Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supplementary Information

Eucalmaidials A and B, phloroglucinol-coupled sesquiterpenoids from the juvenile leaves of *Eucalyptus maideni*

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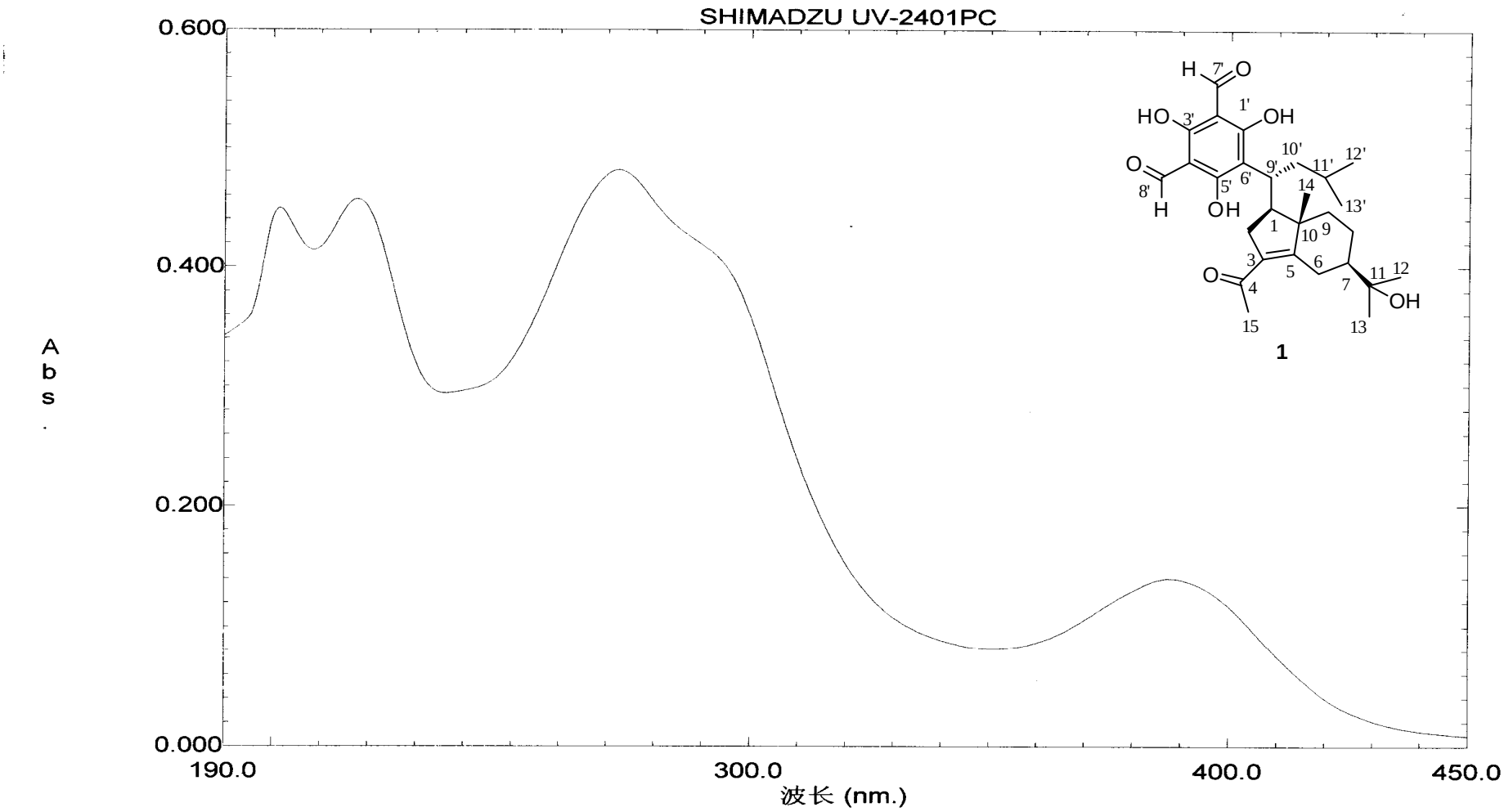
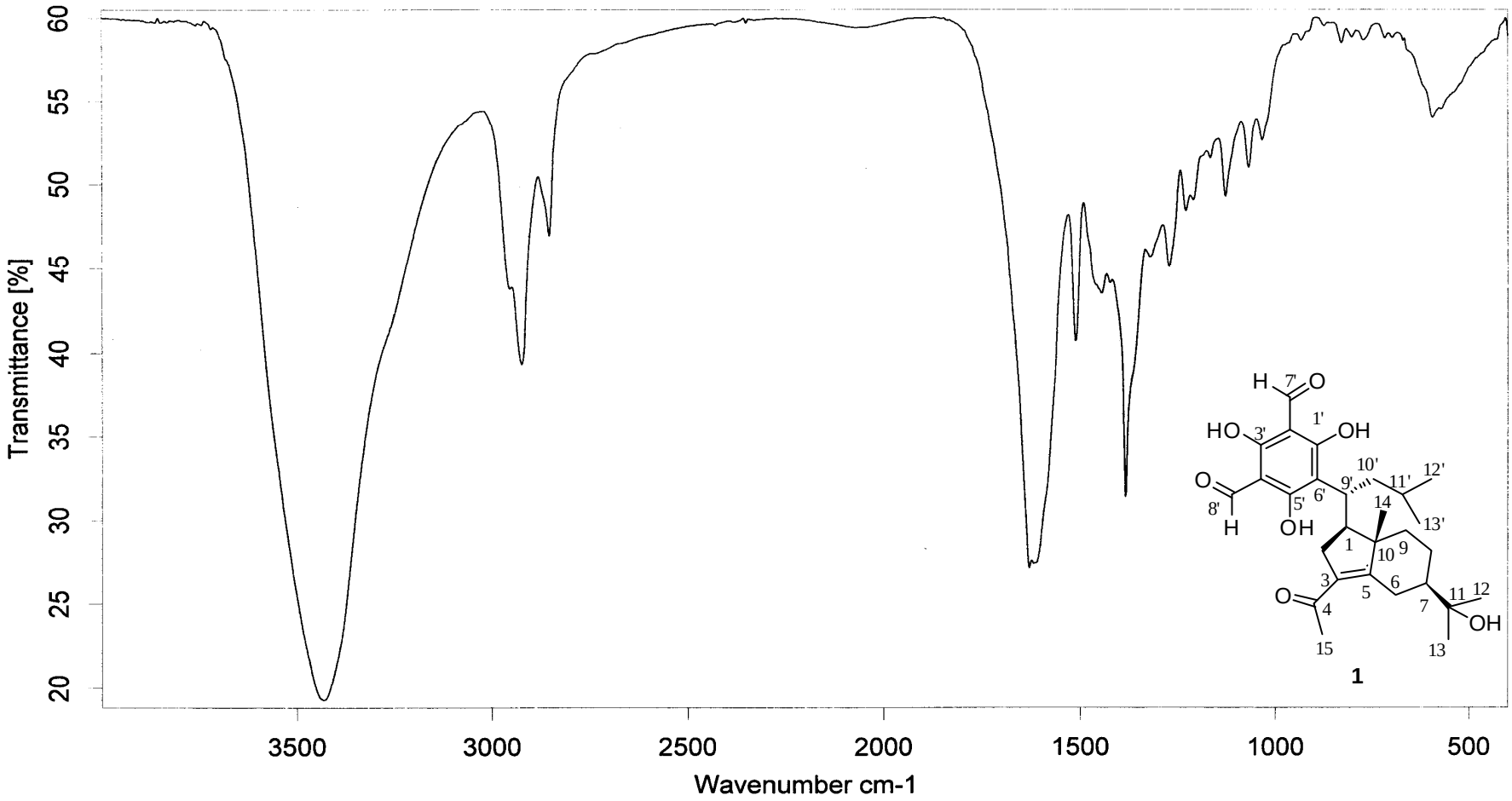
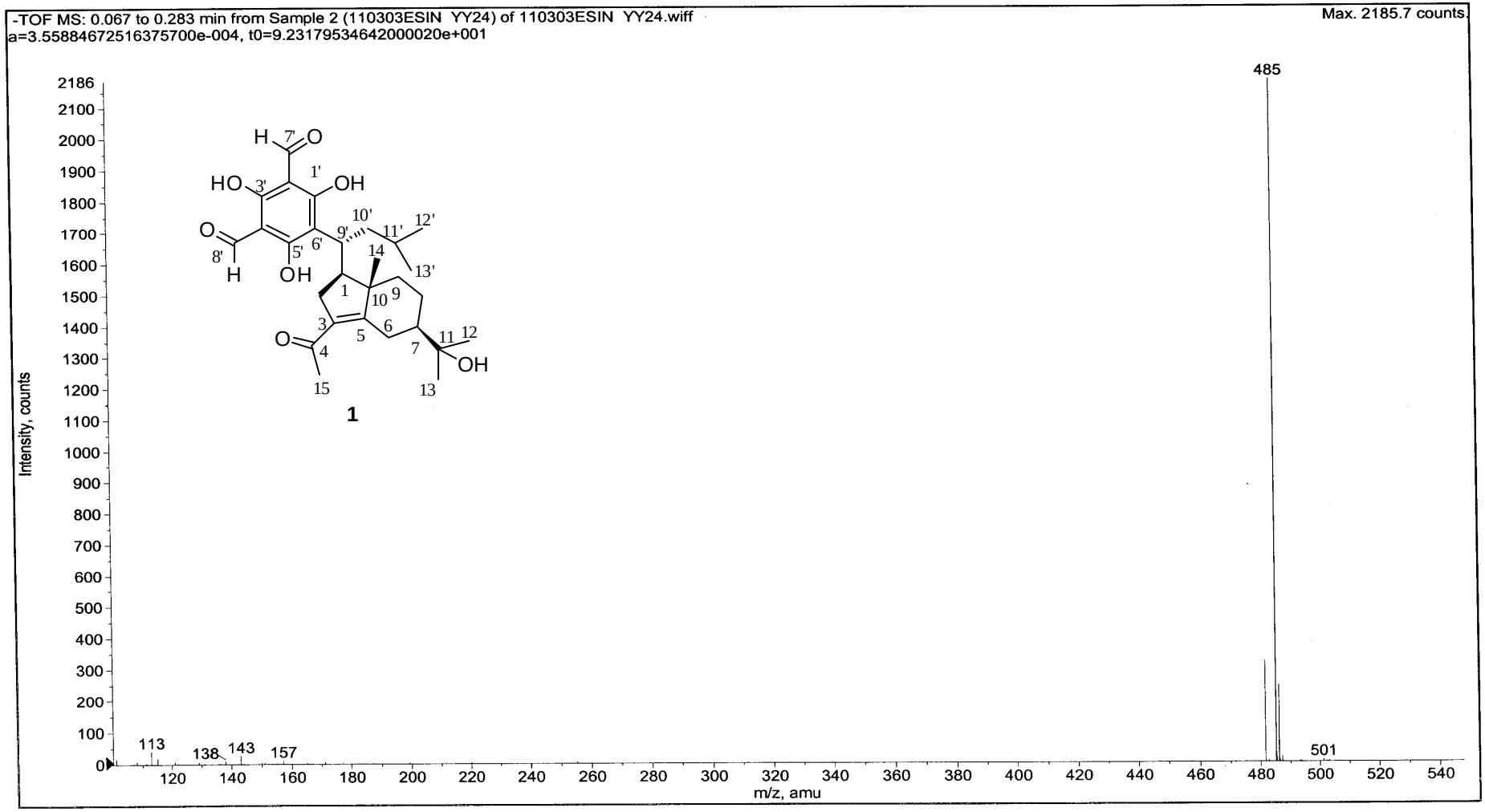
S1 UV spectrum of compound 1



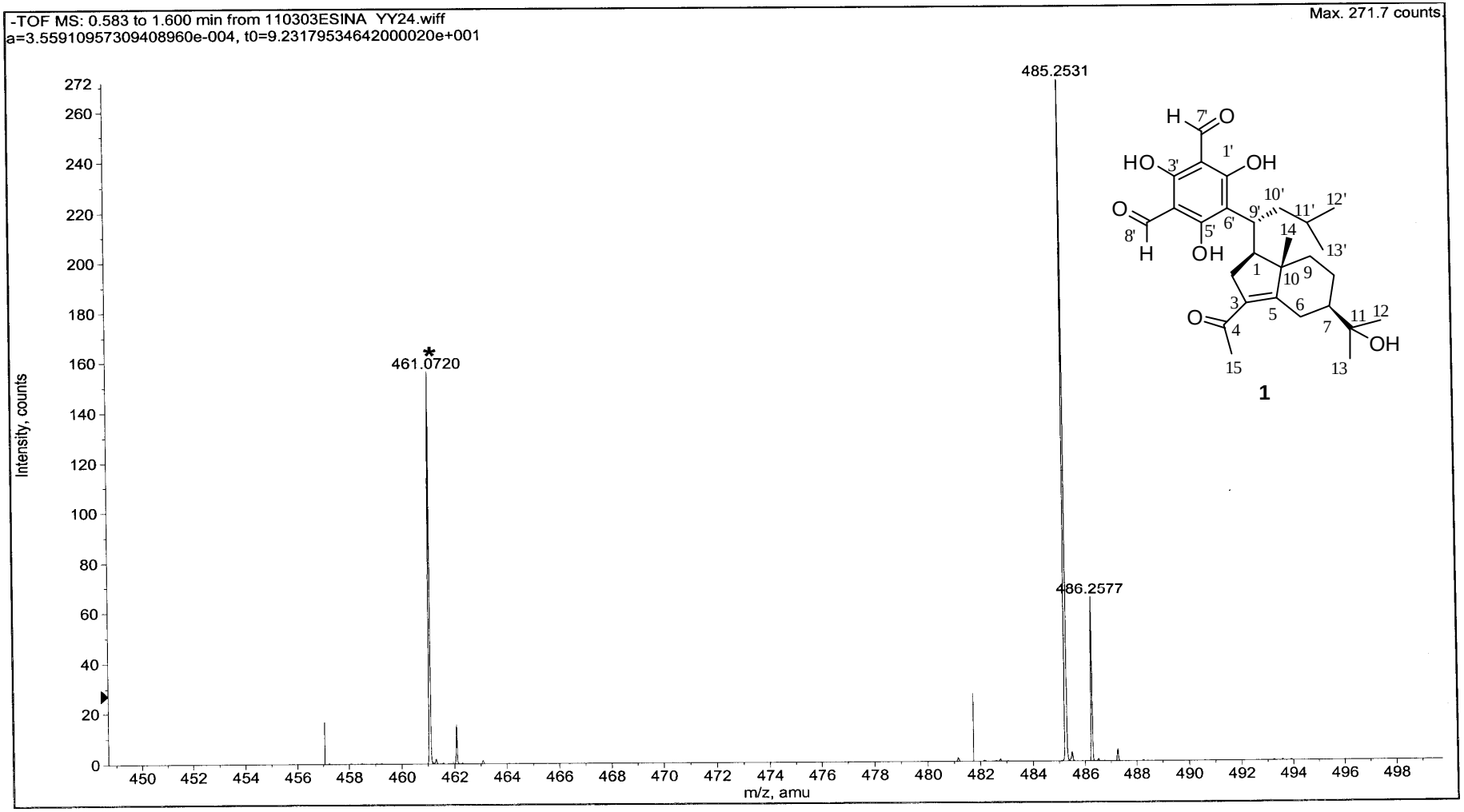
S2 IR spectrum of compound 1



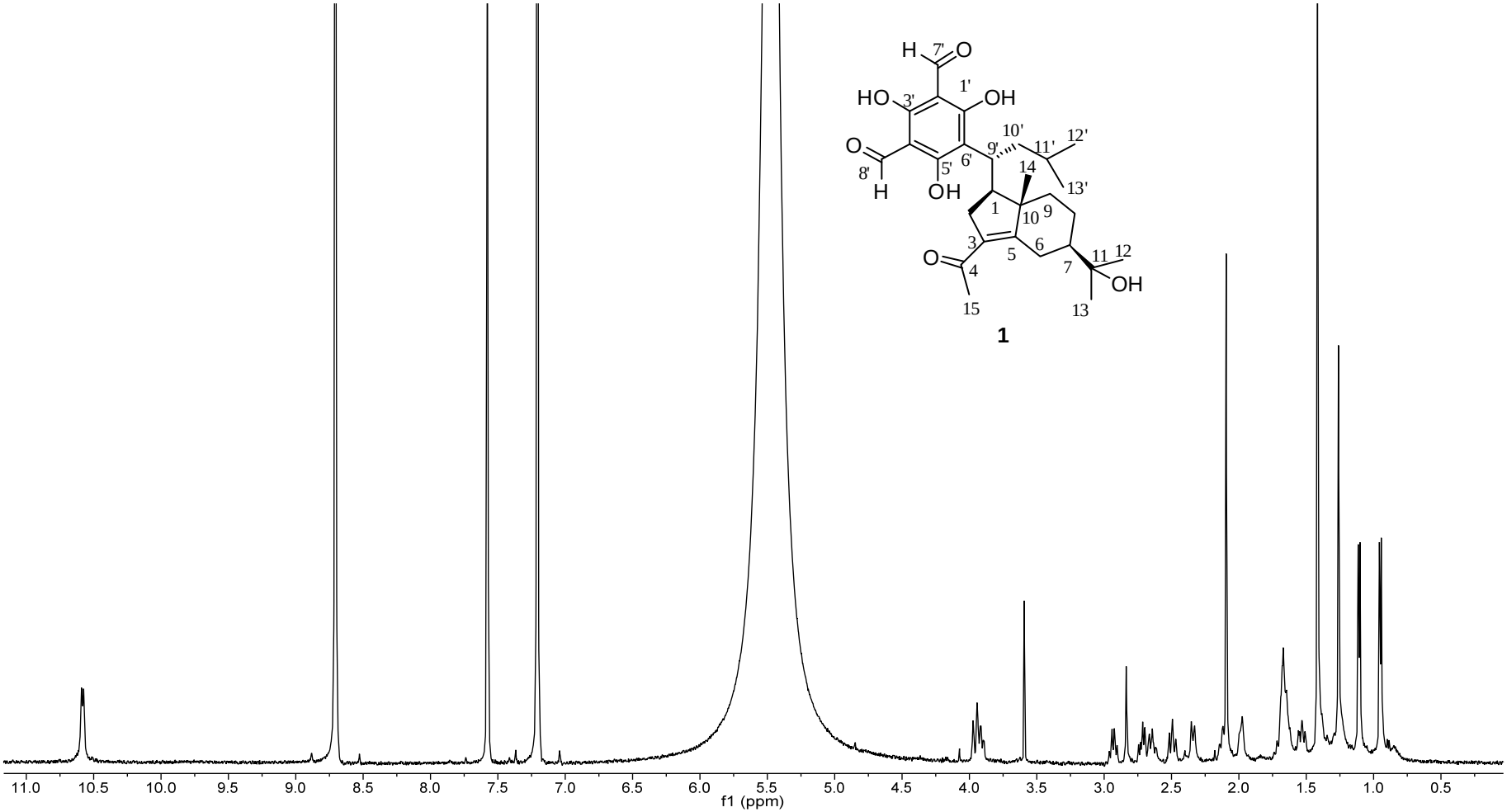
S3 ESI-MS spectrum of compound 1



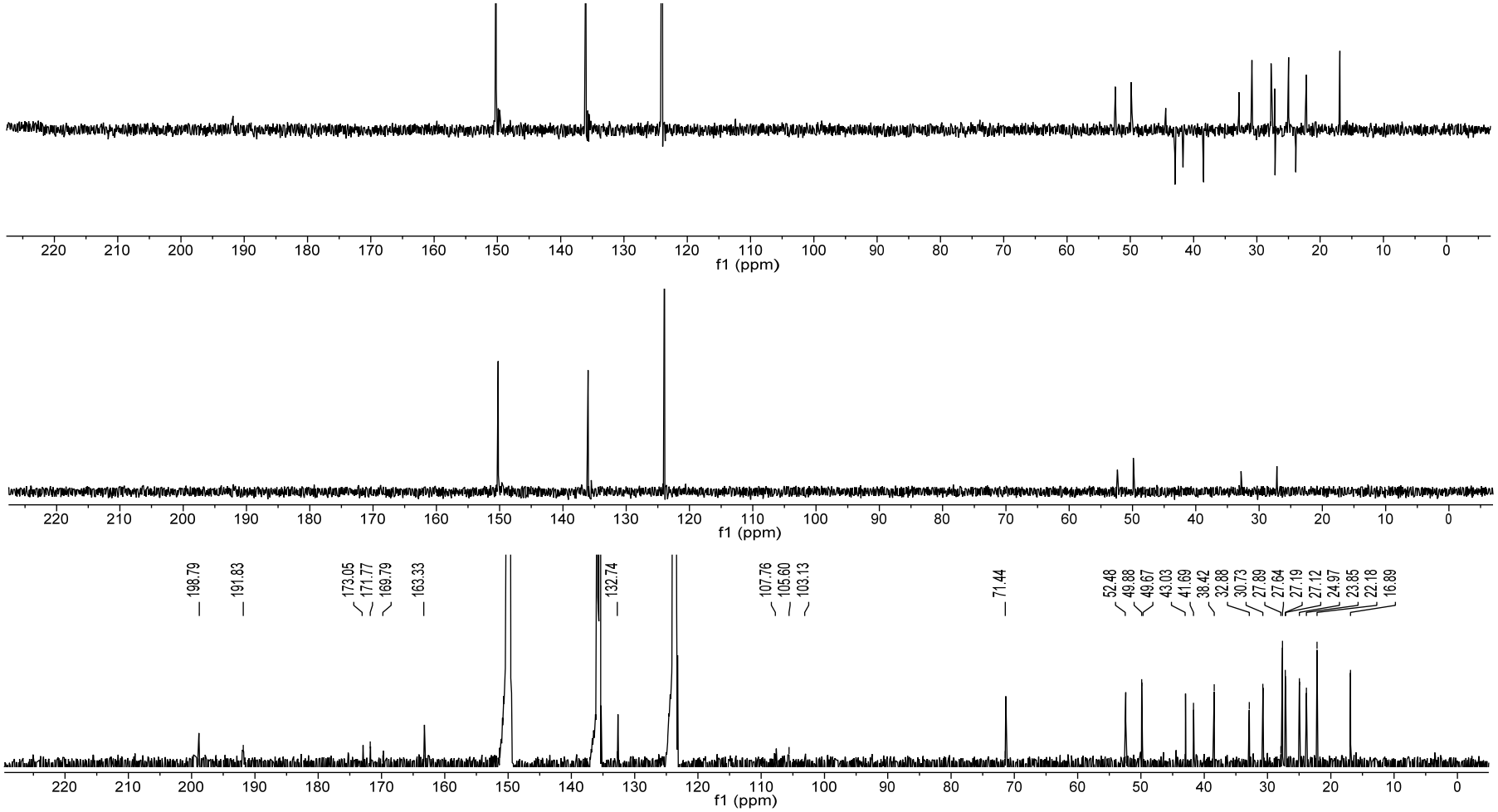
S4 HRESI-MS spectrum of compound 1



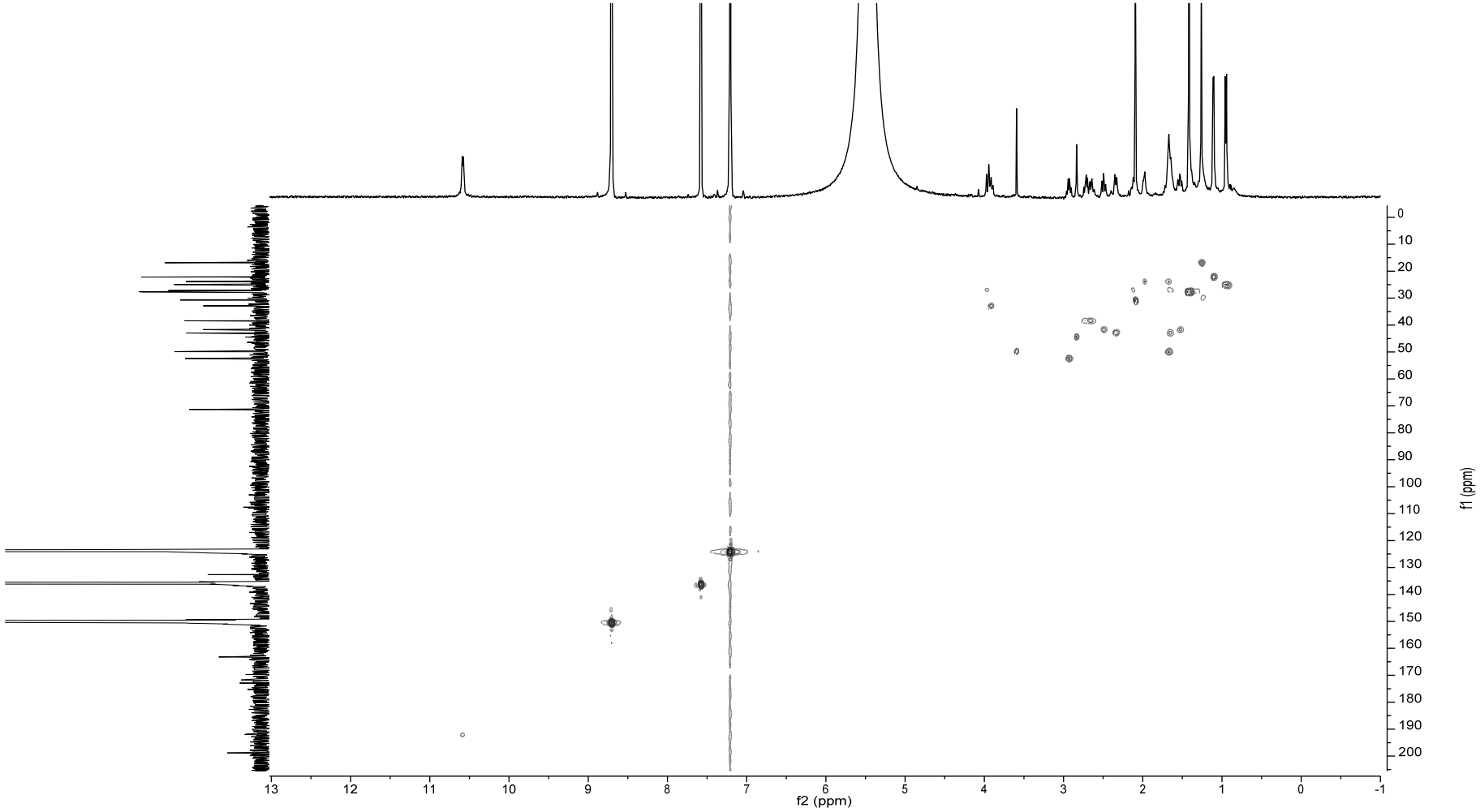
S5 ^{1}H NMR sepctrum of compound 1



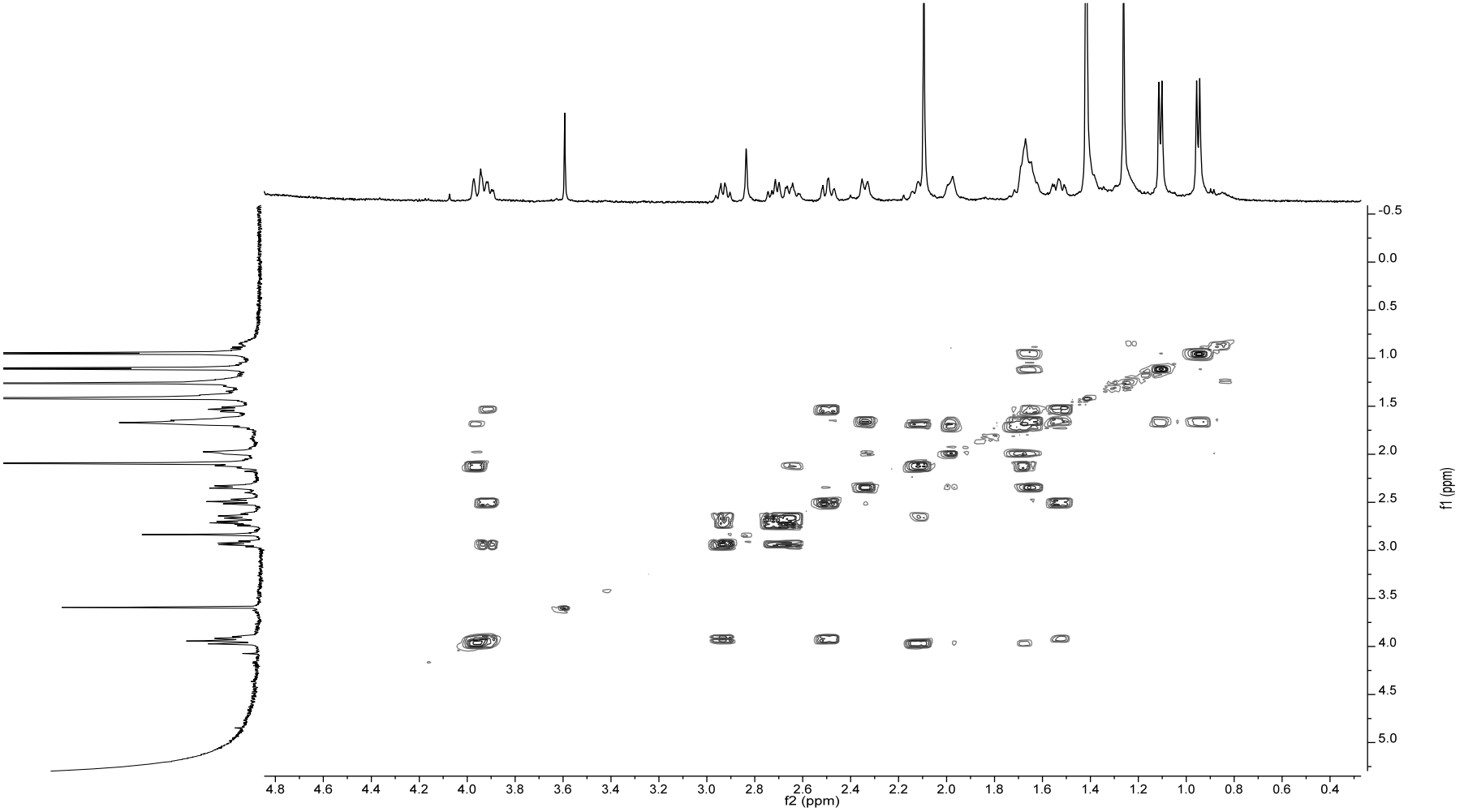
S6 ^{13}C NMR and DEPT spectra of compound 1



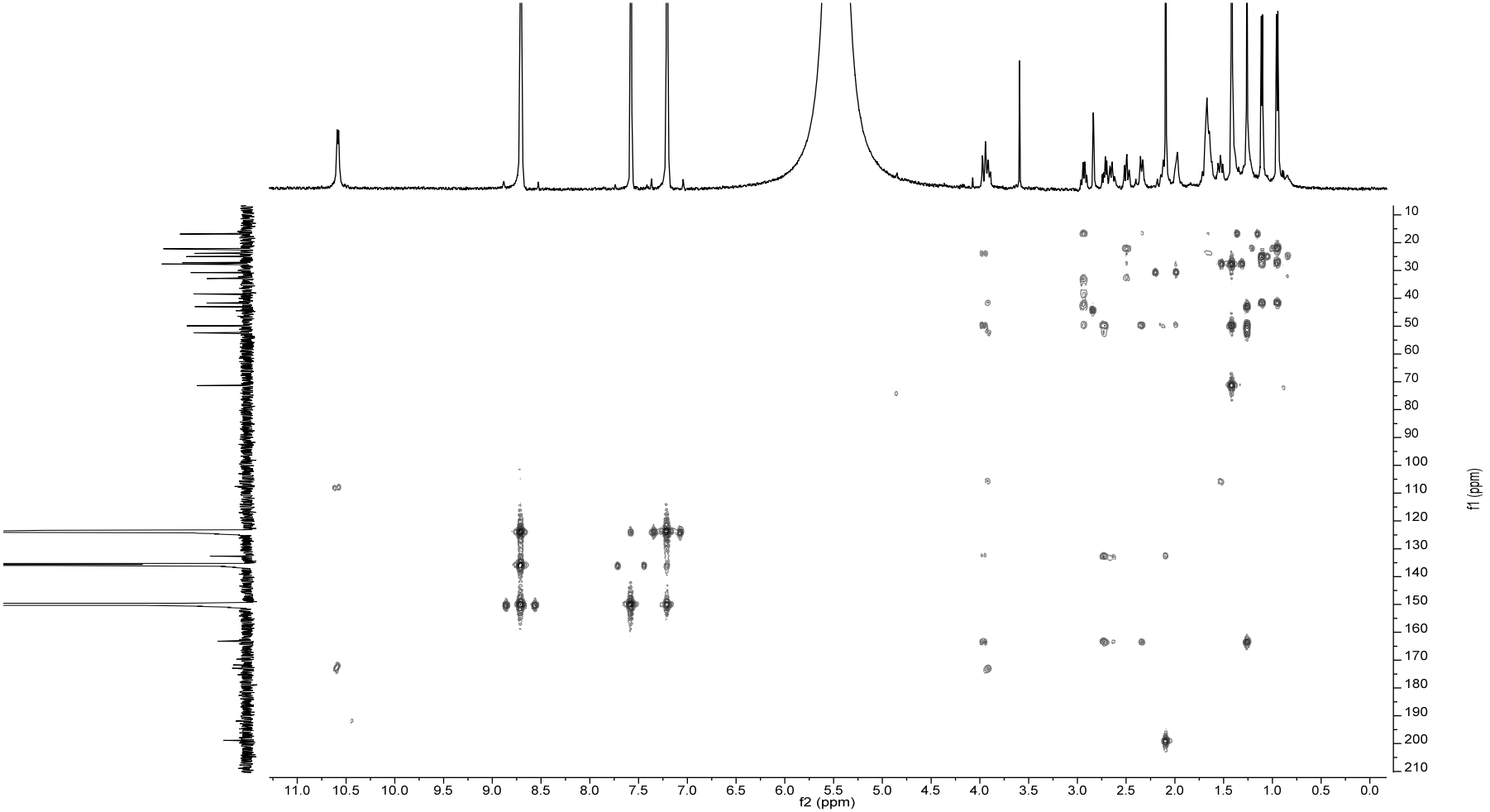
S7 HSQC spectrum of compound 1



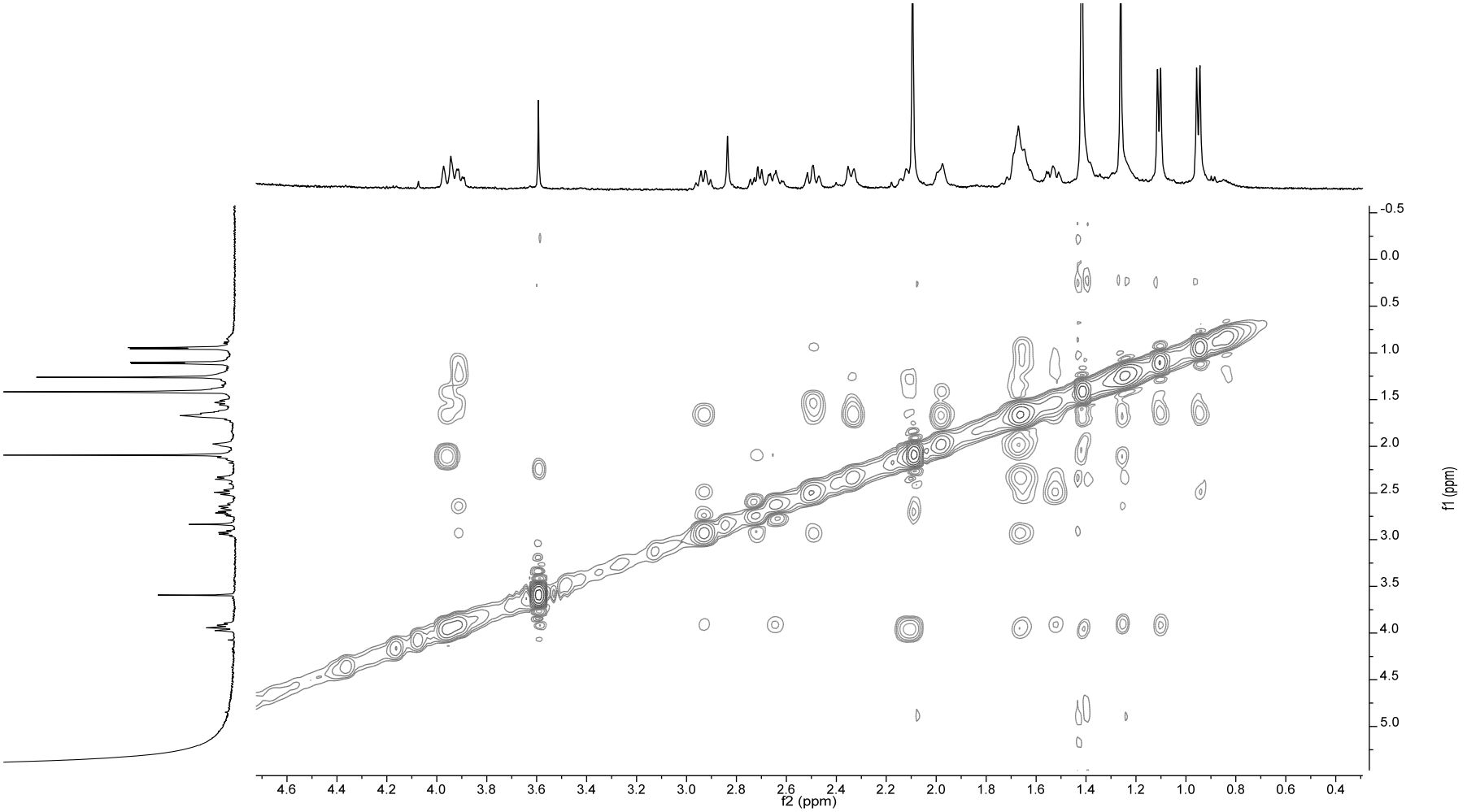
S8 ^{1}H-^{1}H COSY spectrum of compound 1



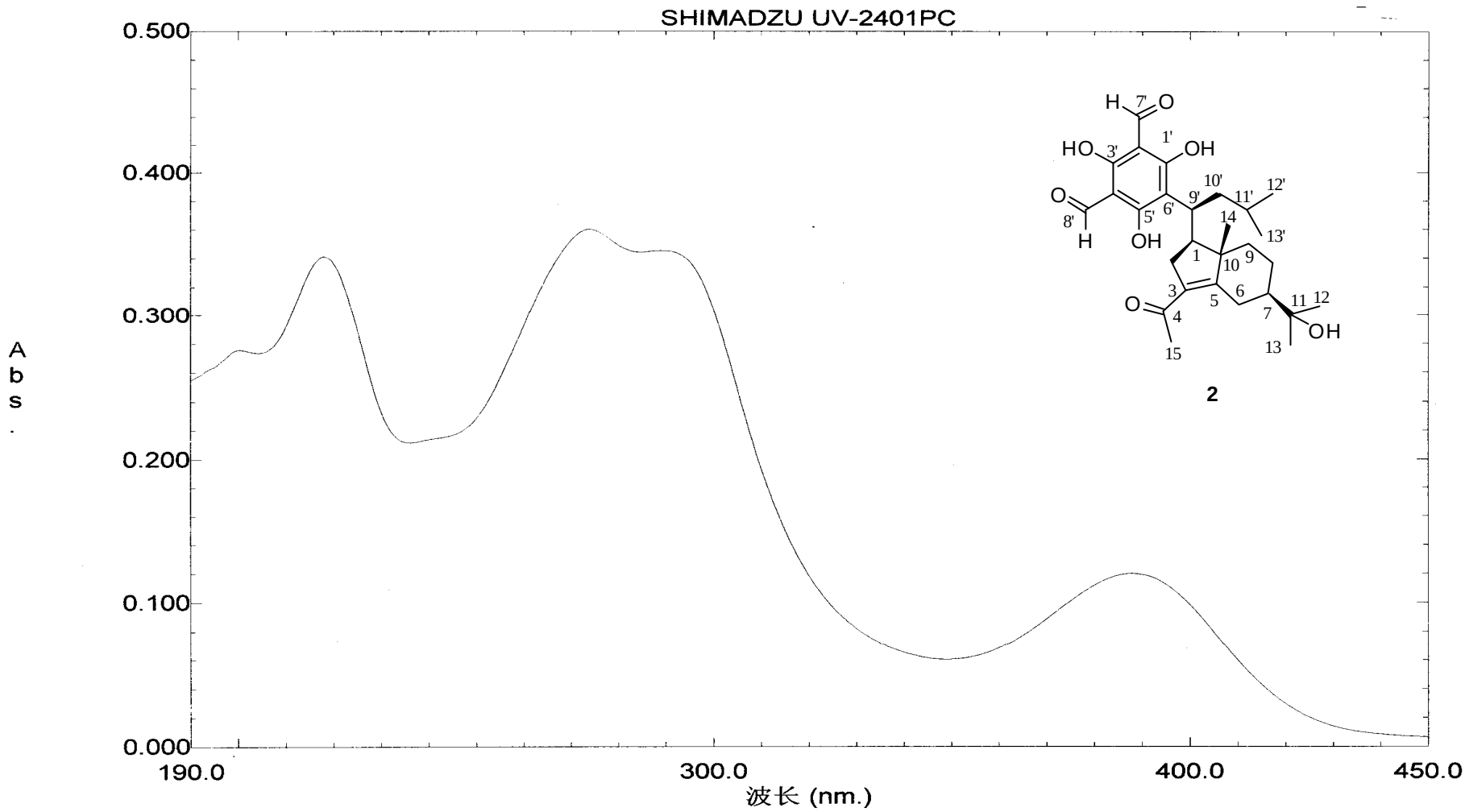
S9 HMBC spectrum of compound 1



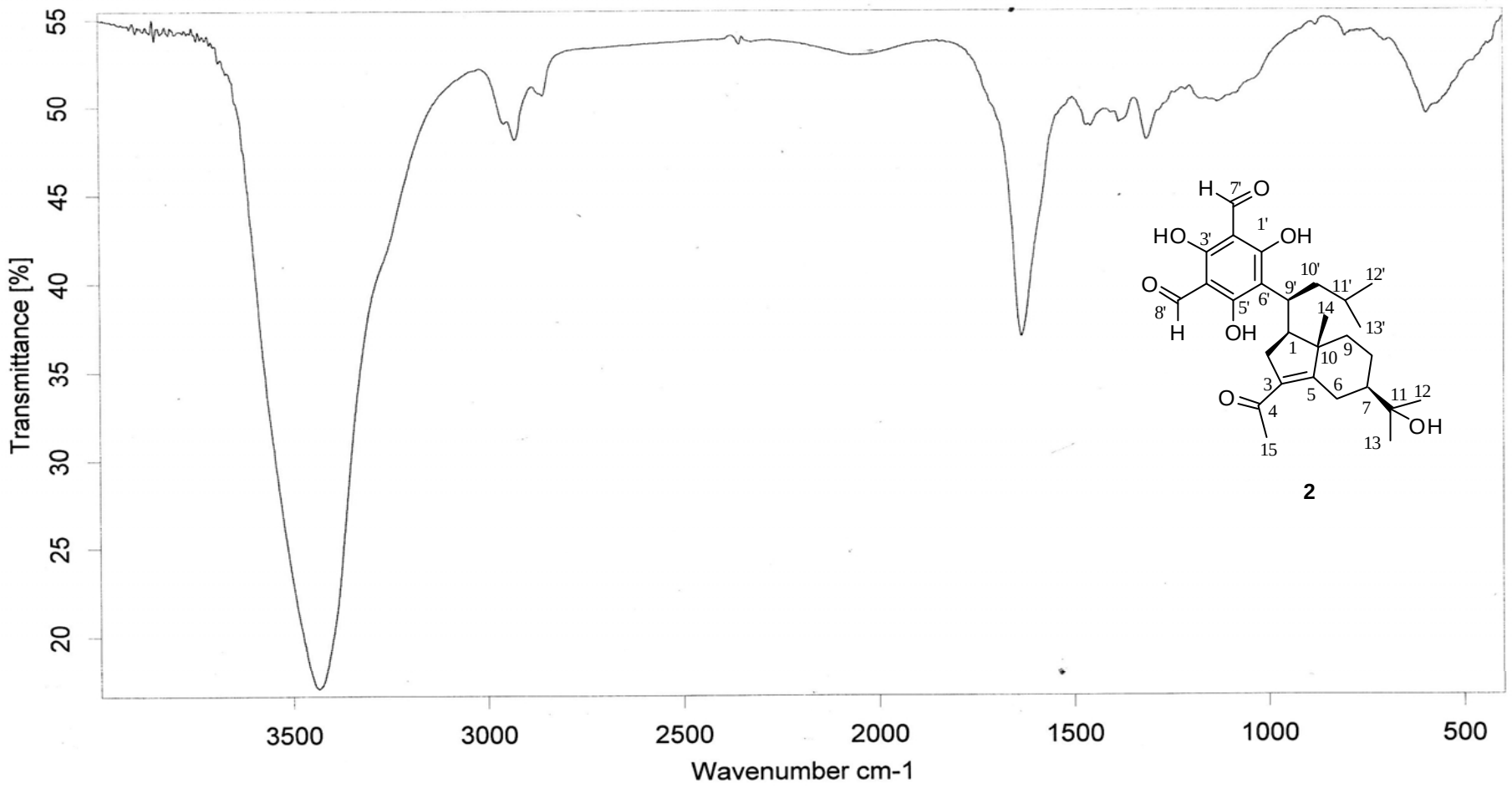
S10 ROESY spectrum of compound 1



S11 UV spectrum of compound 2

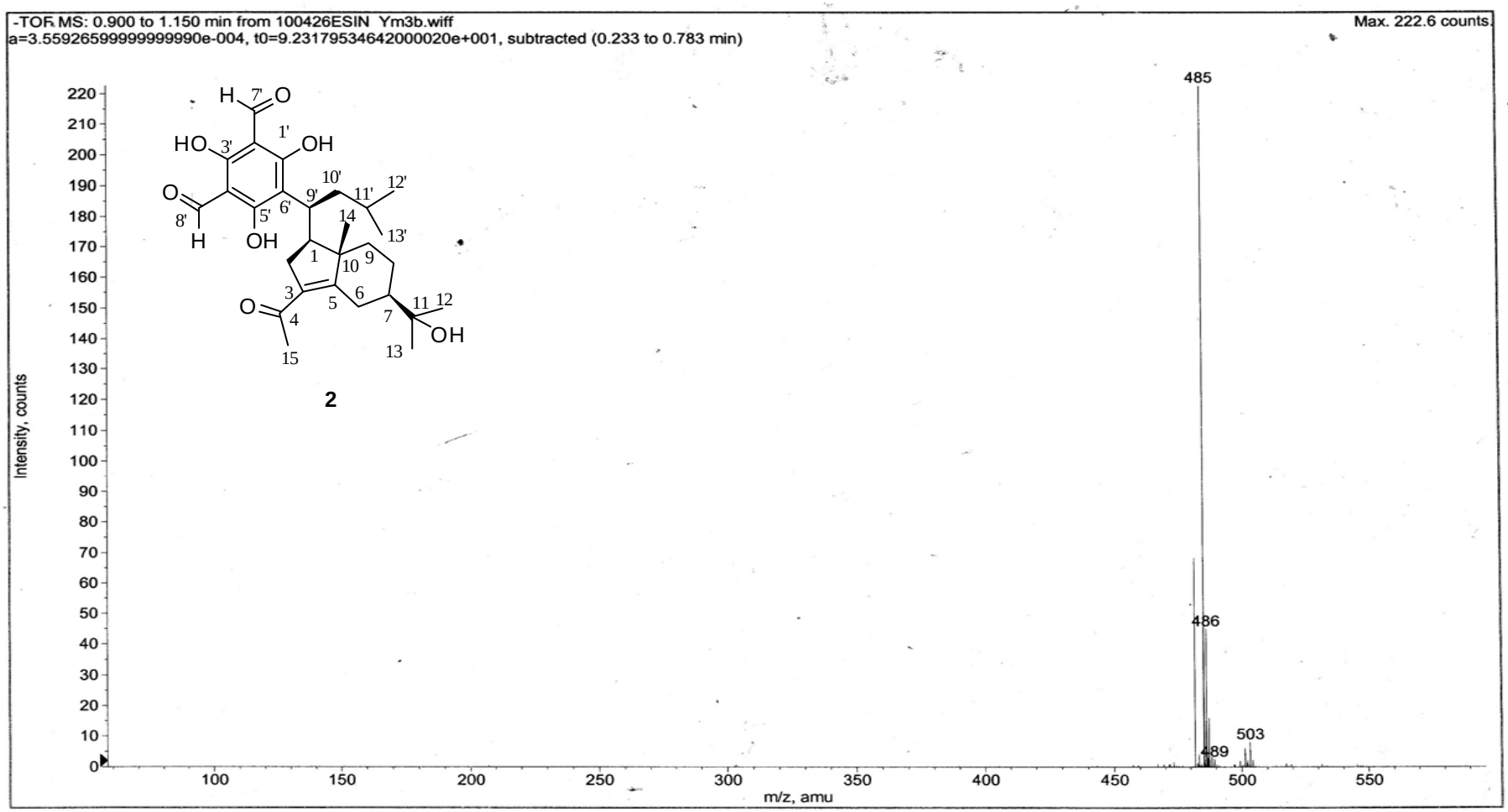


S12 IR spectrum of compound 2

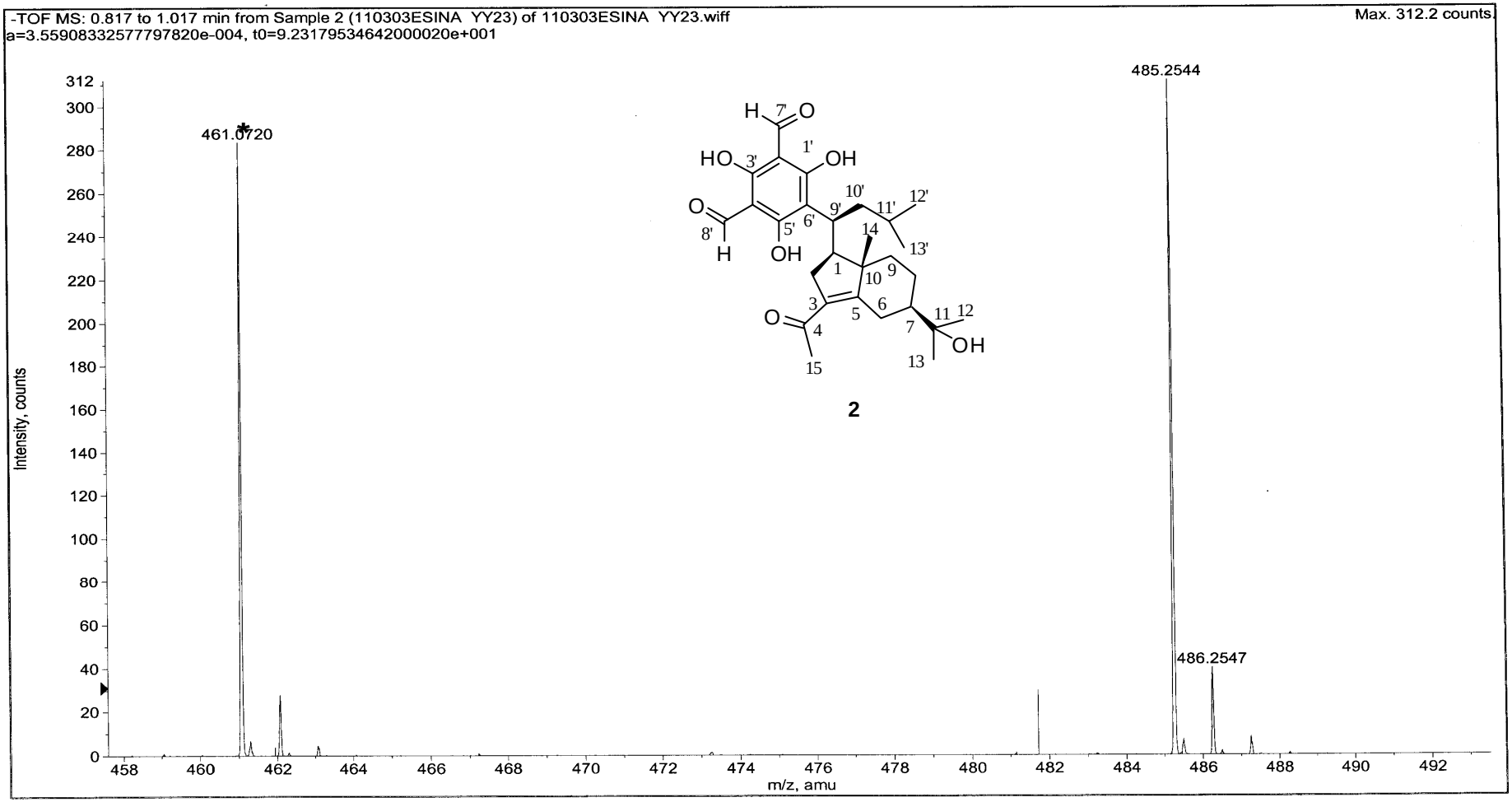


2

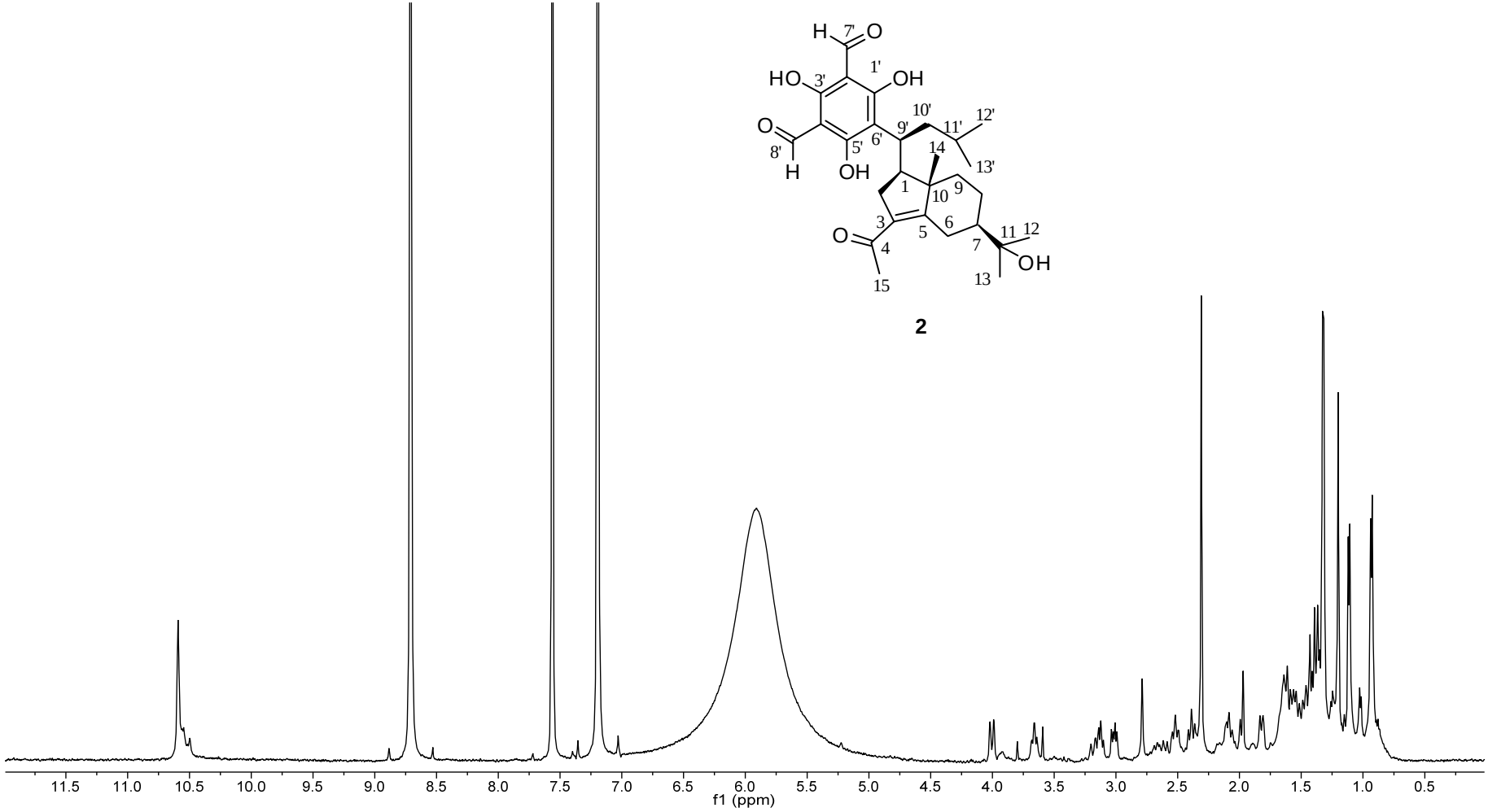
S13 ESI-MS spectrum of compound 2



S14 HRESI-MS spectrum of compound 2

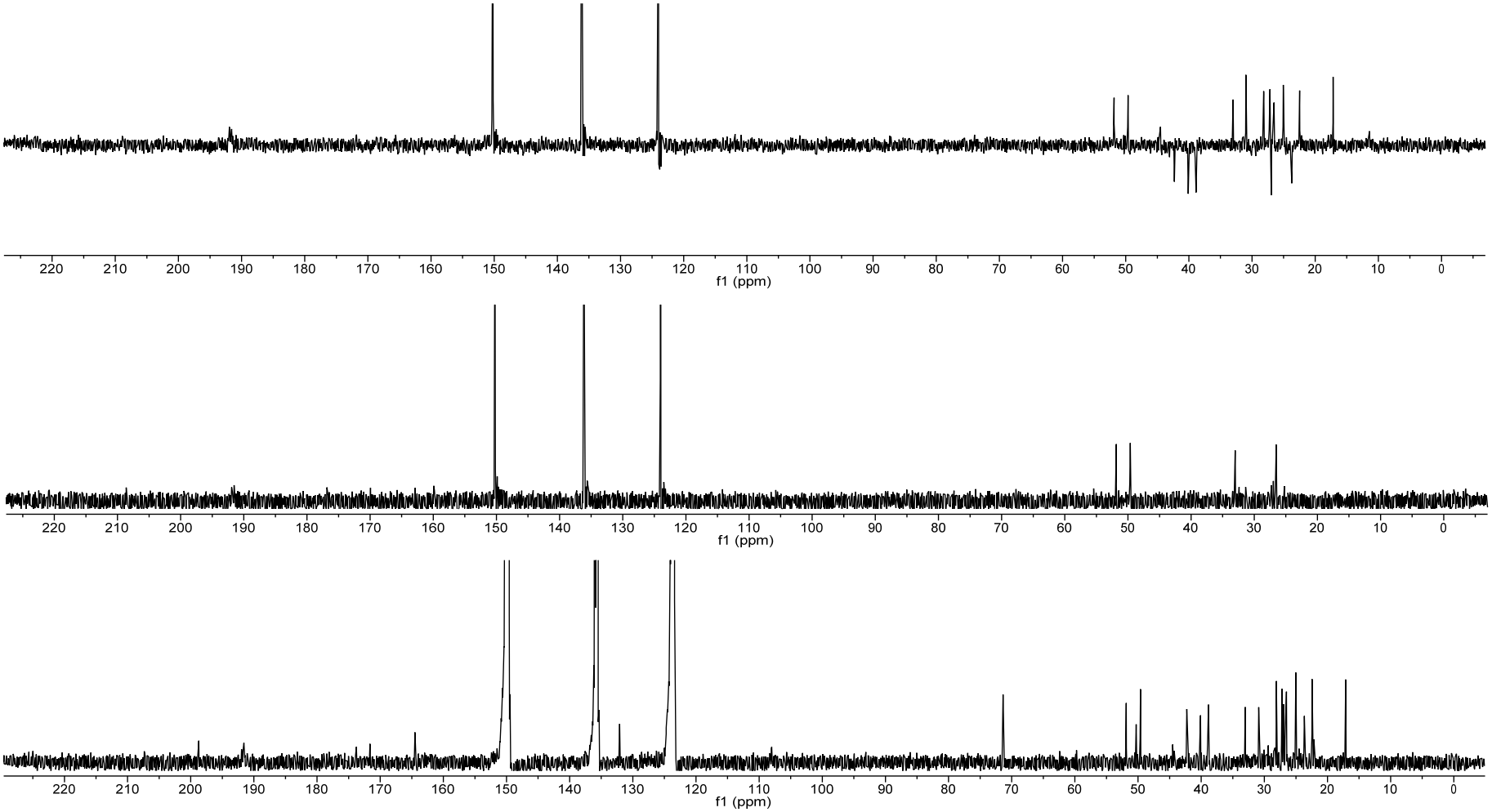


S15 ^{1}H NMR spectrum of compound 2

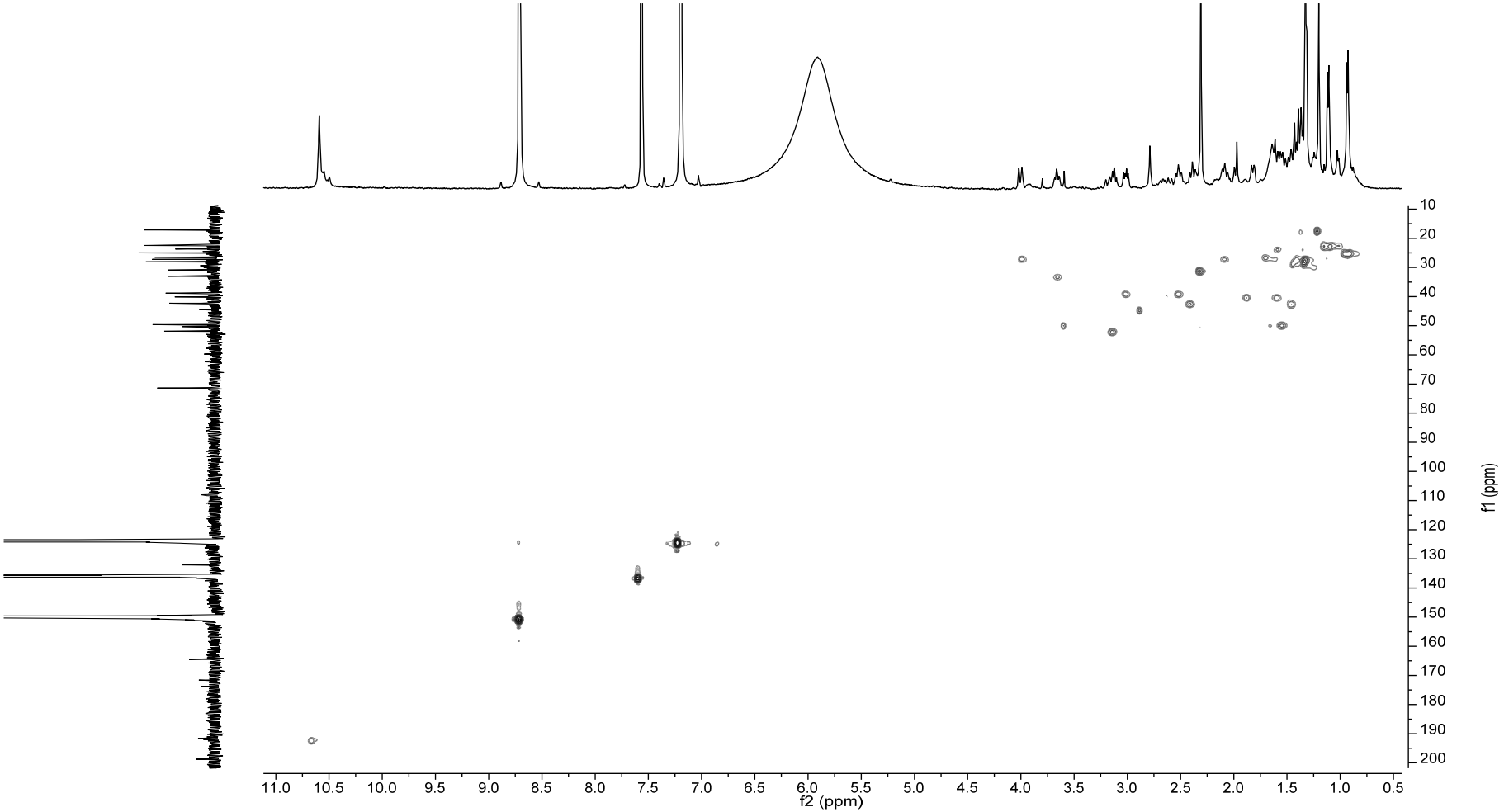


2

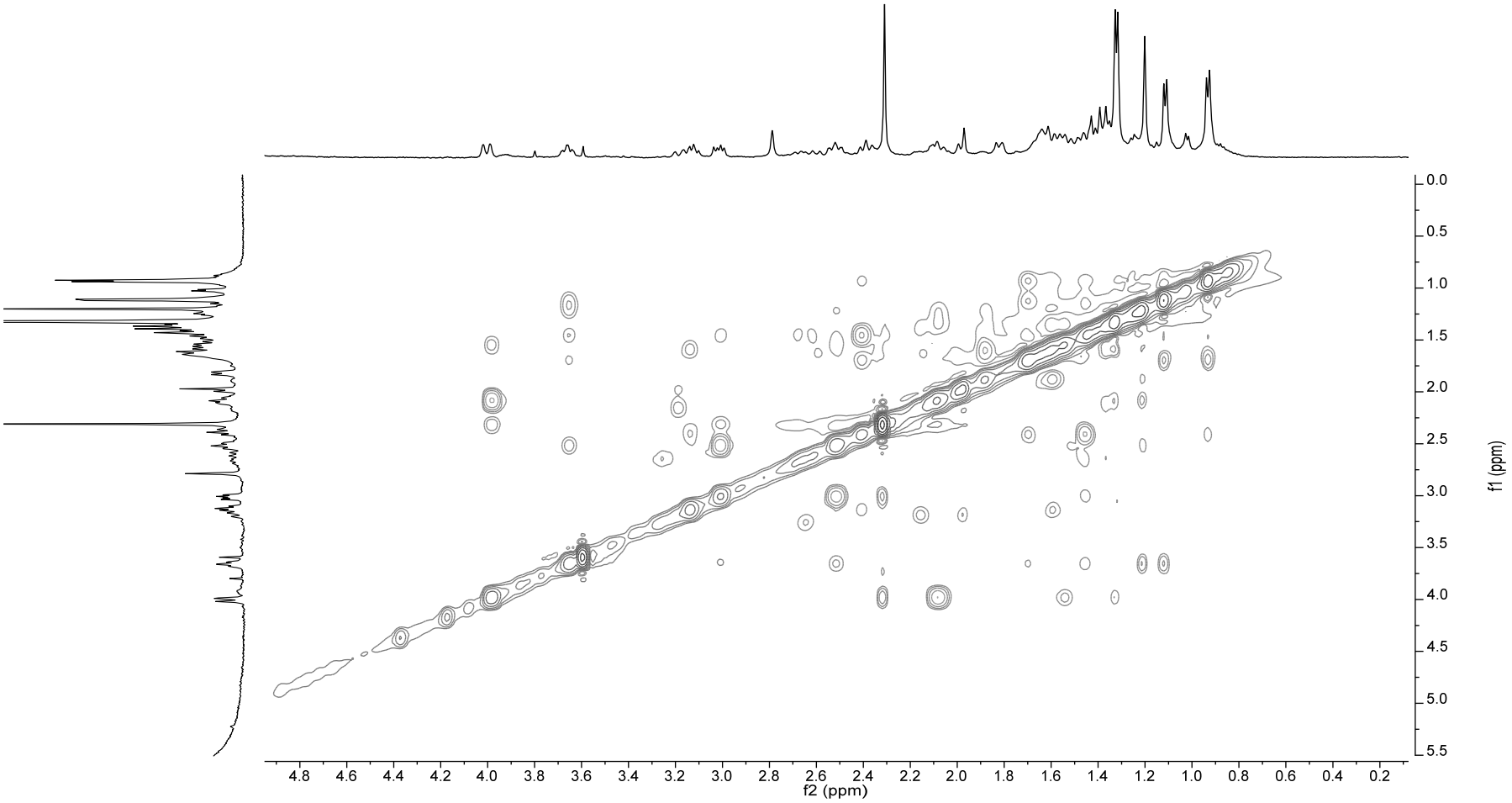
S16 ^{13}C NMR and DEPT spectra of compound 2



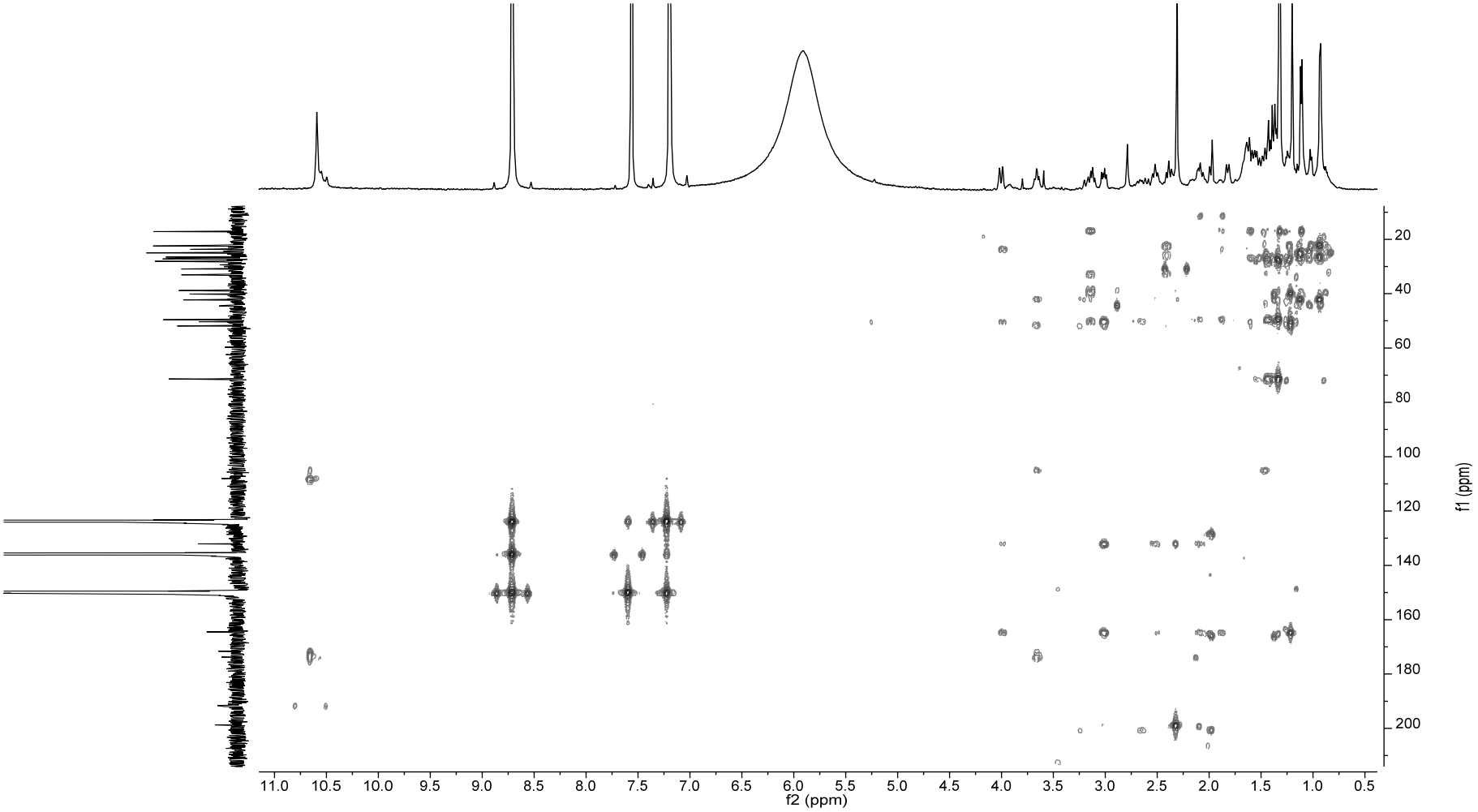
S17 HSQC spectrum of compound 2



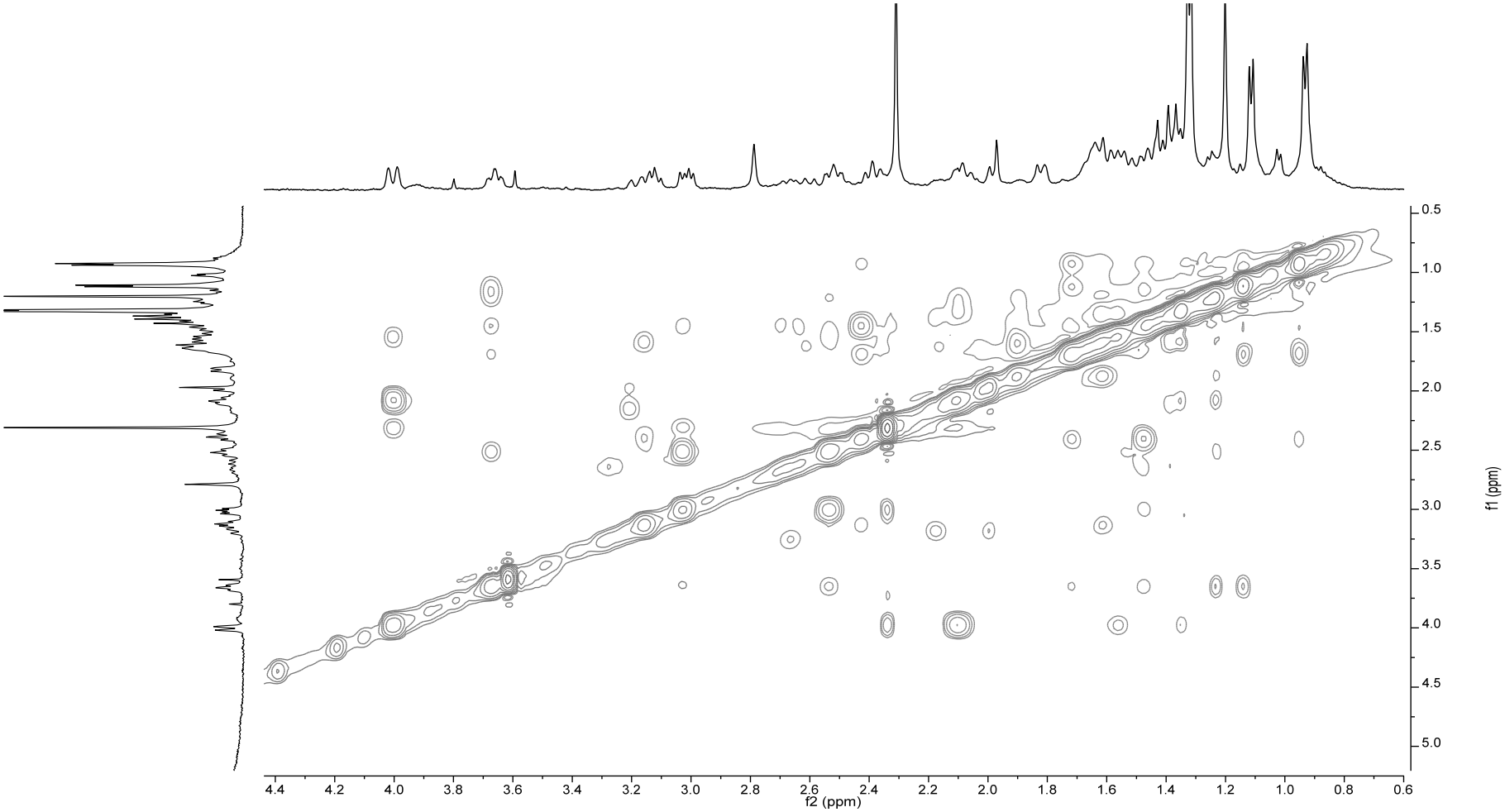
S18 ^{1}H - ^{1}H COSY spectrum of compound 2



S19 HMBC spectrum of compound 2



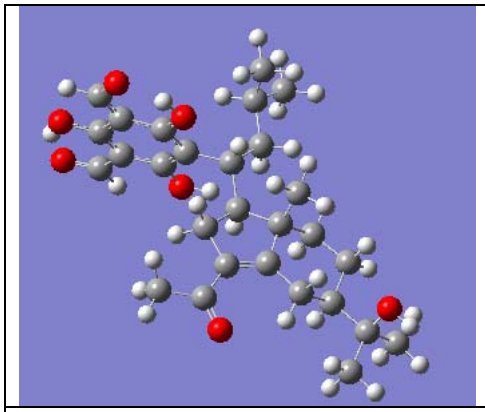
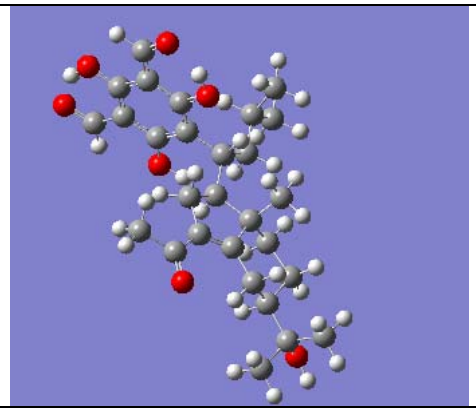
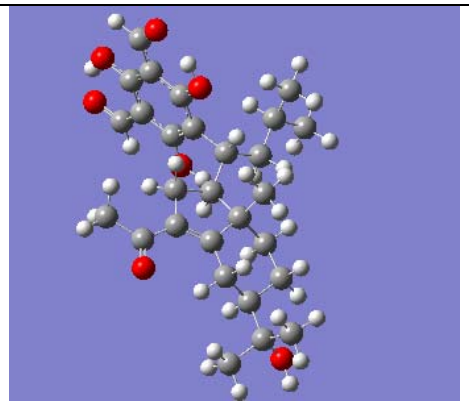
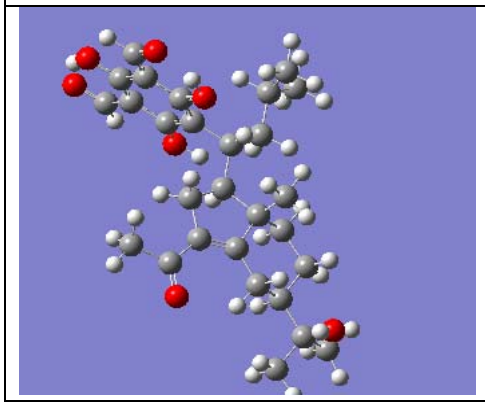
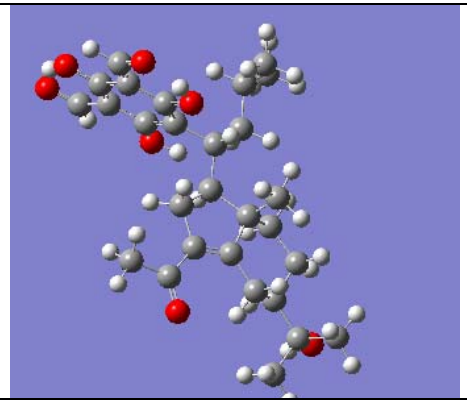
S20 ROESY spectrum of compound 2



S21 ^{13}C NMR calculation details for compounds 1 and 2

The conformational searches were performed using MMFF94S force field, total 48 conformations were found for **1** and 50 for **2,** respectively, they all were used in the optimizations at the B3LYP/6-31+G(d) level. Then the low energy geometries from 0-1.5 kcal/mol were used for NMR computations at the B3LYP/6-311++G(2d,p) level. Total 5 low energy conformations were found for **1** in NMR computations, and 6 conformations for **2**. The optimized conformers, atomic coordinates and calculated ^{13}C NMR chemical shifts are illustrated below:

5 low energy conformers of compound **1**

		
z2b-5	z2b-6	z2b-16
		
Z2b-21	Z2b-26	

The internal energy data for each conformer of **1**:

	z2b-5	z2b-6	z2b-16	Z2b-21	Z2b-26
Energy (a.u.)	-1616.9459998	-1616.9461618	-1616.9461606	-1616.9457654	-1616.9460058

Coordinates for z2b-5:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.992463	-0.435980	1.536736
2	6	0	2.748029	0.202930	1.259065
3	6	0	2.232603	0.366678	-0.030777
4	6	0	3.015453	-0.158521	-1.084323
5	6	0	4.269482	-0.809224	-0.874247
6	6	0	4.747453	-0.939612	0.448843
7	6	0	5.029371	-1.327610	-1.991845
8	1	0	5.986385	-1.815801	-1.760021
9	6	0	4.490176	-0.575844	2.888976
10	1	0	3.872098	-0.170246	3.701890
11	6	0	0.888974	1.038058	-0.346607
12	6	0	0.800495	2.515847	0.132202
13	1	0	-0.095241	2.958262	-0.319573
14	6	0	1.999143	3.430811	-0.195255
15	1	0	-1.222036	0.289588	-2.500062
16	6	0	-0.314675	0.170489	0.135291
17	6	0	-1.756673	0.536705	-0.382409
18	6	0	-0.165250	-1.332510	-0.204245
19	6	0	-2.472380	-0.813370	-0.299940
20	6	0	-1.595296	-1.843218	-0.203138
21	1	0	0.305156	-1.470255	-1.189734
22	1	0	0.477496	-1.846922	0.518567
23	6	0	1.812632	4.800455	0.478287
24	1	0	2.669275	5.455618	0.279850
25	1	0	0.913771	5.306281	0.100283
26	1	0	1.710568	4.705521	1.566906

27	6	0	2.203401	3.597893	-1.710054
28	1	0	3.055850	4.257159	-1.913856
29	1	0	2.393950	2.644343	-2.212470
30	1	0	1.316676	4.052022	-2.173919
31	6	0	-1.921090	-3.292902	-0.170615
32	6	0	-0.755065	-4.266795	-0.257600
33	1	0	-0.135816	-4.206577	0.647321
34	1	0	-1.143360	-5.282862	-0.354883
35	1	0	-0.101164	-4.035780	-1.107585
36	6	0	-3.969448	-0.858202	-0.391436
37	1	0	-4.270299	-0.620617	-1.423093
38	1	0	-4.305281	-1.871851	-0.184160
39	6	0	-4.648715	0.175630	0.544320
40	1	0	-4.445145	-0.128456	1.583130
41	6	0	-4.023996	1.567186	0.323714
42	1	0	-4.445188	2.293936	1.027307
43	1	0	-4.284887	1.922352	-0.680193
44	6	0	-2.498293	1.557360	0.517904
45	1	0	-2.285602	1.312606	1.569548
46	1	0	-2.108506	2.568412	0.348505
47	6	0	-6.198323	0.167200	0.392508
48	6	0	-6.866523	1.153151	1.368708
49	1	0	-6.591336	2.187123	1.145313
50	1	0	-7.958955	1.075920	1.294011
51	1	0	-6.590802	0.932552	2.407615
52	6	0	-6.785728	-1.237138	0.619416
53	1	0	-7.882634	-1.197432	0.580937
54	1	0	-6.448578	-1.945030	-0.141718
55	1	0	-6.505044	-1.629820	1.604218
56	8	0	4.656625	-1.247579	-3.175219
57	8	0	5.570195	-1.126480	3.165868
58	8	0	5.918721	-1.545846	0.650571

59	1	0	6.089288	-1.545092	1.638030
60	8	0	2.088079	0.644982	2.360131
61	1	0	1.269264	1.096985	2.104437
62	8	0	-3.068303	-3.723480	-0.072443
63	8	0	-6.462514	0.588318	-0.964718
64	1	0	-7.415187	0.513808	-1.132305
65	1	0	0.610868	2.571163	1.217710
66	1	0	-0.382310	0.229288	1.233769
67	6	0	-1.756182	1.001213	-1.860509
68	1	0	2.908332	2.974870	0.222071
69	1	0	-2.776086	1.087905	-2.246612
70	1	0	-1.280276	1.982243	-1.971232
71	1	0	0.838100	1.060984	-1.436525
72	8	0	2.550109	-0.039715	-2.333014
73	1	0	3.221145	-0.457894	-2.950702

Coordinates for z2b-6:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.952908	-0.424532	1.573894
2	6	0	2.719625	0.221844	1.265515
3	6	0	2.227165	0.369211	-0.035437
4	6	0	3.022781	-0.179213	-1.067252
5	6	0	4.267016	-0.837745	-0.825979
6	6	0	4.720971	-0.952659	0.507014
7	6	0	5.040585	-1.380223	-1.922431
8	1	0	5.989257	-1.872838	-1.667164
9	6	0	4.426938	-0.547475	2.936363

10	1	0	3.800118	-0.122361	3.732378
11	6	0	0.892585	1.042390	-0.384189
12	6	0	0.796265	2.524249	0.080484
13	1	0	-0.082265	2.967587	-0.402882
14	6	0	2.008511	3.432083	-0.215620
15	1	0	-1.195069	0.276074	-2.563156
16	6	0	-0.320515	0.178068	0.079630
17	6	0	-1.754823	0.550880	-0.453775
18	6	0	-0.171265	-1.324049	-0.264964
19	6	0	-2.475491	-0.799457	-0.375774
20	6	0	-1.601829	-1.832041	-0.285284
21	1	0	0.310903	-1.459719	-1.245012
22	1	0	0.460830	-1.843036	0.463605
23	6	0	1.800580	4.811123	0.431958
24	1	0	2.665850	5.461555	0.256853
25	1	0	0.917714	5.313767	0.014197
26	1	0	1.657740	4.731172	1.517161
27	6	0	2.268235	3.577812	-1.724127
28	1	0	3.126693	4.235749	-1.905672
29	1	0	2.478337	2.617722	-2.205875
30	1	0	1.398682	4.023752	-2.226925
31	6	0	-1.933198	-3.281647	-0.269708
32	6	0	-0.768063	-4.258902	-0.229124
33	1	0	-0.206373	-4.153528	0.708307
34	1	0	-1.152445	-5.278266	-0.303844
35	1	0	-0.061283	-4.069436	-1.046828
36	6	0	-3.975842	-0.839852	-0.452915
37	1	0	-4.272537	-0.596614	-1.486053
38	1	0	-4.318368	-1.854332	-0.255446
39	6	0	-4.612187	0.194090	0.508017
40	1	0	-4.321903	-0.085537	1.532458
41	6	0	-4.022452	1.589012	0.235396

42	1	0	-4.472653	2.319181	0.914472
43	1	0	-4.273293	1.912292	-0.784142
44	6	0	-2.496131	1.594386	0.423156
45	1	0	-2.280563	1.381153	1.480462
46	1	0	-2.109288	2.600713	0.222925
47	6	0	-6.166401	0.160564	0.512242
48	6	0	-6.691977	-1.209505	0.970262
49	1	0	-6.240820	-1.494971	1.926895
50	1	0	-7.781303	-1.168780	1.105398
51	1	0	-6.485096	-1.997942	0.239600
52	6	0	-6.796524	0.547195	-0.835829
53	1	0	-7.891440	0.538457	-0.753957
54	1	0	-6.494039	1.552981	-1.142760
55	1	0	-6.526389	-0.159395	-1.628769
56	8	0	4.688377	-1.314772	-3.113060
57	8	0	5.496369	-1.104858	3.239493
58	8	0	5.882041	-1.567640	0.738184
59	1	0	6.035377	-1.553264	1.728609
60	8	0	2.046285	0.688273	2.347988
61	1	0	1.243419	1.156314	2.071194
62	8	0	-3.086102	-3.707670	-0.287504
63	8	0	-6.529254	1.149750	1.504854
64	1	0	-7.492445	1.129291	1.621154
65	1	0	0.569992	2.590140	1.158585
66	1	0	-0.400123	0.232289	1.177262
67	6	0	-1.731749	0.998234	-1.937810
68	1	0	2.901035	2.980788	0.240885
69	1	0	-2.746000	1.088777	-2.338416
70	1	0	-1.248091	1.974868	-2.052978
71	1	0	0.864704	1.056810	-1.475169
72	8	0	2.579651	-0.076181	-2.325543
73	1	0	3.257902	-0.509689	-2.924931

Coordinates for z2b-16:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.954077	-0.444977	1.565674
2	6	0	2.719604	0.203259	1.266087
3	6	0	2.226982	0.367722	-0.032675
4	6	0	3.023708	-0.164827	-1.071965
5	6	0	4.269200	-0.824206	-0.839731
6	6	0	4.723381	-0.956464	0.491586
7	6	0	5.043902	-1.350083	-1.943521
8	1	0	5.993505	-1.844410	-1.694954
9	6	0	4.428120	-0.586030	2.926413
10	1	0	3.800110	-0.173645	3.728196
11	6	0	0.892176	1.044992	-0.372265
12	6	0	0.799055	2.522507	0.106820
13	1	0	-0.082635	2.970253	-0.366592
14	6	0	2.009786	3.432468	-0.188910
15	1	0	-1.243756	1.985858	-2.038436
16	6	0	-0.321665	0.178768	0.086176
17	6	0	-1.755185	0.553676	-0.448376
18	6	0	-0.171336	-1.322108	-0.263269
19	6	0	-2.475445	-0.797498	-0.379765
20	6	0	-1.601616	-1.830158	-0.292554
21	1	0	0.315276	-1.454287	-1.241647
22	1	0	0.457420	-1.843926	0.466107
23	6	0	1.812773	4.801778	0.482247
24	1	0	2.676218	5.453937	0.304541

25	1	0	0.924682	5.311503	0.084596
26	1	0	1.685293	4.705680	1.568030
27	6	0	2.252332	3.601124	-1.697896
28	1	0	3.113685	4.255325	-1.879281
29	1	0	2.449159	2.647423	-2.197708
30	1	0	1.380245	4.061977	-2.182496
31	6	0	-1.933396	-3.279662	-0.282129
32	6	0	-0.771385	-4.257260	-0.191714
33	1	0	-0.240650	-4.141760	0.762417
34	1	0	-1.154424	-5.277030	-0.267926
35	1	0	-0.038081	-4.078055	-0.988095
36	6	0	-3.975721	-0.838974	-0.457937
37	1	0	-4.272056	-0.594952	-1.491034
38	1	0	-4.317254	-1.854463	-0.263841
39	6	0	-4.614510	0.191452	0.504930
40	1	0	-4.327047	-0.091948	1.529160
41	6	0	-4.024565	1.587544	0.239463
42	1	0	-4.477216	2.315082	0.919862
43	1	0	-4.272027	1.914405	-0.779730
44	6	0	-2.498914	1.592349	0.432165
45	1	0	-2.286598	1.373510	1.488994
46	1	0	-2.111698	2.599784	0.238501
47	6	0	-6.168572	0.157856	0.505766
48	6	0	-6.695436	-1.220532	0.937043
49	1	0	-6.238597	-1.529033	1.883779
50	1	0	-7.783512	-1.178832	1.081172
51	1	0	-6.496901	-1.993145	0.187361
52	6	0	-6.796447	0.569900	-0.835714
53	1	0	-7.891622	0.548352	-0.759524
54	1	0	-6.502446	1.585494	-1.117409
55	1	0	-6.515607	-0.115228	-1.643644
56	8	0	4.691472	-1.269451	-3.133110

57	8	0	5.498643	-1.145303	3.221975
58	8	0	5.885814	-1.572119	0.714153
59	1	0	6.039369	-1.571245	1.704535
60	8	0	2.045275	0.653530	2.354826
61	1	0	1.238541	1.118775	2.084732
62	8	0	-3.085008	-3.705286	-0.342258
63	8	0	-6.532190	1.128272	1.516411
64	1	0	-7.496606	1.113990	1.623188
65	1	0	0.580871	2.577341	1.187037
66	1	0	-0.404128	0.229356	1.183889
67	6	0	-1.729082	1.009274	-1.929811
68	1	0	2.906423	2.971971	0.249938
69	1	0	-1.192536	0.289915	-2.558481
70	1	0	-2.742587	1.103525	-2.331449
71	1	0	0.861883	1.069295	-1.462977
72	8	0	2.580368	-0.045074	-2.328691
73	1	0	3.259382	-0.468688	-2.934091

Coordinates for Z2b-21:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.984769	-0.426616	1.548864
2	6	0	2.744698	0.215908	1.260785
3	6	0	2.233626	0.367831	-0.032353
4	6	0	3.016836	-0.172605	-1.077929
5	6	0	4.266751	-0.827389	-0.857167
6	6	0	4.740056	-0.946285	0.468726
7	6	0	5.026894	-1.362056	-1.967007

8	1	0	5.980743	-1.852629	-1.727438
9	6	0	4.478419	-0.553671	2.904045
10	1	0	3.861023	-0.134701	3.710664
11	6	0	0.893242	1.040183	-0.359577
12	6	0	0.804505	2.521445	0.108156
13	1	0	-0.088226	2.962145	-0.351188
14	6	0	2.006243	3.432097	-0.220208
15	1	0	-1.221444	0.286480	-2.518511
16	6	0	-0.313734	0.177169	0.121851
17	6	0	-1.753679	0.545704	-0.400747
18	6	0	-0.166070	-1.327569	-0.212578
19	6	0	-2.470409	-0.803672	-0.318792
20	6	0	-1.596721	-1.835884	-0.222217
21	1	0	0.310899	-1.469992	-1.194187
22	1	0	0.469855	-1.841394	0.516454
23	6	0	1.816449	4.808351	0.438679
24	1	0	2.675274	5.460523	0.240055
25	1	0	0.920945	5.311531	0.049424
26	1	0	1.706550	4.724135	1.527409
27	6	0	2.220718	3.583857	-1.735233
28	1	0	3.073922	4.241829	-1.939817
29	1	0	2.415815	2.625428	-2.226518
30	1	0	1.336915	4.032371	-2.210007
31	6	0	-1.928385	-3.284805	-0.196206
32	6	0	-0.763564	-4.263026	-0.200146
33	1	0	-0.190532	-4.182451	0.733105
34	1	0	-1.149629	-5.280155	-0.294422
35	1	0	-0.066892	-4.052881	-1.021110
36	6	0	-3.968140	-0.843143	-0.405871
37	1	0	-4.251814	-0.584620	-1.439706
38	1	0	-4.307540	-1.860429	-0.220364
39	6	0	-4.639151	0.181241	0.545181

40	1	0	-4.408720	-0.126118	1.577856
41	6	0	-4.023601	1.573664	0.315045
42	1	0	-4.439396	2.298330	1.023465
43	1	0	-4.301175	1.927330	-0.686005
44	6	0	-2.495090	1.573052	0.492440
45	1	0	-2.272489	1.342777	1.545091
46	1	0	-2.111724	2.583841	0.307526
47	6	0	-6.198958	0.163243	0.422572
48	6	0	-6.843980	1.226414	1.321922
49	1	0	-6.627149	2.234815	0.959441
50	1	0	-7.931785	1.101877	1.322316
51	1	0	-6.484344	1.138813	2.354117
52	6	0	-6.775875	-1.216959	0.779782
53	1	0	-7.869316	-1.186328	0.720019
54	1	0	-6.422666	-2.004578	0.104617
55	1	0	-6.496106	-1.509731	1.798873
56	8	0	4.657356	-1.293072	-3.152061
57	8	0	5.554264	-1.107700	3.189735
58	8	0	5.907160	-1.556863	0.680341
59	1	0	6.075099	-1.546372	1.668229
60	8	0	2.083939	0.673443	2.355074
61	1	0	1.273839	1.136529	2.091612
62	8	0	-3.081753	-3.709841	-0.168996
63	8	0	-6.601914	0.524146	-0.918352
64	1	0	-6.525278	-0.255470	-1.490428
65	1	0	0.608569	2.585941	1.192168
66	1	0	-0.383518	0.239671	1.219782
67	6	0	-1.747877	1.005296	-1.880611
68	1	0	2.912288	2.979468	0.207426
69	1	0	-2.766903	1.103788	-2.266697
70	1	0	-1.261939	1.980852	-1.993899
71	1	0	0.848262	1.055878	-1.449937

72	8	0	2.555261	-0.065548	-2.329188
73	1	0	3.226264	-0.493671	-2.940303

Coordinates for Z2b-26:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.954489	-0.438536	1.572139
2	6	0	2.720741	0.209341	1.269425
3	6	0	2.228323	0.368221	-0.030138
4	6	0	3.024968	-0.169214	-1.067009
5	6	0	4.269905	-0.828316	-0.831585
6	6	0	4.723584	-0.955373	0.500415
7	6	0	5.044603	-1.359431	-1.933035
8	1	0	5.993635	-1.853691	-1.682218
9	6	0	4.428255	-0.573716	2.933666
10	1	0	3.800731	-0.156581	3.733397
11	6	0	0.893718	1.044283	-0.372982
12	6	0	0.800496	2.523490	0.100259
13	1	0	-0.083708	2.968290	-0.371301
14	6	0	2.009261	3.433125	-0.204315
15	1	0	-1.188552	0.293800	-2.558874
16	6	0	-0.320533	0.179793	0.087676
17	6	0	-1.753747	0.553004	-0.449716
18	6	0	-0.170117	-1.322250	-0.256396
19	6	0	-2.473835	-0.797897	-0.379271
20	6	0	-1.600803	-1.829757	-0.278412
21	1	0	0.314002	-1.457107	-1.235518
22	1	0	0.460524	-1.841791	0.473275

23	6	0	1.813280	4.805603	0.460637
24	1	0	2.676120	5.457121	0.277925
25	1	0	0.924238	5.313195	0.062414
26	1	0	1.688273	4.714800	1.547185
27	6	0	2.246428	3.594141	-1.714973
28	1	0	3.105103	4.250041	-1.902594
29	1	0	2.444898	2.638283	-2.209983
30	1	0	1.371446	4.049512	-2.199507
31	6	0	-1.931701	-3.279584	-0.261596
32	6	0	-0.768787	-4.256586	-0.344730
33	1	0	-1.159339	-5.270383	-0.455328
34	1	0	-0.104684	-4.020091	-1.185206
35	1	0	-0.159447	-4.206462	0.567488
36	6	0	-3.973502	-0.838994	-0.473268
37	1	0	-4.263379	-0.578855	-1.504047
38	1	0	-4.318185	-1.854696	-0.287855
39	6	0	-4.619362	0.184170	0.494839
40	1	0	-4.324142	-0.115385	1.515864
41	6	0	-4.025524	1.580231	0.240372
42	1	0	-4.482849	2.308143	0.918755
43	1	0	-4.271688	1.908853	-0.778149
44	6	0	-2.500102	1.588485	0.433938
45	1	0	-2.285256	1.367145	1.489974
46	1	0	-2.115133	2.597272	0.242617
47	6	0	-6.179319	0.159438	0.498059
48	6	0	-6.716674	-1.239860	0.838359
49	1	0	-6.245809	-1.636266	1.748510
50	1	0	-7.797639	-1.182048	1.005903
51	1	0	-6.534678	-1.960313	0.034618
52	6	0	-6.805457	0.664516	-0.805441
53	1	0	-7.896621	0.605335	-0.734760
54	1	0	-6.540435	1.709239	-0.993136

55	1	0	-6.485628	0.060166	-1.660892
56	8	0	4.692339	-1.283512	-3.122923
57	8	0	5.498022	-1.132772	3.231980
58	8	0	5.885513	-1.570824	0.725759
59	1	0	6.039286	-1.565713	1.715996
60	8	0	2.046138	0.664761	2.356091
61	1	0	1.243016	1.134269	2.082790
62	8	0	-3.081852	-3.704995	-0.179567
63	8	0	-6.642015	1.090446	1.505487
64	1	0	-6.425551	0.729332	2.380779
65	1	0	0.586842	2.583319	1.181237
66	1	0	-0.403442	0.234422	1.185074
67	6	0	-1.726810	1.011578	-1.929833
68	1	0	2.907790	2.975418	0.233643
69	1	0	-2.739882	1.105022	-2.332669
70	1	0	-1.242685	1.988824	-2.036998
71	1	0	0.864099	1.064958	-1.463794
72	8	0	2.581578	-0.054974	-2.324250
73	1	0	3.260272	-0.481840	-2.927732

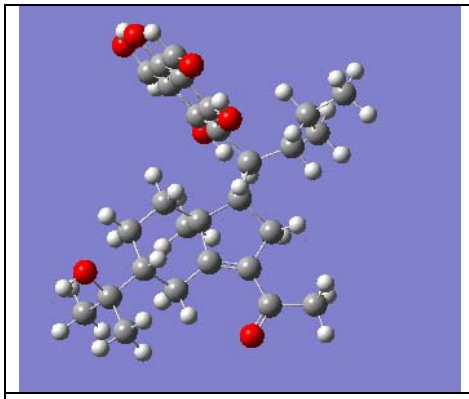
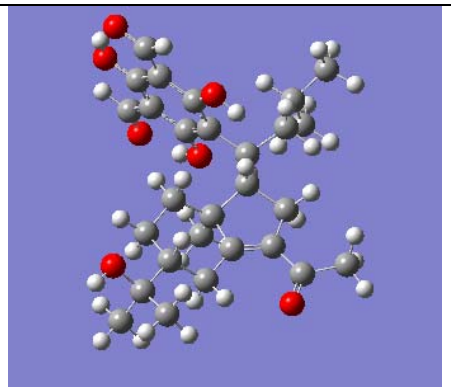
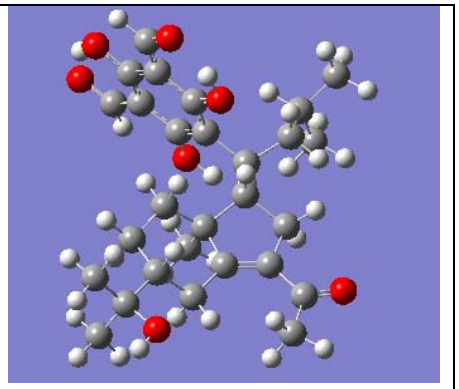
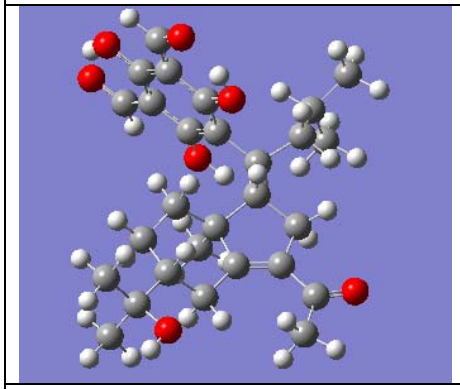
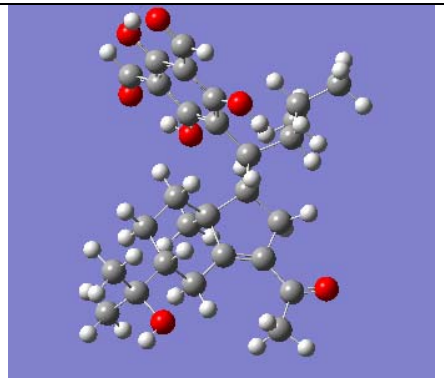
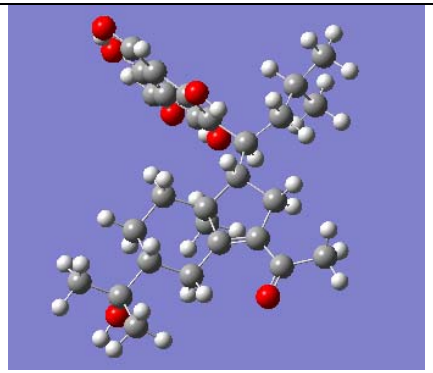
The calculated ^{13}C NMR data for compound **1**

Position	Z2b-5	Z2b-6	Z2b-16	Z2b-21	Z2b-26	Averaged for **1**[a]	Recorded for **1**
1	57.4	57.6	57.7	57.6	57.6	57.6	52.4
2	38.3	38.4	38.5	38.5	38.5	38.4	38.4
3	130.3	130.0	130.0	130.5	130.1	130.2	132.6
4	196.0	196.2	196.1	196.2	196.0	196.1	198.9
5	171.6	170.6	170.7	171.1	169.9	170.8	163.2
6	25.5	27.5	27.7	25.2	27.8	26.9	27.1
7	48.5	49.2	49.3	49.9	53.6	50.1	49.8
8	23.7	23.7	23.9	24.0	24.2	23.9	23.9
9	44.0	44.1	44.3	44.3	44.4	44.2	43.0
10	50.1	51.1	51.3	50.2	51.0	50.8	49.9
11	73.8	74.2	74.2	73.5	75.0	74.2	71.4
12	28.4	29.3	29.4	27.7	28.6	28.8	27.8
13	28.0	21.6	21.6	25.6	17.9	22.7	27.6
14	13.9	14.4	14.6	14.3	14.2	14.3	16.9
15	28.7	29.0	29.2	28.9	28.8	29.0	30.7
7'	189.9	189.9	190.0	188.2	188.1	189.4	192.0
8'	188.3	188.4	188.4	189.9	189.8	188.9	191.9
9'	32.5	33.0	33.0	32.9	32.9	32.9	32.9
10'	44.4	44.6	44.5	44.6	44.5	44.5	41.7
11'	29.3	29.4	29.5	29.5	29.5	29.5	27.2
12'	23.1	23.2	23.3	23.3	23.3	23.2	24.9
13'	18.4	18.5	18.7	18.6	18.5	18.6	22.2

[a]: their ^{13}C NMR chemical shifts were in ppm

The correlation value of plots (experimental versus calculated) for **1** is 0.9990

6 low energy conformers of compound **2**

		
Z1b-1	Z1b-18	z1b-32
		
z1b-2	z1b-3	Z1b-23

The internal energy data for each conformer of **2**:

	z1b-1	z1b-18	z1b-32	Z1b-2	Z1b-3	Z1b-23
Energy (a.u.)	-1616.945256	-1616.944986	-1616.945256	-1616.9447551	-1616.9442829	-1616.9451673

Coordinate for z1b-1:
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.034113	-1.652755	-1.356054
2	6	0	2.250535	-0.465623	-1.247003
3	6	0	2.026828	0.208749	-0.039611
4	6	0	2.672655	-0.331922	1.096644
5	6	0	3.471833	-1.515638	1.054024
6	6	0	3.639250	-2.171434	-0.185593
7	6	0	4.098491	-2.029374	2.253177
8	1	0	4.697474	-2.944879	2.148164
9	6	0	3.219651	-2.326297	-2.624248
10	1	0	2.736244	-1.887480	-3.507843
11	6	0	1.191056	1.490335	0.089469
12	1	0	1.200246	1.747487	1.150867
13	6	0	1.850046	2.691026	-0.656181
14	1	0	1.826300	2.529578	-1.746059
15	6	0	3.300679	3.036995	-0.255955
16	1	0	-0.973317	1.311430	2.398257
17	6	0	-0.309768	1.334922	-0.308974
18	6	0	-1.197736	0.292261	0.463501
19	6	0	-1.120280	2.645930	-0.208884
20	6	0	-2.608084	0.859980	0.238618
21	6	0	-2.556177	2.168033	-0.115887
22	1	0	-0.850063	3.229101	0.685151
23	1	0	-0.970877	3.313914	-1.061533
24	6	0	3.386455	3.599534	1.173001
25	1	0	4.424814	3.840900	1.431418

26	1	0	2.800110	4.524689	1.260458
27	1	0	3.018111	2.890411	1.920793
28	6	0	3.897098	4.035452	-1.262075
29	1	0	4.931857	4.287235	-1.000205
30	1	0	3.899613	3.628470	-2.281213
31	1	0	3.321437	4.970921	-1.276460
32	6	0	-3.626876	3.172810	-0.342591
33	6	0	-5.101292	2.808039	-0.353891
34	1	0	-5.426567	2.446497	0.628780
35	1	0	-5.671389	3.704759	-0.607977
36	1	0	-5.319563	2.019995	-1.083405
37	6	0	-3.779790	-0.042987	0.510439
38	1	0	-3.842798	-0.198505	1.598739
39	1	0	-4.723921	0.399098	0.204143
40	6	0	-3.609071	-1.419383	-0.180017
41	1	0	-3.551209	-1.228536	-1.262670
42	6	0	-2.276417	-2.052484	0.255443
43	1	0	-2.126325	-3.022832	-0.231955
44	1	0	-2.287916	-2.247094	1.336477
45	6	0	-1.087645	-1.144722	-0.104465
46	1	0	-1.023514	-1.088084	-1.200596
47	1	0	-0.156146	-1.608985	0.239724
48	6	0	-4.853282	-2.334365	-0.000211
49	6	0	-5.133866	-2.719572	1.461242
50	1	0	-5.301871	-1.835257	2.083392
51	1	0	-6.036642	-3.341761	1.518794
52	1	0	-4.311016	-3.300460	1.892741
53	6	0	-4.736664	-3.599281	-0.867134
54	1	0	-5.680865	-4.159523	-0.845146
55	1	0	-4.523421	-3.335264	-1.908904
56	1	0	-3.952840	-4.274694	-0.508546
57	8	0	3.992583	-1.495208	3.370927

58	8	0	3.891126	-3.365101	-2.754127
59	8	0	4.379412	-3.280728	-0.230322
60	1	0	4.387314	-3.595517	-1.181833
61	8	0	1.728143	-0.039822	-2.424900
62	1	0	1.222480	0.777637	-2.298294
63	8	0	-3.297154	4.343402	-0.529623
64	8	0	-5.949672	-1.533553	-0.501002
65	1	0	-6.758953	-2.068696	-0.480843
66	1	0	1.232716	3.580733	-0.485818
67	1	0	-0.383040	1.030735	-1.365789
68	6	0	-0.921741	0.296409	1.988360
69	1	0	3.904557	2.119118	-0.299871
70	1	0	-1.660010	-0.308805	2.524722
71	1	0	0.067521	-0.108632	2.216809
72	8	0	2.519034	0.297031	2.267058
73	1	0	3.033678	-0.213689	2.960576

Coordinate for z1b-18:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.504267	-1.551324	-1.056161
2	6	0	-2.714379	-0.367476	-1.157768
3	6	0	-2.030031	0.205488	-0.077478
4	6	0	-2.204418	-0.435328	1.172687
5	6	0	-2.985412	-1.618907	1.340452
6	6	0	-3.627044	-2.172177	0.209982
7	6	0	-3.120784	-2.235947	2.643214

8	1	0	-3.732630	-3.147019	2.701327
9	6	0	-4.179622	-2.115904	-2.206002
10	1	0	-4.062912	-1.598939	-3.168451
11	6	0	-1.194438	1.484578	-0.209617
12	1	0	-1.158714	1.772910	-1.271146
13	6	0	-1.872778	2.671479	0.535952
14	1	0	-1.914409	2.423455	1.601738
15	6	0	-3.285056	3.064637	0.049281
16	1	0	0.895081	1.146319	-2.500940
17	6	0	0.296882	1.324920	0.213685
18	6	0	1.179966	0.243342	-0.511337
19	6	0	1.116239	2.631939	0.069104
20	6	0	2.586525	0.822501	-0.338527
21	6	0	2.550442	2.145044	-0.041852
22	1	0	0.822913	3.201113	-0.829821
23	1	0	0.960991	3.303098	0.920241
24	6	0	-3.262330	3.772258	-1.316510
25	1	0	-4.278740	4.006928	-1.654393
26	1	0	-2.704704	4.716712	-1.255751
27	1	0	-2.795233	3.168290	-2.104496
28	6	0	-3.969559	3.963520	1.092642
29	1	0	-4.978361	4.248612	0.769812
30	1	0	-4.056769	3.455722	2.060616
31	1	0	-3.397659	4.888176	1.250522
32	6	0	3.716856	3.049826	0.126322
33	6	0	3.430403	4.487978	0.533616
34	1	0	2.967636	4.524275	1.528664
35	1	0	4.367782	5.047863	0.552683
36	1	0	2.729764	4.966828	-0.162157
37	6	0	3.783089	-0.062480	-0.544061
38	1	0	3.887491	-0.250123	-1.624973
39	1	0	4.680567	0.470719	-0.234110

40	6	0	3.619293	-1.415555	0.189801
41	1	0	3.564528	-1.200702	1.268031
42	6	0	2.285045	-2.072293	-0.207257
43	1	0	2.174426	-3.026336	0.316882
44	1	0	2.281654	-2.302716	-1.281534
45	6	0	1.094178	-1.162146	0.136431
46	1	0	1.052105	-1.043237	1.227797
47	1	0	0.159319	-1.652434	-0.161147
48	6	0	4.850310	-2.352617	0.034523
49	6	0	6.123612	-1.696593	0.593753
50	1	0	5.957674	-1.343219	1.617451
51	1	0	6.944490	-2.426251	0.614353
52	1	0	6.456760	-0.850897	-0.016541
53	6	0	5.088744	-2.828073	-1.408106
54	1	0	5.949584	-3.509008	-1.440238
55	1	0	4.220782	-3.369944	-1.795480
56	1	0	5.312527	-1.992677	-2.081165
57	8	0	-2.589515	-1.791406	3.675585
58	8	0	-4.874728	-3.145455	-2.151972
59	8	0	-4.352522	-3.280947	0.363395
60	1	0	-4.731509	-3.516456	-0.533944
61	8	0	-2.678495	0.163639	-2.406692
62	1	0	-2.142666	0.972868	-2.411219
63	8	0	4.878730	2.686920	-0.046845
64	8	0	4.519248	-3.494463	0.859099
65	1	0	5.279898	-4.096967	0.869449
66	1	0	-1.230514	3.556167	0.447199
67	1	0	0.309511	1.063982	1.276256
68	6	0	0.892887	0.154184	-2.032777
69	1	0	-3.890344	2.151393	-0.046549
70	1	0	1.652708	-0.443014	-2.546472
71	1	0	-0.072983	-0.323949	-2.227198

72	8	0	-1.607473	0.096518	2.243074
73	1	0	-1.828133	-0.479234	3.035617

Coordinate for z1b-32:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.023756	-1.703702	-1.312149
2	6	0	2.212062	-0.534052	-1.231218
3	6	0	2.007131	0.187861	-0.048303
4	6	0	2.693421	-0.289584	1.092652
5	6	0	3.520210	-1.454309	1.077791
6	6	0	3.674312	-2.155965	-0.138429
7	6	0	4.190687	-1.900872	2.280232
8	1	0	4.808644	-2.805983	2.198451
9	6	0	3.189687	-2.428664	-2.555035
10	1	0	2.663952	-2.046075	-3.440537
11	6	0	1.168562	1.470073	0.048068
12	1	0	1.187718	1.756811	1.101829
13	6	0	1.826037	2.642759	-0.742391
14	1	0	1.816829	2.425770	-1.822051
15	6	0	3.269509	3.017855	-0.341364
16	1	0	-0.930766	1.222500	2.394420
17	6	0	-0.338092	1.313686	-0.326296
18	6	0	-1.209856	0.251739	0.438229
19	6	0	-1.148097	2.626822	-0.183242
20	6	0	-2.617907	0.827011	0.264634
21	6	0	-2.583304	2.144828	-0.054454
22	1	0	-0.834517	3.191808	0.709923

23	1	0	-0.999263	3.294877	-1.038069
24	6	0	3.335732	3.654803	1.056846
25	1	0	4.370551	3.908896	1.317027
26	1	0	2.750129	4.584348	1.087580
27	1	0	2.956710	2.985822	1.835618
28	6	0	3.875430	3.964156	-1.391156
29	1	0	4.905293	4.234909	-1.129138
30	1	0	3.893657	3.503410	-2.386860
31	1	0	3.296501	4.895252	-1.463133
32	6	0	-3.748082	3.052272	-0.217857
33	6	0	-3.456478	4.504379	-0.568672
34	1	0	-2.992653	4.577470	-1.561337
35	1	0	-4.392561	5.066701	-0.569673
36	1	0	-2.756162	4.955381	0.145635
37	6	0	-3.811921	-0.052183	0.505596
38	1	0	-3.902657	-0.212037	1.592172
39	1	0	-4.712735	0.471852	0.190081
40	6	0	-3.653069	-1.423373	-0.194303
41	1	0	-3.604562	-1.236362	-1.278195
42	6	0	-2.317175	-2.070389	0.213126
43	1	0	-2.210983	-3.039901	-0.282779
44	1	0	-2.306170	-2.267638	1.293616
45	6	0	-1.127078	-1.173186	-0.164917
46	1	0	-1.093689	-1.094031	-1.261259
47	1	0	-0.190763	-1.653236	0.143155
48	6	0	-4.883099	-2.356365	-0.009371
49	6	0	-6.161347	-1.711049	-0.569707
50	1	0	-6.004253	-1.375425	-1.600761
51	1	0	-6.981430	-2.441749	-0.570929
52	1	0	-6.490365	-0.855156	0.028450
53	6	0	-5.107888	-2.803088	1.444459
54	1	0	-5.971596	-3.478891	1.499445

55	1	0	-4.238227	-3.341275	1.833020
56	1	0	-5.320403	-1.953799	2.103568
57	8	0	4.101408	-1.320593	3.376268
58	8	0	3.889919	-3.450682	-2.660315
59	8	0	4.443894	-3.245286	-0.157456
60	1	0	4.434147	-3.601036	-1.094499
61	8	0	1.647137	-0.171067	-2.410480
62	1	0	1.076091	0.602842	-2.290680
63	8	0	-4.912348	2.680885	-0.085010
64	8	0	-4.559089	-3.513680	-0.815109
65	1	0	-5.314565	-4.122503	-0.796771
66	1	0	1.202618	3.536671	-0.619225
67	1	0	-0.435812	1.038949	-1.390224
68	6	0	-0.898951	0.218159	1.956624
69	1	0	3.877182	2.101755	-0.329757
70	1	0	-1.631417	-0.393303	2.492895
71	1	0	0.091002	-0.202330	2.151462
72	8	0	2.556458	0.386692	2.238610
73	1	0	3.100343	-0.083172	2.939130

Coordinate for Z1b-2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.531504	-1.500109	-1.094096
2	6	0	-2.742851	-0.312026	-1.154333
3	6	0	-2.043489	0.213771	-0.059701
4	6	0	-2.204965	-0.478485	1.164348
5	6	0	-2.985390	-1.668298	1.291334

6	6	0	-3.640002	-2.173742	0.145921
7	6	0	-3.107387	-2.339494	2.567925
8	1	0	-3.723759	-3.249095	2.594637
9	6	0	-4.221326	-2.014893	-2.258261
10	1	0	-4.118203	-1.455999	-3.198530
11	6	0	-1.207966	1.496565	-0.150483
12	1	0	-1.176378	1.820361	-1.201955
13	6	0	-1.887829	2.654635	0.637494
14	1	0	-1.960024	2.353494	1.687951
15	6	0	-3.281511	3.088661	0.131748
16	1	0	-0.110353	-0.277255	-2.192326
17	6	0	0.286589	1.333450	0.259881
18	6	0	1.167149	0.264667	-0.486422
19	6	0	1.098478	2.640876	0.119157
20	6	0	2.579590	0.845782	-0.317346
21	6	0	2.531506	2.163420	-0.002076
22	1	0	0.810615	3.220555	-0.772693
23	1	0	0.972827	3.317410	0.968916
24	6	0	-3.205291	3.887383	-1.181077
25	1	0	-4.207544	4.143178	-1.545187
26	1	0	-2.653378	4.824982	-1.032557
27	1	0	-2.700861	3.339421	-1.987321
28	6	0	-3.998519	3.919367	1.209053
29	1	0	-4.990991	4.239377	0.868471
30	1	0	-4.128855	3.344838	2.134002
31	1	0	-3.423877	4.822599	1.455010
32	6	0	3.605762	3.177364	0.160919
33	6	0	5.080029	2.811821	0.186134
34	1	0	5.406705	2.424225	-0.786270
35	1	0	5.650087	3.715463	0.414721
36	1	0	5.297451	2.043922	0.936820
37	6	0	3.749267	-0.062167	-0.583563

38	1	0	3.785018	-0.265632	-1.665264
39	1	0	4.698563	0.397530	-0.322673
40	6	0	3.604839	-1.407689	0.171581
41	1	0	3.572788	-1.168850	1.245514
42	6	0	2.264988	-2.064690	-0.200874
43	1	0	2.132570	-3.012348	0.333988
44	1	0	2.250942	-2.308733	-1.272122
45	6	0	1.082009	-1.145834	0.149698
46	1	0	1.045614	-1.034760	1.241746
47	1	0	0.144443	-1.631016	-0.146771
48	6	0	4.849491	-2.323621	0.001248
49	6	0	5.099423	-2.767597	-1.449093
50	1	0	5.253503	-1.908366	-2.108816
51	1	0	6.001444	-3.391384	-1.500808
52	1	0	4.268077	-3.365058	-1.839781
53	6	0	4.759113	-3.551893	0.922406
54	1	0	5.706151	-4.107635	0.903823
55	1	0	4.565744	-3.246078	1.956590
56	1	0	3.972056	-4.245531	0.608564
57	8	0	-2.560247	-1.943337	3.611924
58	8	0	-4.914224	-3.047532	-2.240393
59	8	0	-4.363251	-3.289115	0.260214
60	1	0	-4.753756	-3.484777	-0.641960
61	8	0	-2.722483	0.272600	-2.379020
62	1	0	-2.198195	1.089306	-2.351392
63	8	0	3.278971	4.357307	0.282450
64	8	0	5.952912	-1.497916	0.442658
65	1	0	6.763169	-2.031831	0.432142
66	1	0	-1.231309	3.532246	0.611673
67	1	0	0.307530	1.059205	1.319053
68	6	0	0.862124	0.189899	-2.004495
69	1	0	-3.887987	2.188233	-0.046787

70	1	0	0.866588	1.186495	-2.462230
71	1	0	1.610143	-0.409027	-2.534157
72	8	0	-1.594493	0.006474	2.248967
73	1	0	-1.807988	-0.600071	3.019428

Coordinate for Z1b-3:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.053765	-1.620714	-1.377131
2	6	0	2.271187	-0.434449	-1.252883
3	6	0	2.026122	0.209833	-0.033474
4	6	0	2.649327	-0.360744	1.100901
5	6	0	3.447516	-1.544485	1.043245
6	6	0	3.636345	-2.169672	-0.208959
7	6	0	4.052045	-2.088604	2.240451
8	1	0	4.651385	-3.002464	2.123727
9	6	0	3.261078	-2.262794	-2.657983
10	1	0	2.794370	-1.800980	-3.538868
11	6	0	1.190486	1.489741	0.111892
12	1	0	1.179693	1.719962	1.179445
13	6	0	1.864048	2.707355	-0.592368
14	1	0	1.850449	2.576692	-1.686634
15	6	0	3.311777	3.036618	-0.168809
16	1	0	-1.016882	1.263973	2.372197
17	6	0	-0.302489	1.348403	-0.319737
18	6	0	-1.208120	0.291027	0.409597
19	6	0	-1.111293	2.658506	-0.203048
20	6	0	-2.611441	0.864188	0.169277

21	6	0	-2.550045	2.182852	-0.148330
22	1	0	-0.856874	3.218612	0.710162
23	1	0	-0.944835	3.347203	-1.035790
24	6	0	3.386280	3.552714	1.278141
25	1	0	4.422440	3.786311	1.552066
26	1	0	2.798437	4.474217	1.390887
27	1	0	3.012755	2.819596	1.999616
28	6	0	3.918450	4.065860	-1.137168
29	1	0	4.951859	4.305933	-0.859420
30	1	0	3.927645	3.692722	-2.169173
31	1	0	3.345368	5.002951	-1.124945
32	6	0	-3.609084	3.201352	-0.360649
33	6	0	-5.090386	2.858905	-0.362602
34	1	0	-5.405383	2.443578	0.601717
35	1	0	-5.650906	3.776472	-0.556219
36	1	0	-5.330498	2.122284	-1.138410
37	6	0	-3.794434	-0.037040	0.395736
38	1	0	-3.923209	-0.188823	1.477232
39	1	0	-4.708251	0.433209	0.040512
40	6	0	-3.628586	-1.436537	-0.254301
41	1	0	-3.615250	-1.300891	-1.347434
42	6	0	-2.277576	-2.047991	0.161956
43	1	0	-2.119124	-3.005829	-0.345331
44	1	0	-2.295627	-2.265354	1.236558
45	6	0	-1.097705	-1.129367	-0.190714
46	1	0	-1.040271	-1.045459	-1.286251
47	1	0	-0.162418	-1.599187	0.135222
48	6	0	-4.844870	-2.362078	0.050028
49	6	0	-4.666223	-3.757640	-0.574350
50	1	0	-3.828648	-4.294178	-0.121535
51	1	0	-5.571854	-4.358562	-0.419888
52	1	0	-4.496157	-3.691725	-1.656147

53	6	0	-6.166788	-1.755543	-0.456825
54	1	0	-6.993947	-2.456566	-0.285268
55	1	0	-6.411162	-0.825394	0.063106
56	1	0	-6.124914	-1.554826	-1.534653
57	8	0	3.927426	-1.581394	3.368687
58	8	0	3.933036	-3.299501	-2.801994
59	8	0	4.375465	-3.279038	-0.267924
60	1	0	4.400086	-3.570143	-1.226567
61	8	0	1.772212	0.022786	-2.429386
62	1	0	1.267870	0.839103	-2.291185
63	8	0	-3.269592	4.370669	-0.538004
64	8	0	-4.893226	-2.481888	1.488824
65	1	0	-5.622820	-3.074818	1.728605
66	1	0	1.248847	3.594961	-0.403847
67	1	0	-0.354865	1.069640	-1.384936
68	6	0	-0.964055	0.258191	1.940023
69	1	0	3.914299	2.119393	-0.237224
70	1	0	-1.716227	-0.354832	2.446722
71	1	0	0.018554	-0.158031	2.177418
72	8	0	2.474583	0.238899	2.283468
73	1	0	2.974832	-0.290329	2.973683

Coordinate for Z1b-23:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.035932	-1.671419	-1.342181
2	6	0	2.234239	-0.496143	-1.241769
3	6	0	2.010035	0.190146	-0.041538

4	6	0	2.668619	-0.328603	1.098019
5	6	0	3.485079	-1.500380	1.063858
6	6	0	3.656917	-2.166486	-0.169621
7	6	0	4.126684	-1.990171	2.265428
8	1	0	4.737639	-2.898560	2.168319
9	6	0	3.220384	-2.359264	-2.602925
10	1	0	2.718679	-1.942383	-3.486969
11	6	0	1.175012	1.473005	0.077266
12	1	0	1.172156	1.727126	1.139530
13	6	0	1.852431	2.666707	-0.663264
14	1	0	1.858847	2.486360	-1.749812
15	6	0	3.291659	3.019649	-0.228531
16	1	0	-0.973604	1.180463	2.370046
17	6	0	-0.323086	1.331277	-0.335375
18	6	0	-1.215701	0.257881	0.387278
19	6	0	-1.134567	2.642160	-0.185706
20	6	0	-2.617300	0.835221	0.189071
21	6	0	-2.573413	2.157814	-0.112927
22	1	0	-0.847693	3.183986	0.730518
23	1	0	-0.958482	3.330713	-1.018957
24	6	0	3.339733	3.608120	1.191474
25	1	0	4.371436	3.849546	1.475020
26	1	0	2.756325	4.537946	1.245537
27	1	0	2.947385	2.914081	1.941028
28	6	0	3.917966	3.998015	-1.236214
29	1	0	4.944872	4.254591	-0.949482
30	1	0	3.949469	3.571303	-2.246695
31	1	0	3.344293	4.933835	-1.285282
32	6	0	-3.730880	3.068797	-0.298435
33	6	0	-3.426531	4.541867	-0.534872
34	1	0	-2.762746	4.944075	0.240734
35	1	0	-2.916214	4.681697	-1.497161

36	1	0	-4.363357	5.102977	-0.544381
37	6	0	-3.815496	-0.040810	0.406002
38	1	0	-3.943114	-0.199148	1.487666
39	1	0	-4.702867	0.484018	0.057983
40	6	0	-3.671886	-1.433787	-0.259905
41	1	0	-3.689425	-1.286962	-1.351526
42	6	0	-2.314386	-2.062547	0.111560
43	1	0	-2.175391	-3.012862	-0.415695
44	1	0	-2.307864	-2.299756	1.181837
45	6	0	-1.132348	-1.148807	-0.250891
46	1	0	-1.103701	-1.038106	-1.345327
47	1	0	-0.193803	-1.635978	0.038983
48	6	0	-4.883210	-2.356294	0.068360
49	6	0	-4.767207	-3.717756	-0.641138
50	1	0	-3.901956	-4.283366	-0.285822
51	1	0	-5.662971	-4.321500	-0.445799
52	1	0	-4.684119	-3.594153	-1.728218
53	6	0	-6.221170	-1.702392	-0.319863
54	1	0	-7.048321	-2.402423	-0.141257
55	1	0	-6.415185	-0.798766	0.263346
56	1	0	-6.239245	-1.437616	-1.384158
57	8	0	4.020668	-1.442551	3.376463
58	8	0	3.910109	-3.386695	-2.725851
59	8	0	4.415474	-3.263261	-0.206540
60	1	0	4.421819	-3.589864	-1.153990
61	8	0	1.697861	-0.091338	-2.421122
62	1	0	1.139028	0.689730	-2.290296
63	8	0	-4.899204	2.686764	-0.273763
64	8	0	-4.842378	-2.559319	1.498923
65	1	0	-5.621453	-3.074273	1.761750
66	1	0	1.232287	3.559935	-0.520020
67	1	0	-0.395832	1.077590	-1.406466

68	6	0	-0.938769	0.185912	1.910477
69	1	0	3.894663	2.100448	-0.239178
70	1	0	-1.687349	-0.432023	2.415644
71	1	0	0.044471	-0.245031	2.116979
72	8	0	2.513836	0.313296	2.260849
73	1	0	3.037949	-0.183081	2.958076

The calculated ^{13}C NMR data for compound **2**

Position	Z1b-1	Z1b-18	Z1b-32	Z1b-2	Z1b-3	Z1b-23	Averaged for **2** [a]	Recorded for **2**
1	57.1	52.9	59.6	51.1	56.6	59.2	56.6	51.9
2	37.6	39.4	39.3	38.6	37.4	39.3	38.7	38.9
3	135.3	128.8	127.8	136.1	135.2	128.1	131.3	132.1
4	195.3	195.5	194.9	195.9	194.5	195.1	195.3	198.7
5	166.3	173.0	173.7	165.3	168.2	174.7	170.8	164.5
6	27.4	28.6	28.2	27.4	27.2	26.0	27.5	26.9
7	49.8	49.5	49.2	50.2	48.3	48.5	49.3	49.6
8	24.9	22.9	22.4	25.7	21.7	22.2	23.3	23.8
9	41.2	41.4	41.3	41.3	40.4	40.9	41.1	40.1
10	53.7	51.7	52.2	53.1	53.7	51.9	52.6	50.3
11	73.9	74.2	73.7	74.4	72.6	72.8	73.7	71.4
12	29.1	29.9	29.4	29.5	27.6	28.3	29.1	28.1
13	21.3	22.8	22.0	22.1	27.5	27.9	23.6	27.3
14	15.8	16.3	16.5	15.7	15.3	15.9	16.0	17.1
15	29.2	30.2	29.6	29.8	29.2	29.5	29.6	30.9
7'	190.4	190.3	189.6	190.3	189.9	188.6	189.9	191.9
8'	189.8	189.2	189.0	191.0	190.6	189.3	189.8	191.6
9'	32.4	37.6	32.8	37.8	37.0	32.5	34.4	33.0
10'	43.2	39.8	43.3	39.3	43.2	43.5	42.2	42.3
11'	29.3	28.6	29.4	28.1	28.9	29.3	29.0	26.5
12'	23.3	23.8	23.6	23.4	23.1	23.1	23.4	25.0
13'	19.1	20.7	19.6	20.5	19.1	19.6	19.7	22.5

[a]: their ^{13}C NMR chemical shifts were in ppm

The correlation value of plots (experimental versus calculated) for **2** is 0.9989