

Supporting Information

Eremophilane-type Sesquiterpenoids from the Endophytic Fungus *Rhizopycnis vagum* and Their Antibacterial, Cytotoxic, and Phytotoxic Activities

Ali Wang¹, Ruya Yin¹, Zhiyao Zhou¹, Gan Gu¹, Jungui Dai², Daowan Lai^{1} and
Ligang Zhou^{1*}*

¹ Department of Plant Pathology, College of Plant Protection, China Agricultural University, Beijing 100193, China, ² State Key Laboratory of Bioactive Substance and Function of Natural Medicines, Institute of Materia Medica, Chinese Academy of Medical Science & Peking Union Medical College, Beijing 100050, China

*** Corresponding Authors**

Daowan Lai: dwlai@cau.edu.cn; Ligang Zhou: lgzhou@cau.edu.cn

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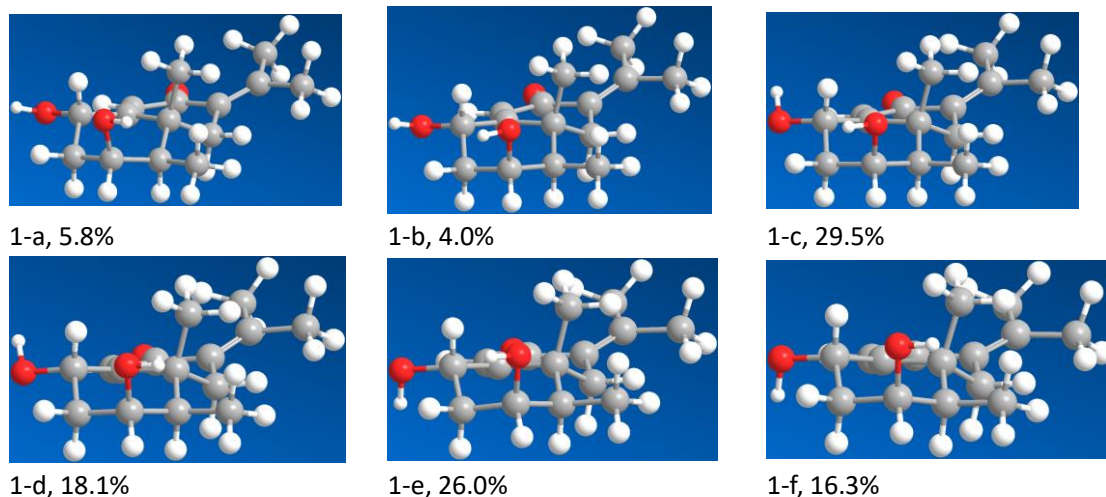


Figure S1. Optimized geometries of the predominant conformers of **1** at the B3LYP/6-31G(d) level in the gas phase.

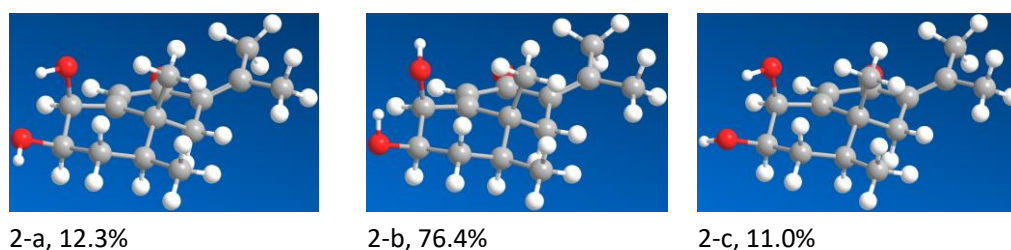


Figure S2. Optimized geometries of the predominant conformers of **2** at the B3LYP/6-31G(d) level in the gas phase.

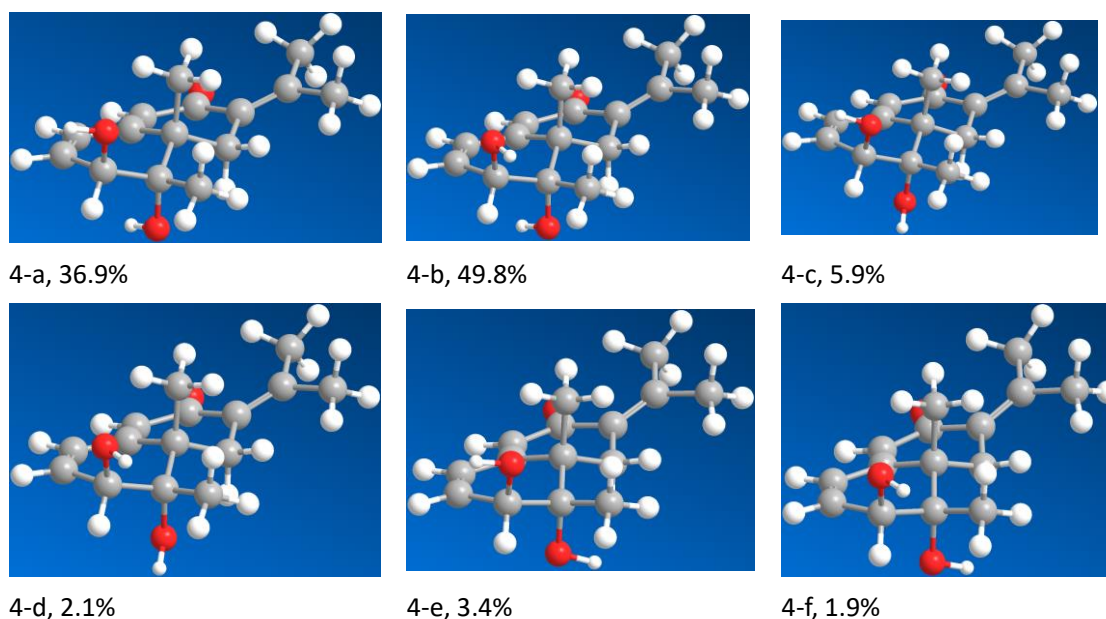


Figure S3. Optimized geometries of the predominant conformers of **4** at the B3LYP/6-31G(d) level in the gas phase.

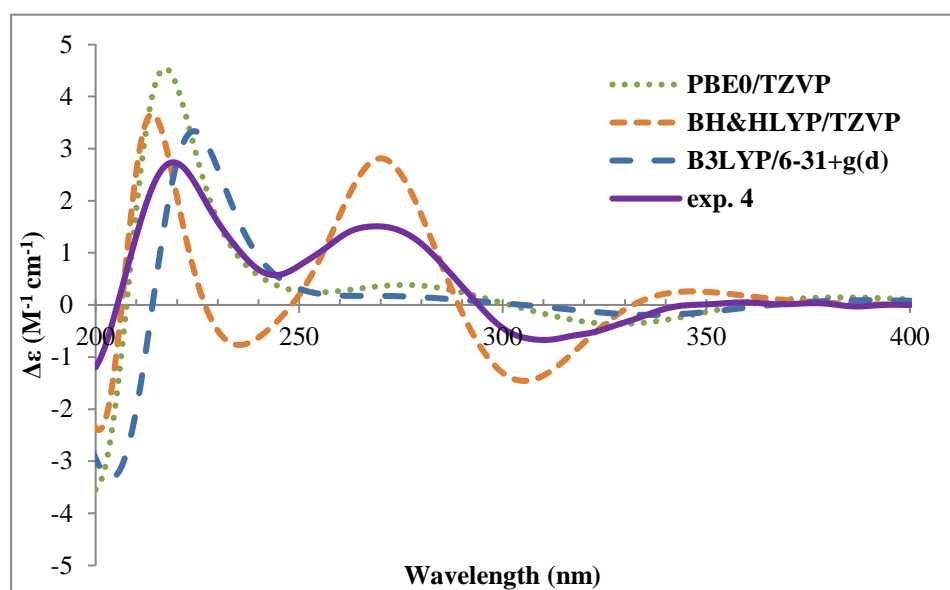
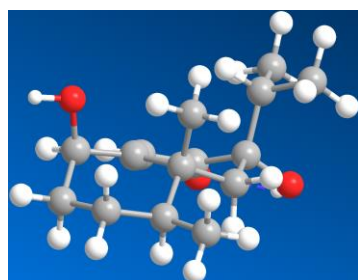
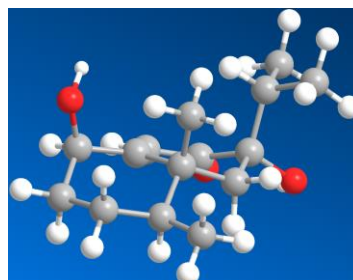


Figure S4. The experiment ECD and the calculated spectra of **4** using three different methods.



5-a, 9.9%



5-b, 90.1%

Figure S5. Optimized geometries of the predominant conformers of **5** at the B3LYP/6-31G(d) level in the gas phase.

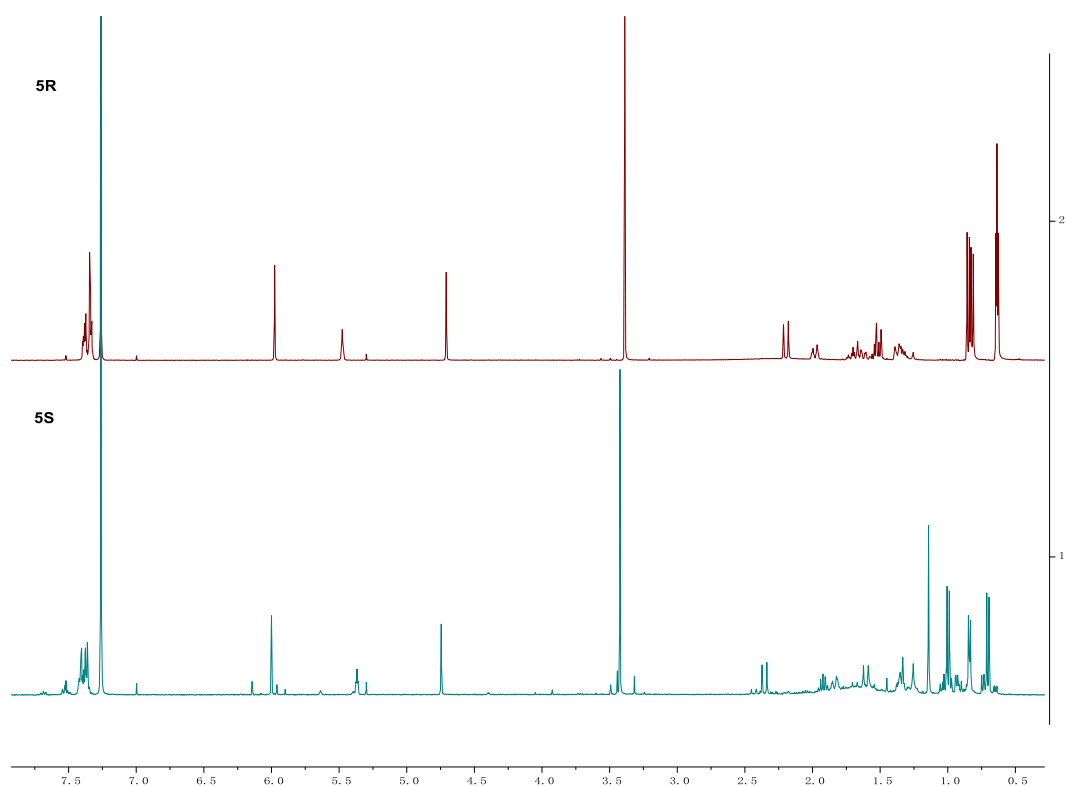


Figure S6. Comparison of the ^1H NMR spectra of the (*R/S*)-MPA esters of **5**.

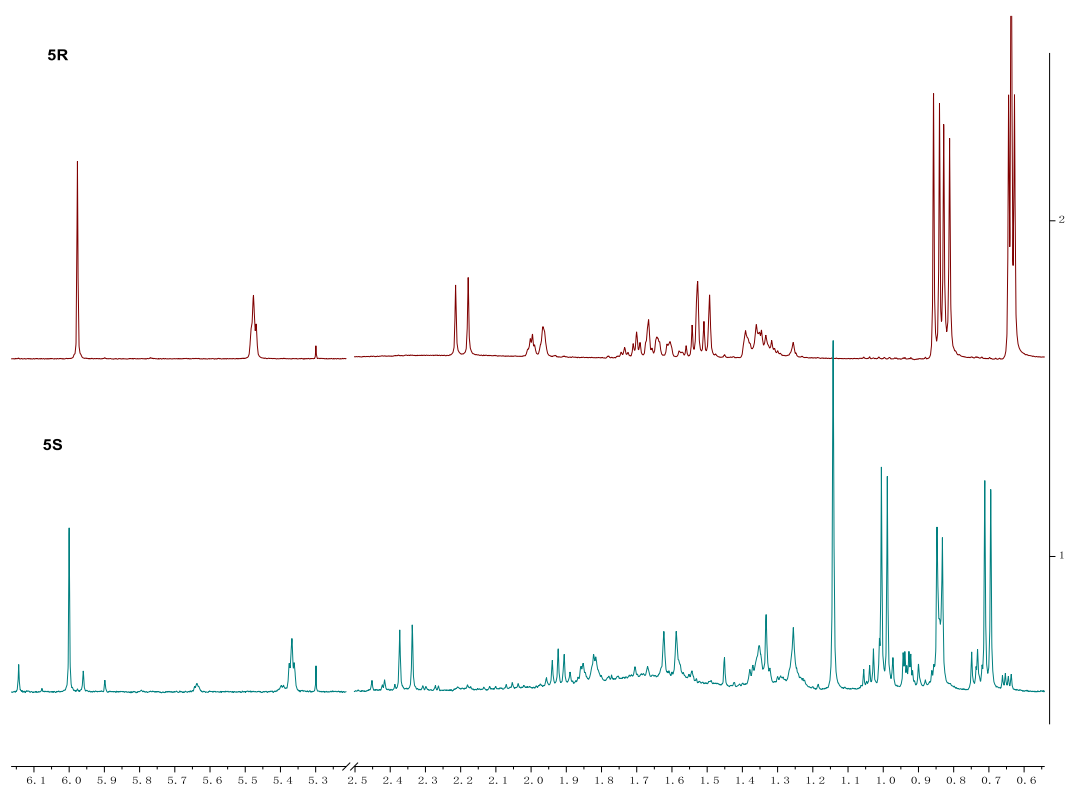
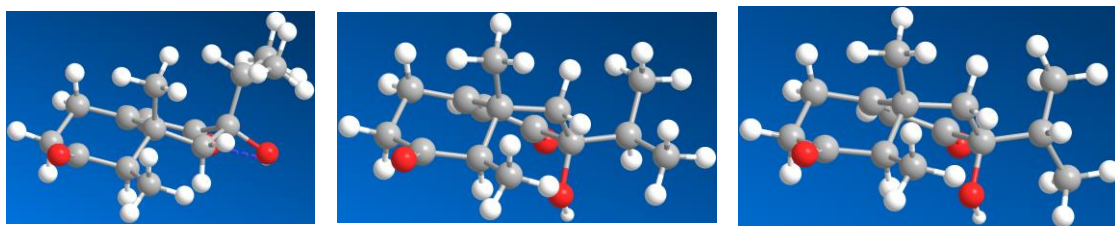


Figure S6-1. Comparison of the ^1H NMR spectra of the (*R/S*)-MPA esters of **5** (Expansion).



6-a, 75.2%

6-b, 23.4%

6-c, 1.1%

Figure S7. Optimized geometries of the predominant conformers of **6** at the B3LYP/6-31G(d) level in the gas phase.

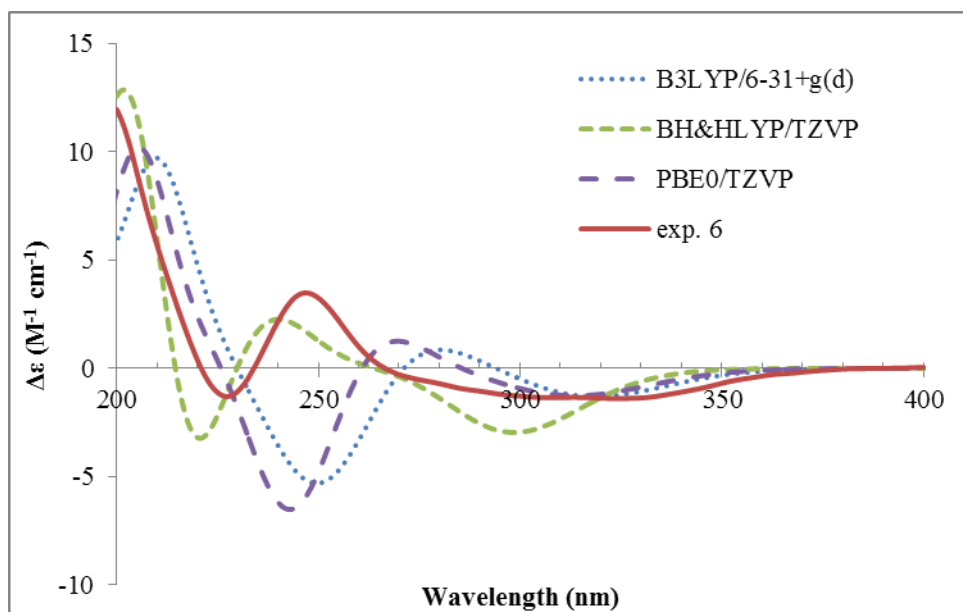
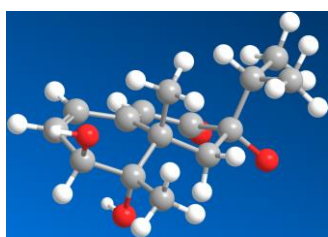
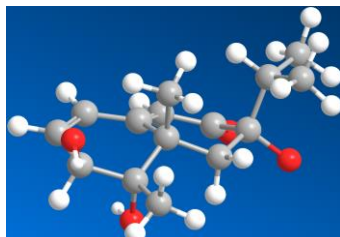


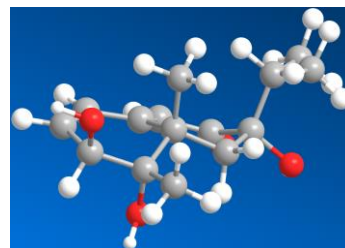
Figure S8. The experiment ECD and the calculated spectra of **6** using three different methods.



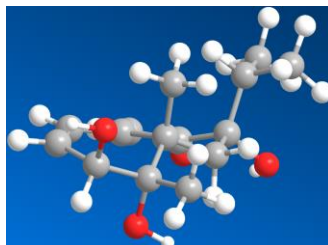
7-a, 12.0%



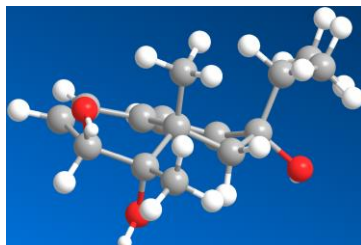
7-b, 32.4%



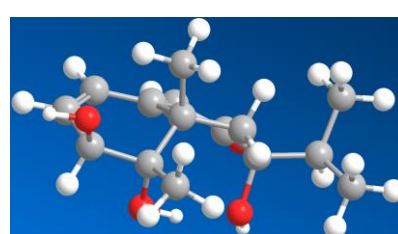
7-c, 2.6%



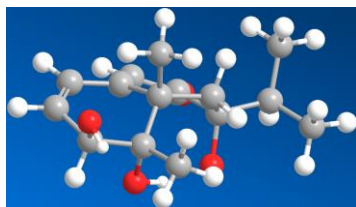
7-d, 2.4%



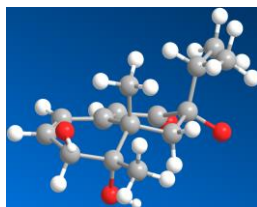
7-e, 2.1%



7-f, 11.5%



7-g, 32.4%



7-h, 4.3%

Figure S9. Optimized geometries of the predominant conformers of **7** at the B3LYP/6-31G(d) level in the gas phase.

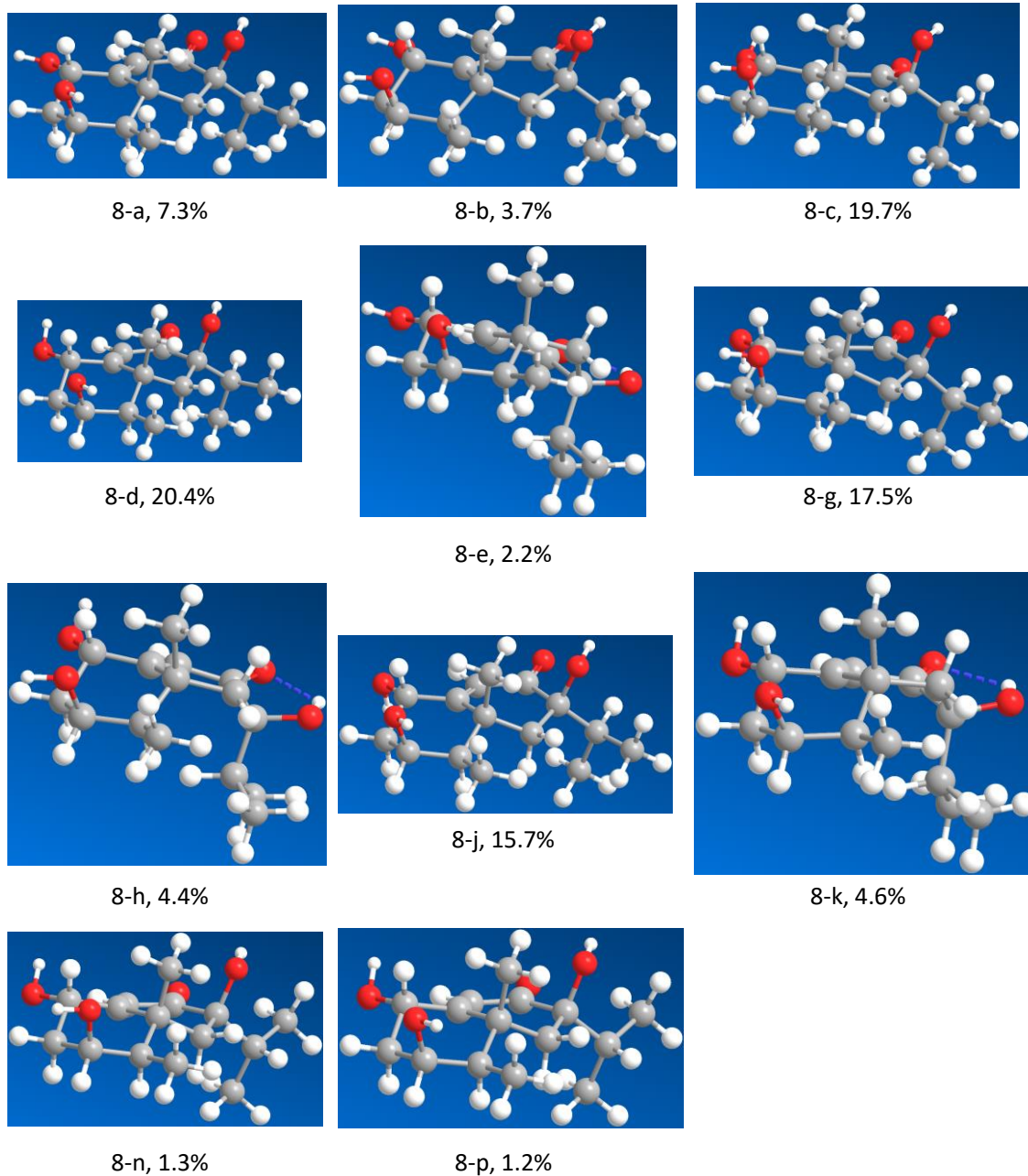


Figure S10. Optimized geometries of the predominant conformers of **8** at the B3LYP/6-31G(d) level in the gas phase.

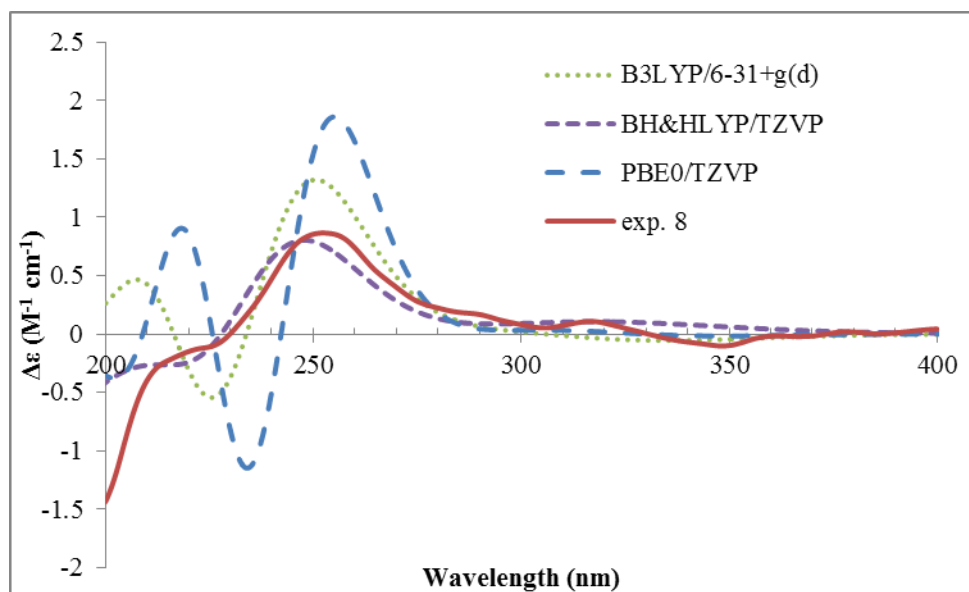


Figure S11. The experiment ECD and the calculated spectra of **8** using three different methods.

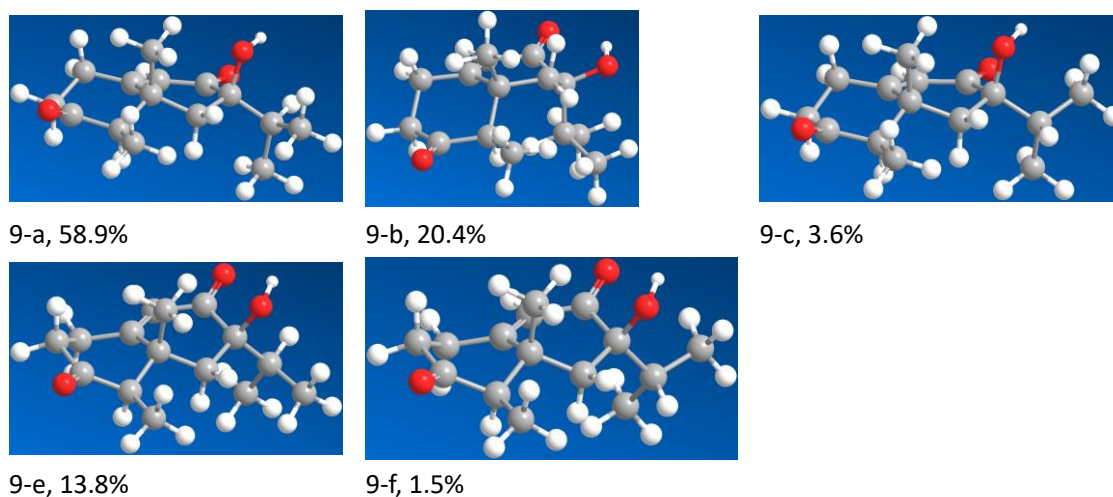
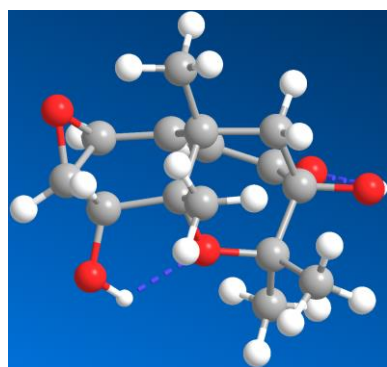


Figure S12. Optimized geometries of the predominant conformers of **9** at the B3LYP/6-31G(d) level in the gas phase.



10-a, 100%

Figure S13. Optimized geometries of the predominant conformers of **10** at the B3LYP/6-31G(d) level in the gas phase.

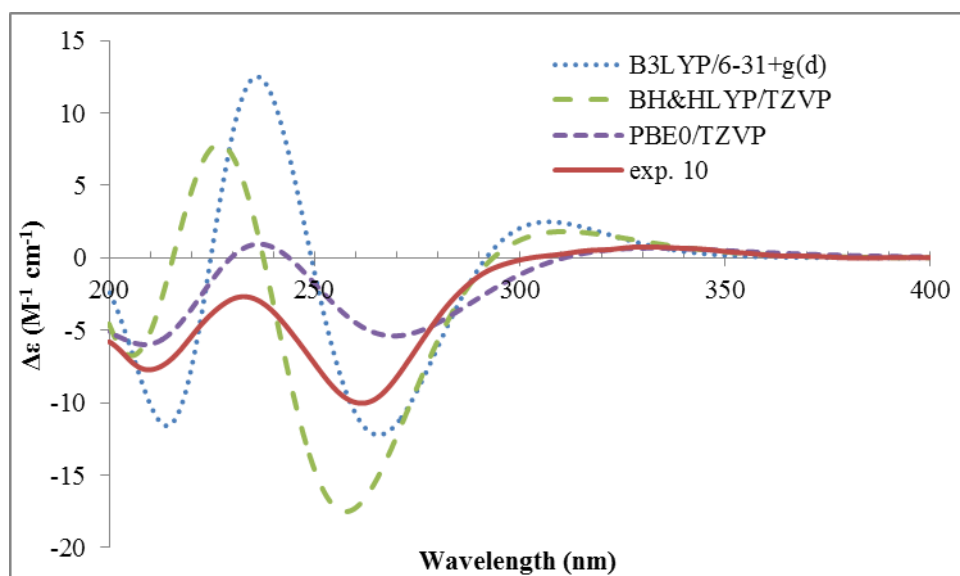


Figure S14. The experiment ECD and the calculated spectra of **10** using three different methods.

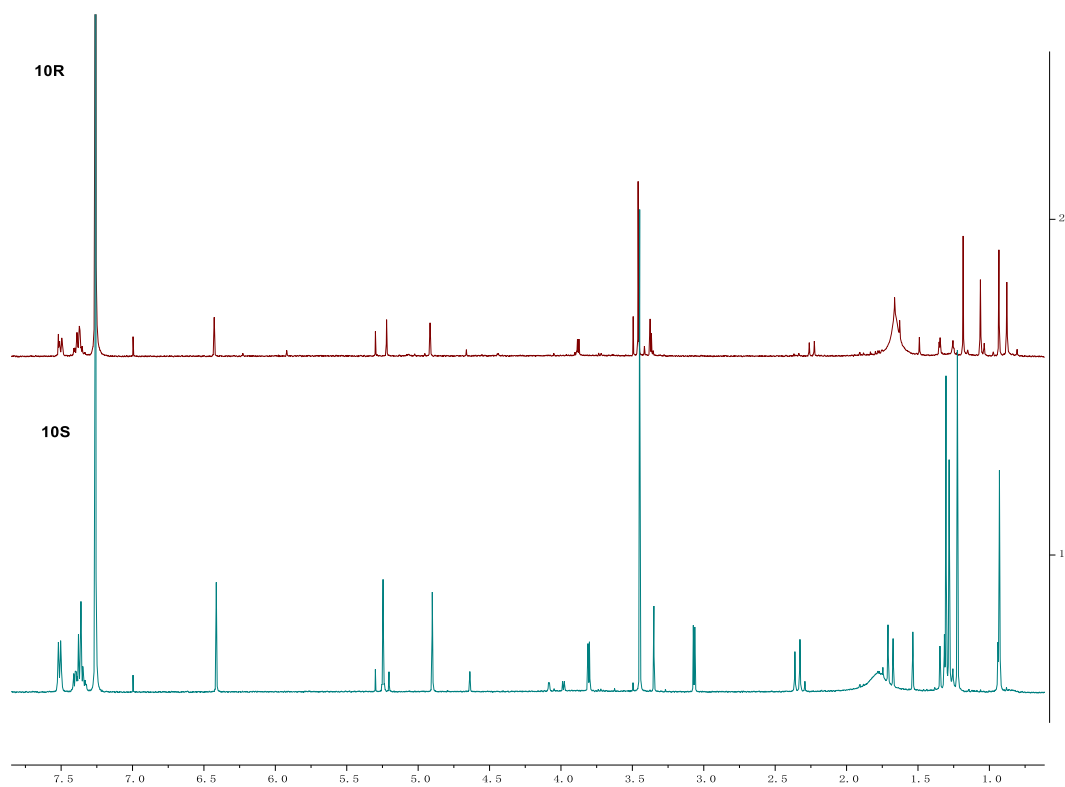


Figure S15. Comparison of the ^1H NMR spectra of the (*R/S*)-MPA esters of **10**.

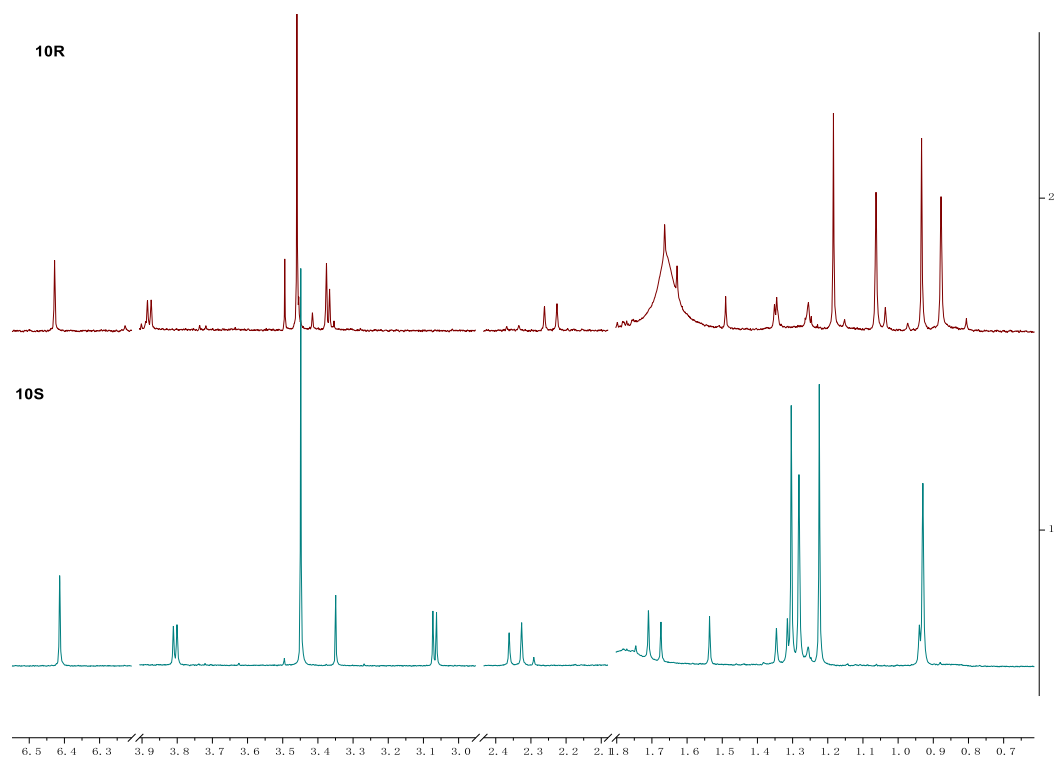
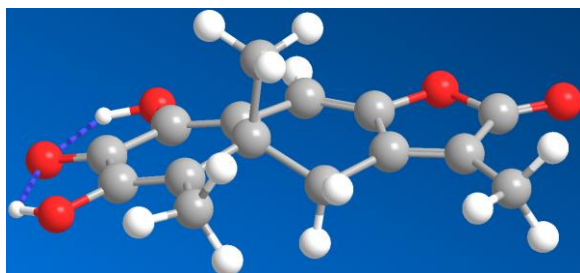


Figure S15-1. Comparison of the ^1H NMR spectra of the (*R/S*)-MPA esters of **10** (Expansion).



11-a, 100%.

Figure S16. Optimized geometries of the predominant conformers of **11** at the B3LYP/6-31G(d) level in the gas phase.

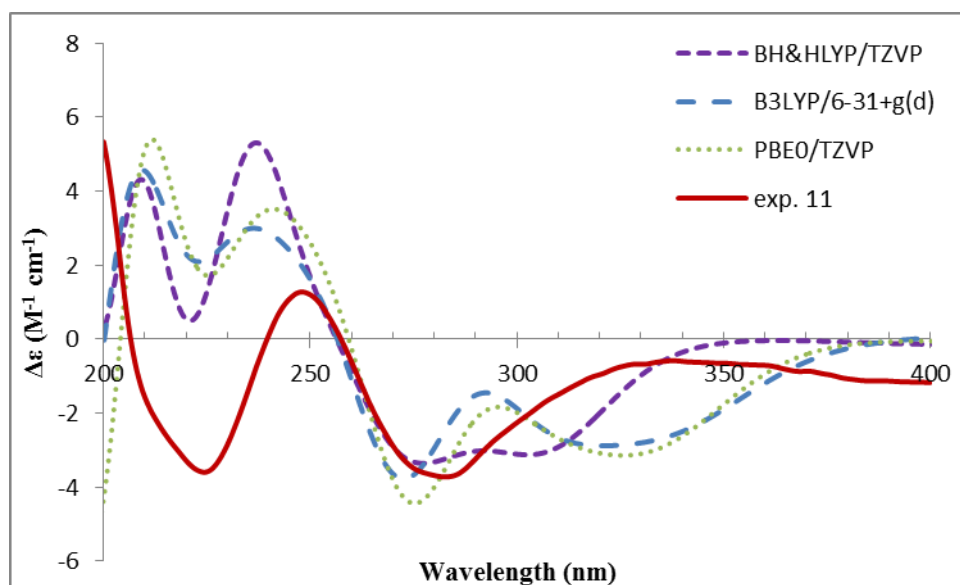
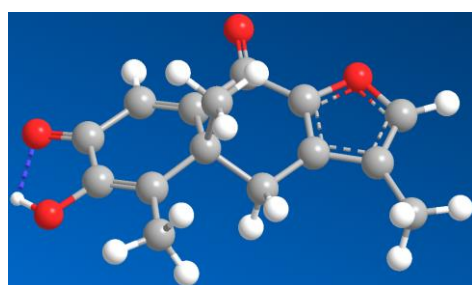
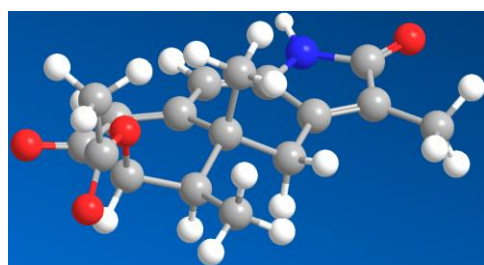


Figure S17. The experiment ECD and the calculated spectra of **11** using three different methods.



12-a, 100%

Figure S18. Optimized geometries of the predominant conformers of **12** at the B3LYP/6-31G(d) level in the gas phase.



13-a, 100%

Figure S19. Optimized geometries of the predominant conformers of **13** at the B3LYP/6-31G(d) level in the gas phase.

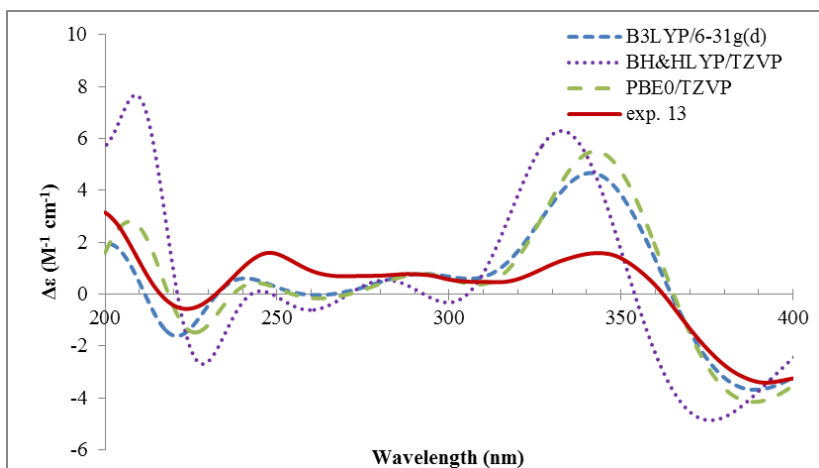
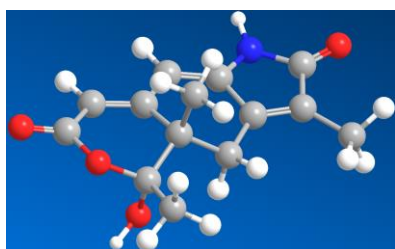
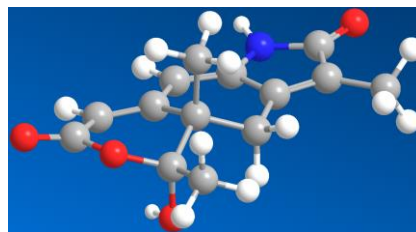


Figure S20. The experiment ECD and the calculated spectra of **13** using three different methods.



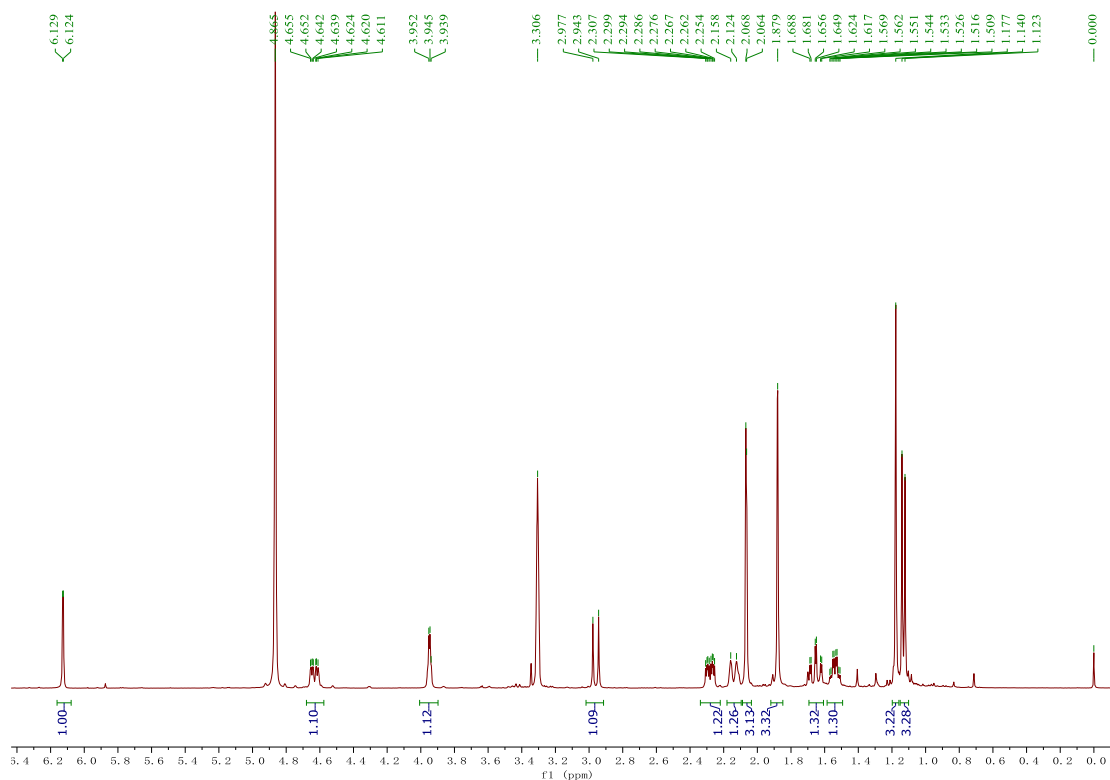
14-a, 85.3%



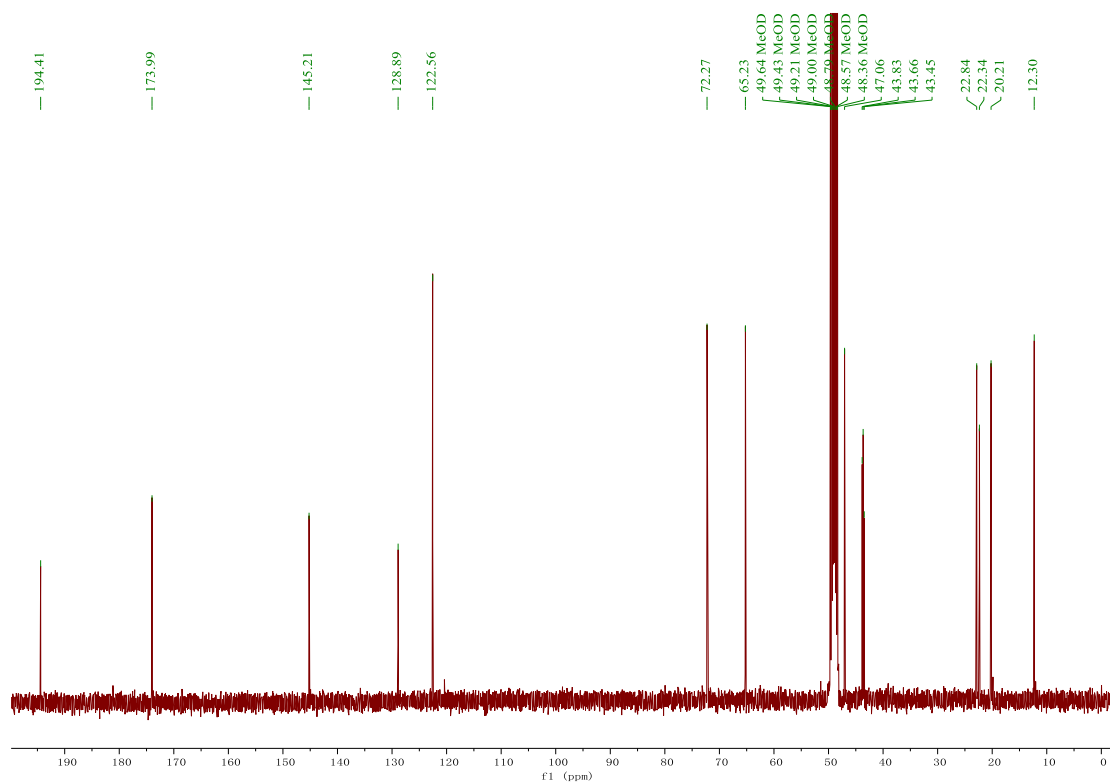
14-b, 14.7%

Figure S21. Optimized geometries of the predominant conformers of **14** at the B3LYP/6-31G(d) level in the gas phase.

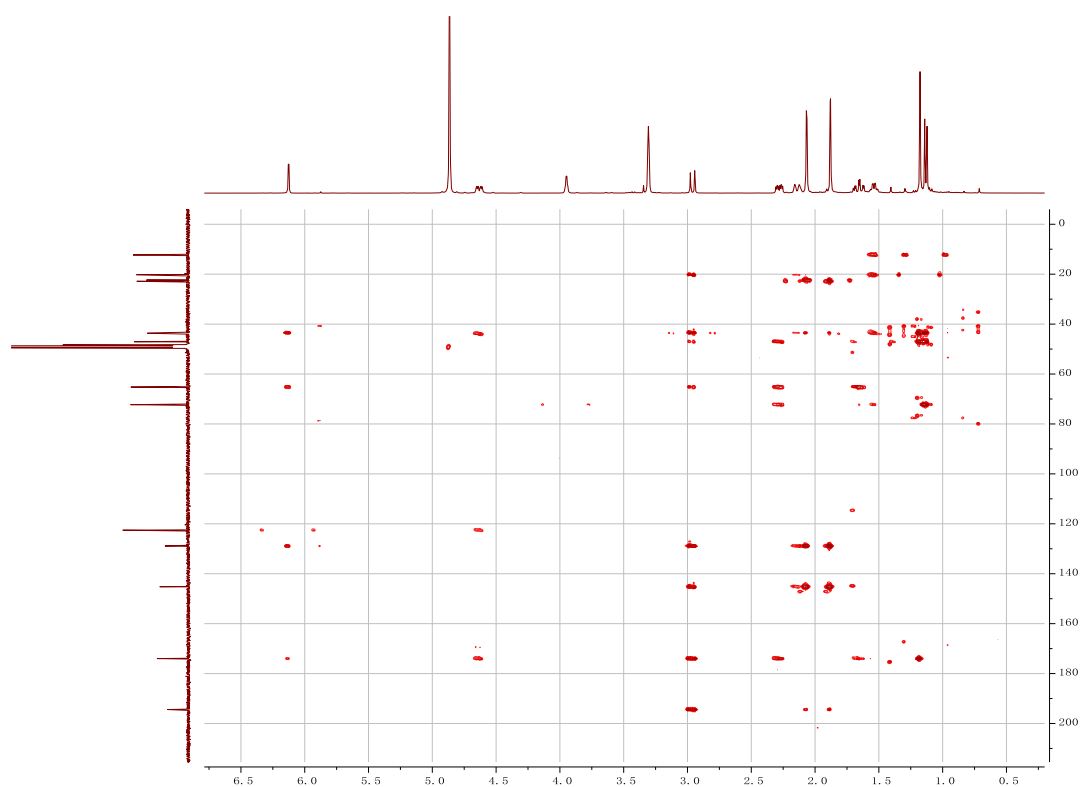
NMR, HRMS spectra of the compounds



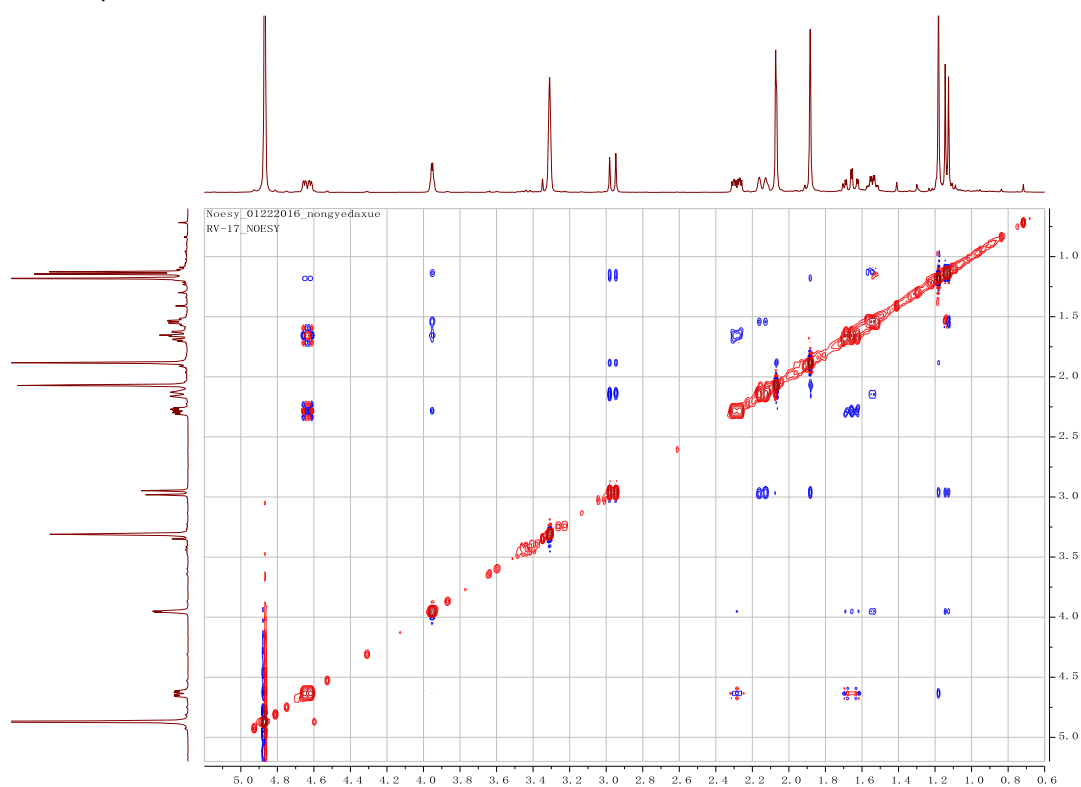
¹H NMR spectrum of **1**



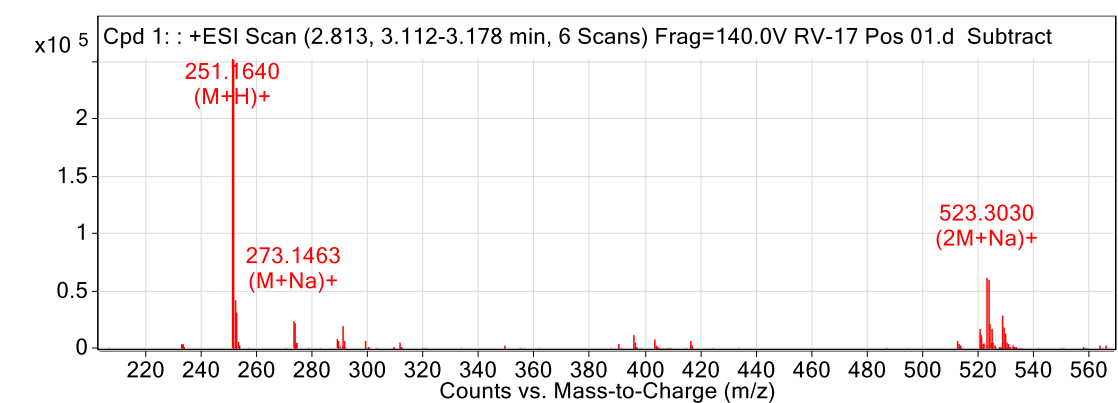
¹³C NMR spectrum of **1**



HMBC spectrum of **1**

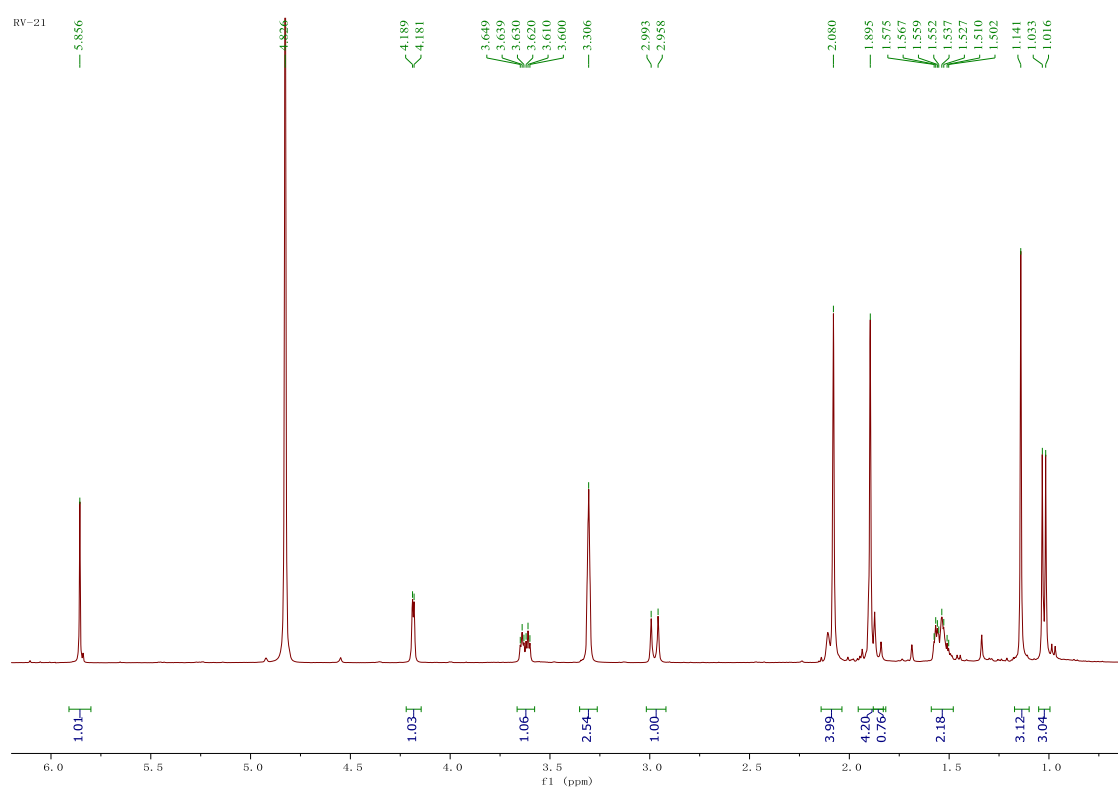


NOESY spectrum of **1**

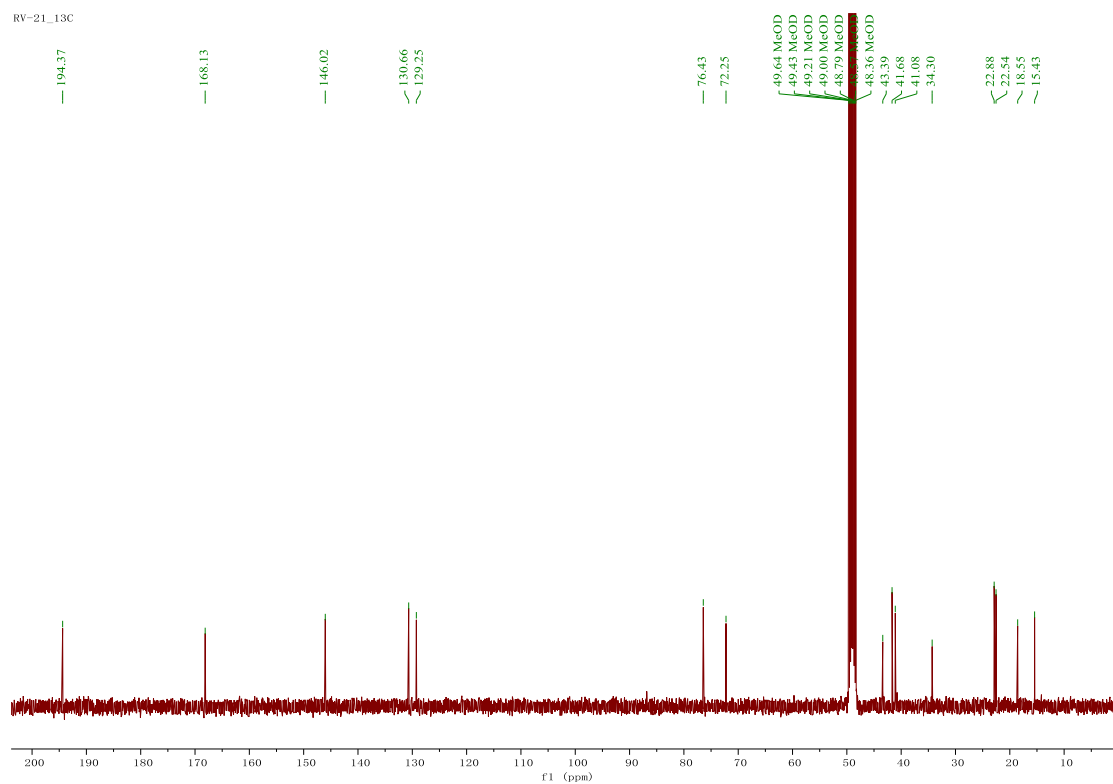


m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
251.1640	251.1642	-0.8	1	252280.2	$C_{15}H_{23}O_3$	$(M+H)^+$
273.1463	273.1461	0.51	1	23876.4	$C_{15}H_{22}NaO_3$	$(M+Na)^+$
523.3030	523.303	0.01	1	61058.6	$C_{30}H_{44}NaO_6$	$(2M+Na)^+$

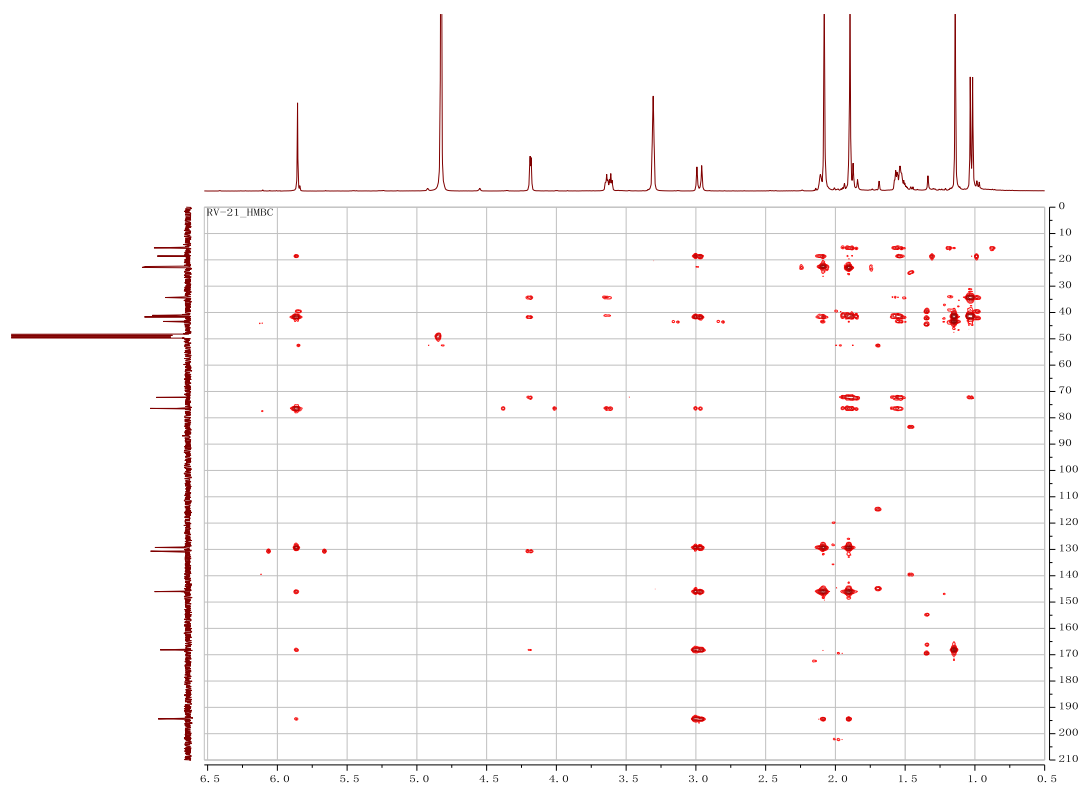
HRMS spectrum of **1**



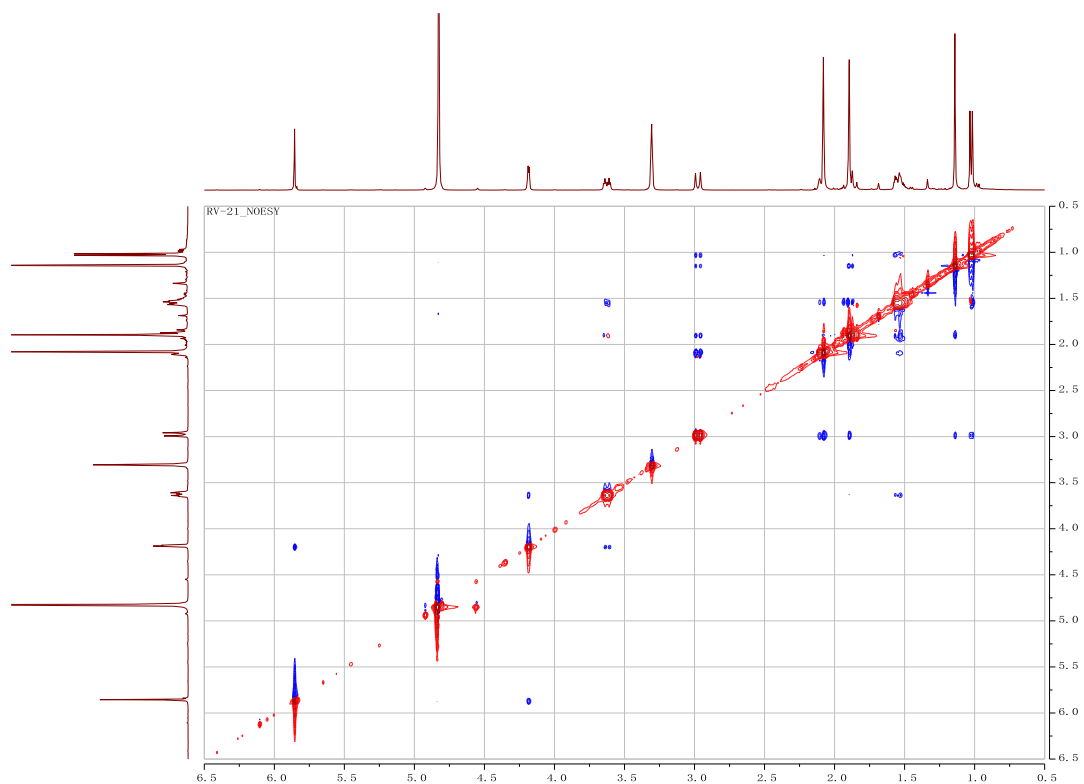
1H NMR spectrum of **2**



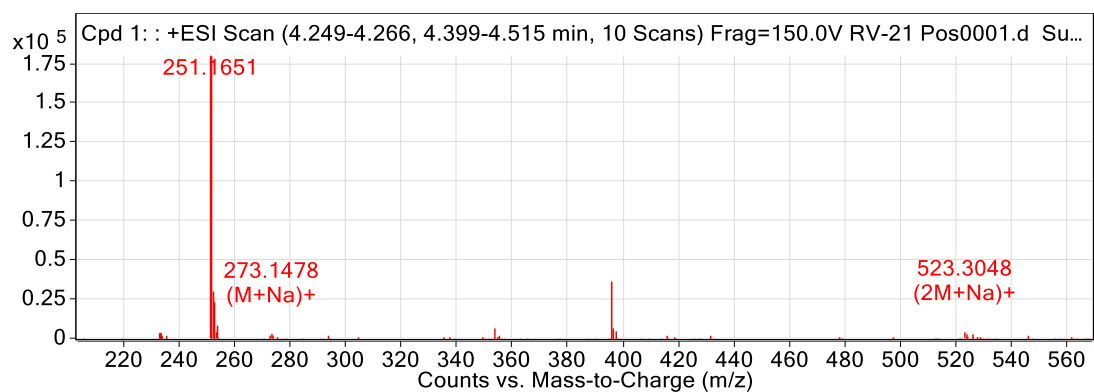
^{13}C NMR spectrum of **2**



HMBC spectrum of **2**

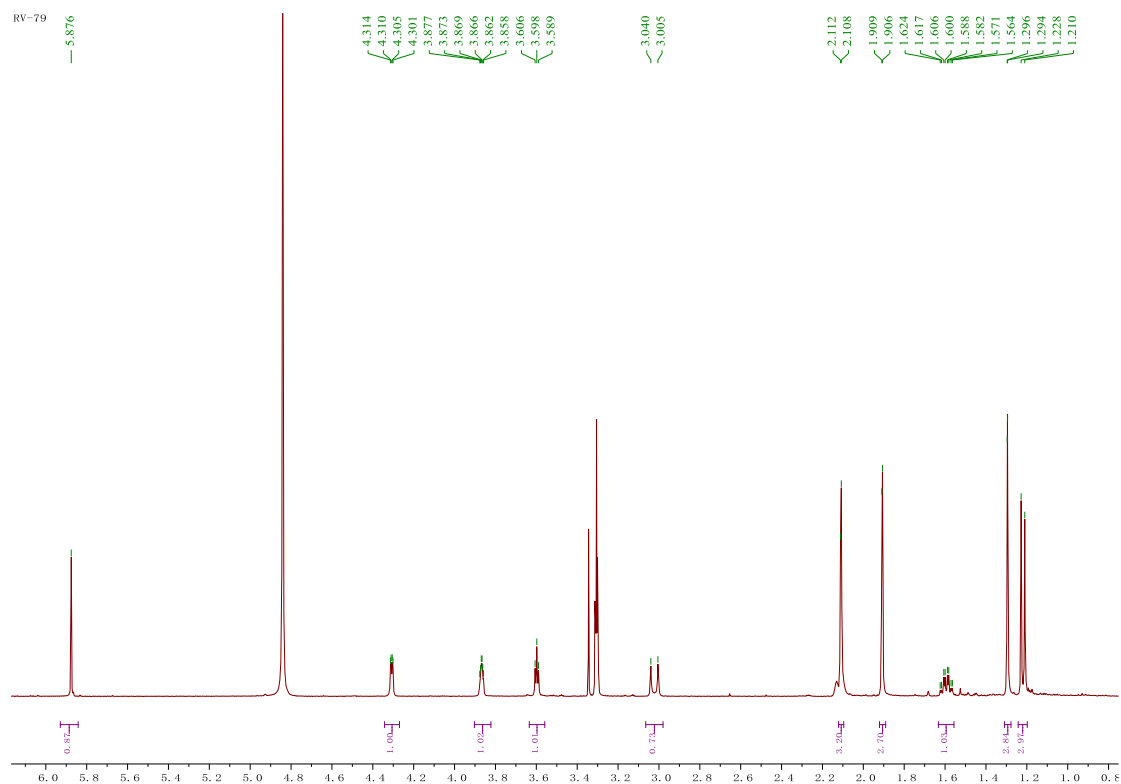


NOESY spectrum of **2**

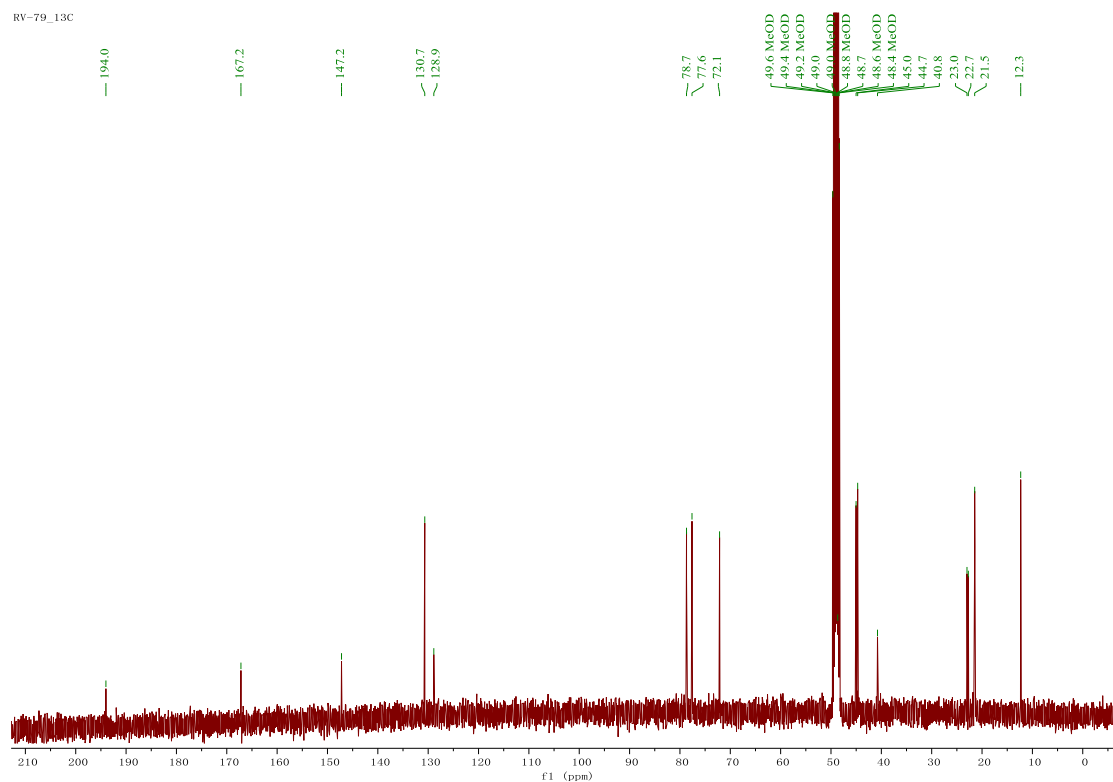


<i>m/z</i>	<i>Calc m/z</i>	Diff(ppm)	<i>z</i>	Abund	Formula	Ion
251.1651	251.1642	3.76	1	180122.1	C ₁₅ H ₂₃ O ₃	(M+H) ⁺

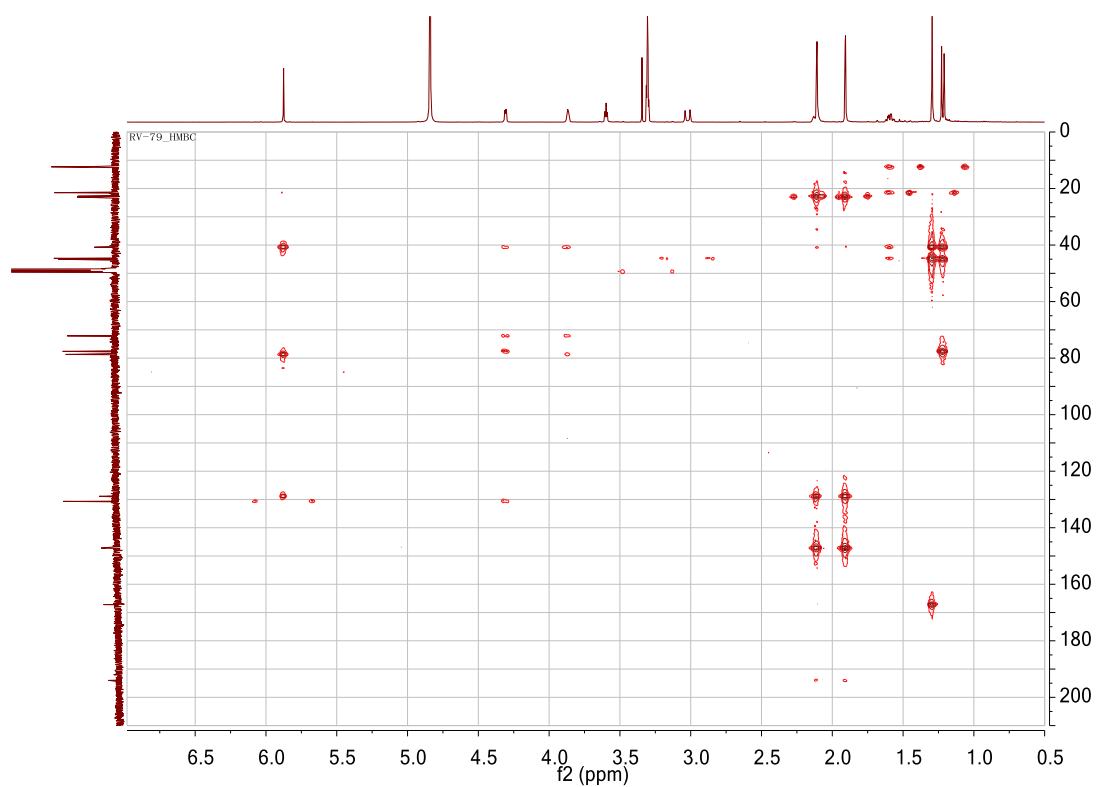
HRESIMS spectrum of **2**



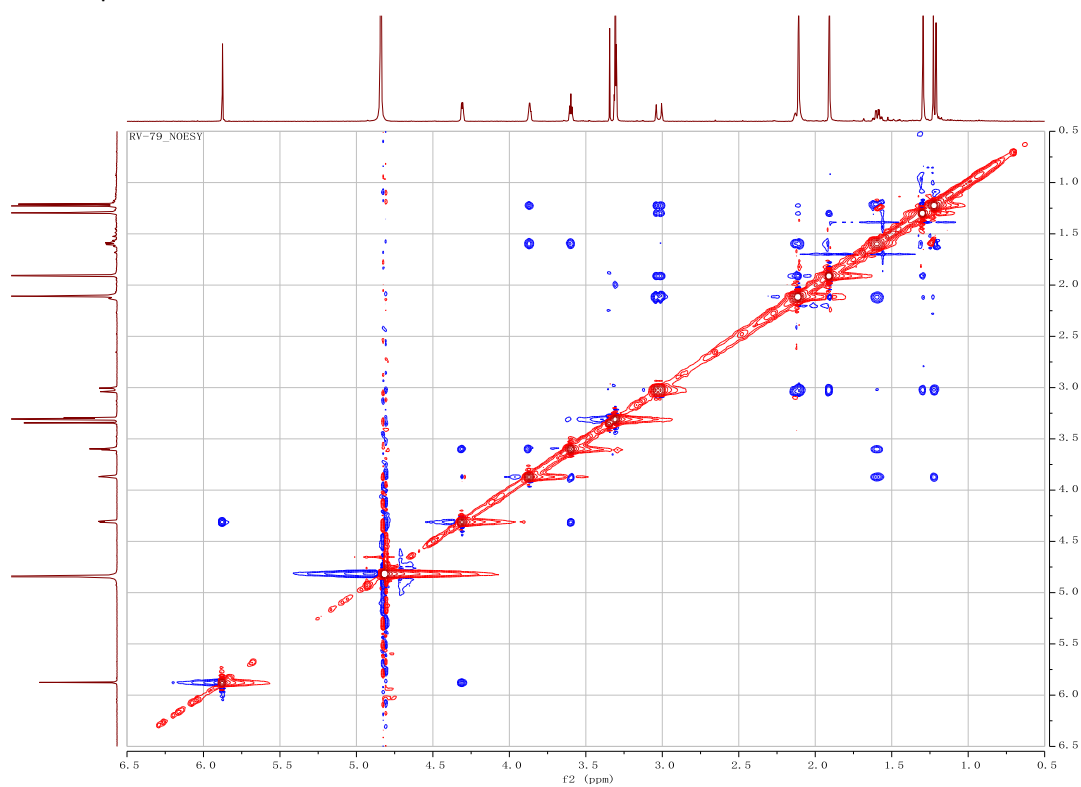
^1H NMR spectrum of **3**



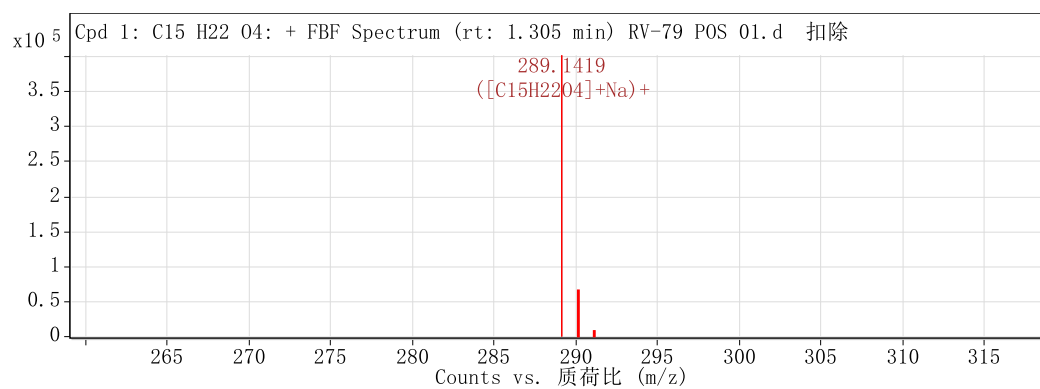
^{13}C NMR spectrum of **3**



HMBC spectrum of **3**

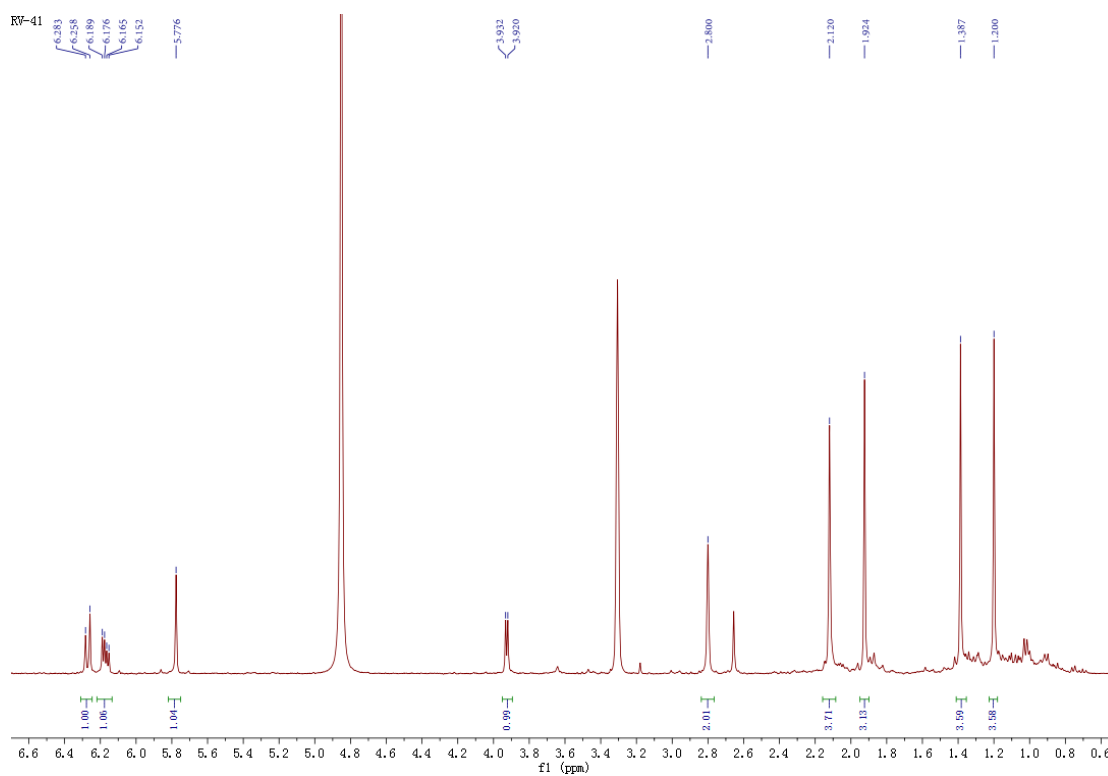


NOESY spectrum of **3**

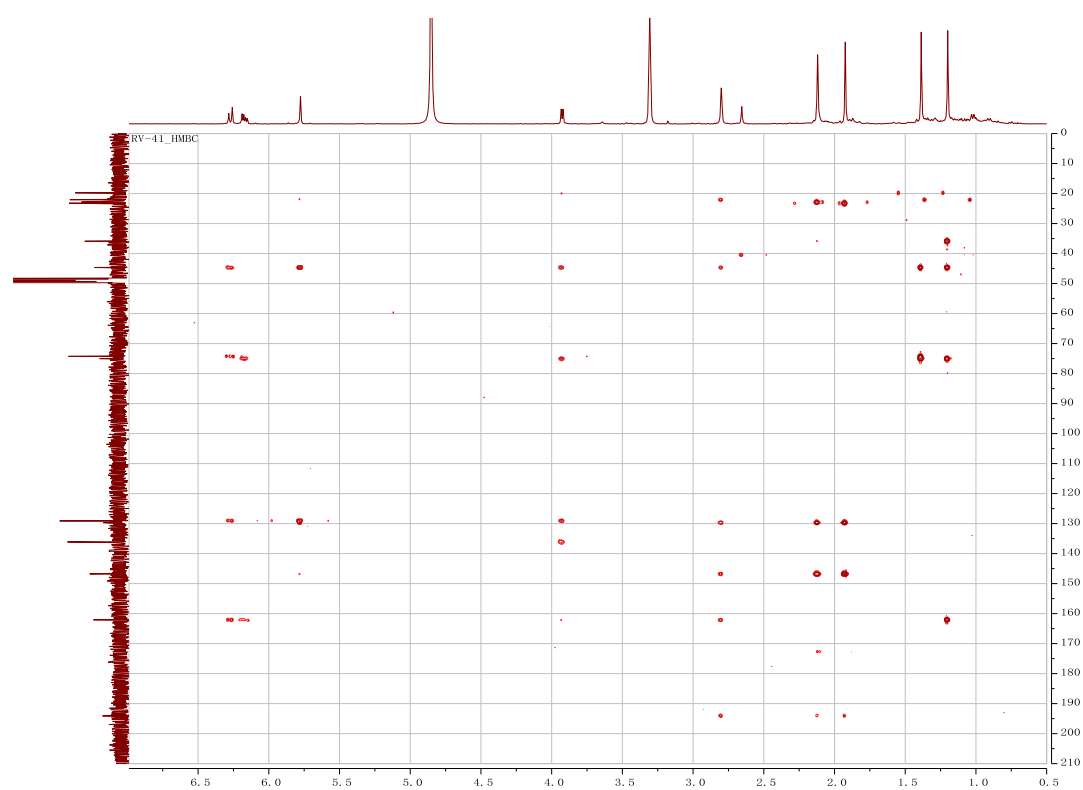
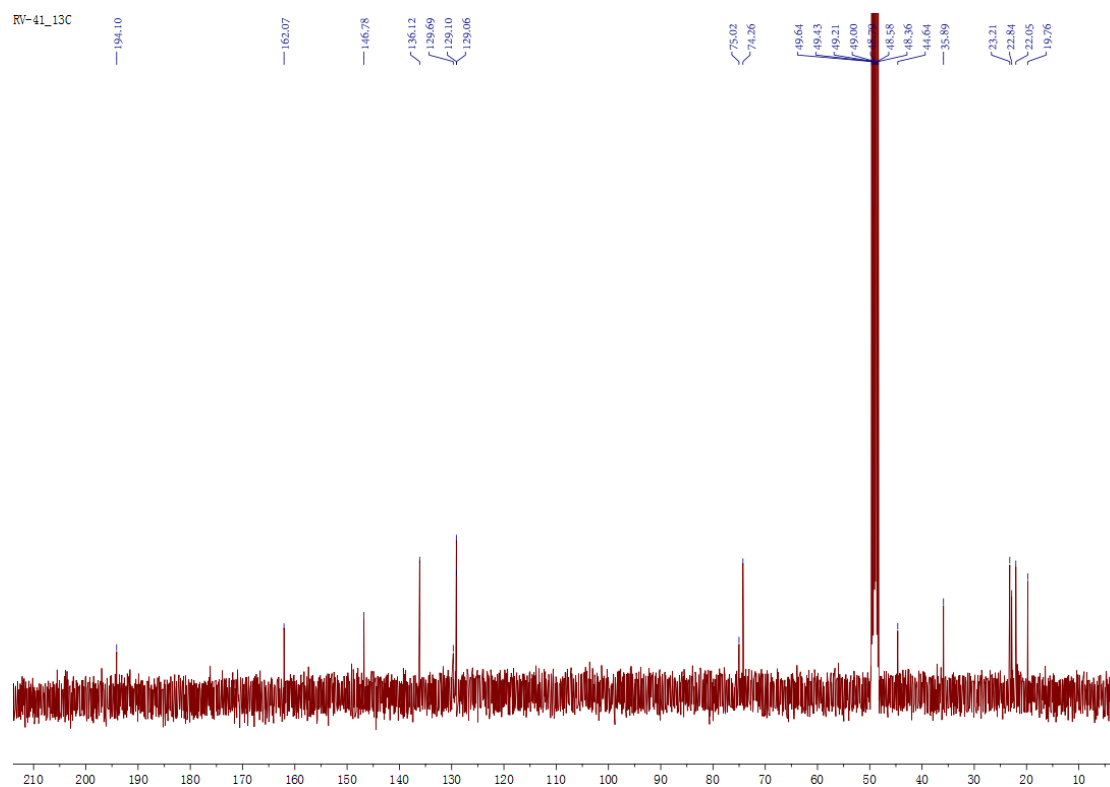


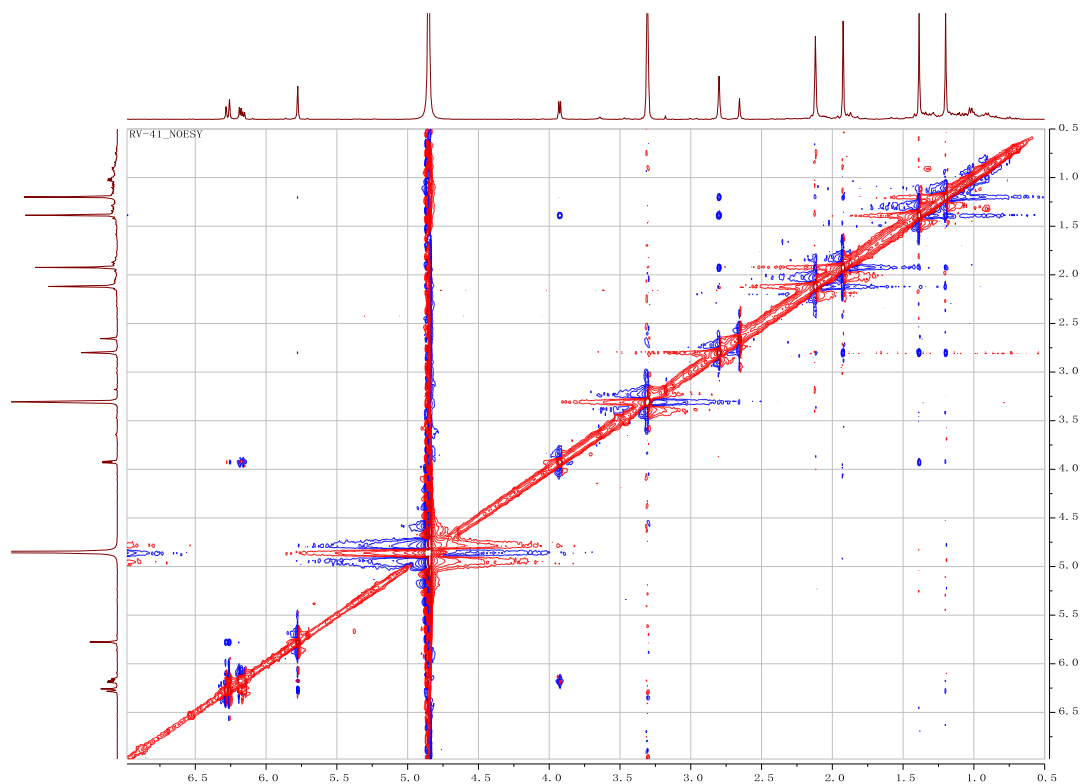
<i>m/z</i>	<i>Calc m/z</i>	Diff(ppm)	<i>z</i>	Abund	Formula	Ion
289.1419	289.1410	3.11	1	402304.38	C ₁₅ H ₂₂ O ₄ Na	(M+ Na) ⁺

HRESIMS spectrum of **3**

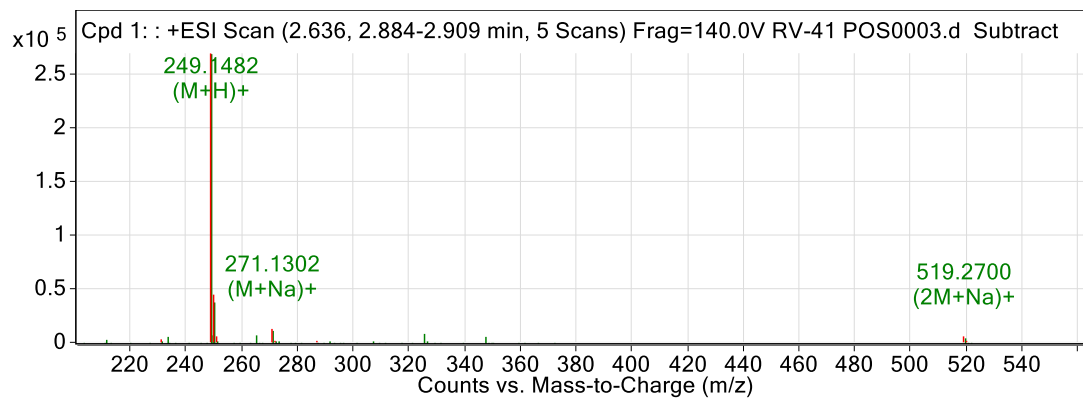


¹H NMR spectrum of **4**



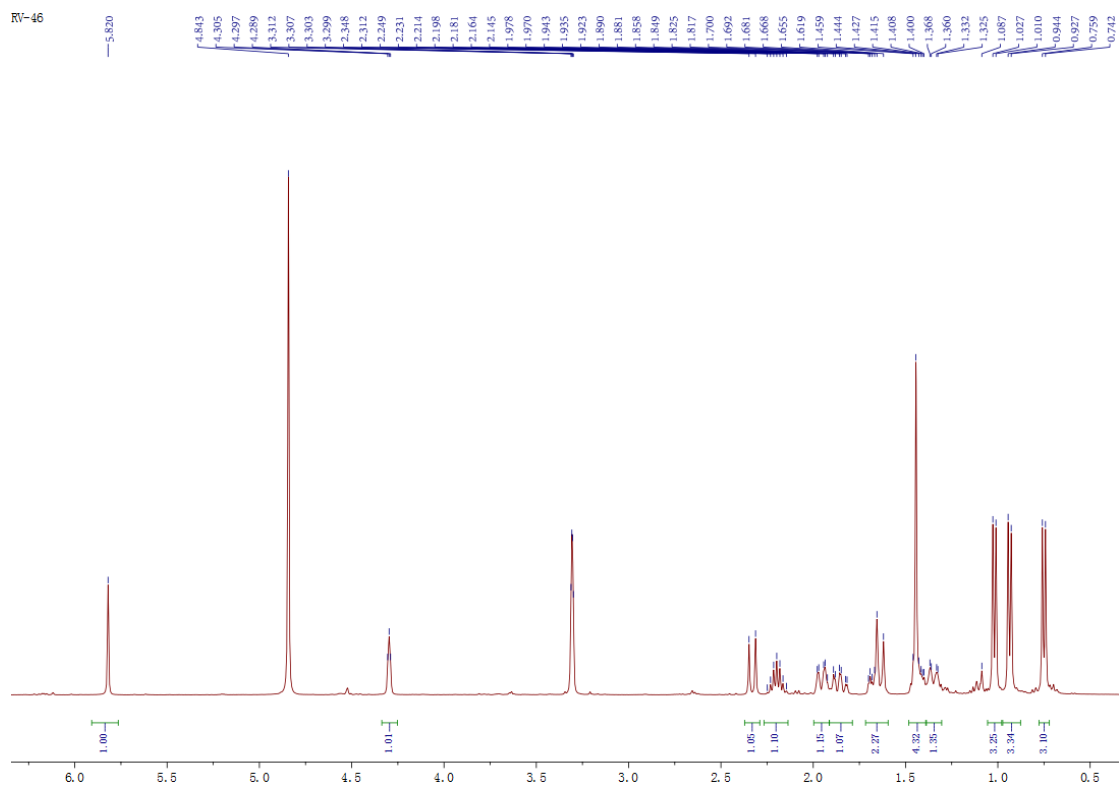


NOESY spectrum of **4**

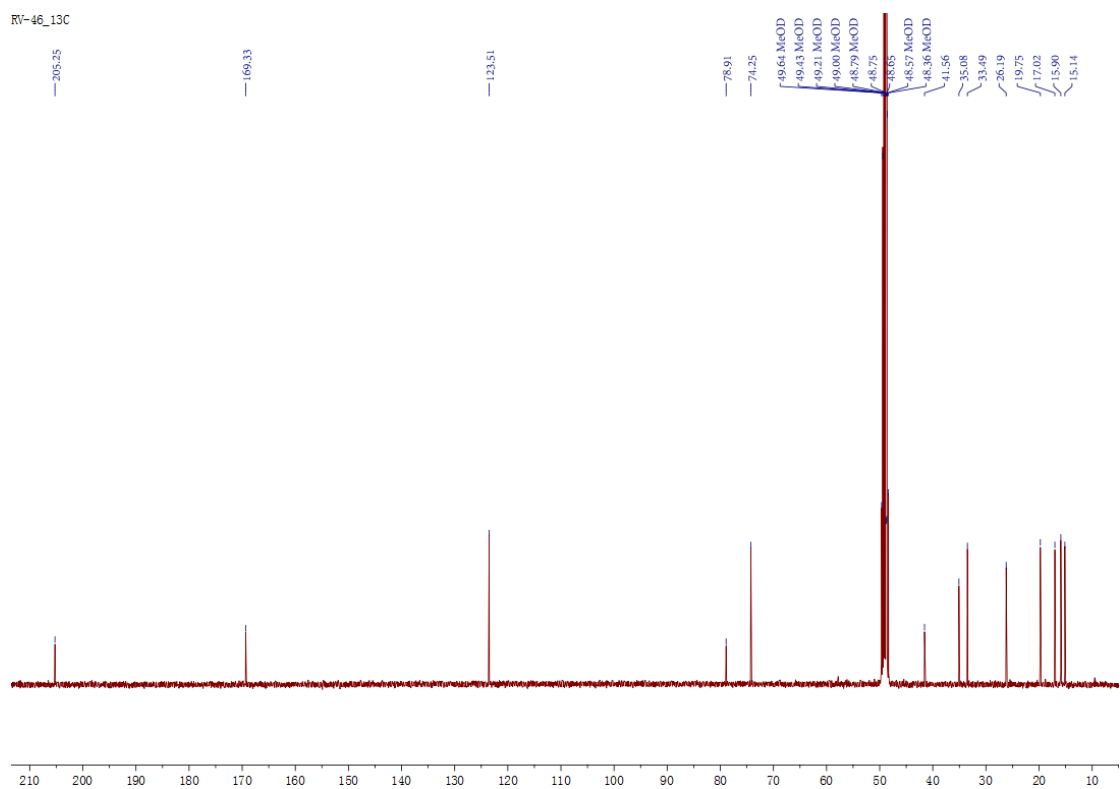


<i>m/z</i>	<i>Calc m/z</i>	Diff(ppm)	<i>z</i>	Abund	Formula	Ion
249.1482	249.1485	-1.33		270074.8	C ₁₅ H ₂₁ O ₃	(M+H) ⁺
271.1302	271.1305	-0.95	1	12518.7	C ₁₅ H ₂₀ NaO ₃	(M+Na) ⁺

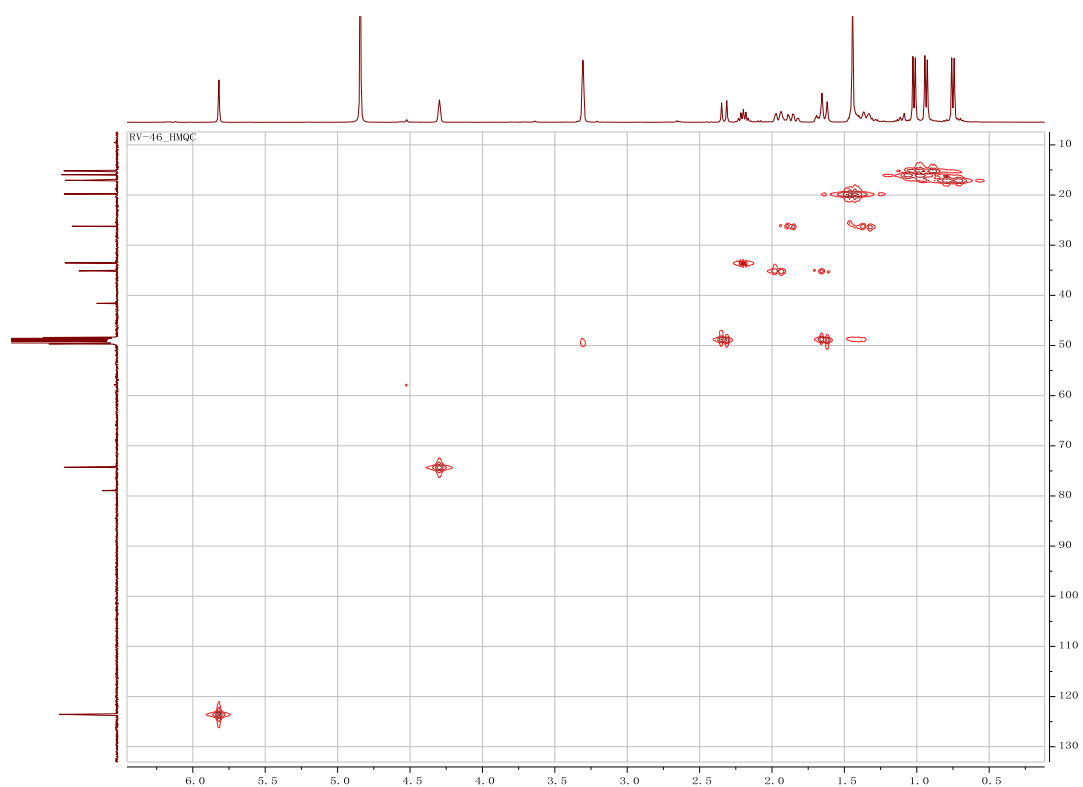
HRESIMS spectrum of **4**



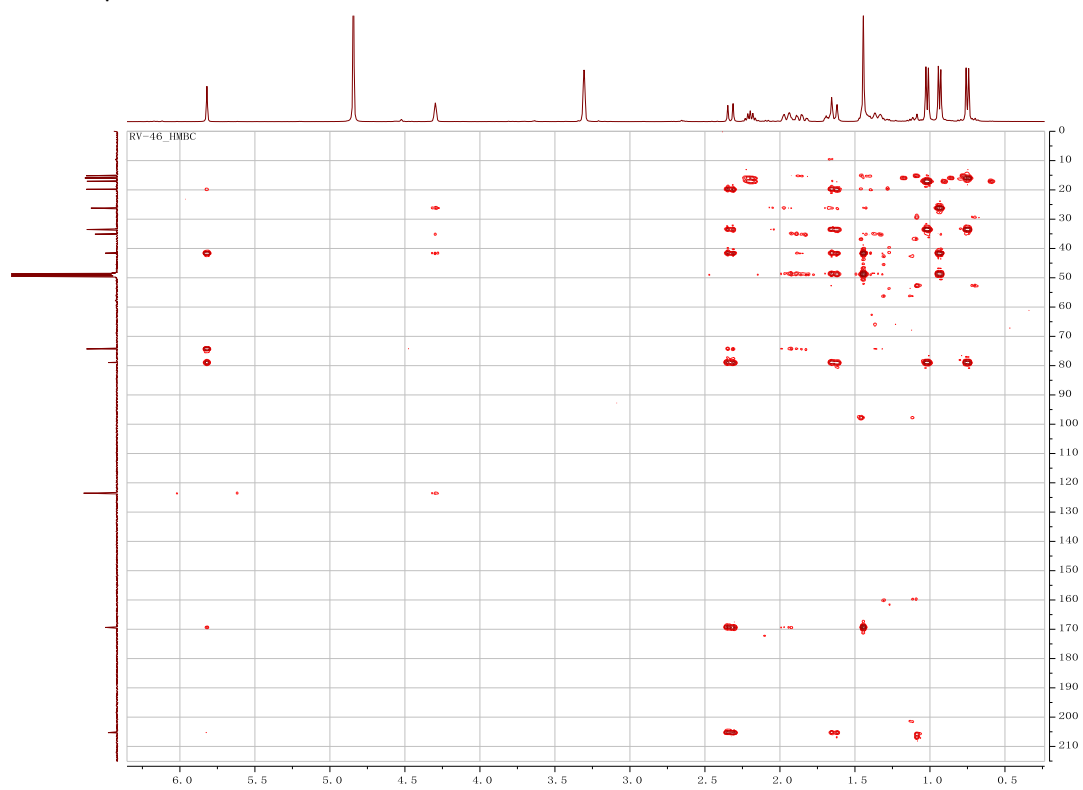
^1H NMR spectrum of **5**



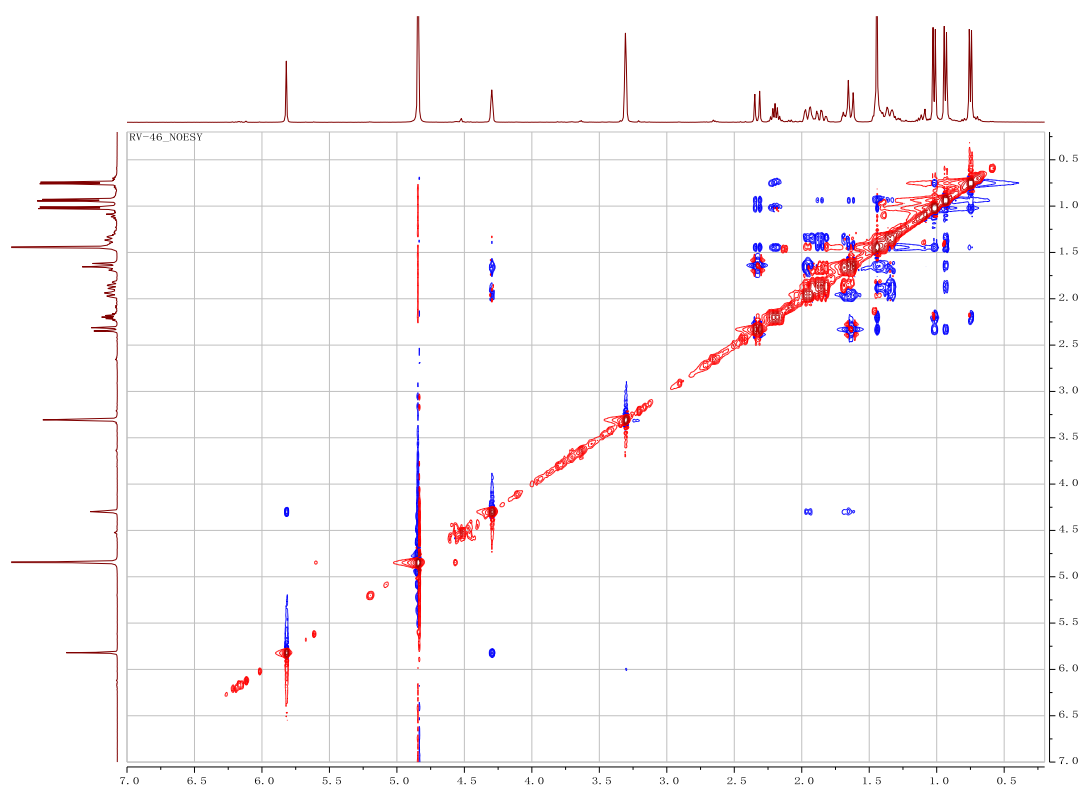
^{13}C NMR spectrum of **5**



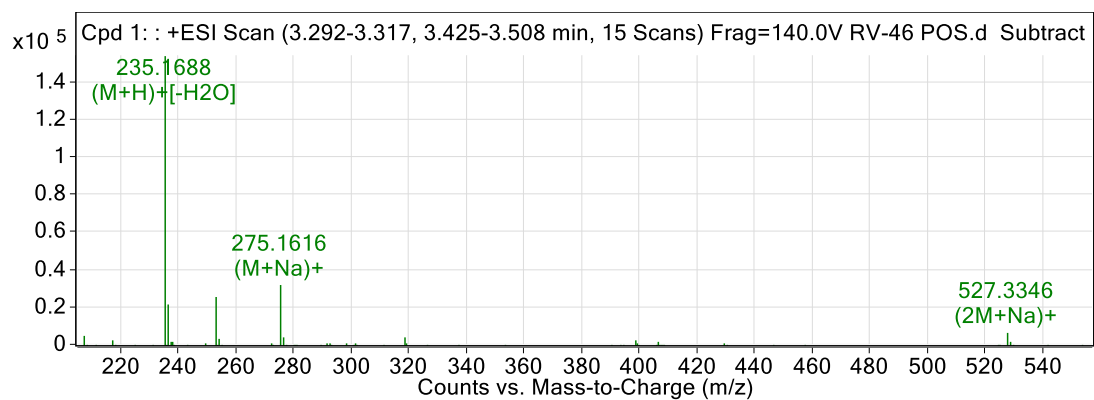
HMQC spectrum of **5**



HMBC spectrum of **5**



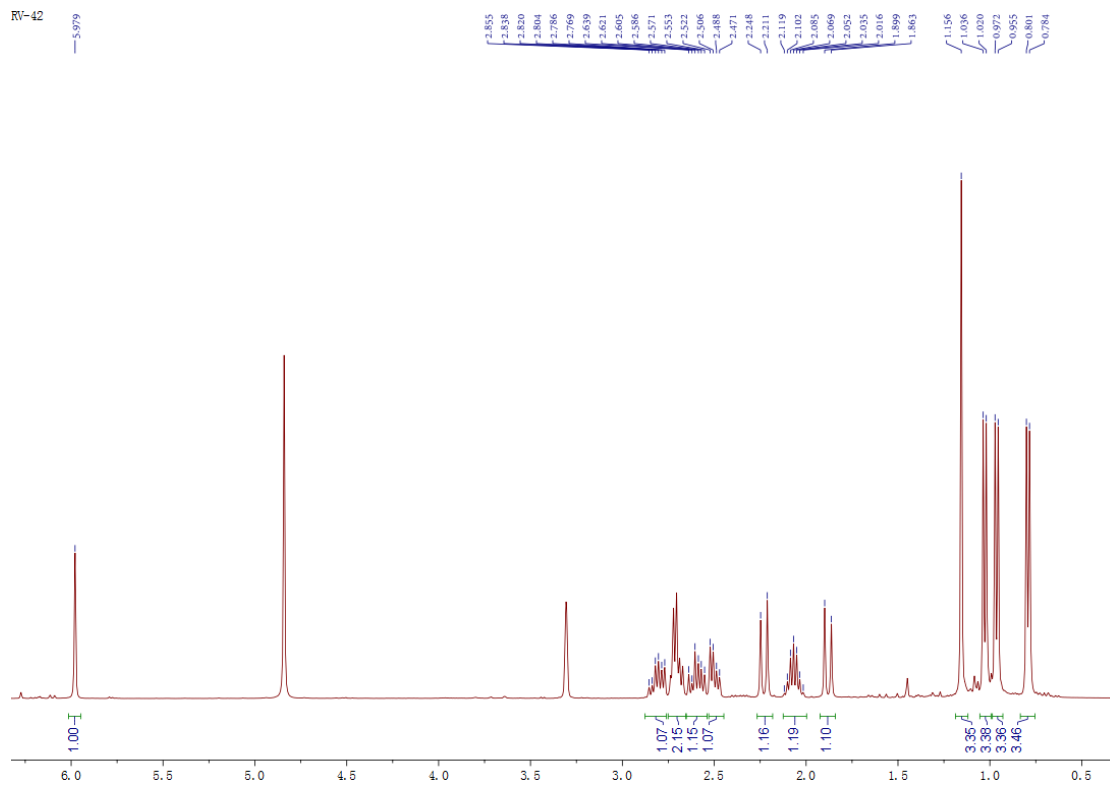
NOESY spectrum of **5**



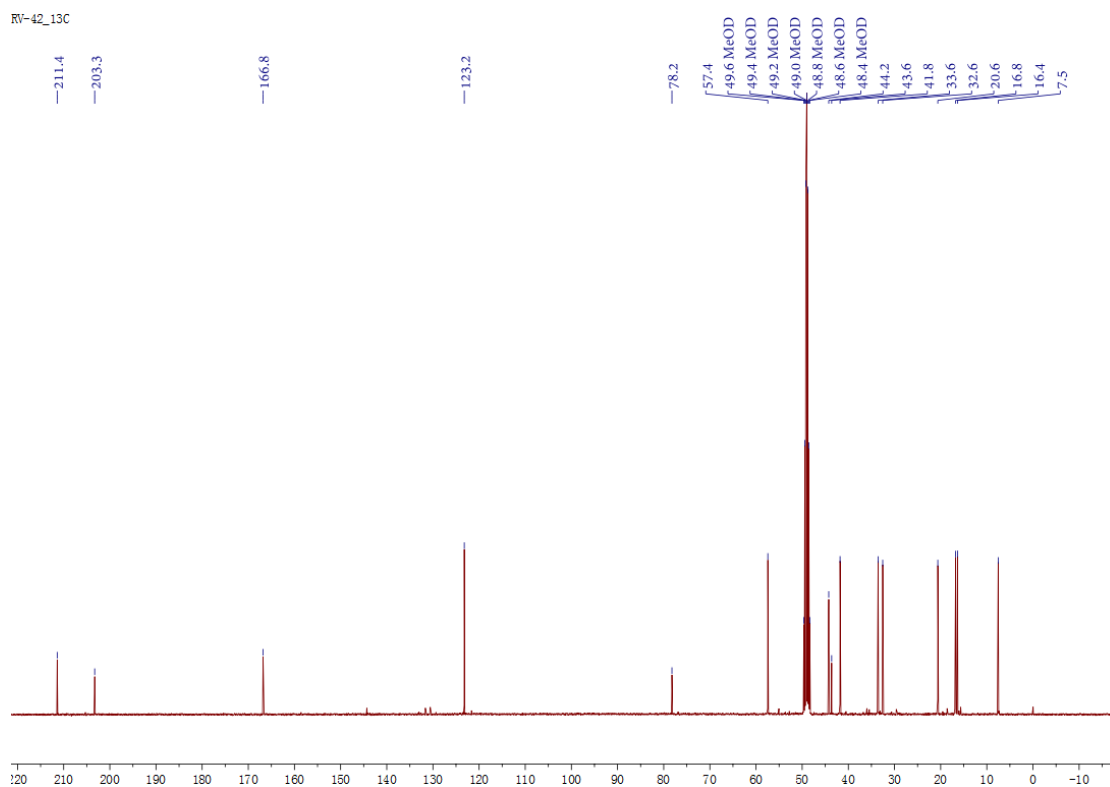
<i>m/z</i>	<i>Calc m/z</i>	Diff(ppm)	<i>z</i>	Abund	Formula	Ion
235.1688	235.1693	-2.02	1	153907.2	C ₁₅ H ₂₃ O ₂	(M+H) ⁺ [-H ₂ O]
253.1798	253.1798	-0.08	1	25897.4	C ₁₅ H ₂₅ O ₃	(M+H) ⁺
275.1616	275.1618	-0.76	1	32605.2	C ₁₅ H ₂₄ NaO ₃	(M+Na) ⁺
527.3346	527.3343	0.47	1	7395.4	C ₃₀ H ₄₈ NaO ₆	(2M+Na) ⁺

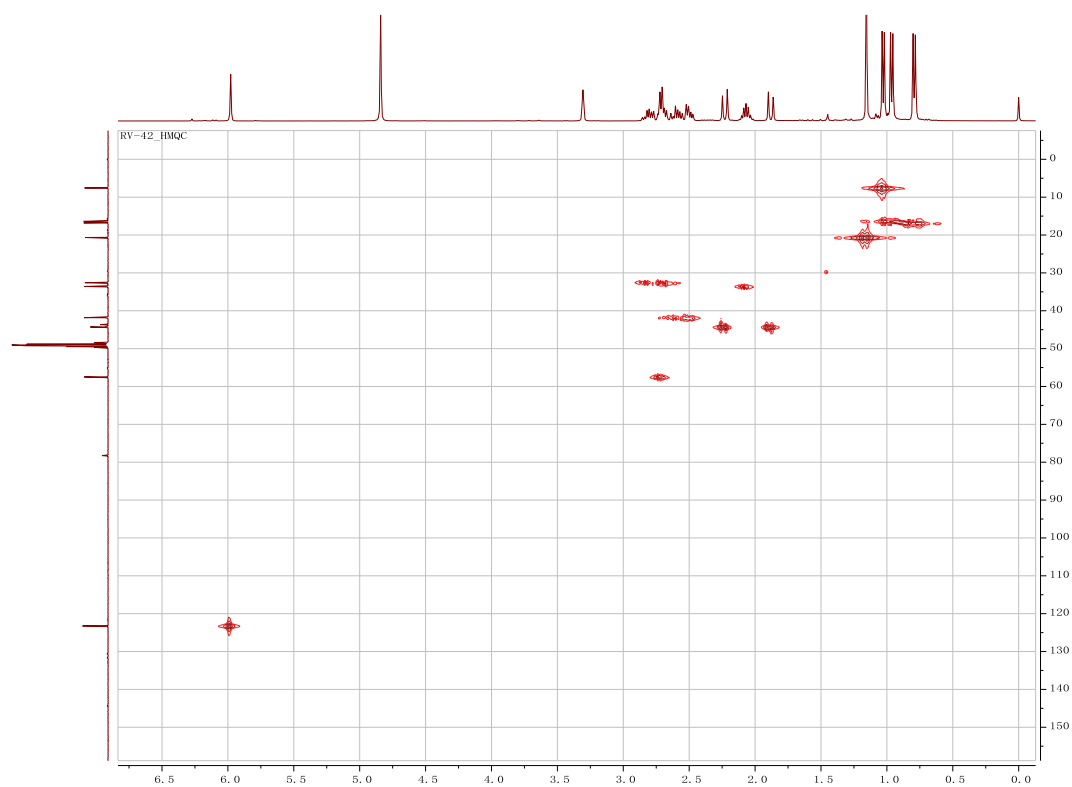
HRESIMS spectrum of **5**

RV-42

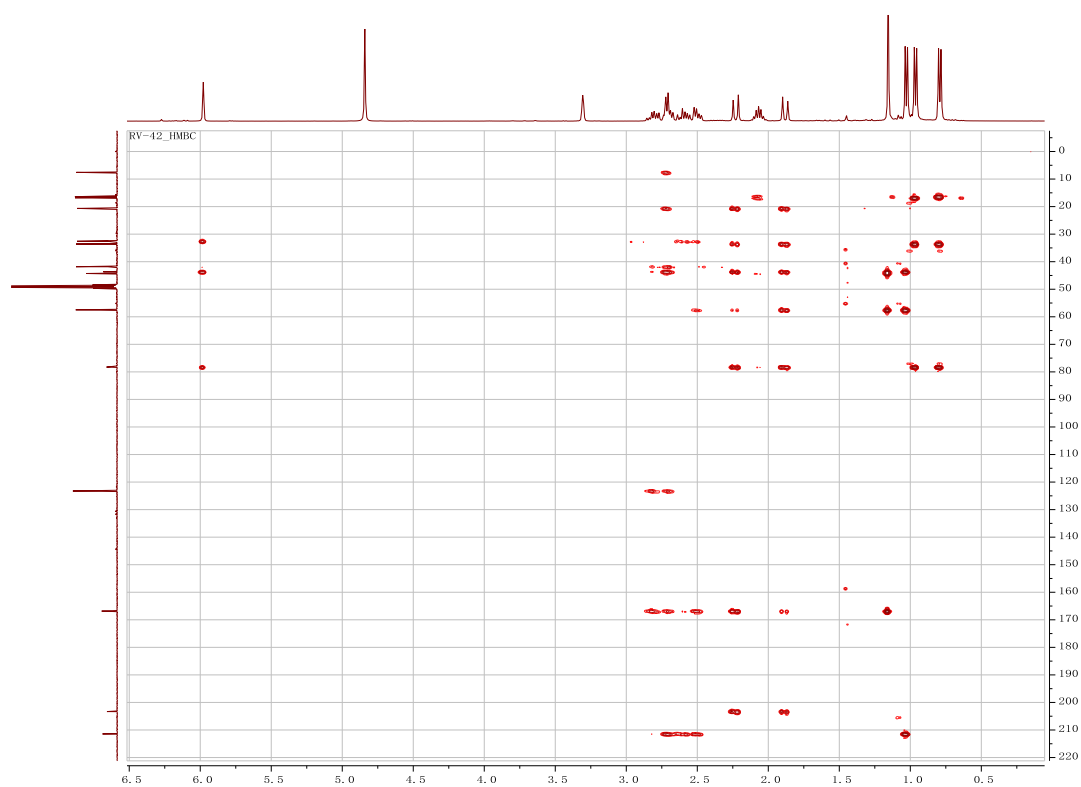
¹H NMR spectrum of **6**

RV-42_13C

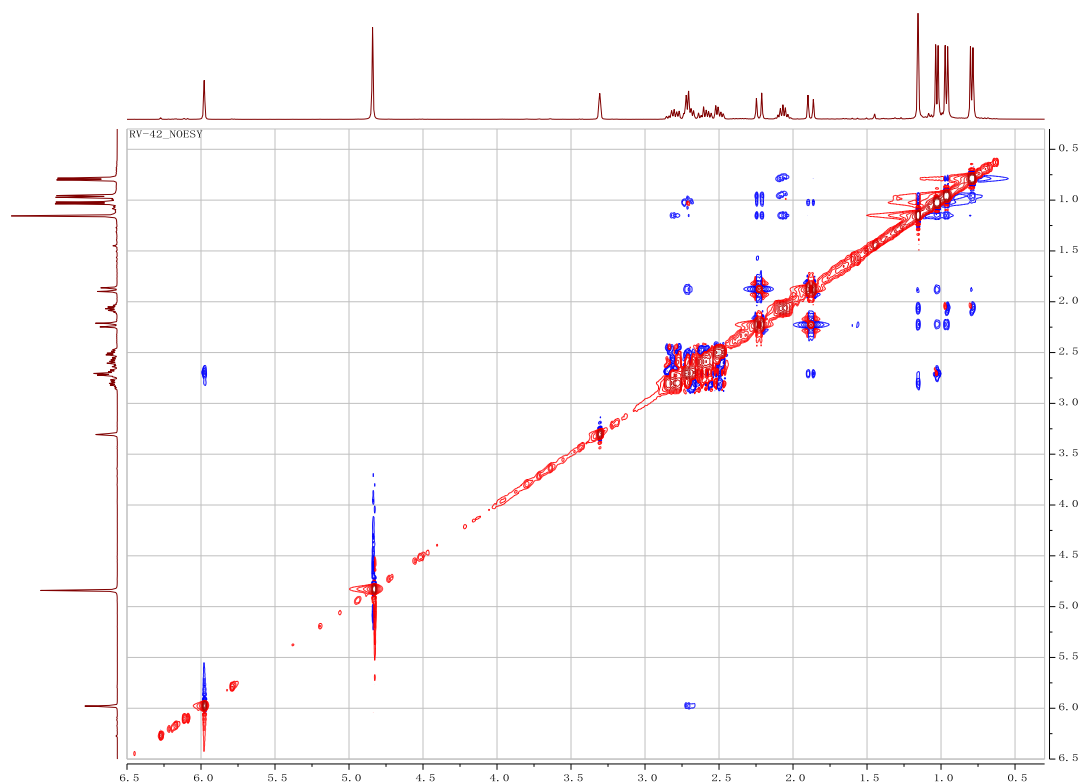
¹³C NMR spectrum of **6**



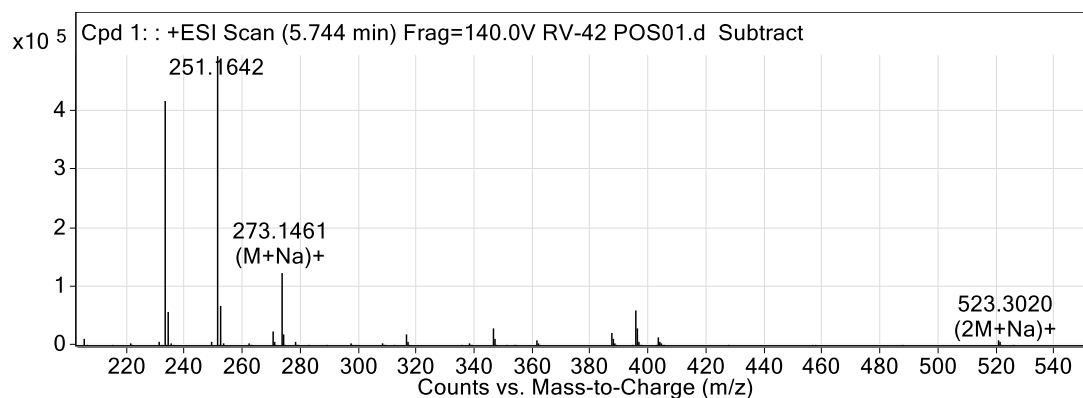
HMQC of **6**



HMBC spectrum of **6**

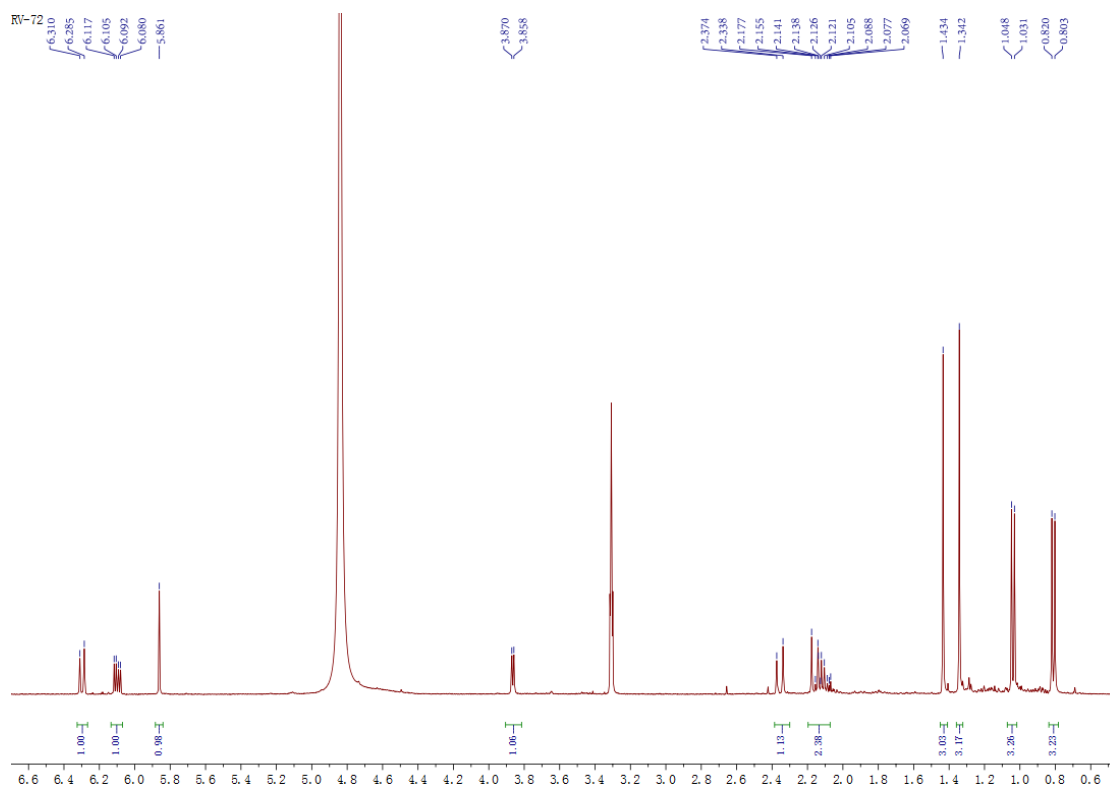


NOESY spectrum of **6**

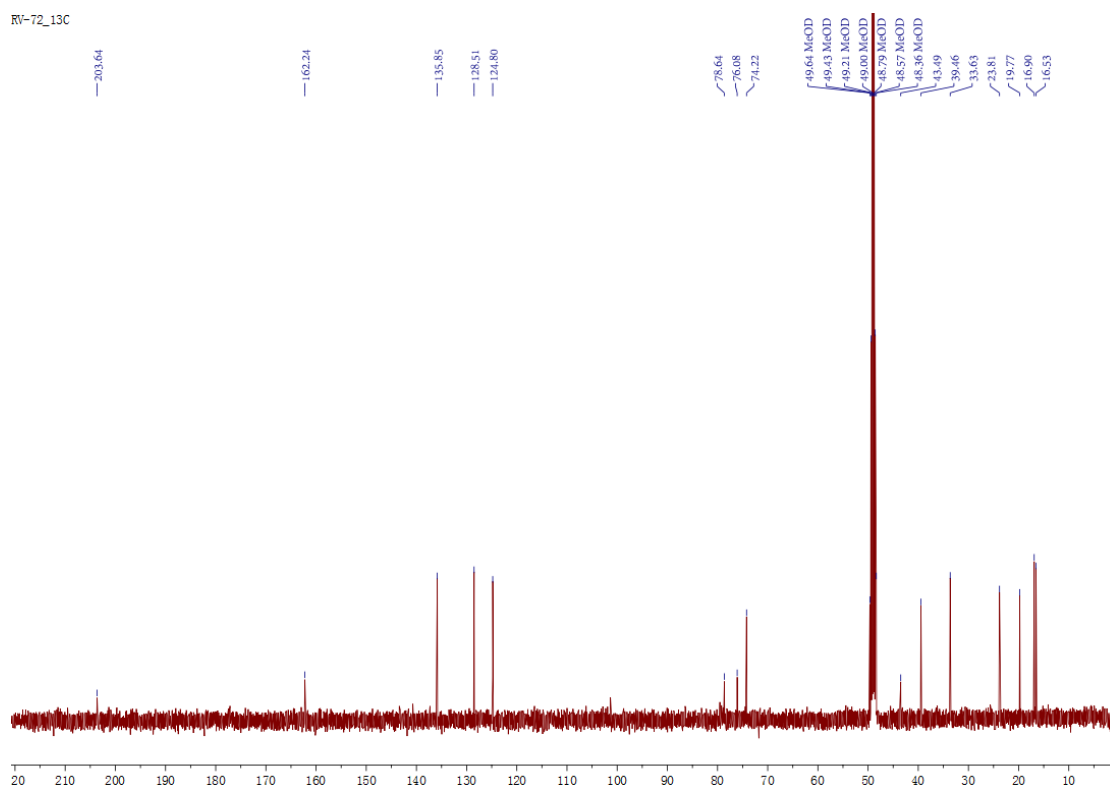


<i>m/z</i>	<i>Calc m/z</i>	Diff(ppm)	<i>Z</i>	Abund	Formula	Ion
233.1535	233.1536	-0.58	1	419769.5	C ₁₅ H ₂₁ O ₂	(M+H) ⁺ [-H ₂ O]
251.1642	251.1642	0.06		495166.2	C ₁₅ H ₂₃ O ₃	(M+H) ⁺
273.1461	273.1461	-0.19	1	125710.6	C ₁₅ H ₂₂ NaO ₃	(M+Na) ⁺
523.3020	523.3030	-1.94	1	695.4	C ₃₀ H ₄₄ NaO ₆	(2M+Na) ⁺

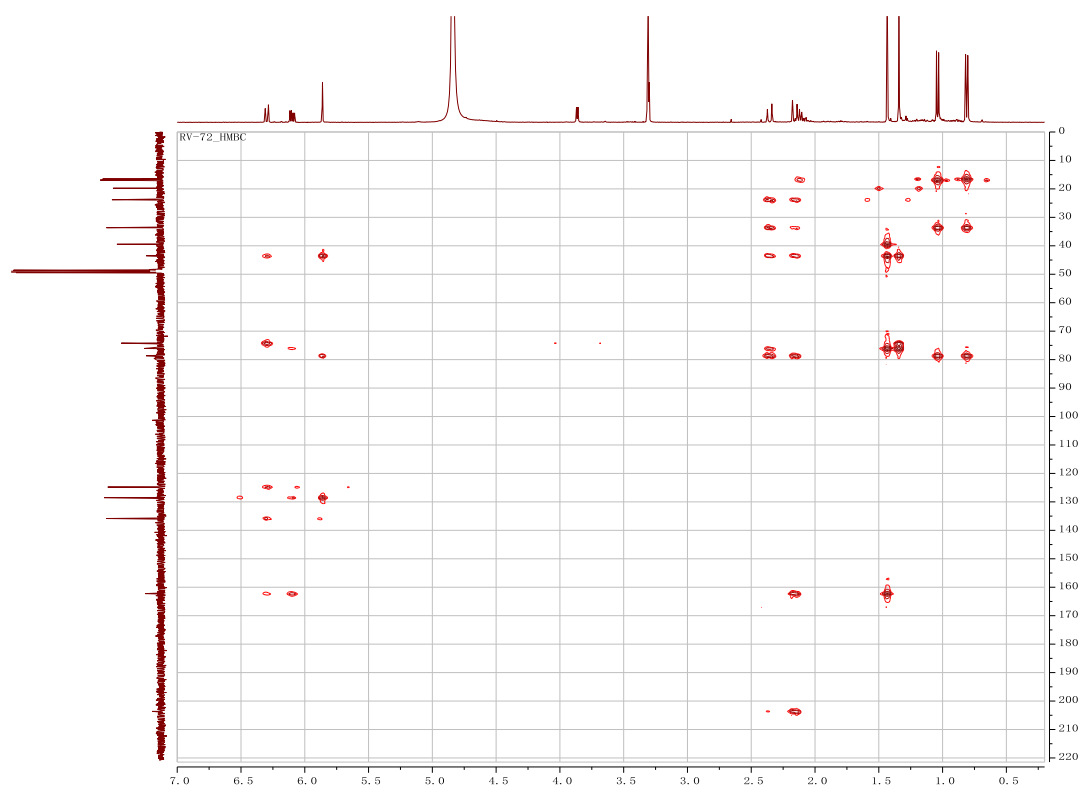
HRESIMS spectrum of **6**



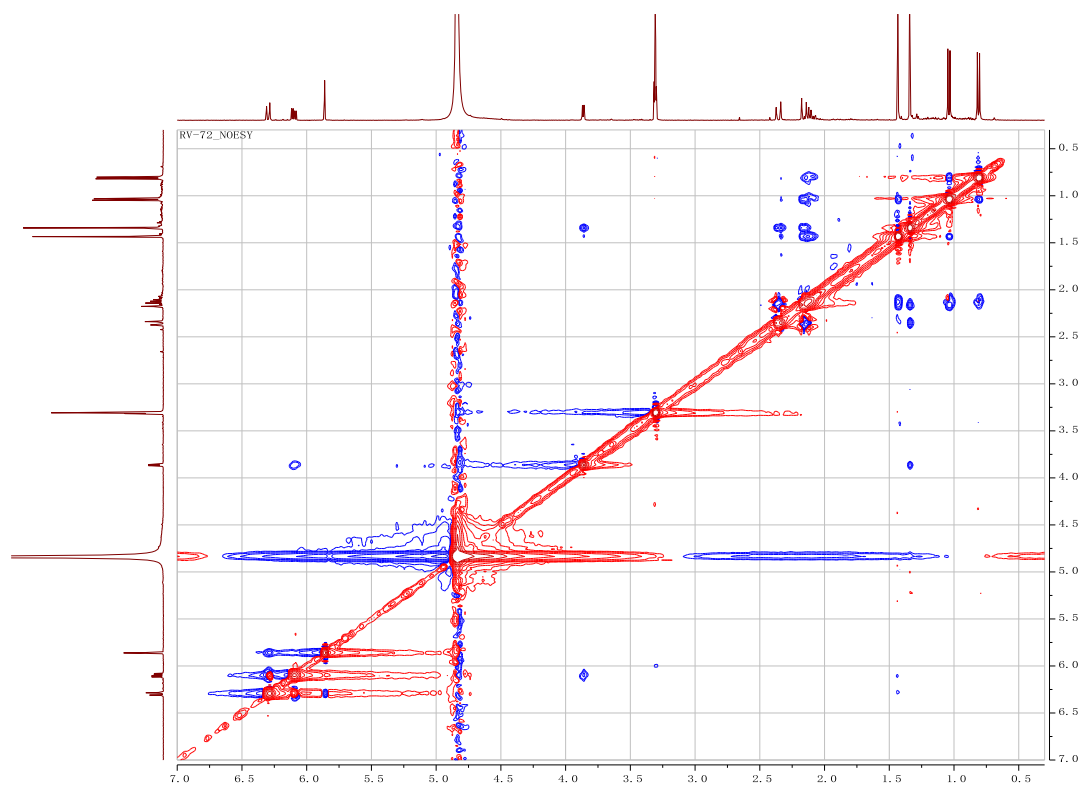
^1H NMR spectrum of **7**



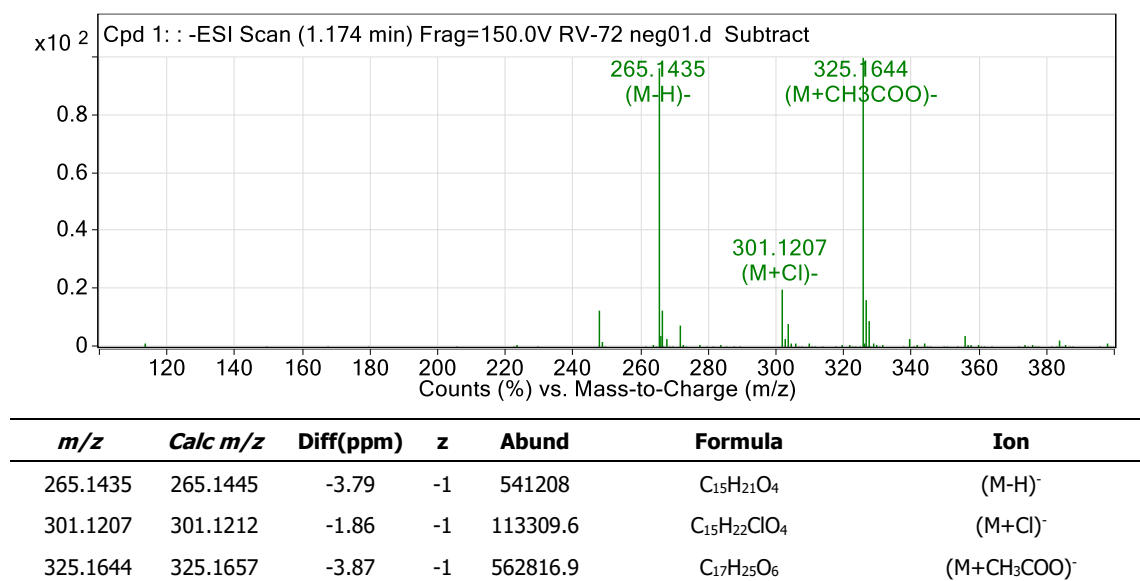
^{13}C NMR spectrum of **7**



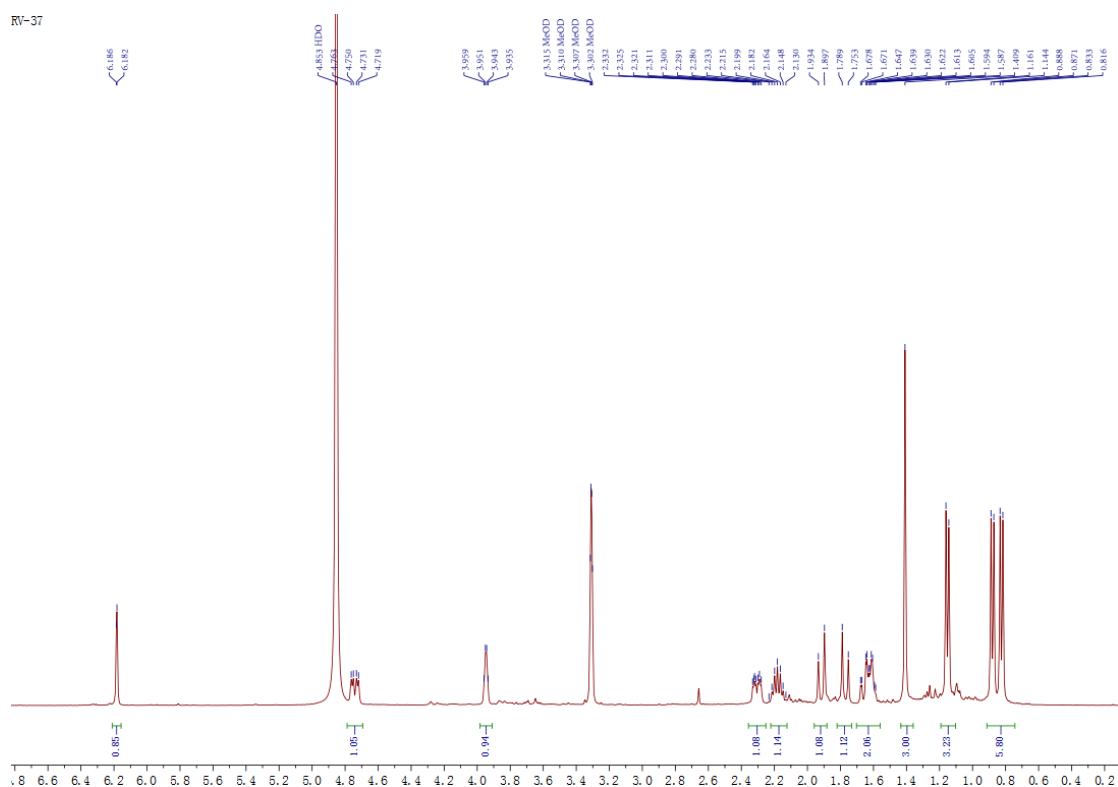
HMBC spectrum of **7**



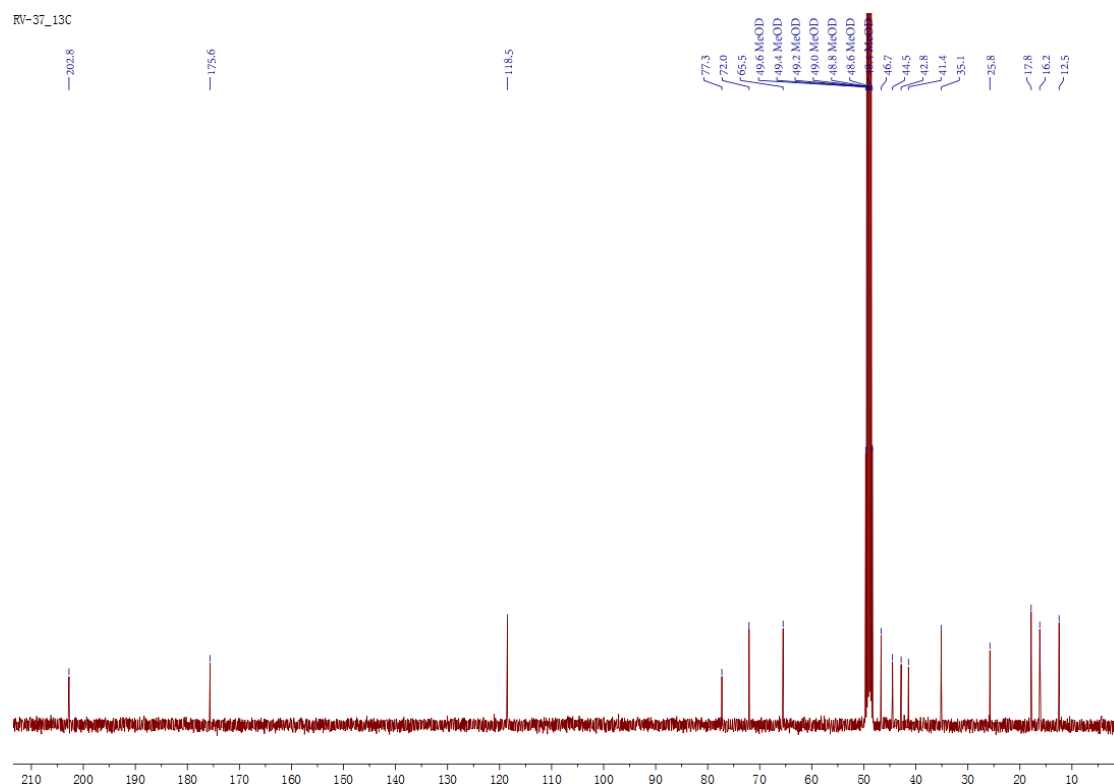
NOESY spectrum of **7**



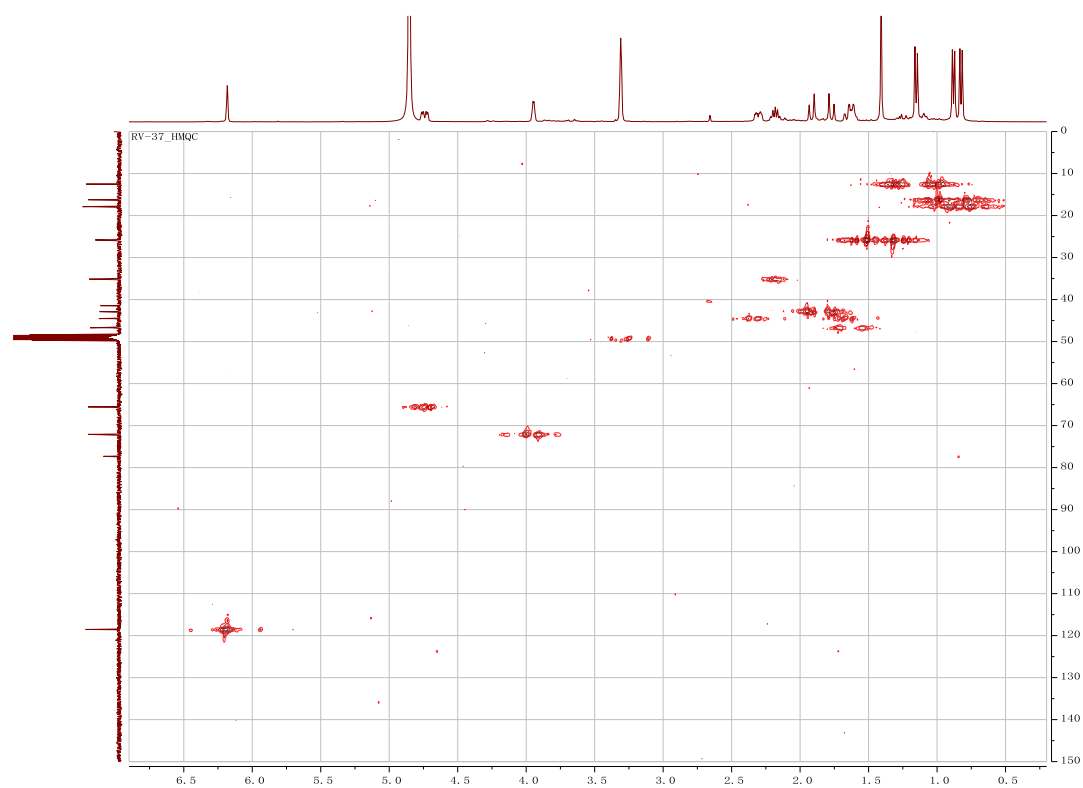
HRESIMS spectrum of **7**



¹H NMR spectrum of **8**



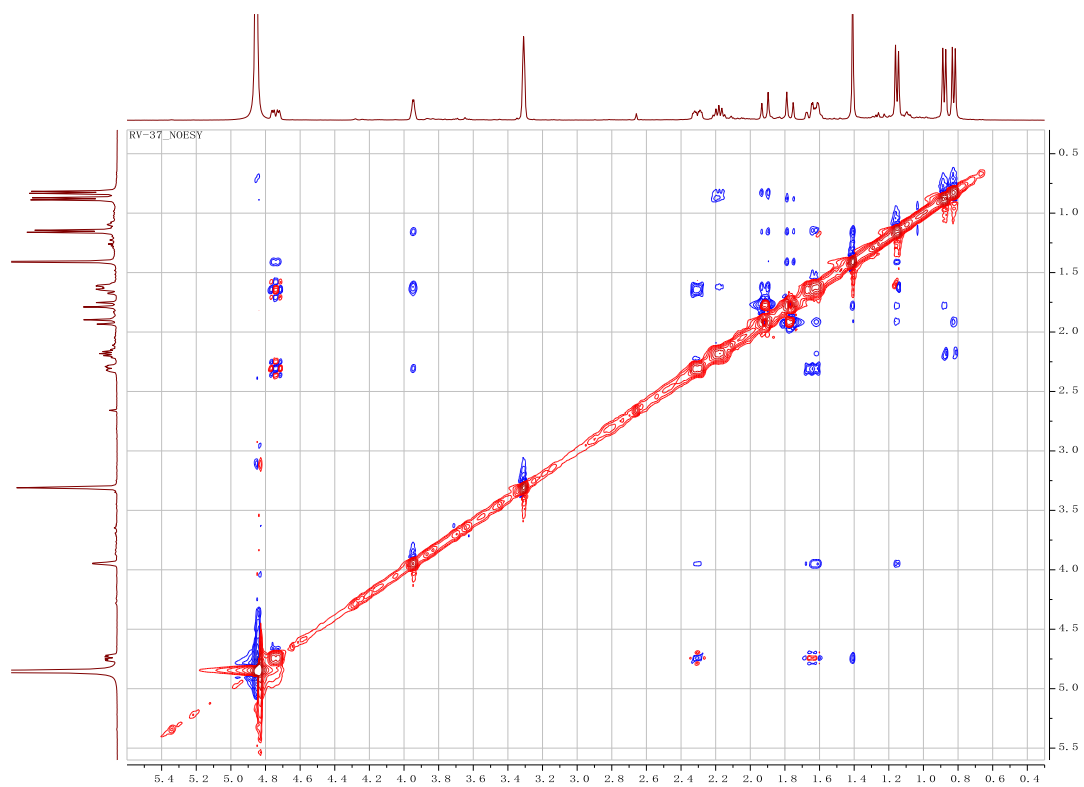
^{13}C NMR spectrum of **8**



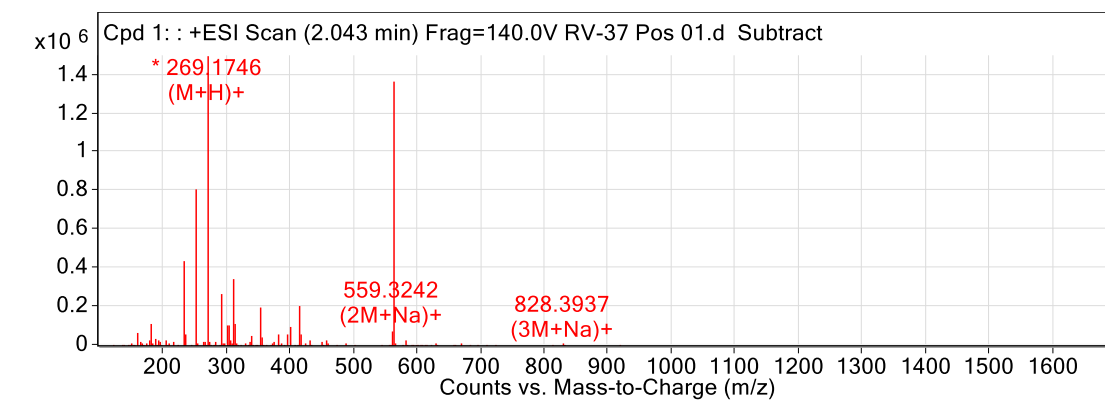
HMQC spectrum of **8**



HMBC spectrum of **8**

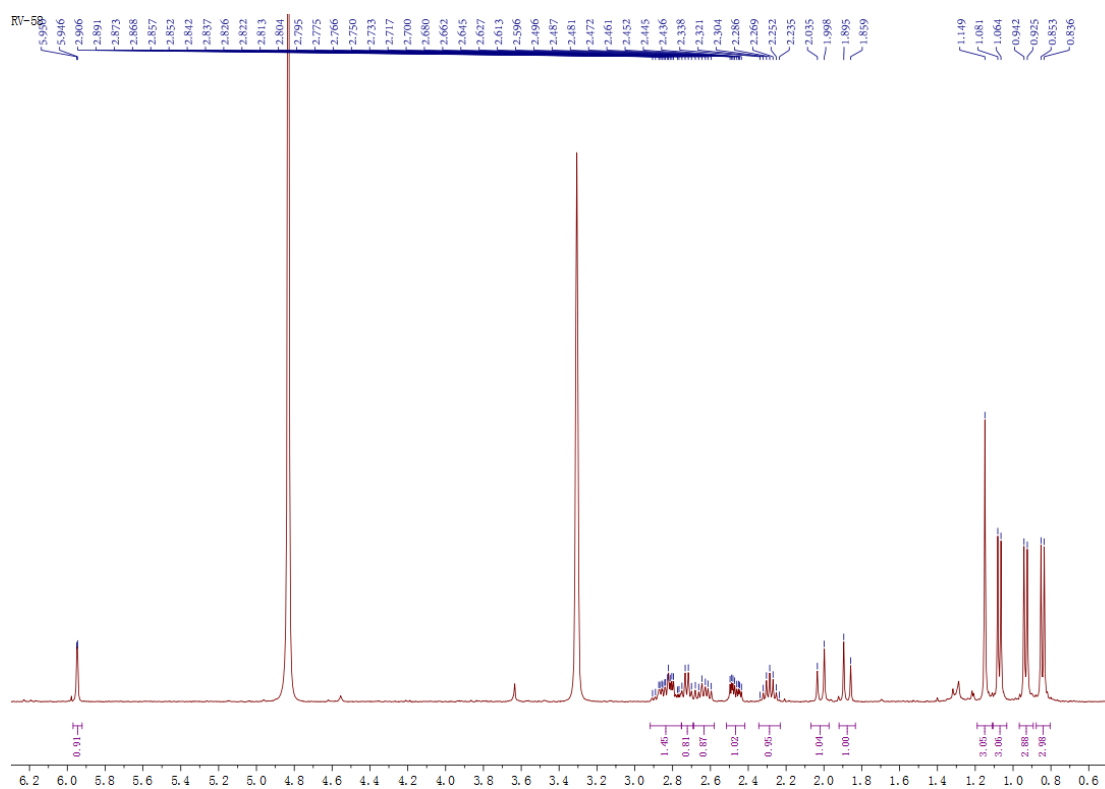


NOESY spectrum of **8**



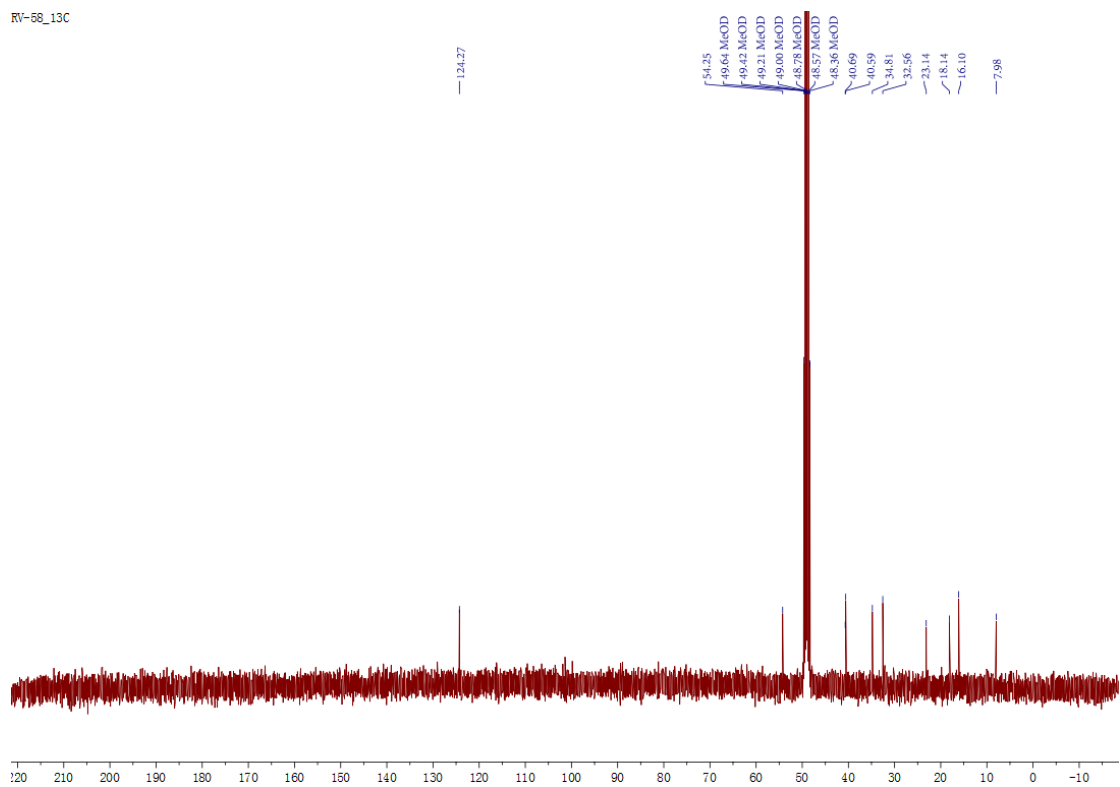
<i>m/z</i>	<i>Calc m/z</i>	Diff(ppm)	<i>z</i>	Abund	Formula	Ion
269.1746	269.1747	-0.57		1497296	C ₁₅ H ₂₅ O ₄	(M+H) ⁺
291.1563	291.1567	-1.24	1	269051.4	C ₁₅ H ₂₄ NaO ₄	(M+Na) ⁺
559.3242	559.3241	0.07	1	74474.2	C ₃₀ H ₄₈ NaO ₈	(2M+Na) ⁺

HRESIMS spectrum of **8**

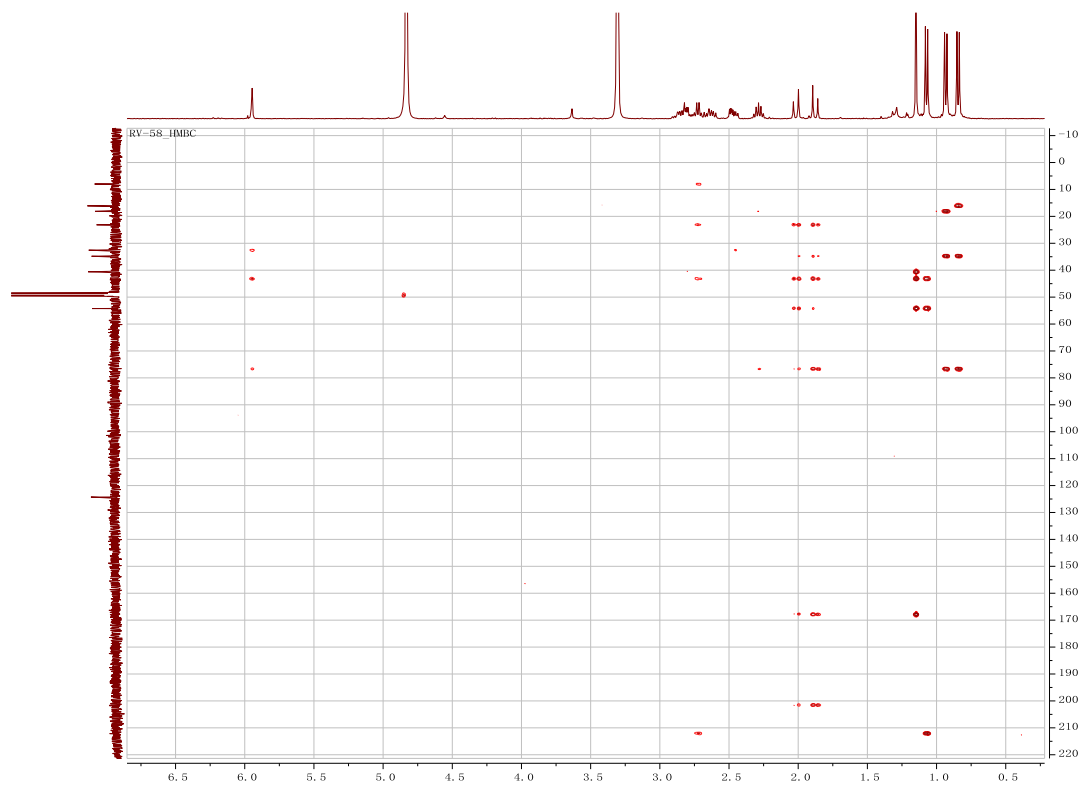


¹H NMR spectrum of **9**

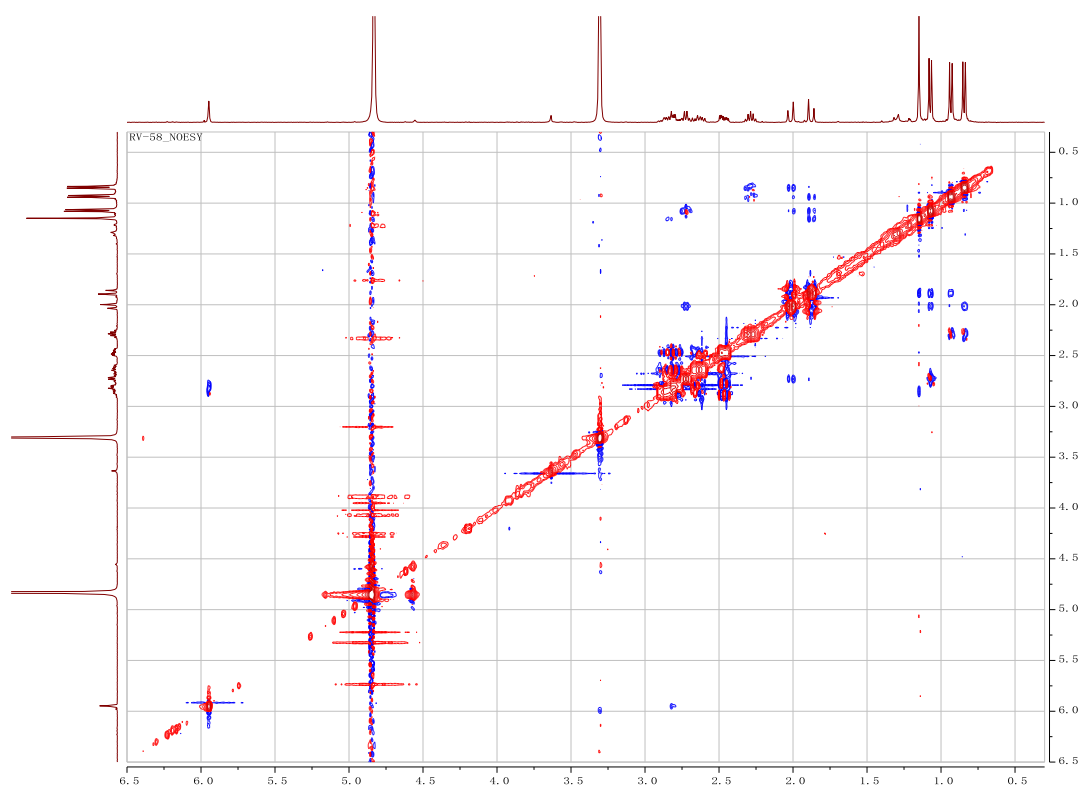
RV-58_13C



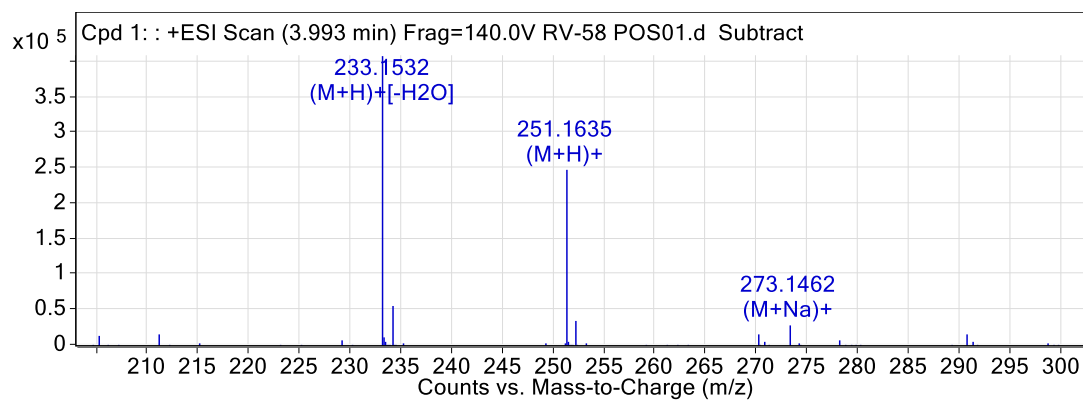
^{13}C NMR spectrum of **9**



HMBC spectrum of **9**

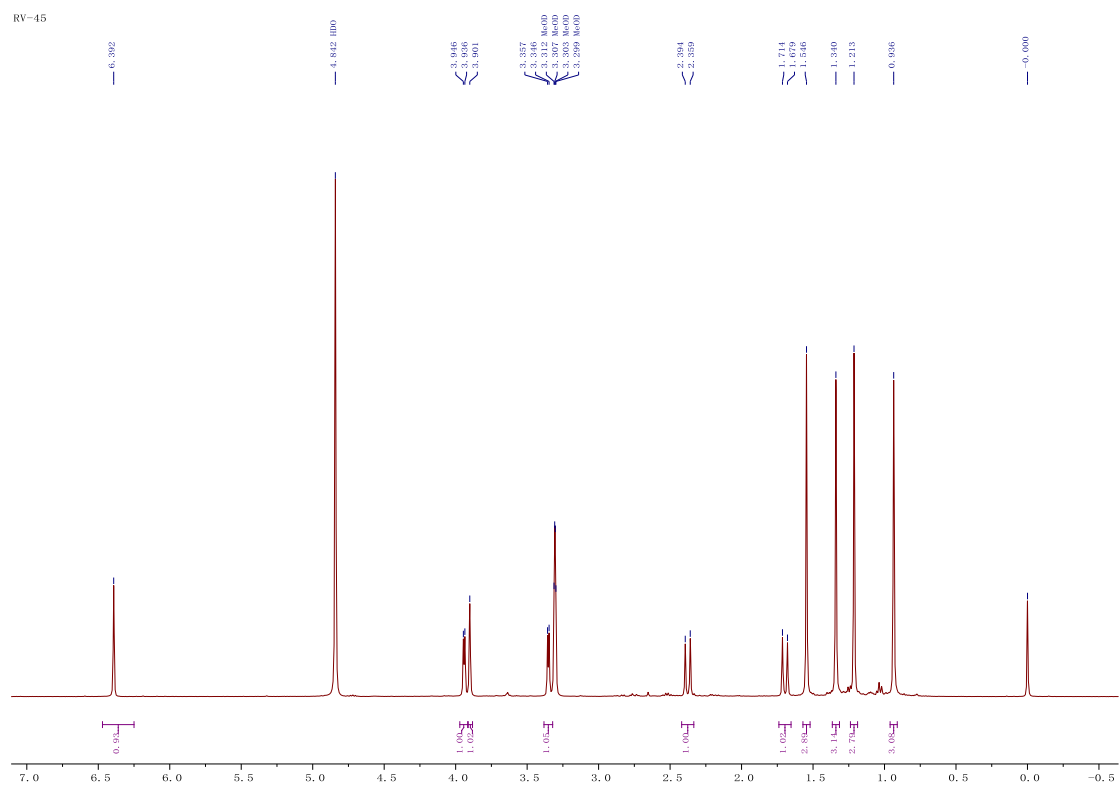


NOESY spectrum of **9**

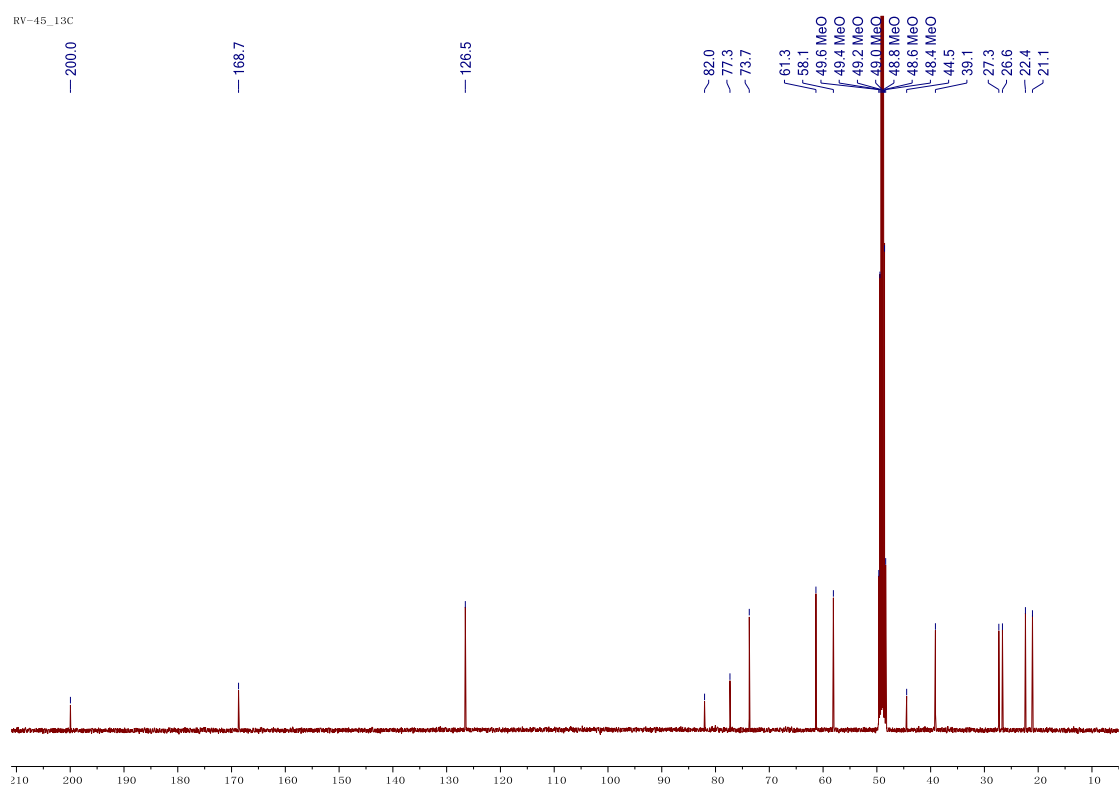


<i>m/z</i>	<i>Calc m/z</i>	Diff(ppm)	<i>z</i>	Abund	Formula	Ion
233.1532	233.1536	-1.89	1	408255.1	C ₁₅ H ₂₁ O ₂	(M+H) ⁺ [-H ₂ O]
251.1635	251.1642	-2.65	1	247640.1	C ₁₅ H ₂₃ O ₃	(M+H) ⁺
273.1462	273.1461	0.25	1	28448.9	C ₁₅ H ₂₂ NaO ₃	(M+Na) ⁺

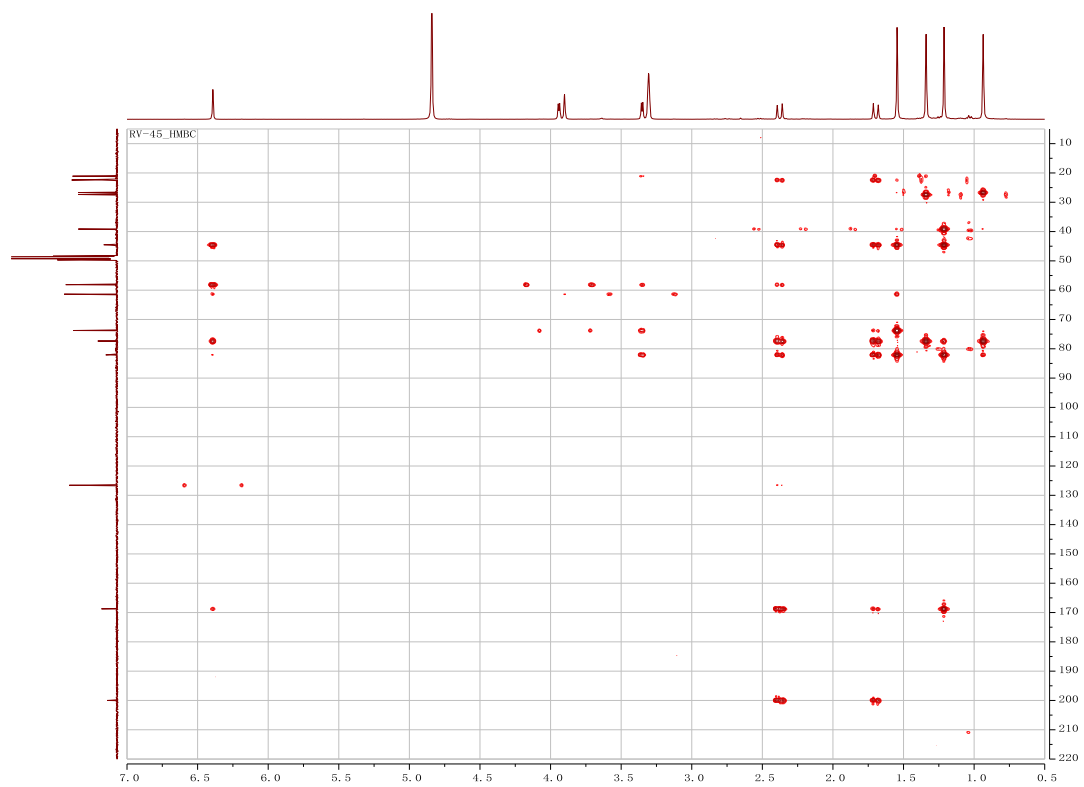
HRESIMS spectrum of **9**



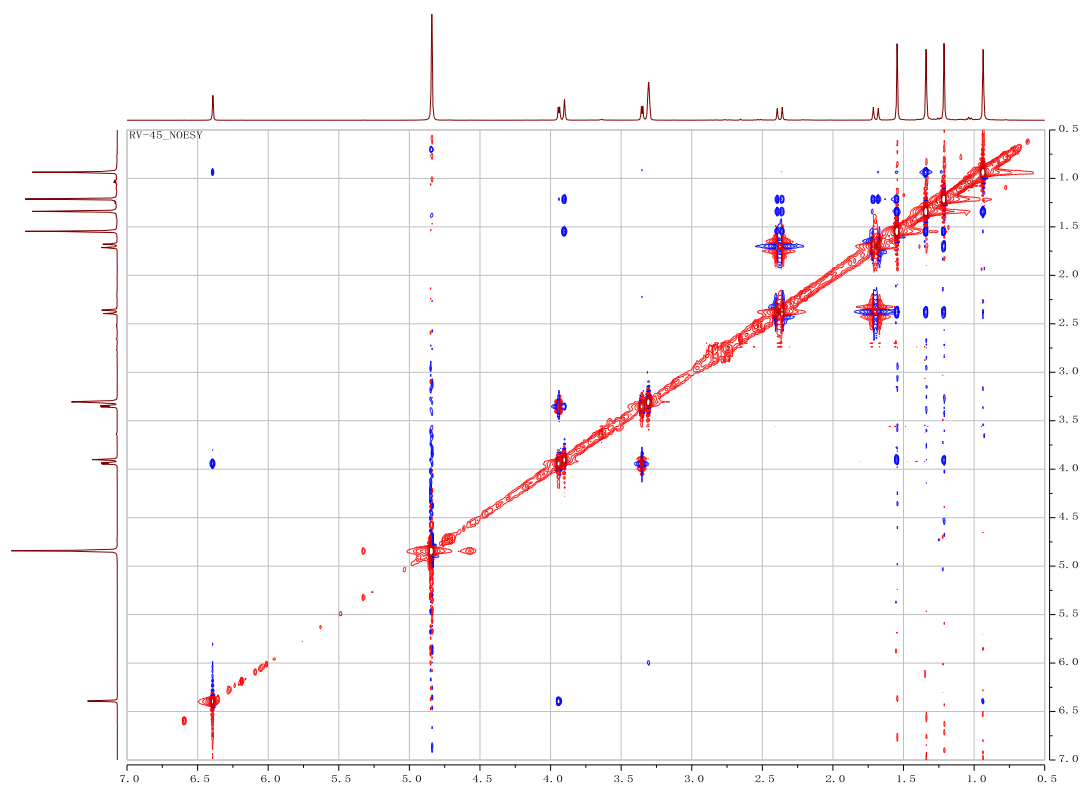
¹H NMR spectrum of **10**



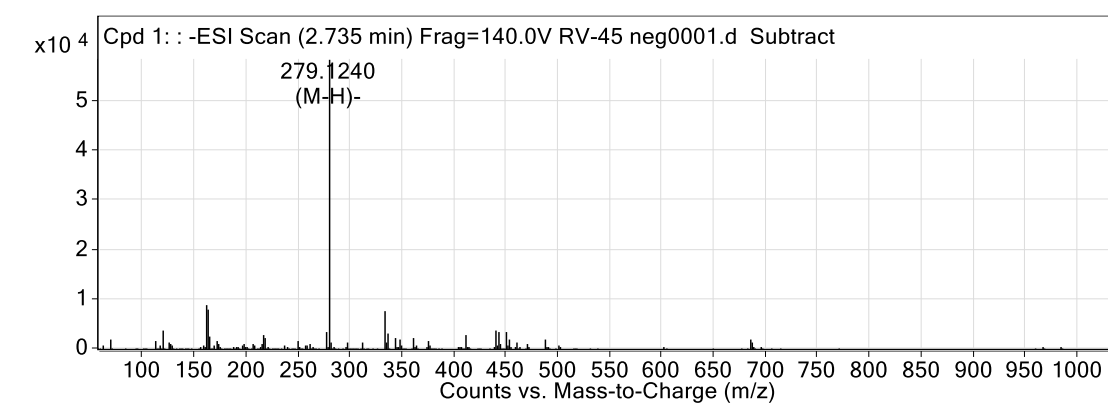
¹³C NMR spectrum of **10**



HMBC spectrum of **10**

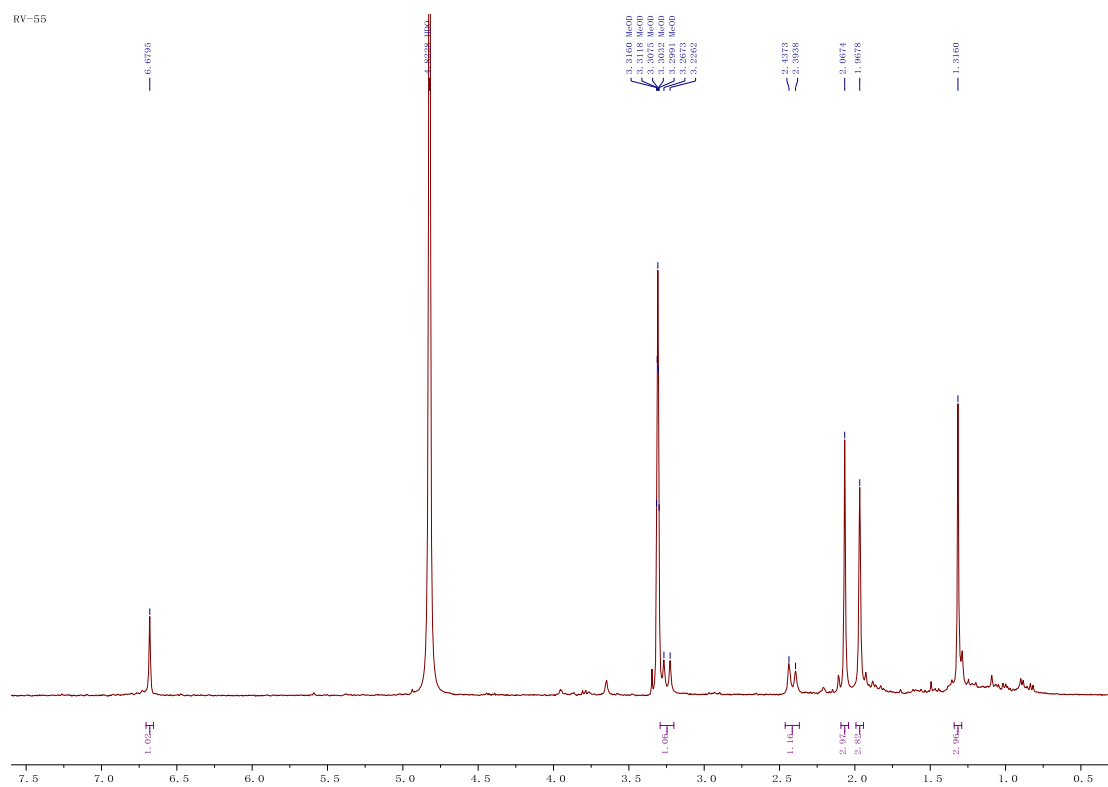


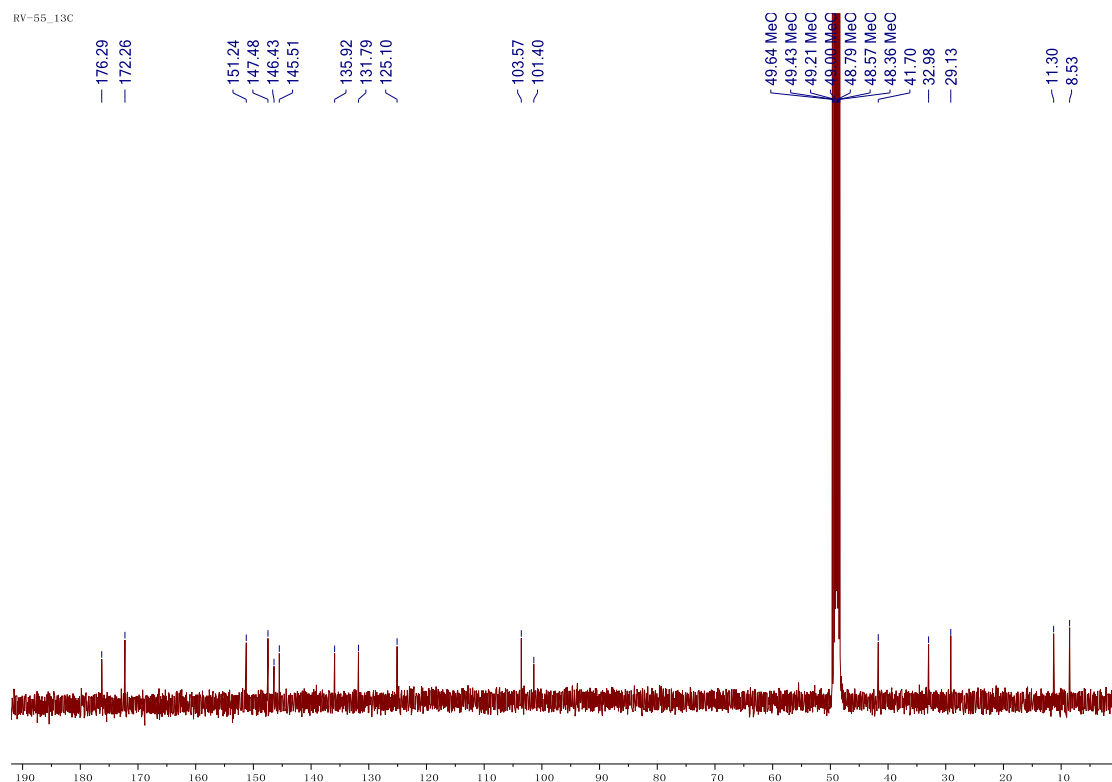
NOESY spectrum of **10**



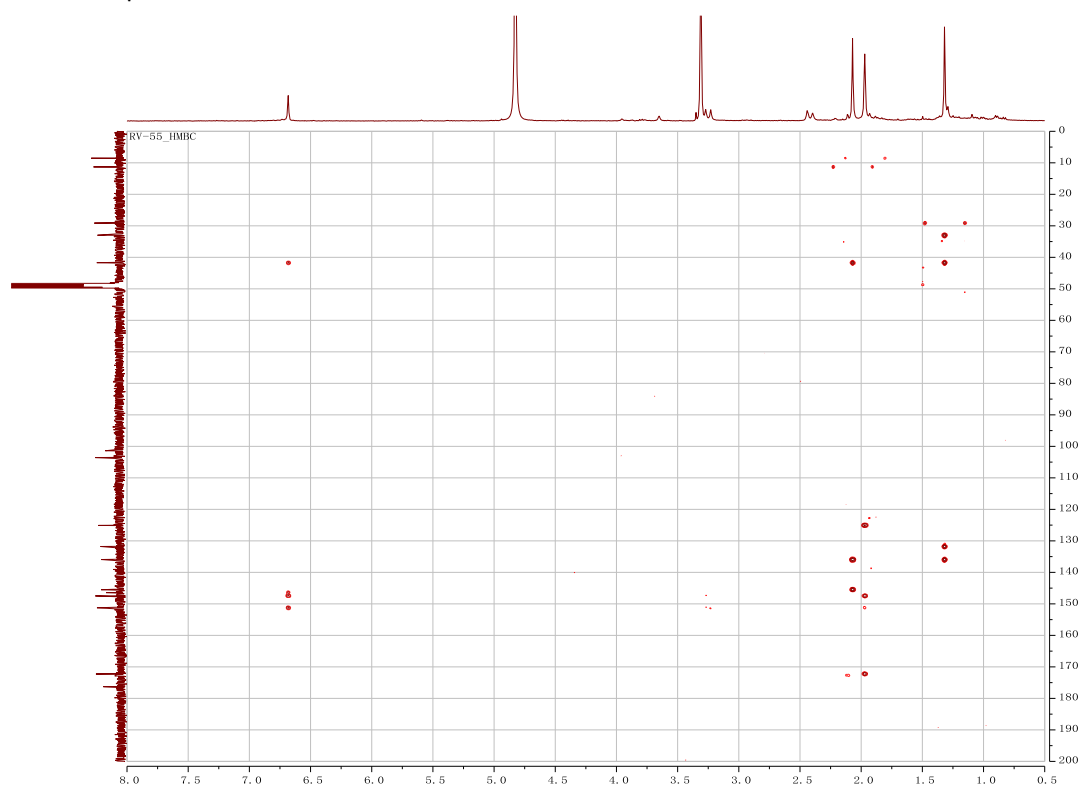
<i>m/z</i>	<i>Calc m/z</i>	Diff(ppm)	<i>z</i>	Abund	Formula	Ion
279.124	279.1238	0.72	-1	58422	C ₁₅ H ₁₉ O ₅	(M-H) ⁻

HRESIMS spectrum of **10**

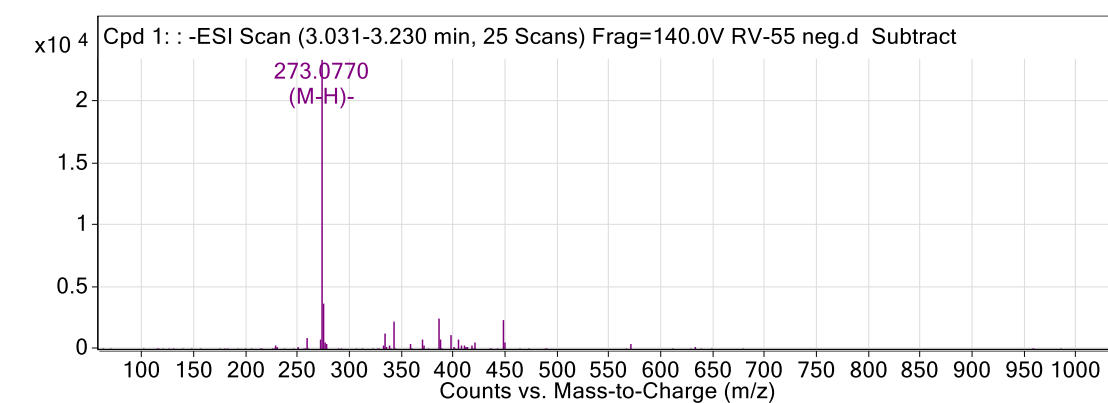




^{13}C NMR spectrum of **11**

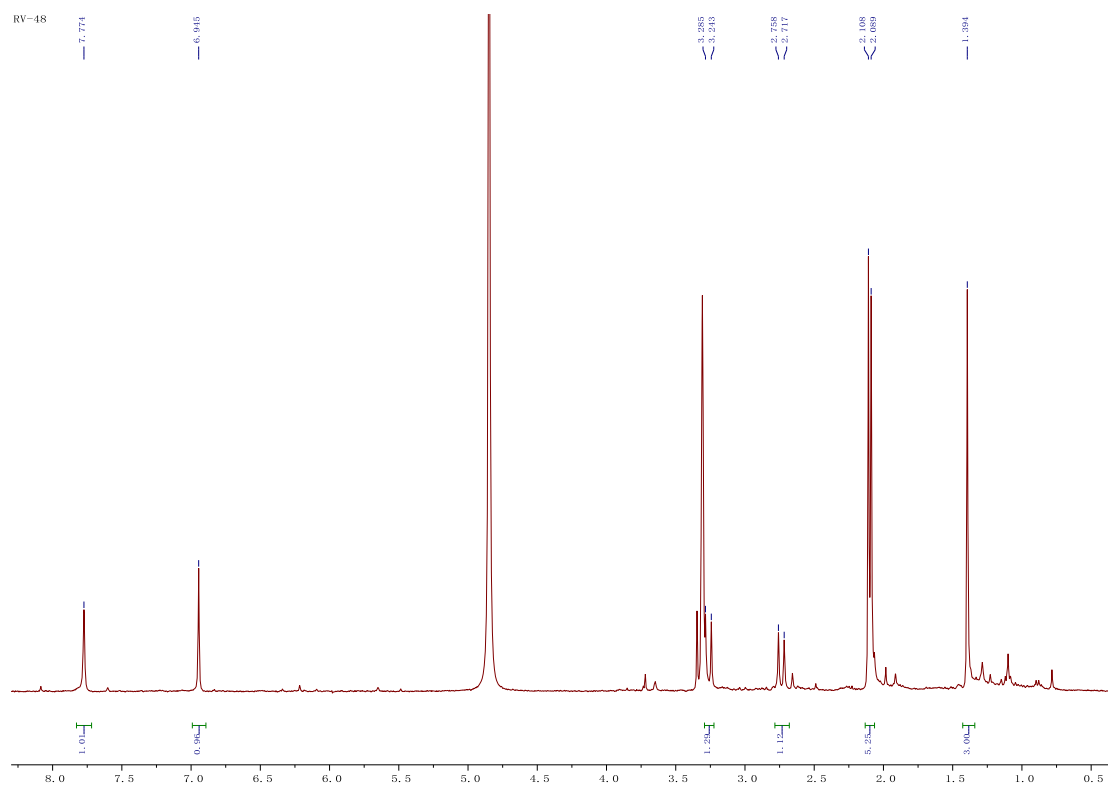


HMBC spectrum of **11**

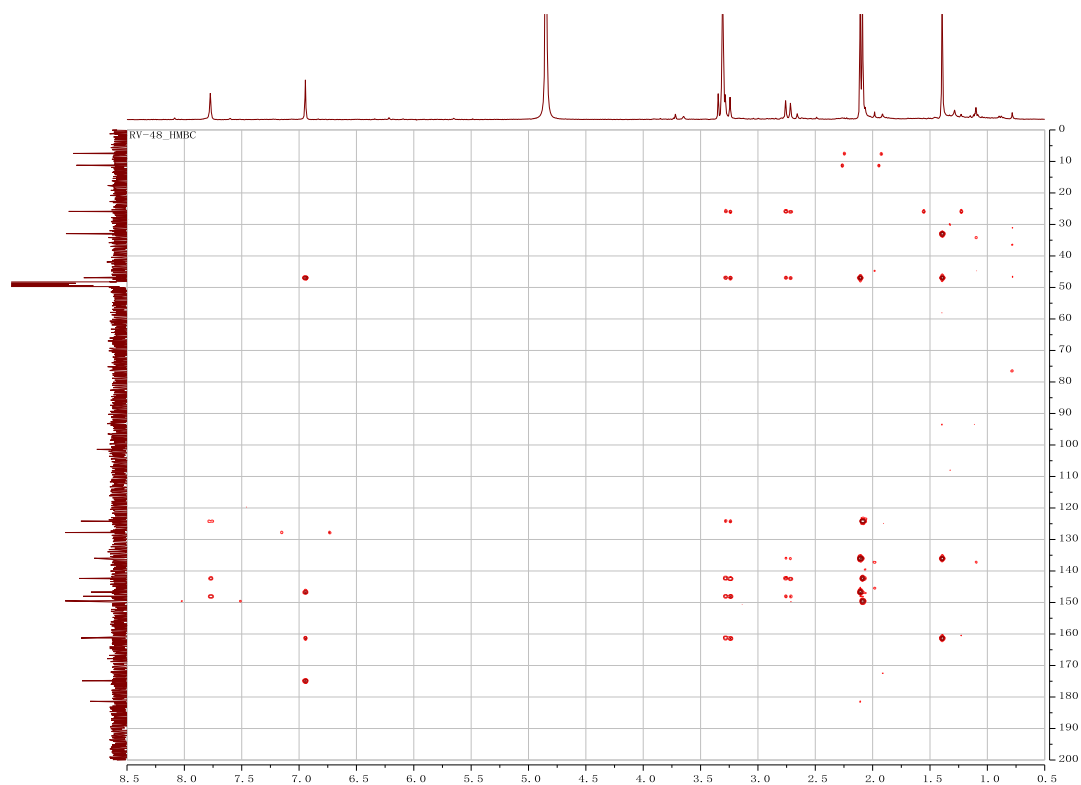
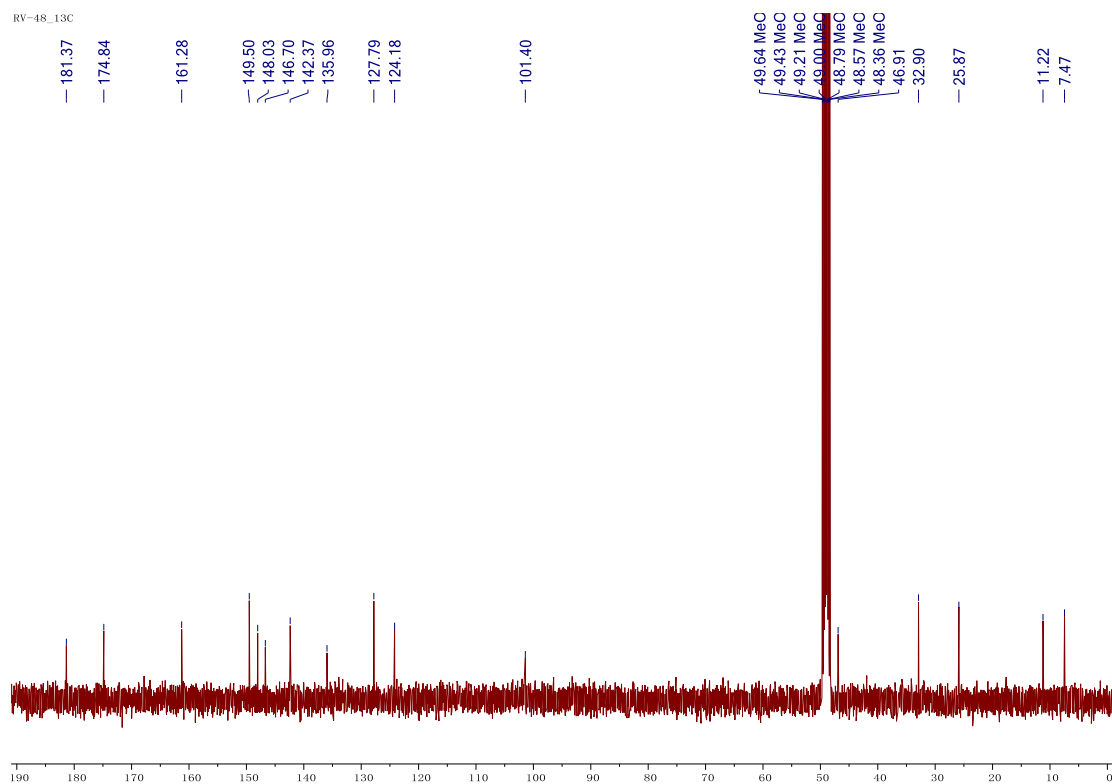


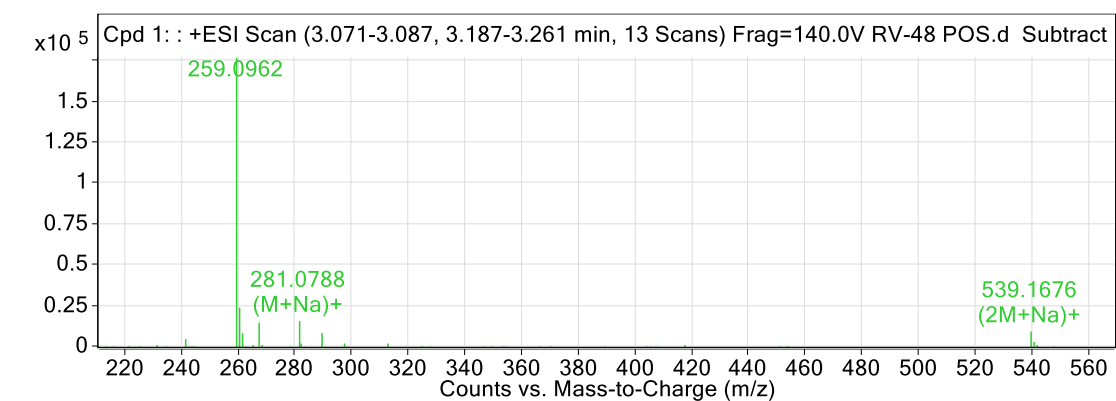
<i>m/z</i>	<i>Calc m/z</i>	Diff(ppm)	<i>z</i>	Abund	Formula	Ion
273.0770	273.0768	0.43	-1	23393	C ₁₅ H ₁₃ O ₅	(M-H) ⁻

HRESIMS spectrum of **11**



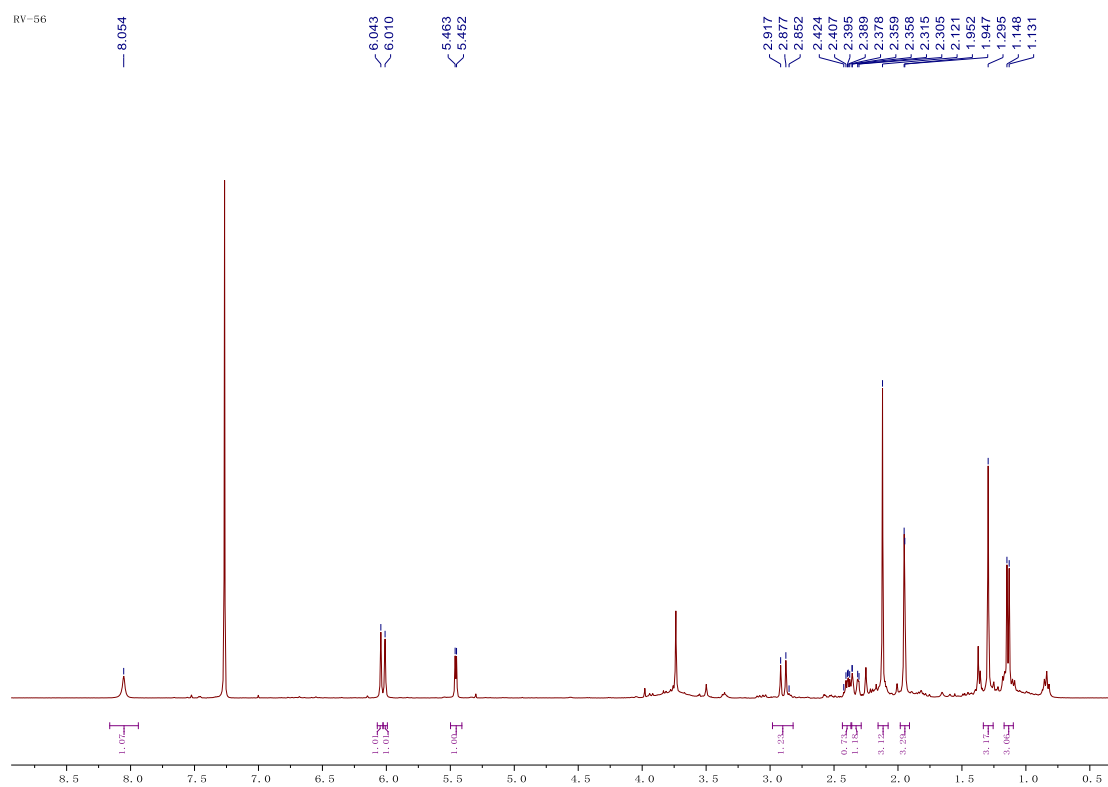
¹H NMR spectrum of **12**



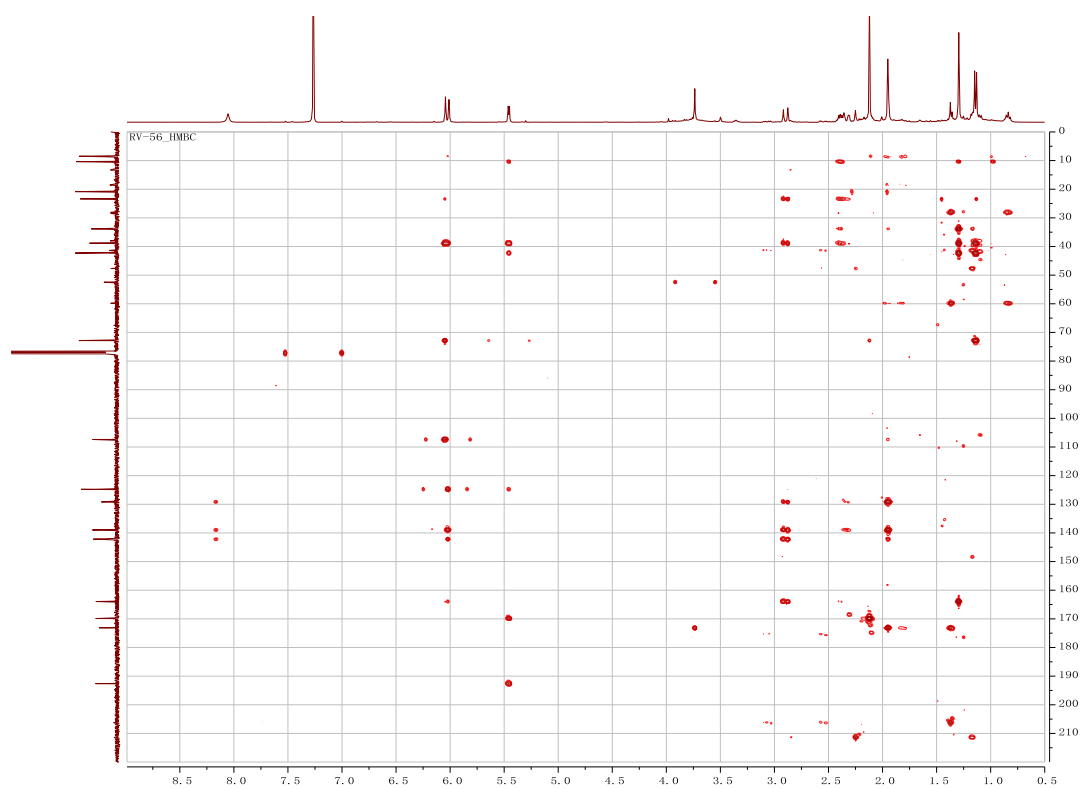
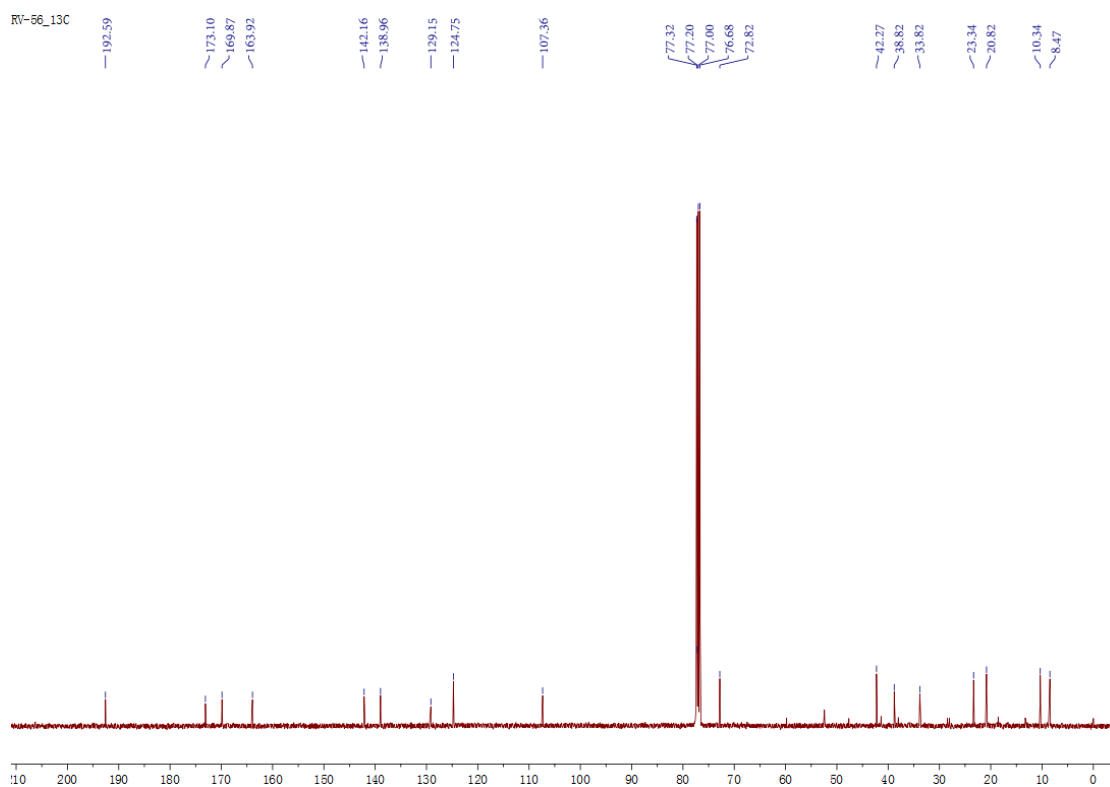


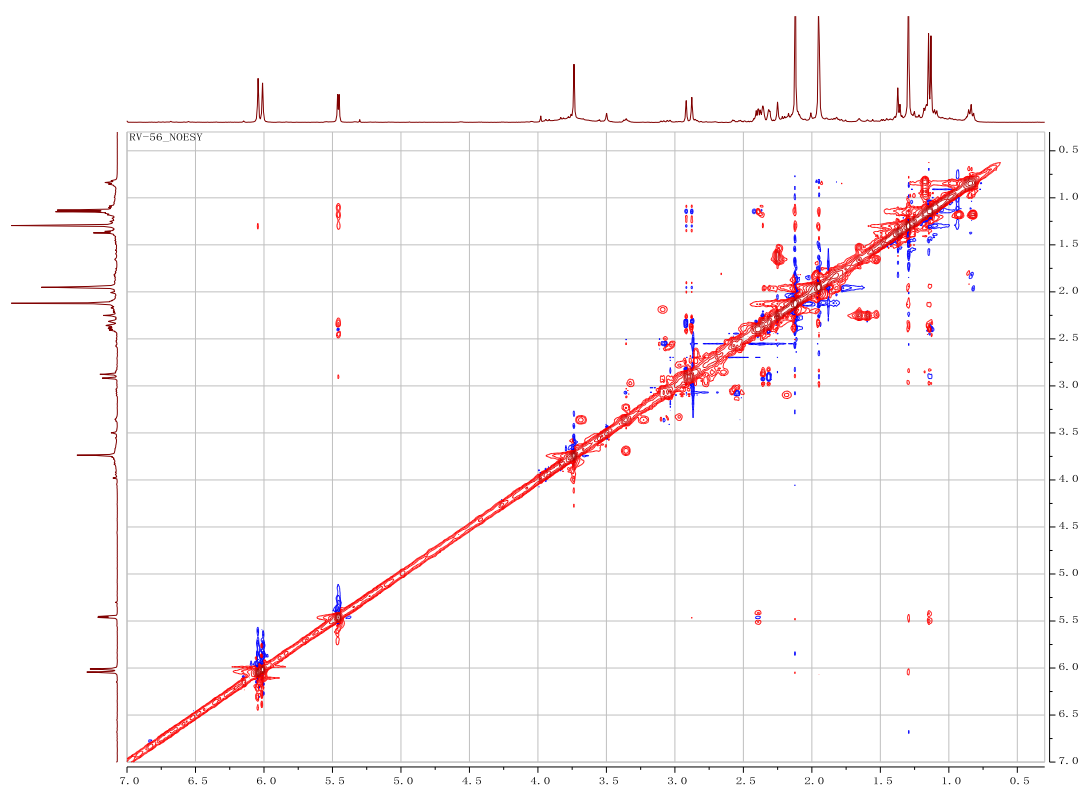
<i>m/z</i>	<i>Calc m/z</i>	Diff(ppm)	<i>z</i>	Abund	Formula	Ion
259.0962	259.0965	-1.21	1	176911.6	C ₁₅ H ₁₅ O ₄	(M+H) ⁺
281.0788	281.0784	1.41	1	16374.6	C ₁₅ H ₁₄ NaO ₄	(M+Na) ⁺
539.1676	539.1676	-0.13	1	10018.4	C ₃₀ H ₂₈ NaO ₈	(2M+Na) ⁺

HRESIMS spectrum of **12**

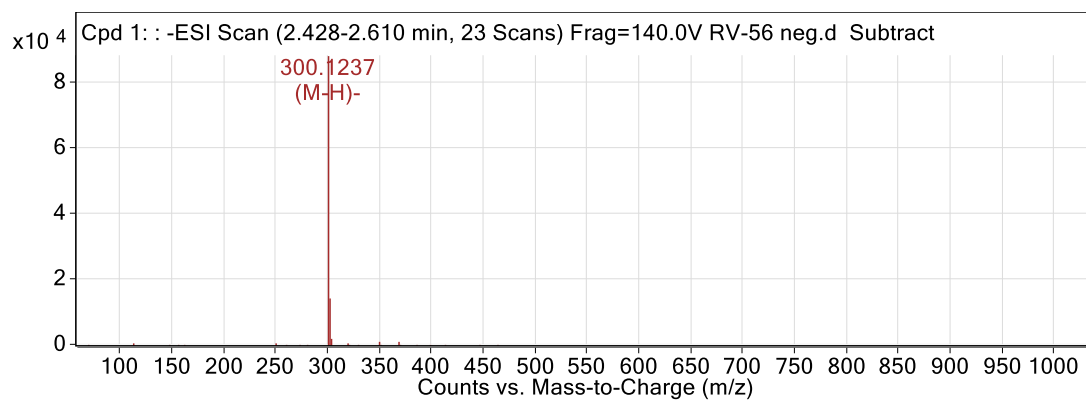


¹H NMR spectrum of **13** (CDCl₃, 400 MHz)



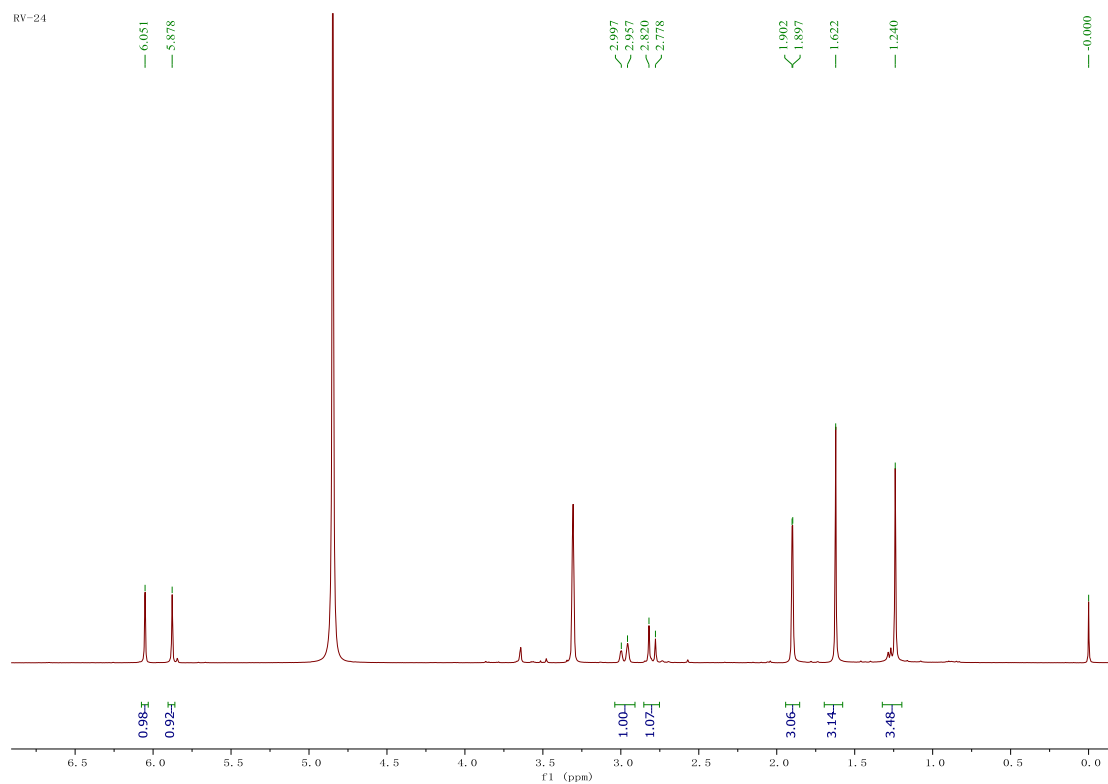


NOESY spectrum of **13**

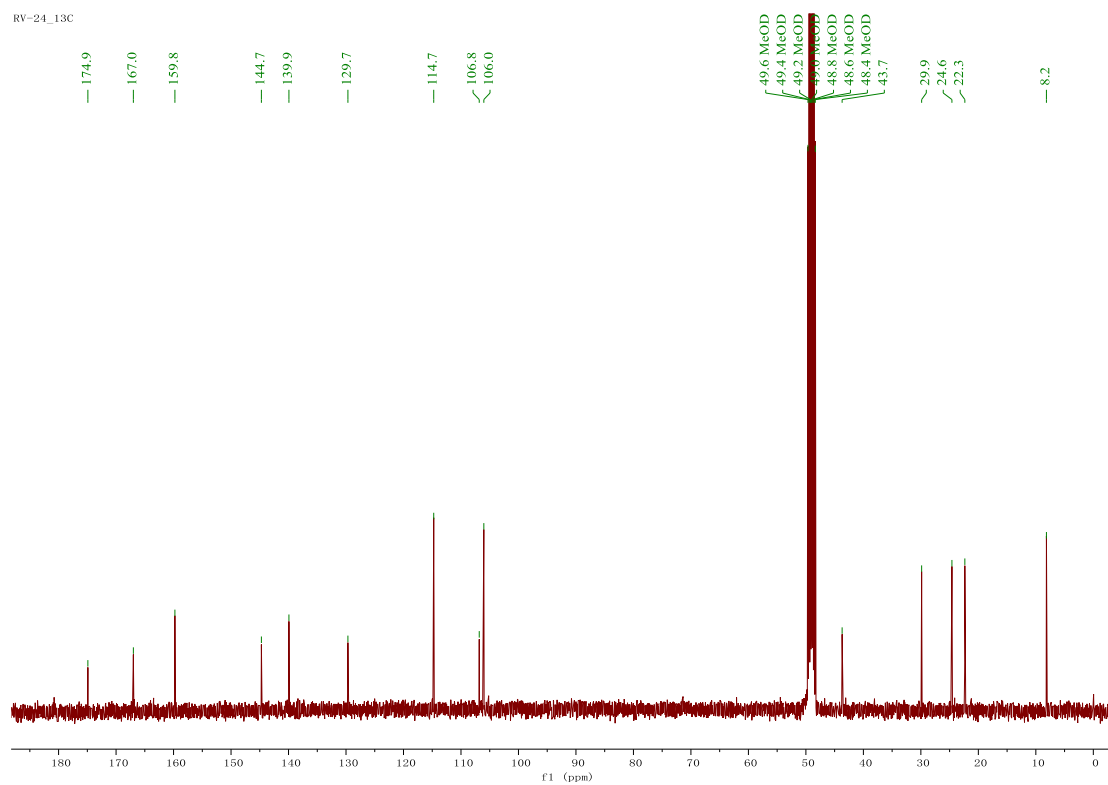


<i>m/z</i>	<i>Calc m/z</i>	Diff(ppm)	<i>z</i>	Abund	Formula	Ion
300.1237	300.1241	-1.34	-1	88045	C ₁₇ H ₁₈ NO ₄	(M-H) ⁻

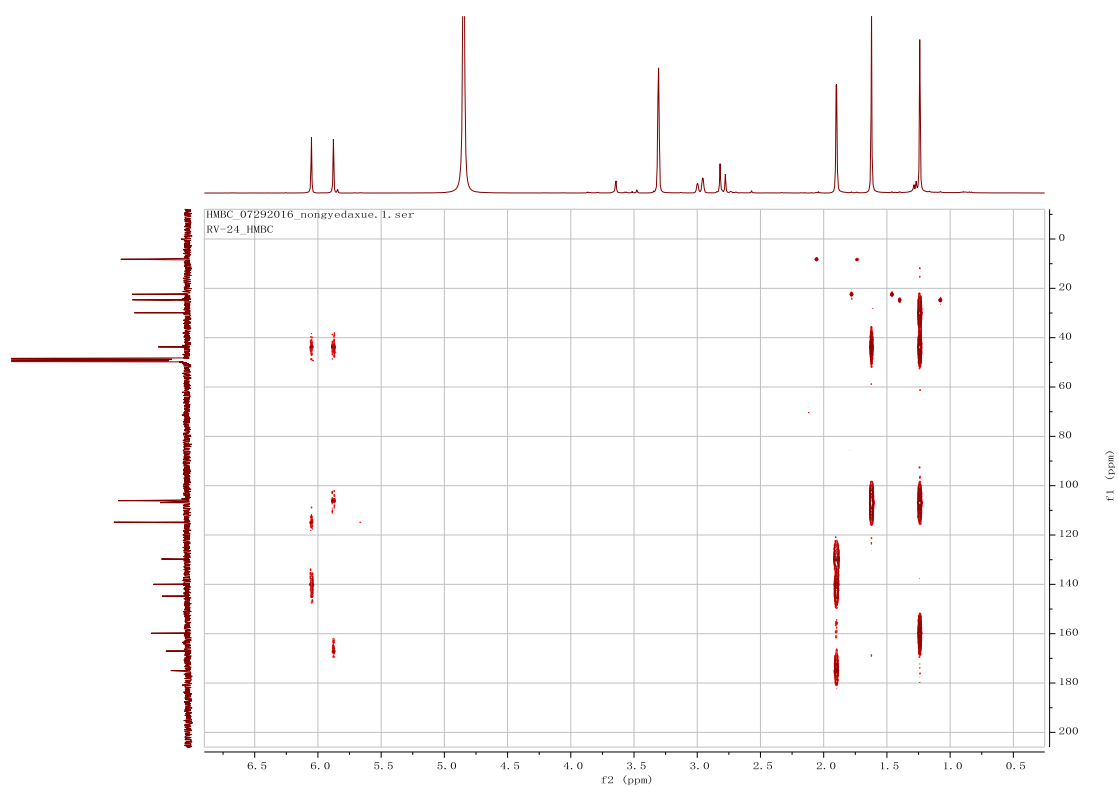
HRESIMS spectrum of **13**



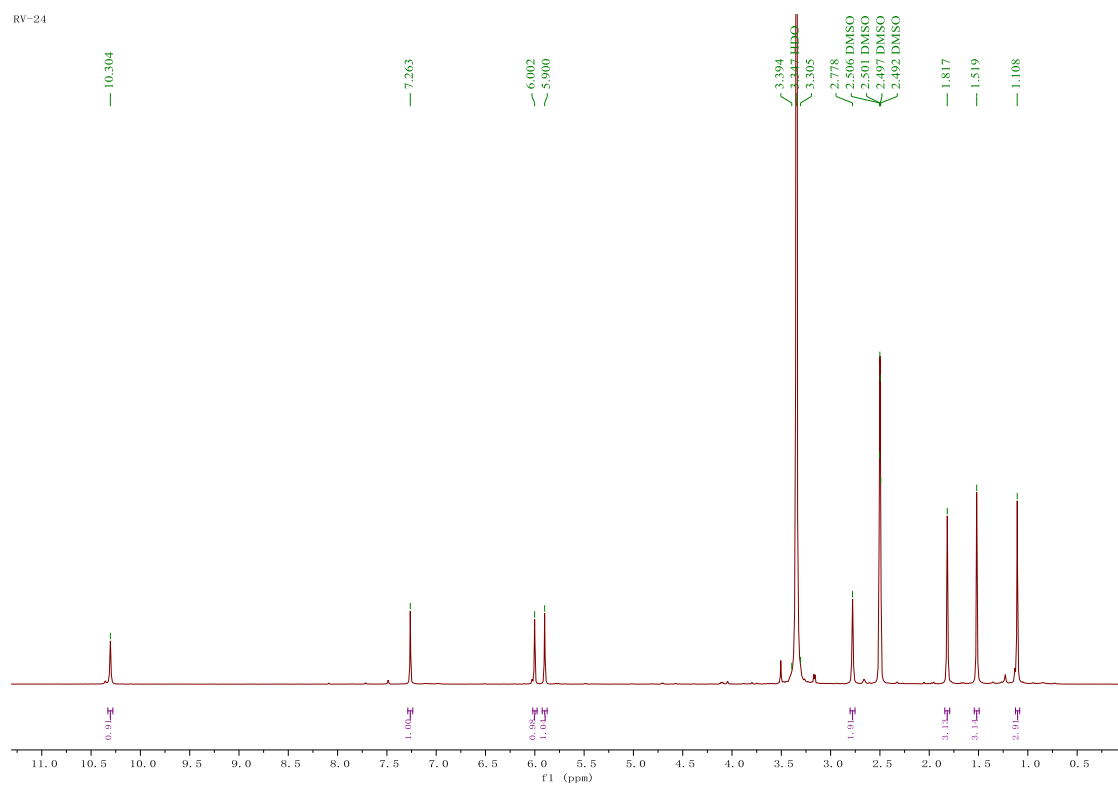
^1H NMR spectrum of **14** (CD_3OD , 400 MHz)



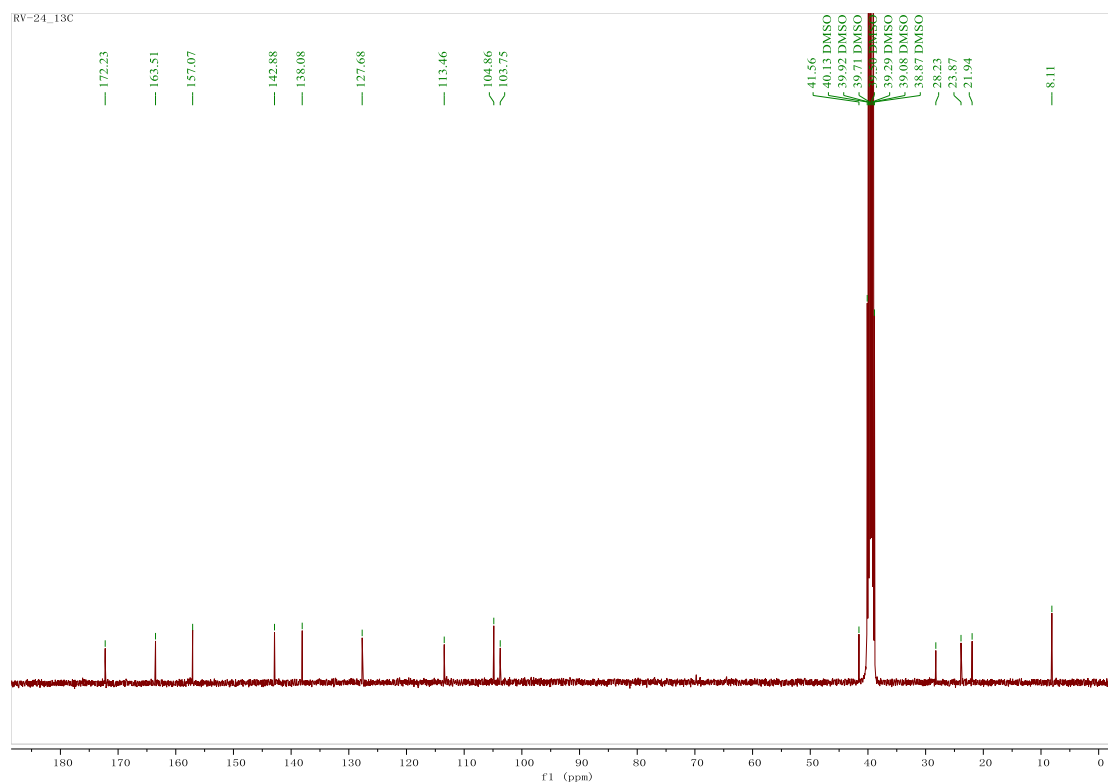
^{13}C NMR spectrum of **14** (CD_3OD , 100 MHz)



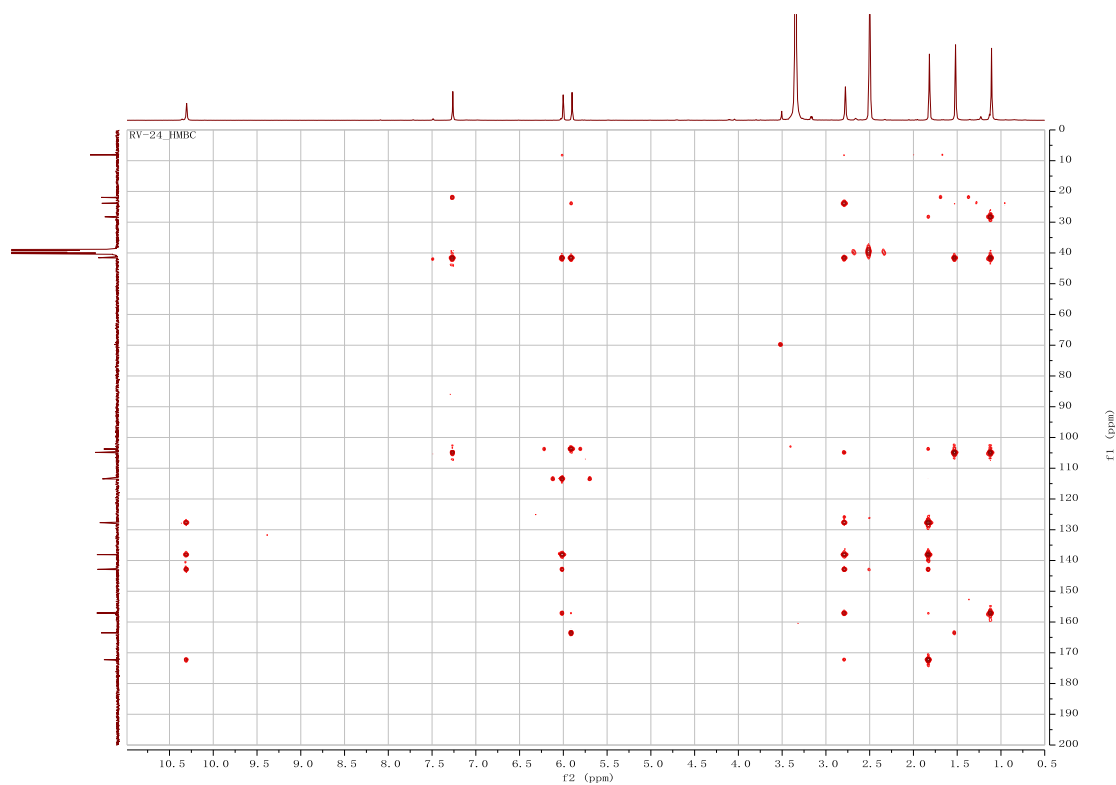
HMBC spectrum of **14** (CD_3OD)



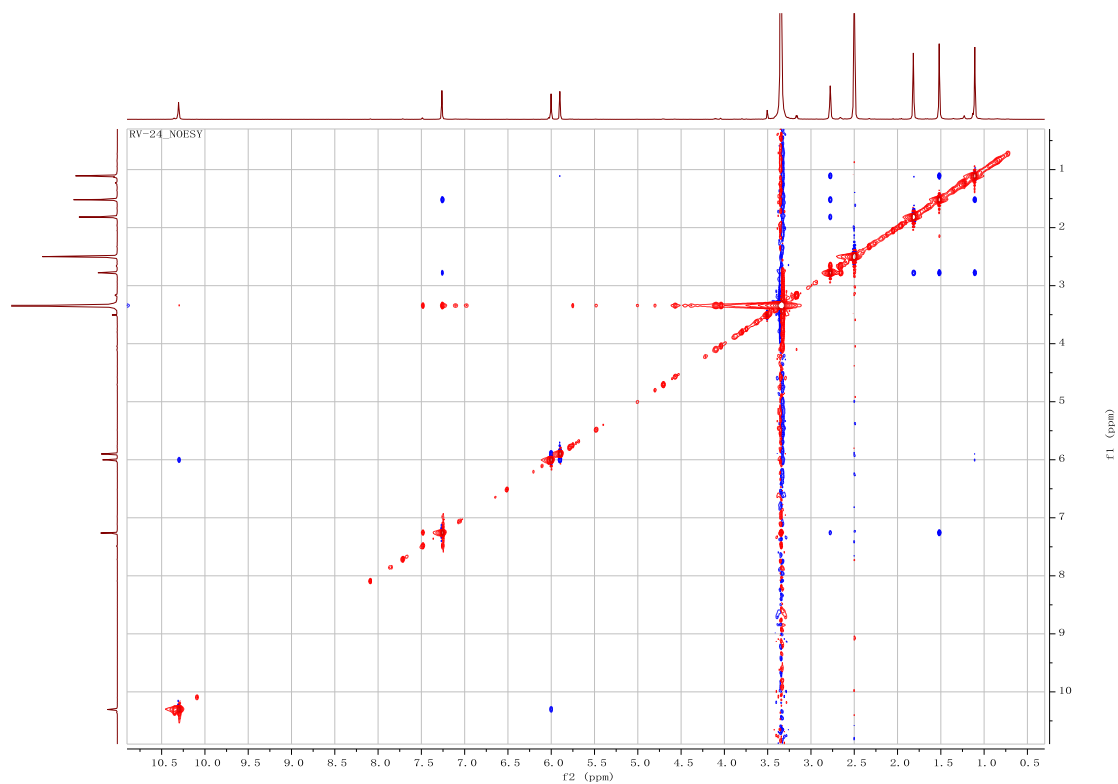
^1H NMR spectrum of **14** ($\text{DMSO}-d_6$, 400 MHz)



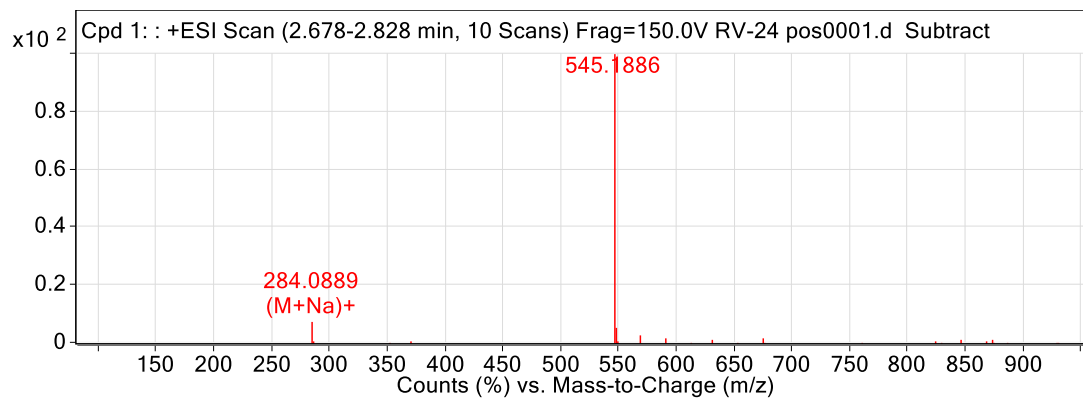
^{13}C NMR spectrum of **14** ($\text{DMSO}-d_6$, 100 MHz)



HMBC spectrum of **14** ($\text{DMSO}-d_6$)



NOESY spectrum of **14** (DMSO-*d*₆)



<i>m/z</i>	<i>Calc m/z</i>	Diff(ppm)	<i>z</i>	Abund	Formula	Ion
284.0889	284.0893	-1.55	1	2326.7	C ₁₄ H ₁₅ NNaO ₄	(M+Na) ⁺
545.1886	545.1894	-1.51	1	30926	C ₂₈ H ₃₀ N ₂ NaO ₈	(2M+Na) ⁺

HRESIMS spectrum of **14**