Supplementary Information

Biswulfenioidins A–E, dioxygen-bridged abietane-type diterpenoid dimers with anti-zika virus potential from *Orthosiphon wulfenioides*

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Contents

Table S1. ^{1}H and ^{13}C NMR data of compound **6**−**8** in $CDCl_3$ (J in Hz, δ in ppm)

No.	**6** [b]		**7** [a]		**8** [a]	
	δ_H (J in Hz)	δ_C	δ_H (J in Hz)	δ_C	δ_H (J in Hz)	δ_C
1	2.86 m	37.3	2.85 d (13.7)	35.1	2.63 m	35.7
	1.76 m		1.66 dd (13.7, 3,4)		1.05 m	
2	1.71 m	19.1	1.55 m	18.8	1.63 m	18.5
	1.62		1.15 m		1.48 m	
3	1.64 m	41.4	1.48 dd (13.2, 3,3)	40.8	1.44 m	42.7
	1.35 m		1.31 dd (13.2, 4.9)		1.24 m	
4		33.7		33.2		33.3
5	2.26 d (12.5)	43.6	2.11 t (3.2)	52.6	1.40 d (11.9)	53.1
6	4.46 dd (12.5, 4.5)	72.5	6.53 dd (9.5, 3.2)	142.0	4.02 dd (11.9, 8.1)	73.7
7	4.63 d (4.5)	75.7	6.22 dd (9.5, 3.2)	126.9	4.22 d (8.1)	77.6
8		126.9		139.5		144.5
9		132.7		141.5		144.7
10		41.4		38.5		41.5
11		142.0		182.1		181.4
12		140.4		182.0		180.8
13		131.7		148.0		147.5
14	6.86 br s	119.9	6.57 d (1.3)	136.6	7.02 br s	134.0
15	3.04 sept (6.7)	27.0	2.92 sept (6.8)	27.2	2.92 sept (7.0)	27.3
16	1.27 d (6.7)	22.5	1.11 d (6.8)	21.6	1.11 d (6.9)	21.4
17	1.29 d (6.7)	22.4	1.11 d (6.8)	21.7	1.12 d (6.9)	21.4
18	1.28 s	34.4	0.98 s	32.8	1.20 s	36.2
19	1.40 s	23.5	0.99 s	23.0	1.13 s	22.7
20	1.42 s	23.4	1.00 s	15.5	1.36 s	21.5
1′	2.90 m	36.5				
	1.54 m					
2′	1.71 m	19.1				
	1.55 m					
3′	1.52 m	41.3				
	1.26 m					
4′		33.1				
5′	1.73 d (11.3)	51.6				
6′	3.94 dd (11.3, 8.7)	77.5				
7′	4.58 d (8.7)	73.7				
8′		127.3				
9′		131.7				
10′		42.1				
11′		140.9				
12′		140.1				
13′		132.0				
14′	7.09 br s	114.1				
15′	3.01 sept (6.8)	27.4				
16′	1.26 d (6.8)	22.6				
17′	1.24 d (6.8)	22.6				
18′	1.12 s	35.3				
19′	1.30 s	23.8				
20′	1.52 s	23.2				

[a]Measured at 400 MHz, [b]Measured at 600 MHz.

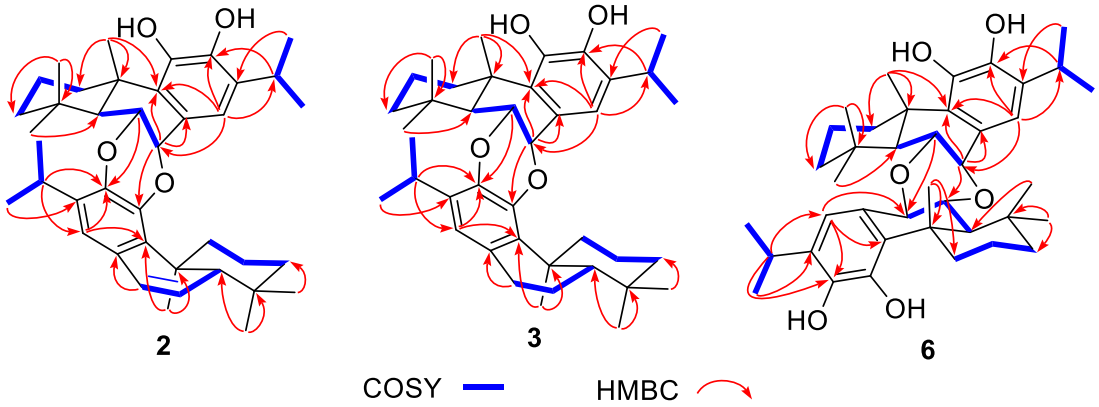

Figure S1. Key HMBC and COSY correlations of compounds **2**, **3**, and **6**

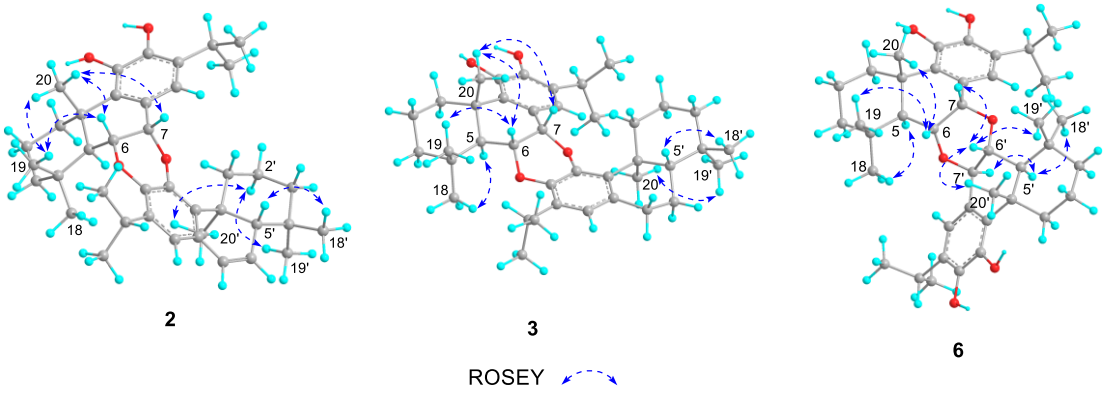

Figure S2. Key ROESY correlations of compounds **2**, **3**, and **6**.

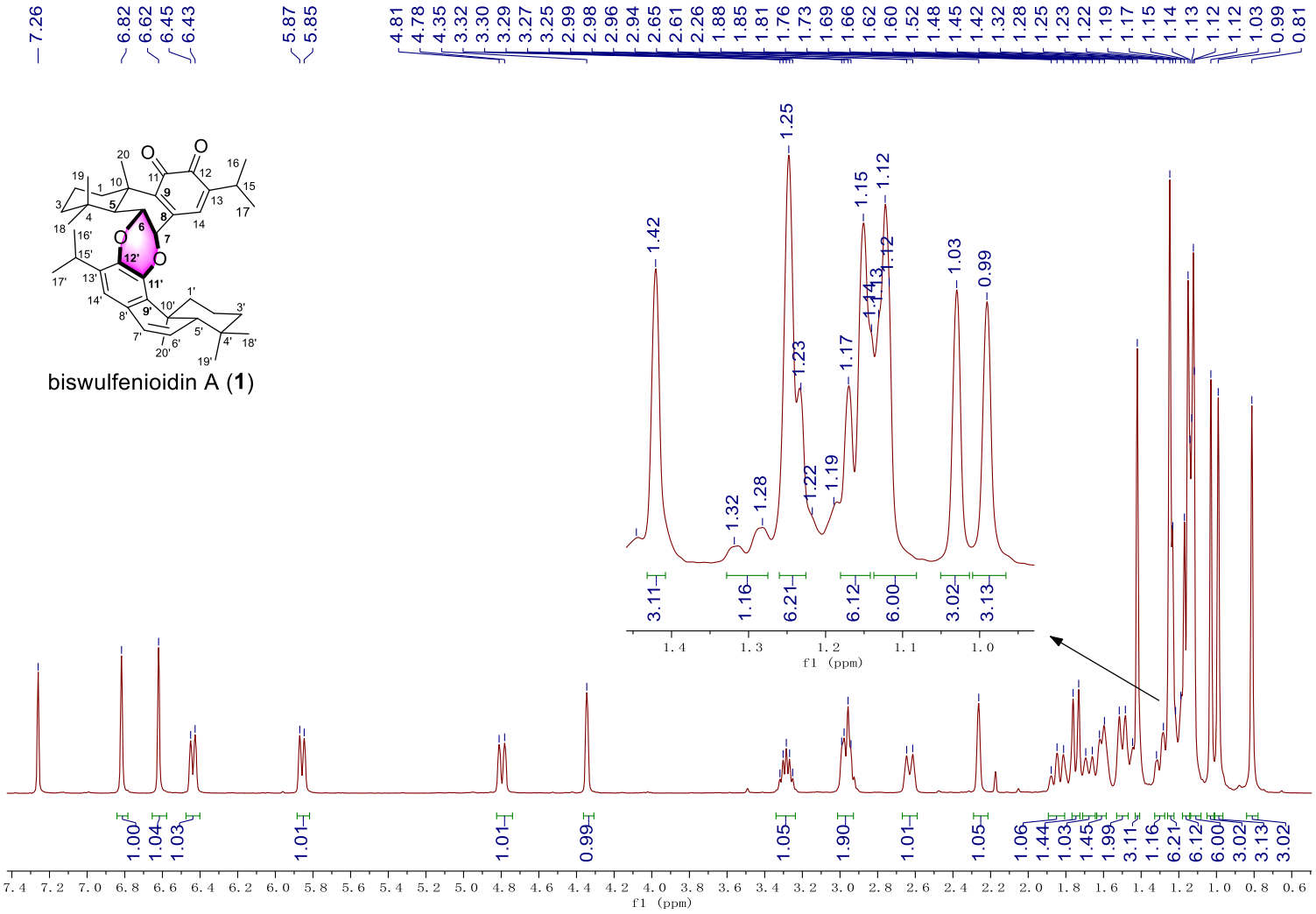

Figure S3. ^{1}H NMR spectrum of biswulfenioidin A (**1**) in chloroform (400 MHz)

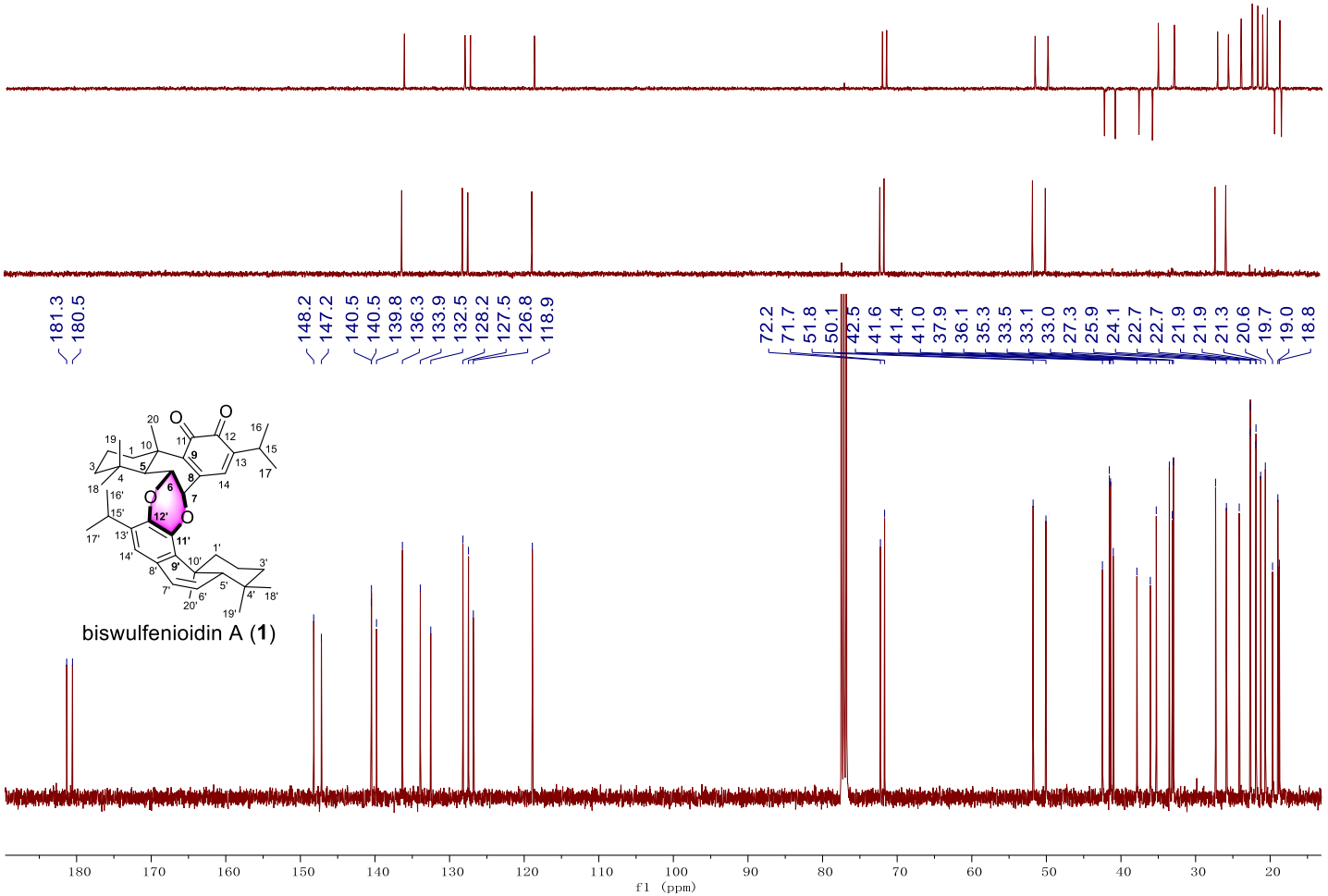

Figure S4. ^{13}C and DEPT NMR spectra of biswulfenioidin A (**1**) in chloroform (100 MHz)

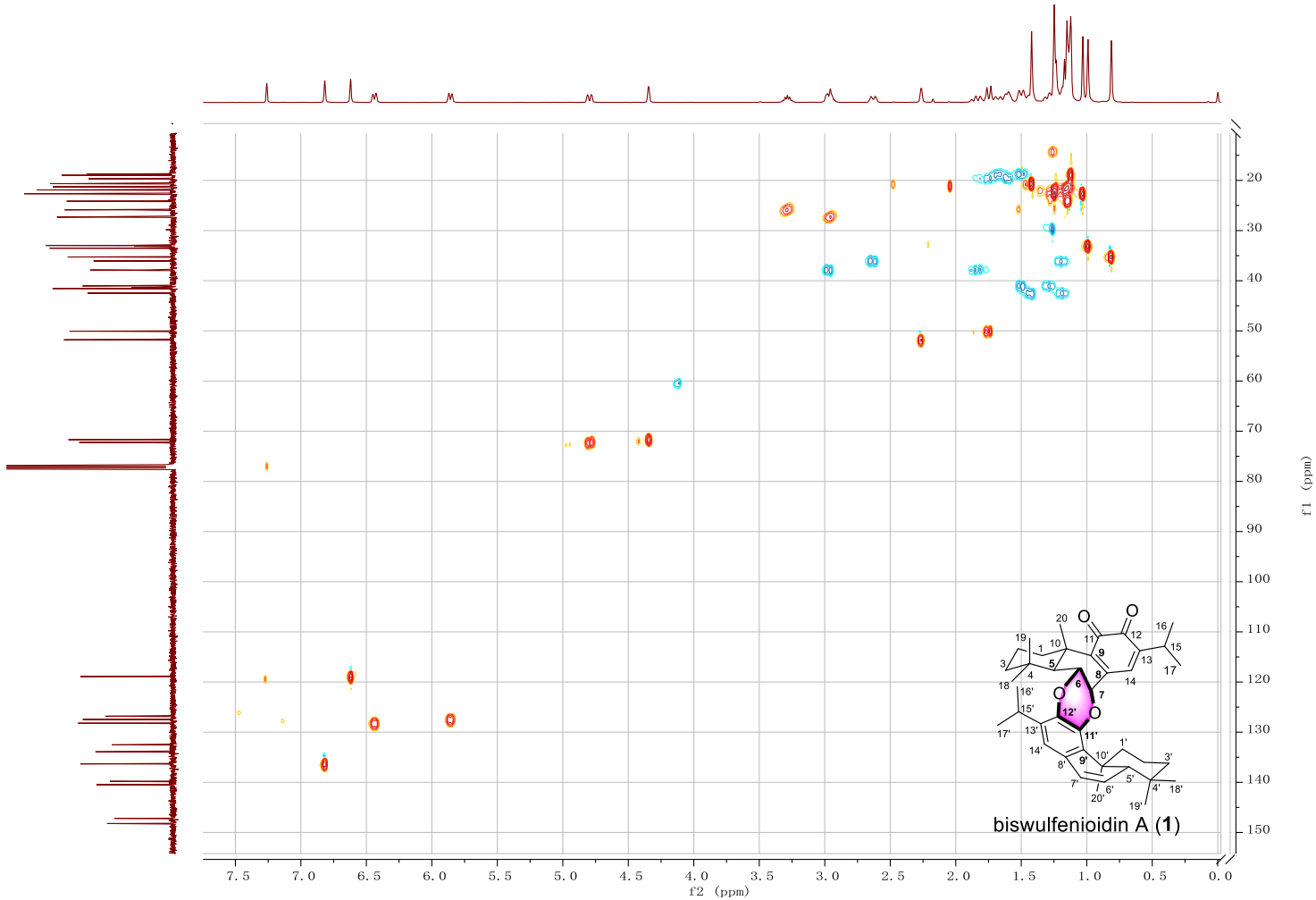

Figure S5. HSQC spectrum of biswulfenioidin A (**1**) in chloroform (400 MHz)

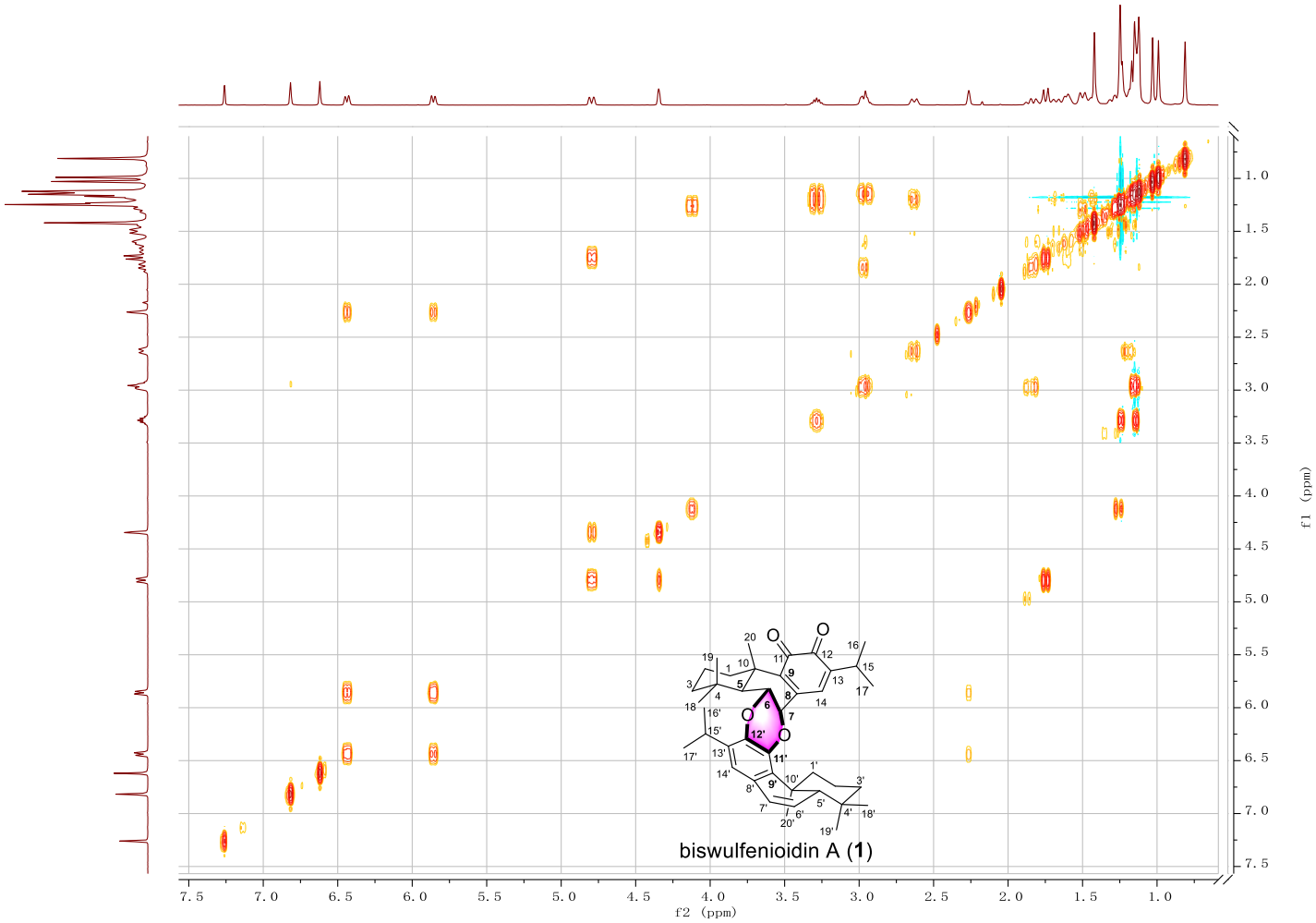

Figure S6. ^{1}H-^{1}H COSY spectrum of biswulfenioidin A (**1**) in chloroform (400 MHz)

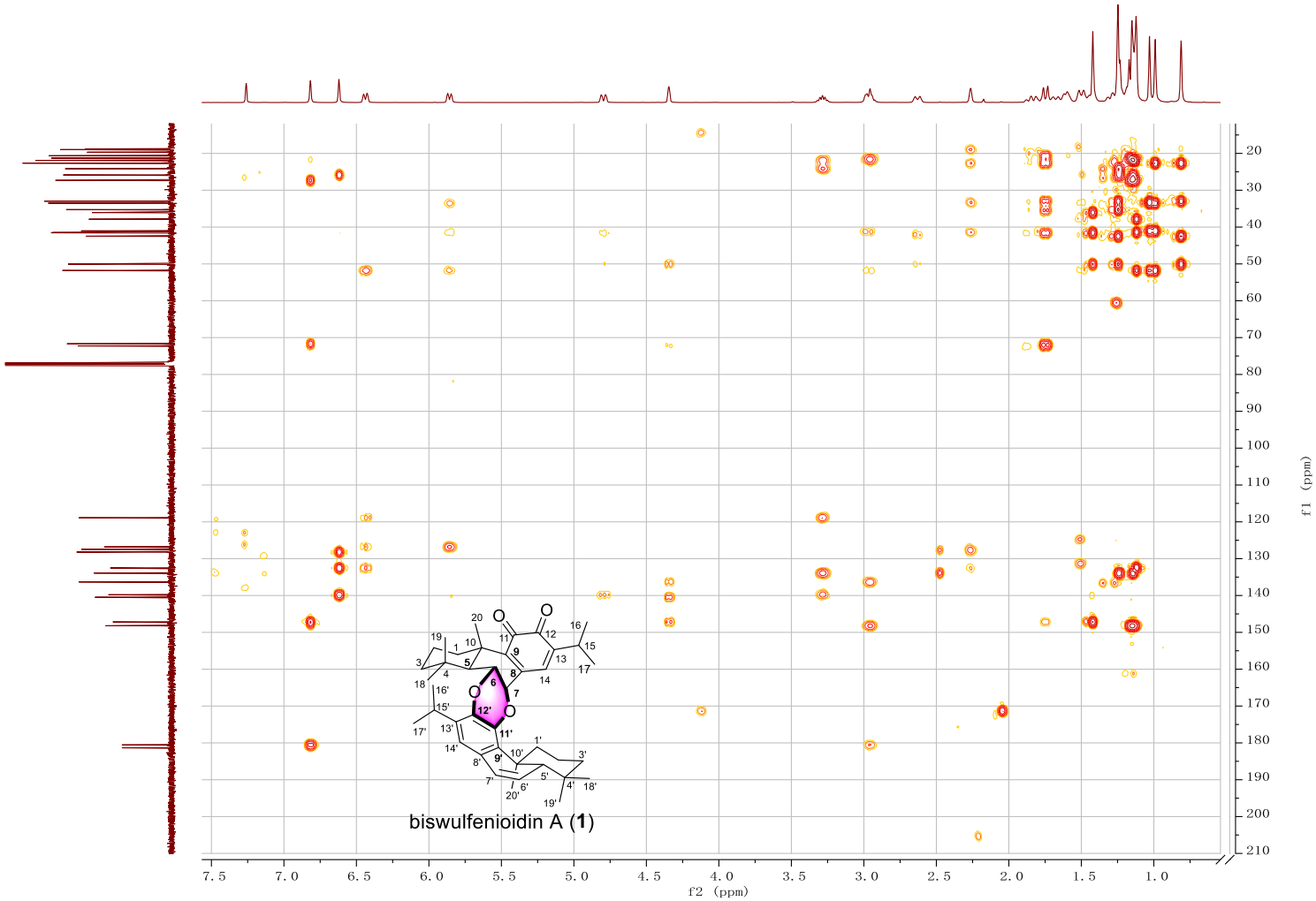

Figure S7. HMBC spectrum of biswulfenioidin A (**1**) in chloroform (400 MHz)

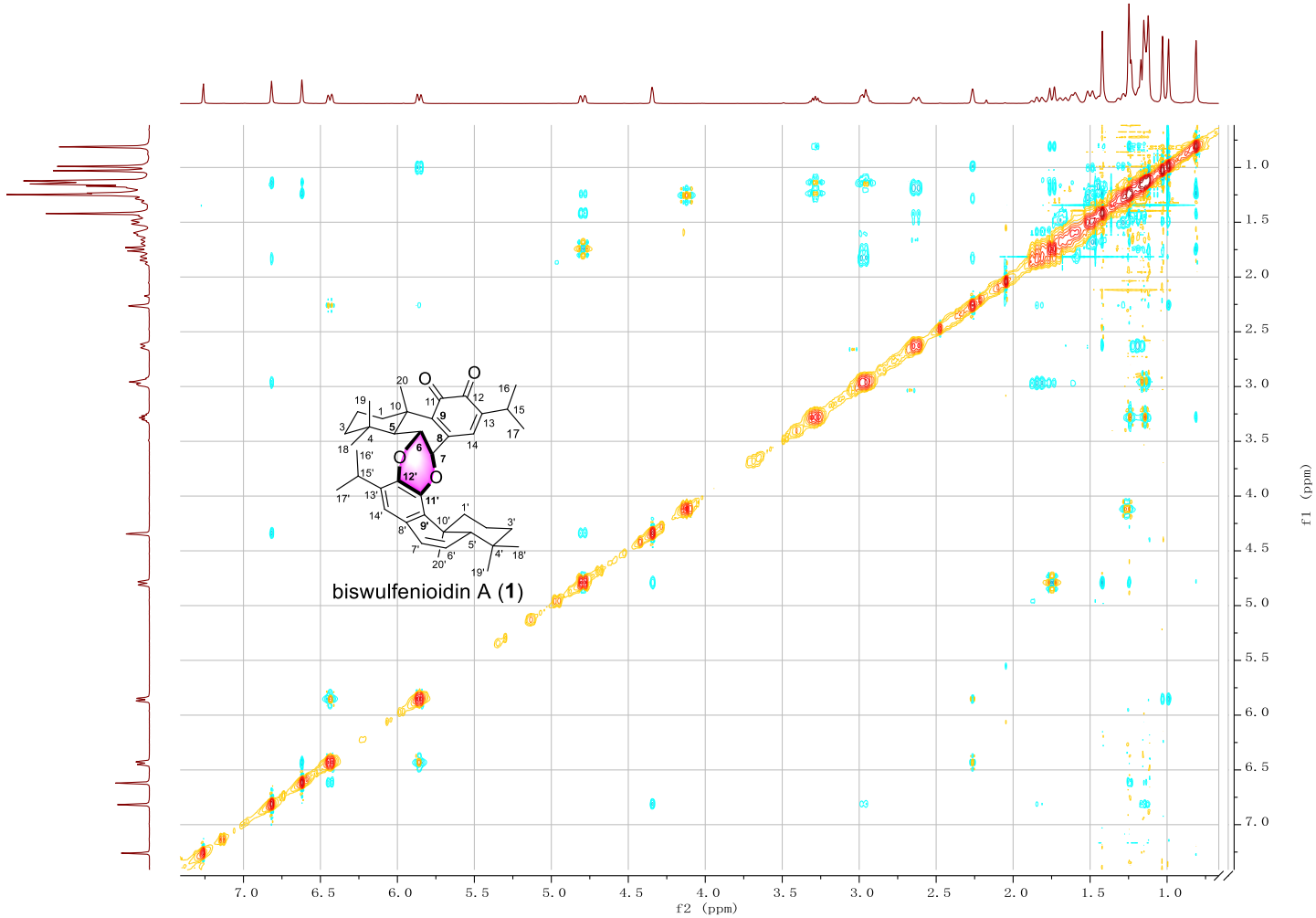

Figure S8. ROESY spectrum of biswulfenioidin A (**1**) in chloroform (400 MHz)

MS Formula Results: + Scan (0.225 min) Sub (JJS-16+++.d)

m/z	Ion	Formula	Abundance
597.394	(M+H)+	C40 H53 O4	110126.5

Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
☑	C40 H52 O4	C40 H53 O4	86.78		597.3938	-0.63	99.51	74.35	76.24

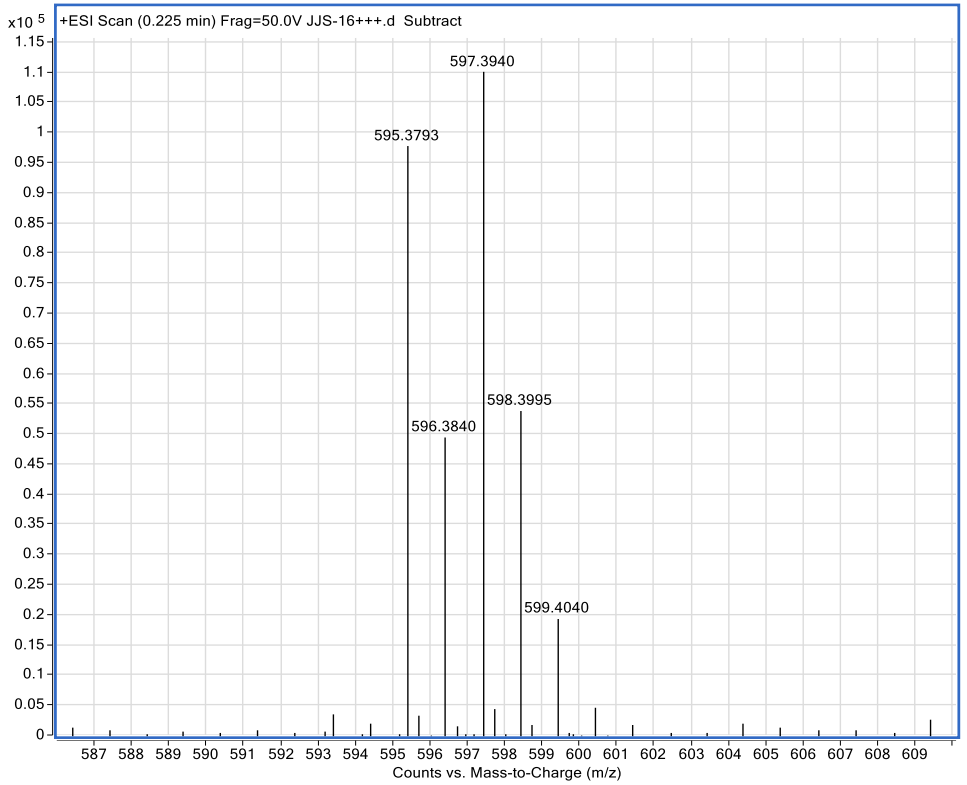

Figure S9. HRESIMS spectrum of biswulfenioidin A (**1**)

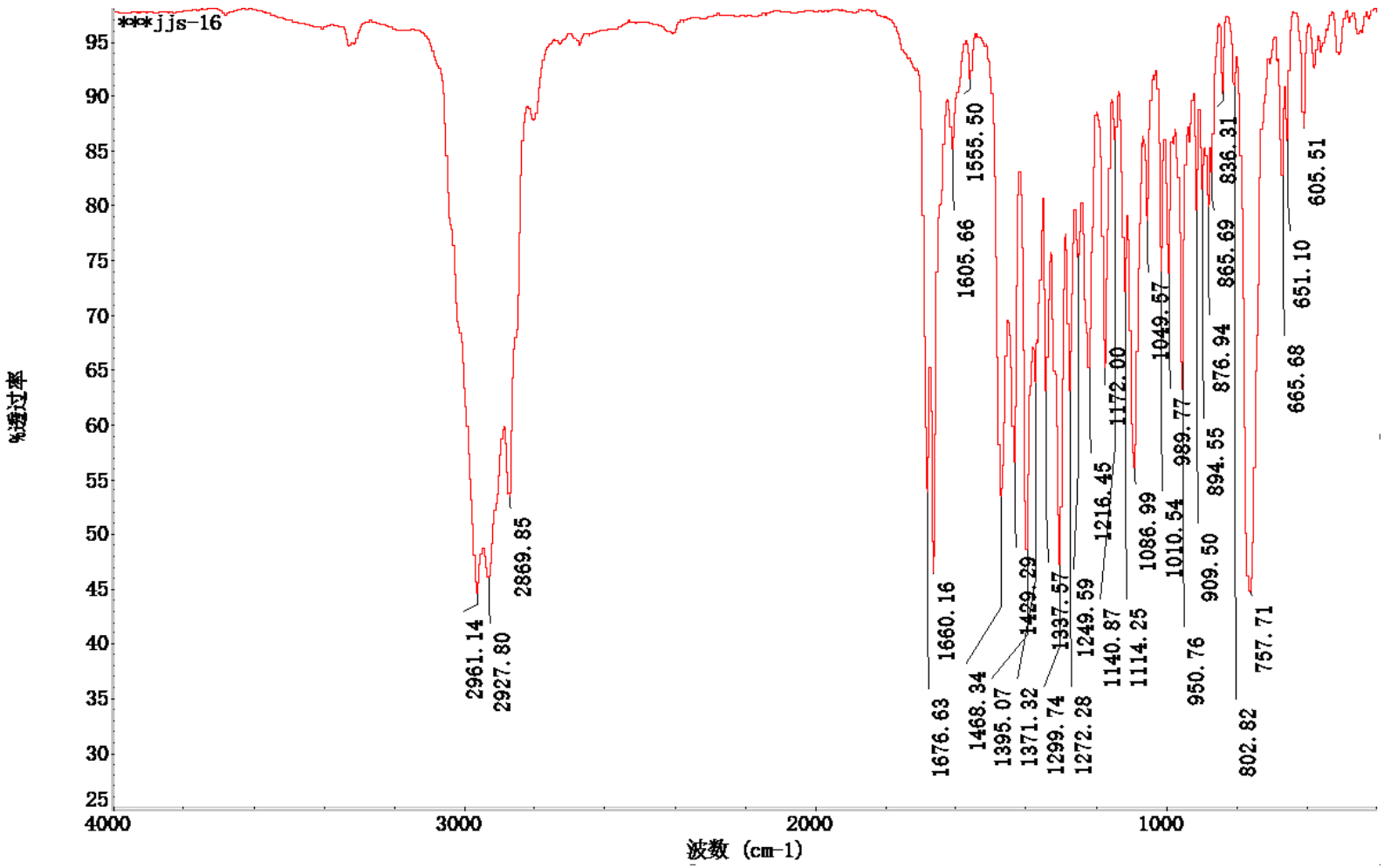

Figure S10. IR spectrum of biswulfenioidin A (**1**)

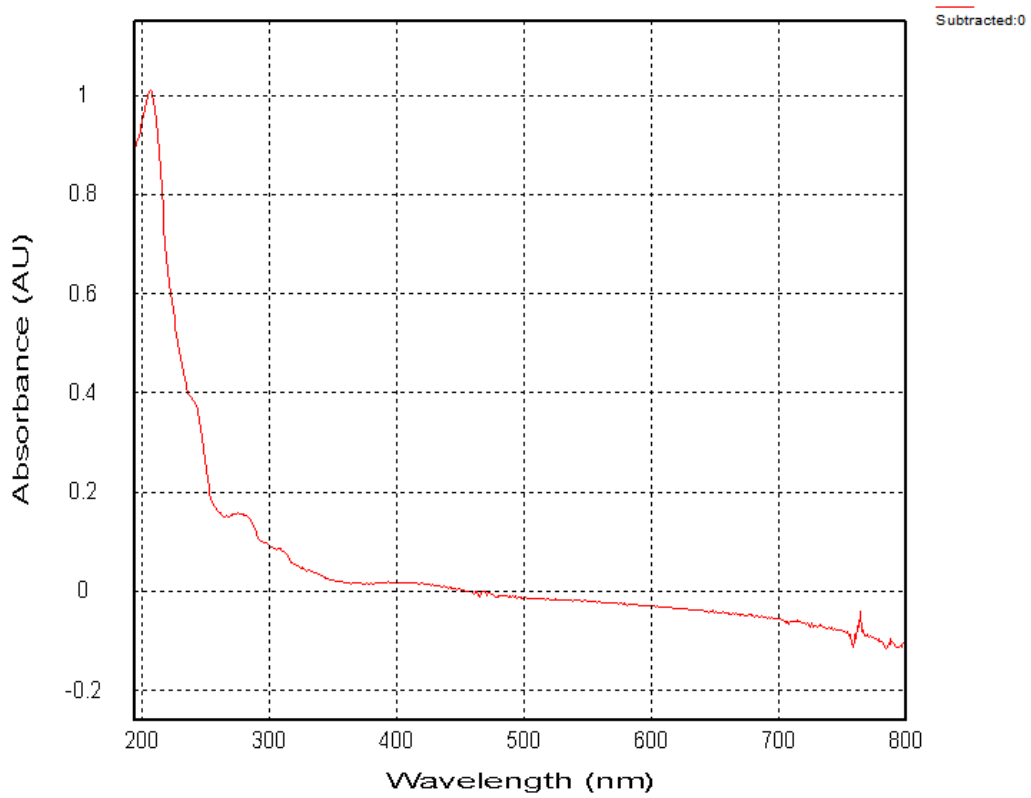

Figure S11. UV spectrum of biswulfenioidin A (**1**)

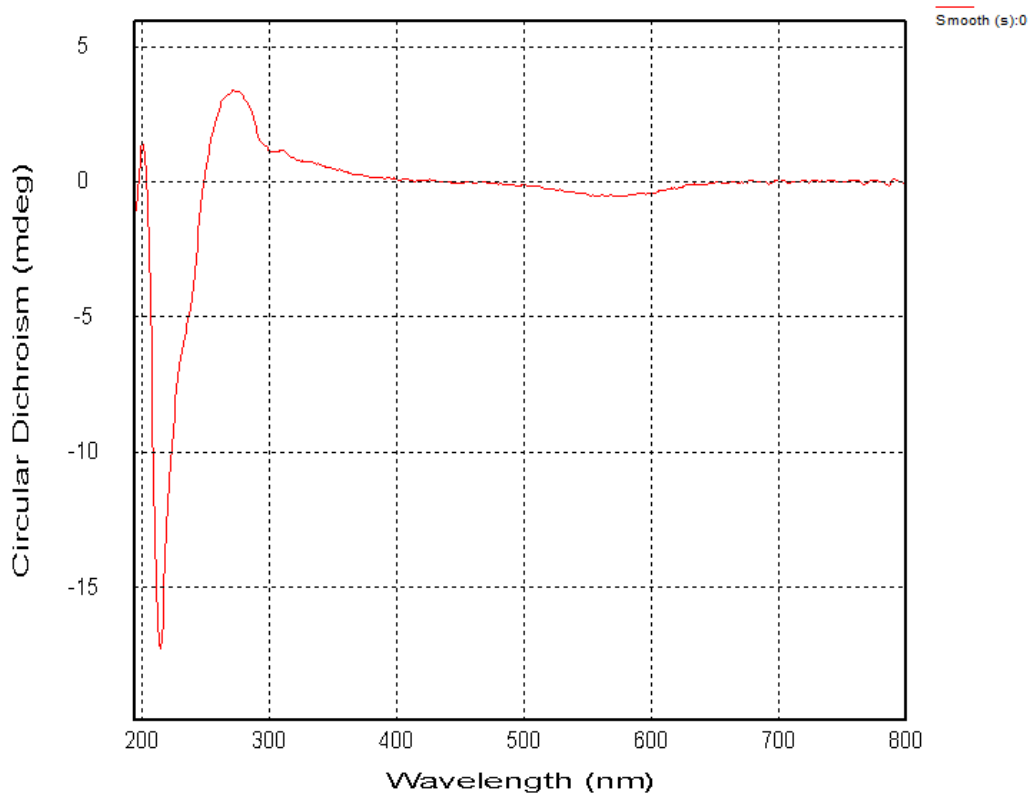

Figure S12. CD spectrum of biswulfenioidin A (**1**)

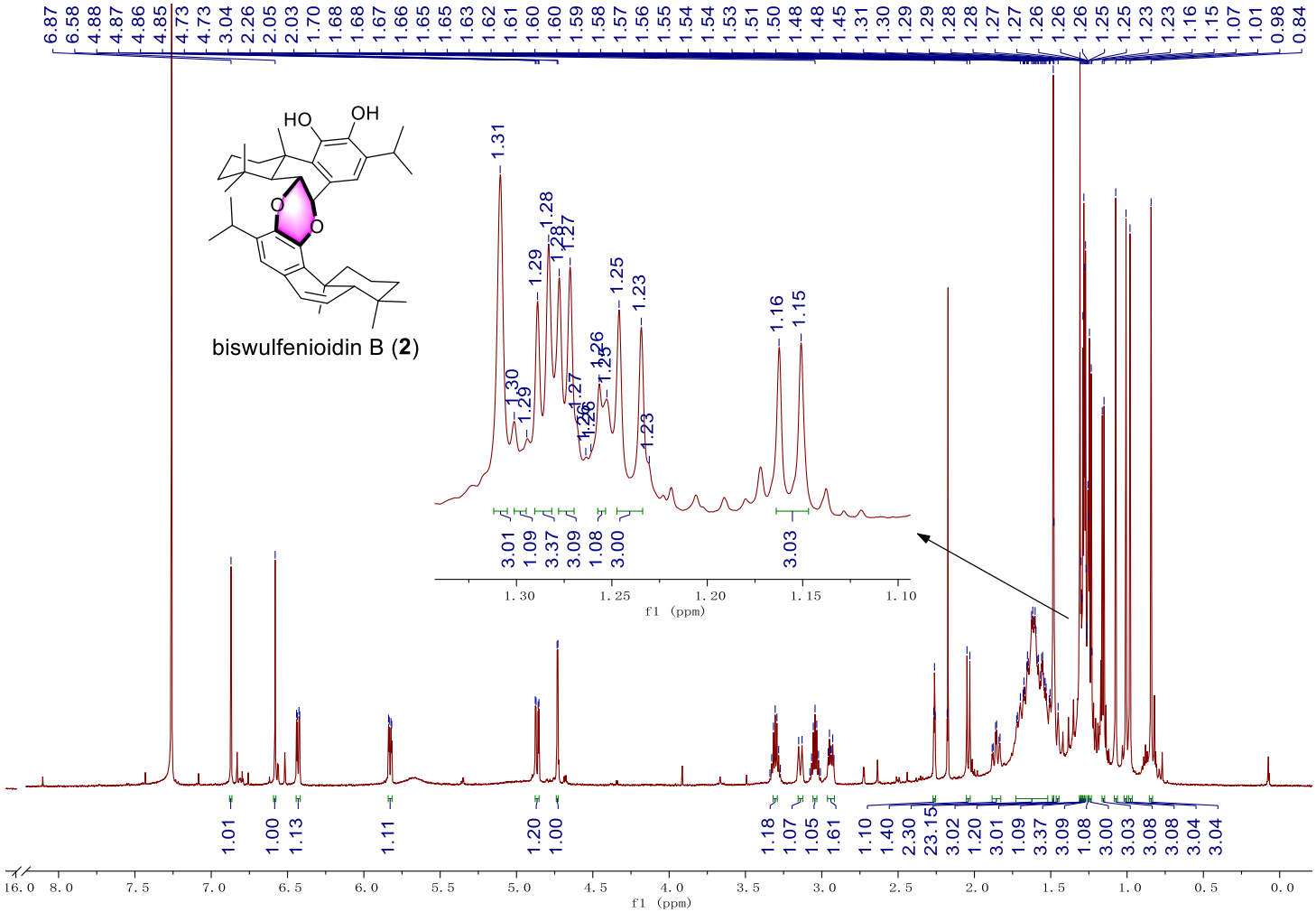

Figure S13. ^{1}H NMR spectrum of biswulfenioidin B (**2**) in chloroform (600 MHz)

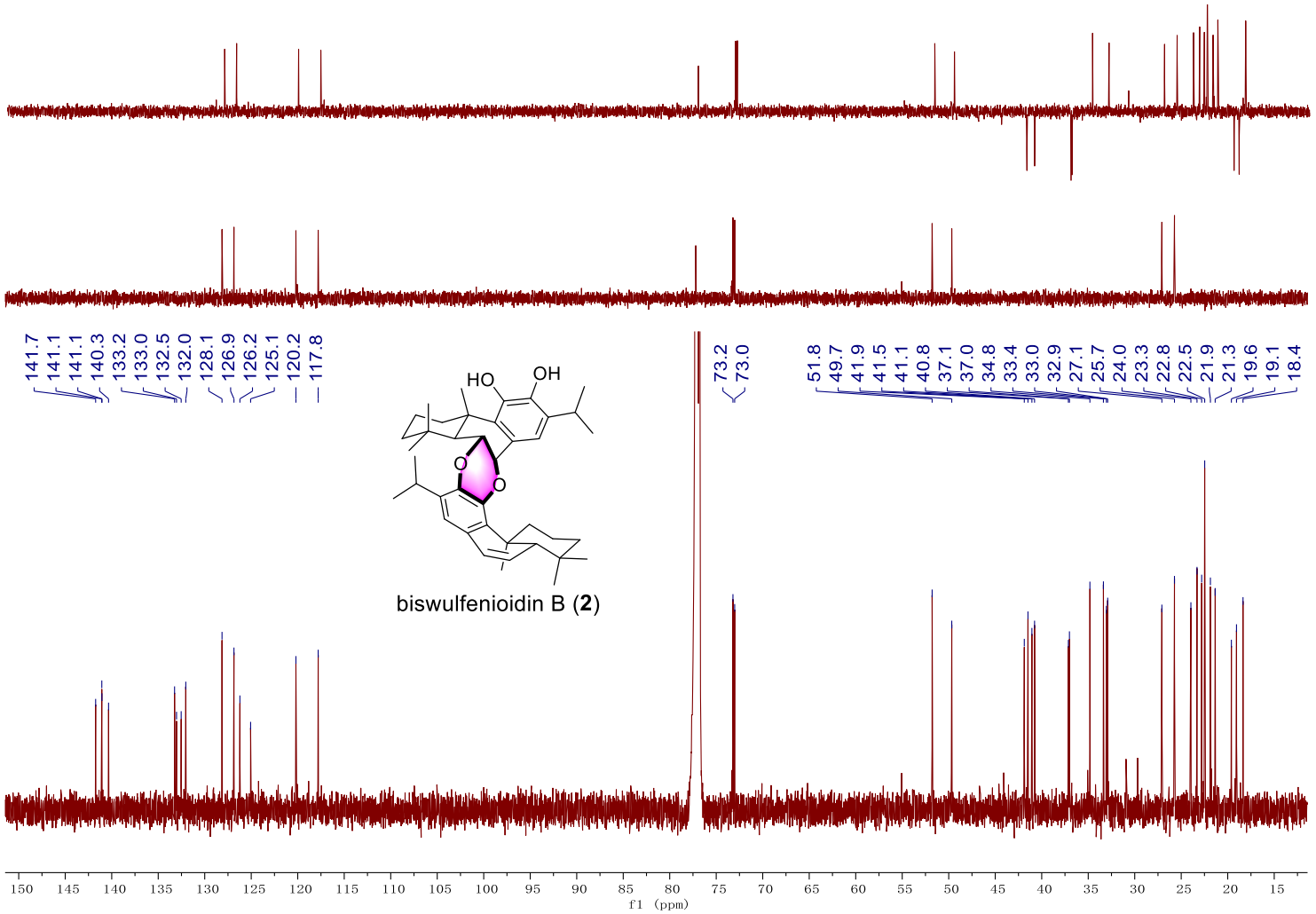

Figure S14. ^{13}C and DEPT NMR spectra of biswulfenioidin B (**2**) in chloroform (150 MHz)

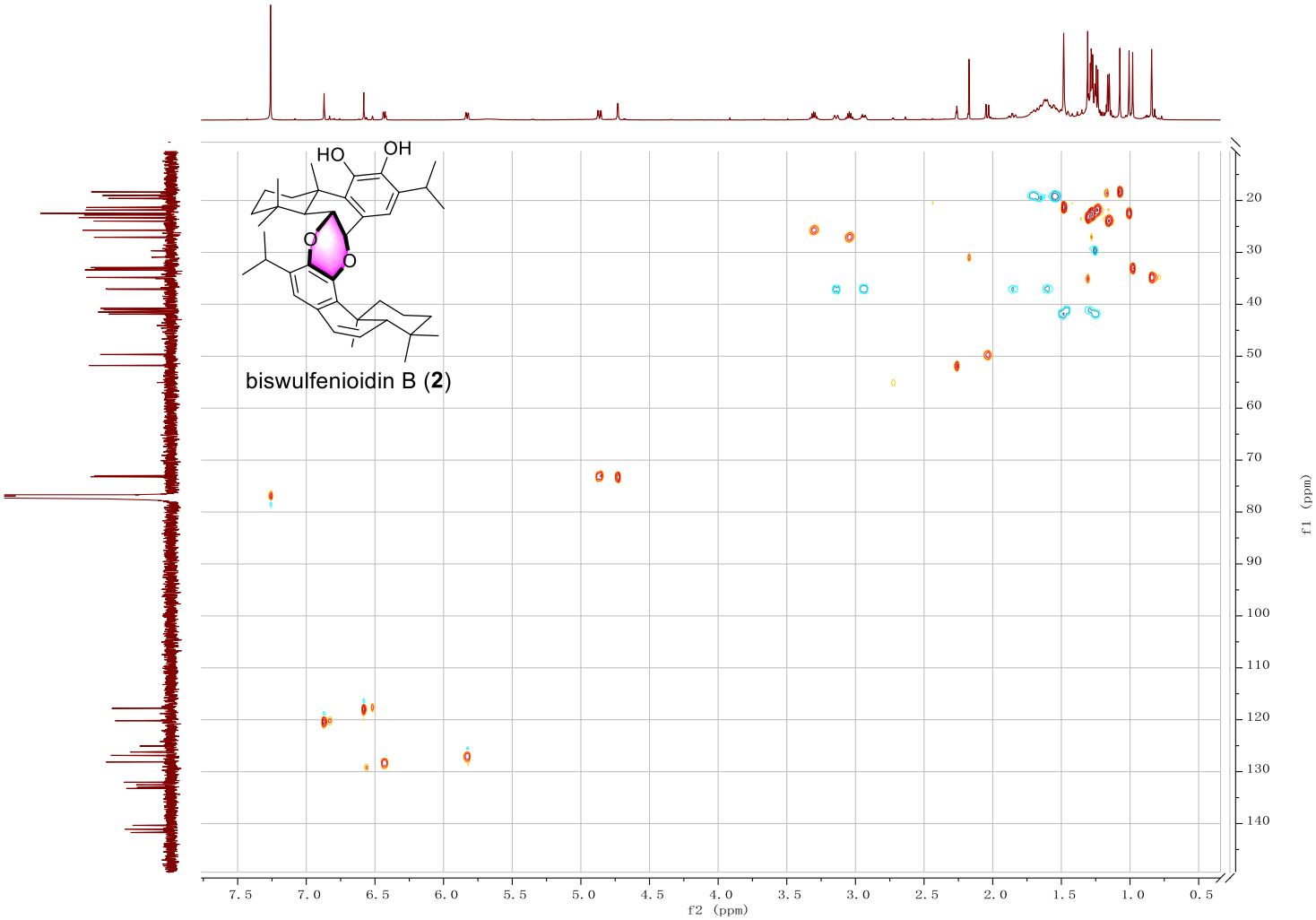

Figure S15. HSQC spectrum of biswulfenioidin B (**2**) in chloroform (600 MHz)

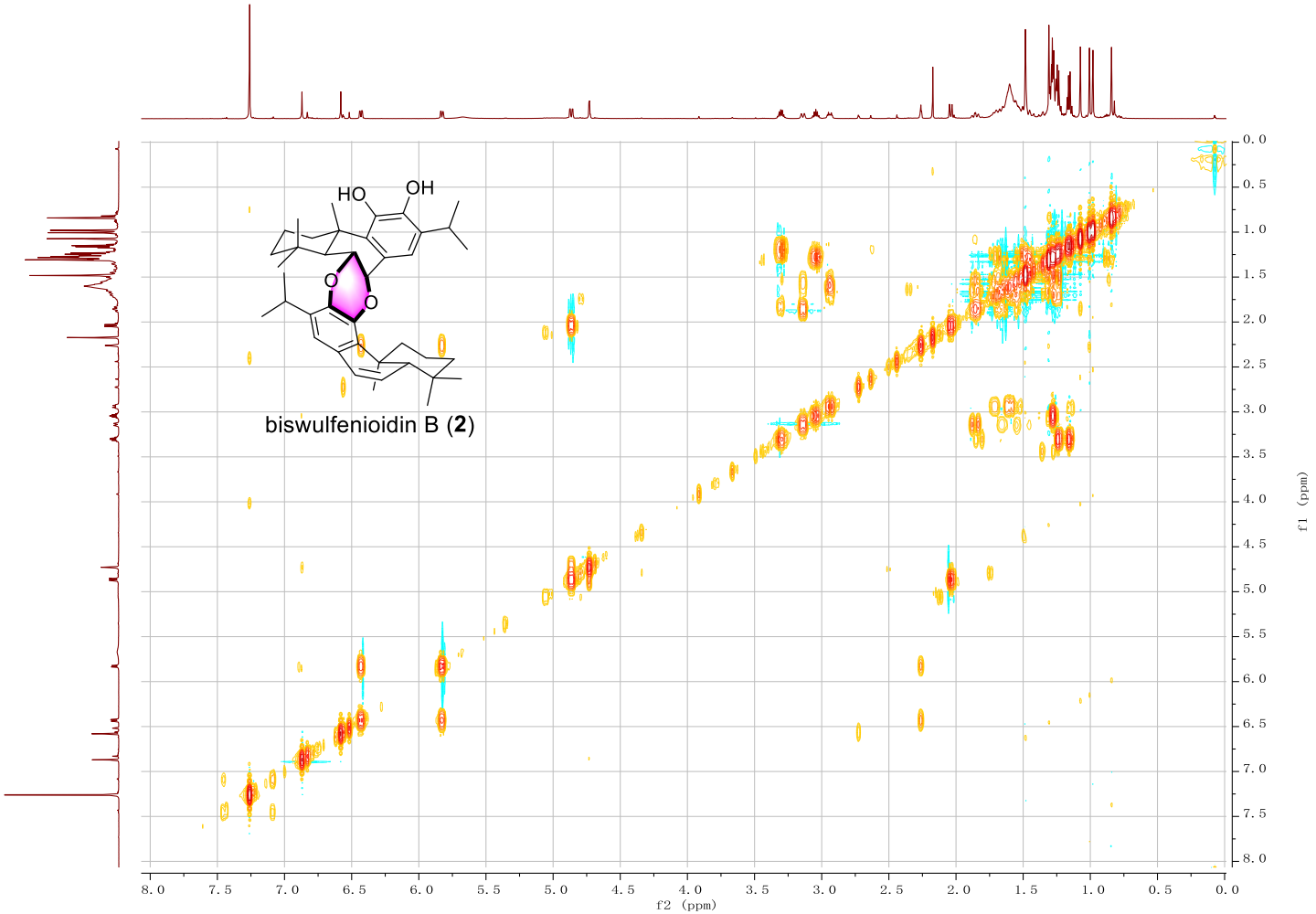

Figure S16. ^{1}H-^{1}H COSY spectrum of biswulfenioidin B (**2**) in chloroform (600 MHz)

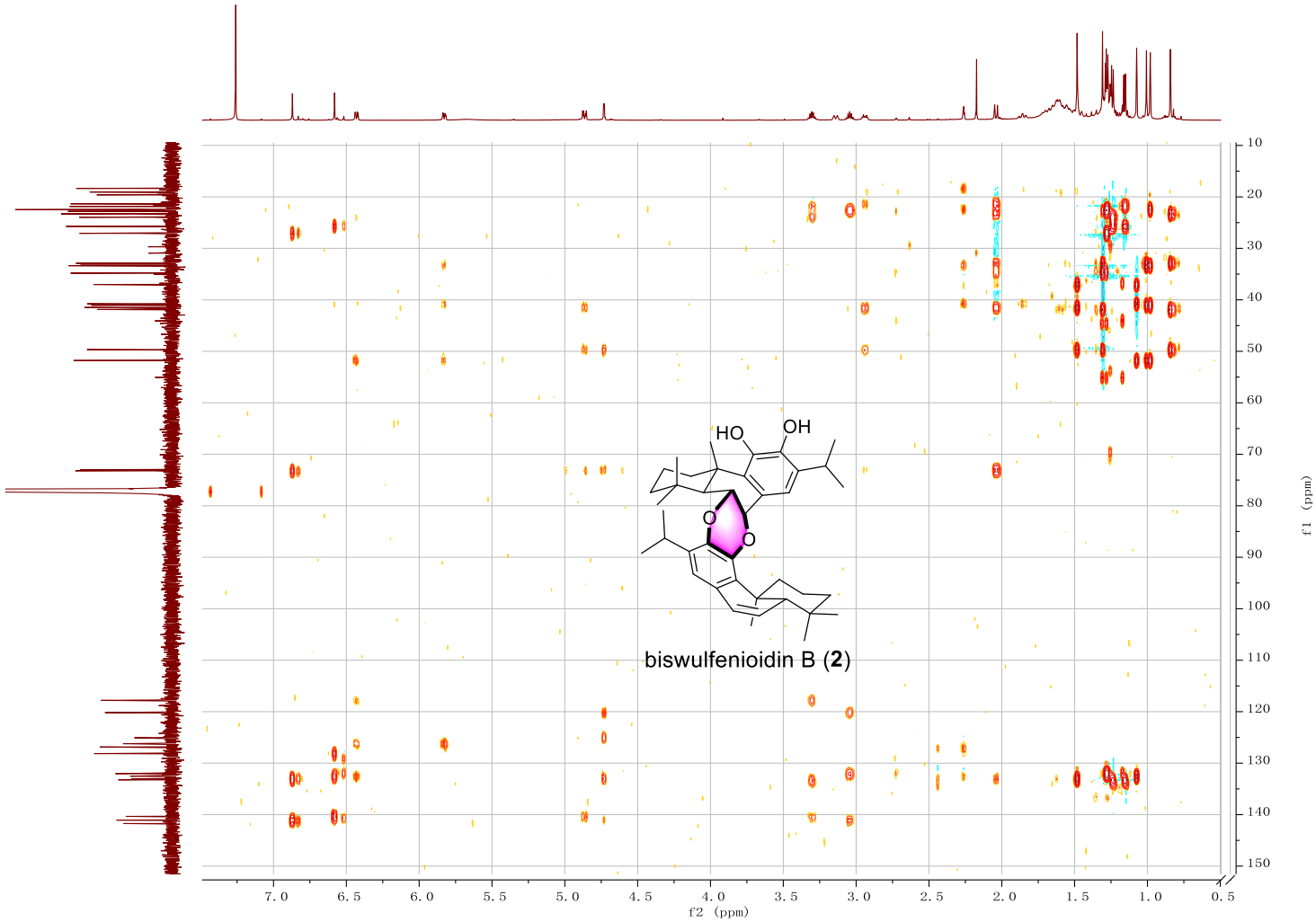

Figure S17. HMBC spectrum of biswulfenioidin B (**2**) in chloroform (600 MHz)

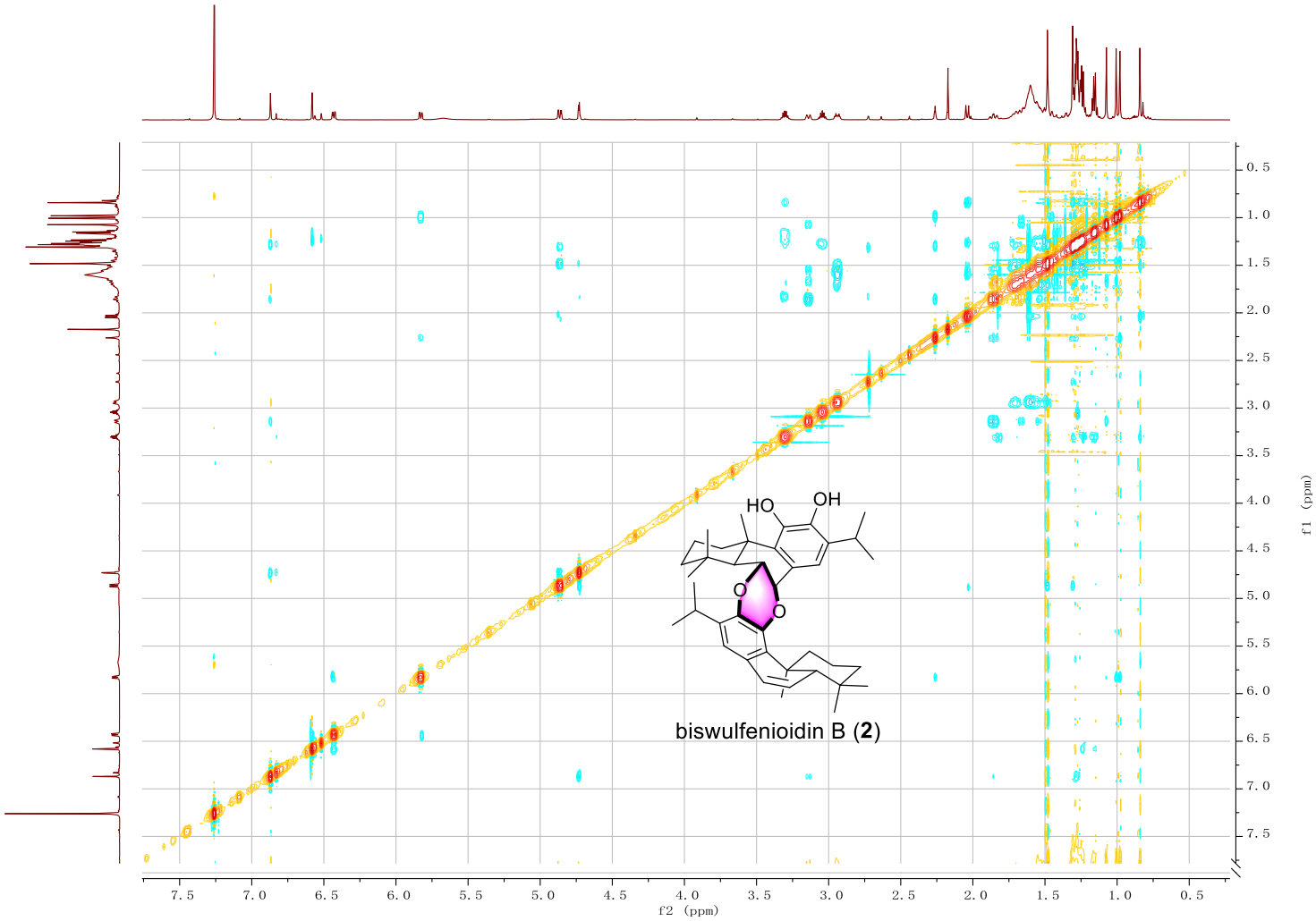

Figure S18. ROESY spectrum of biswulfenioidin B (**2**) in chloroform (600 MHz)

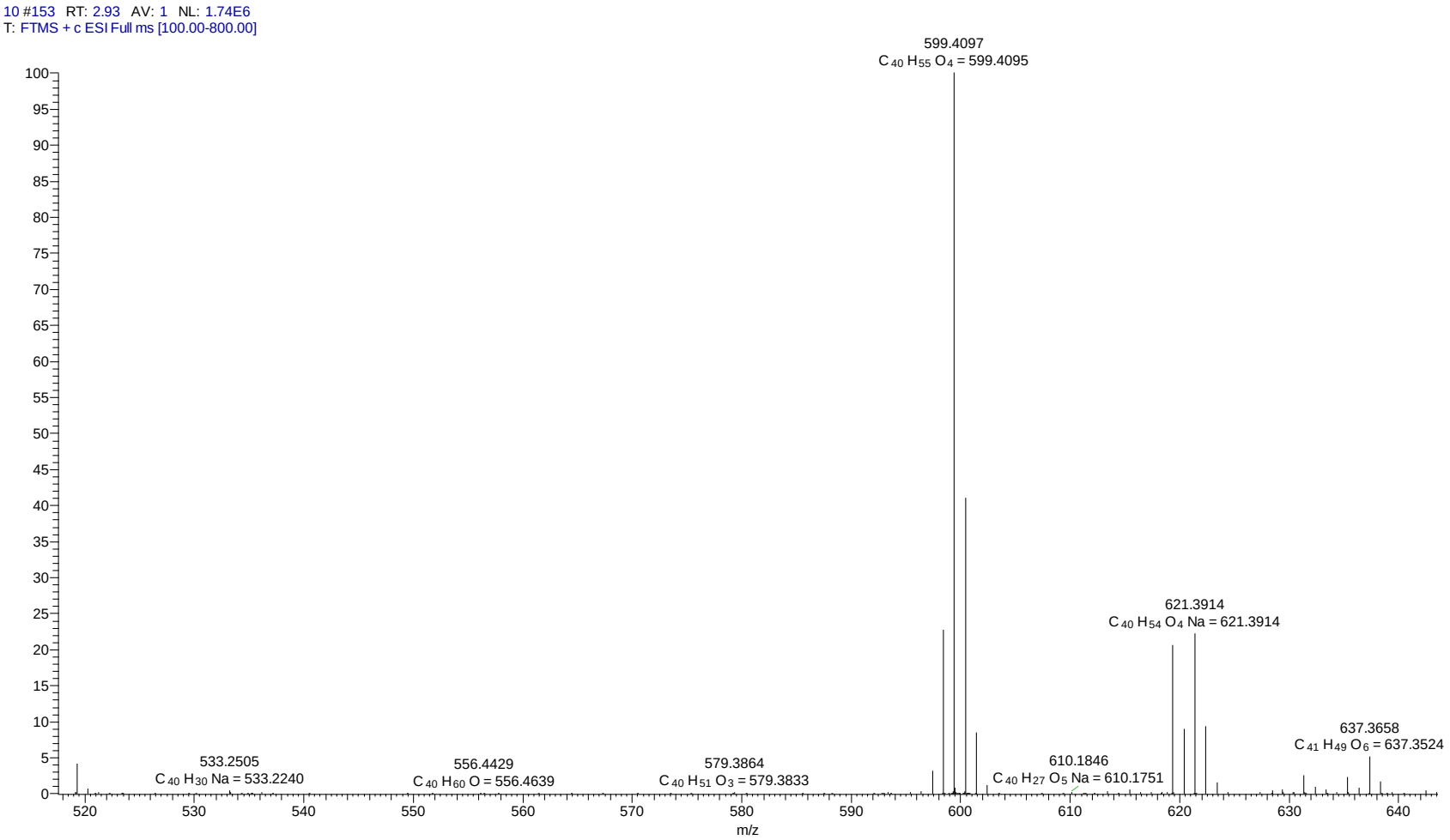

Figure S19. HRESIMS spectrum of biswulfenioidin B (**2**)

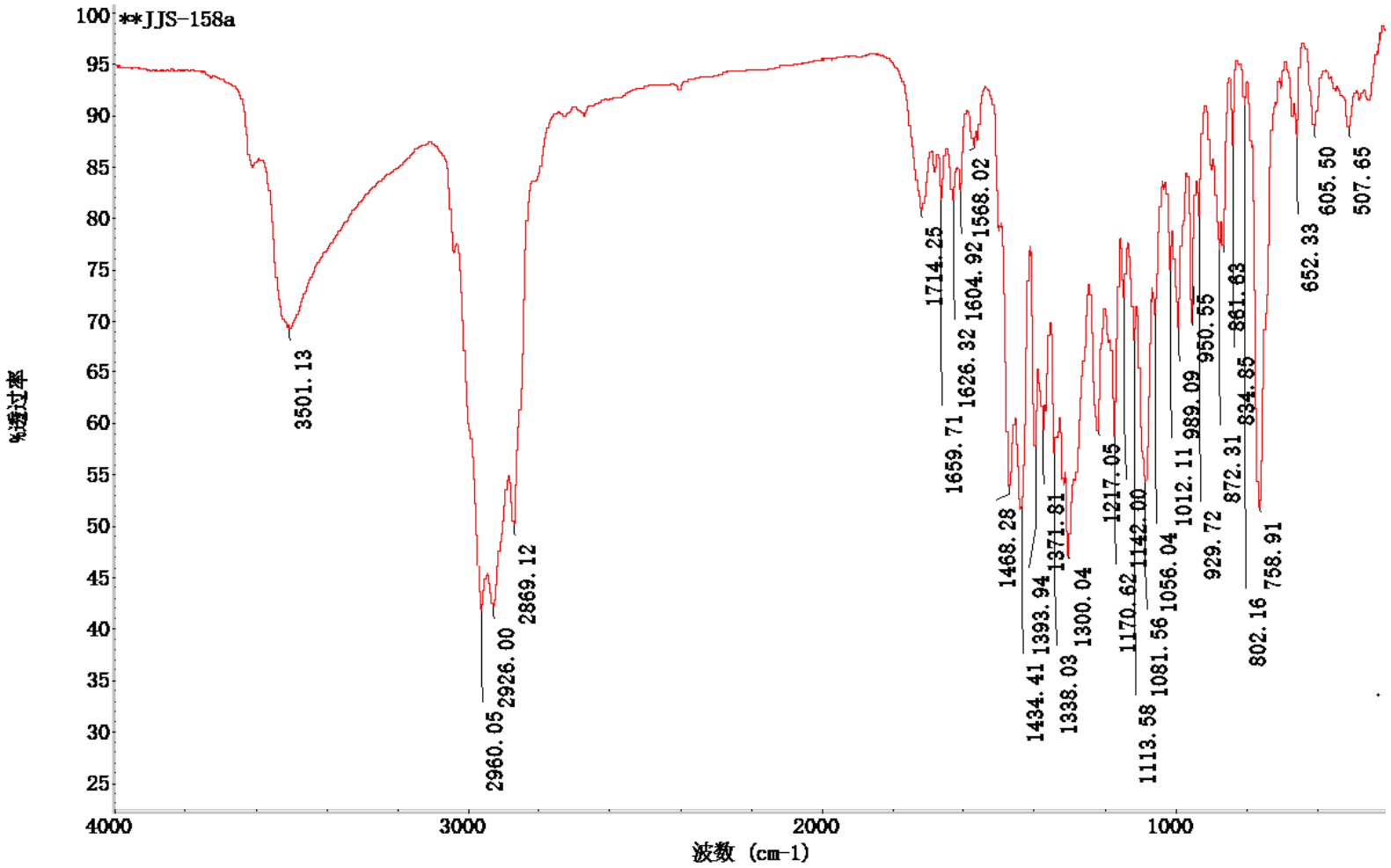

Figure S20. IR spectrum of biswulfenioidin B (**2**)

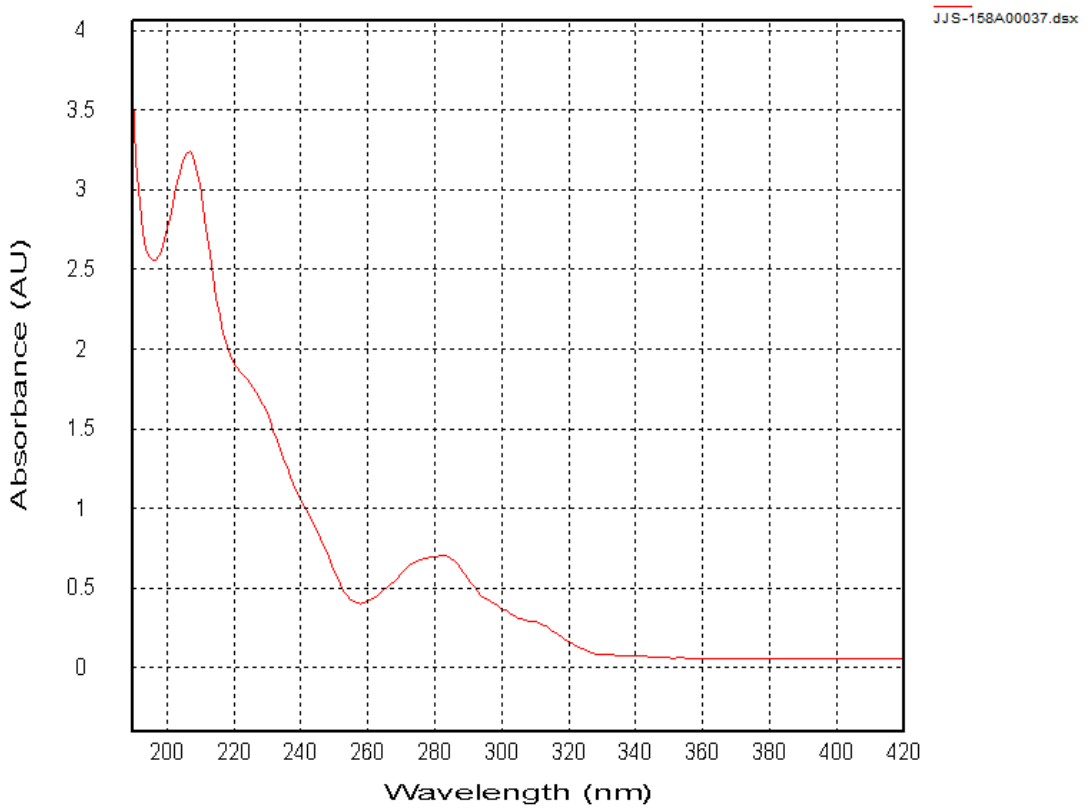

Figure S21. UV spectrum of biswulfenioidin B (**2**)

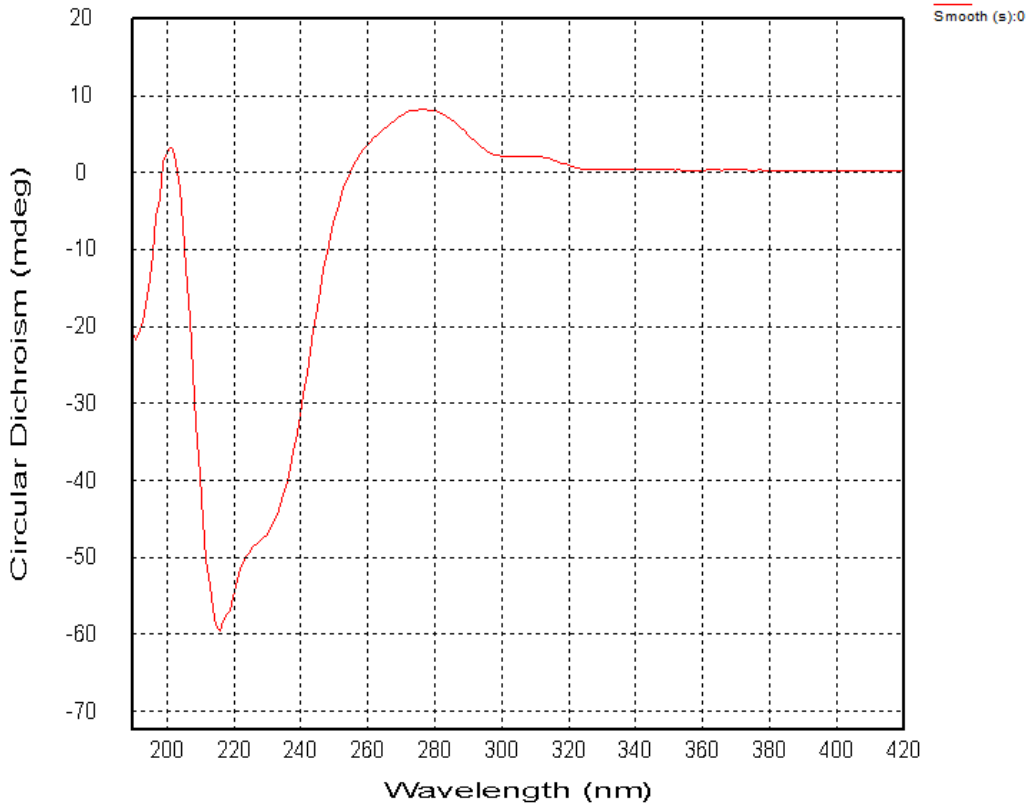

Figure S22. CD spectrum of biswulfenioidin B (**2**)

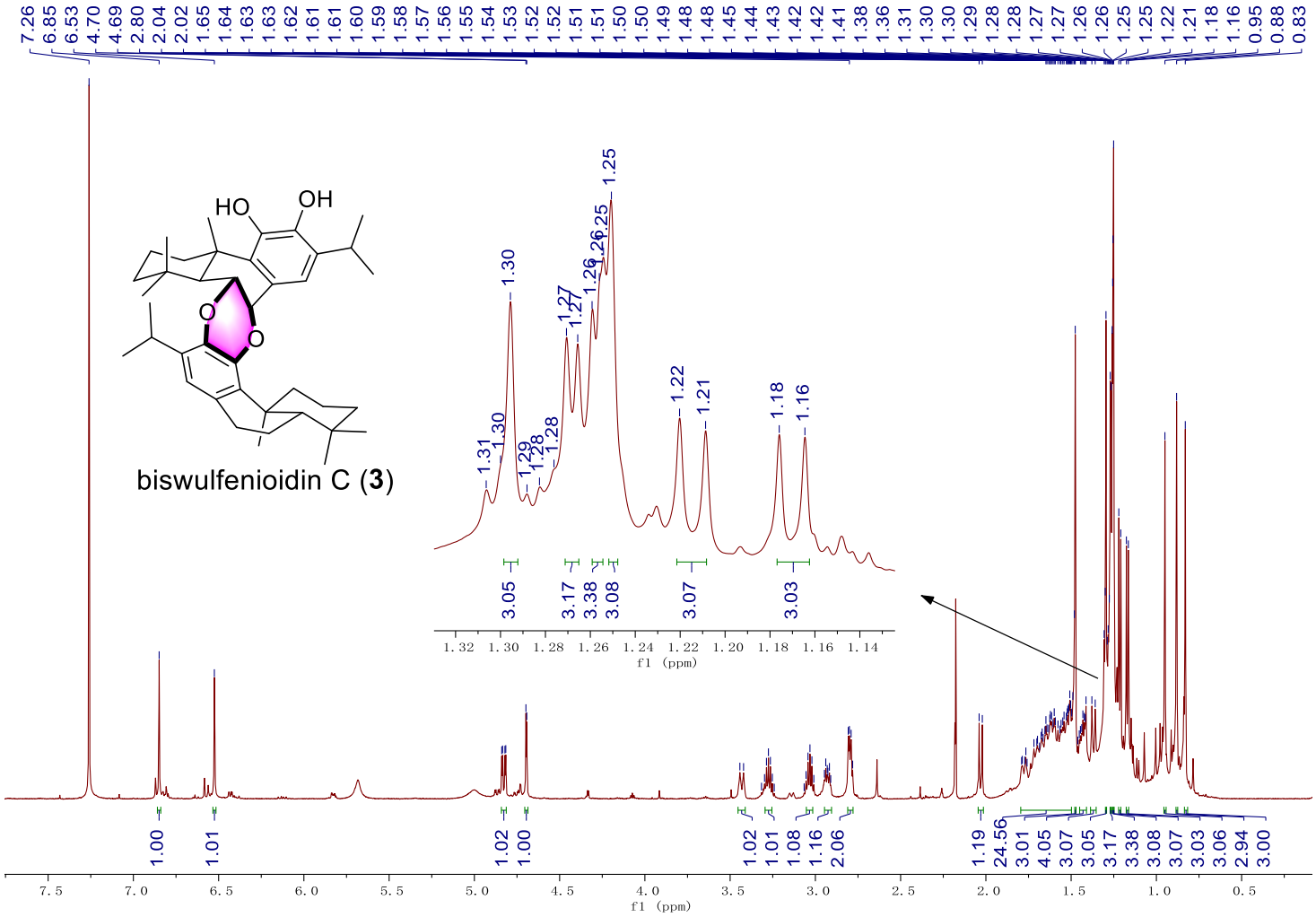

Figure S23. ^{1}H NMR spectrum of biswulfenioidin C (**3**) in chloroform (600 MHz)

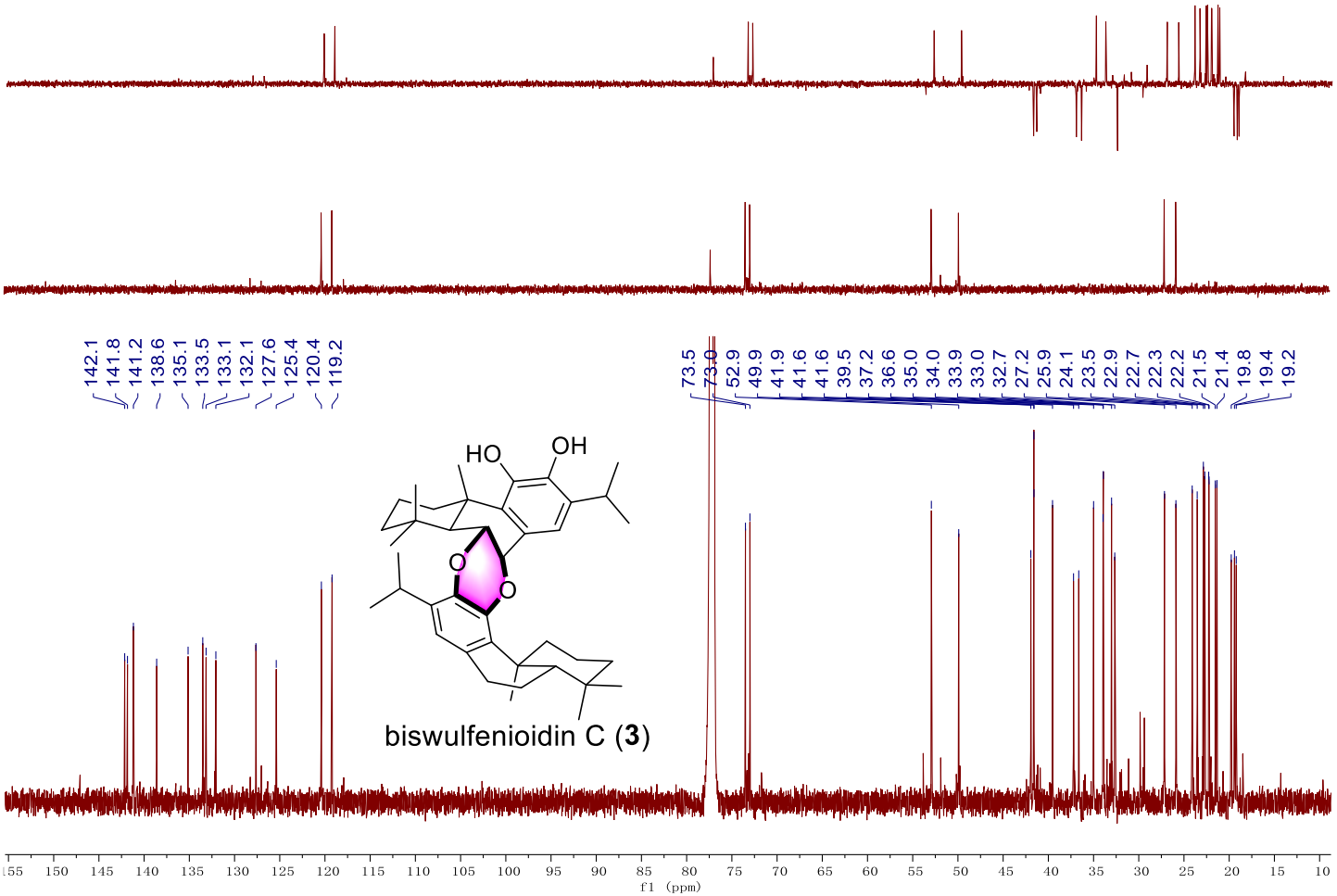

Figure S24. ^{13}C and DEPT NMR spectra of biswulfenioidin C (**3**) in chloroform (150 MHz)

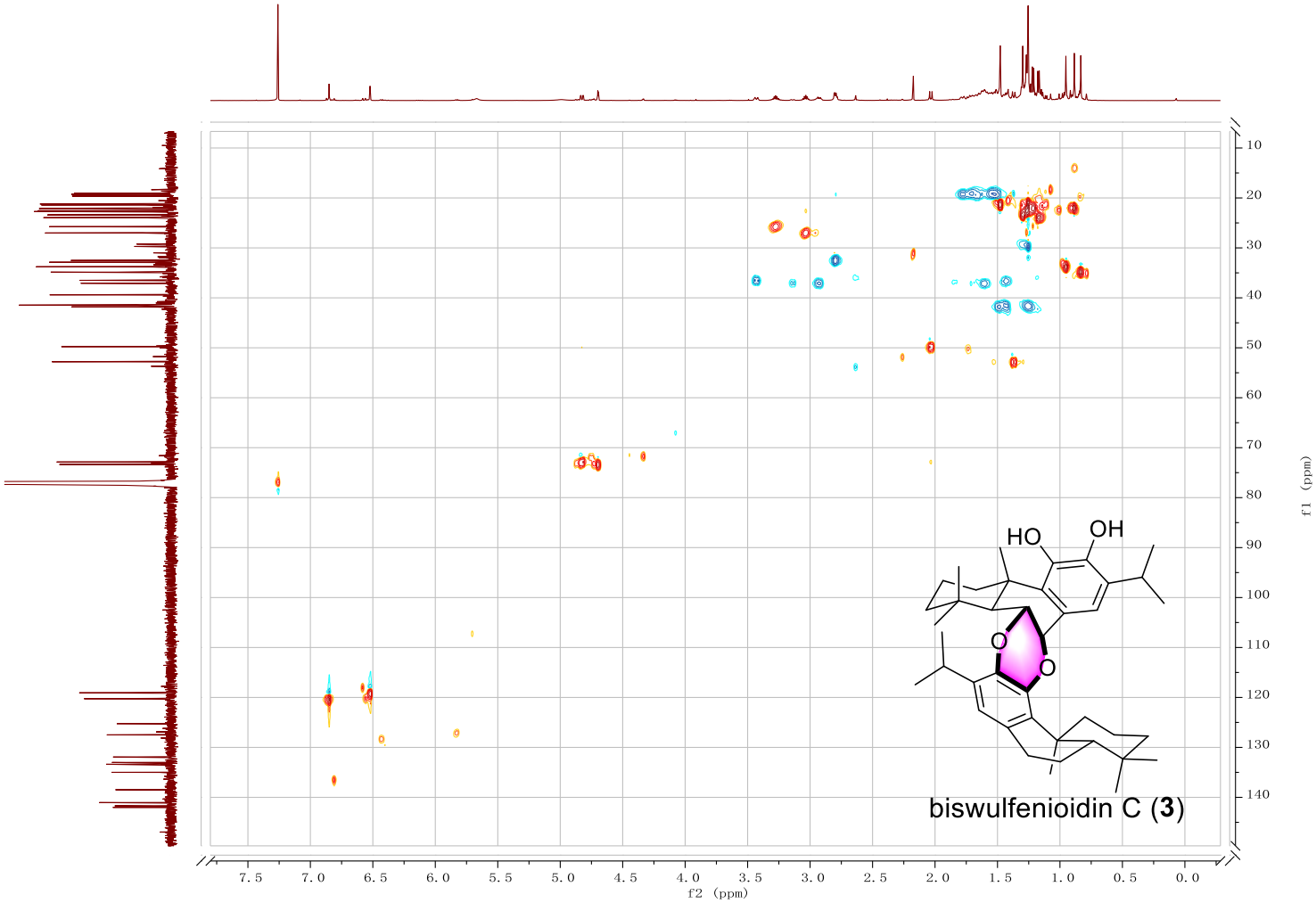

Figure S25. HSQC spectrum of biswulfenioidin C (**3**) in chloroform (600 MHz)

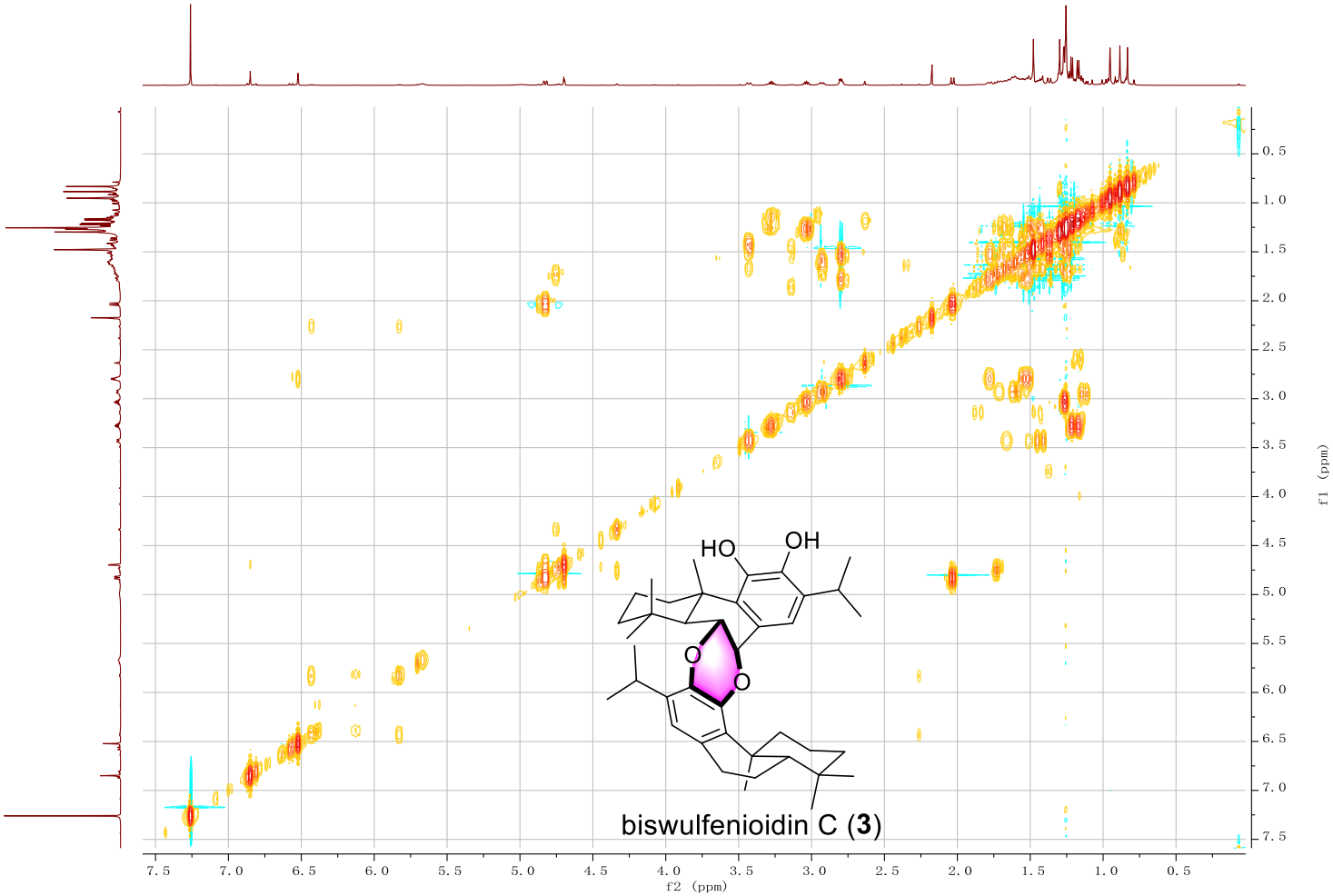

Figure S26. ^{1}H-^{1}H COSY spectrum of biswulfenioidin C (**3**) in chloroform (600 MHz)

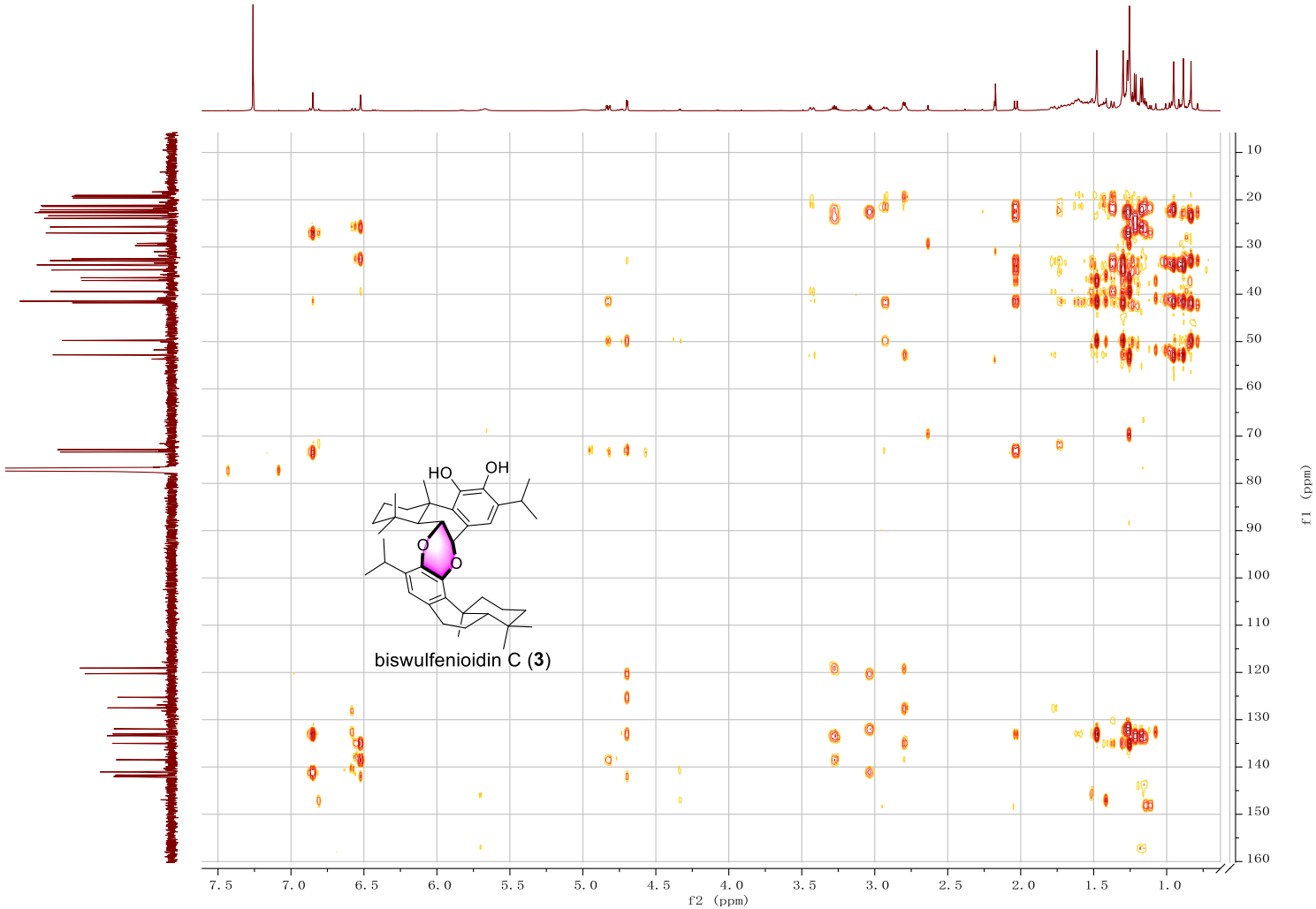

Figure S27. HMBC spectrum of biswulfenioidin C (**3**) in chloroform (600 MHz)

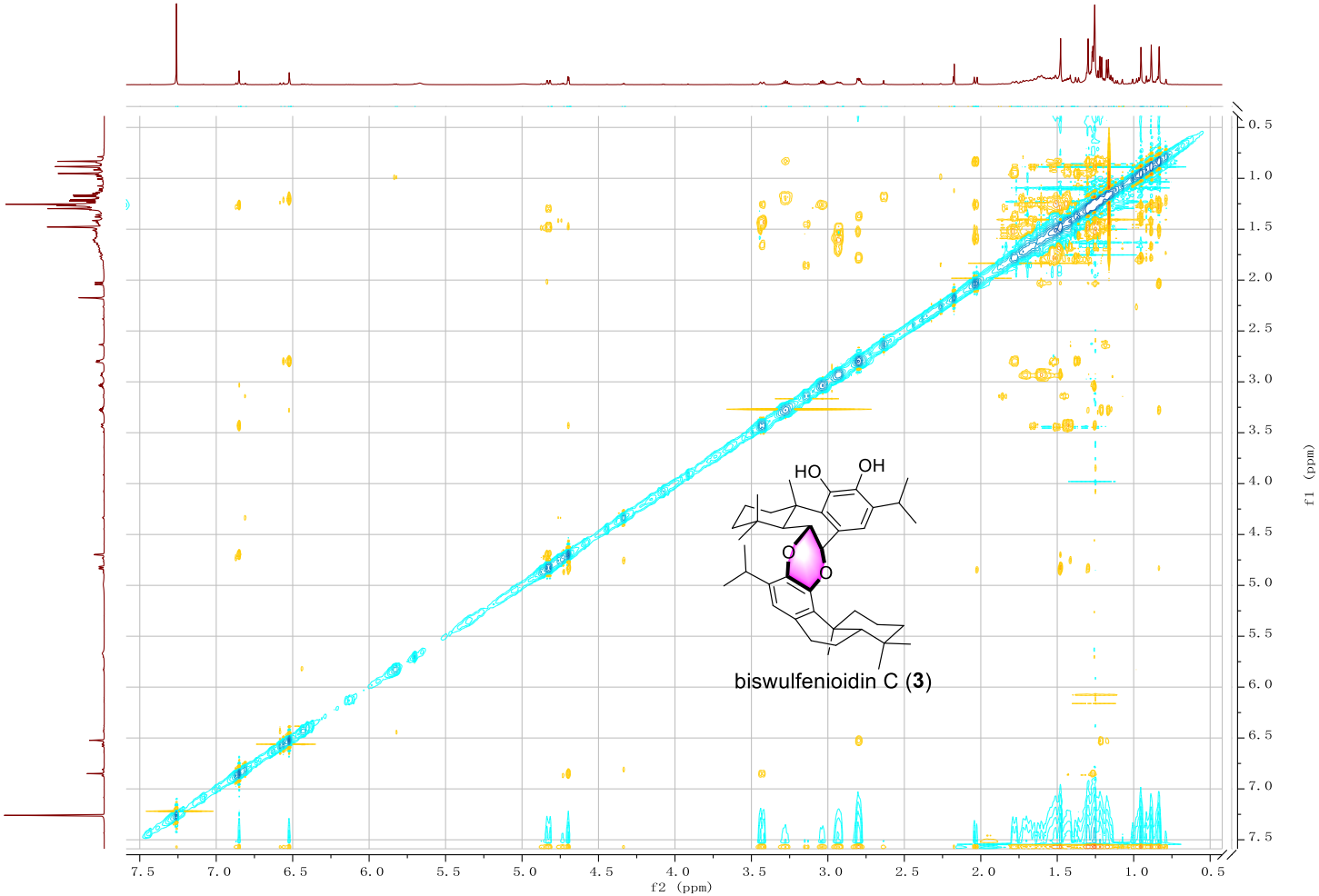

Figure S28. ROESY spectrum of biswulfenioidin C (**3**) in chloroform (600 MHz)

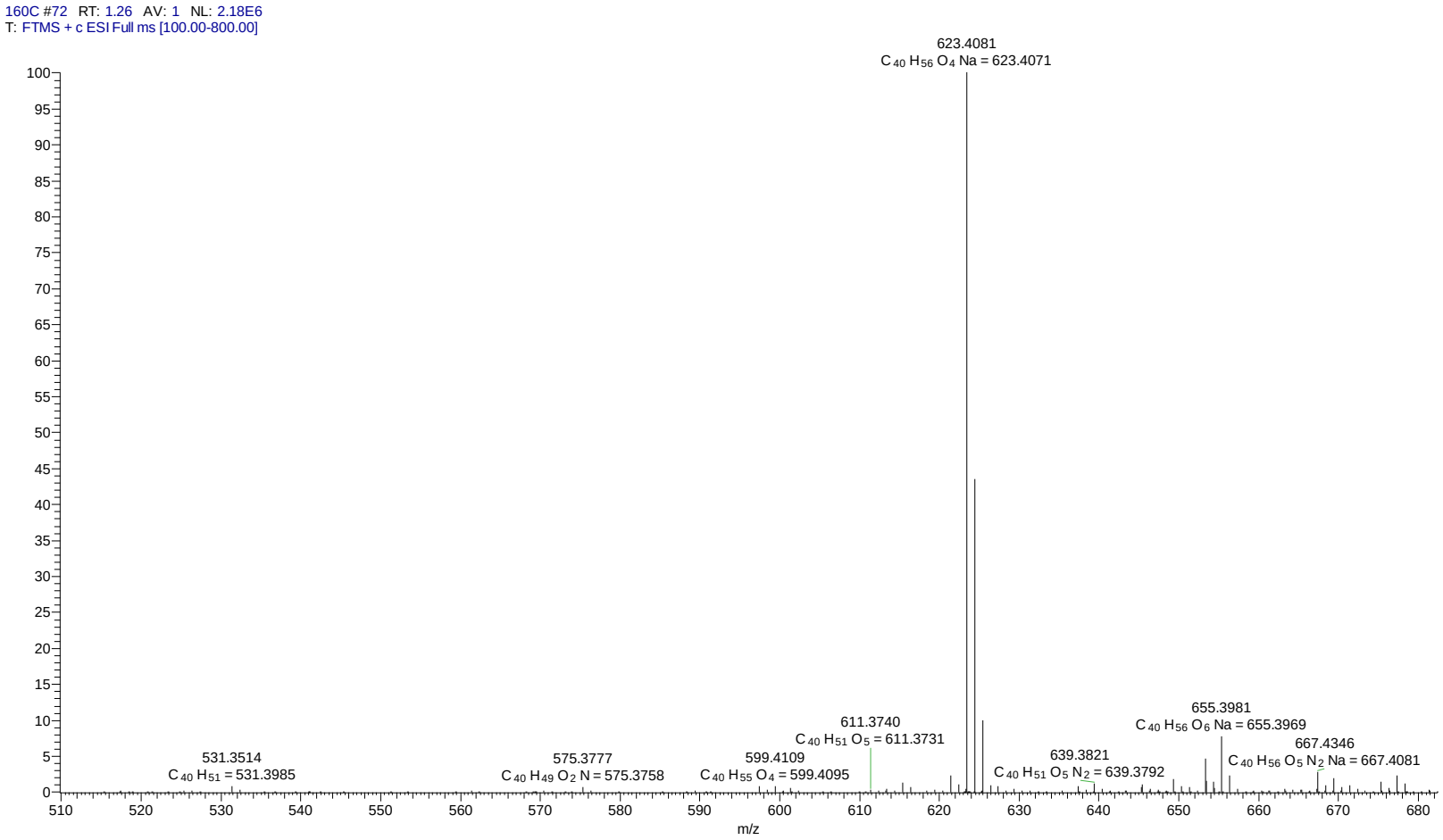

Figure S29. HRESIMS spectrum of biswulfenioidin C (**3**)

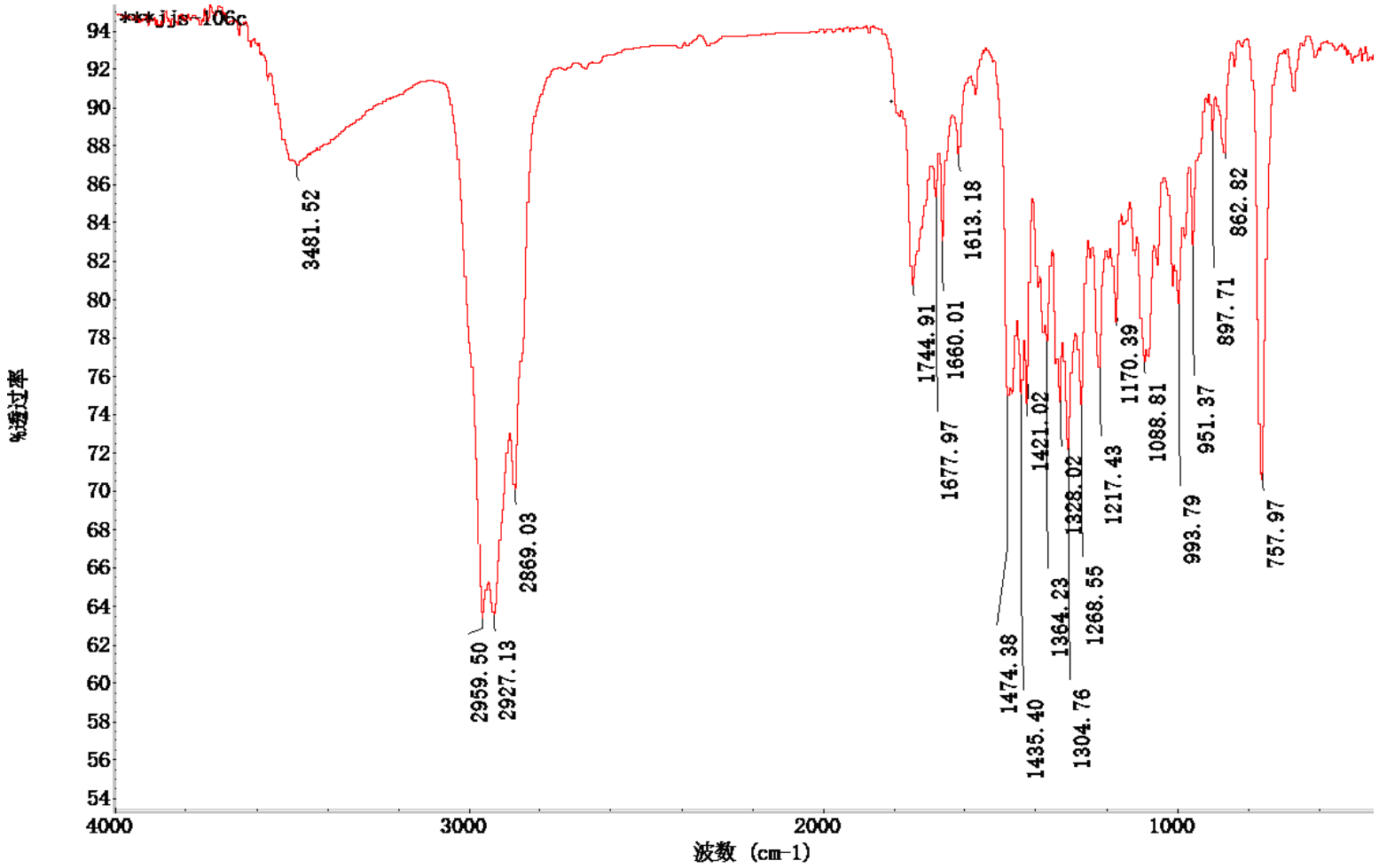

Figure S30. IR spectrum of biswulfenioidin C (**3**)

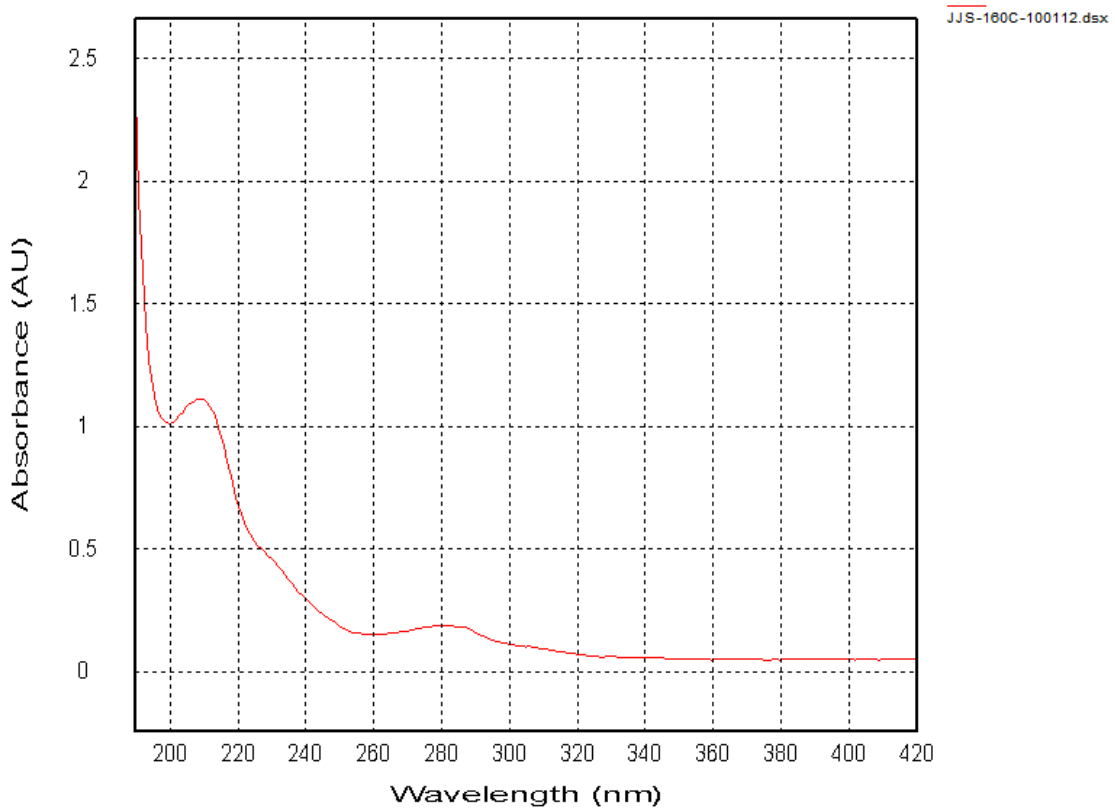

Figure S31. UV spectrum of biswulfenioidin C (**3**)

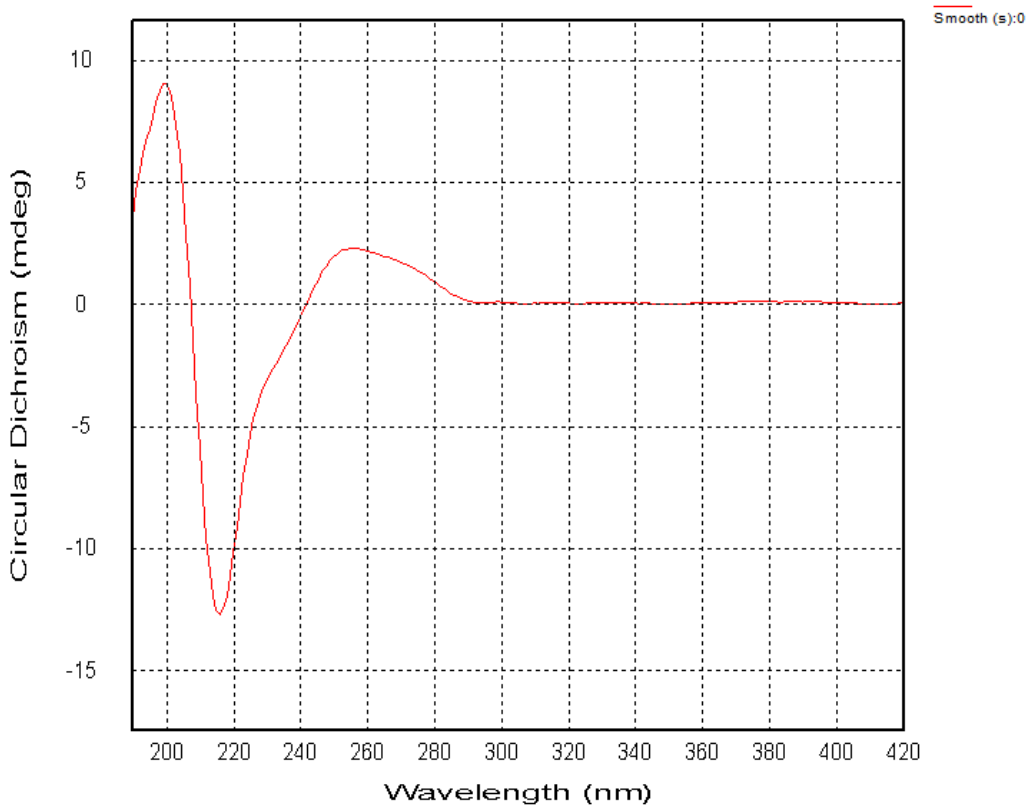

Figure S32. CD spectrum of biswulfenioidin C (**3**)

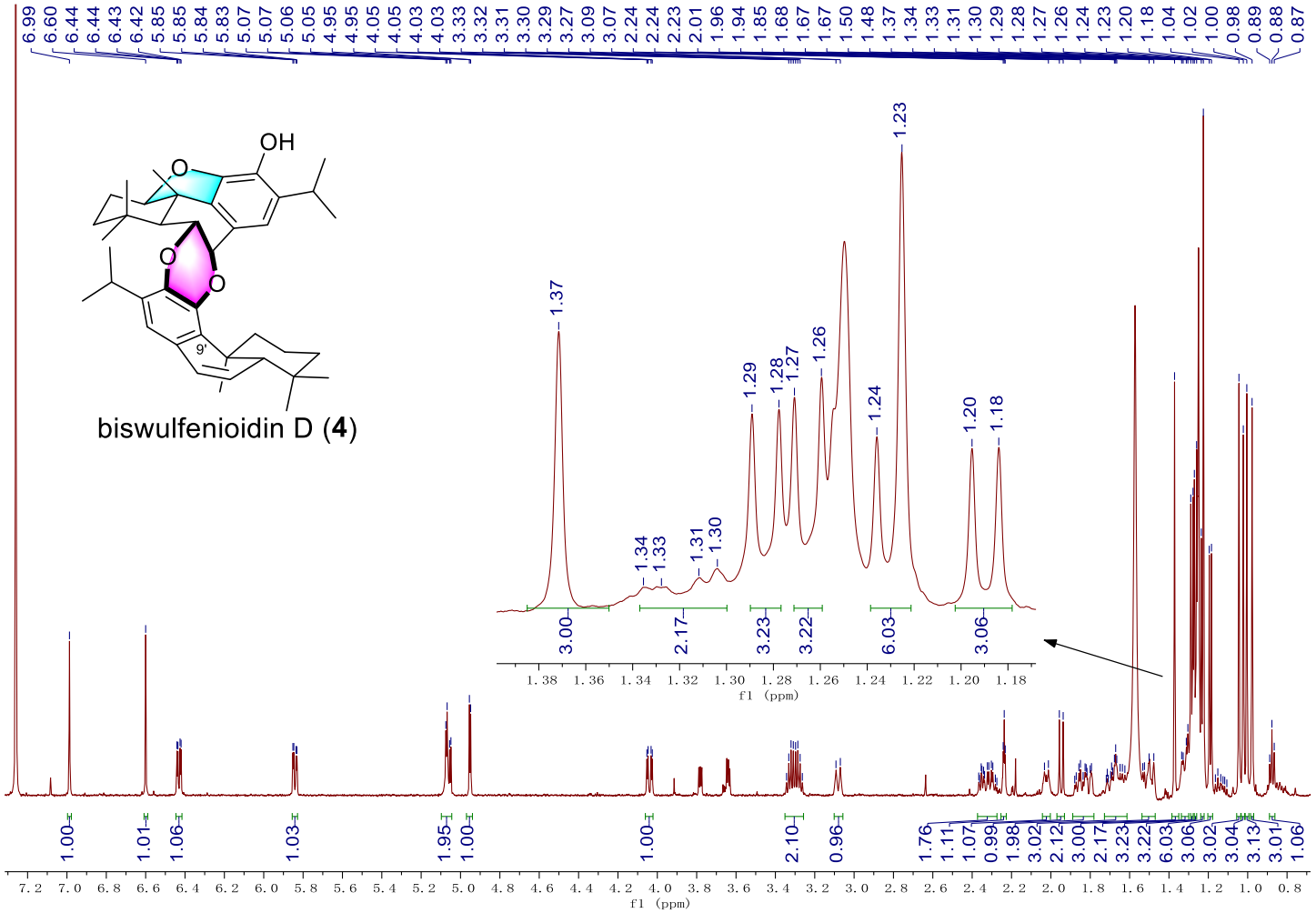

Figure S33. ^{1}H NMR spectrum of biswulfenioidin D (**4**) in chloroform (600 MHz)

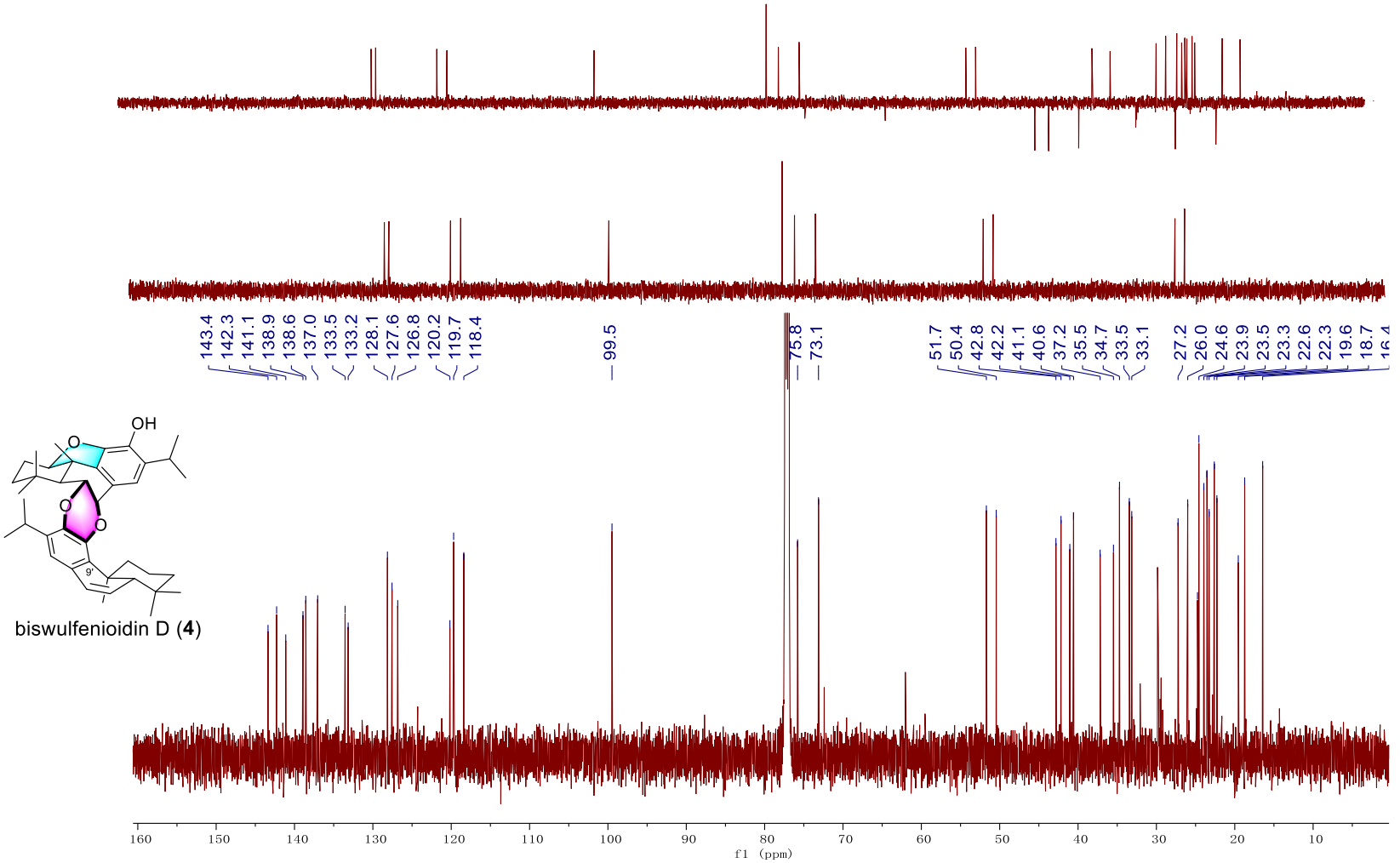

Figure S34. ^{13}C and DEPT NMR spectra of biswulfenioidin D (**4**) in chloroform (100 MHz)

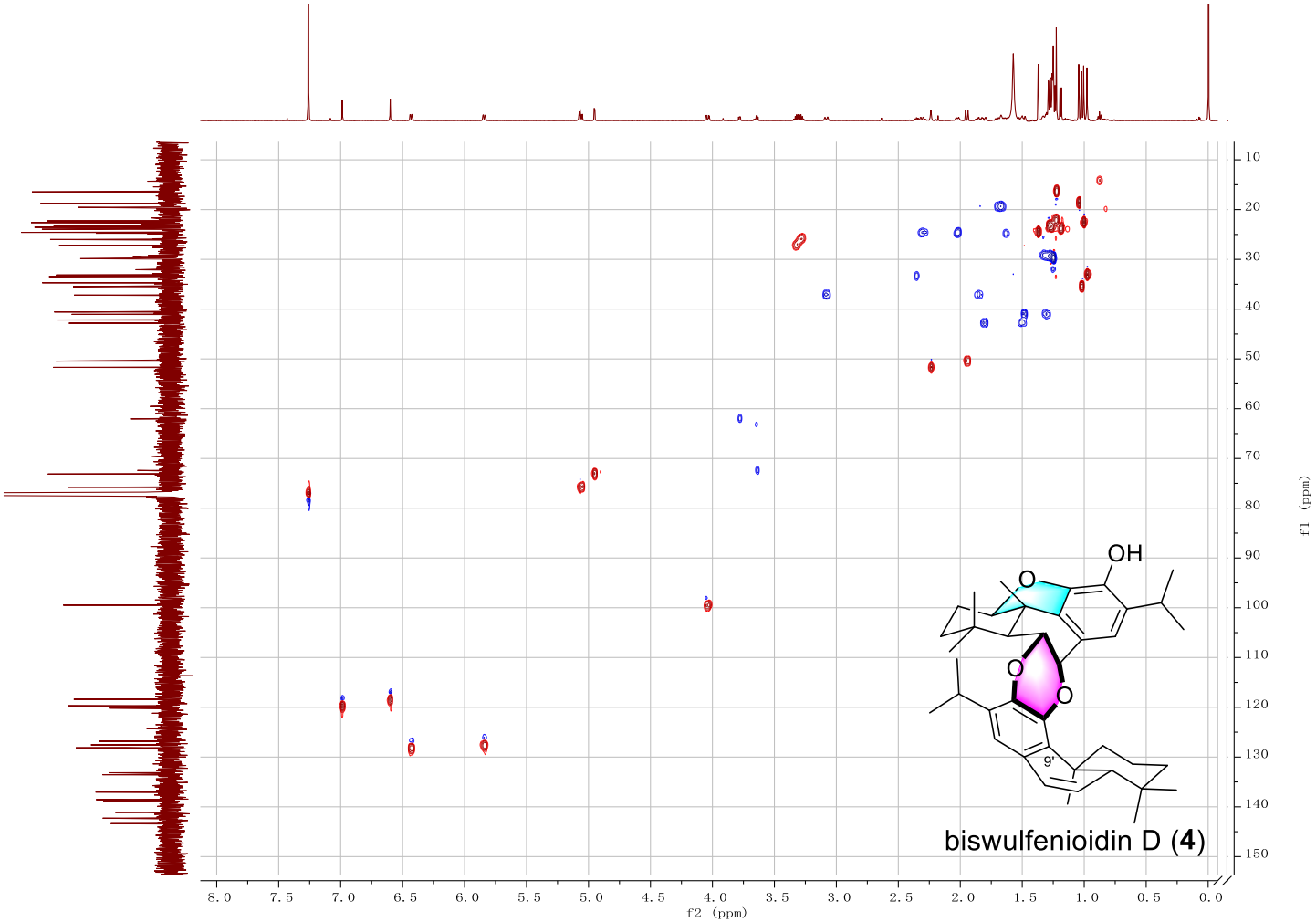

Figure S35. HSQC spectrum of biswulfenioidin D (**4**) in chloroform (600 MHz)

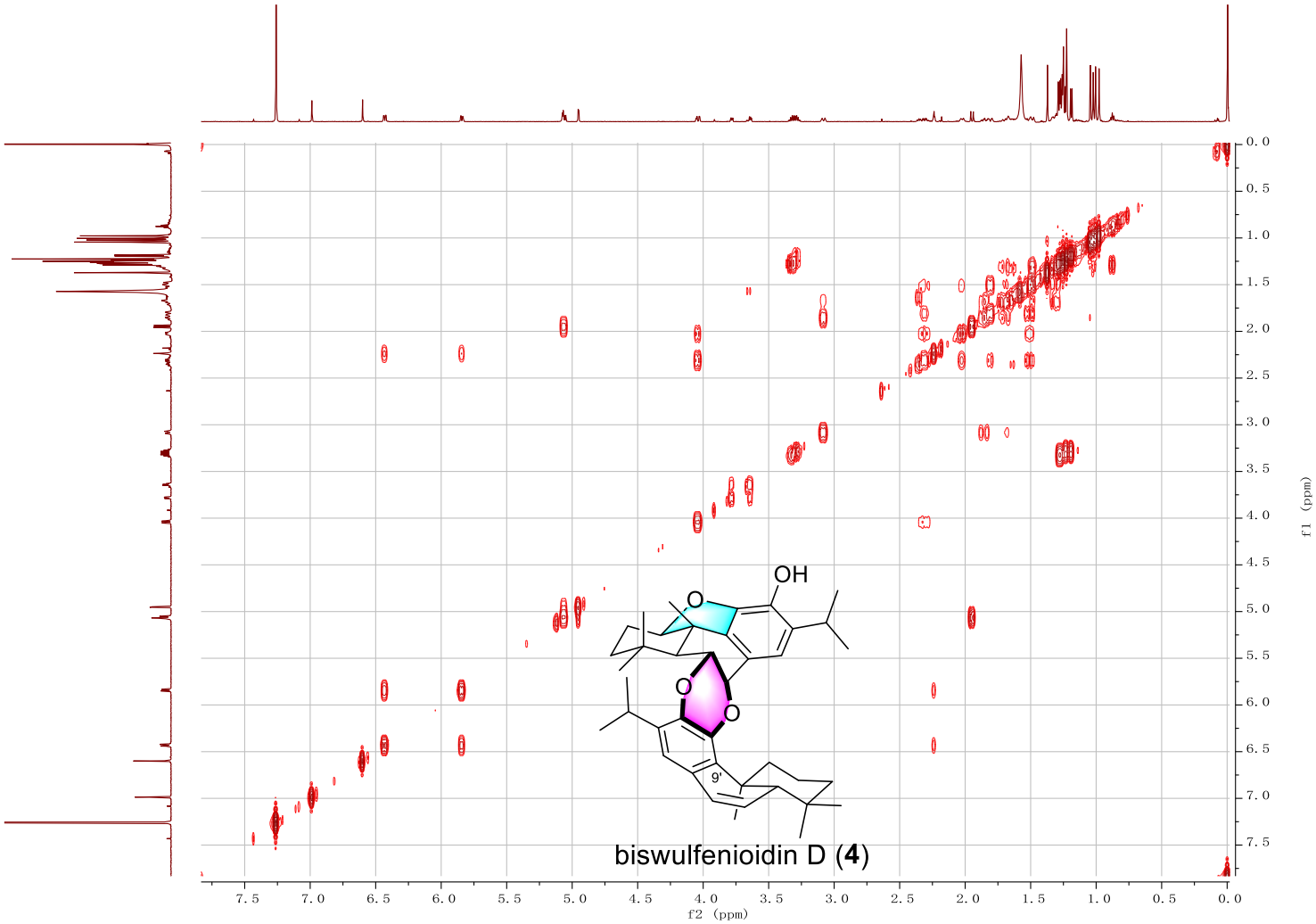

Figure S36. ^{1}H-^{1}H COSY spectrum of biswulfenioidin D (**4**) in chloroform (600 MHz)

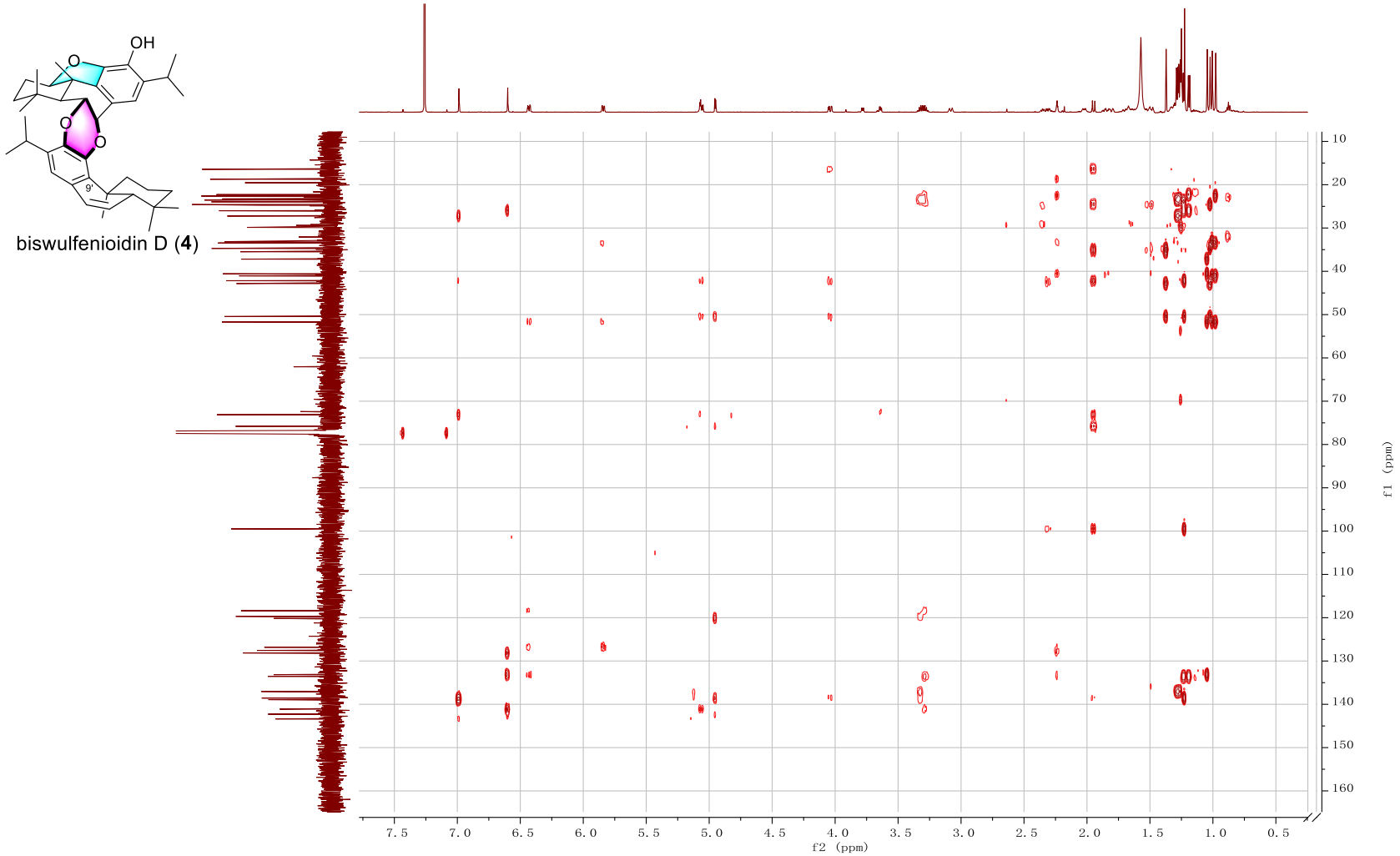

Figure S37. HMBC spectrum of biswulfenioidin D (**4**) in chloroform (600 MHz)

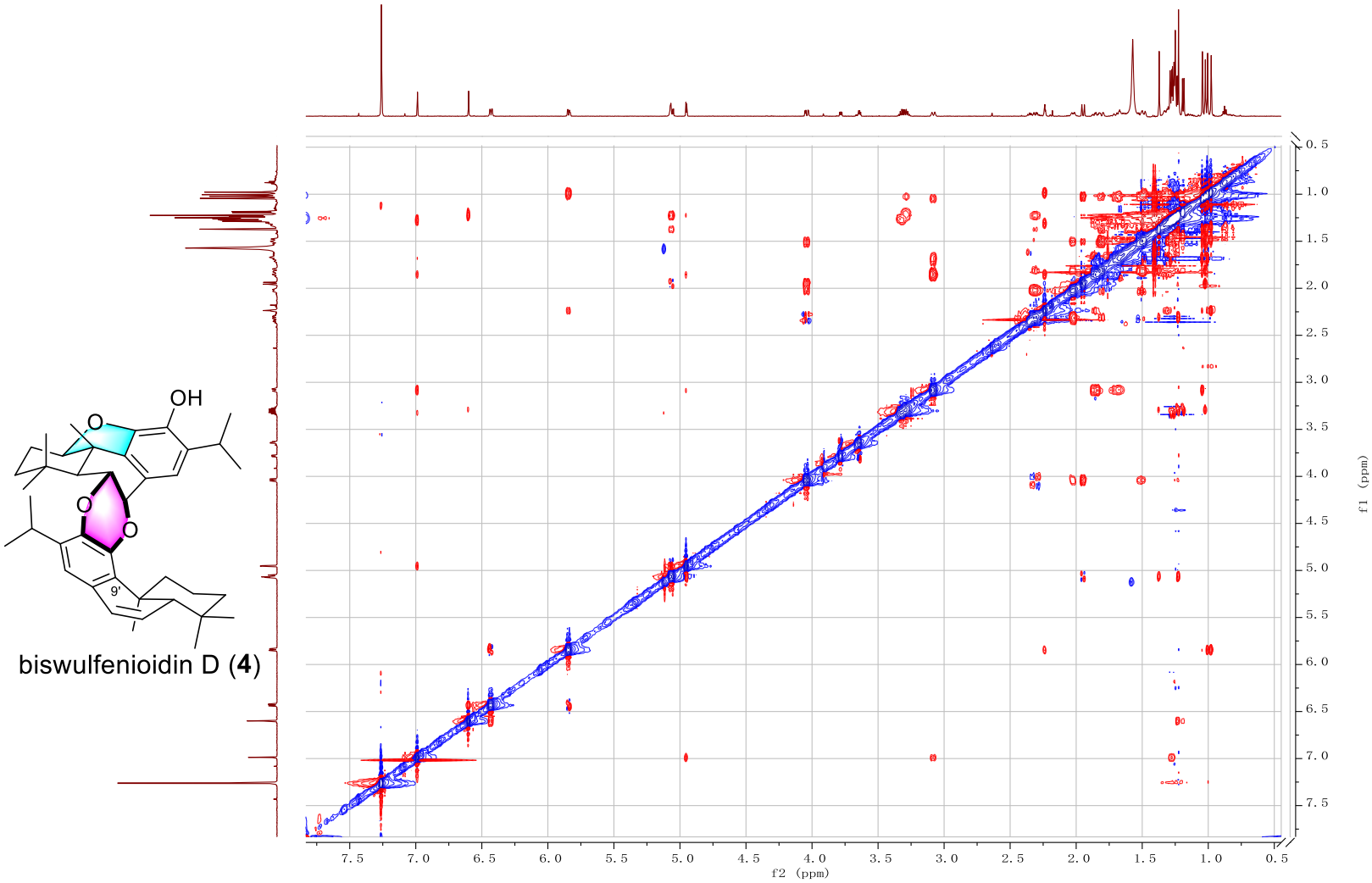

Figure S38. ROESY spectrum of biswulfenioidin D (**4**) in chloroform (600 MHz)

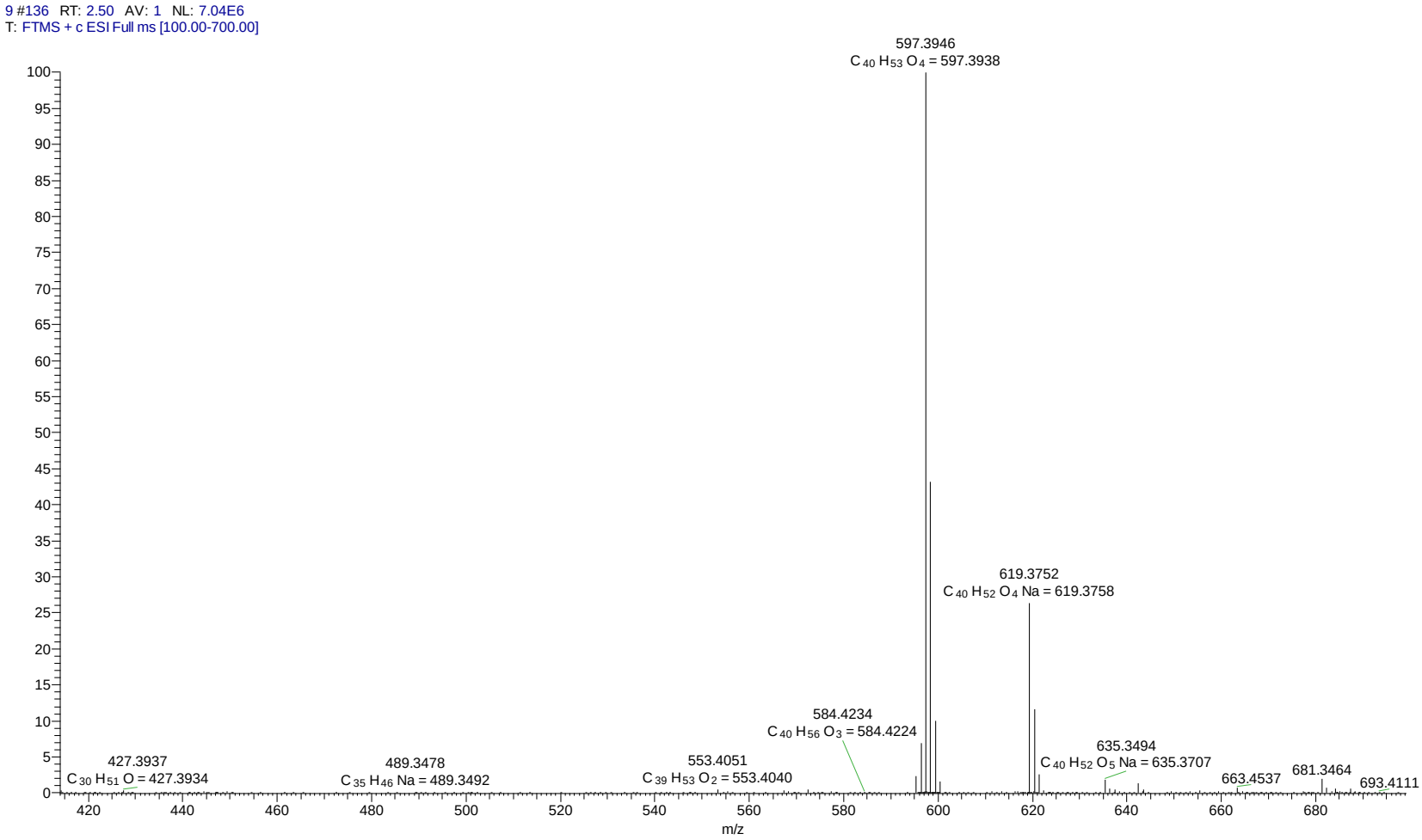

Figure S39. HRESIMS spectrum of biswulfenioidin D (**4**)

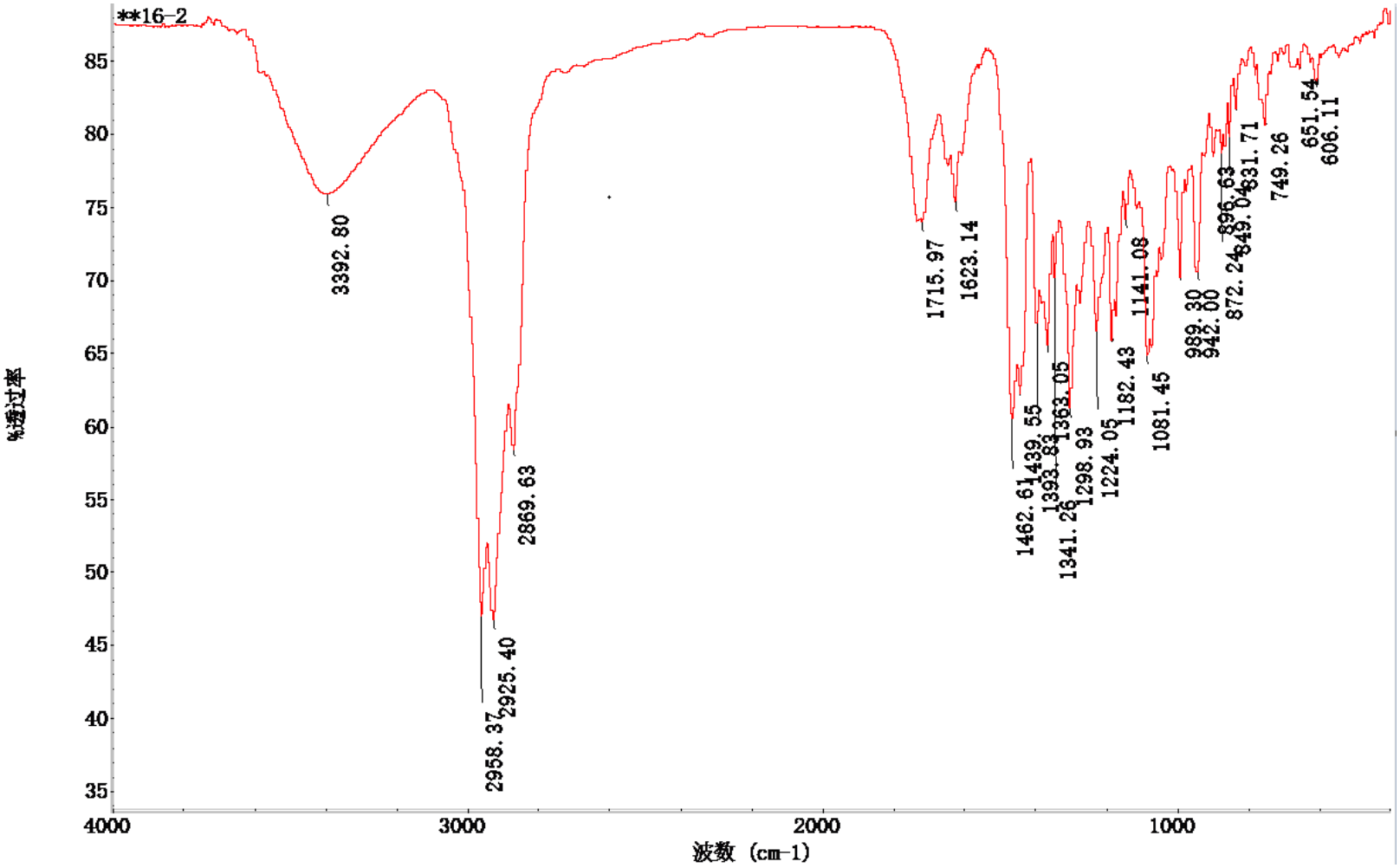

Figure S40. IR spectrum of biswulfenioidin D (**4**)

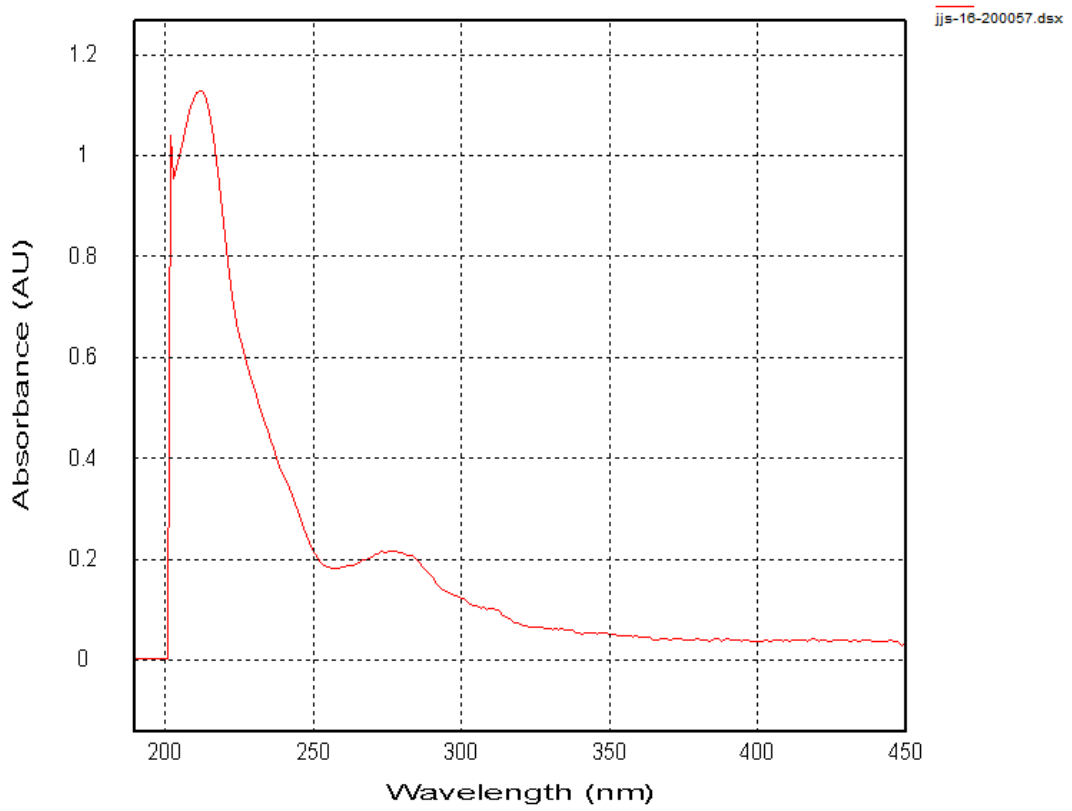

Figure S41. UV spectrum of biswulfenioidin D (**4**)

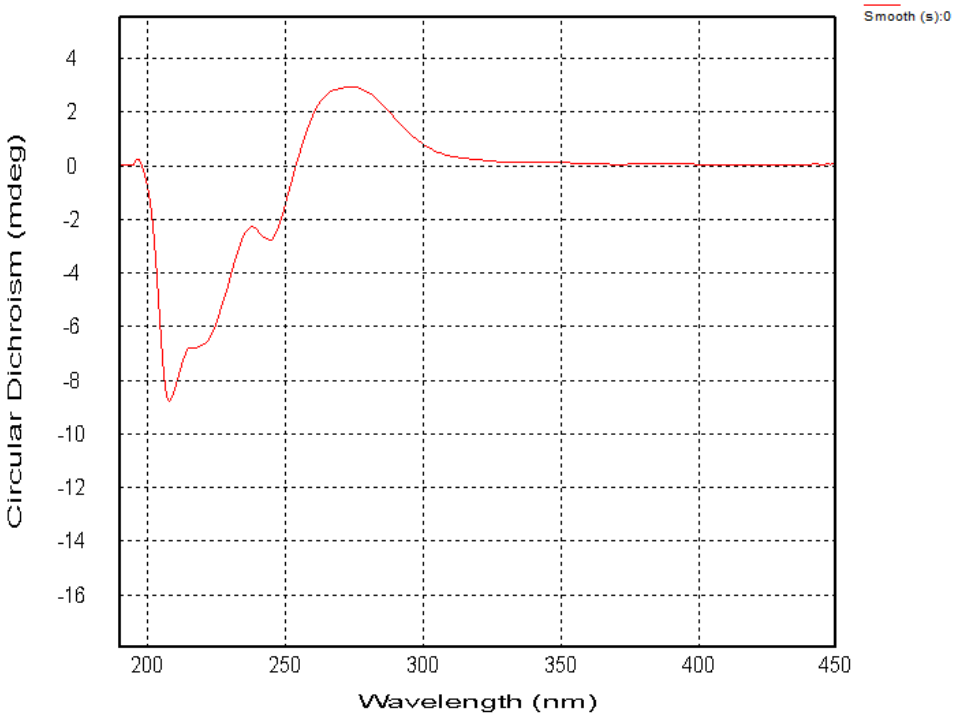

Figure S42. CD spectrum of biswulfenioidin D (**4**)

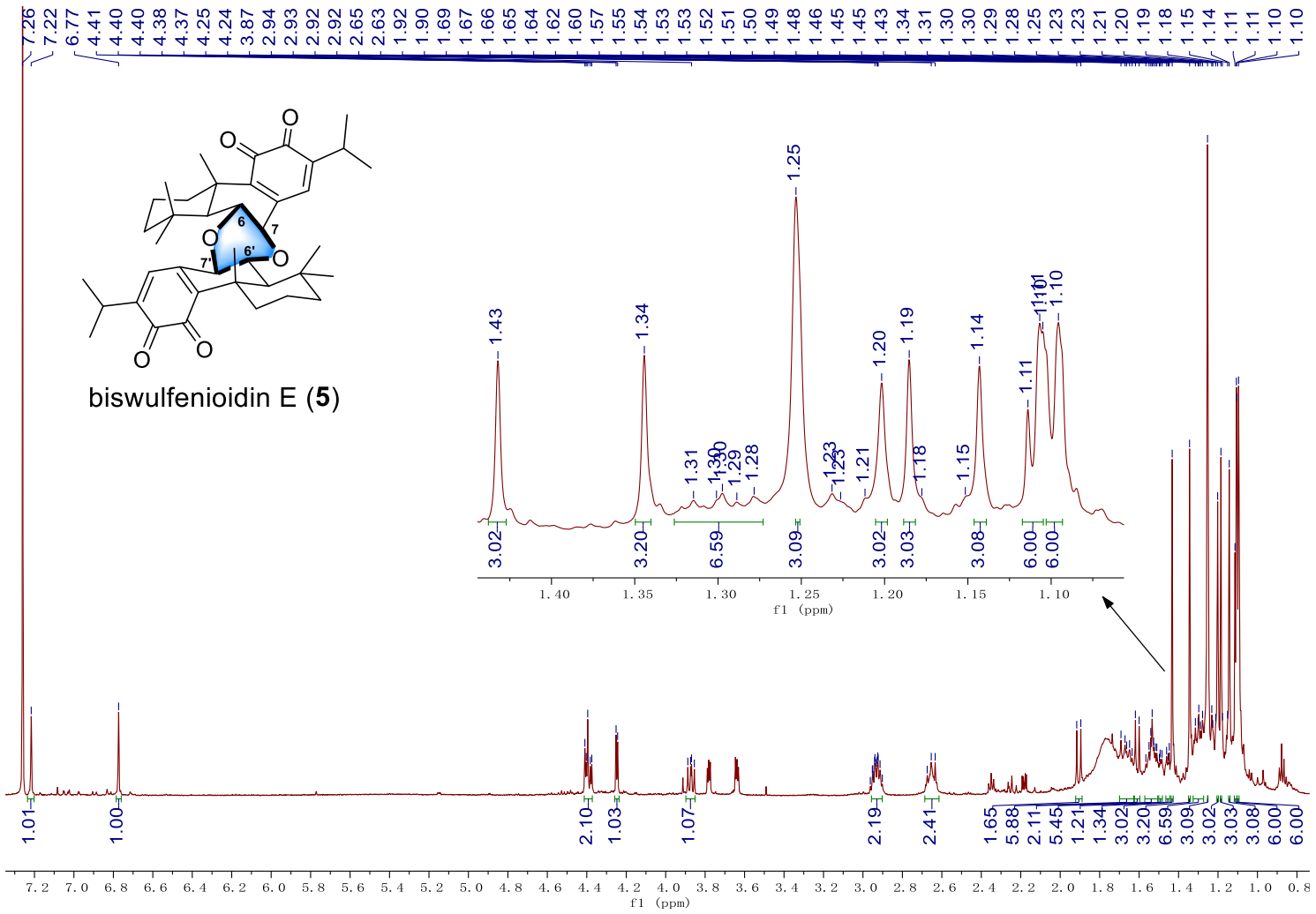

Figure S43. ^{1}H NMR spectrum of biswulfenioidin E (**5**) in chloroform (600 MHz)

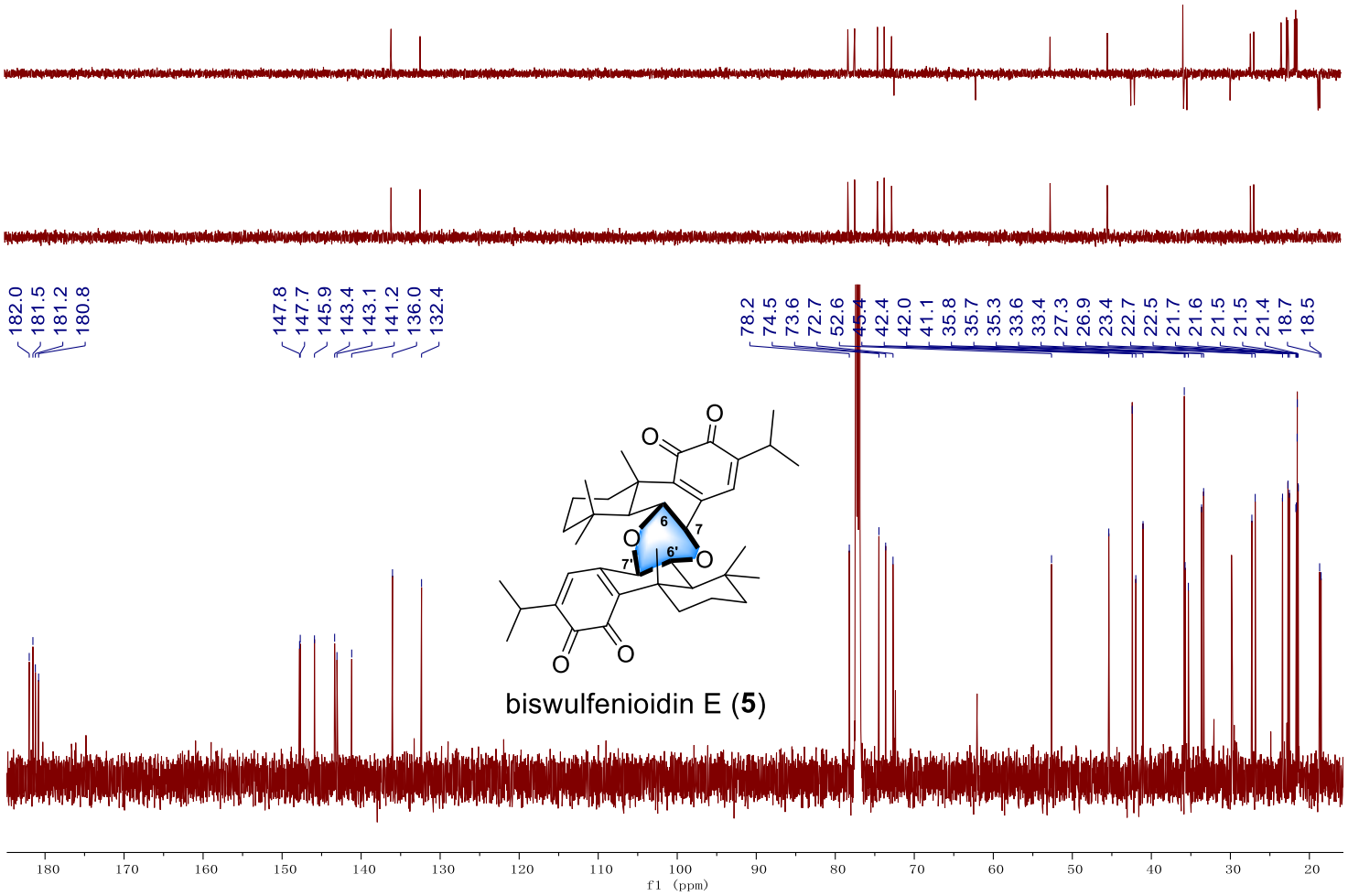

Figure S44. ^{13}C and DEPT NMR spectra of biswulfenioidin E (**5**) in chloroform (150 MHz)

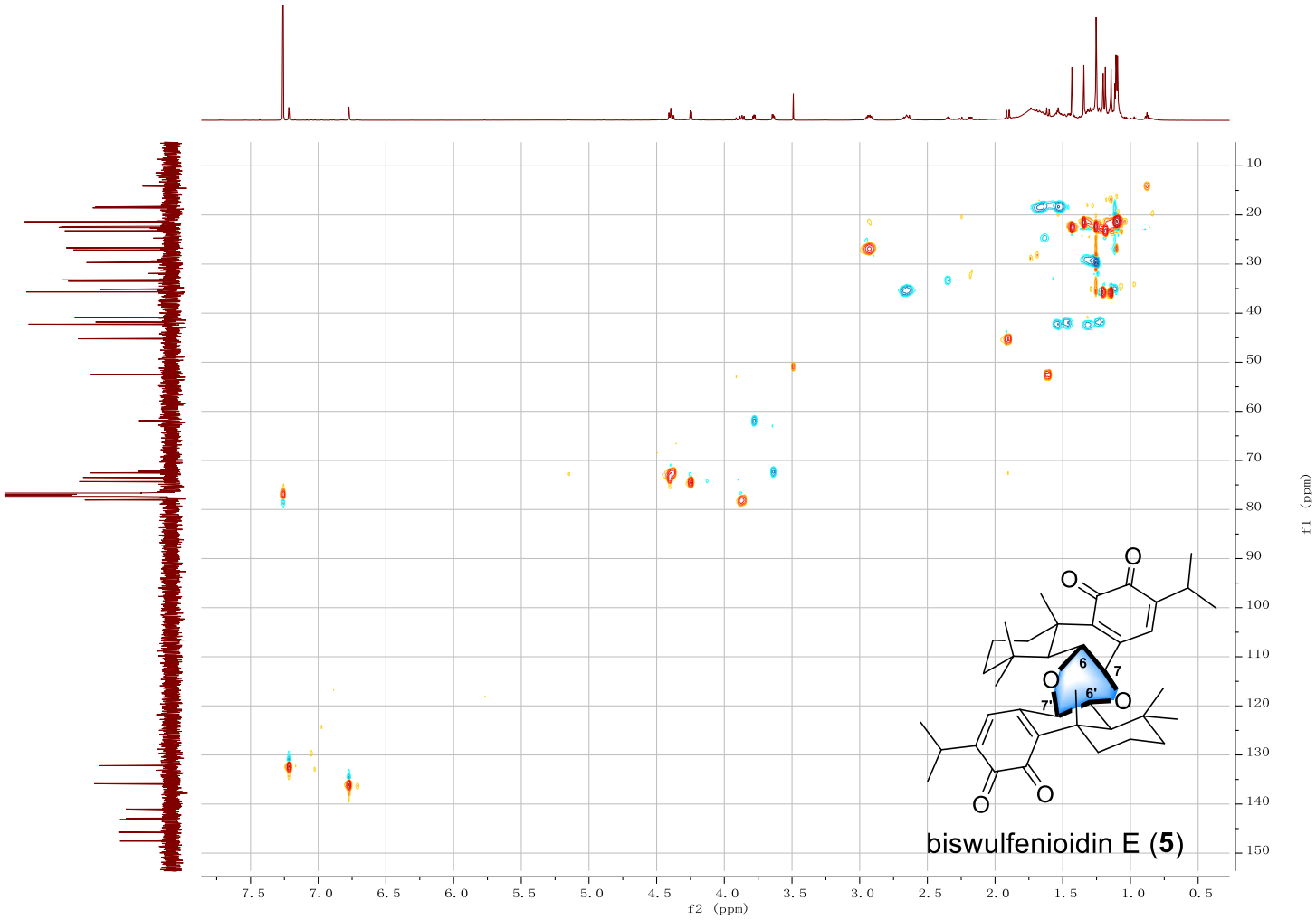

Figure S45. HSQC spectrum of biswulfenioidin E (**5**) in chloroform (600 MHz)

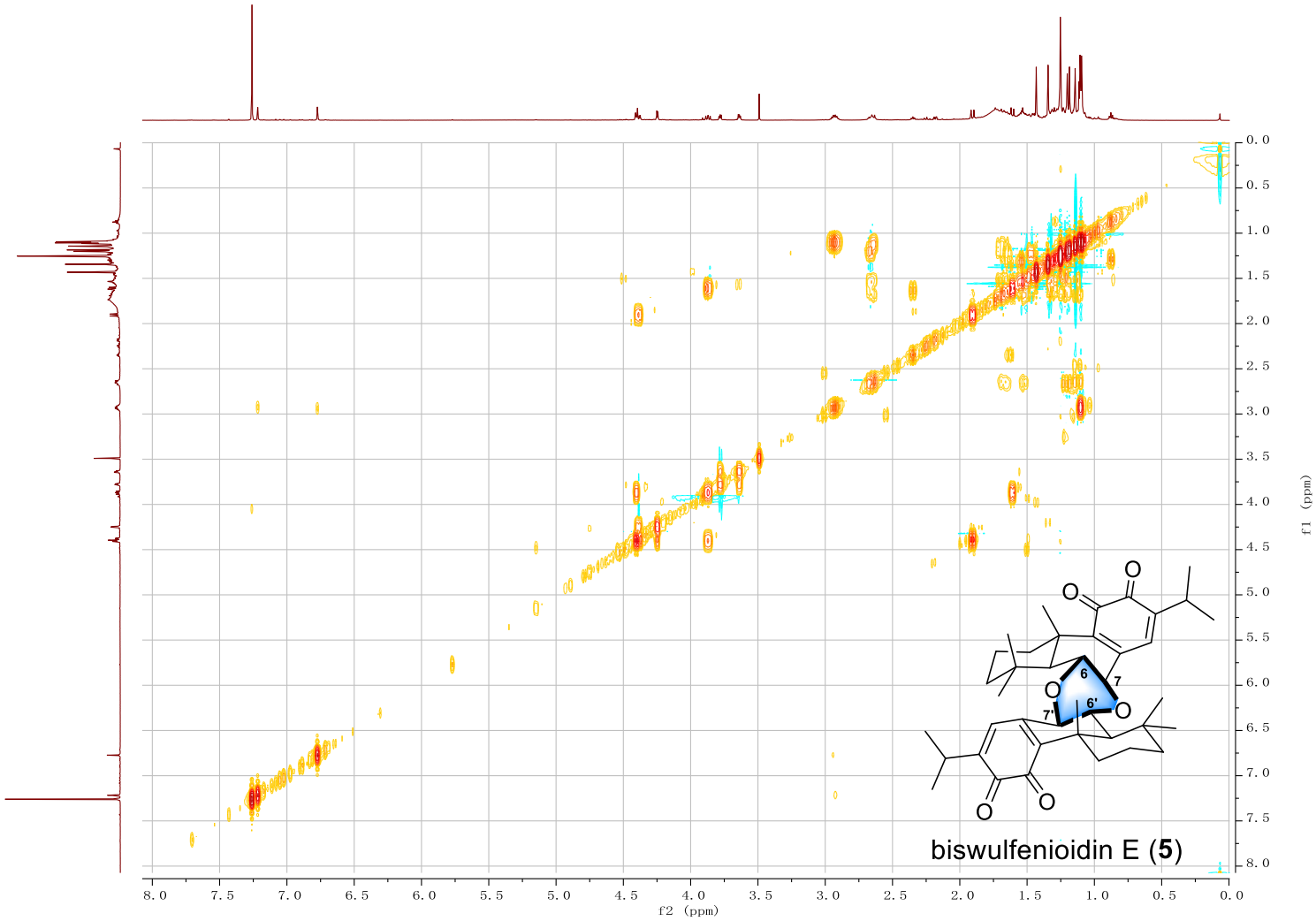

Figure S46. ^{1}H-^{1}H COSY spectrum of biswulfenioidin E (**5**) in chloroform (600 MHz)

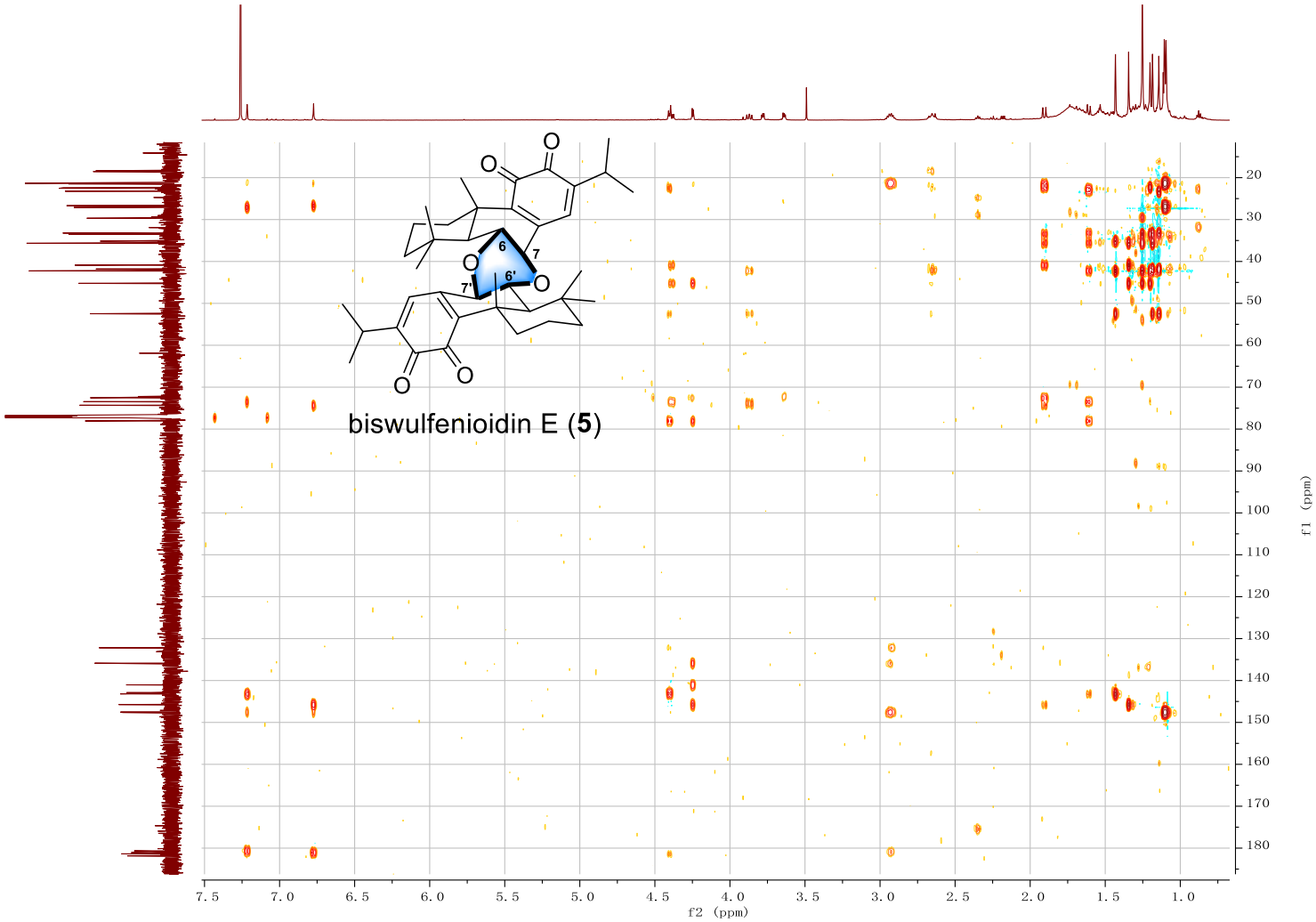

Figure S47. HMBC spectrum of biswulfenioidin E (**5**) in chloroform (600 MHz)

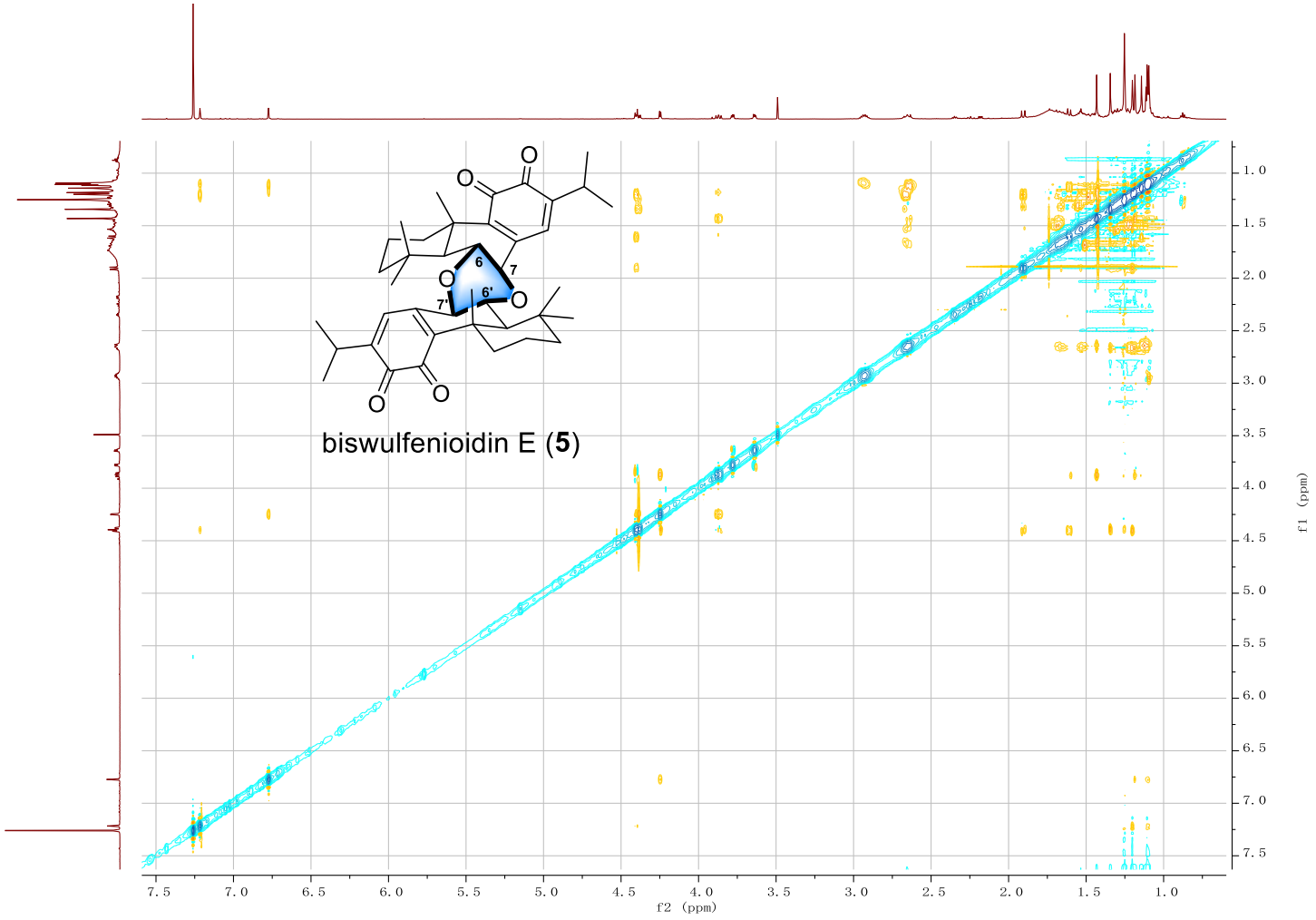

Figure S48. ROESY spectrum of biswulfenioidin E (**5**) in chloroform (600 MHz)

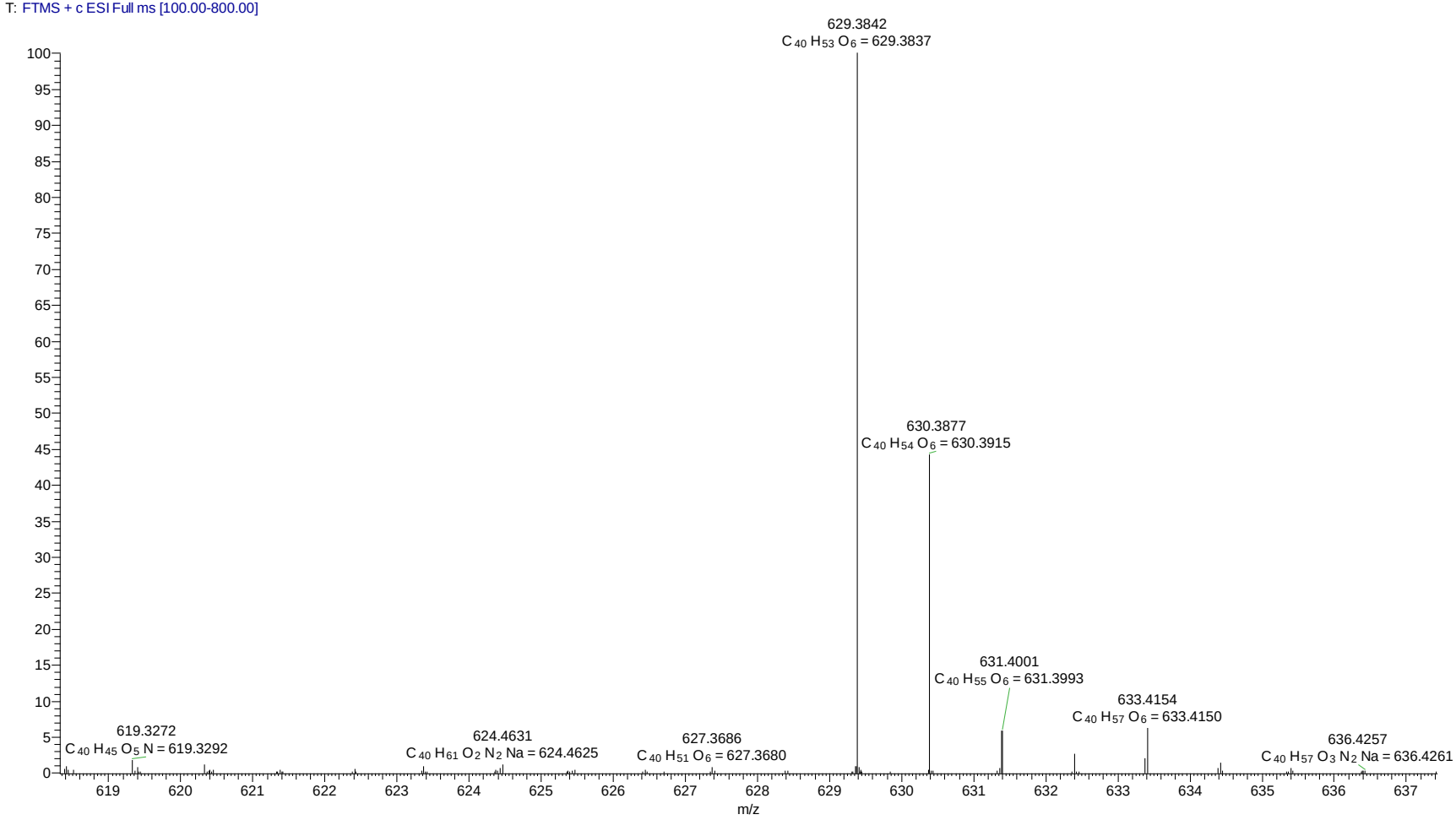

Figure S49. HRESIMS spectrum of biswulfenioidin E (**5**)

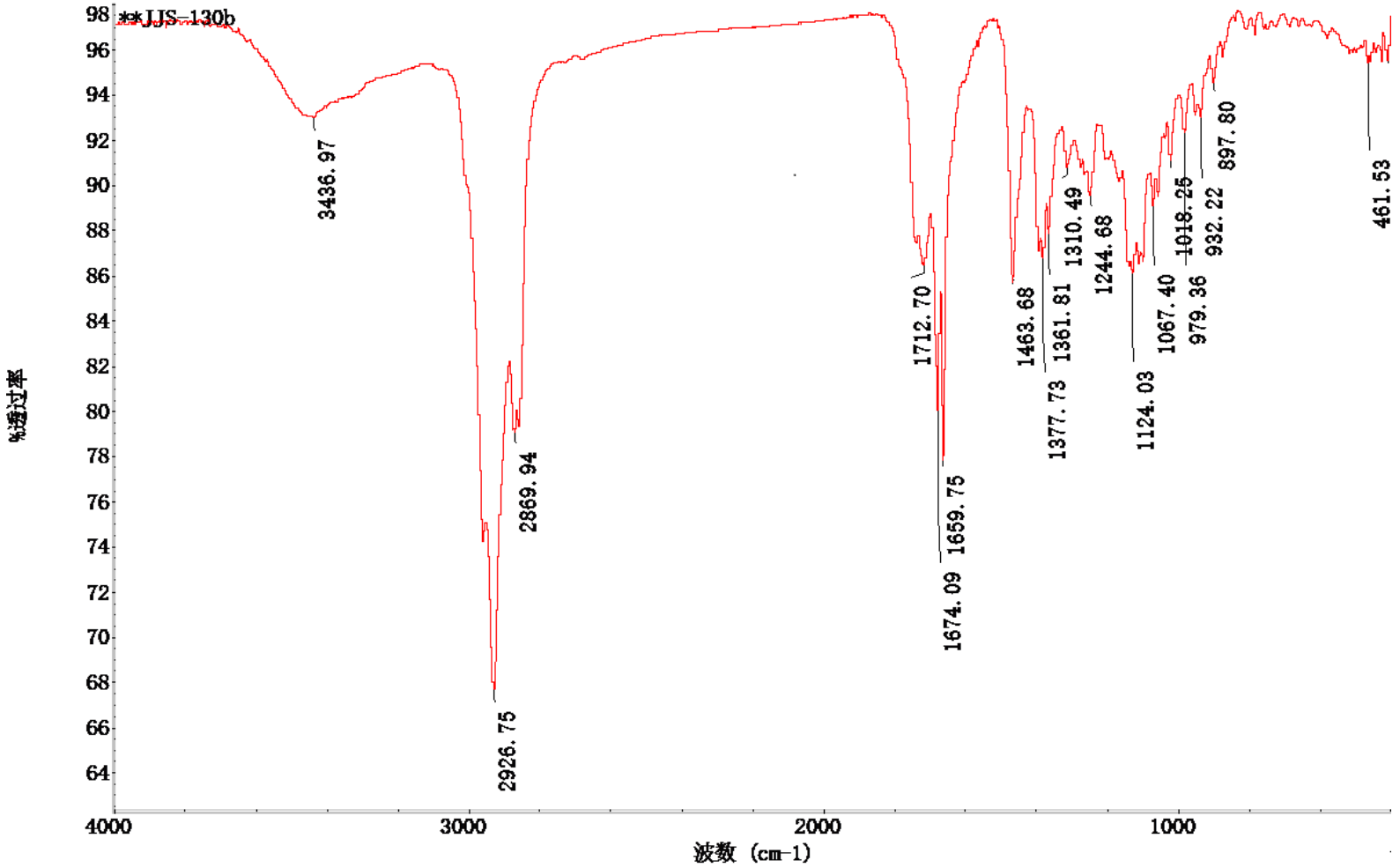

Figure S50. IR spectrum of biswulfenioidin E (**5**)

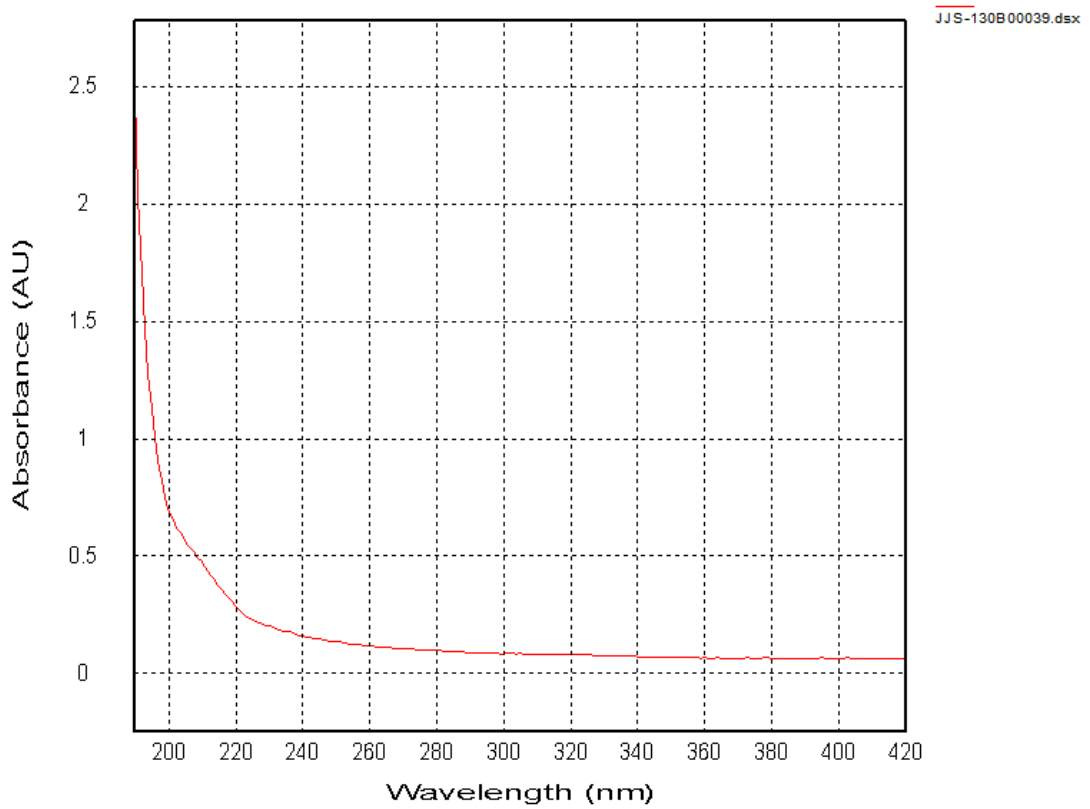

Figure S51. UV spectrum of biswulfenioidin E (**5**)

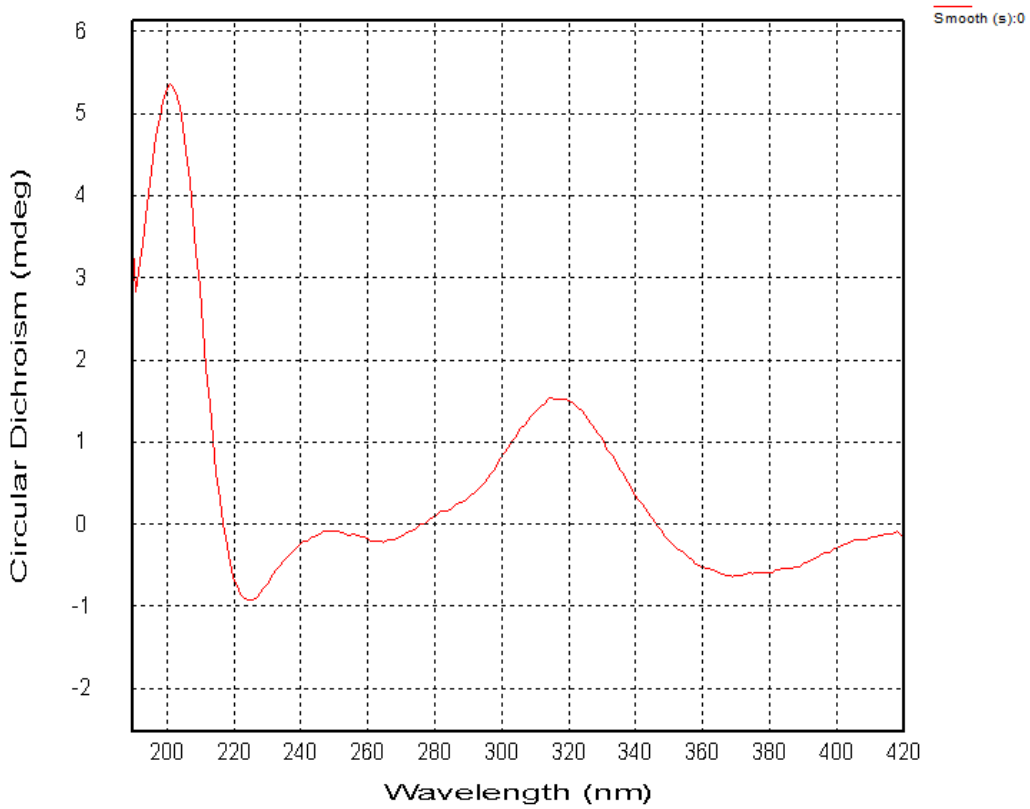

Figure S52. CD spectrum of biswulfenioidin E (**5**)

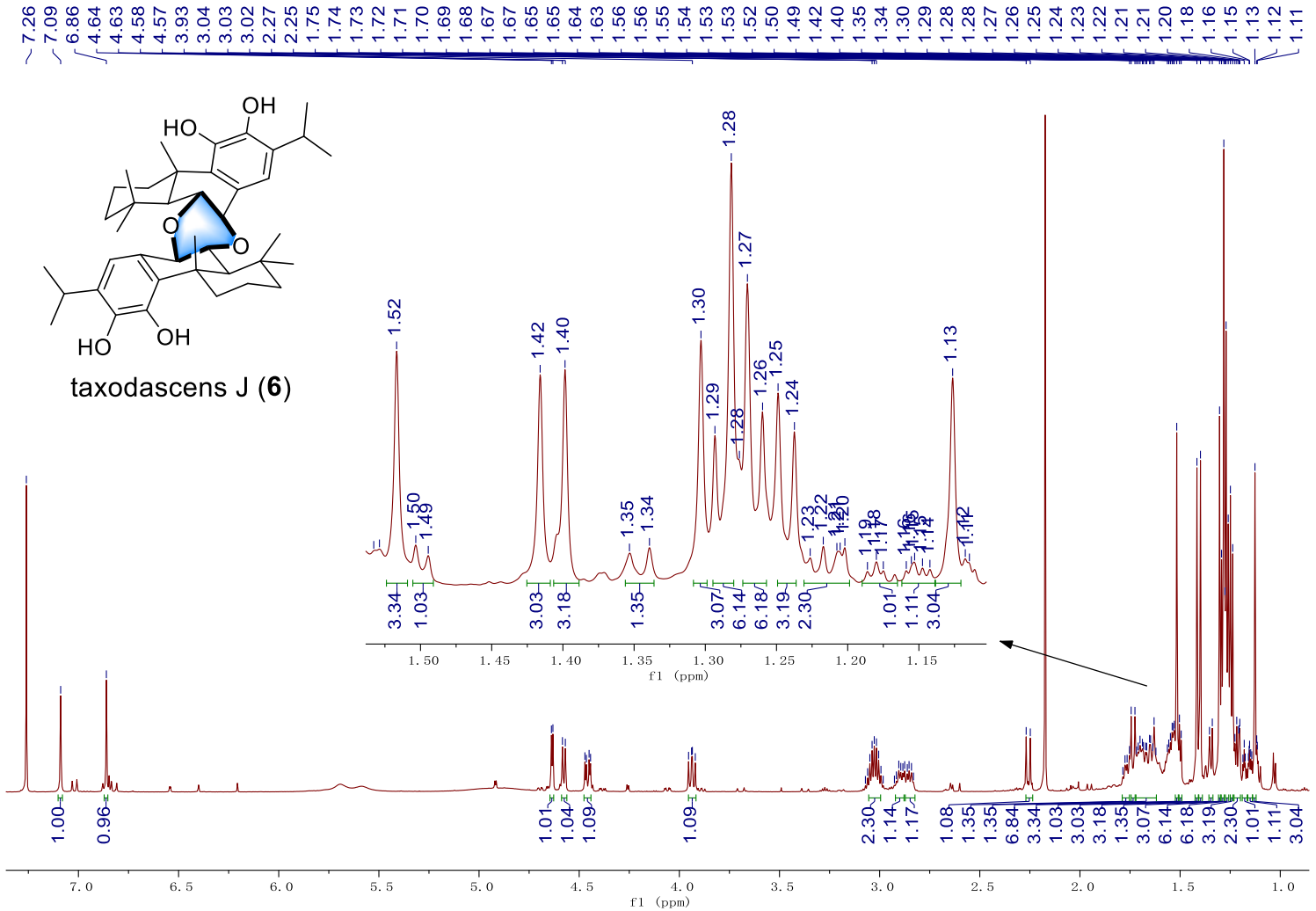

Figure S53. ^{1}H NMR spectrum of taxodascens J (**6**) in chloroform (600 MHz)

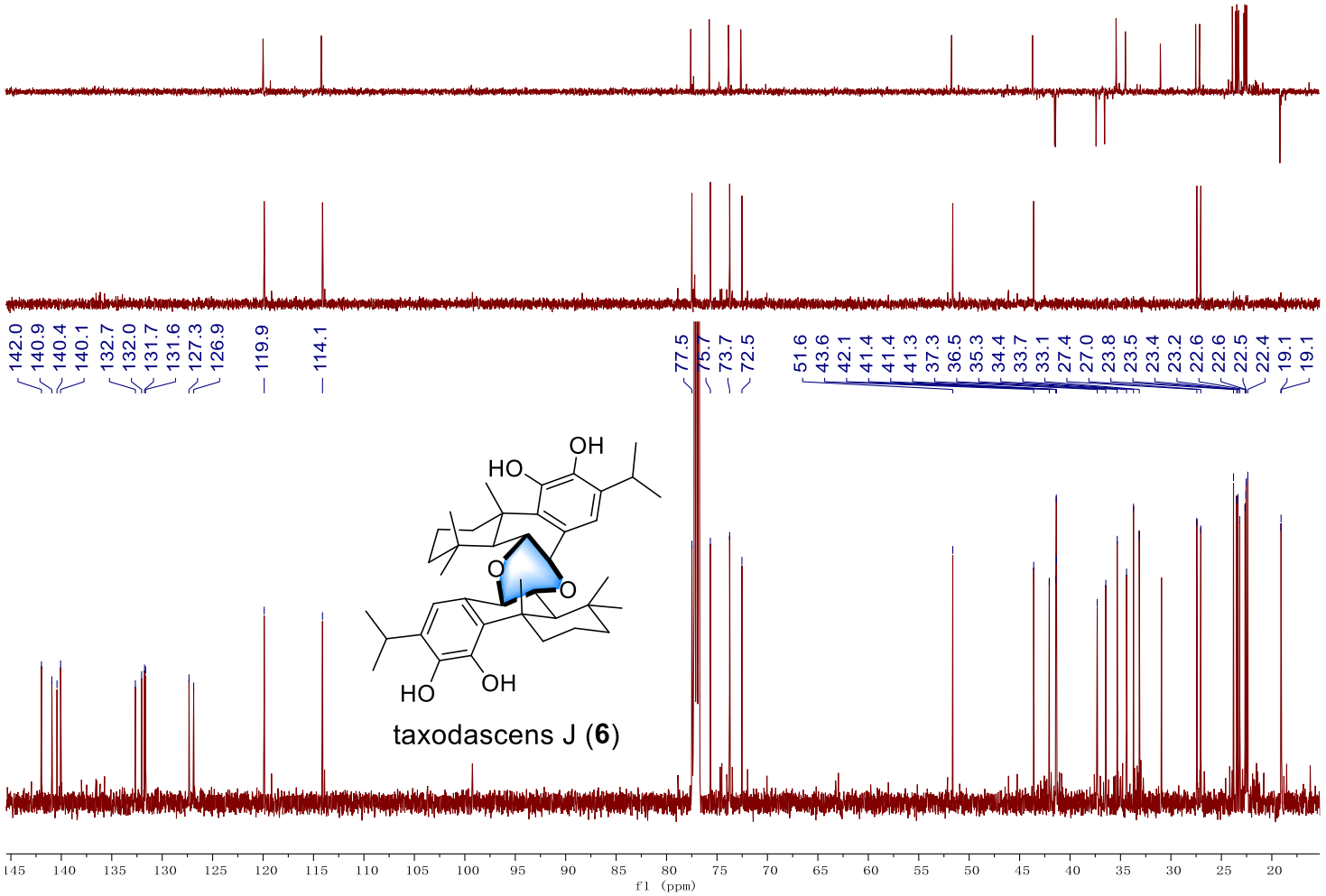

Figure S54. ^{13}C and DEPT NMR spectra of taxodascens J (**6**) in chloroform (150 MHz)

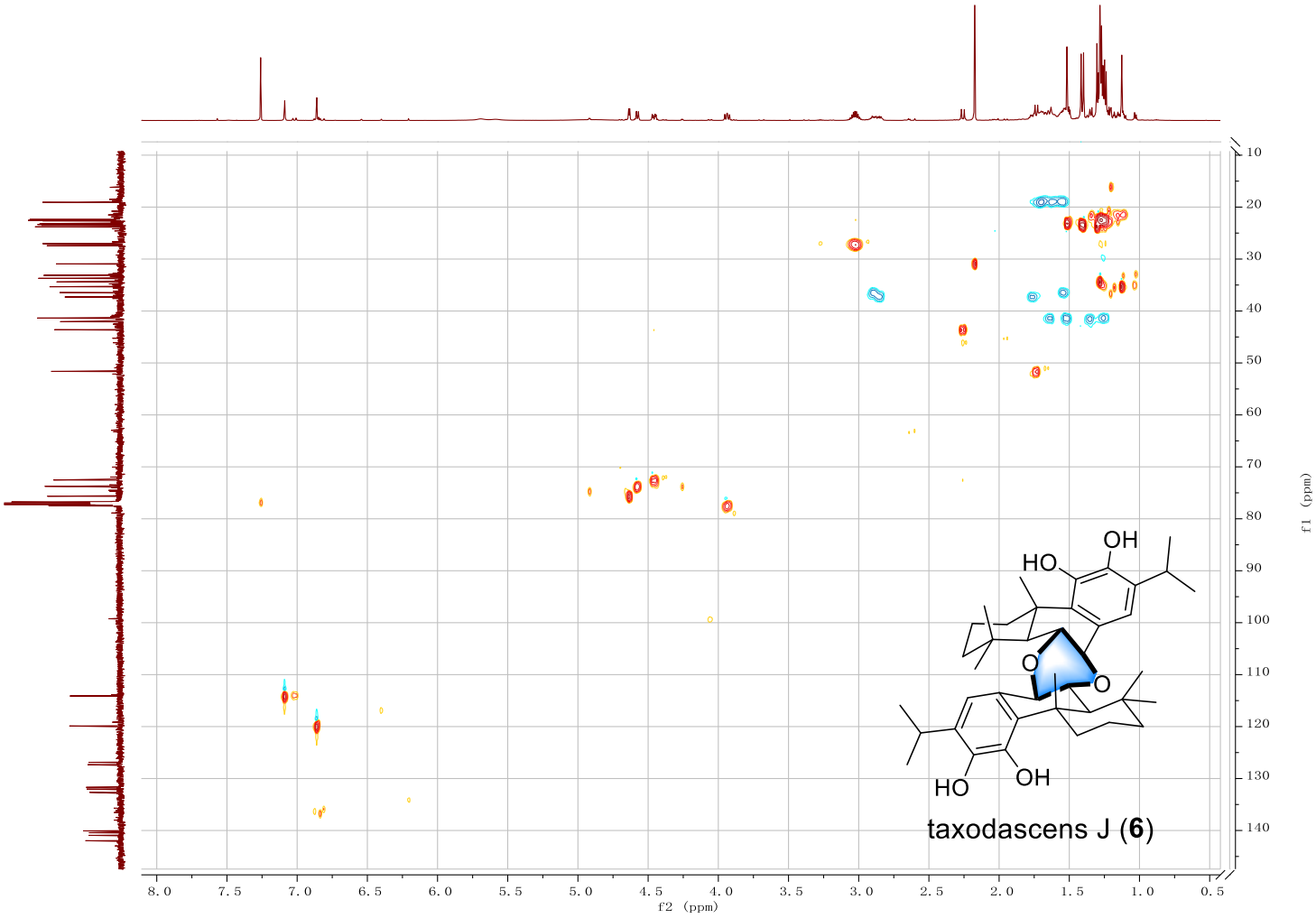

Figure S55. HSQC spectrum of taxodascens J (**6**) in chloroform (600 MHz)

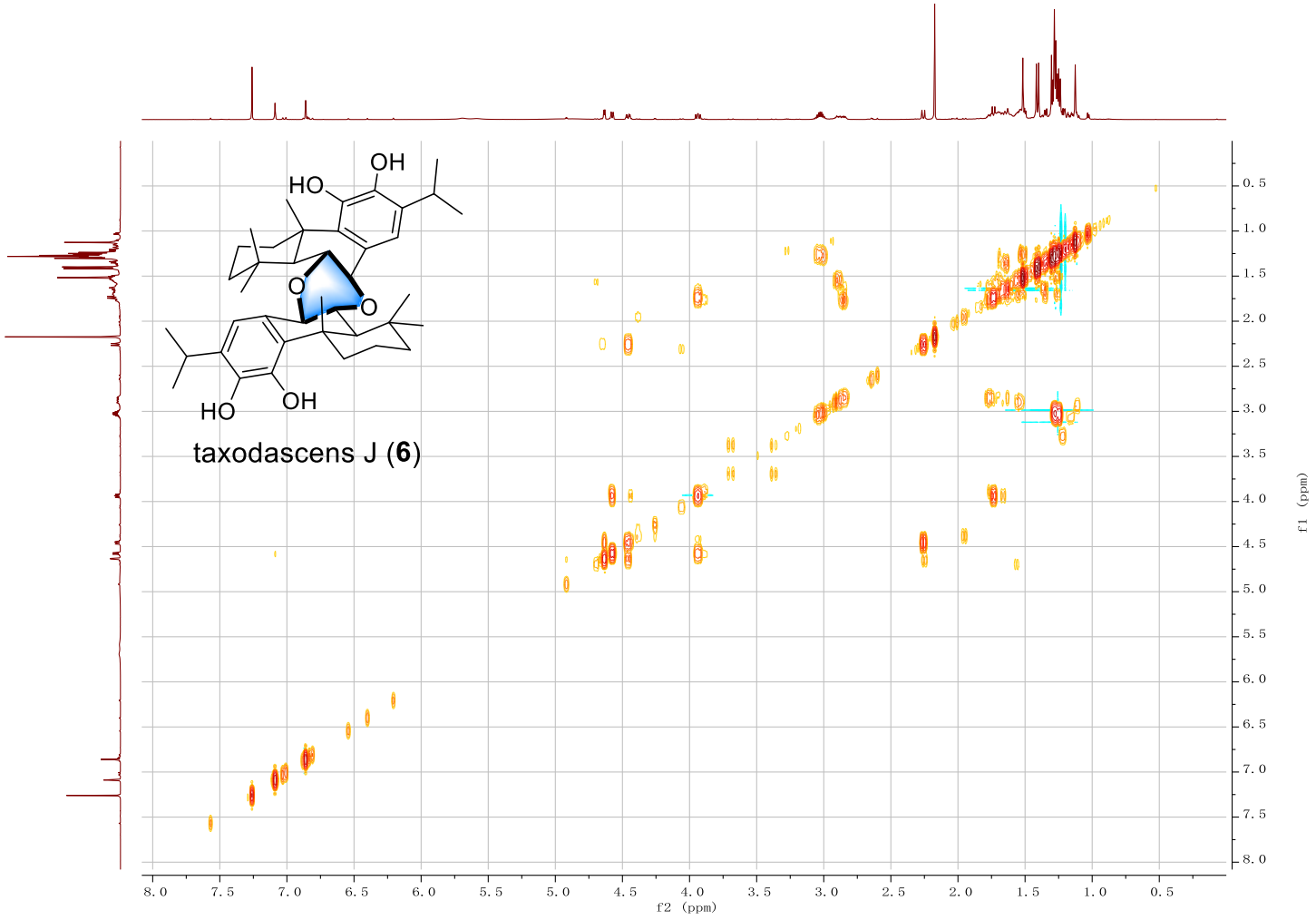

Figure S56. ^{1}H-^{1}H COSY spectrum of taxodascens J (**6**) in chloroform (600 MHz)

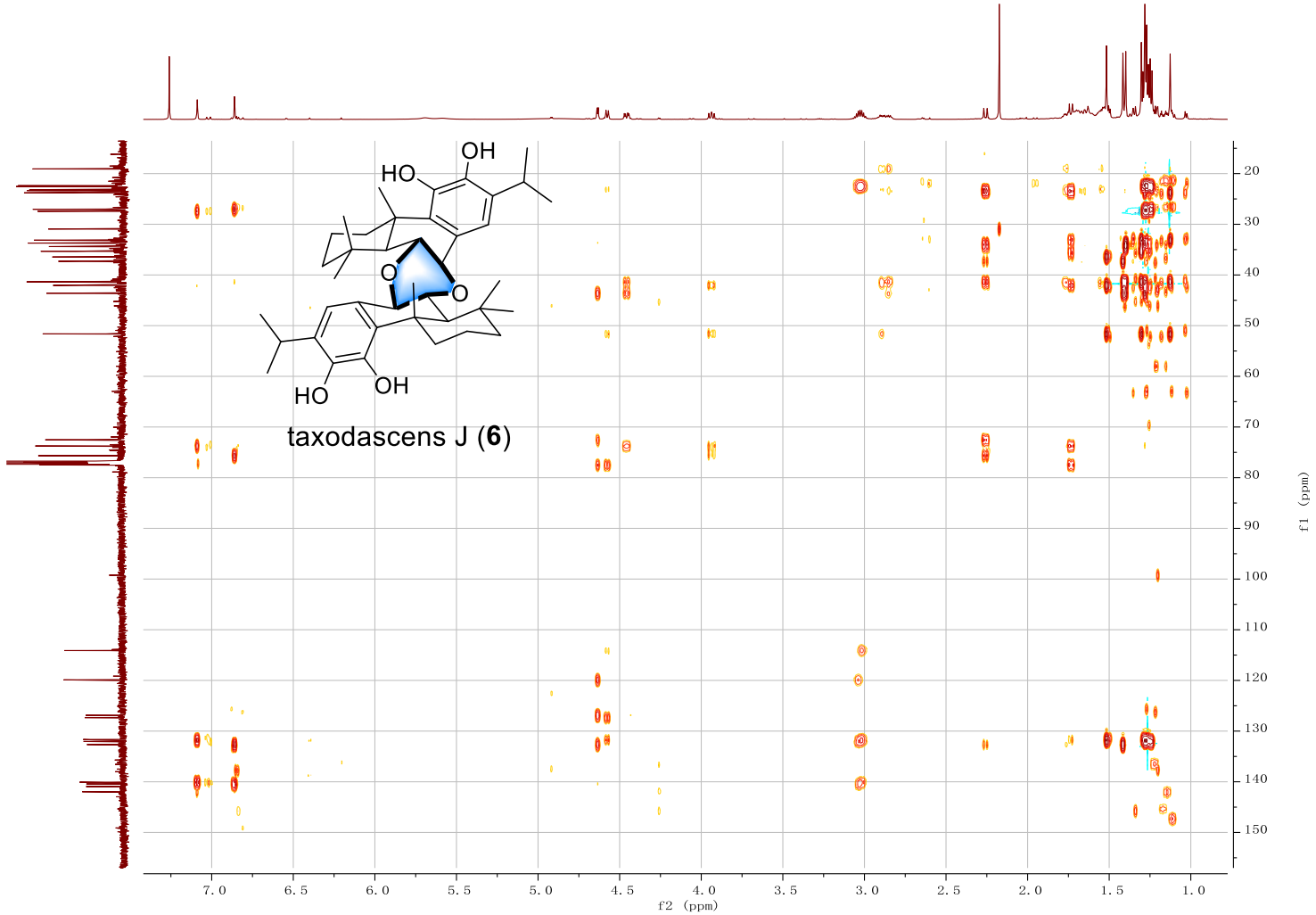

Figure S57. HMBC spectrum of taxodascens J (**6**) in chloroform (600 MHz)

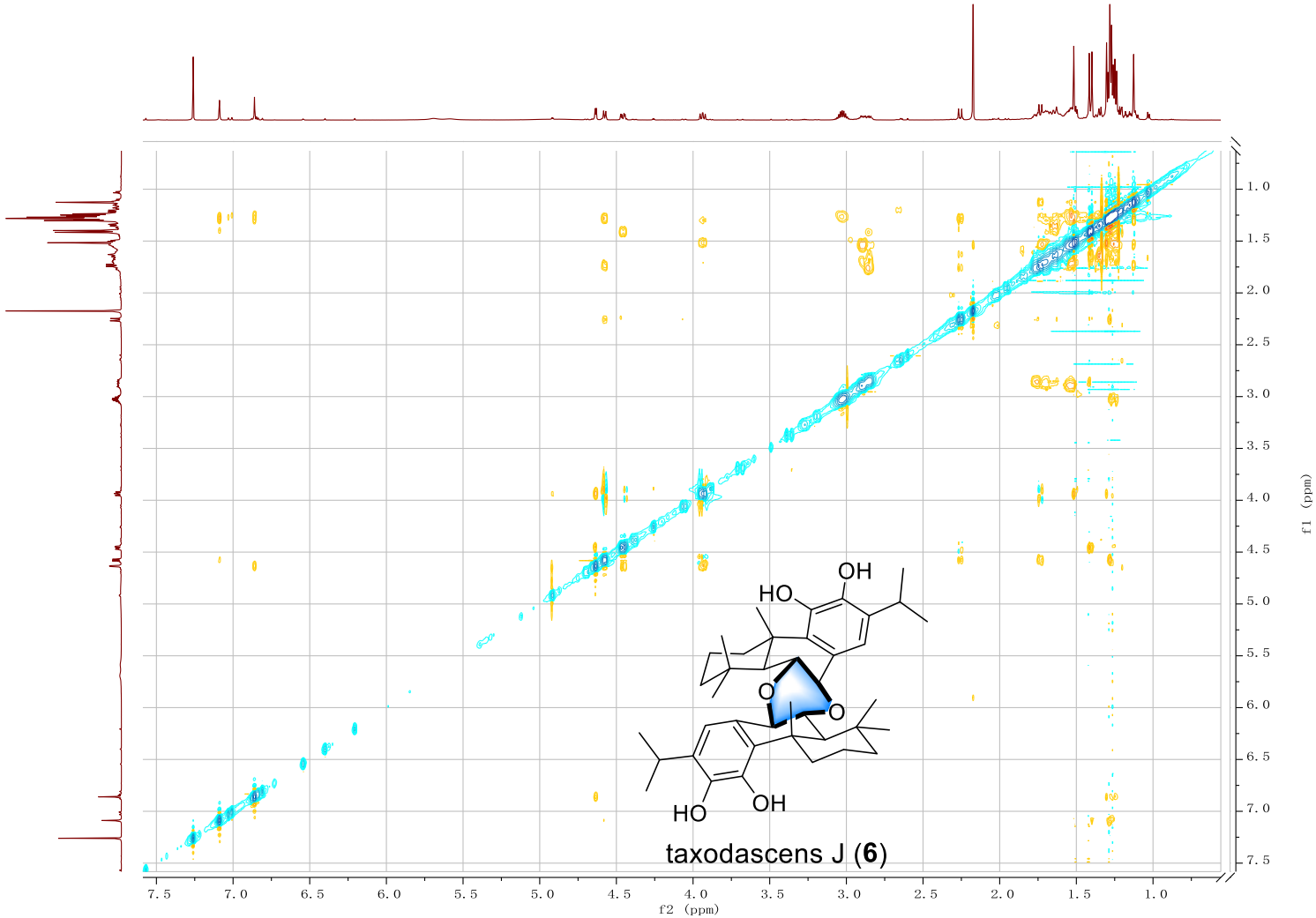

Figure S58. ROESY spectrum of taxodascens J (**6**) in chloroform (600 MHz)

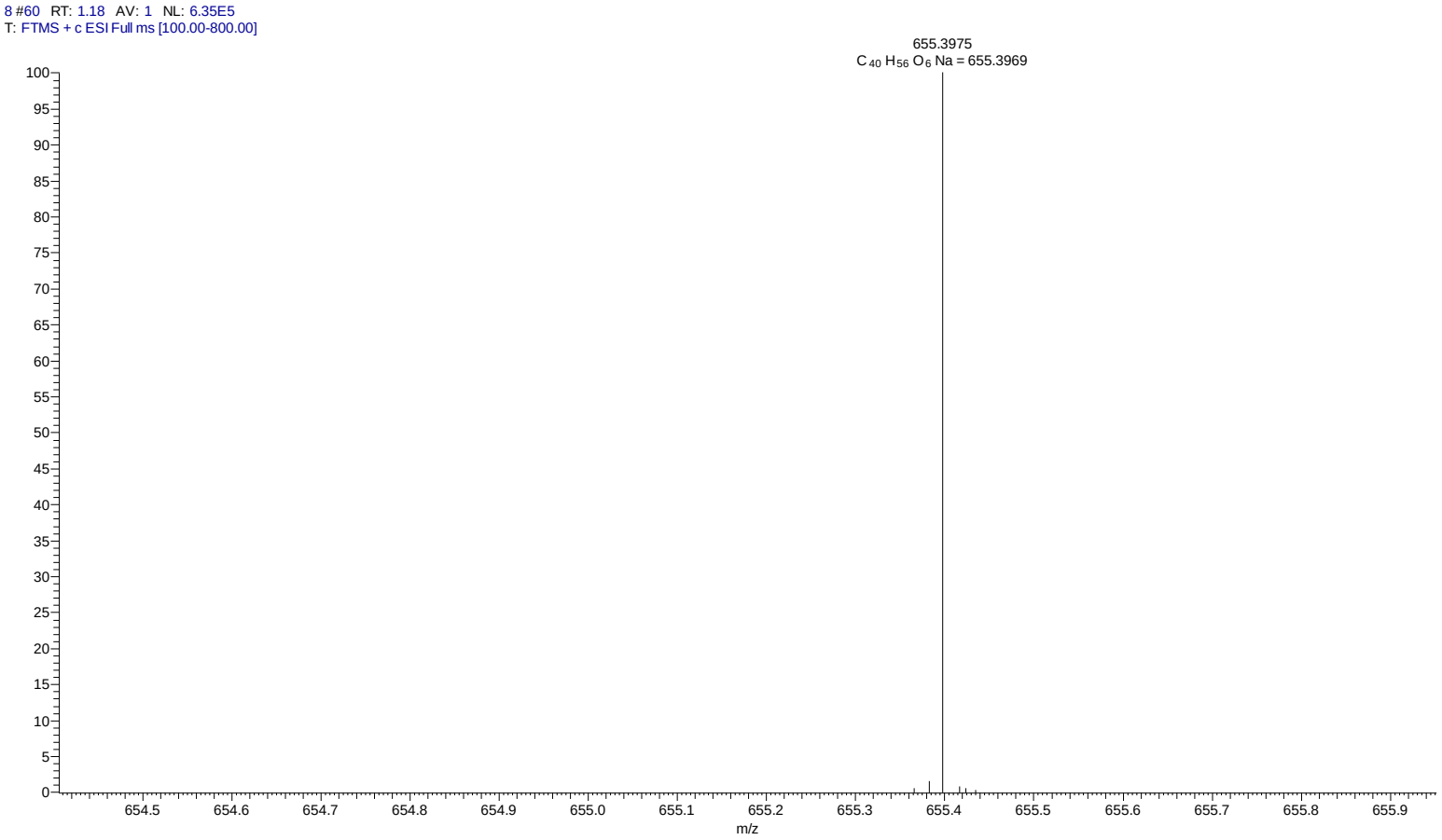

Figure S59. HRESIMS spectrum of taxodascens J (**6**)

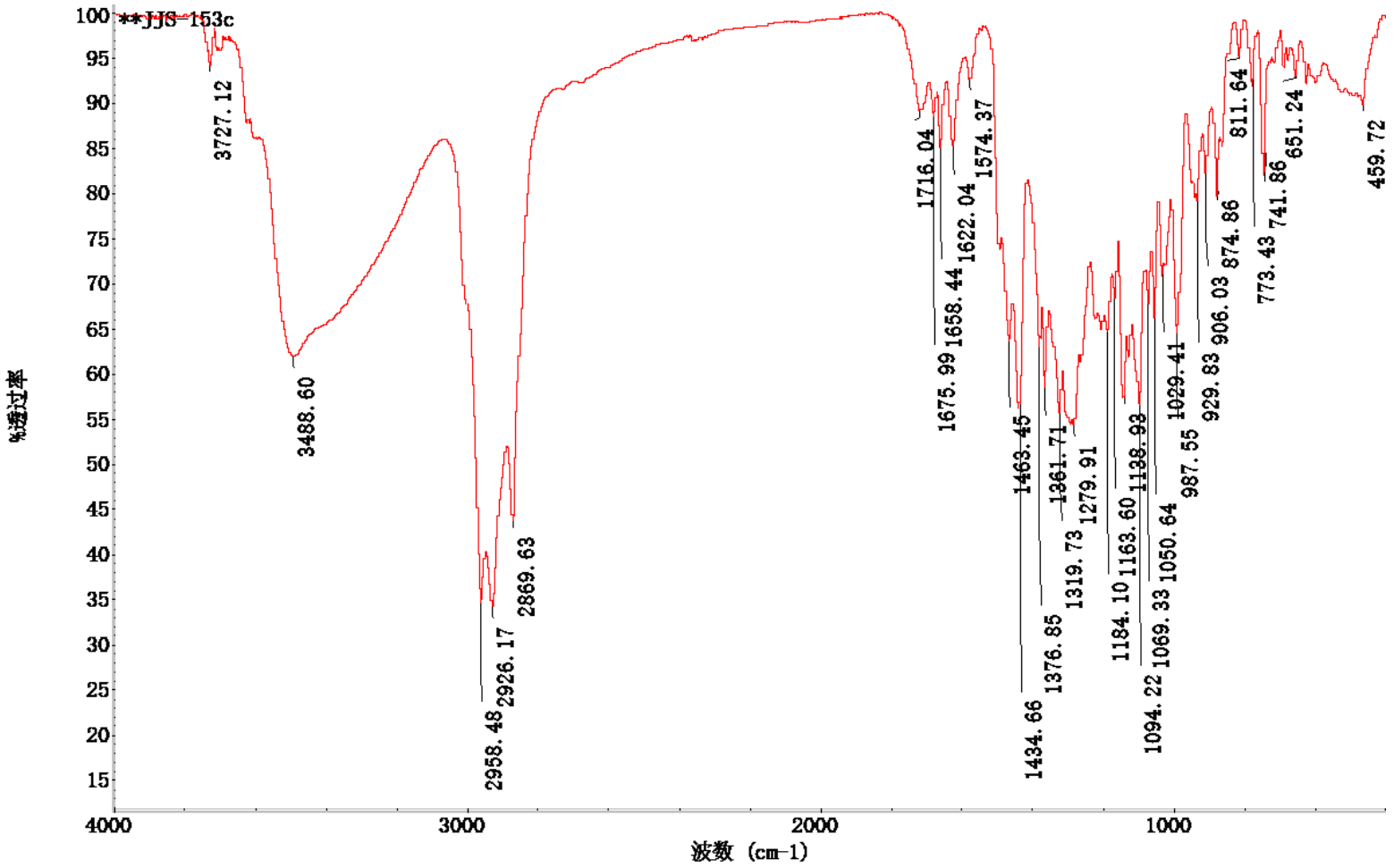

Figure S60. IR spectrum of taxodascens J (**6**)

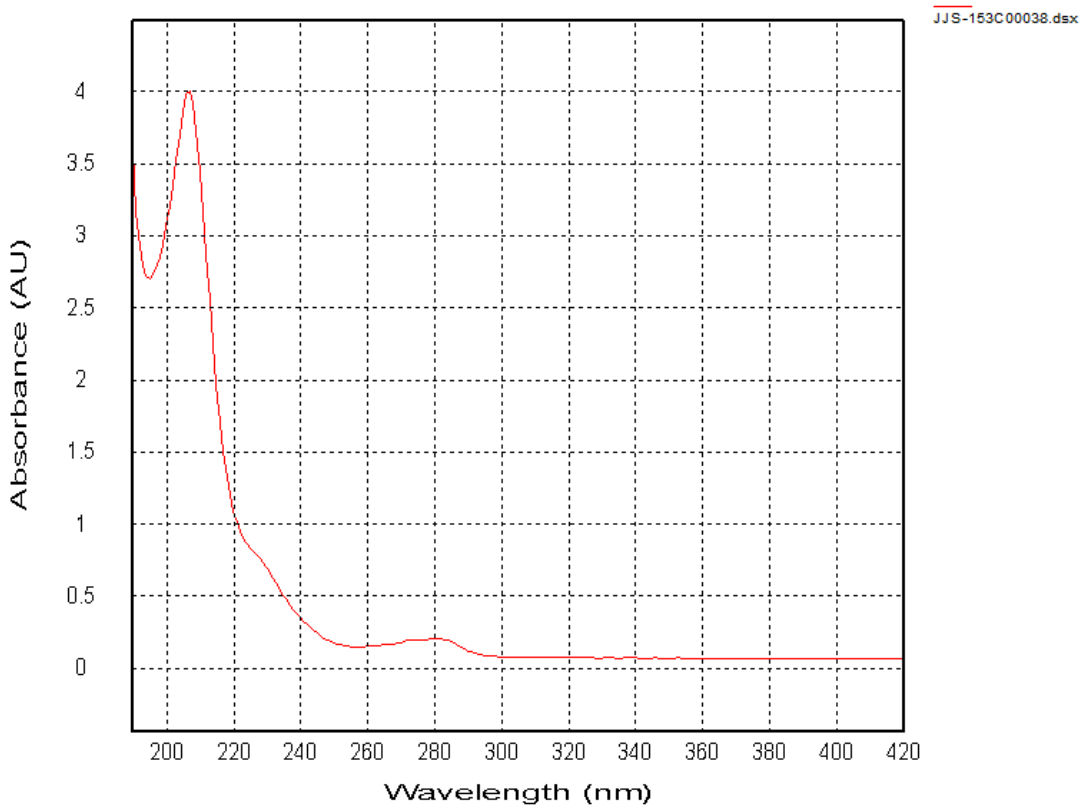

Figure S61. UV spectrum of taxodascens J (**6**)

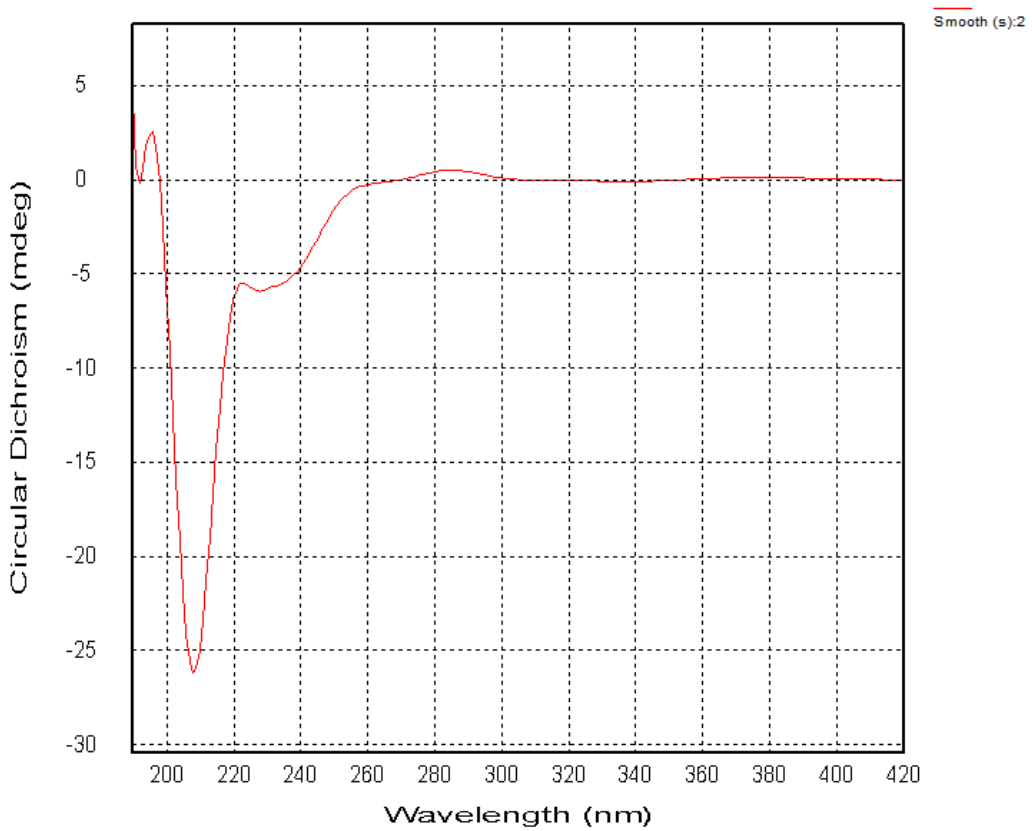

Figure S62. CD spectrum of taxodascens J (**6**)

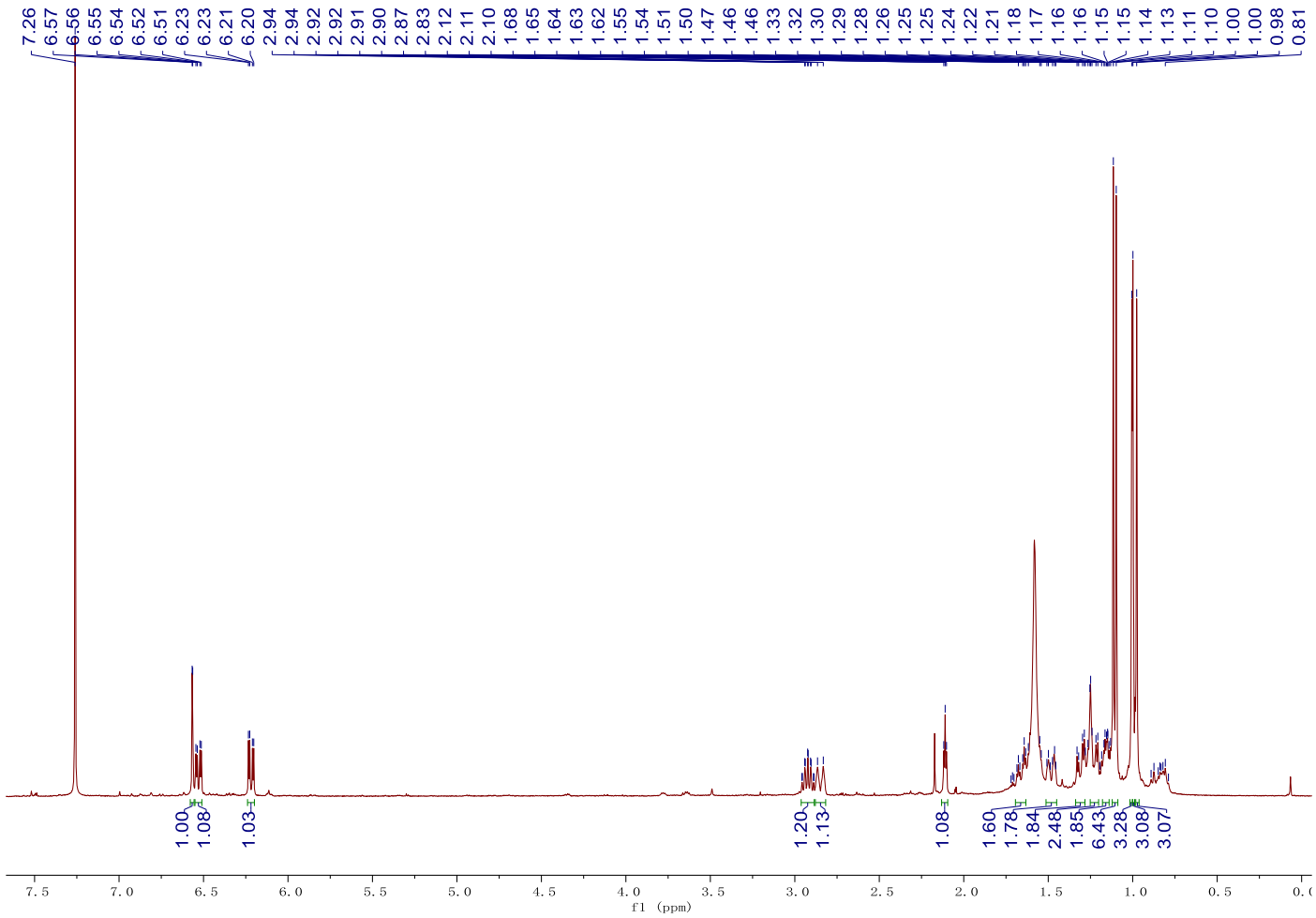

Figure S63. ^{1}H NMR spectrum of abieta-6,8,13-triene-11,12-dione (**7**) in chloroform (400 MHz)

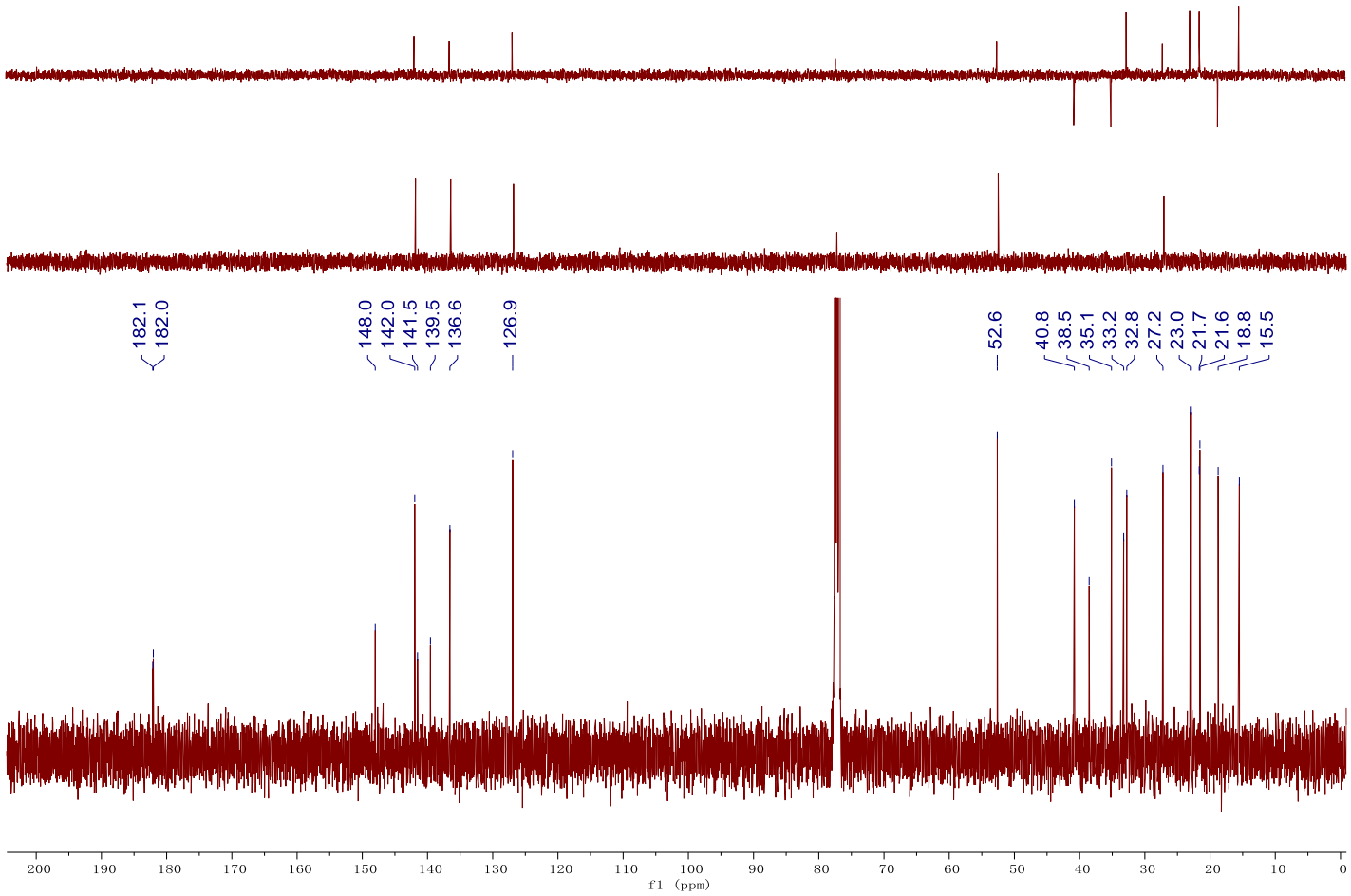

Figure S64. ^{13}C NMR spectrum of abieta-6,8,13-triene-11,12-dione (**7**) in chloroform (100 MHz)

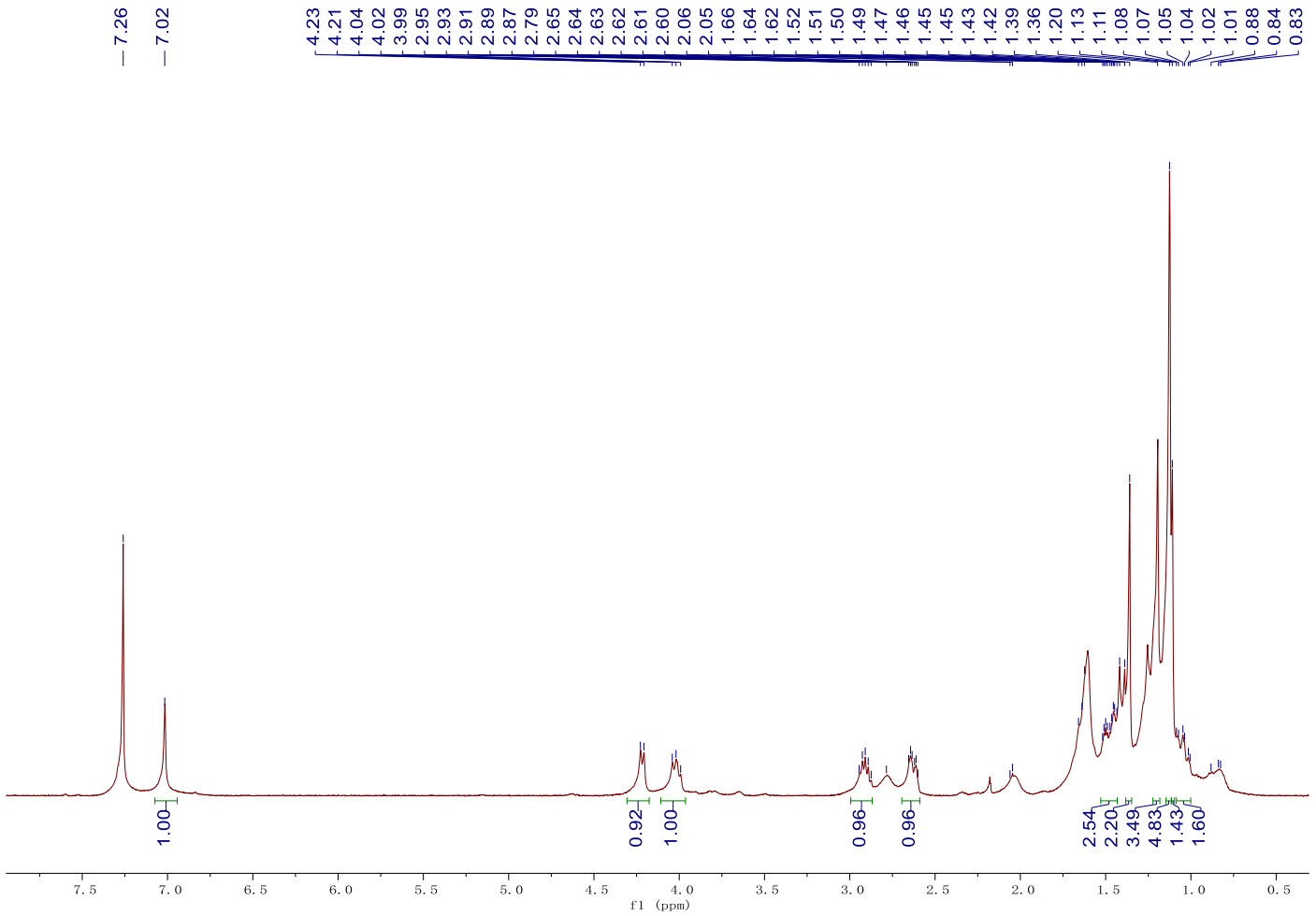

Figure S65. ^{1}H NMR spectrum of salviphlomone (**8**) in chloroform (400 MHz)

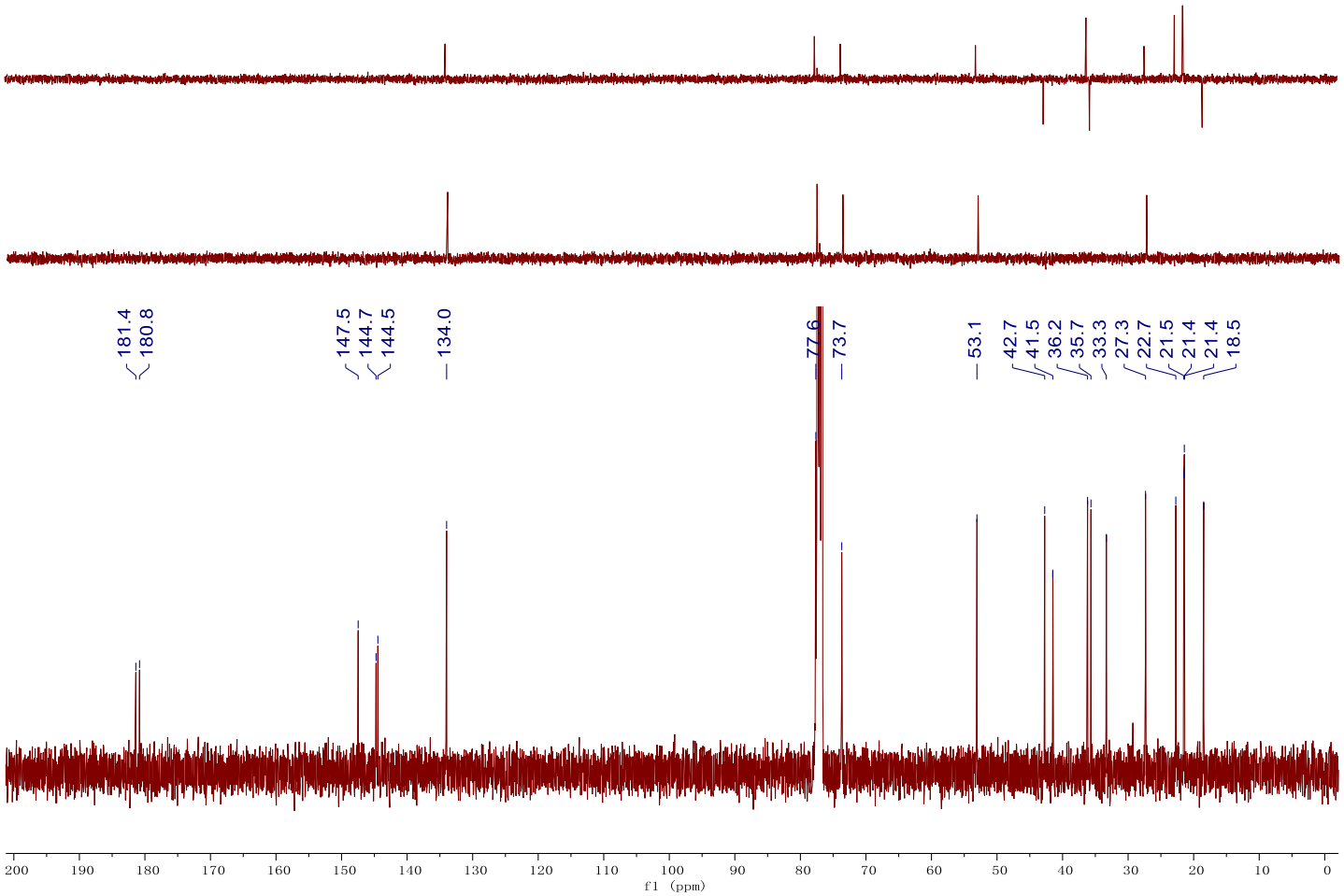

Figure S66. ^{13}C NMR spectrum of salviphlomone (**8**) in chloroform (100 MHz)

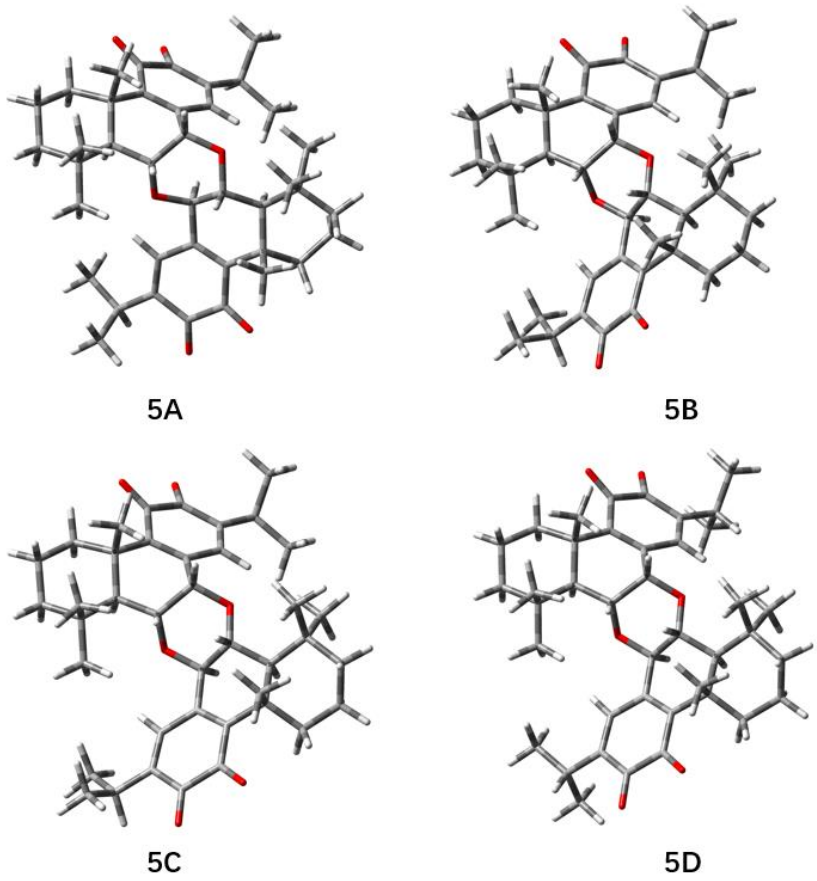

Figure S67. Possible conformers of **5** for ECD calculation.

Table S2. Important thermodynamic parameters and Boltzmann distributions of the optimized isomer **5** at m062x /6-311 + G (d, p) level in the methanol.

Conformations	Energy (a.u)	*Δ*G(kcal/mol)	%	Number of imaginary frequencies
5A	-2005.777588	0.00	4.1	0
5B	-2005.780499	-1.83	89.3	0
5C	-2005.777855	-0.17	5.4	0
5D	-2005.776388	0.75	1.1	0

Table S3. Optimized Z-matrixes of isomer **5** in the methanol (Å) at m062x/6-311 G (d, p) level.

5A				**5B**			
C	-4.91538	3.123233	-0.78195	C	-2.8832	-4.72578	1.017085
C	-3.60214	3.858185	-1.02858	C	-1.4261	-4.77413	0.572737
C	-2.40884	1.668998	-0.98193	C	-1.38274	-2.27607	0.528428
C	-3.72443	0.851671	-0.7489	C	-2.87333	-2.15803	0.988582

C	-4.70915	1.805825	-0.03062	C	-3.58603	-3.45528	0.536851
C	-1.18344	0.843964	-1.42935	C	-0.55307	-0.99164	0.684172
C	-1.42384	-0.67044	-1.36506	C	-1.39961	0.289142	0.884153
C	-2.19486	-1.0325	-0.11091	C	-2.72291	0.20875	0.162385
C	-3.31802	-0.32329	0.147518	C	-3.43777	-0.93419	0.264667
C	-1.71735	-2.15782	0.702422	C	-3.18663	1.411647	-0.54526
C	-2.32624	-2.59422	1.816835	C	-4.37126	1.515049	-1.16821
C	-3.56281	-1.88814	2.213236	C	-5.2483	0.329015	-1.12089
C	-4.18075	-0.85862	1.219449	C	-4.84163	-0.85202	-0.19069
C	-1.8439	-3.71713	2.698745	C	-4.86037	2.72281	-1.92649
C	-0.41793	-4.15568	2.378251	C	-3.75953	3.743621	-2.20088
C	-2.80782	-4.91134	2.606757	C	-6.02881	3.377639	-1.17197
C	-2.55325	3.003528	-1.76177	C	-0.61747	-3.54209	1.014705
C	-1.21743	3.762441	-1.70986	C	0.749484	-3.61274	0.31635
C	-2.9389	2.828889	-3.23793	C	-0.36292	-3.59399	2.529836
C	-4.42642	0.28055	-2.00808	C	-3.10641	-1.95271	2.504567
O	-5.35466	-0.60868	1.360845	O	-5.72919	-1.59449	0.158436
O	-4.13254	-2.07529	3.260911	O	-6.27216	0.225553	-1.75253
C	4.177586	-3.42637	-0.33877	C	3.463977	4.679552	0.716817
C	3.588756	-3.66907	-1.72413	C	2.010767	4.984001	0.370274
C	2.100435	-1.75542	-0.94919	C	1.539694	2.536822	0.257951
C	3.451411	-0.98354	-0.80741	C	3.016568	2.169719	0.652696
C	4.472648	-1.93678	-0.10891	C	3.913487	3.328775	0.156582
C	0.991695	-0.77237	-1.31415	C	0.696684	1.289811	0.516518
C	0.775812	0.201451	-0.17603	C	1.030443	0.300828	-0.58157
C	2.052009	0.824017	0.319775	C	2.508019	-0.01421	-0.5863
C	3.249358	0.26736	0.045602	C	3.396321	0.853491	-0.04622
C	1.869437	2.036665	1.135297	C	2.874338	-1.27015	-1.25856
C	2.867789	2.734612	1.697004	C	4.127938	-1.72624	-1.39577
C	4.236708	2.221921	1.488943	C	5.20327	-0.8746	-0.85207
C	4.441396	0.989094	0.553534	C	4.816478	0.422824	-0.0706
C	2.708242	3.984696	2.524699	C	4.52519	-3.02173	-2.05546
C	1.274618	4.215224	2.993837	C	3.415289	-3.62399	-2.91192
C	3.220417	5.200407	1.735189	C	4.984205	-4.02492	-0.98447
C	2.182967	-3.03053	-1.85484	C	0.999635	3.894383	0.783879
C	1.168852	-4.07171	-1.34714	C	-0.32328	4.252747	0.076301
C	1.875453	-2.74701	-3.33189	C	0.730156	3.918736	2.294775
C	4.025433	-0.49166	-2.15766	C	3.261311	1.95207	2.166313
O	-0.24689	-1.44307	-1.5448	O	-0.70672	1.464948	0.471139
O	-0.10244	1.239714	-0.5717	O	0.207262	-0.85771	-0.51673
O	5.580679	0.699005	0.278648	O	5.718466	0.988084	0.50072
O	5.214827	2.702308	2.007683	O	6.37732	-1.12358	-0.97829
H	-2.13175	1.975273	0.034018	H	-1.4618	-2.39463	-0.5601

H	1.864642	-2.1142	0.064159	H	1.577104	2.672625	-0.8325
H	-5.58443	3.757276	-0.19435	H	-3.41784	-5.59151	0.617693
H	-5.43089	2.944466	-1.73005	H	-2.95045	-4.80951	2.105811
H	-3.77761	4.776533	-1.59878	H	-0.93713	-5.6767	0.954087
H	-3.18011	4.159739	-0.0617	H	-1.39221	-4.83178	-0.52251
H	-4.31973	2.024435	0.971096	H	-3.62812	-3.46598	-0.55936
H	-5.66717	1.306554	0.102507	H	-4.61346	-3.44858	0.895142
H	-0.89368	1.080431	-2.45772	H	0.130417	-1.08588	1.533274
H	-2.0633	-0.92733	-2.21147	H	-1.61225	0.388193	1.956493
H	-0.7966	-2.62052	0.366702	H	-2.48256	2.232631	-0.57694
H	-1.87895	-3.34071	3.72692	H	-5.24788	2.354122	-2.88244
H	-0.09177	-4.90679	3.099585	H	-4.15452	4.555021	-2.81457
H	0.283056	-3.31776	2.414144	H	-2.91441	3.294848	-2.72775
H	-0.36457	-4.60619	1.383031	H	-3.38937	4.182694	-1.26966
H	-3.82512	-4.62366	2.873869	H	-6.4215	4.21876	-1.74711
H	-2.81246	-5.31068	1.589101	H	-6.84049	2.669185	-1.00273
H	-2.48569	-5.70436	3.284775	H	-5.68546	3.753533	-0.20453
H	-0.86308	3.865285	-0.68079	H	1.428088	-2.82585	0.657041
H	-0.43538	3.259056	-2.28354	H	1.216952	-4.57762	0.533675
H	-1.353	4.762048	-2.13205	H	0.638503	-3.51671	-0.76668
H	-2.27801	2.123942	-3.7499	H	0.333516	-4.40996	2.741849
H	-2.84616	3.791762	-3.74795	H	-1.26373	-3.77812	3.11141
H	-3.96271	2.484548	-3.37286	H	0.094104	-2.67392	2.902808
H	-5.02327	-0.58916	-1.72422	H	-3.08714	-2.89621	3.046661
H	-3.73759	-0.02144	-2.79684	H	-4.09543	-1.51478	2.657691
H	-5.10987	1.007731	-2.44364	H	-2.36817	-1.29475	2.965545
H	3.476696	-3.79257	0.418312	H	4.104812	5.463135	0.304062
H	5.098204	-3.9985	-0.20532	H	3.612394	4.711587	1.799843
H	4.270666	-3.27883	-2.48434	H	1.701285	5.932891	0.82077
H	3.498883	-4.74136	-1.92089	H	1.934875	5.112959	-0.71704
H	4.483109	-1.73782	0.966345	H	3.868042	3.360604	-0.93889
H	5.471058	-1.69726	-0.47728	H	4.948496	3.138688	0.435348
H	1.258675	-0.20763	-2.21613	H	0.962639	0.878931	1.495212
H	0.327258	-0.35521	0.665352	H	0.784326	0.78088	-1.53753
H	0.841581	2.352361	1.270456	H	2.040846	-1.83571	-1.65828
H	3.352824	3.862615	3.401588	H	5.386045	-2.79826	-2.69413
H	0.885038	3.352862	3.539089	H	3.788733	-4.50964	-3.42878
H	0.611345	4.416672	2.147749	H	3.05353	-2.916	-3.66067
H	1.239252	5.08323	3.654363	H	2.568714	-3.93551	-2.29336
H	3.158309	6.099908	2.351265	H	5.323084	-4.94919	-1.45718
H	4.257792	5.066537	1.426542	H	5.804077	-3.62307	-0.38795
H	2.606723	5.351852	0.843129	H	4.151045	-4.26468	-0.31782
H	0.150728	-3.68626	-1.37965	H	-1.16766	3.716029	0.503962

H	1.217985	-4.96638	-1.97413	H	-0.50585	5.325471	0.191087
H	1.397488	-4.37036	-0.3195	H	-0.27741	4.030589	-0.99429
H	2.029119	-3.66315	-3.90978	H	0.146291	4.810658	2.539175
H	2.52297	-1.97753	-3.75407	H	1.636739	3.949406	2.896349
H	0.837902	-2.43438	-3.46249	H	0.144014	3.045977	2.597995
H	4.910545	0.115812	-1.96756	H	4.216195	1.446547	2.307303
H	3.308748	0.121141	-2.70771	H	2.489653	1.341949	2.636794
H	4.331647	-1.31847	-2.7943	H	3.319116	2.892621	2.707958
5C				**5D**			
C	-2.87002	-4.74047	0.96796	C	3.108839	-4.5565	-1.16921
C	-1.41265	-4.78181	0.524535	C	1.652715	-4.68782	-0.73978
C	-1.37551	-2.28259	0.491995	C	1.477185	-2.19614	-0.6458
C	-2.86669	-2.17235	0.95152	C	2.964575	-1.99439	-1.08756
C	-3.57559	-3.46953	0.493617	C	3.739961	-3.26214	-0.6561
C	-0.55154	-0.9962	0.659712	C	0.587235	-0.95152	-0.79371
C	-1.40286	0.28433	0.853668	C	1.373386	0.376019	-0.94364
C	-2.72862	0.200004	0.137305	C	2.689696	0.340818	-0.20605
C	-3.43691	-0.94734	0.235008	C	3.46049	-0.7622	-0.33082
C	-3.20555	1.405572	-0.55716	C	3.0933	1.539163	0.543406
C	-4.39109	1.504491	-1.17907	C	4.258501	1.678369	1.197653
C	-5.257	0.309977	-1.14232	C	5.199377	0.544606	1.114325
C	-4.84314	-0.86968	-0.21494	C	4.855954	-0.61995	0.135487
C	-4.89225	2.713679	-1.92715	C	4.6035	2.900757	2.013245
C	-3.80376	3.751029	-2.18771	C	5.88702	3.576148	1.513211
C	-6.07171	3.346844	-1.17129	C	4.698886	2.569968	3.509052
C	-0.60832	-3.54972	0.974087	C	0.78541	-3.49056	-1.16668
C	0.7601	-3.61464	0.278863	C	-0.58339	-3.64908	-0.48836
C	-0.35604	-3.60948	2.489473	C	0.55125	-3.52589	-2.68578
C	-3.10029	-1.97353	2.468208	C	3.199467	-1.74329	-2.59659
O	-5.72677	-1.61533	0.137172	O	5.782807	-1.29856	-0.23968
O	-6.27726	0.199938	-1.77856	O	6.232589	0.464399	1.734642
C	3.116803	4.721451	-0.03175	C	-3.37513	4.564062	-0.05569
C	2.129677	4.871244	1.123266	C	-2.39263	4.768298	-1.20597
C	1.51671	2.548956	0.309522	C	-1.66561	2.474474	-0.40076
C	3.016371	2.211644	0.603167	C	-3.14535	2.065603	-0.70315
C	3.872927	3.382992	0.027242	C	-4.0618	3.189502	-0.12464
C	0.697018	1.283767	0.5227	C	-0.78116	1.255605	-0.62384
C	1.050393	0.303561	-0.57808	C	-1.09221	0.237085	0.454928
C	2.527204	-0.00565	-0.57866	C	-2.55336	-0.14003	0.452925
C	3.403235	0.890618	-0.07089	C	-3.47027	0.723748	-0.03856
C	2.915315	-1.27039	-1.22016	C	-2.88464	-1.42413	1.089266
C	4.177396	-1.70917	-1.33948	C	-4.13126	-1.88833	1.264896
C	5.240754	-0.82466	-0.82291	C	-5.23307	-1.04913	0.75332

C	4.8362	0.517035	-0.13128	C	-4.88596	0.291223	0.030392
C	4.595798	-3.02211	-1.95027	C	-4.5012	-3.17412	1.959607
C	3.502471	-3.6649	-2.79872	C	-5.06864	-2.86929	3.355244
C	5.051036	-3.98418	-0.84059	C	-3.3399	-4.15989	2.050712
C	0.986887	3.828947	1.027147	C	-1.19889	3.785247	-1.10798
C	-0.1256	4.439444	0.156509	C	-0.12517	4.449084	-0.22826
C	0.402839	3.554852	2.420173	C	-0.59404	3.549878	-2.49923
C	3.325911	2.03216	2.108558	C	-3.44005	1.878555	-2.21082
O	-0.70778	1.454892	0.430313	O	0.611842	1.499557	-0.50958
O	0.224909	-0.85521	-0.53032	O	-0.21377	-0.88147	0.386437
O	5.733929	1.178919	0.33217	O	-5.81095	0.903616	-0.44723
O	6.417598	-1.0754	-0.91625	O	-6.39795	-1.34935	0.850763
H	-1.45169	-2.39496	-0.59746	H	1.548698	-2.33046	0.44152
H	1.477919	2.770231	-0.76546	H	-1.64083	2.687695	0.676374
H	-3.40188	-5.60558	0.563543	H	3.683966	-5.40183	-0.78259
H	-2.9381	-4.82998	2.056175	H	3.189594	-4.61341	-2.25872
H	-0.92089	-5.68471	0.901447	H	1.213729	-5.60659	-1.1426
H	-1.37759	-4.83342	-0.57098	H	1.612223	-4.76807	0.353827
H	-3.61715	-3.47512	-0.60267	H	3.77285	-3.29375	0.440063
H	-4.60309	-3.46726	0.851564	H	4.768682	-3.19378	-1.0041
H	0.120963	-1.09161	1.51725	H	-0.06616	-1.06088	-1.66407
H	-1.61176	0.390944	1.926804	H	1.595469	0.516527	-2.0101
H	-2.51115	2.234231	-0.58058	H	2.362602	2.337155	0.587239
H	-5.27141	2.349058	-2.88802	H	3.775272	3.602811	1.875068
H	-4.20615	4.561422	-2.79786	H	6.053965	4.504497	2.063767
H	-2.94939	3.318014	-2.71279	H	5.815846	3.816994	0.450498
H	-3.44634	4.188629	-1.25098	H	6.750262	2.926925	1.666389
H	-5.73722	3.716849	-0.1985	H	3.777346	2.106569	3.867285
H	-6.47147	4.189196	-1.73968	H	5.529019	1.88868	3.700149
H	-6.87591	2.627414	-1.01315	H	4.866345	3.486129	4.079823
H	1.227038	-4.58141	0.489047	H	-0.49424	-3.57277	0.598491
H	0.65144	-3.50945	-0.8036	H	-1.29911	-2.89256	-0.82207
H	1.43742	-2.83081	0.628761	H	-0.99447	-4.6328	-0.73385
H	0.345203	-4.42246	2.69705	H	1.466868	-3.65008	-3.25996
H	-1.25626	-3.80346	3.068639	H	0.048878	-2.62512	-3.04723
H	0.09478	-2.68925	2.869444	H	-0.09757	-4.374	-2.92145
H	-3.07211	-2.91801	3.008053	H	4.162566	-1.24547	-2.73052
H	-4.09301	-1.54473	2.623228	H	2.428	-1.11975	-3.05116
H	-2.36747	-1.30964	2.929638	H	3.240219	-2.67466	-3.15819
H	2.572836	4.802982	-0.97809	H	-2.83948	4.66818	0.893173
H	3.839772	5.539924	-0.0247	H	-4.13861	5.344901	-0.06177
H	2.662071	4.782692	2.07398	H	-2.91612	4.656491	-2.15914
H	1.685895	5.871324	1.117633	H	-1.99997	5.789465	-1.19505

H	4.21707	3.124995	-0.97827	H	-4.3964	2.909278	0.878165
H	4.767104	3.489464	0.642729	H	-4.95777	3.253739	-0.74334
H	0.938651	0.871678	1.509125	H	-0.98904	0.850054	-1.62045
H	0.812086	0.792914	-1.53138	H	-0.87814	0.718977	1.417997
H	2.092535	-1.86159	-1.60445	H	-2.03288	-2.00163	1.429457
H	5.462281	-2.81191	-2.58577	H	-5.30331	-3.62744	1.367818
H	3.892891	-4.56053	-3.28499	H	-5.39399	-3.79358	3.83746
H	3.138614	-2.98477	-3.57189	H	-5.92209	-2.1927	3.297467
H	2.654261	-3.96934	-2.17893	H	-4.29839	-2.40832	3.979212
H	5.404257	-4.92051	-1.27783	H	-2.91286	-4.36704	1.067044
H	5.859645	-3.55464	-0.24811	H	-2.54502	-3.77715	2.697267
H	4.211814	-4.2095	-0.1765	H	-3.68847	-5.10087	2.480067
H	-0.54776	5.316053	0.655717	H	0.713222	3.775185	-0.05534
H	0.265707	4.759133	-0.81382	H	0.250621	5.350265	-0.72064
H	-0.92706	3.721559	-0.01636	H	-0.53849	4.741704	0.741404
H	1.11193	3.059454	3.084037	H	-1.27213	3.020486	-3.16932
H	-0.49588	2.938208	2.352728	H	0.336399	2.982453	-2.43036
H	0.124578	4.506212	2.883146	H	-0.36508	4.517238	-2.95602
H	4.36223	1.71477	2.222934	H	-4.45954	1.512064	-2.32997
H	2.690958	1.276129	2.574484	H	-2.76801	1.155614	-2.67729
H	3.212303	2.963319	2.658692	H	-3.36913	2.816315	-2.75696

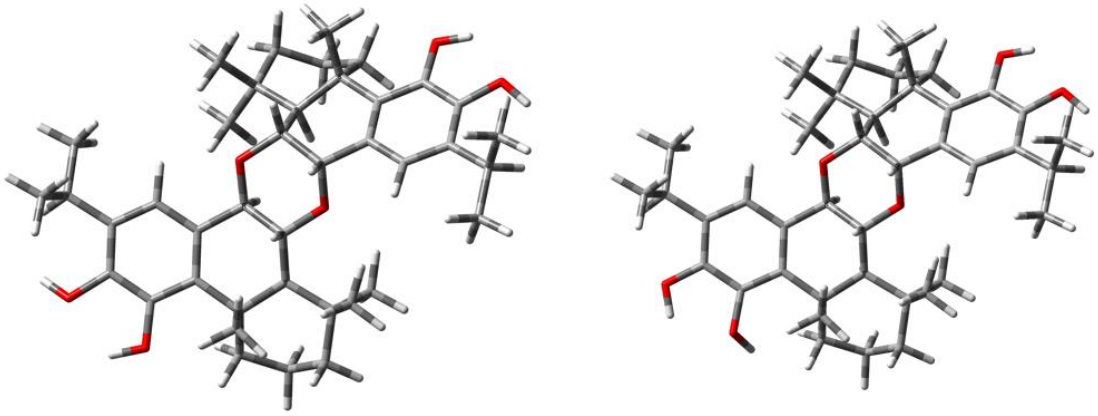

Figure S68. Possible conformers of **6** for ECD calculation.

Table S4. Important thermodynamic parameters and Boltzmann distributions of the optimized isomer 6 at m062x/6-311 G (d, p) level in the methanol.

Conformations	Energy (a.u)	*Δ*G(kcal/mol)	%	Number of imaginary frequencies
6A	-2008.227616	0	57.2	0

6B	-2008.227344	0.17	42.8	0

Table S5. Optimized Z-matrixes of isomer **6** in the methanol (Å) at m062x/6-311 G (d, p) level.

6A				**6B**			
C	2.129613	-3.589133	2.591788	C	2.123656	-3.585167	2.595625
C	1.186119	-4.380193	1.696427	C	1.182866	-4.378448	1.699356
C	1.164796	-2.129103	0.487587	C	1.162592	-2.12923	0.487574
C	2.706797	-2.385847	0.363826	C	2.705018	-2.384787	0.36723
C	3.209216	-2.8937	1.7544	C	3.204717	-2.890243	1.759653
C	0.659705	-1.355968	-0.738672	C	0.658971	-1.35772	-0.740147
C	1.324056	0.016866	-0.848011	C	1.323006	0.015097	-0.851135
C	2.806816	-0.002817	-0.608183	C	2.805283	-0.003259	-0.608792
C	3.447282	-1.099949	-0.027832	C	3.445238	-1.098825	-0.024813
C	3.507962	1.149204	-0.967177	C	3.506344	1.148467	-0.968715
C	4.880786	1.262508	-0.794069	C	4.878672	1.263239	-0.79259
C	5.532152	0.151204	-0.259461	C	5.529664	0.153502	-0.254333
C	4.842614	-1.006501	0.106208	C	4.840164	-1.004057	0.112059
C	5.678293	2.484886	-1.209293	C	5.676049	2.485552	-1.208231
C	6.466839	2.193634	-2.495626	C	6.466623	2.193211	-2.493089
C	4.817613	3.735491	-1.383161	C	4.814818	3.735399	-1.384954
C	0.339635	-3.427536	0.814898	C	0.337606	-3.428004	0.814226
C	-0.906253	-3.065884	1.64401	C	-0.911374	-3.066958	1.639141
C	-0.14436	-4.177089	-0.436034	C	-0.142036	-4.179705	-0.437086
C	3.073828	-3.410882	-0.736707	C	3.075237	-3.410984	-0.73112
O	5.569303	-2.054135	0.586181	O	5.566576	-2.050244	0.595497
O	6.892965	0.077934	-0.082701	O	6.889921	0.081658	-0.073779
C	-2.432058	4.019528	2.37092	C	-2.421016	4.019465	2.371083
C	-1.299452	4.597141	1.528891	C	-1.295333	4.596408	1.520775
C	-1.24295	2.173618	0.755945	C	-1.24419	2.171316	0.750928
C	-2.728077	2.430045	0.338701	C	-2.731079	2.42456	0.33561
C	-3.410836	3.208826	1.508521	C	-3.403527	3.221213	1.50143
C	-0.618112	1.142584	-0.177463	C	-0.620609	1.138905	-0.181981
C	-1.293139	-0.191352	0.049911	C	-1.293809	-0.194805	0.048967
C	-2.785442	-0.115551	-0.139179	C	-2.785957	-0.119394	-0.139091
C	-3.454816	1.100649	0.065826	C	-3.462409	1.092153	0.073367
C	-3.474581	-1.277241	-0.481983	C	-3.474584	-1.277132	-0.500443
C	-4.857824	-1.297983	-0.631221	C	-4.855233	-1.306923	-0.650678
C	-5.527689	-0.096192	-0.423379	C	-5.537787	-0.11239	-0.427845
C	-4.847694	1.079145	-0.090624	C	-4.855245	1.05754	-0.084003
C	-5.628638	-2.53581	-1.051834	C	-5.629347	-2.541938	-1.063281

C	-6.088026	-2.402977	-2.512228	C	-6.057807	-2.428199	-2.533705
C	-4.842721	-3.831944	-0.857286	C	-4.860716	-3.841637	-0.828593
C	-0.394285	3.471087	0.971	C	-0.394056	3.469163	0.960107
C	0.680975	3.185678	2.03622	C	0.6852	3.185079	2.021762
C	0.316958	3.953872	-0.301435	C	0.311333	3.950068	-0.316137
C	-2.854743	3.243698	-0.971676	C	-2.864282	3.228909	-0.979674
O	0.76306	0.940217	0.085602	O	0.760489	0.940139	0.080524
O	-0.759786	-1.18852	-0.810852	O	-0.760544	-1.19046	-0.813251
O	-5.580991	2.218124	0.05589	O	-5.682262	2.161098	0.003118
O	-6.886381	0.057573	-0.568306	O	-6.891095	-0.082064	-0.561731
H	2.609079	-4.241263	3.32559	H	2.601926	-4.235767	3.331554
H	1.553987	-2.853758	3.163006	H	1.546115	-2.849366	3.164372
H	0.506913	-4.996423	2.29243	H	0.502901	-4.994355	2.294792
H	1.766187	-5.076121	1.084385	H	1.764962	-5.074818	1.089746
H	1.059127	-1.459465	1.351781	H	1.054872	-1.459051	1.351067
H	4.033837	-3.587439	1.588401	H	4.030164	-3.583678	1.596522
H	3.622719	-2.054051	2.31883	H	3.616375	-2.049479	2.323766
H	0.90029	-1.919815	-1.64334	H	0.900179	-1.922629	-1.643958
H	1.126587	0.407505	-1.856756	H	1.126448	0.404233	-1.860586
H	2.948714	1.971697	-1.397993	H	2.947601	1.969649	-1.402663
H	6.397771	2.708682	-0.409981	H	6.394125	2.710777	-0.408058
H	5.771384	1.996692	-3.315606	H	5.772447	1.995061	-3.313856
H	7.086321	3.051109	-2.767536	H	7.086146	3.05064	-2.765028
H	7.114273	1.321922	-2.382949	H	7.114294	1.321875	-2.378699
H	4.213657	3.934402	-0.49507	H	5.454978	4.600247	-1.567863
H	4.146704	3.633749	-2.240089	H	4.209324	3.934938	-0.498048
H	5.458045	4.600137	-1.566078	H	4.145377	3.63224	-2.242856
H	-1.423202	-3.983747	1.938343	H	-1.426679	-3.985287	1.934776
H	-0.638835	-2.524428	2.556591	H	-0.647784	-2.522194	2.550873
H	-1.613078	-2.463254	1.078664	H	-1.618513	-2.468028	1.070089
H	0.671831	-4.448151	-1.106773	H	-0.862818	-3.58402	-1.001065
H	-0.639448	-5.102676	-0.125974	H	0.676235	-4.451051	-1.10513
H	-0.866121	-3.579861	-0.997121	H	-0.637285	-5.105227	-0.127139
H	4.161319	-3.466693	-0.8106	H	2.712887	-4.412003	-0.508592
H	2.710631	-4.411799	-0.515076	H	2.690781	-3.114523	-1.709757
H	2.688043	-3.112507	-1.714228	H	4.162916	-3.465598	-0.80302
H	6.49027	-1.766615	0.640563	H	6.487326	-1.762257	0.650958
H	7.274378	0.958069	-0.004112	H	7.271617	0.96234	-0.003356
H	-2.979317	4.816259	2.880172	H	-2.966203	4.812279	2.887281
H	-2.007451	3.388705	3.15839	H	-1.998437	3.377455	3.149385
H	-1.719204	5.202724	0.720717	H	-1.721937	5.20016	0.714619
H	-0.680283	5.27421	2.125405	H	-0.674183	5.274944	2.112806
H	-1.301975	1.689997	1.741447	H	-1.300158	1.689295	1.737162

H	-4.157688	3.880425	1.083663	H	-4.109197	3.939879	1.07071
H	-3.956183	2.505419	2.143168	H	-3.961463	2.534777	2.148077
H	-0.732176	1.441868	-1.229661	H	-0.73658	1.435782	-1.234582
H	-1.070813	-0.462845	1.091579	H	-1.067954	-0.465914	1.08996
H	-2.902025	-2.178364	-0.653187	H	-2.897674	-2.174677	-0.679583
H	-6.52264	-2.61204	-0.417978	H	-6.538869	-2.565244	-0.45409
H	-5.215021	-2.352817	-3.168181	H	-6.660568	-3.291905	-2.825271
H	-6.689743	-3.266282	-2.805008	H	-6.644946	-1.523854	-2.699973
H	-6.681465	-1.499847	-2.666693	H	-5.174894	-2.393486	-3.178273
H	-3.992334	-3.881083	-1.54249	H	-3.998517	-3.917956	-1.497071
H	-5.48678	-4.68768	-1.067577	H	-5.509583	-4.696297	-1.030236
H	-4.466704	-3.925244	0.163955	H	-4.501861	-3.917694	0.200701
H	0.22147	2.953016	3.001713	H	0.229992	2.952767	2.989362
H	1.31307	2.348553	1.744639	H	1.317107	2.348623	1.728525
H	1.30924	4.071492	2.169308	H	1.312631	4.071856	2.15142
H	0.817379	4.90461	-0.092765	H	0.811835	4.901436	-0.111142
H	1.075286	3.234929	-0.617345	H	1.068838	3.231035	-0.633407
H	-0.371442	4.116535	-1.131511	H	-0.38003	4.110807	-1.144124
H	-3.908337	3.30671	-1.247028	H	-3.919187	3.292917	-1.252031
H	-2.485314	4.26115	-0.861055	H	-2.490677	4.245882	-0.878781
H	-2.319094	2.770263	-1.79725	H	-2.336385	2.746101	-1.804053
H	-6.510636	1.980109	-0.057826	H	-5.47225	2.6828	0.783111
H	-7.338692	-0.782279	-0.439674	H	-7.176427	0.817907	-0.353091

Table S6. Key transitions, oscillator strengths, and rotatory strengths in the ECD spectra of conformers **6A** at the pbe1pbe/aug-ccpvdz level in MeOH with PCM.

Num	*Excited states*	*CI Coefficient*	*ΔE (eV)*	*λ (nm)*	*f*	*R(vel)*	*R(len)*
1	169 -> 176	0.11986	4.9614	249.90	0.0413	-0.1303	0.0005
	170 -> 176	0.31883					
	171 -> 173	0.19523					
	172 -> 173	0.47508					
	172 -> 174	0.27880					
	172 -> 175	0.11840					
2	169 -> 173	-0.13033	4.9774	249.10	0.0322	1.0073	1.1243
	169 -> 175	0.31592					
	170 -> 175	-0.11310					
	171 -> 173	-0.23626					
	171 -> 174	0.47365					
	171 -> 175	-0.14739					
	172 -> 173	0.12856					
	172 -> 174	-0.18794					
3	169 -> 173	0.12903	5.4591	227.12	0.0365	-6.1716	-7.6939
	169 -> 174	-0.23990					

	171 -> 173	-0.27508					
	171 -> 175	0.49892					
	172 -> 173	0.10651					
	172 -> 175	-0.24689					
4	170 -> 173	-0.39420	5.5100	225.02	0.0141	5.0601	5.3078
	170 -> 174	-0.20478					
	171 -> 176	0.15935					
	172 -> 176	0.48540					
5	168 -> 173	-0.14097	5.6260	220.38	0.0063	8.7160	8.7747
	168 -> 174	0.12038					
	170 -> 173	-0.11677					
	170 -> 174	0.13463					
	171 -> 174	0.21590					
	172 -> 173	-0.33967					
	172 -> 174	0.45561					
	172 -> 175	0.17834					
6	171 -> 173	0.49878	5.6884	217.96	0.0032	-0.5138	-1.7957
	171 -> 174	0.29579					
	171 -> 175	0.20054					
	172 -> 173	-0.16703					
	172 -> 174	-0.16779					
	172 -> 175	-0.11526					
7	170 -> 173	-0.10469	5.7479	215.70	0.0135	-8.6540	-11.3495
	171 -> 175	0.15968					
	171 -> 178	-0.16476					
	172 -> 174	-0.23615					
	172 -> 175	0.40664					
	172 -> 177	-0.15103					
	172 -> 178	-0.36981					
8	171 -> 177	0.58068	5.7632	215.13	0.0026	-5.4310	-11.5393
	171 -> 178	-0.17852					
	172 -> 177	-0.18725					
	172 -> 178	0.18187					
9	170 -> 175	0.10799	5.7667	215.00	0.0310	-27.8327	-29.7901
	171 -> 175	0.16493					
	171 -> 178	0.20274					
	172 -> 174	-0.17405					
	172 -> 175	0.36446					
	172 -> 177	0.19753					
	172 -> 178	0.42279					
10	168 -> 173	-0.26737	5.8211	212.99	0.0348	36.8778	38.2690
	168 -> 174	0.22527					
	168 -> 175	0.14293					

	170 -> 173	-0.29920					
	170 -> 174	0.32799					
	170 -> 175	0.11374					
	171 -> 174	-0.11373					
	171 -> 175	-0.16569					
	172 -> 173	0.15291					
	172 -> 174	-0.11969					
	172 -> 175	-0.16689					
11	168 -> 173	0.28001	5.8815	210.80	0.0582	-76.5344	-72.0277
	168 -> 174	0.24766					
	169 -> 173	-0.16238					
	169 -> 174	-0.14645					
	170 -> 173	0.19085					
	170 -> 174	0.26973					
	170 -> 176	-0.20719					
	171 -> 173	0.17771					
	171 -> 176	0.23137					
	172 -> 176	0.17408					
12	168 -> 176	-0.17181	5.9026	210.05	0.0869	-20.8966	-20.2393
	170 -> 173	-0.15507					
	170 -> 174	-0.15008					
	170 -> 176	-0.13364					
	171 -> 176	0.51070					
	172 -> 176	-0.34476					
13	168 -> 174	-0.12241	5.9849	207.16	0.3022	11.0801	11.9403
	168 -> 175	0.28311					
	169 -> 173	0.10020					
	169 -> 175	-0.15906					
	170 -> 173	0.11333					
	170 -> 174	-0.14680					
	170 -> 175	0.49115					
	171 -> 174	0.15509					
	171 -> 176	0.14504					
	172 -> 175	-0.14092					
14	168 -> 176	0.24279	6.0179	206.02	0.2764	-71.1011	-70.5892
	169 -> 173	0.11082					
	170 -> 173	0.20004					
	170 -> 174	0.16705					
	170 -> 175	-0.11789					
	170 -> 176	0.40324					
	171 -> 176	0.34214					
	172 -> 173	-0.11585					
15	168 -> 173	0.18147	6.0954	203.41	0.1846	-244.5149	-241.3950

	168 -> 175	-0.10300					
	169 -> 173	-0.31222					
	169 -> 174	0.37632					
	170 -> 173	-0.21634					
	170 -> 174	0.23598					
	170 -> 175	0.19488					
	170 -> 176	0.12451					
	171 -> 175	0.13233					
16	168 -> 174	-0.17222	6.1401	201.92	0.2533	-264.1220	-261.7917
	168 -> 175	-0.12939					
	168 -> 176	-0.12848					
	169 -> 173	0.43789					
	169 -> 174	0.22878					
	169 -> 175	-0.15426					
	170 -> 174	0.21800					
	170 -> 176	-0.17971					
	171 -> 174	0.14715					
	172 -> 176	0.15608					
17	168 -> 173	-0.28922	6.1667	201.05	0.7461	406.2533	407.6805
	168 -> 174	0.36254					
	169 -> 174	0.31220					
	169 -> 175	-0.16828					
	170 -> 173	0.16677					
	170 -> 174	-0.15902					
	171 -> 175	0.20091					
18	168 -> 173	-0.18956	6.1842	200.49	0.6234	290.6693	292.0323
	168 -> 174	-0.22102					
	169 -> 174	0.17764					
	169 -> 175	0.42853					
	170 -> 175	0.17541					
	170 -> 176	-0.18220					
	171 -> 174	-0.16237					
	171 -> 175	0.10252					
	172 -> 174	0.12300					
	172 -> 176	0.16252					
19	168 -> 173	0.32970	6.2291	199.04	0.0808	-12.7105	-12.1106
	168 -> 174	0.32171					
	169 -> 173	0.30285					
	169 -> 174	0.15258					
	169 -> 175	0.28180					
	169 -> 176	-0.10767					
	170 -> 173	-0.11424					
	170 -> 174	-0.16668					

	170 -> 175	0.11226					
20	168 -> 175	0.34005	6.2711	197.71	0.0582	-22.0180	-22.1873
	168 -> 178	-0.10010					
	169 -> 174	0.12615					
	169 -> 178	0.16234					
	170 -> 175	-0.17149					
	170 -> 177	0.18527					
	170 -> 178	0.45971					

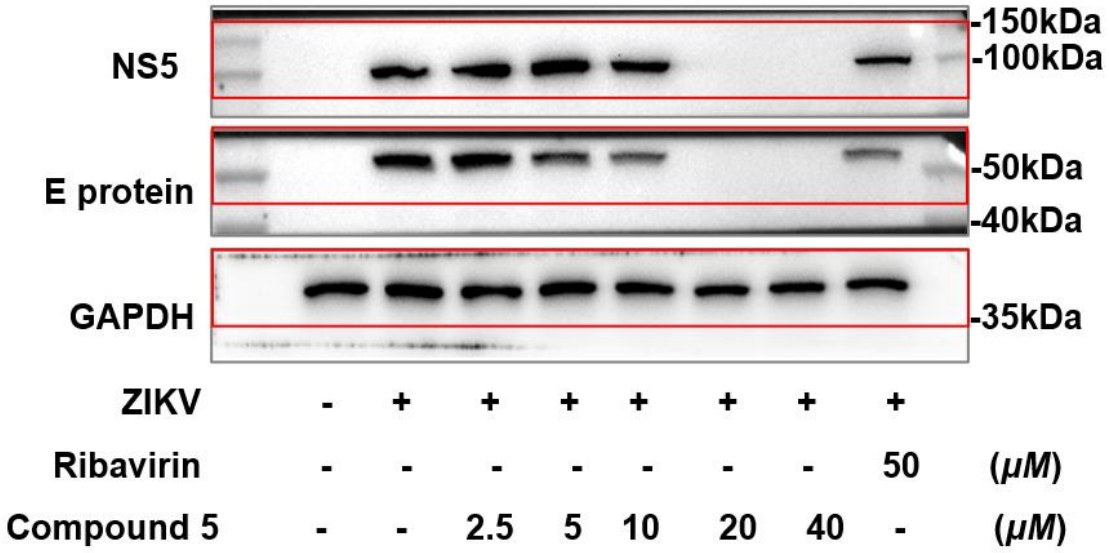

Figure S69. The full raw data of western blots (E and F) of compound **5**