

## Supplementary information

### Insights into the daily functions of Radix *Panax notoginseng*

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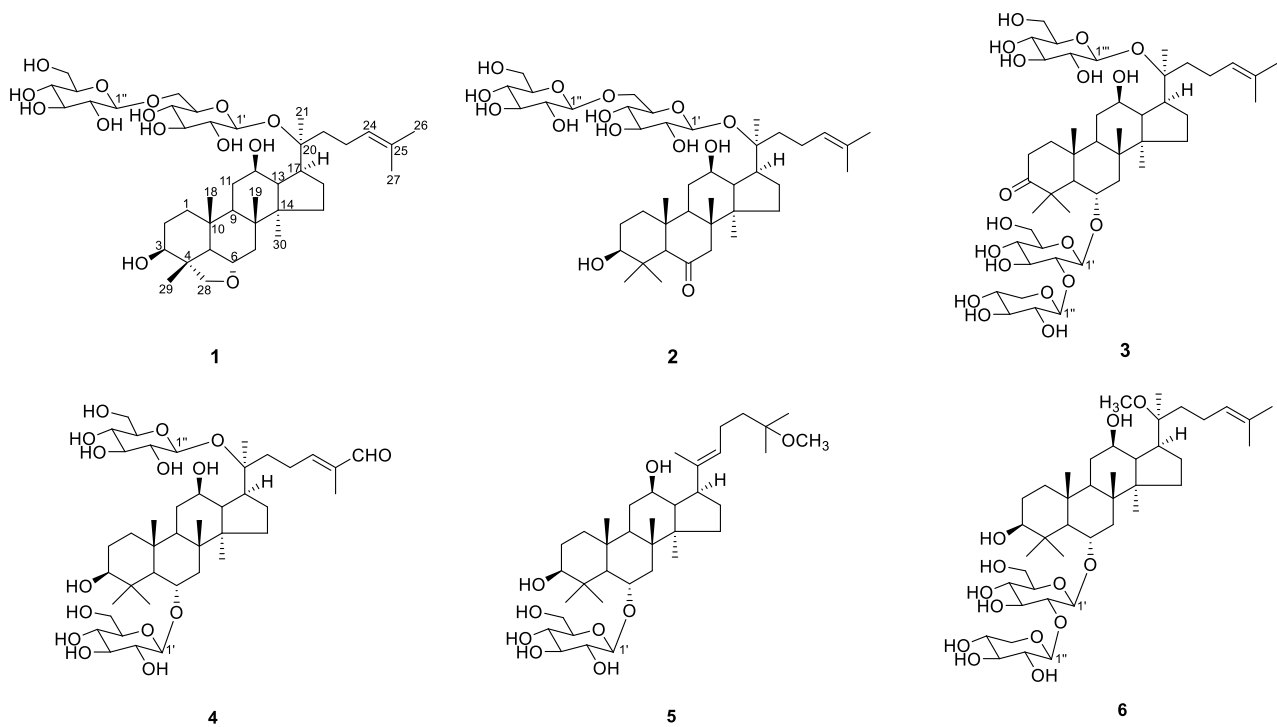
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#These authors contributed equally to this work.

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Triterpenoids saponins notoginsenoside V1-V6 (1-6) from *Panax notoginseng*

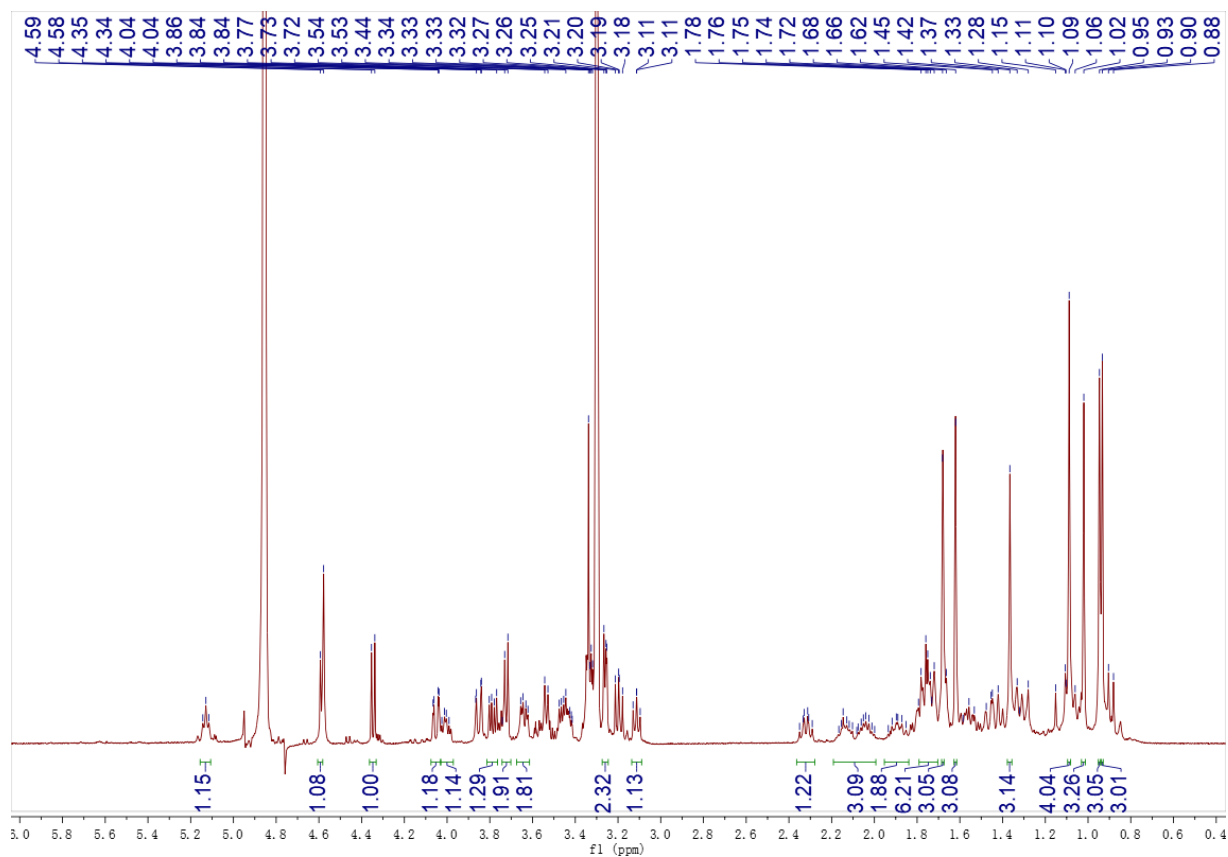


Figure 1  $^1\text{H}$  NMR spectroscopic spectrum of **1**

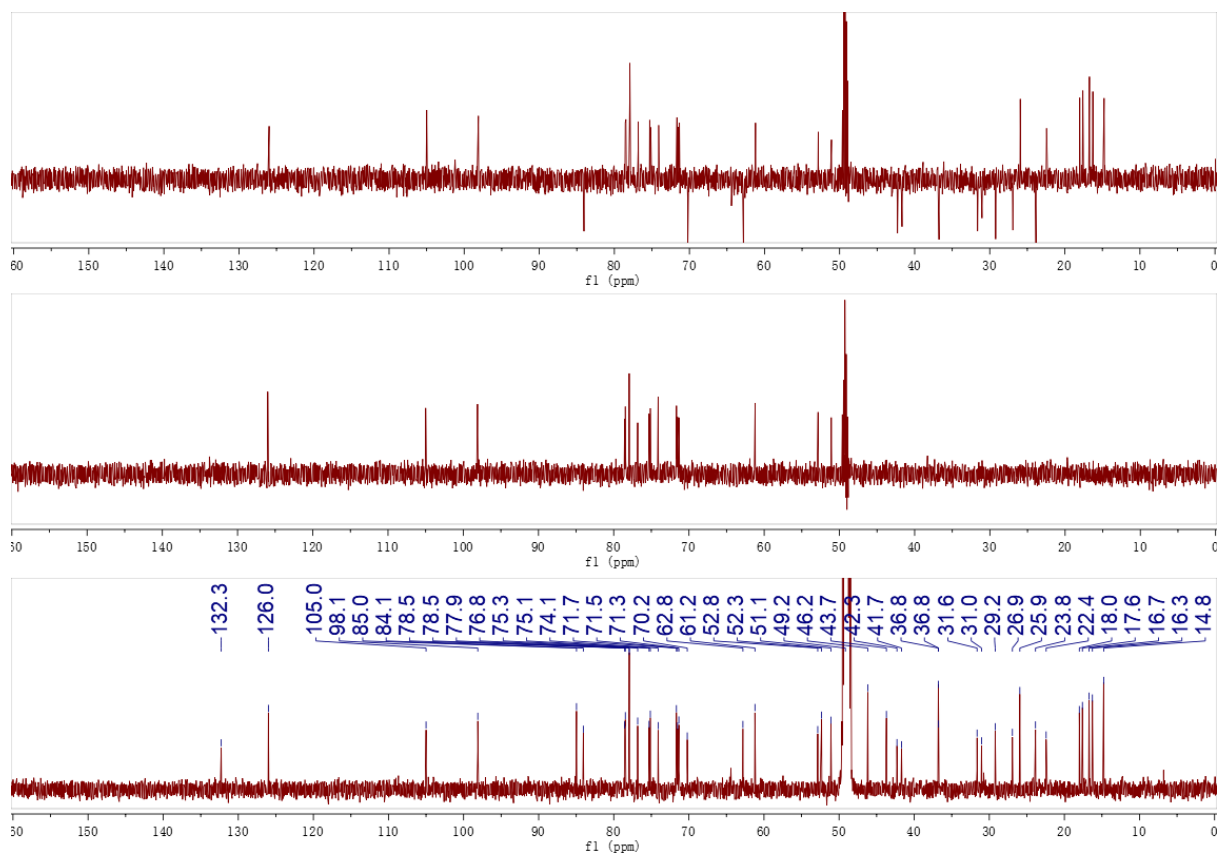
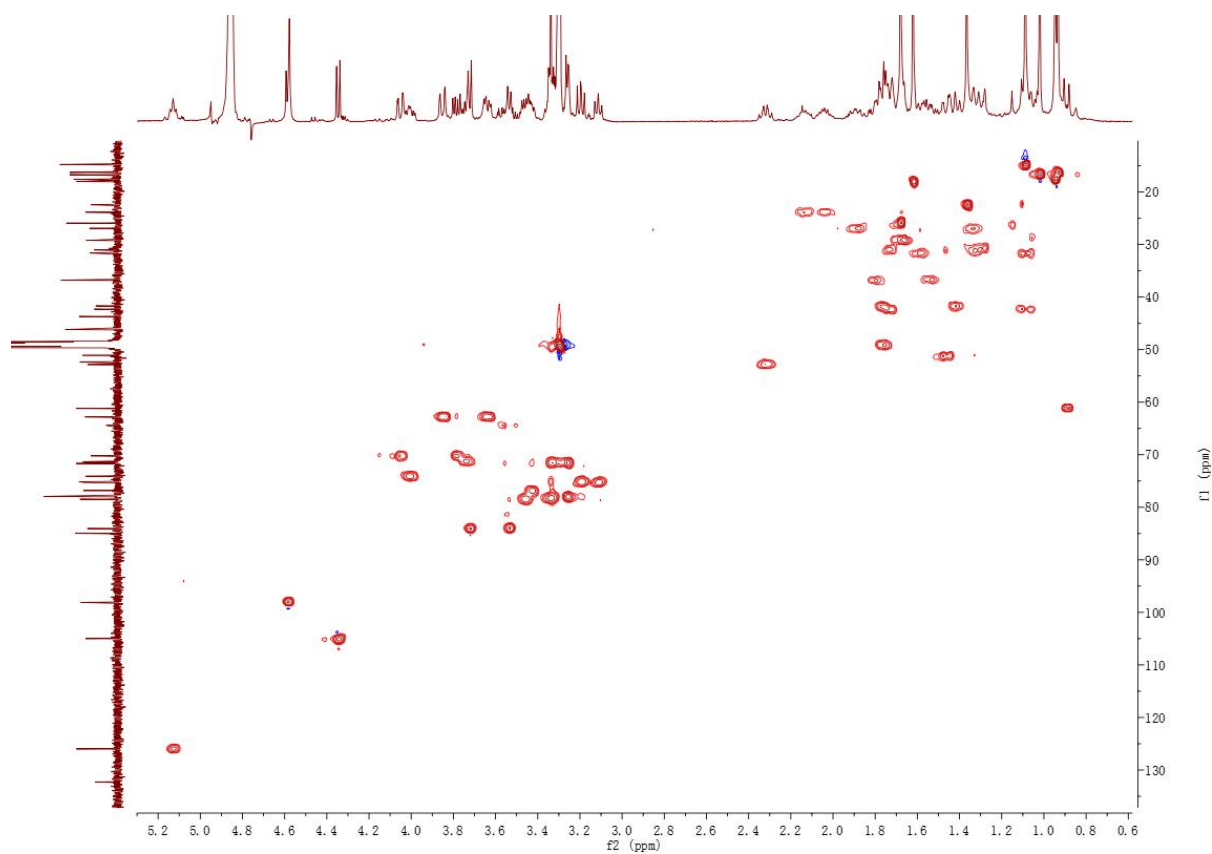
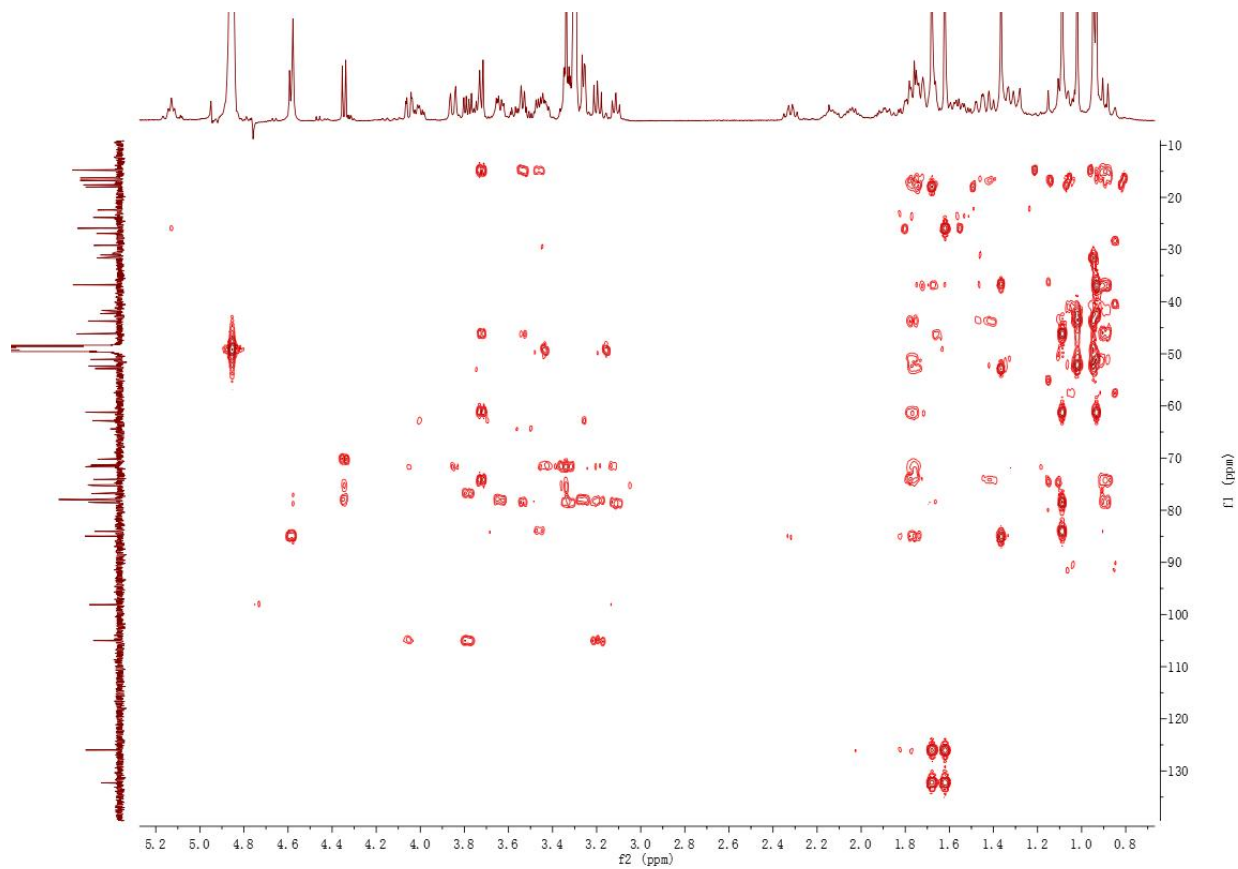


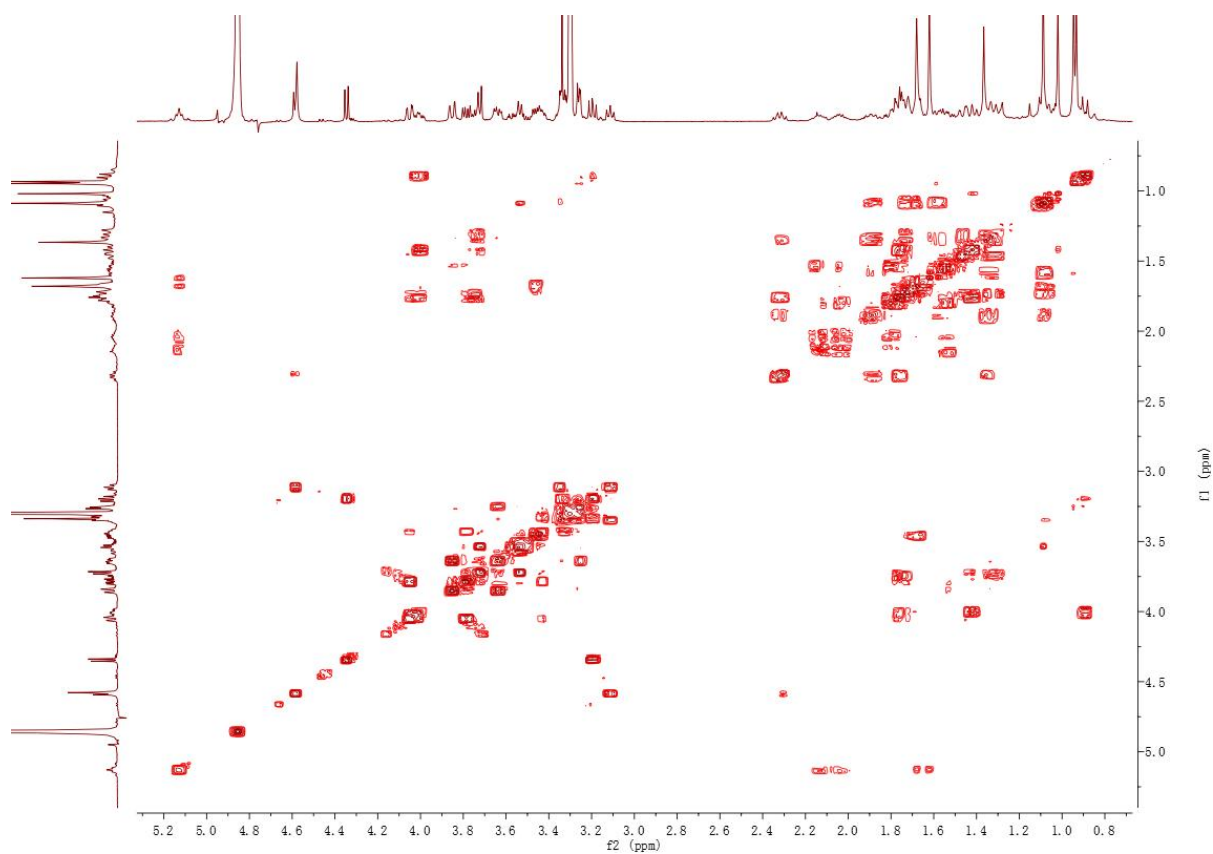
Figure 2  $^{13}\text{C}$  and DEPT NMR spectroscopic spectrum of **1**



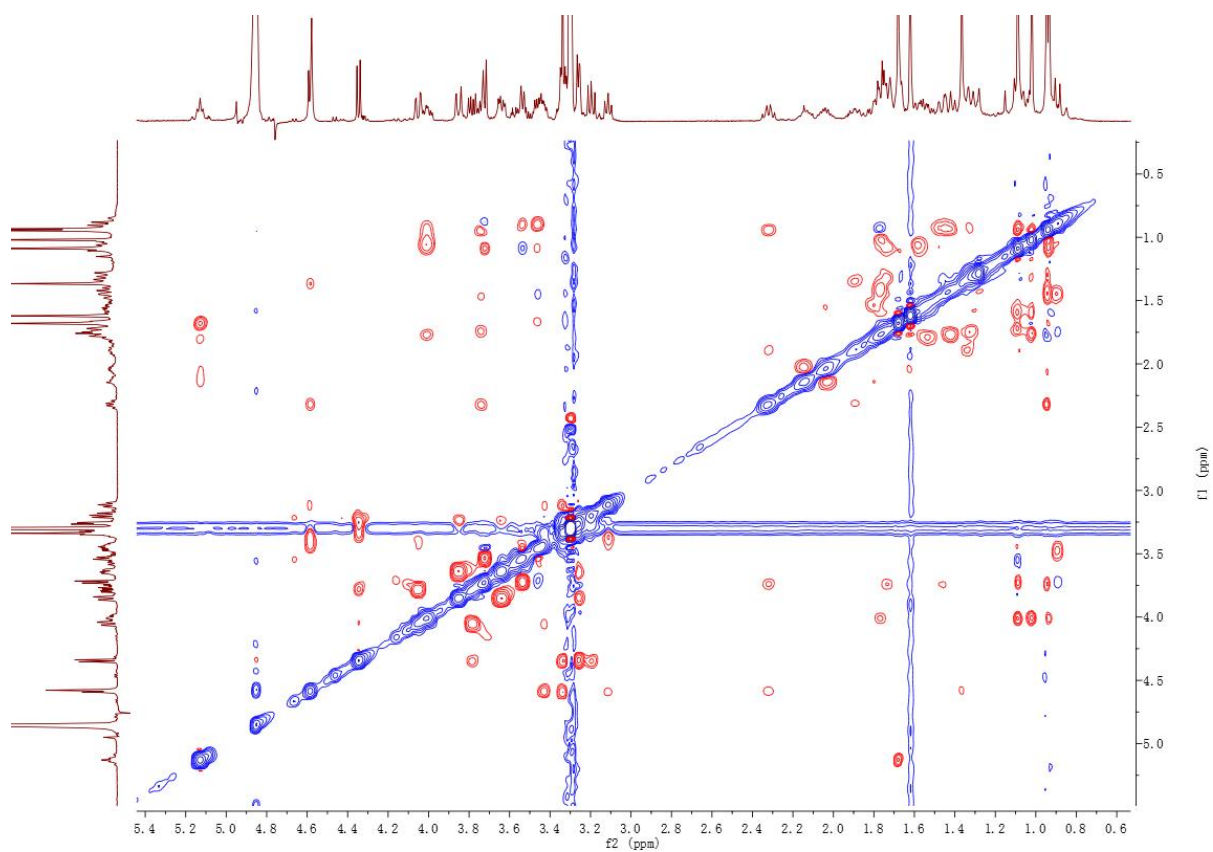
**Figure 3.** HSQC spectrum of **1**



**Figure 4** HMBC spectrum of **1**



**Figure 5**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **1**



**Figure 6** ROESY spectrum of **1**

Data File: E:\DATA\2023\0818\wpr-82a.lcd

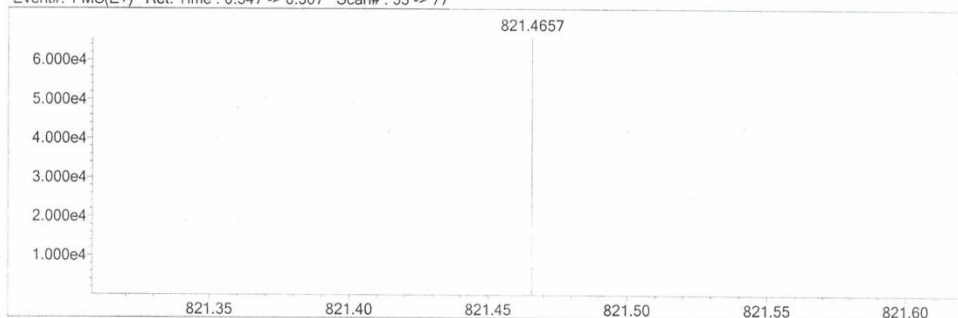
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B	3	0	0	Mg	2	0	0	Cu	2	0	0	Ir	3	0	0	
C	4	5	100	Si	4	0	0	Se	2	0	0	Pt	2	0	0	
N	3	0	10	P	3	0	0	Br	1	0	0					
O	2	0	30	S	2	0	0	Pd	2	0	0					

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 MSn Iso RI (%): 75.00

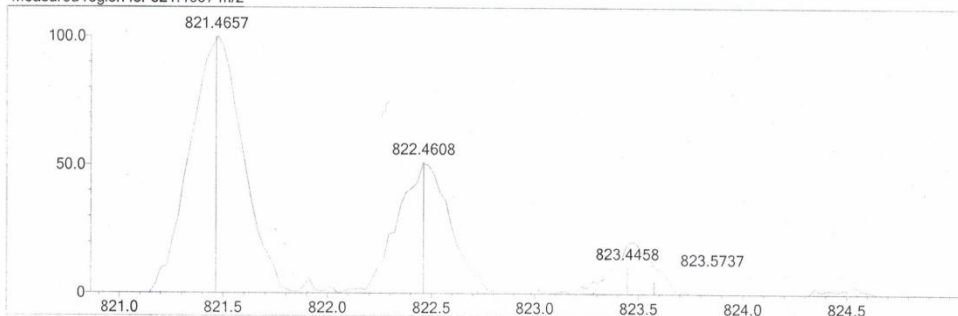
DBE Range: not fixed  
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 MSn Logic Mode: OR

Electron Ions: both  
 Use MSn Info: yes  
 Isotope Res: 10000  
 Max Results: 30

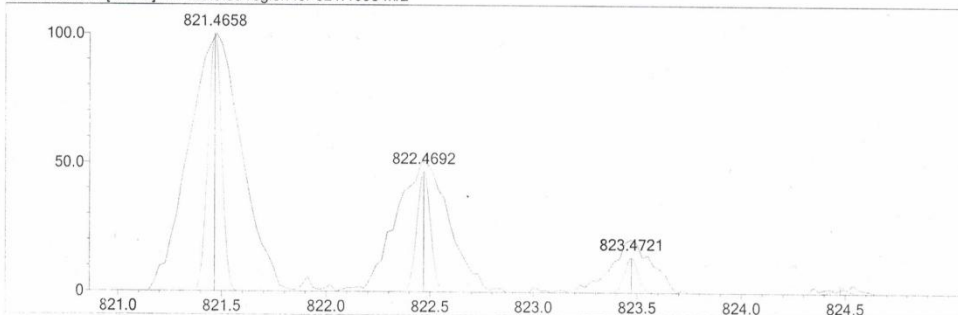
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Measured region for 821.4657 m/z



C42 H70 O14 [M+Na]+ : Predicted region for 821.4658 m/z



Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C42 H70 O14	[M+Na]+	821.4657	821.4658	-0.1	-0.12	8.0

Figure 7 HRESIMS spectrum of 1

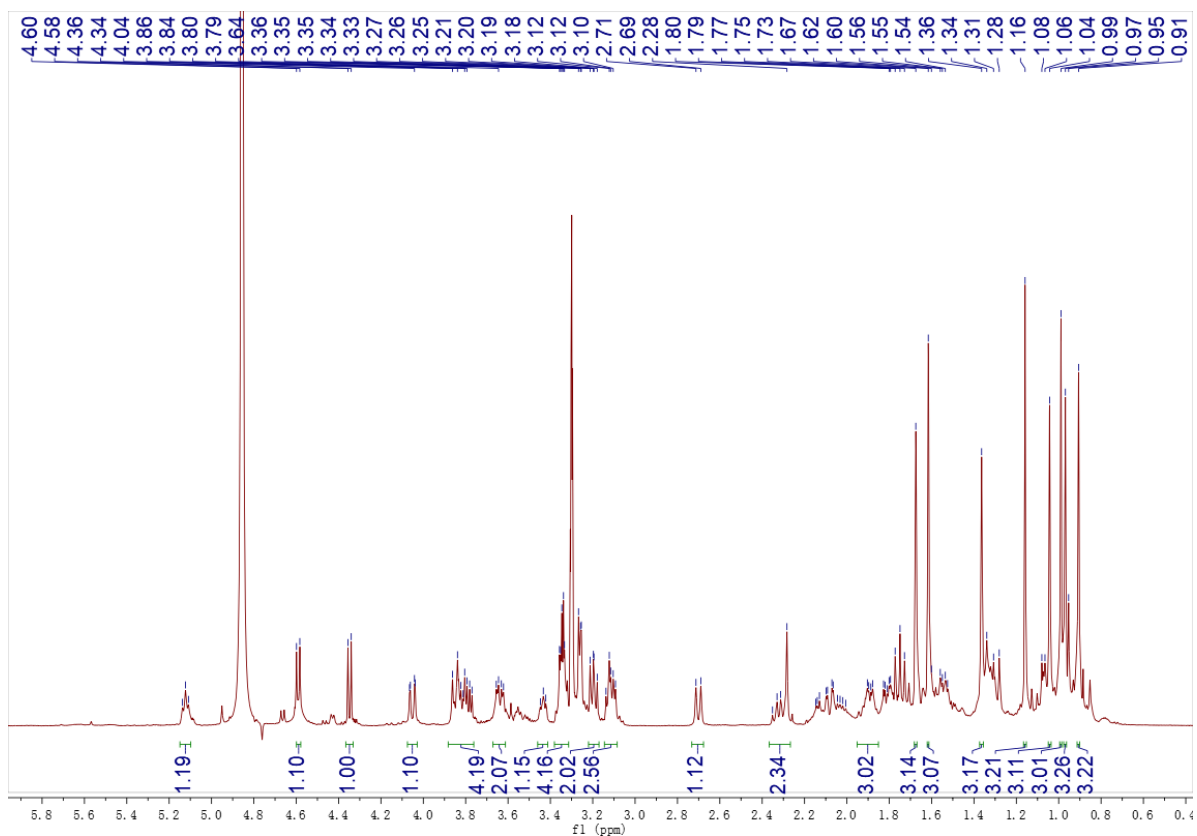


Figure 8  $^1\text{H}$  NMR spectroscopic spectrum of 2

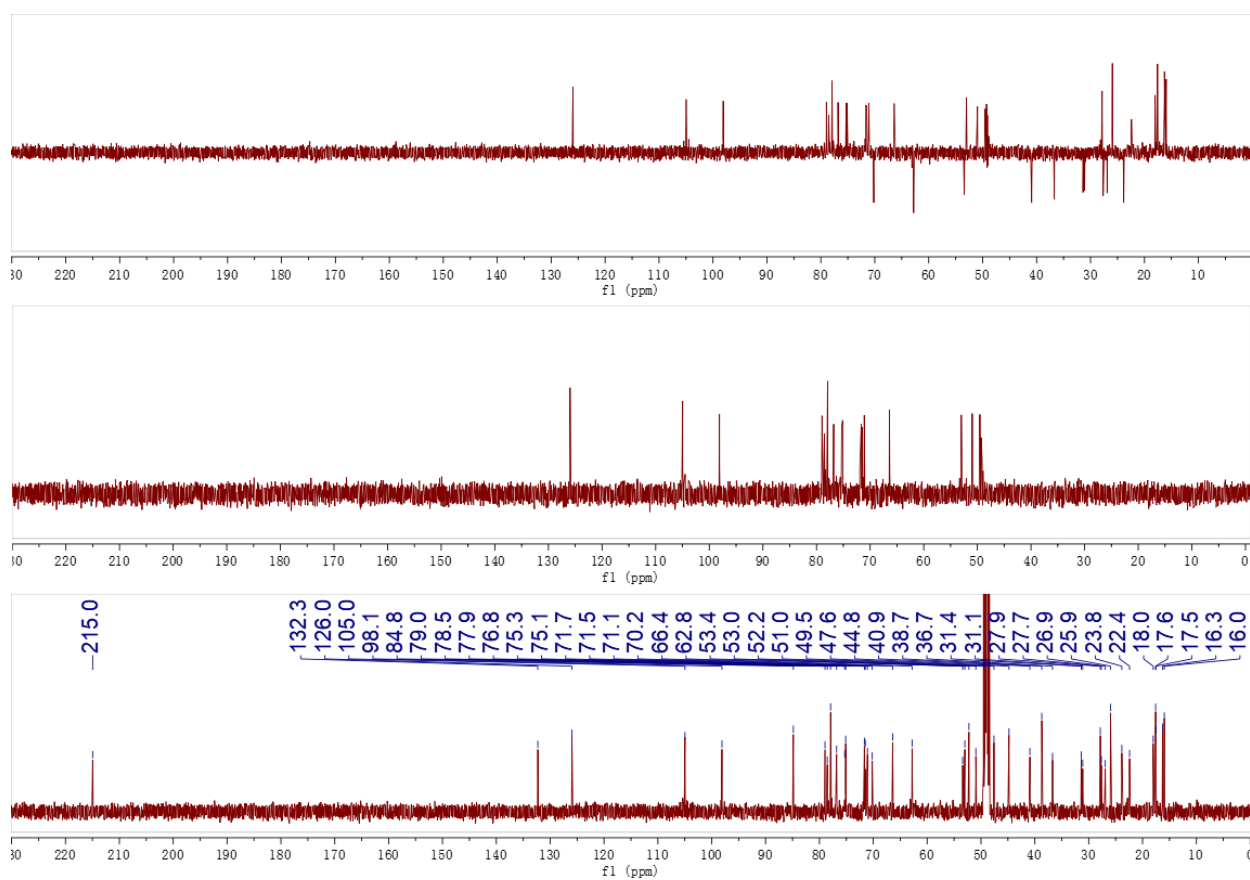
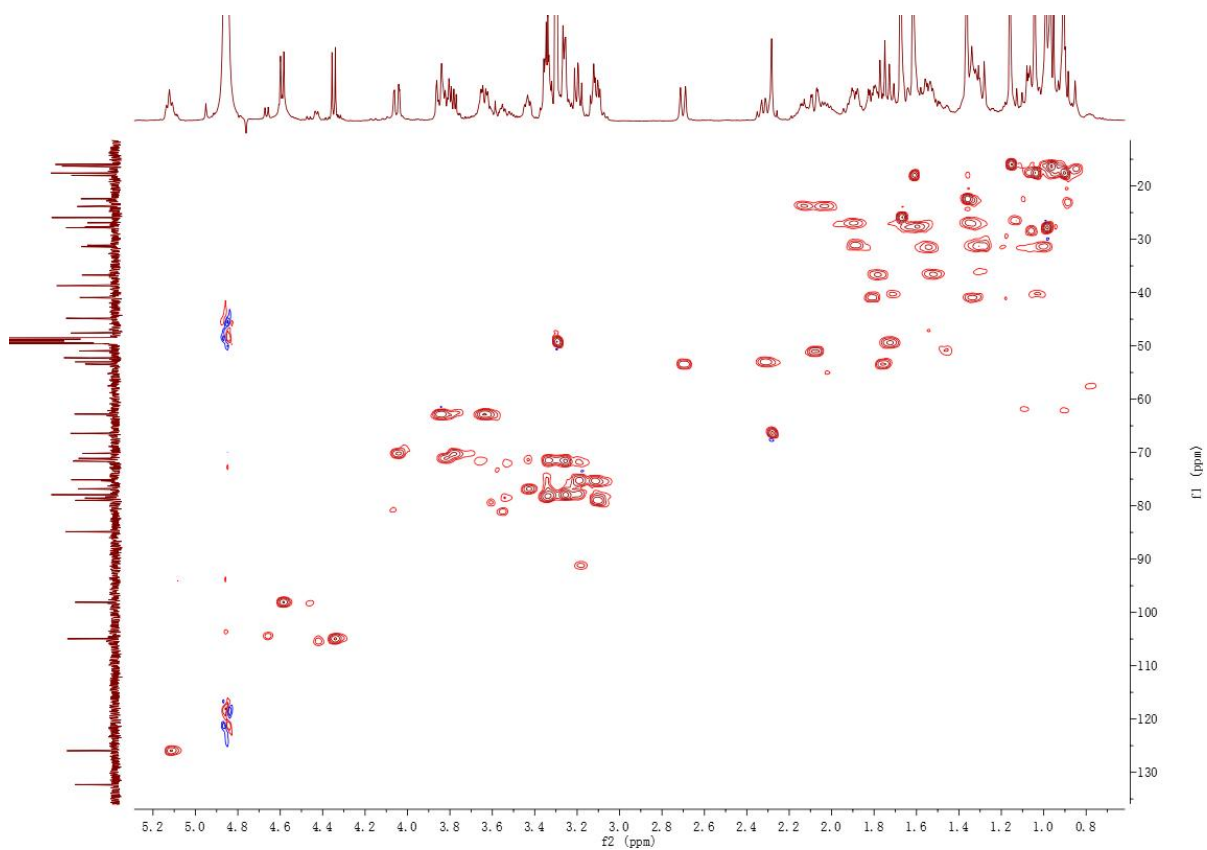
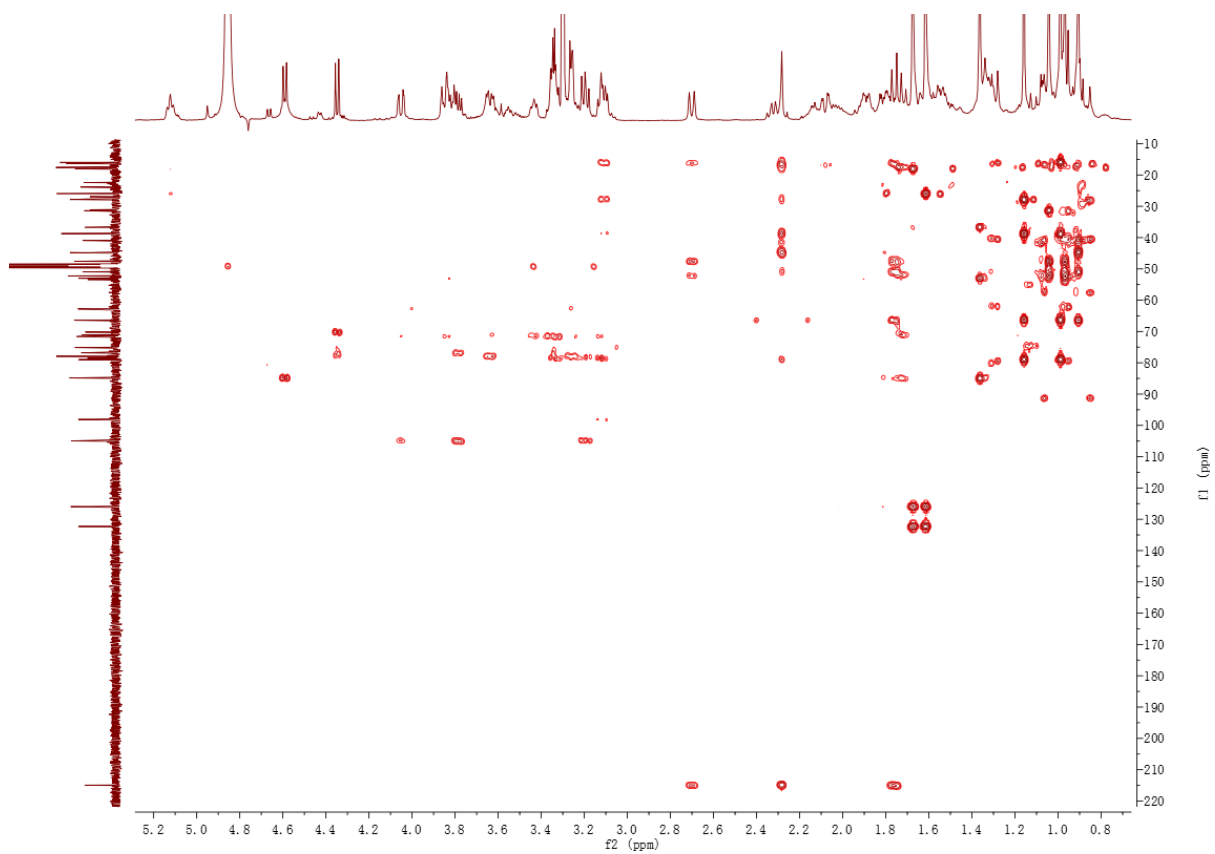


Figure 9  $^{13}\text{C}$  and DEPT NMR spectroscopic spectrum of 2



**Figure 10** HSQC spectrum of **2**



**Figure 11** HMBC spectrum of **2**

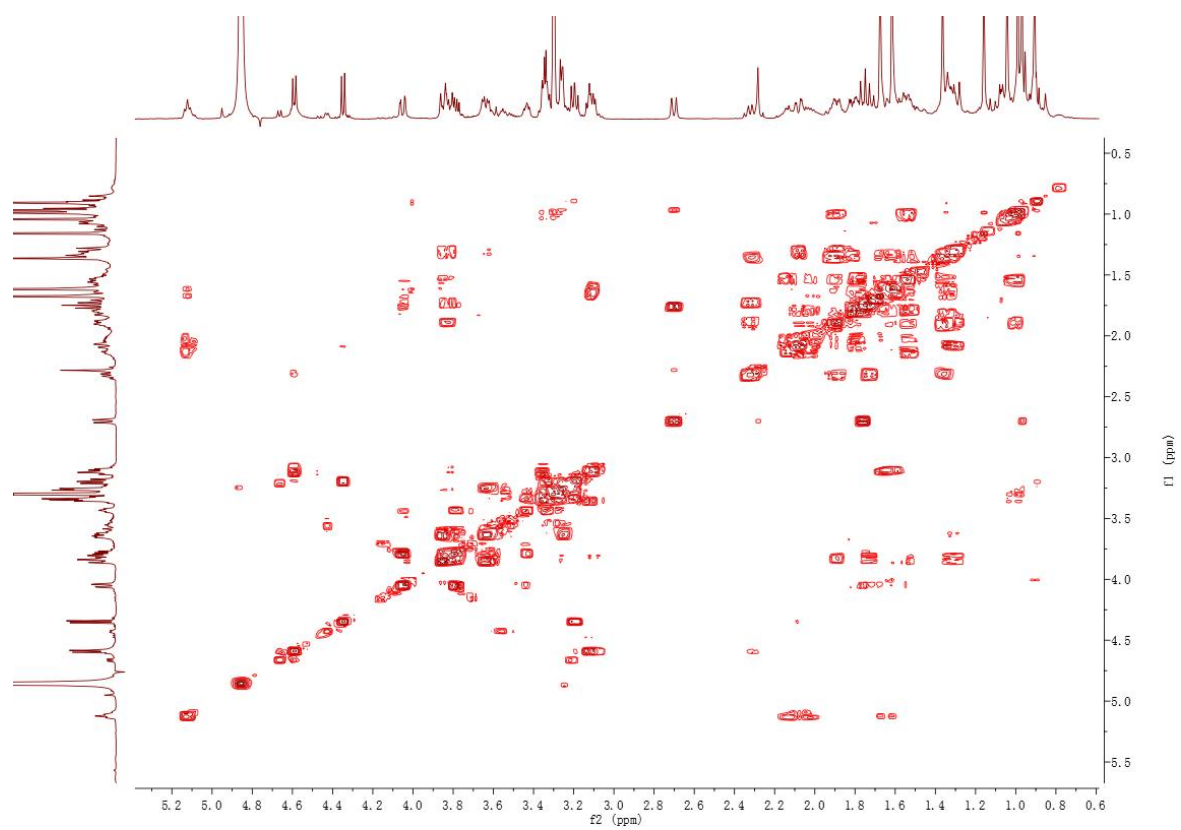


Figure 12  $^1\text{H}$ - $^1\text{H}$  COSY s spectrum of **2**

Data File: E:\DATA\2023\0818\wpn-82f.lcd

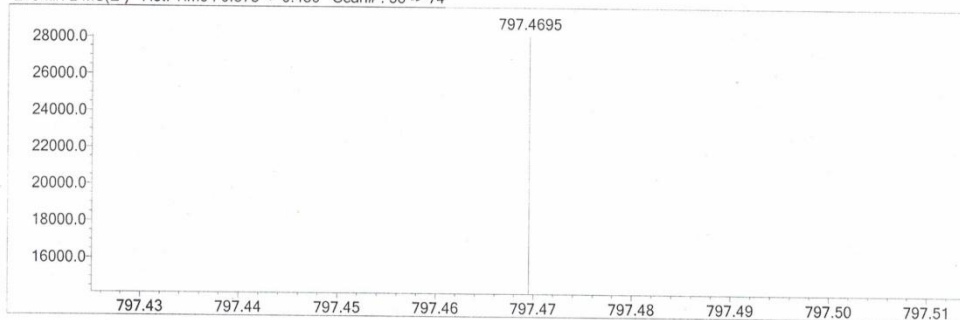
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B	3	0	0	Mg	2	0	0	Cu	2	0	0	Ir	3	0	0	Cl
C	4	5	100	Si	4	0	0	Se	2	0	0	Pt	2	0	0	
N	3	0	10	P	3	0	0	Br	1	0	0					
O	2	0	30	S	2	0	0	Pd	2	0	0					

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 MSn Iso RI (%): 75.00

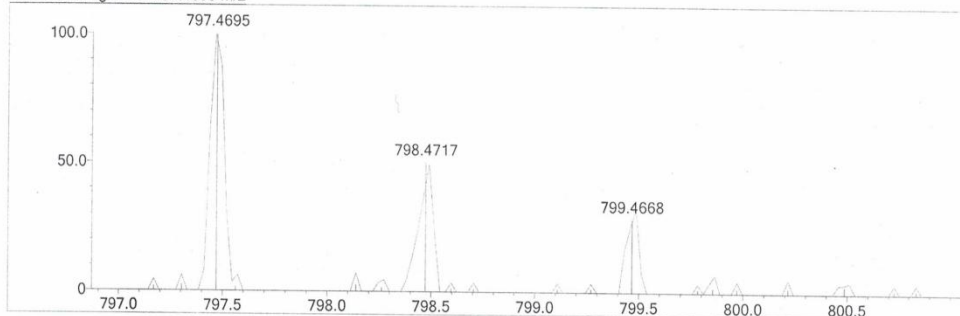
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Electron Ions: both  
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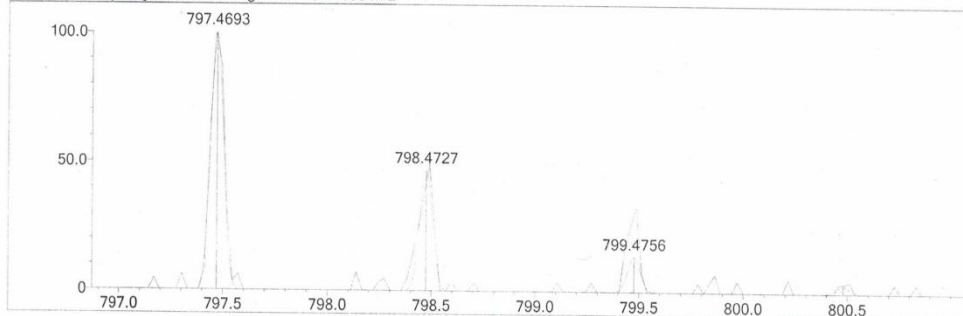
Event#: 2 MS(E-) Ret. Time : 0.373 -> 0.480 Scan# : 58 -> 74



Measured region for 797.4695 m/z



C42 H70 O14 [M-H]- : Predicted region for 797.4693 m/z



Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C42 H70 O14	[M-H]-	797.4695	797.4693	0.2	0.25	8.0

Figure 13 HRESIMS spectrum of 2

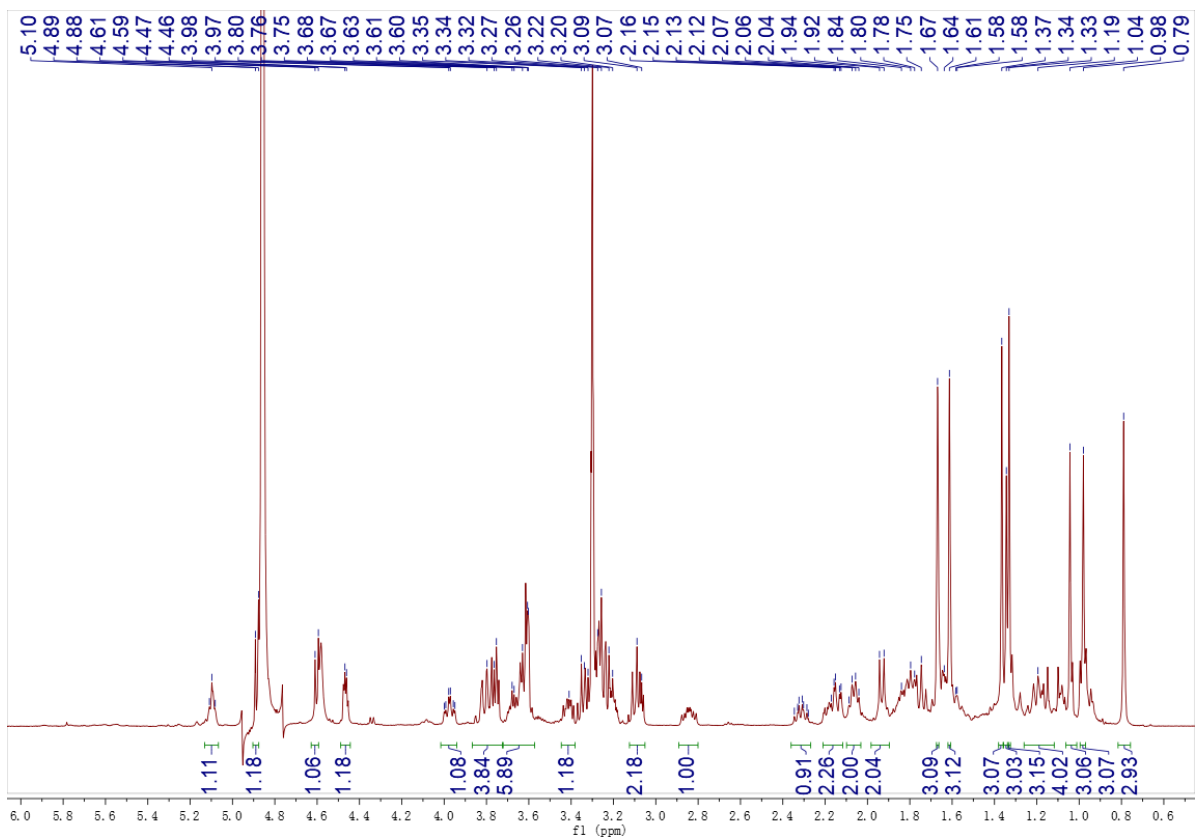


Figure 14  $^1\text{H}$  NMR spectroscopic spectrum of **3**

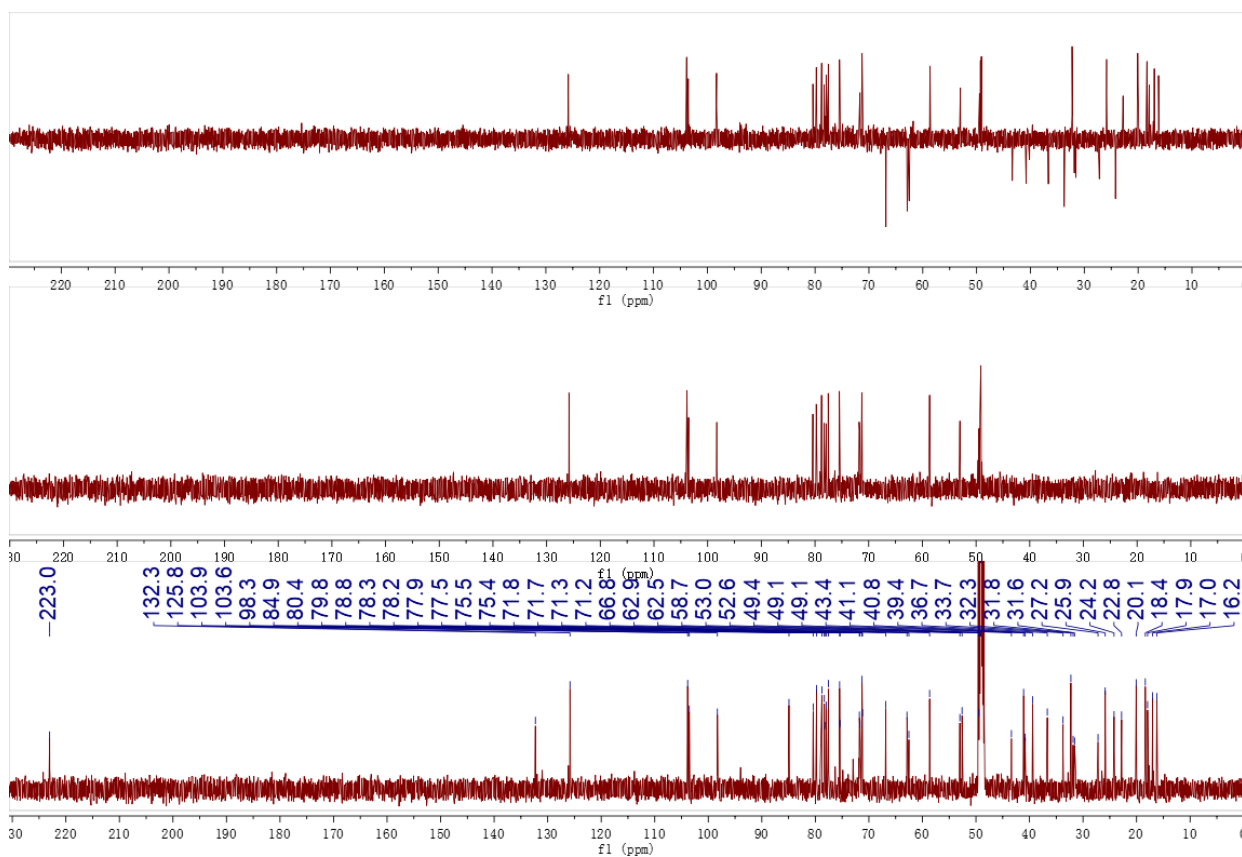


Figure 15  $^{13}\text{C}$  and DEPT NMR spectroscopic spectrum of **3**

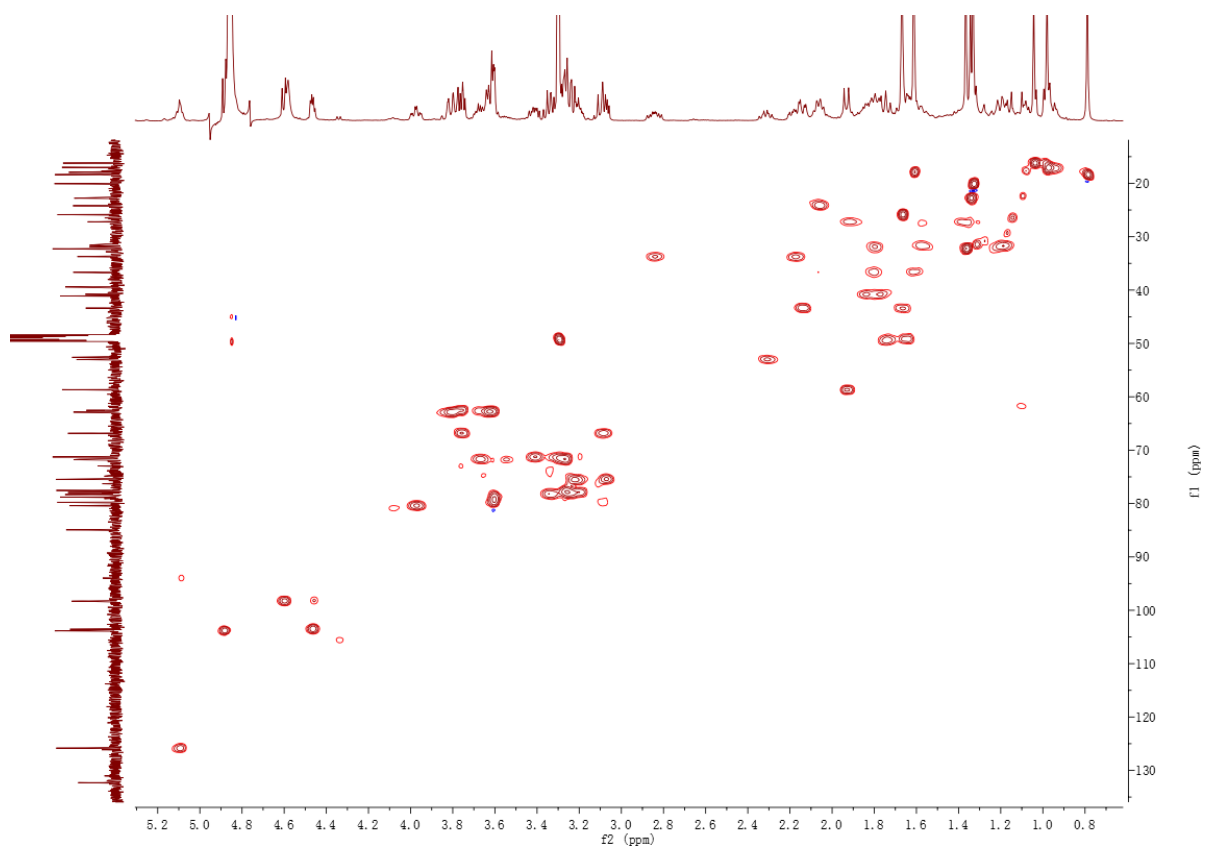


Figure 16 HSQC spectrum of 3

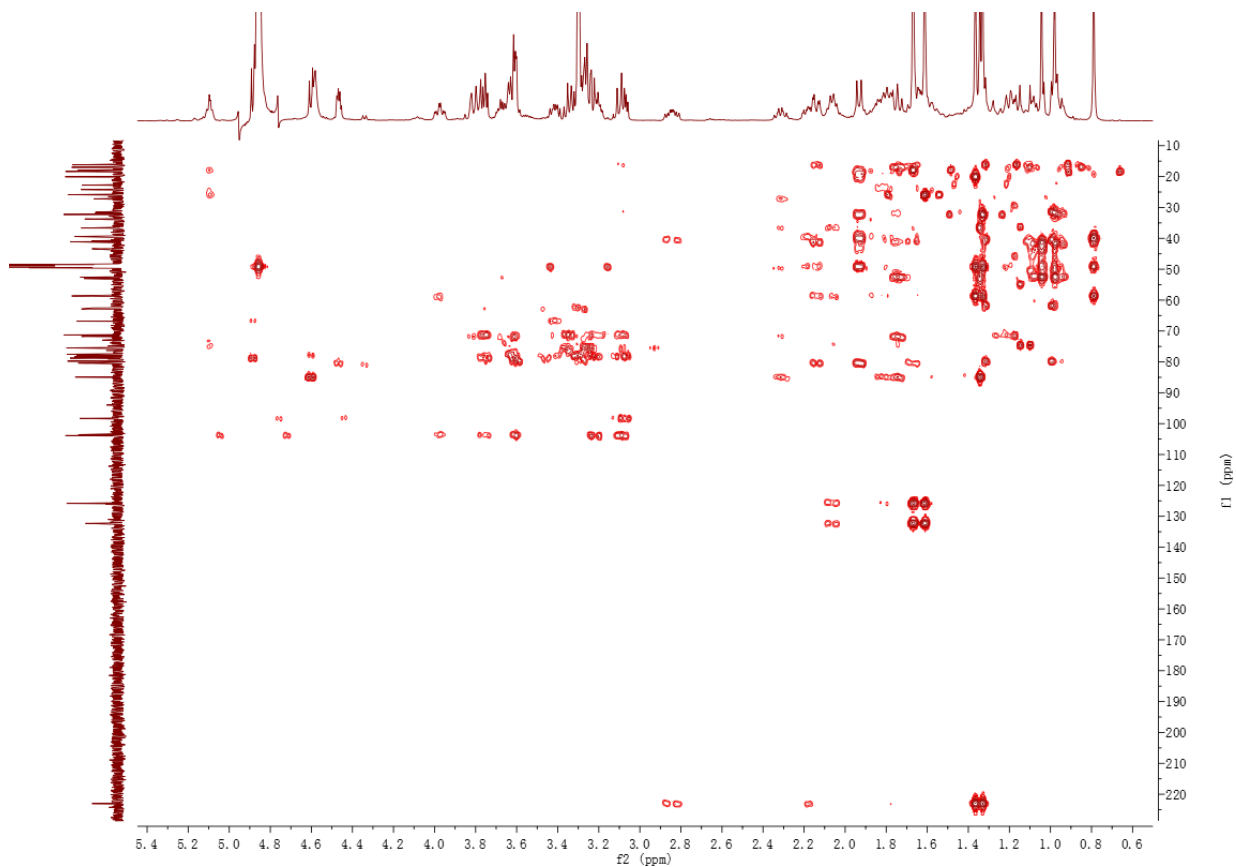


Figure 17 HMBC spectrum of 3

Data File: E:\DATA\2023\1205\2\wpn-45c.lcd

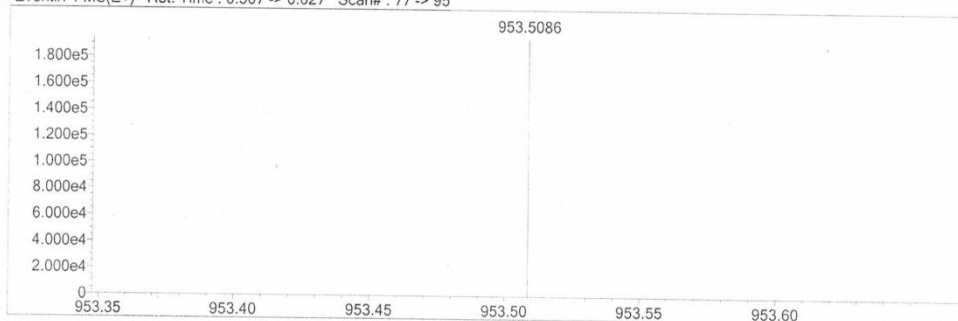
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B	3	0	0	Mg	2	0	0	Cu	2	0	0	Ir	3	0	0	
C	4	5	100	Si	4	0	0	Se	2	0	0	Pt	2	0	0	
N	3	0	10	P	3	0	0	Br	1	0	0					
O	2	0	30	S	2	0	0	Pd	2	0	0					

Error Margin (ppm): 5  
 HC Ratio: unlimited  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

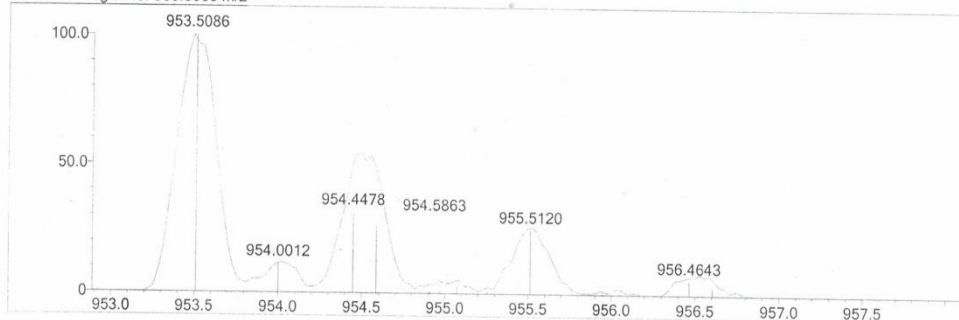
DBE Range: not fixed  
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 MSn Logic Mode: OR

Electron Ions: both  
 Use MSn Info: yes  
 Isotope Res: 10000  
 Max Results: 30

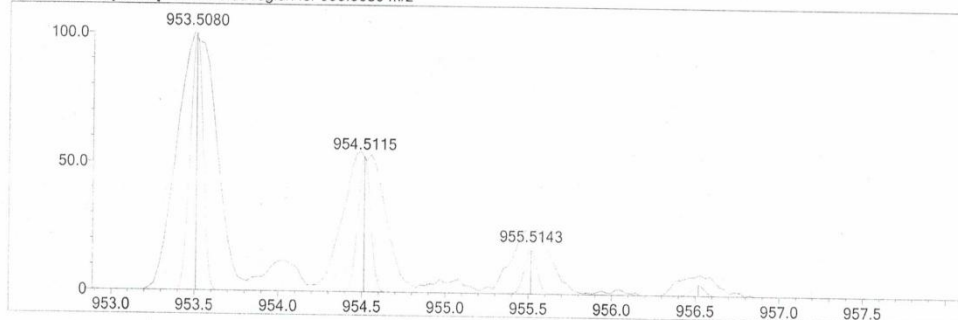
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Measured region for 953.5086 m/z



C47 H78 O18 [M+Na]+ : Predicted region for 953.5080 m/z



Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C47 H78 O18	[M+Na]+	953.5086	953.5080	0.6	0.63	9.0

Figure 18 HRESIMS of 3

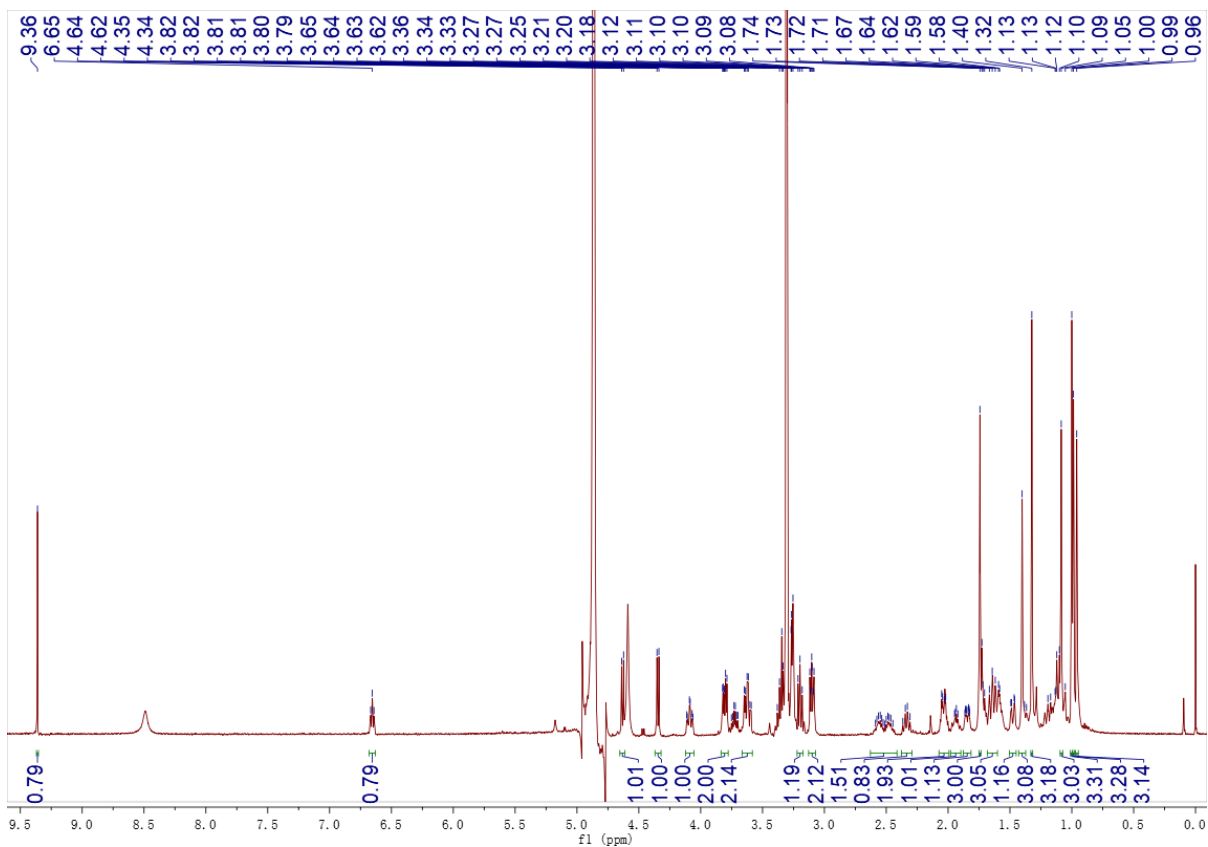


Figure 19  $^1\text{H}$  NMR spectroscopic spectrum of 4

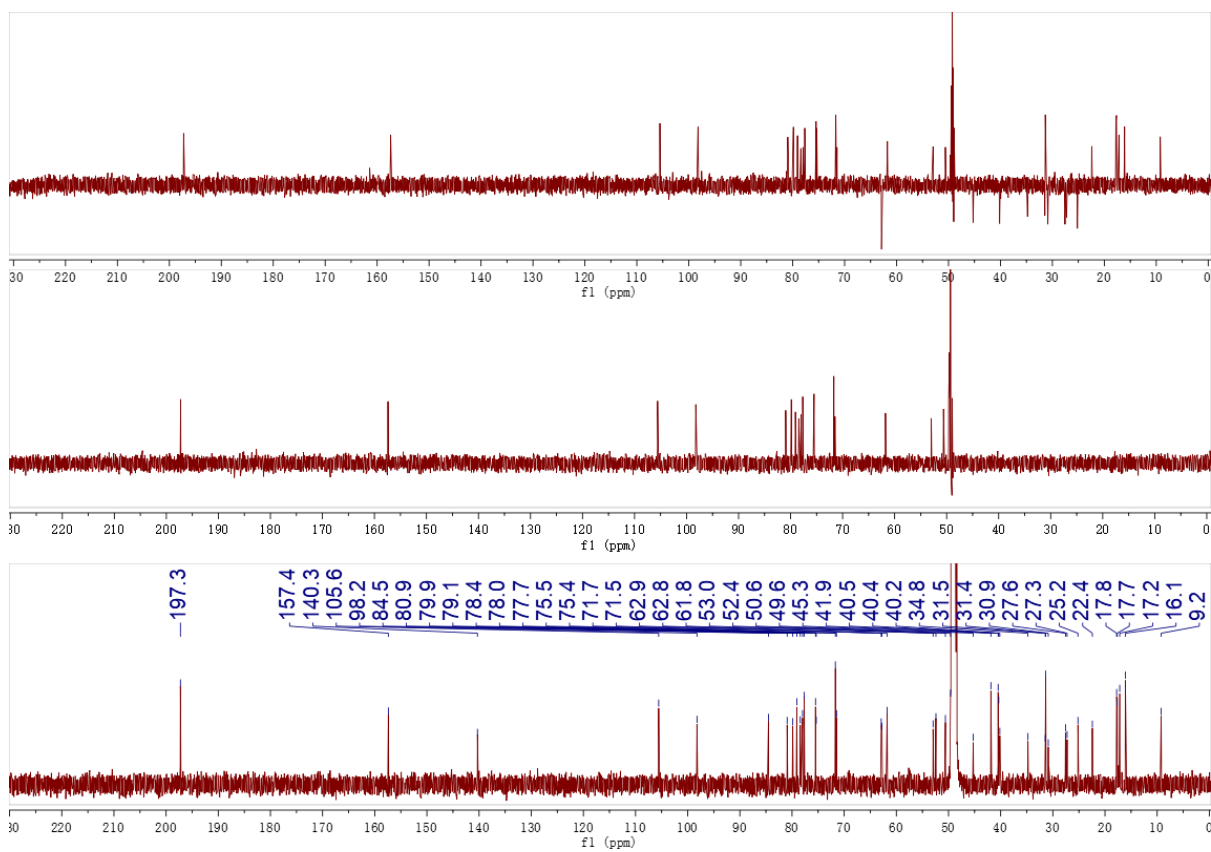


Figure 20  $^{13}\text{C}$  and DEPT NMR spectrum of 4

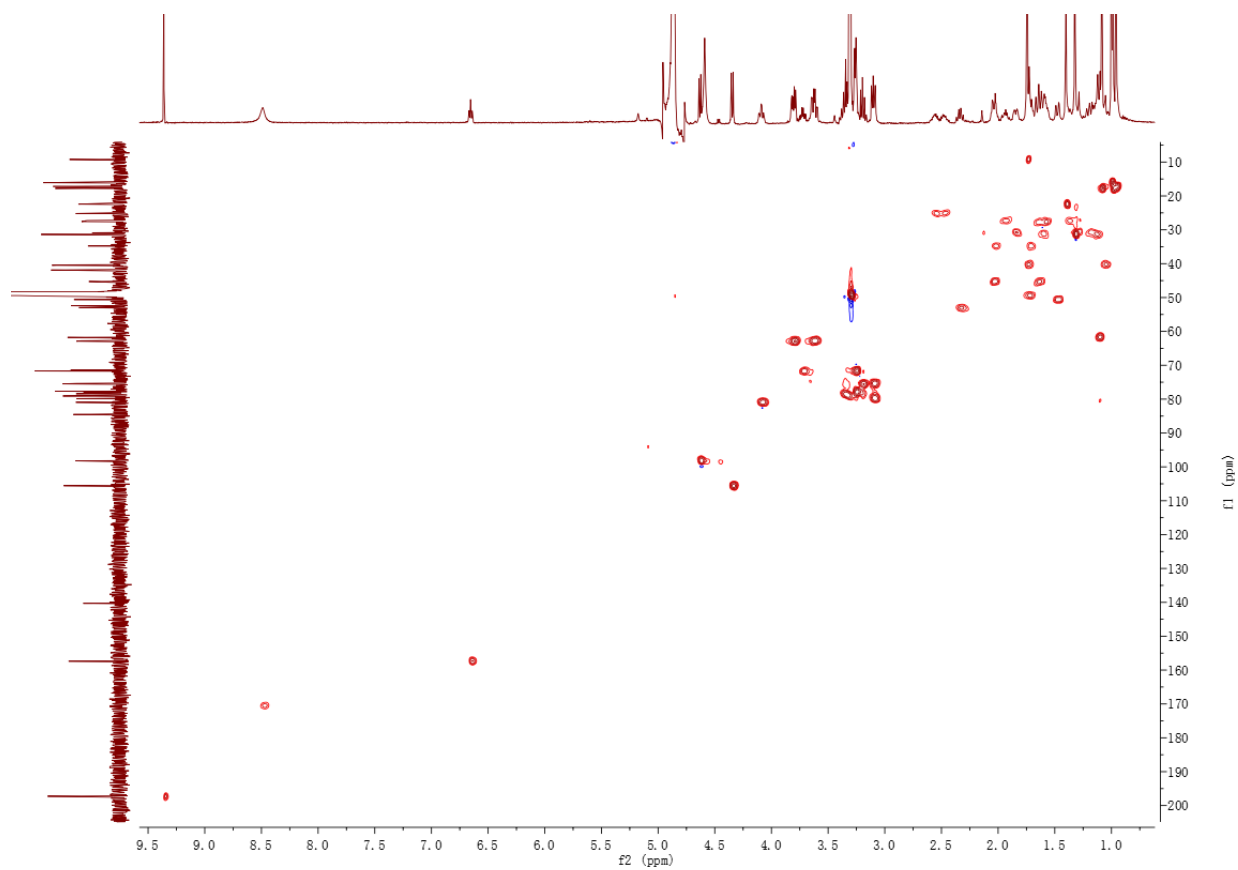


Figure 21 HSQC spectrum of 4

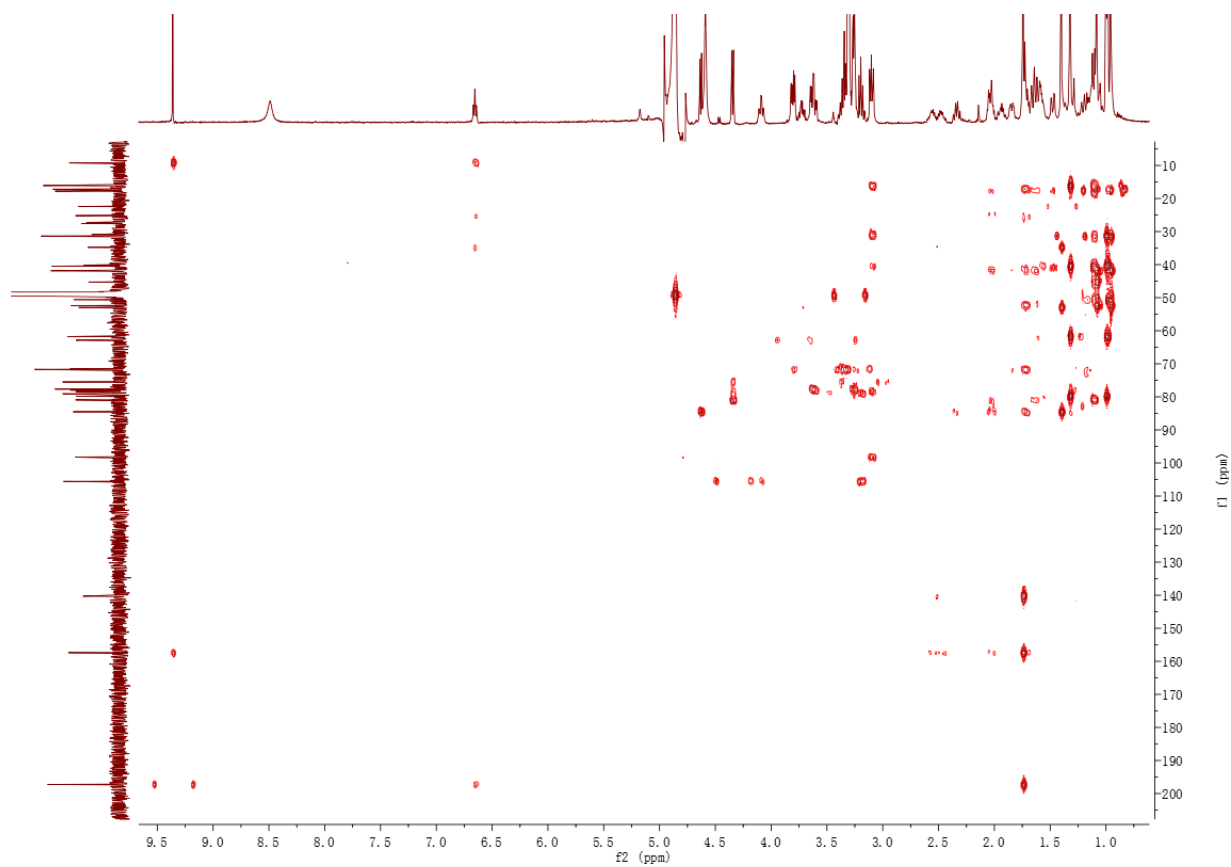


Figure 22 HMBC spectrum of 4

Data File: E:\DATA\2023\0614\wpr-62.lcd

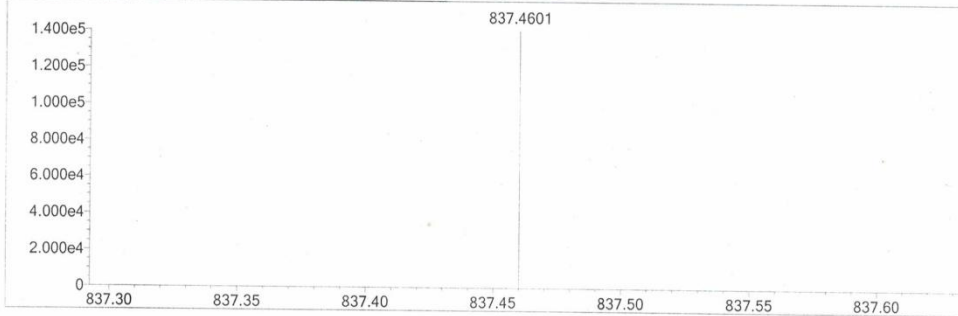
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B	3	0	0	Mg	2	0	0	Cu	2	0	0	Ir	3	0	0	
C	4	5	100	Si	4	0	0	Se	2	0	0	Pt	2	0	0	
N	3	0	10	P	3	0	0	Br	1	0	0					
O	2	0	30	S	2	0	0	Pd	2	0	0					

Error Margin (ppm): 5  
 HC Ratio: unlimited  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

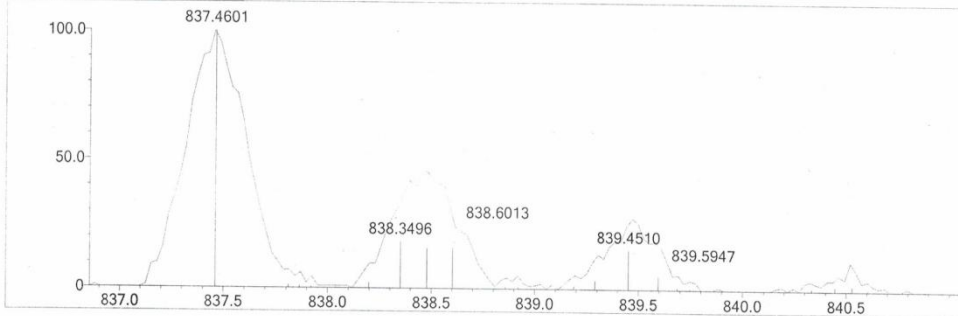
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 MSn Logic Mode: OR

Electron Ions: both  
 Use MSn Info: yes  
 Isotope Res: 10000  
 Max Results: 30

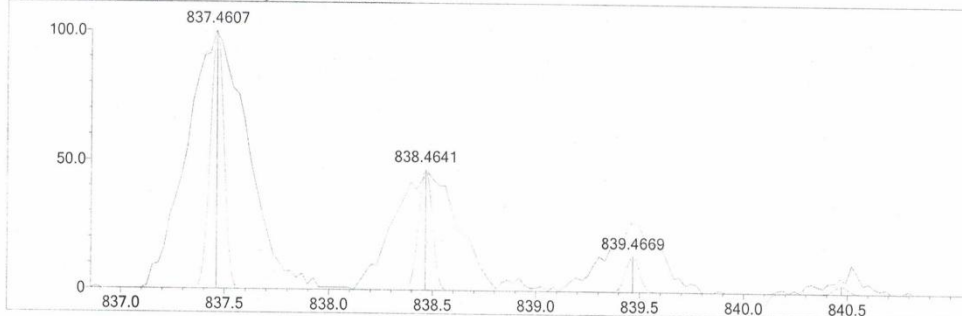
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Measured region for 837.4601 m/z



C42 H70 O15 [M+Na]+ : Predicted region for 837.4607 m/z



Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C42 H70 O15	[M+Na]+	837.4601	837.4607	-0.6	-0.72	8.0

Figure 23 HRMS spectrum of 4

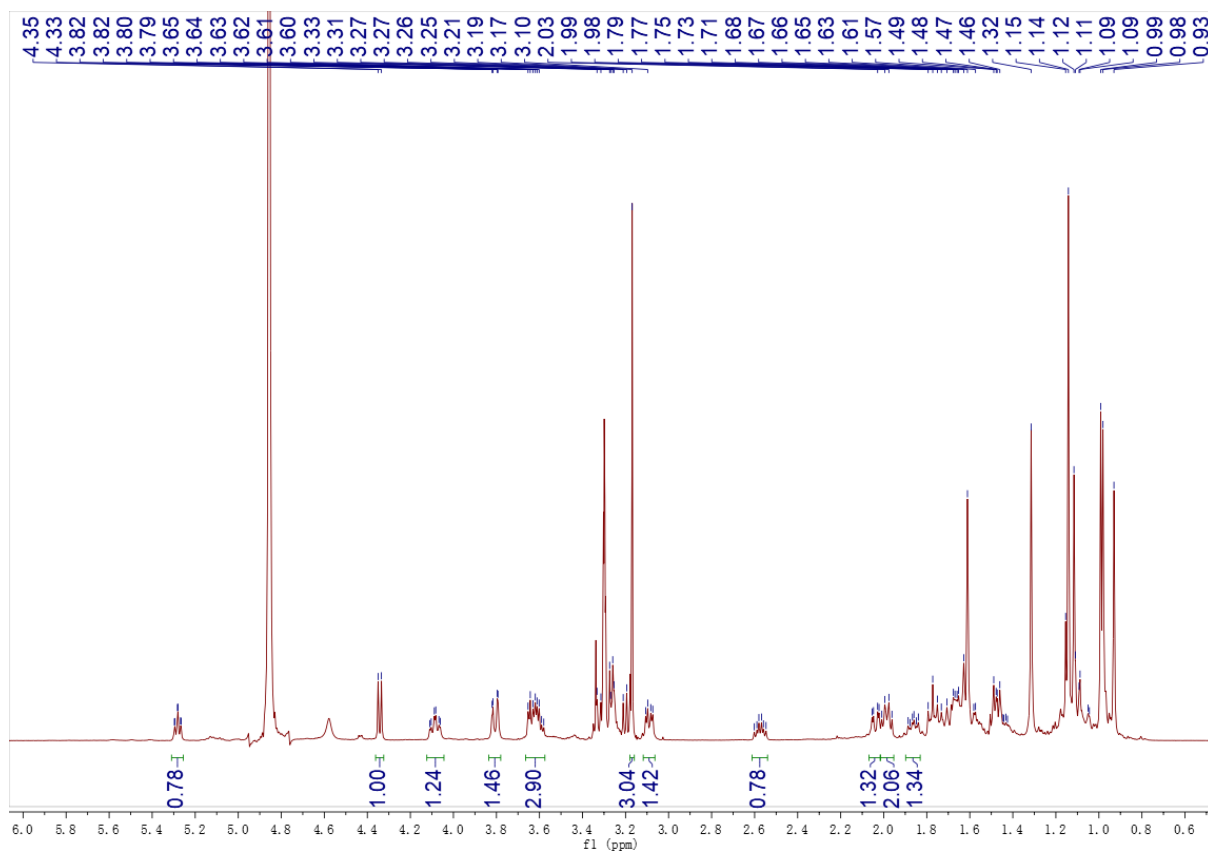


Figure 24  $^1\text{H}$  NMR spectroscopic spectrum of **5**

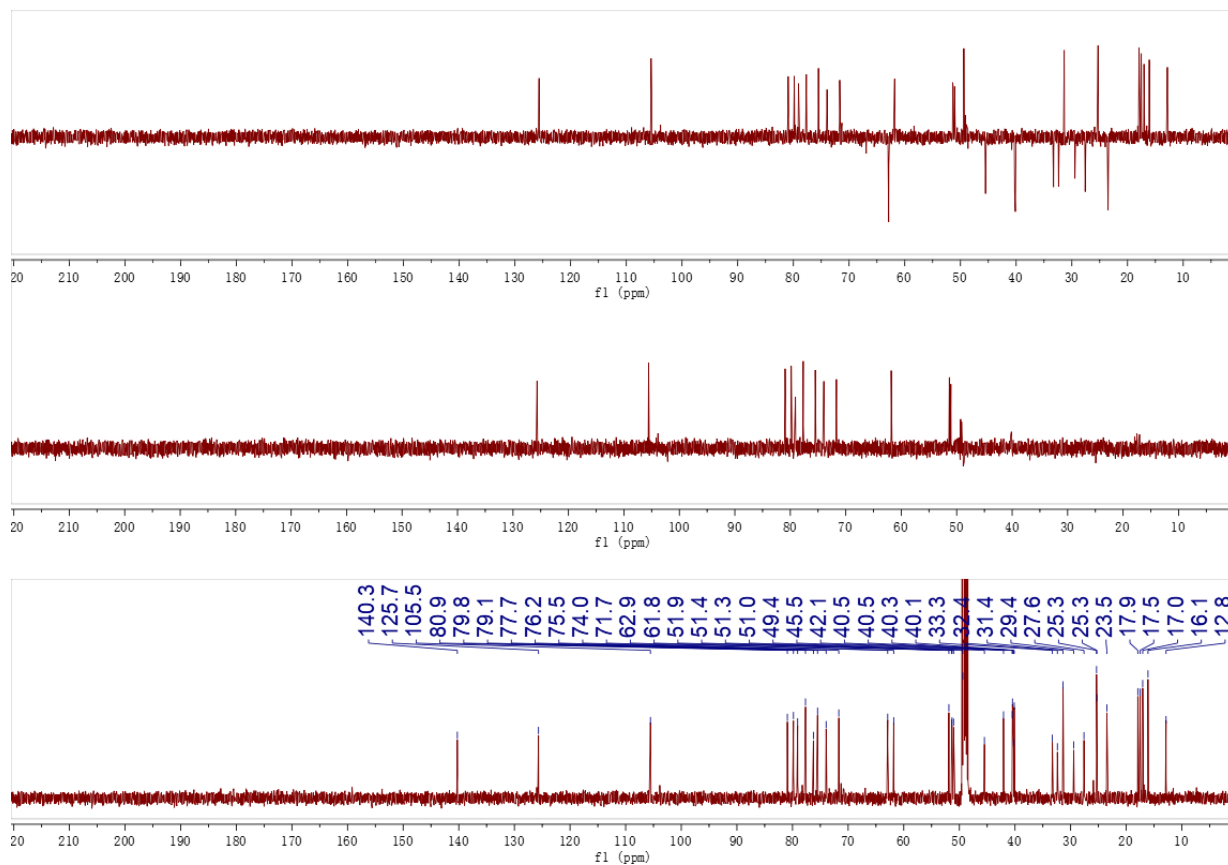


Figure 25  $^{13}\text{C}$  and DEPT NMR spectrum of **5**

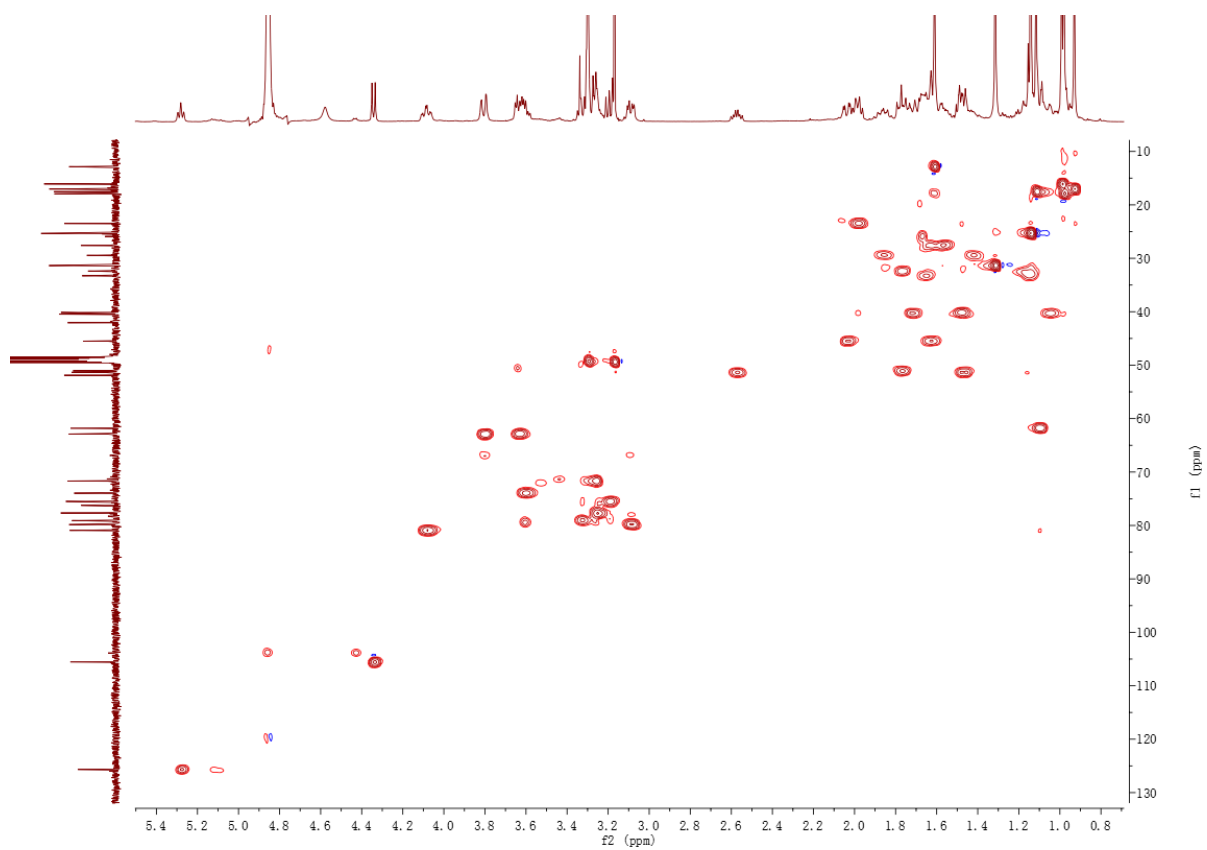


Figure 26 HSQC spectrum of 5

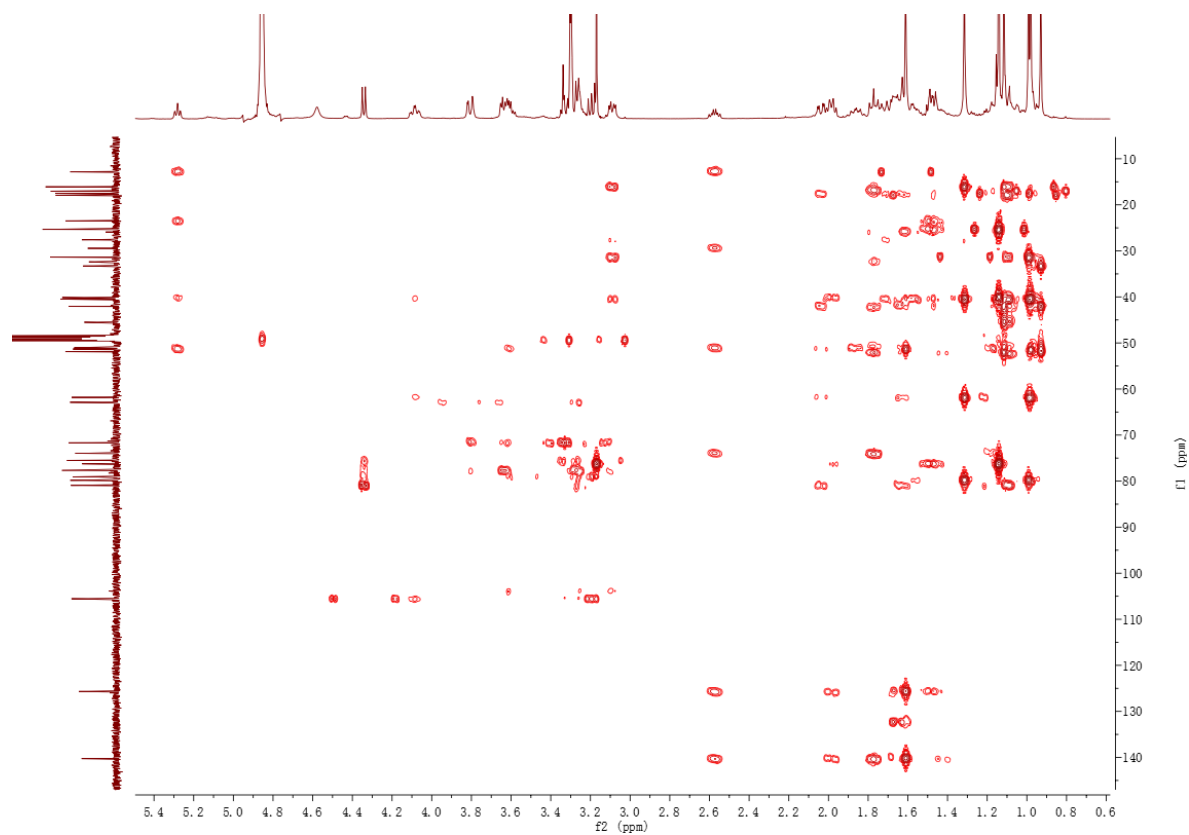


Figure 27 HMBC spectrum of 5

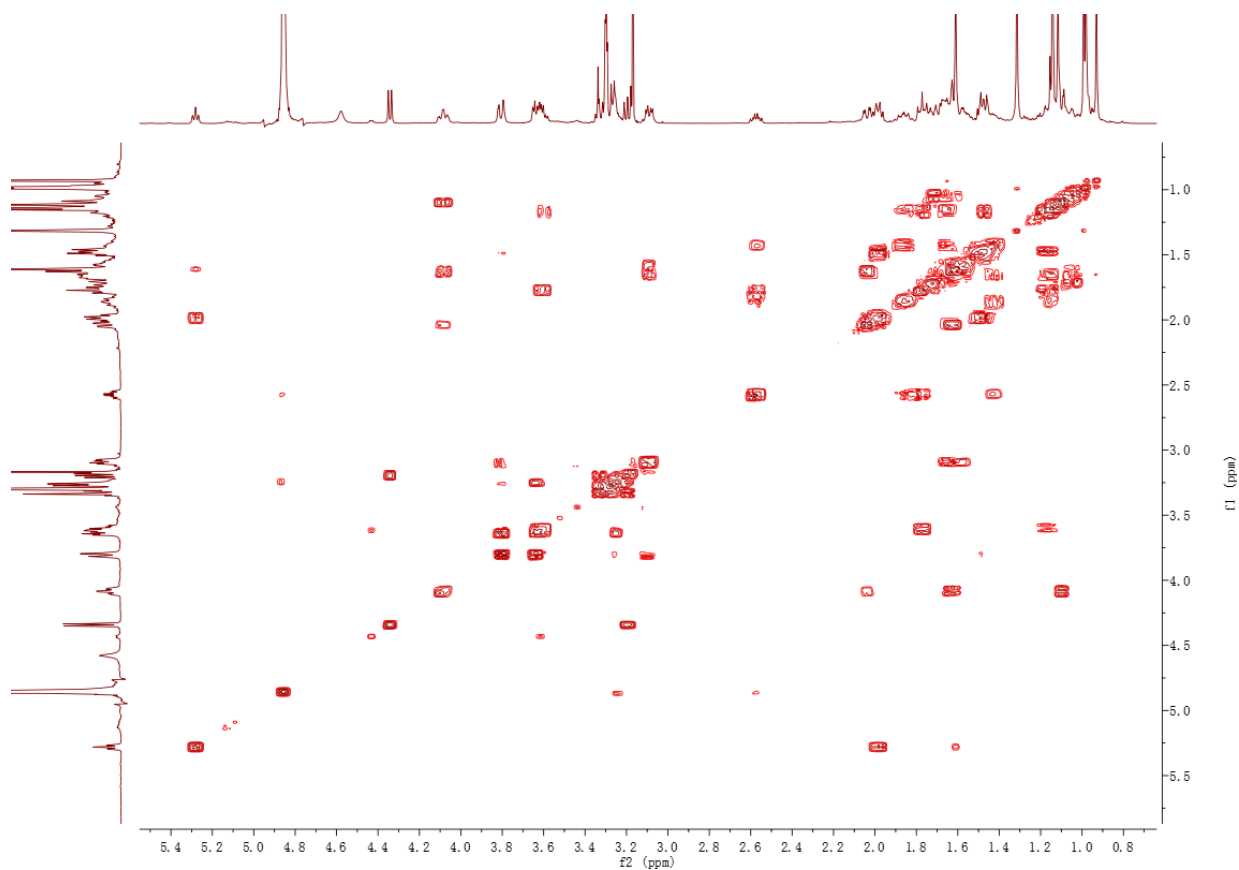


Figure 28  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **5**

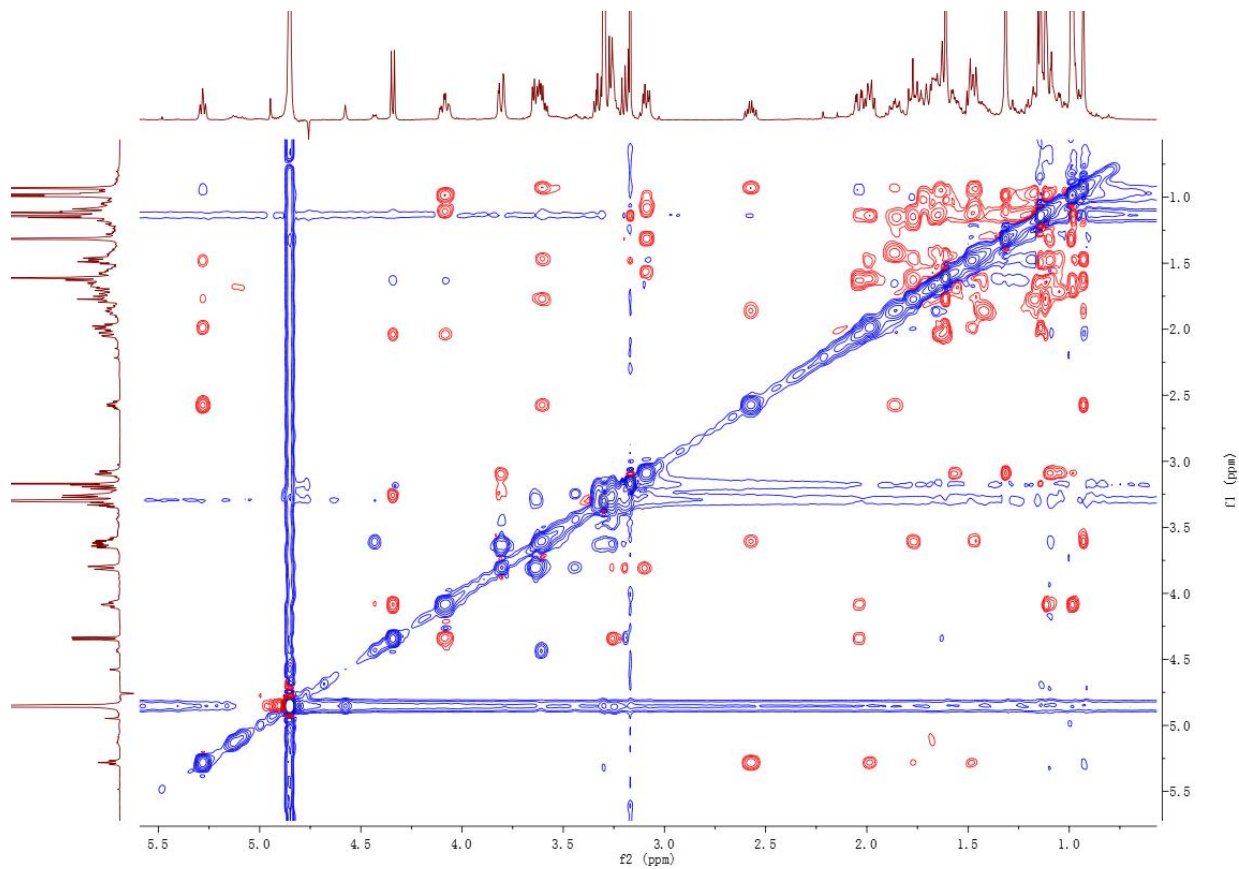


Figure 29 ROESY spectrum of **5**

Data File: E:\DATA\2023\0927\wpn-92d.lcd

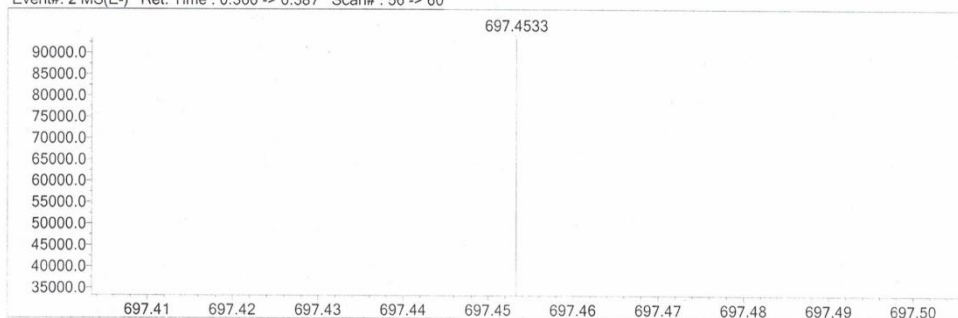
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B	3	0	0	Mg	2	0	0	Cu	2	0	0	Ir	3	0	0	Cl
C	4	5	100	Si	4	0	0	Se	2	0	0	Pt	2	0	0	
N	3	0	10	P	3	0	0	Br	1	0	0					
O	2	0	30	S	2	0	0	Pd	2	0	0					

Error Margin (ppm): 5  
 HC Ratio: unlimited  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

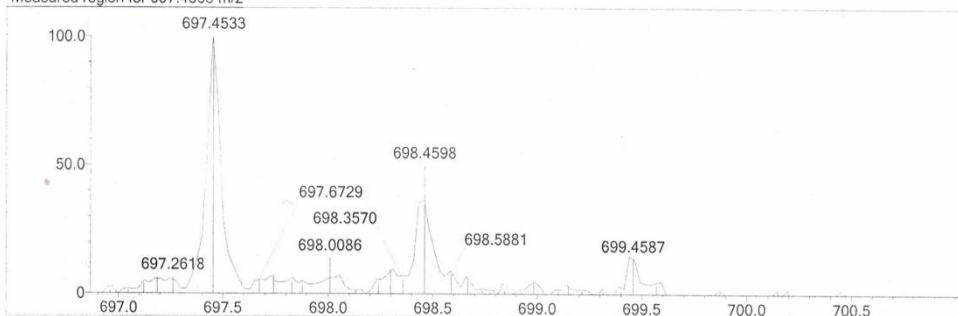
DBE Range: not fixed  
 Apply N Rule: no  
 Isotope RI (%): 1.00  
 MSn Logic Mode: OR

Electron Ions: both  
 Use MSn Info: yes  
 Isotope Res: 10000  
 Max Results: 30

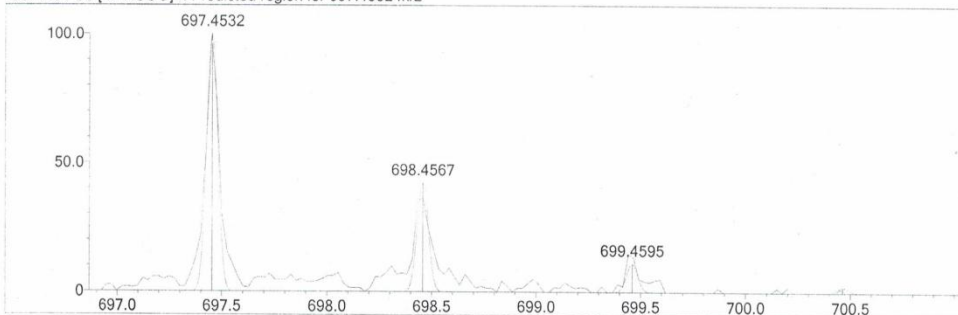
Event#: 2 MS(E-) Ret. Time : 0.360 -> 0.387 Scan# : 56 -> 60



Measured region for 697.4533 m/z



C37 H64 O9 [M+HCOO]- : Predicted region for 697.4532 m/z



Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C37 H64 O9	[M+HCOO]-	697.4533	697.4532	0.1	0.14	6.0

Figure 30 HRESIMS spectrum of 5

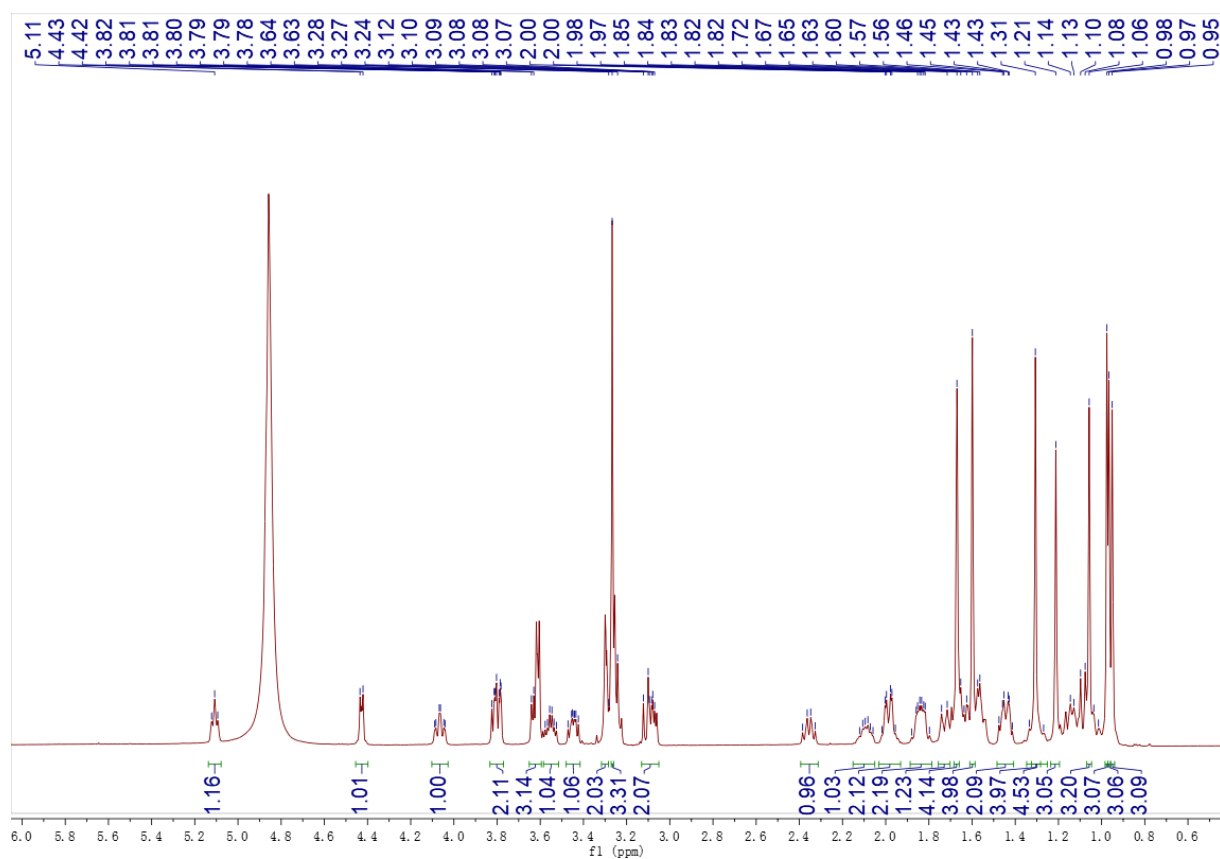


Figure 31  $^1\text{H}$  NMR spectrum of **6**

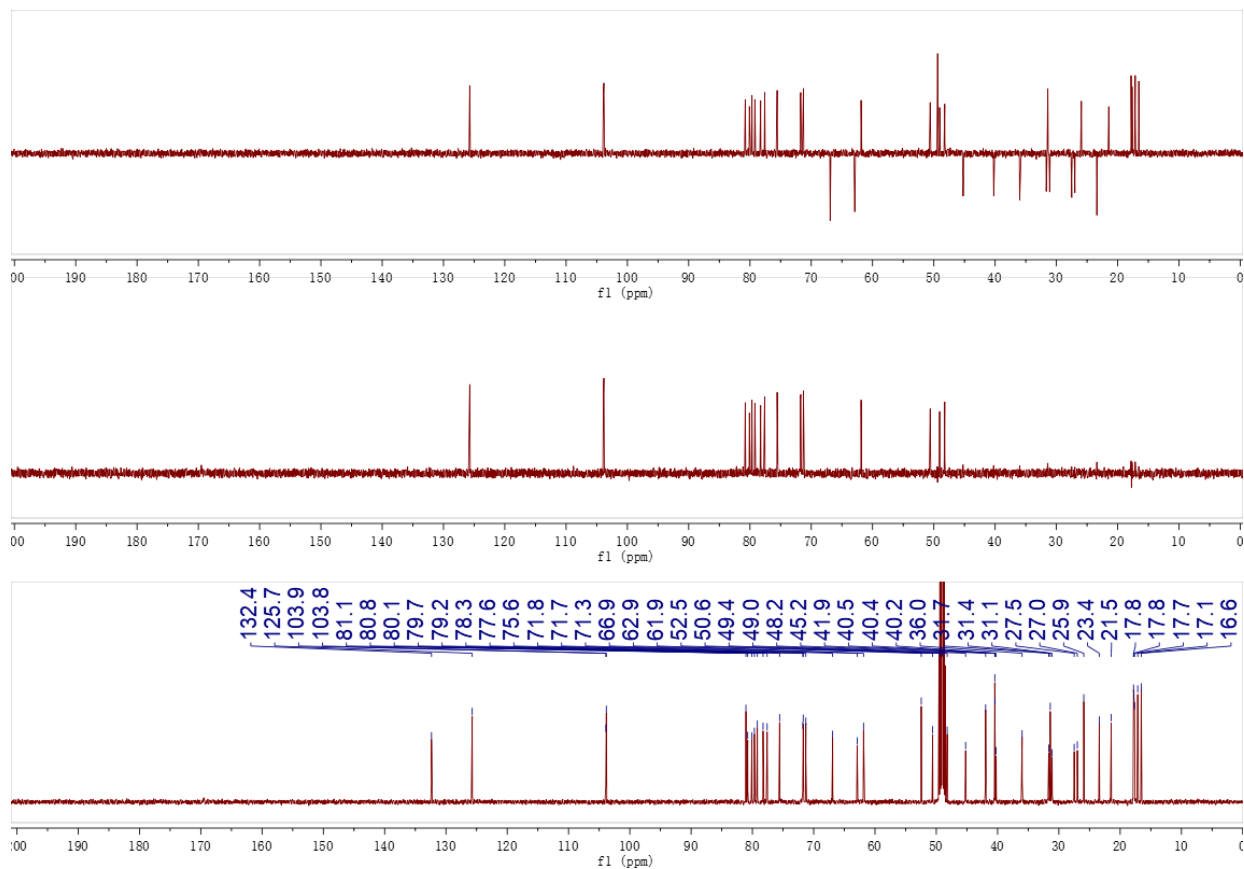


Figure 32  $^{13}\text{C}$  and DEPT NMR spectrum of **6**

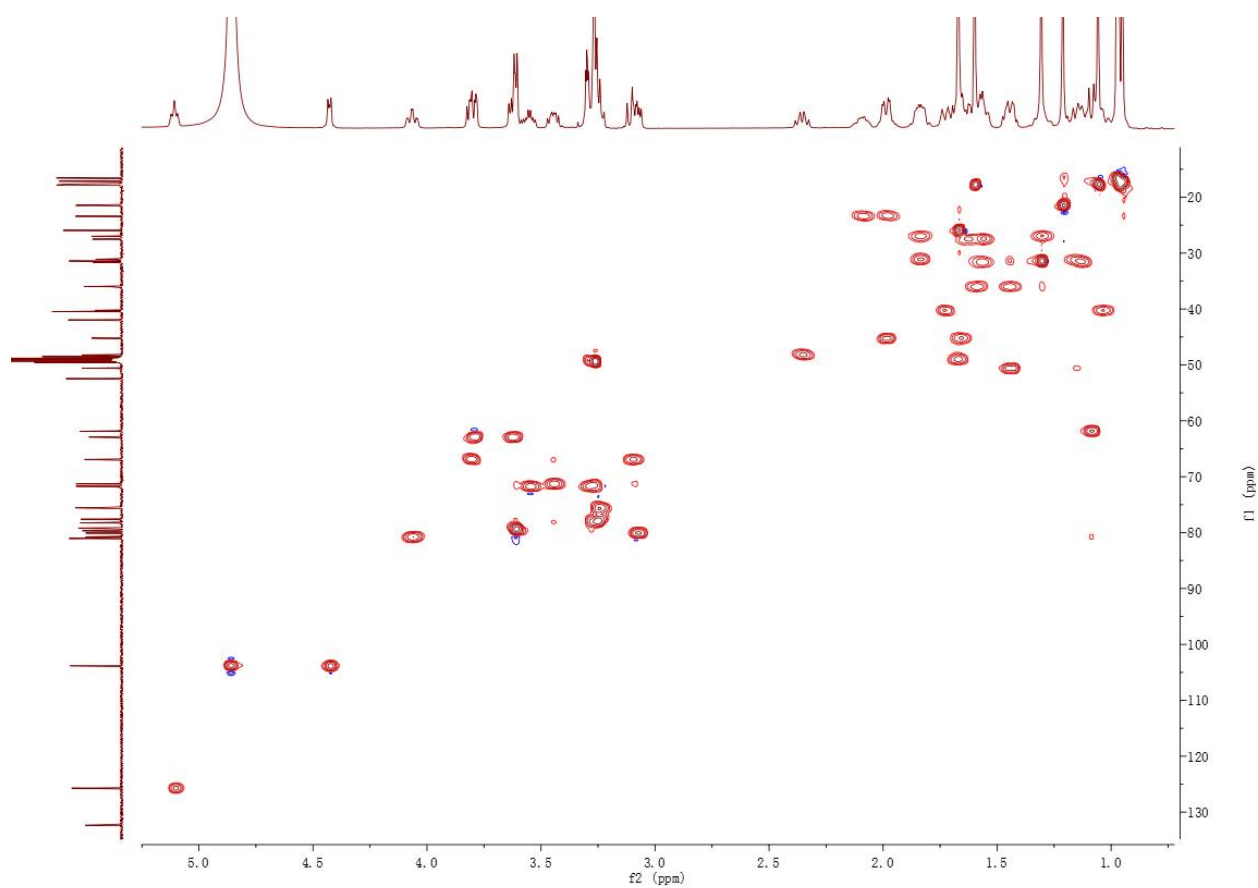


Figure 33 HSQC spectrum of 6

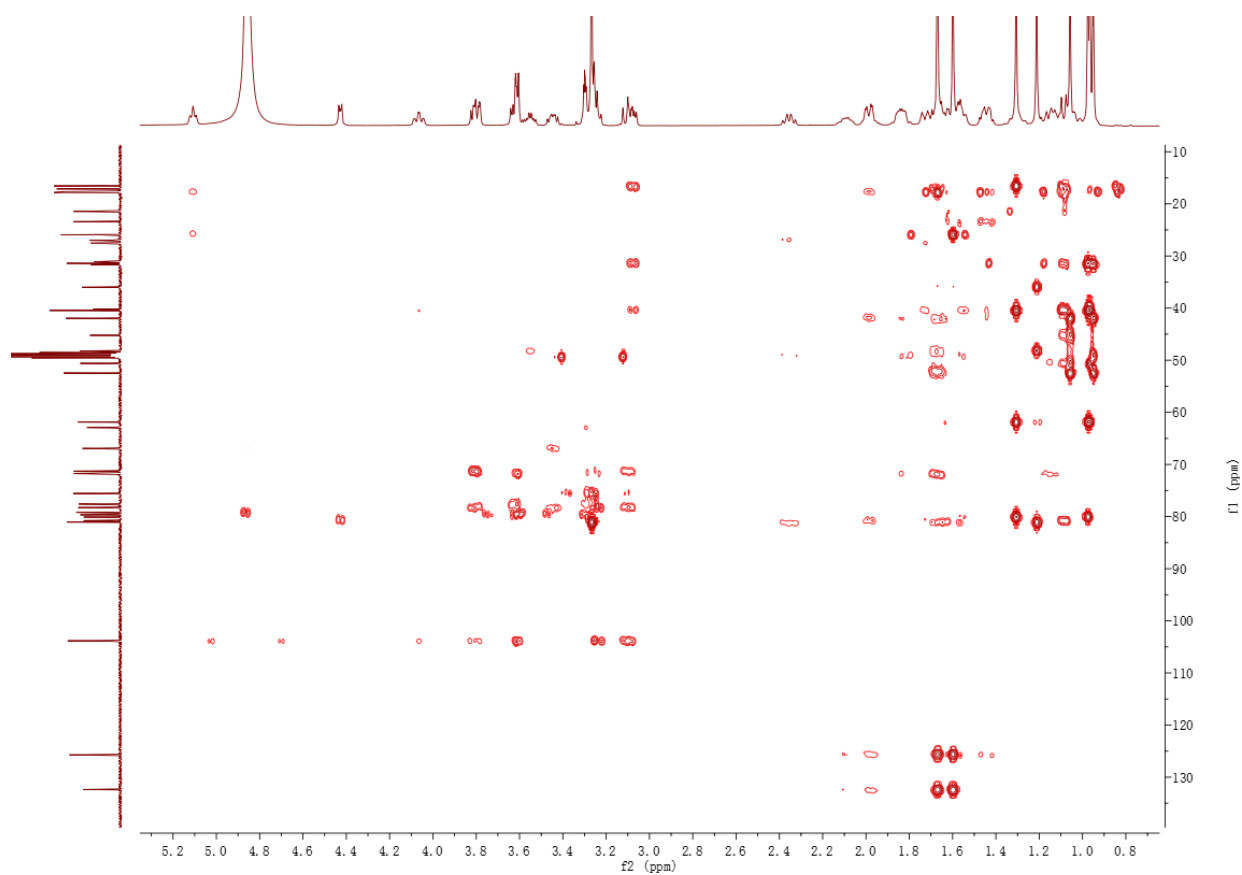


Figure 34 HMBC spectrum of 6

Data File: E:\DATA\2023\0927\wpn-92e.lcd

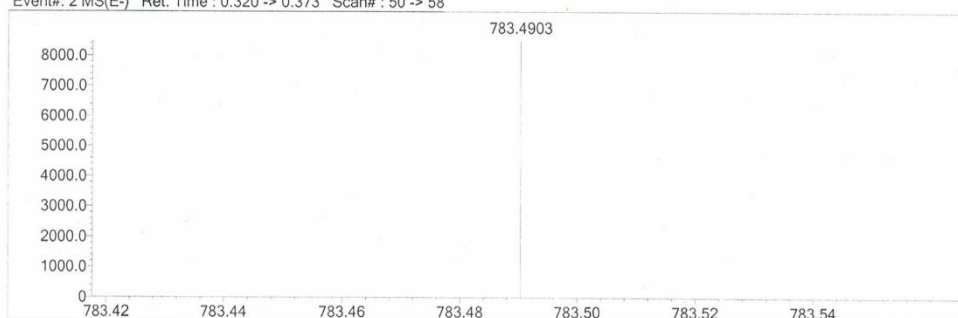
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	10	100	F	1	0	0	Cl	1	0	0	Ag	1	0	0	H
2H	1	0	0	Na	1	0	0	Co	2	0	0	I	3	0	0	HCOO
B	3	0	0	Mg	2	0	0	Cu	2	0	0	Ir	3	0	0	Cl
C	4	5	100	Si	4	0	0	Se	2	0	0	Pt	2	0	0	
N	3	0	10	P	3	0	0	Br	1	0	0					
O	2	0	30	S	2	0	0	Pd	2	0	0					

Error Margin (ppm): 5  
 HC Ratio: unlimited  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

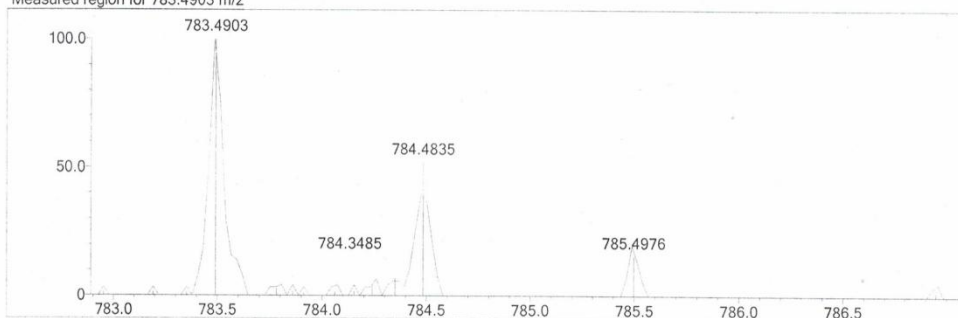
DBE Range: not fixed  
 Apply N Rule: no  
 Isotope RI (%): 1.00  
 MSn Logic Mode: OR

Electron Ions: both  
 Use MSn Info: yes  
 Isotope Res: 10000  
 Max Results: 30

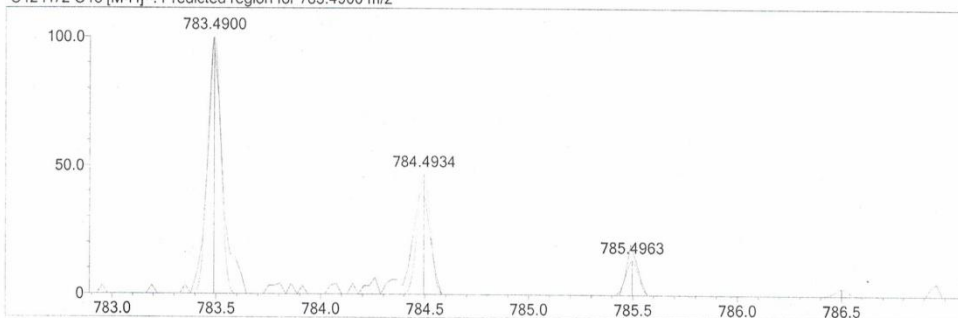
Event#: 2 MS(E-) Ret. Time : 0.320 -> 0.373 Scan# : 50 -> 58



Measured region for 783.4903 m/z



C42 H72 O13 [M-H]- : Predicted region for 783.4900 m/z



Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C42 H72 O13	[M-H]-	783.4903	783.4900	0.3	0.38	7.0

Figure 35 HRESIMS spectrum of 6