

SUPPLEMENTARY MATERIAL

Chemical constituents of *Thesium chinense* Turcz and their in vitro antioxidant, anti-inflammatory and cytotoxic activities

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Content

Fig. S1. The ¹ H NMR spectrum of compound 1	1
Fig. S2. The ³ C-DEPT-135 spectrum of compound 1	1
Fig. S3. The ¹³ C NMR spectrum of compound 1	1
Fig. S4. The HSQC spectrum of compound 1	2
Fig. S5. The HMBC spectrum of compound 1	2
Fig. S6. ¹ H- ¹ H COSY spectrum of compound 1	3
Fig. S7. The NOESY spectrum of compound 1	3
Fig. S8. The MS-ESI spectrum of compound 1	4
Fig. S9. The HRMS-ESI spectrum of compound 1	4
Fig. S10. The IR spectrum of compound 1	5
Fig. S11. The UV spectrum of compound 1	5
Fig. S12. The rotation spectrum of compound 1	5
Table S1. “GIAO” method results of 1a and 1b	6
Table S2. Energies of the calculated configuration of 1a	6
Table S3. Energies of the calculated configuration of 1b	7
Fig. S13. The ¹ H NMR spectrum of compound 2	8
Fig. S14. The ³ C-DEPT-135 spectrum of compound 2	8
Fig. S15. The ¹³ C NMR spectrum of compound 2	8
Fig. S16. The HSQC spectrum of compound 2	9
Fig. S17. The HMBC spectrum of compound 2	9

Fig. S18. ^1H - ^1H COSY spectrum of compound 2	10
Fig. S19. The MS-ESI spectrum of compound 2	11
Fig. S20. The HRMS-ESI spectrum of compound 2	11
Fig. S21. The IR spectrum of compound 2	12
Fig. S22. The UV spectrum of compound 2	12
Fig. S23. The rotation spectrum of compound 2	12
Fig. S24. The ^1H NMR spectrum of compound 3	13
Fig. S25. The ^{13}C -DEPT-135 spectrum of compound 3	13
Fig. S26. The ^{13}C NMR spectrum of compound 3	13
Fig. S27. The HSQC spectrum of compound 3	14
Fig. S28. The HMBC spectrum of compound 3	14
Fig. S29. ^1H - ^1H COSY spectrum of compound 3	15
Fig. S30. The MS-ESI spectrum of compound 3	16
Fig. S31. The HRMS-ESI spectrum of compound 3	16
Fig. S32. The IR spectrum of compound 3	17
Fig. S33. The UV spectrum of compound 3	17
Fig. S34. The rotation spectrum of compound 3	17

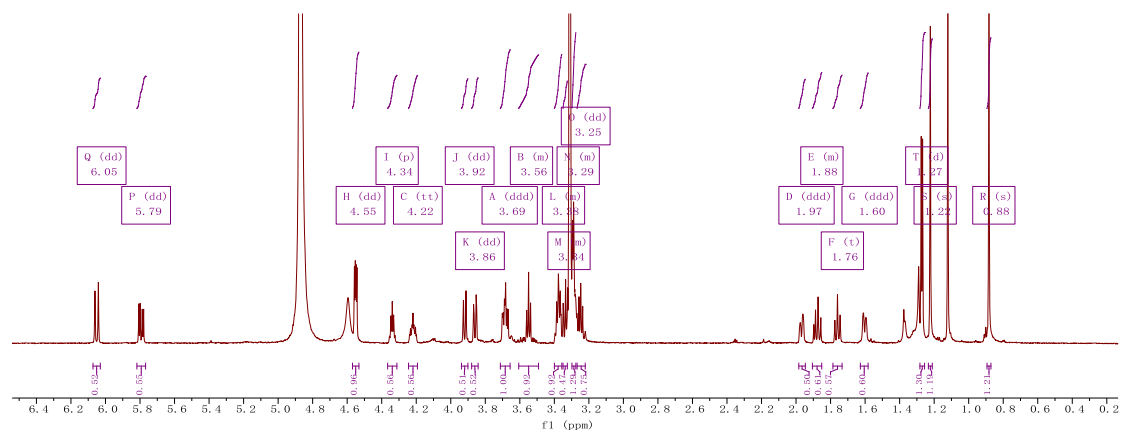


Fig. S1. The ^1H NMR spectrum (800 MHz, CD_3OD) of compound **1**.

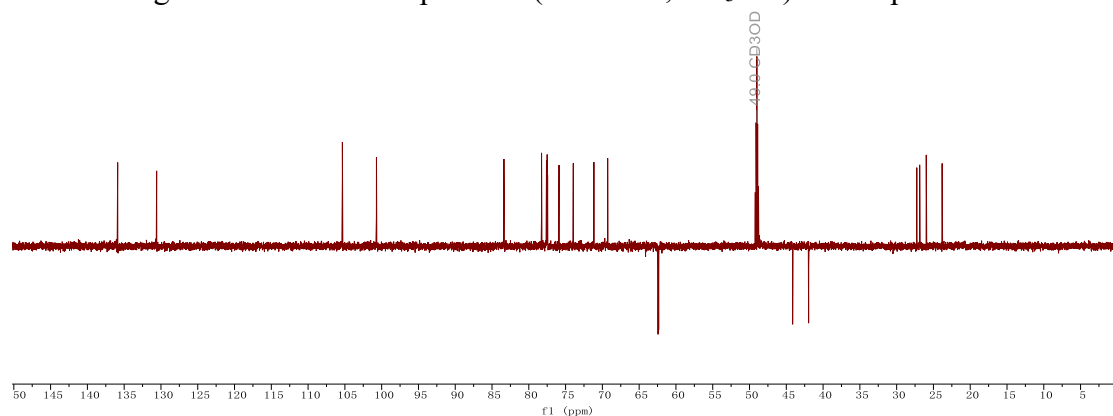


Fig. S2. The ^{13}C -DEPT-135 spectrum (2000 MHz, CD_3OD) of compound **1**.

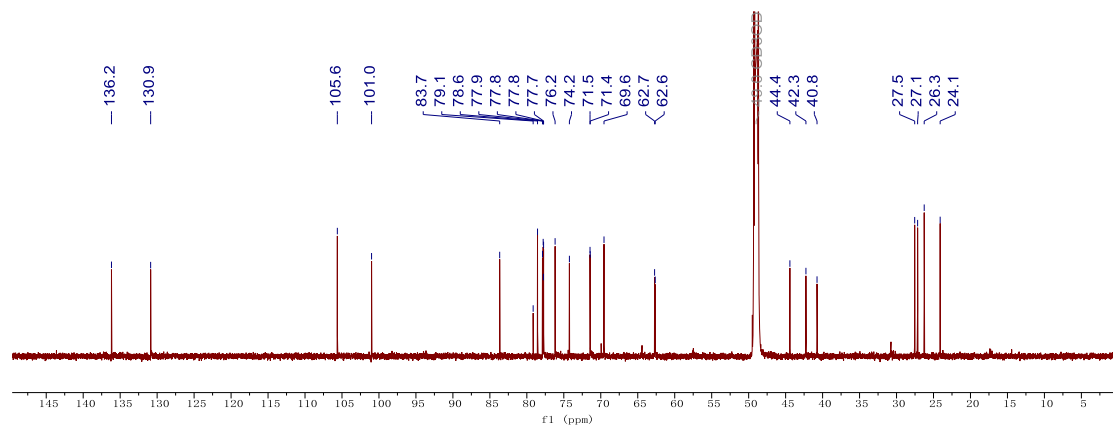


Fig. S3. The ^{13}C NMR spectrum (200 MHz, CD_3OD) of compound **1**.

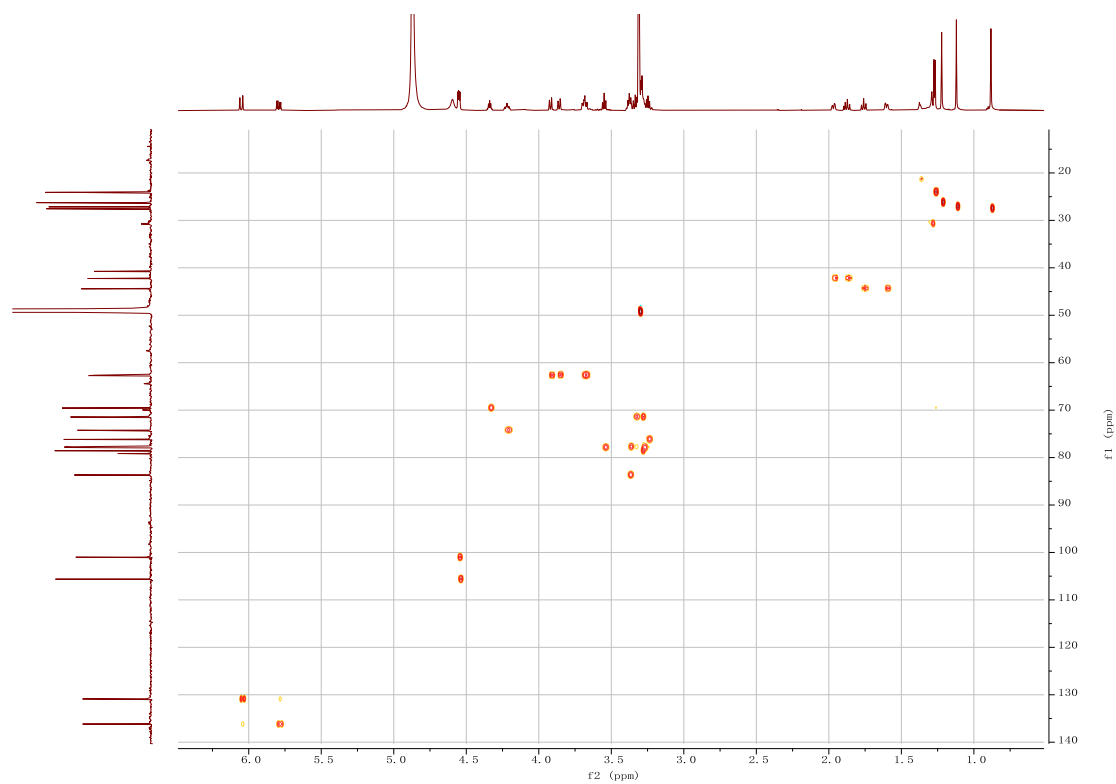


Fig. S4. The HSQC spectrum of compound **1**.

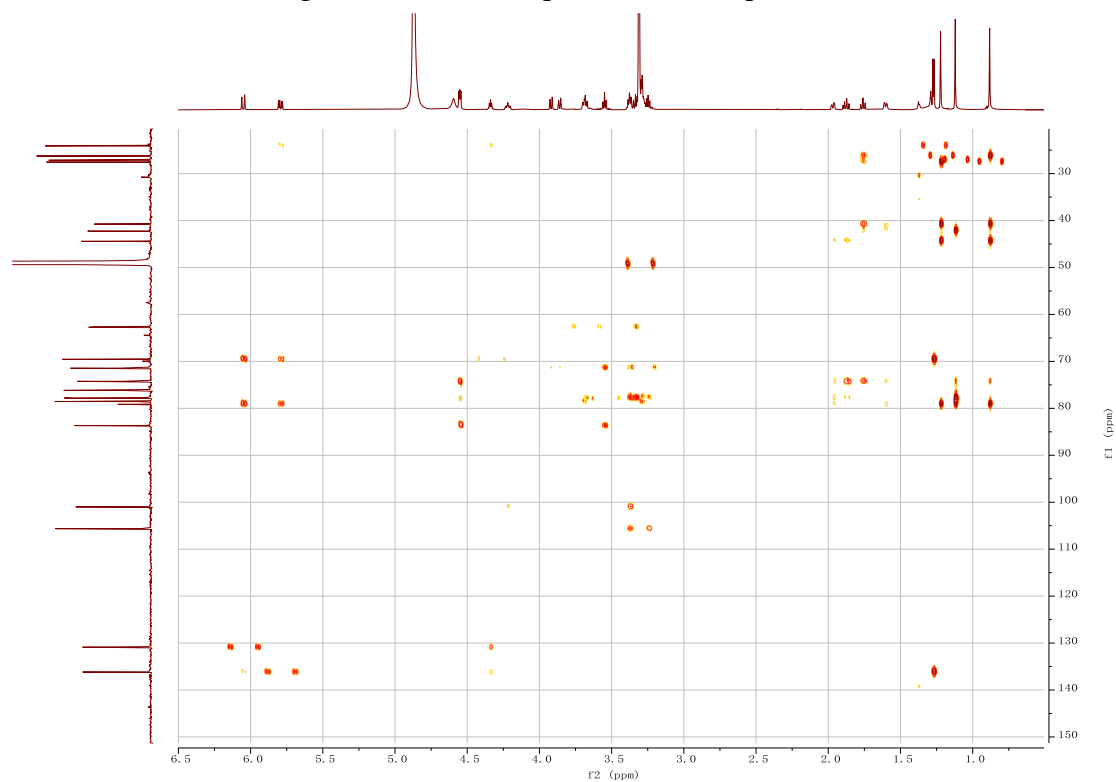


Fig. S5. The HMBC spectrum of compound **1**.

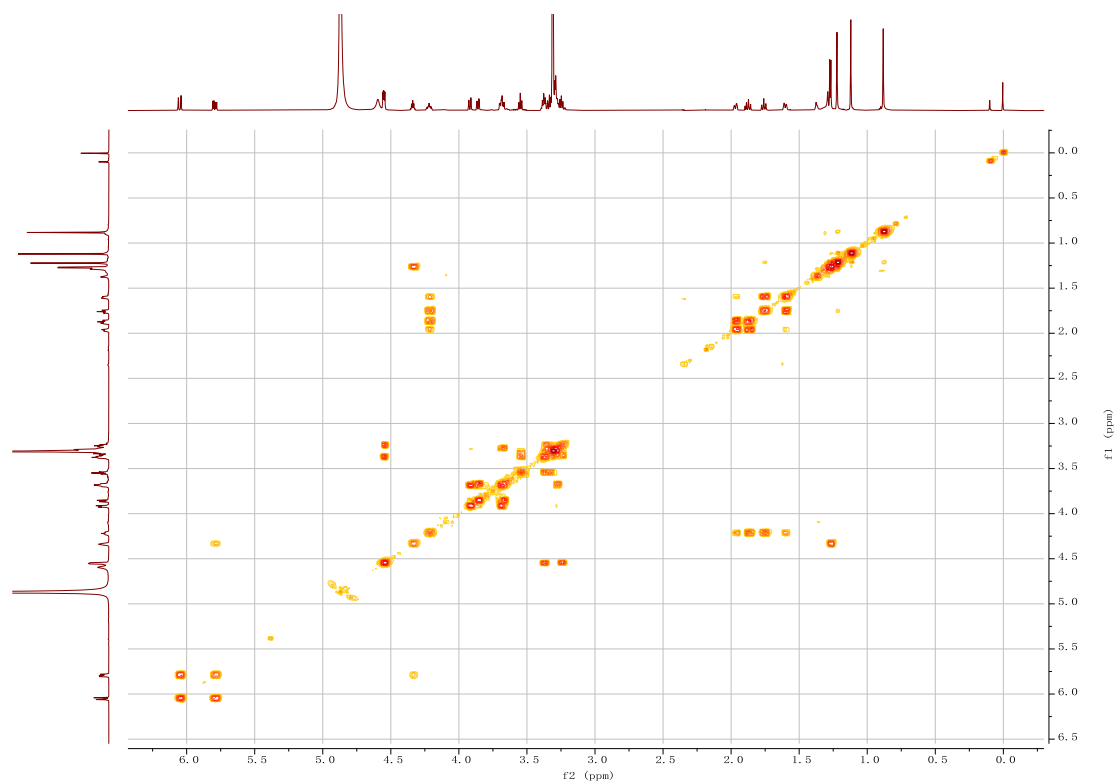


Fig. S6. ^1H - ^1H COSY spectrum of compound **1**.

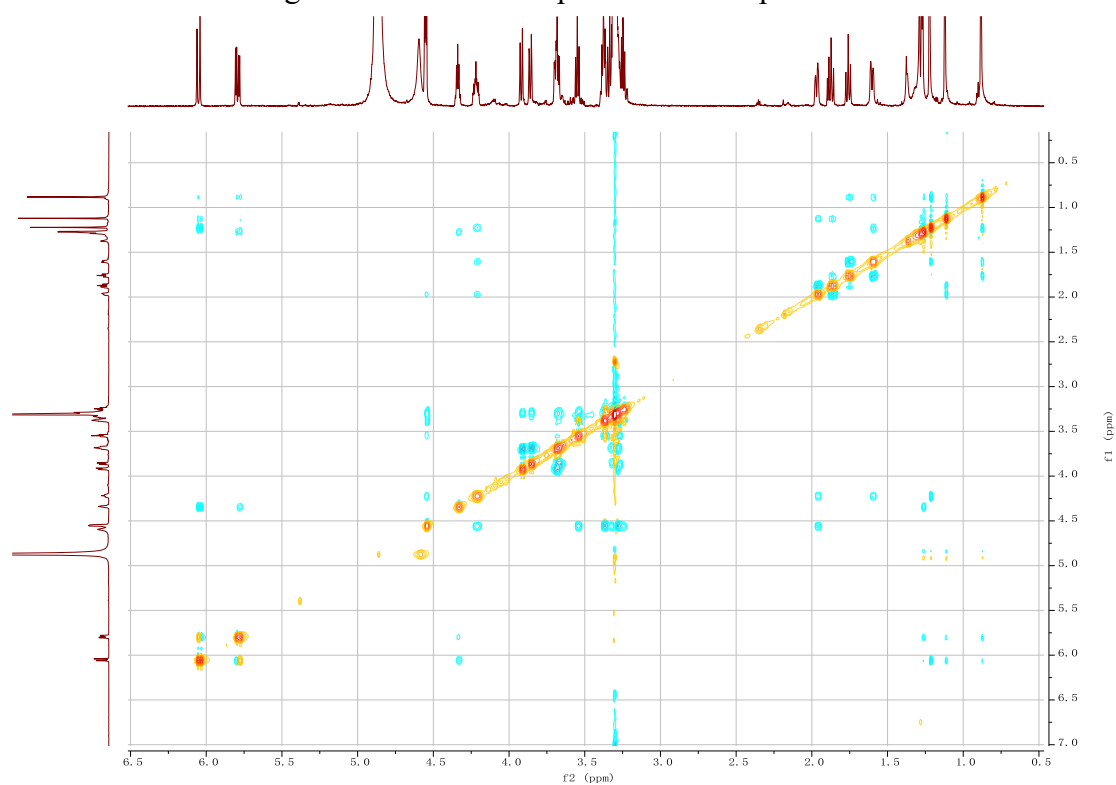


Fig. S7. The NOESY spectrum of compound **1**.

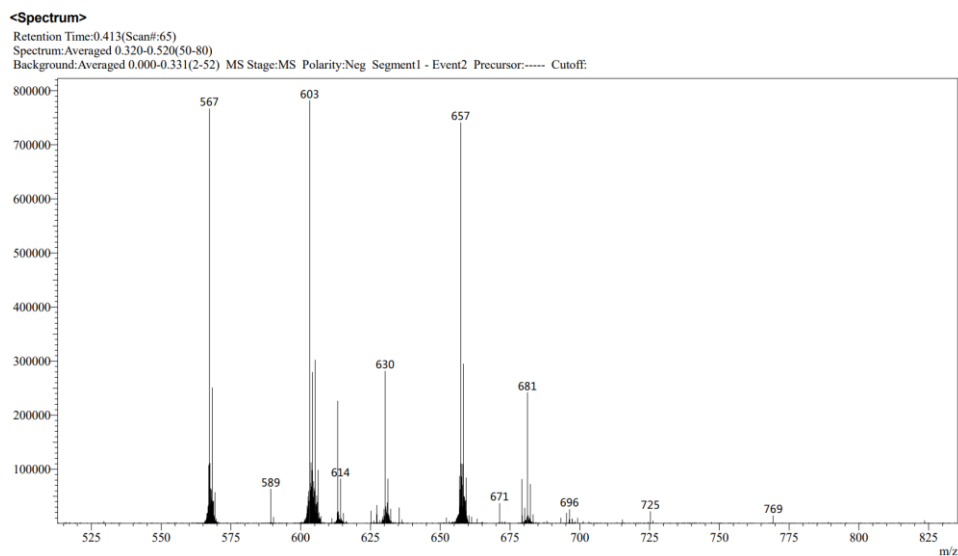


Fig. S8. MS-ESI (-) spectrum of compound **1**.

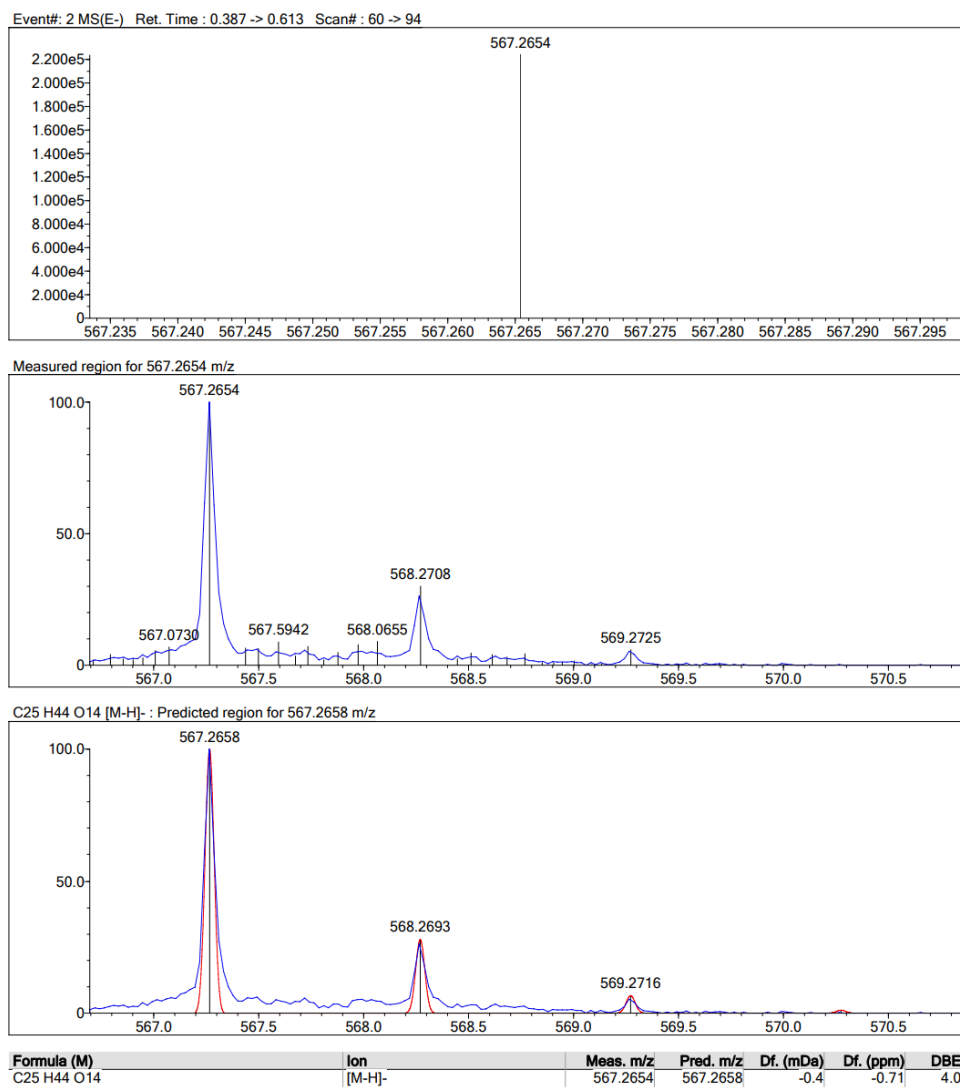


Fig. S9. HRMS-ESI (-) spectrum of compound **1**.

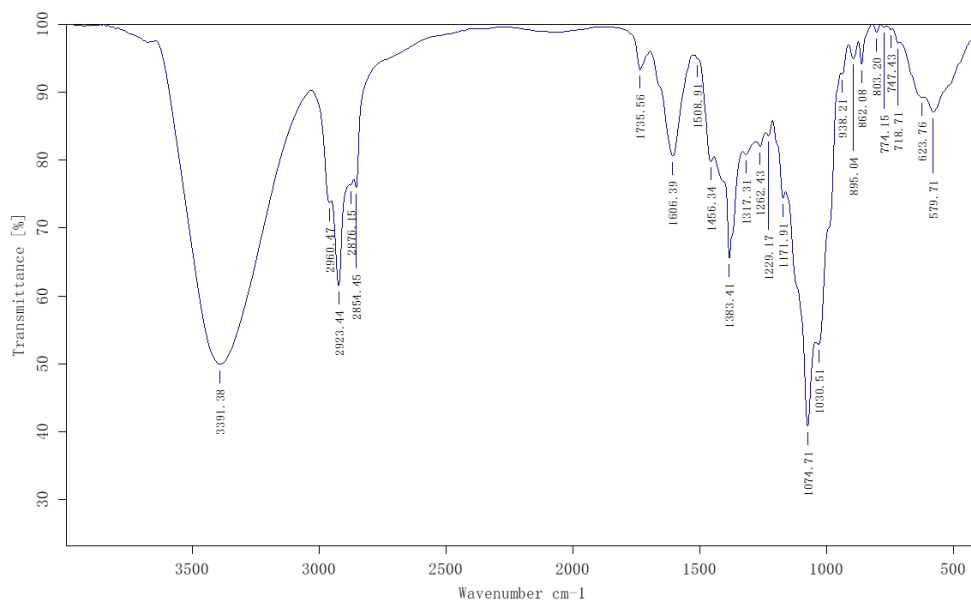


Fig. S10. IR spectrum of compound 1.

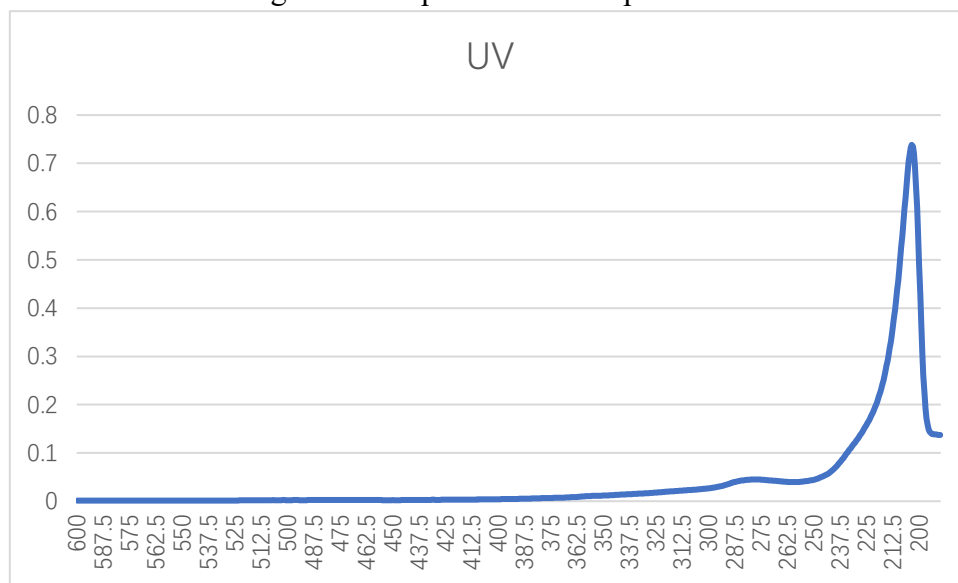


Fig. S11. UV spectrum of compound 1.

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Friday, 22-JUL-2022

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	-26.70	0.23	-0.86	-26.50	-27.10

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lq.mm	Conc.g/100ml	Temp.
1	ZL-3	01:59:44 PM	-27.10	SR	-0.0271	589	100.00	0.100	25.4
2	ZL-3	01:59:52 PM	-26.70	SR	-0.0267	589	100.00	0.100	25.5
3	ZL-3	02:00:01 PM	-26.60	SR	-0.0266	589	100.00	0.100	25.4
4	ZL-3	02:00:09 PM	-26.50	SR	-0.0265	589	100.00	0.100	25.4
5	ZL-3	02:00:17 PM	-26.60	SR	-0.0266	589	100.00	0.100	25.4

Fig. S12. Rotation spectrum of compound 1.

Table S1 Statistics of Ordinary Least Squares (OLS) Linear Regression of experimental and computed ^{13}C -NMR chemical shifts.

Configuration	DP4+ probability (%)	R^2	RMSE
1a	99.96	0.9904	3.13
1b	0.04	0.9861	3.63

Energies at M062X/6-31G(d) theory level

Energies of the calculated configuration of **1a**.

Table S2 Energies and populations of conformers of the calculated configuration.

Conformer	Population (%)	E (Hartree)
1	1.47	-2031.385069
6	44.86	-2031.388295
12	5.14	-2031.386251
18	45.94	-2031.388317
19	1.35	-2031.384992
21	1.24	-2031.384912

Energies of the calculated configuration of **1b**.

Table S3 Energies and populations of conformers of the calculated configuration.

Conformer	Population (%)	E (Hartree)
1	3.87	-2031.387785
2	5.2	-2031.388062
3	5.49	-2031.388113
4	6.49	-2031.388271
5	3.18	-2031.3876
6	4.53	-2031.387933
7	7.1	-2031.388357
8	3.44	-2031.387673
9	1.13	-2031.386623
10	1.55	-2031.386921
11	2.17	-2031.387239
12	4.15	-2031.387849
17	1.24	-2031.386711
20	3.05	-2031.387559
22	1.18	-2031.386662
24	5.55	-2031.388125
25	4.84	-2031.387995
53	1.58	-2031.386941
62	1.98	-2031.387152
66	2	-2031.387161
90	3.15	-2031.38759
92	4.61	-2031.387949
94	3.87	-2031.387784
116	5.94	-2031.388188
120	5.65	-2031.388141
122	7.07	-2031.388352

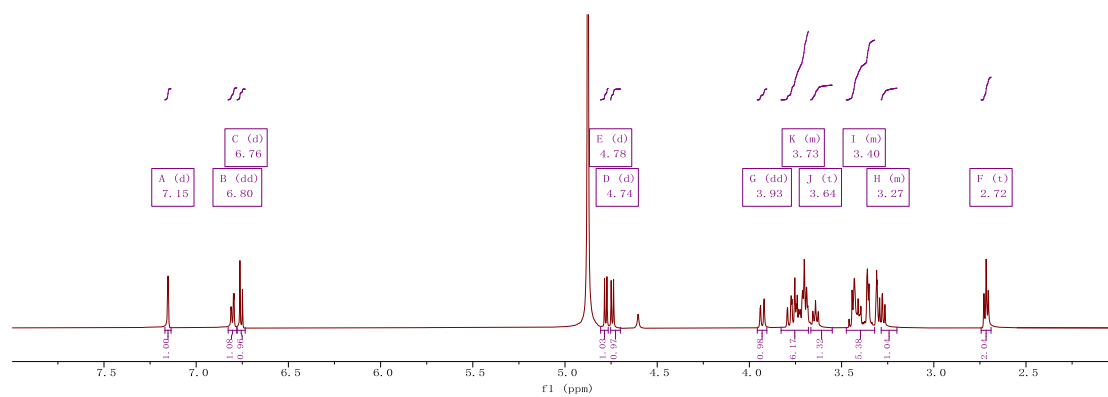


Fig. S13. The ¹H NMR spectrum (600 MHz, CD₃OD) of compound **2**.

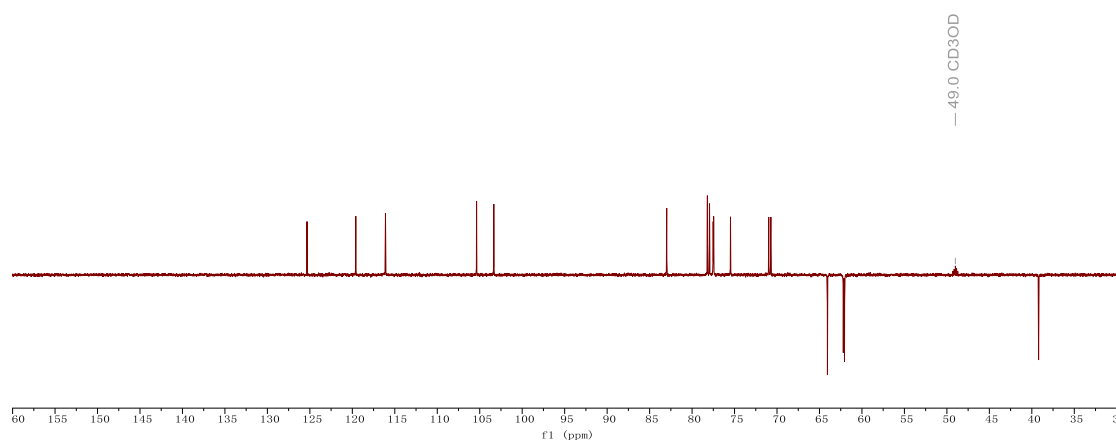


Fig. S14. The ¹³C-DEPT-135 spectrum (150 MHz, CD₃OD) of compound **2**.

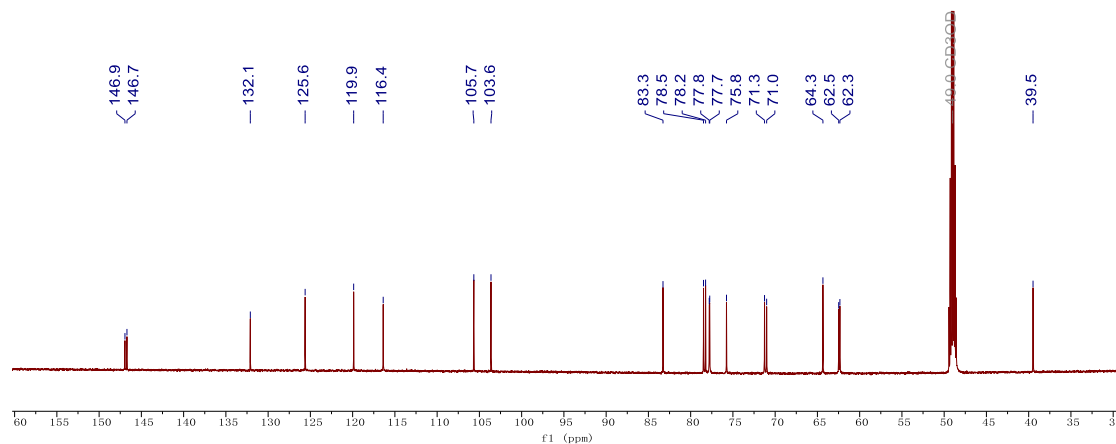


Fig. S15. The ¹³C NMR spectrum (150 MHz, CD₃OD) of compound **2**.

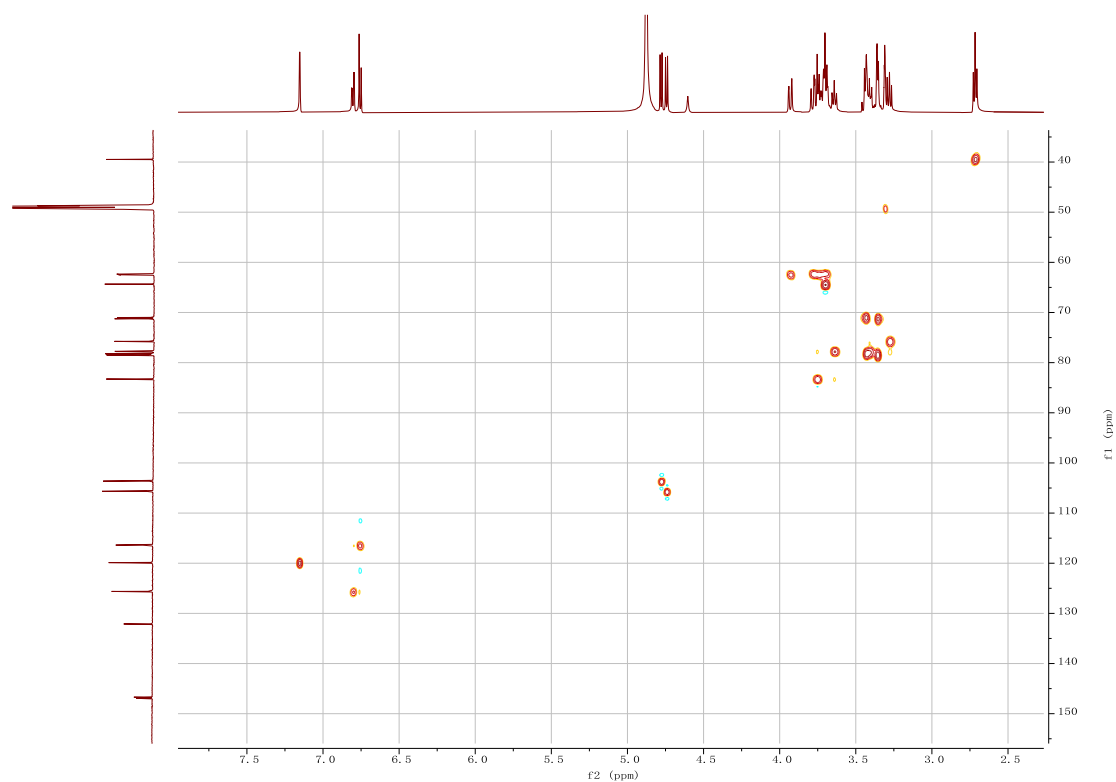


Fig. S16. The HSQC spectrum of compound **2**.

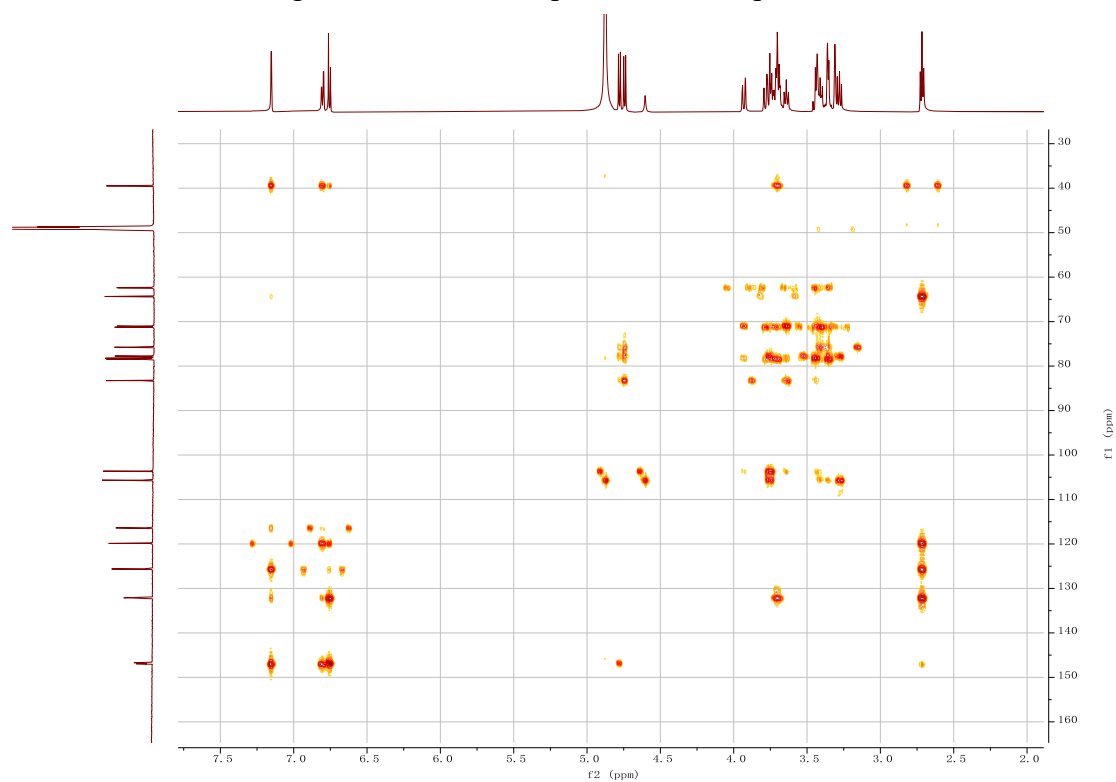


Fig. S17. The HMBC spectrum of compound **2**.

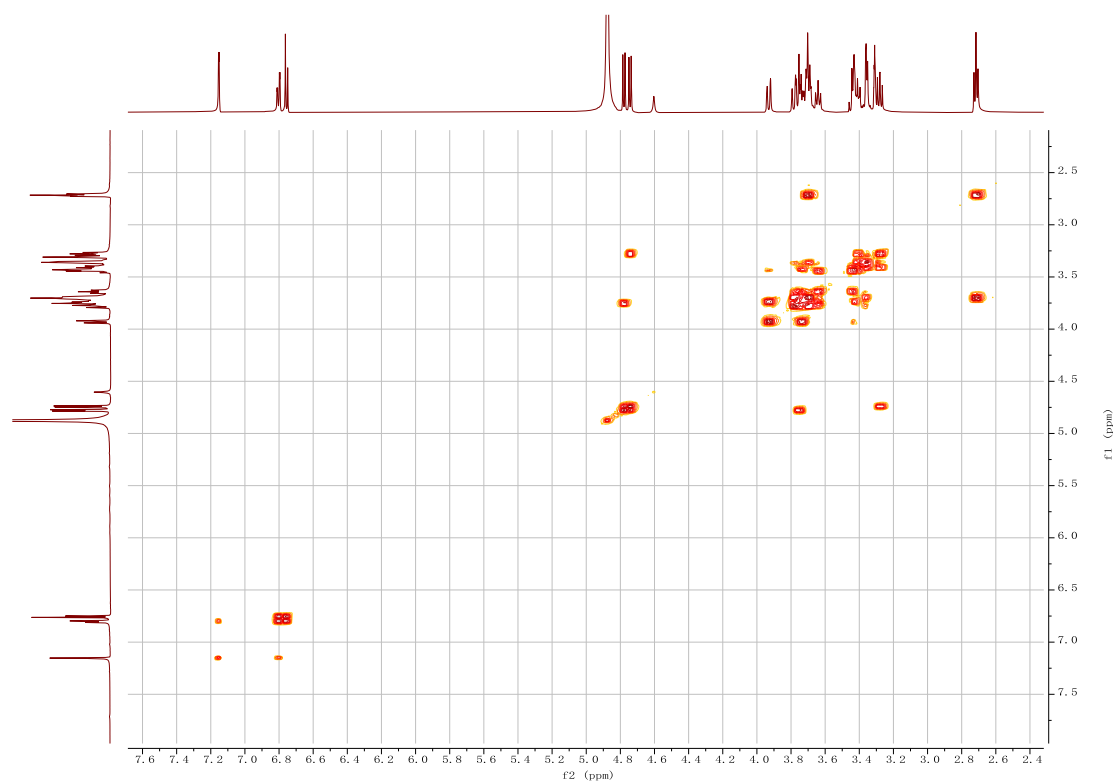


Fig. S18. ^1H - ^1H COSY spectrum of compound **2**.

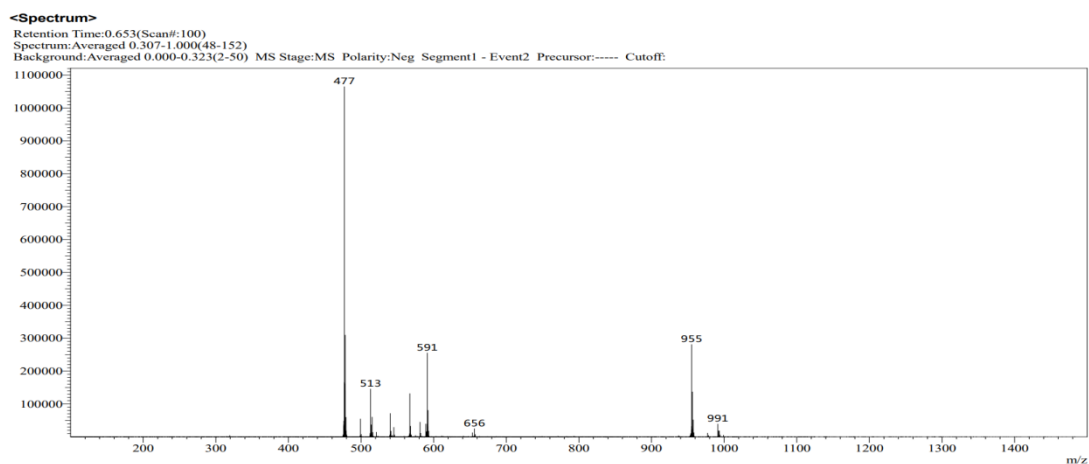


Fig. S19. MS-ESI (-) spectrum of compound **2**.

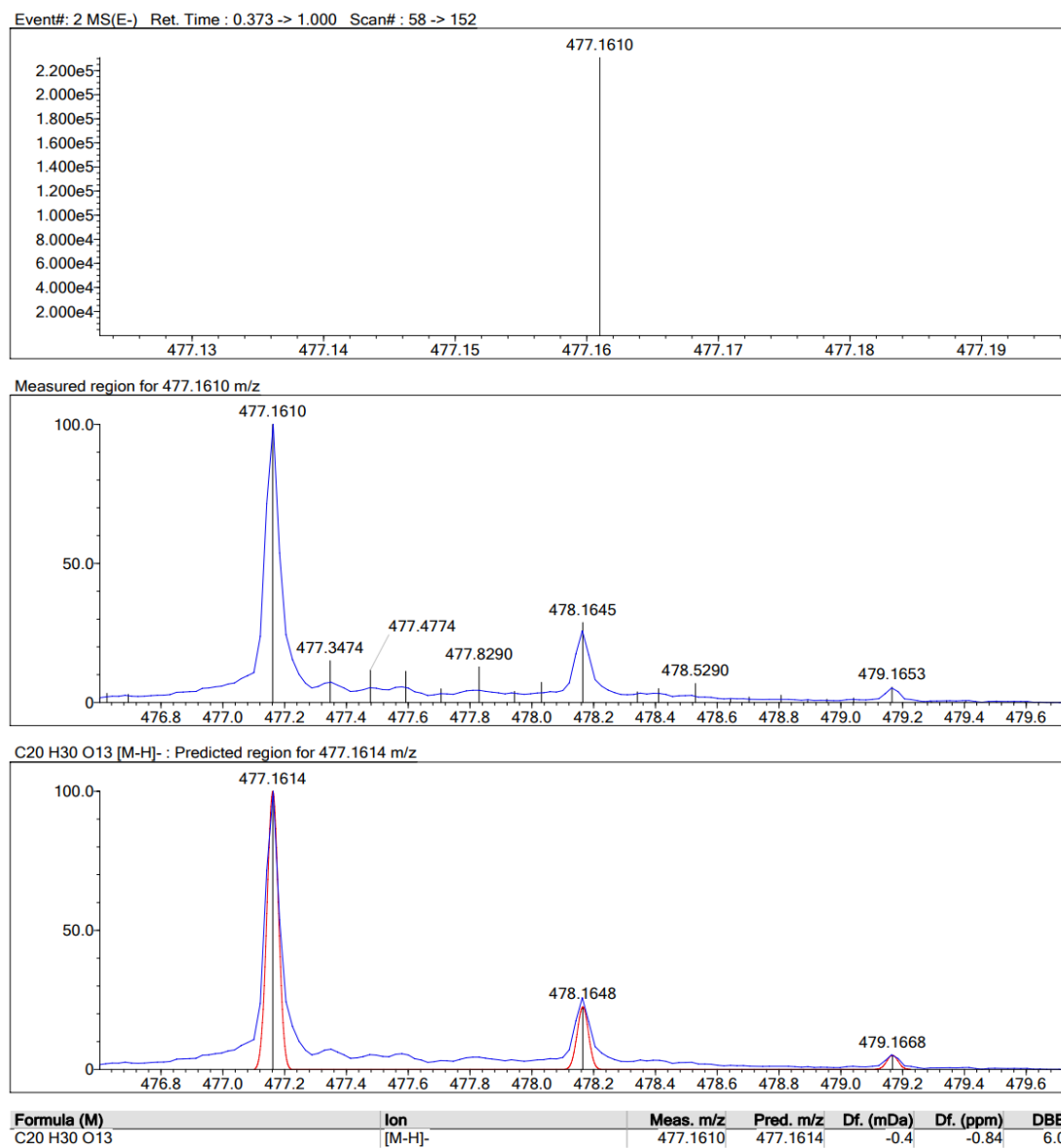


Fig. S20. HRMS-ESI (-) spectrum of compound **2**.

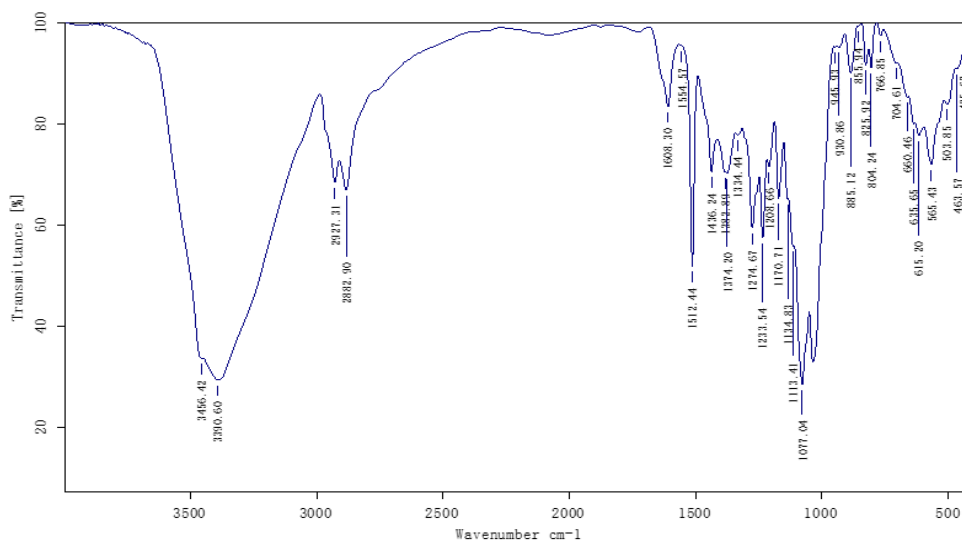


Fig. S21. IR spectrum of compound 2.

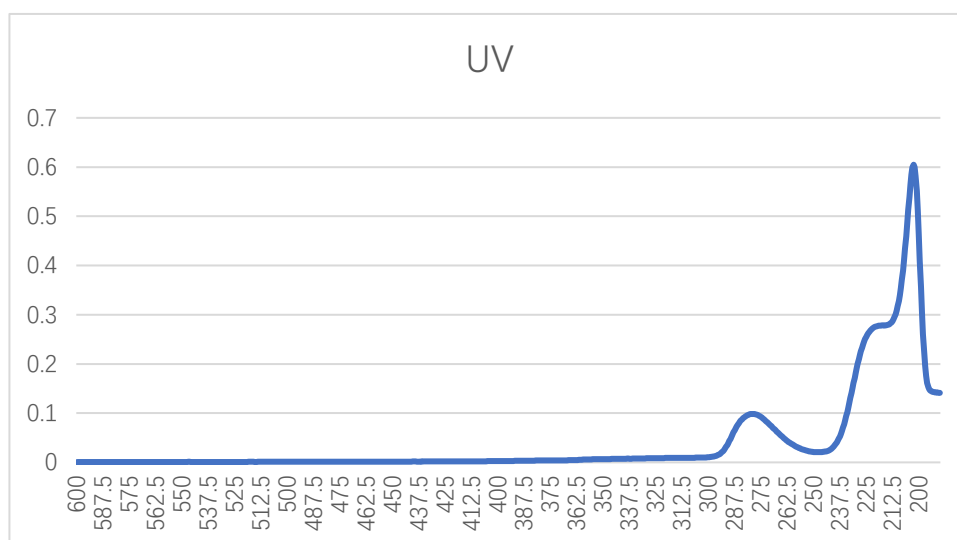


Fig. S22. UV spectrum of compound 2.

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Friday, 22-JUL-2022

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

<u>n</u>	<u>Average</u>	<u>Std.Dev.</u>	<u>% RSD</u>	<u>Maximum</u>	<u>Minimum</u>				
5	-1.20	0.10	-8.33	-1.07	-1.27				
<u>S.No</u>	<u>Sample ID</u>	<u>Time</u>	<u>Result</u>	<u>Scale</u>	<u>OR °Arc</u>	<u>WLg.nm</u>	<u>Lg.mm</u>	<u>Conc.g/100ml</u>	<u>Temp.</u>
1	ZL-5	02:06:13 PM	-1.27	SR	-0.0038	589	100.00	0.300	25.5
2	ZL-5	02:06:21 PM	-1.27	SR	-0.0038	589	100.00	0.300	25.5
3	ZL-5	02:06:30 PM	-1.27	SR	-0.0038	589	100.00	0.300	25.5
4	ZL-5	02:06:38 PM	-1.07	SR	-0.0032	589	100.00	0.300	25.5
5	ZL-5	02:06:46 PM	-1.10	SR	-0.0033	589	100.00	0.300	25.5

Fig. S23. Rotation spectrum of compound 2.

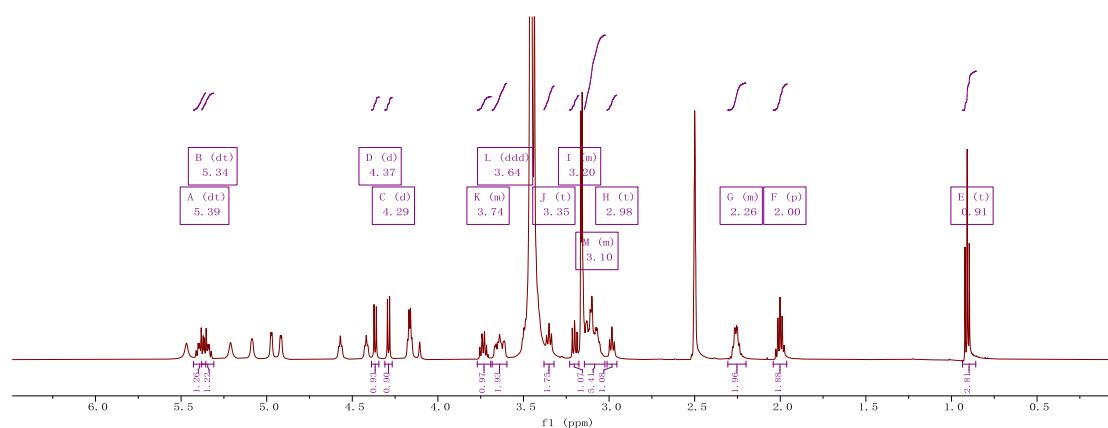


Fig. S24. The ^1H NMR spectrum (600 MHz, CD_3OD) of compound **3**.

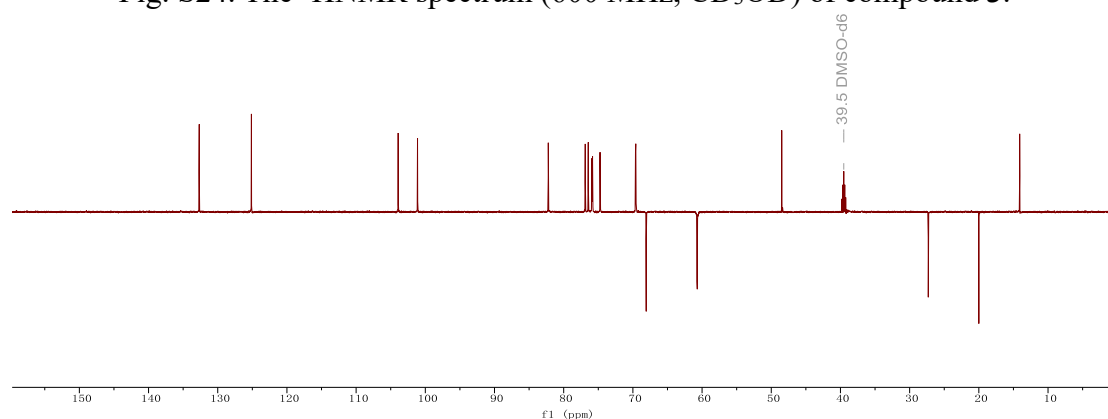


Fig. S25. The ^{13}C -DEPT-135 spectrum (150 MHz, CD_3OD) of compound **3**.

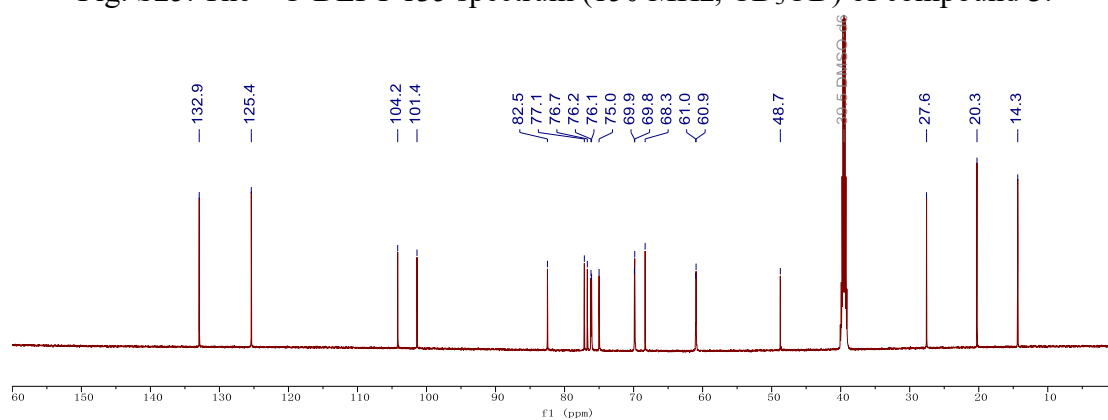


Fig. S26. The ^{13}C NMR spectrum (150 MHz, CD_3OD) of compound **3**.

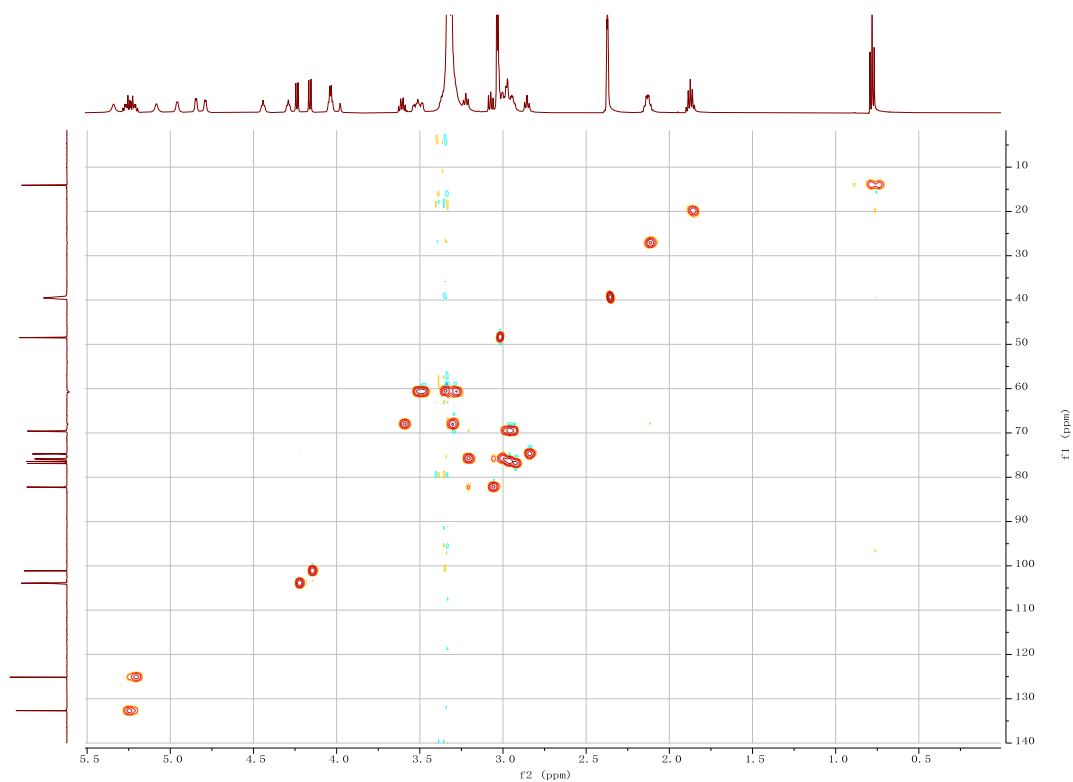


Fig. S27 The HSQC spectrum of compound **3**.

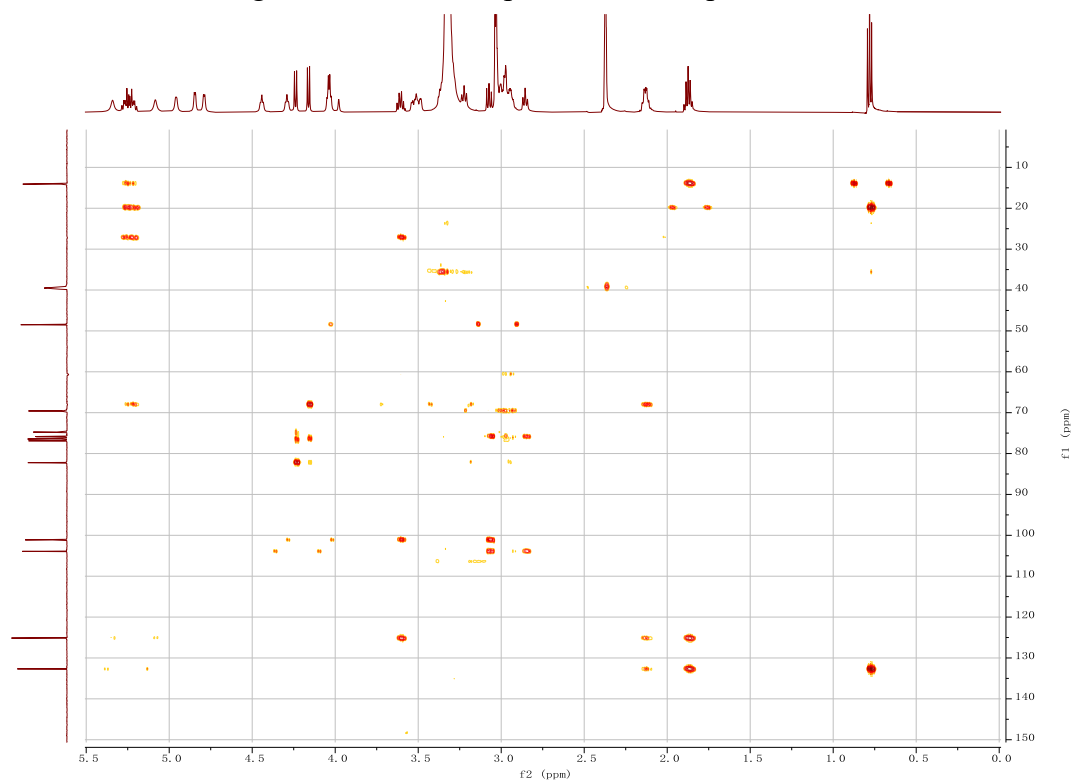


Fig. S28. The HMBC spectrum of compound **3**.

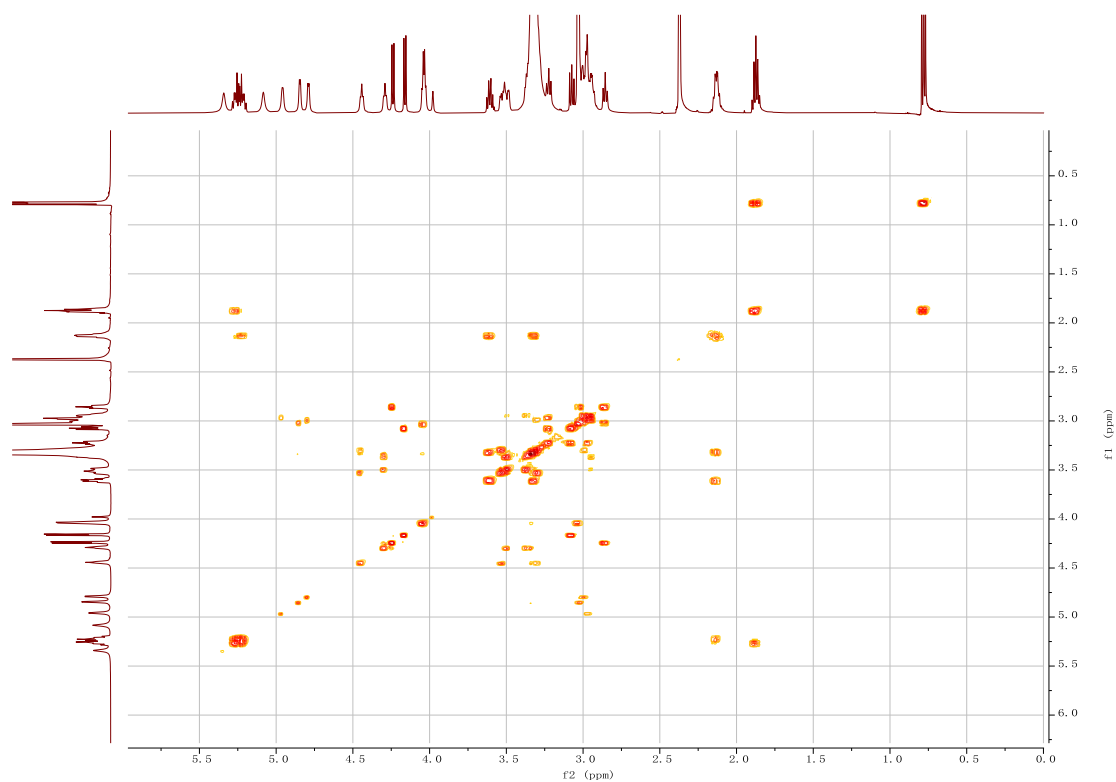


Fig. S29. ^1H - ^1H COSY spectrum of compound **3**.

<Spectrum>

Retention Time: 0.493 (Scan#: 76)
Spectrum: Averaged 0.320-0.667 (50-102)
Background: Averaged 0.000-0.303 (2-48) MS Stage: MS Polarity: Neg Segment1 - Event2 Precursor: ----- Cutoff:

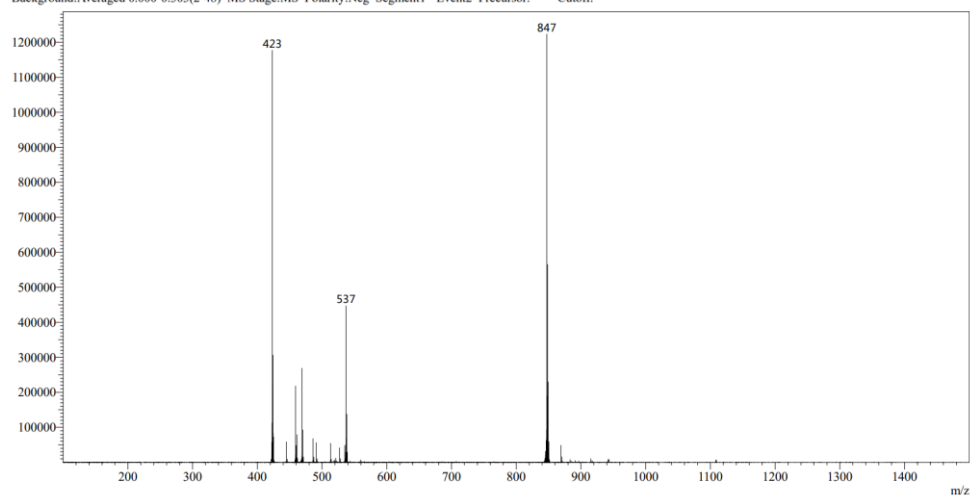
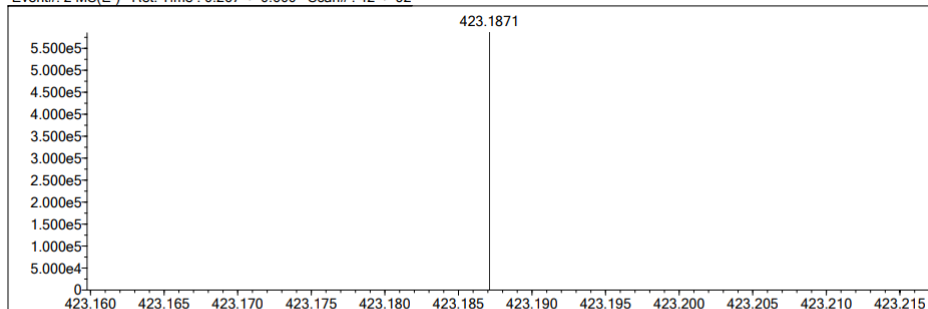
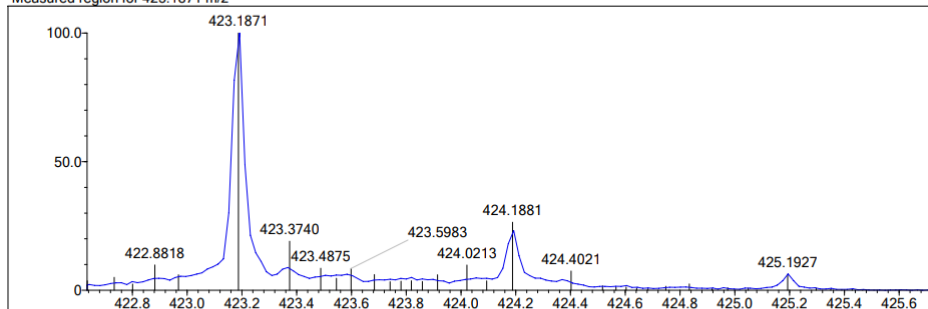


Fig. S30. MS-ESI (-) spectrum of compound **3**.

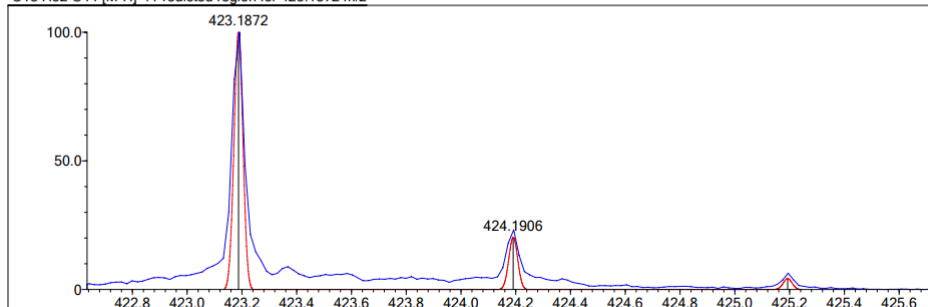
Event#: 2 MS(E-) Ret. Time : 0.267 -> 0.600 Scan#: 42 -> 92



Measured region for 423.1871 m/z



C18 H32 O11 [M-H]- : Predicted region for 423.1872 m/z



Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C18 H32 O11	[M-H]-	423.1871	423.1872	-0.1	-0.24	3.0

Fig. S31. HRMS-ESI (-) spectrum of compound **3**.

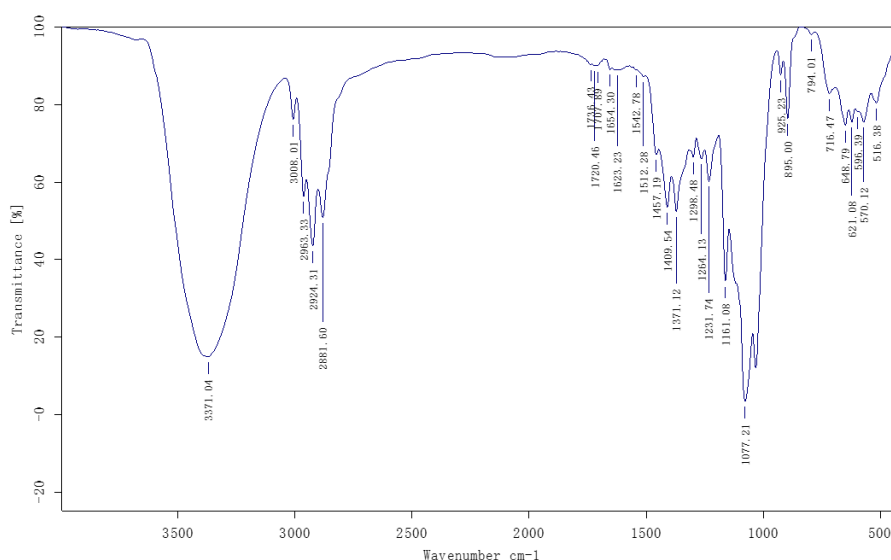


Fig..S32. IR spectrum of compound 3.

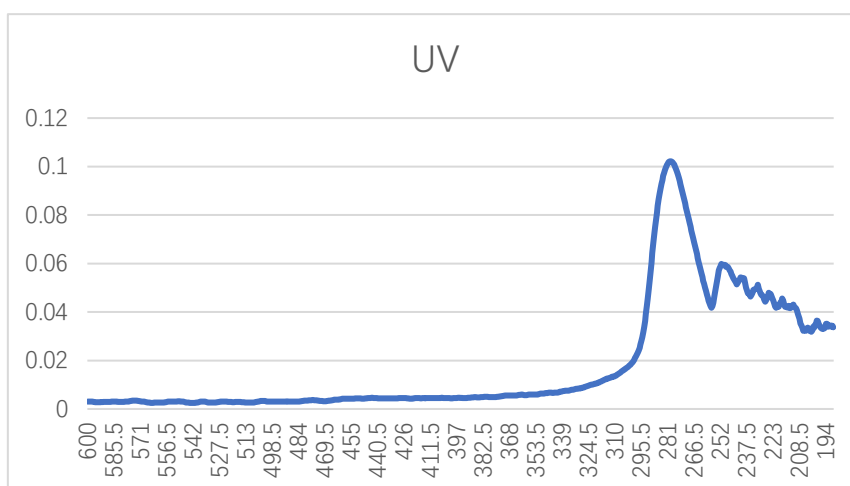


Fig. S33. UV spectrum of compound 3.

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Friday, 22-JUL-2022

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

<u>n</u>	<u>Average</u>	<u>Std.Dev.</u>	<u>% RSD</u>	<u>Maximum</u>	<u>Minimum</u>				
5	-14.22	0.13	-0.91	-14.06	-14.36				
<u>S.No</u>	<u>Sample ID</u>	<u>Time</u>	<u>Result</u>	<u>Scale</u>	<u>OR °Arc</u>	<u>WLG.nm</u>	<u>Lg.mm</u>	<u>Conc.g/100ml</u>	<u>Temp.</u>
1	ZL-2	01:28:22 PM	-14.06	SR	-0.1406	589	100.00	1.000	24.6
2	ZL-2	01:28:30 PM	-14.13	SR	-0.1413	589	100.00	1.000	24.6
3	ZL-2	01:28:38 PM	-14.36	SR	-0.1436	589	100.00	1.000	24.6
4	ZL-2	01:28:55 PM	-14.33	SR	-0.1433	589	100.00	1.000	24.6
5	ZL-2	01:29:04 PM	-14.21	SR	-0.1421	589	100.00	1.000	24.7

Fig. S34. Rotation spectrum of compound 3.