Electronic Supplementary Information for

(+)- and (–)-Ganodilactone, a Pair of Meroterpenoid Dimers with Pancreatic Lipase Inhibitory Activities from the Macromycete *Ganoderma leucocontextum*

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Contents

Table 1S Results of inhibitory activities of compounds (±)-**1** and **2** against pancreatic lipase.[a]

Compound	Concentration (μM)	PPL inhibitory rate (%)	IC_{50} (μM)	Concentration (μM)[b]	PPL inhibitory rate (%)[b]	IC_{50} (μM)[b]
Orlistat	0.010	80.570	0.003604	0.005	86.024	0.0018
	0.005	63.444		0.002	51.526	
	0.0025	34.988		0.001	28.284	
	0.00125	2.637				
	0.000625	-10.594				
	0.0003125	-16.698				
Vibralactone				10000	91.800	48.668
				1000	87.038	
				100	57.678	
				10	33.130	
(±)-**1**	50	64.917	27.269			
	25	47.862				
	12.5	37.007				
	6.25	30.879				
	3.125	24.228				
2	50	42.090	＞50			
	25	26.152				
	12.5	7.767				
	6.25	-5.321				
	3.125	-18.670				

[a] Orlistat used as positive control [b] Data reported in the literature: Chen, H. P.; Zhao, Z. Z.; Li, Z. H.; Dong, Z. J.; Wei, K.; Bai, X.; Zhang, L.; Wen, C. N.; Feng, T.; Liu, J. K. *ChemistryOpen* **2016**. DOI: 10.1002/open.201500198.

Table 2S Results of inhibitory activities of compounds (+)-**1**, (−)-**1** against pancreatic lipase.[a]

Compound	Concentration (μM)	PPL inhibitory rate (%)	IC_{50} (μM)	Compound	Concentration (μM)	PPL inhibitory rate (%)	IC_{50} (μM)
Orlistat	0.005	78.985	0.002434	**(+)-1**	12.5	65.715	3.956
	0.0025	51.003			3.125	46.778	
	0.00125	25.057			0.78125	4.494	
	0.000625	11.066			0.1953125	-21.311	
	0.0003125	1.908					
Vibralactone	50	41.601	>50	**(−)-1**	12.5	73.036	2.518
	25	21.472			3.125	56.868	
	12.5	7.304			0.78125	12.761	
	6.25	0.643			0.1953125	-13.228	
	3.125	-1.461					

[a] Orlistat and vibralactone used as positive control.

Fig. 1S ^{1}H NMR spectrum of 1 (800 MHz, DMSO-d_6)

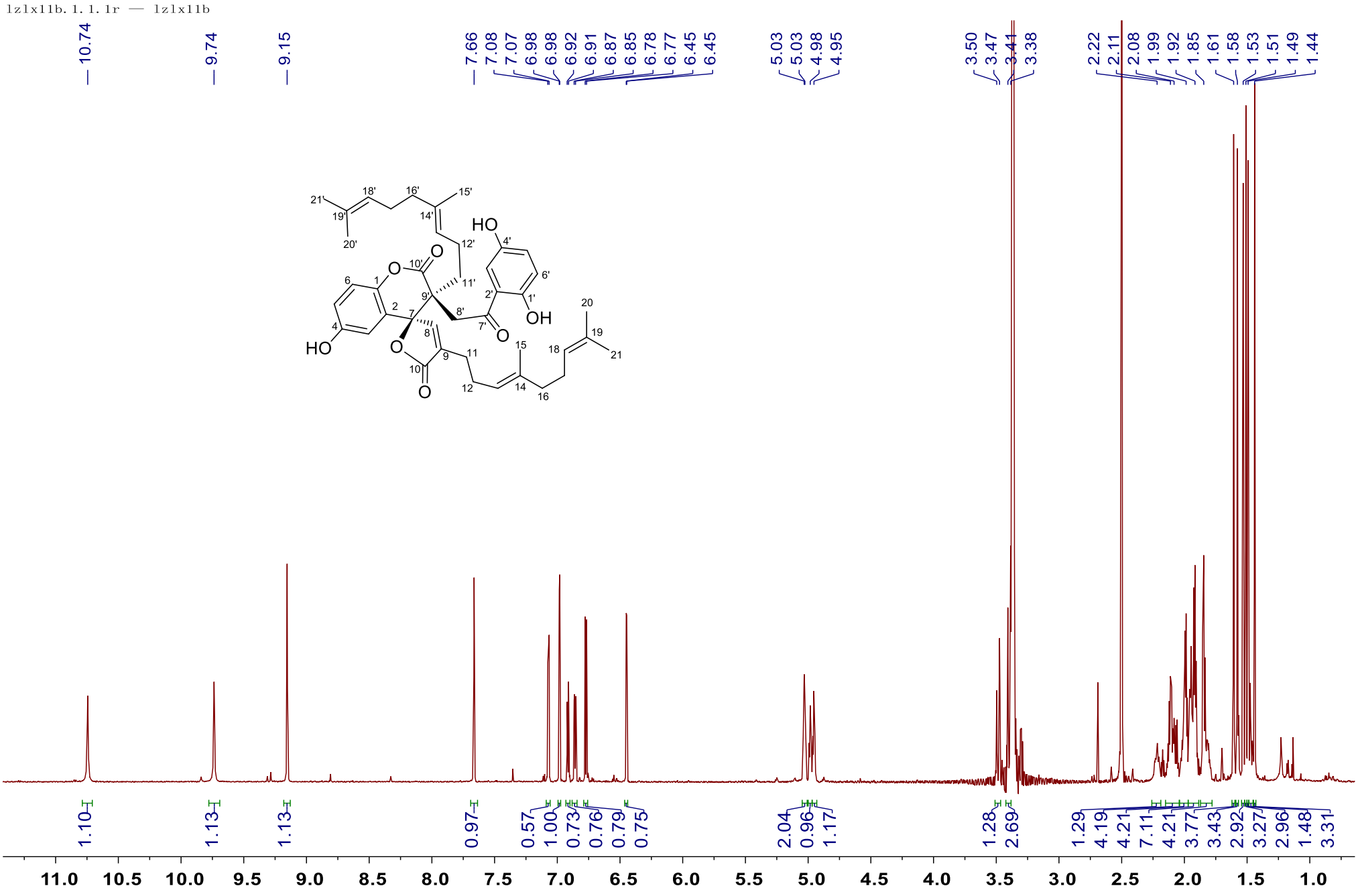


Fig. 2S Enlarged ^{1}H NMR spectra of **1** (800 MHz, DMSO-d_6)

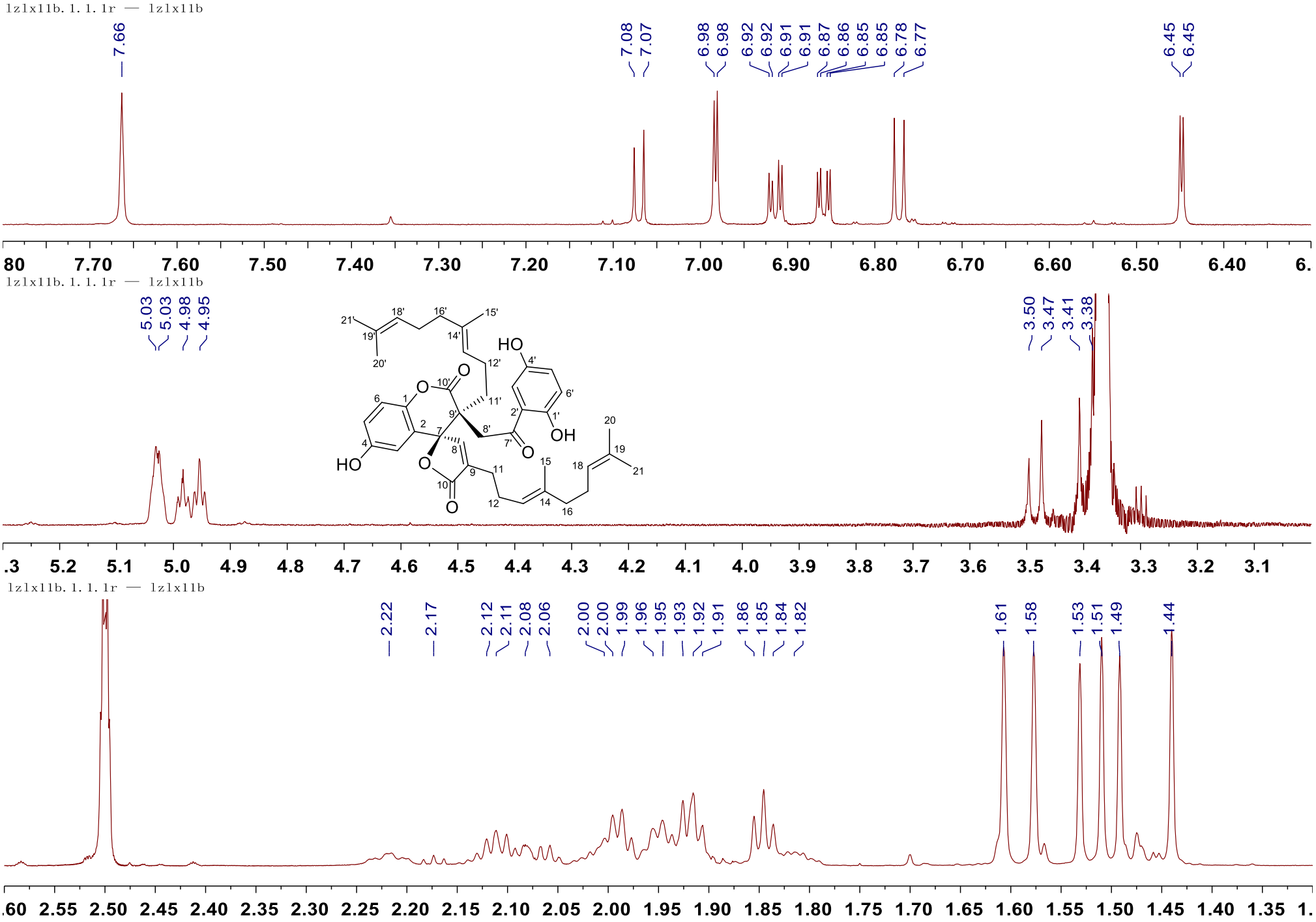


Fig. 3S ^{13}C NMR and DEPT spectra of **1** (200 MHz, DMSO-d_6)

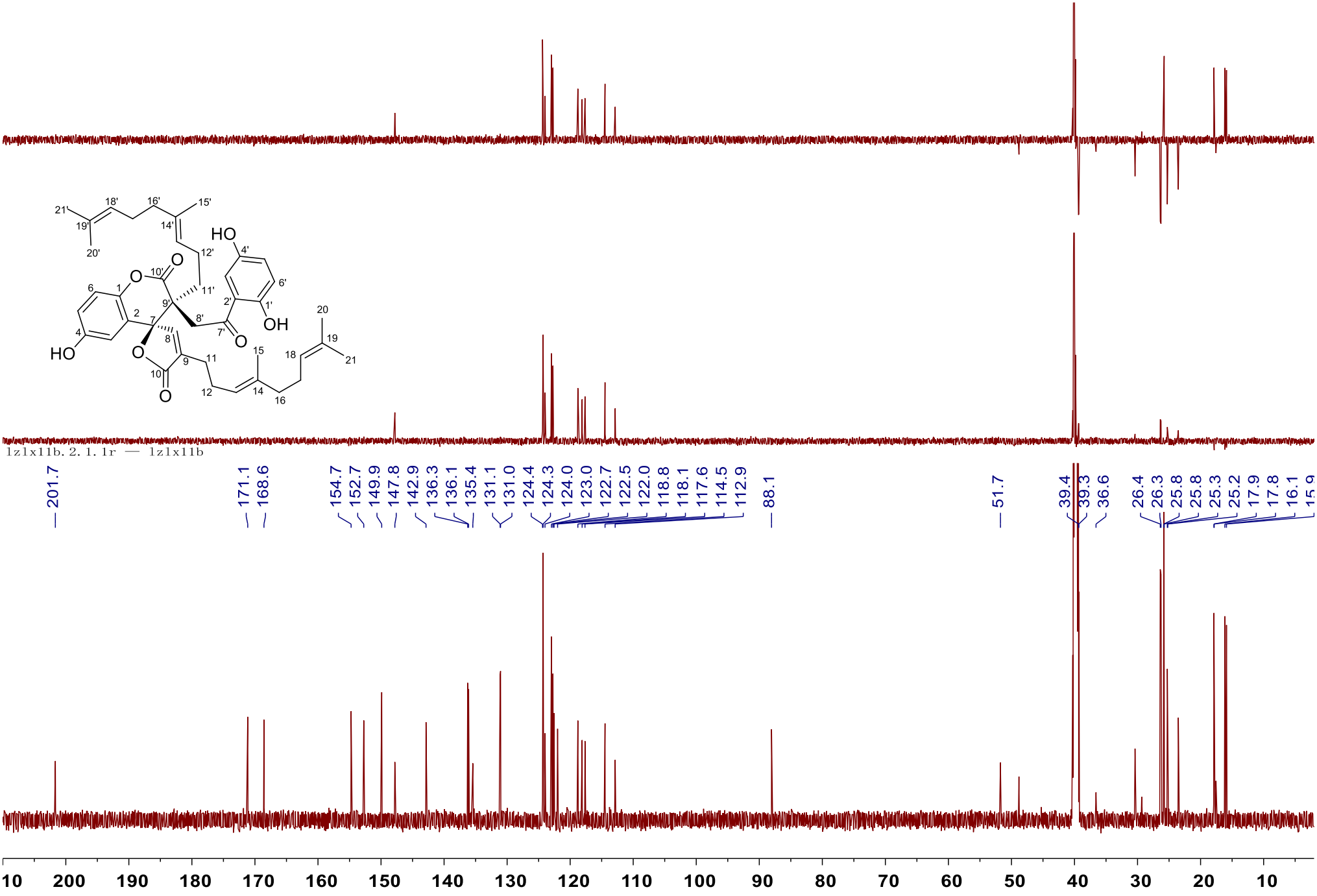


Fig. 4S Enlarged ^{13}C NMR spectra of **1** (200 MHz, DMSO-d_6)

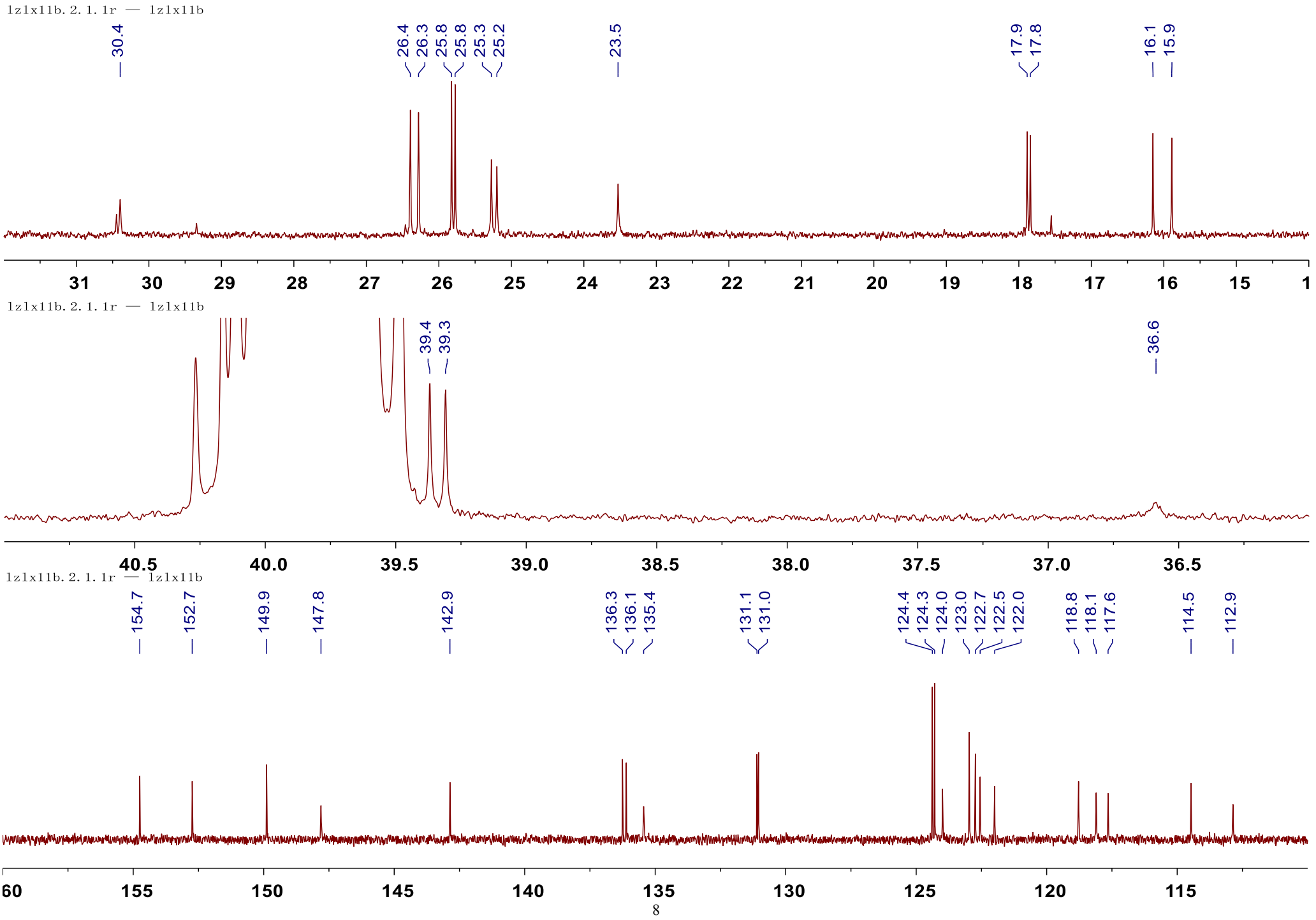


Fig. 5S HSQC spectrum of **1** (DMSO-d_6)

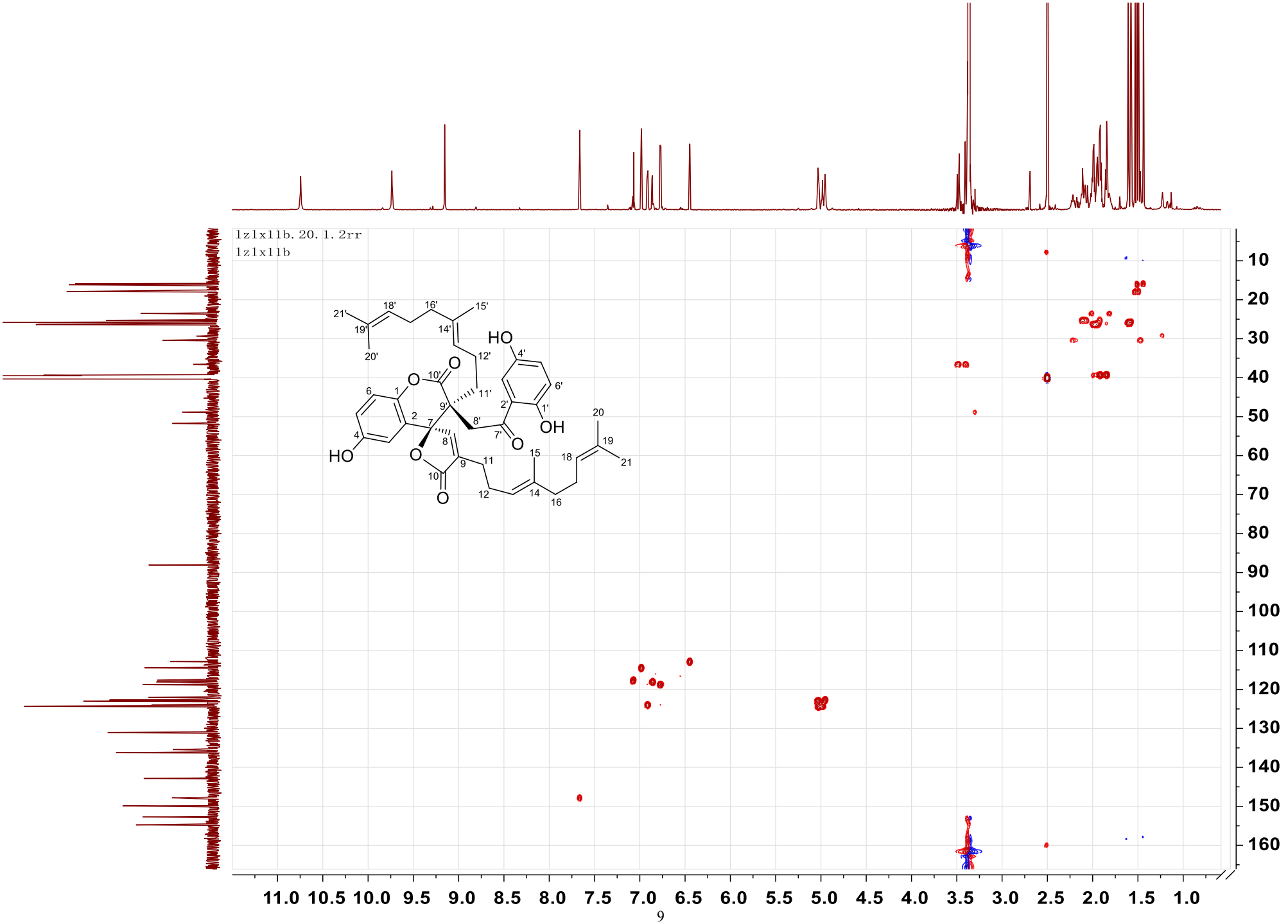


Fig. 6S Enlarged HSQC spectra of **1** (DMSO-d_6)

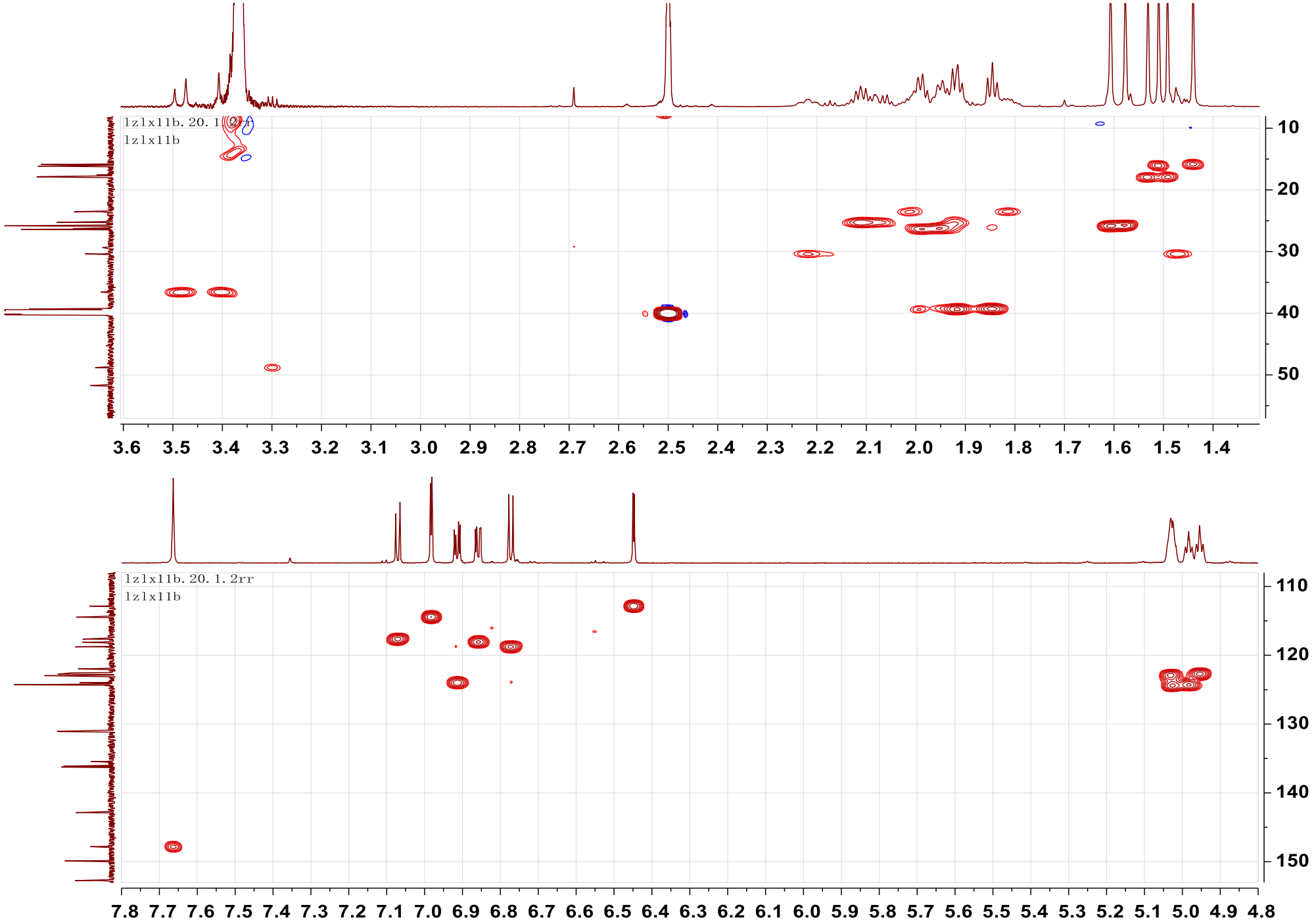


Fig. 7S ^{1}H-^{1}H COSY spectrum of **1** (DMSO-d_6)

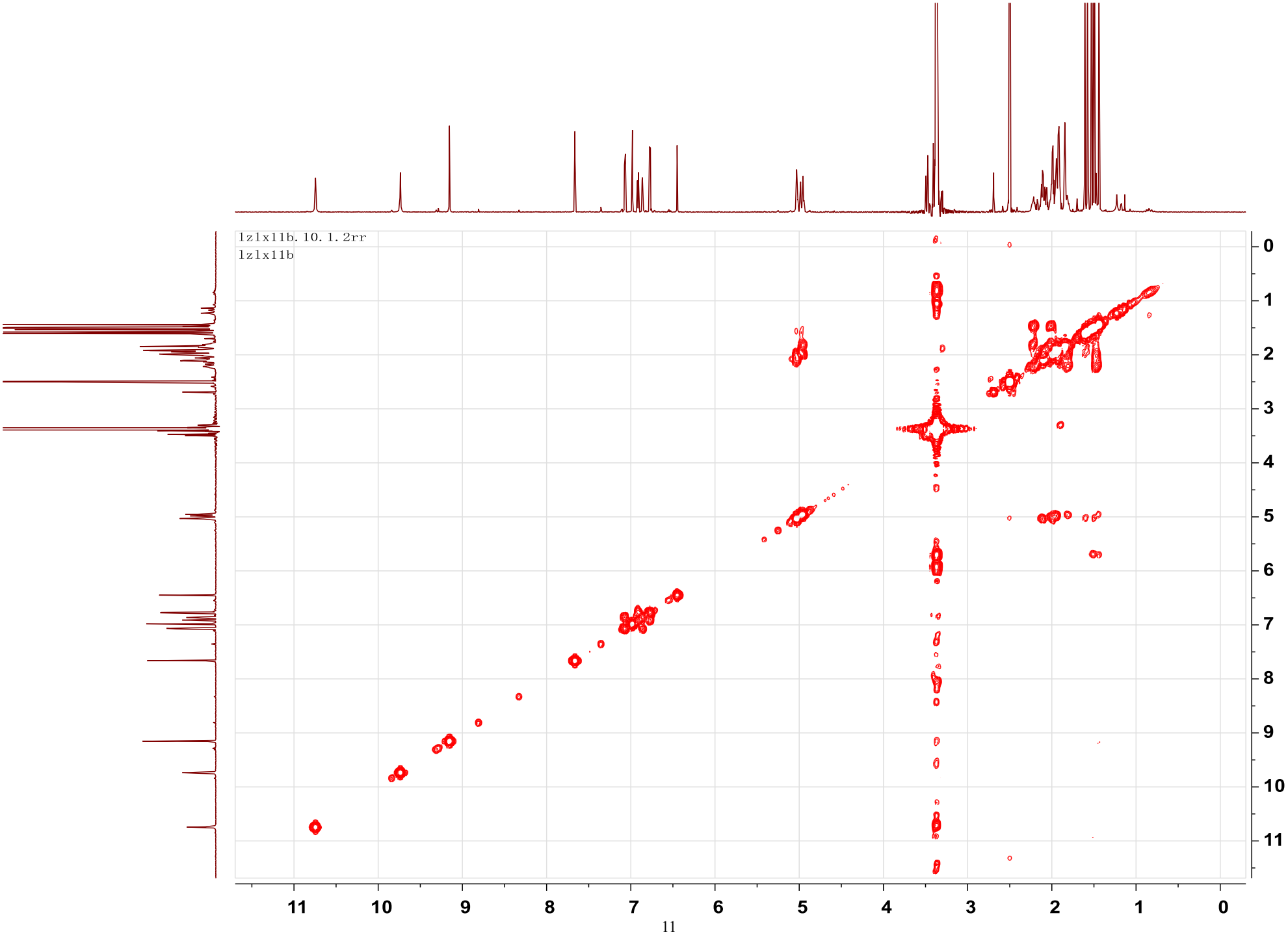


Fig. 8S Enlarged ^{1}H-^{1}H COSY spectra of **1** (DMSO-d_6)

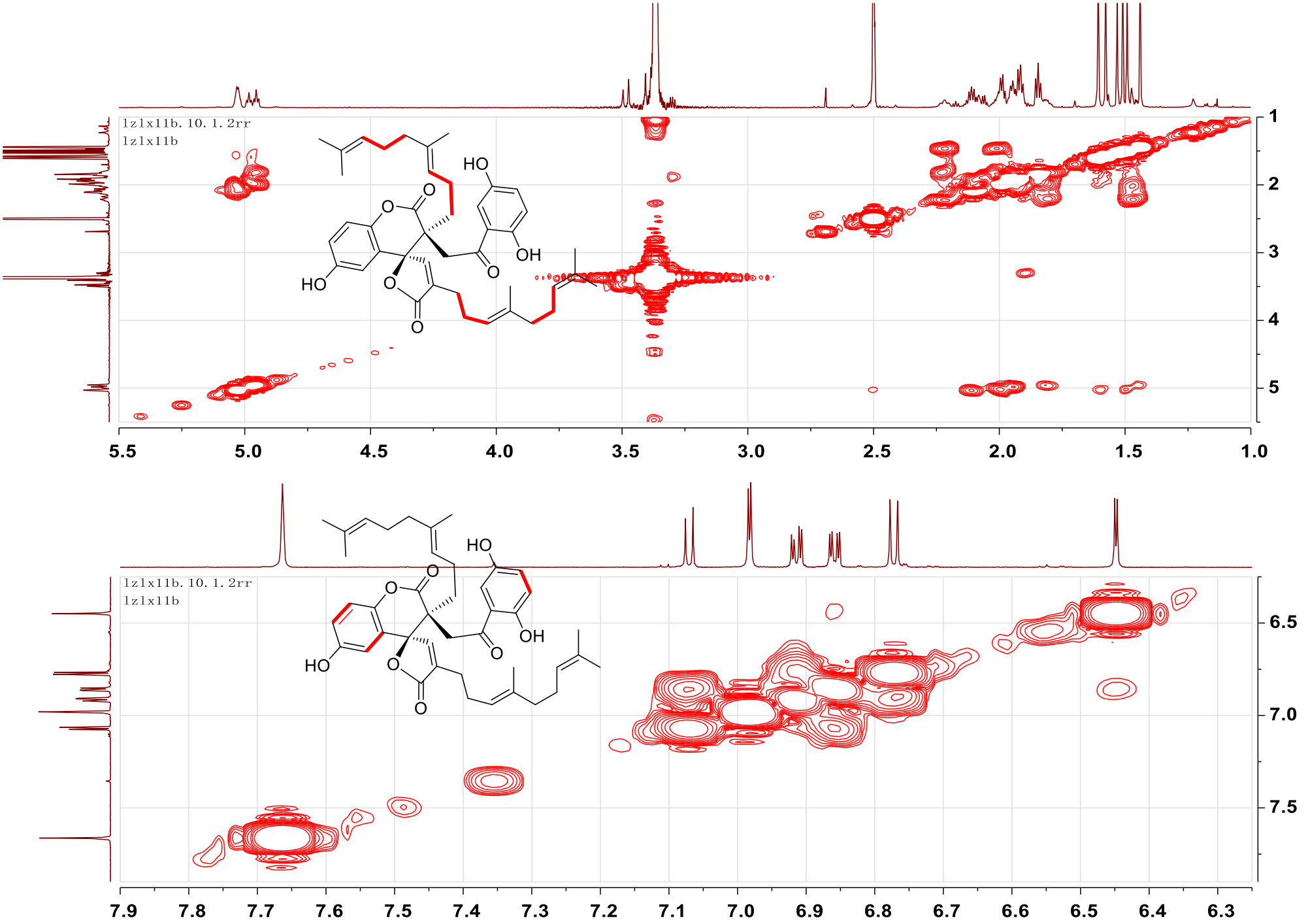


Fig. 9S HMBC spectrum of **1** (DMSO-d_6)

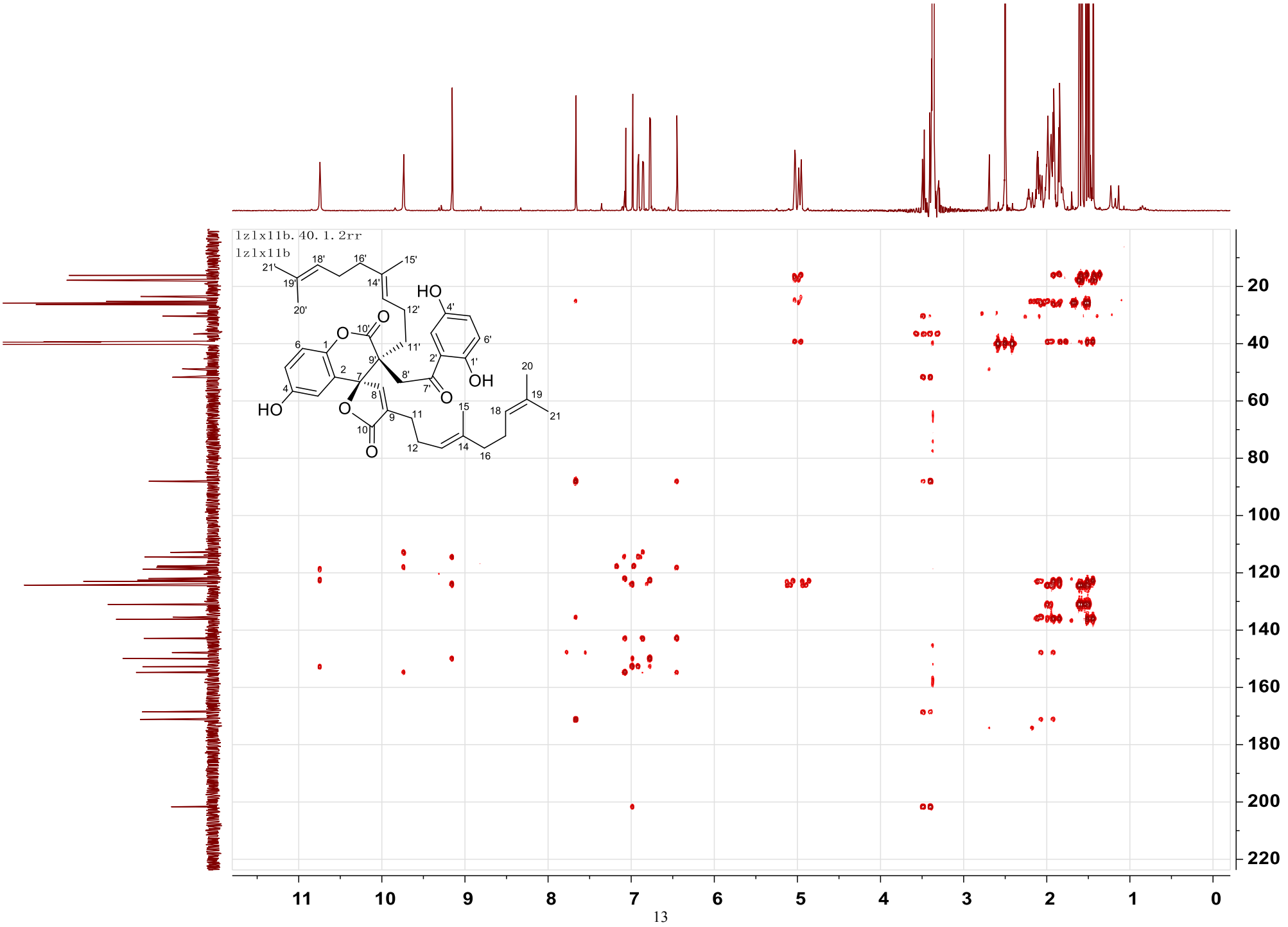


Fig. 10S Enlarged HMBC spectra of **1** (DMSO-d_6) (a)

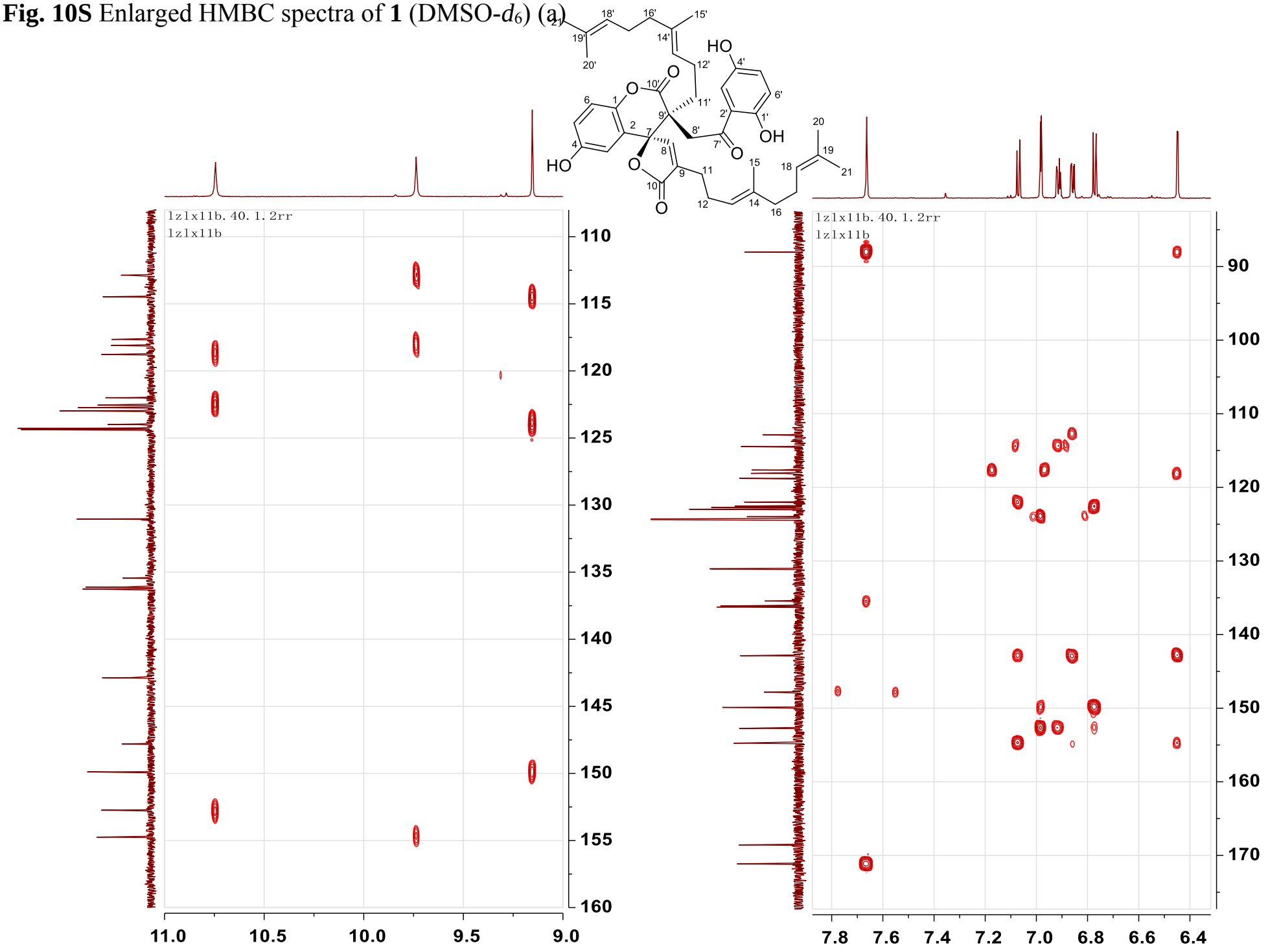


Fig. 11S Enlarged HMBC spectrum of **1** (DMSO-d_6) (b)

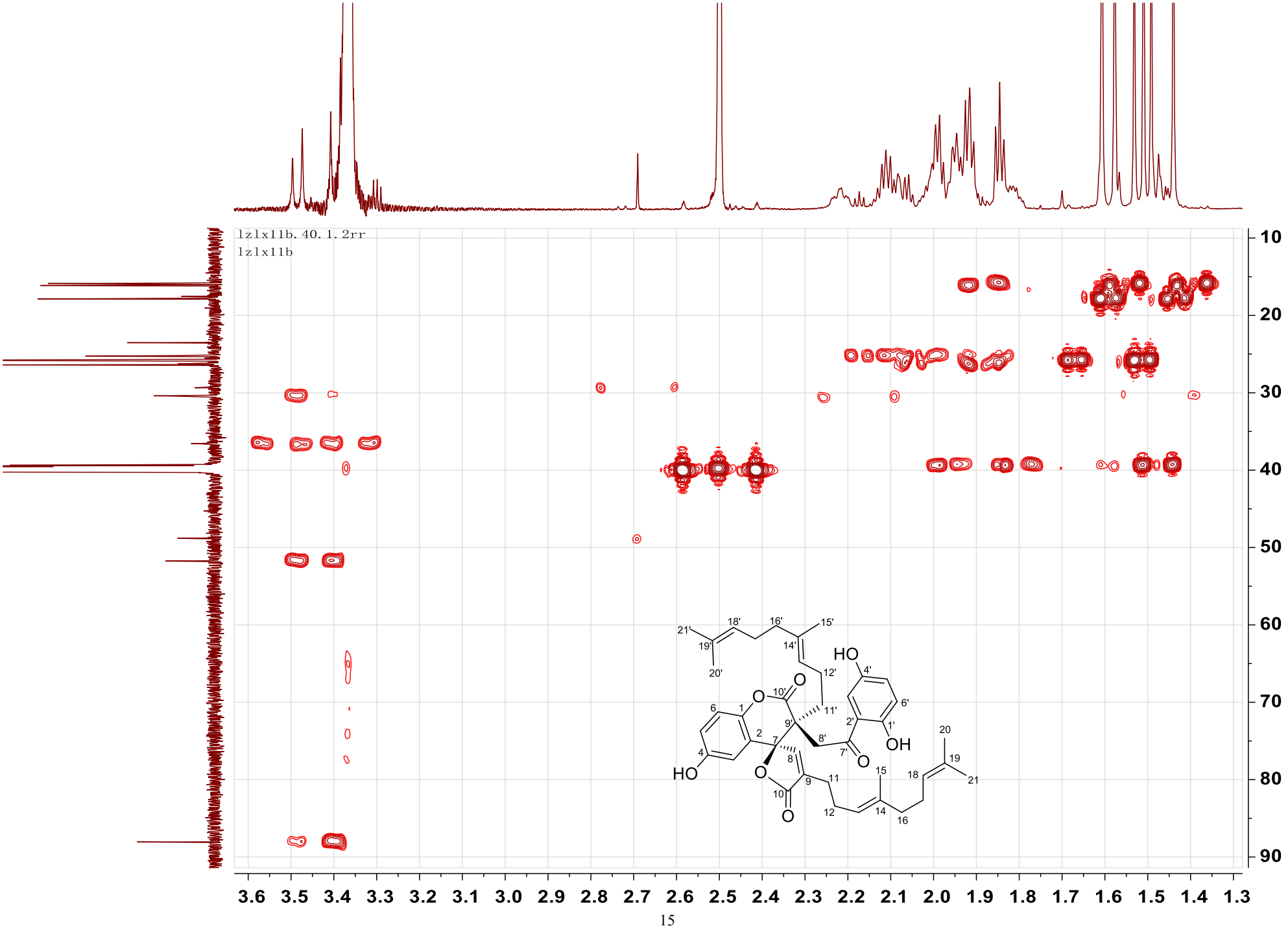


Fig. 12S Enlarged HMBC spectrum of **1** (DMSO-d_6) (c)

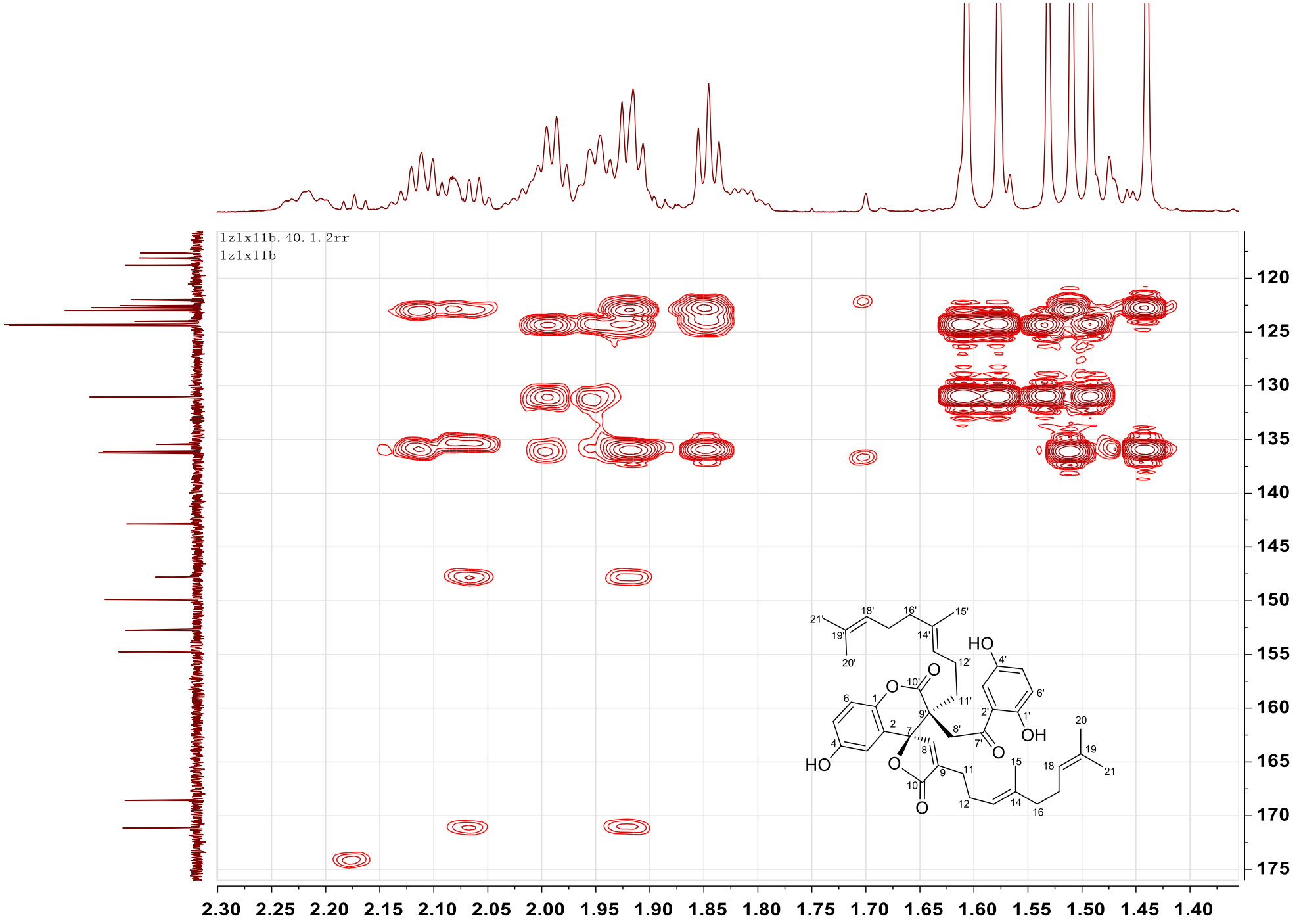


Fig. 13S ROESY spectrum of **1** (DMSO-d_6)

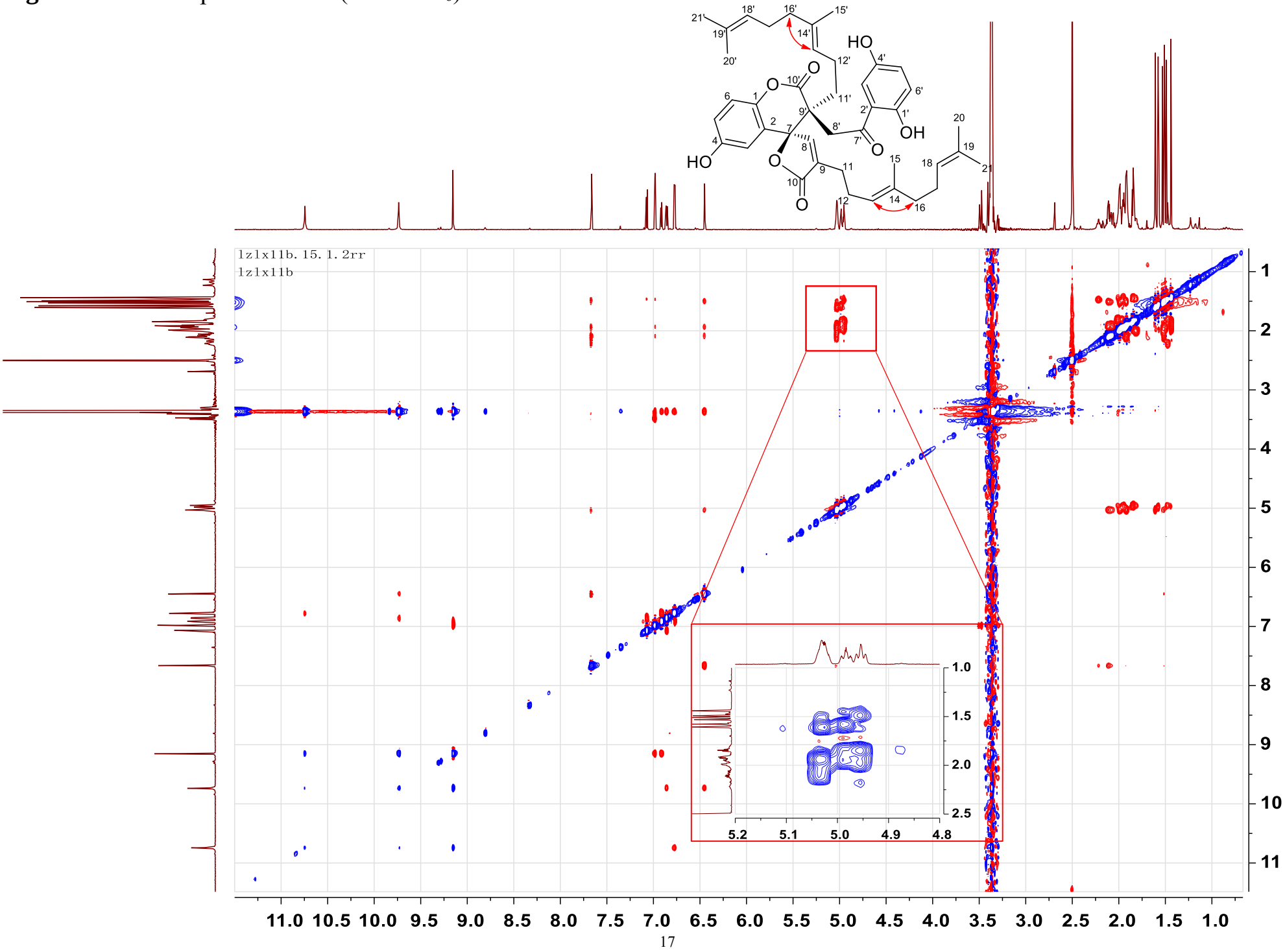


Fig. 14S Enlarged ROESY spectra of **1** (DMSO-d_6)

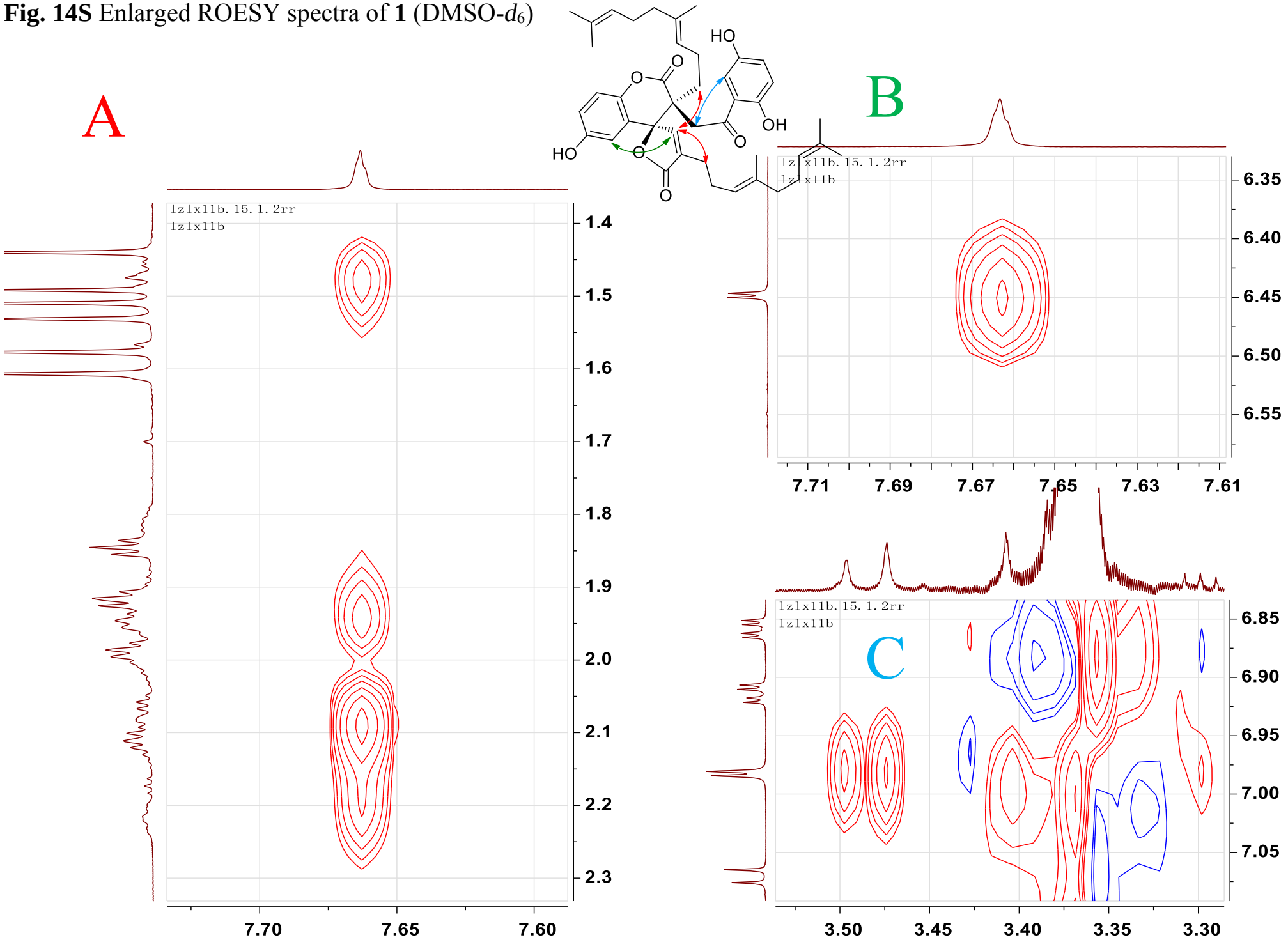


Fig. 15S ^{1}H NMR spectrum of **1** ($CDCl_3$)

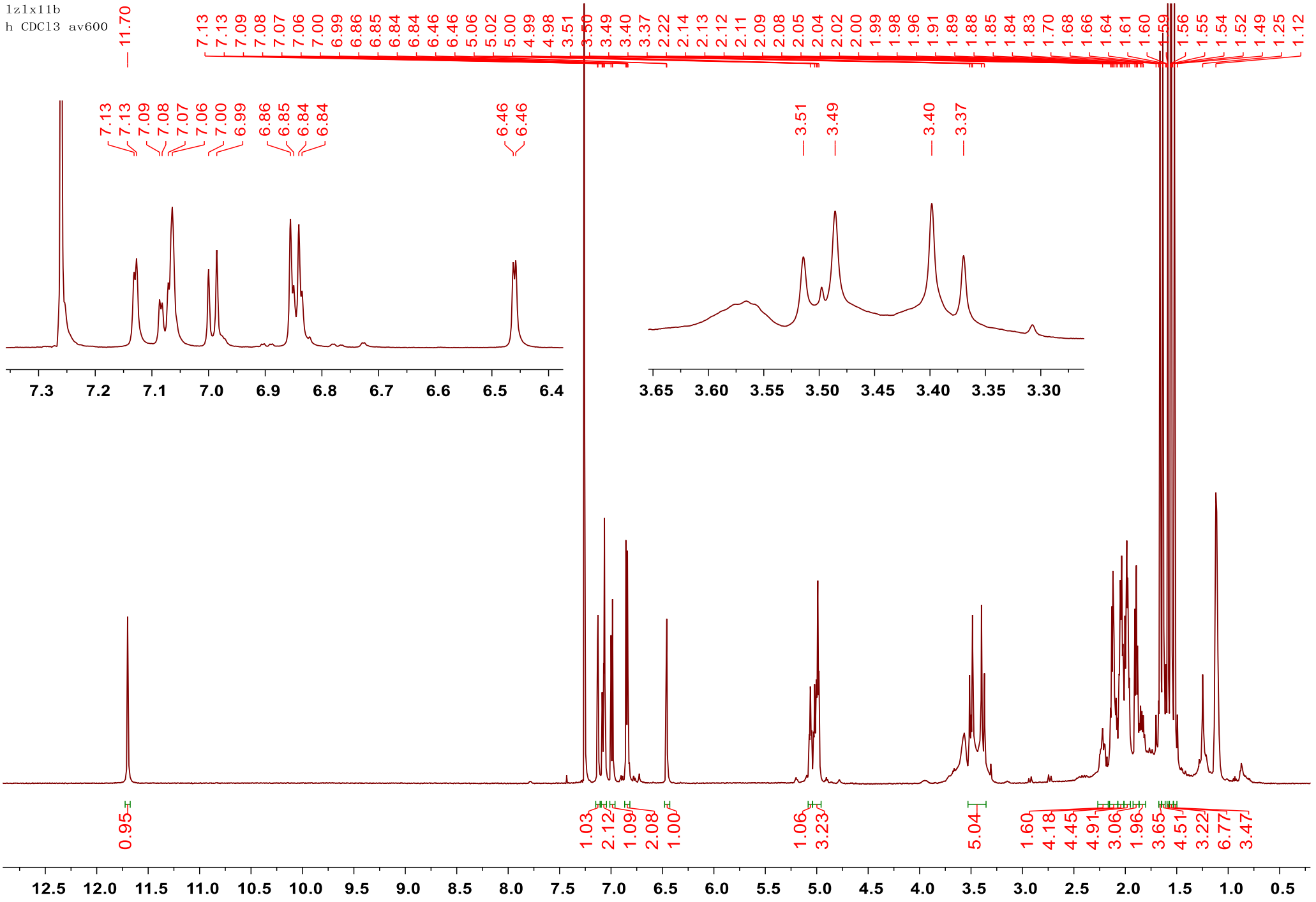


Fig. 16S ^{13}C NMR and DEPT spectra of **1** ($CDCl_3$)

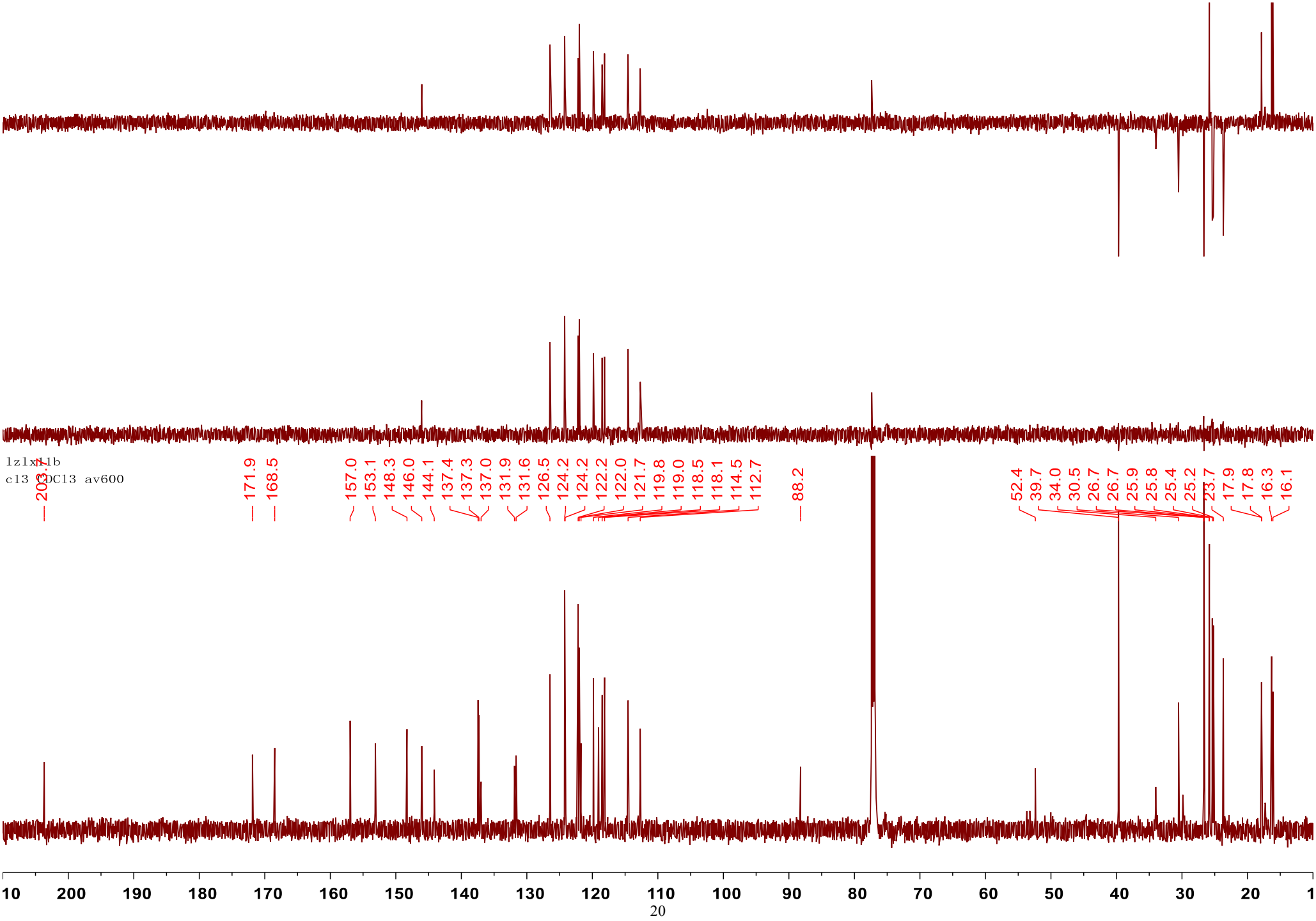


Fig. 17S HSQC spectrum of **1** ($CDCl_3$)

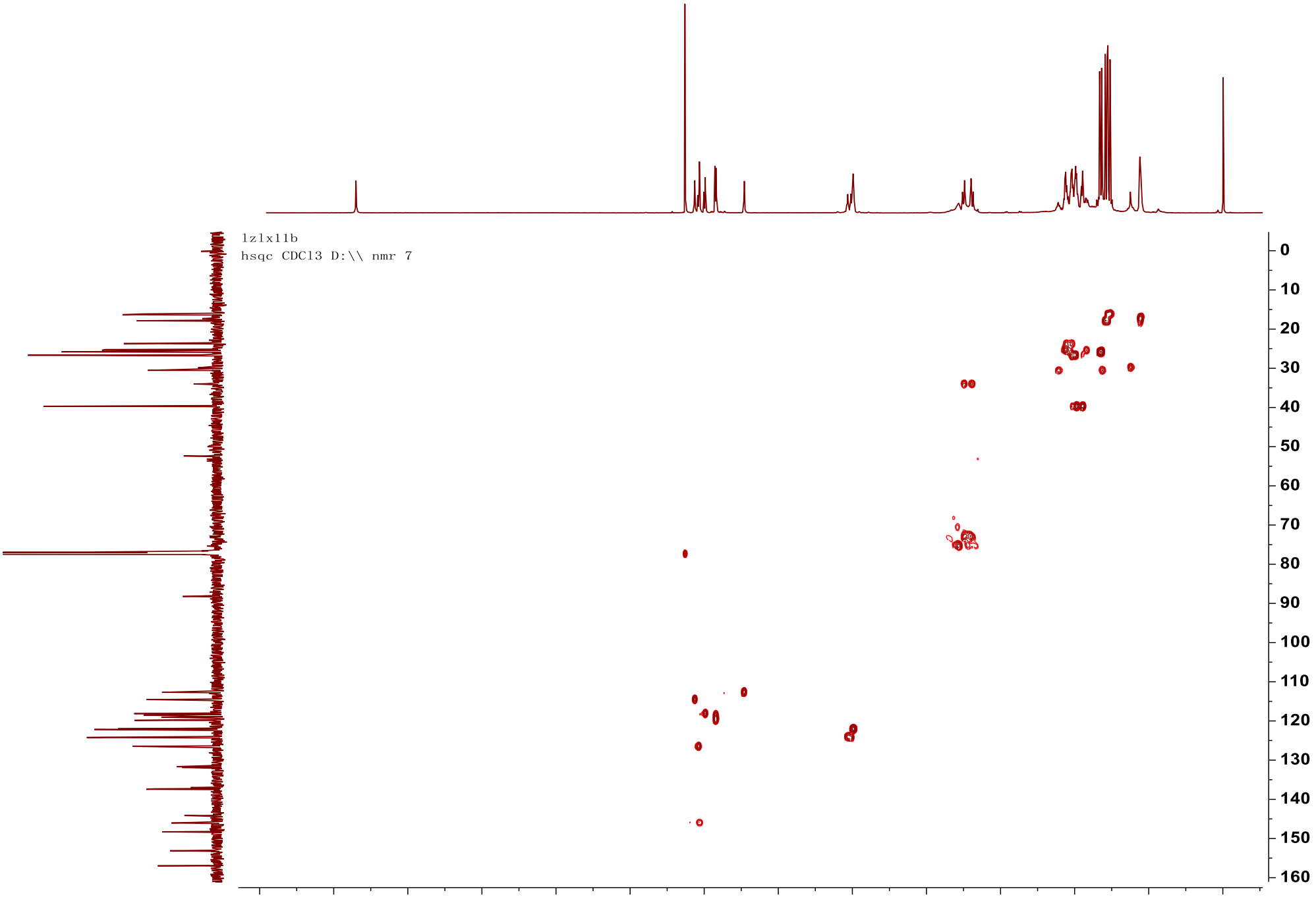


Fig. 18S ^{1}H-^{1}H COSY spectrum of **1** ($CDCl_3$)

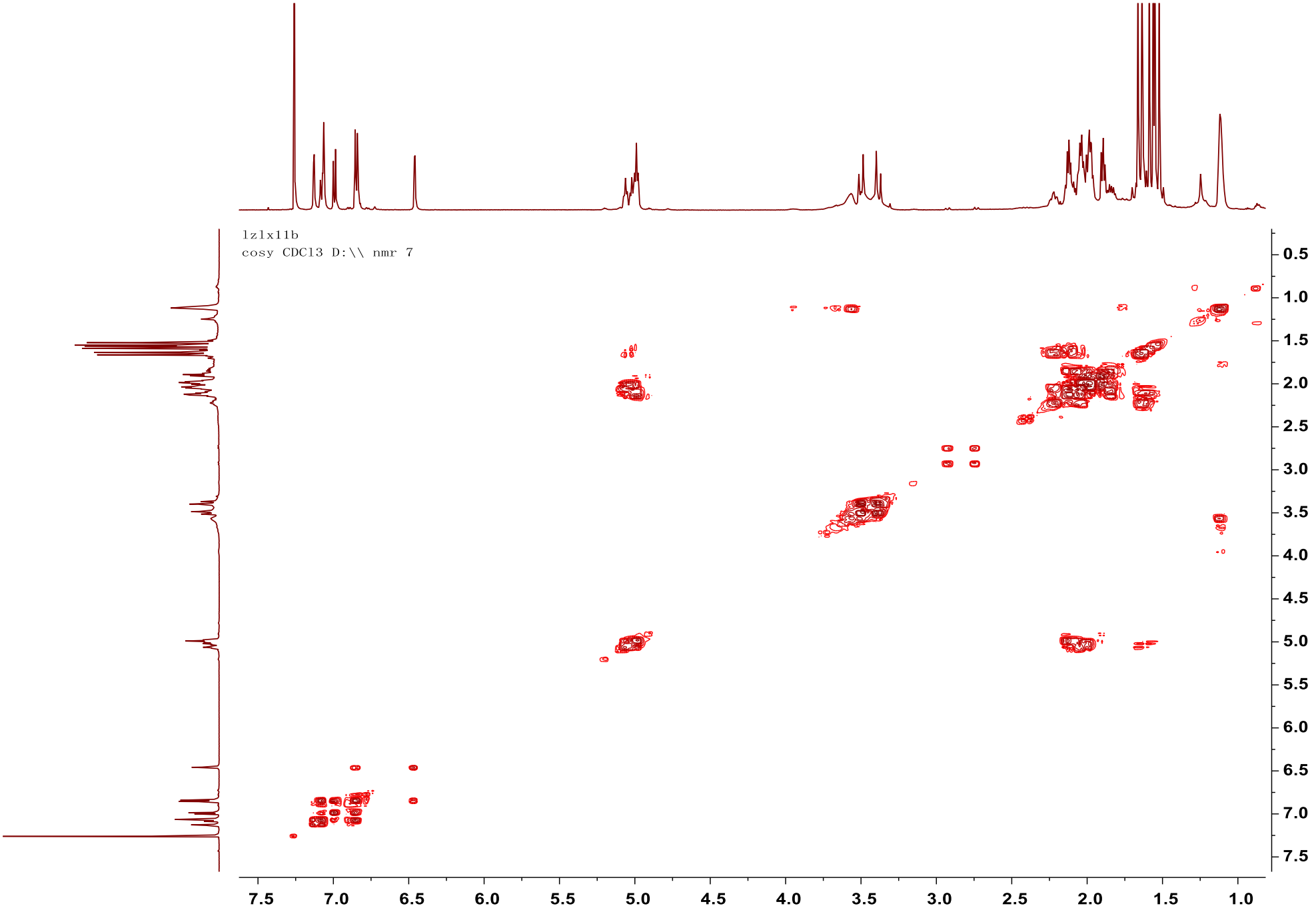


Fig. 19S HMBC spectrum of **1** ($CDCl_3$)

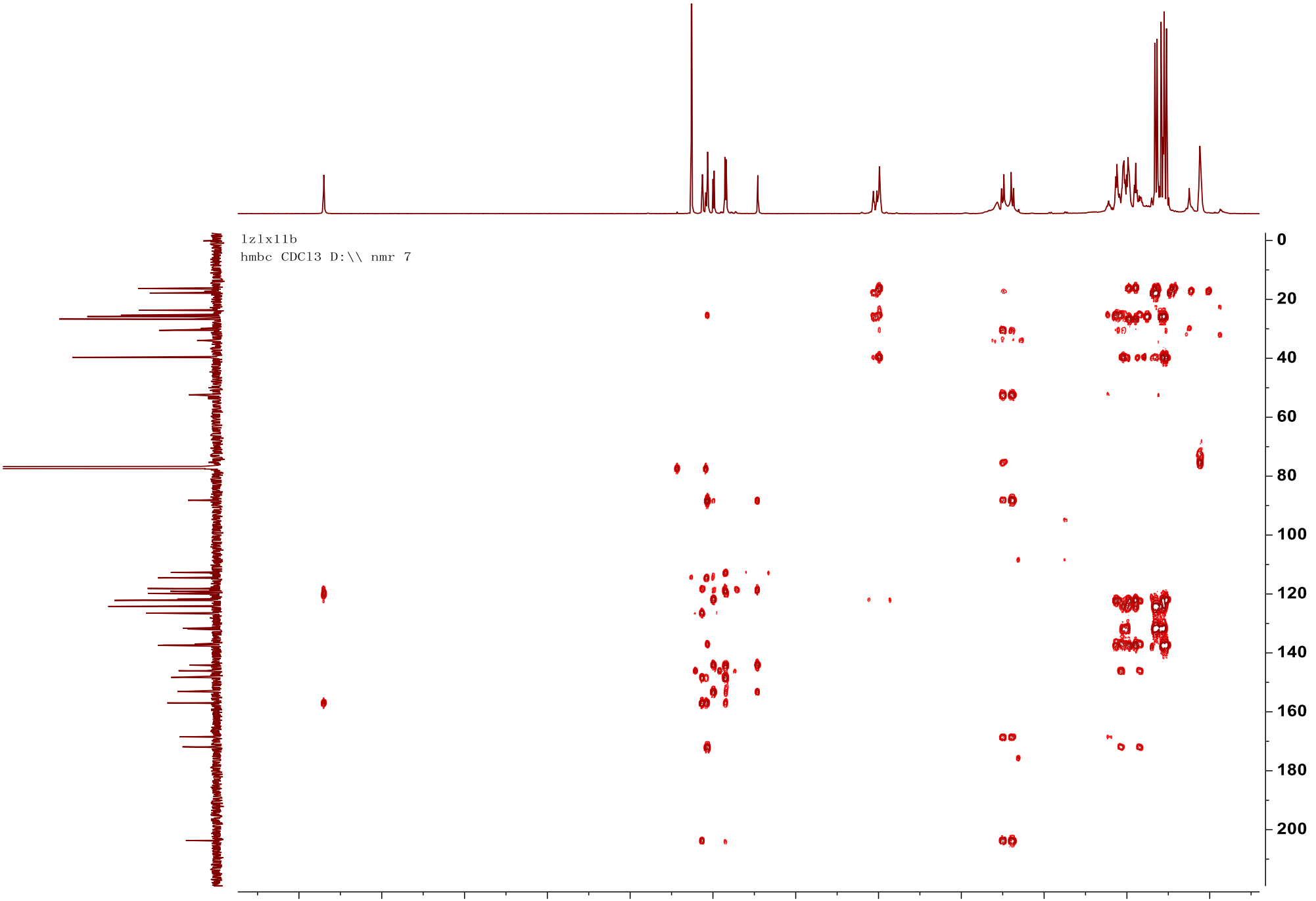


Fig. 20S ROESY spectrum of **1** ($CDCl_3$)

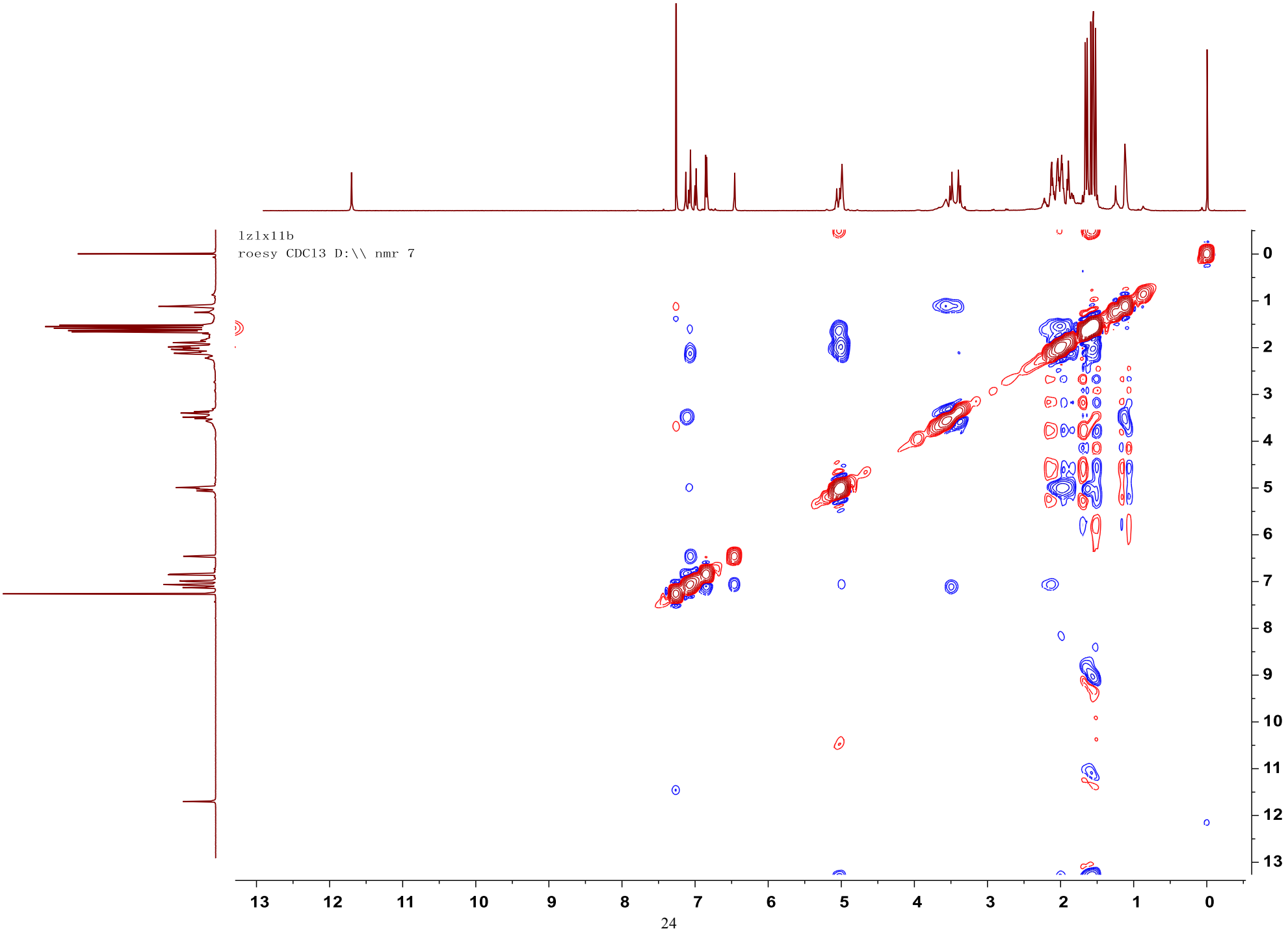


Fig. 21S Chiral phase HPLC chromatograph of **1**.

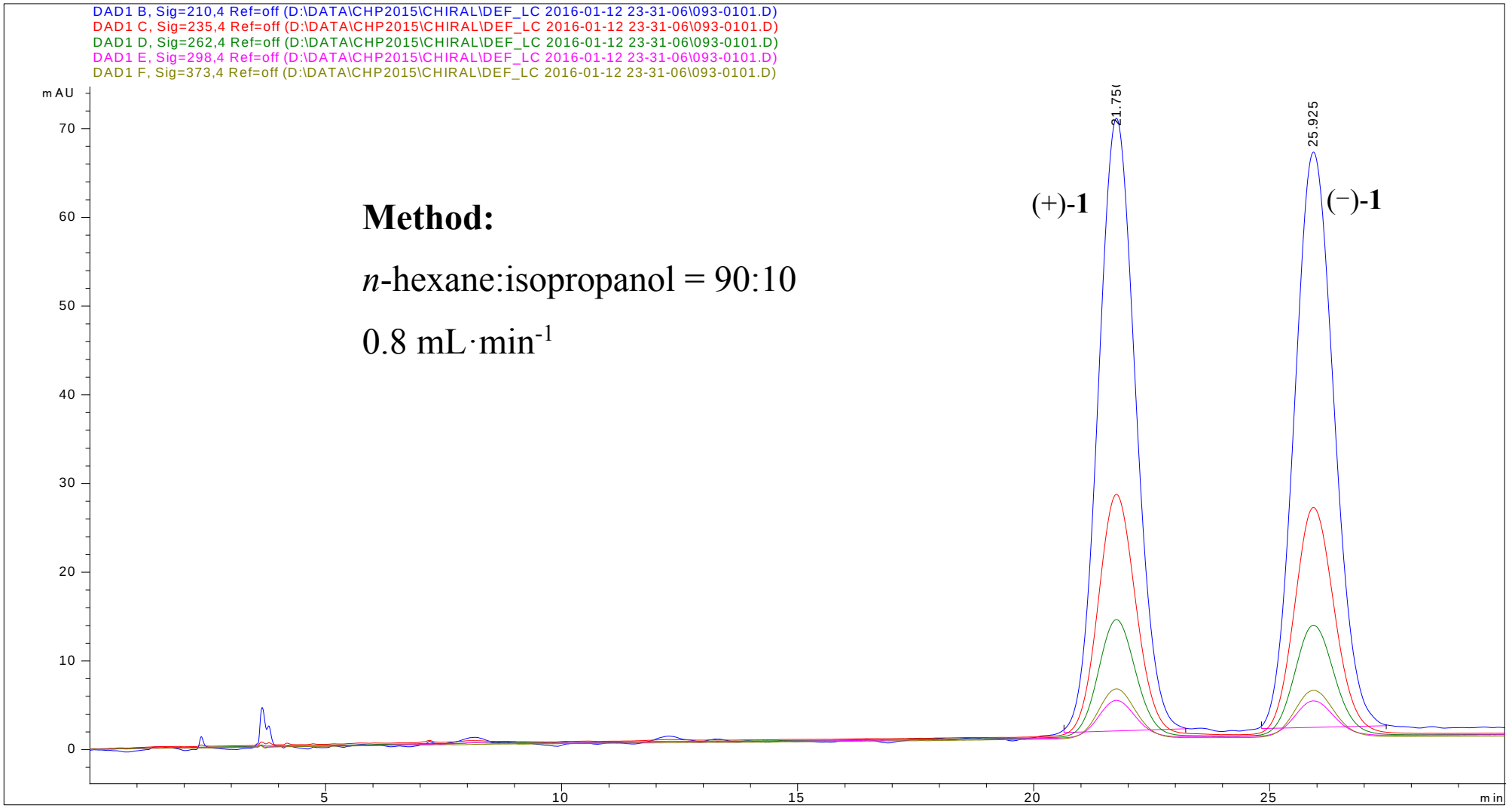
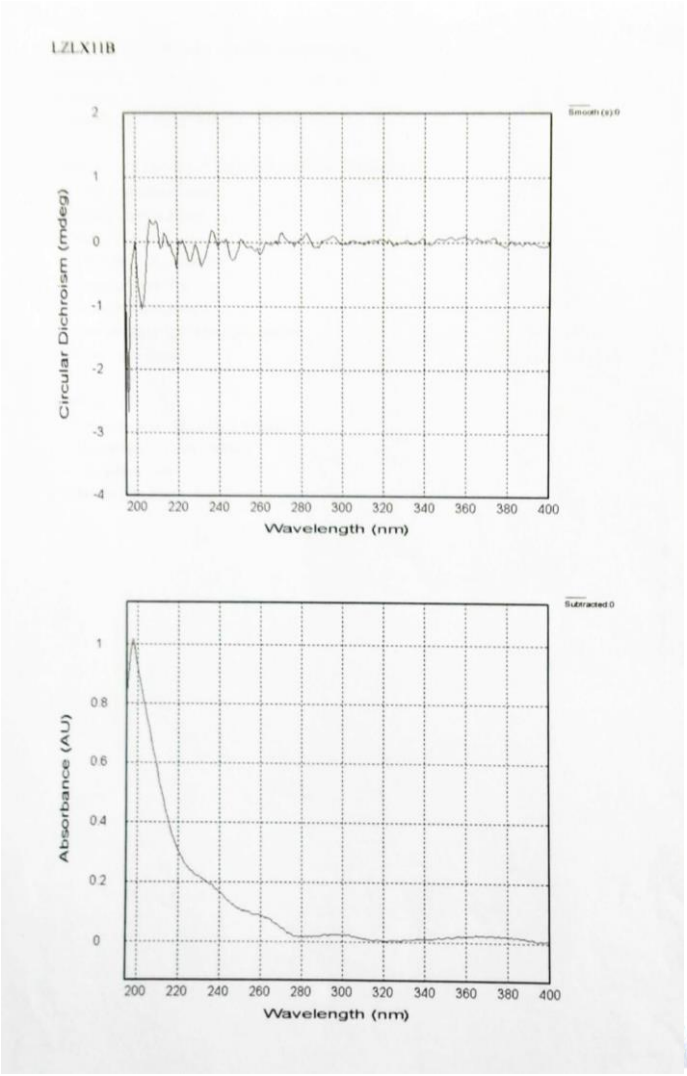


Fig. 22S The CD spectrum of (±)-**1**.



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ProBinaryX
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- Is CFR Compliant : false
- Original unaltered data
Remarks:
- HV (CDDC channel): 0 v
- Time per point: 1 s
- Description: Sample 1
- Concentration: 0.0735mg/mL MeOH
- Pathlength: 1 mm

Settings:
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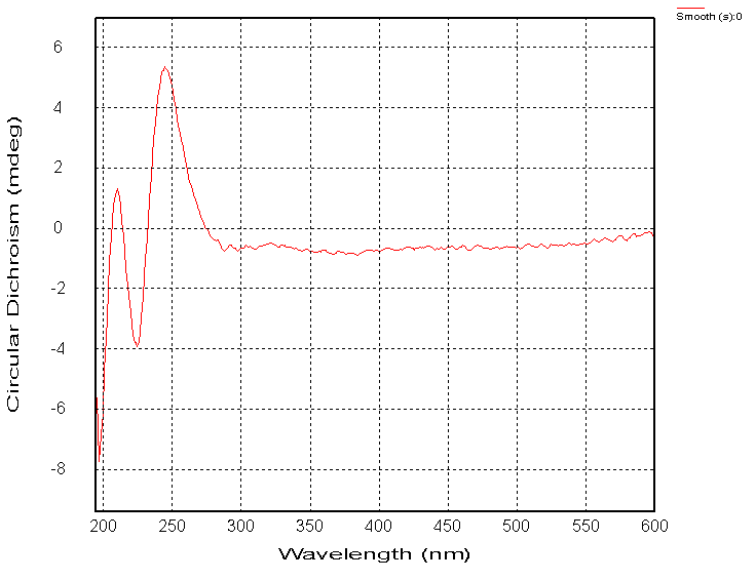
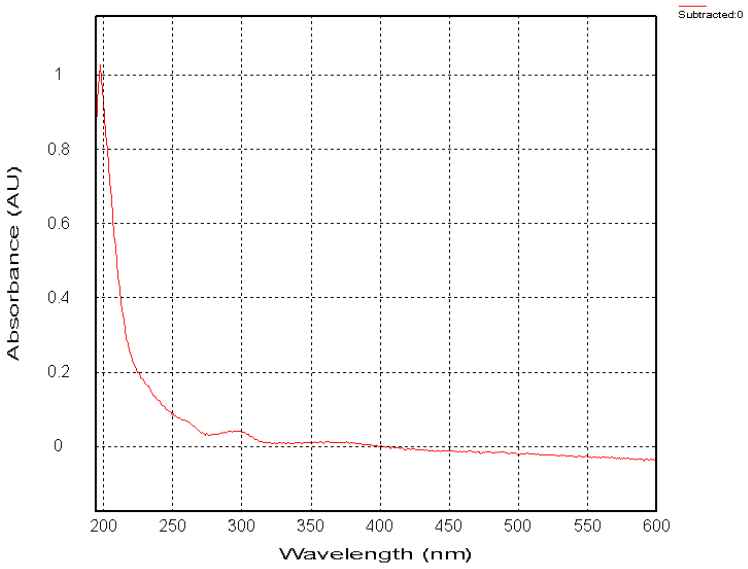
- Wavelength: 195nm - 400nm
- Step Size: 1nm
- Bandwidth: 2nm

Fig. 23S The CD spectrum of (+)-**1**.





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- Is CFR Compliant : false
- Original unaltered data

Remarks:
- HV (CDDC channel): 0 v
- Time per point: 1 s
- Description: Sample 1
- Concentration: 0.0690mg/mL MeOH
- Pathlength: 1 mm

Settings:
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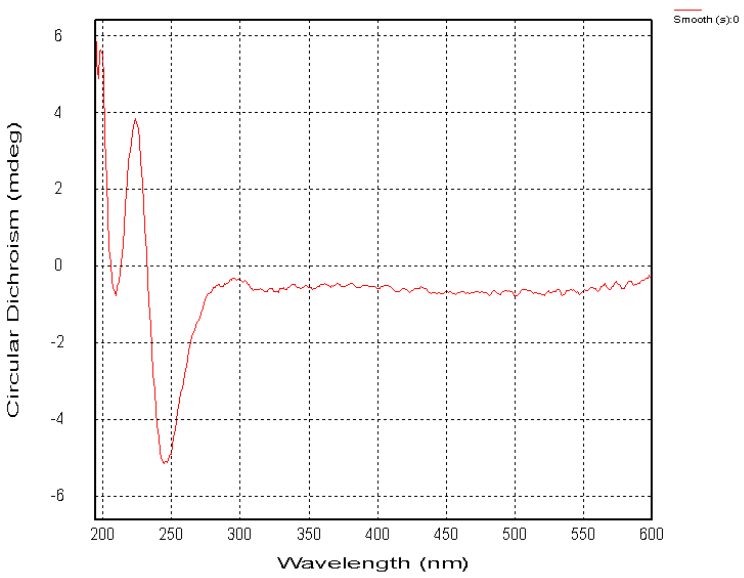
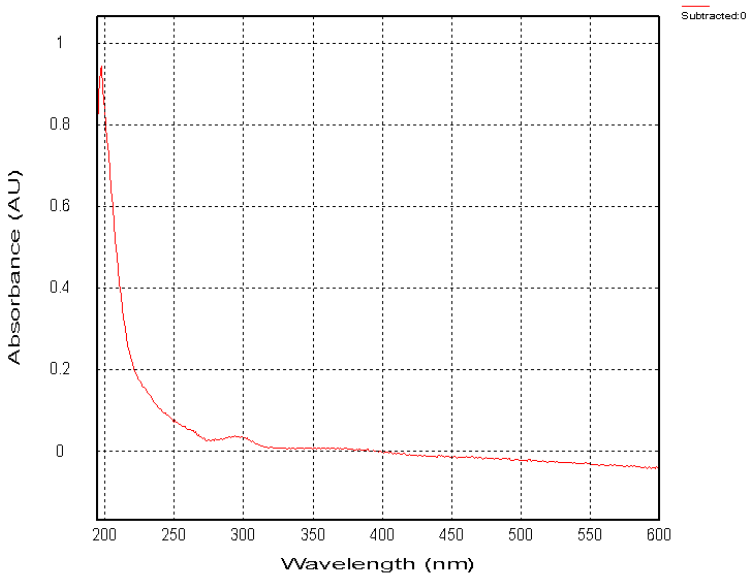
- Wavelength: 195nm - 600nm
- Step Size: 1nm
- Bandwidth: 2nm

Fig. 24S The CD spectrum of (-)-**1**.





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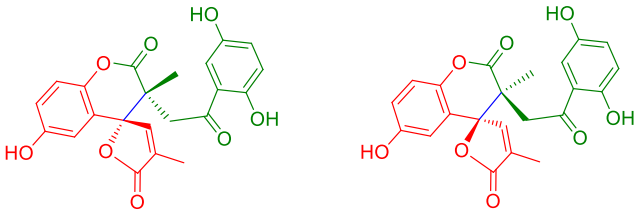
- Is CFR Compliant : false
- Original unaltered data
Remarks:
- HV (CDDC channel): 0 v
- Time per point: 1 s
- Description: Sample 1
- Concentration: 0.0720mg/mL MeOH
- Pathlength: 1 mm

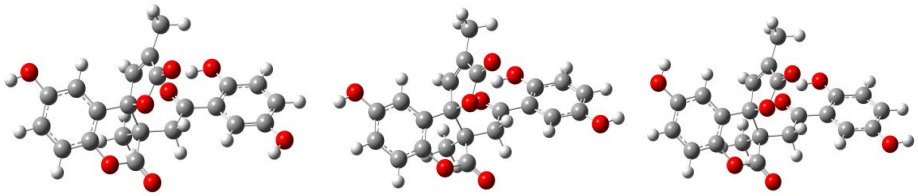
Settings:
- Time-per-point: 1s (25us x 40000)
- Wavelength: 195nm - 600nm
- Step Size: 1nm
- Bandwidth: 2nm

Computational details of the simplified model compound 1a.



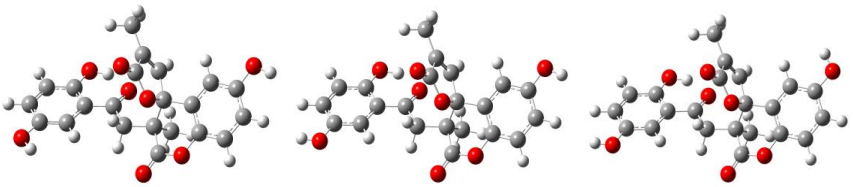
(7*R*,9'*R*)-1a (7*S*,9'*S*)-1a

The CONFLEX searches based on molecular mechanics with MMFF94S force fields were performed for (7*R*,9′*R*)-**1a** and (7*S*,9′*S*)-**1a**, which gave 54 and 54 stable conformers, respectively.[1,2] Selected conformers (10 and 10) with distributions higher than 1% were further optimized by the density functional theory method at the B3LYP/6-31G* level in Gaussian 09 program package,[3] leading to three minimum geometries, respectively, which were further checked by frequency calculation and resulted in no imaginary frequencies. The ECD were calculated using TD-DFT-B3LYP/6-31G (d,p) of theory on B3LYP/6-31G(d) optimized geometry through the IEFPCM model (in MeOH). The calculated ECD curves for (7*R*,9′*R*)-**1a** and (7*S*,9′*S*)-**1a**, and weighted ECD were all generated using SpecDis 1.60 with σ = 0.16 eV, and UV shift 0 nm, respectively.[4]



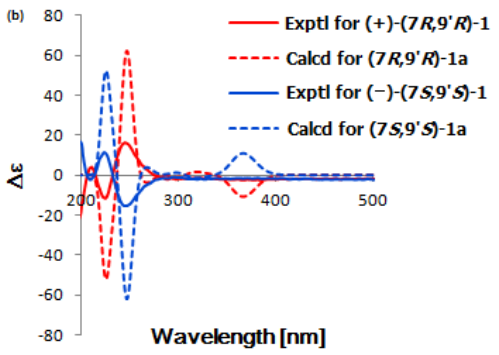
(7*R*,9'*R*)-**1a1** (42.23%) (7*R*,9'*R*)-**1a2** (30.65%) (7*R*,9'*R*)-**1a3** (27.12%)

Three optimized conformers of (7*R*,9'*R*)-**1a** at B3LYP/6-31G(d) level.



(7*S*,9'*S*)-**1a1** (42.23%) (7*S*,9'*S*)-**1a2** (30.65%) (7*S*,9'*S*)-**1a3** (27.12%)

Three optimized conformers of (7*S*,9'*S*)-**1a** at B3LYP/6-31G(d) level.



Experimental CD spectra of **1** and calculated ECD spectra of the model compounds **1a**.

Table 3S Standard orientation of (7*R*,9'*R*)-1a at B3LYP/6-31G(d,p) level.

Standard orientation of (7*R*,9'*R*)-**1a1**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.673471	-1.616910	-0.063233
2	6	0	-5.572608	-0.587726	-0.292351
3	6	0	-5.118233	0.714024	-0.406079
4	6	0	-3.762627	0.987171	-0.286346
5	6	0	-2.861112	-0.035336	-0.056092
6	6	0	-3.332273	-1.332467	0.051269
7	8	0	-2.485973	-2.383031	0.291694
8	6	0	-1.369105	0.169054	0.140713
9	6	0	-0.885210	1.546560	-0.232897
10	6	0	-0.468267	2.192082	0.838622
11	6	0	-0.618601	1.274950	1.998306
12	8	0	-0.351087	1.466220	3.131896
13	6	0	3.766358	-0.907900	0.428709
14	6	0	3.257431	-0.046659	-0.569214
15	6	0	4.139527	0.823541	-1.212528
16	6	0	5.491922	0.823670	-0.847927
17	6	0	5.958873	-0.017315	0.123174
18	6	0	5.088537	-0.898874	0.773170
19	8	0	5.626250	-1.705476	1.721432
20	8	0	3.790311	1.682327	-2.172487
21	6	0	1.817839	-0.055992	-0.939751
22	8	0	1.403747	0.665673	-1.816352
23	6	0	0.905715	-1.016617	-0.198864
24	6	0	-0.605473	-1.019803	-0.514131
25	6	0	-1.162455	-2.309409	0.113593
26	6	0	-0.889115	-1.141757	-2.032585
27	8	0	-0.502011	-3.251286	0.383680
28	8	0	-1.116426	0.110985	1.544804
29	8	0	-5.939854	1.762992	-0.635073
30	6	0	0.088256	3.570615	1.000896
31	1	0	-5.005845	-2.633530	0.029115
32	1	0	-6.622432	-0.807044	-0.382893
33	1	0	-3.439997	2.006813	-0.368630
34	1	0	-0.903141	1.909258	-1.240027
35	1	0	3.108144	-1.591017	0.931540
36	1	0	6.148819	1.504045	-1.356009
37	1	0	6.996351	-0.016449	0.401699
38	1	0	4.960576	-2.244160	2.126037
39	1	0	2.859400	1.589337	-2.359928
40	1	0	1.276537	-2.013035	-0.401868
41	1	0	1.040646	-0.874727	0.865338
42	1	0	-0.257752	-1.917732	-2.449885
43	1	0	-1.918070	-1.413283	-2.227718
44	1	0	-0.669617	-0.221966	-2.549218

45	1	0	-6.844409	1.484549	-0.668305
46	1	0	0.134210	4.085330	0.049455
47	1	0	-0.524975	4.148746	1.683375
48	1	0	1.086450	3.528216	1.422468

Standard orientation of (7*R*,9'*R*)-**1a2**:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.675381	-1.617626	-0.054603
2	6	0	-5.573300	-0.588953	-0.290470
3	6	0	-5.117433	0.711542	-0.411994
4	6	0	-3.761704	0.983924	-0.293054
5	6	0	-2.861322	-0.038135	-0.055942
6	6	0	-3.333782	-1.334106	0.058930
7	8	0	-2.489139	-2.383930	0.305179
8	6	0	-1.369311	0.165936	0.142309
9	6	0	-0.885089	1.541384	-0.238769
10	6	0	-0.473448	2.194498	0.830085
11	6	0	-0.629377	1.285612	1.995675
12	8	0	-0.372586	1.488091	3.129685
13	6	0	3.768237	-0.913085	0.417581
14	6	0	3.259689	-0.051337	-0.566539
15	6	0	4.138442	0.834223	-1.207055
16	6	0	5.483092	0.838979	-0.843773
17	6	0	5.956152	-0.014351	0.124115
18	6	0	5.096282	-0.902675	0.763262
19	8	0	5.512729	-1.770270	1.720222
20	8	0	3.777703	1.698469	-2.160380
21	6	0	1.815966	-0.066475	-0.934411
22	8	0	1.401810	0.651622	-1.812938
23	6	0	0.906017	-1.023916	-0.187570
24	6	0	-0.605273	-1.026735	-0.505079
25	6	0	-1.165108	-2.314692	0.123453
26	6	0	-0.887282	-1.154721	-2.023643
27	8	0	-0.507984	-3.259614	0.388645
28	8	0	-1.120227	0.116857	1.547223
29	8	0	-5.938127	1.760001	-0.648127
30	6	0	0.079868	3.575044	0.985809
31	1	0	-5.008789	-2.633345	0.043748
32	1	0	-6.623344	-0.807682	-0.380228
33	1	0	-3.437993	2.002735	-0.381111
34	1	0	-0.900169	1.897591	-1.248248
35	1	0	3.132538	-1.608829	0.927743
36	1	0	6.139356	1.526106	-1.343450
37	1	0	7.000866	0.006840	0.385274
38	1	0	6.434628	-1.656669	1.901985
39	1	0	2.848863	1.593699	-2.350108
40	1	0	1.276850	-2.021562	-0.384316
41	1	0	1.042680	-0.876986	0.875809

42	1	0	-0.253240	-1.930307	-2.437504
43	1	0	-1.915237	-1.430510	-2.218356
44	1	0	-0.671133	-0.236236	-2.543993
45	1	0	-6.842889	1.481980	-0.678589
46	1	0	0.128220	4.084171	0.031434
47	1	0	-0.536858	4.156048	1.662681
48	1	0	1.076621	3.537140	1.411262

Standard orientation of (7*R*,9'*R*)-**1a3**:

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	-4.680774	-1.628474	-0.060967
2	6	0	-5.580651	-0.607543	-0.279125
3	6	0	-5.128616	0.701025	-0.387350
4	6	0	-3.777977	0.976208	-0.275553
5	6	0	-2.865412	-0.049455	-0.054761
6	6	0	-3.332592	-1.340411	0.050243
7	8	0	-2.489569	-2.393939	0.286114
8	6	0	-1.373291	0.162583	0.135702
9	6	0	-0.894515	1.535868	-0.261123
10	6	0	-0.479790	2.201179	0.799026
11	6	0	-0.628440	1.303464	1.974608
12	8	0	-0.368413	1.520231	3.105245
13	6	0	3.766285	-0.915802	0.426221
14	6	0	3.260200	-0.053027	-0.558388
15	6	0	4.140708	0.832763	-1.196155
16	6	0	5.484518	0.836905	-0.829819
17	6	0	5.955068	-0.017242	0.138538
18	6	0	5.093492	-0.905943	0.775008
19	8	0	5.507301	-1.774056	1.732433
20	8	0	3.782214	1.698066	-2.149502
21	6	0	1.817397	-0.067309	-0.929338
22	8	0	1.405230	0.652068	-1.807977
23	6	0	0.905574	-1.024936	-0.184932
24	6	0	-0.604904	-1.030290	-0.506849
25	6	0	-1.164388	-2.319681	0.118549
26	6	0	-0.881383	-1.160739	-2.026387
27	8	0	-0.505561	-3.261661	0.389659
28	8	0	-1.117369	0.129405	1.540231
29	8	0	-6.053669	1.662733	-0.605280
30	6	0	0.076554	3.582404	0.937845
31	1	0	-5.006774	-2.647355	0.029757
32	1	0	-6.632095	-0.805647	-0.367033
33	1	0	-3.434925	1.992231	-0.352327
34	1	0	-0.911275	1.880309	-1.274745
35	1	0	3.129341	-1.611950	0.934266
36	1	0	6.142161	1.524125	-1.327546
37	1	0	6.999157	0.003500	0.402160
38	1	0	6.429771	-1.664041	1.913556

39	1	0	2.854203	1.592226	-2.342437
40	1	0	1.277790	-2.022313	-0.380178
41	1	0	1.039220	-0.877777	0.878786
42	1	0	-0.249116	-1.940473	-2.435167
43	1	0	-1.909688	-1.432253	-2.224633
44	1	0	-0.658000	-0.245066	-2.548592
45	1	0	-5.656451	2.522276	-0.612410
46	1	0	0.115899	4.084211	-0.020906
47	1	0	-0.530827	4.169786	1.617752
48	1	0	1.077927	3.546169	1.352365

Table 4S Standard orientation of (7*S*,9'*S*)-1a at B3LYP/6-31G(d,p) level.

Standard orientation of (7*S*,9'*S*)-**1a1**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.673471	-1.616910	-0.063233
2	6	0	5.572608	-0.587726	-0.292351
3	6	0	5.118233	0.714024	-0.406079
4	6	0	3.762627	0.987171	-0.286346
5	6	0	2.861112	-0.035336	-0.056092
6	6	0	3.332273	-1.332467	0.051269
7	8	0	2.485973	-2.383031	0.291694
8	6	0	1.369105	0.169054	0.140713
9	6	0	0.885210	1.546560	-0.232897
10	6	0	0.468267	2.192082	0.838622
11	6	0	0.618601	1.274950	1.998306
12	8	0	0.351087	1.466220	3.131896
13	6	0	-3.766358	-0.907900	0.428709
14	6	0	-3.257431	-0.046659	-0.569214
15	6	0	-4.139527	0.823541	-1.212528
16	6	0	-5.491922	0.823670	-0.847927
17	6	0	-5.958873	-0.017315	0.123174
18	6	0	-5.088537	-0.898874	0.773170
19	8	0	-5.626250	-1.705476	1.721432
20	8	0	-3.790311	1.682327	-2.172487
21	6	0	-1.817839	-0.055992	-0.939751
22	8	0	-1.403747	0.665673	-1.816352
23	6	0	-0.905715	-1.016617	-0.198864
24	6	0	0.605473	-1.019803	-0.514131
25	6	0	1.162455	-2.309409	0.113593
26	6	0	0.889115	-1.141757	-2.032585
27	8	0	0.502011	-3.251286	0.383680
28	8	0	1.116426	0.110985	1.544804
29	8	0	5.939854	1.762992	-0.635073
30	6	0	-0.088256	3.570615	1.000896
31	1	0	5.005845	-2.633530	0.029115
32	1	0	6.622432	-0.807044	-0.382893
33	1	0	3.439997	2.006813	-0.368630

34	1	0	0.903141	1.909258	-1.240027
35	1	0	-3.108144	-1.591017	0.931540
36	1	0	-6.148819	1.504045	-1.356009
37	1	0	-6.996351	-0.016449	0.401699
38	1	0	-4.960576	-2.244160	2.126037
39	1	0	-2.859400	1.589337	-2.359928
40	1	0	-1.040646	-0.874727	0.865338
41	1	0	-1.276537	-2.013035	-0.401868
42	1	0	0.257752	-1.917732	-2.449885
43	1	0	0.669617	-0.221966	-2.549218
44	1	0	1.918070	-1.413283	-2.227718
45	1	0	6.844409	1.484549	-0.668305
46	1	0	-0.134210	4.085330	0.049455
47	1	0	-1.086450	3.528216	1.422468
48	1	0	0.524975	4.148746	1.683375

Standard orientation of (7*S*,9'*S*)-**1a2**

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	4.675381	-1.617626	-0.054603
2	6	0	5.573300	-0.588953	-0.290470
3	6	0	5.117433	0.711542	-0.411994
4	6	0	3.761704	0.983924	-0.293054
5	6	0	2.861322	-0.038135	-0.055942
6	6	0	3.333782	-1.334106	0.058930
7	8	0	2.489139	-2.383930	0.305179
8	6	0	1.369311	0.165936	0.142309
9	6	0	0.885089	1.541384	-0.238769
10	6	0	0.473448	2.194498	0.830085
11	6	0	0.629377	1.285612	1.995675
12	8	0	0.372586	1.488091	3.129685
13	6	0	-3.768237	-0.913085	0.417581
14	6	0	-3.259689	-0.051337	-0.566539
15	6	0	-4.138442	0.834223	-1.207055
16	6	0	-5.483092	0.838979	-0.843773
17	6	0	-5.956152	-0.014351	0.124115
18	6	0	-5.096282	-0.902675	0.763262
19	8	0	-5.512729	-1.770270	1.720222
20	8	0	-3.777703	1.698469	-2.160380
21	6	0	-1.815966	-0.066475	-0.934411
22	8	0	-1.401810	0.651622	-1.812938
23	6	0	-0.906017	-1.023916	-0.187570
24	6	0	0.605273	-1.026735	-0.505079
25	6	0	1.165108	-2.314692	0.123453
26	6	0	0.887282	-1.154721	-2.023643
27	8	0	0.507984	-3.259614	0.388645
28	8	0	1.120227	0.116857	1.547223
29	8	0	5.938127	1.760001	-0.648127
30	6	0	-0.079868	3.575044	0.985809

31	1	0	5.008789	-2.633345	0.043748
32	1	0	6.623344	-0.807682	-0.380228
33	1	0	3.437993	2.002735	-0.381111
34	1	0	0.900169	1.897591	-1.248248
35	1	0	-3.132538	-1.608829	0.927743
36	1	0	-6.139356	1.526106	-1.343450
37	1	0	-7.000866	0.006840	0.385274
38	1	0	-6.434628	-1.656669	1.901985
39	1	0	-2.848863	1.593699	-2.350108
40	1	0	-1.042680	-0.876986	0.875809
41	1	0	-1.276850	-2.021562	-0.384316
42	1	0	0.253240	-1.930307	-2.437504
43	1	0	0.671133	-0.236236	-2.543993
44	1	0	1.915237	-1.430510	-2.218356
45	1	0	6.842889	1.481980	-0.678589
46	1	0	-0.128220	4.084171	0.031434
47	1	0	-1.076621	3.537140	1.411262
48	1	0	0.536858	4.156048	1.662681

Standard orientation of (7*S*,9'*S*)-**1a3**:

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	4.715389	-1.643636	-0.062703
2	6	0	5.619245	-0.607517	-0.267577
3	6	0	5.156354	0.708480	-0.367268
4	6	0	3.789328	0.976755	-0.263032
5	6	0	2.874010	-0.059523	-0.058387
6	6	0	3.355449	-1.363682	0.041371
7	8	0	2.515185	-2.443421	0.277582
8	6	0	1.382631	0.158504	0.127290
9	6	0	0.902461	1.519325	-0.299992
10	6	0	0.477505	2.223463	0.754834
11	6	0	0.619701	1.370922	1.961555
12	8	0	0.352970	1.625185	3.109281
13	6	0	-3.779760	-0.906946	0.470912
14	6	0	-3.261802	-0.078385	-0.548948
15	6	0	-4.149144	0.800419	-1.232872
16	6	0	-5.504666	0.823877	-0.874597
17	6	0	-5.985923	-0.000050	0.130330
18	6	0	-5.123097	-0.874599	0.810708
19	8	0	-5.550328	-1.711831	1.809888
20	8	0	-3.751975	1.623829	-2.221148
21	6	0	-1.836239	-0.096040	-0.915289
22	8	0	-1.406475	0.657360	-1.808990
23	6	0	-0.909628	-1.028391	-0.155519
24	6	0	0.599439	-1.049944	-0.494095
25	6	0	1.158587	-2.347844	0.127144
26	6	0	0.856930	-1.180394	-2.020093
27	8	0	0.489906	-3.310618	0.407722

28	8	0	1.128730	0.149047	1.568552
29	8	0	6.088584	1.689885	-0.570150
30	6	0	-0.082836	3.603928	0.849909
31	1	0	5.048678	-2.672162	0.022714
32	1	0	6.683284	-0.799947	-0.351262
33	1	0	3.431641	2.000864	-0.332192
34	1	0	0.921009	1.842433	-1.332356
35	1	0	-3.138687	-1.589830	1.014964
36	1	0	-6.162265	1.501865	-1.407725
37	1	0	-7.041843	0.031879	0.392623
38	1	0	-6.500083	-1.579094	1.954300
39	1	0	-2.782387	1.458053	-2.339488
40	1	0	-1.025430	-0.840848	0.917453
41	1	0	-1.282142	-2.048867	-0.293923
42	1	0	0.316619	-2.053056	-2.400930
43	1	0	0.490441	-0.301690	-2.548798
44	1	0	1.918164	-1.318733	-2.239356
45	1	0	5.646258	2.553129	-0.591818
46	1	0	-0.119360	4.092135	-0.127164
47	1	0	-1.096371	3.578012	1.266665
48	1	0	0.516095	4.218021	1.532331

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(1) Goto, H.; Osawa, E.; *J. Am. Chem. Soc.* **1989**, *111*, 8950–8951.

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(3) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A.; Jr., Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; and Fox, D. J.; Gaussian *09*, Revision B.01,Gaussian, Inc., Wallingford CT, 2010.

(4) Bruhn, T.; Schaumlöffel, A.; Hemberger, Y.; Bringmann, G. *Spec Dis*, version 1.60, University of Würzburg, Germany, 2012.

Fig. 25S ESIMS (−) report of **1**.

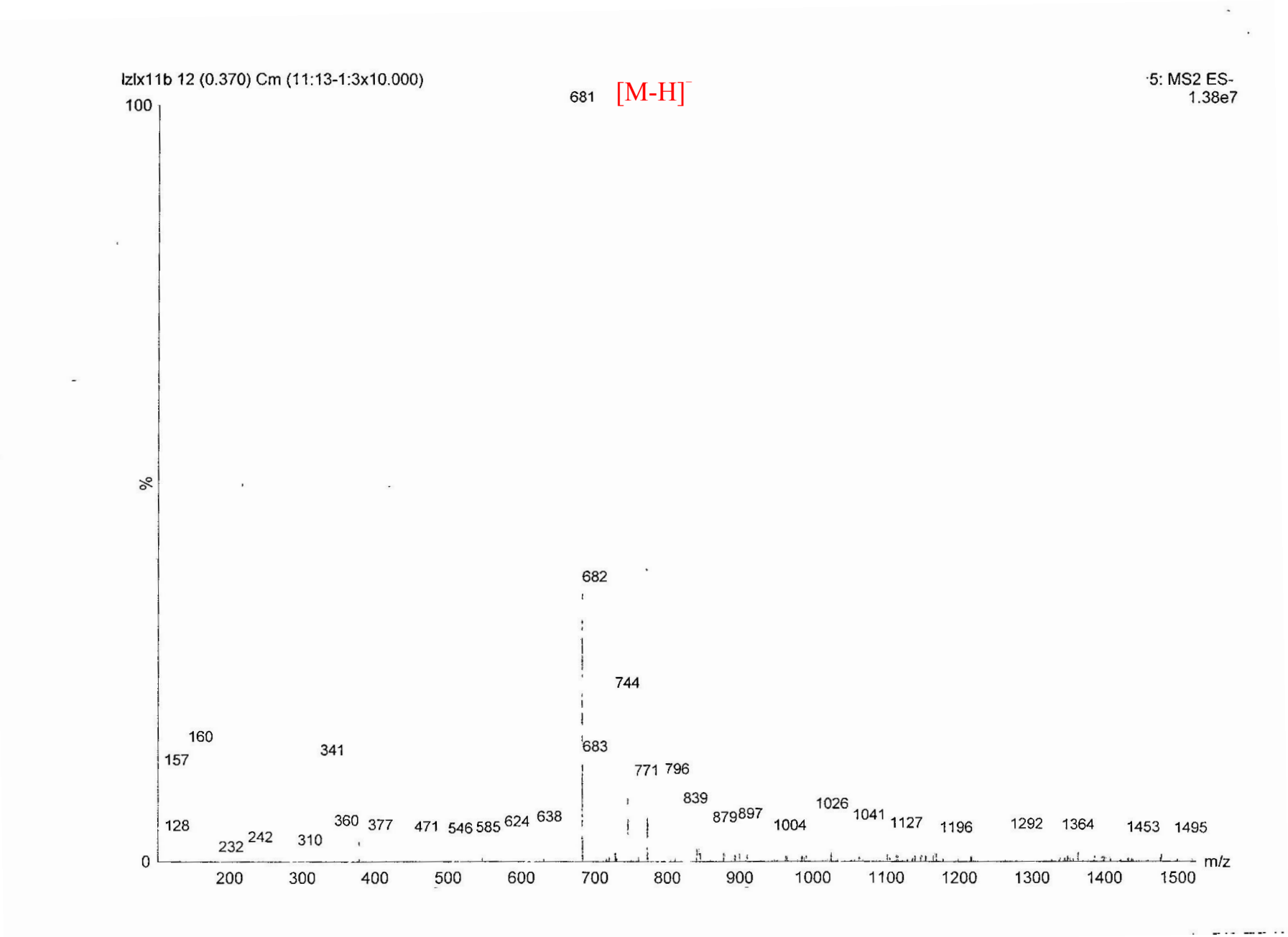


Fig. 26S HRESIMS (−) report of **1**.

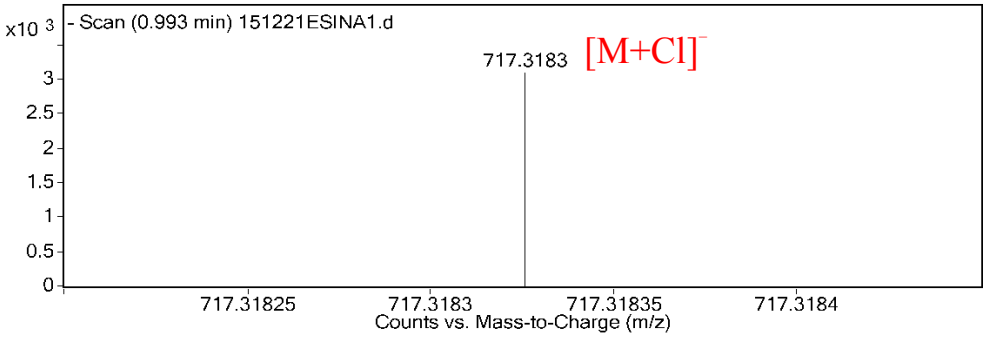
Qualitative Analysis Report

Data Filename	151221ESINA1.d	**Sample Name**	lzlx11b
Sample Type	Sample	**Position**	
Instrument Name	Agilent G6230 TOF MS	**User Name**	KIB
Acq Method	ESIN.m	**Acquired Time**	12/21/2015 9:31:18 AM
IRM Calibration Status	Success	**DA Method**	ESI.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
112.9856		2562.6		
717.3183	1	3088.09	C42 H50 Cl O8	M-
718.3214	1	983.84	C42 H50 Cl O8	M-
733.3116	1	1256.88		
744.3381	1	2690.58		
745.3394	1	862.47		
1033.9881	1	95864.88		
1034.9896	1	12841.06		
1933.927	1	16671.82		
1934.9301	1	3335.57		

Formula Calculator Element Limits

Element	Min	Max
C	0	200
H	0	400
O	0	13
Cl	1	1

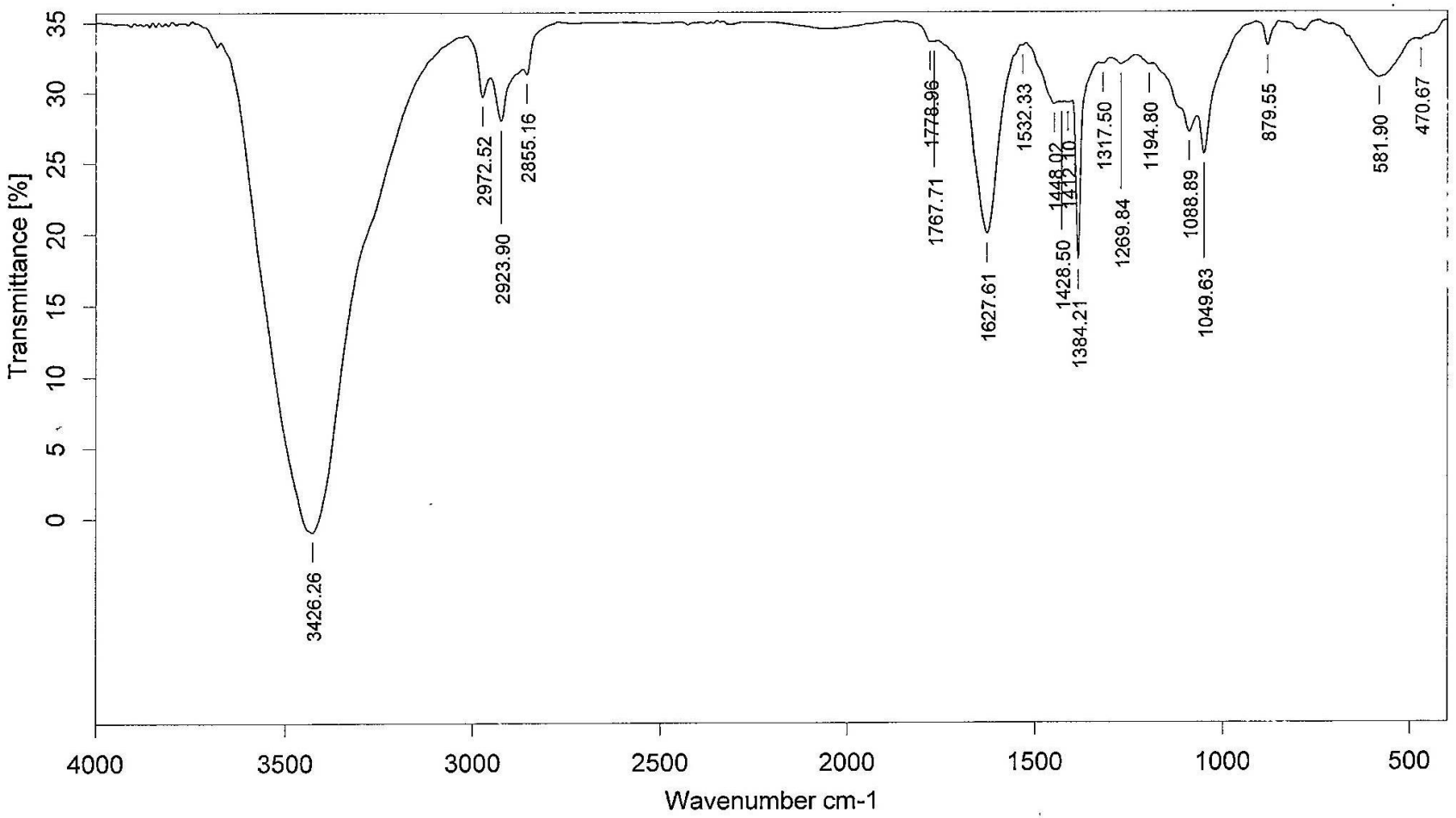
Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C42 H50 Cl O8	717.3194	717.3200	717.3183	1.8	2.5	17.5000

[M+Cl]⁻

--- End Of Report ---

Fig. 27S IR spectrum of **1**.



Sample : lzlx11b	Frequency Range : 399.246 - 3996.32	Measured on : 05/01/2016	
Technique : KBr压片	Resolution : 4	Instrument : Tensor27	Sample Scans : 16
Customer : 160105IR1	Zerofilling : 2	Acquisition : Double Sided,For	

Fig. 28S Optical rotatory data of (±)-**1**.

Optical rotation measurement

Model : P-1020 (A060460638)

No.	Sample	Mode	Data	Monitor Blank	Temp. Cell Temp Point	Date Comment Sample Name	Light Filter Operator	Cycle Time Integ Time
No.1	2 (1/3)	Sp.Rot	-17.1430	-0.0012 0.0000	19.6 10.00 Cell	Thu Jan 07 16:09:30 2016 0.00070g/mL MeOH LZLX11B	Na 589nm	2 sec 10 sec
No.2	2 (2/3)	Sp.Rot	-15.7140	-0.0011 0.0000	19.6 10.00 Cell	Thu Jan 07 16:09:43 2016 0.00070g/mL MeOH LZLX11B	Na 589nm	2 sec 10 sec
No.3	2 (3/3)	Sp.Rot	-17.1430	-0.0012 0.0000	19.6 10.00 Cell	Thu Jan 07 16:09:57 2016 0.00070g/mL MeOH LZLX11B	Na 589nm	2 sec 10 sec

$-16.666)^{\circ}$

Fig. 29S Optical rotatory data of (+)-**1**.

Optical rotation measurement

Model : P-1020 (A060460638)

No.	Sample	Mode	Data	Monitor Blank	Temp. Cell Temp Point	Date Comment Sample Name	Light Filter Operator	Cycle Time Integ Time
No.1	18 (1/3)	Sp.Rot	32.0000	0.0048 0.0000	18.3 10.00 Cell	Sun Jan 17 16:28:49 2016 0.00150g/mL MeOH LZLX11BA	Na 589nm	2 sec 10 sec
No.2	18 (2/3)	Sp.Rot	30.6670	0.0046 0.0000	18.3 10.00 Cell	Sun Jan 17 16:29:02 2016 0.00150g/mL MeOH LZLX11BA	Na 589nm	2 sec 10 sec
No.3	18 (3/3)	Sp.Rot	36.6670	0.0055 0.0000	18.3 10.00 Cell	Sun Jan 17 16:29:16 2016 0.00150g/mL MeOH LZLX11BA	Na 589nm	2 sec 10 sec
No.4	19 (1/3)	Sp.Rot	28.0000	0.0042 0.0000	18.3 10.00 Cell	Sun Jan 17 16:29:59 2016 0.00150g/mL MeOH LZLX11BA	Na 589nm	2 sec 10 sec
No.5	19 (2/3)	Sp.Rot	36.6670	0.0055 0.0000	18.3 10.00 Cell	Sun Jan 17 16:30:13 2016 0.00150g/mL MeOH LZLX11BA	Na 589nm	2 sec 10 sec
No.6	19 (3/3)	Sp.Rot	32.0000	0.0048 0.0000	18.3 10.00 Cell	Sun Jan 17 16:30:26 2016 0.00150g/mL MeOH LZLX11BA	Na 589nm	2 sec 10 sec

$+32.666)^{\circ}$

Fig. 30S Optical rotatory data of (−)-**1**.

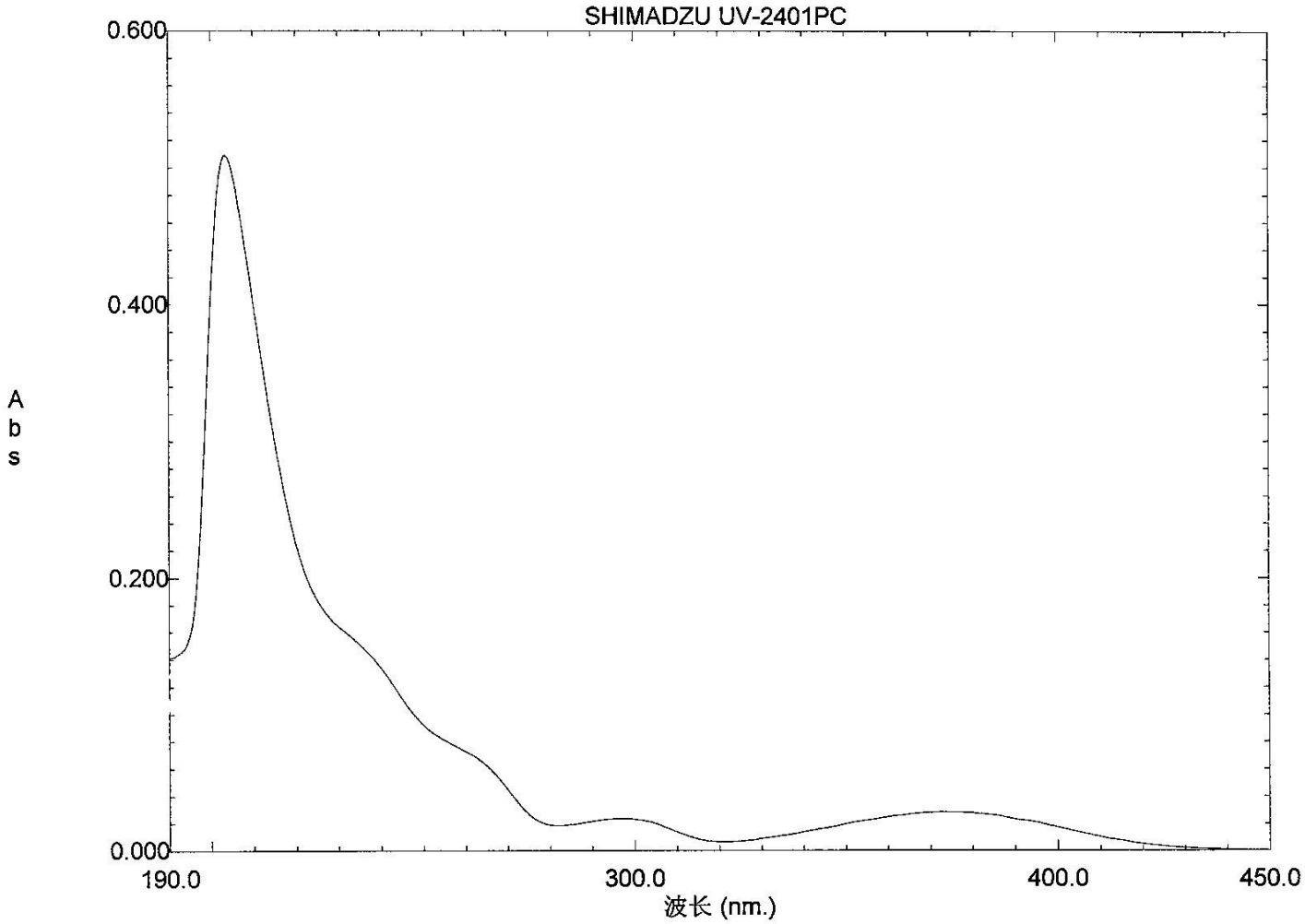
Optical rotation measurement

Model : P-1020 (A060460638)

No.	Sample	Mode	Data	Monitor Blank	Temp. Cell Temp Point	Date Comment Sample Name	Light Filter Operator	Cycle Time Integ Time
No.1	20 (1/3)	Sp.Rot	9.3330	0.0014 0.0000	18.5 10.00 Cell	Sun Jan 17 16:43:49 2016 0.00150g/mL MeOH LZLX11BB	Na 589nm	2 sec 10 sec
No.2	20 (2/3)	Sp.Rot	4.6670	0.0007 0.0000	18.5 10.00 Cell	Sun Jan 17 16:44:03 2016 0.00150g/mL MeOH LZLX11BB	Na 589nm	2 sec 10 sec
No.3	20 (3/3)	Sp.Rot	2.6670	0.0004 0.0000	18.5 10.00 Cell	Sun Jan 17 16:44:16 2016 0.00150g/mL MeOH LZLX11BB	Na 589nm	2 sec 10 sec
No.4	21 (1/3)	Sp.Rot	9.3330	0.0014 0.0000	18.5 10.00 Cell	Sun Jan 17 16:45:11 2016 0.00150g/mL MeOH LZLX11BB	Na 589nm	2 sec 10 sec
No.5	21 (2/3)	Sp.Rot	0.6670	0.0001 0.0000	18.4 10.00 Cell	Sun Jan 17 16:45:24 2016 0.00150g/mL MeOH LZLX11BB	Na 589nm	2 sec 10 sec
No.6	21 (3/3)	Sp.Rot	4.0000	0.0006 0.0000	18.5 10.00 Cell	Sun Jan 17 16:45:38 2016 0.00150g/mL MeOH LZLX11BB	Na 589nm	2 sec 10 sec

+2.111 °

Fig. 31S UV spectrum of **1**.



文件名: LZLX11B

LZLX11B

样品浓度：0.0067毫克/毫升
溶剂：甲醇

创建于: 14:43 16-01-08
数据: 原始

测量模式: Abs.
扫描速度: 中速
狭缝: 5.0
采样间隔: 0.5

否.	波长 (nm.)	Abs.
1	373.50	0.0283
2	297.00	0.0236
3	203.50	0.5090