Novel metabolites from the marine-derived fungus *Peniophora* sp. SCSIO41203 shows promising in vitro antitumor activity as methuosis inducers in PC-3 cells

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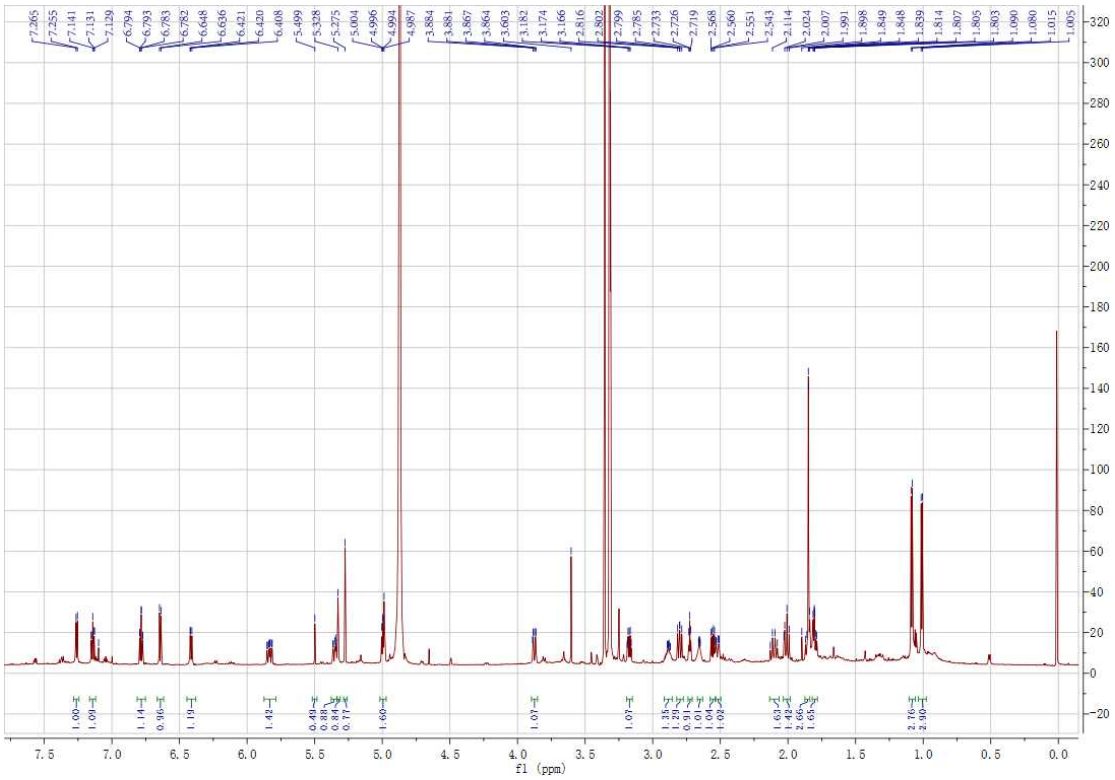


Figure S1. ^{1}H NMR spectrum of **1** (CD_3OD, 700 MHz)

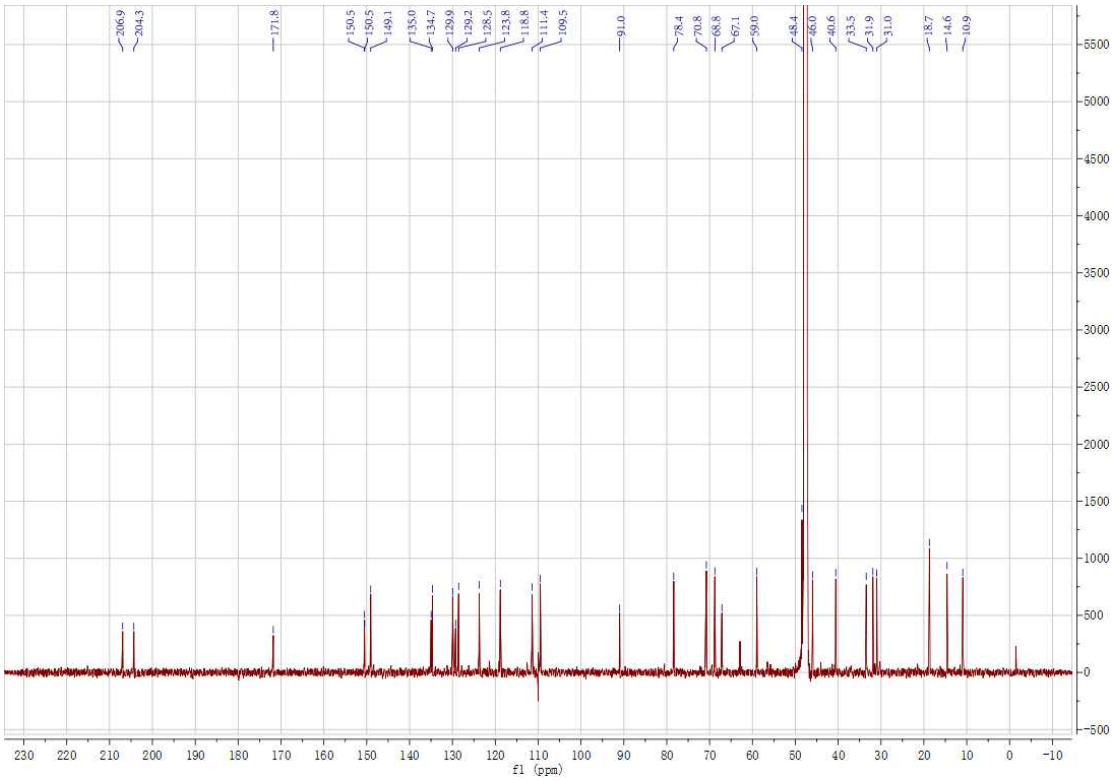


Figure S2. ^{13}C NMR spectrum of **1** (CD_3OD, 175 MHz)

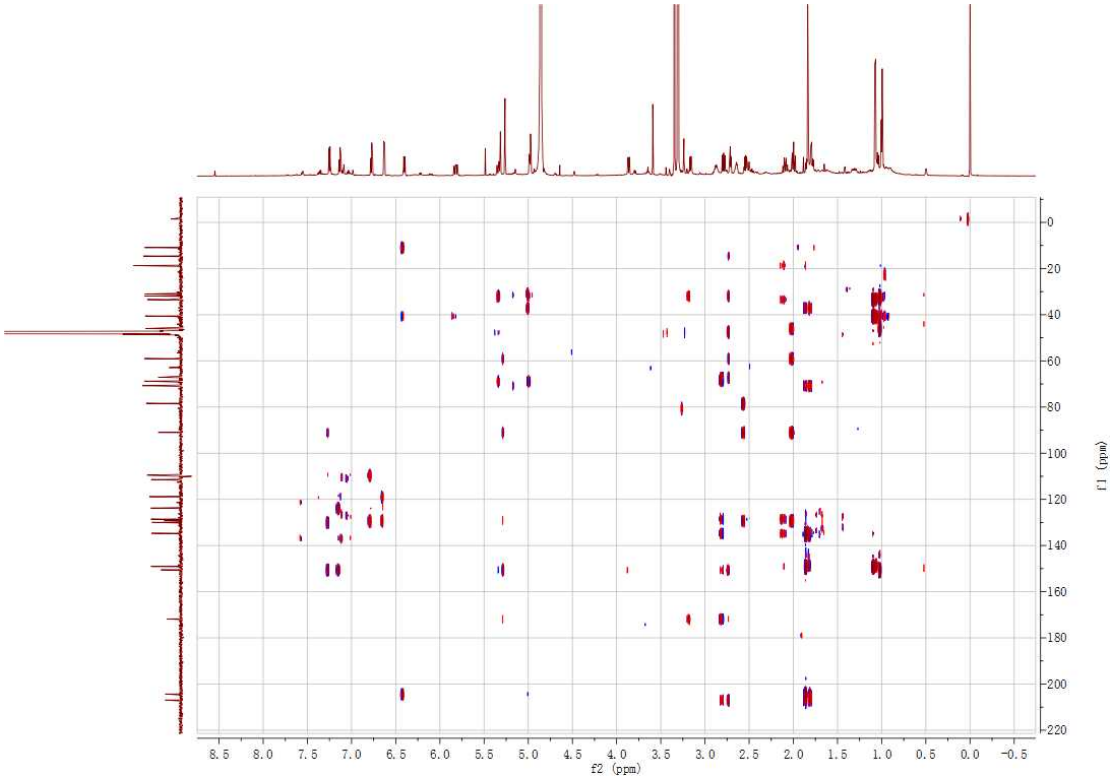


Figure S3. HSQC spectrum of **1** (CD_3OD)

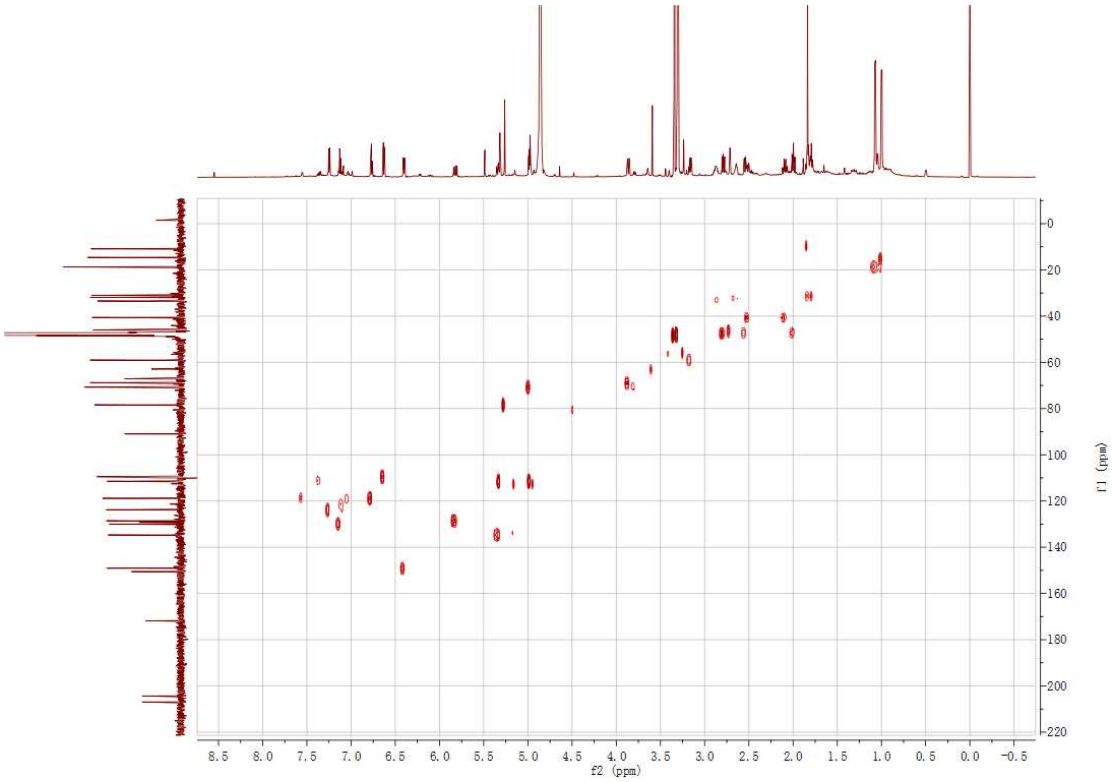


Figure S4. HMBC spectrum of **1** (CD_3OD)

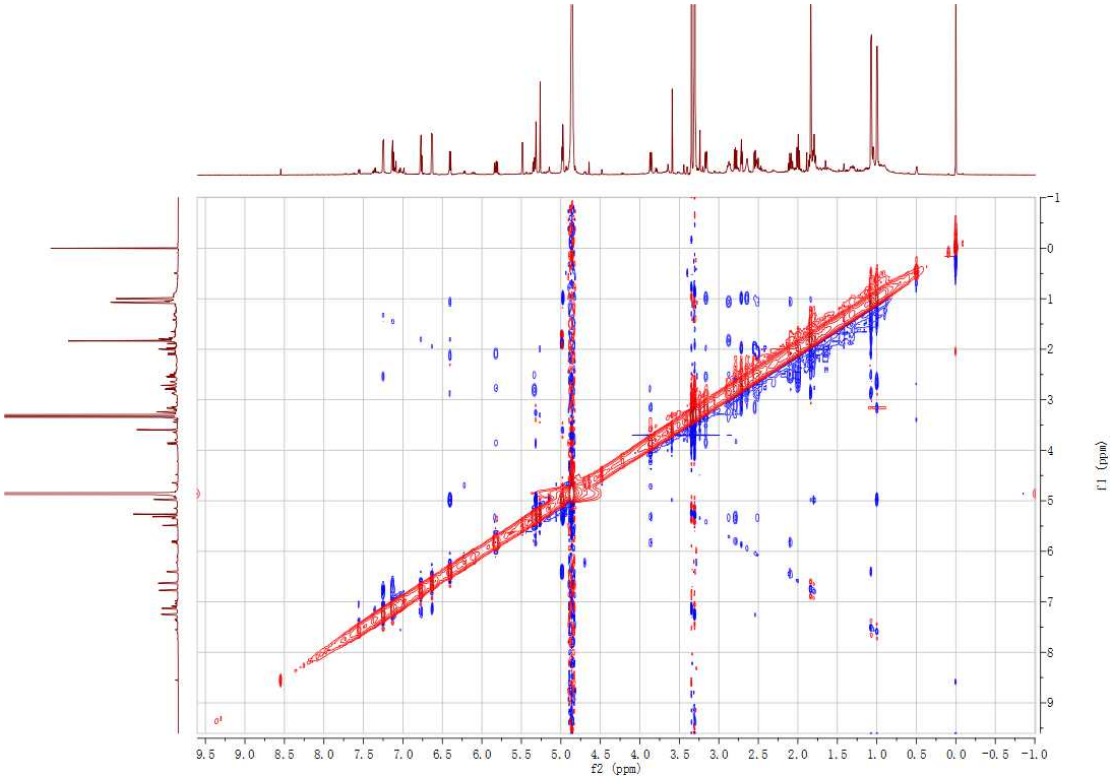


Figure S5. NOESY spectrum of **1** (CD_3OD)

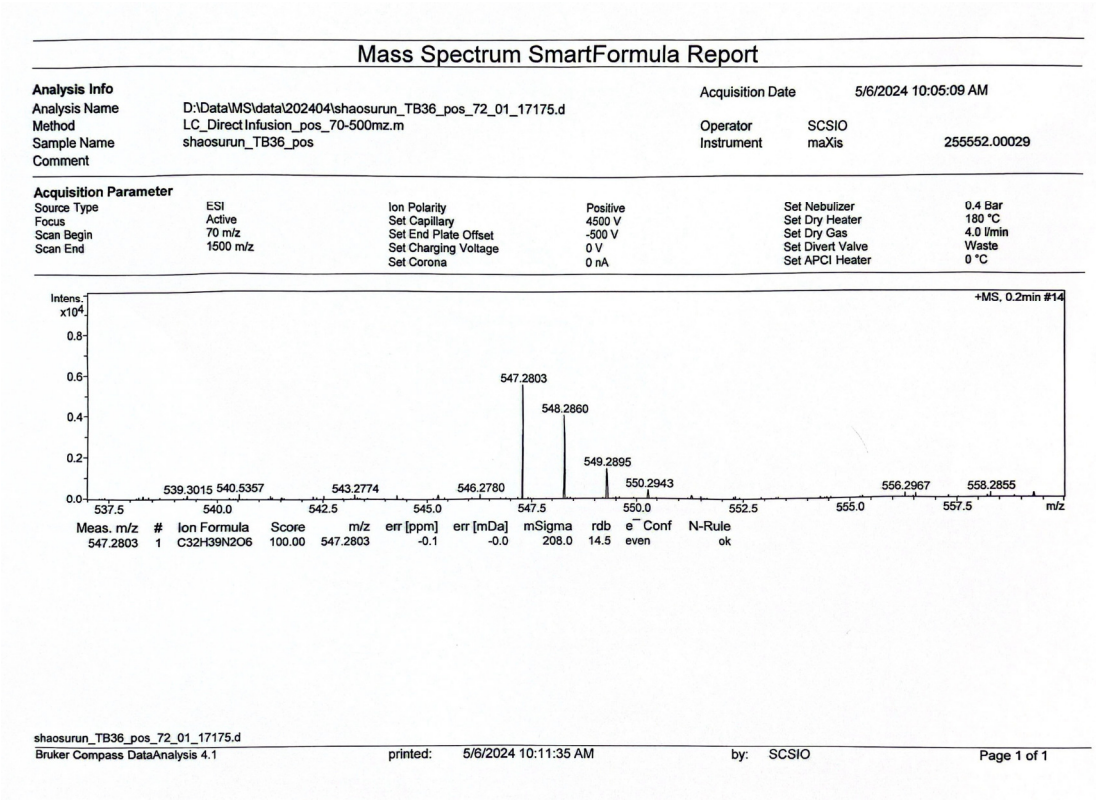


Figure S6. HRESIMS spectrum of **1**

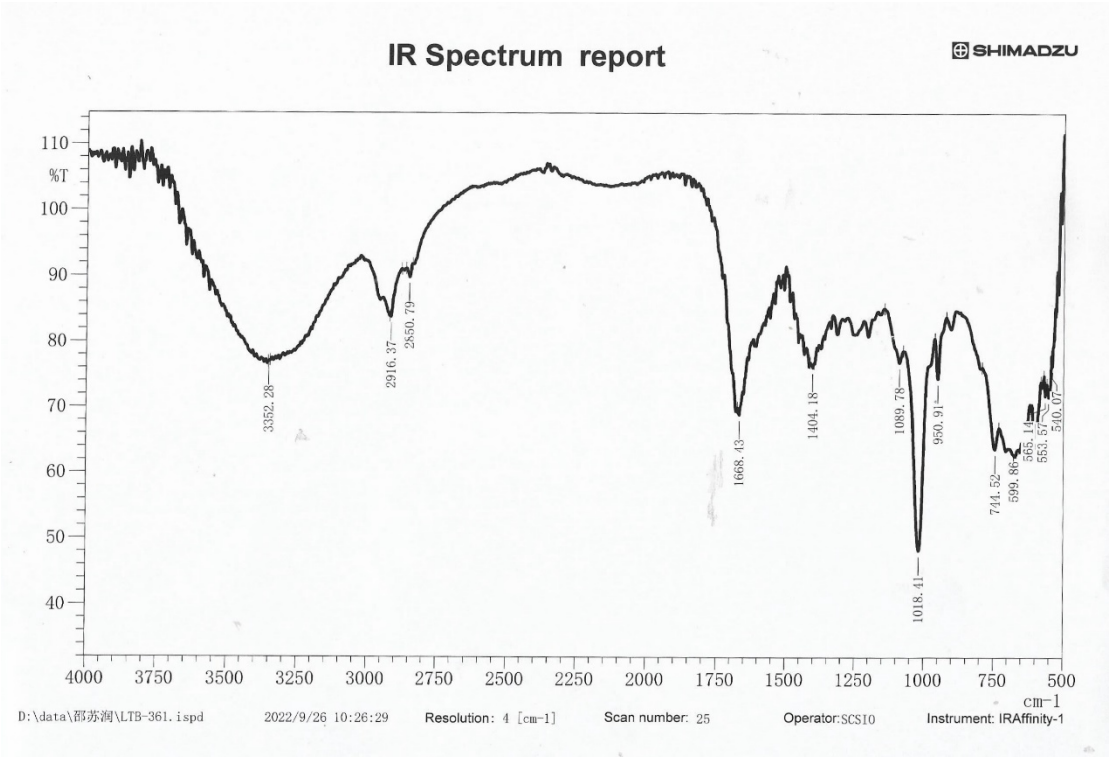
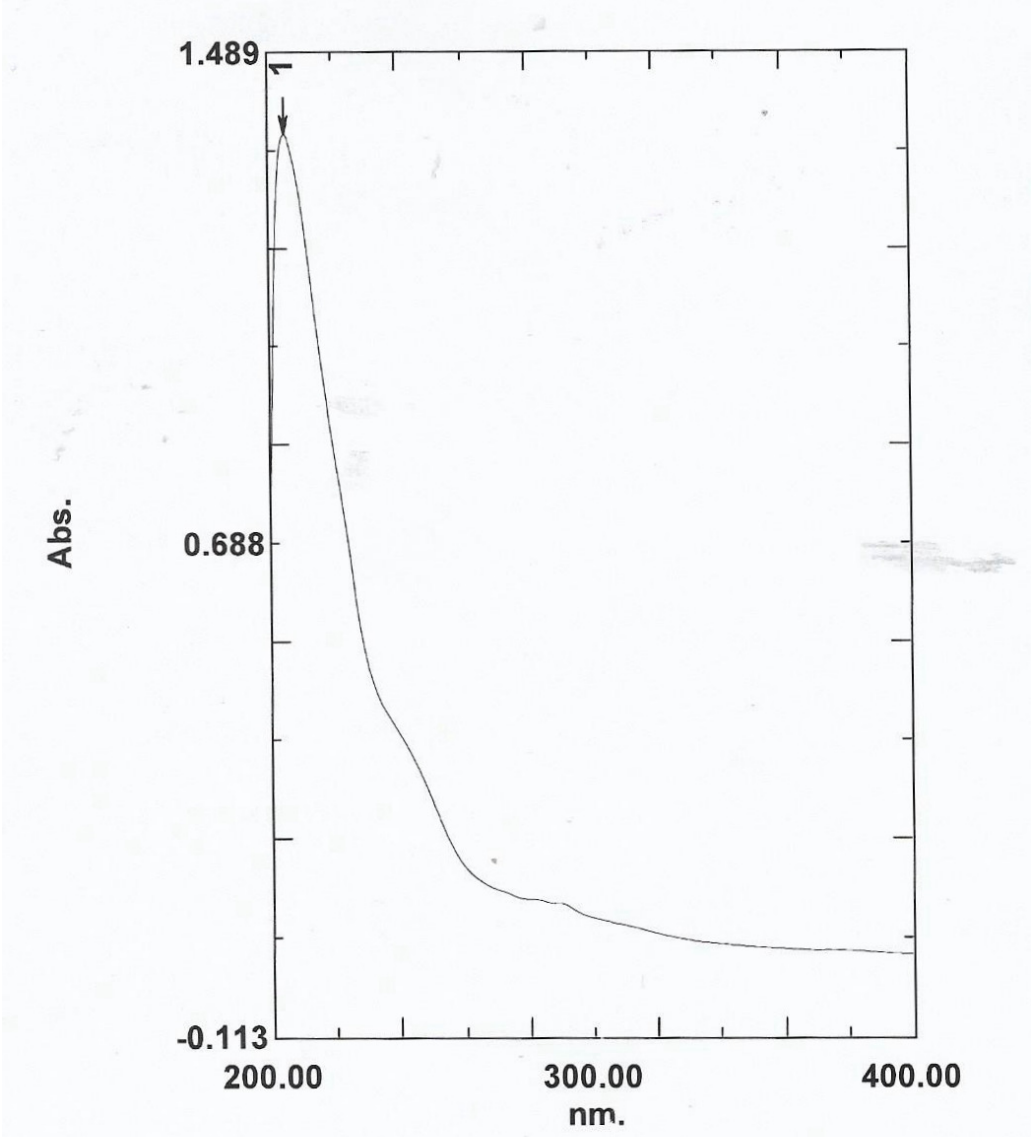


Figure S7. IR spectrum of **1**



Wavelength （nm）

No.	P/V	波长(nm)	Abs.	描述
1		205.20	1.355	

Figure S8. UV spectrum of **1**

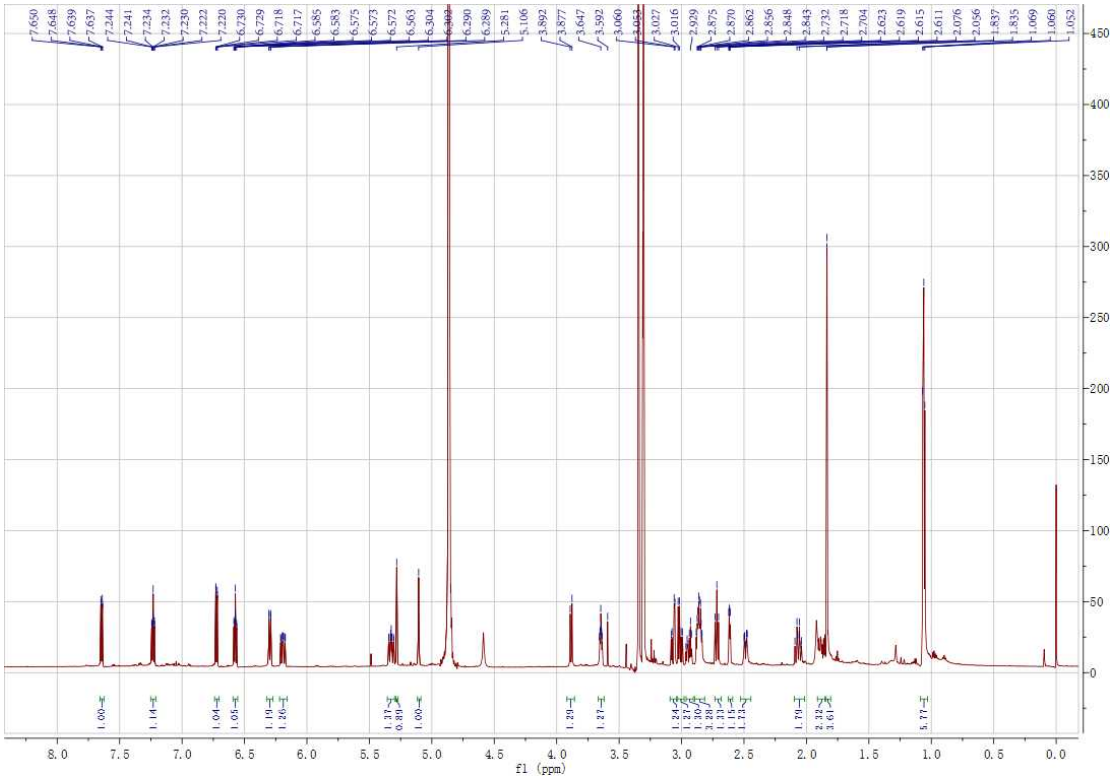


Figure S9. ^{1}H NMR spectrum of **2** (CD_3OD, 700 MHz)

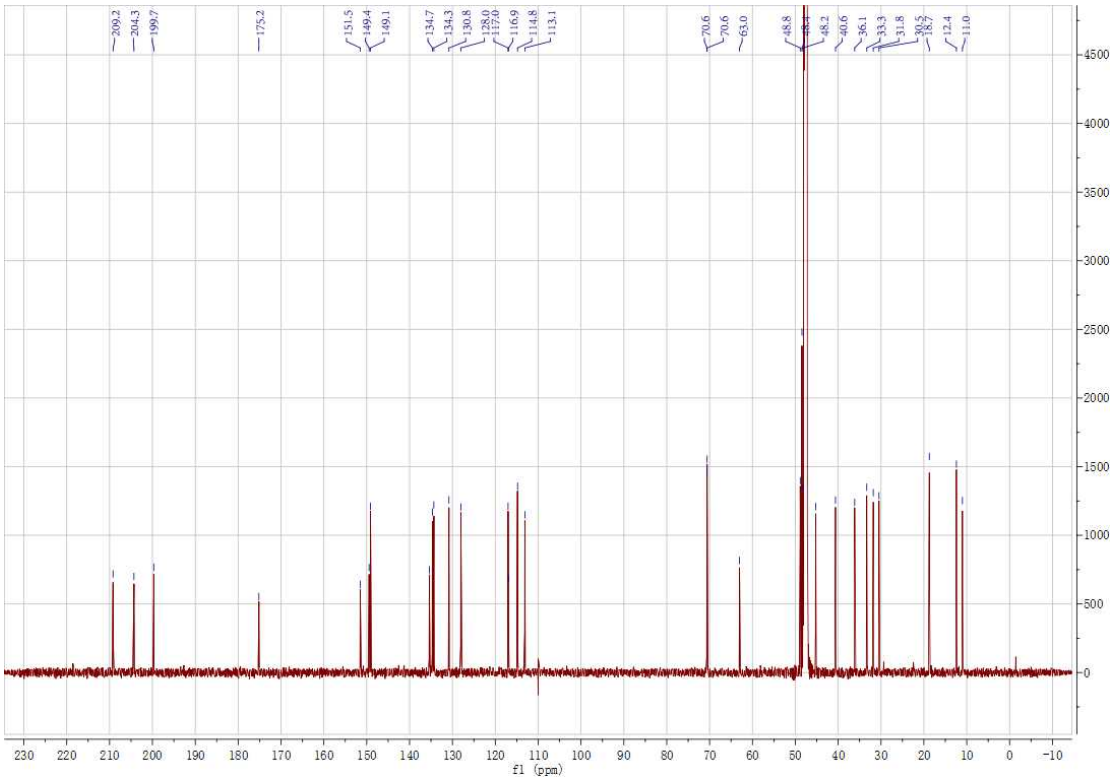


Figure S10. ^{13}C NMR spectrum of **2** (CD_3OD, 175 MHz)

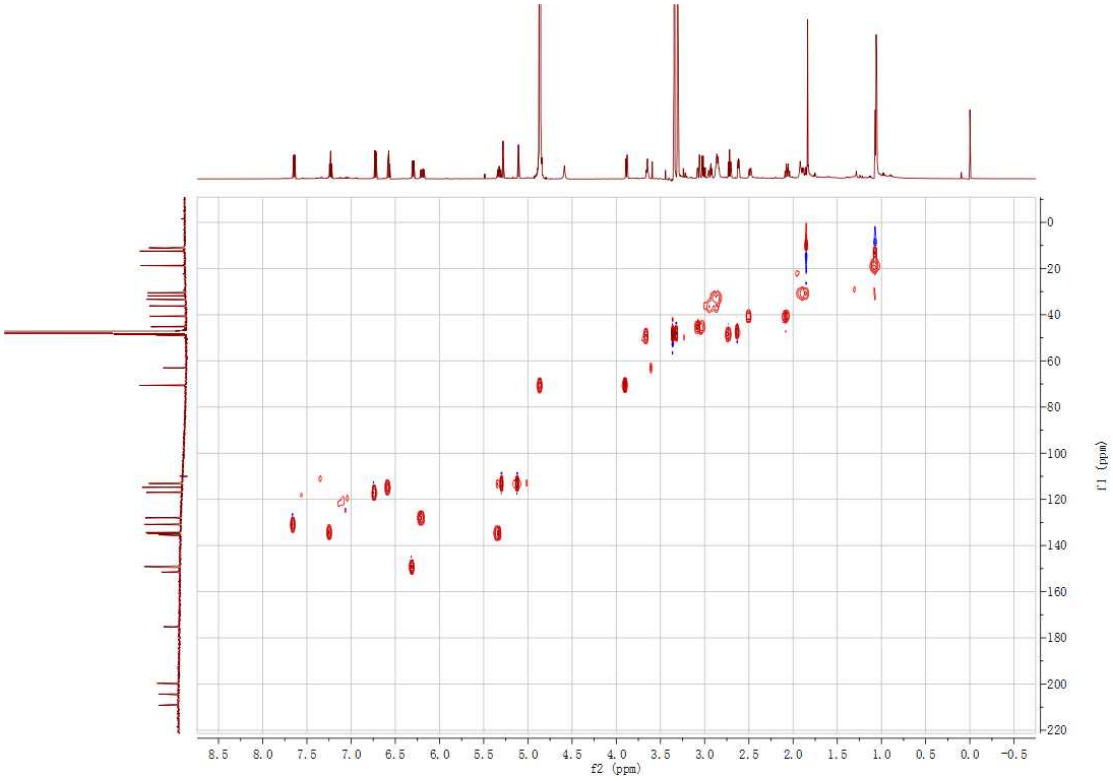


Figure S11. HSQC spectrum of **2** (CD_3OD)

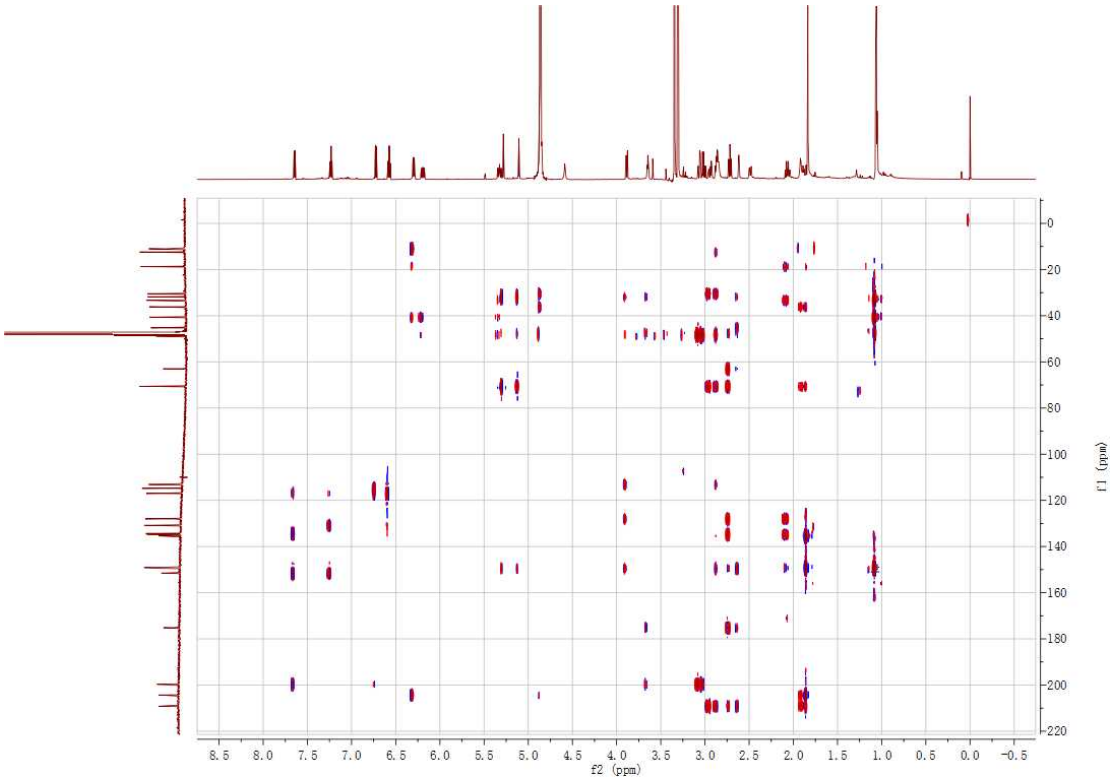


Figure S12. HMBC spectrum of **2** (CD_3OD)

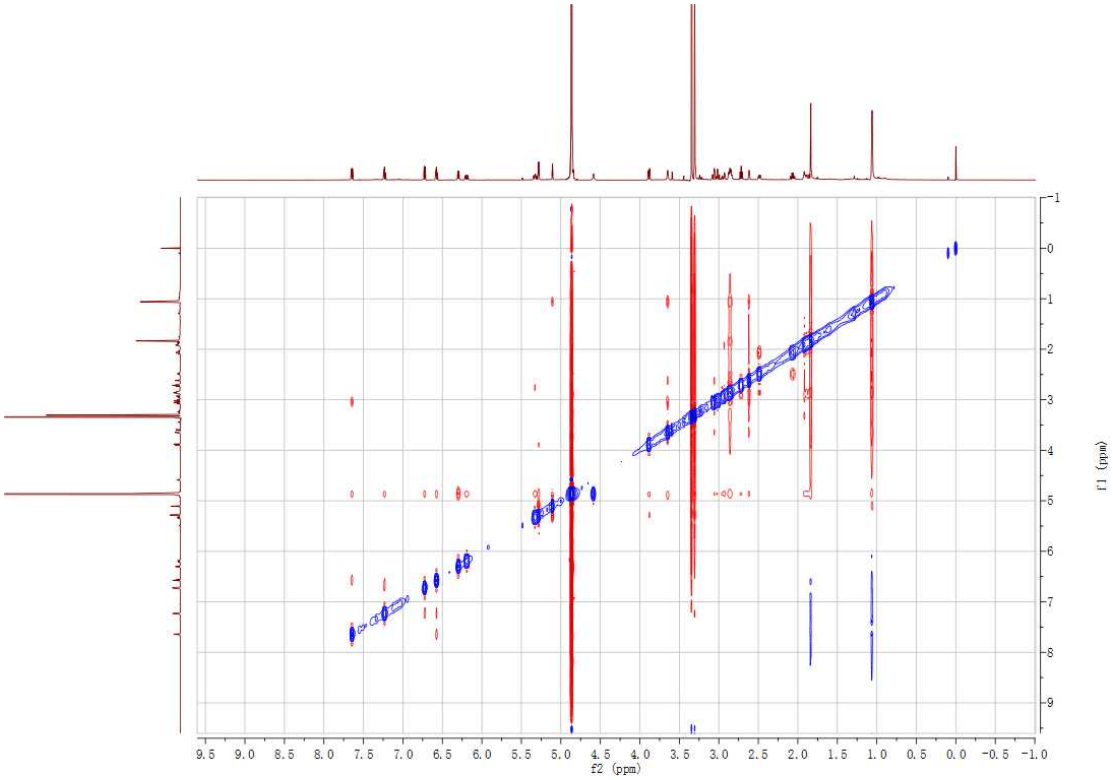


Figure S13. NOESY spectrum of **2** (CD_3OD)

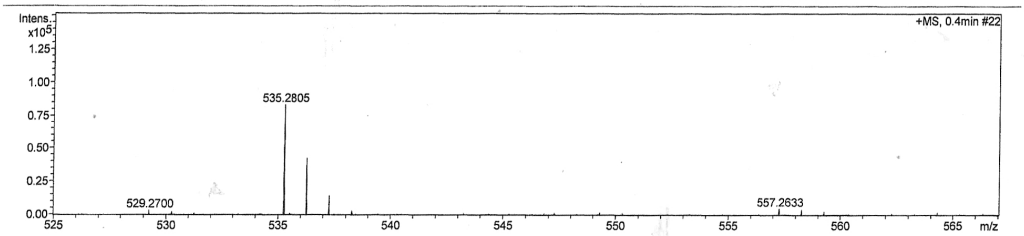
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\MS\data\202109\shaosurun_TB37_pos_2_01_11599.d	Acquisition Date	9/28/2021 10:33:23 AM
Method	LC_Direct Infusion_pos_70-500mz.m	Operator	SCSIO
Sample Name	shaosurun_TB37_pos	Instrument	maXis 255552.00029
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	70 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	err [mDa]	mSigma	rdb	e⁻ Conf	N-Rule
535.2805	1	C31H39N2O6	100.00	535.2803	0.4	0.2	92.6	13.5	even	ok
557.2633	1	C31H38N2NaO6	100.00	557.2622	1.9	1.1	173.9	13.5	even	ok

Figure S14. HRESIMS spectrum of **2**

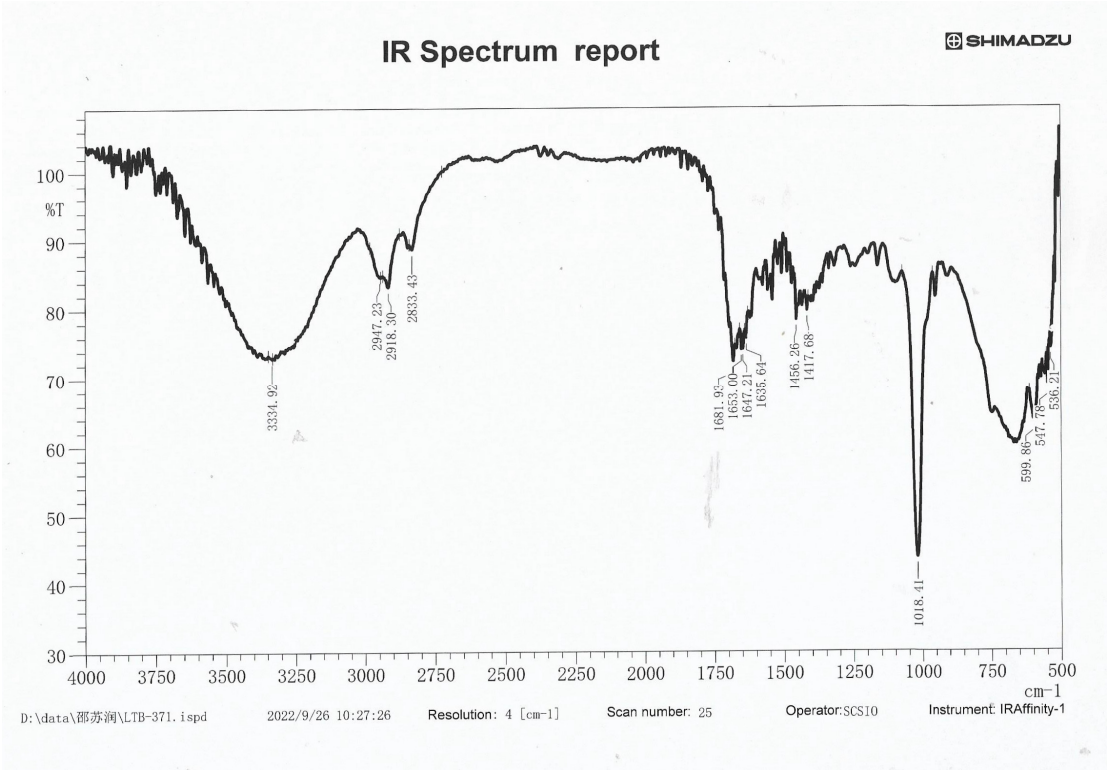
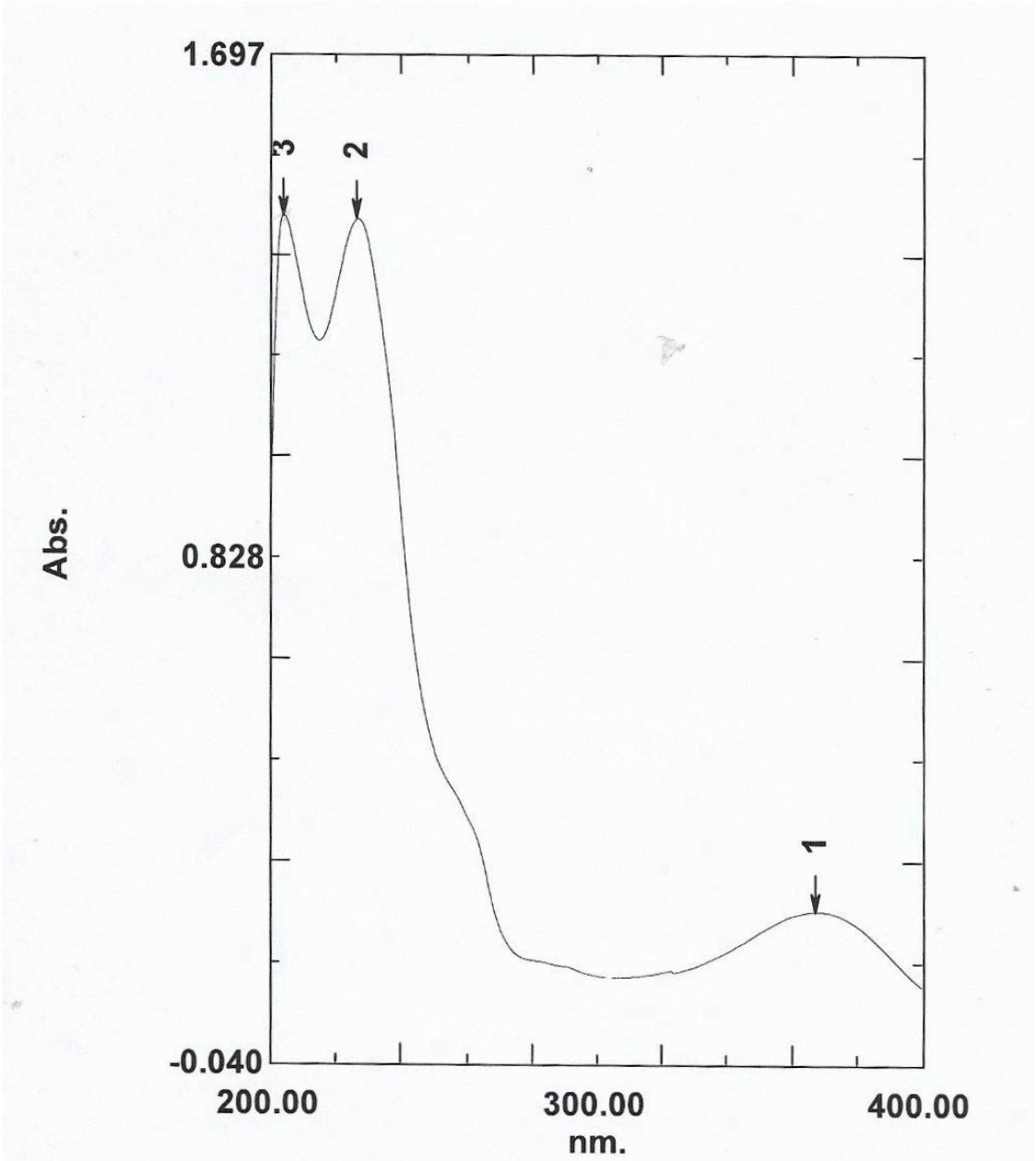


Figure S15. IR spectrum of **2**



Wavelength （nm）

No.	P/V	波长(nm)	Abs.	描述
1		367.40	0.222	
2		226.60	1.413	
3		203.80	1.419	

Figure S16. UV spectrum of **2**

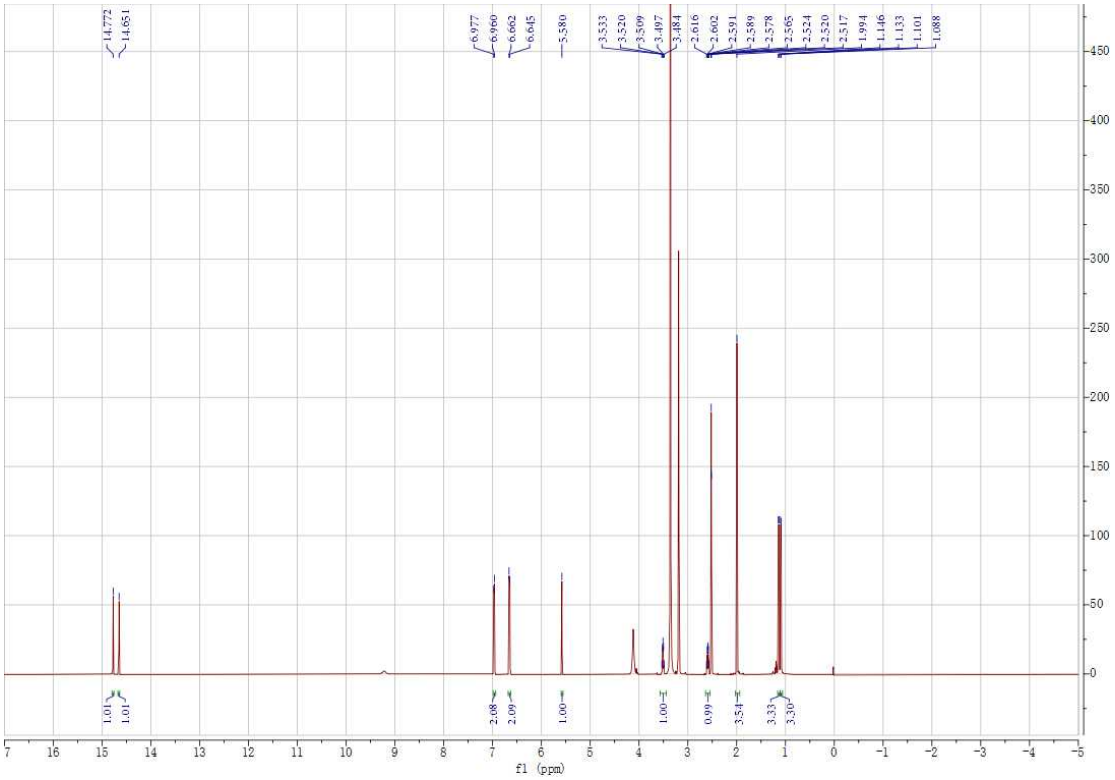


Figure S17. ^{1}H NMR spectrum of **4** (DMSO-d_6, 500 MHz)

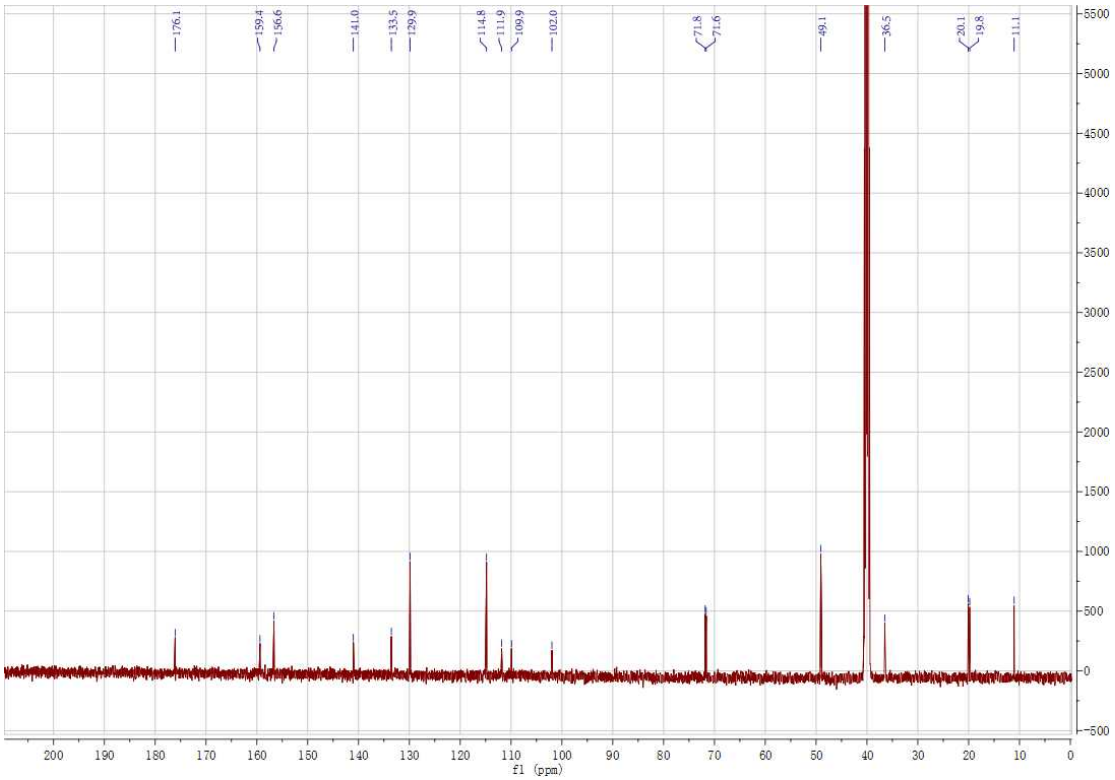


Figure S18. ^{13}C NMR spectrum of **4** (DMSO-d_6, 125 MHz)

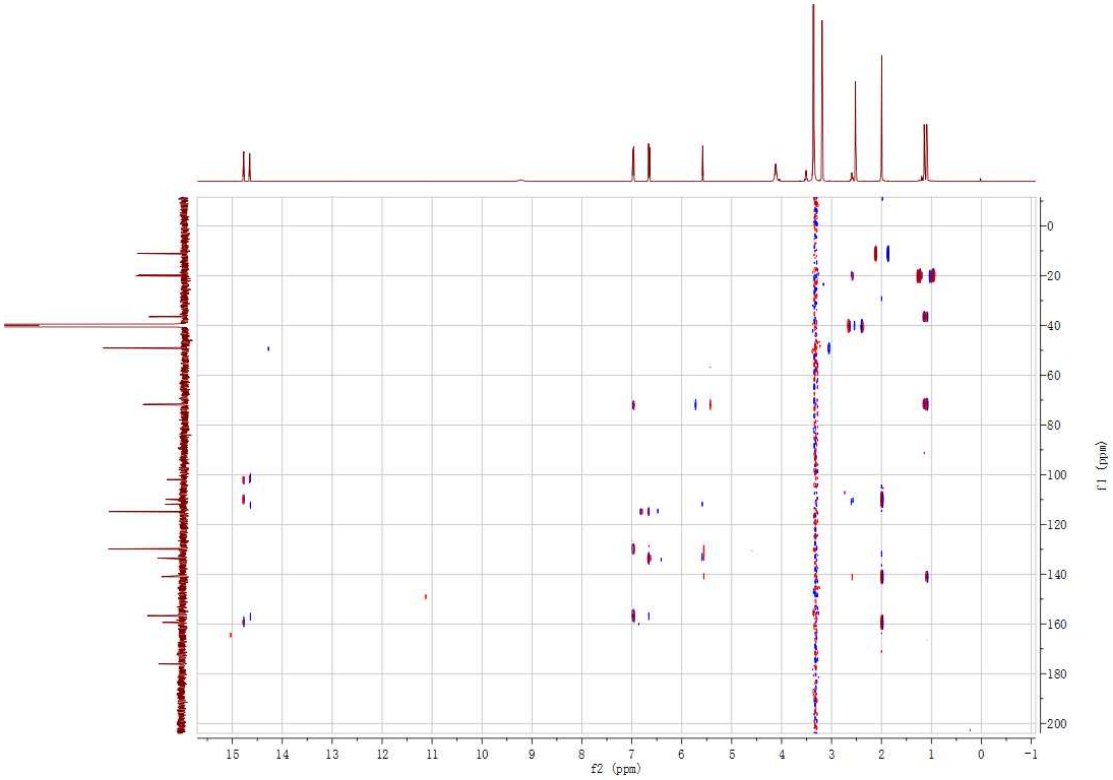


Figure S19. HSQC spectrum of **4** (DMSO-d_6)

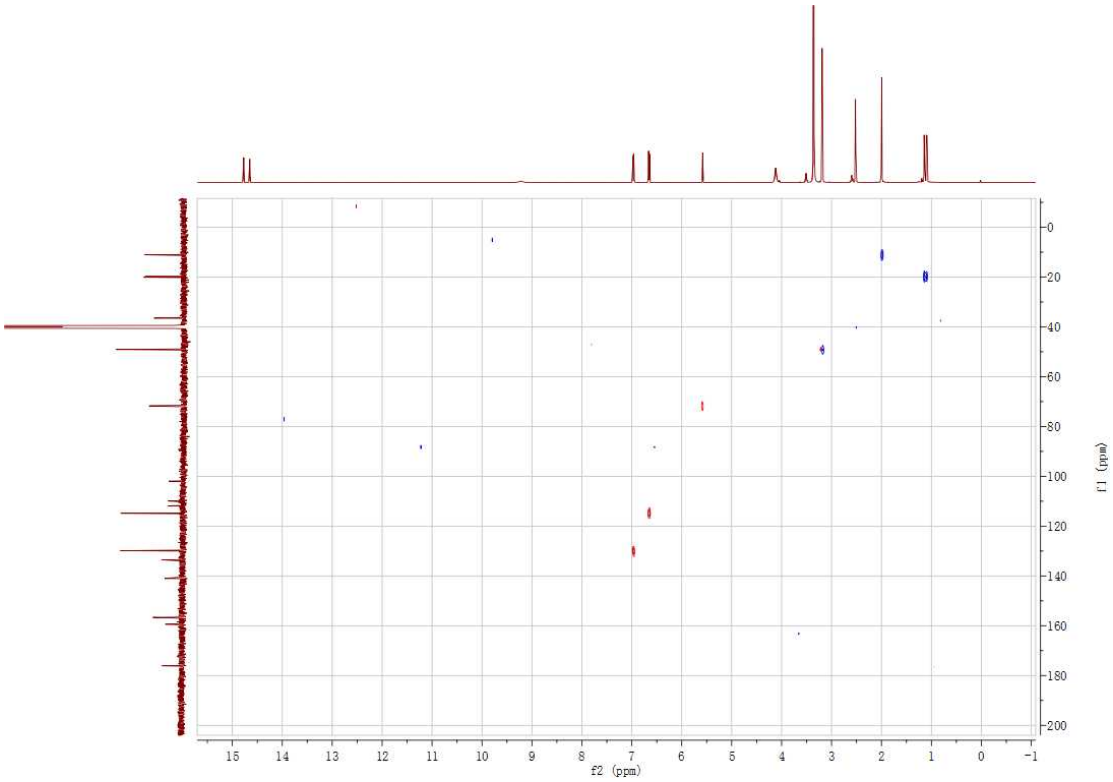


Figure S20. HMBC spectrum of **4** (DMSO-d_6)

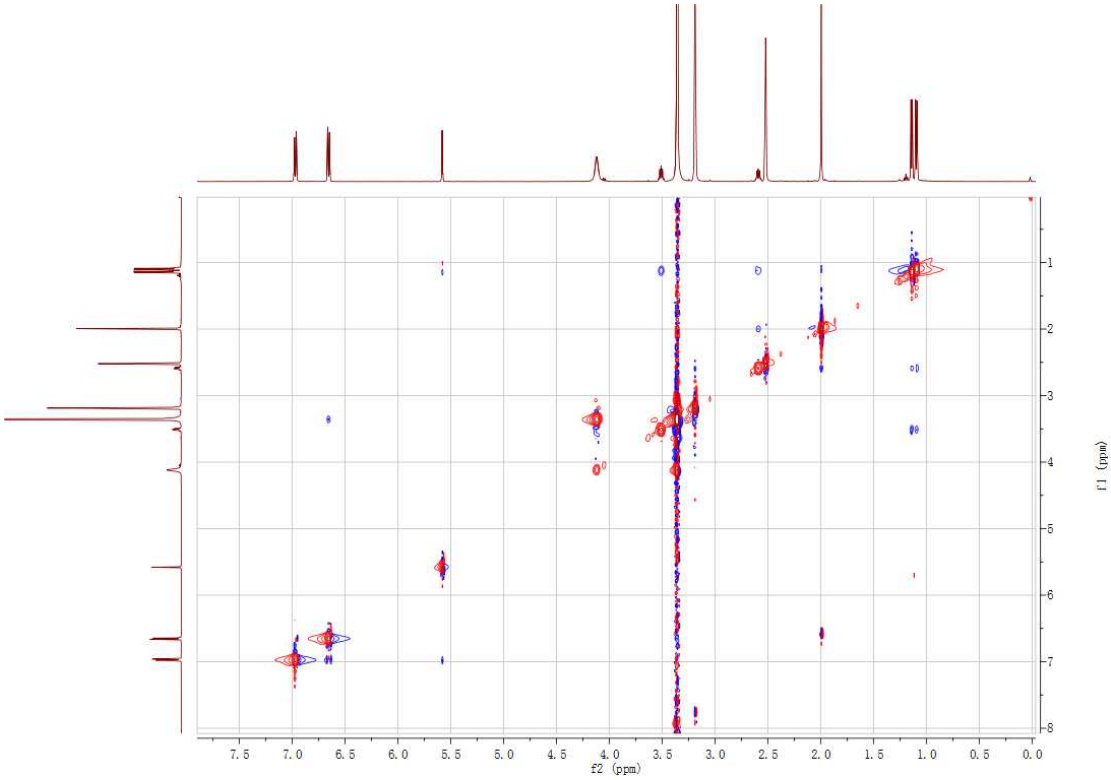


Figure S21. NOESY spectrum of **4** (DMSO-d_6)

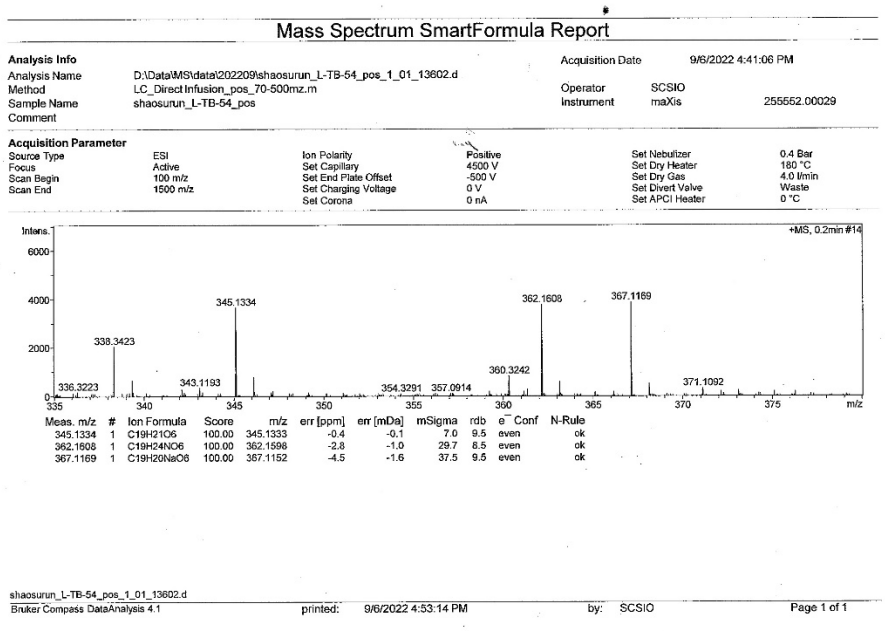


Figure S22. HRESIMS spectrum of **4**

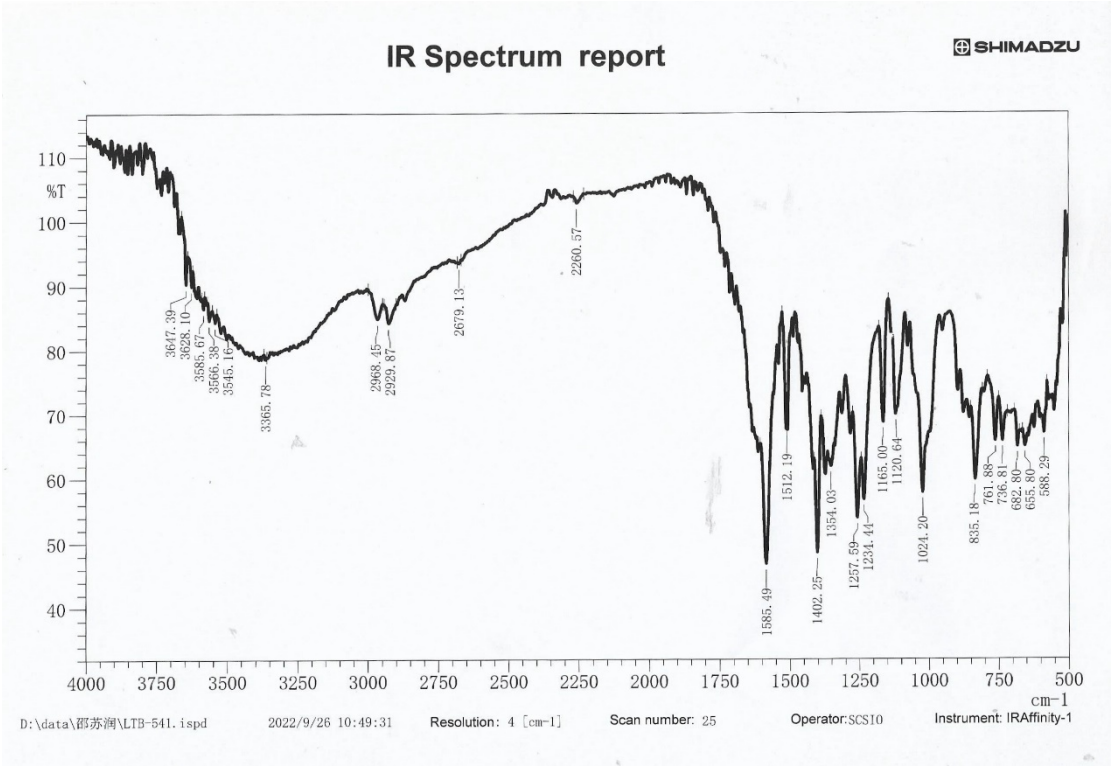
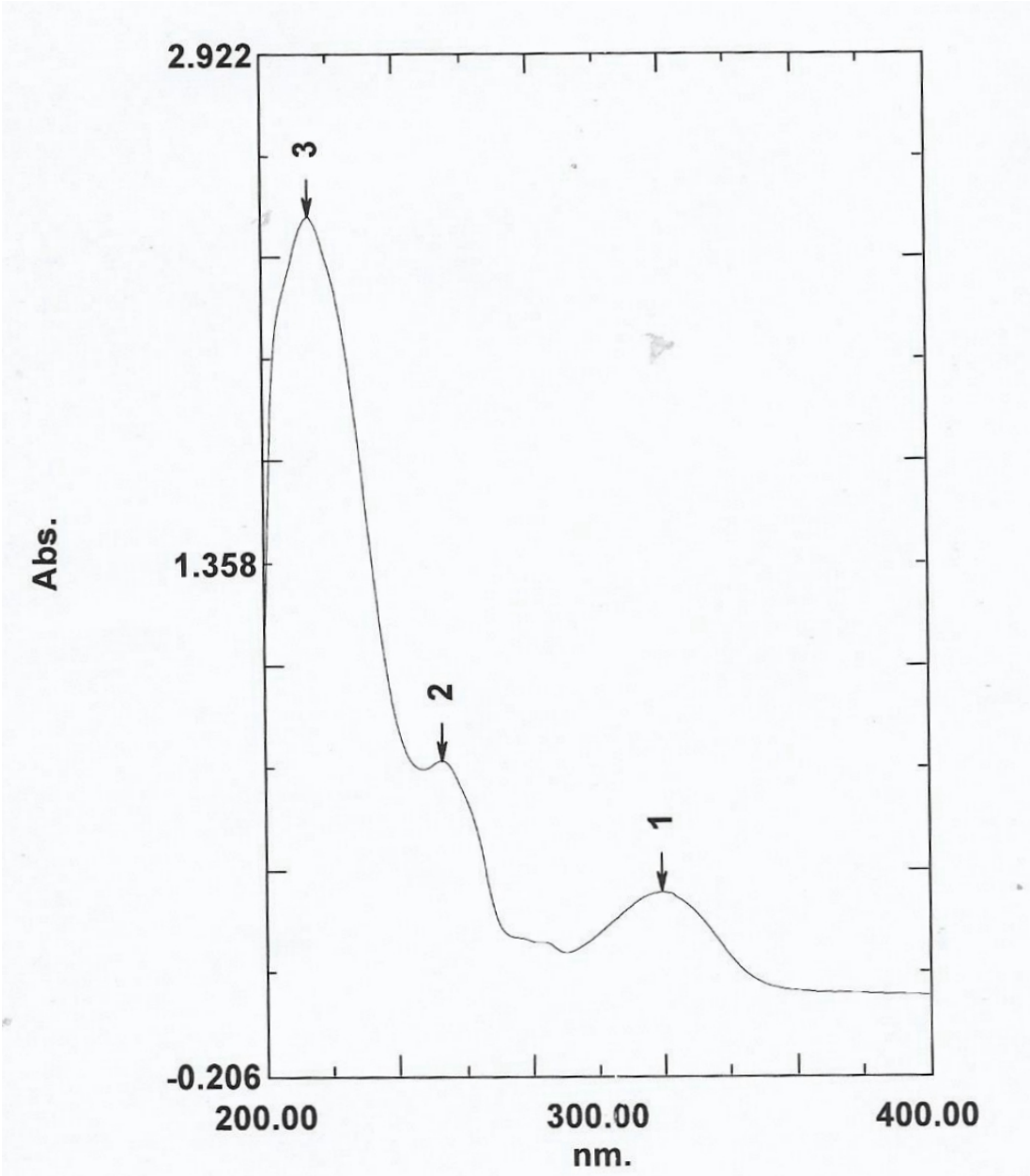


Figure S23. IR spectrum of **4**



Wavelength （nm）

No.	P/V	波长(nm)	Abs.	描述
1		319.20	0.352	
2		253.00	0.753	
3		214.00	2.421	

Figure S24. UV spectrum of **4**

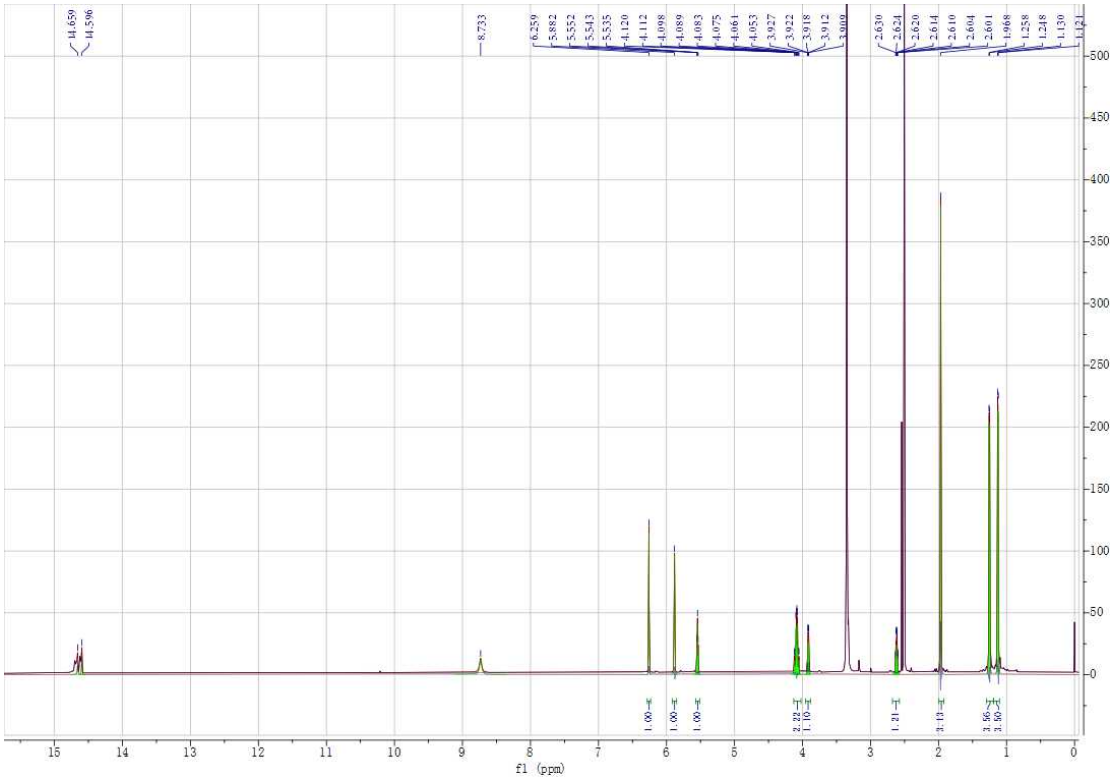


Figure S25. ^{1}H NMR spectrum of **5** (DMSO-d_6, 700 MHz)

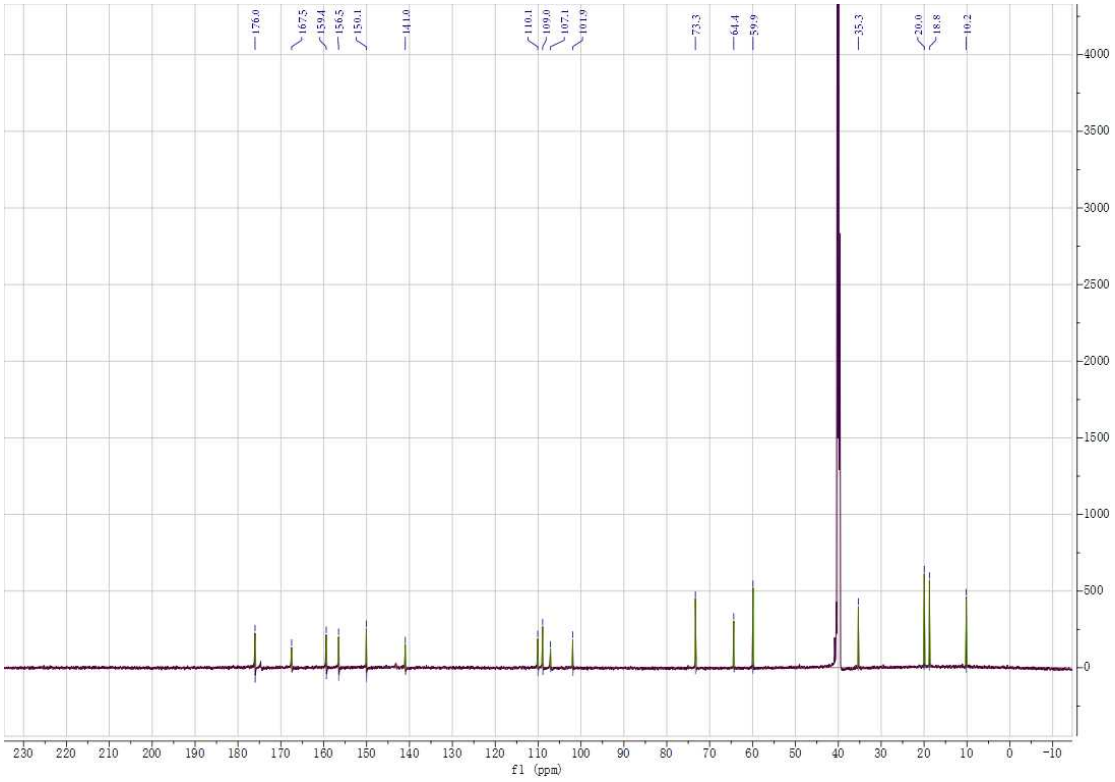


Figure S26. ^{13}C NMR spectrum of **5** (DMSO-d_6, 175 MHz)

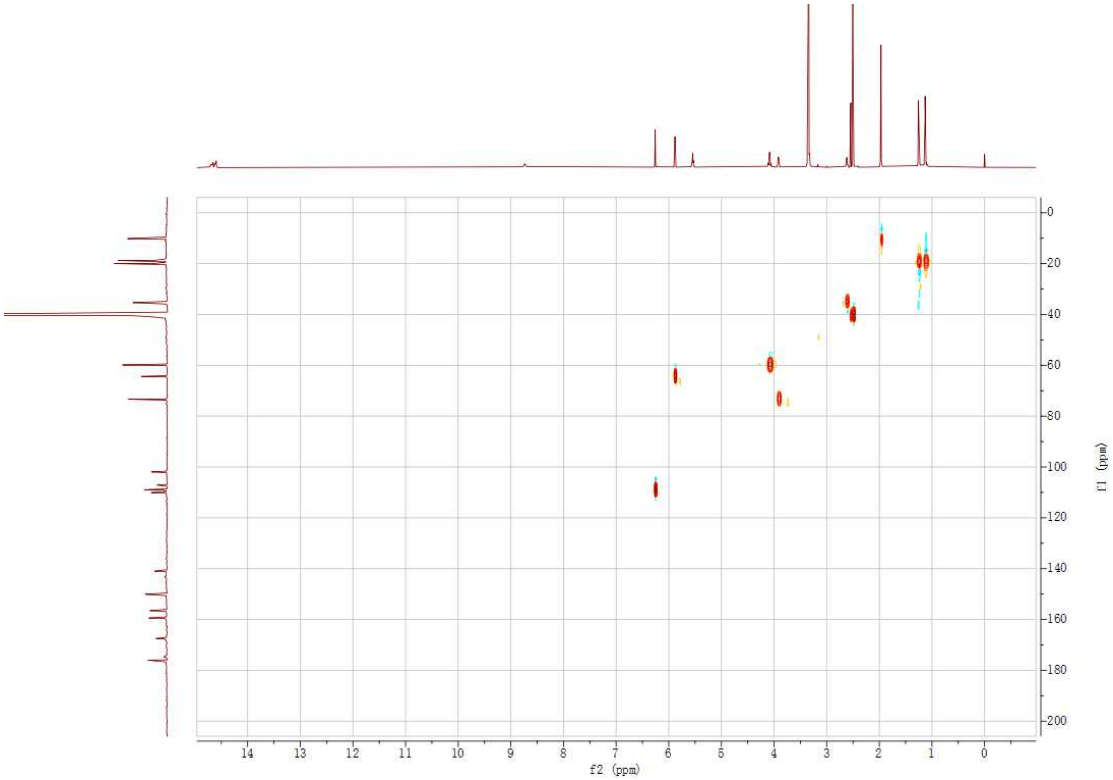


Figure S27. HSQC spectrum of **5** (DMSO-d_6)

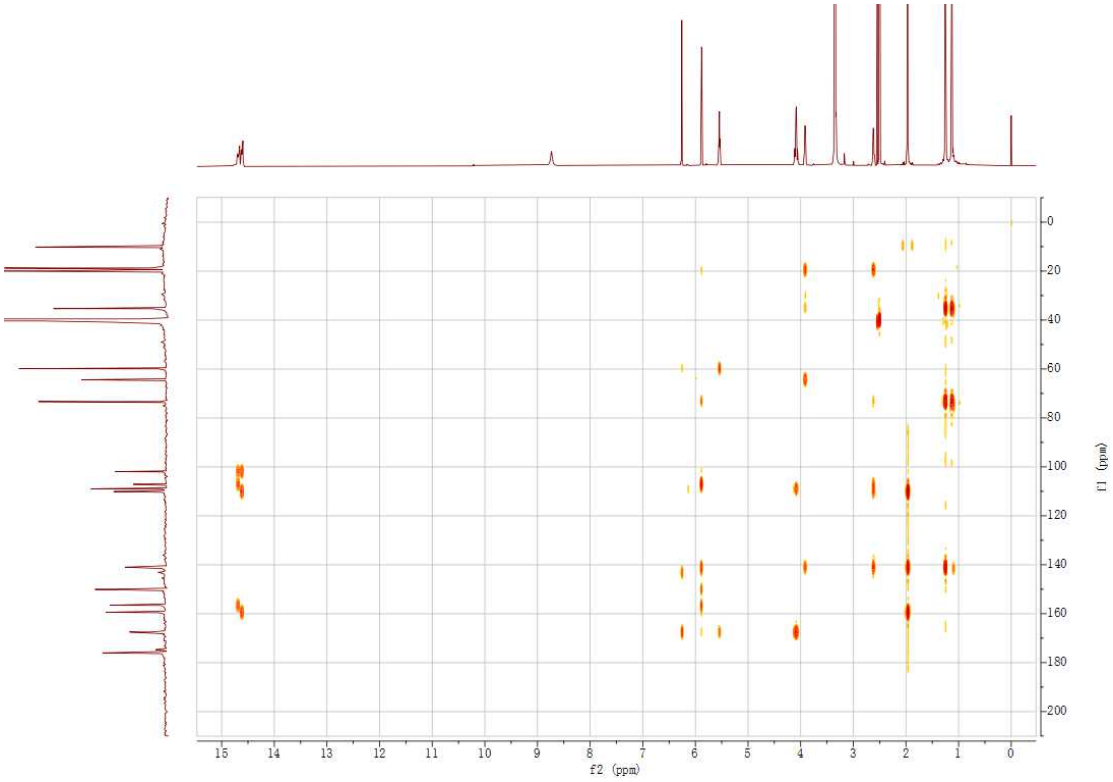


Figure S28. HMBC spectrum of **5**(DMSO-d_6)

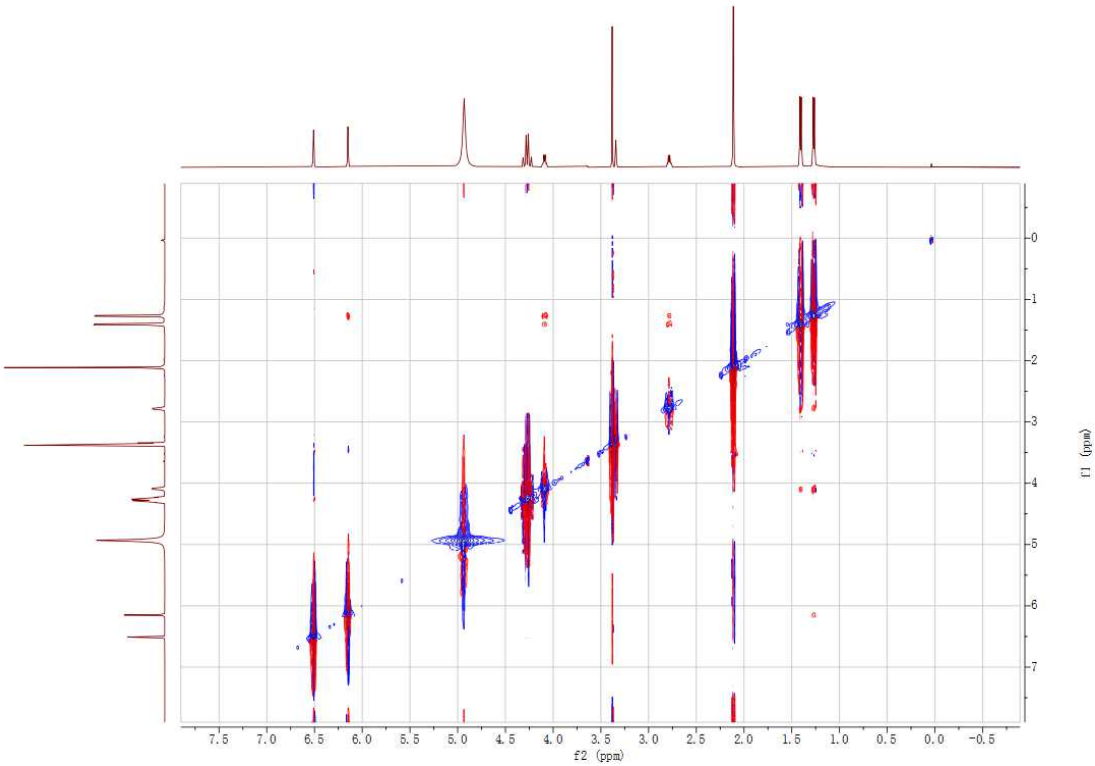


Figure S29. NOESY spectrum of **5** (CD_3OD)

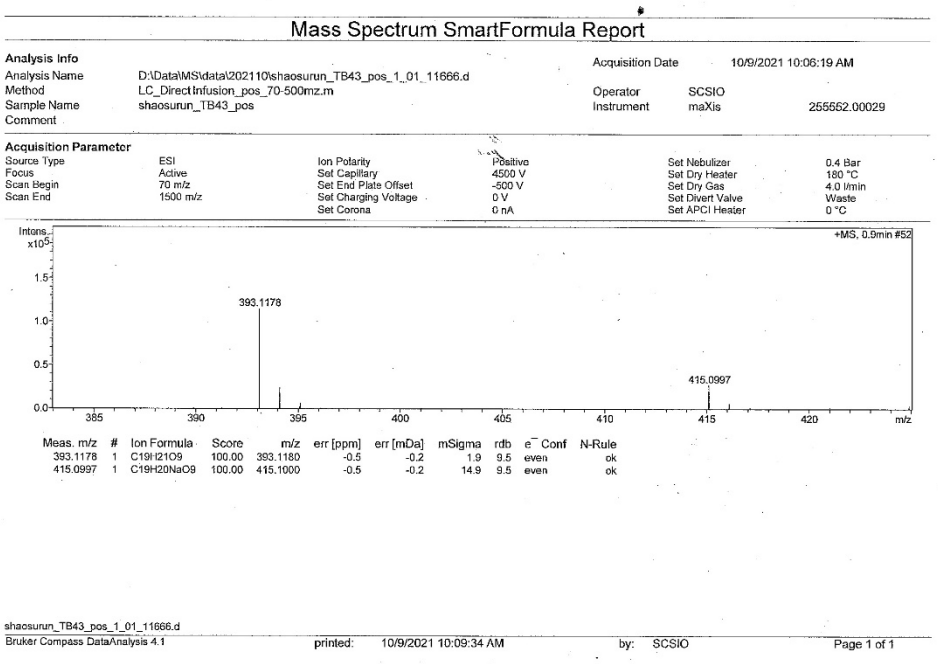


Figure S30. HRESIMS spectrum of **5**

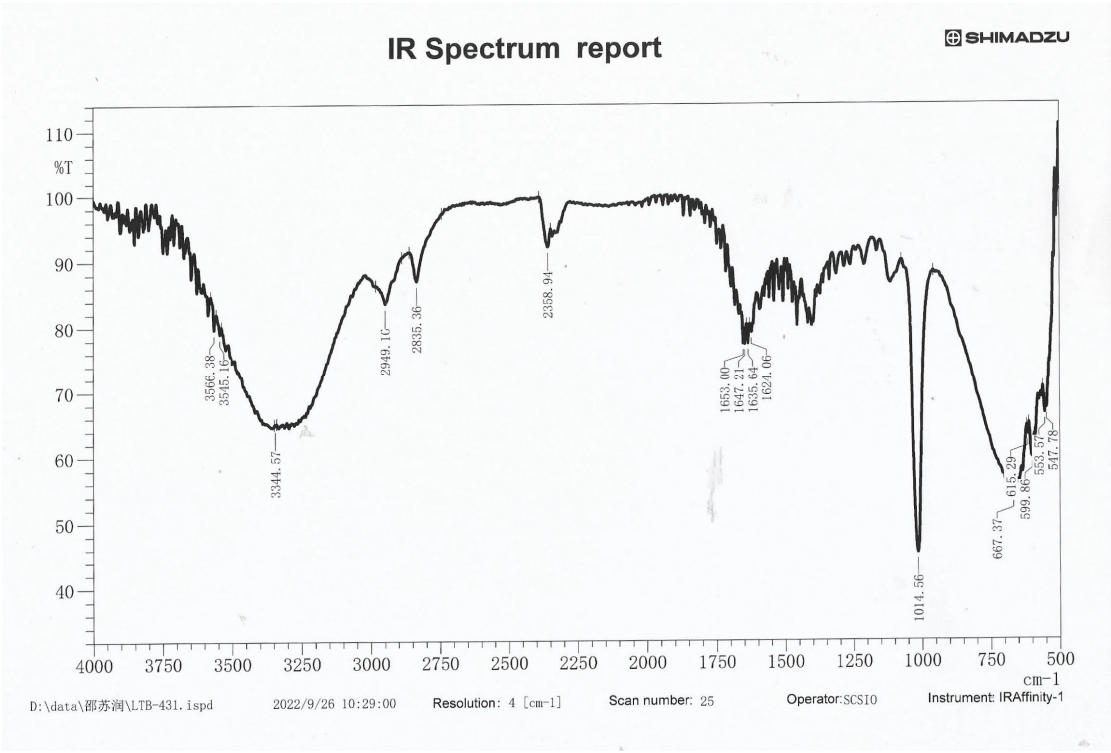
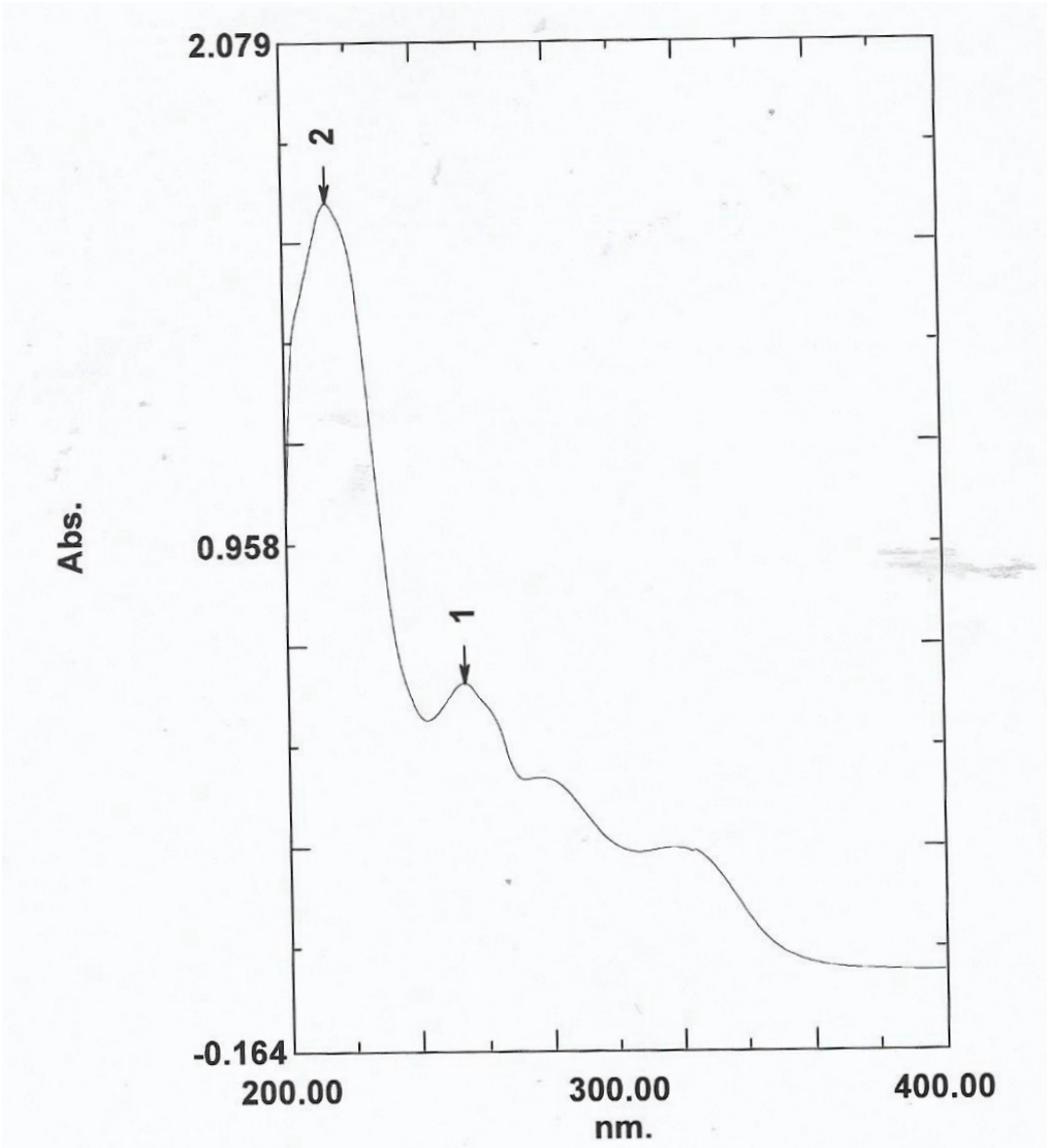


Figure S31. IR spectrum of **5**



Wavelength （nm）

No.	P/V	波长(nm)	Abs.	描述
1		253.60	0.651	
2		213.20	1.720	

Figure S32. UV spectrum of **5**

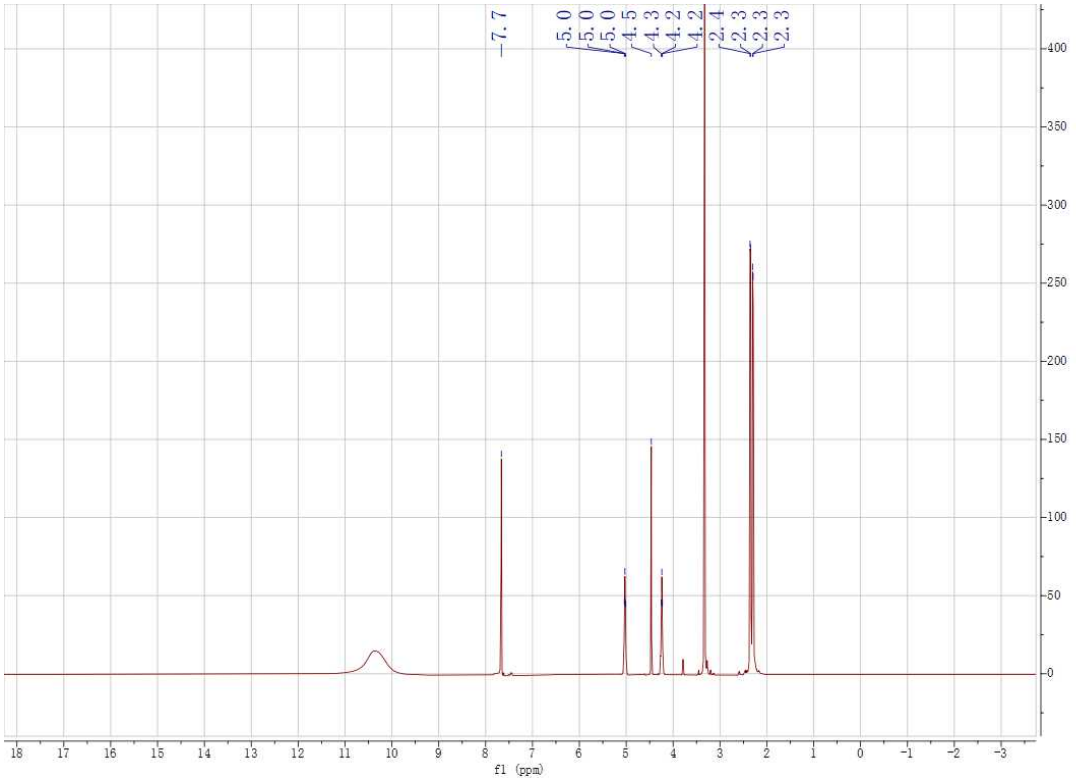


Figure S33. ^{1}H NMR spectrum of **7** (DMSO-d_6, 700 MHz)

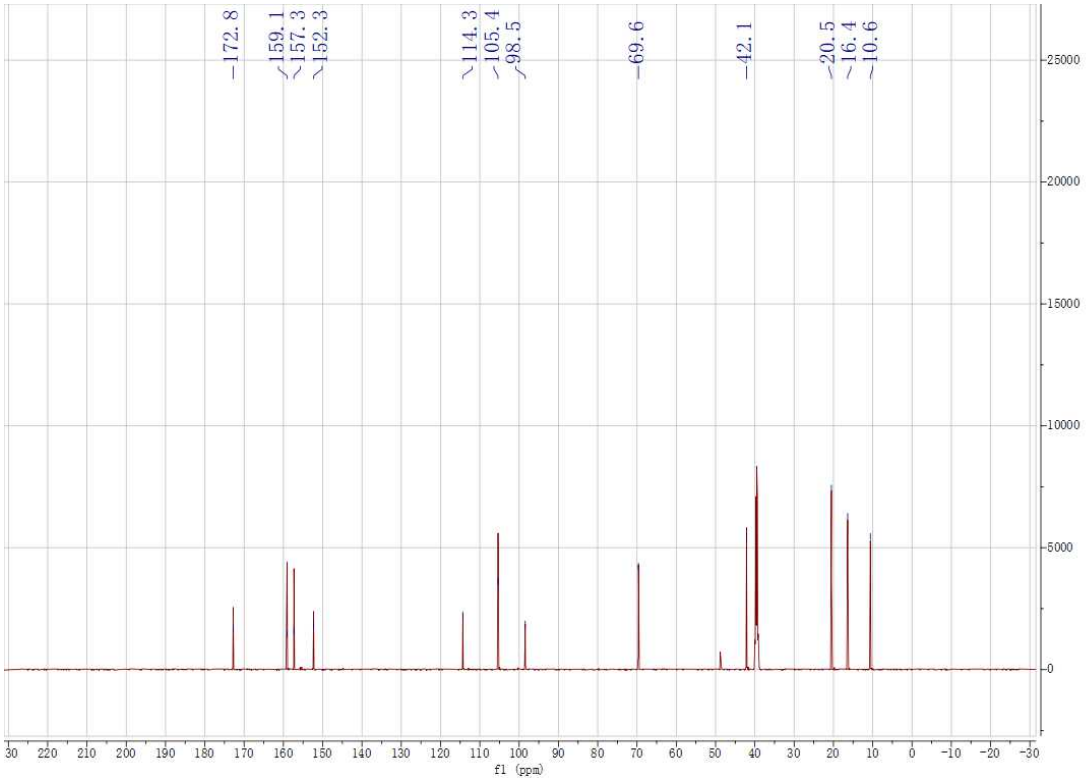


Figure S34. ^{13}C NMR spectrum of **7** (DMSO-d_6, 175 MHz)

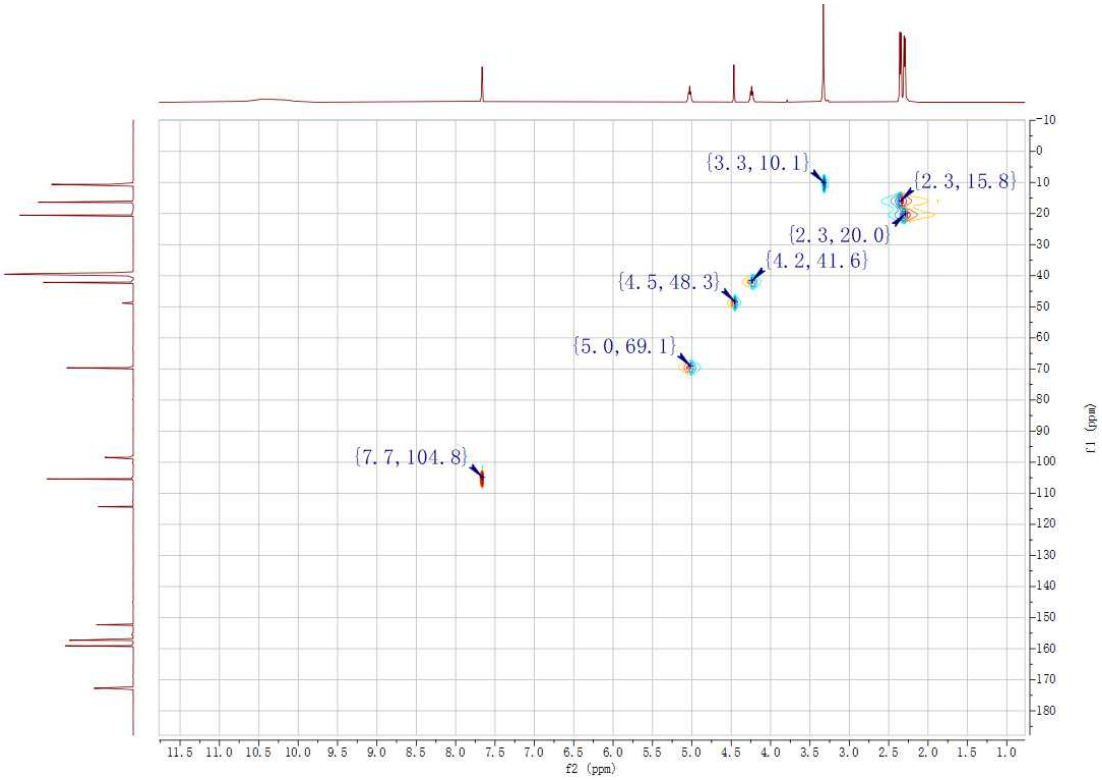


Figure S35. HSQC spectrum of **7** (DMSO-d_6)

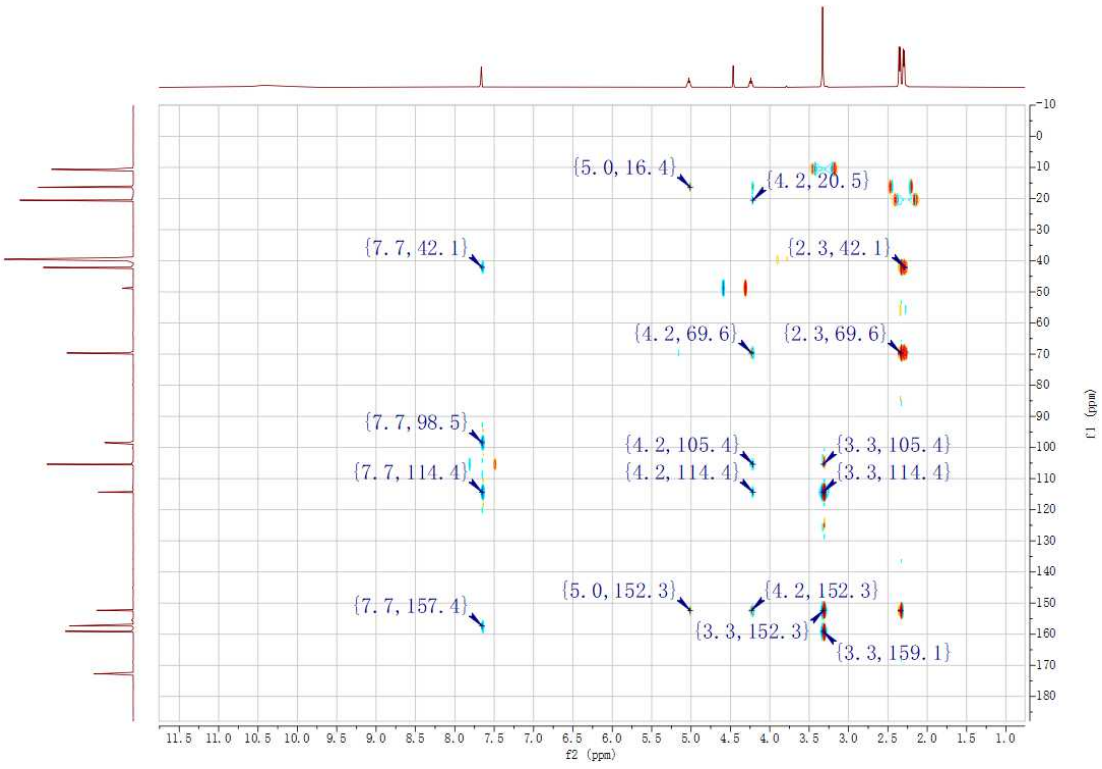


Figure S36. HMBC spectrum of **7** (DMSO-d_6)

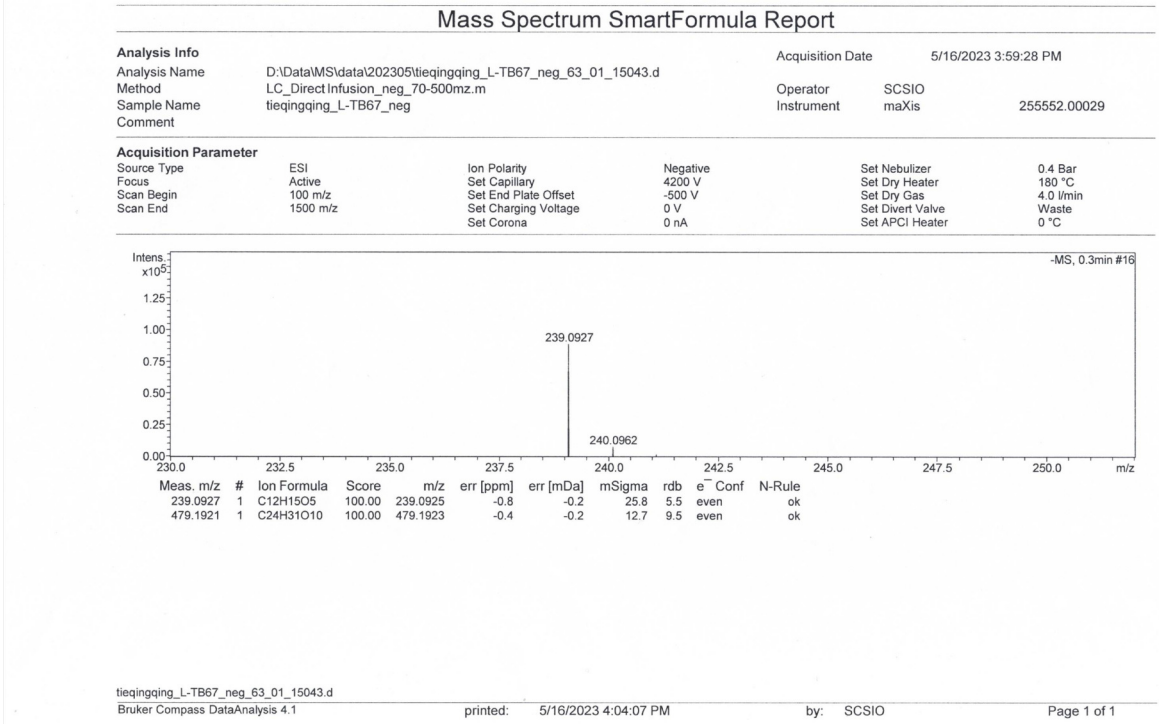


Figure S37. HRESIMS spectrum of **7**

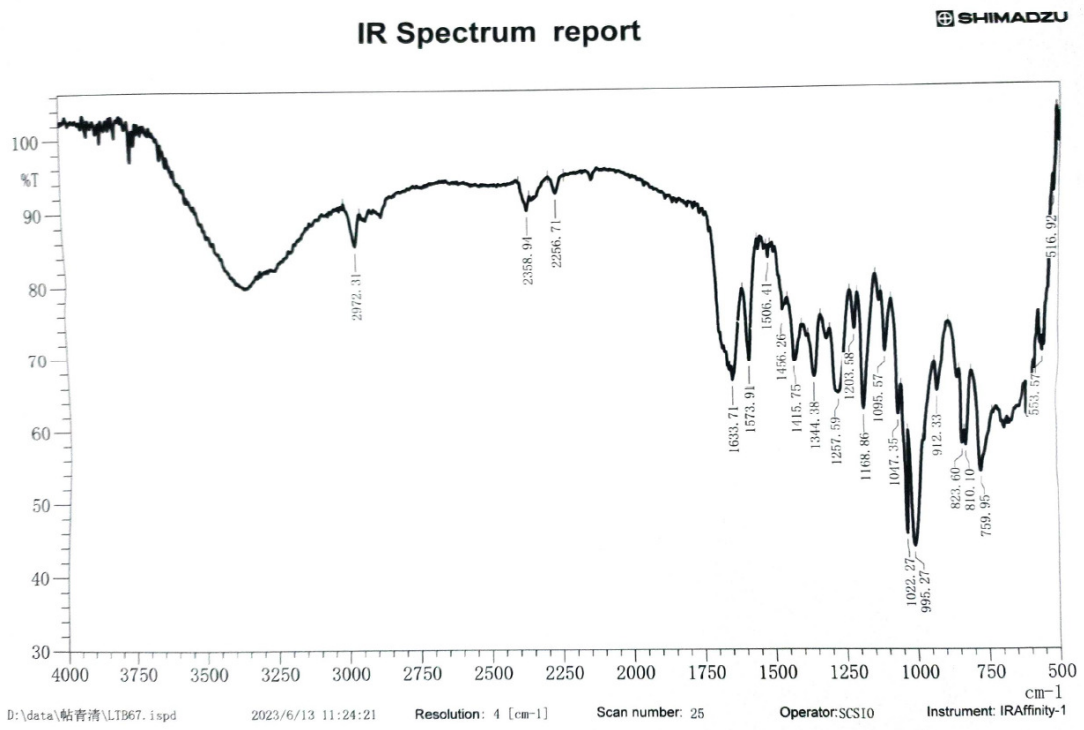
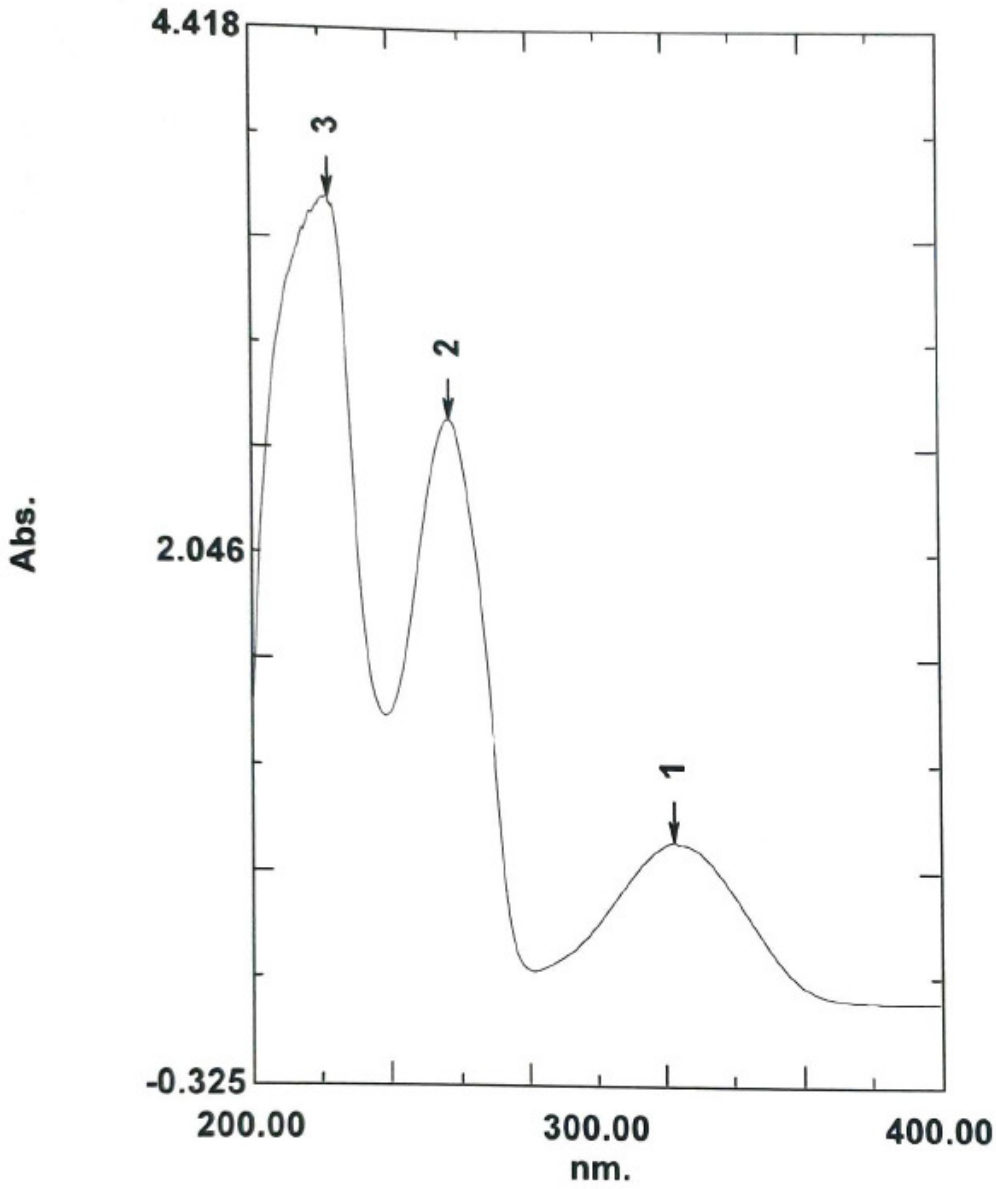


Figure S38. IR spectrum of **7**



Wavelenth (nm)

No.	P/V	波长(nm)	Abs.	描述
1	↑	322.60	0.757	
2	↑	256.80	2.656	
3	↑	222.20	3.658	

Figure S39. UV spectrum of **7**

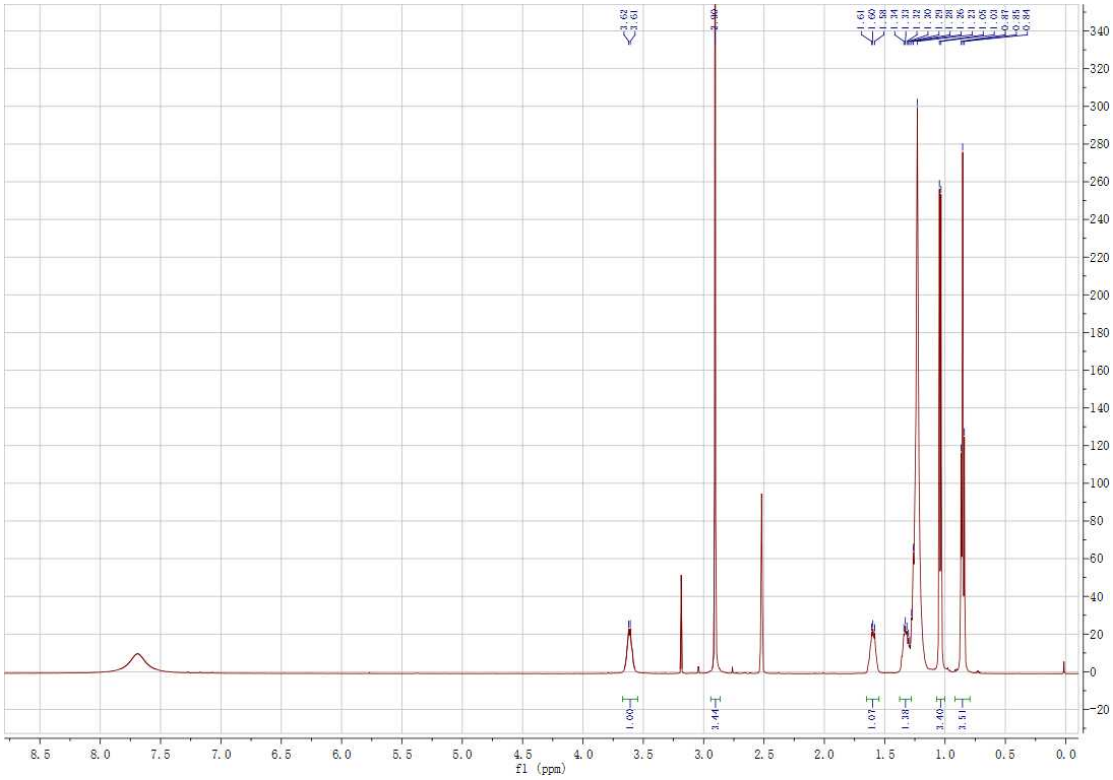


Figure S40. ^{1}H NMR spectrum of **12** (DMSO-d_6, 500 MHz)

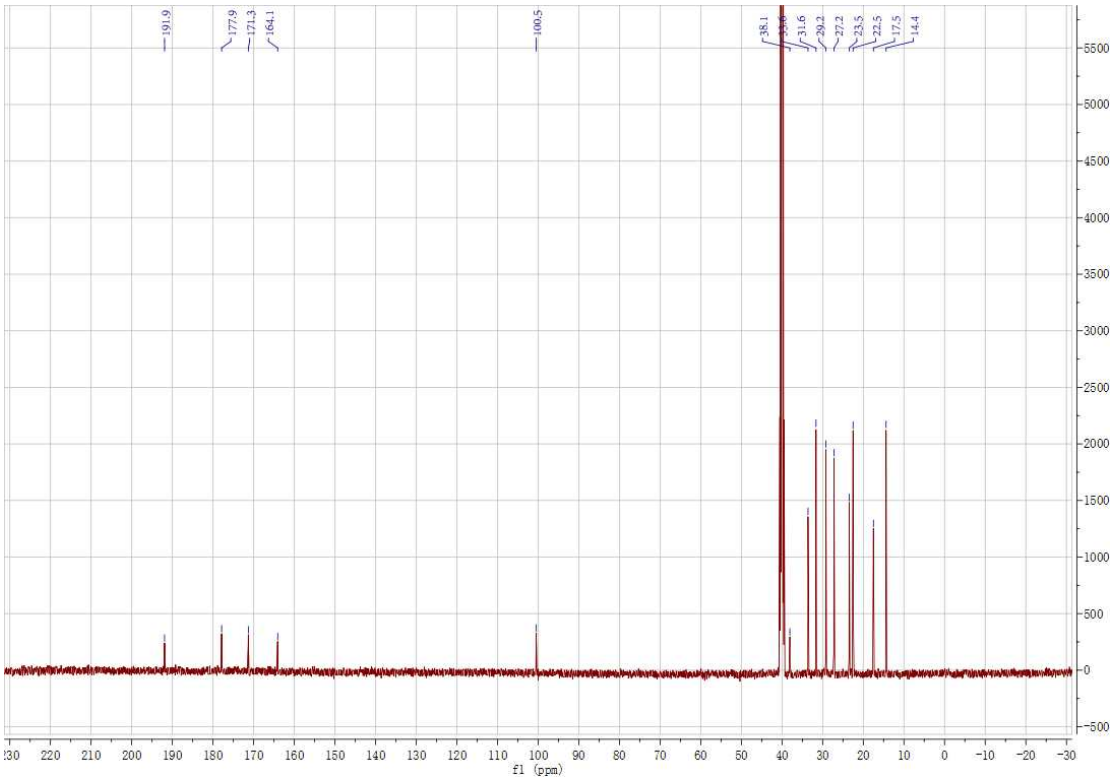


Figure S41. ^{13}C NMR spectrum of **12** (DMSO-d_6, 125 MHz)

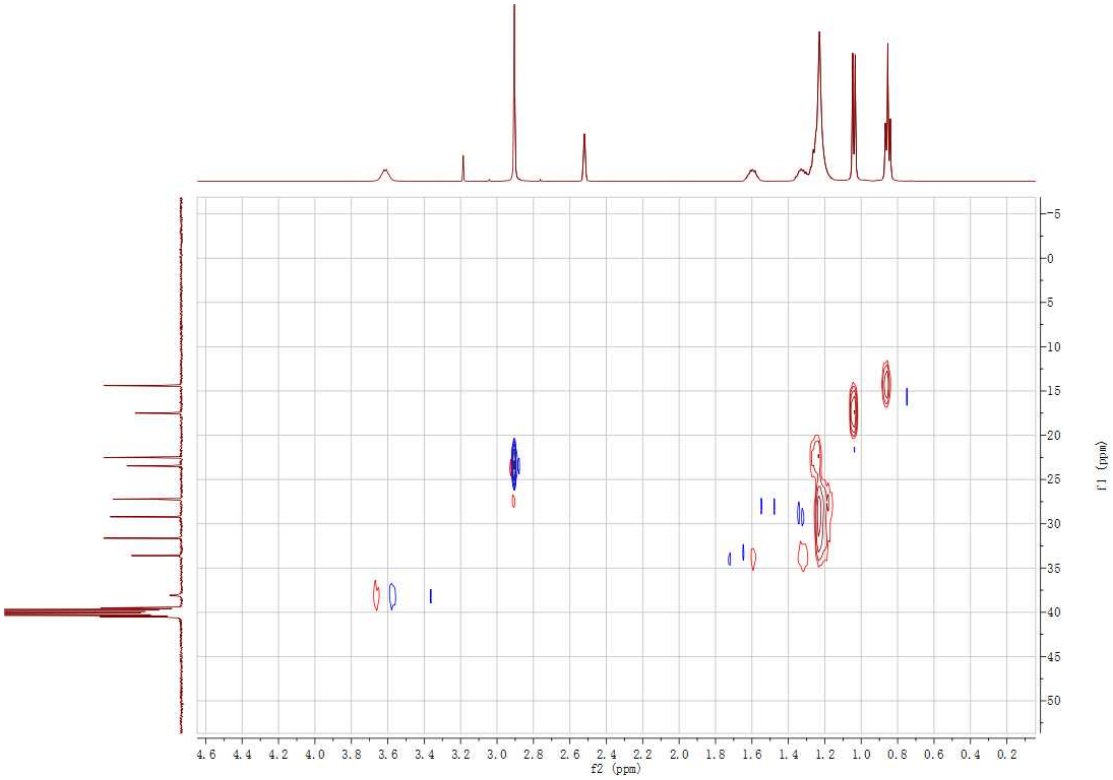


Figure S42. HSQC spectrum of **12** (DMSO-d_6)

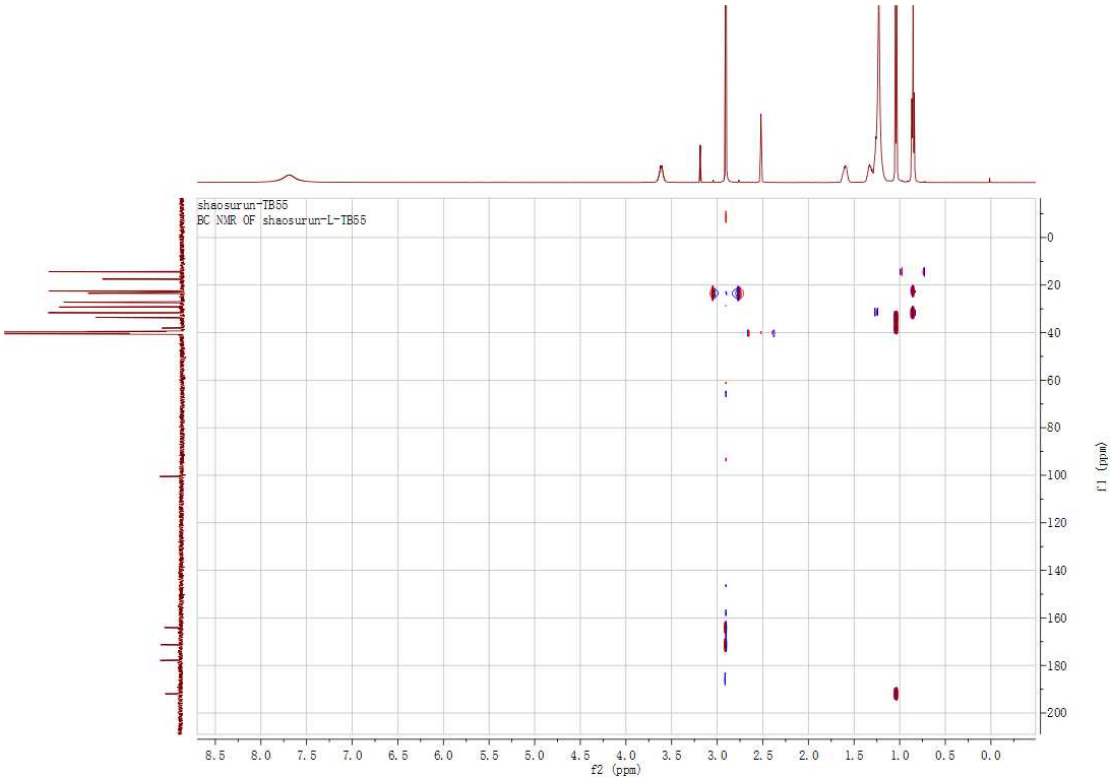


Figure S43. HMBC spectrum of **12** (DMSO-d_6)

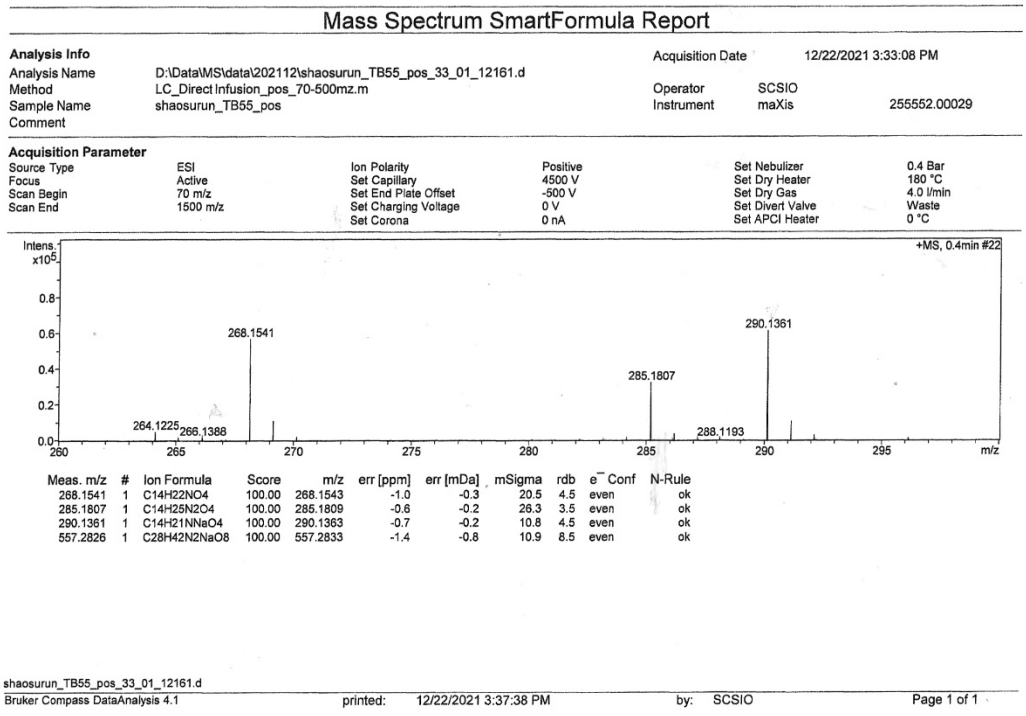


Figure S44. HRESIMS spectrum of **12**

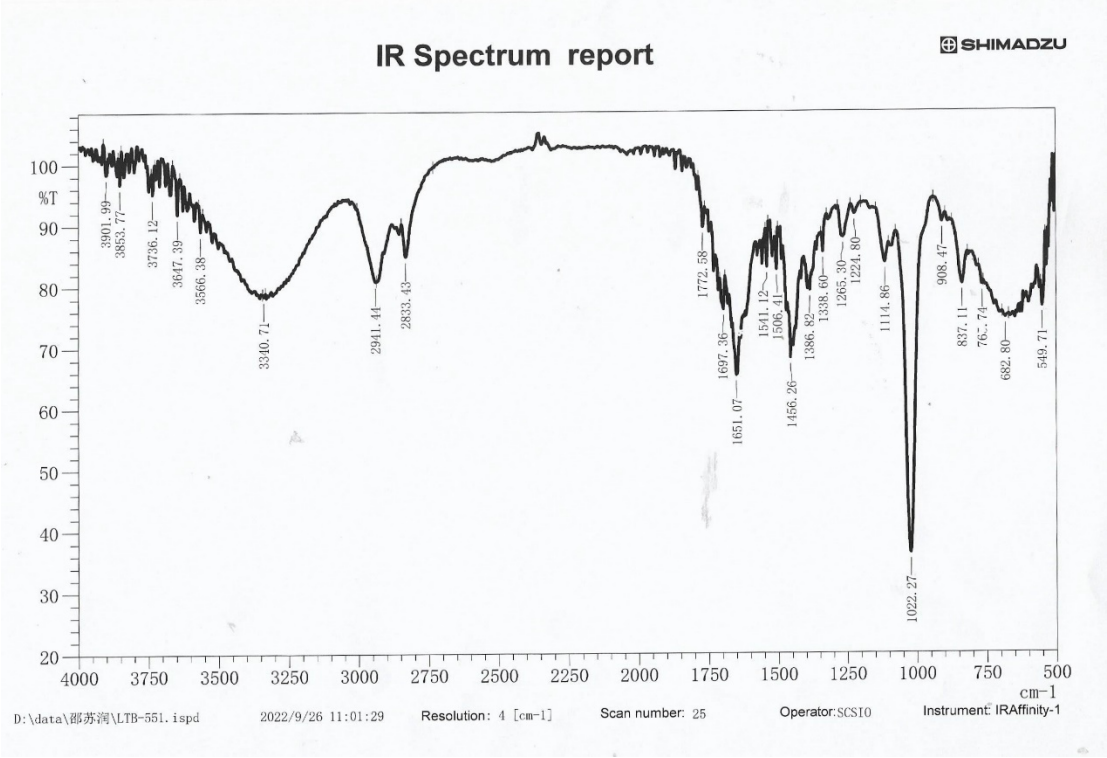
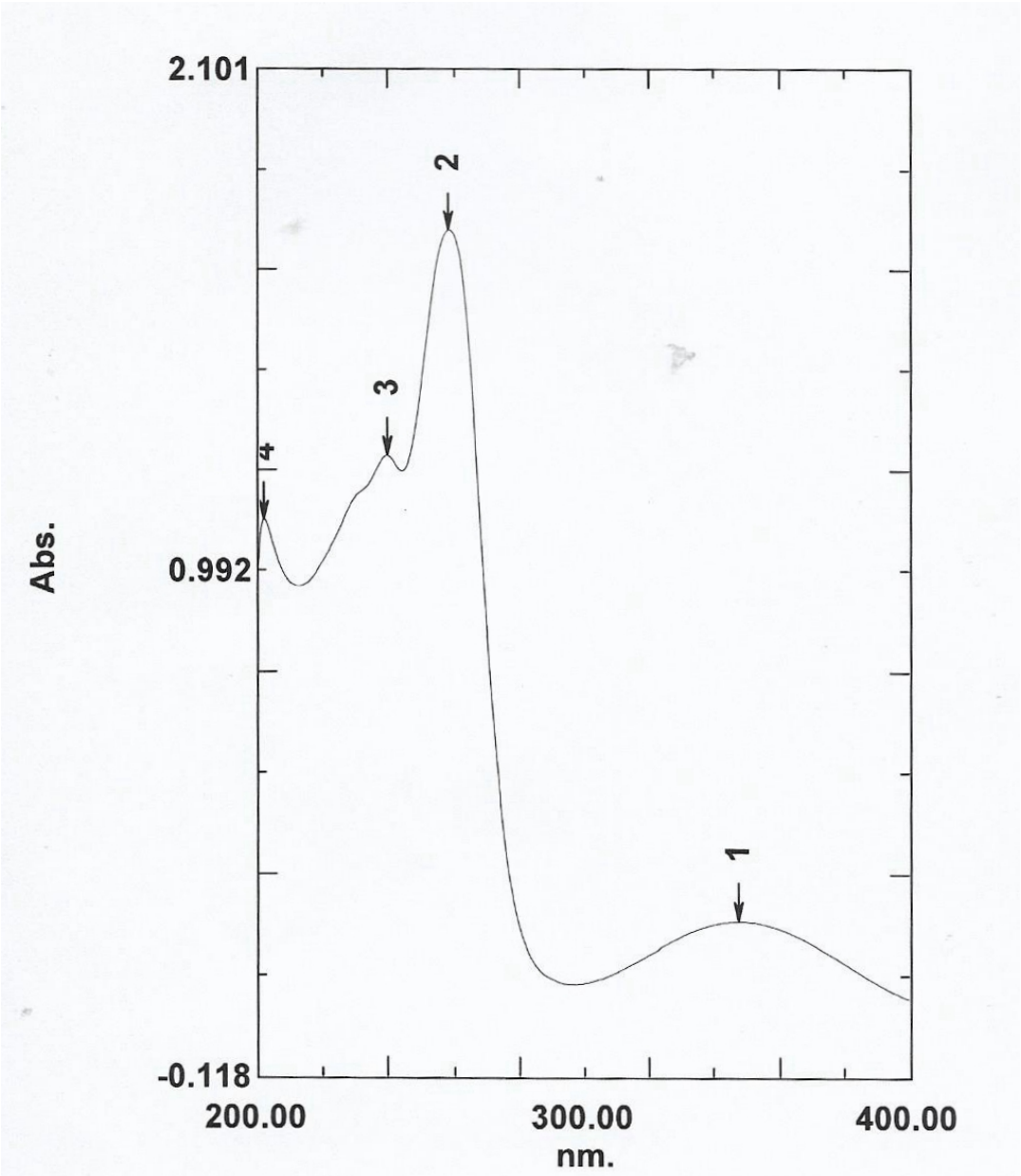
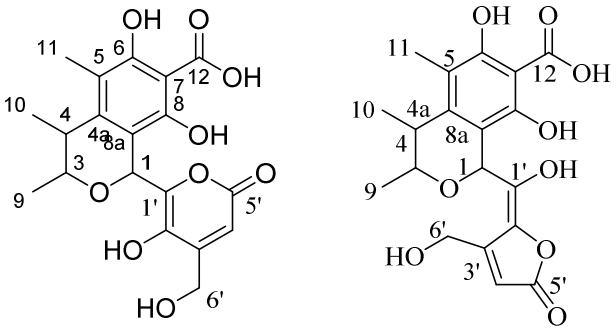


Figure S45. IR spectrum of **12**



No.	P/V	波长(nm)	Abs.	描述
1		347.20	0.223	
2		258.60	1.746	
3		239.60	1.245	
4		202.20	1.105	

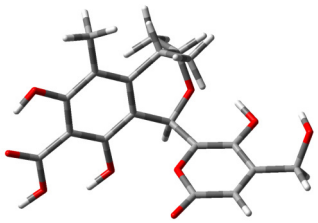
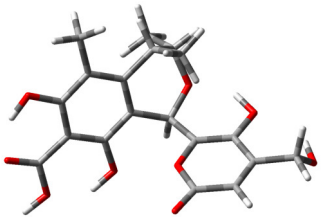
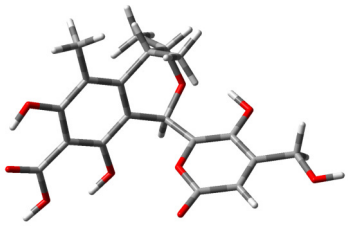
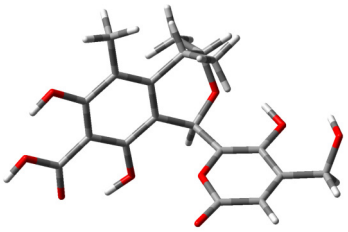
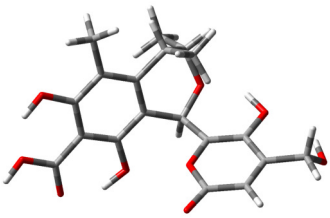
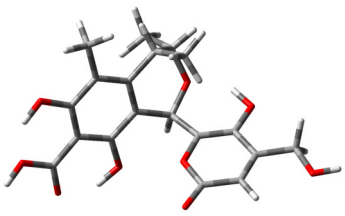
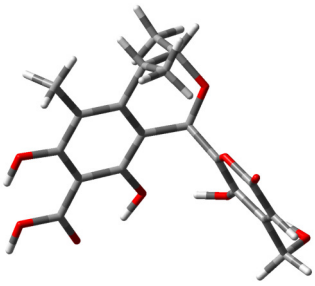
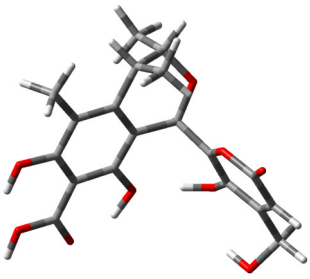
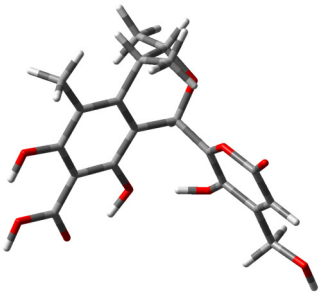
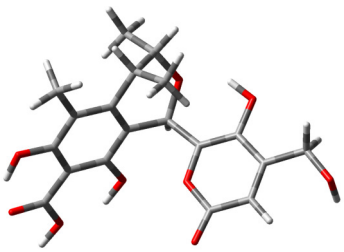
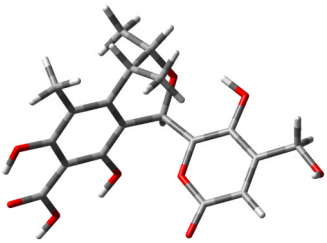
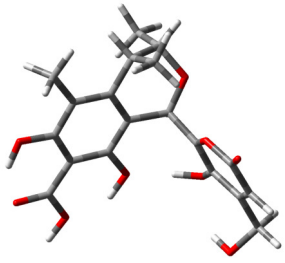
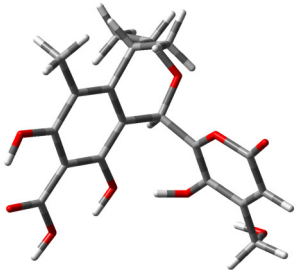
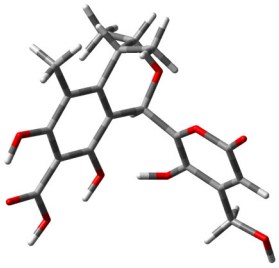
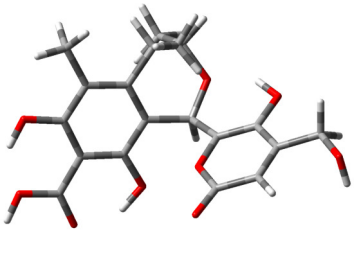
Figure S46. UV spectrum of **12**



5a 5b

Figure S47. The NMR calculations of two candidate structures (**5**a and **5**b)

5a

		
Conf.1 (7.6%)	Conf.2 (6.2%)	Conf.3 (2.0%)
		
Conf.4 (6.2%)	Conf.5 (5.1%)	Conf.6 (1.7%)
		
Conf.7 (17.1%)	Conf.8 (18.8%)	Conf.9 (5.3%)
		
Conf.10 (3.5%)	Conf.11 (3.4%)	Conf.12 (9.5%)
		
Conf.13 (7.8%)	Conf.14 (2.6%)	Conf.15 (2.9%)

5b

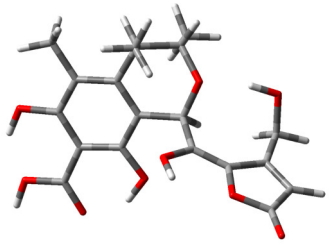
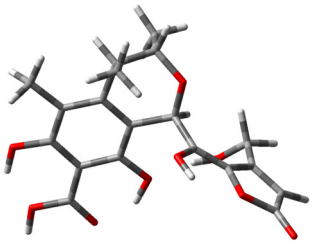
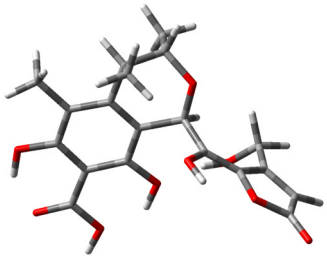
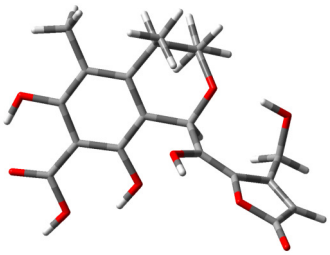
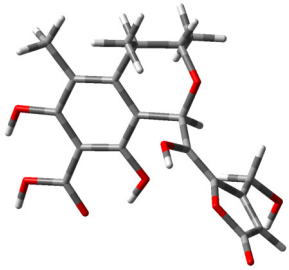
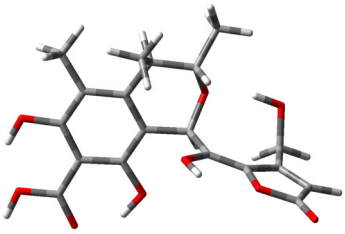
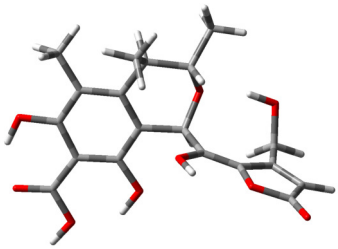
		
Conf.1 (25.3%)	Conf.2 (3.5%)	Conf.3 (2.1%)
		
Conf.4 (31.1%)	Conf.11 (5.8%)	Conf.12 (13.9%)
		
Conf.13 (17.0%)		

Figure S48. The optimized conformers and equilibrium populations of **5**a and **5**b

Table S1. Energies of **5** at MMFF94 force field

Configuration	Conformer	Energy (kJ/mol)	Population (%)
5a	1	245.12	18.1
5a	2	245.29	16.9
5a	3	245.71	14.3
5a	4	246.47	10.5
5a	5	246.92	8.8
5a	6	247.46	7.1
5a	7	249.52	3.1
5a	8	249.69	2.9
5a	9	250.03	2.5
5a	10	250.41	2.1
5a	11	250.55	2.0
5a	12	250.61	2.0
5a	13	251.11	1.6
5a	14	251.56	1.3
5a	15	251.83	1.2
5b	1	270.60	18.8
5b	2	270.77	17.5
5b	3	270.85	17.0
5b	4	271.10	15.4
5b	5	272.58	8.4
5b	6	273.03	7.1
5b	7	274.88	3.3
5b	8	275.42	2.7
5b	9	276.76	1.6
5b	10	276.93	1.5
5b	11	277.49	1.2
5b	12	277.65	1.1
5b	13	278.25	0.9

Table S2. Energies of **5** at B3LYP/6–31+G(d, p) level in methanol

Configuration	Conformer	E (Hartree)	E (kcal/mol)	Population (%)
5a	1	-1413.2151505	-886806.639090255	7.6
5a	2	-1413.2149512	-886806.514027512	6.2
5a	3	-1413.2139306	-886805.873590806	2.0
5a	4	-1413.2149615	-886806.520490865	6.2
5a	5	-1413.2147744	-886806.403083744	5.1
5a	6	-1413.2137505	-886805.760576255	1.7
5a	7	-1413.2159133	-886807.117754883	17.1
5a	8	-1413.2160064	-886807.176176064	18.9
5a	9	-1413.2148047	-886806.422097297	5.3
5a	10	-1413.2144186	-886806.179815686	3.5
5a	11	-1413.2144315	-886806.187910565	3.4
5a	12	-1413.2153618	-886806.771683118	9.5
5a	13	-1413.2151724	-886806.652832724	7.8
5a	14	-1413.2141327	-886806.000410577	2.6
5a	15	-1413.2142439	-886806.070189689	2.9
5b	1	-1413.21398	-886805.9045898	25.3
5b	2	-1413.2121165	-886804.735224915	3.5
5b	3	-1413.2116154	-886804.420779654	2.1
5b	4	-1413.2141763	-886806.027770013	31.1
5b	5	-1413.2088589	-886802.691048339	0.1
5b	6	-1413.2087708	-886802.635764708	0.1
5b	7	-1413.2096562	-886803.191362062	0.2
5b	8	-1413.2100148	-886803.416387148	0.4
5b	9	-1413.2094884	-886803.086065884	0.2
5b	10	-1413.209393	-886803.02620143	0.2
5b	11	-1413.2093962	-886803.028209462	5.8
5b	12	-1413.2134105	-886805.547222855	13.9
5b	13	-1413.2136055	-886805.669587305	17.0

Table S3. DP4+ analysis of calculated ^{1}H & ^{13}C NMR data of **5a** and **5b** (experimental for **5**, isomers **1** and **2** for **5a** and **5b**, respectively)

A	B	C	D	E	F	G	H
Functional		Solvent?		Basis Set		Type of Data	
mPW1PW91		PCM		6-311G(d,p)		Unscaled Shifts	
		DP4+	0.02%	99.98%	–	–	–
Nuclei	sp2?	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5
C		64.4	69.8	71.5			
C		73.3	79.6	79.1			
C		35.3	41.0	40.8			
C	x	141	156.9	157.5			
C	x	110.1	123.0	122.0			
C	x	159.4	166.6	167.1			
C	x	101.9	100.5	100.0			
C	x	156.5	162.5	162.0			
C	x	107.3	115.4	114.6			
C		18.8	22.1	20.3			
C		20	19.57	20.25			
C		10.3	12.07	12.73			
C		176	177.51	177.48			
C	x	150.1	156.65	154.52			
C	x	143.2	144.47	140.94			
C	x	167.5	163.56	166.36			
C	x	109	115.78	118.55			
C	x	174.7	168.95	176.16			
C		59.9	66.93	61.89			
H		5.88	6.26	5.99			
H		3.93	4.28	3.97			
H		2.63	2.88	2.84			
H		1.13	1.09	1.30			
H		1.26	1.50	1.23			
H		1.97	2.20	2.00			
H	x	6.26	6.17	6			
H		4.12	4.67	4.58			

A	B	C	D	E	F	G	H
Functional		Solvent?		Basis Set		Type of Data	
mPW1PW91		PCM		6-311G(d,p)		Unscaled Shifts	
		Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
sDP4+ (H data)		52.38%	47.62%	–	–	–	–
sDP4+ (C data)		2.77%	97.23%	–	–	–	–
sDP4+ (all data)		3.04%	96.96%	–	–	–	–
uDP4+ (H data)		0.69%	99.31%	–	–	–	–
uDP4+ (C data)		47.35%	52.65%	–	–	–	–
uDP4+ (all data)		0.62%	99.38%	–	–	–	–
DP4+ (H data)		0.75%	99.25%	–	–	–	–
DP4+ (C data)		2.50%	97.50%	–	–	–	–
DP4+ (all data)		0.02%	99.98%	–	–	–	–