

SUPPORTING INFORMATION

Article

Isomalabaricane Triterpenes from the Marine Sponge *Rhabdastrella* sp.

Kuei-Hung Lai ^{1,2,3,*}, Zheng-Hao Huang ^{4,5}, Mohamed El-Shazly ^{6,7}, Bo-Rong Peng ^{4,5}, Wen-Chi Wei ^{8,*} and Jui-Hsin Su ^{4,5,*}

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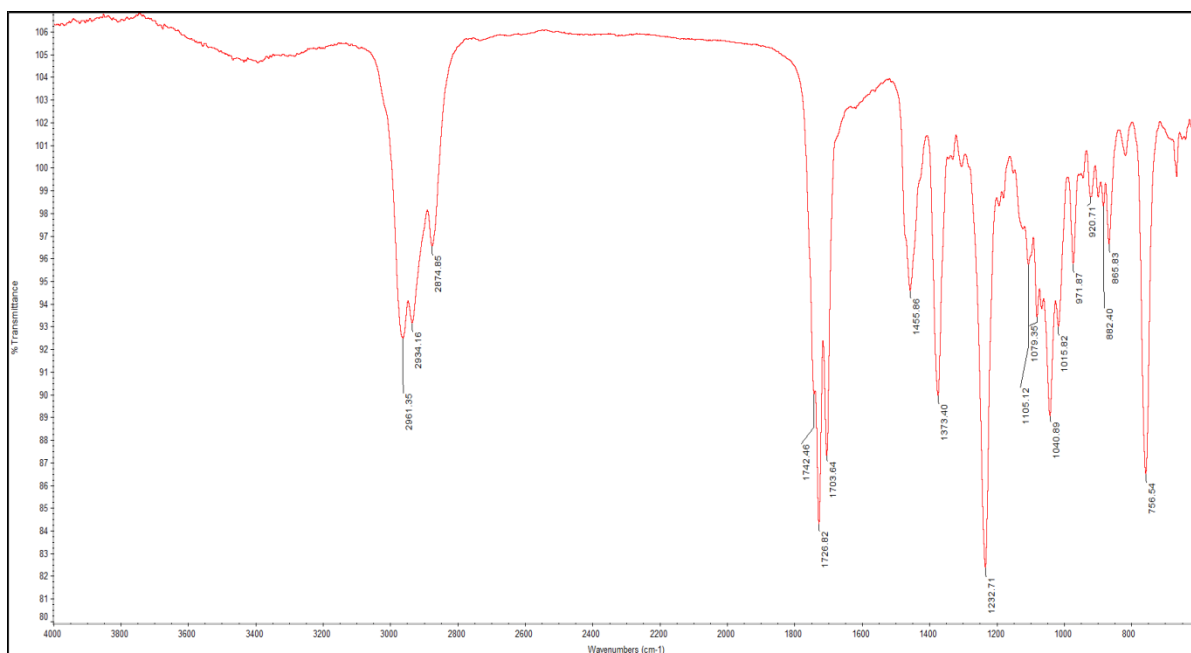


Figure S1. IR spectrum of **1**

F:\Exp_data\...\2018\20181102\38-MSP-2P

2018/11/2 下午 03:06:00

38-MSP-2P #1-20 RT: 0.00-0.06 AV: 20 NL: 3.91E6
T: ITMS + c ESI Full ms [150.00-2000.00]

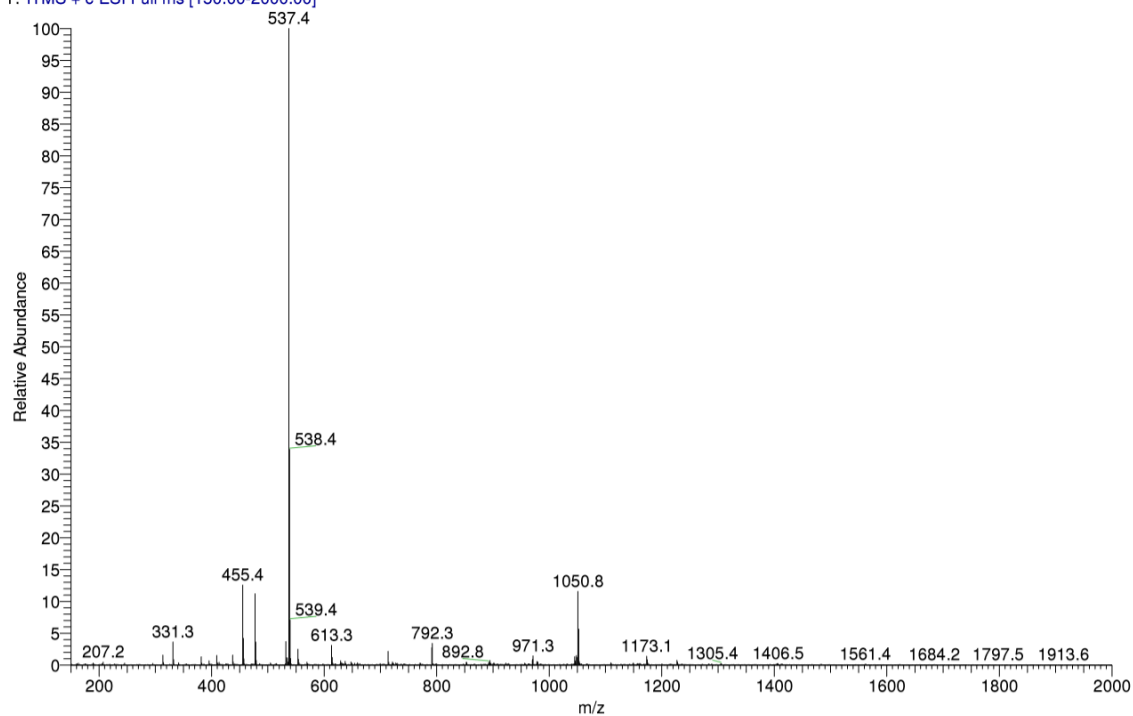


Figure S2. ESIMS spectrum of **1**

35-MSP-2P-H#1-20 RT: 0.00-0.27 AV: 20
T: FTMS + p ESI Full ms [150.00-2000.00]

m/z= 537.2468-537.4527

Isotope Min Max

C-12 0 32

H-1 0 51

O-16 0 5

Na-23 0 1

Charge 1

Mass tolerance 1000.00 ppm

Nitrogen rule not used

RDB equiv -1.00-100.00

max results 1

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
537.3539	48065596.0	100.00	537.3550	-2.09	C ₃₂ H ₅₀ O ₅ Na

Figure S3. HRESIMS spectrum of 1

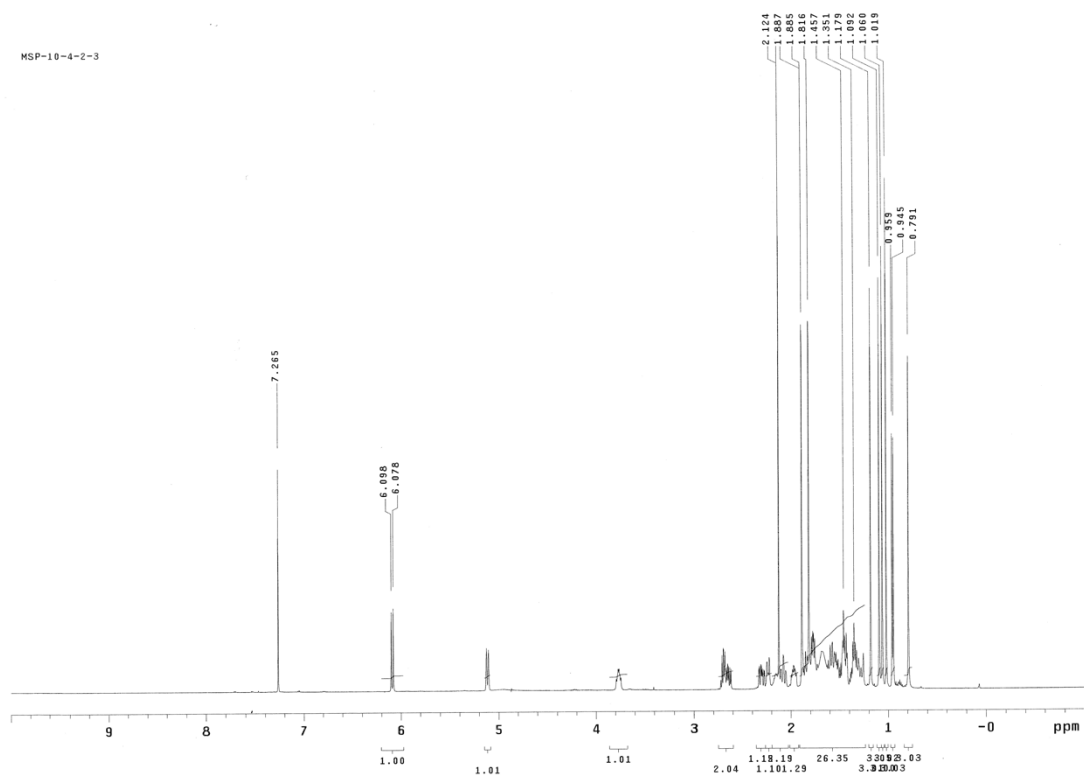


Figure S4. ¹H NMR (500 MHz, CDCl₃) spectrum of 1

MSP-10-4-2-3

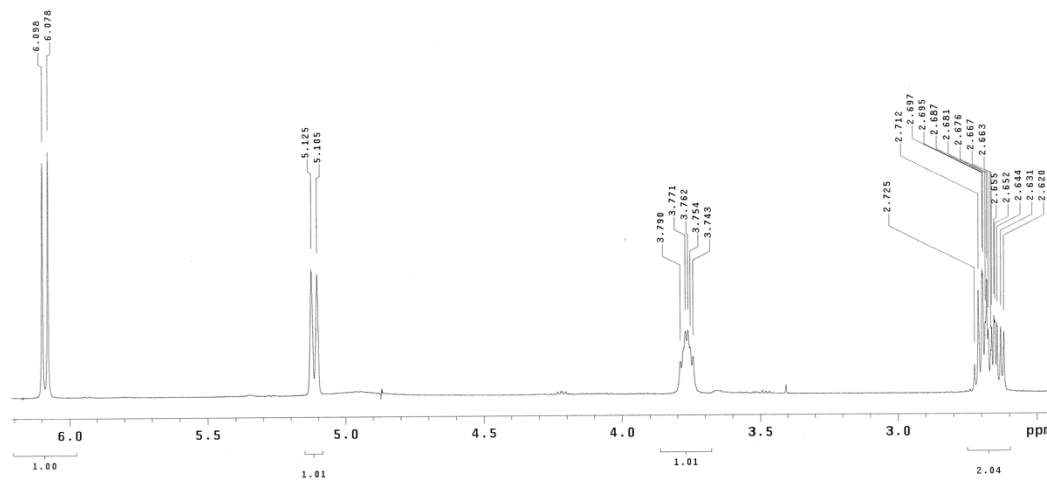


Figure S5. ^1H NMR (500 MHz, CDCl_3) spectrum of **1** (Partial enlarged view)

MSP-10-4-2-3

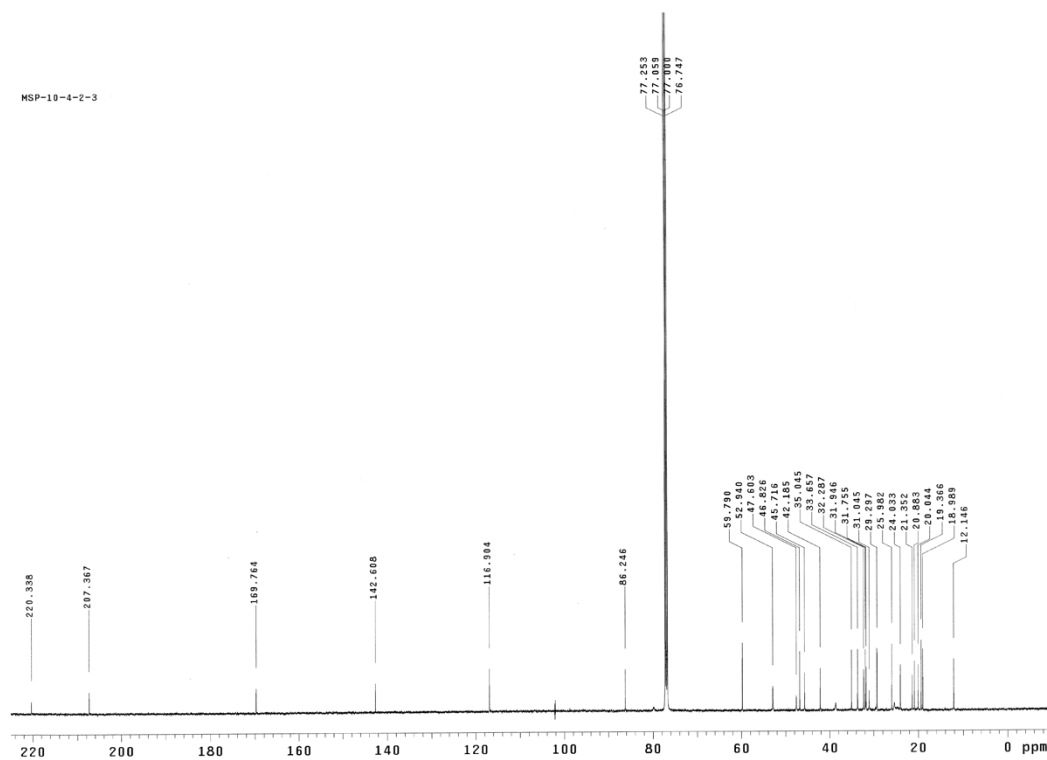


Figure S6. ^{13}C NMR (125 MHz, CDCl_3) spectrum of **1**

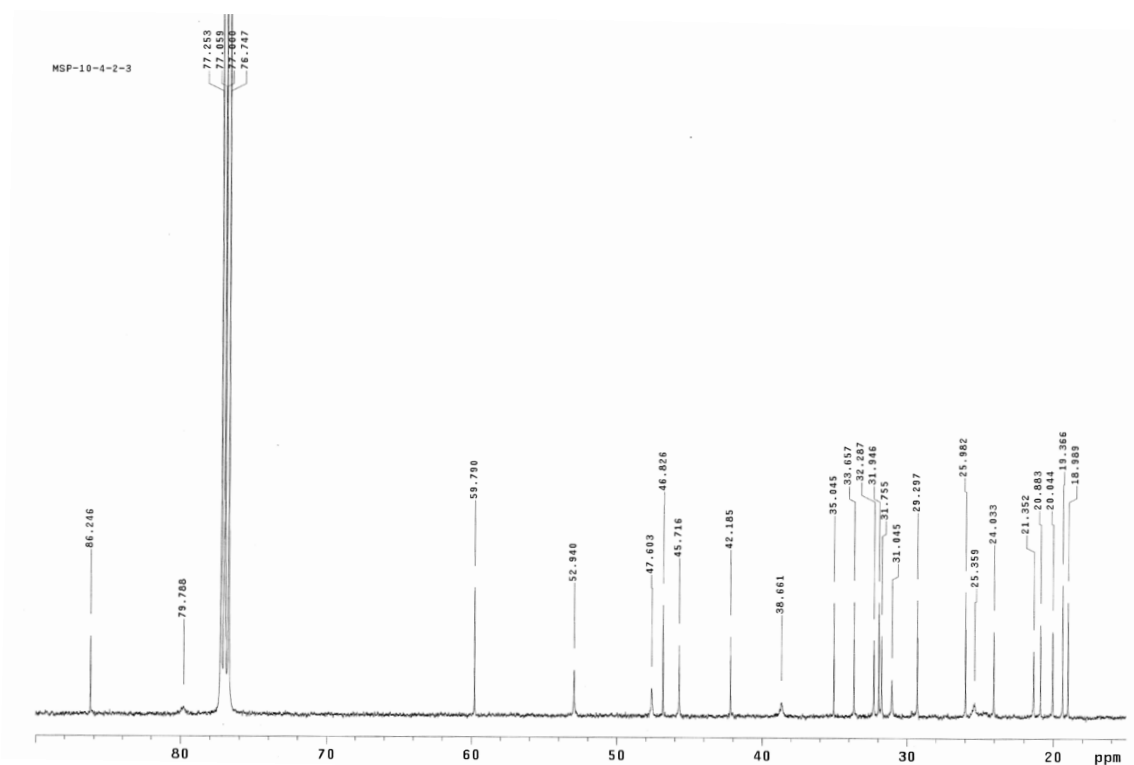


Figure S7. ^{13}C NMR (125 MHz, CDCl_3) spectrum of **1** (Partial enlarged view)

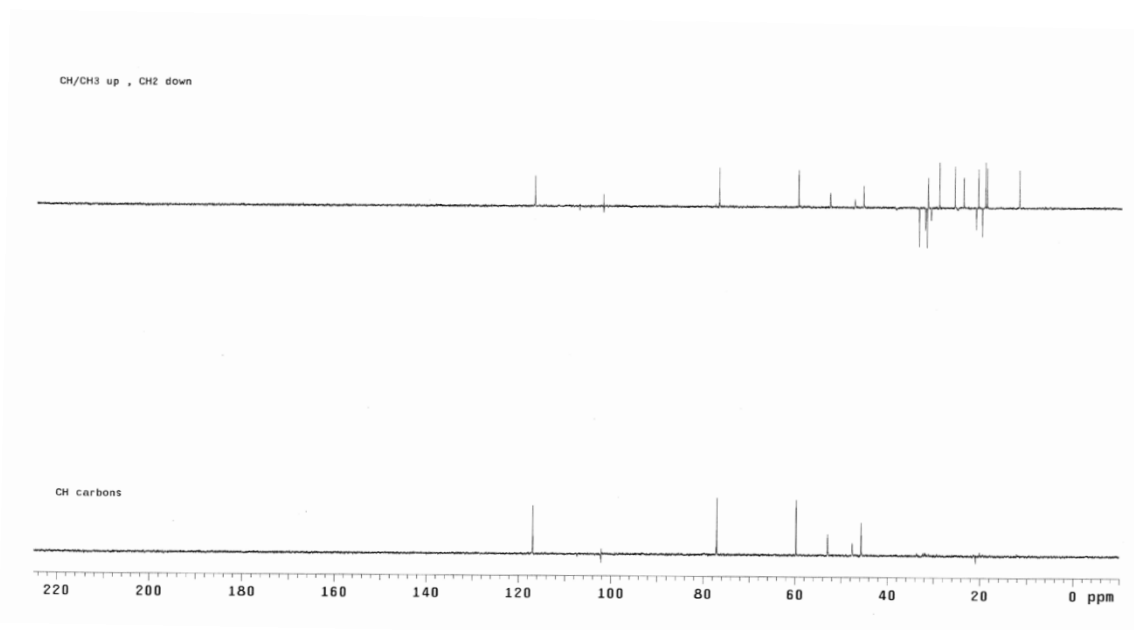


Figure S8. DEPT spectrum of **1**

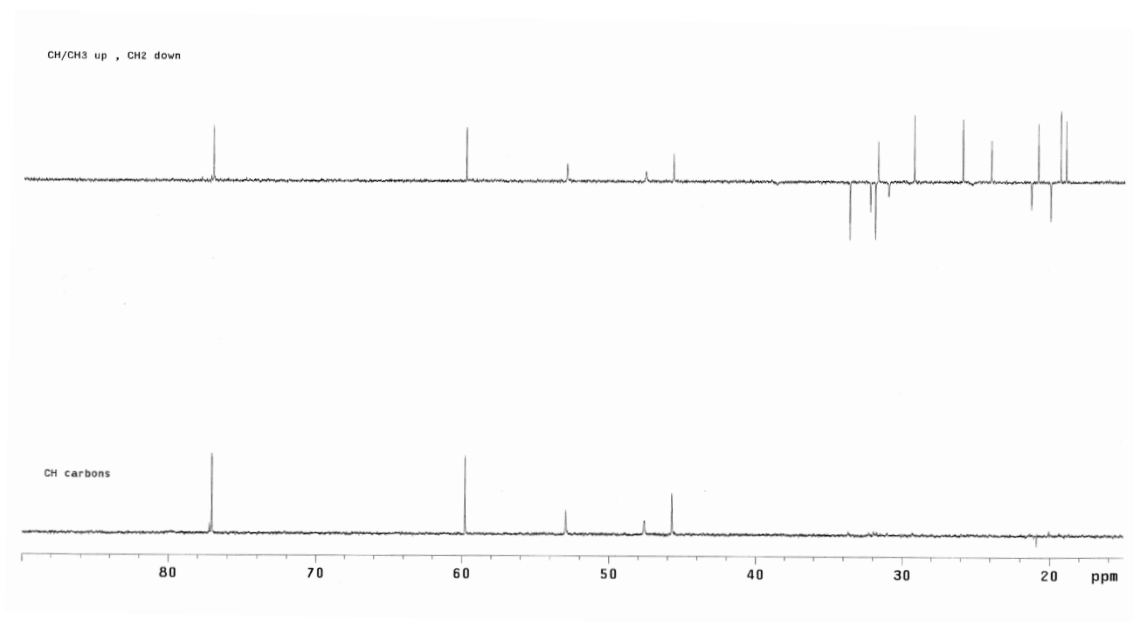


Figure S9. DEPT spectrum of **1** (Partial enlarged view)

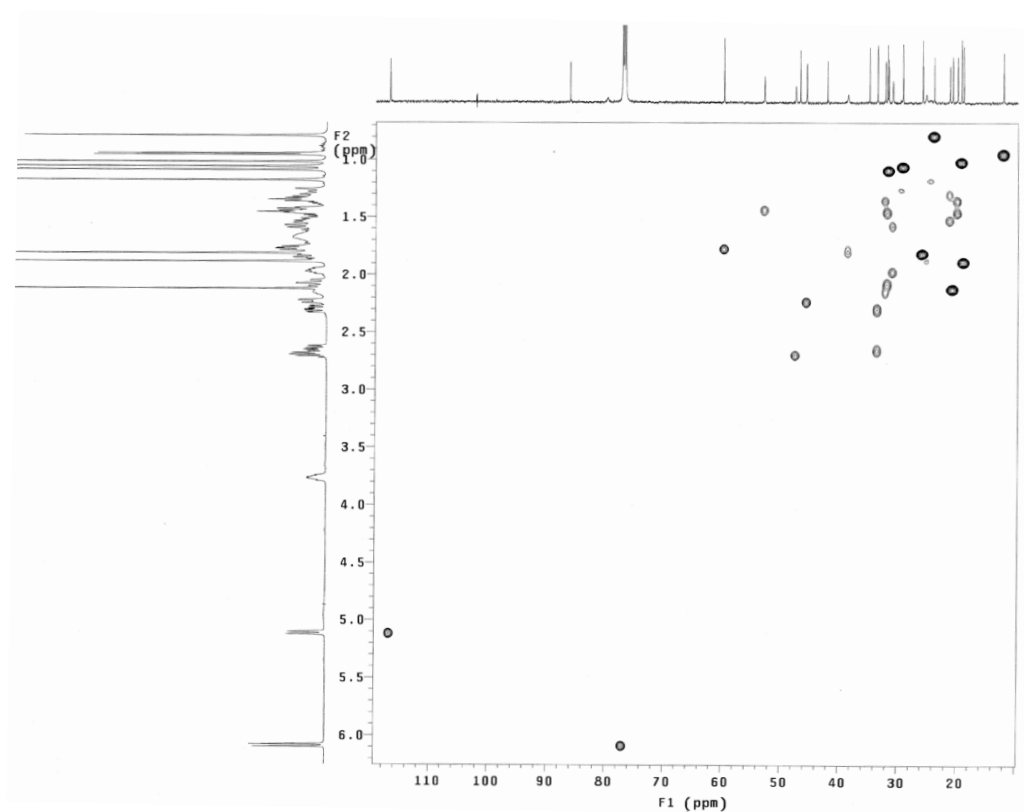


Figure S10. HSQC spectrum of **1**

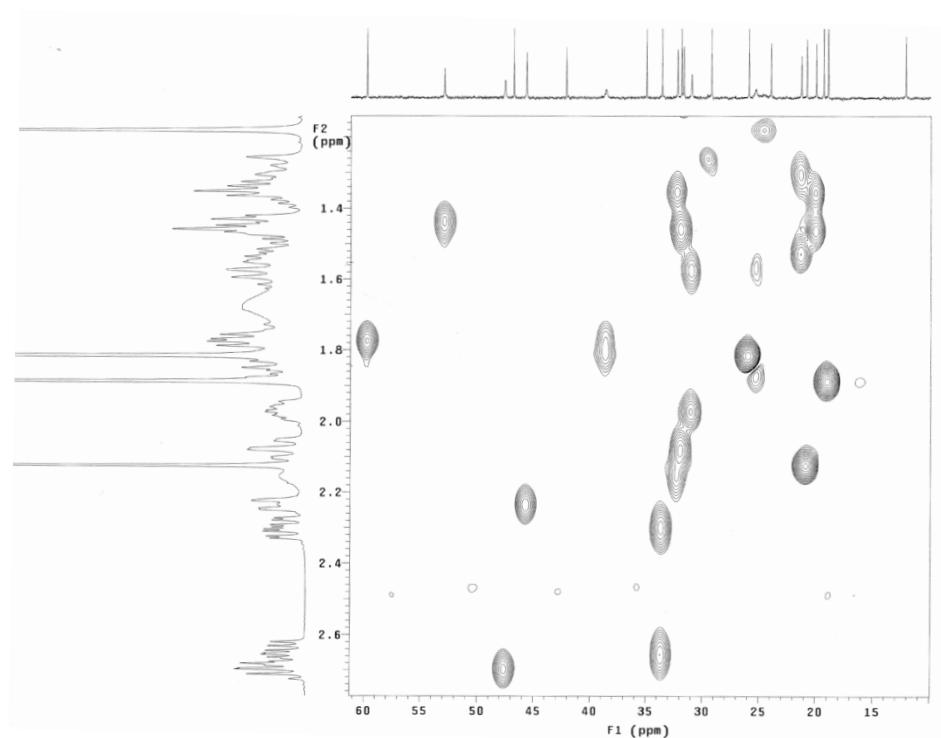


Figure S11. HSQC spectrum of **1** (Partial enlarged view)

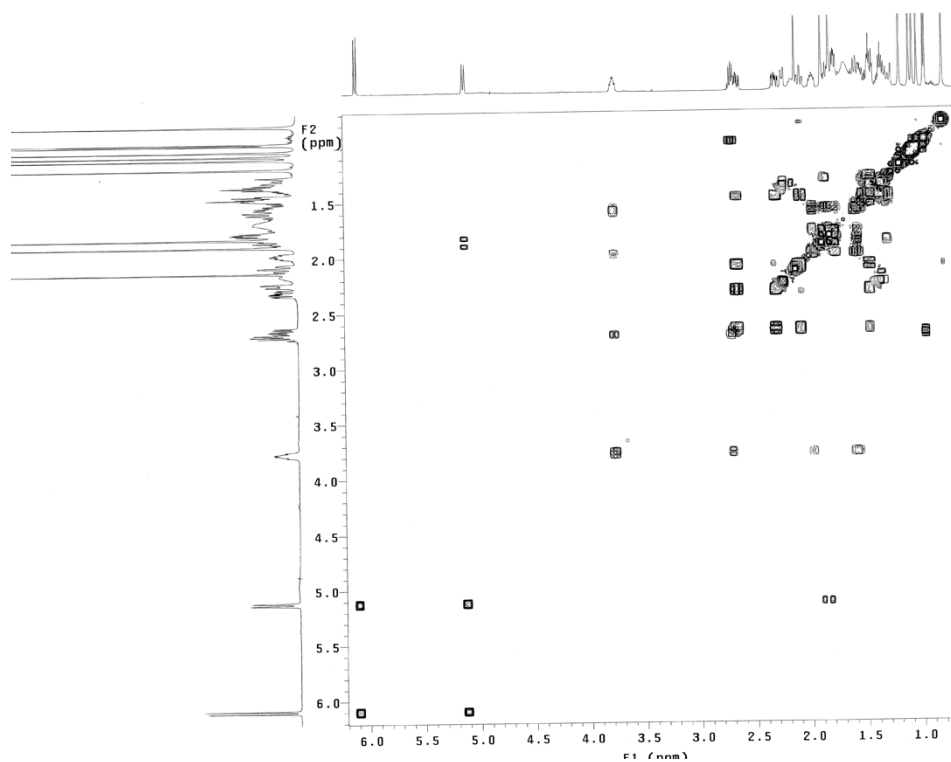


Figure S12. COSY spectrum of **1**

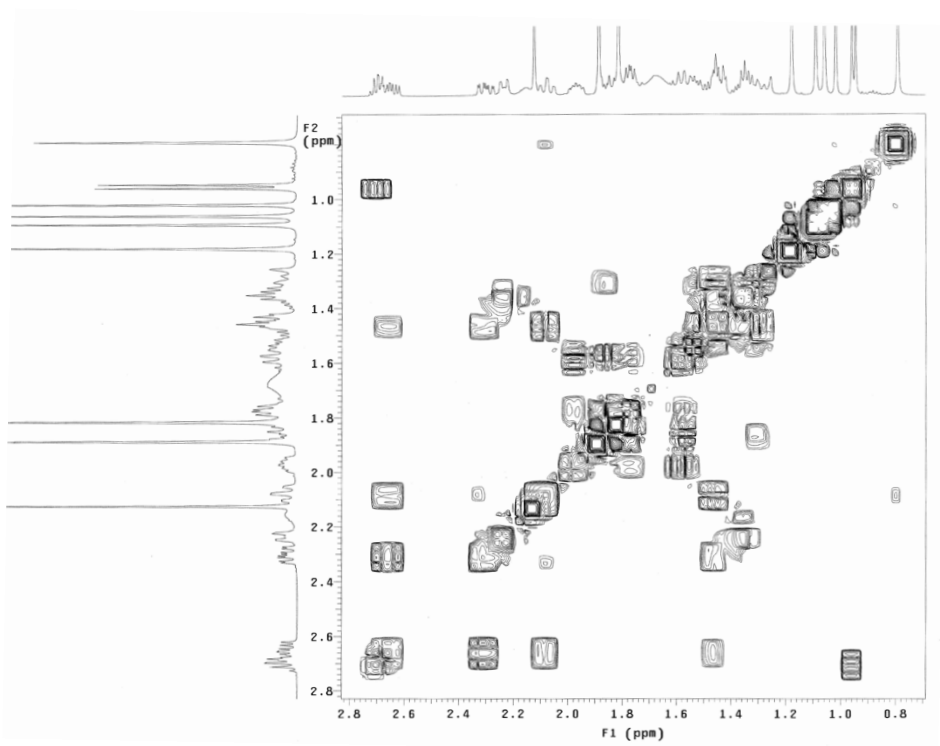


Figure S13. COSY spectrum of **1** (Partial enlarged view)

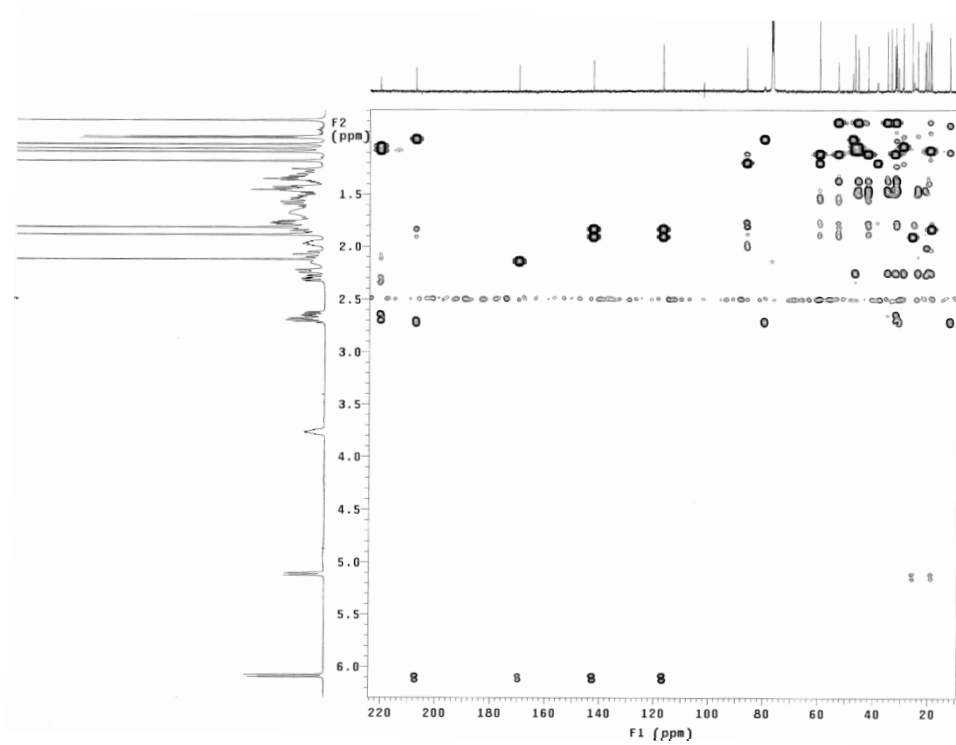


Figure S14. HMBC spectrum of **1**

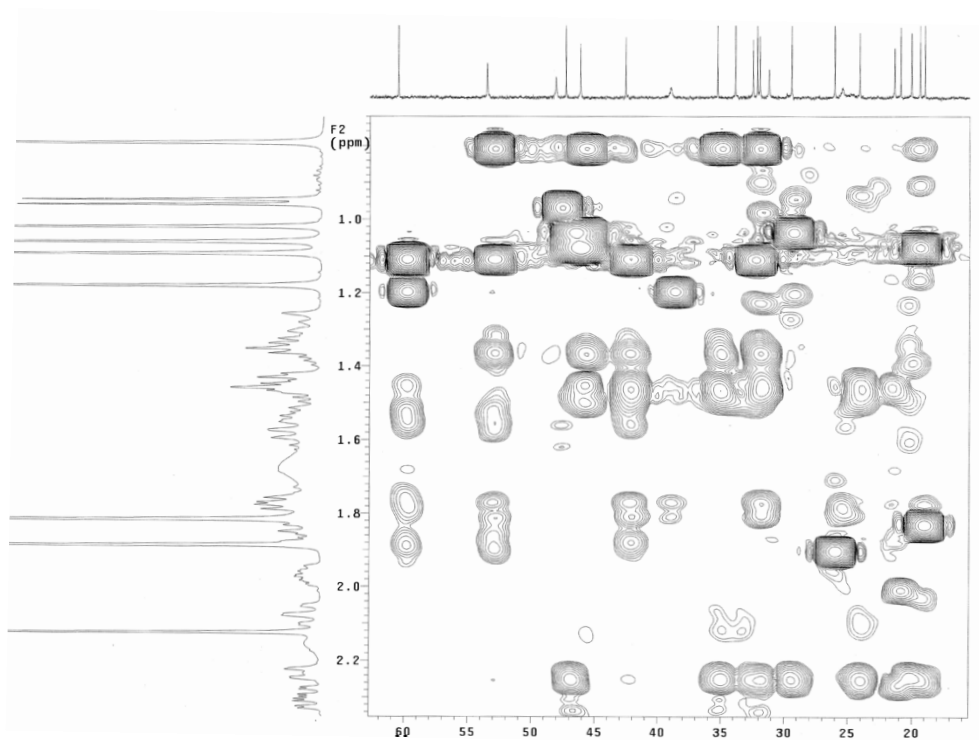


Figure S15. HMBC spectrum of **1** (Partial enlarged view)

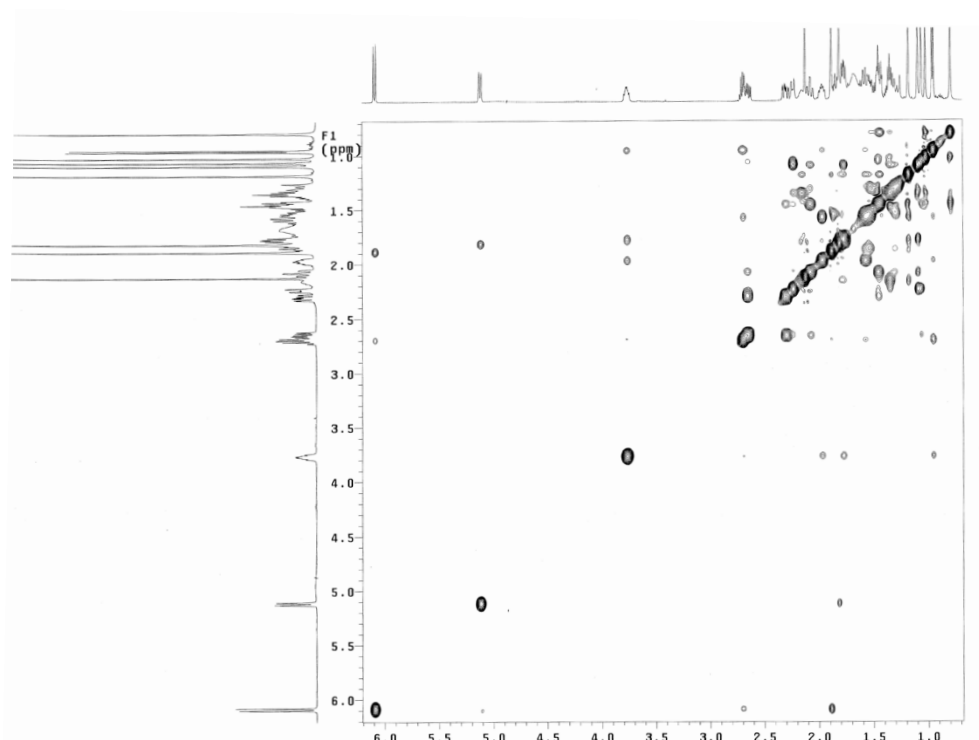


Figure S16. NOESY spectrum of **1**

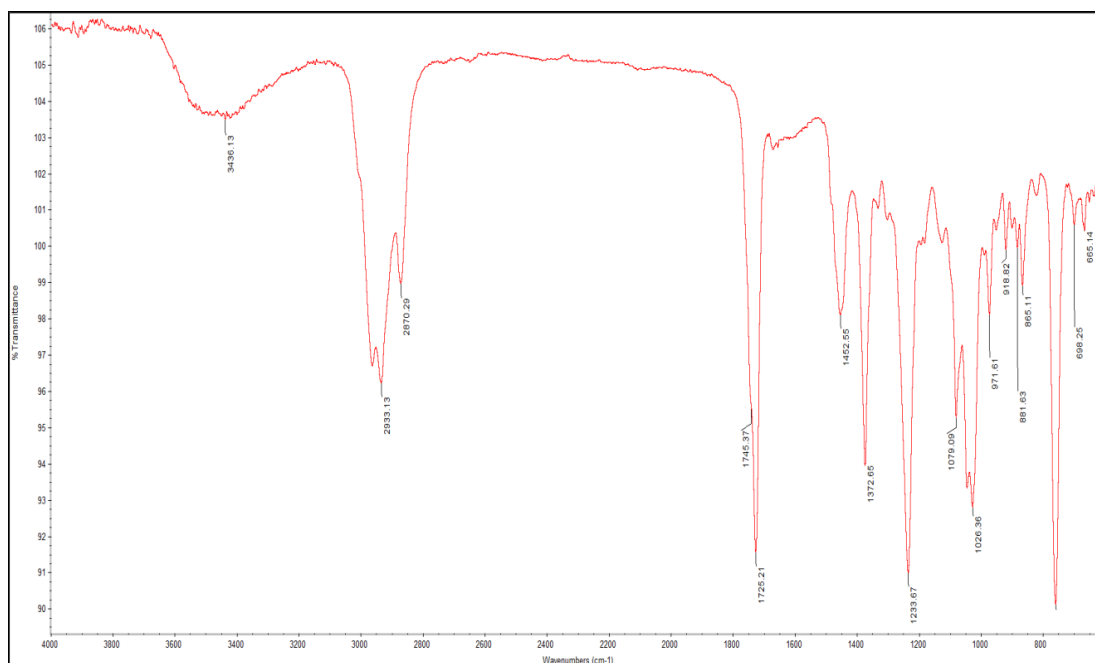


Figure S17. IR spectrum of 2

F:\Exp_data...\20181030-LTQ-K09-MSP-1P

2018/10/30 上午 11:00:42

09-MSP-1P #1-30 RT: 0.00-0.09 AV: 30 NL: 4.91E5
T: ITMS + c ESI Full ms [150.00-2000.00]

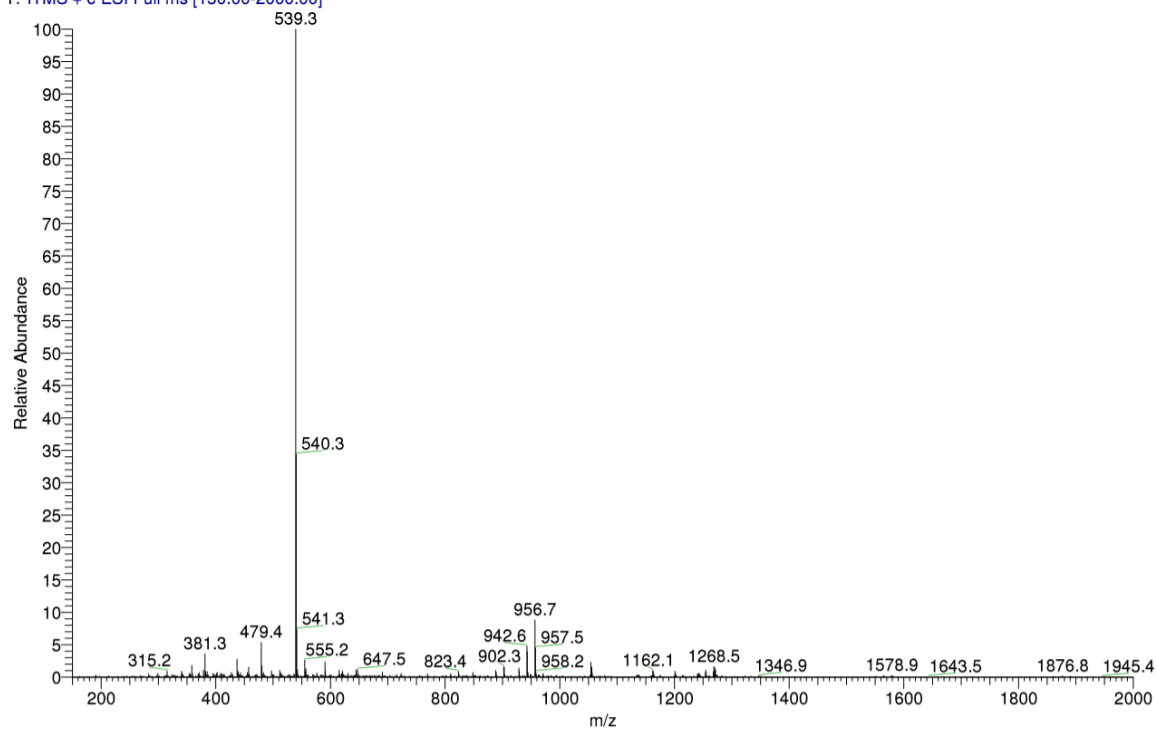


Figure S18. ESIMS spectrum of 2

45-MSP-1P-H#1-20 RT: 0.01-0.28 AV: 20
T: FTMS + p ESI Full ms [150.00-2000.00]
m/z= 539.0505-539.6632

Isotope	Min	Max
C-12	0	32
H-1	0	53
O-16	0	5
Na-23	0	1

Charge 1

Mass tolerance 1000.00 ppm

Nitrogen rule not used

RDB equiv -1.00-100.00

max results 1

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
539.3696	55447880.0	100.00	539.3707	-2.04	C ₃₂ H ₅₂ O ₅ Na

Figure S19. HRESIMS spectrum of 2

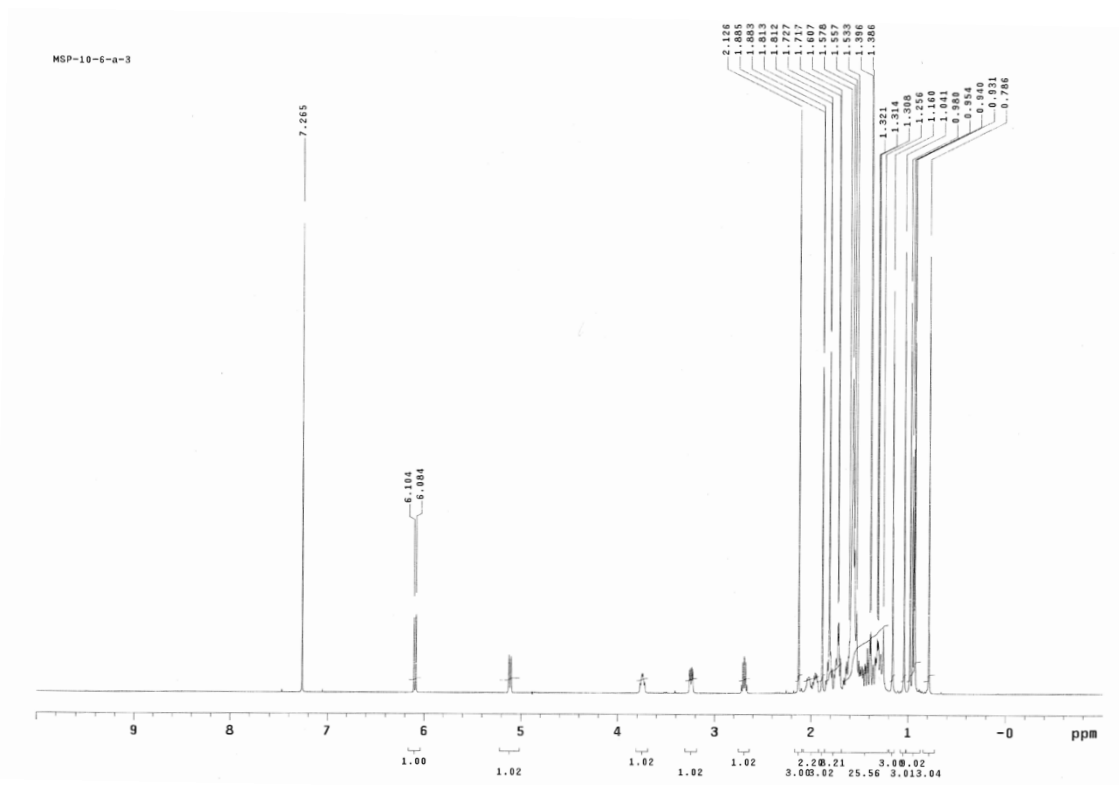


Figure S20. ¹H NMR (500 MHz, CDCl₃) spectrum of 2

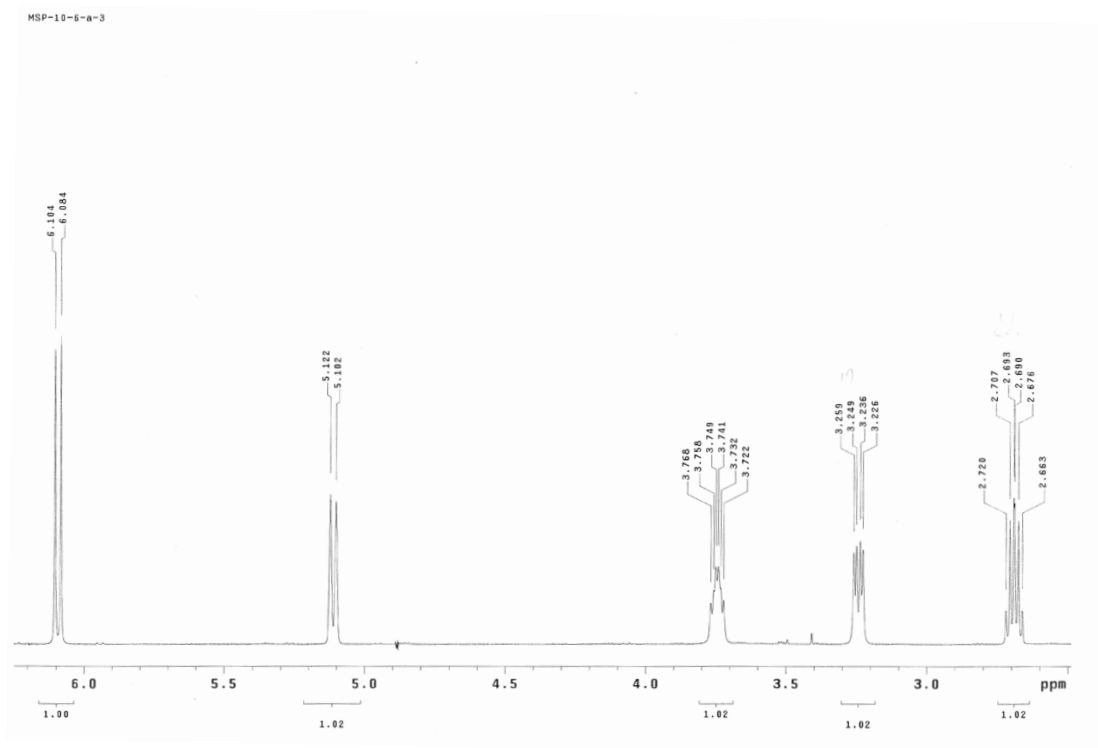


Figure S21. ^1H NMR (500 MHz, CDCl_3) spectrum of **2** (Partial enlarged view)

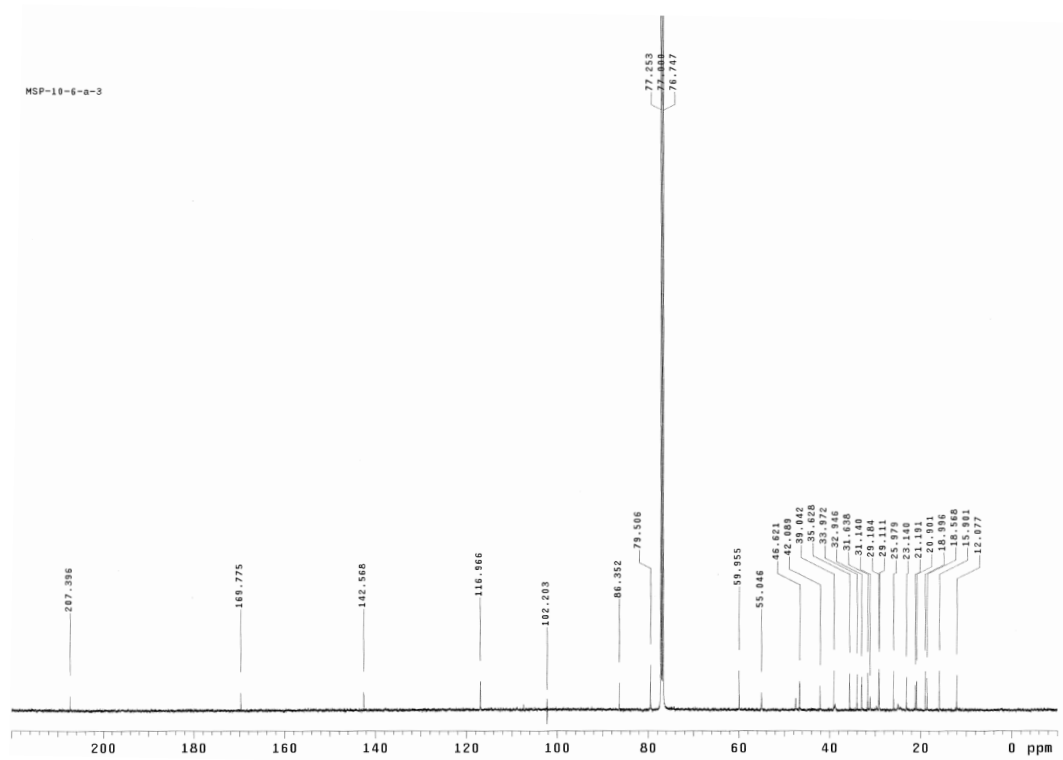


Figure S22. ^{13}C NMR (125 MHz, CDCl_3) spectrum of **2**

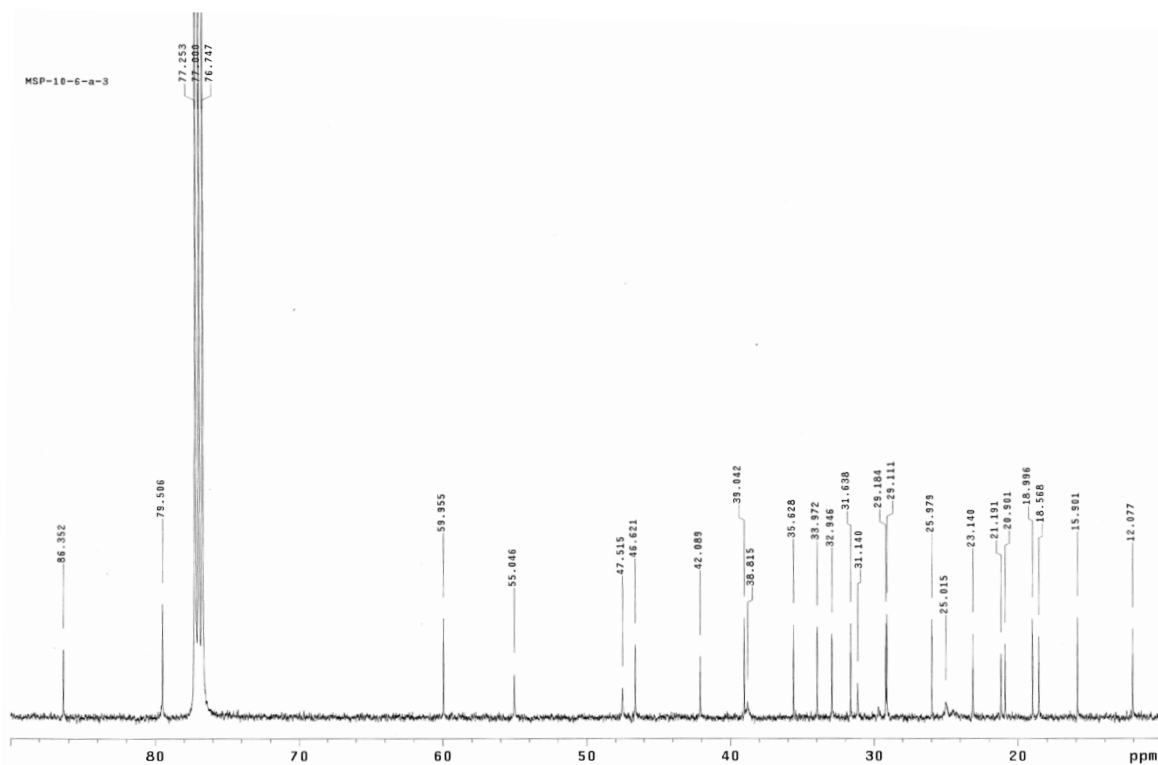


Figure S23. ^{13}C NMR (125 MHz, CDCl_3) spectrum of **2** (Partial enlarged view)

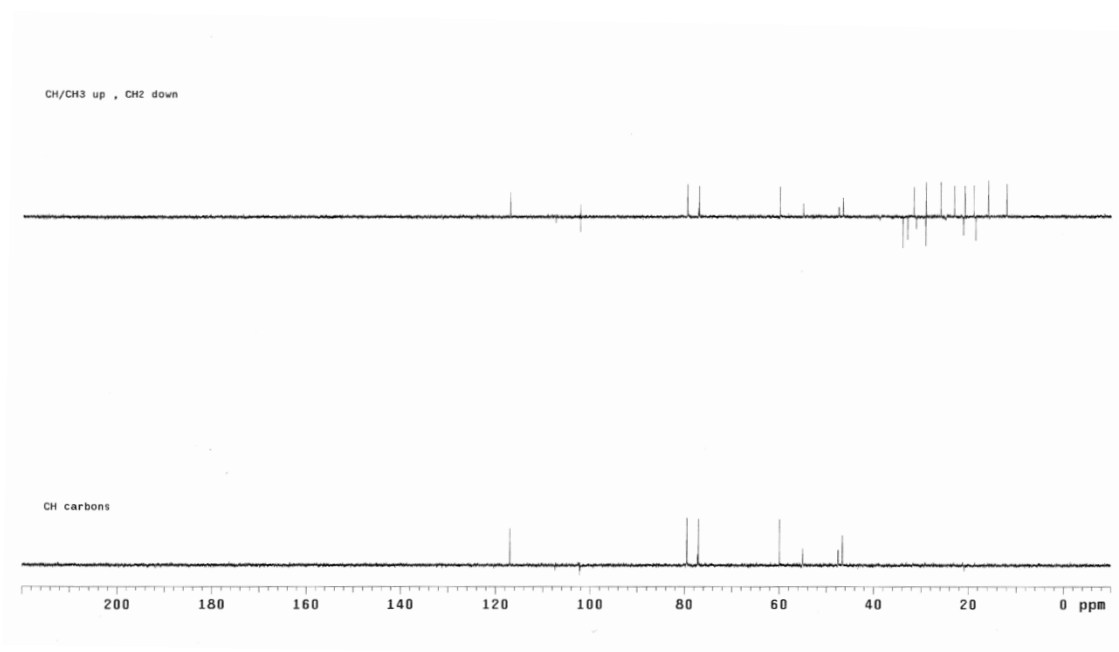


Figure S24. DEPT spectrum of **2**

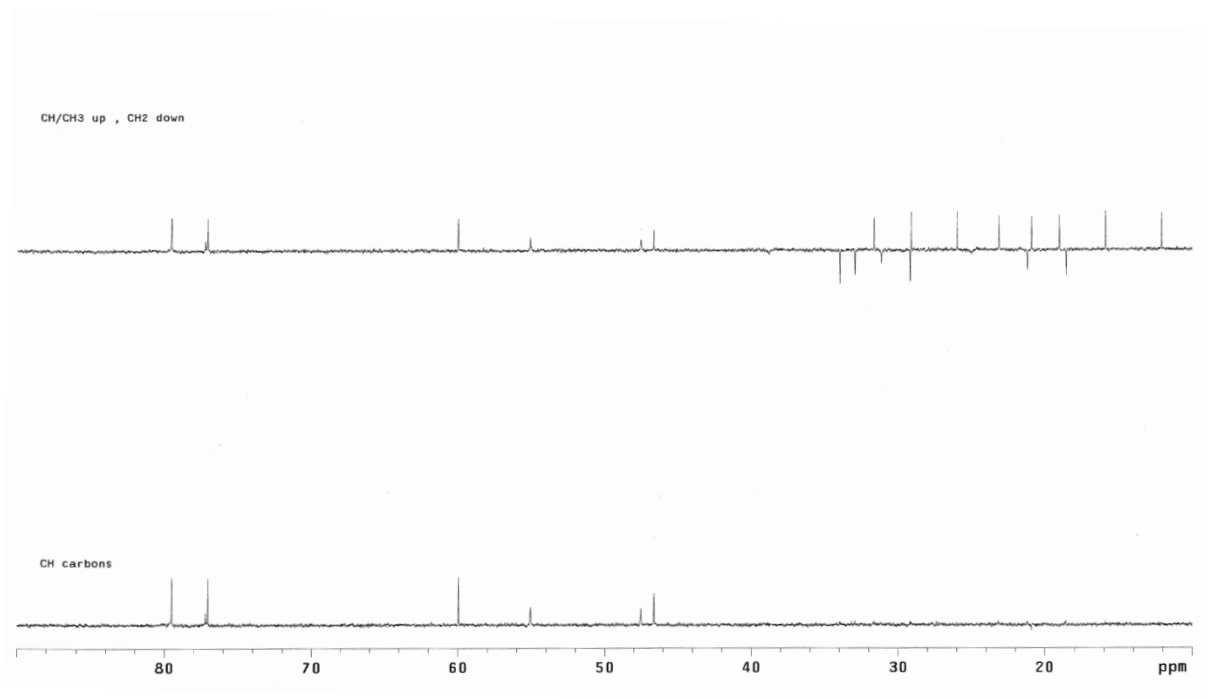


Figure S25. DEPT spectrum of **2** (Partial enlarged view)

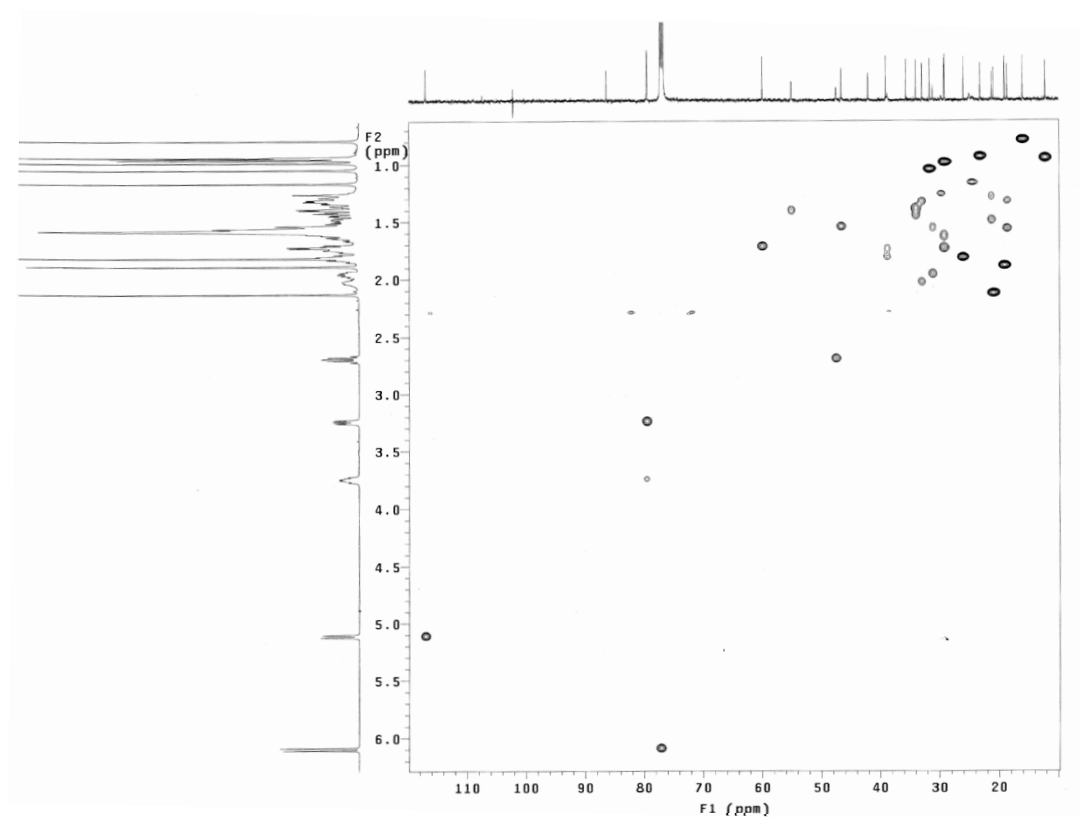


Figure S26. HSQC spectrum of **2**

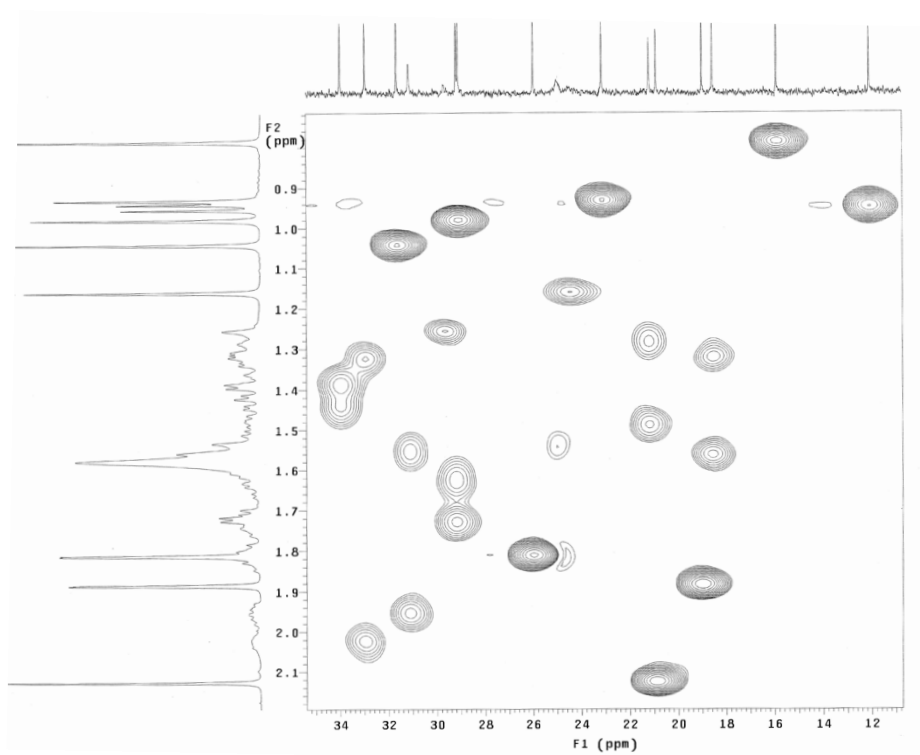


Figure S27. HSQC spectrum of 2 (Partial enlarged view)

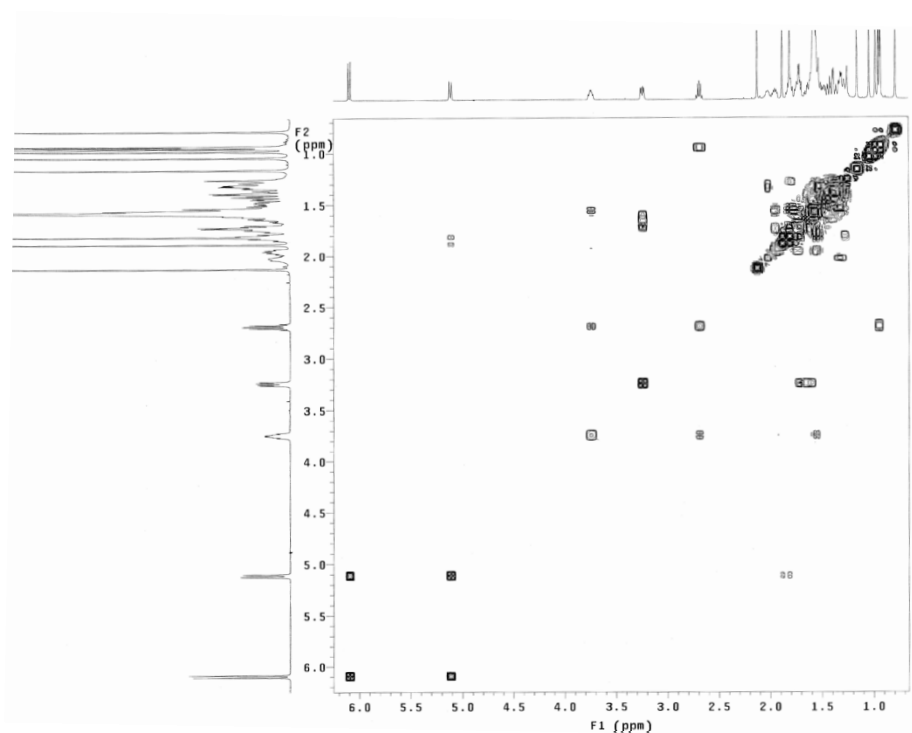


Figure S28. COSY spectrum of 2

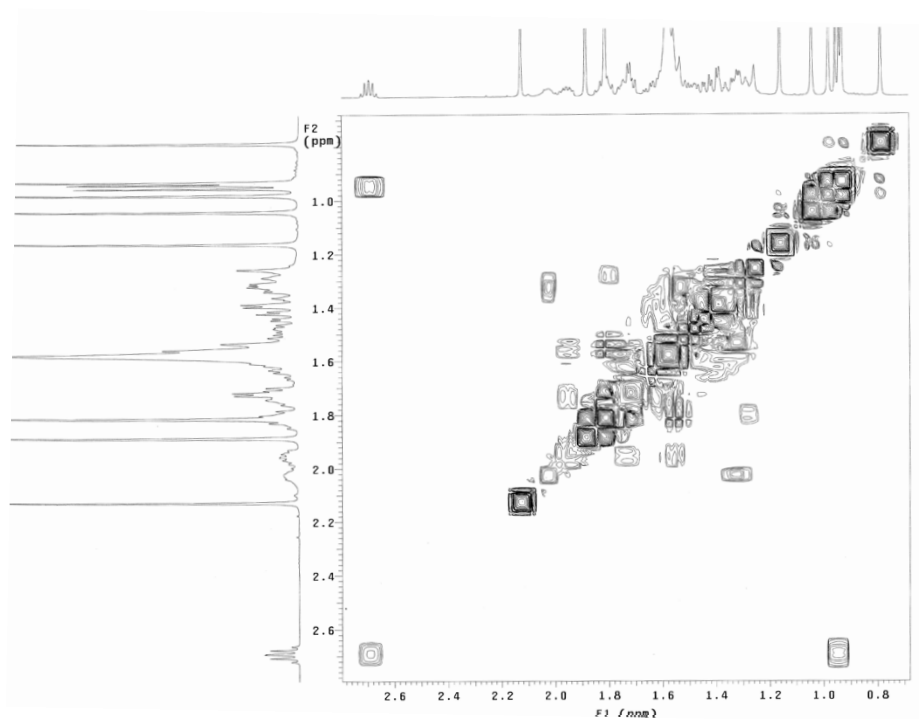


Figure S29. COSY spectrum of **2** (Partial enlarged view)

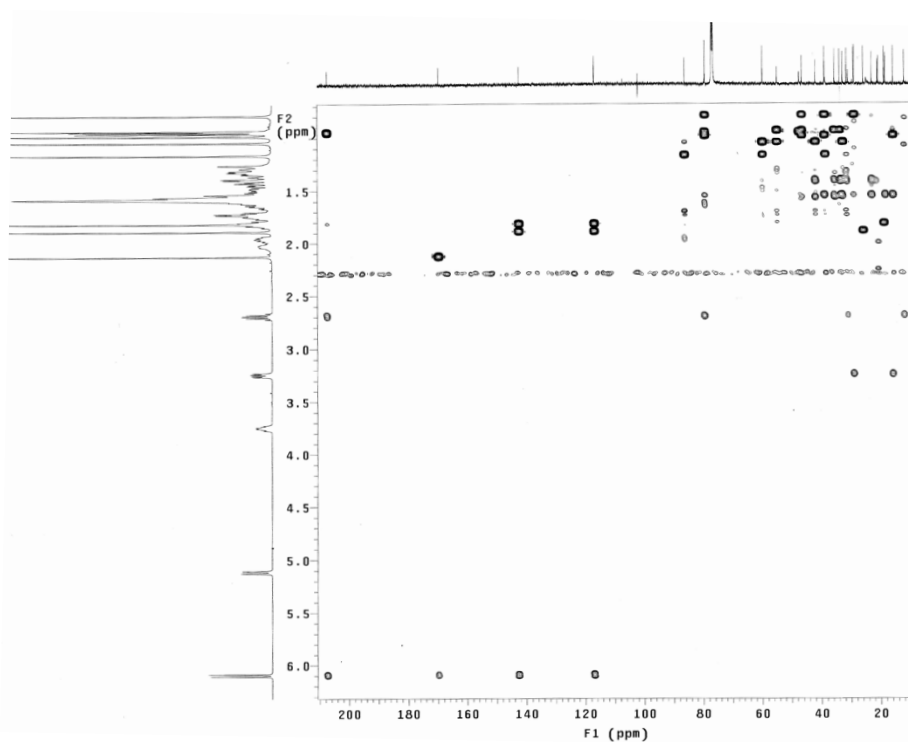


Figure S30. HMBC spectrum of **2**

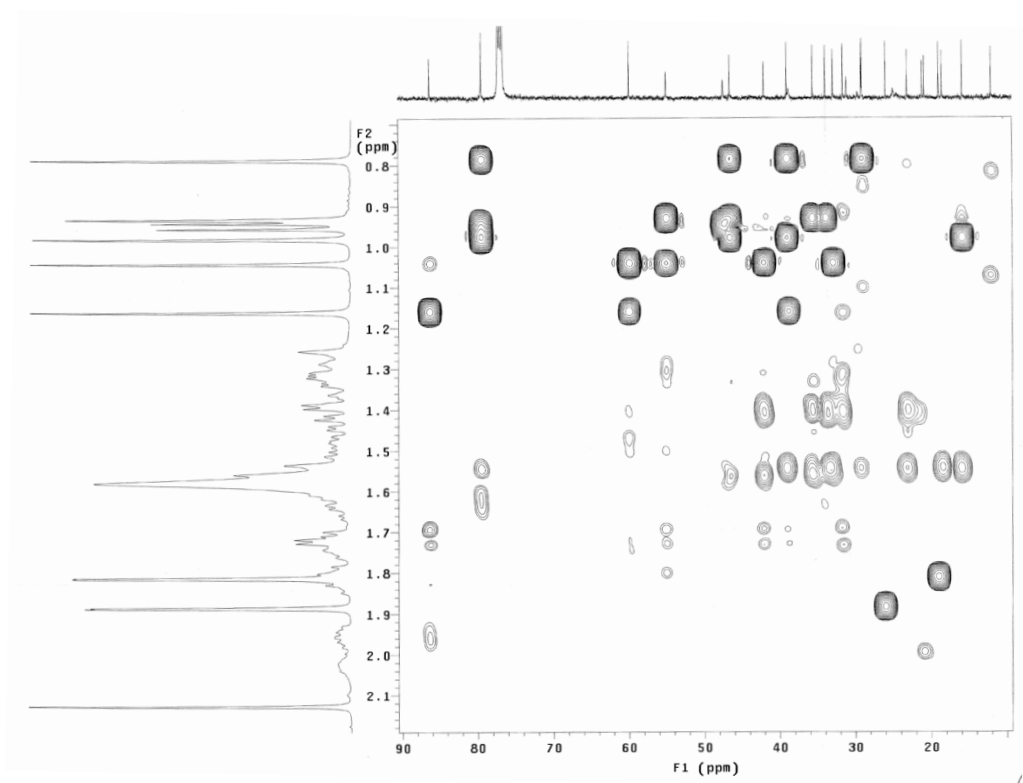


Figure S31. HMBC spectrum of **2** (Partial enlarged view)

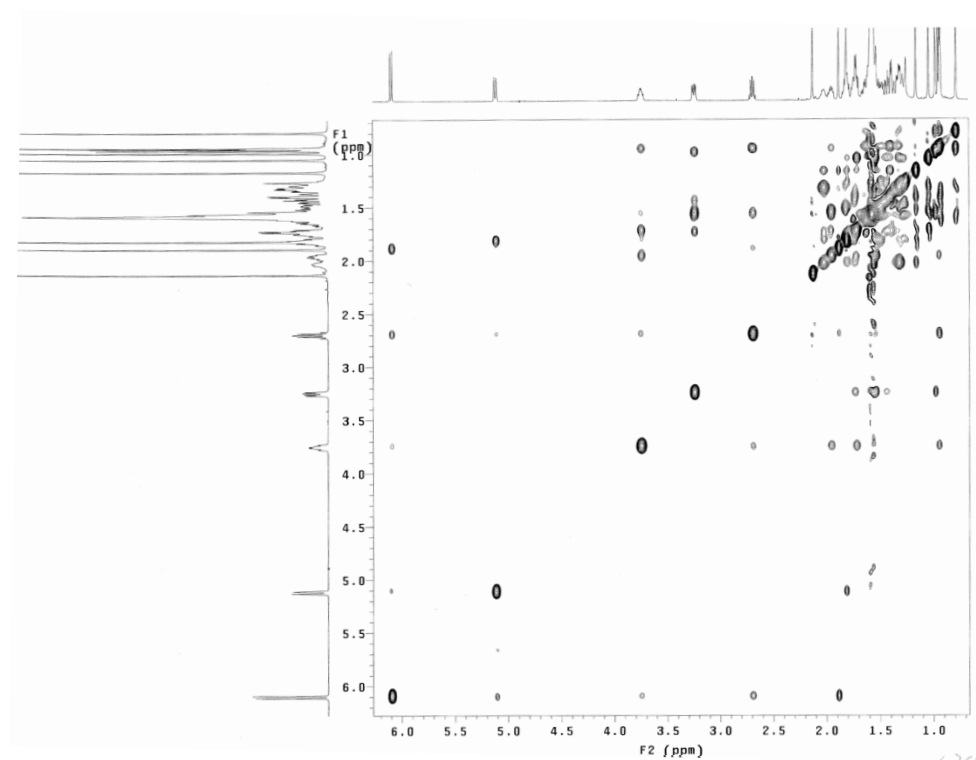


Figure S32. NOESY spectrum of **2**