

Supplementary Materials

# Croargoids A–G, Eudesmane Sesquiterpenes from the Bark of *Croton argyratus*

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## Tables

**Table S1.** NO inhibitory effects of compounds 1~7.

Compound	Concentration ( $\mu$ M)	NO Inhibition Rate (%)
1	50	-28.60 $\pm$ 2.84
2	50	-19.03 $\pm$ 3.52
3	50	-9.29 $\pm$ 2.36
4	50	-9.18 $\pm$ 2.25
5	50	41.62 $\pm$ 0.95
6	50	4.62 $\pm$ 2.53
7	50	10.34 $\pm$ 2.17
L-NMMA <sup>a</sup>	50	54.94 $\pm$ 1.43

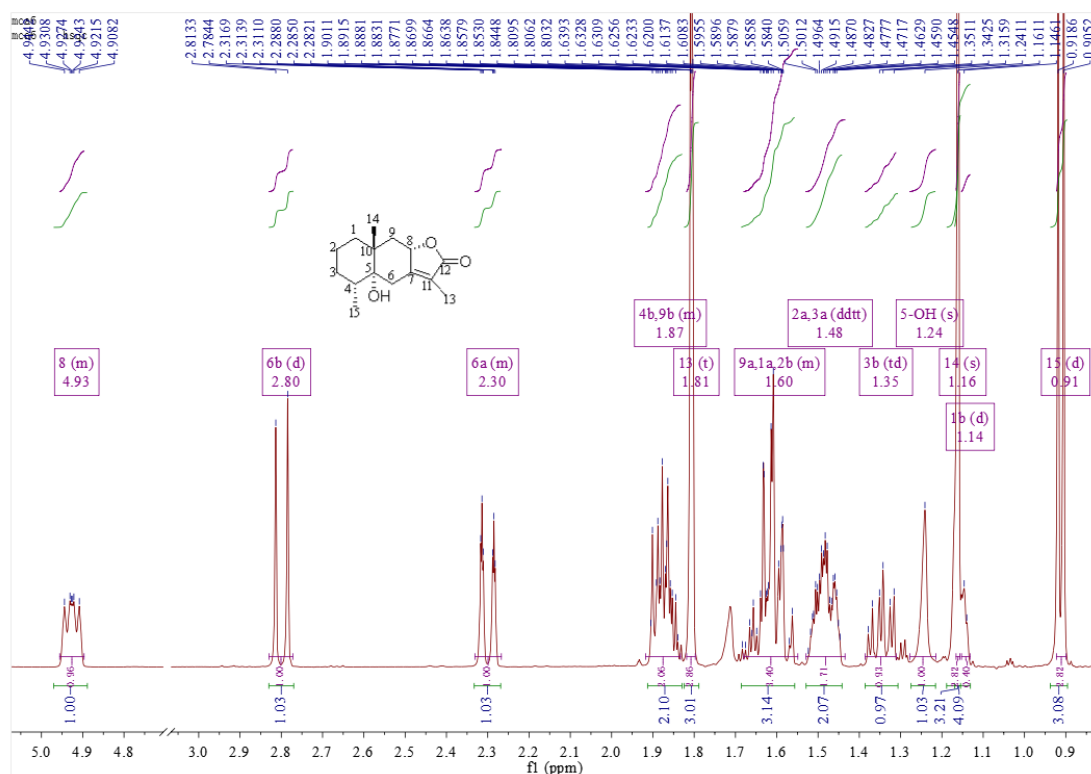
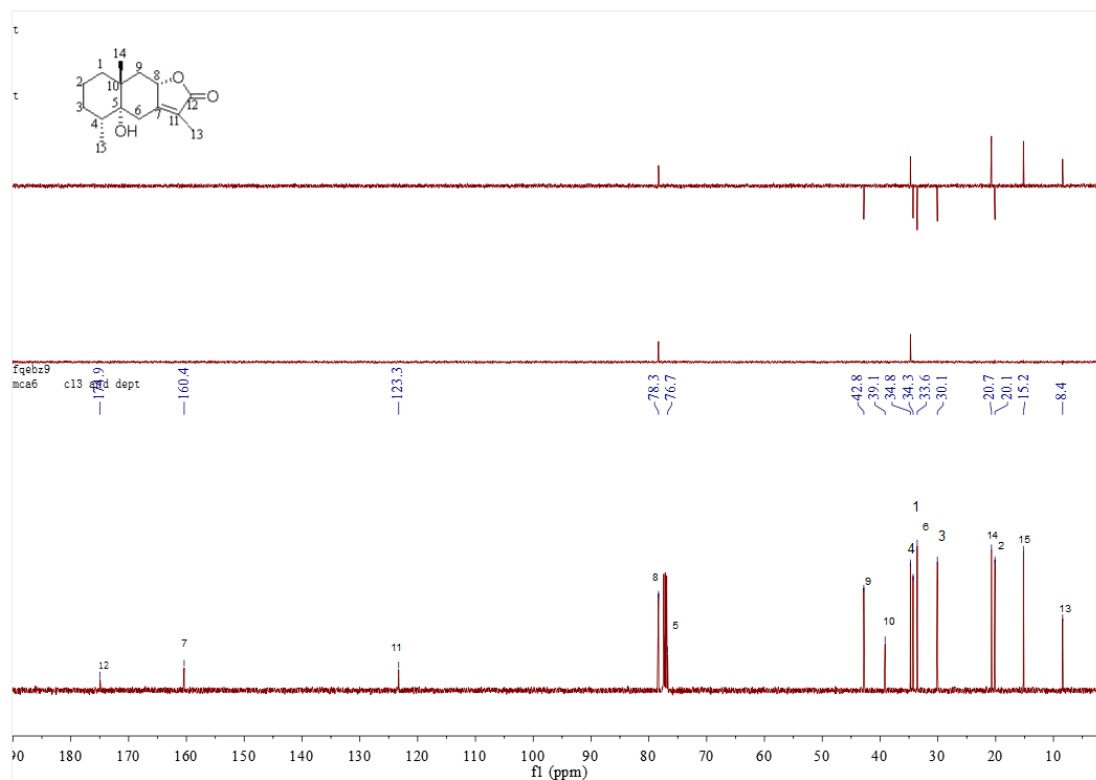
<sup>a</sup>Positive control.

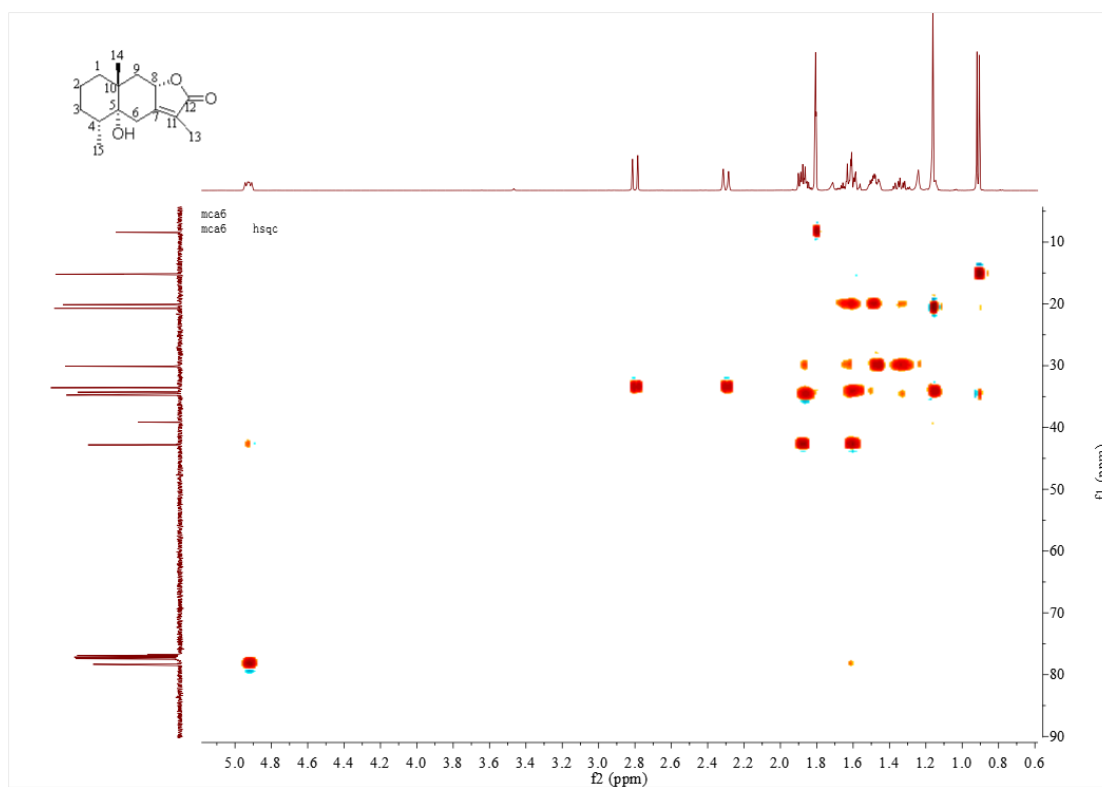
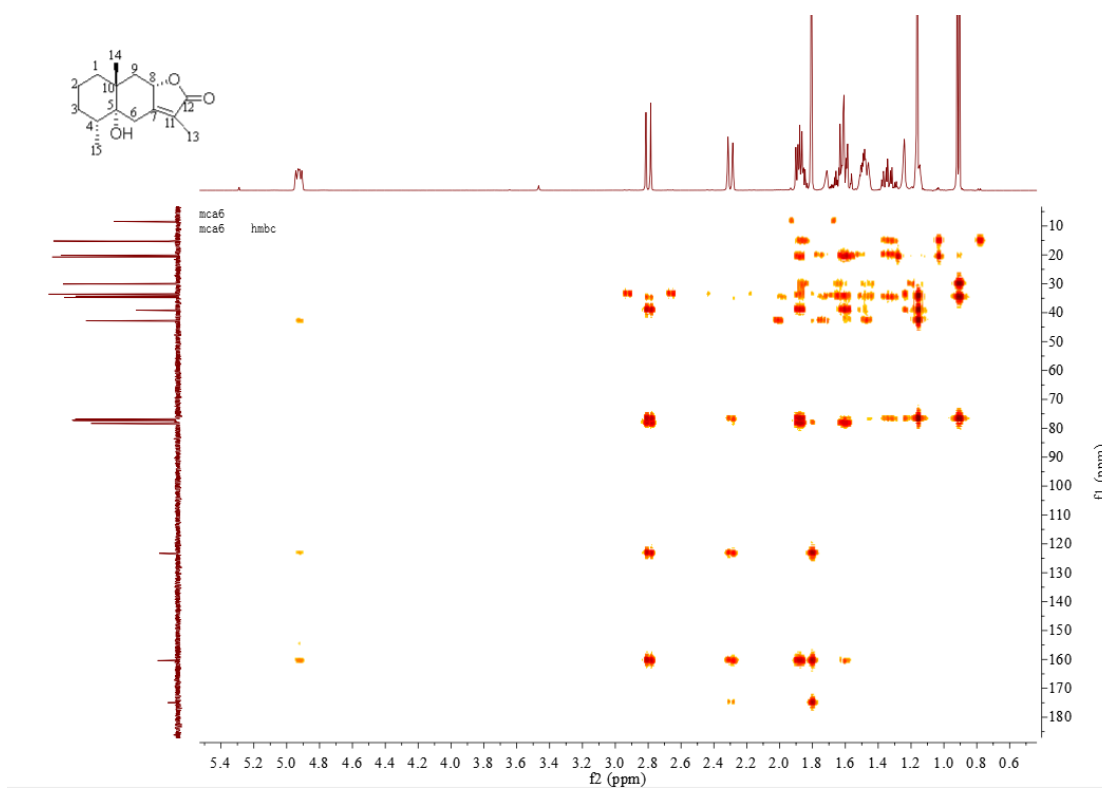
**Table S2.** Cytotoxic activity of compounds 1~7 (IC<sub>50</sub>,  $\mu$ M).

Compound	HL-60	SMMC-7721	A-549	MCF-7	SW480
1	>40	>40	>40	>40	>40
2	>40	>40	>40	>40	>40
3	>40	>40	>40	>40	>40
4	>40	>40	>40	>40	>40
5	>40	>40	>40	>40	>40
6	>40	>40	>40	>40	>40
7	>40	>40	>40	>40	>40
Cisplatin <sup>a</sup>	2.75	4.78	3.56	16.20	10.69

<sup>a</sup>Positive control.

## Figures

Figure S1.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of 1.Figure S2.  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of 1.

Figure S3. HSQC (500 MHz, CDCl<sub>3</sub>) spectrum of 1.Figure S4. HMBC (500 MHz, CDCl<sub>3</sub>) spectrum of 1.

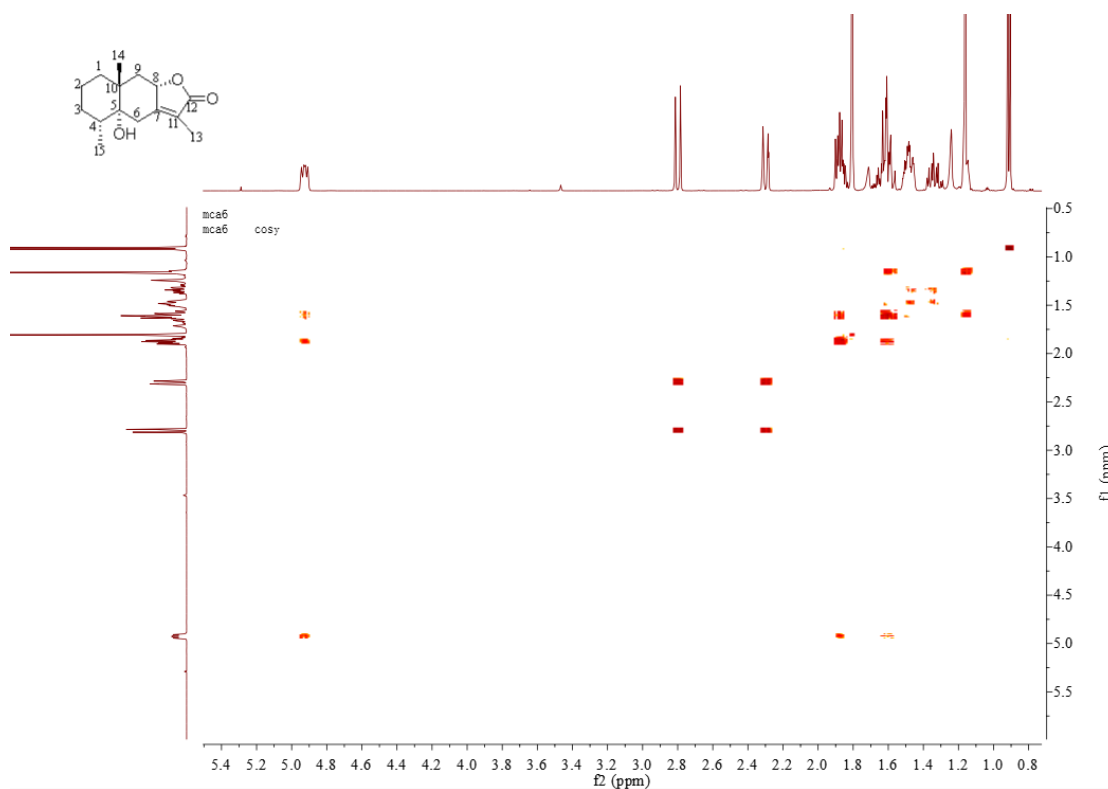


Figure S5.  $^1\text{H}$ - $^1\text{H}$  COSY (500 MHz,  $\text{CDCl}_3$ ) spectrum of **1**.

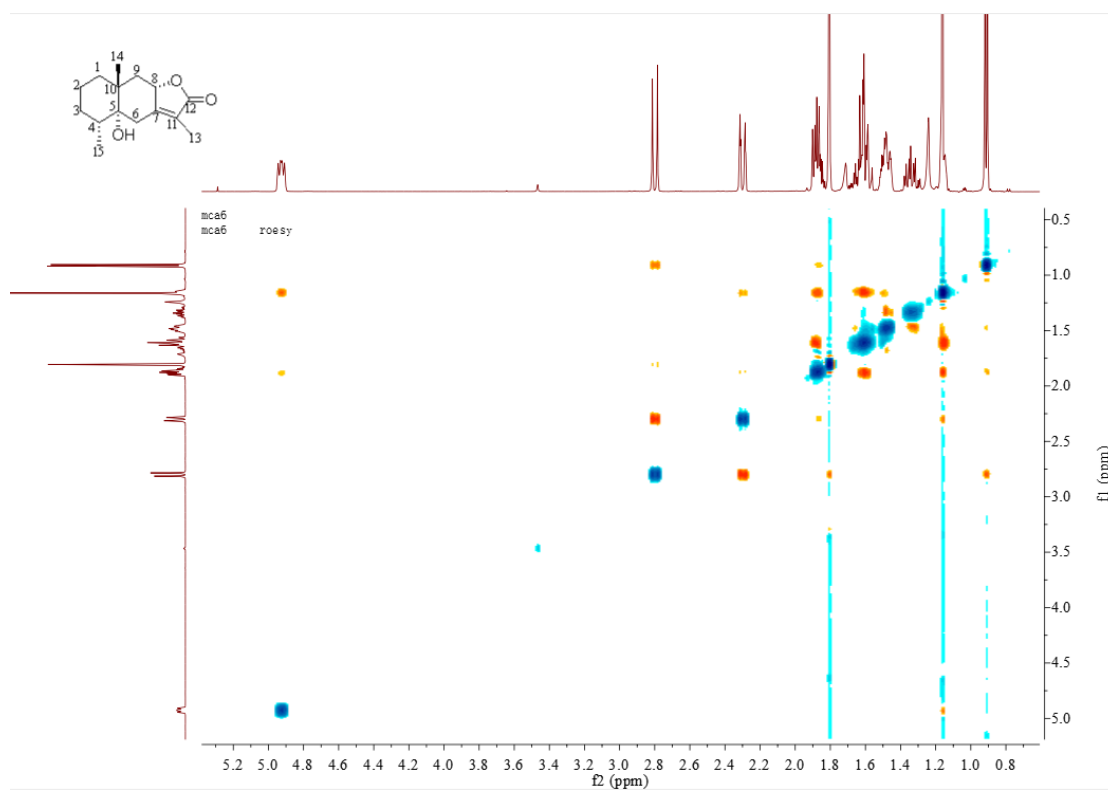


Figure S6. NOESY (500 MHz,  $\text{CDCl}_3$ ) spectrum of **1**.

Formula Predictor Report - MCA-6.lcd

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Data File: E:\DATA\2021\0714\MCA-6.lcd

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B	3	0	0	Na	1	0	0	Cl	1	0	0	Pd	2	0	0	
C	4	10	150	Mg	2	0	0	Co	2	0	0	Ag	1	0	0	
N	3	0	10	Si	4	0	0	Cu	2	0	0	I	3	0	0	

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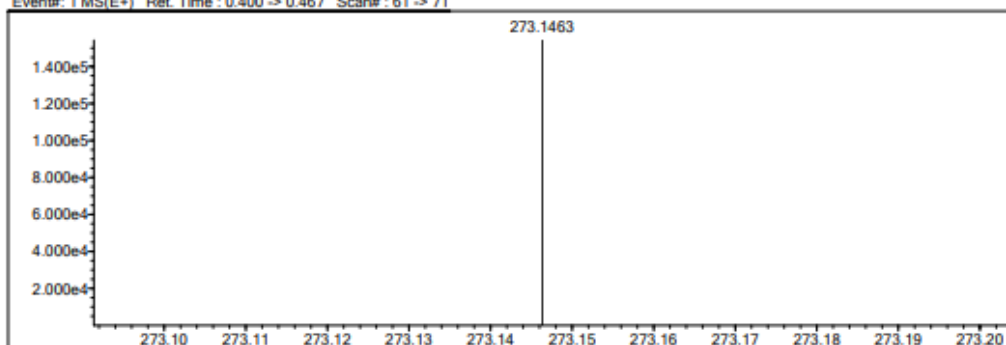
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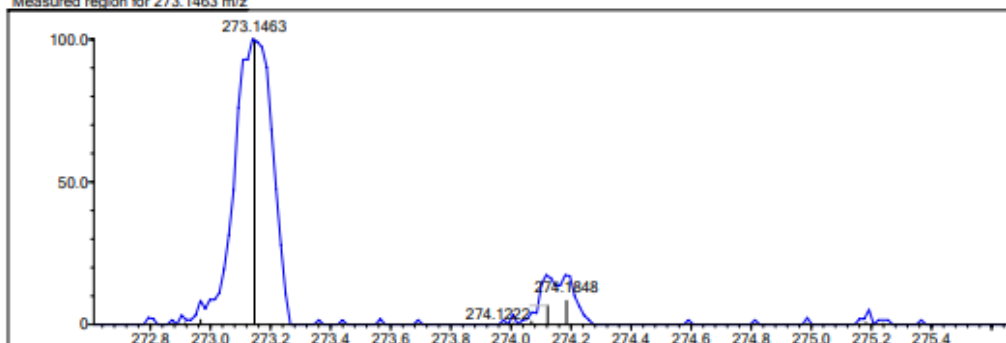
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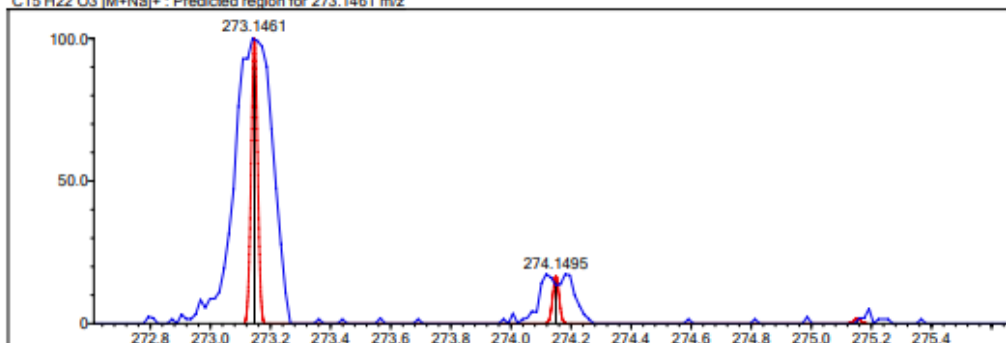
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Measured region for 273.1463 m/z

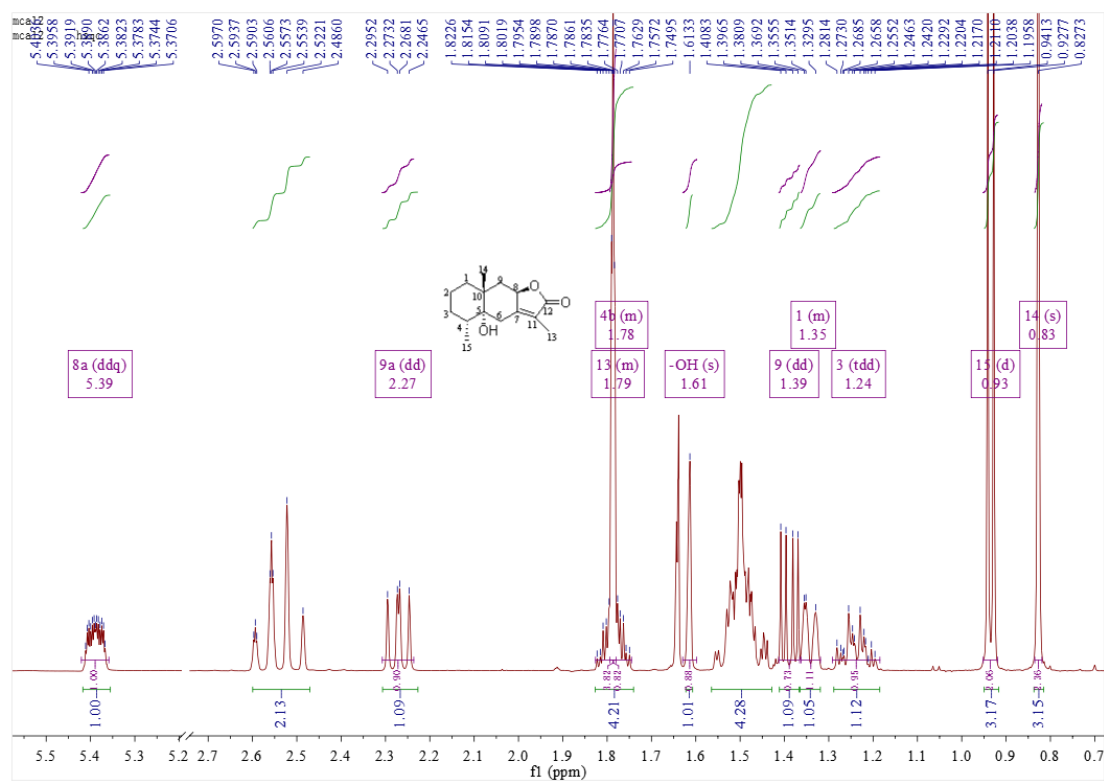
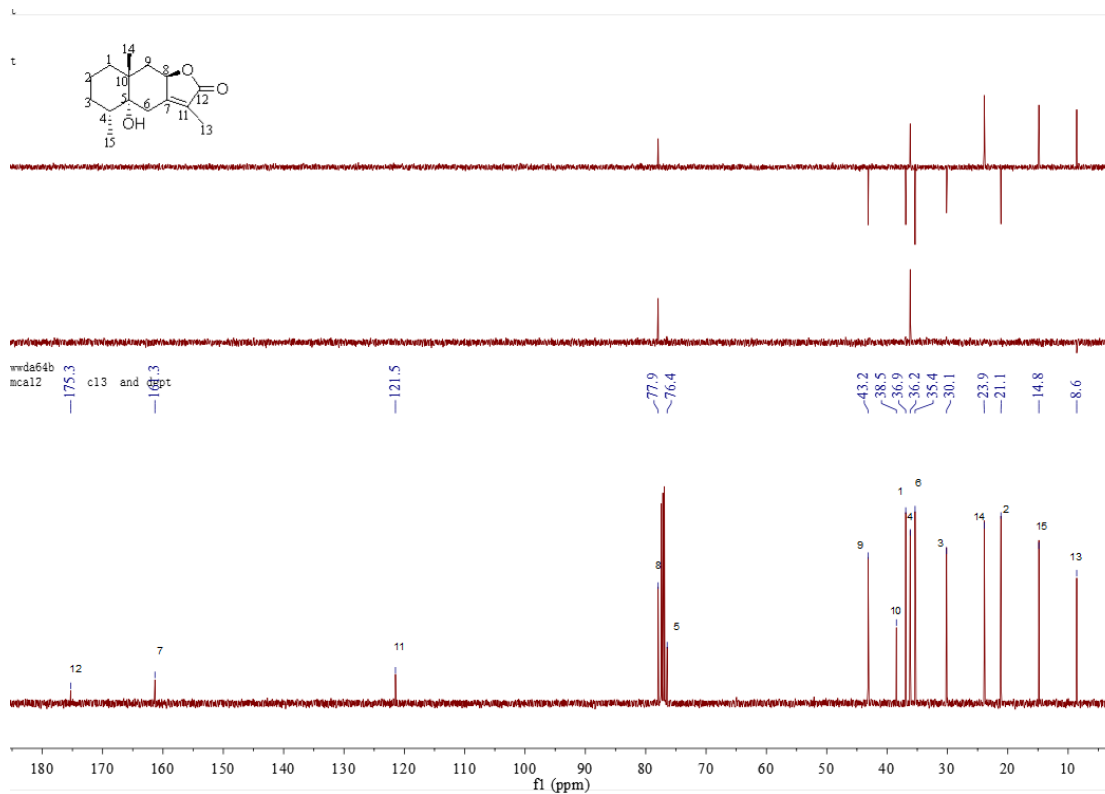


C15 H22 O3 [M+Na]+ : Predicted region for 273.1461 m/z



Formula (M)	Ion	Mass, m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C15 H22 O3	[M+Na]+	273.1463	273.1461	0.2	0.73	5.0

Figure S7. HR-ESI-MS spectrum of 1.

Figure S8.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of 2.Figure S9.  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of 2.

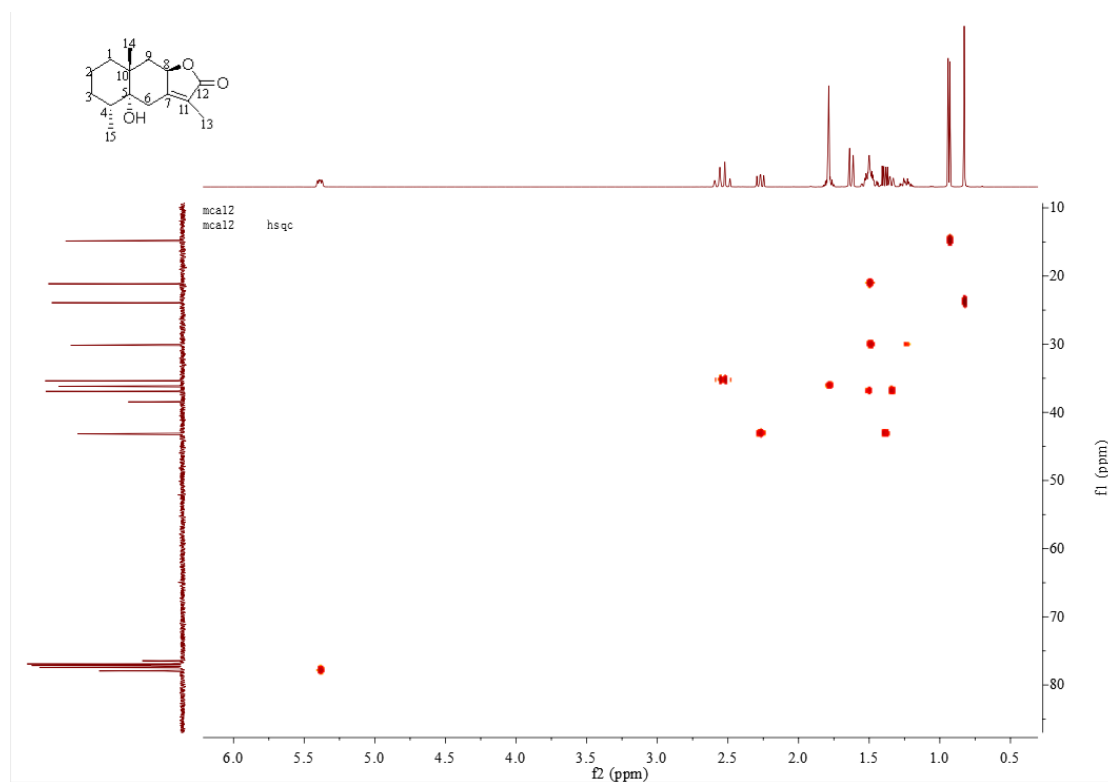


Figure S10. HSQC (500 MHz, CDCl<sub>3</sub>) spectrum of **2**.

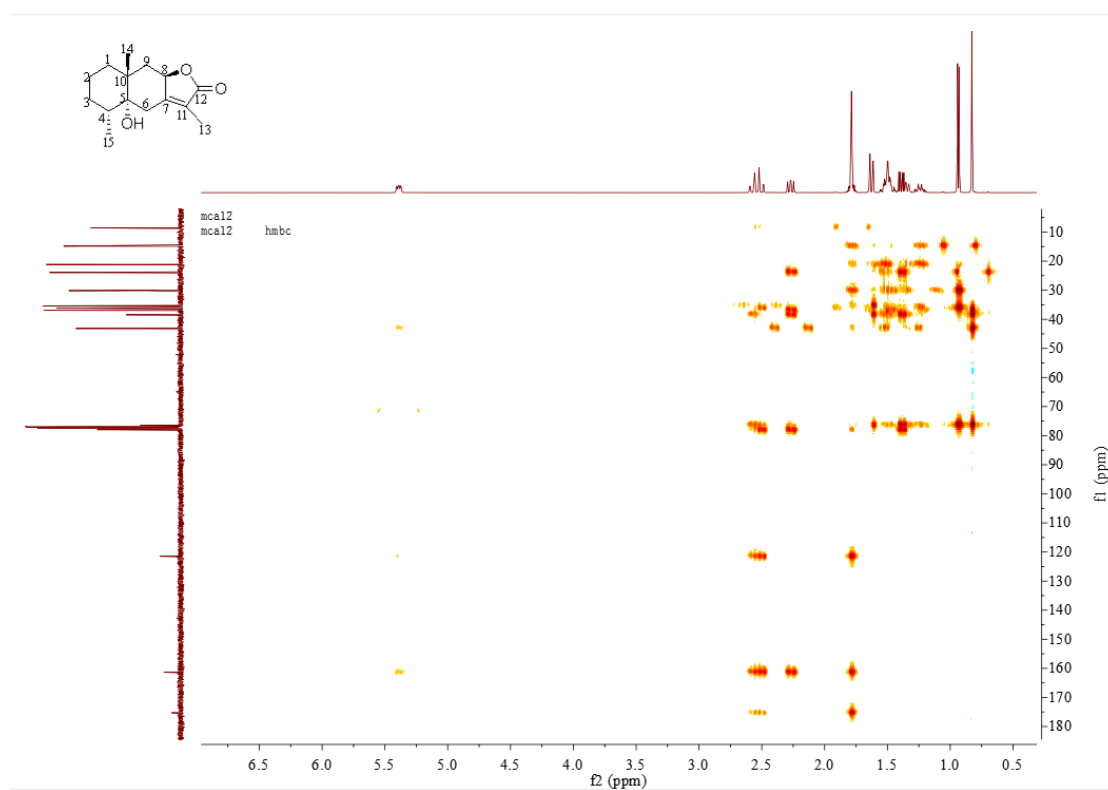


Figure S11. HMBC (500 MHz, CDCl<sub>3</sub>) spectrum of **2**.

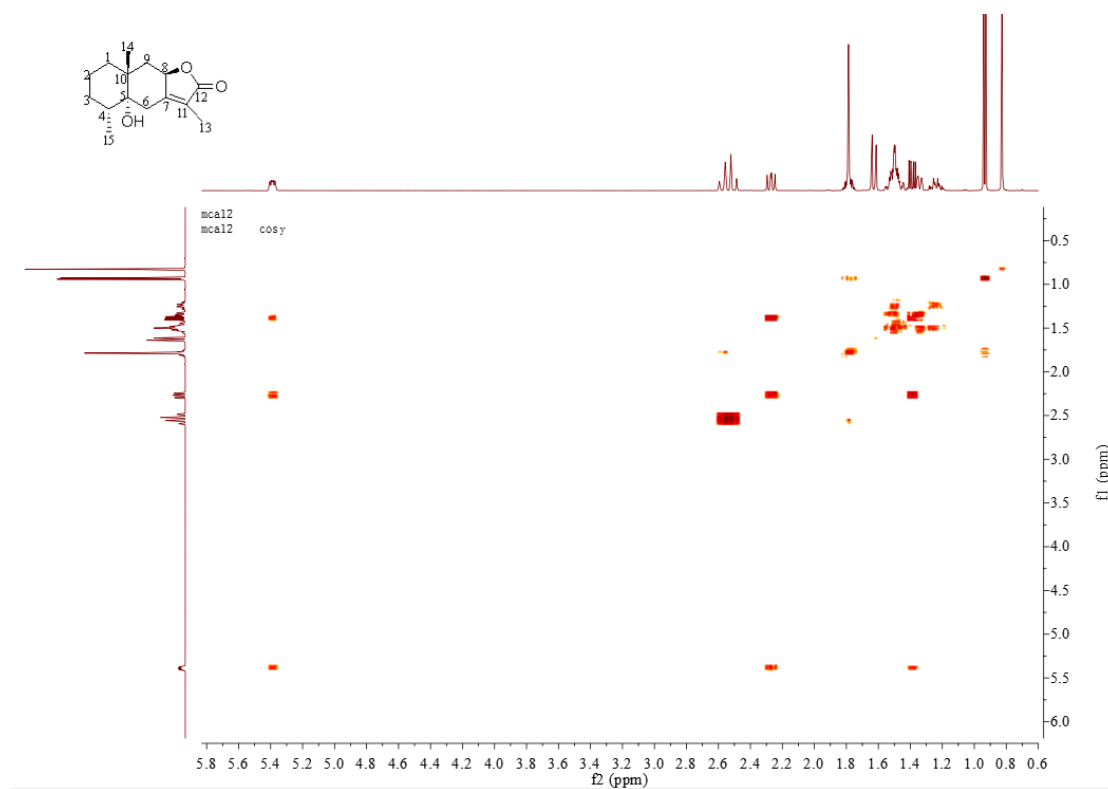


Figure S12.  $^1\text{H}$ - $^1\text{H}$  COSY (500 MHz,  $\text{CDCl}_3$ ) spectrum of 2.

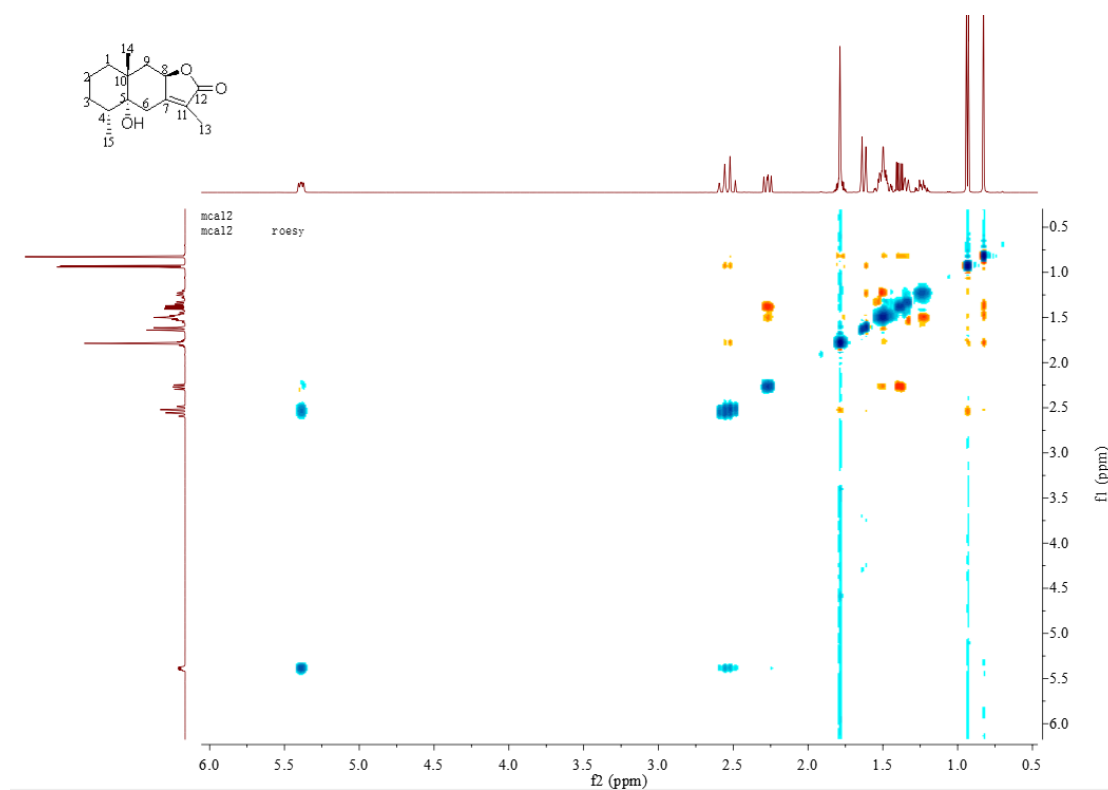


Figure S13. NOESY (500 MHz,  $\text{CDCl}_3$ ) spectrum of 2.

Formula Predictor Report - MCA-12.lcd

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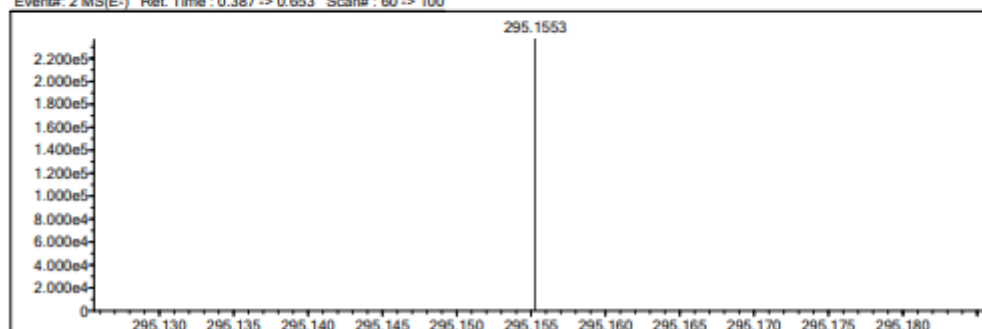
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B	3	0	0	Mg	2	0	0	Cu	2	0	0	Ir	3	0	0	
C	4	5	50	Si	4	0	0	Se	2	0	0					
N	3	0	10	P	3	0	0	Br	1	0	0					
O	2	0	30	S	2	0	0	Pd	2	0	0					

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 Max Isotopes: all  
 MSn Iso RI (%): 75.00

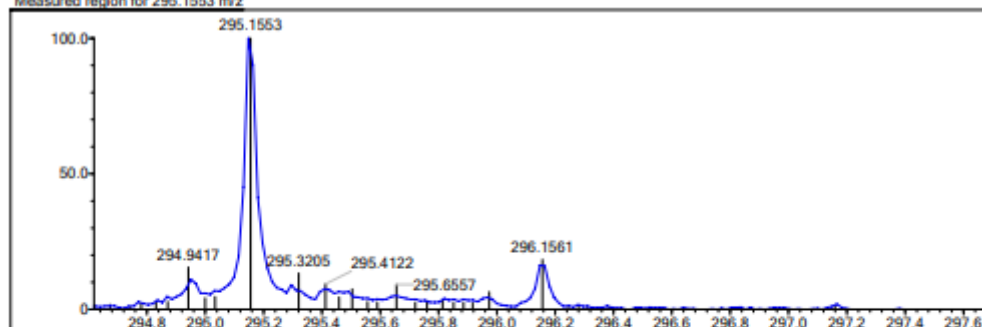
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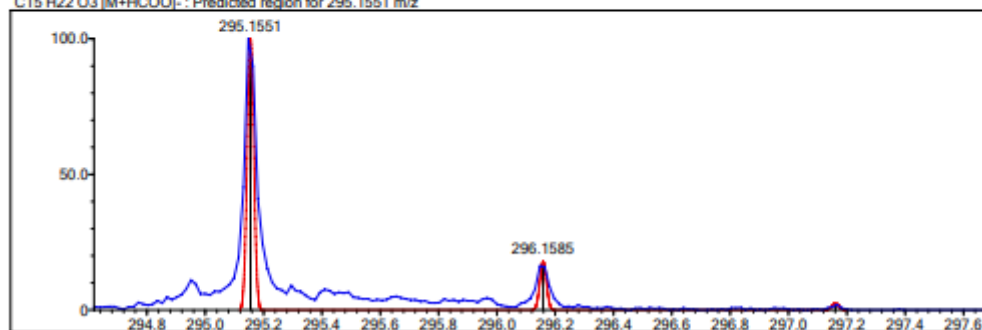
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Measured region for 295.1553 m/z

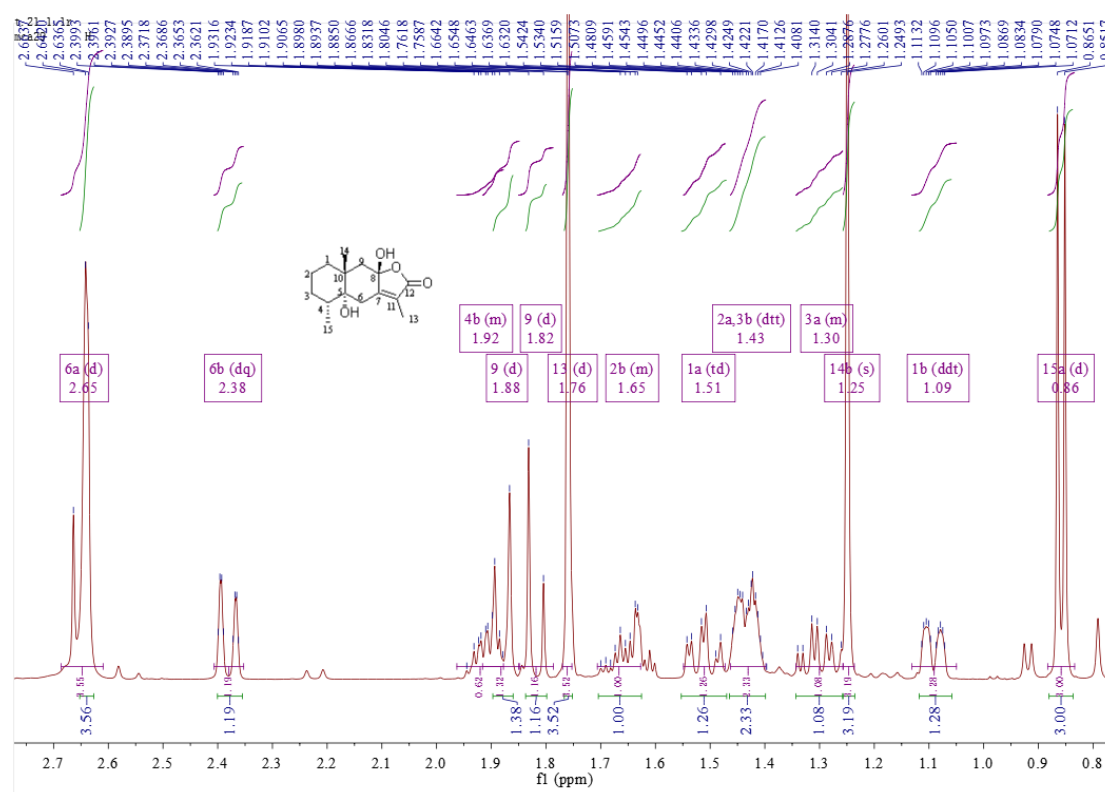
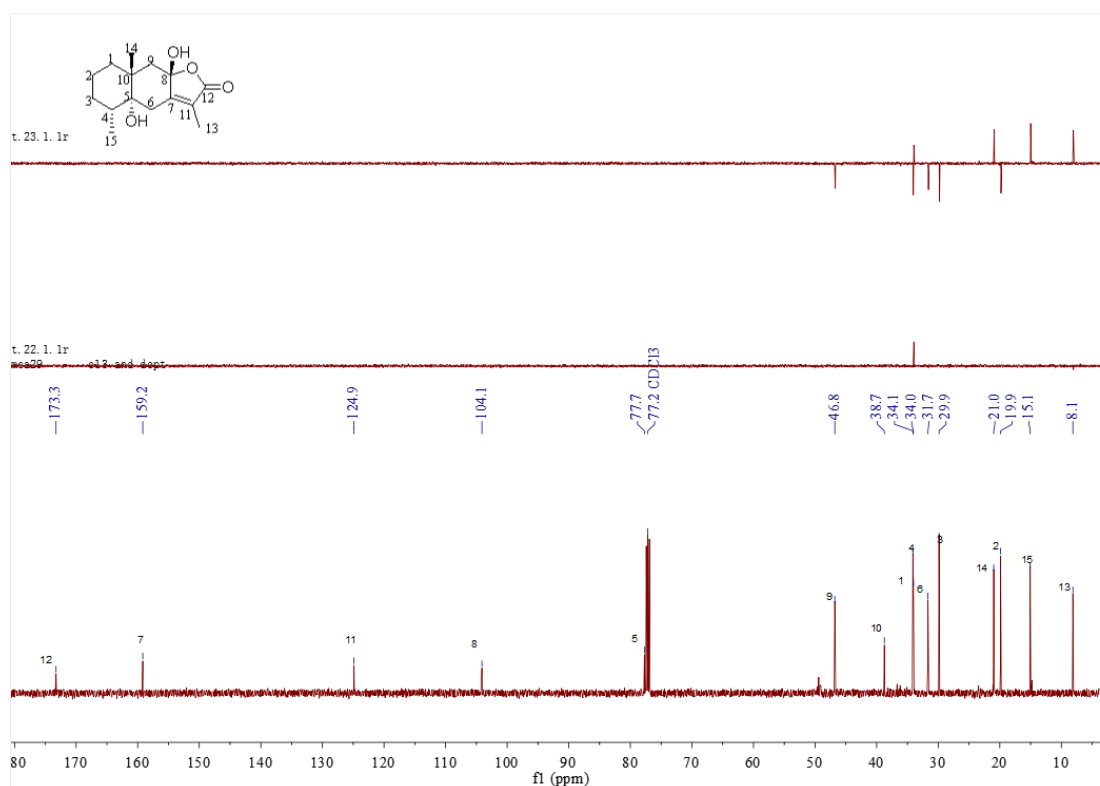


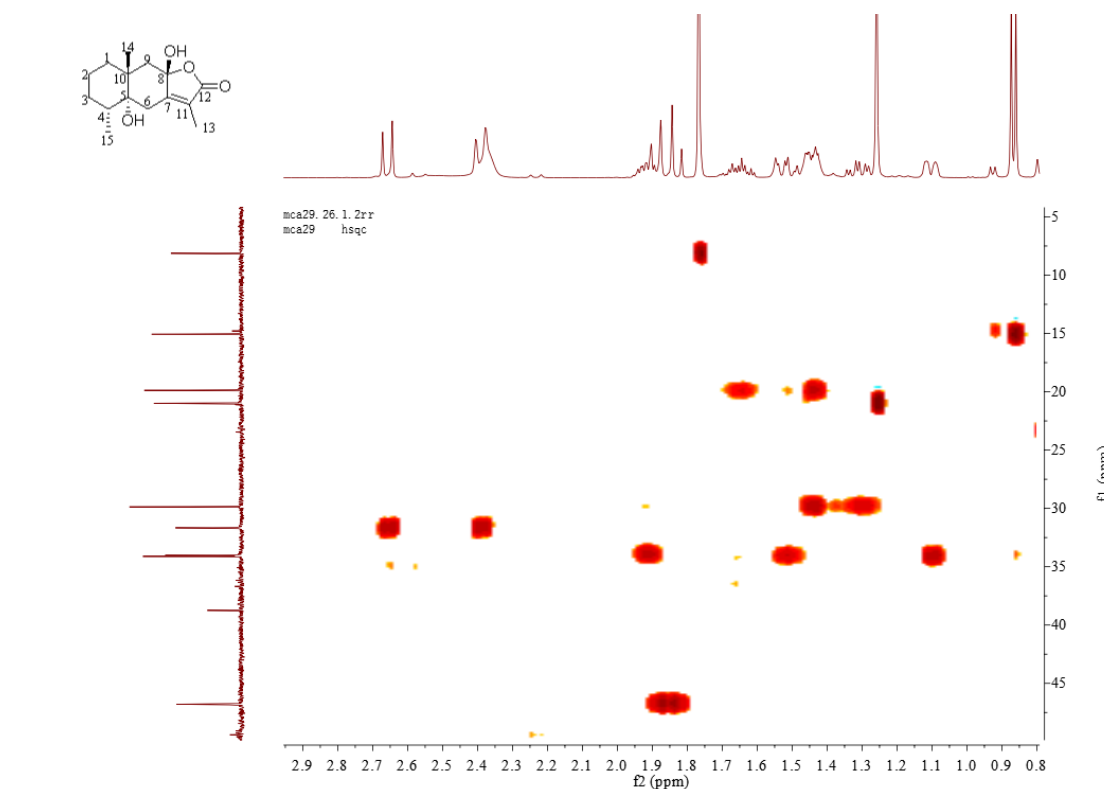
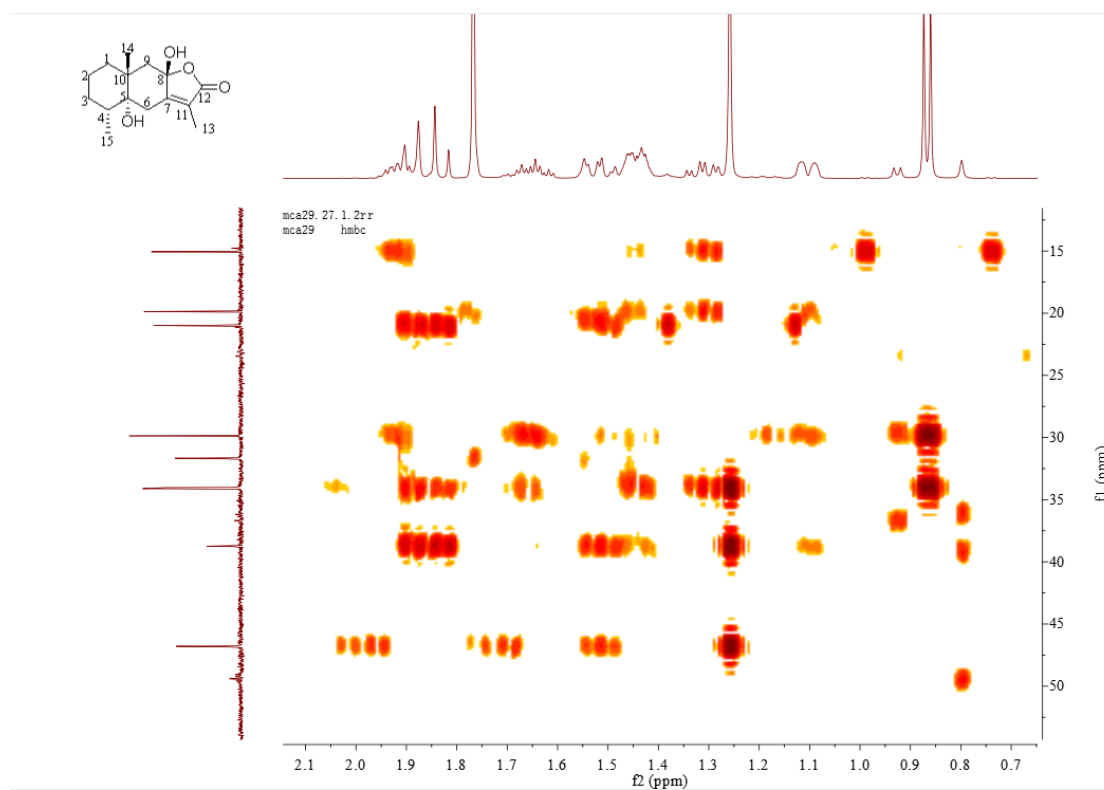
C15 H22 O3 [M+HCOO]-: Predicted region for 295.1551 m/z



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C15 H22 O3	[M+HCOO]-	295.1553	295.1551	0.2	0.68	5.0

Figure S14. HR-ESI-MS spectrum of 2.

Figure S15. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of 3.Figure S16. <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) spectrum of 3.

Figure S17. HSQC (500 MHz, CDCl<sub>3</sub>) spectrum of 3.Figure S18. HMBC (500 MHz, CDCl<sub>3</sub>) spectrum of 3.

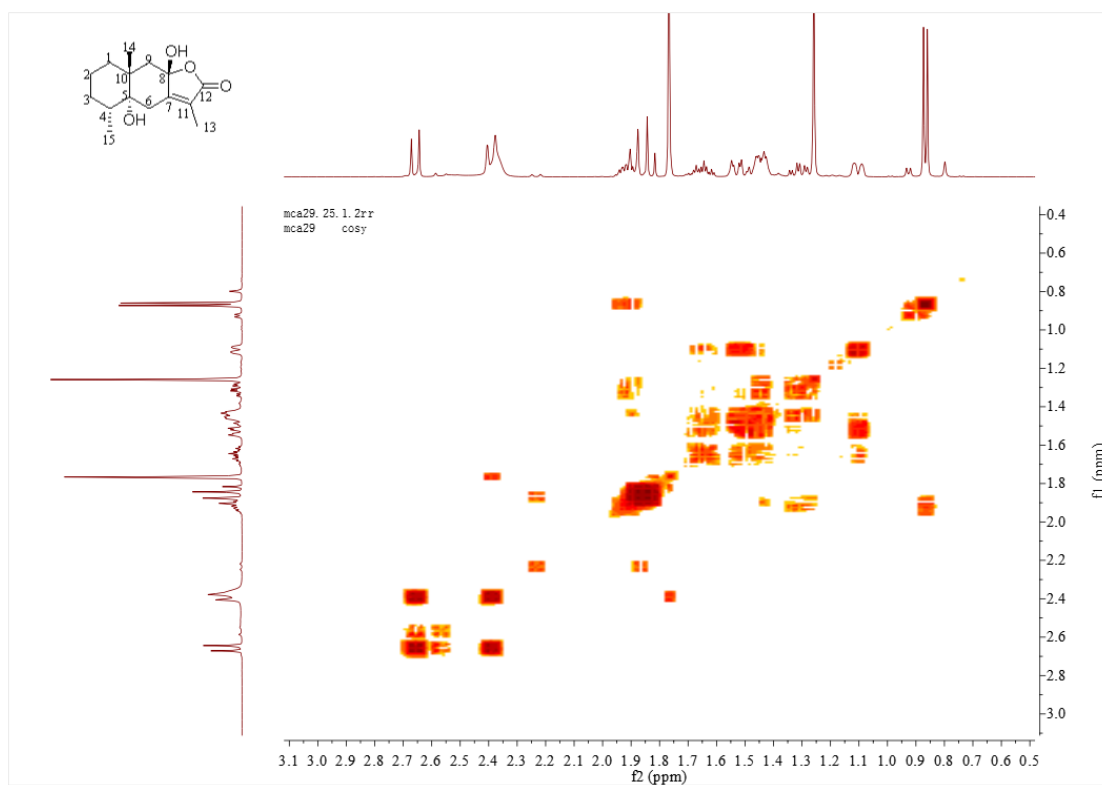


Figure S19.  $^1\text{H}$ - $^1\text{H}$  COSY (500 MHz,  $\text{CDCl}_3$ ) spectrum of **3**.

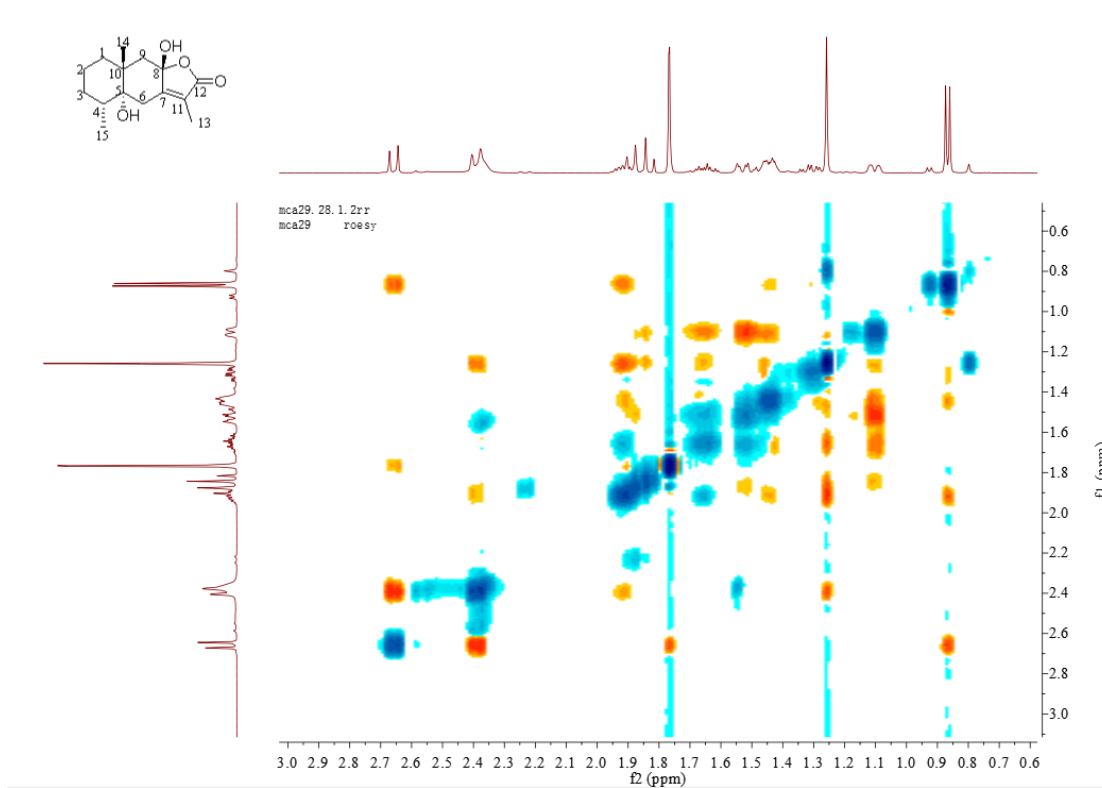


Figure S20. NOESY (500 MHz,  $\text{CDCl}_3$ ) spectrum of **3**.

Formula Predictor Report - MCA-29.lcd

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B	3	0	0	Mg	2	0	0	Cu	2	0	0	Ir	3	0	0	
C	4	5	50	Si	4	0	0	Se	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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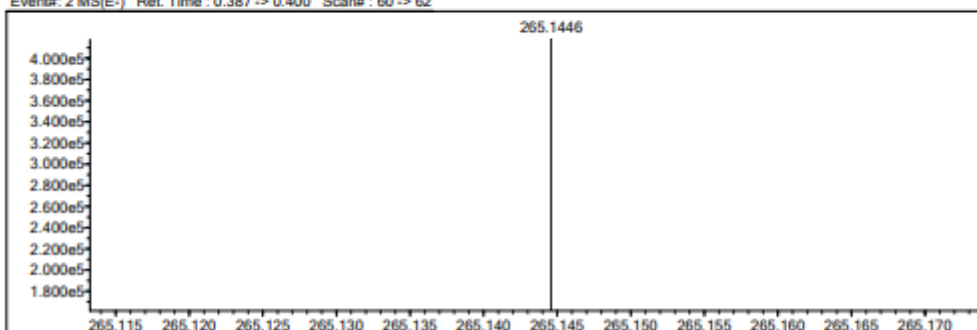
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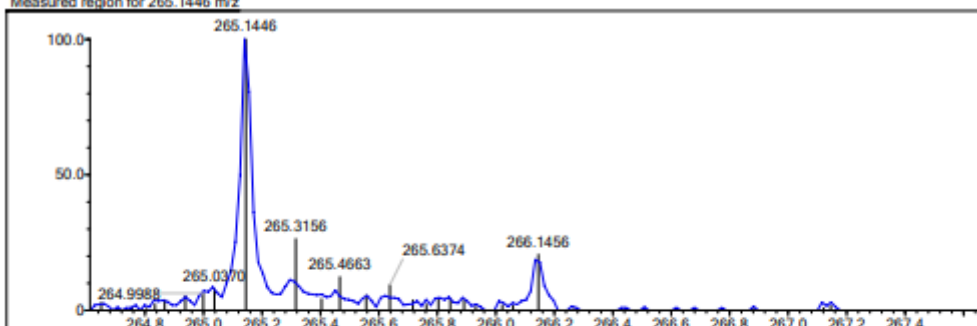
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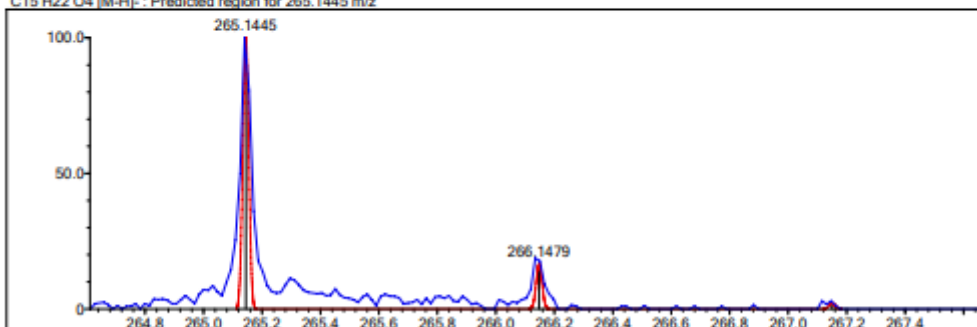
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Measured region for 265.1446 m/z

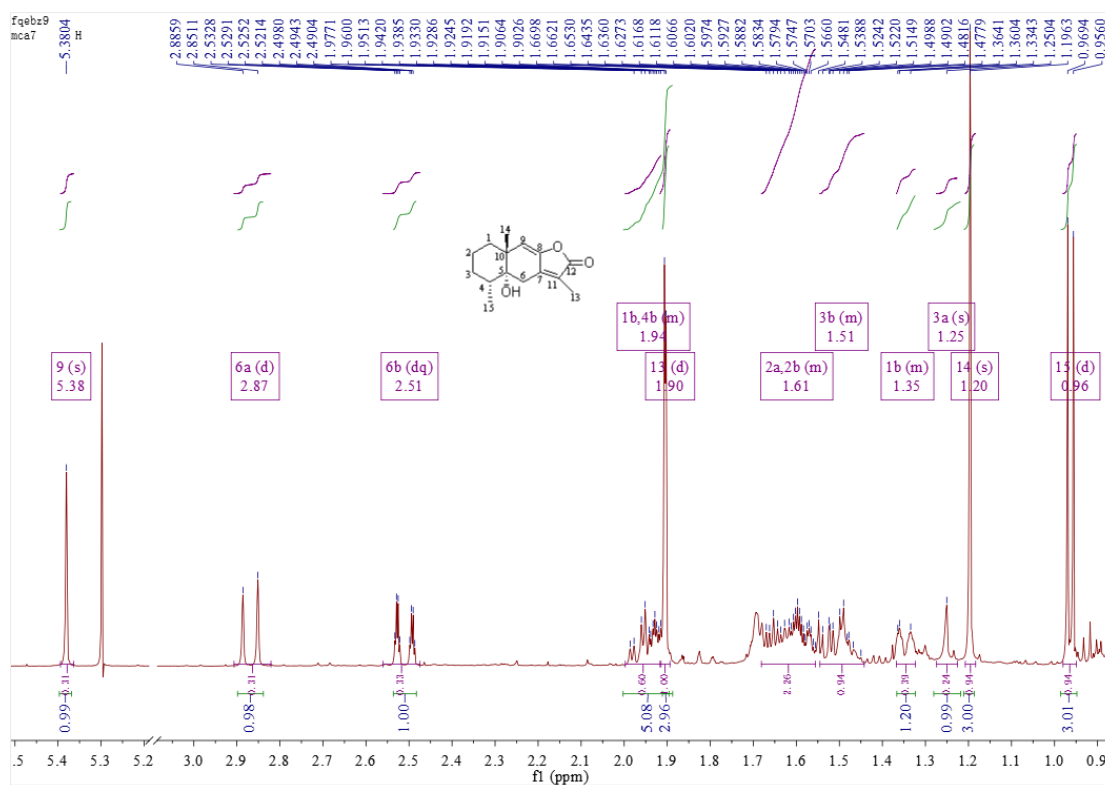


C15 H22 O4 [M-H]- : Predicted region for 265.1445 m/z

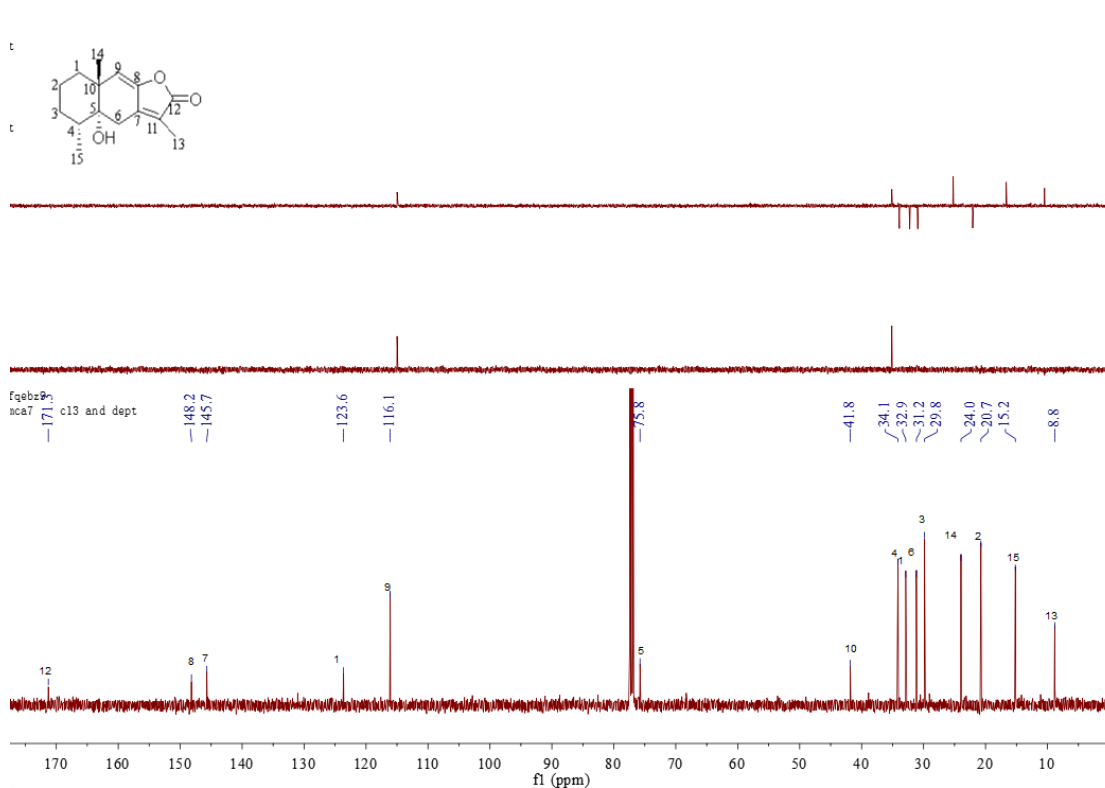


Formula (M)	Ion	Mass. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
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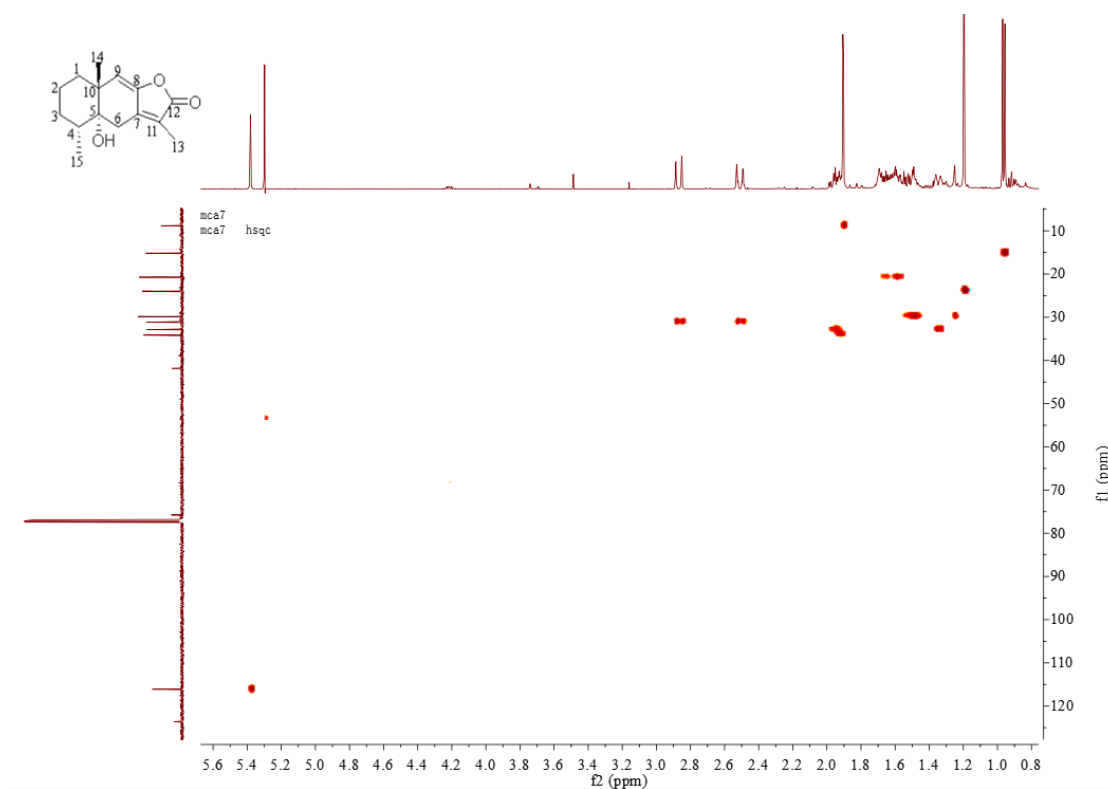
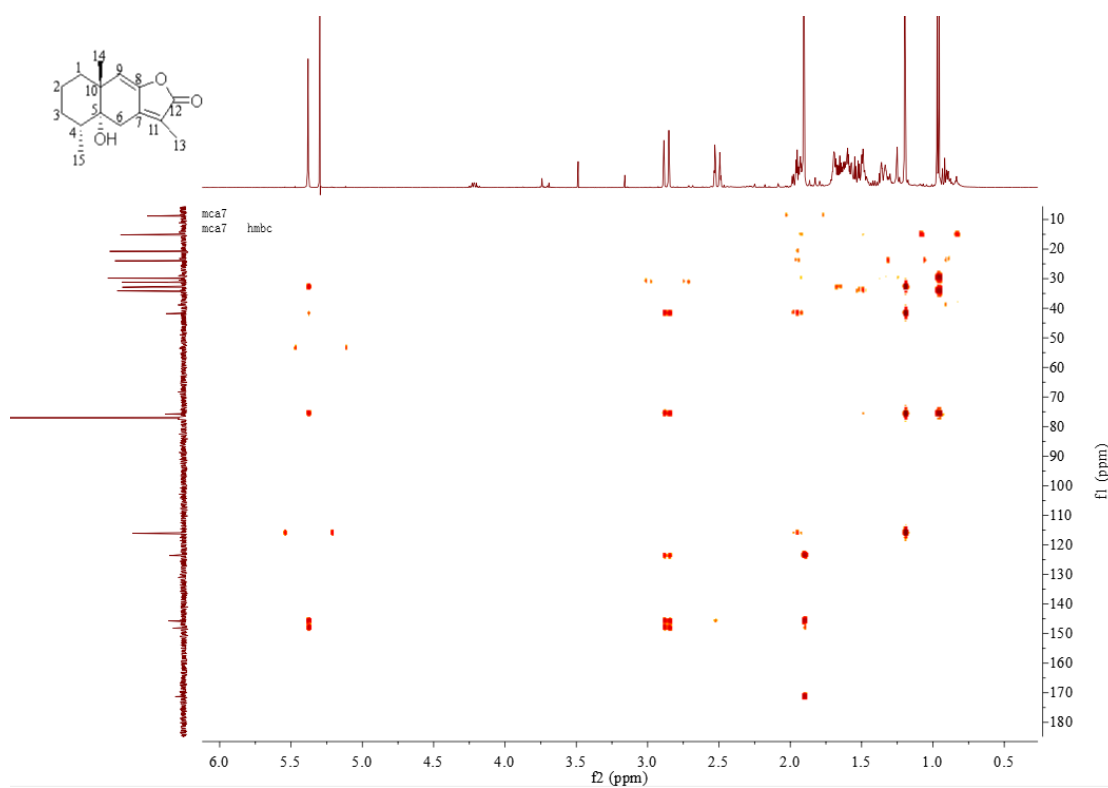
Figure S21. HR-ESI-MS spectrum of 3.

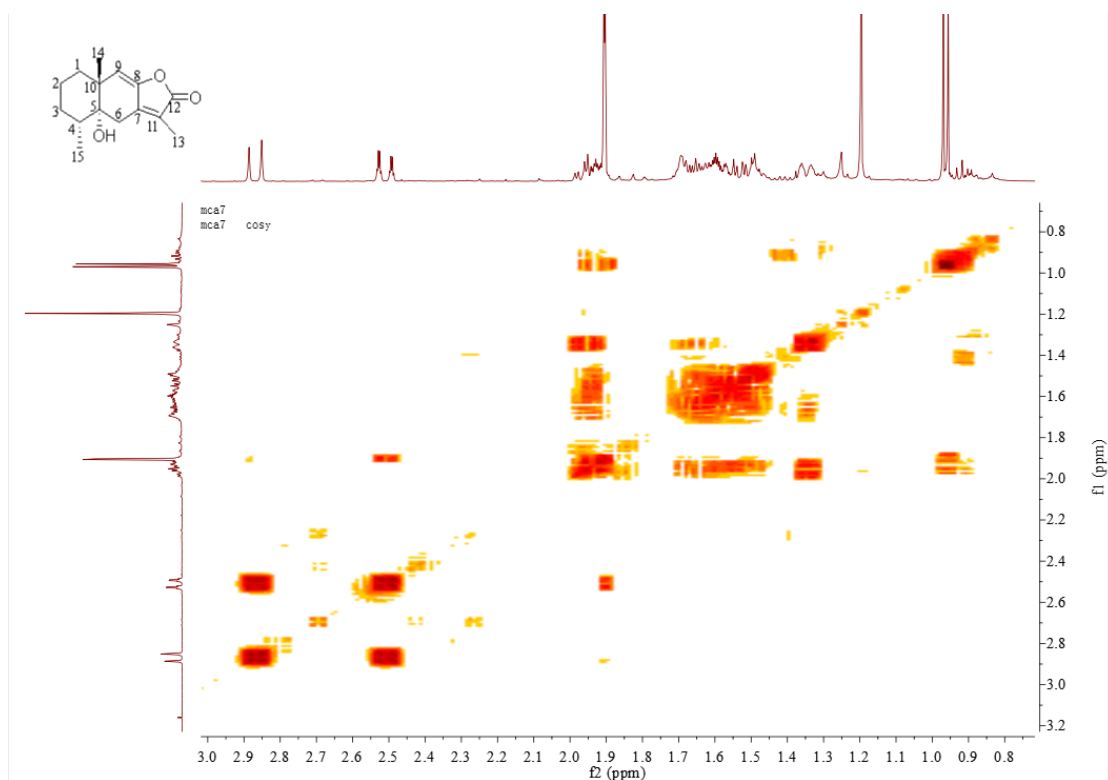
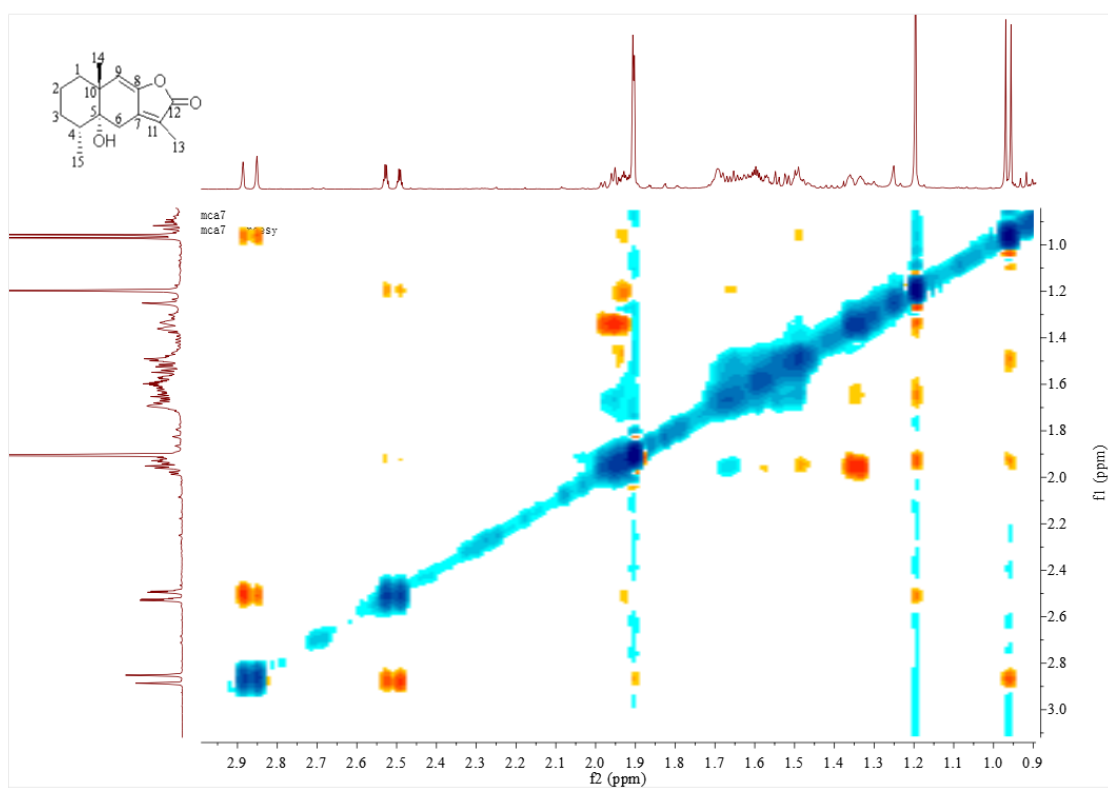


**Figure S22.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **4**.



**Figure S23.**  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of **4**.

Figure S24. HSQC (500 MHz, CDCl<sub>3</sub>) spectrum of 4.Figure S25. HMBC (500 MHz, CDCl<sub>3</sub>) spectrum of 4.

Figure S26.  $^1\text{H}$ - $^1\text{H}$  COSY (500 MHz,  $\text{CDCl}_3$ ) spectrum of 4.Figure S27. NOESY (500 MHz,  $\text{CDCl}_3$ ) spectrum of 4.

Formula Predictor Report - MCA-7.lcd

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Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	10	150	O	2	0	30	P	3	0	0	Se	2	0	0	H
2H	1	0	0	F	1	0	0	S	2	0	0	Br	1	0	0	Na
B	3	0	0	Na	1	0	0	Cl	1	0	0	Pd	2	0	0	
C	4	10	150	Mg	2	0	0	Co	2	0	0	Ag	1	0	0	
N	3	0	10	Si	4	0	0	Cu	2	0	0	I	3	0	0	

Error Margin (ppm): 5

DBE Range: not fixed

Electron Ions: both

HC Ratio: unlimited

Apply N Rule: yes

Use MSn Info: yes

Max Isotopes: all

Isotope RI (%): 1.00

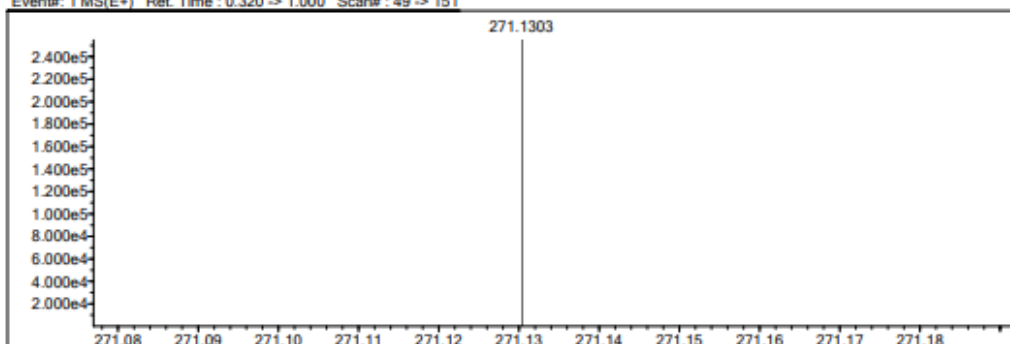
Isotope Res: 10000

MSn Iso RI (%): 75.00

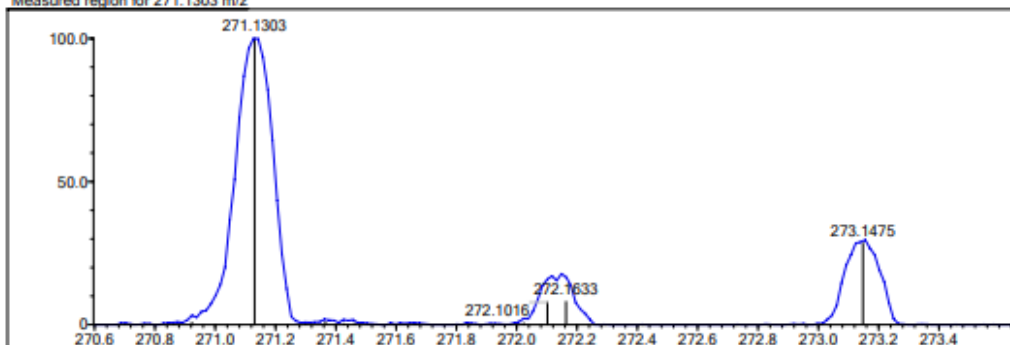
MSn Logic Mode: OR

Max Results: 20

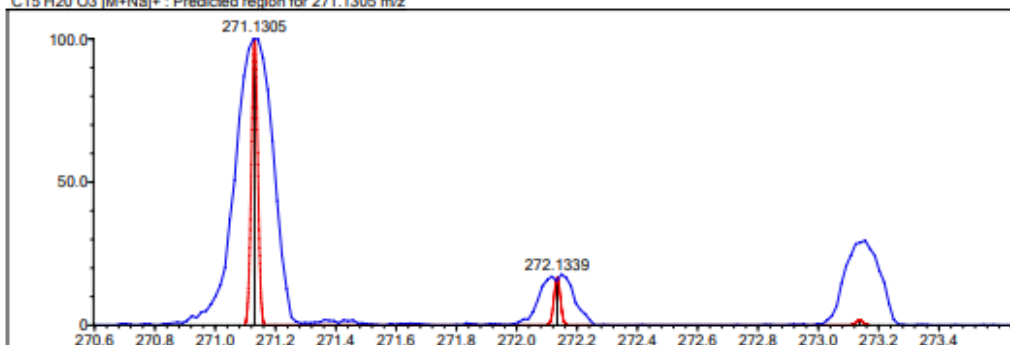
Event#: 1 MS(E+) Ret. Time : 0.320 -&gt; 1.000 Scan#: 49 -&gt; 151



Measured region for 271.1303 m/z

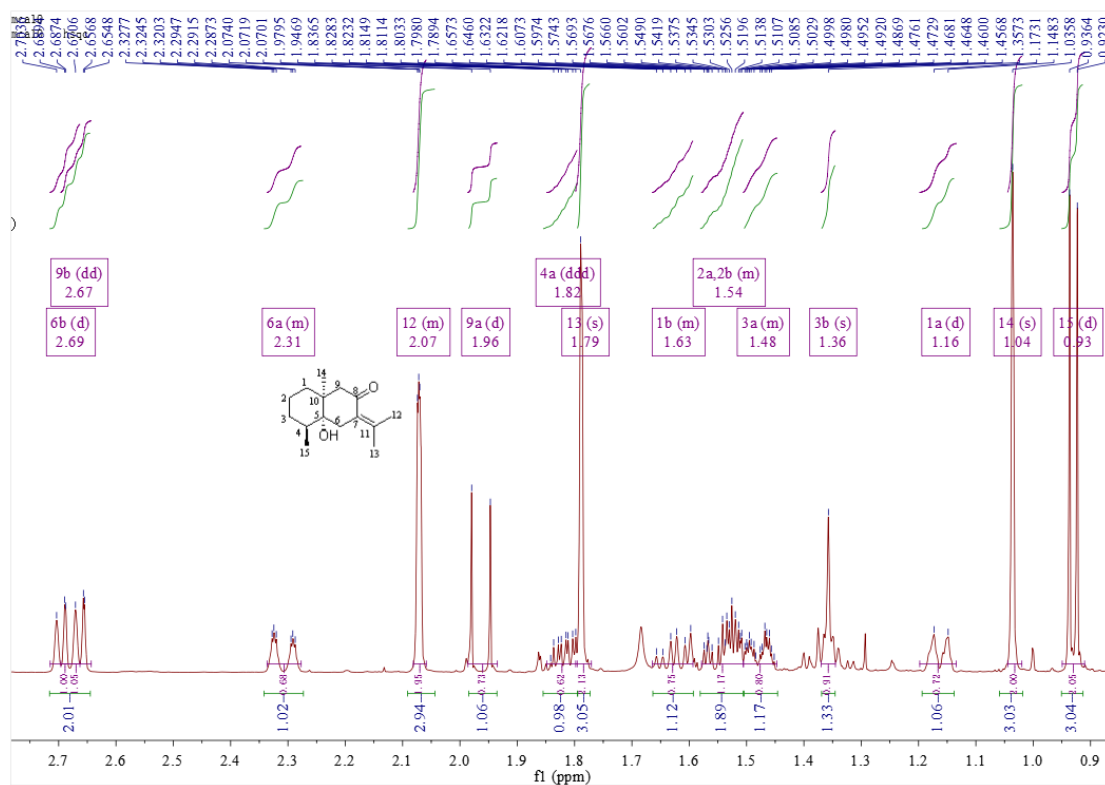
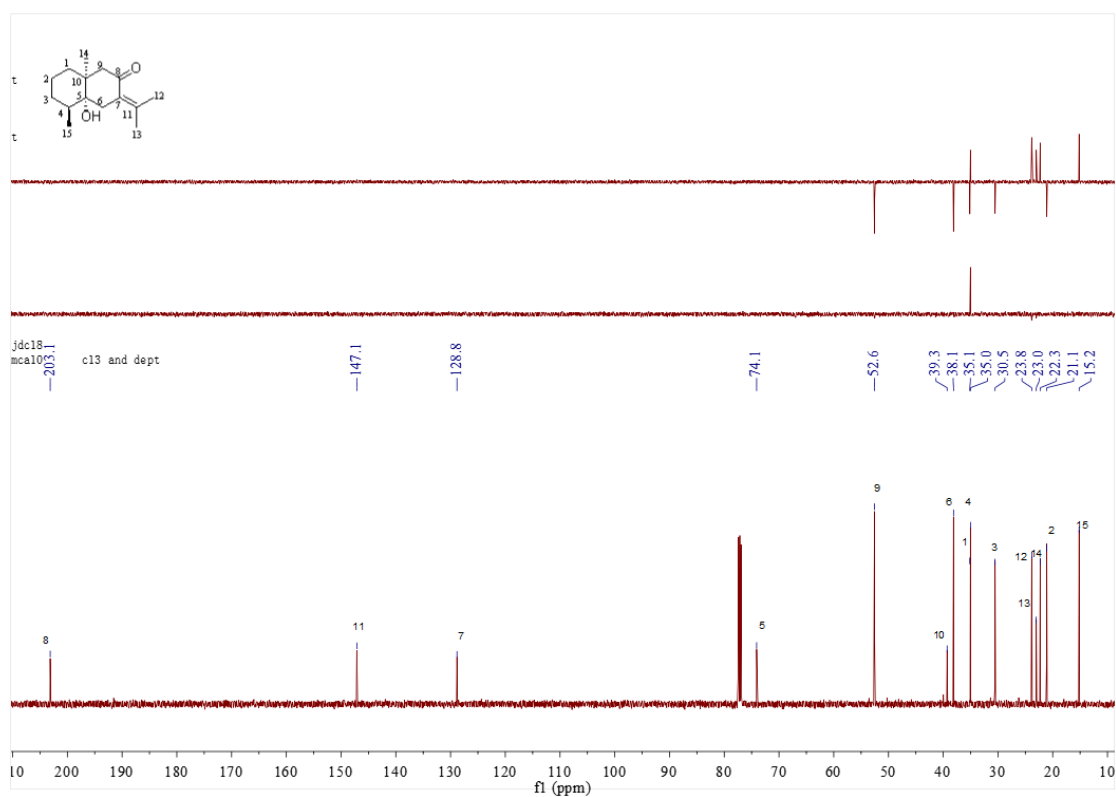


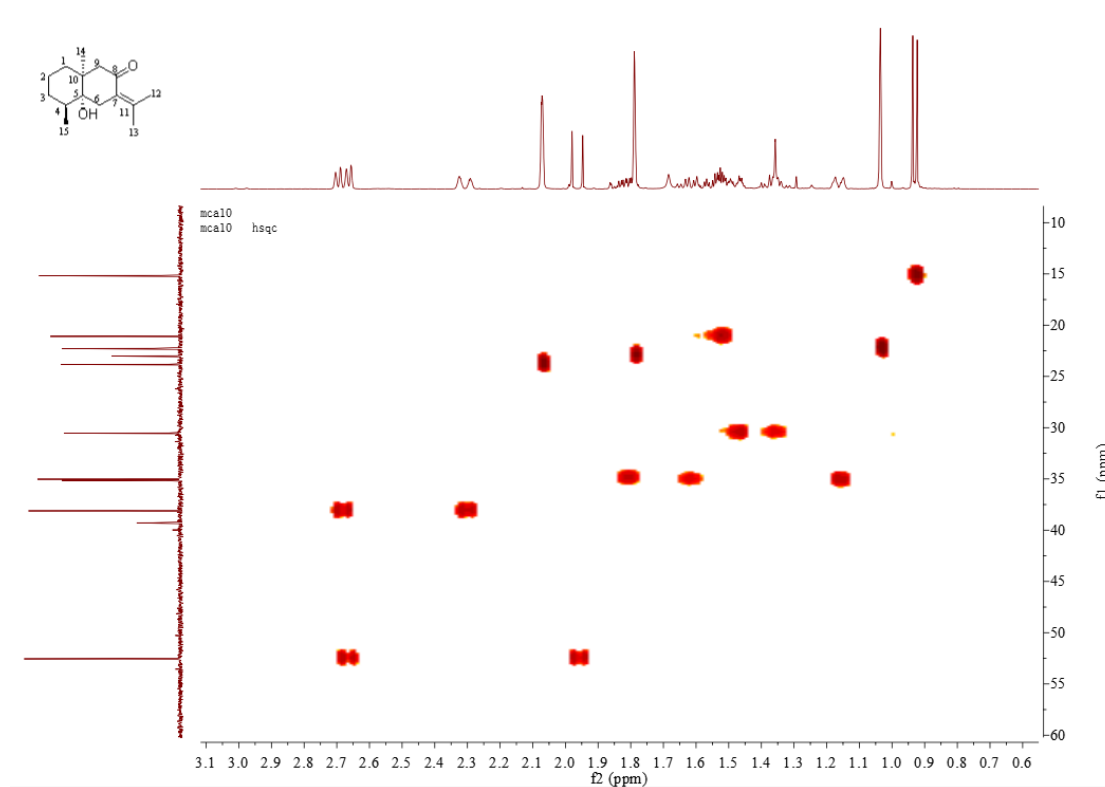
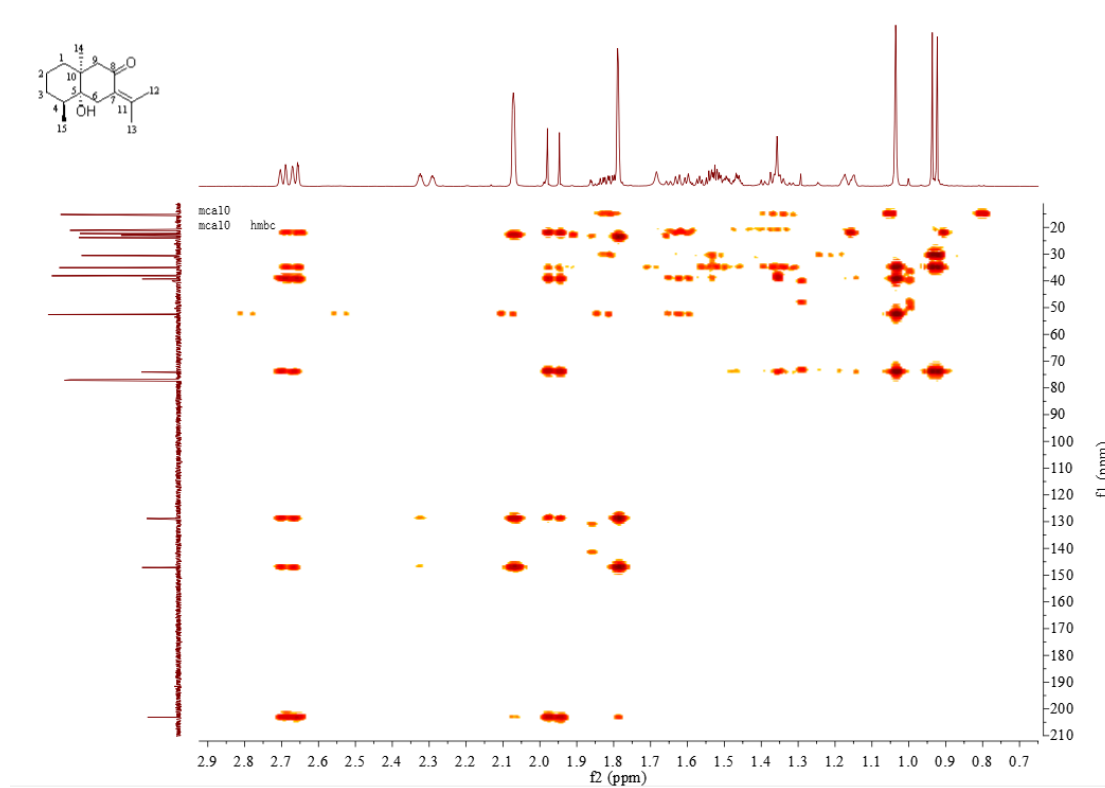
C15 H20 O3 [M+Na]+ : Predicted region for 271.1305 m/z



Formula (M)	Ion	Mass, m/z	Pred. m/z	Df, (mDa)	Df, (ppm)	DBE
C15 H20 O3	[M+Na]+	271.1303	271.1305	-0.2	-0.74	6.0

Figure S28. HR-ESI-MS spectrum of 4.

Figure S29.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of 5.Figure S30.  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of 5.

Figure S31. HSQC (500 MHz,  $\text{CDCl}_3$ ) spectrum of 5.Figure S32. HMBC (500 MHz,  $\text{CDCl}_3$ ) spectrum of 5.

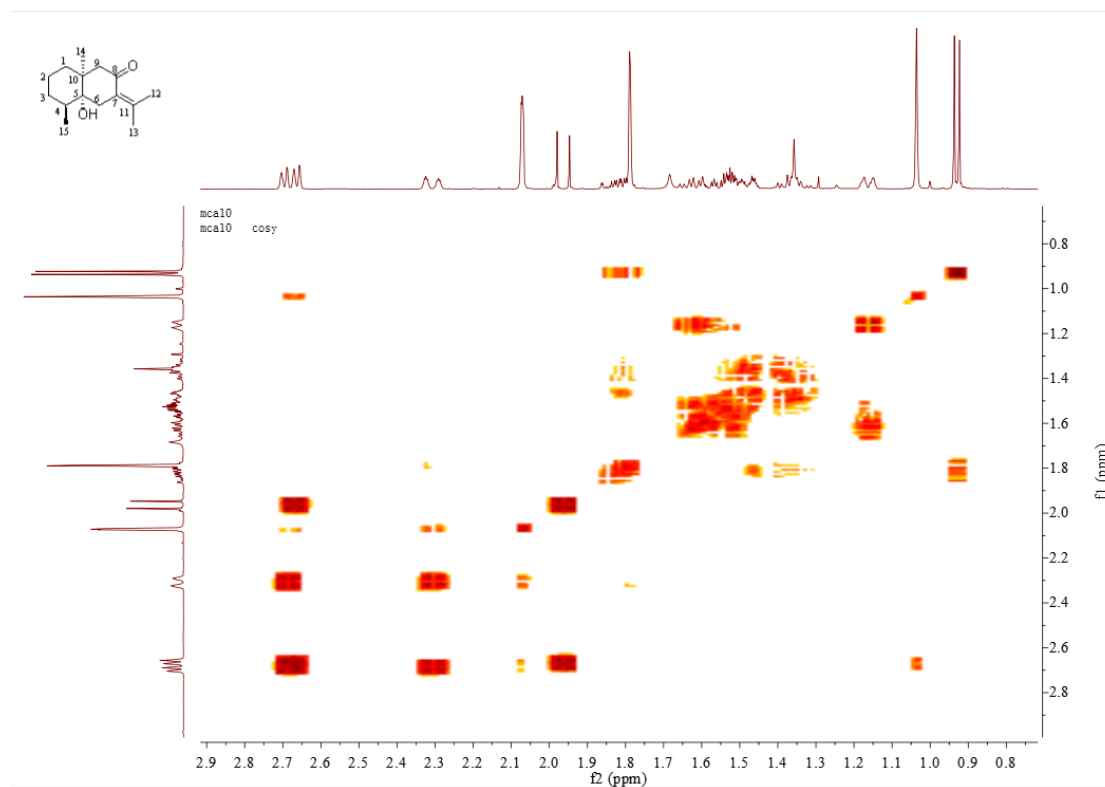


Figure S33.  $^1\text{H}$ - $^1\text{H}$  COSY (500 MHz,  $\text{CDCl}_3$ ) spectrum of 5.

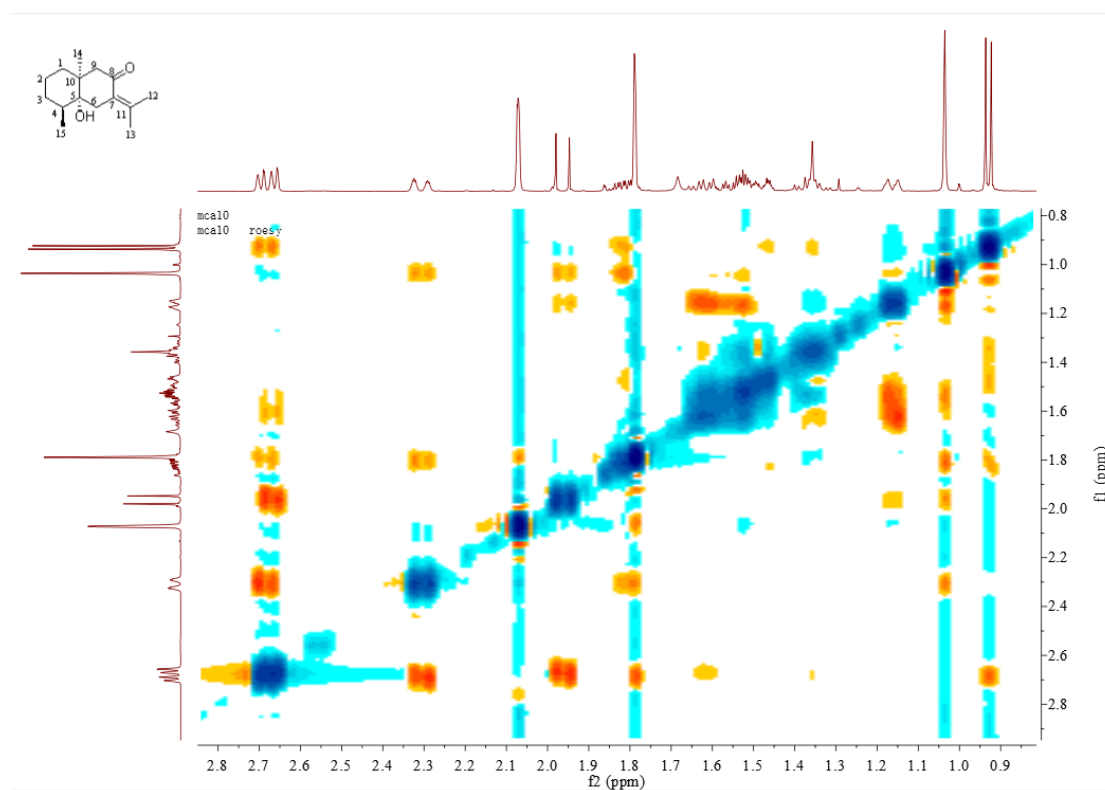


Figure S34. NOESY (500 MHz,  $\text{CDCl}_3$ ) spectrum of 5.

Formula Predictor Report - MCA-10.lcd

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Data File: E:\DATA\2021\0720\MCA-10.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	10	150	O	2	0	30	P	3	0	0	Se	2	0	0	Na
2H	1	0	0	F	1	0	0	S	2	0	0	Br	1	0	5	
B	3	0	0	Na	1	0	0	Cl	1	0	0	Pd	2	0	0	
C	4	10	150	Mg	2	0	0	Co	2	0	0	Ag	1	0	0	
N	3	0	10	Si	4	0	0	Cu	2	0	0	I	3	0	0	

Error Margin (ppm): 5

DBE Range: not fixed

Electron Ions: both

HC Ratio: unlimited

Apply N Rule: yes

Use MSn Info: yes

Max Isotopes: all

Isotope RI (%): 1.00

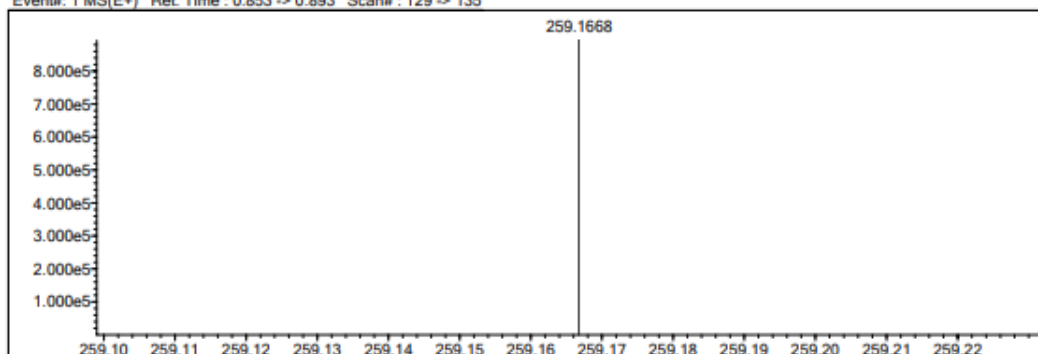
Isotope Res: 10000

MSn Iso RI (%): 75.00

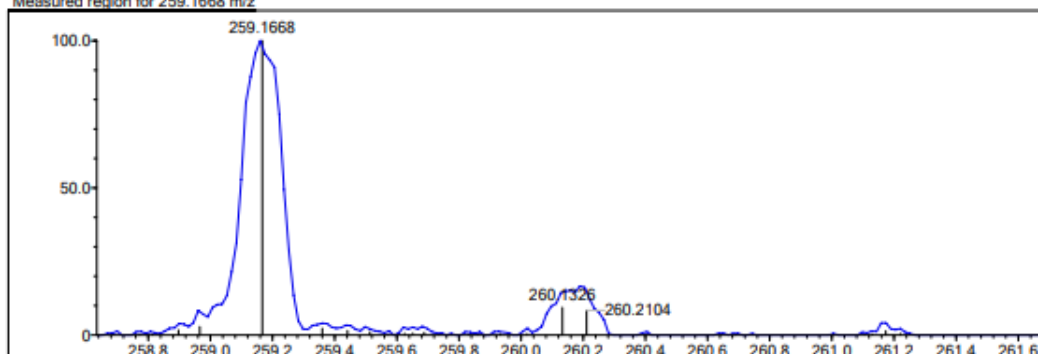
MSn Logic Mode: OR

Max Results: 20

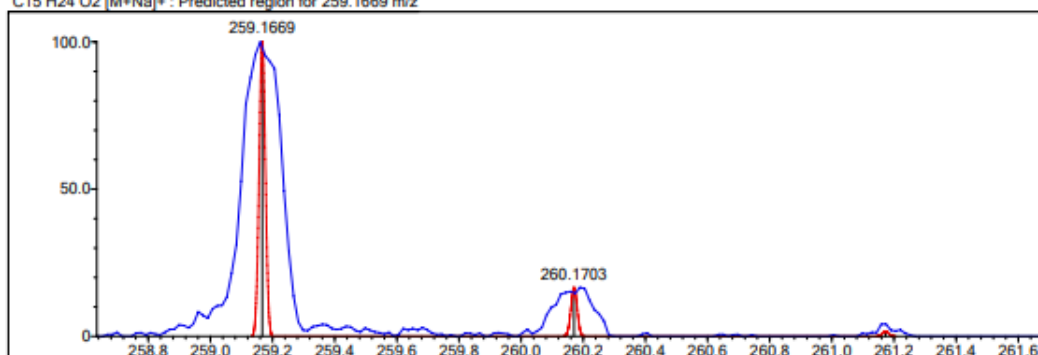
Event#: 1 MS(E+) Ret. Time : 0.853 -&gt; 0.893 Scan#: 129 -&gt; 135



Measured region for 259.1668 m/z

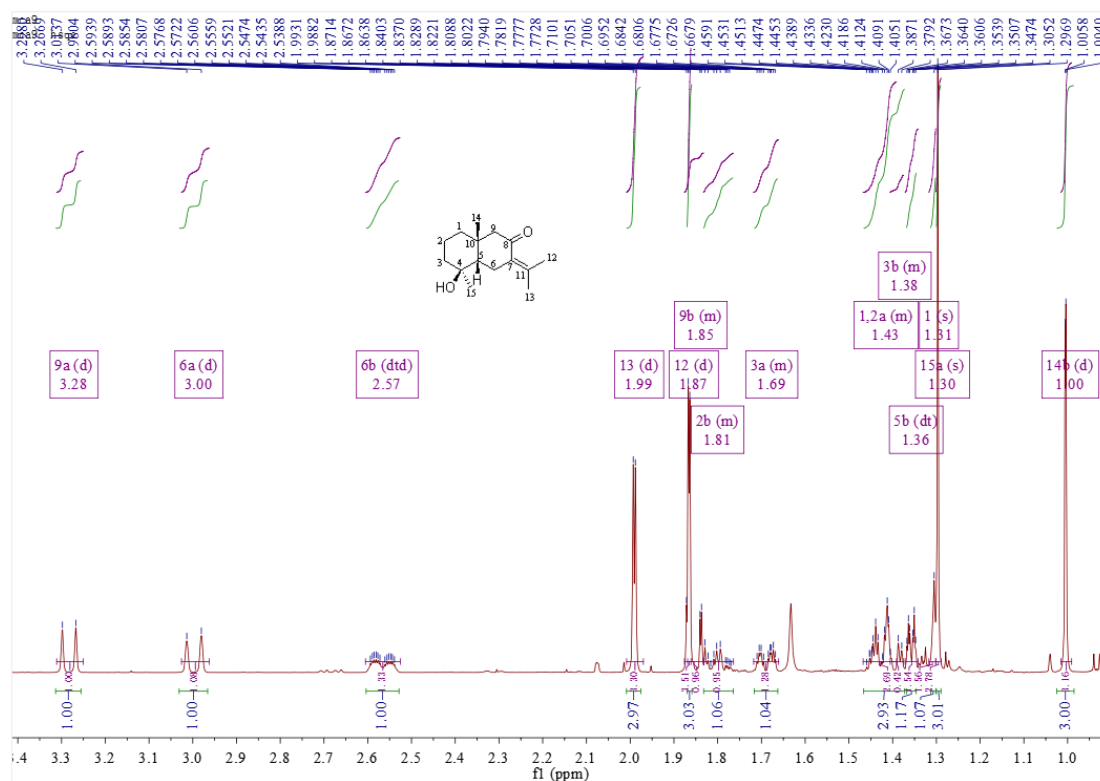


C15 H24 O2 [M+Na]+ : Predicted region for 259.1669 m/z

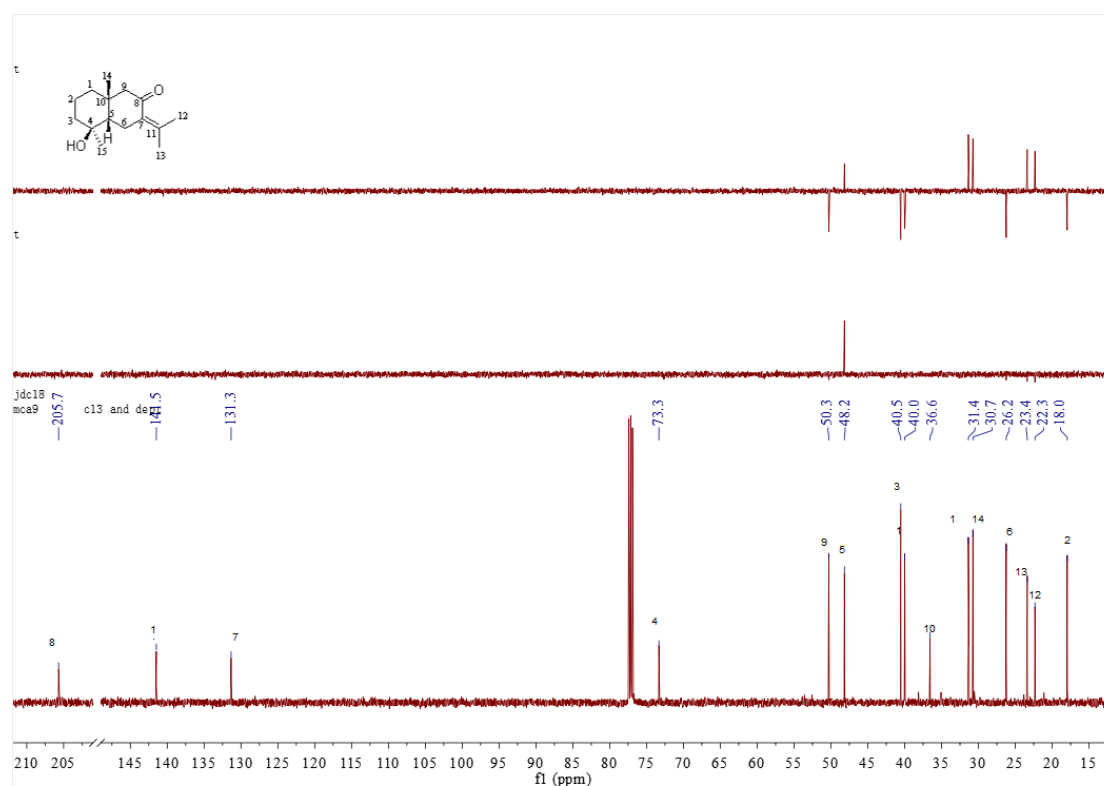


Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C15 H24 O2	[M+Na]+	259.1668	259.1669	-0.1	-0.39	4.0

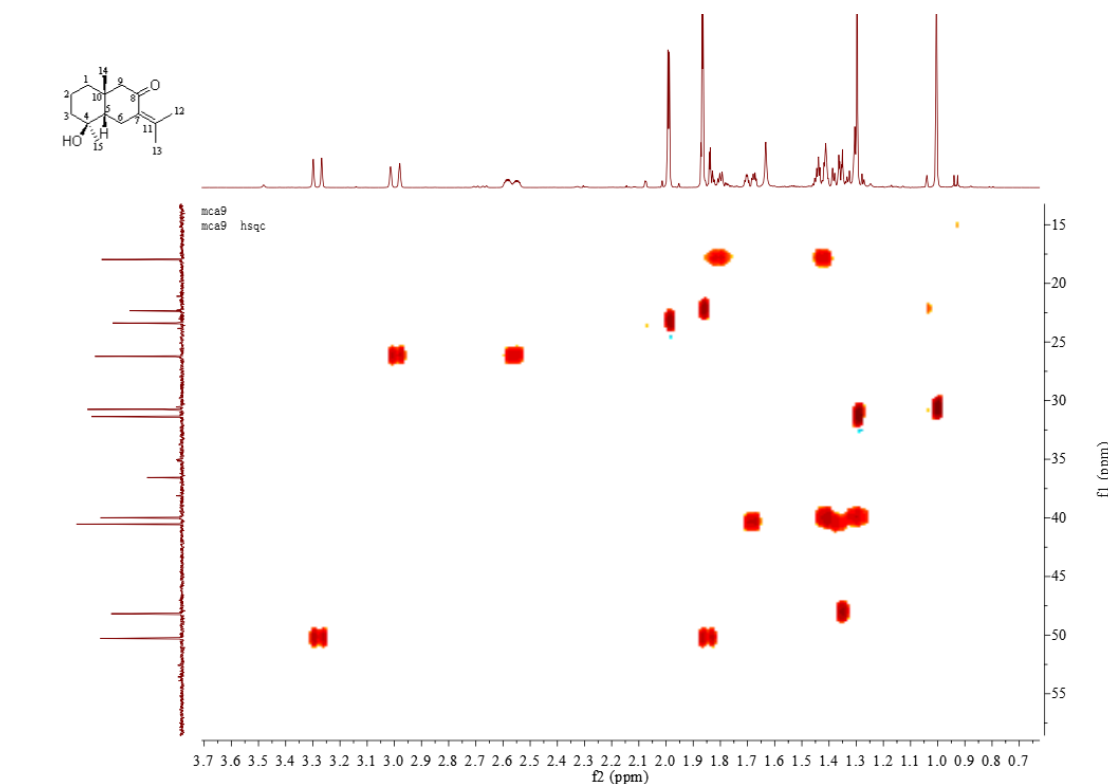
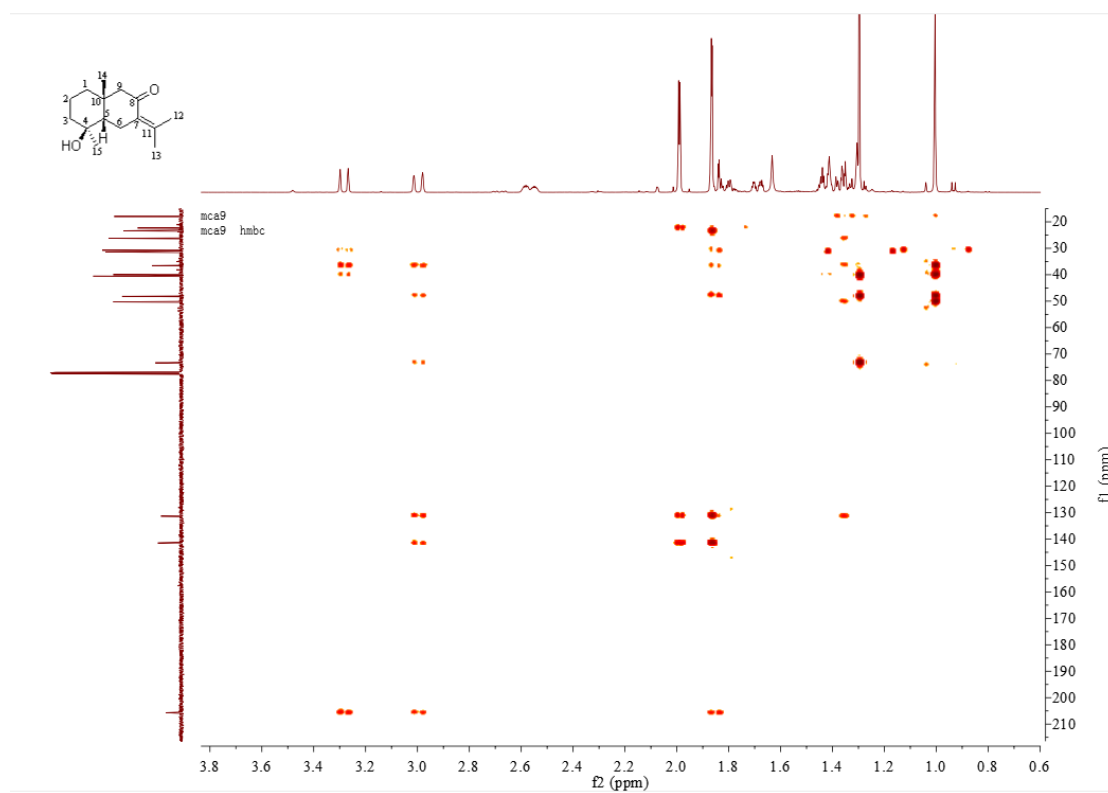
Figure S35. HR-ESI-MS spectrum of 5.



**Figure S36.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **6**.



**Figure S37.**  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of **6**.

Figure S38. HSQC (500 MHz, CDCl<sub>3</sub>) spectrum of 6.Figure S39. HMBC (500 MHz, CDCl<sub>3</sub>) spectrum of 6.

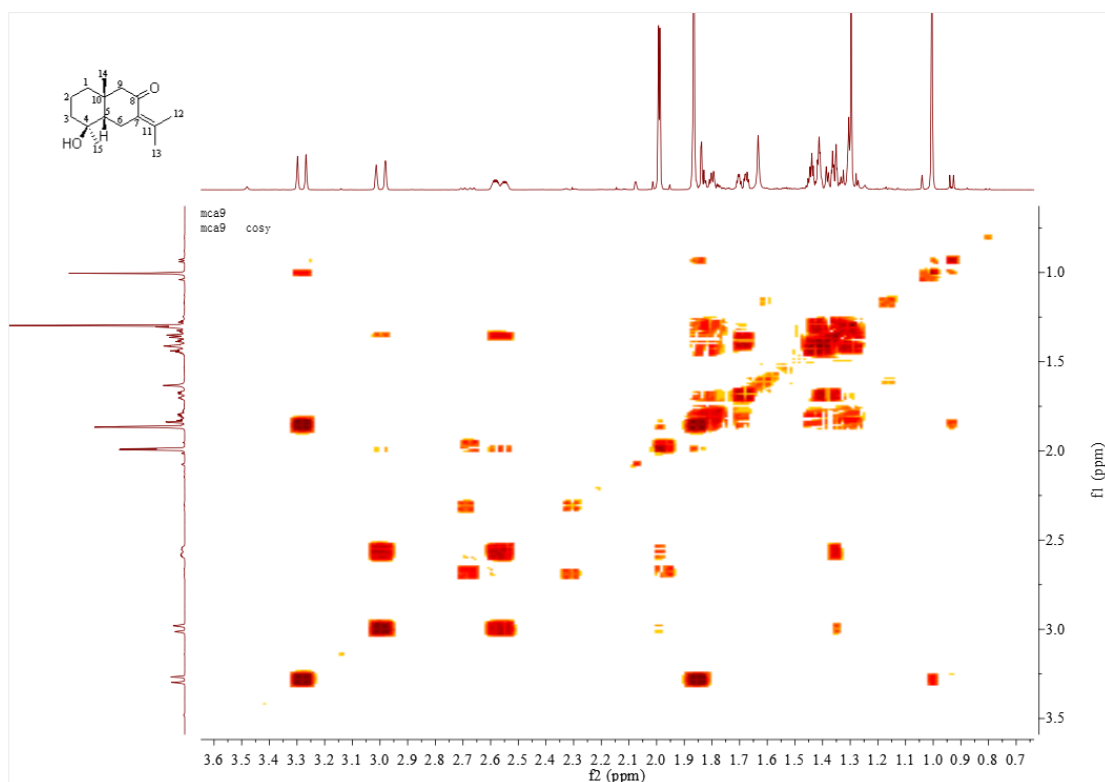


Figure S40.  $^1\text{H}$ - $^1\text{H}$  COSY (500 MHz,  $\text{CDCl}_3$ ) spectrum of **6**.

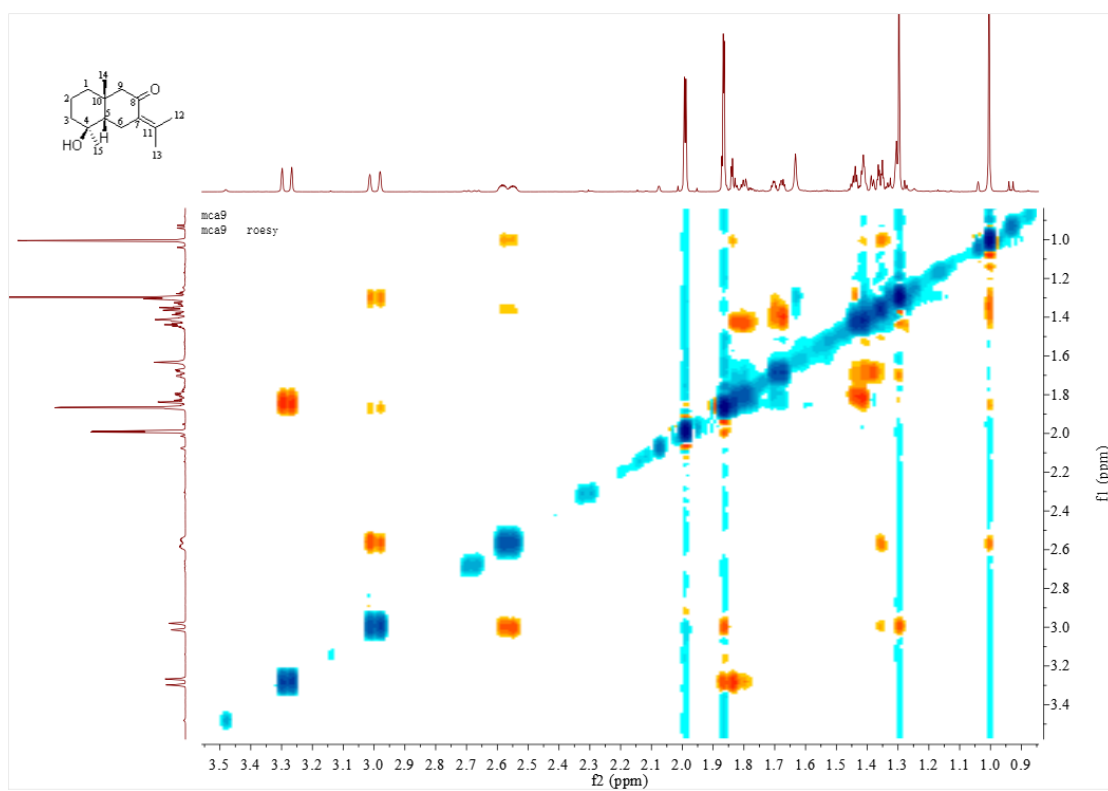


Figure S41. NOESY (500 MHz,  $\text{CDCl}_3$ ) spectrum of **6**.

Formula Predictor Report - MCA-9.lcd

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Data File: E:\DATA\2021\0720\MCA-9.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	10	150	O	2	0	30	P	3	0	0	Se	2	0	0	Na
2H	1	0	0	F	1	0	0	S	2	0	0	Br	1	0	5	
B	3	0	0	Na	1	0	0	Cl	1	0	0	Pd	2	0	0	
C	4	10	150	Mg	2	0	0	Co	2	0	0	Ag	1	0	0	
N	3	0	10	Si	4	0	0	Cu	2	0	0	I	3	0	0	

Error Margin (ppm): 5

HC Ratio: unlimited

Max Isotopes: all

MSn Iso RI (%): 75.00

DBE Range: not fixed

Apply N Rule: yes

Isotope RI (%): 1.00

MSn Logic Mode: OR

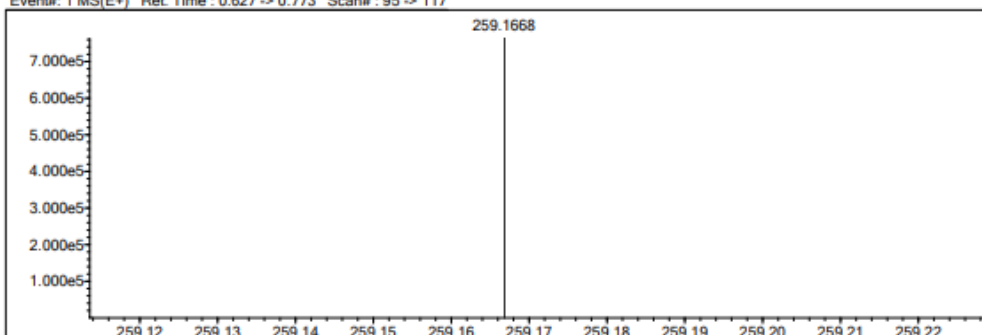
Electron Ions: both

Use MSn Info: yes

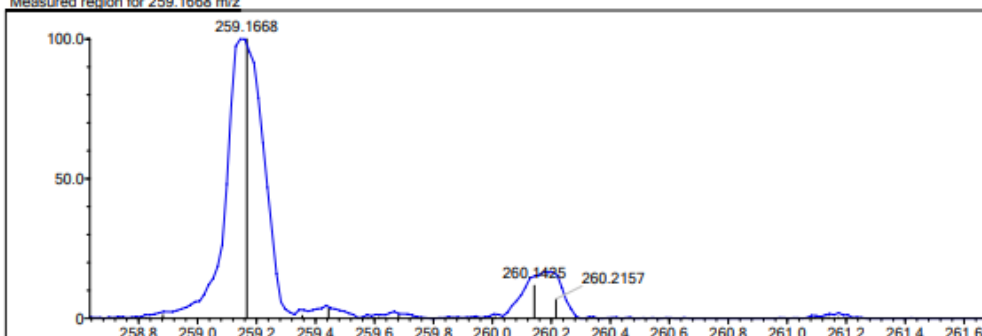
Isotope Res: 10000

Max Results: 20

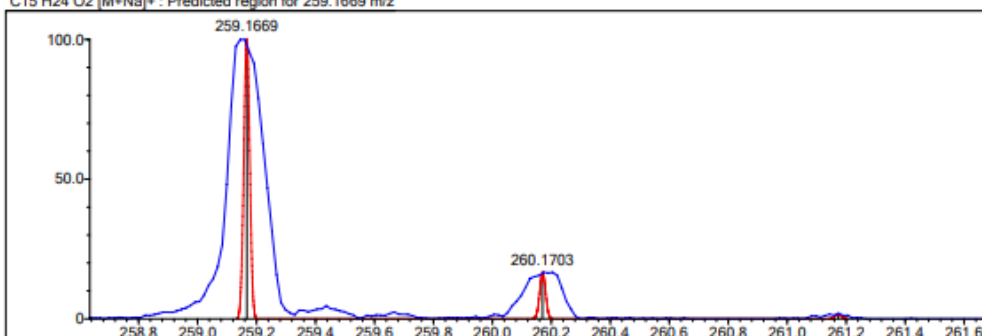
Event#: 1 MS(E+) Ret. Time : 0.627 -&gt; 0.773 Scan#: 95 -&gt; 117



Measured region for 259.1668 m/z

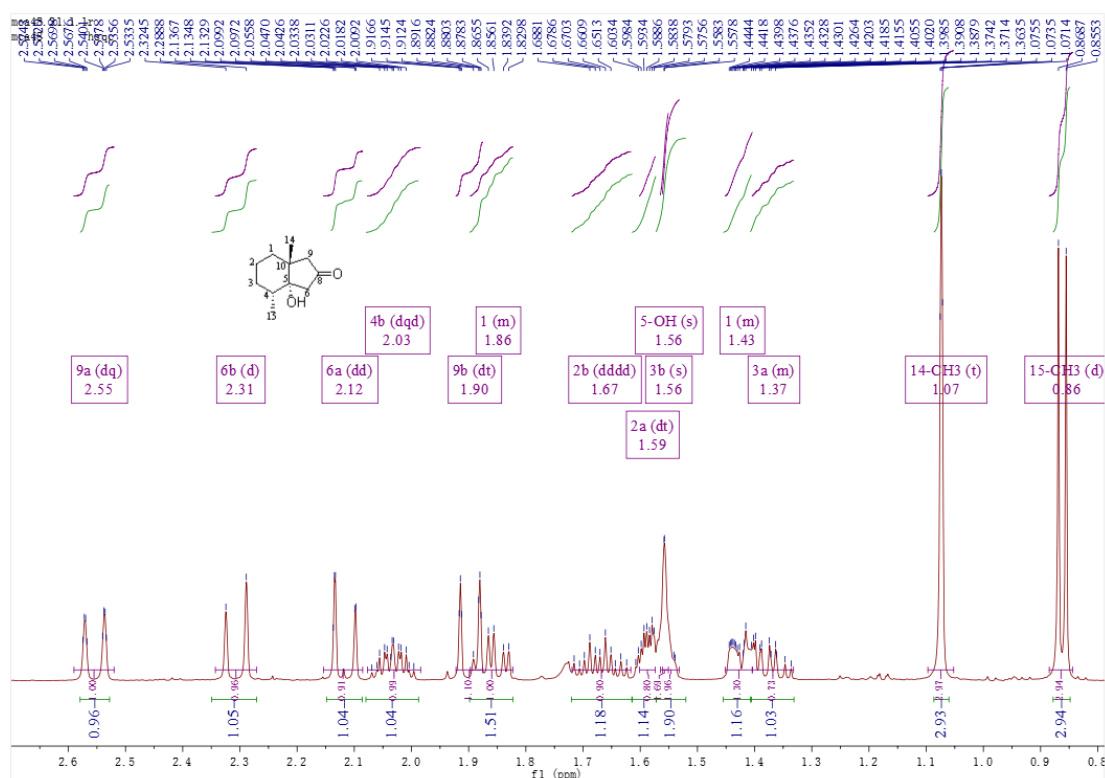


C15 H24 O2 [M+Na]+ : Predicted region for 259.1669 m/z

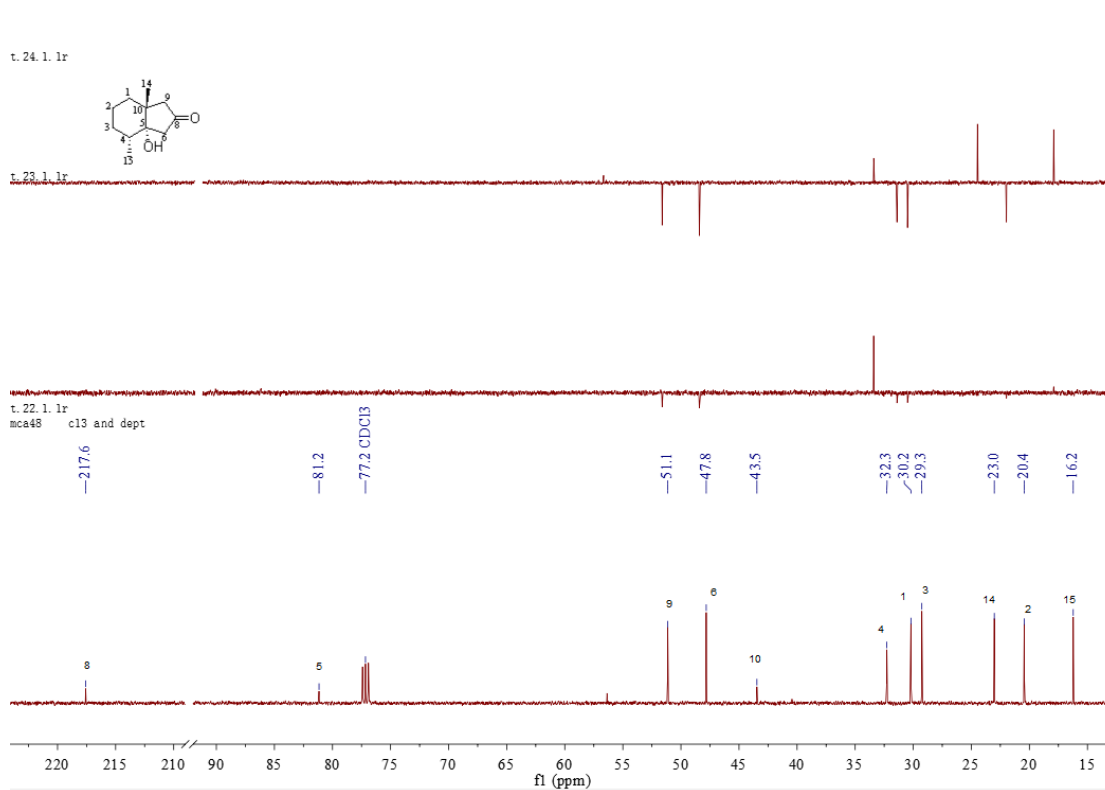


Formula (M)	Ion	Mass. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C15 H24 O2	[M+Na]+	259.1668	259.1669	-0.1	-0.39	4.0

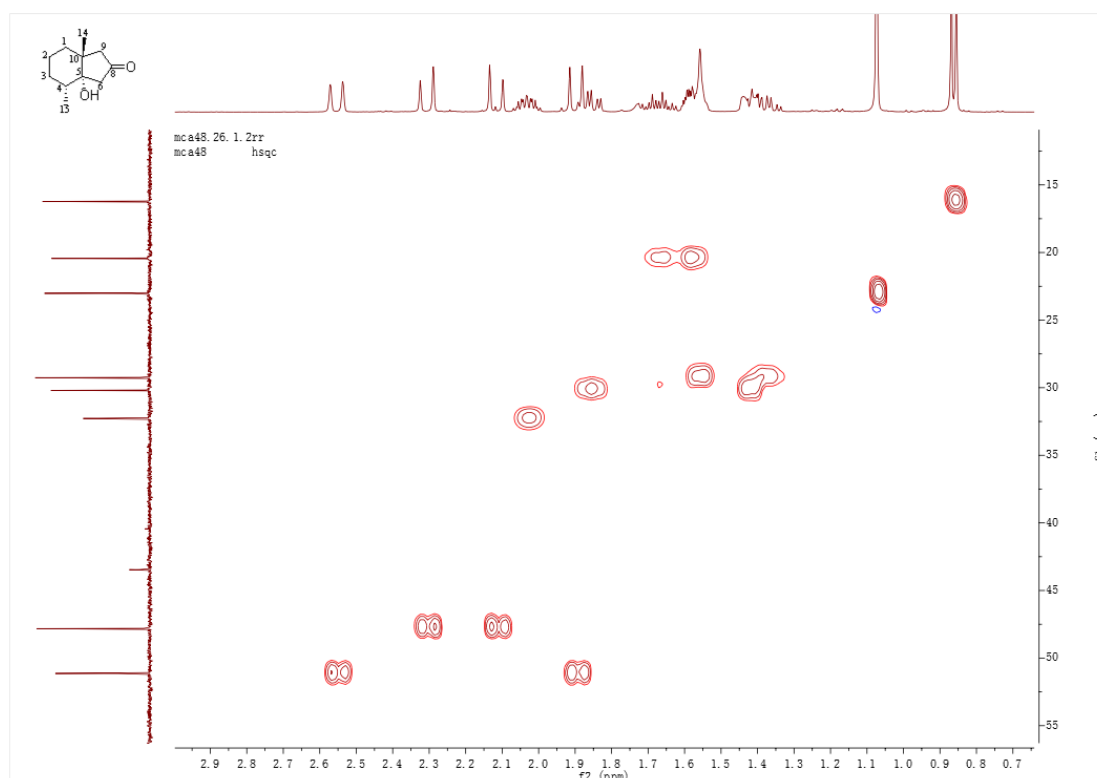
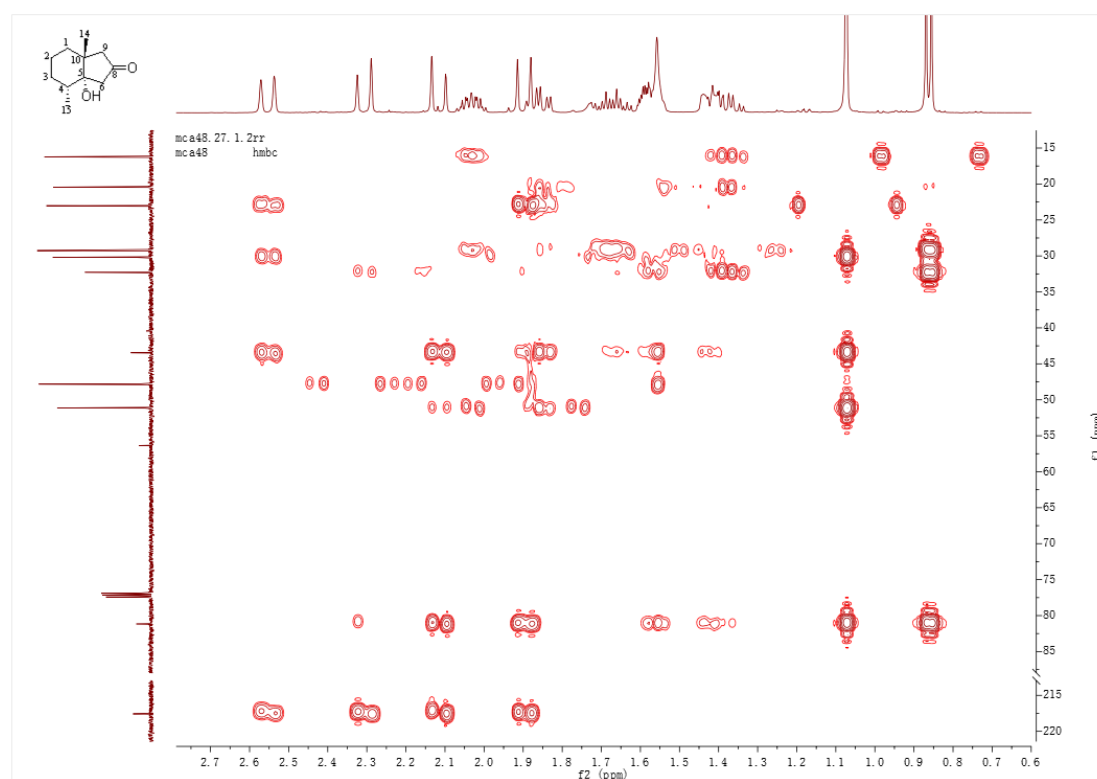
Figure S42. HR-ESI-MS spectrum of 6.

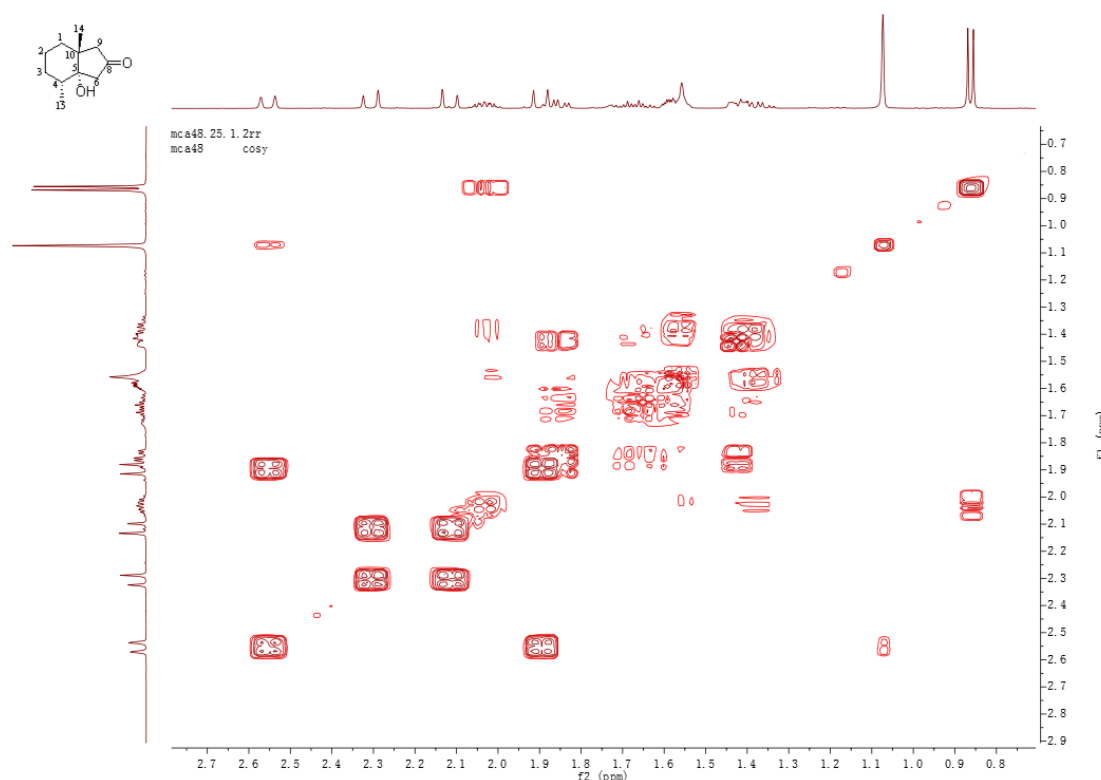
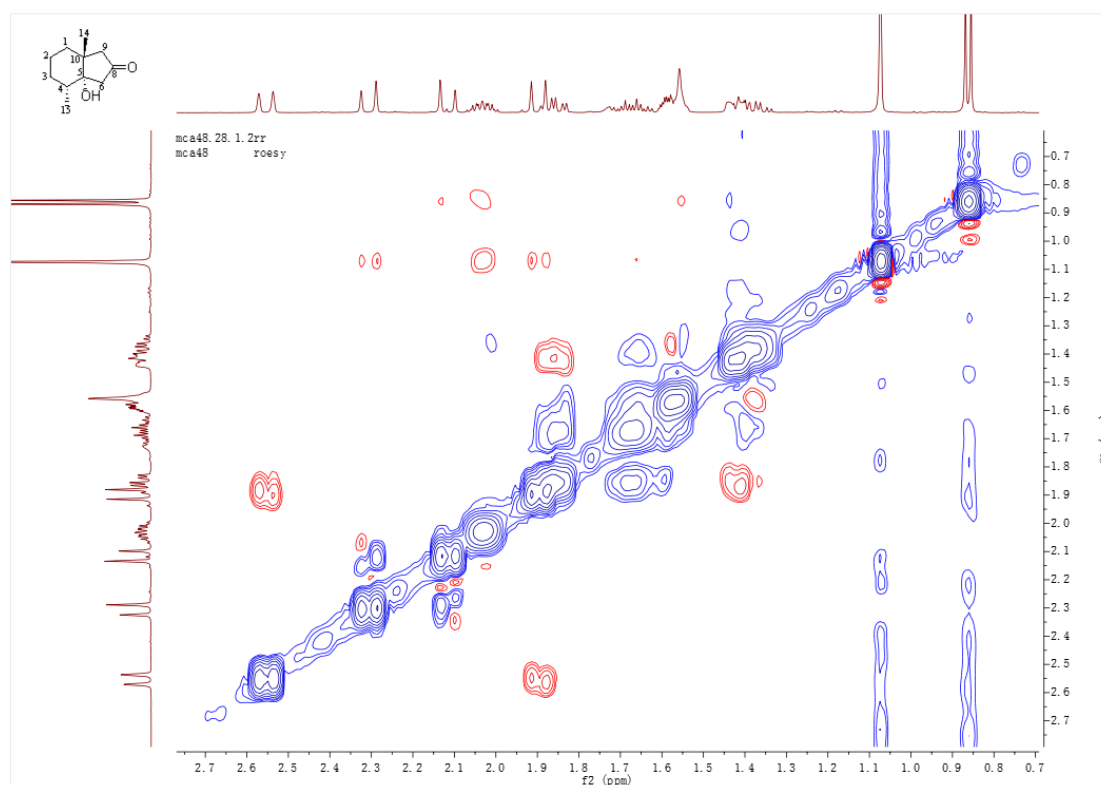


**Figure S43.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of 7.



**Figure S44.**  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of 7.

Figure S45. HSQC (500 MHz, CDCl<sub>3</sub>) spectrum of 7.Figure S46. HMBC (500 MHz, CDCl<sub>3</sub>) spectrum of 7.

Figure S47.  $^1\text{H}$ - $^1\text{H}$  COSY (500 MHz,  $\text{CDCl}_3$ ) spectrum of 7.Figure S48. NOESY (500 MHz,  $\text{CDCl}_3$ ) spectrum of 7.

Formula Predictor Report - MCA-48.lcd

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Data File: E:\DATA\2021\1206\MCA-48.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	Na
2H	1	0	0	Na	1	0	0	Co	2	0	0	I	3	0	0	
B	3	0	0	Mg	2	0	0	Cu	2	0	0	Ir	3	0	0	
C	4	5	50	Si	4	0	0	Se	2	0	0					
N	3	0	10	P	3	0	0	Br	1	0	5					
O	2	0	30	S	2	0	0	Pd	2	0	0					

Error Margin (ppm): 5

DBE Range: not fixed

Electron Ions: both

HC Ratio: unlimited

Apply N Rule: yes

Use MSn Info: yes

Max Isotopes: all

Isotope RI (%): 1.00

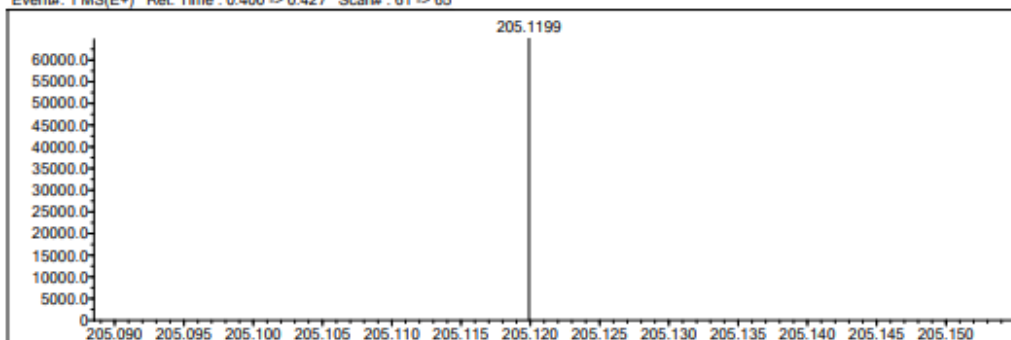
Isotope Res: 10000

MSn Iso RI (%): 75.00

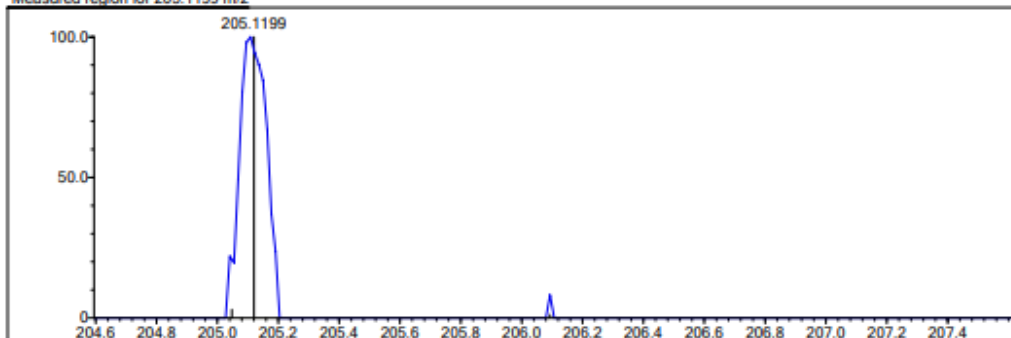
MSn Logic Mode: OR

Max Results: 20

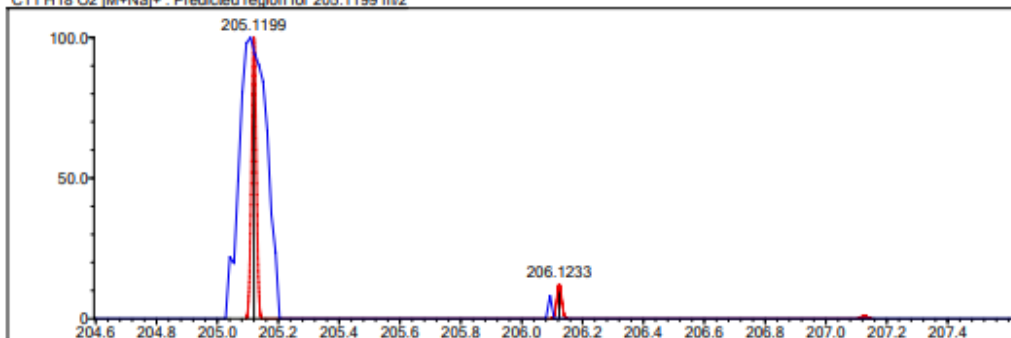
Event#: 1 MS(E+) Ret. Time : 0.400 -&gt; 0.427 Scan#: 61 -&gt; 65



Measured region for 205.1199 m/z



C11 H18 O2 [M+Na]+ : Predicted region for 205.1199 m/z



Formula (M)	Ion	Mass. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C11 H18 O2	[M+Na]+	205.1199	205.1199	-0.0	0.00	3.0

Figure S49. HR-ESI-MS spectrum of 7.