

Supplementary Materials

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Figure S45. ^1H - ^1H COSY spectrum (600 MHz) of compound **6** in CDCl_3 .

Figure S46. NOESY spectrum (600 MHz) of compound **6** in CDCl_3 .

Figure S47. HR-EIMS spectrum of compound **6**.

Figure S48. IR spectrum of compound **6**.

1. Spectra of compound 1

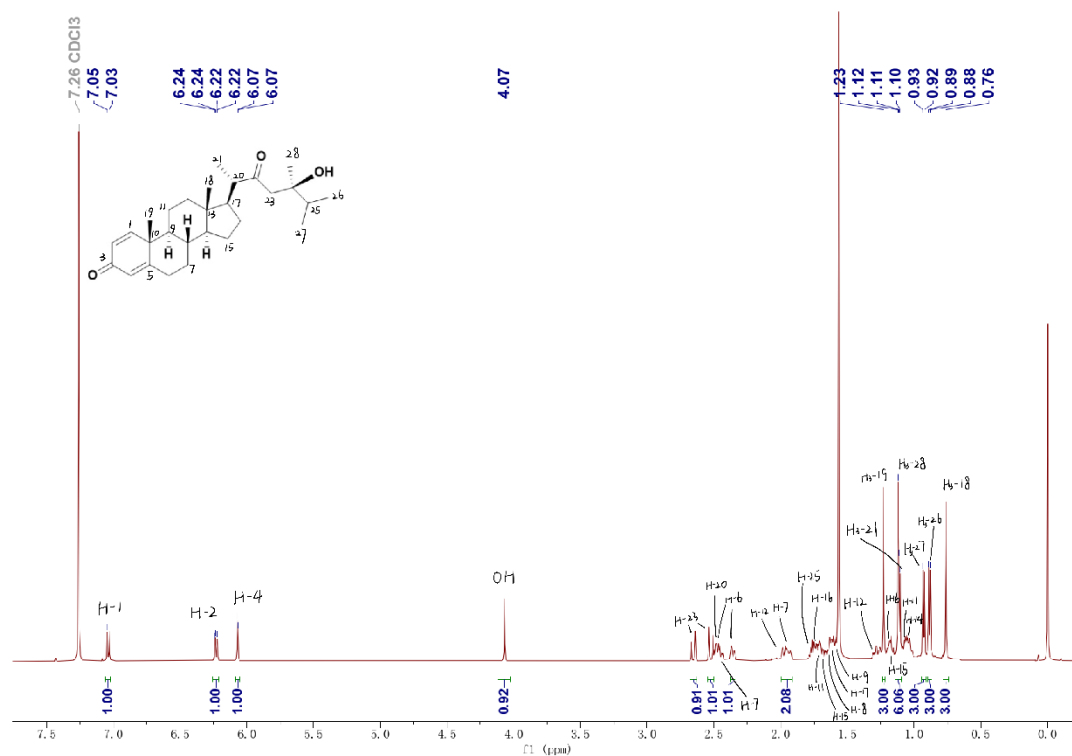


Figure S1. ¹H NMR spectrum (600 MHz) of compound 1 in CDCl₃.

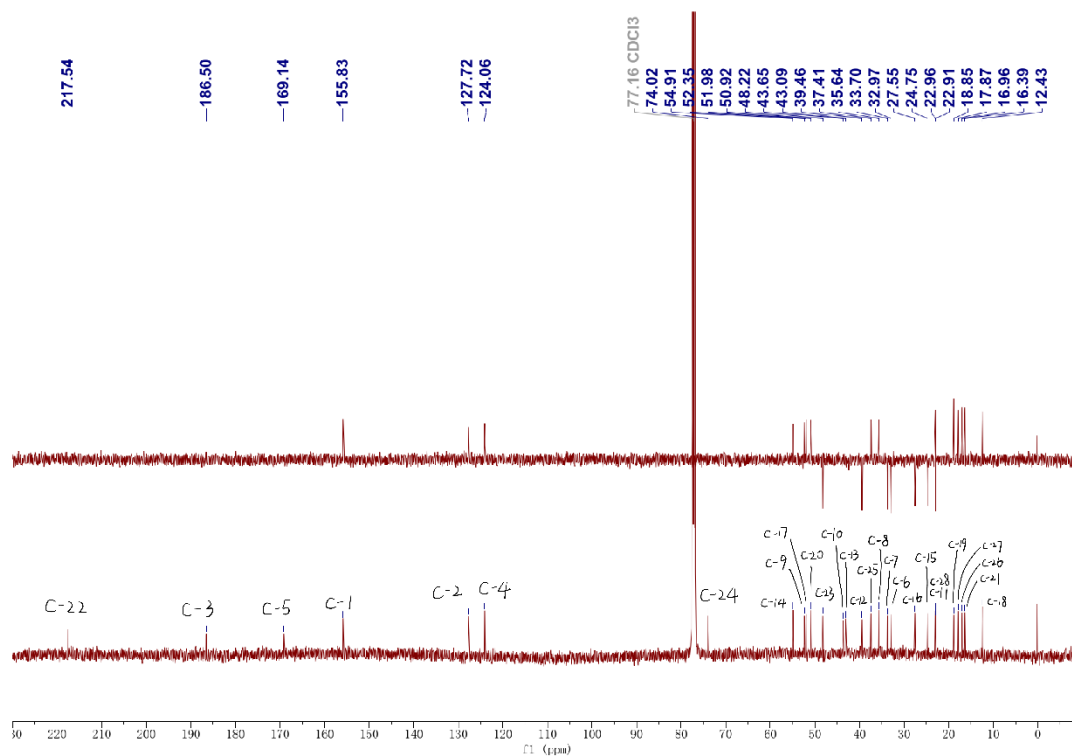


Figure S2. ¹³C NMR spectrum (125 MHz) of compound 1 in CDCl₃.

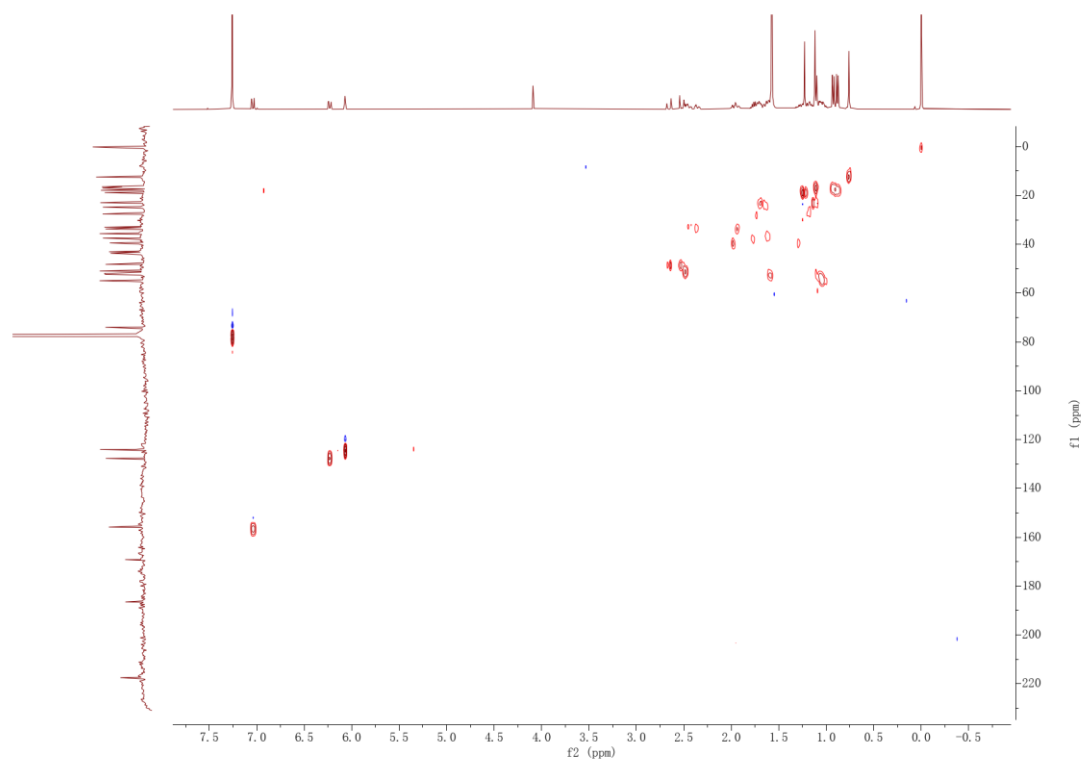


Figure S3. HSQC spectrum (600 MHz) of compound **1** in CDCl₃.

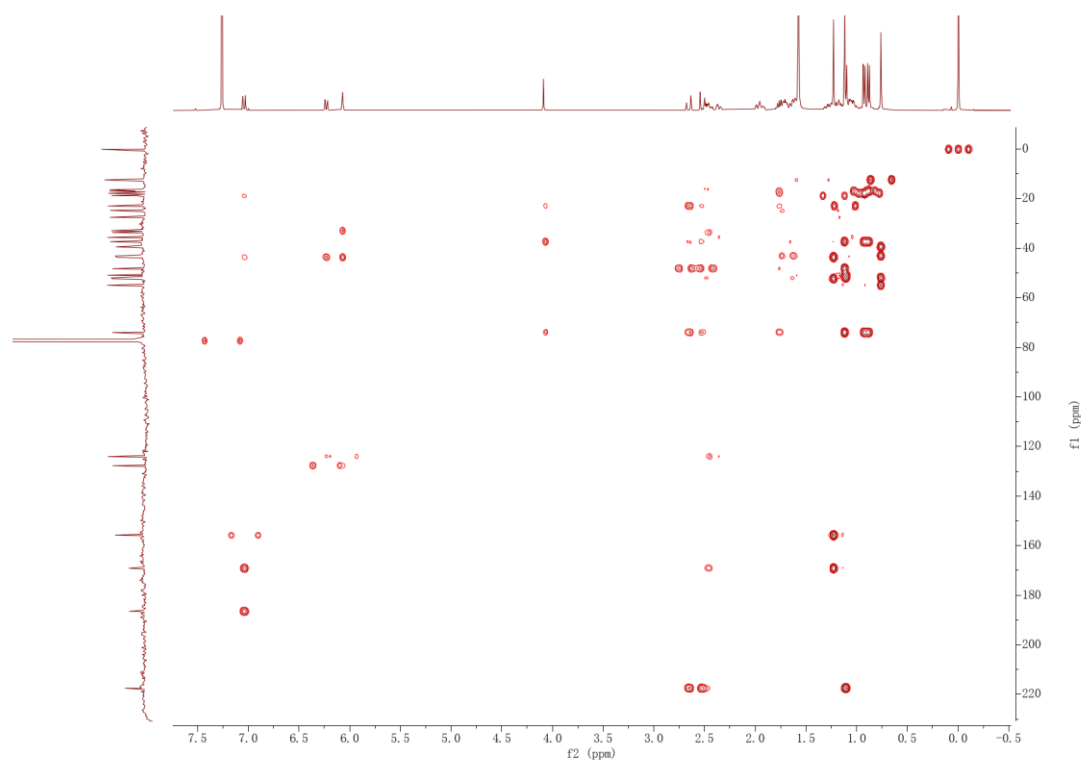


Figure S4. HMBC spectrum (600 MHz) of compound **1** in CDCl₃.

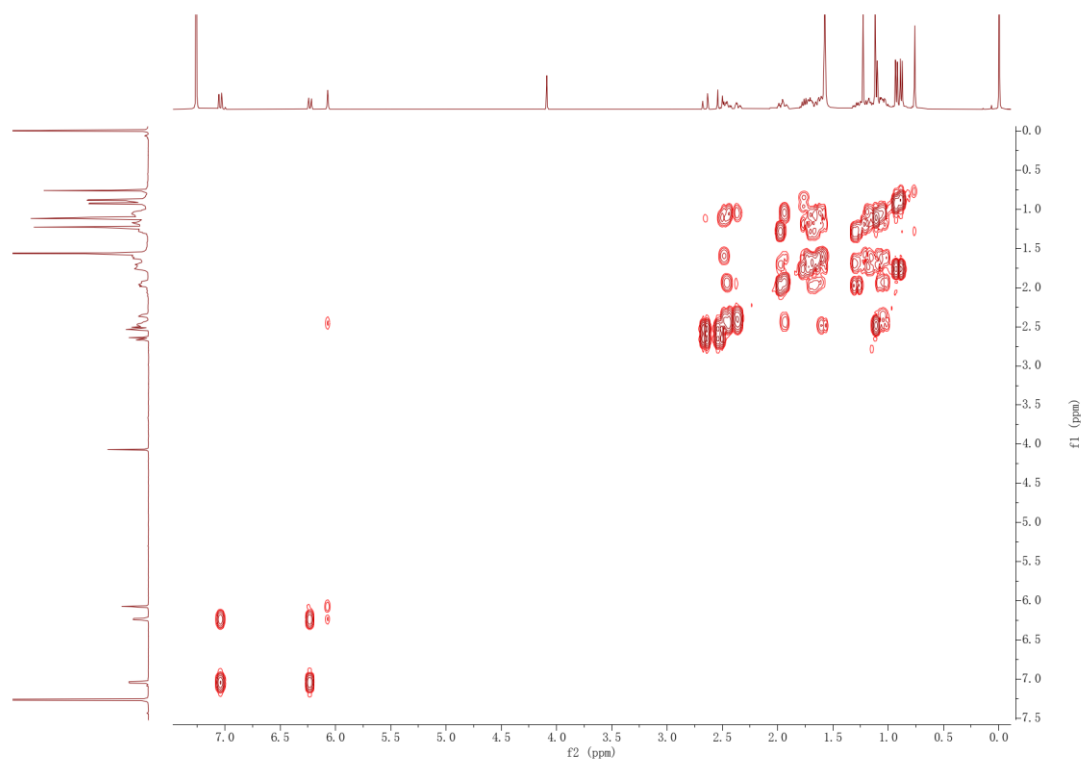


Figure S5. ^1H - ^1H COSY spectrum (600 MHz) of compound **1** in CDCl_3 .

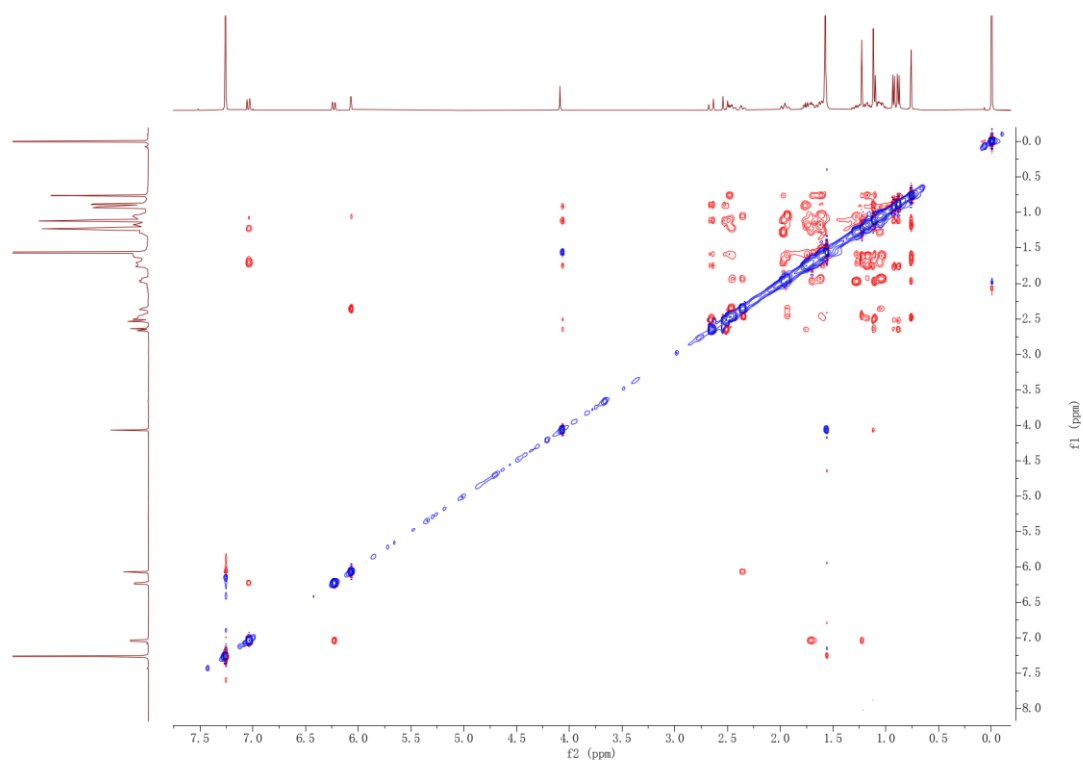
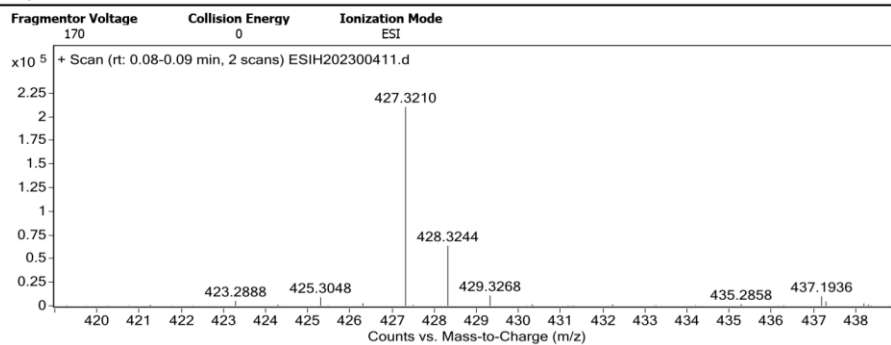


Figure S6. NOESY spectrum (600 MHz) of compound **1** in CDCl_3 .

Data Filename	ESI202300411.d	Sample Name	A8-A8-AFBBBE-4
Sample ID		Position	P1-D8
Instrument Name	Agilent G6520 Q-TOF	Acq Method	20160322_MS_ESIH_POS_1min.m
Acquired Time	1/11/2023 14:00:02	IRM Calibration Status	Success
DA Method	small molecular data analysis method.m	Comment	ESIH by fangsu

User Spectra



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
427.321	427.3207	-0.3	-0.7	C ₂₈ H ₄₃ O ₃	(M+H) ⁺

Figure S7. HR-ESIMS spectrum of compound **1**.

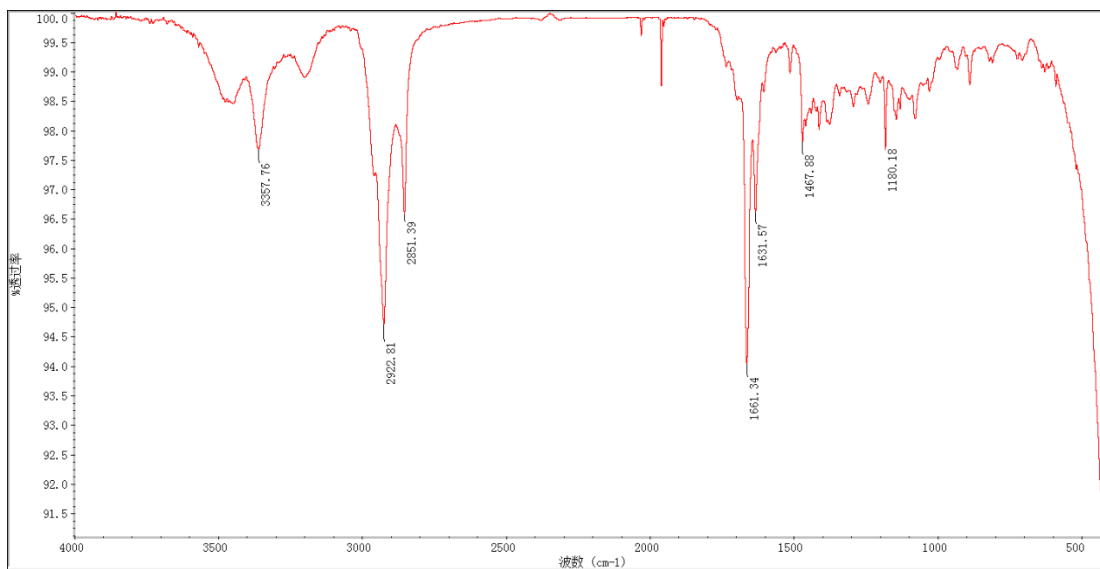


Figure S8. IR spectrum of compound **1**.

2. Spectra of compound 2

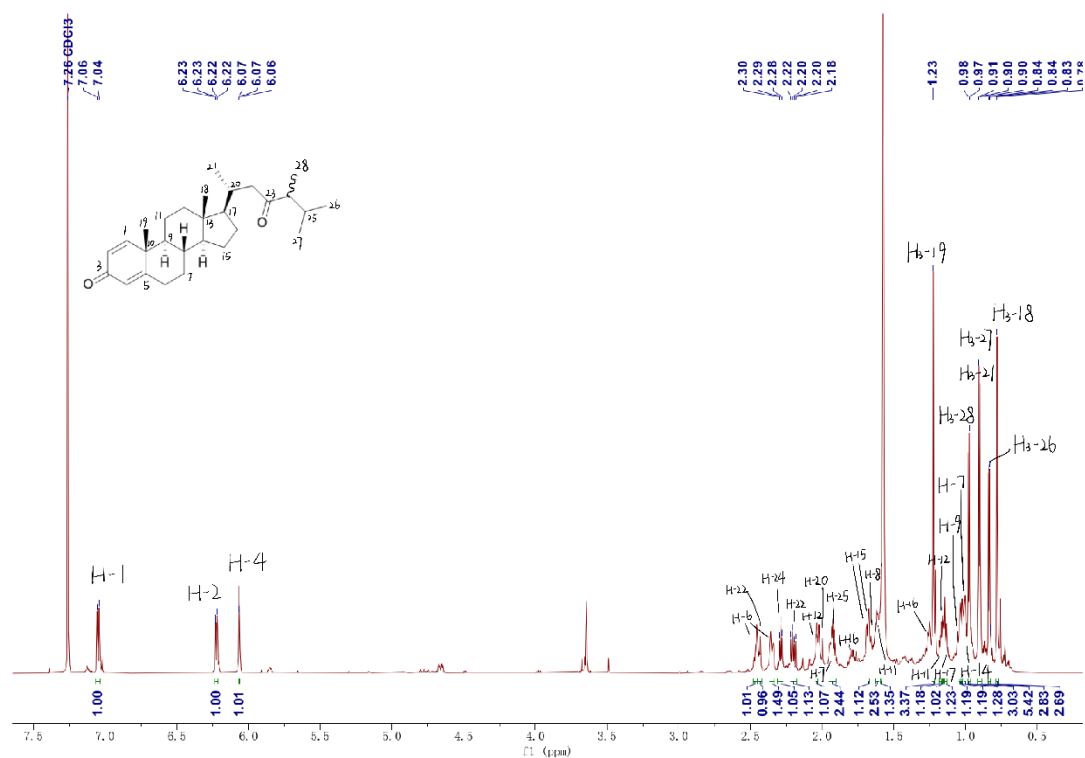


Figure S9. ^1H NMR spectrum (800 MHz) of compound **2** in CDCl_3 .

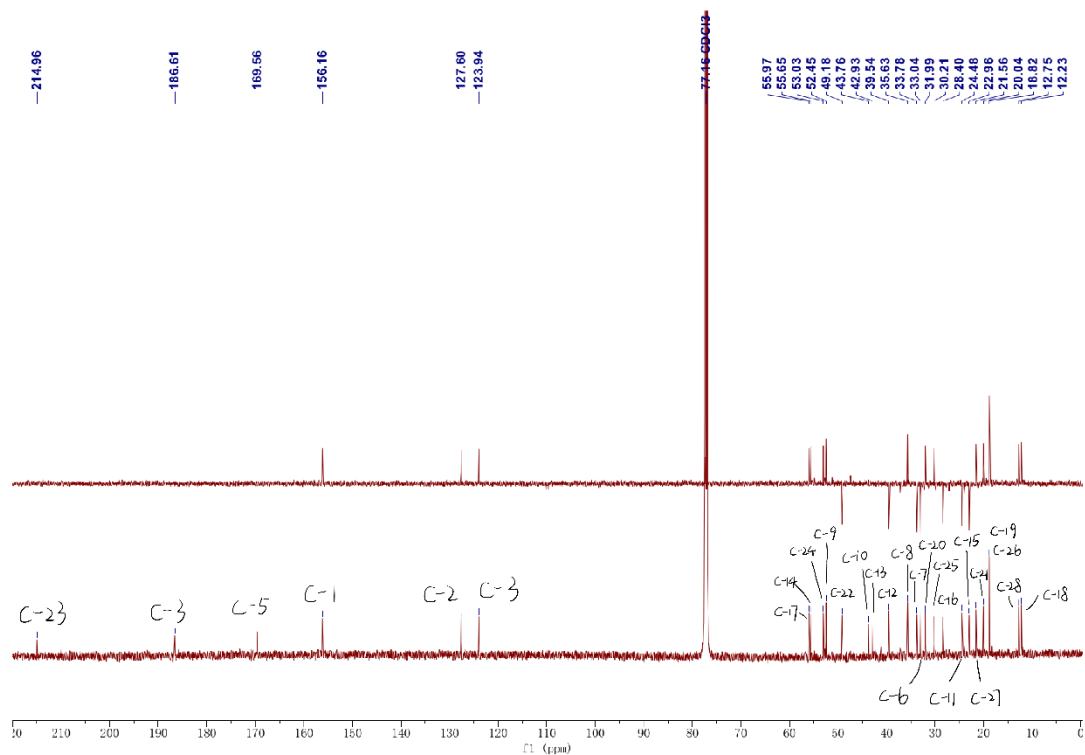


Figure S10. ^{13}C NMR spectrum (150 MHz) of compound **2** in CDCl_3 .

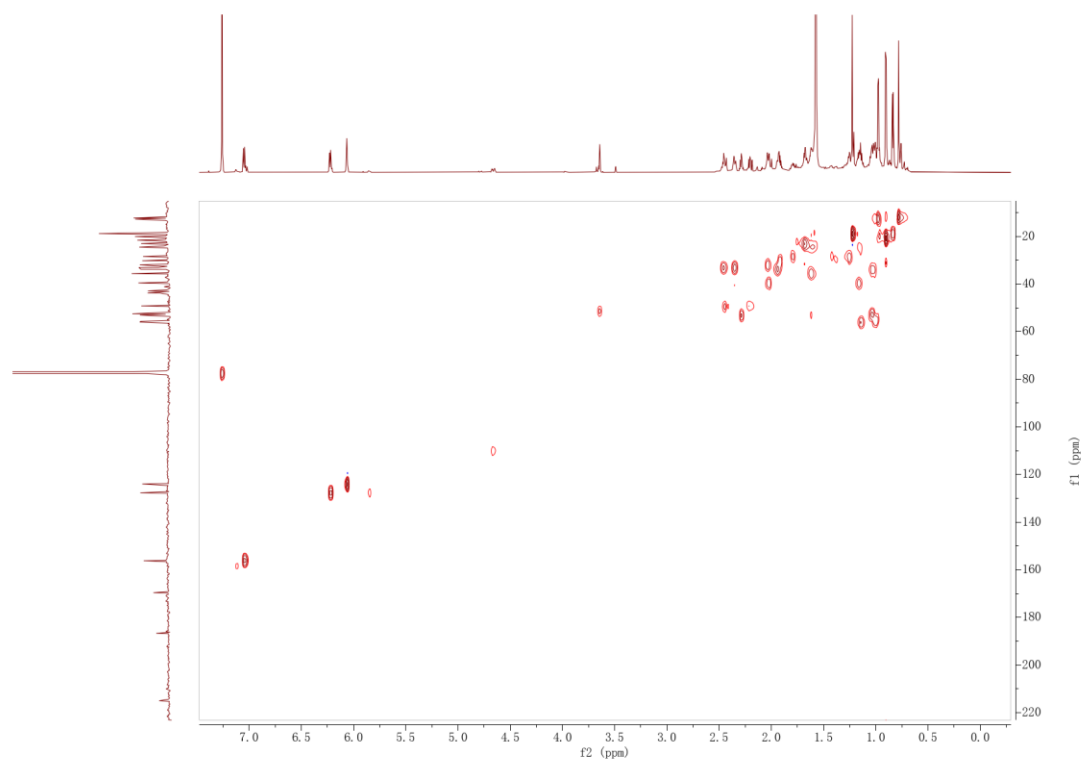


Figure S11. HSQC spectrum (800 MHz) of compound **2** in CDCl₃.

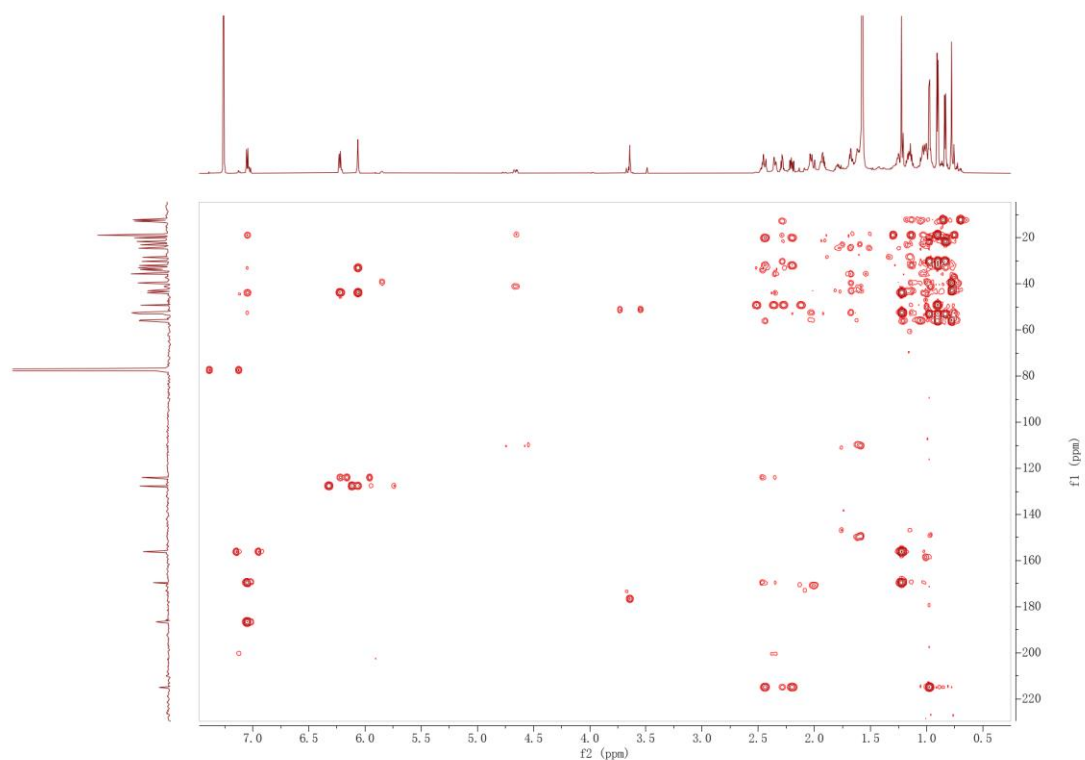


Figure S12. HMBC spectrum (800 MHz) of compound **2** in CDCl₃.

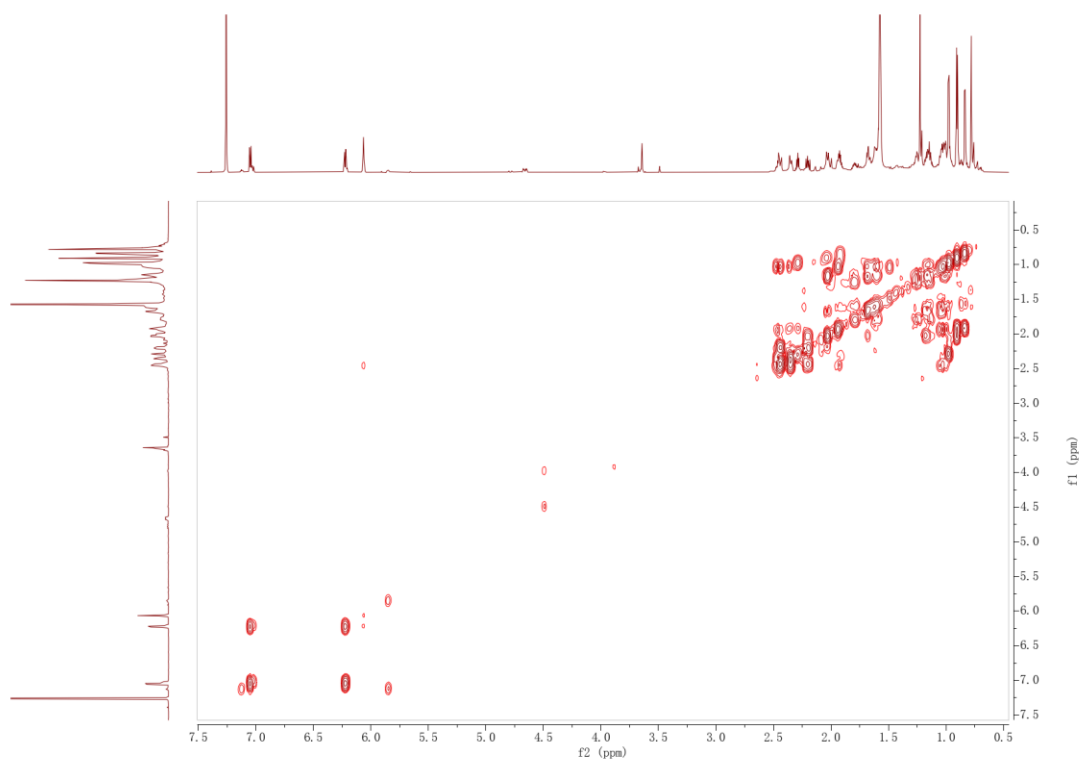


Figure S13. ^1H - ^1H COSY spectrum (800 MHz) of compound **2** in CDCl_3 .

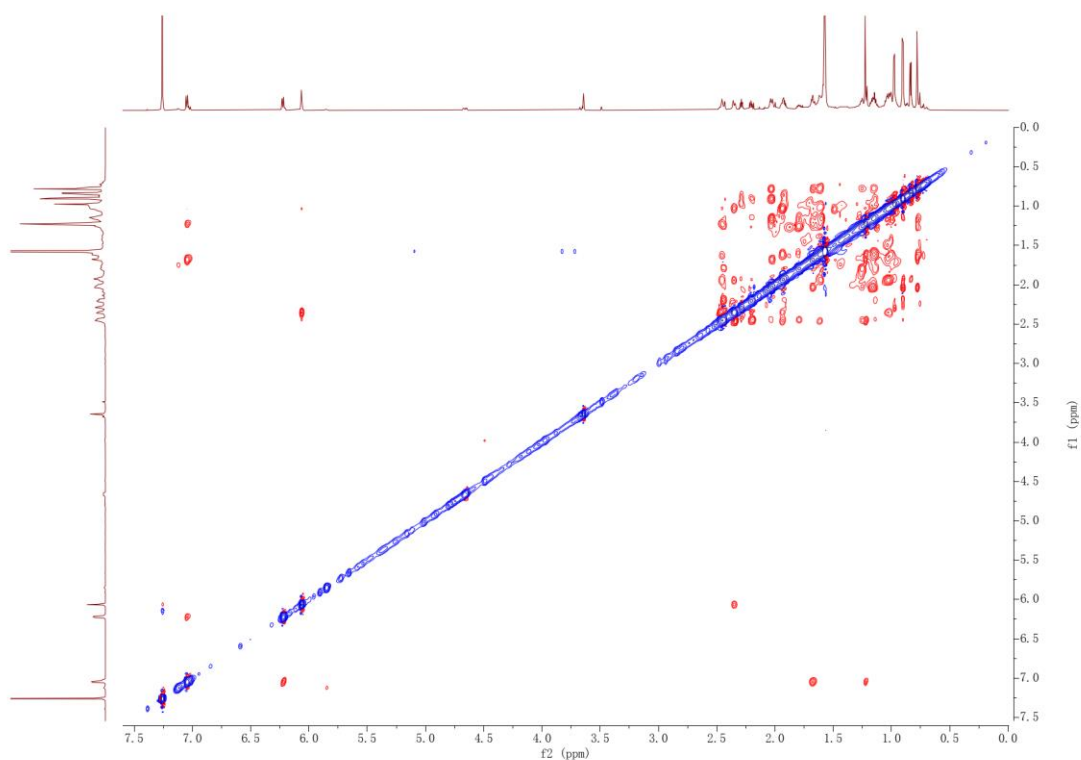
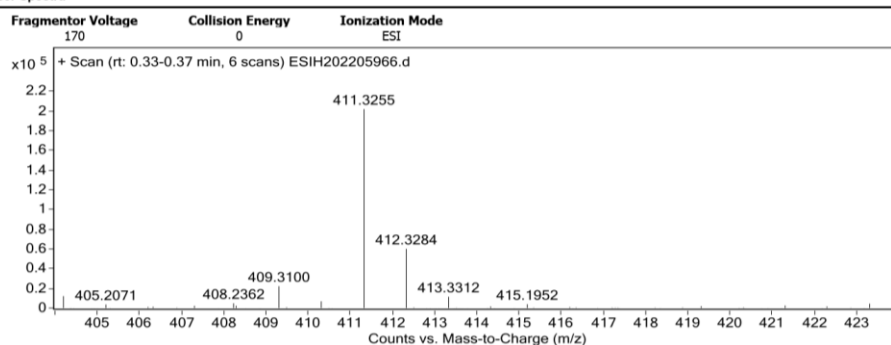


Figure S14. NOESY spectrum (800 MHz) of compound **2** in CDCl_3 .

Data Filename	ESI202205966.d	Sample Name	A8-2DCA-8
Sample ID		Position	P1-E7
Instrument Name	Agilent G6520 Q-TOF	Acq Method	20160322_MS_ESIH_POS_1min.m
Acquired Time	12/27/2022 10:35:10	IRM Calibration Status	Success
DA Method	small molecular data analysis method.m	Comment	ESIH by fangsu

User Spectra



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
411.3255	411.3258	0.24	0.57	C ₂₈ H ₄₃ O ₂	(M+H) ⁺

Figure S15. HR-ESIMS spectrum of compound **2**.

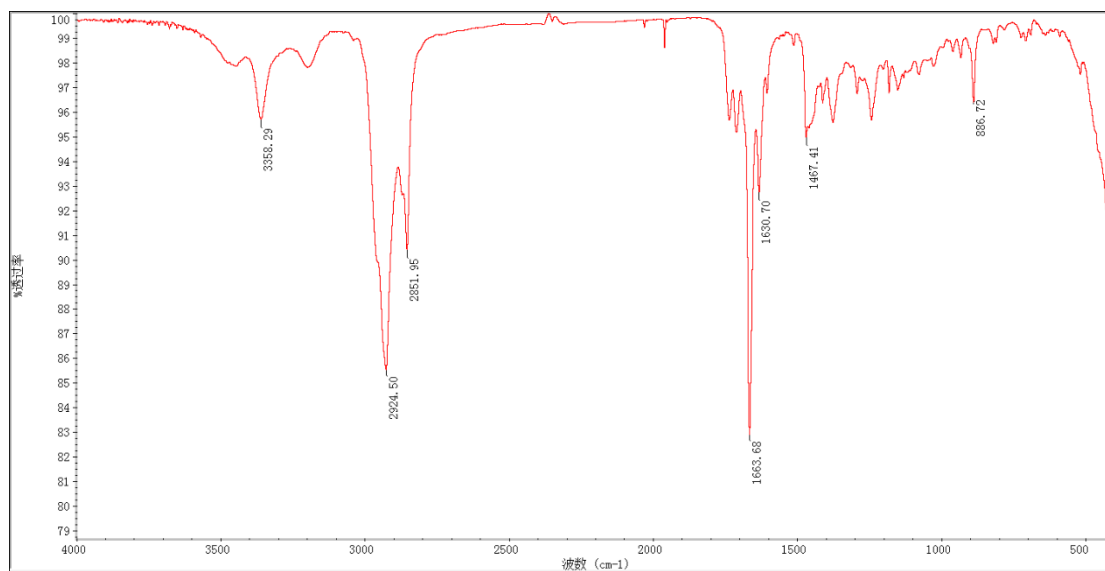


Figure S16. IR spectrum of compound **2**.

3. Spectra of compound 3

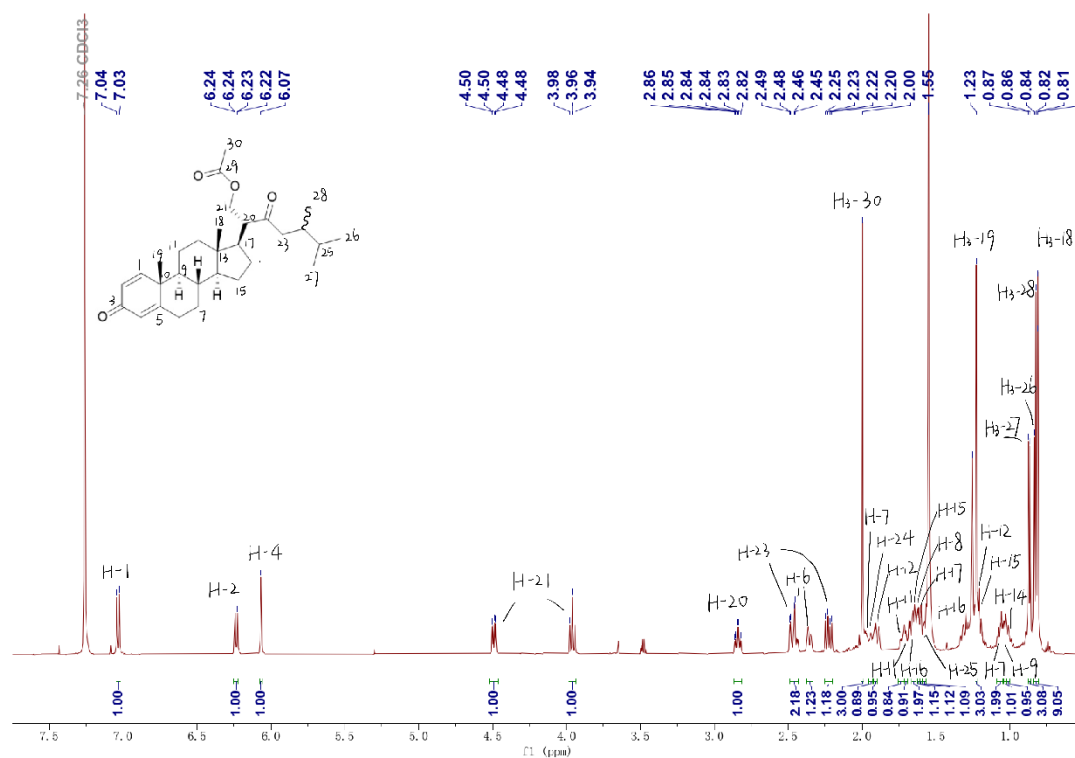


Figure S17. ¹H NMR spectrum (600 MHz) of compound **3** in CDCl₃.

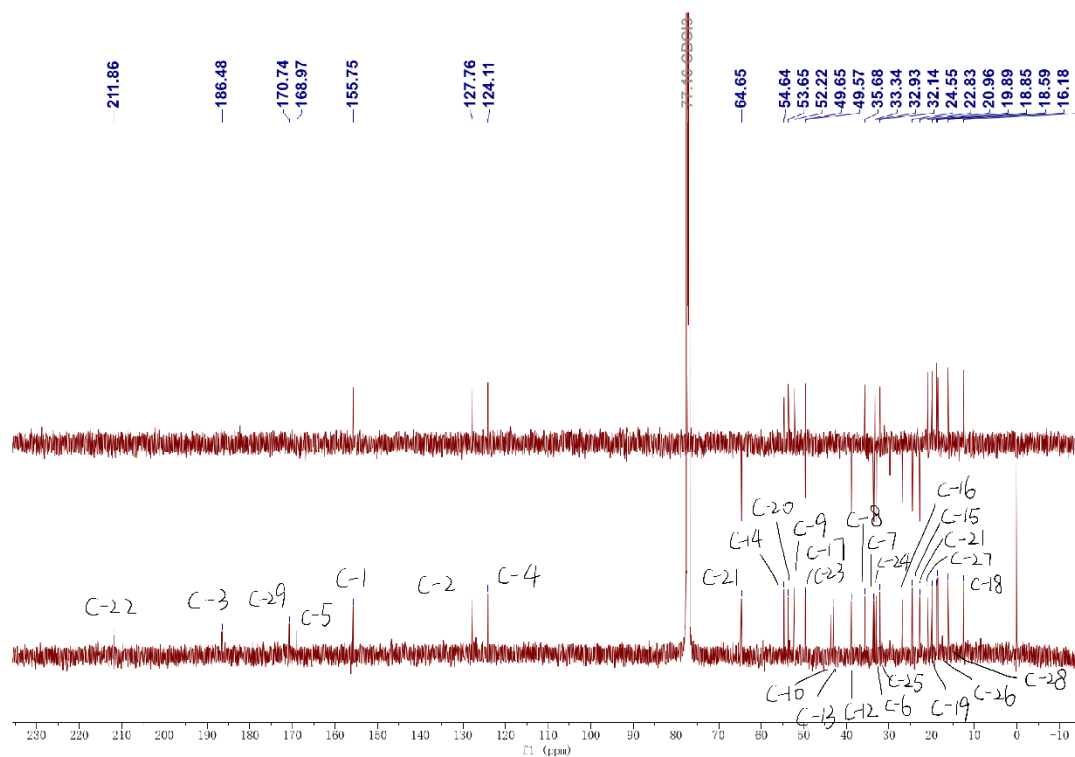


Figure S18. ¹³C NMR spectrum (150 MHz) of compound **3** in CDCl₃.

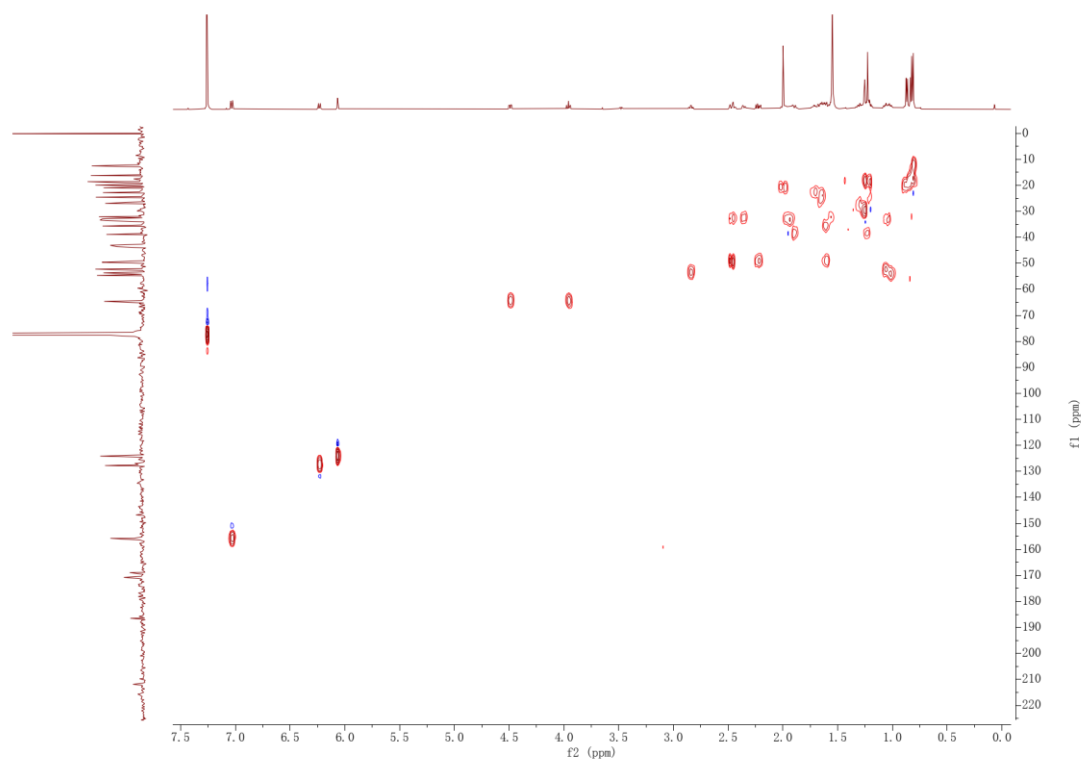


Figure S19. HSQC spectrum (600 MHz) of compound **3** in CDCl₃.

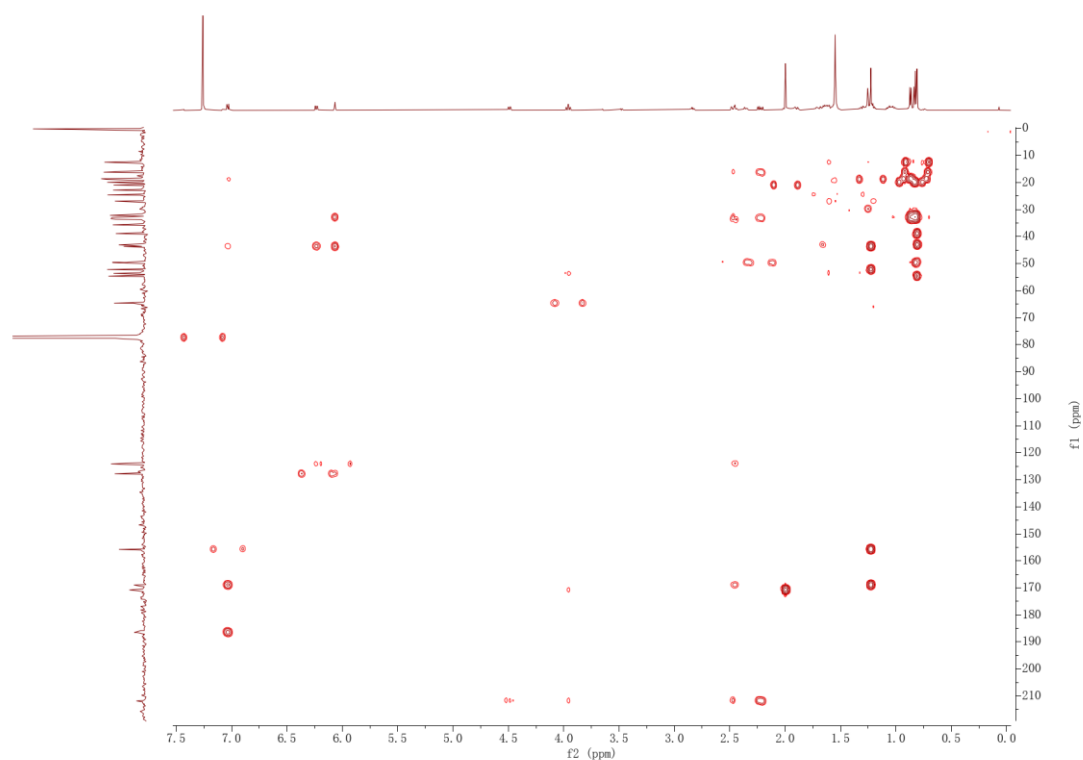


Figure S20. HMBC spectrum (600 MHz) of compound **3** in CDCl₃.

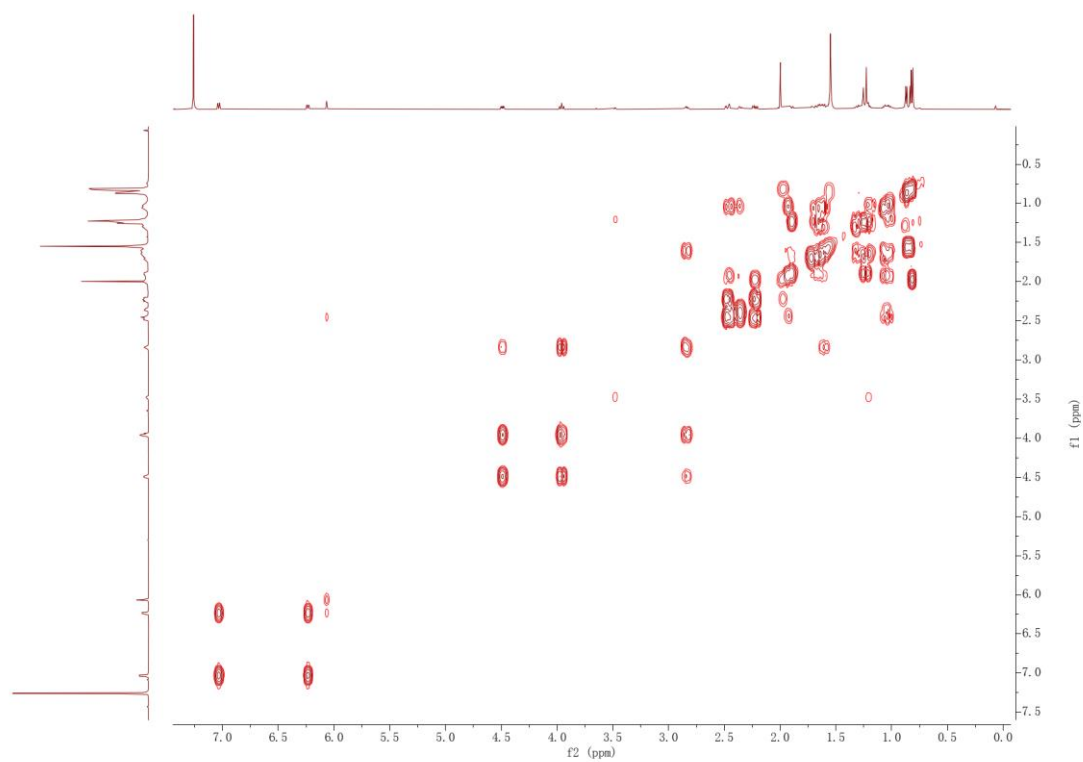


Figure S21. ^1H - ^1H COSY spectrum (600 MHz) of compound **3** in CDCl_3 .

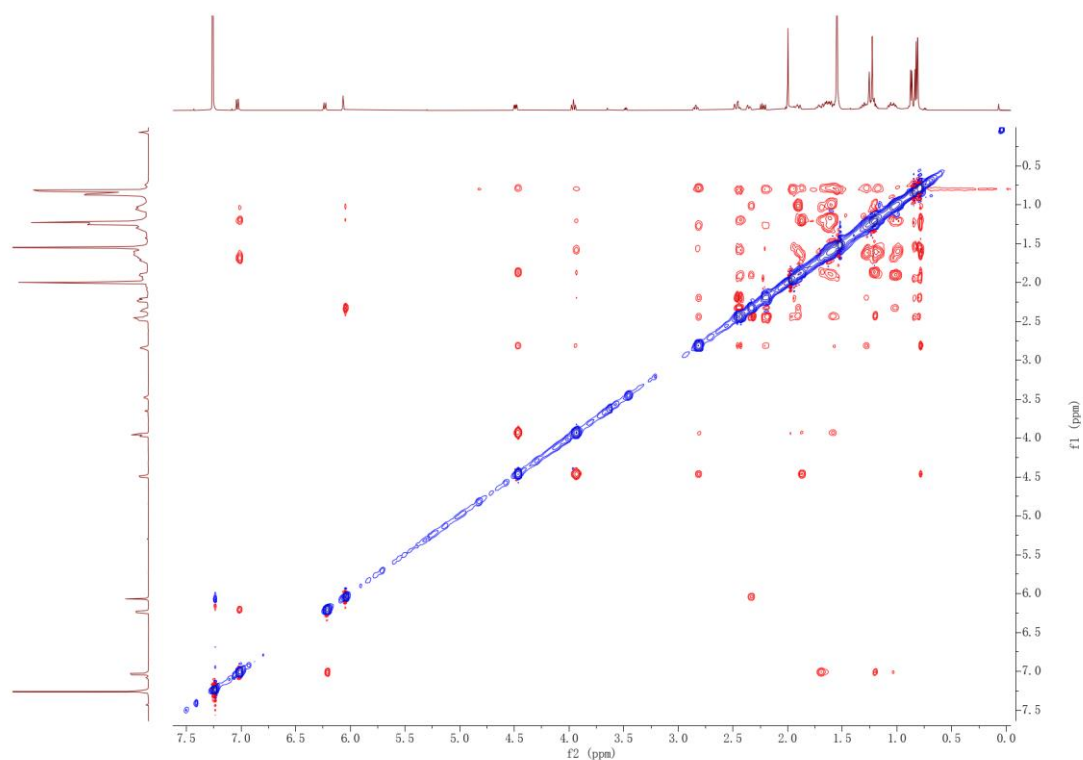
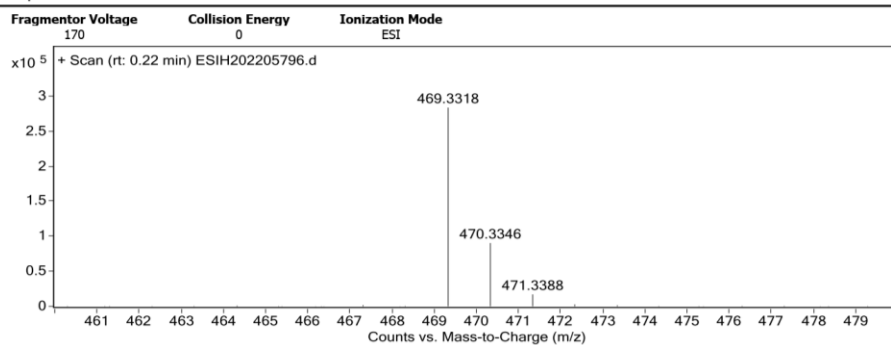


Figure S22. NOESY spectrum (600 MHz) of compound **3** in CDCl_3 .

Data Filename	ESI202205796.d	Sample Name	A8-AFB8BE-6
Sample ID		Position	P1-D2
Instrument Name	Agilent G6520 Q-TOF	Acq Method	20160322_MS_ESIH_POS_1min.m
Acquired Time	12/20/2022 15:04:07	IRM Calibration Status	Success
DA Method	small molecular data analysis method.m	Comment	ESIH by zhuzhenyun

User Spectra



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
469.3318	469.3312	-0.56	-1.19	C30 H45 O4	(M+H)+

Figure S23. HR-ESIMS spectrum of compound **3**.

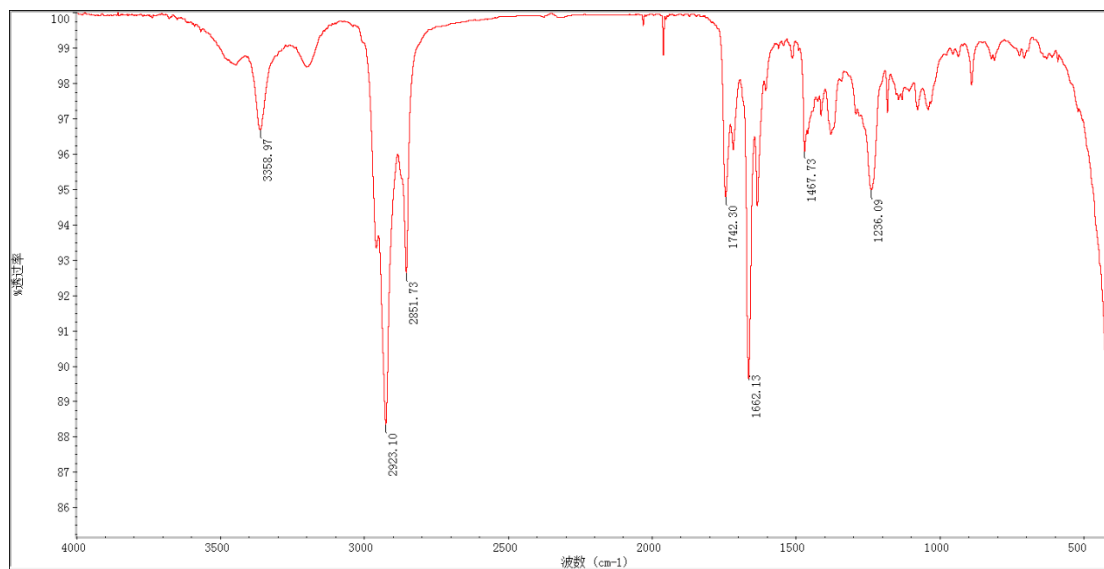


Figure S24. IR spectrum of compound **3**.

4. Spectra of compound 4

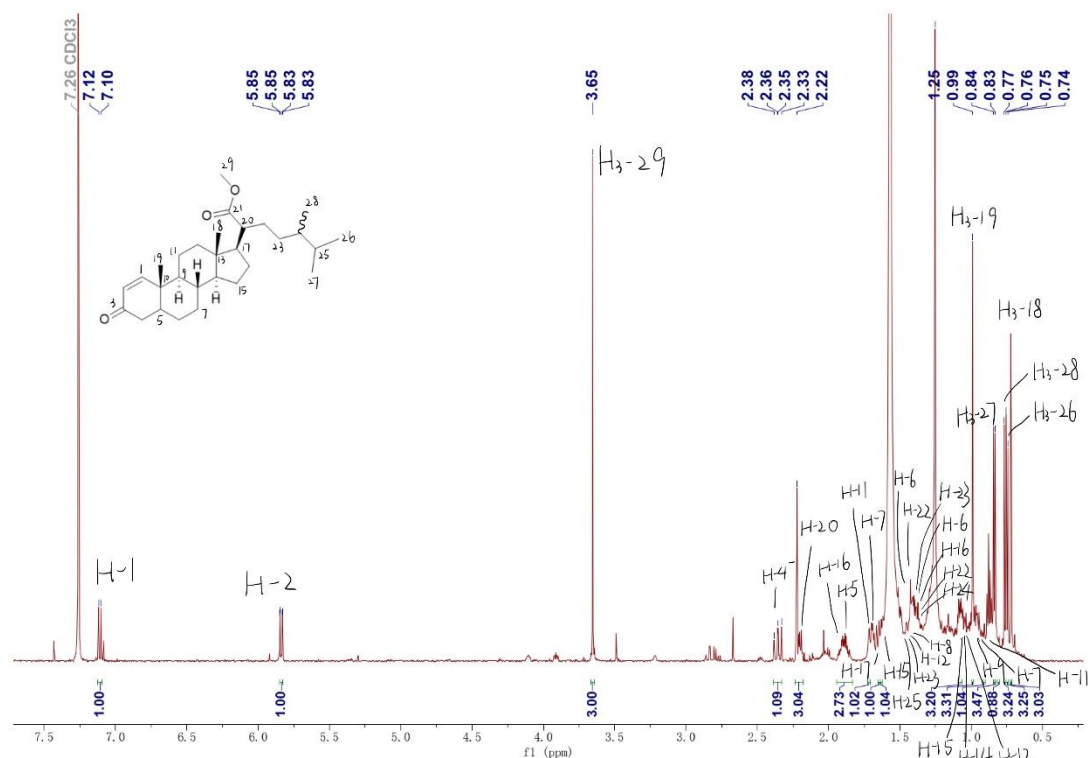


Figure S25. ^1H NMR spectrum (600 MHz) of compound **4** in CDCl_3 .

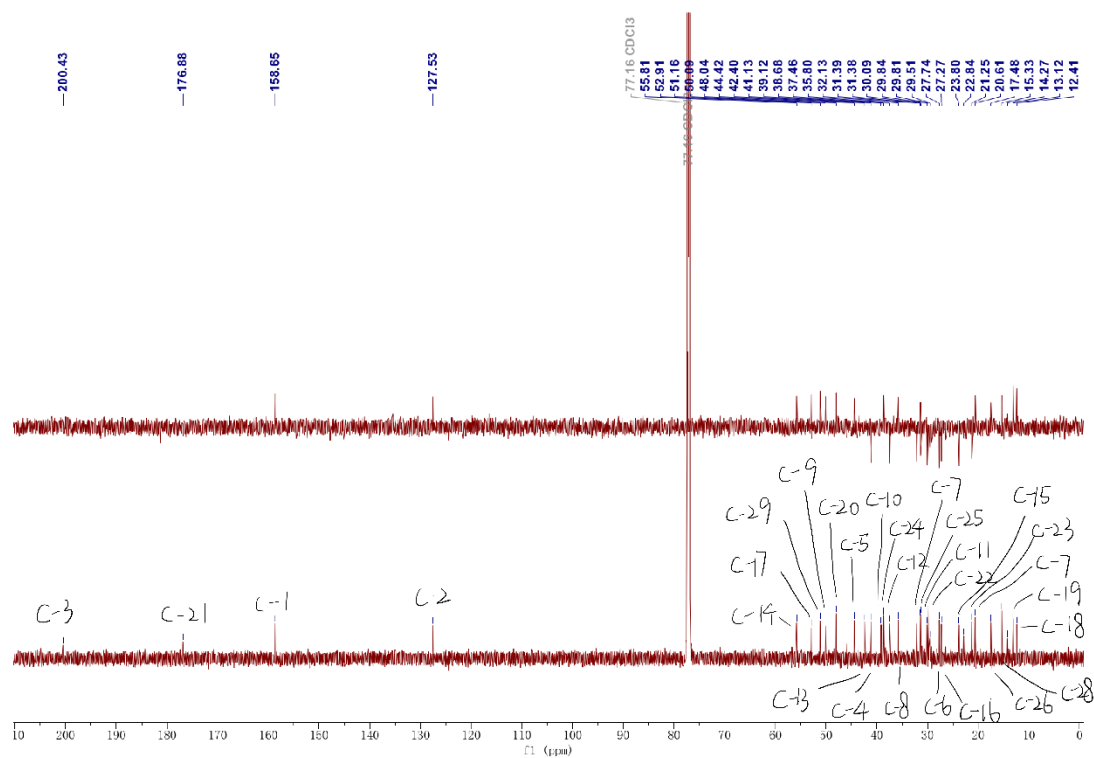


Figure S26. ^{13}C NMR spectrum (200 MHz) of compound **4** in CDCl_3 .

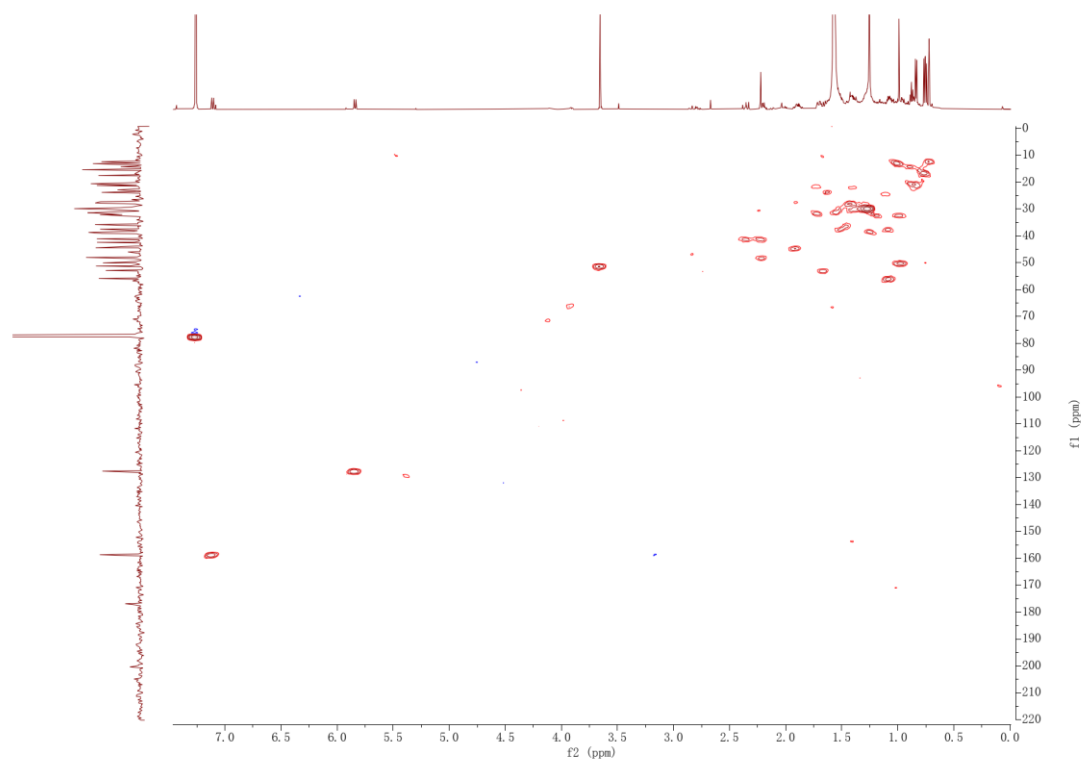


Figure S27. HSQC spectrum (600 MHz) of compound **4** in CDCl₃.

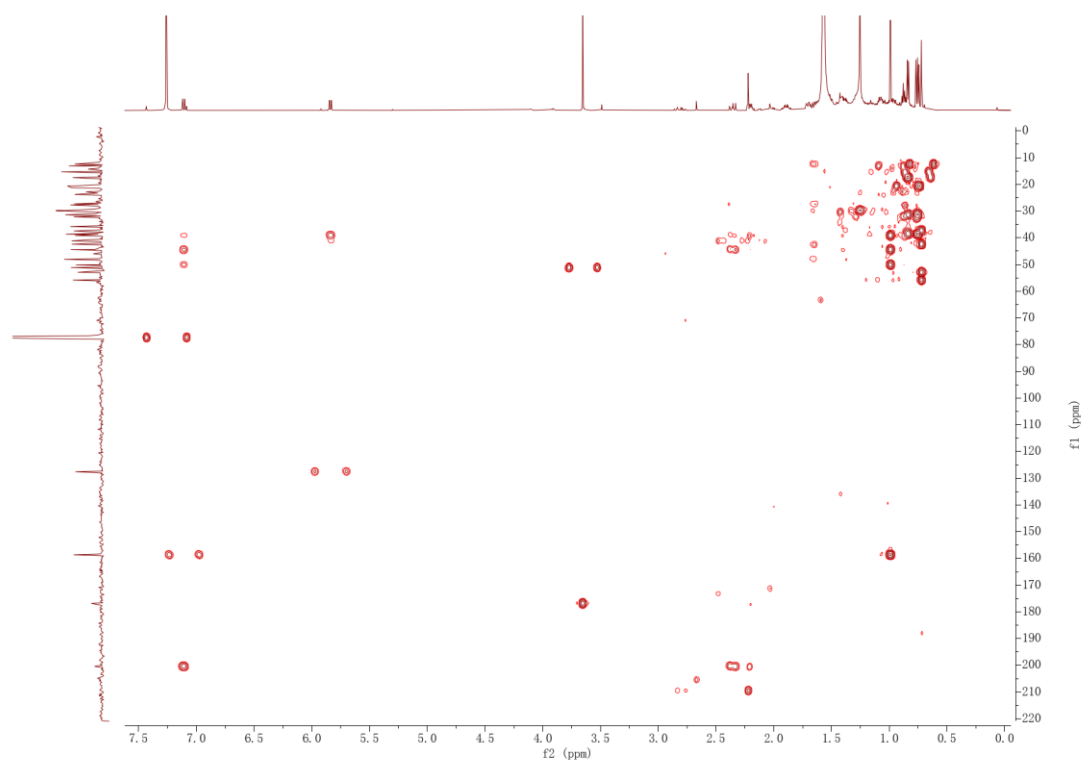


Figure S28. HMBC spectrum (600 MHz) of compound **4** in CDCl₃.

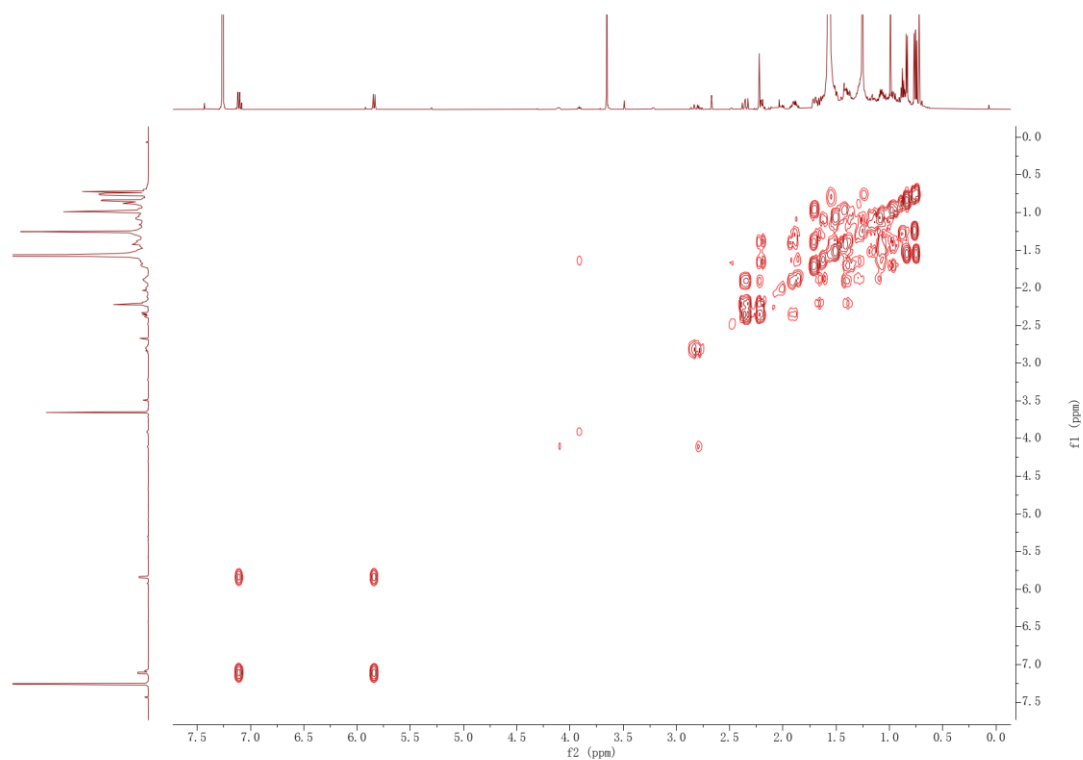


Figure S29. ^1H - ^1H COSY spectrum (600 MHz) of compound **4** in CDCl_3 .

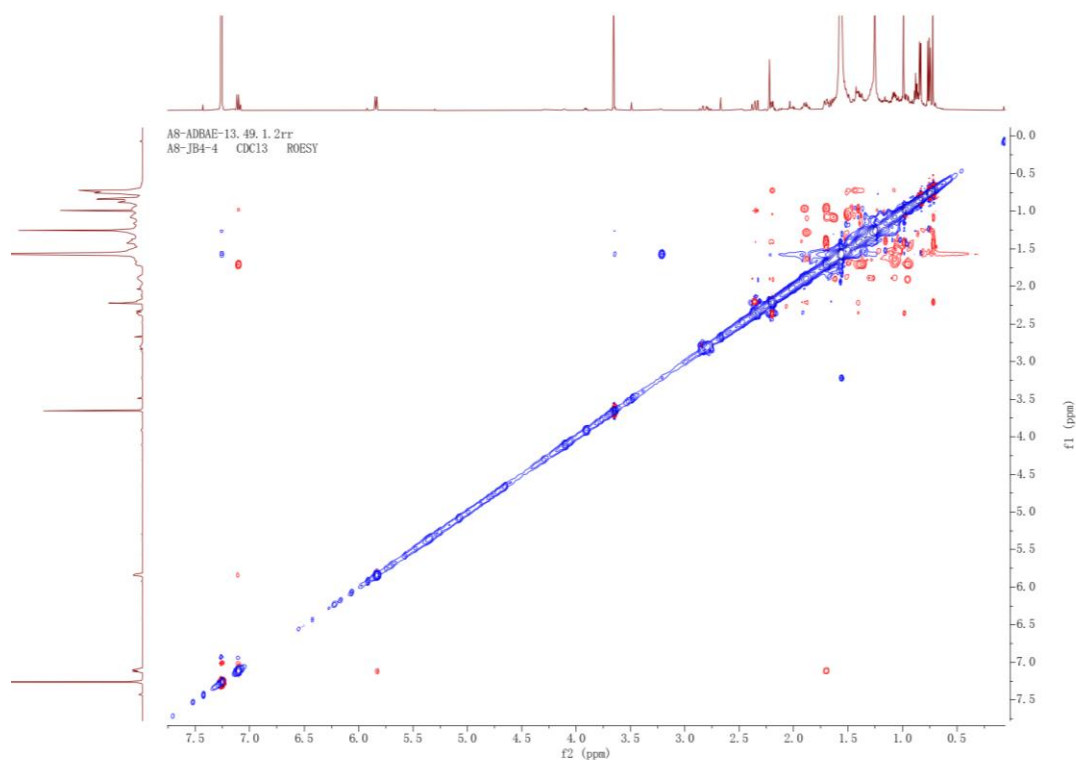
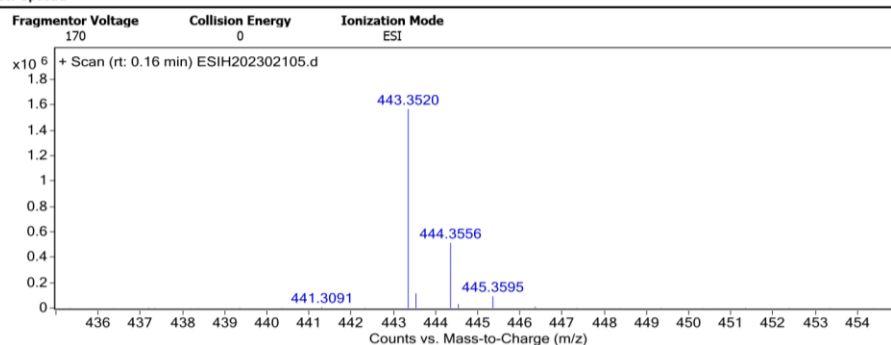


Figure S30. ROESY spectrum (600 MHz) of compound **4** in CDCl_3 .

Data Filename	ESI202302105.d	Sample Name	A8-A8-ADBAE-13
Sample ID		Position	P1-A1
Instrument Name	Agilent 6520 Q-TOF	Acq Method	20160322_MS_ESIH_POS_1min.m
Acquired Time	3/28/2023 14:46:28	IRM Calibration Status	Success
DA Method	small molecular data analysis method.m	Comment	ESIH by fangsu

User Spectra



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
443.352	443.352	0	-0.01	C ₂₉ H ₄₇ O ₃	(M+H) ⁺

Figure S31. HR-ESIMS spectrum of compound **4**.

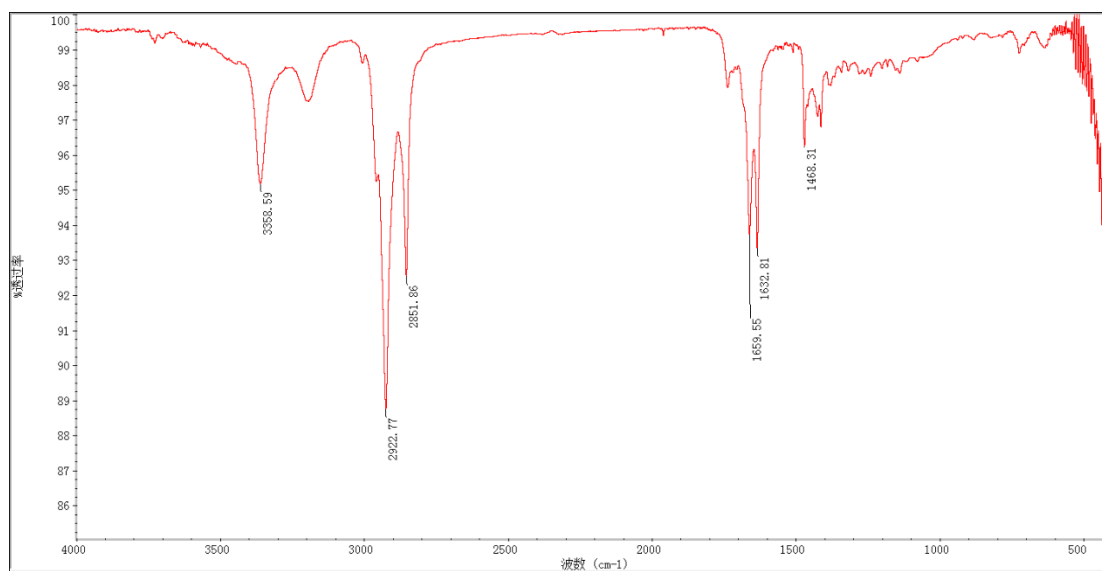
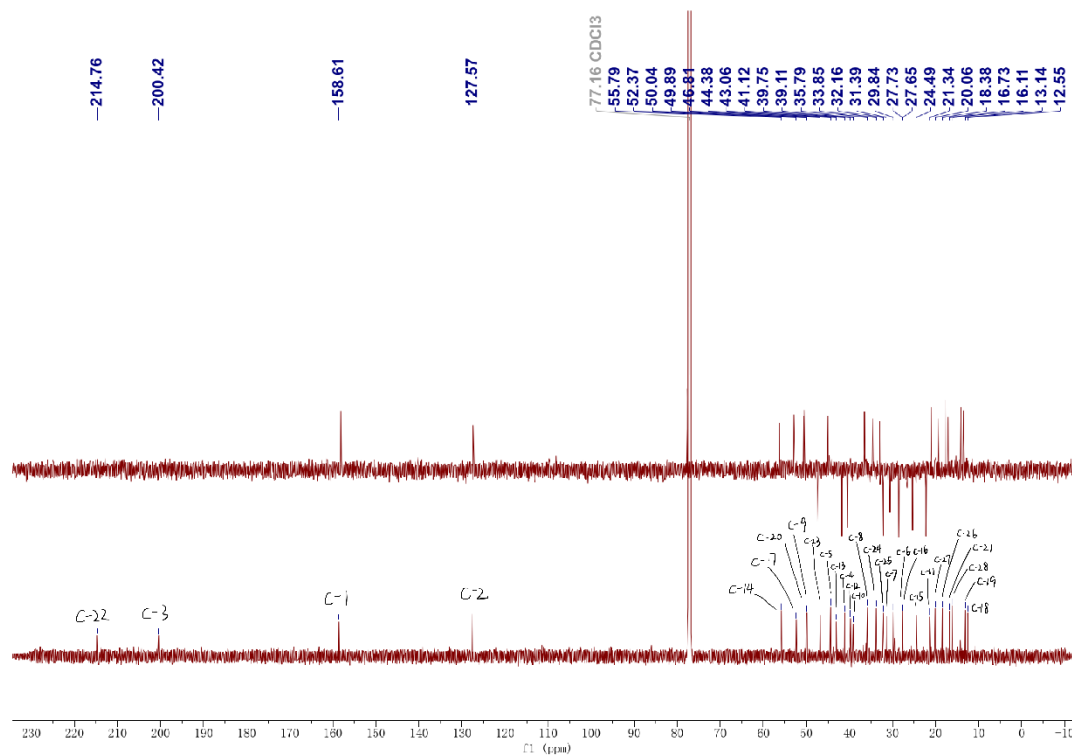
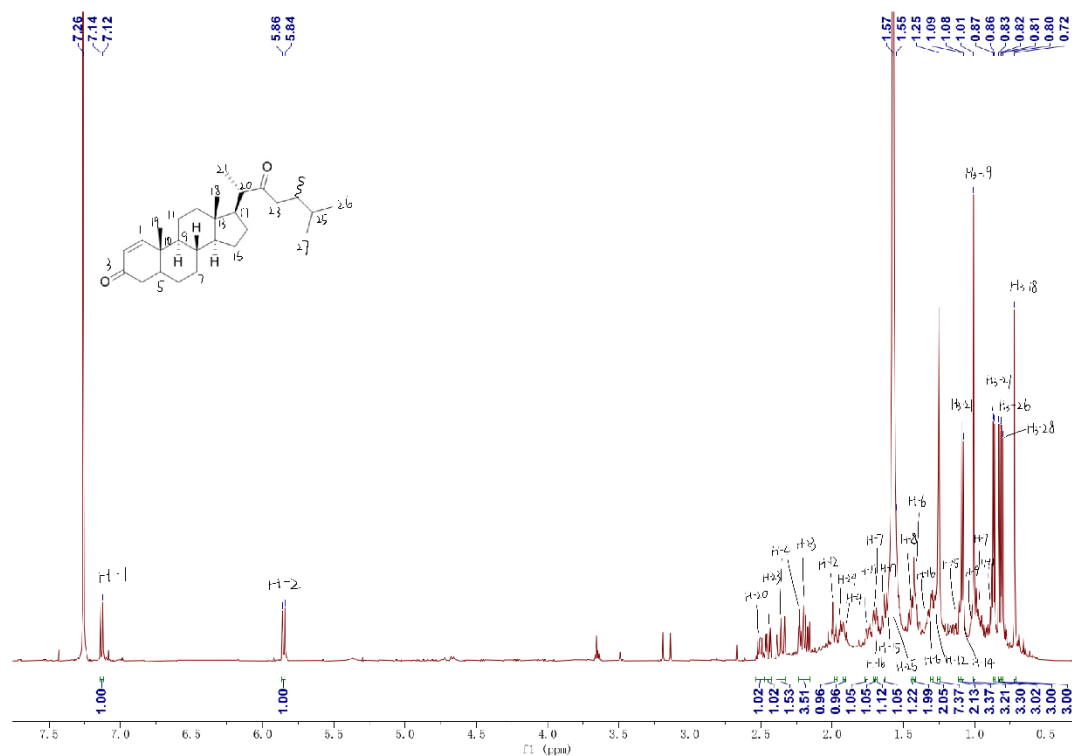


Figure S32. IR spectrum of compound **4**.

5. Spectra of compound 5



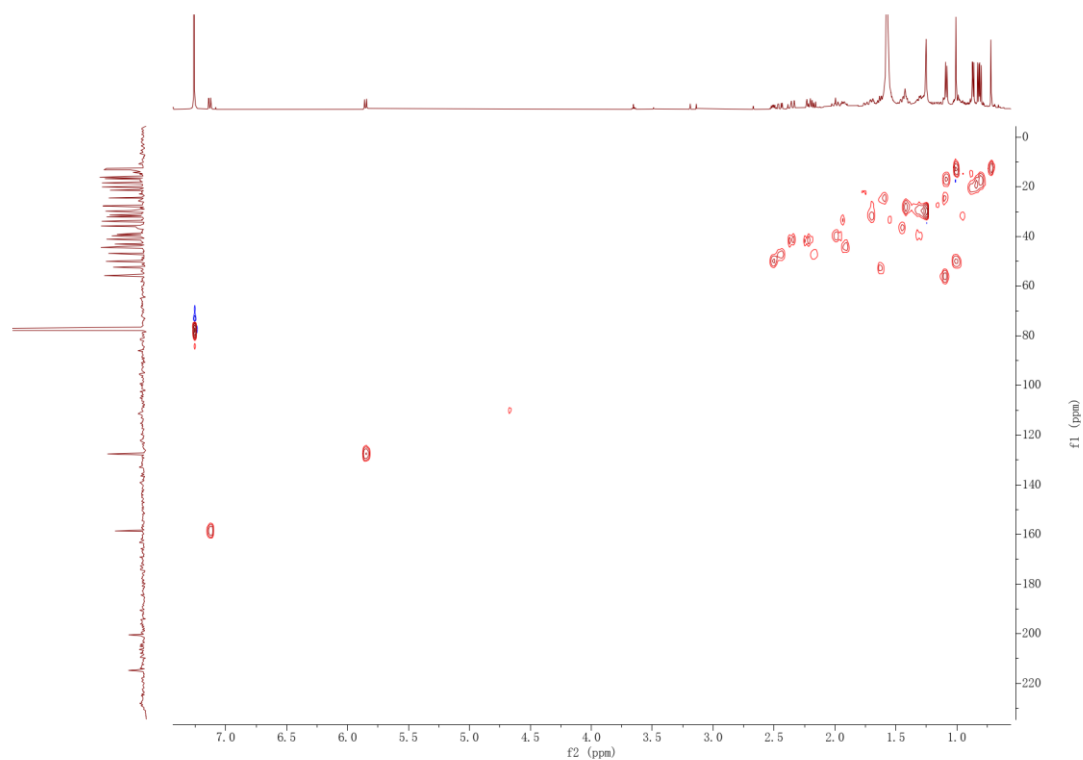


Figure S35. HSQC spectrum (600 MHz) of compound **5** in CDCl_3 .

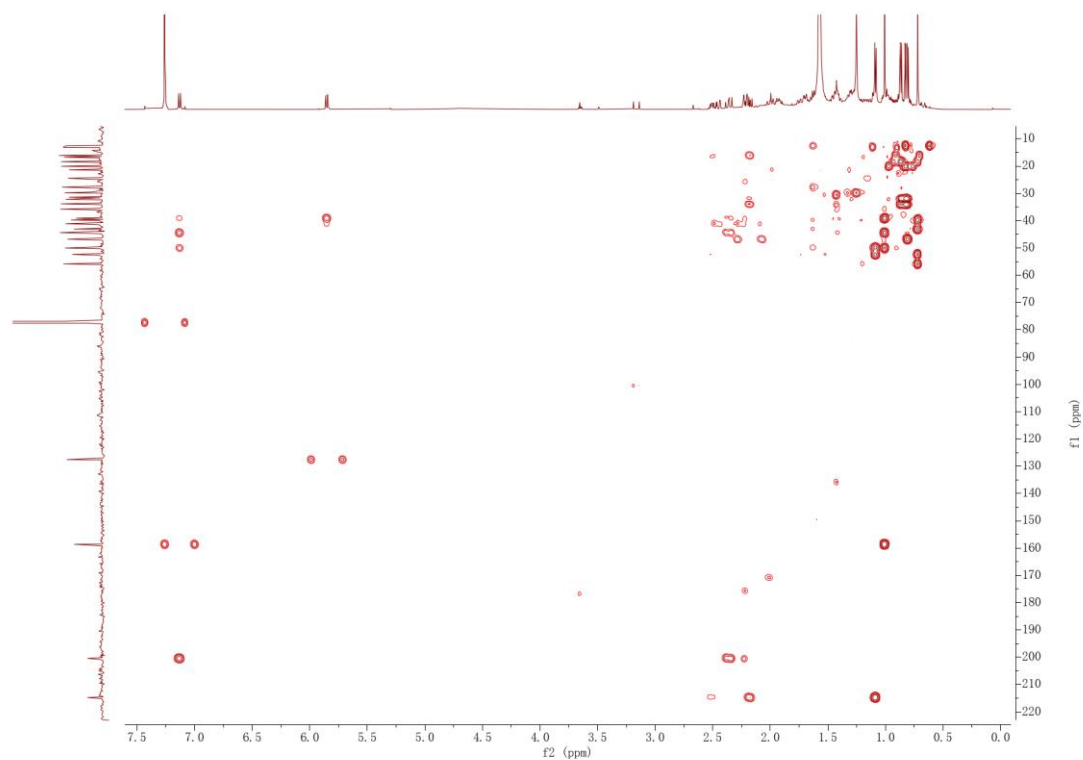


Figure S36. HMBC spectrum (600 MHz) of compound **5** in CDCl_3 .

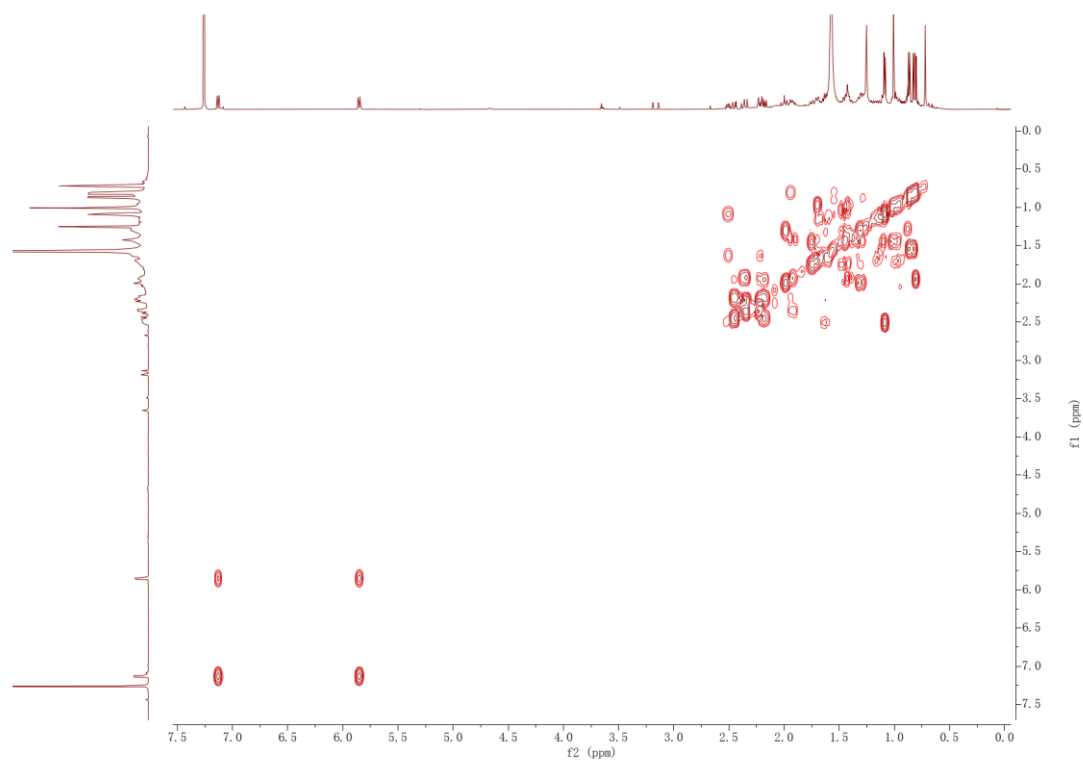


Figure S37. ^1H - ^1H COSY spectrum (600 MHz) of compound **5** in CDCl_3 .

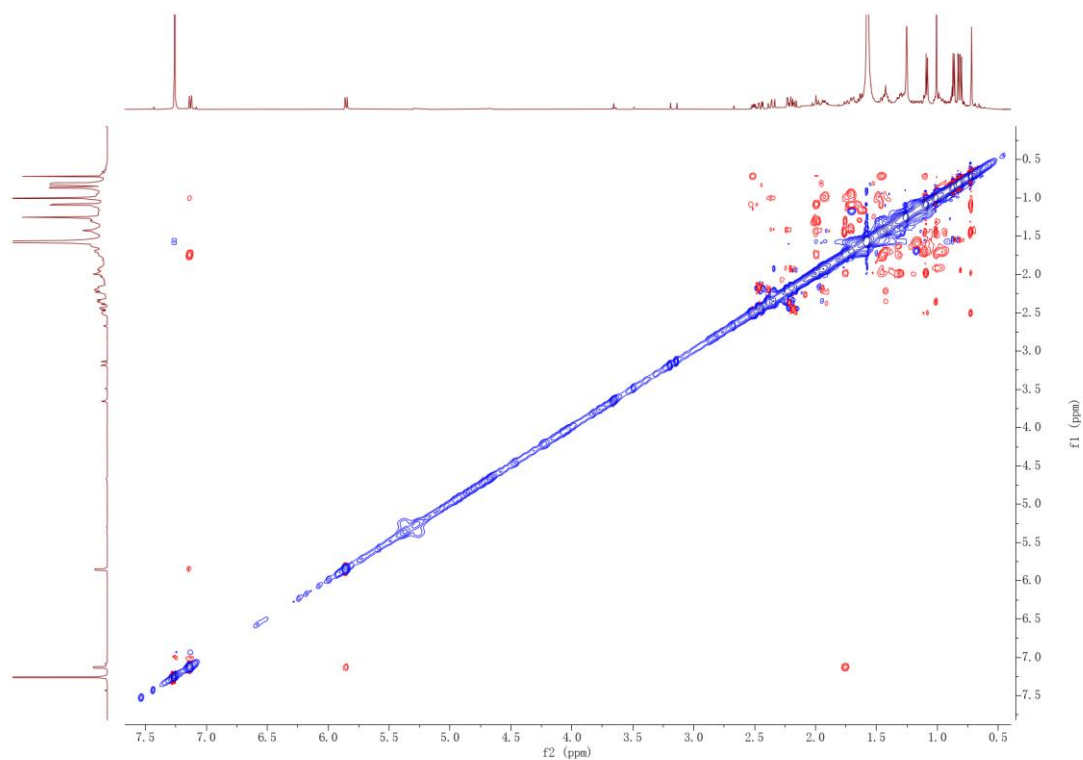
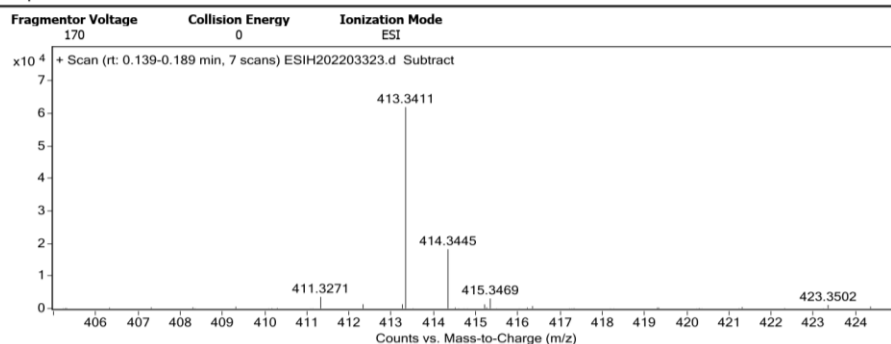


Figure S38. ROESY spectrum (600 MHz) of compound **5** in CDCl_3 .

Data Filename	ESI202203323.d	Sample Name	A8-A8-ADBAE12
Sample ID		Position	P1-F4
Instrument Name	Agilent G6520 Q-TOF	Acq Method	20160322_MS_ESIH_POS_1min.m
Acquired Time	9/14/2022 15:22:02	IRM Calibration Status	Success
DA Method	small molecular data analysis method.m	Comment	ESIH by fangsu

User Spectra



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
413.3411	413.3414	0.27	0.65	C28 H45 O2	(M+H)+

Figure S39. HR-ESIMS spectrum of compound **5**.

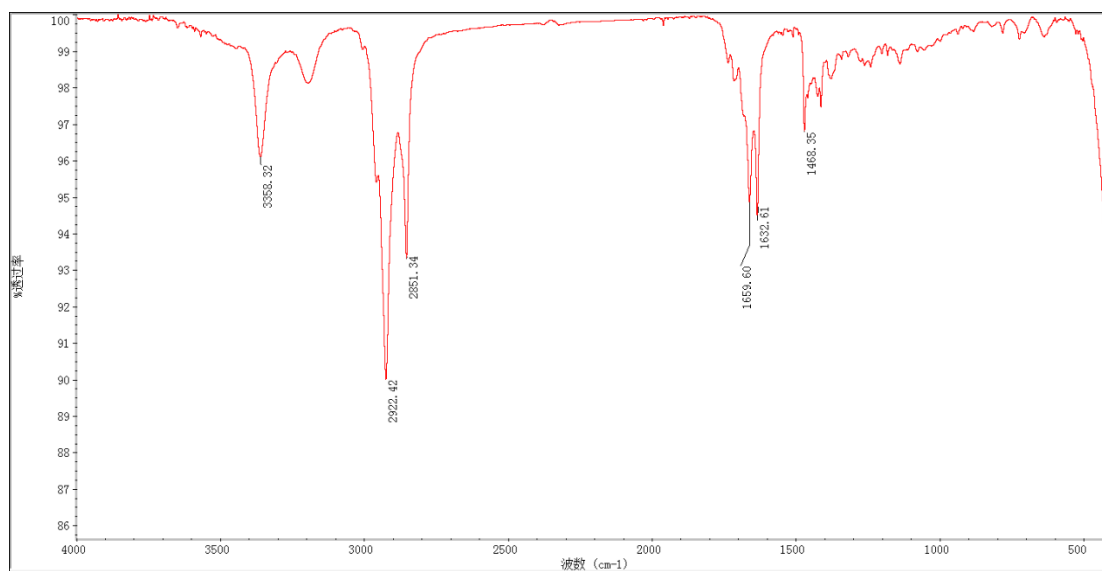
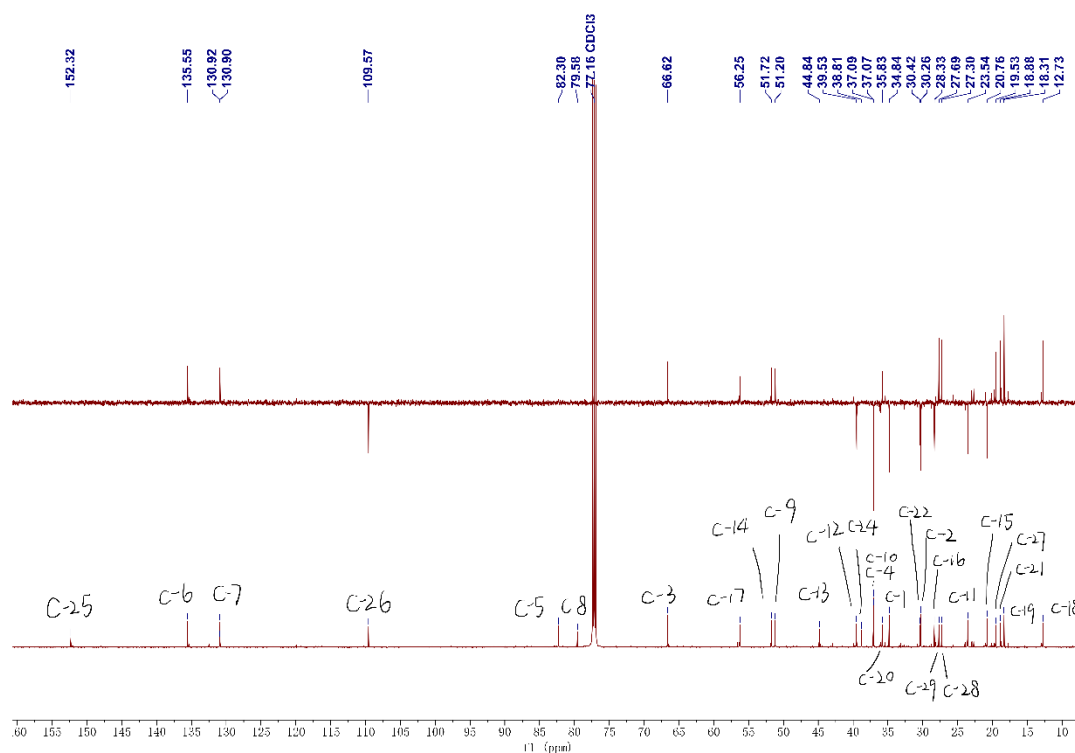
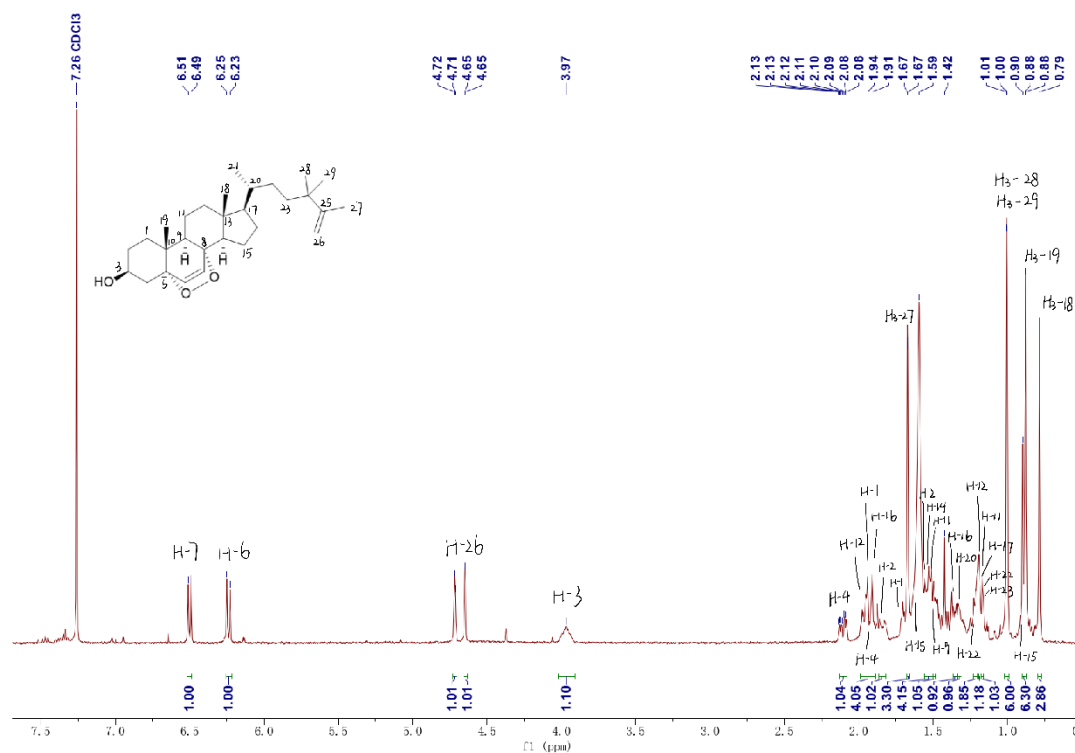


Figure S40. IR spectrum of compound **5**.

6. Spectra of compound 6



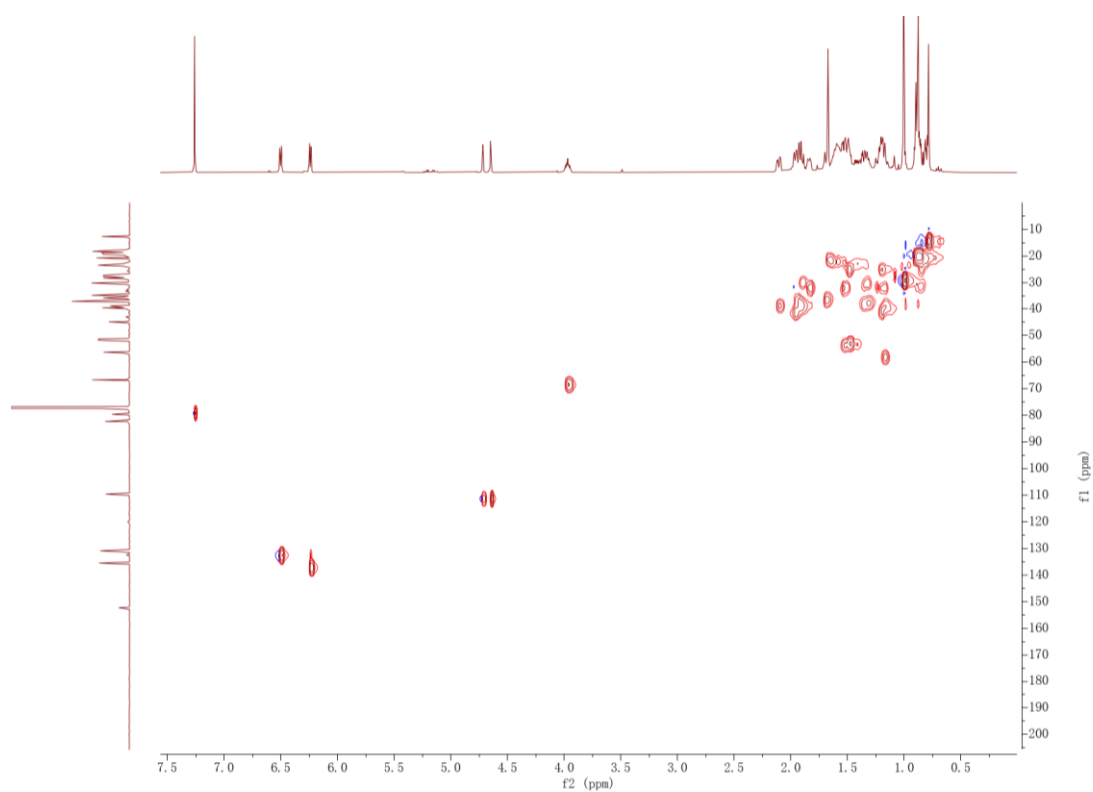


Figure S43. HSQC spectrum (600 MHz) of compound **6** in CDCl₃.

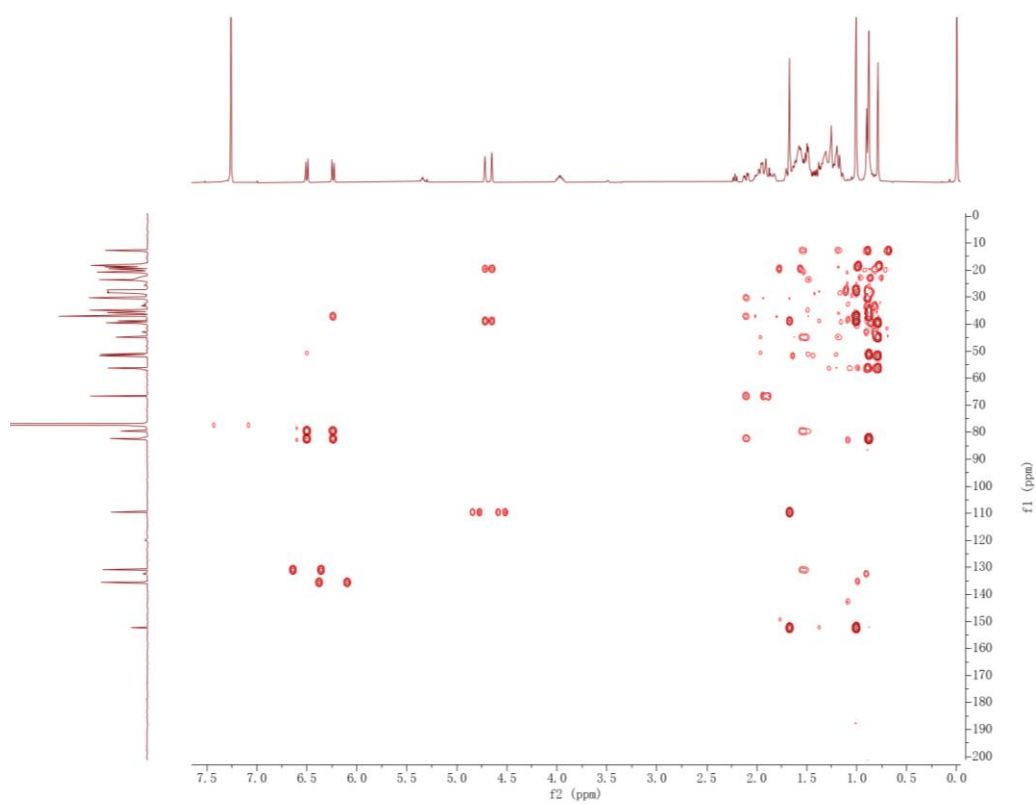


Figure S44. HMBC spectrum (600 MHz) of compound **6** in CDCl₃.

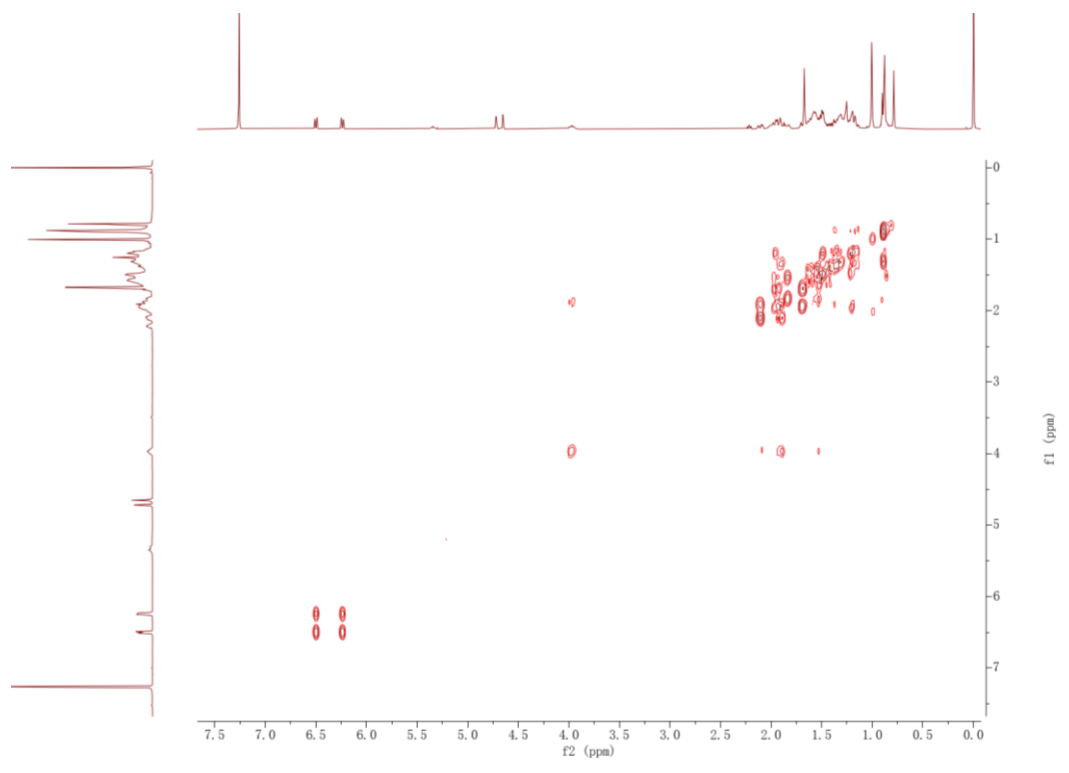


Figure S45. ^1H - ^1H COSY spectrum (600 MHz) of compound **6** in CDCl_3 .

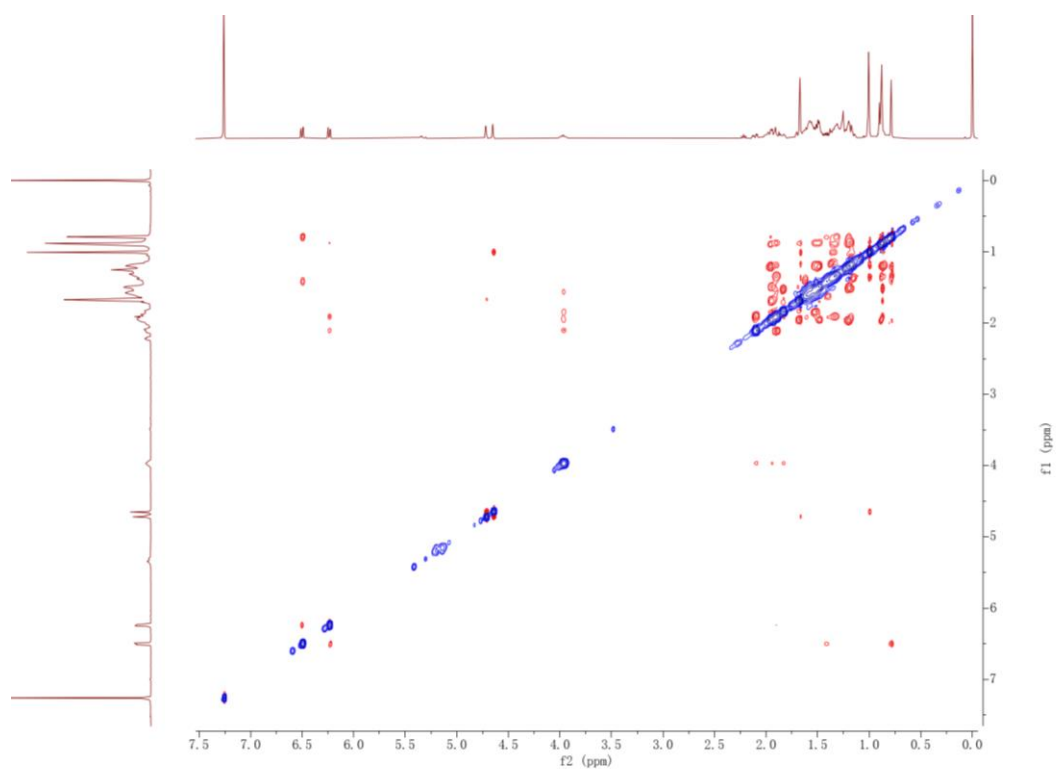


Figure S46. NOESY spectrum (600 MHz) of compound **6** in CDCl_3 .

EI202300247_A8-2CBgCD-7 -c1#17 RT: 3.30

T: + c EI Full ms [49.50-800.50]

m/z= 48-803

m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	RDB equiv.	Composition
69.0692	2526253.0	14.16	69.0699	-0.67	1.5	C ₅ H ₉
79.0176	1227372.0	6.88	79.0178	-0.23	4.5	C ₅ H ₃ O ₁
93.0697	1596930.0	8.95	93.0699	-0.15	3.5	C ₇ H ₉
95.0865	1721079.0	9.65	95.0855	0.97	2.5	C ₇ H ₁₁
119.0858	1105517.0	6.20	119.0855	0.27	4.5	C ₉ H ₁₁
121.1009	849310.0	4.76	121.1012	-0.23	3.5	C ₉ H ₁₃
123.1161	662506.0	3.71	123.1168	-0.69	2.5	C ₉ H ₁₅
131.0844	863563.0	4.84	131.0855	-1.09	5.5	C ₁₀ H ₁₁
133.1005	884241.0	4.96	133.1012	-0.70	4.5	C ₁₀ H ₁₃
137.1317	646525.0	3.62	137.1325	-0.77	2.5	C ₁₀ H ₁₇
143.0848	1464170.0	8.21	143.0855	-0.71	6.5	C ₁₁ H ₁₁
145.1009	1483471.0	8.32	145.1012	-0.29	5.5	C ₁₁ H ₁₃
152.0828	1155889.0	6.48	152.0832	-0.35	4.0	C ₉ H ₁₂ O ₂
157.1010	1241274.0	6.96	157.1012	-0.20	6.5	C ₁₂ H ₁₃
158.1074	1285518.0	7.21	158.1090	-1.55	6.0	C ₁₂ H ₁₄
159.1150	1343098.0	7.53	159.1168	-1.79	5.5	C ₁₂ H ₁₅
161.0947	745542.0	4.18	161.0961	-1.39	5.5	C ₁₁ H ₁₃ O ₁
171.1161	1103951.0	6.19	171.1168	-0.71	6.5	C ₁₃ H ₁₅
183.1162	778880.0	4.37	183.1168	-0.63	7.5	C ₁₄ H ₁₅
185.1315	889154.0	4.99	185.1325	-1.01	6.5	C ₁₄ H ₁₇
197.1324	1271589.0	7.13	197.1325	-0.06	7.5	C ₁₅ H ₁₇
199.1478	937934.0	5.26	199.1481	-0.32	6.5	C ₁₅ H ₁₉
209.1330	627898.0	3.52	209.1325	0.51	8.5	C ₁₆ H ₁₇
211.1466	1328899.0	7.45	211.1481	-1.50	7.5	C ₁₆ H ₁₉
249.1640	669200.0	3.75	249.1638	0.25	9.5	C ₁₉ H ₂₁
251.1779	1080331.0	6.06	251.1794	-1.50	8.5	C ₁₉ H ₂₃
253.1954	798748.0	4.48	253.1951	0.36	7.5	C ₁₉ H ₂₅
267.1750	725700.0	4.07	267.1743	0.68	8.5	C ₁₉ H ₂₃ O ₁
271.2060	683373.0	3.83	271.2056	0.40	6.5	C ₁₉ H ₂₇ O ₁
293.1911	626252.0	3.51	293.1900	1.13	9.5	C ₂₁ H ₂₅ O ₁
341.2836	751534.0	4.21	341.2839	-0.32	6.5	C ₂₄ H ₃₇ O ₁
351.3039	3330212.0	18.67	351.3046	-0.69	7.5	C ₂₆ H ₃₉
377.3198	7690815.0	43.12	377.3203	-0.48	8.5	C ₂₈ H ₄₁
390.3278	639938.0	3.59	390.3281	-0.29	9.0	C ₂₉ H ₄₂
391.3008	912396.0	5.12	391.2995	1.21	9.5	C ₂₈ H ₃₉ O ₁
392.3418	643150.0	3.61	392.3438	-1.96	8.0	C ₂₉ H ₄₄
395.3318	706885.0	3.96	395.3308	0.99	7.5	C ₂₈ H ₄₃ O ₁
406.3231	953240.0	5.34	406.3230	0.06	9.0	C ₂₉ H ₄₂ O ₁
410.3547	17835264.0	100.00	410.3543	0.36	7.0	C ₂₉ H ₄₆ O ₁
424.3325	1101792.0	6.18	424.3336	-1.11	8.0	C ₂₉ H ₄₄ O ₂

Figure S47. HR-EIMS spectrum of compound 6.

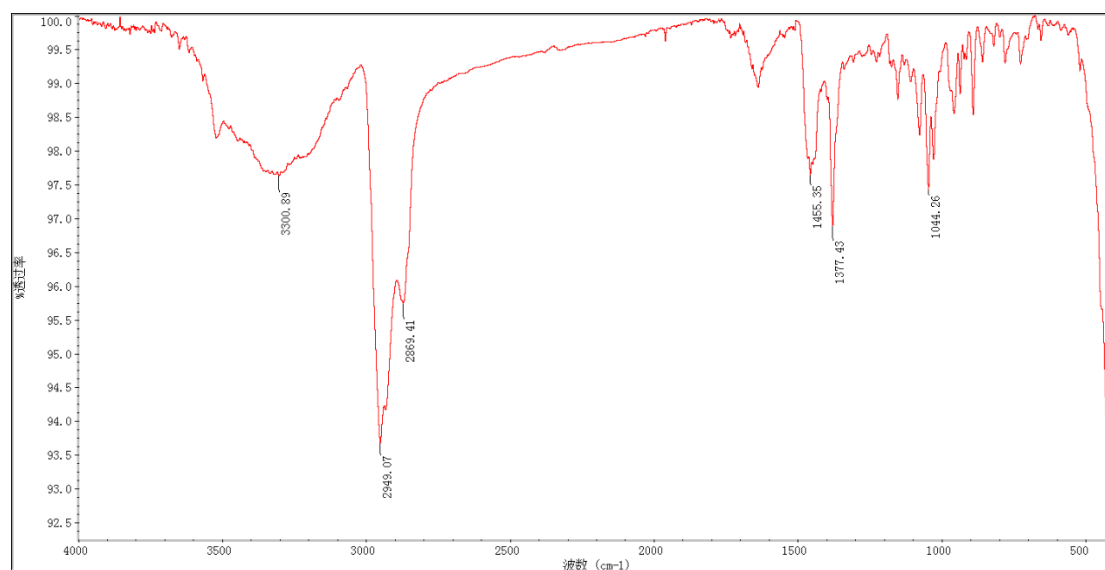


Figure S48. IR spectrum of compound **6**.