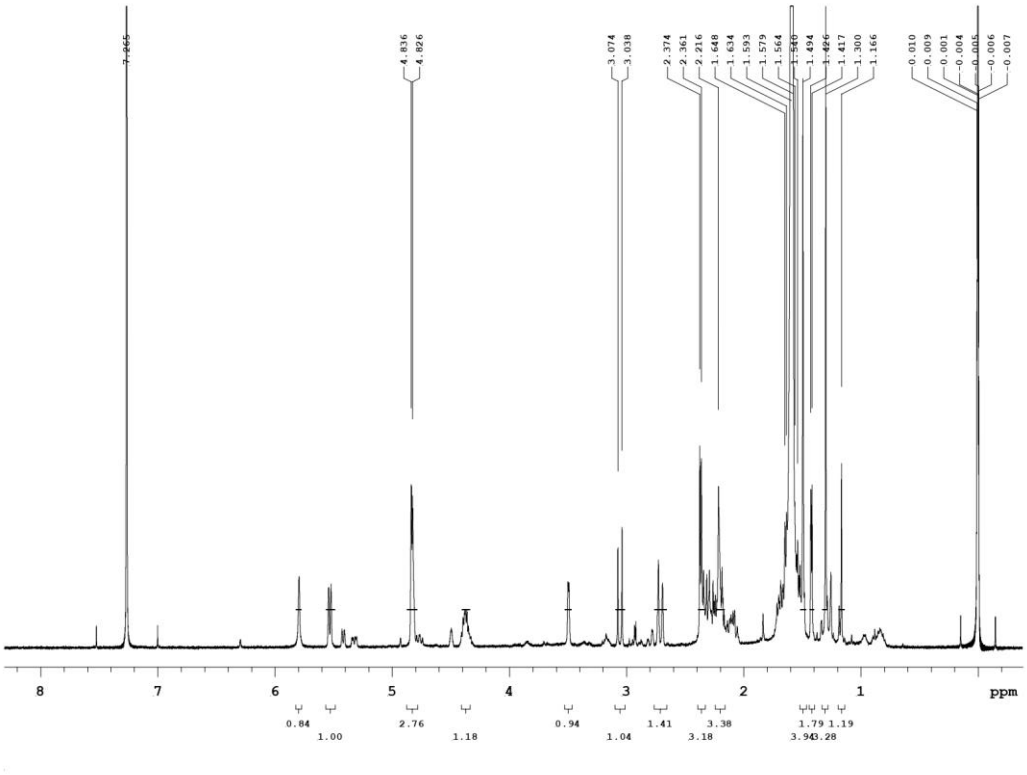

Figure S53. ^{1}H NMR spectrum (400MHz) of compound **10** in $CDCl_3$

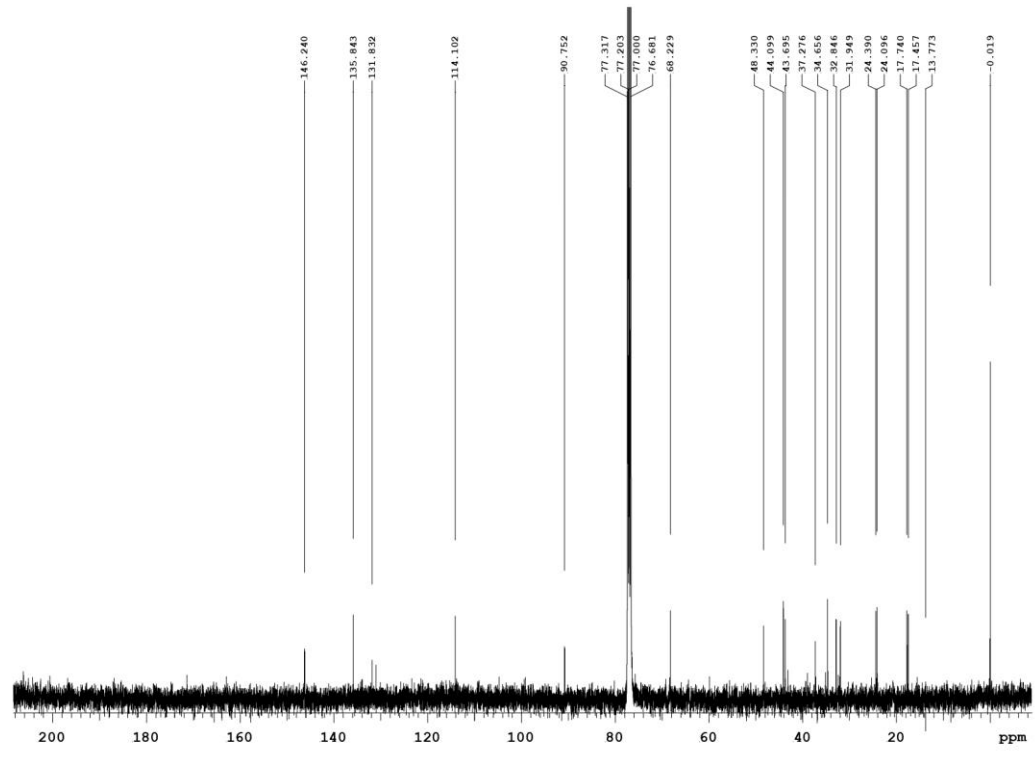

Figure S54. ^{13}C NMR spectrum (100 MHz) of compound **10** in $CDCl_3$

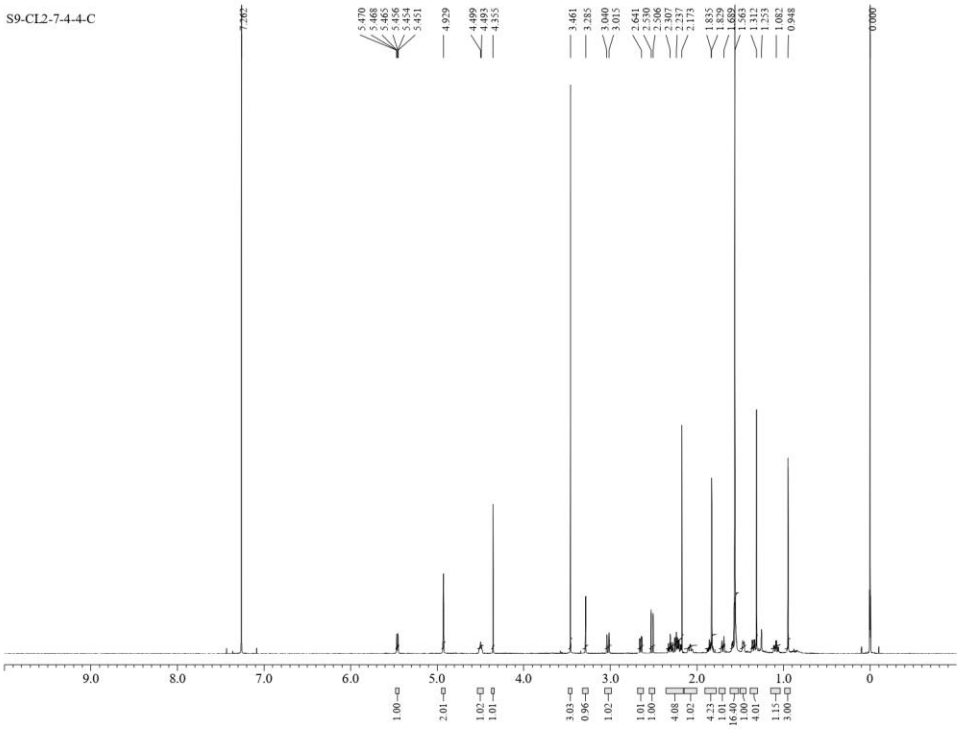

Figure S55. ^{1}H NMR spectrum (600MHz) of compound **11** in $CDCl_3$

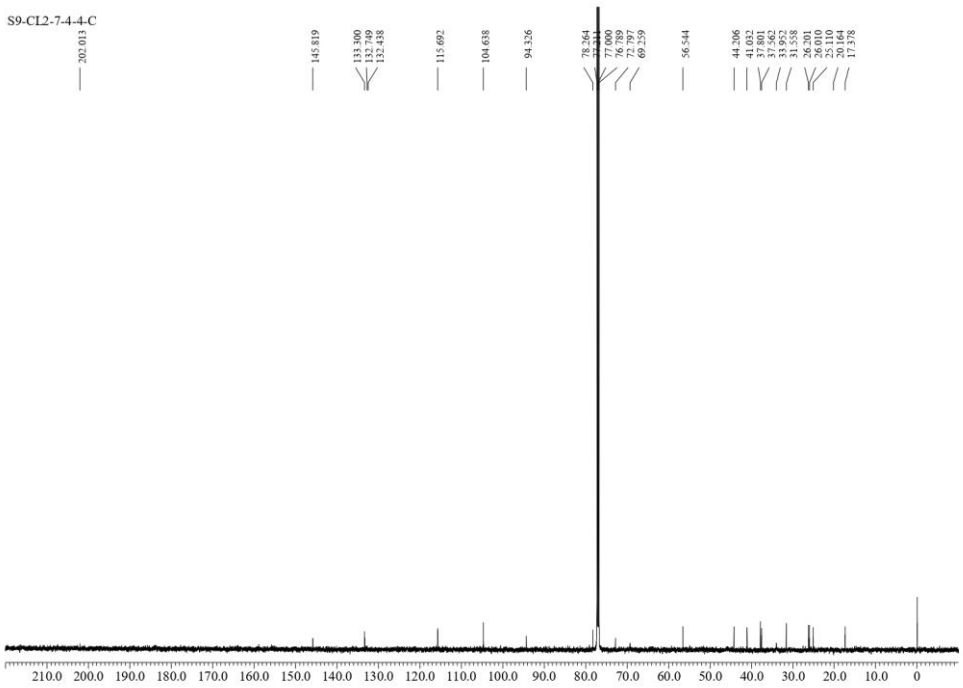

Figure S56. ^{13}C NMR spectrum (150 MHz) of compound **11** in $CDCl_3$

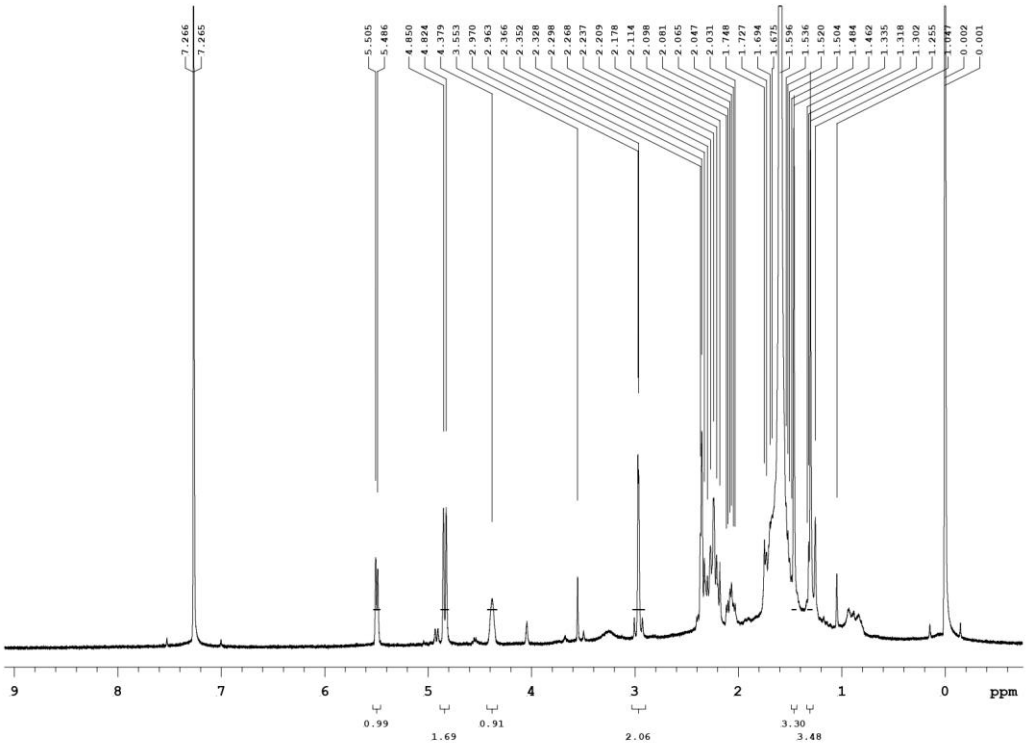

Figure S57. ^{1}H NMR spectrum (400MHz) of compound **12** in $CDCl_3$

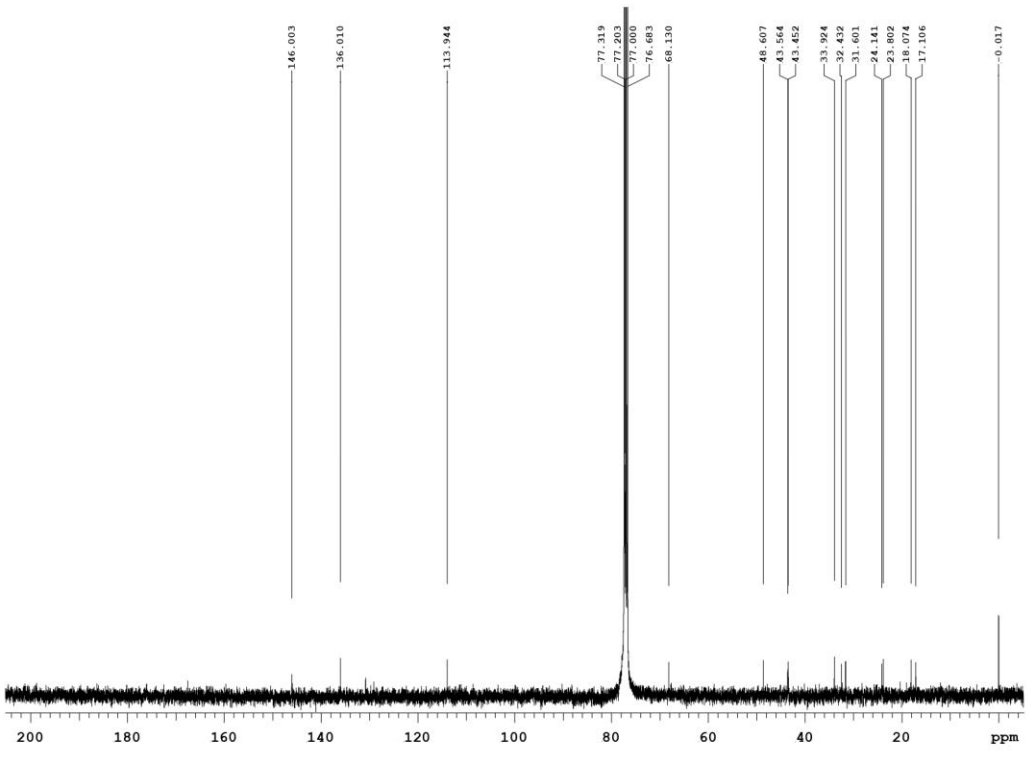

Figure S58. ^{13}C NMR spectrum (100 MHz) of compound **12** in $CDCl_3$

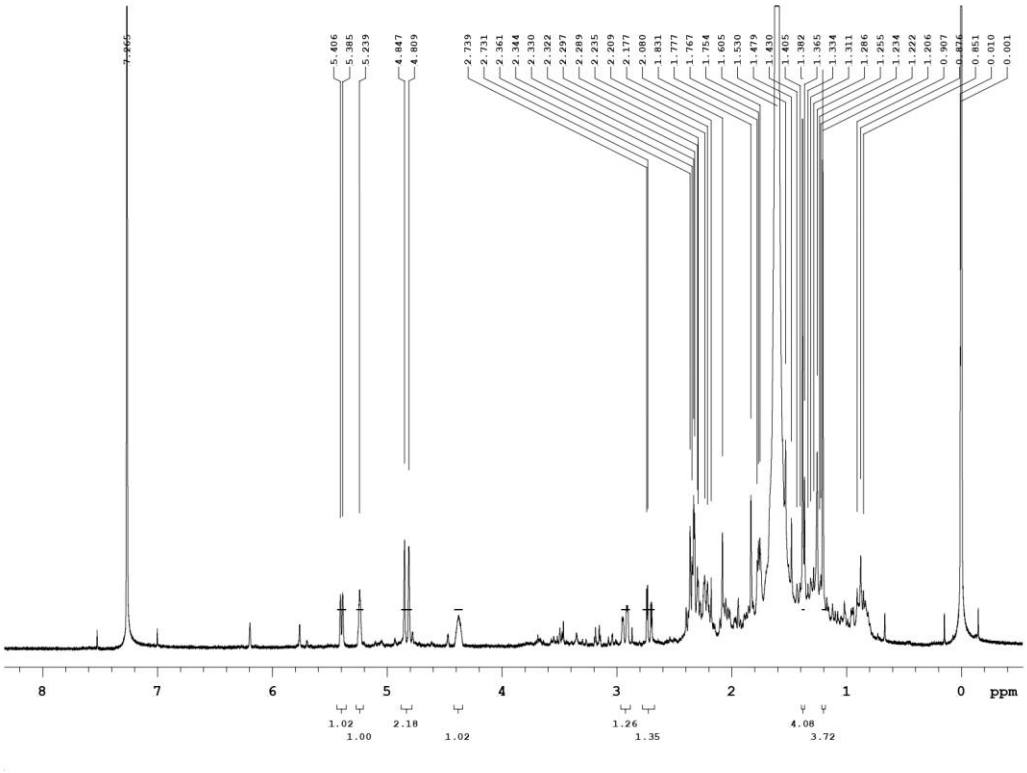

Figure S59. ^{1}H NMR spectrum (400MHz) of compound **13** in $CDCl_3$

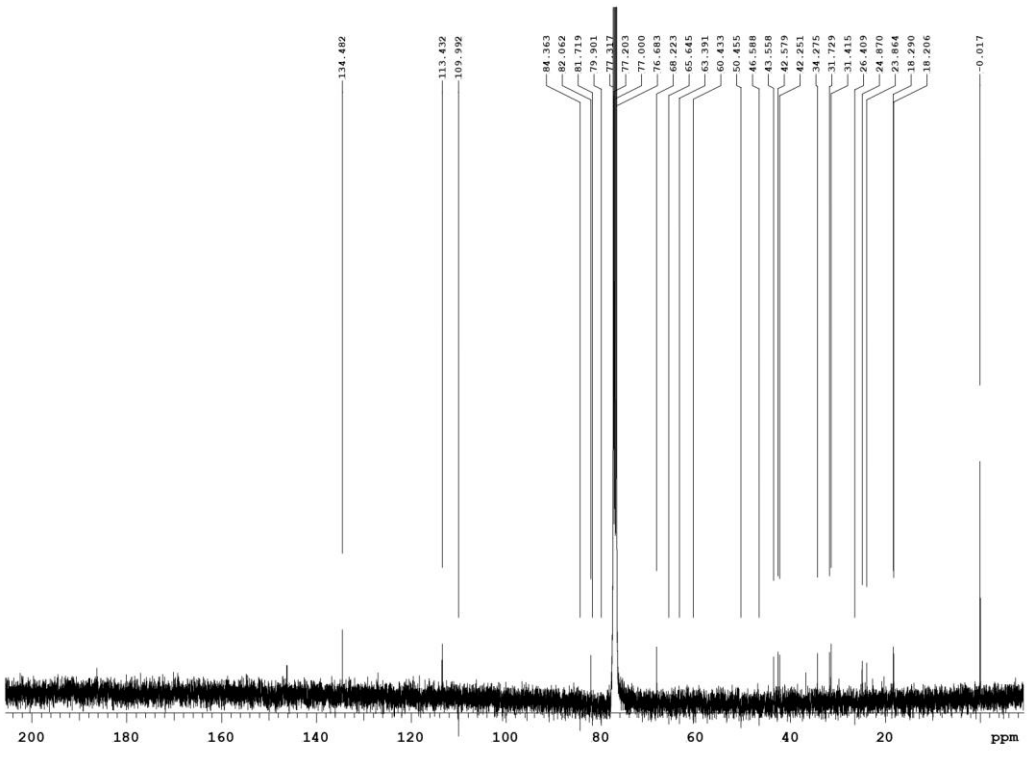

Figure S60. ^{13}C NMR spectrum (100 MHz) of compound **13** in $CDCl_3$

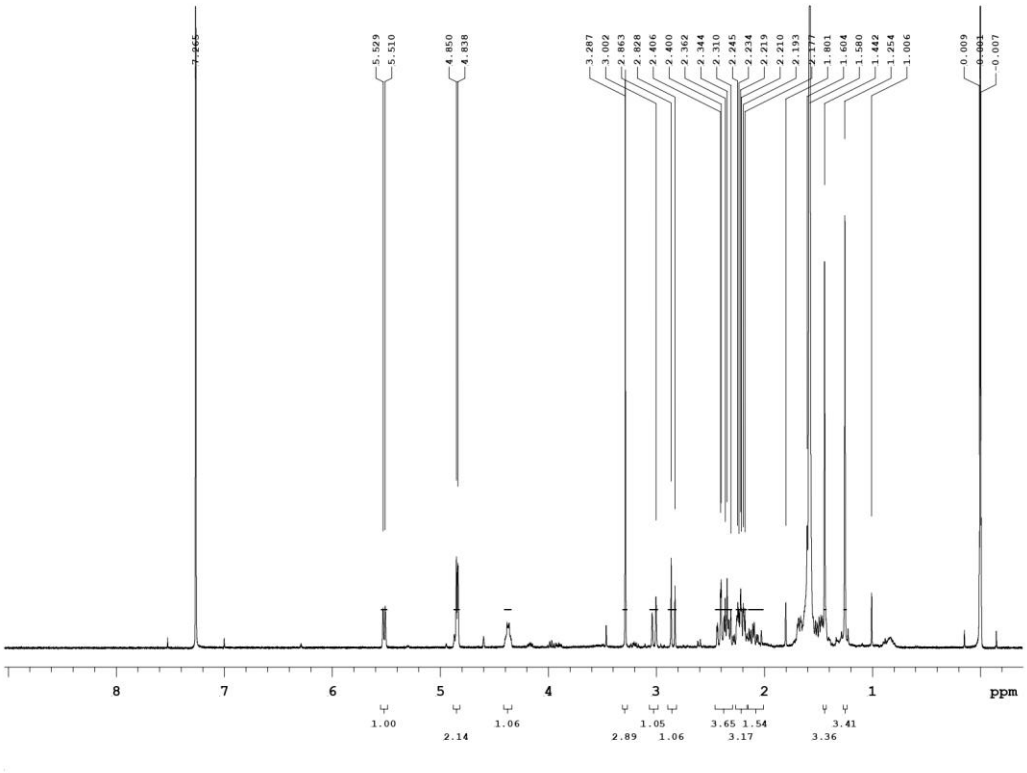

Figure S61. ^{1}H NMR spectrum (400MHz) of compound **14** in $CDCl_3$

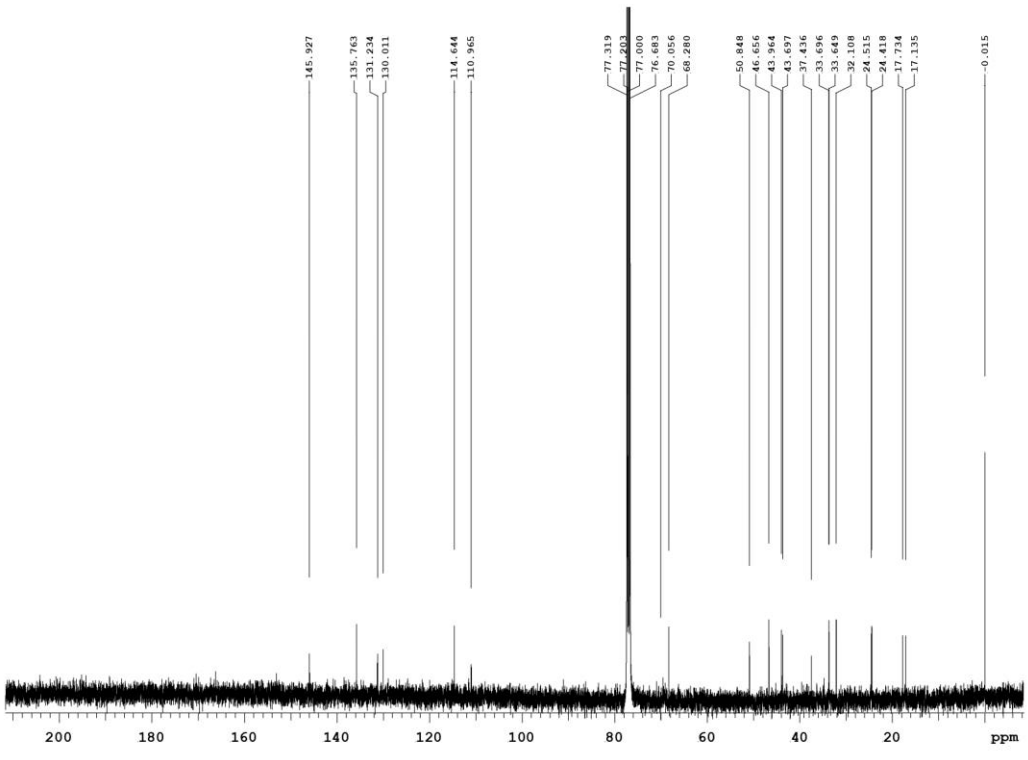

Figure S62. ^{13}C NMR spectrum (100 MHz) of compound **14** in $CDCl_3$

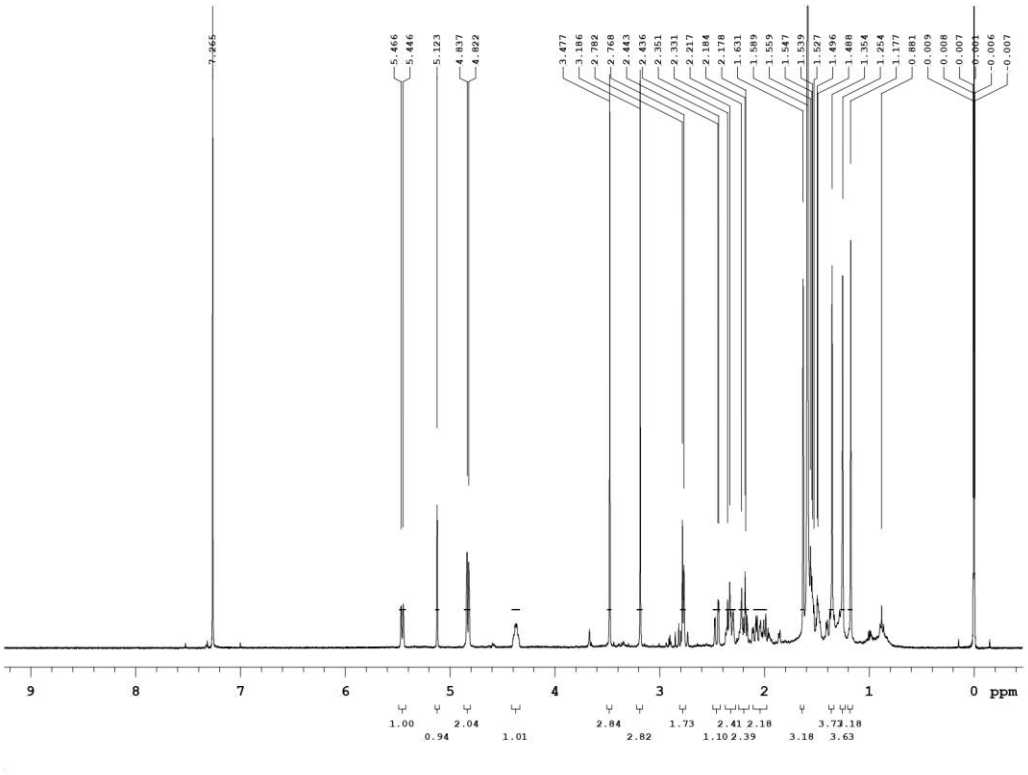

Figure S63. ^{1}H NMR spectrum (400MHz) of compound **15** in $CDCl_3$

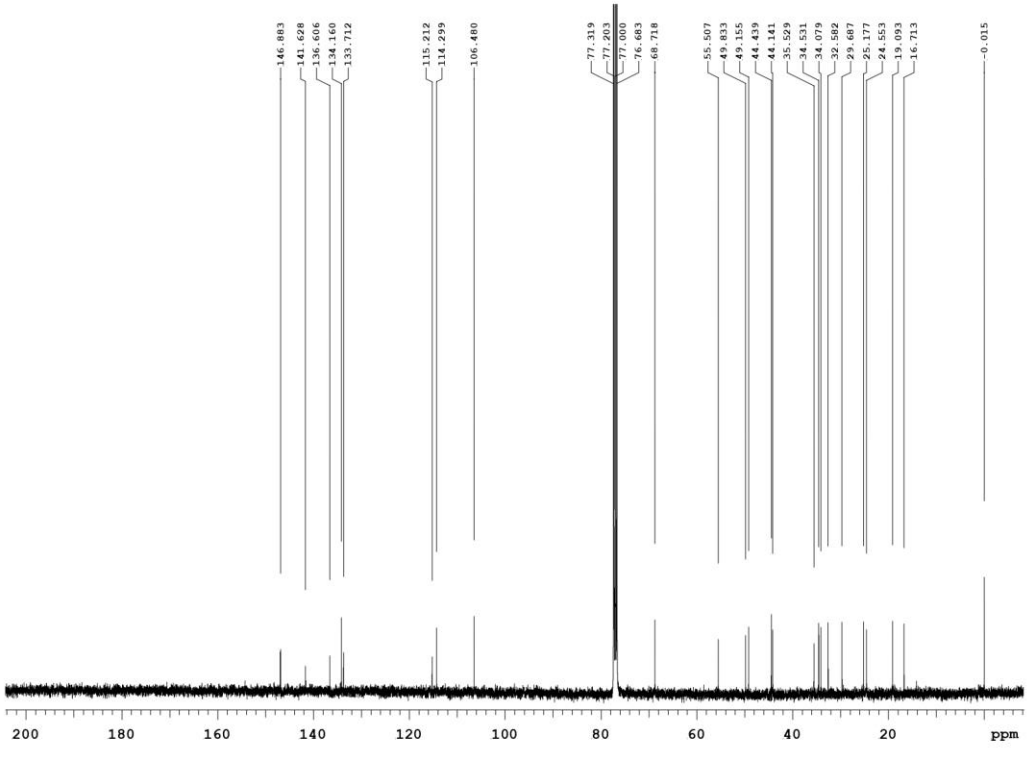

Figure S64. ^{13}C NMR spectrum (100 MHz) of compound **15** in $CDCl_3$

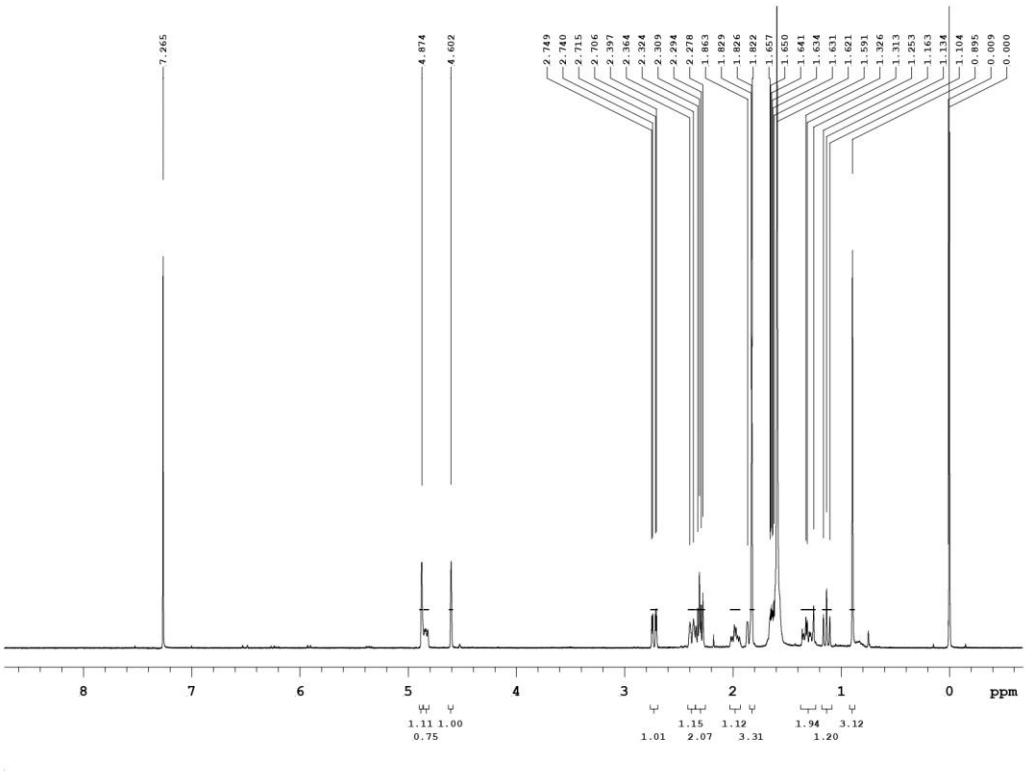

Figure S65. ^{1}H NMR spectrum (400MHz) of compound **16** in $CDCl_3$

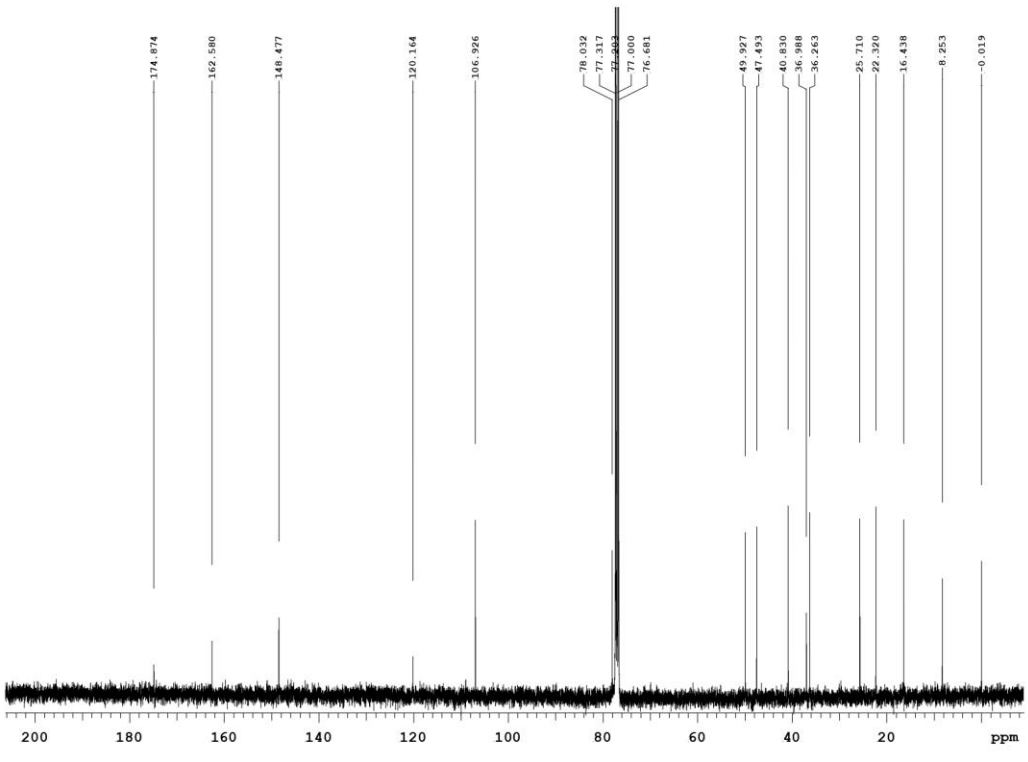

Figure S66. ^{13}C NMR spectrum (100 MHz) of compound **16** in $CDCl_3$

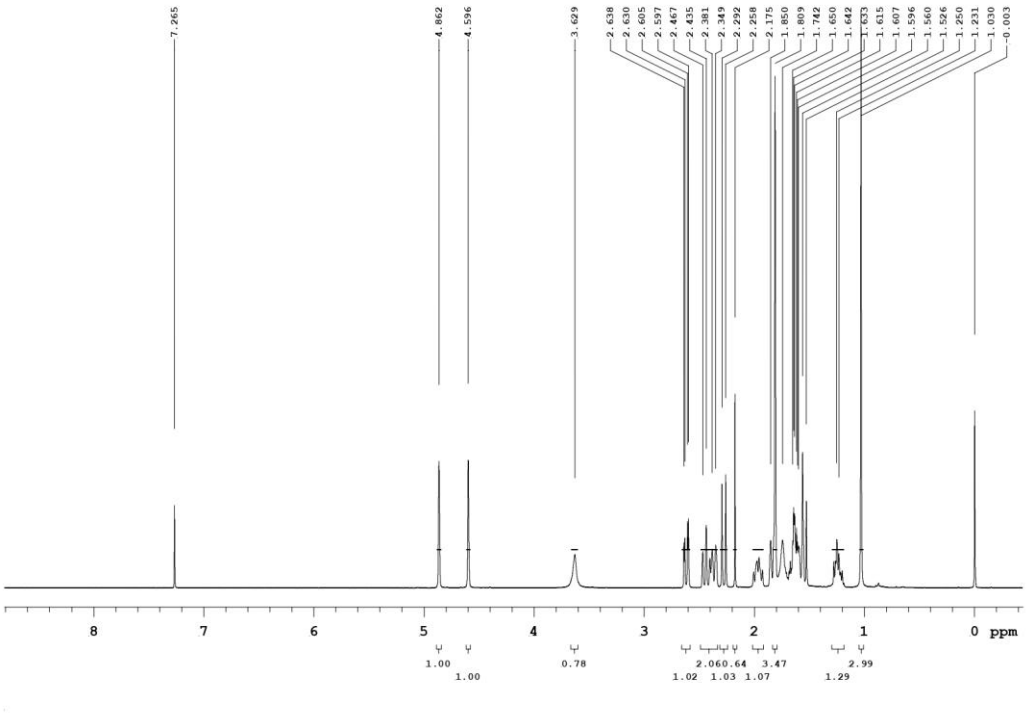

Figure S67. ^{1}H NMR spectrum (400MHz) of compound **17** in $CDCl_3$

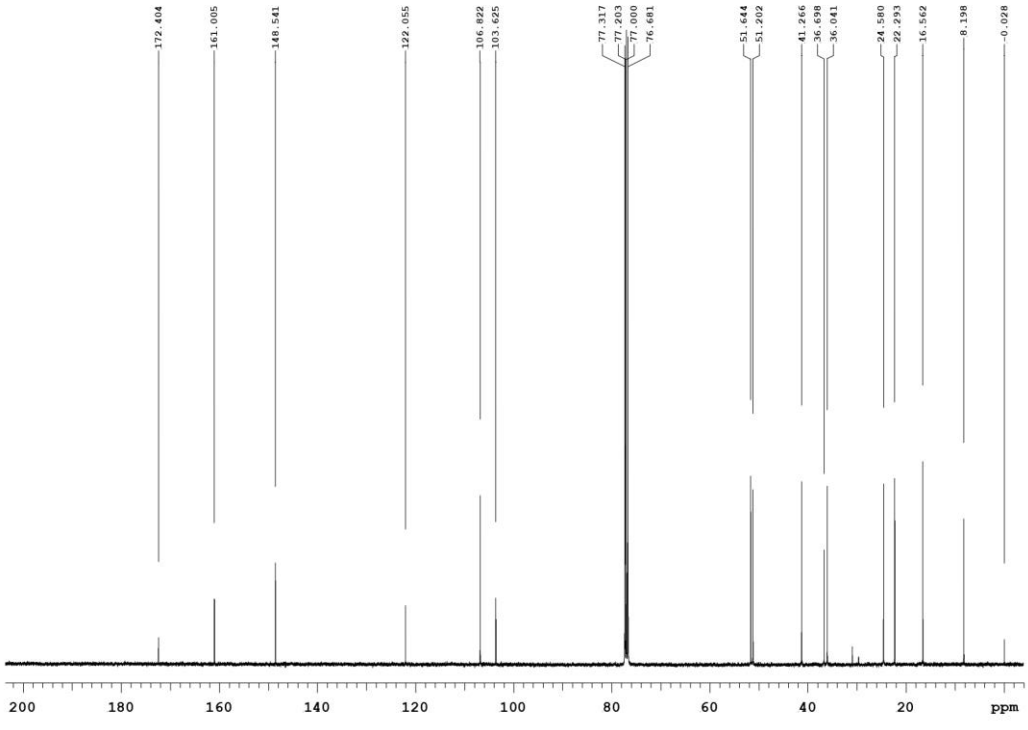

Figure S68. ^{13}C NMR spectrum (100 MHz) of compound **17** in $CDCl_3$

Table S1. The cytotoxicity data of compounds **1–16** and **1a**.

Cell lines IC_{50} (μg/mL)			
Compounds	HepG2	MDA-MB231	A549
1	> 20	> 20	> 20
1a	> 20	> 20	> 20
2	> 20	> 20	> 20
3	> 20	> 20	> 20
4	> 20	> 20	> 20
5	> 20	15.40	18.74
6	> 20	> 20	> 20
7	> 20	> 20	> 20
8	> 20	> 20	> 20
9	> 20	> 20	> 20
10	> 20	> 20	> 20
11	> 20	> 20	> 20
12	> 20	> 20	> 20
13	> 20	> 20	> 20
14	> 20	> 20	> 20
15	> 20	> 20	> 20
16	> 20	> 20	> 20
Doxorubicin	0.37	0.30	0.15

Table S2. Antibacterial activity (zone of inhibition in mm).

	Inhibition zone (mm)									
Compounds (25 μg/disk)	*B. s.*	*S. a.*	*S. e.*	*E. a.*	*E. c.*	*K. p.*	*S. m.*	*S. s.*	*S. t.*	*Y. e.*
3	–	–	–	–	–	–	–	–	–	–
4	–	–	–	–	–	–	–	–	–	–
5	–	–	6	–	–	5	–	–	–	–
6	–	–	–	–	–	–	–	–	–	–
7	–	–	–	–	–	–	–	–	–	–
9	–	–	–	–	–	9	–	–	–	–
12	–	–	–	–	–	–	–	–	–	–
Ampicillin	9	12	10	5	5	5	8	9	8	18

–: Inactive

Ampicillin: Positive control

B. s.: *Bacillus subtilis* (ATCC6051)

S. a.: *Staphylococcus aureus* (ATCC9144)

S. e.: *Salmonella enterica* (ATCC13076)

E. a.: *Enterobacter aerogenes* (ATCC13048)

E. c.: *Escherichia coli* (ATCC25922)

K. p.: *Klebsiella pneumoniae* (ATCC10031)

S. m.: *Serratia marcescens* (ATCC25419)

S. s.: *Shigella sonnei* (ATCC11060)

S. t.: *Salmonella typhimurium* (ATCC14028)

Y. e.: *Yersinia enterocolitica* (ATCC23715)

Table S3. Inhibitory effects of compounds **1–10**, **1a**, **14**, and **15** on TNF-α expression, PGE_2, and NO production in LPS induced dendritic cells.

	Inh %[1]		
Compounds	TNF-α	PGE_2	NO
1	2.3 ± 2.0	2.9 ± 1.5	11.0 ± 2.4
1a	–0.1 ± 1.6	–0.8 ± 5.9	14.0 ± 1.5 *
2	7.3 ± 3.2	12.8 ± 3.5	19.6 ± 4.0 ***
3	8.0 ± 3.0	11.4 ± 2.1	33.8 ± 1.5 ***
4	3.8 ± 2.7	2.4 ± 2.1	34.9 ± 3.9 ***
5	0.8 ± 1.8	3.5 ± 4.2	16.0 ± 3.7 **
6	5.0 ± 2.9	–4.4 ± 0.4	14.6 ± 3.9 *
7	1.9 ± 5.1	–7.6 ± 2.8	3.7 ± 5.7
8	0.2 ± 0.5	–4.9 ± 3.2	10.2 ± 3.2
9	3.3 ± 1.7	1.2 ± 5.9	16.8 ± 4.7 **
10	–3.9 ± 1.1	–11.5 ± 4.6	11.9 ± 2.7
14	5.2 ± 1.8	–8.8 ± 6.3	24.8 ± 1.4***
15	23.6 ± 2.5 ***	21.2 ± 0.9 *	35.0 ± 3.7 ***
DEX[2]	85.6 ± 3.4 ****	–	73.4 ± 1.3 ****

1. Percentage of inhibition (Inh %) at the concentration 100 μM for **1–3**, **5, 7**, **9**, **11**, **14** and **15** and 25 μM for **4**, **6**, and **8** compared with the control group (100 % for stimulated LPS alone). Results are presented as mean ± SEM. (n = 3). * $p < 0.05$, ** $p < 0.01$, *** $p < 0.001$, **** $p < 0.0001$.

2. Positive control: dexamethasone (DEX) at 100 μM.