Sarcanolides C–E: Three new lindenane sesquiterpenoid dimers with anti-inflammatory activities from *Sarcandra glabra*

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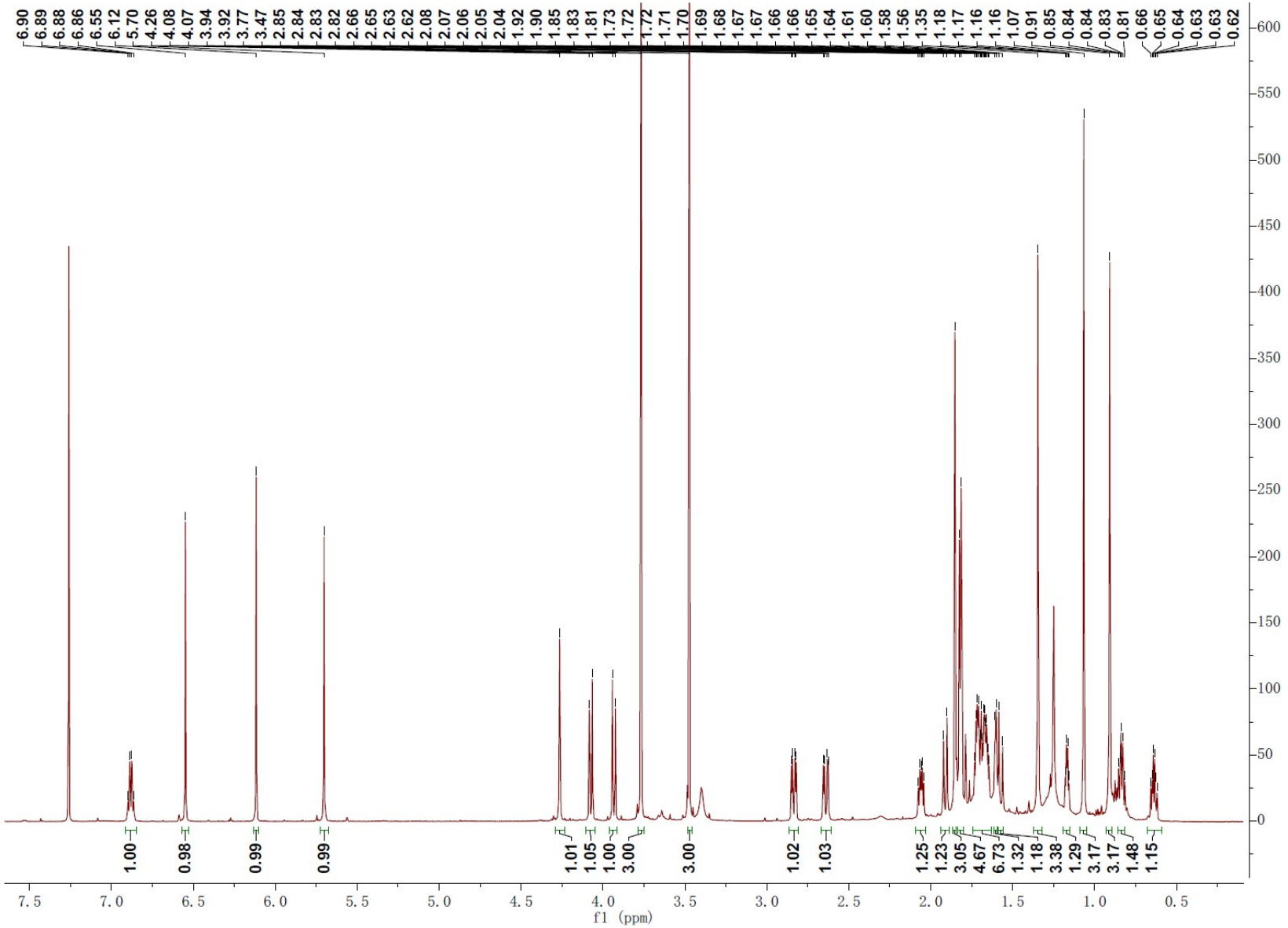

Fig. S1 ^{1}H NMR spectrum (600 MHz) of compound **1** in $CDCl_3$.

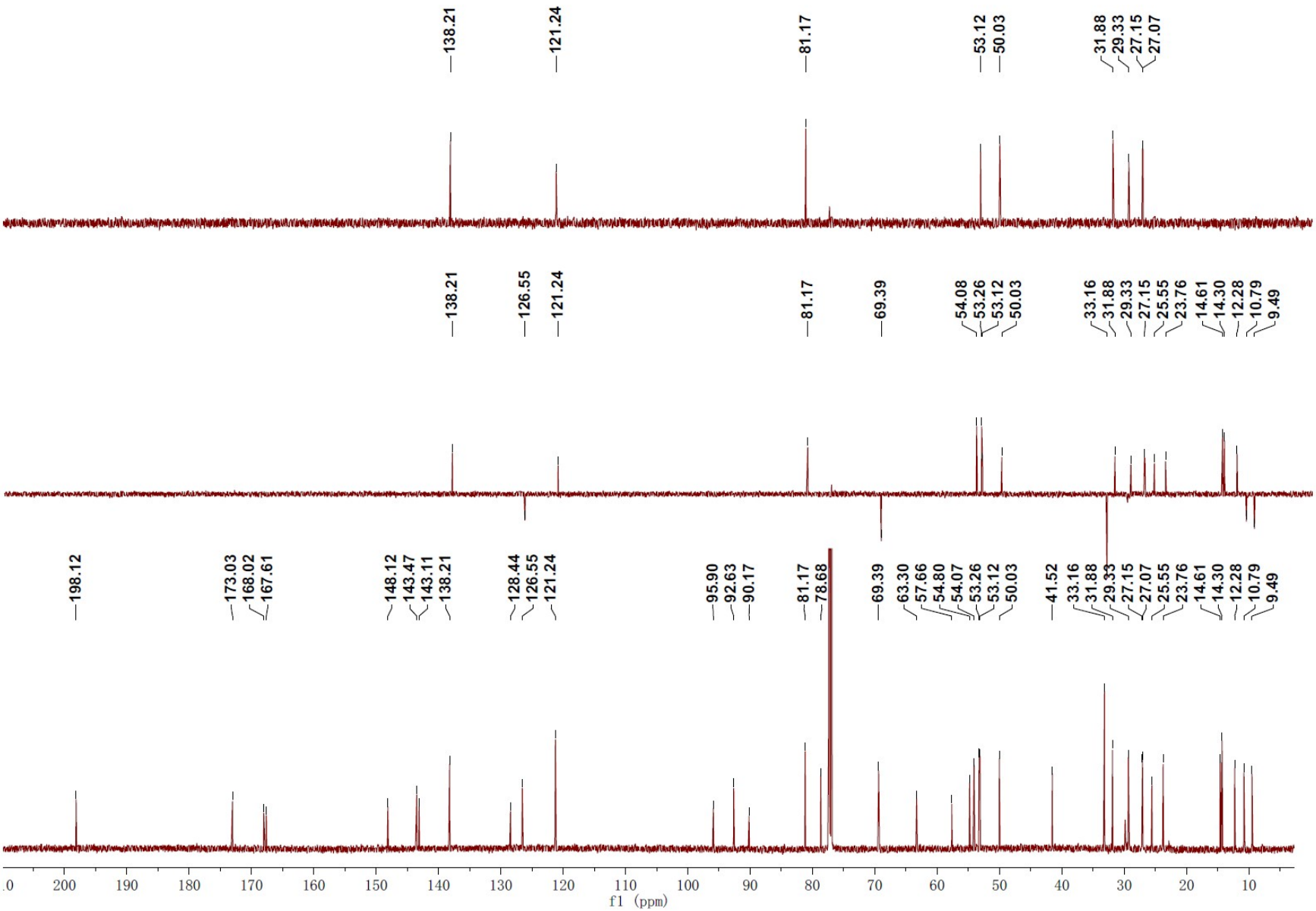

Fig. S2 ^{13}C NMR spectrum (150 MHz) of compound **1** in $CDCl_3$.

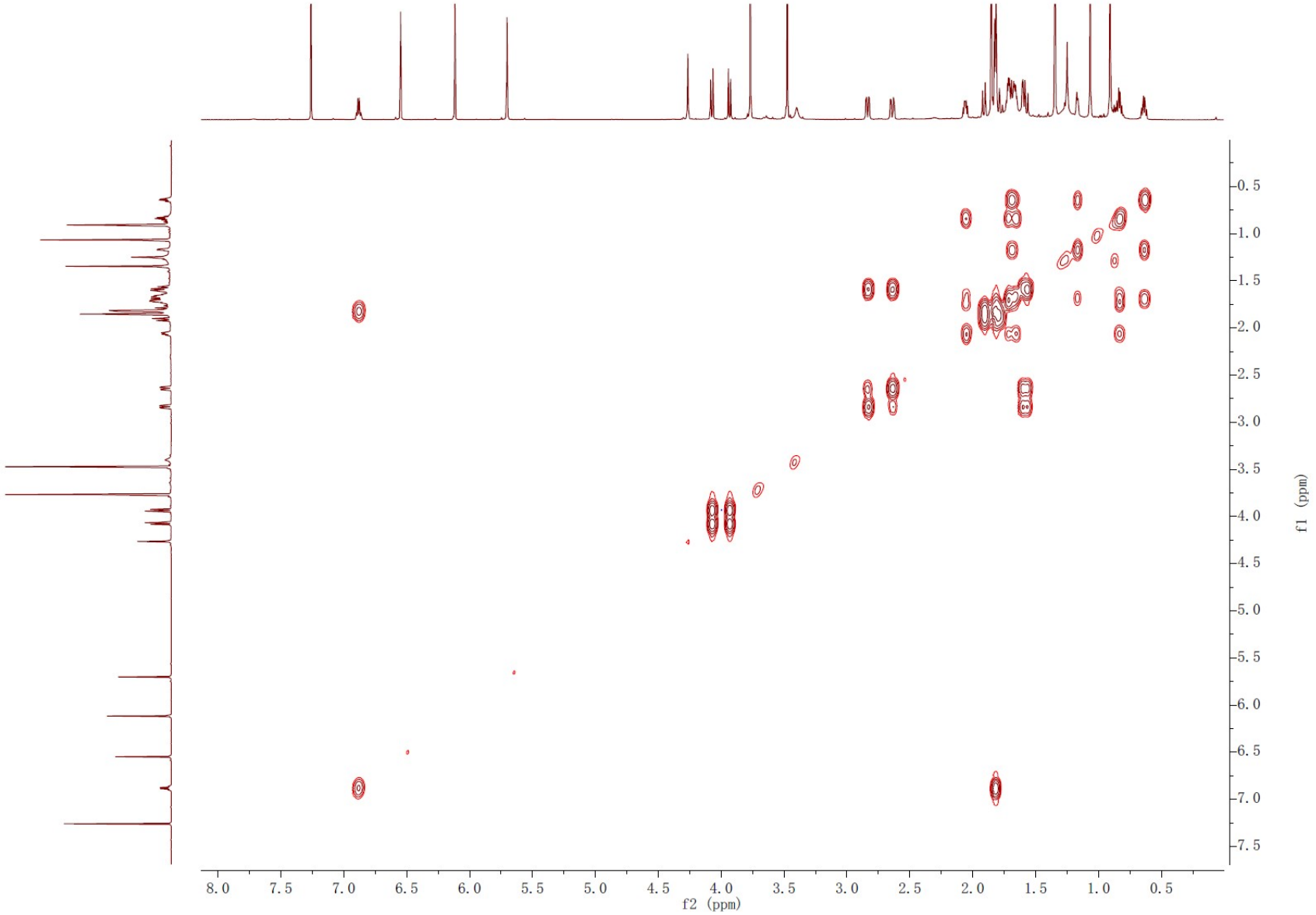

Fig. S3 ^{1}H–^{1}H COSY spectrum of compound **1** in $CDCl_3$.

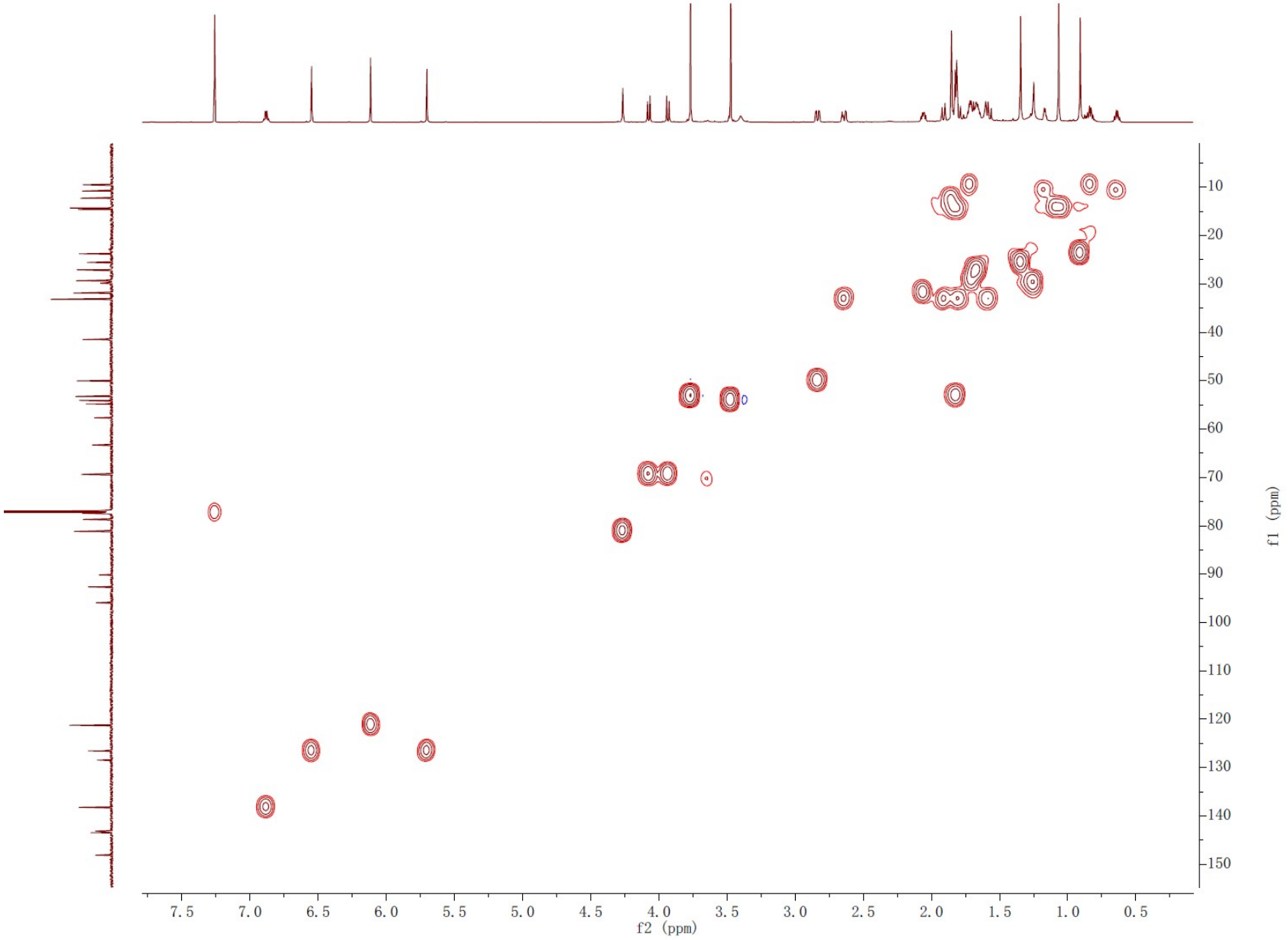

Fig. S4 HSQC spectrum of compound **1** in $CDCl_3$.

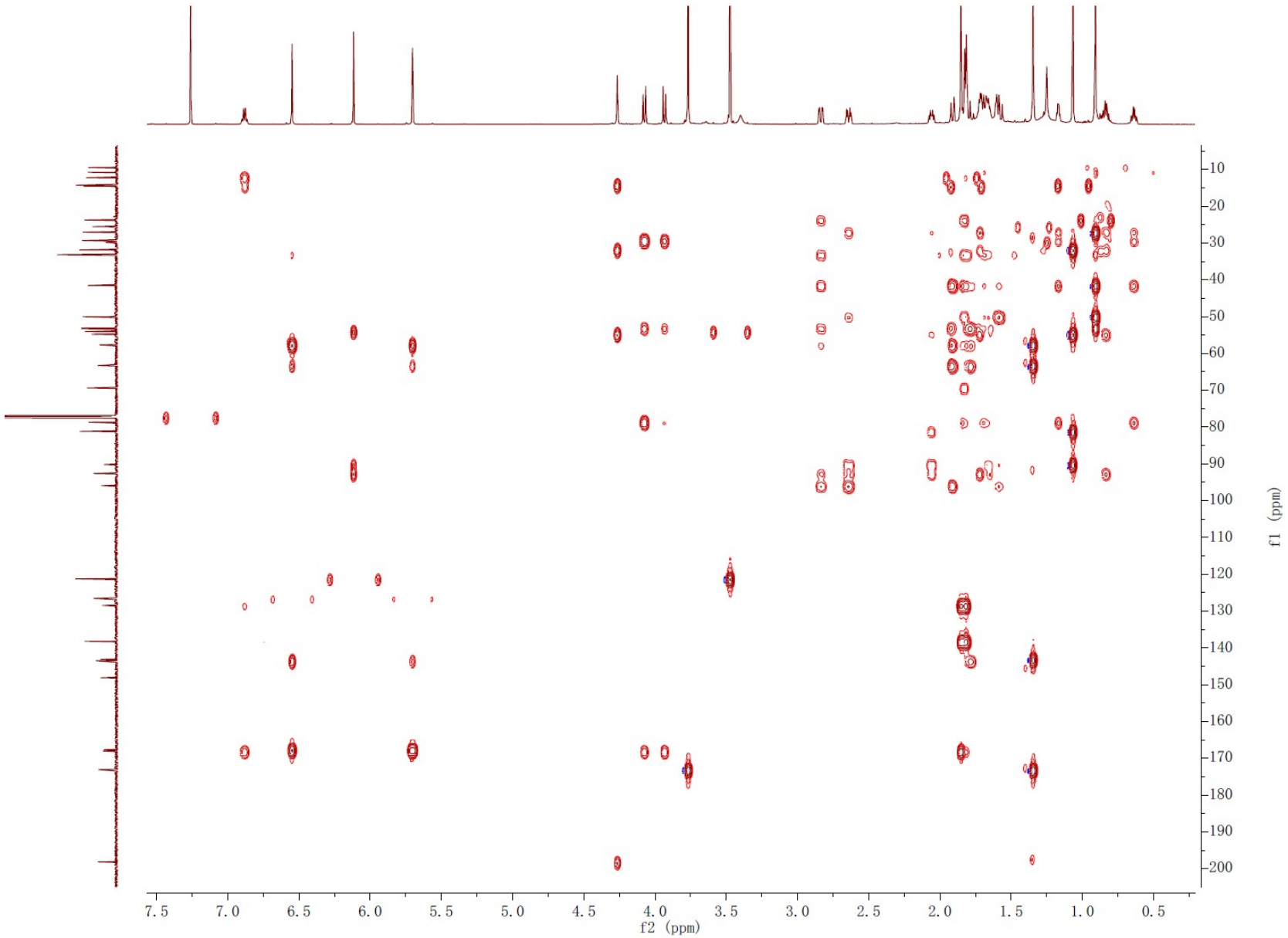

Fig. S5 HMBC spectrum of compound **1** in $CDCl_3$.

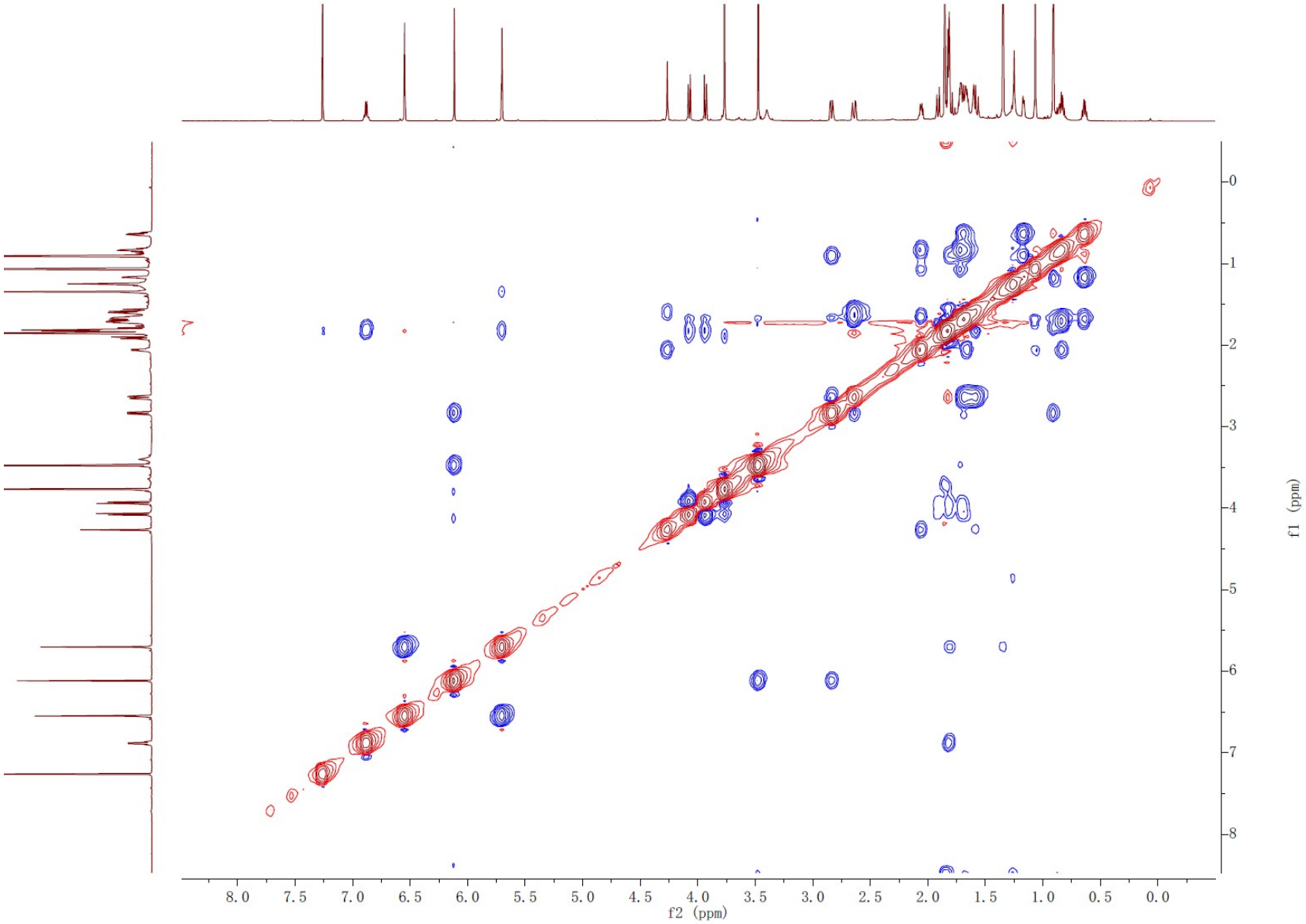

Fig. S6 ROESY spectrum of compound **1** in $CDCl_3$.

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
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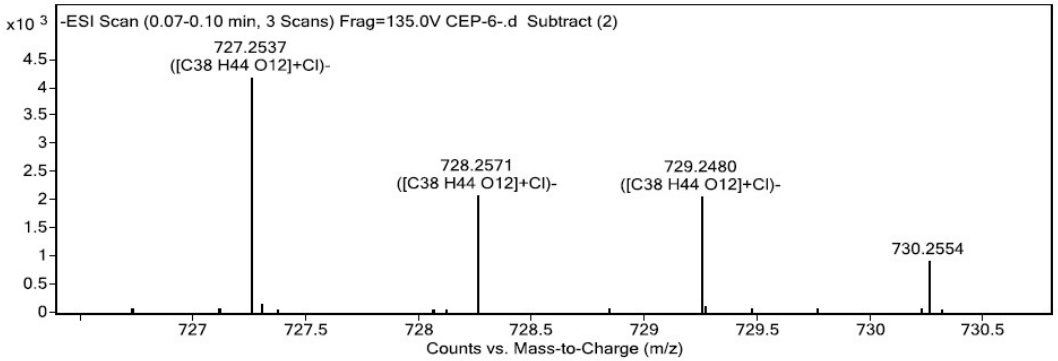

Peak List

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340.2361	1	23672.75		
375.275	1	5875.43		
403.3064	1	5329.96		
613.2284	1	4510.04		
681.2542	1	7694.38		
695.2703	1	11740.21		
696.274	1	4995.23		
709.2492	1	5317.38		
723.2644	1	9660.23		
727.2537	1	4187.47	C38 H44 O12	(M+Cl)-
737.2806	1	6794.96		
740.2577	1	6090.63		
754.2713	1	7473.97		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C38 H44 O12	692.2833	727.2527	727.2537	-1.00	-1.38	17.0000

Fig. S7 HRESI (+) MS spectrum of compound **1**.

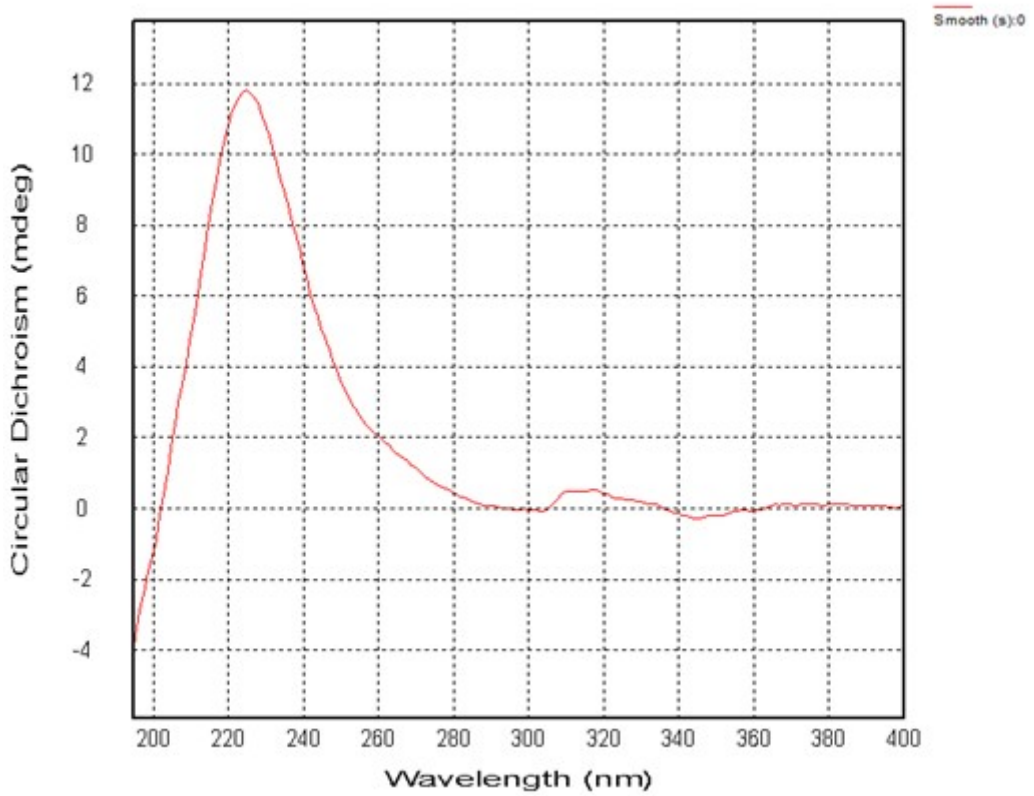
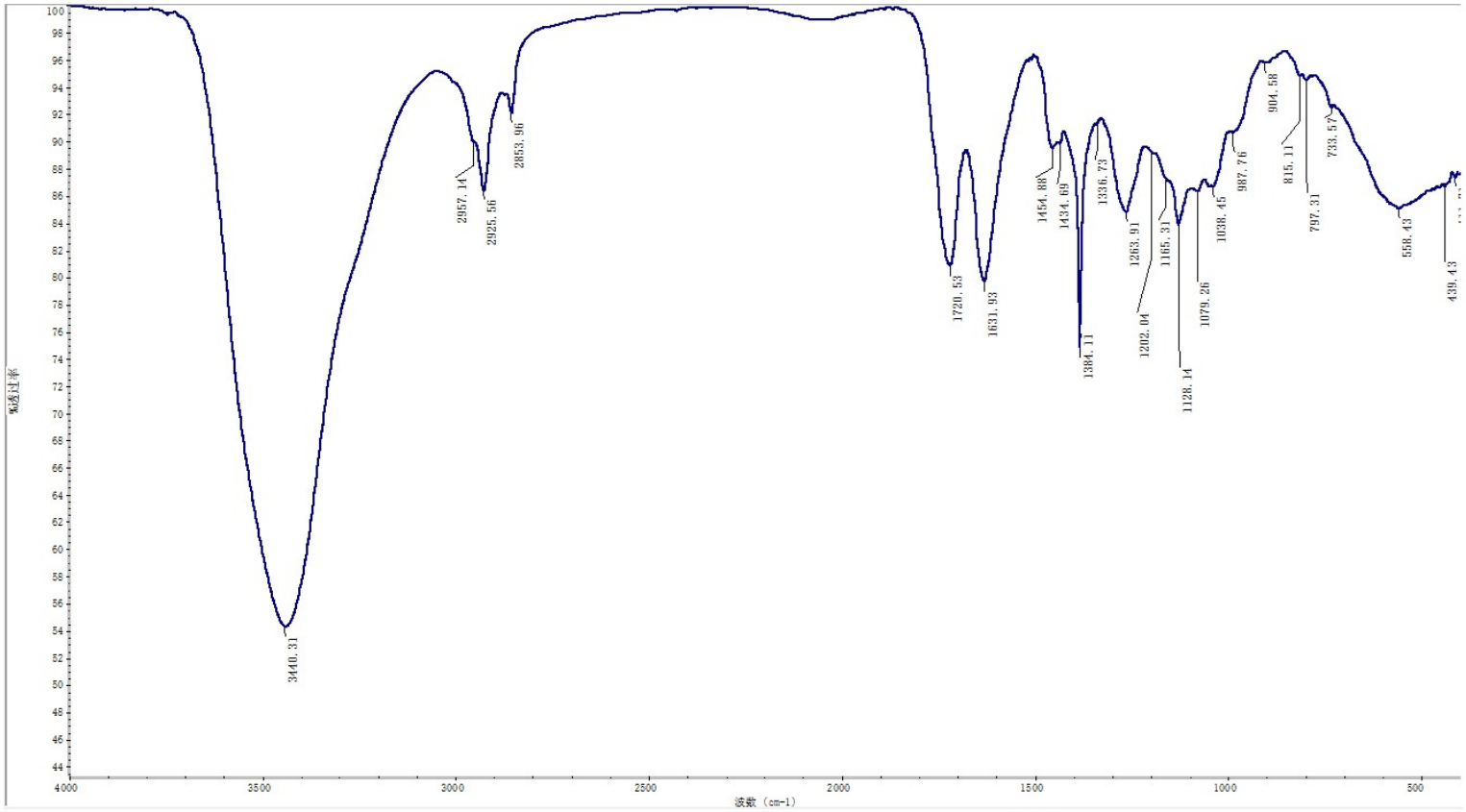


Fig. S8 CD spectrum of compound **1**.



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背景扫描次数: 16
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Fig. S9 IR spectrum of compound **1**.

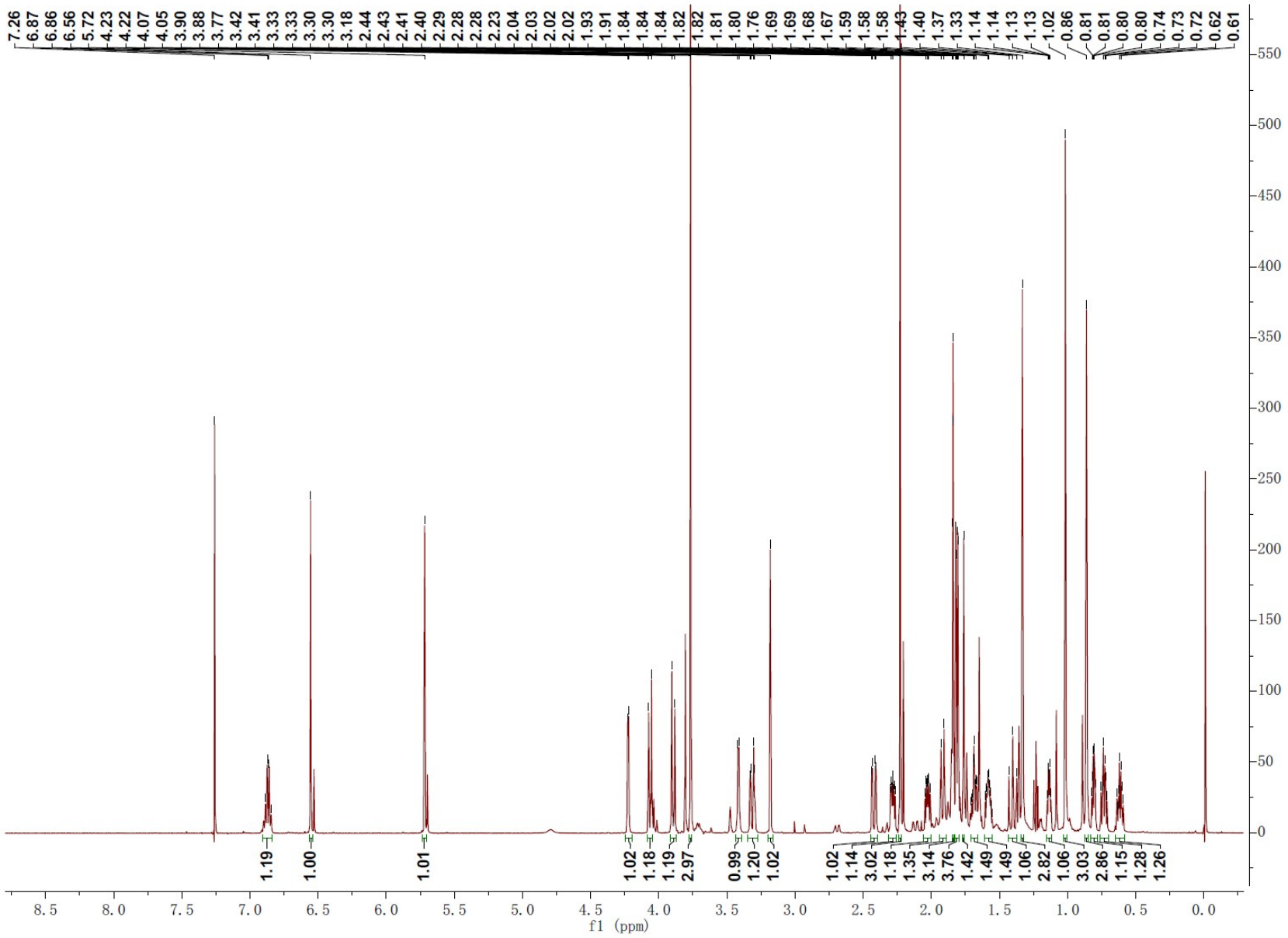

Fig. S10 ^{1}H NMR spectrum (500 MHz) of compound **2** in $CDCl_3$.

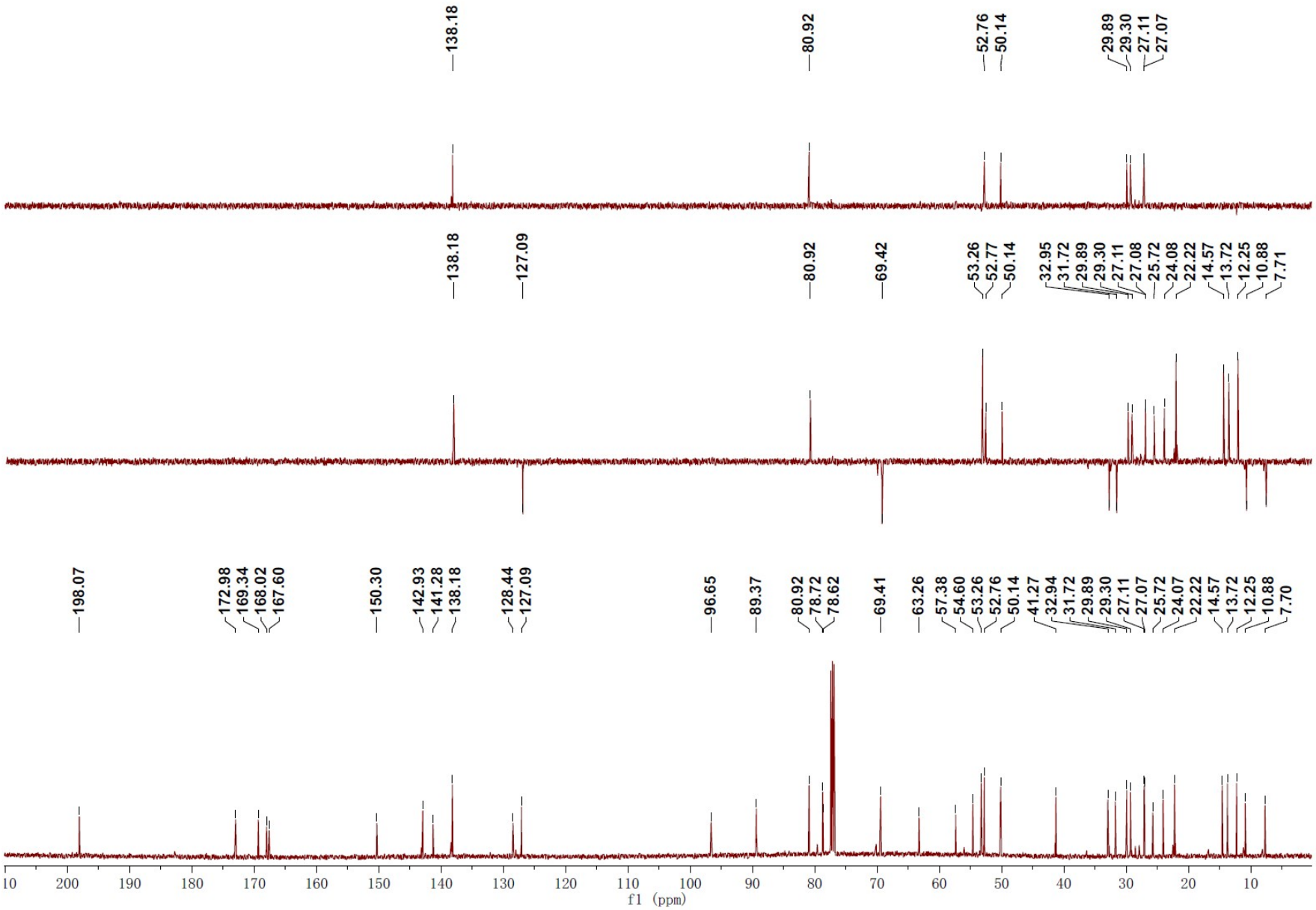

Fig. S11 ^{13}C NMR spectrum (125 MHz) of compound **2** in $CDCl_3$.

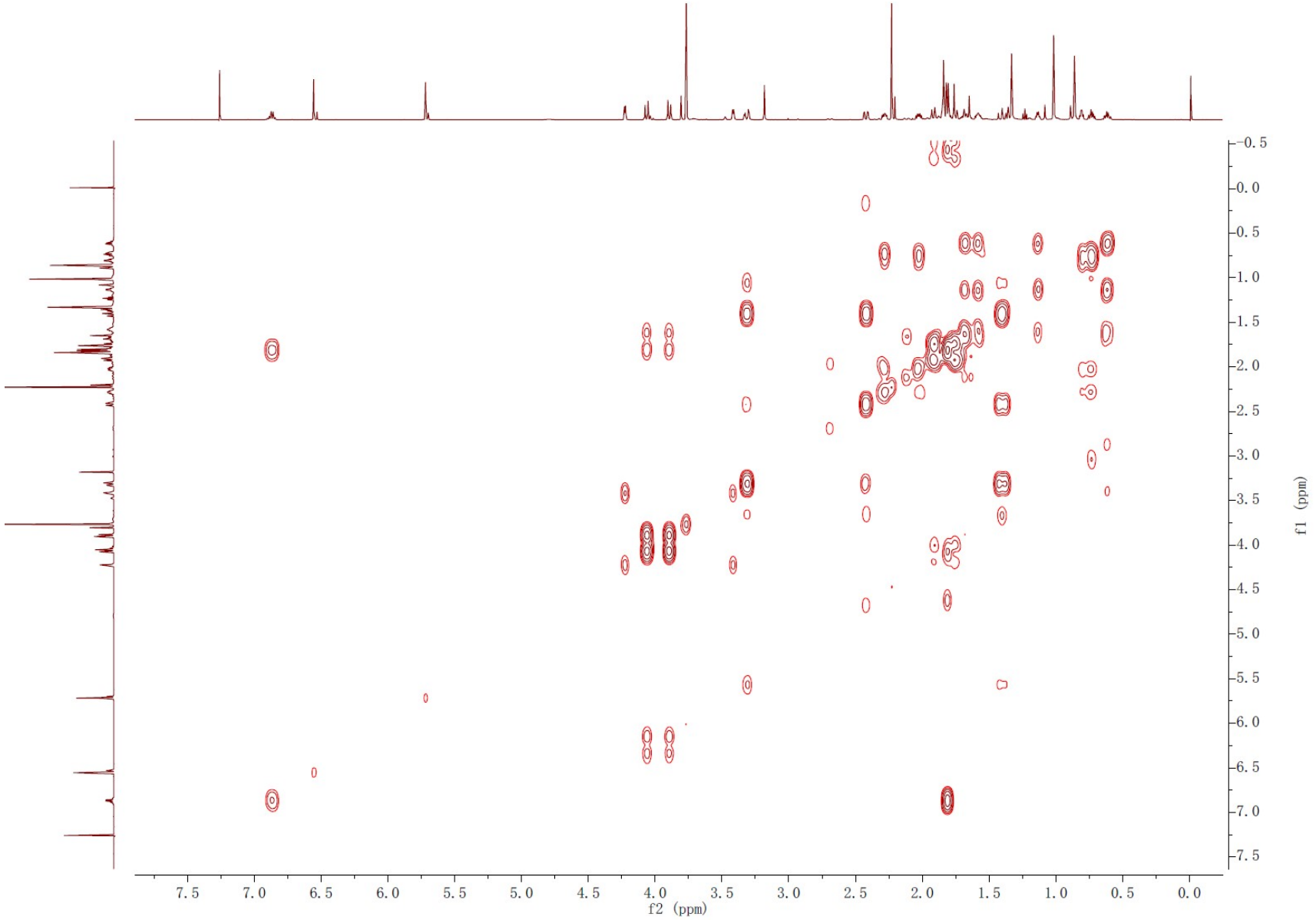

Fig. S12 ^{1}H–^{1}H COSY spectrum of compound **2** in $CDCl_3$.

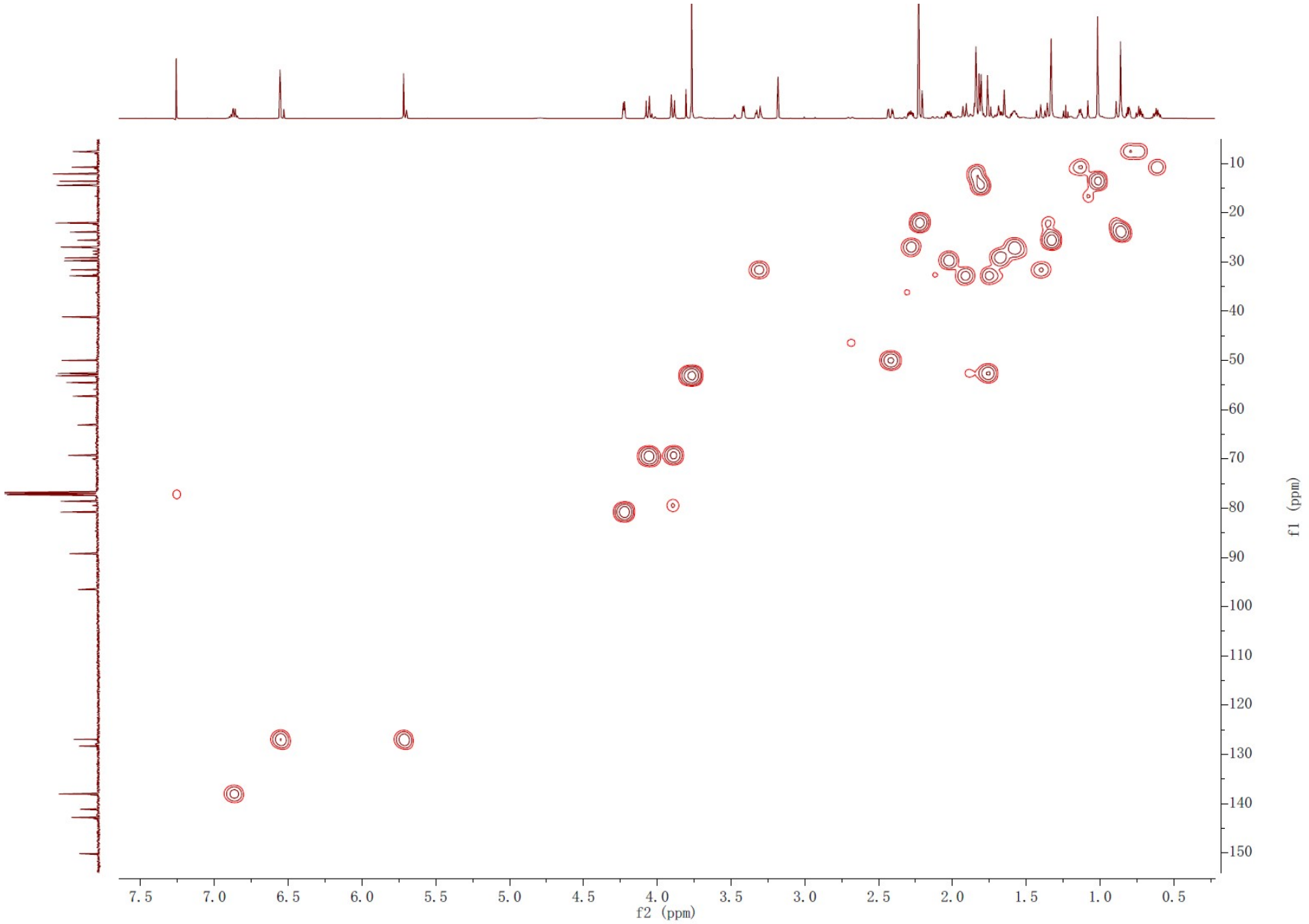

Fig. S13 HSQC spectrum of compound **2** in $CDCl_3$.

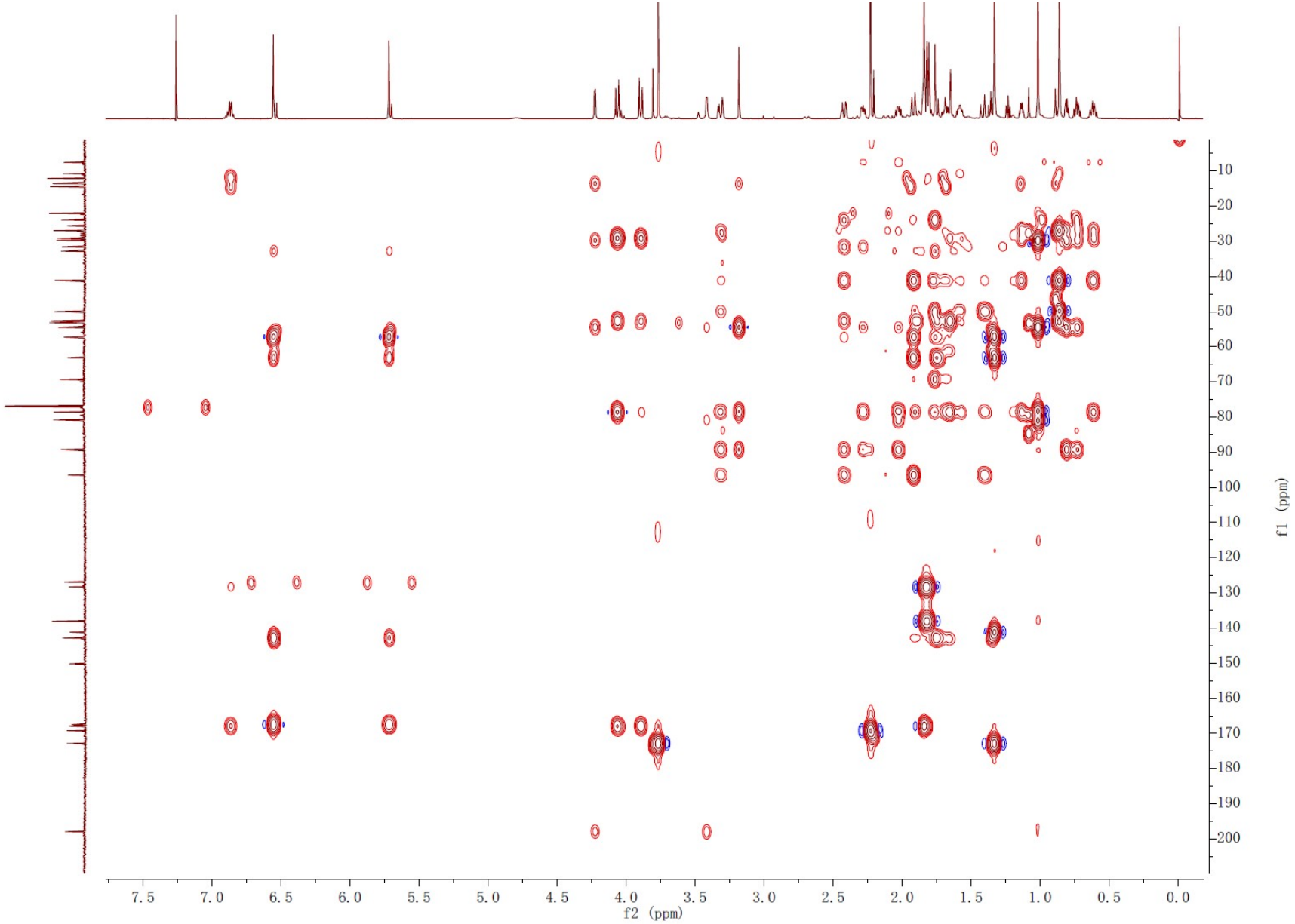

Fig. S14 HMBC spectrum of compound **2** in $CDCl_3$.

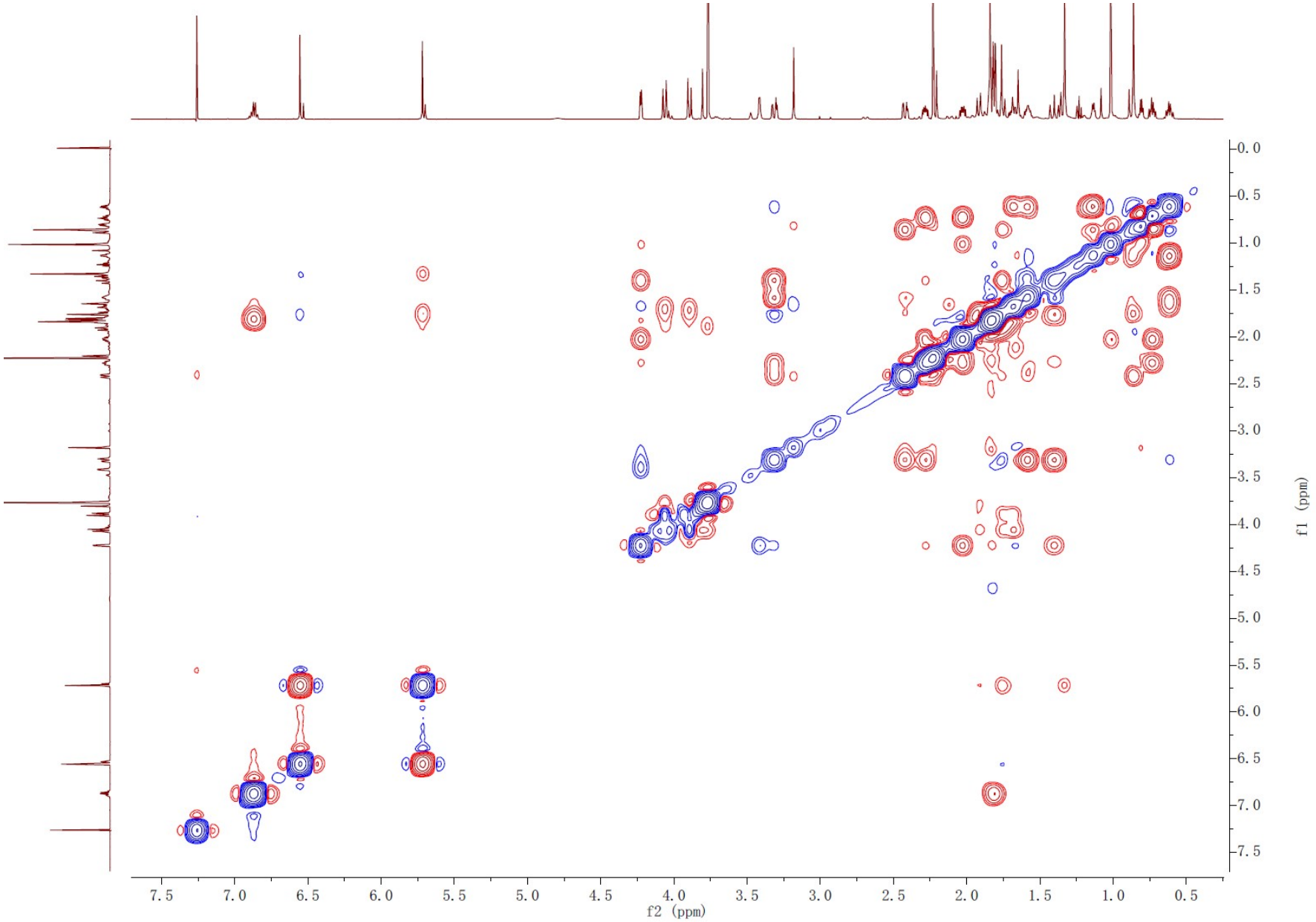

Fig. S15 ROESY spectrum of compound **2** in $CDCl_3$.

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
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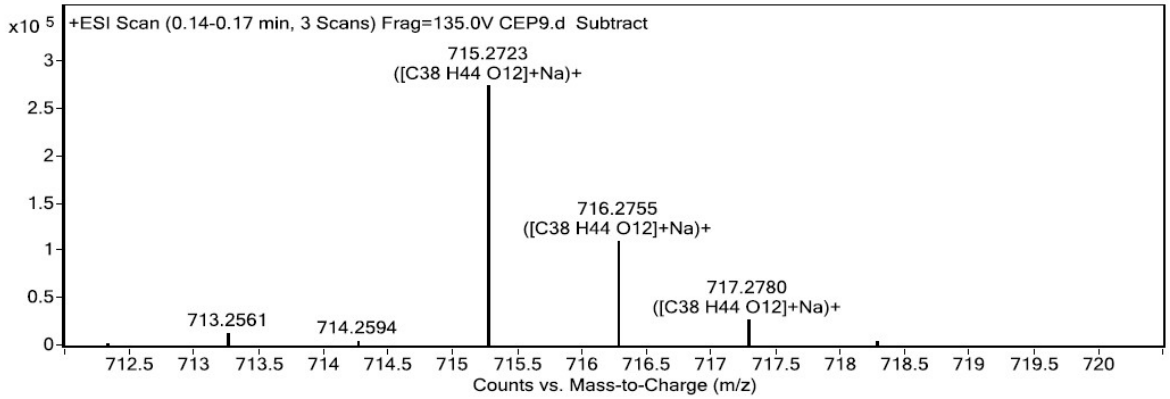

Peak List

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655.2505	1	29179.3		
710.3165	1	31586.91		
715.2723	1	275452.88	C38 H44 O12	(M+Na)+
716.2755	1	111275.16	C38 H44 O12	(M+Na)+
717.278	1	27890.61	C38 H44 O12	(M+Na)+
731.2462	1	62875.49		
1407.5551	1	311097.28		
1408.5584	1	252286.73		
1409.5608	1	114043.63		
1410.5632	1	35389.04		

Formula Calculator Element Limits

Element	Min	Max
C	3	120
H	0	240
O	0	50

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C38 H44 O12	692.2833	715.2725	715.2723	0.20	0.28	17.0000

Fig. S16 HRESI (+) MS spectrum of compound **2**.

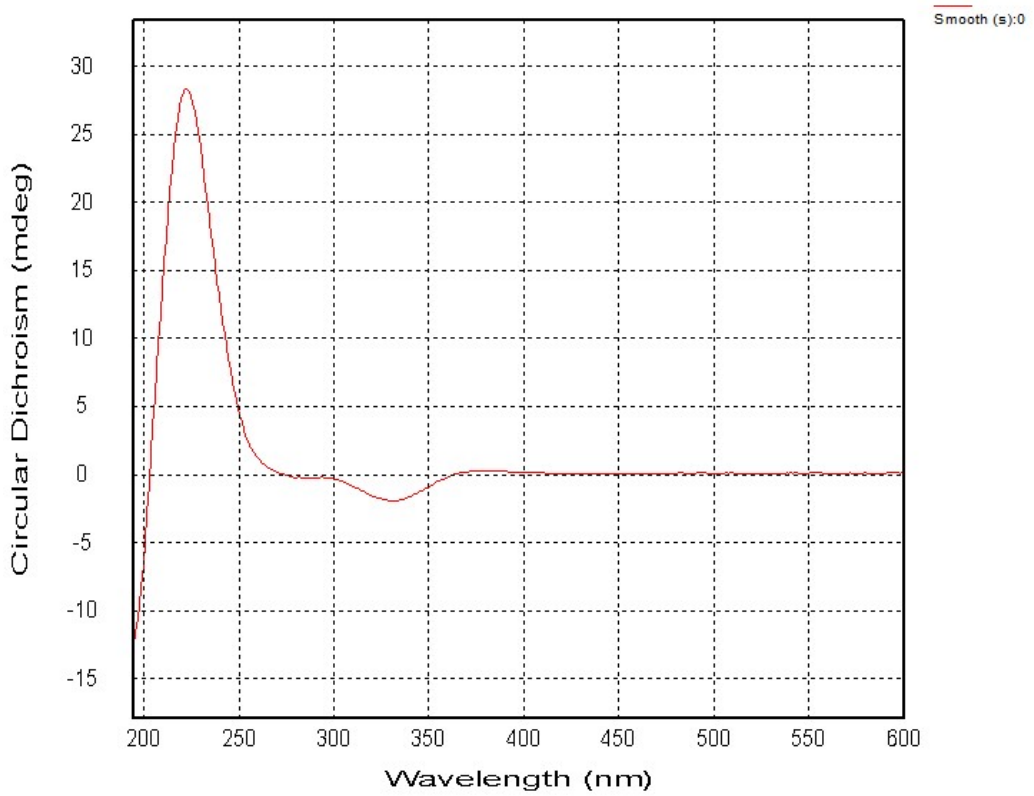

Fig. S17 CD spectrum of compound **2**.

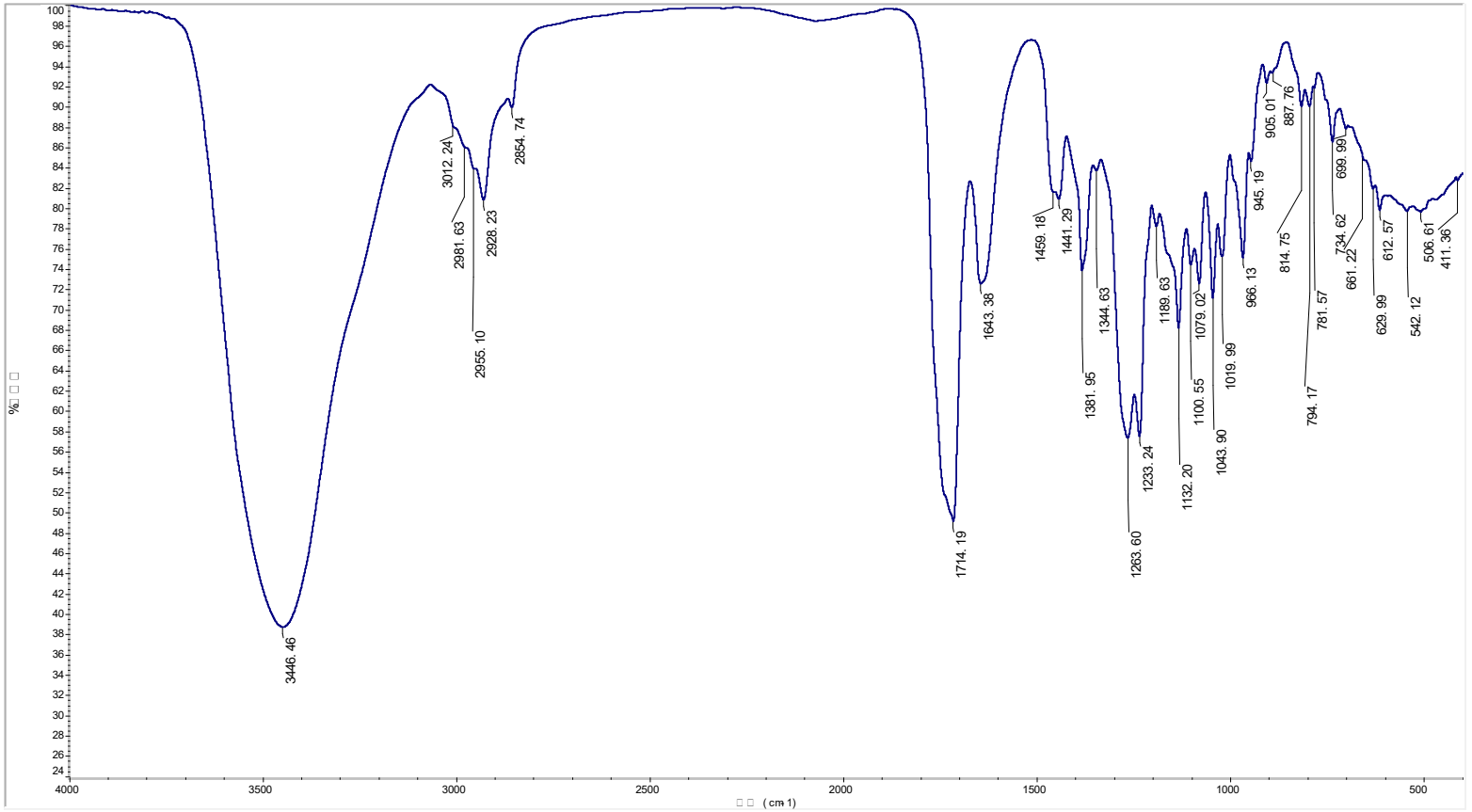

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Fig. S18 IR spectrum of compound **2**.

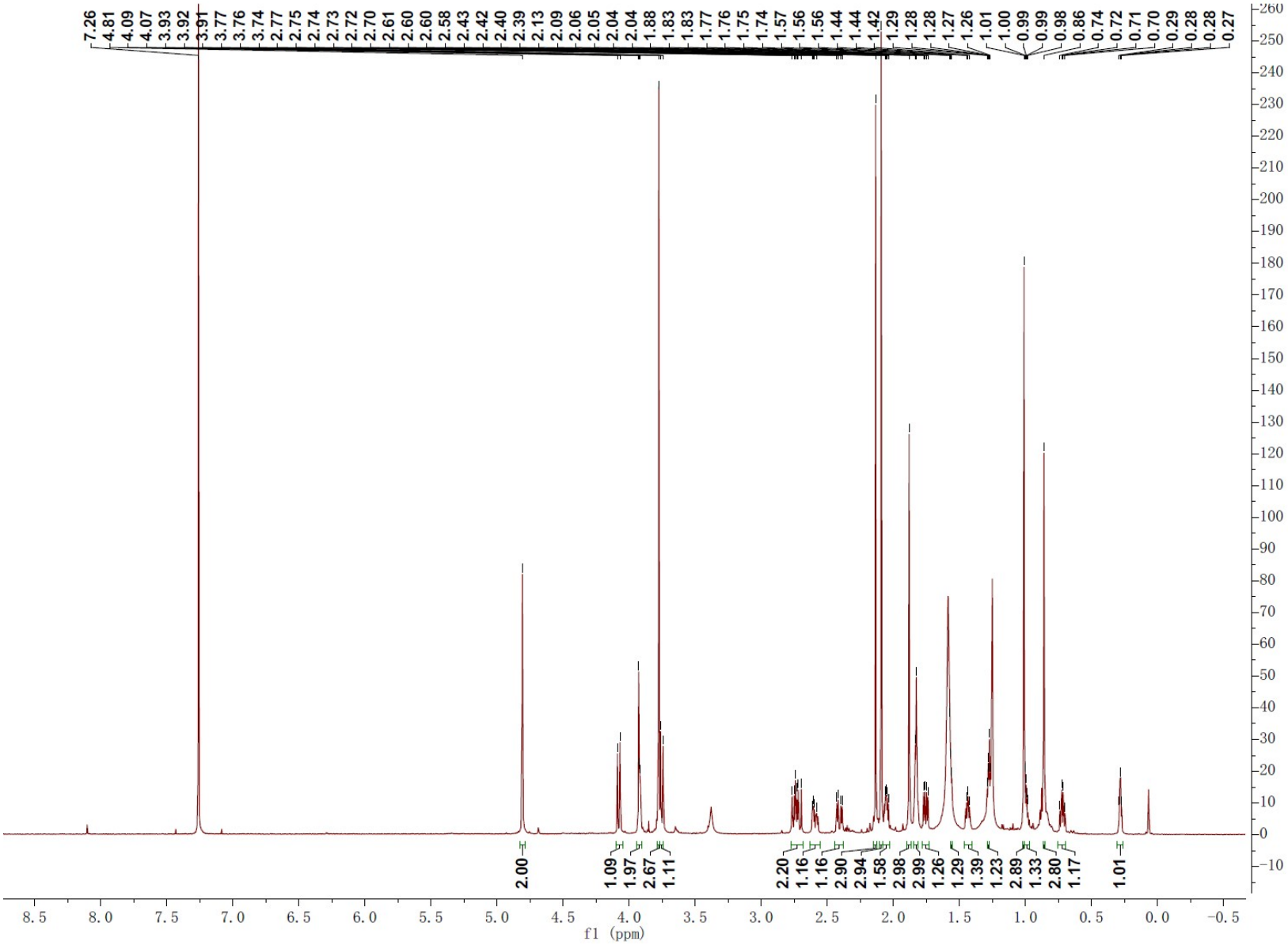

Fig. S19 ^{1}H NMR spectrum (600 MHz) of compound **3** in $CDCl_3$.

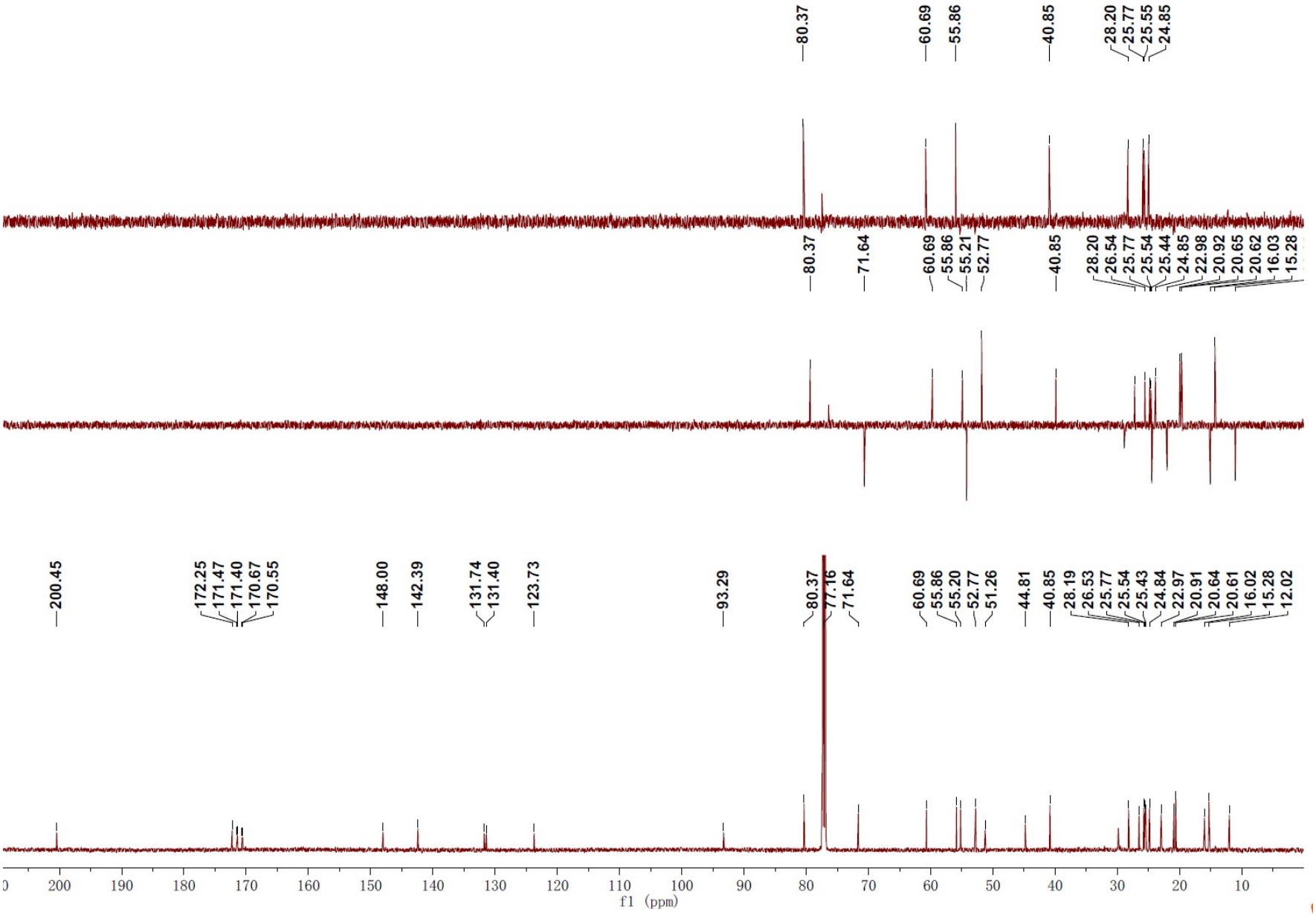

Fig. S20 ^{13}C NMR spectrum (150 MHz) of compound **3** in $CDCl_3$.

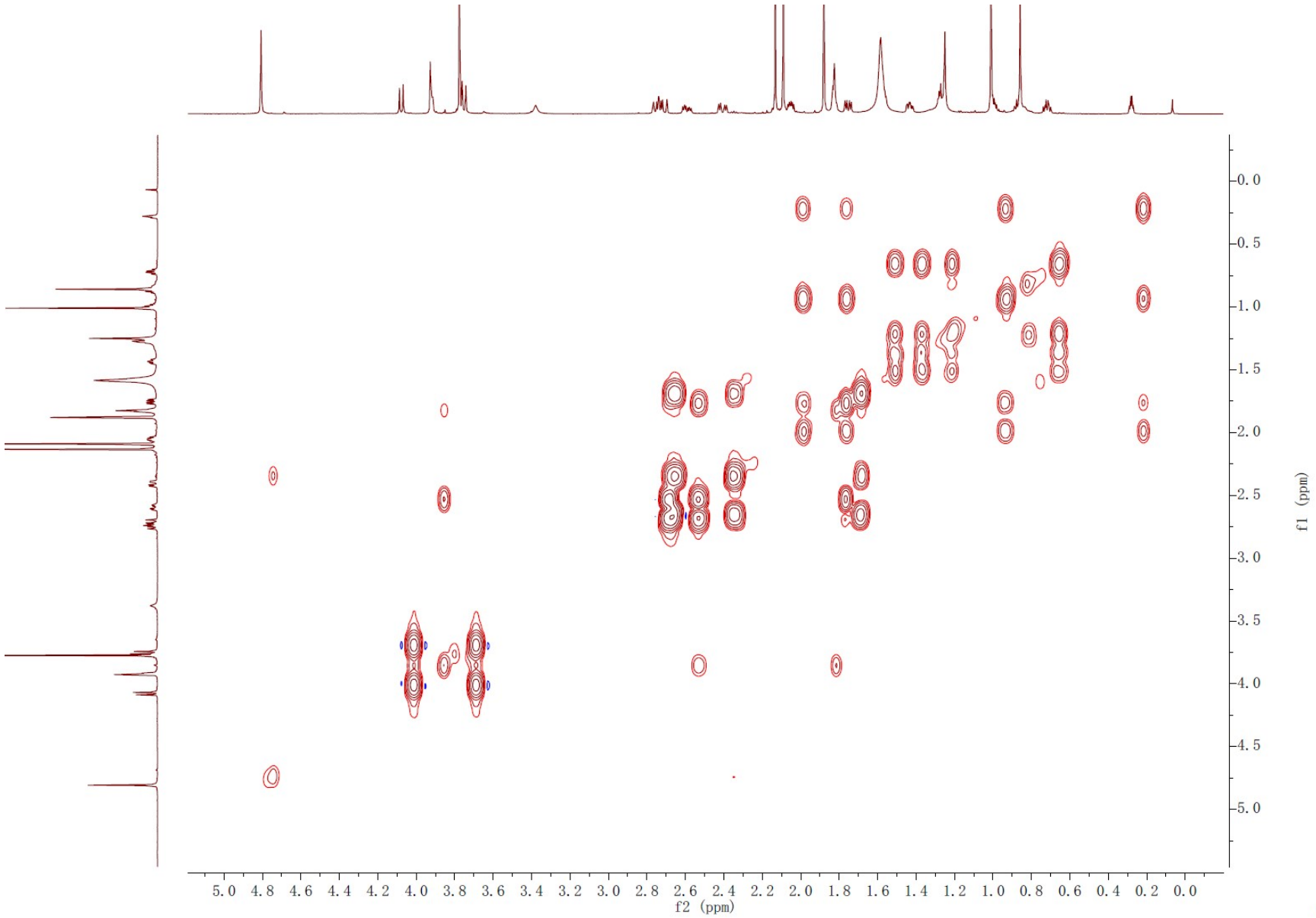

Fig. S21 ^{1}H–^{1}H COSY spectrum of compound **3** in $CDCl_3$.

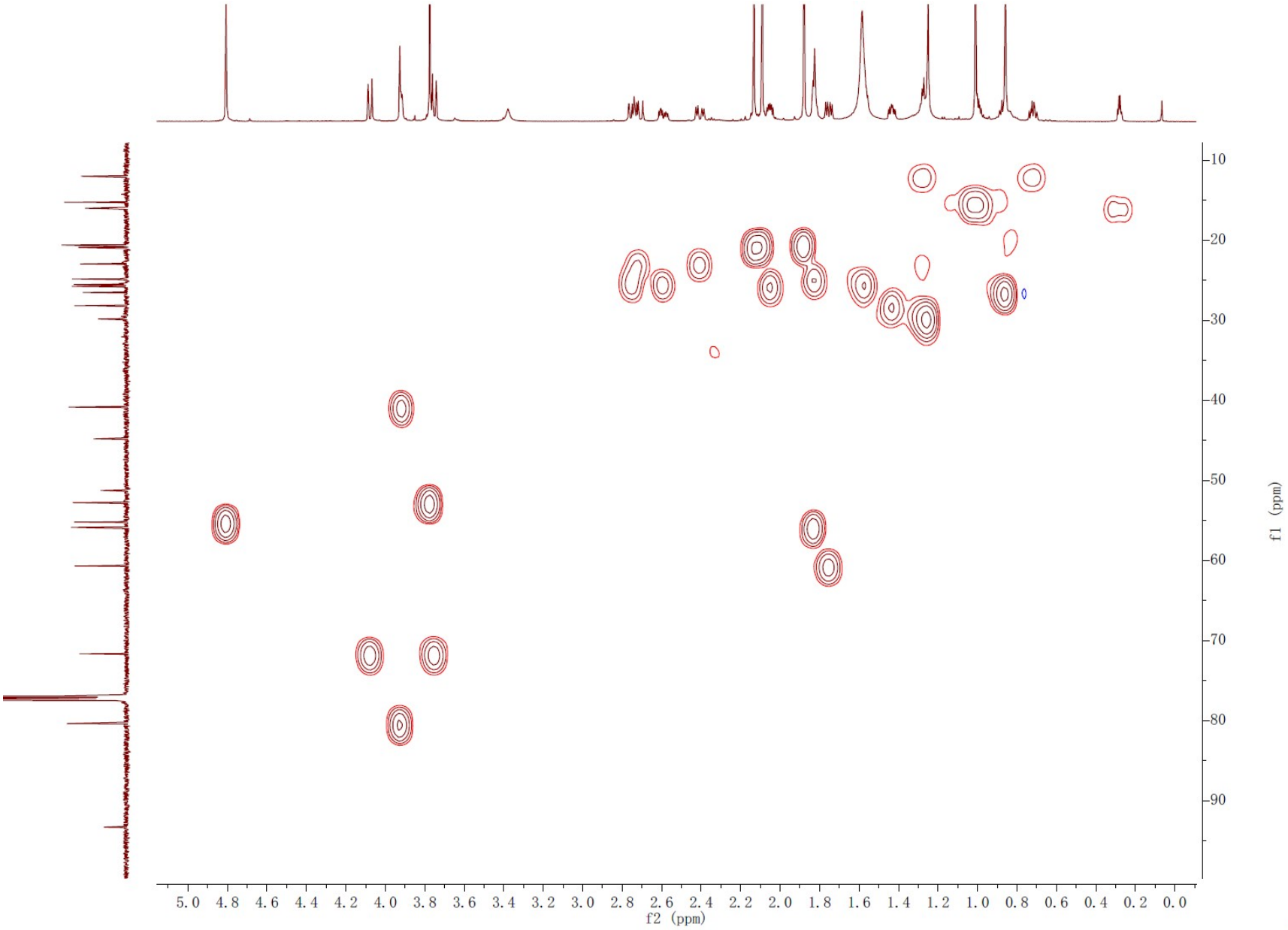

Fig. S22 HSQC spectrum of compound **3** in $CDCl_3$.

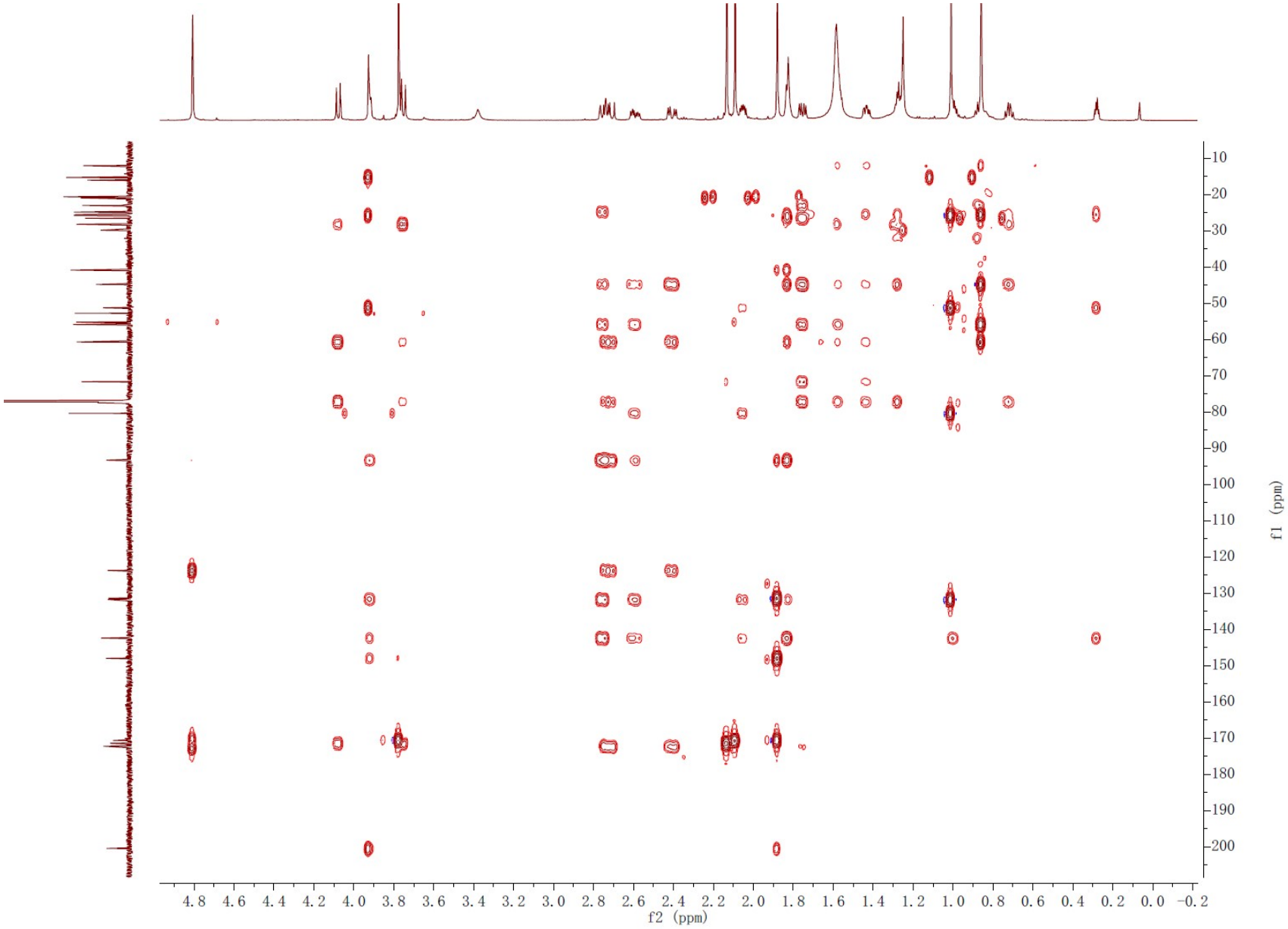

Fig. S23 HMBC spectrum of compound **3** in $CDCl_3$.

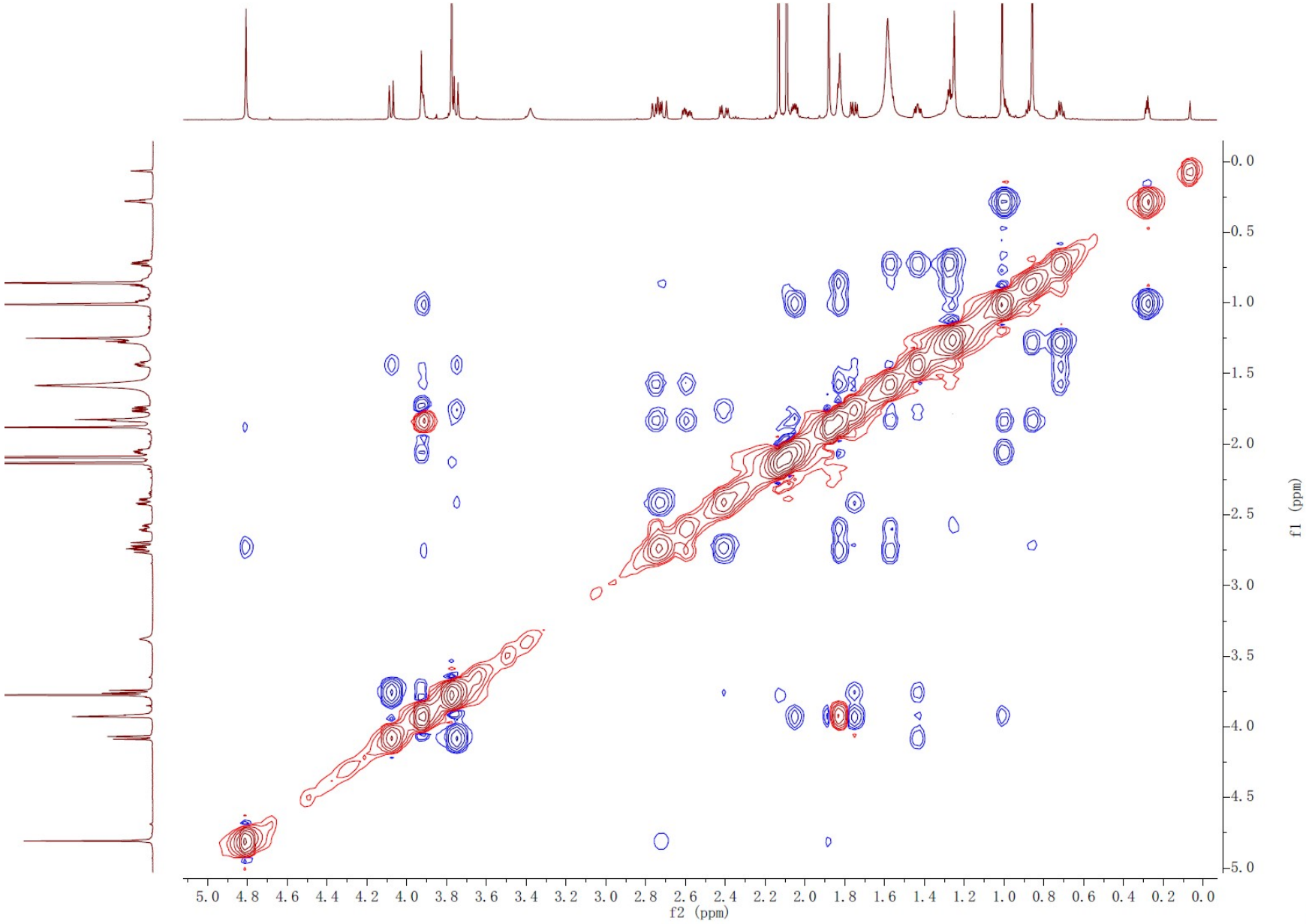

Fig. S24 ROESY spectrum of compound **3** in $CDCl_3$.

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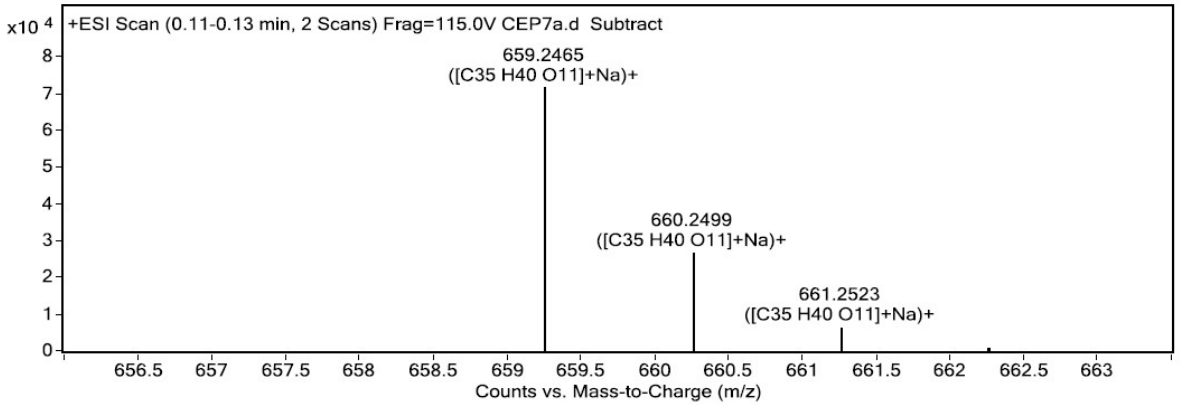

Peak List

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631.2507	1	5749.18		
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659.2465	1	71883.18	C35 H40 O11	(M+Na)+
660.2499	1	26964.39	C35 H40 O11	(M+Na)+
661.2523	1	6738.39	C35 H40 O11	(M+Na)+
675.2205	1	23385.72		
676.2236	1	8955.44		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
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Fig. S25 HRESI (+) MS spectrum of compound **3**.

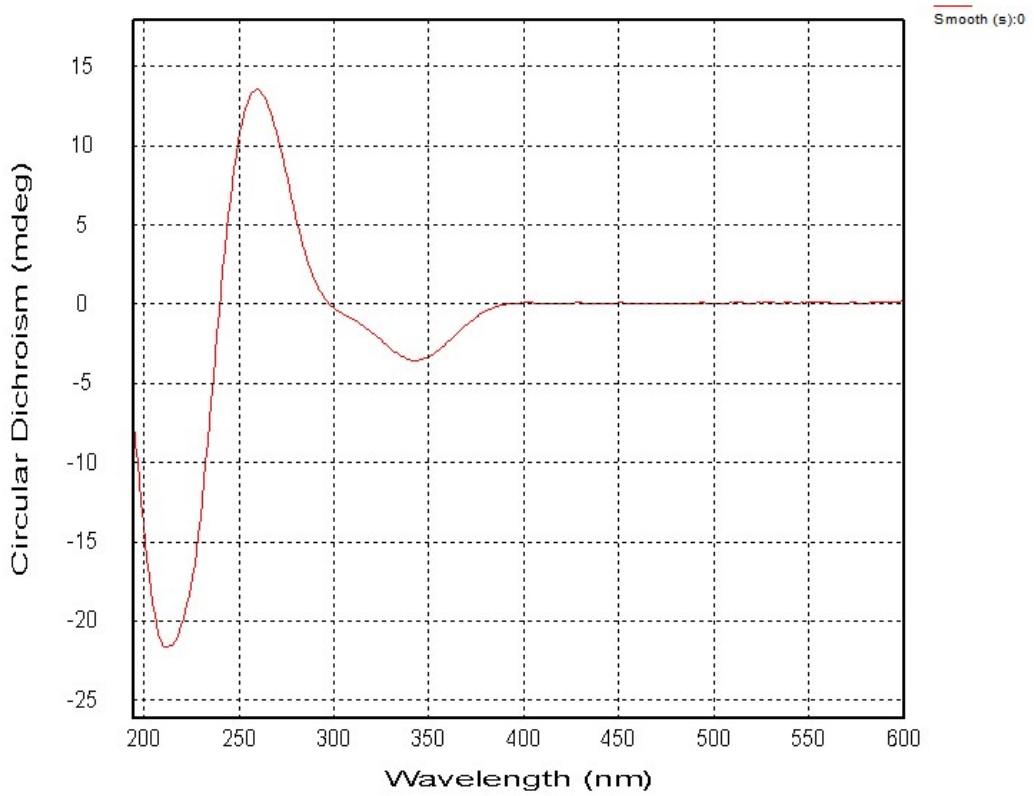

Fig. S26 CD spectrum of compound **3**.

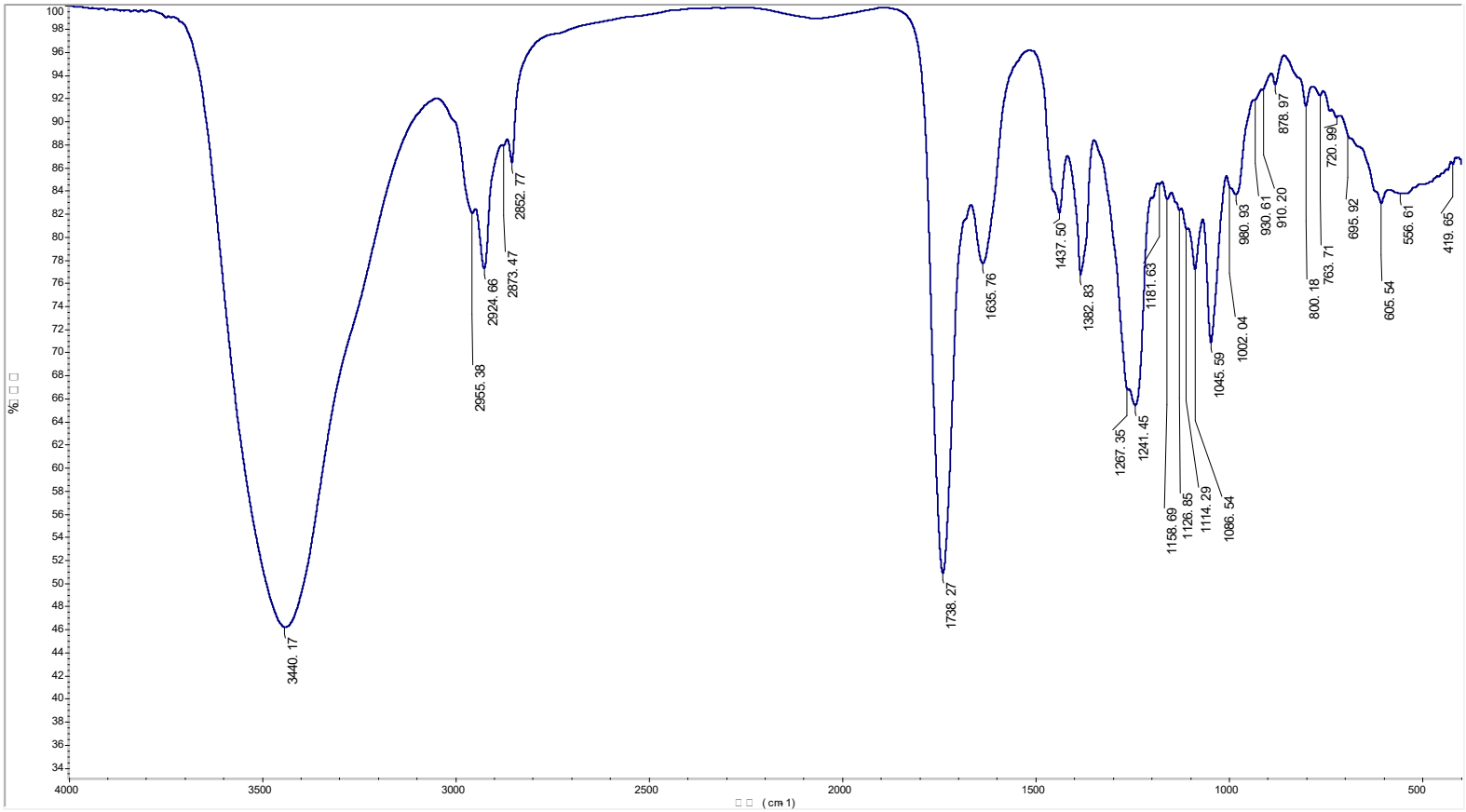

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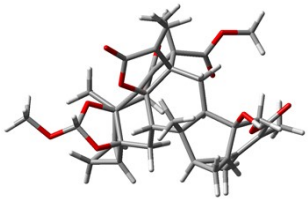
Fig. S27 IR spectrum of compound **3**.

Table S1 Standard orientations of **1a** (1*R*,3*S*,4*S*,5*S*,9*R*,10*R*,11*R*,1′*R*,3′*S*,4′*S*,5′*R*,7′*R*,8′*R*,9′*S*,10′*S*,1‴*S*)-**1** at B3LYP/6–311+G(2d,p) level in methanol.

Conformation **1a-1**



SCF Energy (B3LYP): −2377.125183 Hartree

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2	6	0	-2.491608	0.816507	-0.077633
3	6	0	-1.446864	0.006434	0.650748
4	6	0	-0.737642	0.421485	1.706274
5	6	0	-0.834632	1.818746	2.154425
6	6	0	-1.220435	2.777229	1.042264
7	6	0	-2.244616	0.737368	-1.621132
8	6	0	-0.898596	0.084301	-1.960411
9	6	0	-0.761925	-1.345689	-1.386548
10	6	0	-1.036851	-1.369860	0.177921
11	6	0	-2.600210	3.106452	-0.993385
12	6	0	-2.364952	2.159107	-2.153747
13	6	0	-3.701261	2.842137	-1.978754
14	8	0	-0.572390	2.233848	3.277959
15	8	0	-1.295572	4.095771	1.529942
16	6	0	0.553097	-2.093069	-1.761728
17	1	0	-1.597514	-1.908415	-1.812426
18	6	0	0.089043	-1.843919	1.235966
19	6	0	1.472651	-2.235227	0.609698
20	6	0	1.660341	-1.626481	-0.771769
21	6	0	0.190514	-0.612810	2.298523
22	6	0	-0.263161	-0.955389	3.736980
23	8	0	-2.169041	-2.284758	0.373832
24	6	0	-0.567103	-3.062546	1.853009
25	6	0	-1.953409	-3.205207	1.344062
26	6	0	-0.045849	-3.979837	2.672417
27	8	0	-2.804824	-4.007228	1.662976
28	6	0	1.171685	-1.717616	-3.135455
29	6	0	2.668154	-1.523100	-2.959689
30	6	0	3.015865	-1.823923	-1.489206
31	6	0	2.144939	-2.661350	-3.798476
32	8	0	3.458588	-3.171574	-1.262567
33	6	0	0.248932	-3.610114	-1.696178
34	8	0	-3.758647	0.168999	0.109707
35	1	0	1.564417	-0.536063	-0.690255

36	8	0	-3.291117	-0.140557	-2.094813
37	6	0	-4.221074	-0.414643	-1.095476
38	8	0	-5.452422	0.119913	-1.472902
39	1	0	-4.317685	-1.498449	-0.947259
40	6	0	4.132108	-0.921007	-0.949452
41	8	0	3.777072	0.457672	-1.155403
42	6	0	4.462783	1.378792	-0.438722
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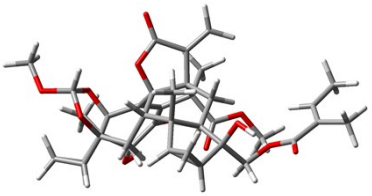
52	8	0	2.390267	-0.551870	3.261437
53	6	0	3.704296	0.033286	3.425583
54	1	0	-0.406565	2.714419	0.302003
55	1	0	-0.828603	0.041700	-3.049655
56	1	0	-0.093422	0.747009	-1.619914
57	1	0	-2.148744	4.094772	-0.991285
58	1	0	-1.734527	2.436317	-2.994066
59	1	0	-3.929343	3.642174	-2.677918
60	1	0	-4.556881	2.236976	-1.697901
61	1	0	-1.077968	4.030313	2.481926
62	1	0	1.528991	-3.321700	0.533058
63	1	0	2.280355	-1.952726	1.288848
64	1	0	0.364026	-1.729757	4.181237
65	1	0	-0.198325	-0.056031	4.354437
66	1	0	-1.300167	-1.300285	3.742843
67	1	0	-0.655028	-4.815042	3.005753
68	1	0	0.978415	-3.931932	3.028961
69	1	0	0.623909	-1.062766	-3.803109
70	1	0	3.193076	-0.705497	-3.444824
71	1	0	2.255693	-2.564422	-4.875472
72	1	0	2.258747	-3.675298	-3.432179
73	1	0	4.140675	-3.372662	-1.924860
74	1	0	-0.308692	-3.885627	-0.796800
75	1	0	-0.367230	-3.893719	-2.556644
76	1	0	1.159217	-4.212275	-1.708403
77	1	0	4.292299	-1.109909	0.113629
78	1	0	5.071184	-1.128414	-1.476432
79	1	0	2.757402	2.221659	-2.229562
80	1	0	5.825868	3.734424	0.080408
81	1	0	4.425959	4.816221	-0.033299
82	1	0	4.516073	3.591353	1.243986

83	1	0	1.541857	4.427496	-1.980752
84	1	0	3.051750	5.233861	-1.513761
85	1	0	2.845205	4.575080	-3.148845
86	1	0	-7.453544	0.042493	-1.145300
87	1	0	-6.583116	-1.436824	-0.652596
88	1	0	-6.478788	0.039667	0.350977
89	1	0	-3.693544	2.058629	2.187536
90	1	0	-3.718552	3.707477	1.534315
91	1	0	-4.682938	2.425344	0.770248
92	1	0	4.212015	-0.604286	4.148021
93	1	0	4.241006	0.055747	2.475775
94	1	0	3.606696	1.049986	3.813596

Conformation **1a-2**



SCF Energy (B3LYP): −2377.124003 Hartree

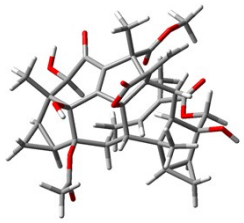
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.970417	0.500948	0.937087
2	6	0	0.945512	1.801470	0.028656
3	6	0	-0.380231	-0.278967	1.346347
4	6	0	1.720657	1.573680	-1.290676
5	6	0	-0.486965	2.408558	-0.107227
6	1	0	1.549667	2.522017	0.586660
7	6	0	1.840852	-0.560401	0.299665
8	8	0	1.592865	0.909337	2.203424
9	6	0	-1.711032	0.375972	0.846700
10	6	0	-0.169421	-1.792380	0.788209
11	6	0	-0.318914	-0.215761	2.861146
12	6	0	3.161119	1.098145	-1.048152
13	1	0	1.783975	2.515815	-1.839430
14	1	0	1.217709	0.856392	-1.951052
15	6	0	-0.769089	3.187328	1.200786
16	6	0	-0.714590	3.306316	-1.354425
17	6	0	-1.489835	1.248964	-0.378636
18	6	0	3.215885	-0.238955	-0.233095
19	6	0	1.214421	-1.736432	0.179578
20	6	0	0.935791	0.447247	3.293306
21	1	0	-2.132496	0.984325	1.648388
22	1	0	-2.452657	-0.402423	0.650959
23	6	0	-0.246795	-2.898785	1.861546
24	6	0	-1.127045	-2.119806	-0.380984
25	6	0	-1.242519	-0.559370	3.763393

26	6	0	3.934817	0.852880	-2.336909
27	8	0	3.801511	2.058689	-0.177842
28	1	0	-0.504692	2.608451	2.090729
29	1	0	-0.162642	4.099927	1.218493
30	1	0	-1.819756	3.466298	1.292708
31	6	0	-1.840443	4.312281	-1.376160
32	6	0	-2.053077	2.947858	-1.975729
33	1	0	0.124768	3.531306	-2.001667
34	6	0	-2.721585	1.883696	-1.070580
35	1	0	-1.029424	0.637301	-1.164450
36	6	0	3.845515	-1.353821	-1.158666
37	8	0	4.068506	0.062628	0.880521
38	6	0	1.804691	-2.810277	-0.633833
39	8	0	1.355851	0.628039	4.416269
40	1	0	-1.227755	-2.927382	2.339476
41	1	0	0.510788	-2.739067	2.631900
42	1	0	-0.061290	-3.867403	1.392760
43	8	0	-2.184004	-2.853383	-0.014358
44	8	0	-0.919857	-1.777154	-1.532268
45	1	0	-1.044818	-0.405321	4.820269
46	1	0	-2.200832	-0.989694	3.490899
47	6	0	5.399554	0.508177	-2.194417
48	6	0	4.394299	-0.591042	-2.374351
49	1	0	3.595124	1.364559	-3.233122
50	6	0	4.392007	1.441481	0.922091
51	1	0	-2.375074	4.555804	-0.465389
52	1	0	-1.730894	5.143418	-2.068379
53	1	0	-2.169921	2.850923	-3.052858
54	6	0	-3.537389	0.905580	-1.940201
55	8	0	-3.566955	2.443783	-0.061983
56	6	0	4.906551	-2.190843	-0.428102
57	6	0	2.733413	-2.302230	-1.720065
58	8	0	1.529757	-4.003109	-0.554237
59	6	0	-3.053046	-3.292539	-1.086406
60	1	0	5.875934	0.666943	-1.232634
61	1	0	6.032604	0.730535	-3.049253
62	1	0	4.405502	-1.138529	-3.312796
63	8	0	5.770944	1.636108	0.855787
64	1	0	4.002647	1.866567	1.856730
65	8	0	-4.382123	0.039031	-1.148403
66	1	0	-2.878946	0.235179	-2.495303
67	1	0	-4.169525	1.457339	-2.639573
68	1	0	-4.393156	2.724430	-0.495202
69	1	0	5.288781	-2.960138	-1.102575
70	1	0	4.490778	-2.686155	0.457396
71	1	0	5.735895	-1.562113	-0.100839
72	8	0	3.282413	-3.376448	-2.446049

73	1	0	2.088511	-1.706668	-2.387662
74	1	0	-3.556324	-2.435031	-1.535829
75	1	0	-2.471481	-3.824103	-1.841890
76	1	0	-3.773299	-3.959330	-0.614296
77	6	0	6.456168	1.299238	2.064068
78	6	0	-5.622881	0.500320	-0.855966
79	1	0	2.867220	-4.179056	-2.070326
80	1	0	6.425834	0.220154	2.252481
81	1	0	6.021975	1.827968	2.923352
82	1	0	7.491720	1.616708	1.931355
83	6	0	-6.449317	-0.414082	-0.023548
84	8	0	-6.035796	1.581708	-1.257576
85	6	0	-7.900118	-0.009840	0.069223
86	6	0	-5.876488	-1.455906	0.610181
87	1	0	-8.351896	0.051576	-0.927506
88	1	0	-7.997060	0.984654	0.519104
89	1	0	-8.482926	-0.713802	0.665081
90	6	0	-6.526757	-2.450685	1.520075
91	1	0	-4.809586	-1.602288	0.466923
92	1	0	-6.058723	-2.414453	2.512912
93	1	0	-6.363002	-3.468368	1.141238
94	1	0	-7.600954	-2.299189	1.642376

Table S2 Standard orientations of **2a** (1*R*,3*S*,4*S*,5*S*,9*R*,10*R*,11*R*,1′*R*,3′*S*,4′*S*,5′*R*,7′*R*,8′*R*,9′*S*,10′*S*)-**2** at B3LYP/6–311+G(2d,p) level in methanol.

Conformation **2a-1**



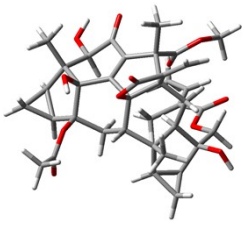
SCF Energy (B3LYP): −2375.954772 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.392451	2.608912	0.660272
2	6	0	-2.543963	1.044391	0.460945
3	6	0	-2.750587	3.206851	-0.701195
4	6	0	-2.822945	2.124525	-1.755140
5	6	0	-2.600028	0.771822	-1.108258
6	6	0	-1.393459	0.250668	1.043679
7	6	0	-0.457023	0.723582	1.873797
8	6	0	-0.344216	2.170468	2.101837
9	6	0	-0.903624	2.998390	0.955619
10	6	0	-3.274784	3.149159	1.798622
11	6	0	-4.073158	2.858402	-1.322319
12	8	0	0.195283	2.710151	3.061811

13	8	0	-0.762651	4.373279	1.225716
14	6	0	-1.171799	-1.196050	0.684119
15	6	0	-1.165727	-1.341124	-0.896798
16	6	0	0.016902	-2.219308	-1.404363
17	6	0	1.303346	-1.771527	-0.651777
18	6	0	1.296389	-2.244796	0.794469
19	6	0	0.080968	-1.655842	1.589498
20	6	0	0.423439	-2.012444	-2.887739
21	6	0	1.938836	-1.943480	-2.971023
22	6	0	2.501628	-2.153328	-1.551794
23	6	0	1.196274	-3.091575	-3.605918
24	6	0	3.761172	-1.319577	-1.286732
25	8	0	3.499123	0.060796	-1.592264
26	6	0	4.397640	0.963975	-1.135086
27	8	0	5.387887	0.635892	-0.498241
28	6	0	4.080628	2.376867	-1.482920
29	6	0	2.994301	2.664155	-2.226033
30	6	0	5.070437	3.374590	-0.935440
31	6	0	2.514710	4.009685	-2.674701
32	8	0	2.866390	-3.513167	-1.266777
33	6	0	-0.379364	-3.694454	-1.144633
34	1	0	1.304814	-0.673853	-0.663522
35	6	0	0.468328	-0.324508	2.447223
36	6	0	-1.325147	0.044686	-1.572318
37	8	0	-3.742568	-0.130811	-1.293239
38	8	0	-3.740804	0.635584	1.116888
39	1	0	-2.088109	-1.886169	-1.115072
40	8	0	-2.322175	-1.976399	1.162550
41	6	0	-0.550191	-2.727495	2.455192
42	6	0	-2.010714	-2.798074	2.197165
43	6	0	0.033757	-3.589307	3.292583
44	8	0	-2.851202	-3.475317	2.747749
45	6	0	0.224173	-0.440838	3.970076
46	6	0	-4.207598	-0.416733	-2.534055
47	6	0	-5.417988	-1.313836	-2.448830
48	8	0	-3.709252	-0.004445	-3.560806
49	6	0	1.914275	0.141461	2.194258
50	8	0	2.225799	0.921589	1.313143
51	8	0	2.789596	-0.386385	3.059429
52	6	0	4.158546	0.069933	2.948803
53	1	0	-2.310630	4.171118	-0.939356
54	1	0	-2.440764	2.278383	-2.757915
55	1	0	-0.297275	2.745190	0.071658
56	1	0	-3.045123	2.666788	2.755289
57	1	0	-3.100045	4.222455	1.904397
58	1	0	-4.331139	2.981823	1.586623
59	1	0	-4.495231	3.567271	-2.028645

60	1	0	-4.807301	2.316791	-0.732962
61	1	0	-0.335670	4.419456	2.105257
62	1	0	1.238680	-3.333753	0.815491
63	1	0	2.229027	-1.997356	1.307017
64	1	0	-0.175625	-1.363017	-3.515561
65	1	0	2.437135	-1.218803	-3.607916
66	1	0	1.134158	-3.090675	-4.691151
67	1	0	1.288886	-4.079797	-3.169689
68	1	0	4.584228	-1.673949	-1.918760
69	1	0	4.070213	-1.418467	-0.244243
70	1	0	2.376765	1.829289	-2.547967
71	1	0	6.081805	3.158547	-1.298152
72	1	0	4.817612	4.398527	-1.215095
73	1	0	5.111894	3.318215	0.158476
74	1	0	3.153937	4.834293	-2.352808
75	1	0	2.440988	4.038250	-3.770024
76	1	0	1.500764	4.193278	-2.294354
77	1	0	3.427151	-3.826293	-1.996117
78	1	0	-1.143781	-3.997166	-1.868859
79	1	0	0.472116	-4.370935	-1.236577
80	1	0	-0.804822	-3.841310	-0.147680
81	1	0	-1.395367	-0.077435	-2.652695
82	1	0	-0.462272	0.694383	-1.381702
83	1	0	-4.005370	-0.213494	0.721959
84	1	0	-0.569139	-4.320760	3.822888
85	1	0	1.104363	-3.596179	3.472245
86	1	0	-0.823164	-0.676560	4.174280
87	1	0	0.849862	-1.212660	4.420993
88	1	0	0.457680	0.517244	4.442027
89	1	0	-6.213202	-0.816708	-1.884073
90	1	0	-5.769754	-1.548302	-3.453894
91	1	0	-5.166294	-2.237917	-1.918671
92	1	0	4.535517	-0.072020	1.934720
93	1	0	4.214215	1.128677	3.213068
94	1	0	4.718959	-0.531869	3.662890

Conformation **2a-2**



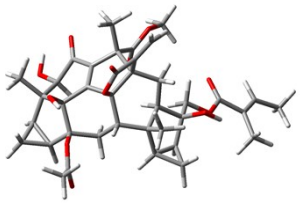
SCF Energy (B3LYP): −2375.954790 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.272120	2.825870	0.357246

2	6	0	-2.525664	1.263267	0.297775
3	6	0	-2.574238	3.318763	-1.058776
4	6	0	-2.702509	2.151303	-2.011817
5	6	0	-2.580035	0.851414	-1.241305
6	6	0	-1.438681	0.452176	0.970877
7	6	0	-0.476862	0.935193	1.765544
8	6	0	-0.265323	2.385760	1.859863
9	6	0	-0.763762	3.142411	0.638659
10	6	0	-3.127795	3.523666	1.428196
11	6	0	-3.908075	3.000147	-1.671197
12	8	0	0.310641	2.972908	2.769614
13	8	0	-0.535175	4.523855	0.787850
14	6	0	-1.317326	-1.033749	0.751714
15	6	0	-1.300510	-1.325866	-0.808359
16	6	0	-0.181199	-2.333485	-1.209505
17	6	0	1.126458	-1.924075	-0.470926
18	6	0	1.056869	-2.255675	1.012715
19	6	0	-0.114300	-1.493607	1.721314
20	6	0	0.265168	-2.292034	-2.695554
21	6	0	1.781937	-2.359589	-2.748571
22	6	0	2.300391	-2.490882	-1.303314
23	6	0	0.952899	-3.490925	-3.301561
24	6	0	3.629722	-1.759695	-1.080721
25	8	0	3.515585	-0.392971	-1.515623
26	6	0	4.512514	0.443192	-1.143368
27	8	0	5.463216	0.066544	-0.473852
28	6	0	4.300716	1.827625	-1.659169
29	6	0	5.274935	2.715163	-1.381063
30	6	0	3.038903	2.112369	-2.433881
31	6	0	5.349825	4.160405	-1.758728
32	8	0	2.532548	-3.847347	-0.890302
33	6	0	-0.698610	-3.743838	-0.829241
34	1	0	1.221565	-0.836623	-0.586194
35	6	0	0.370620	-0.115642	2.445286
36	6	0	-1.352980	-0.001676	-1.612470
37	8	0	-3.779944	0.015128	-1.365278
38	8	0	-3.755558	0.996778	0.965345
39	1	0	-2.257480	-1.821369	-0.992835
40	8	0	-2.528376	-1.681974	1.276019
41	6	0	-0.837011	-2.419310	2.679413
42	6	0	-2.294530	-2.412029	2.396355
43	6	0	-0.332013	-3.231284	3.612527
44	8	0	-3.190850	-2.967577	2.993068
45	6	0	0.123016	-0.063750	3.971239
46	6	0	-4.249482	-0.348679	-2.583658
47	6	0	-5.524077	-1.143790	-2.440416
48	8	0	-3.710427	-0.068766	-3.634270

49	6	0	1.846961	0.217762	2.155208
50	8	0	2.214727	0.875015	1.198532
51	8	0	2.681743	-0.273056	3.079983
52	6	0	4.079498	0.073452	2.935125
53	1	0	-2.069002	4.226994	-1.374926
54	1	0	-2.297276	2.188545	-3.016626
55	1	0	-0.169435	2.772967	-0.212126
56	1	0	-2.937873	3.117268	2.427975
57	1	0	-2.885605	4.588940	1.438656
58	1	0	-4.190787	3.404145	1.216845
59	1	0	-4.273421	3.667084	-2.446600
60	1	0	-4.683788	2.562416	-1.049691
61	1	0	-0.102686	4.619436	1.660707
62	1	0	0.904718	-3.328922	1.133762
63	1	0	1.998438	-2.040126	1.523631
64	1	0	-0.263591	-1.649349	-3.389869
65	1	0	2.350632	-1.736538	-3.432266
66	1	0	0.909007	-3.578531	-4.384154
67	1	0	0.951452	-4.442099	-2.781253
68	1	0	4.425596	-2.248096	-1.655338
69	1	0	3.909573	-1.792217	-0.025784
70	1	0	6.119197	2.338058	-0.806588
71	1	0	2.153382	1.919195	-1.817768
72	1	0	2.997348	3.149925	-2.771082
73	1	0	2.959982	1.465249	-3.314615
74	1	0	4.490964	4.509051	-2.336292
75	1	0	5.432023	4.781740	-0.856827
76	1	0	6.258782	4.350715	-2.345013
77	1	0	3.069366	-4.276153	-1.577461
78	1	0	-1.473965	-4.049258	-1.540628
79	1	0	0.096707	-4.490907	-0.841056
80	1	0	-1.150003	-3.765141	0.166974
81	1	0	-1.418883	-0.219851	-2.677891
82	1	0	-0.448974	0.602093	-1.467507
83	1	0	-4.064527	0.127521	0.655953
84	1	0	-0.996319	-3.858254	4.200175
85	1	0	0.732151	-3.298987	3.816067
86	1	0	-0.937961	-0.200284	4.194287
87	1	0	0.691513	-0.831858	4.497886
88	1	0	0.428905	0.915666	4.348295
89	1	0	-6.290460	-0.535253	-1.949513
90	1	0	-5.873856	-1.453058	-3.425761
91	1	0	-5.352094	-2.024617	-1.813713
92	1	0	4.455730	-0.226142	1.955535
93	1	0	4.205048	1.151581	3.059644
94	1	0	4.590902	-0.465385	3.731569

Conformation **2a-3**



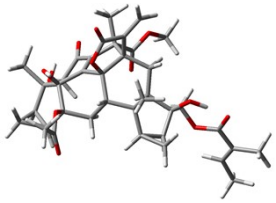
SCF Energy (B3LYP): −2375.951934 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.970417	0.500948	0.937087
2	6	0	0.945512	1.801470	0.028656
3	6	0	-0.380231	-0.278967	1.346347
4	6	0	1.720657	1.573680	-1.290676
5	6	0	-0.486965	2.408558	-0.107227
6	1	0	1.549667	2.522017	0.586660
7	6	0	1.840852	-0.560401	0.299665
8	8	0	1.592865	0.909337	2.203424
9	6	0	-1.711032	0.375972	0.846700
10	6	0	-0.169421	-1.792380	0.788209
11	6	0	-0.318914	-0.215761	2.861146
12	6	0	3.161119	1.098145	-1.048152
13	1	0	1.783975	2.515815	-1.839430
14	1	0	1.217709	0.856392	-1.951052
15	6	0	-0.769089	3.187328	1.200786
16	6	0	-0.714590	3.306316	-1.354425
17	6	0	-1.489835	1.248964	-0.378636
18	6	0	3.215885	-0.238955	-0.233095
19	6	0	1.214421	-1.736432	0.179578
20	6	0	0.935791	0.447247	3.293306
21	1	0	-2.132496	0.984325	1.648388
22	1	0	-2.452657	-0.402423	0.650959
23	6	0	-0.246795	-2.898785	1.861546
24	6	0	-1.127045	-2.119806	-0.380984
25	6	0	-1.242519	-0.559370	3.763393
26	6	0	3.934817	0.852880	-2.336909
27	8	0	3.801511	2.058689	-0.177842
28	1	0	-0.504692	2.608451	2.090729
29	1	0	-0.162642	4.099927	1.218493
30	1	0	-1.819756	3.466298	1.292708
31	6	0	-1.840443	4.312281	-1.376160
32	6	0	-2.053077	2.947858	-1.975729
33	1	0	0.124768	3.531306	-2.001667
34	6	0	-2.721585	1.883696	-1.070580
35	1	0	-1.029424	0.637301	-1.164450
36	6	0	3.845515	-1.353821	-1.158666
37	8	0	4.068506	0.062628	0.880521
38	6	0	1.804691	-2.810277	-0.633833

39	8	0	1.355851	0.628039	4.416269
40	1	0	-1.227755	-2.927382	2.339476
41	1	0	0.510788	-2.739067	2.631900
42	1	0	-0.061290	-3.867403	1.392760
43	8	0	-2.184004	-2.853383	-0.014358
44	8	0	-0.919857	-1.777154	-1.532268
45	1	0	-1.044818	-0.405321	4.820269
46	1	0	-2.200832	-0.989694	3.490899
47	6	0	5.399554	0.508177	-2.194417
48	6	0	4.394299	-0.591042	-2.374351
49	1	0	3.595124	1.364559	-3.233122
50	6	0	4.392007	1.441481	0.922091
51	1	0	-2.375074	4.555804	-0.465389
52	1	0	-1.730894	5.143418	-2.068379
53	1	0	-2.169921	2.850923	-3.052858
54	6	0	-3.537389	0.905580	-1.940201
55	8	0	-3.566955	2.443783	-0.061983
56	6	0	4.906551	-2.190843	-0.428102
57	6	0	2.733413	-2.302230	-1.720065
58	8	0	1.529757	-4.003109	-0.554237
59	6	0	-3.053046	-3.292539	-1.086406
60	1	0	5.875934	0.666943	-1.232634
61	1	0	6.032604	0.730535	-3.049253
62	1	0	4.405502	-1.138529	-3.312796
63	8	0	5.770944	1.636108	0.855787
64	1	0	4.002647	1.866567	1.856730
65	8	0	-4.382123	0.039031	-1.148403
66	1	0	-2.878946	0.235179	-2.495303
67	1	0	-4.169525	1.457339	-2.639573
68	1	0	-4.393156	2.724430	-0.495202
69	1	0	5.288781	-2.960138	-1.102575
70	1	0	4.490778	-2.686155	0.457396
71	1	0	5.735895	-1.562113	-0.100839
72	8	0	3.282413	-3.376448	-2.446049
73	1	0	2.088511	-1.706668	-2.387662
74	1	0	-3.556324	-2.435031	-1.535829
75	1	0	-2.471481	-3.824103	-1.841890
76	1	0	-3.773299	-3.959330	-0.614296
77	6	0	6.456168	1.299238	2.064068
78	6	0	-5.622881	0.500320	-0.855966
79	1	0	2.867220	-4.179056	-2.070326
80	1	0	6.425834	0.220154	2.252481
81	1	0	6.021975	1.827968	2.923352
82	1	0	7.491720	1.616708	1.931355
83	6	0	-6.449317	-0.414082	-0.023548
84	8	0	-6.035796	1.581708	-1.257576
85	6	0	-7.900118	-0.009840	0.069223

86	6	0	-5.876488	-1.455906	0.610181
87	1	0	-8.351896	0.051576	-0.927506
88	1	0	-7.997060	0.984654	0.519104
89	1	0	-8.482926	-0.713802	0.665081
90	6	0	-6.526757	-2.450685	1.520075
91	1	0	-4.809586	-1.602288	0.466923
92	1	0	-6.058723	-2.414453	2.512912
93	1	0	-6.363002	-3.468368	1.141238
94	1	0	-7.600954	-2.299189	1.642376

Conformation **2a-4**



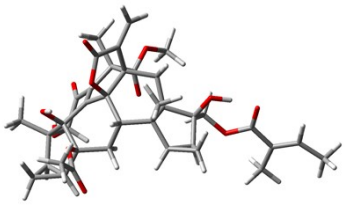
SCF Energy (B3LYP): −2375.952161 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.708505	0.257392	-2.123271
2	6	0	-3.305102	-0.228699	-0.670760
3	6	0	-3.759240	-1.024207	-2.956532
4	6	0	-3.141663	-2.176786	-2.196396
5	6	0	-2.745642	-1.714096	-0.808014
6	6	0	-2.235332	0.626578	-0.026361
7	6	0	-1.814529	1.818341	-0.465487
8	6	0	-2.211519	2.291116	-1.797727
9	6	0	-2.591584	1.163071	-2.744128
10	6	0	-5.036057	1.034076	-2.140363
11	6	0	-4.625546	-2.159819	-2.491753
12	8	0	-2.182080	3.453996	-2.187009
13	8	0	-2.969628	1.678583	-3.998957
14	6	0	-1.483181	0.159785	1.193319
15	6	0	-0.890992	-1.286612	0.911199
16	6	0	0.604710	-1.412692	1.337689
17	6	0	1.352360	-0.134962	0.854369
18	6	0	0.983885	1.078083	1.695930
19	6	0	-0.543176	1.405731	1.594124
20	6	0	1.412442	-2.534384	0.634558
21	6	0	2.763686	-1.979934	0.219376
22	6	0	2.853124	-0.519080	0.731000
23	6	0	2.681657	-3.061481	1.261435
24	6	0	3.585655	0.389399	-0.276491
25	8	0	4.751896	-0.209114	-0.904563
26	6	0	5.901758	-0.296226	-0.211678
27	8	0	5.974986	-0.059829	0.992582
28	6	0	7.080638	-0.711552	-1.014628

29	6	0	6.957682	-0.880568	-2.346665
30	6	0	8.341918	-0.895420	-0.207894
31	6	0	8.014119	-1.291683	-3.322689
32	8	0	3.443241	-0.390377	2.024831
33	6	0	0.615167	-1.602473	2.874744
34	1	0	1.019106	0.035850	-0.177284
35	6	0	-0.870192	2.539029	0.468756
36	6	0	-1.231668	-1.744805	-0.530368
37	8	0	-3.426126	-2.472132	0.248607
38	8	0	-4.470075	-0.169989	0.147165
39	1	0	-1.467793	-1.938804	1.572483
40	8	0	-2.437666	0.001488	2.299848
41	6	0	-1.094156	1.773000	2.957063
42	6	0	-2.279881	0.936431	3.271320
43	6	0	-0.614389	2.634347	3.858624
44	8	0	-3.018122	0.988566	4.230693
45	6	0	-1.560930	3.811004	1.011848
46	6	0	-3.339337	-3.823885	0.298855
47	6	0	-4.169198	-4.362456	1.438384
48	8	0	-2.680317	-4.494344	-0.468492
49	6	0	0.381561	2.929216	-0.338964
50	8	0	0.766028	2.325263	-1.324589
51	8	0	0.998485	4.012154	0.149786
52	6	0	2.155019	4.477241	-0.581631
53	1	0	-3.581948	-0.917803	-4.022982
54	1	0	-2.513845	-2.911849	-2.687019
55	1	0	-1.682372	0.553321	-2.868302
56	1	0	-5.000009	1.914941	-1.489544
57	1	0	-5.239016	1.368653	-3.160378
58	1	0	-5.860409	0.404871	-1.803519
59	1	0	-4.983820	-2.855062	-3.245284
60	1	0	-5.310685	-1.997267	-1.664848
61	1	0	-2.868050	2.648760	-3.919094
62	1	0	1.237892	0.879721	2.737470
63	1	0	1.570502	1.959093	1.423231
64	1	0	0.895443	-3.220501	-0.026288
65	1	0	3.194353	-2.208679	-0.750580
66	1	0	2.988035	-4.061195	0.963272
67	1	0	2.937847	-2.799864	2.281511
68	1	0	3.891810	1.316733	0.216225
69	1	0	2.942985	0.626534	-1.124724
70	1	0	5.978067	-0.700395	-2.782089
71	1	0	8.196400	-1.646880	0.576493
72	1	0	9.181575	-1.208931	-0.829956
73	1	0	8.618816	0.036420	0.298025
74	1	0	8.989178	-1.473429	-2.866571
75	1	0	7.703022	-2.204252	-3.848436

76	1	0	8.132311	-0.519480	-4.094532
77	1	0	4.412619	-0.349953	1.886488
78	1	0	0.272136	-2.614717	3.116295
79	1	0	1.611509	-1.463478	3.297520
80	1	0	-0.057391	-0.904976	3.383539
81	1	0	-0.895778	-2.770466	-0.679193
82	1	0	-0.723920	-1.132217	-1.285239
83	1	0	-4.312229	-0.755728	0.908056
84	1	0	-1.121077	2.757400	4.811451
85	1	0	0.277034	3.228623	3.683876
86	1	0	-2.499996	3.555106	1.508430
87	1	0	-0.925970	4.343582	1.721624
88	1	0	-1.785529	4.479138	0.176403
89	1	0	-5.216531	-4.071085	1.310211
90	1	0	-4.088089	-5.449420	1.466822
91	1	0	-3.824010	-3.940310	2.387698
92	1	0	2.938846	3.717309	-0.577414
93	1	0	1.876802	4.712214	-1.610978
94	1	0	2.485818	5.372246	-0.056861

Conformation **2a-5**



SCF Energy (B3LYP): −2375.952497 Hartree

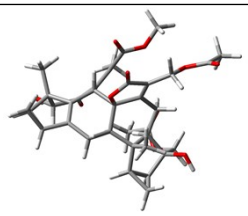
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.784374	0.281072	-2.052236
2	6	0	-3.339340	-0.240675	-0.624367
3	6	0	-3.841380	-0.977109	-2.920018
4	6	0	-3.192418	-2.143219	-2.208265
5	6	0	-2.766830	-1.714894	-0.817609
6	6	0	-2.263352	0.608955	0.017224
7	6	0	-1.867568	1.817625	-0.398298
8	6	0	-2.303850	2.323109	-1.706071
9	6	0	-2.694051	1.217642	-2.674628
10	6	0	-5.120768	1.041689	-2.014439
11	6	0	-4.683344	-2.135251	-2.466205
12	8	0	-2.298979	3.496920	-2.062129
13	8	0	-3.109500	1.763653	-3.904436
14	6	0	-1.474996	0.117195	1.203792
15	6	0	-0.873498	-1.313241	0.865729
16	6	0	0.634358	-1.432625	1.249483
17	6	0	1.353711	-0.132413	0.783455
18	6	0	0.993596	1.051187	1.669548

19	6	0	-0.539389	1.362836	1.616015
20	6	0	1.435932	-2.523788	0.493430
21	6	0	2.768496	-1.940912	0.057401
22	6	0	2.854974	-0.493951	0.607582
23	6	0	2.727995	-3.052080	1.070504
24	6	0	3.548129	0.453117	-0.392935
25	8	0	4.700614	-0.111987	-1.075860
26	6	0	5.866761	-0.230869	-0.416254
27	8	0	5.976670	-0.013658	0.788733
28	6	0	6.976087	-0.651314	-1.315688
29	6	0	8.173678	-0.842416	-0.727079
30	6	0	6.671057	-0.825200	-2.782815
31	6	0	9.461799	-1.257850	-1.361287
32	8	0	3.479396	-0.394265	1.887878
33	6	0	0.687801	-1.665678	2.779617
34	1	0	0.990530	0.063507	-0.233459
35	6	0	-0.907794	2.523021	0.531796
36	6	0	-1.246016	-1.734924	-0.579029
37	8	0	-3.411854	-2.510392	0.233528
38	8	0	-4.484056	-0.218753	0.223442
39	1	0	-1.425039	-1.990847	1.523025
40	8	0	-2.398794	-0.083859	2.329206
41	6	0	-1.059038	1.684581	3.002567
42	6	0	-2.225613	0.823851	3.323536
43	6	0	-0.566645	2.526467	3.915649
44	8	0	-2.938060	0.838335	4.303506
45	6	0	-1.598083	3.771477	1.127474
46	6	0	-3.308519	-3.861923	0.243359
47	6	0	-4.104019	-4.442204	1.386905
48	8	0	-2.660546	-4.502515	-0.558125
49	6	0	0.318396	2.950435	-0.296018
50	8	0	0.682103	2.380791	-1.309566
51	8	0	0.938067	4.023840	0.209726
52	6	0	2.073169	4.519884	-0.534915
53	1	0	-3.691975	-0.838654	-3.987072
54	1	0	-2.569106	-2.857000	-2.734765
55	1	0	-1.781156	0.623054	-2.838799
56	1	0	-5.077900	1.905103	-1.341068
57	1	0	-5.353787	1.401093	-3.019485
58	1	0	-5.928836	0.393646	-1.673884
59	1	0	-5.052820	-2.813309	-3.229913
60	1	0	-5.349312	-2.003716	-1.618374
61	1	0	-3.019524	2.732486	-3.798711
62	1	0	1.276558	0.825705	2.698086
63	1	0	1.562315	1.947284	1.408392
64	1	0	0.909522	-3.197681	-0.172550
65	1	0	3.173892	-2.137482	-0.930384

66	1	0	3.038045	-4.039120	0.736163
67	1	0	3.008776	-2.815797	2.090332
68	1	0	3.862164	1.366465	0.120334
69	1	0	2.878112	0.711474	-1.213255
70	1	0	8.216113	-0.673839	0.347311
71	1	0	6.289179	0.104708	-3.218823
72	1	0	7.557793	-1.123909	-3.344870
73	1	0	5.898737	-1.587116	-2.937516
74	1	0	9.391252	-1.417404	-2.439189
75	1	0	10.233622	-0.499347	-1.174254
76	1	0	9.825921	-2.184720	-0.898269
77	1	0	4.444363	-0.346036	1.724458
78	1	0	0.364051	-2.688818	3.001033
79	1	0	1.693239	-1.525418	3.179808
80	1	0	0.020268	-0.991828	3.325633
81	1	0	-0.902263	-2.751775	-0.765382
82	1	0	-0.764979	-1.095065	-1.328740
83	1	0	-4.301627	-0.825376	0.962159
84	1	0	-1.049697	2.615615	4.884396
85	1	0	0.312288	3.137392	3.735083
86	1	0	-2.523449	3.491948	1.636890
87	1	0	-0.952211	4.289237	1.838332
88	1	0	-1.847800	4.461480	0.317315
89	1	0	-5.156156	-4.154085	1.296780
90	1	0	-4.015291	-5.528917	1.378519
91	1	0	-3.735329	-4.048090	2.339478
92	1	0	2.860757	3.764867	-0.575013
93	1	0	1.767798	4.786322	-1.548772
94	1	0	2.412160	5.399446	0.010318

Table S3 Standard orientations of **3a** (1*R*,3*S*,6*R*,9*R*,10*S*,1′*R*,3′*S*,4′*S*,5′*R*,8′*S*,9′*S*,10′*S*)-**3** at B3LYP/6–311+G(2d,p) level in methanol.

Conformation **3a-1**



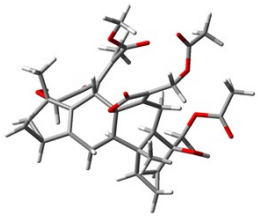
SCF Energy (B3LYP): −-2184.099955 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.400758	1.689439	-1.953918
2	6	0	1.178362	1.740659	-0.586360
3	6	0	1.836424	0.423031	-0.137966
4	6	0	1.065029	-0.725085	-0.734415
5	6	0	-0.416309	-0.621180	-1.107496
6	6	0	-0.822273	0.796034	-1.636377

7	6	0	0.027907	3.187379	-2.106119
8	6	0	0.996058	4.015665	-1.272827
9	6	0	1.991423	3.048800	-0.596320
10	6	0	1.585004	-1.823994	-1.314379
11	6	0	0.561000	-2.429833	-2.183122
12	8	0	-0.542660	-1.634822	-2.162707
13	8	0	0.637053	-3.416374	-2.888102
14	6	0	-3.078059	-0.086127	-1.873870
15	6	0	-2.865419	-0.765399	-0.728579
16	6	0	-4.144570	-0.938017	0.074119
17	6	0	-5.235943	-0.585334	-0.946680
18	6	0	-4.538911	0.015486	-2.166712
19	6	0	-1.535044	-1.101590	-0.097347
20	6	0	-1.499499	-0.581721	1.348643
21	6	0	-2.611498	0.334545	1.761021
22	6	0	-4.004705	0.224925	1.084029
23	6	0	-5.274654	-1.312574	-2.260060
24	6	0	-1.979452	0.617742	-2.633650
25	1	0	-1.289949	1.284612	-0.771984
26	6	0	0.993660	4.132421	-2.775873
27	1	0	0.387247	1.955175	0.143116
28	6	0	2.989445	-2.328334	-1.411648
29	6	0	1.188146	1.172983	-3.178178
30	8	0	-4.995485	0.175079	2.098490
31	8	0	3.201804	2.835151	-1.335666
32	6	0	-4.350930	-2.296390	0.758752
33	6	0	-0.676342	-1.080186	2.314688
34	8	0	-2.531245	1.143027	2.682052
35	6	0	-0.595469	-0.608898	3.748980
36	8	0	3.701026	-2.067365	-0.184762
37	1	0	-1.421168	-2.187464	-0.046386
38	6	0	5.044545	-2.249644	-0.233686
39	8	0	5.625177	-2.624900	-1.231456
40	6	0	2.436265	3.530489	0.796895
41	8	0	1.317501	3.861467	1.648289
42	6	0	5.686226	-1.944767	1.095375
43	6	0	1.054875	3.065159	2.709585
44	6	0	-0.140330	3.552731	3.485607
45	8	0	1.697014	2.067583	2.985179
46	6	0	0.208689	-2.275630	2.038060
47	8	0	-0.119677	-3.264922	1.408393
48	8	0	1.387854	-2.155445	2.663843
49	6	0	2.253533	-3.311836	2.616430
50	1	0	2.873472	0.356185	-0.476899
51	1	0	1.859271	0.378487	0.957658
52	1	0	-1.026966	3.450575	-2.124144
53	1	0	0.643757	4.856457	-0.682674

54	1	0	-6.160294	-0.157934	-0.568921
55	1	0	-4.928992	0.879017	-2.698461
56	1	0	-4.106643	1.157976	0.504435
57	1	0	-6.228124	-1.318894	-2.782309
58	1	0	-4.674170	-2.208769	-2.397280
59	1	0	-2.342970	1.597279	-2.969209
60	1	0	-1.672674	0.068530	-3.531514
61	1	0	0.578774	5.048223	-3.189287
62	1	0	1.833363	3.736433	-3.336732
63	1	0	2.983379	-3.403917	-1.613511
64	1	0	3.522759	-1.846901	-2.239601
65	1	0	2.176542	1.630236	-3.243175
66	1	0	1.330559	0.091608	-3.158989
67	1	0	0.636976	1.412816	-4.094480
68	1	0	-4.726714	0.841257	2.757330
69	1	0	3.566423	3.706160	-1.565735
70	1	0	-4.434095	-3.089577	0.008875
71	1	0	-3.520739	-2.550443	1.427435
72	1	0	-5.266894	-2.286568	1.356124
73	1	0	0.153298	0.189527	3.829623
74	1	0	-1.542131	-0.198817	4.098959
75	1	0	-0.279664	-1.424083	4.403787
76	1	0	3.055195	2.774534	1.280966
77	1	0	3.009614	4.456544	0.692906
78	1	0	6.766962	-1.871940	0.968767
79	1	0	5.289681	-1.016581	1.515123
80	1	0	5.464140	-2.751991	1.802093
81	1	0	-0.416585	4.571192	3.209079
82	1	0	-0.980611	2.878673	3.283708
83	1	0	0.081033	3.498285	4.554831
84	1	0	3.106280	-3.054920	3.243442
85	1	0	1.732465	-4.185346	3.013750
86	1	0	2.573663	-3.499146	1.591244

Conformation **3a-2**



SCF Energy (B3LYP): −2184.095209 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.509075	-2.228322	-1.278594
2	6	0	-1.367828	-1.680527	-0.077126
3	6	0	-1.704100	-0.178872	-0.130295

4	6	0	-0.637893	0.526427	-0.923903
5	6	0	0.793626	0.002214	-1.033696
6	6	0	0.871028	-1.561323	-1.065462
7	6	0	-0.502046	-3.740332	-0.934691
8	6	0	-1.694093	-4.043033	-0.039398
9	6	0	-2.484098	-2.722223	0.167040
10	6	0	-0.837955	1.461738	-1.872926
11	6	0	0.359307	1.529844	-2.728481
12	8	0	1.241188	0.581394	-2.306370
13	8	0	0.572537	2.223827	-3.702545
14	6	0	3.284418	-1.306396	-1.210651
15	6	0	3.166198	-0.274303	-0.350075
16	6	0	4.373882	-0.163528	0.566858
17	6	0	5.412531	-1.054657	-0.128311
18	6	0	4.684433	-1.824782	-1.229121
19	6	0	1.918409	0.523925	-0.048957
20	6	0	1.636501	0.508877	1.462184
21	6	0	2.456975	-0.407705	2.313692
22	6	0	3.845235	-0.894829	1.825035
23	6	0	5.752998	-0.796668	-1.567846
24	6	0	2.104794	-1.955756	-1.894034
25	1	0	1.141956	-1.839597	-0.038993
26	6	0	-1.622015	-4.627983	-1.422218
27	1	0	-0.707191	-1.821105	0.788146
28	6	0	-2.090186	2.167588	-2.302478
29	6	0	-1.062914	-1.974230	-2.697658
30	8	0	4.753624	-0.826666	2.910097
31	8	0	-3.528507	-2.508182	-0.783171
32	6	0	4.880634	1.251620	0.877721
33	6	0	0.863949	1.435632	2.094785
34	8	0	2.143588	-0.738461	3.454477
35	6	0	0.511720	1.452035	3.567118
36	8	0	-2.940314	2.526383	-1.194901
37	1	0	2.079290	1.567375	-0.338148
38	6	0	-2.971478	3.829281	-0.823326
39	8	0	-2.331364	4.703490	-1.373783
40	6	0	-3.054205	-2.714998	1.590872
41	8	0	-3.778034	-1.501408	1.902226
42	6	0	-3.889454	4.028078	0.353567
43	6	0	-5.095746	-1.470497	1.616393
44	6	0	-5.722386	-0.180572	2.075367
45	8	0	-5.689285	-2.379459	1.060154
46	6	0	0.260332	2.618648	1.377324
47	8	0	-0.922033	2.897917	1.439875
48	8	0	1.187247	3.376470	0.778680
49	6	0	0.728445	4.617894	0.188781
50	1	0	-2.669883	-0.003999	-0.611541

51	1	0	-1.785169	0.226836	0.884728
52	1	0	0.457227	-4.210039	-0.730420
53	1	0	-1.593742	-4.708765	0.815057
54	1	0	6.154417	-1.545018	0.495174
55	1	0	4.872403	-2.875329	-1.432820
56	1	0	3.689947	-1.947595	1.531088
57	1	0	6.713215	-1.171598	-1.913132
58	1	0	5.427284	0.126551	-2.041372
59	1	0	2.236924	-3.044989	-1.881024
60	1	0	2.011625	-1.659396	-2.945261
61	1	0	-1.408780	-5.691706	-1.493355
62	1	0	-2.316938	-4.261505	-2.169475
63	1	0	-1.832014	3.059299	-2.875755
64	1	0	-2.699092	1.510359	-2.932956
65	1	0	-2.122331	-2.225488	-2.766989
66	1	0	-0.953313	-0.935442	-3.012185
67	1	0	-0.516113	-2.592723	-3.418425
68	1	0	4.224911	-1.056431	3.697753
69	1	0	-4.351165	-2.883769	-0.419957
70	1	0	5.248315	1.731990	-0.034674
71	1	0	4.093362	1.887312	1.298824
72	1	0	5.698656	1.211594	1.602533
73	1	0	-0.165005	0.627729	3.813776
74	1	0	1.400590	1.316031	4.188818
75	1	0	0.019289	2.389467	3.832133
76	1	0	-3.721451	-3.569357	1.735148
77	1	0	-2.250037	-2.762231	2.327509
78	1	0	-4.815405	3.461057	0.226658
79	1	0	-3.383197	3.659800	1.251664
80	1	0	-4.108125	5.090059	0.472800
81	1	0	-5.551071	-0.037600	3.146665
82	1	0	-5.257107	0.661713	1.552511
83	1	0	-6.792243	-0.196577	1.866674
84	1	0	1.624705	5.086816	-0.214408
85	1	0	-0.000454	4.423055	-0.598516
86	1	0	0.276862	5.247183	0.958884