

Bioactive Azaphilone Derivatives from the Fungus *Talaromyces aculeatus*

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List of Supporting Information

Figure S1. Experimental and calculated ECD spectra for **1**.

Figure S2. Experimental ECD spectra for **1–5**.

Figure S3. Experimental and calculated ECD spectra for **6**.

Figure S4. ^1H NMR (600 MHz, CD_3OD) spectrum of compound **1**

Figure S5. ^{13}C NMR (150 MHz, CD_3OD) spectrum of compound **1**

Figure S6. HSQC (CD_3OD) spectrum of compound **1**

Figure S7. ^1H - ^1H COSY (CD_3OD) spectrum of compound **1**

Figure S8. HMBC (CD_3OD) spectrum of compound **1**

Figure S9. ROESY (CD_3OD) spectrum of compound **1**

Figure S10. HRESIMS spectrum of compound **1**

Figure S11. ^1H NMR (600 MHz, CD_3OD) spectrum of compound **2**

Figure S12. ^{13}C NMR (150 MHz, CD_3OD) spectrum of compound **2**

Figure S13. HSQC (CD_3OD) spectrum of compound **2**

Figure S14. ^1H - ^1H COSY (CD_3OD) spectrum of compound **2**

Figure S15. HMBC (CD_3OD) spectrum of compound **2**

Figure S16. ROESY (CD_3OD) spectrum of compound **2**

Figure S17. HRESIMS spectrum of compound **2**

Figure S18. ^1H NMR (600 MHz, CDCl_3) spectrum of compound **3**

Figure S19. ^{13}C NMR (150 MHz, CDCl_3) spectrum of compound **3**

Figure S20. HSQC (CDCl_3) spectrum of compound **3**

Figure S21. ^1H - ^1H COSY (CDCl_3) spectrum of compound **3**

Figure S22. HMBC (CDCl_3) spectrum of compound **3**

Figure S23. ROESY (CDCl_3) spectrum of compound **3**

Figure S24. HRESIMS spectrum of compound **3**

Figure S25. ^1H NMR (600 MHz, CD_3OD) spectrum of compound **4**

Figure S26. ^{13}C NMR (150MHz, CD_3OD) spectrum of compound **4**

Figure S27. HSQC (CD_3OD) spectrum of compound **4**

Figure S28. ^1H - ^1H COSY (CD_3OD) spectrum of compound **4**

Figure S29. HMBC (CD_3OD) spectrum of compound **4**

Figure S30. ROESY (CD_3OD) spectrum of compound **4**

Figure S31. HRESIMS spectrum of compound **4**

Figure S32. ^1H NMR (600 MHz, CDCl_3) spectrum of compound **5**

Figure S33. ^{13}C NMR (150MHz, CDCl_3) spectrum of compound **5**

Figure S34. HSQC (CDCl_3) spectrum of compound **5**

Figure S35. ^1H - ^1H COSY (CDCl_3) spectrum of compound **5**

Figure S36. HMBC (CDCl_3) spectrum of compound **5**

Figure S37. ROESY (CDCl_3) spectrum of compound **5**

Figure S38. HRESIMS spectrum of compound **5**

Figure S39. ^1H NMR (600 MHz, CD_3OD) spectrum of compound **6**

Figure S40. ^{13}C NMR (150MHz, CD_3OD) spectrum of compound **6**

Figure S41. HSQC (CD₃OD) spectrum of compound **6**

Figure S42. ¹H-¹H COSY (CD₃OD) spectrum of compound **6**

Figure S43 HMBC (CD₃OD) spectrum of compound **6**

Figure S44. ROESY (CD₃OD) spectrum of compound **6**

Figure S45. HRESIMS spectrum of compound **6**

Table S1. Simulated ECD spectrum date of *7S,8S,8aS,12S-1*

Table S1. Simulated ECD spectrum date of *7S,8S,8aS,12R-1*

Table S1. Simulated ECD spectrum date of *7S,8S-6*

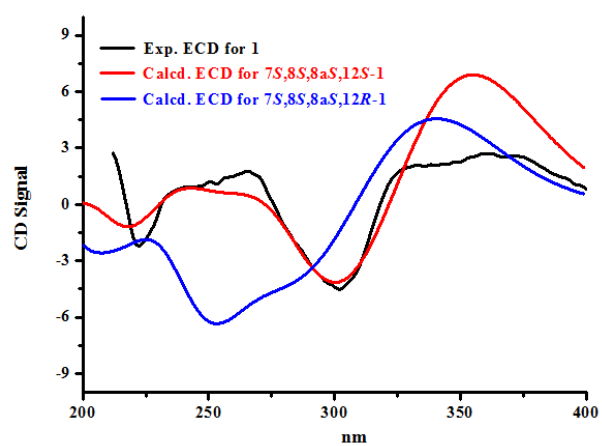


Figure S1. Experimental and calculated ECD spectra for **1**

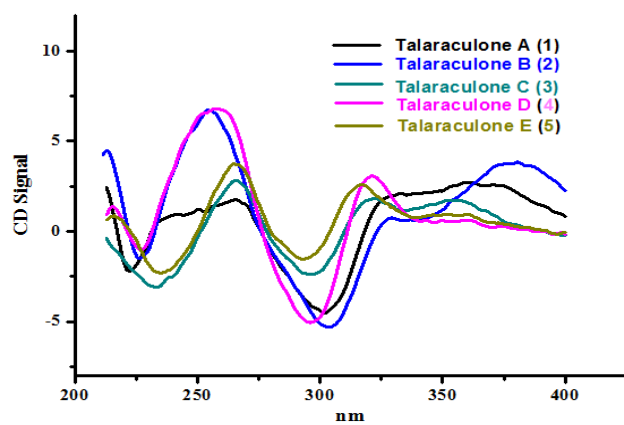


Figure S2. Experimental ECD spectra for **1–5**.

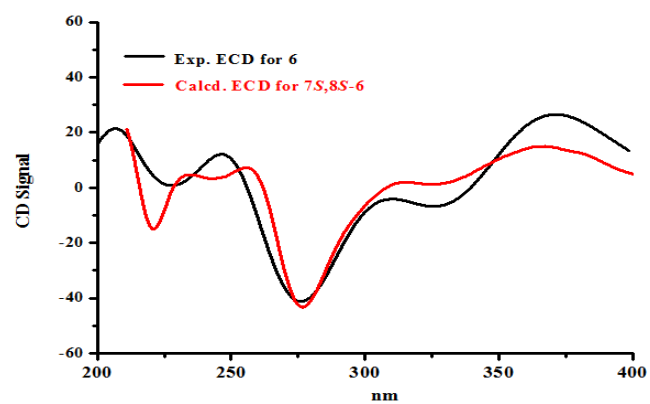


Figure S3 Experimental and calculated ECD spectra for **6**.

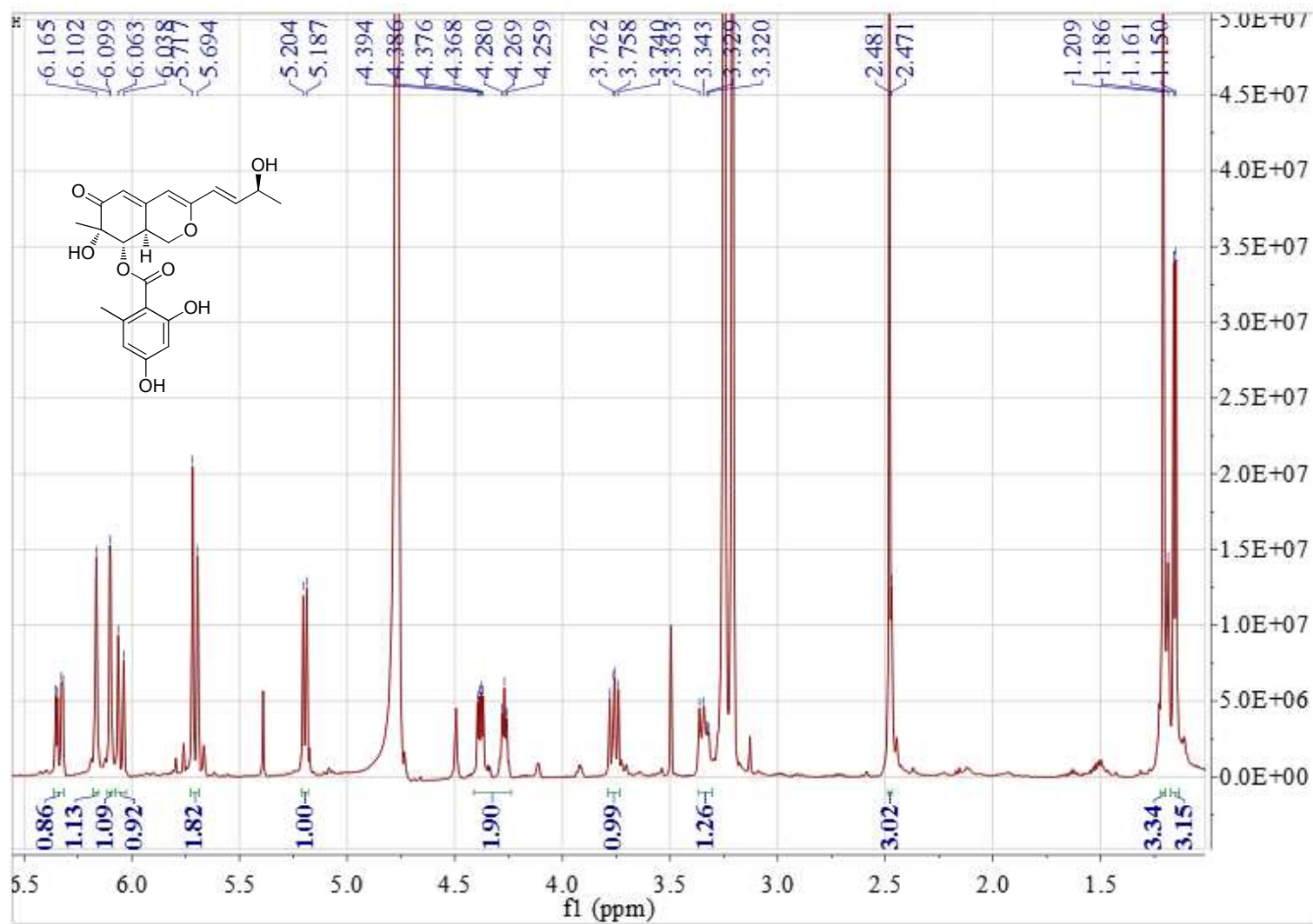


Figure S4. ¹H NMR (600 MHz, CD₃OD) spectrum of compound 1

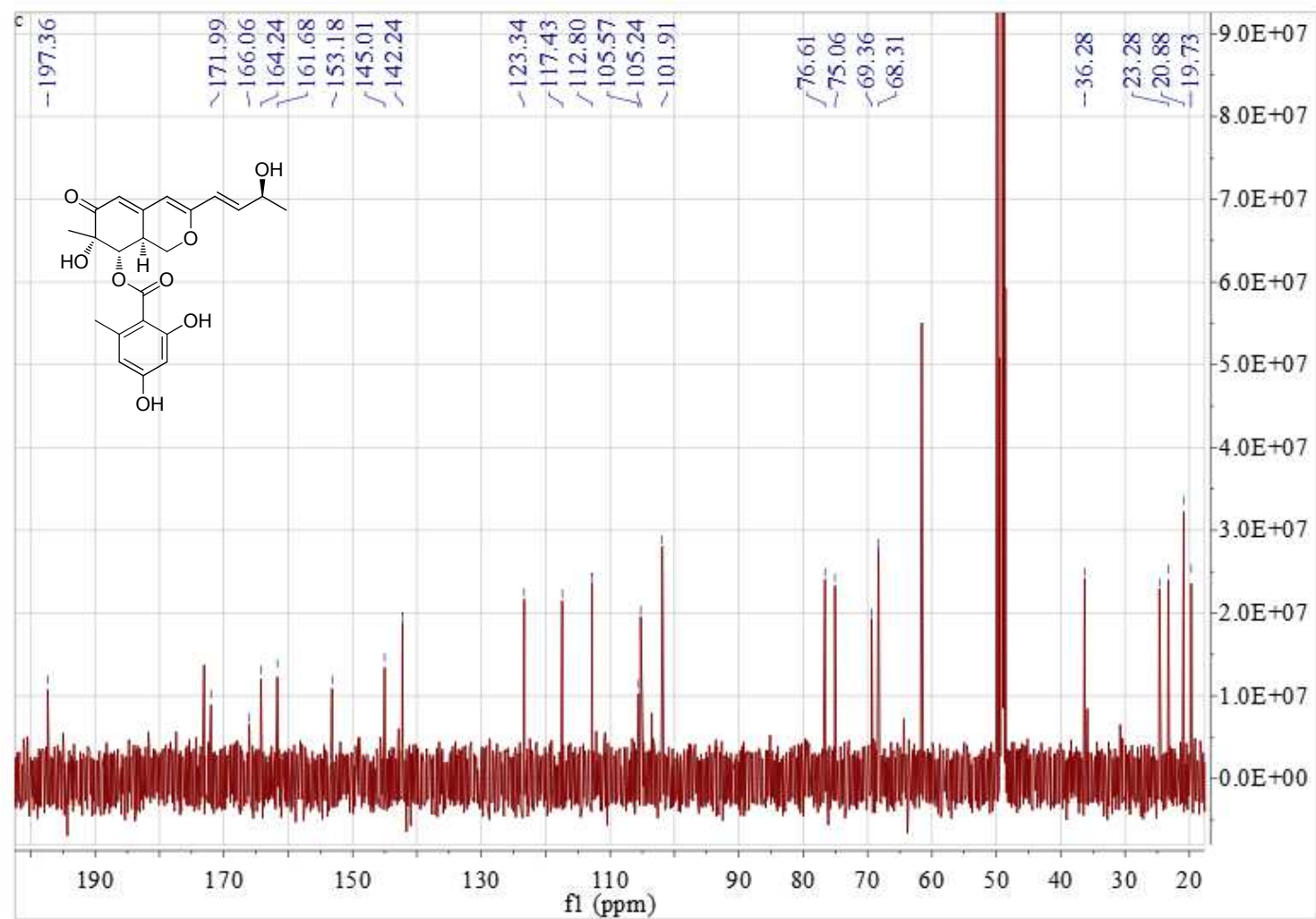


Figure S5. ^{13}C NMR (150 MHz, CD_3OD) spectrum of compound **1**

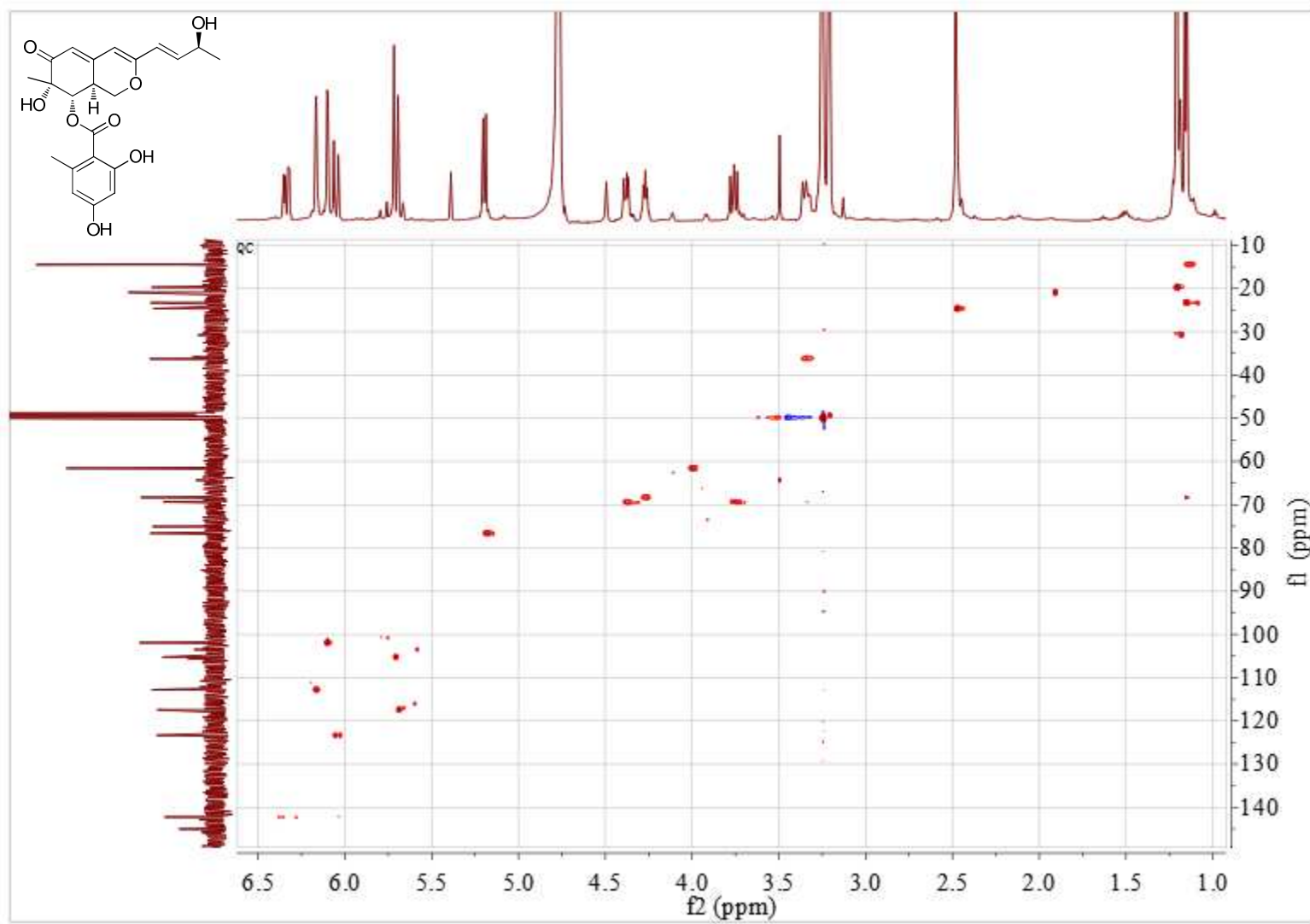


Figure S6. HSQC (CD₃OD) spectrum of compound 1

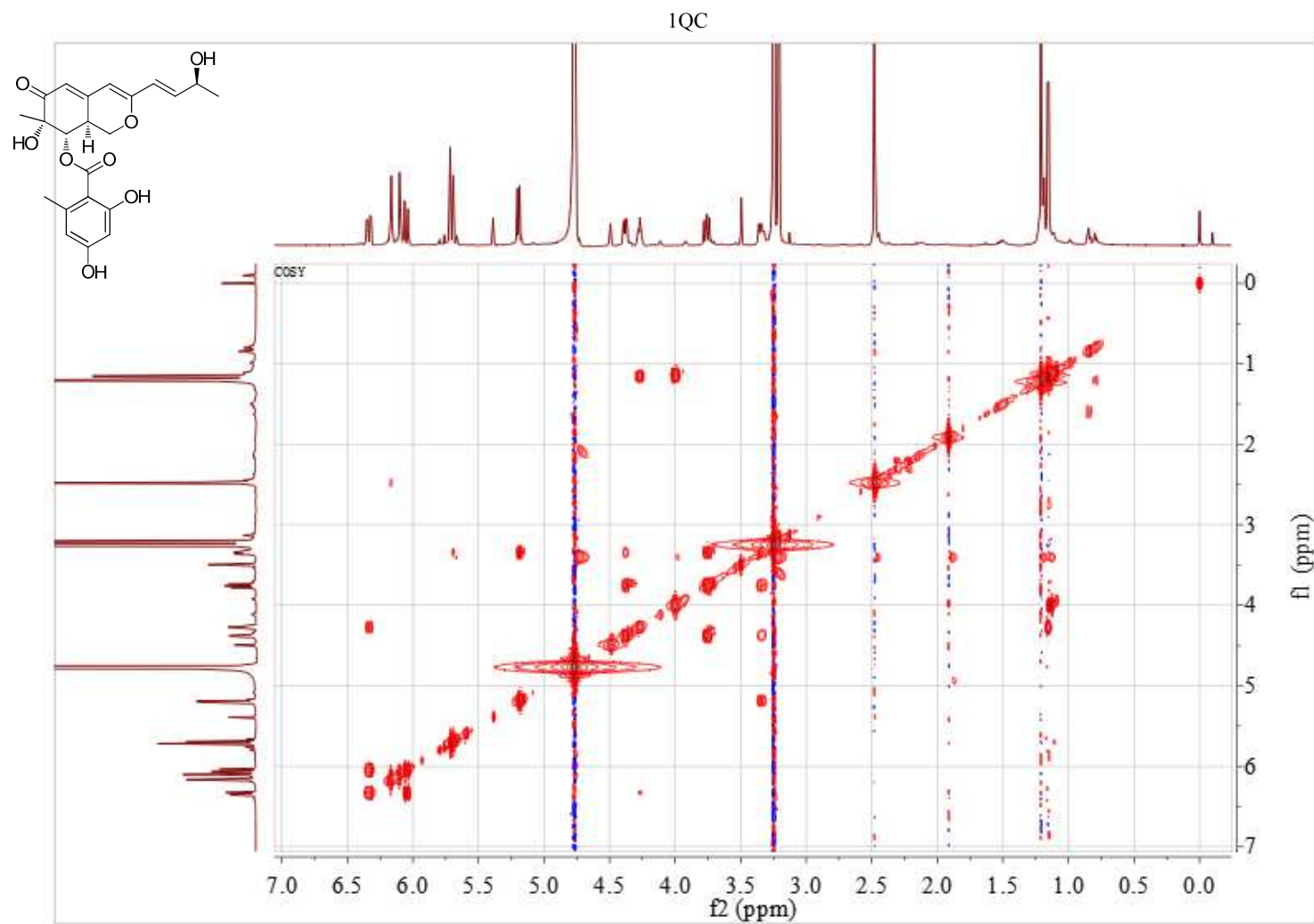


Figure S7. ^1H - ^1H COSY (CD_3OD) spectrum of compound **1**

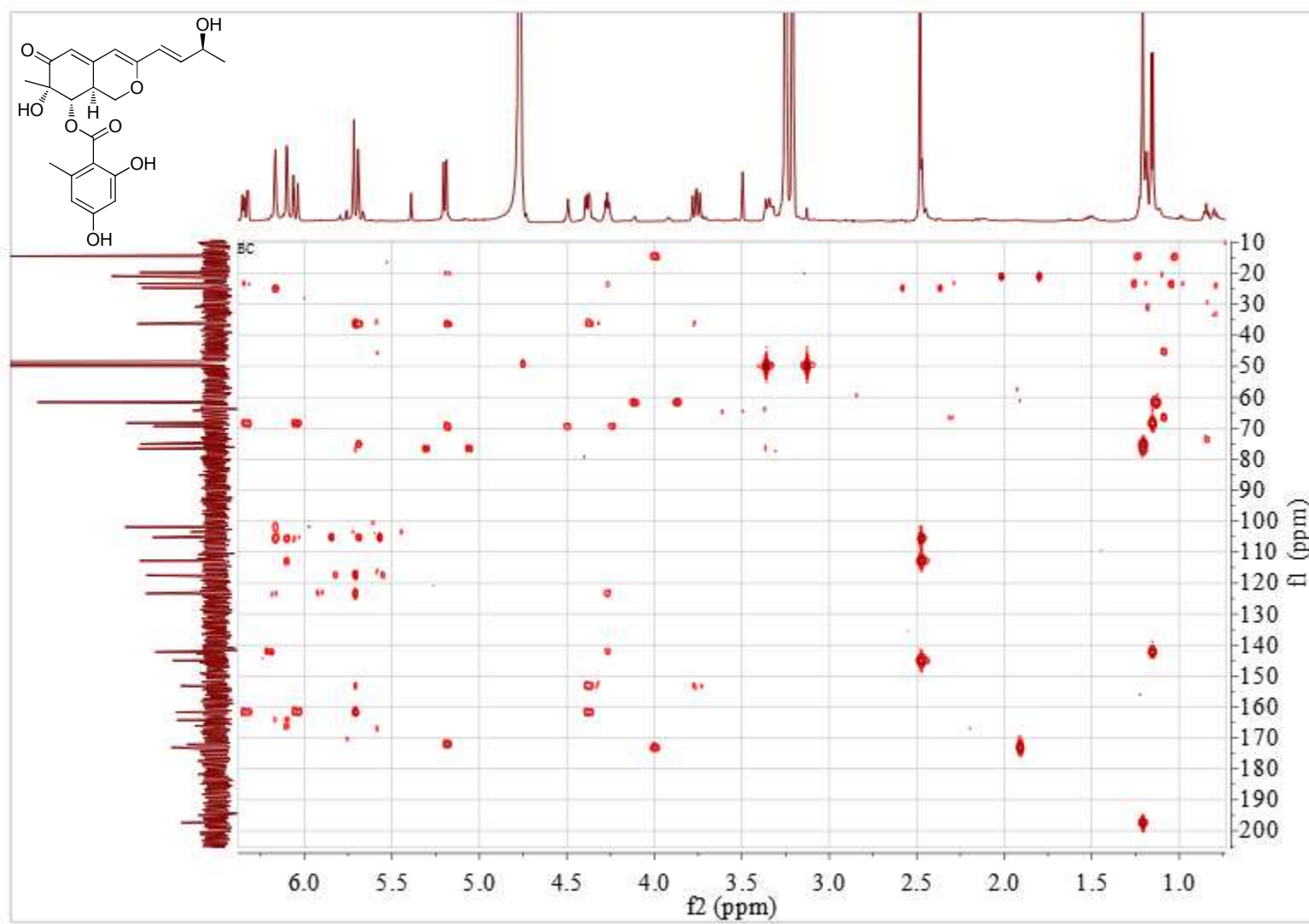


Figure S8. HMBC (CD₃OD) spectrum of compound 1

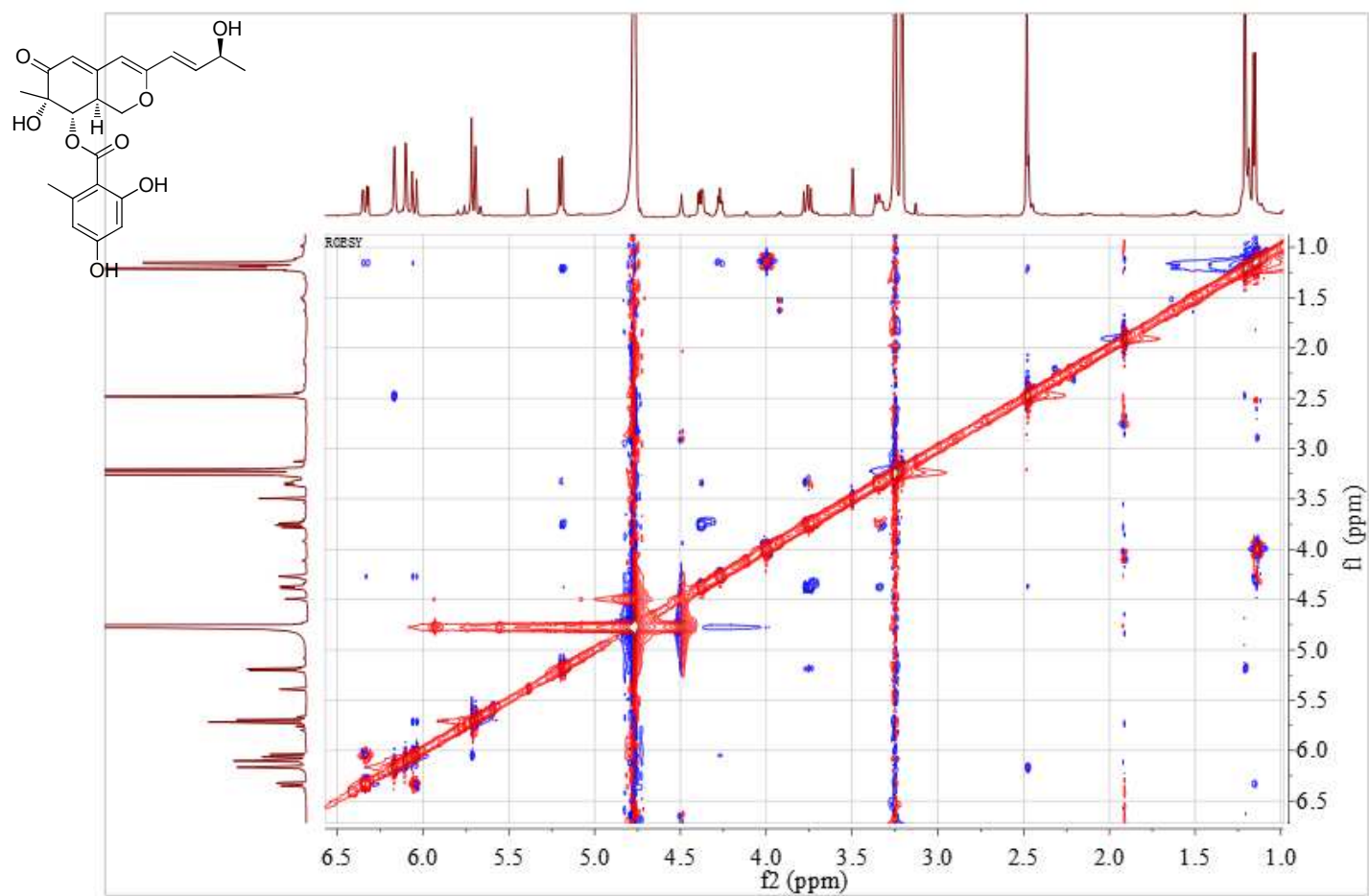


Figure S9. ROESY (CD₃OD) spectrum of compound **1**

20151029-DS-16_151027192708 #126 RT: 1.05 AV: 1 NL: 3.83E6
T: FTMS + p ESI Full ms [100.00-2000.00]

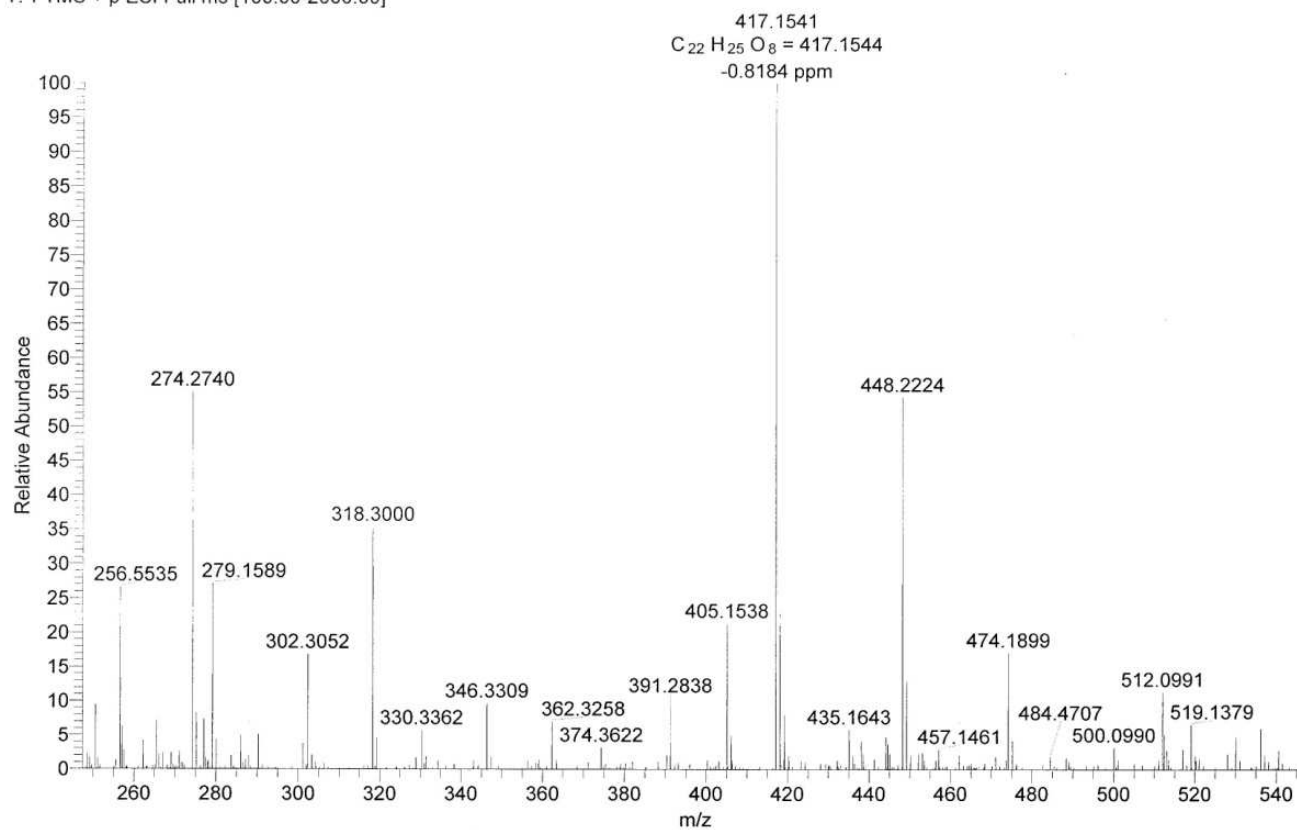


Figure S10. HRESIMS spectrum of compound 1

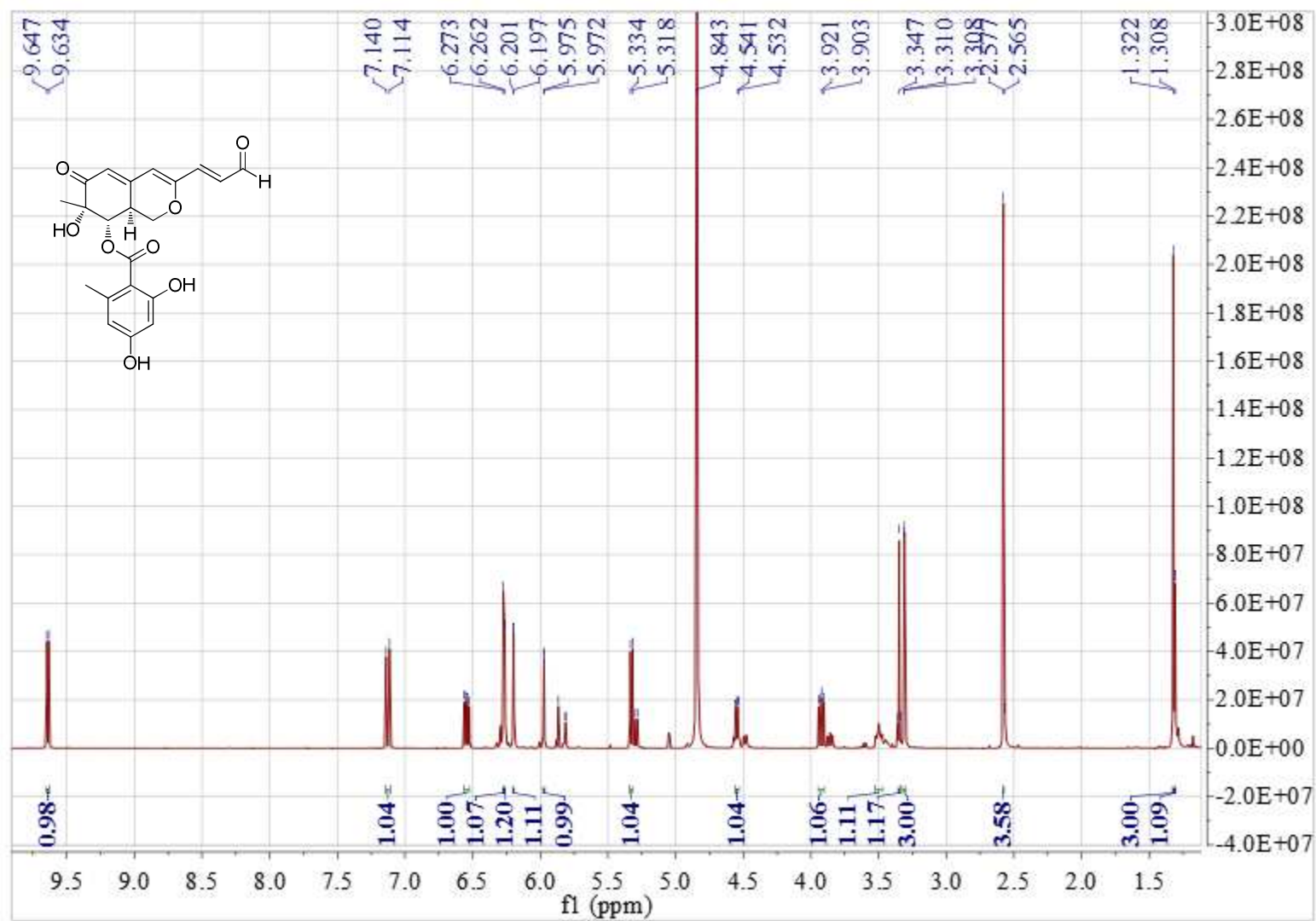


Figure S11. ¹H NMR (600 MHz, CD₃OD) spectrum of compound 2

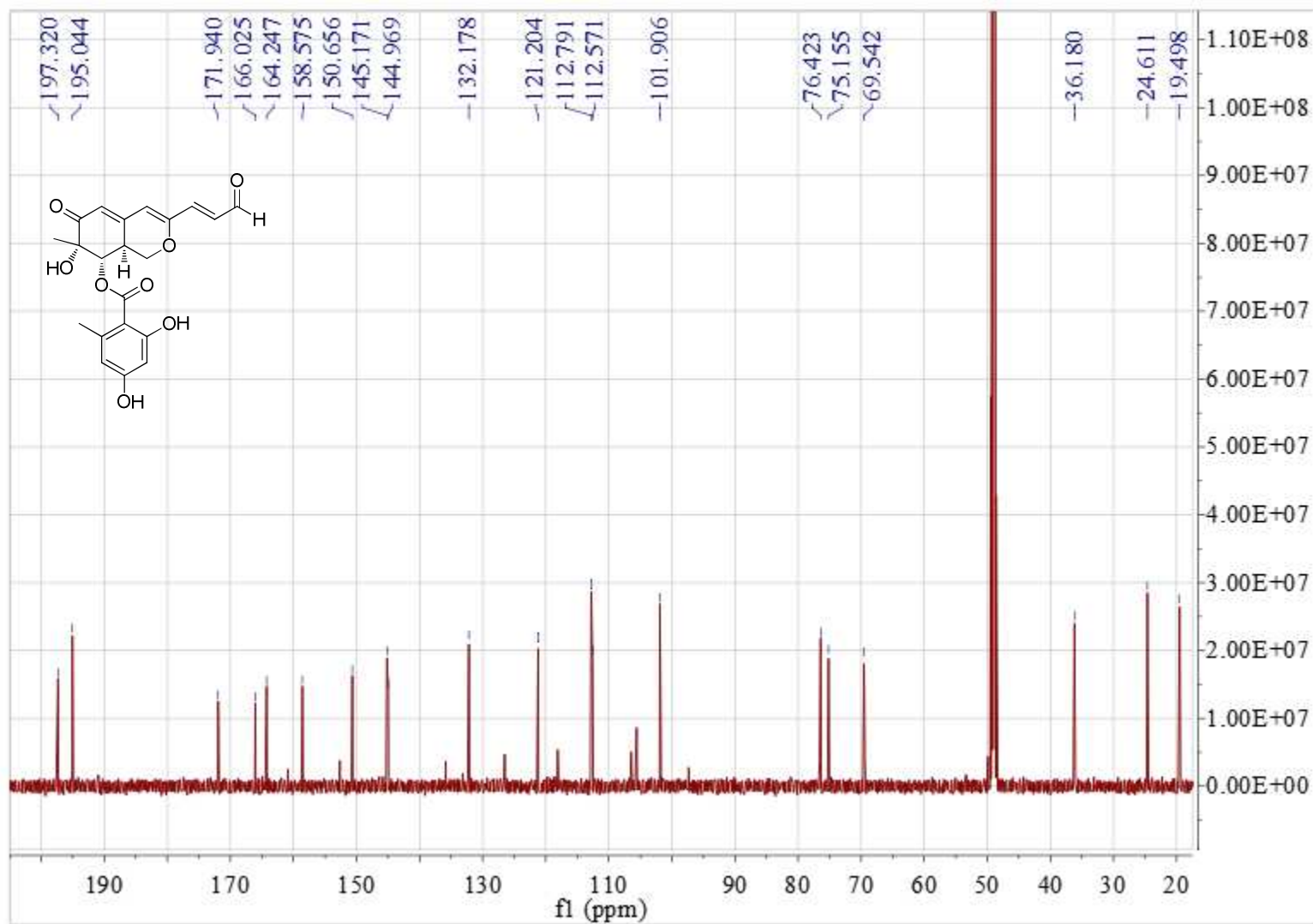


Figure S12. ¹³C NMR (150 MHz, CD₃OD) spectrum of compound 2

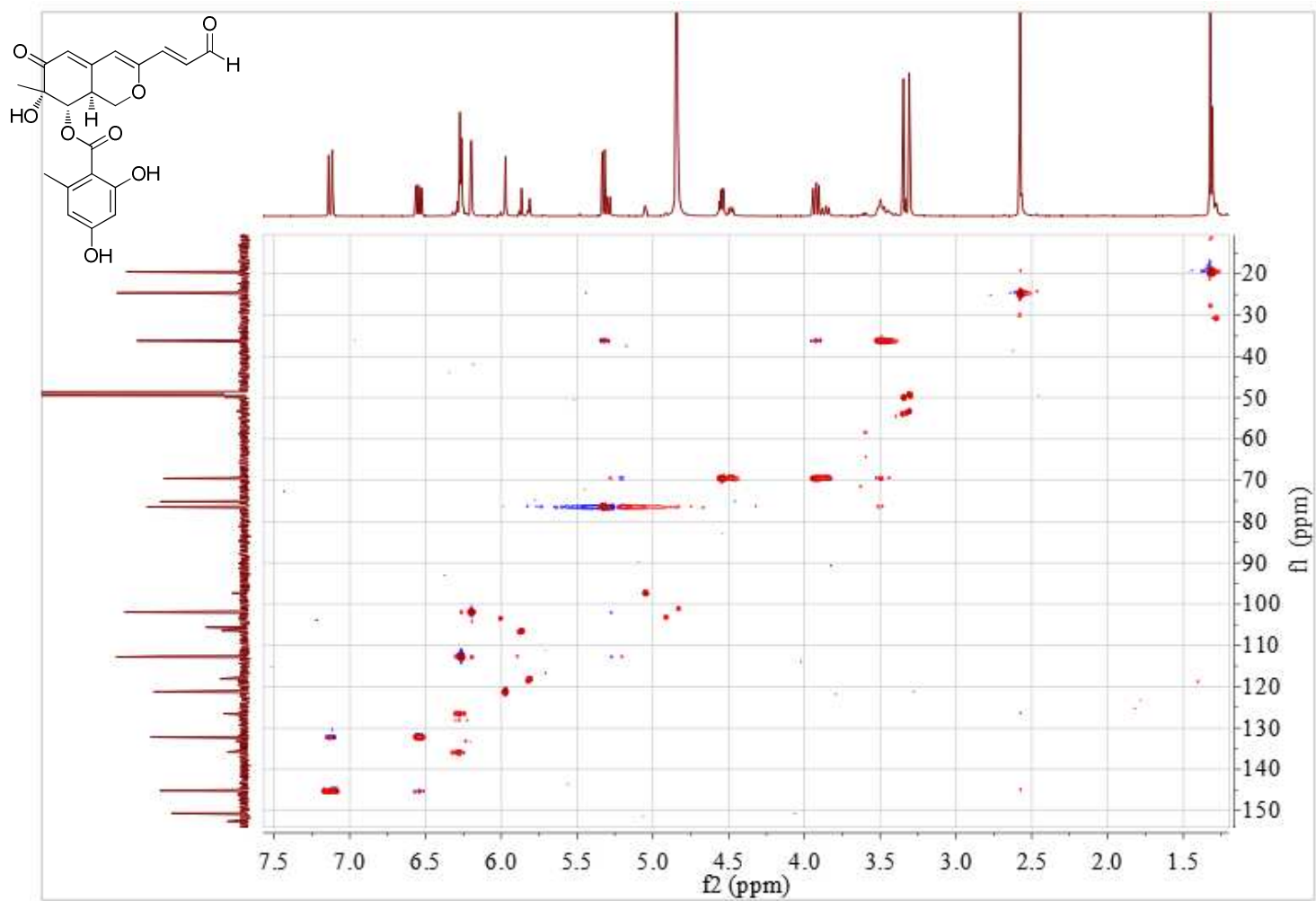


Figure S13. HSQC (CD₃OD) spectrum of compound 2

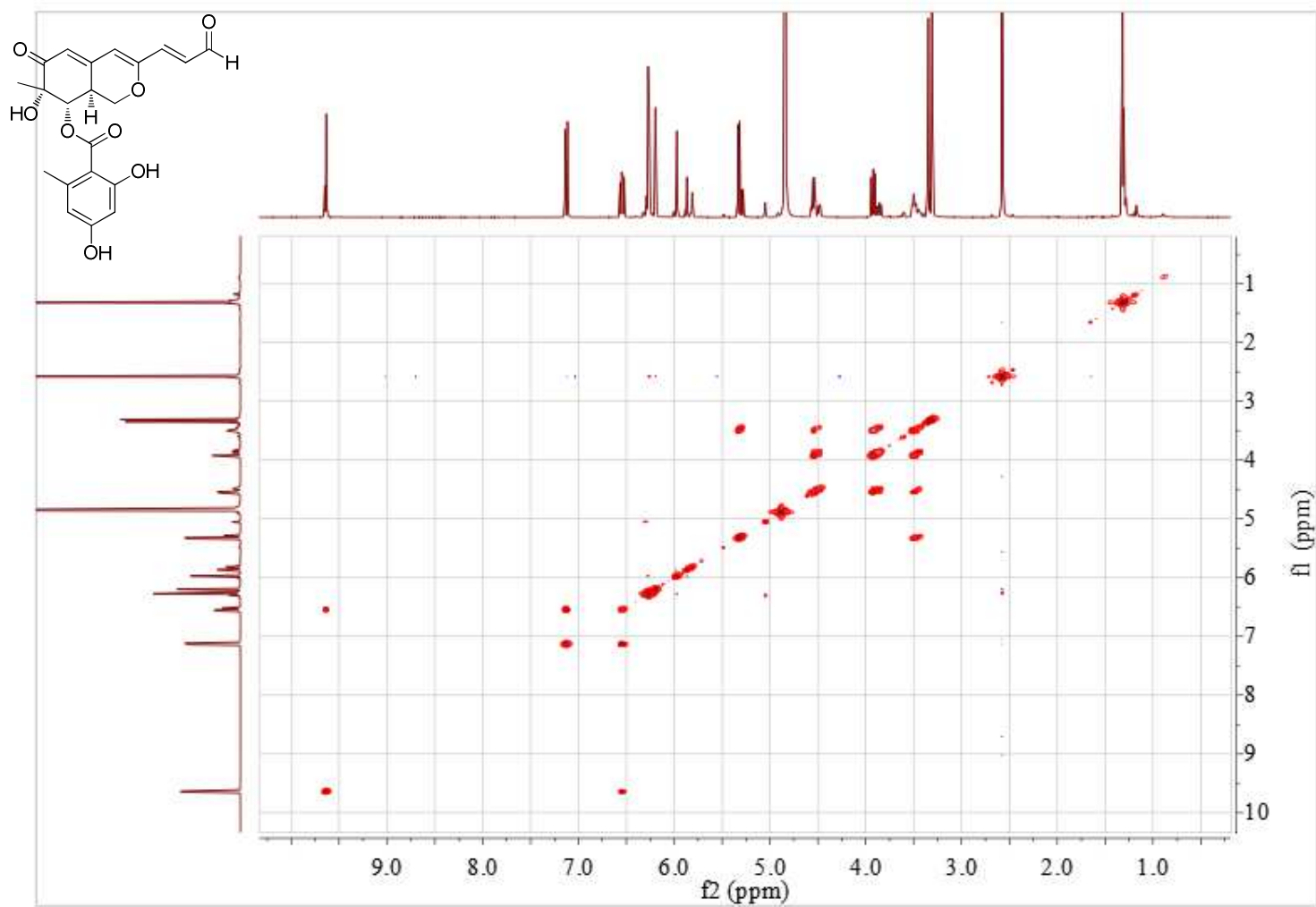


Figure S14. ^1H - ^1H COSY (CD_3OD) spectrum of compound **2**

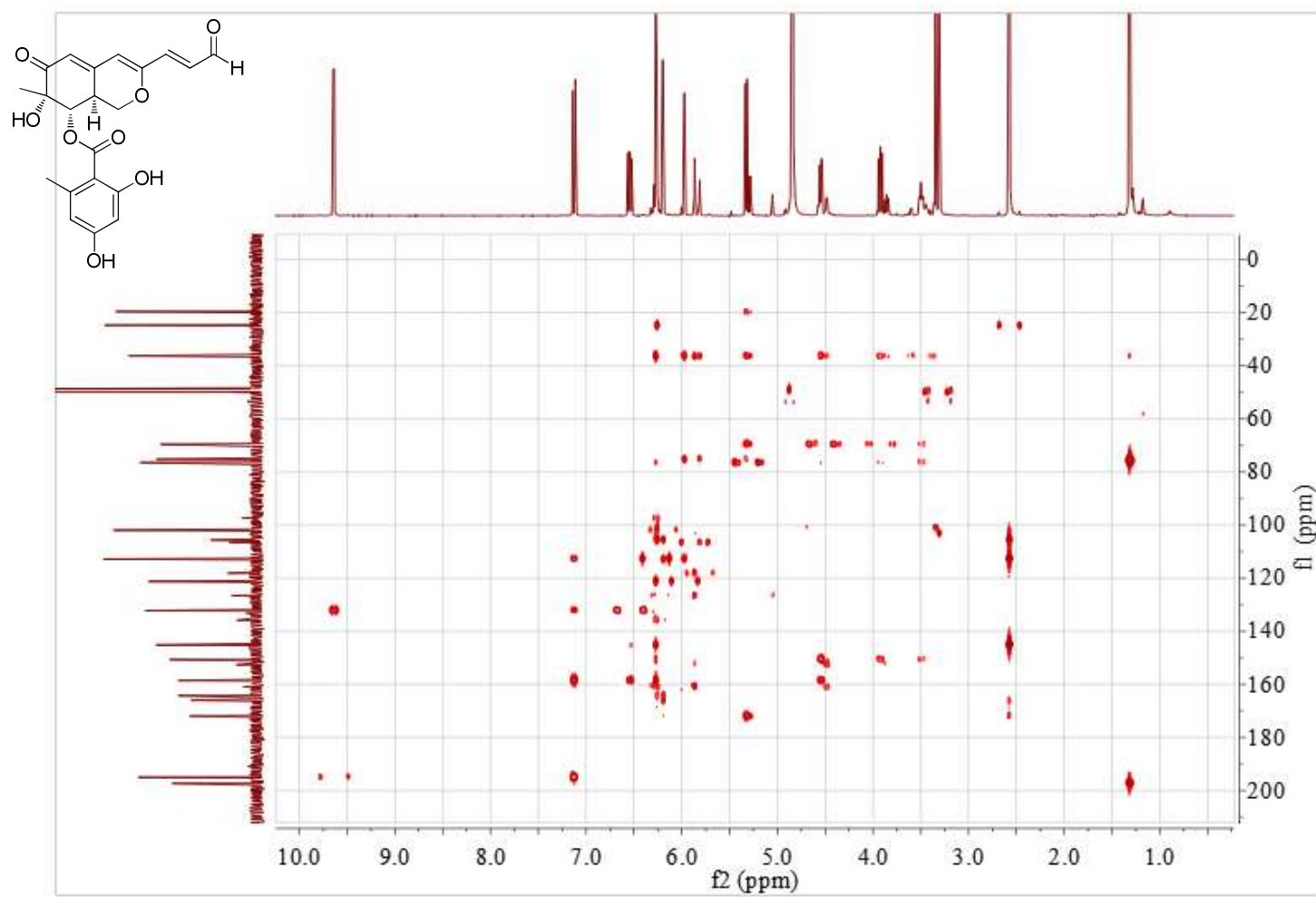


Figure S15. HMBC (CD₃OD) spectrum of compound 2

20160120-DS-05_160120112604 #270-275 RT: 2.70-2.74 AV: 6 NL: 6.11E5
T: FTMS + c ESI Full ms [150.00-1000.00]

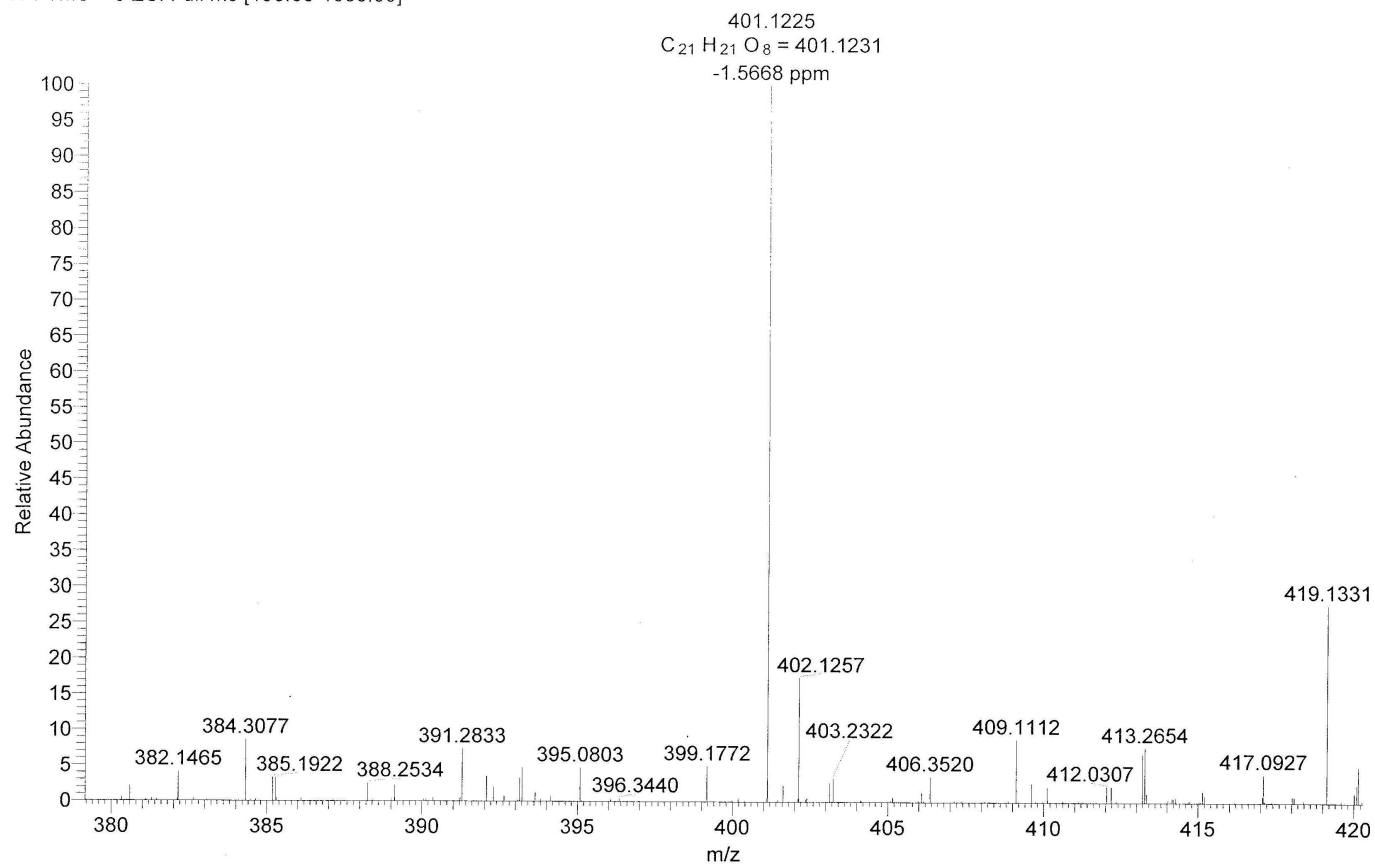


Figure S17. HRESIMS spectrum of compound 2

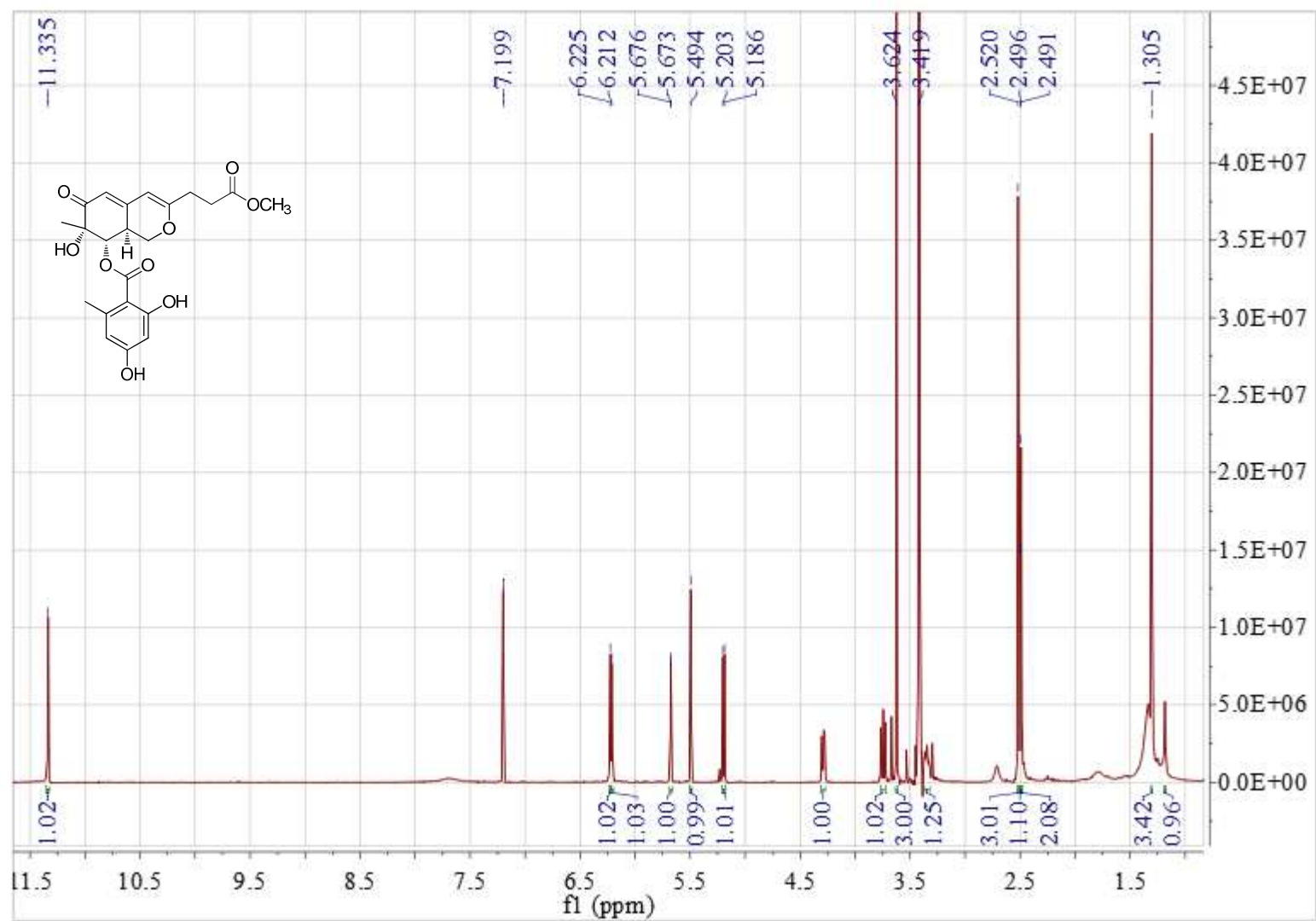


Figure S18. ¹H NMR (600 MHz, CDCl₃) spectrum of compound 3

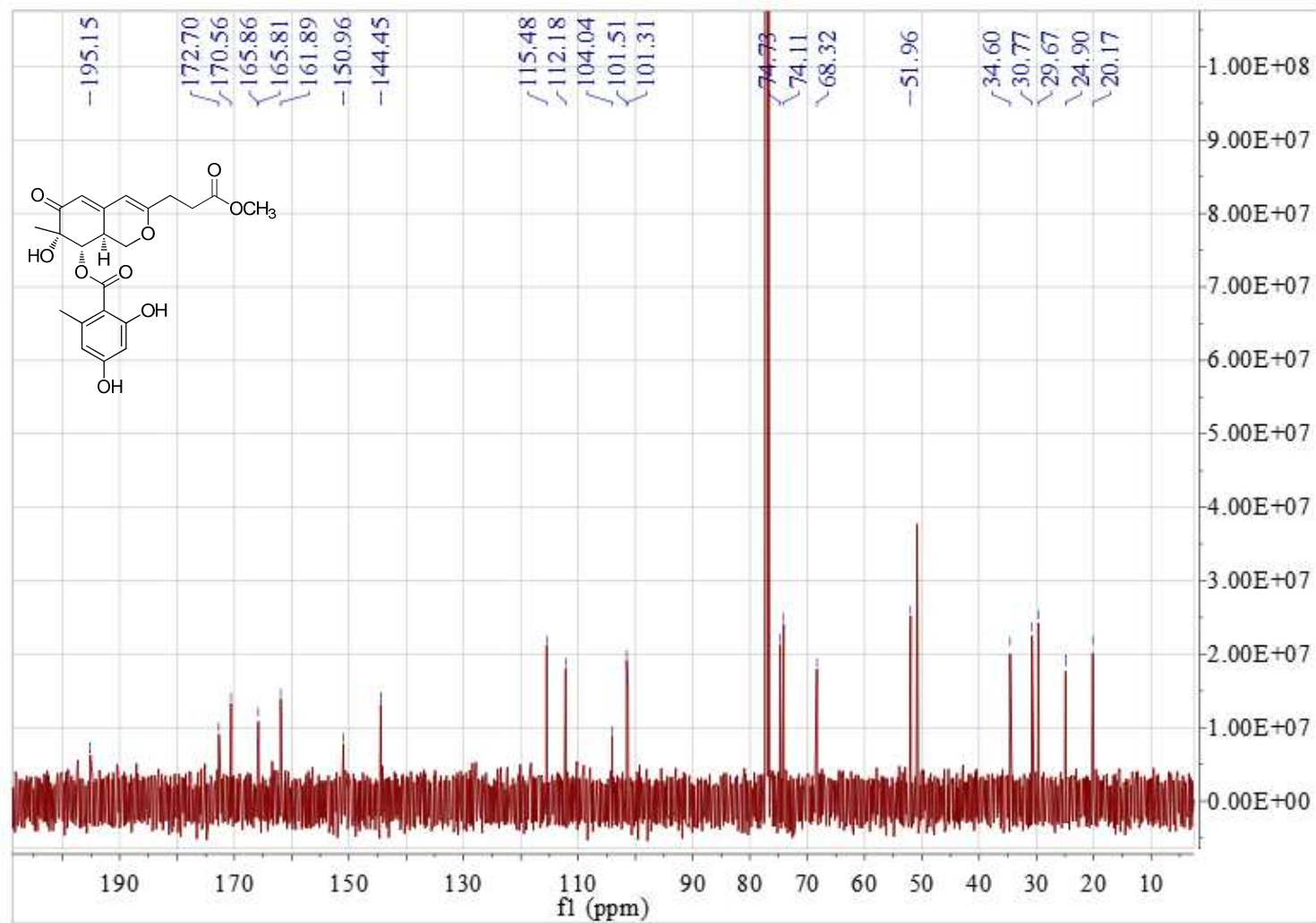


Figure S19. ¹³C NMR (150 MHz, CDCl₃) spectrum of compound 3

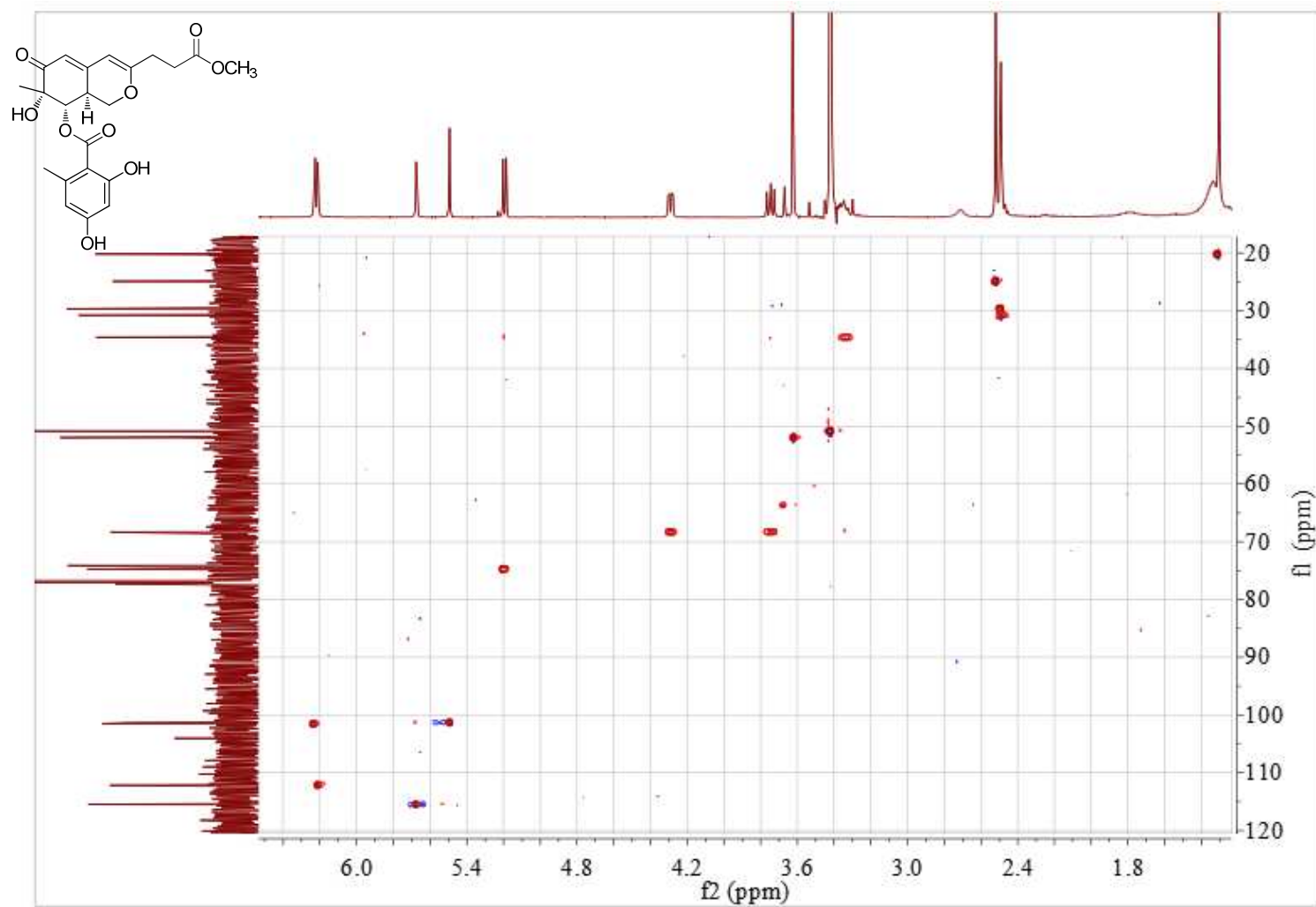


Figure S20. HSQC (CDCl₃) spectrum of compound **3**

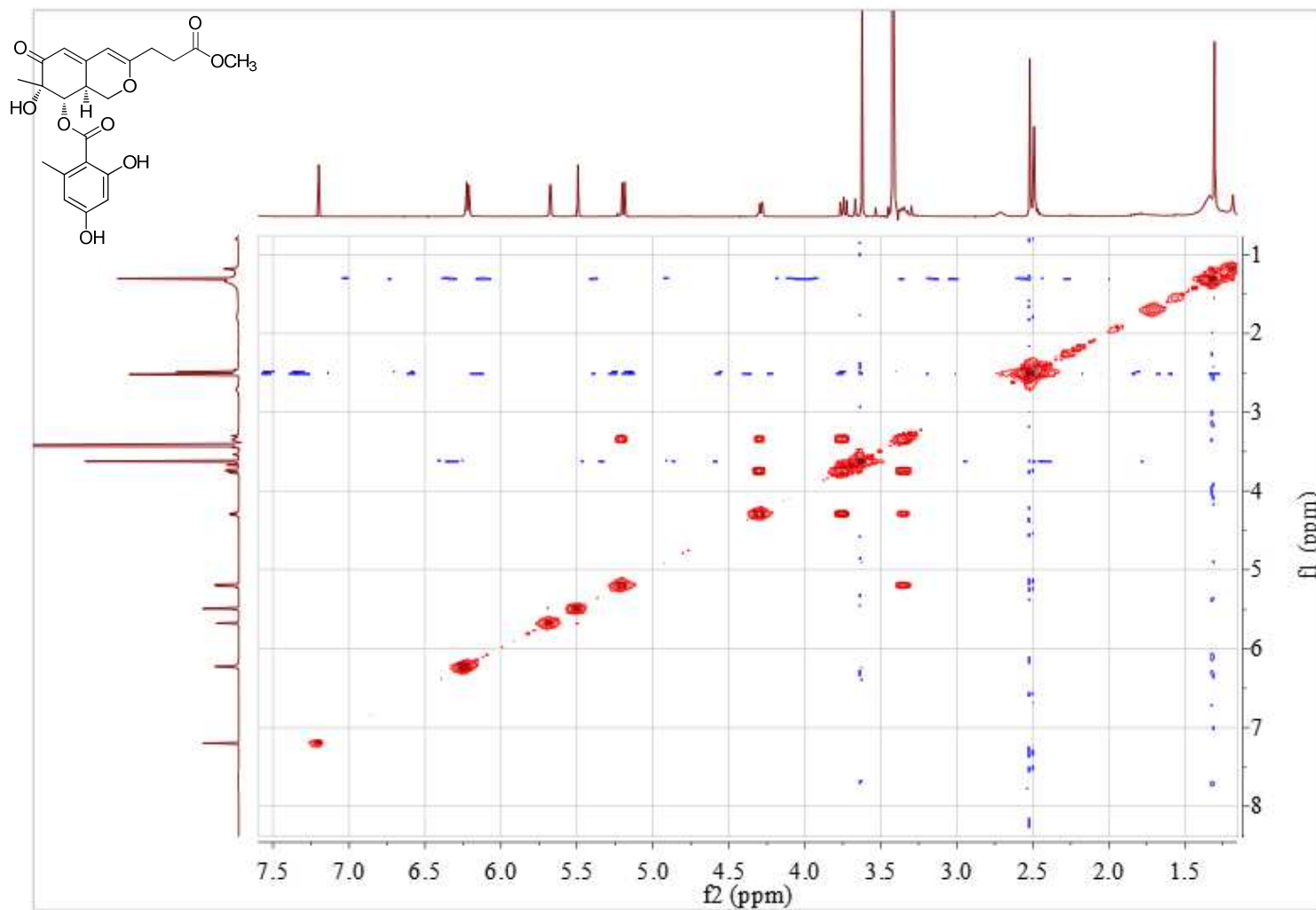


Figure S21. ^1H - ^1H COSY (CDCl_3) spectrum of compound 3

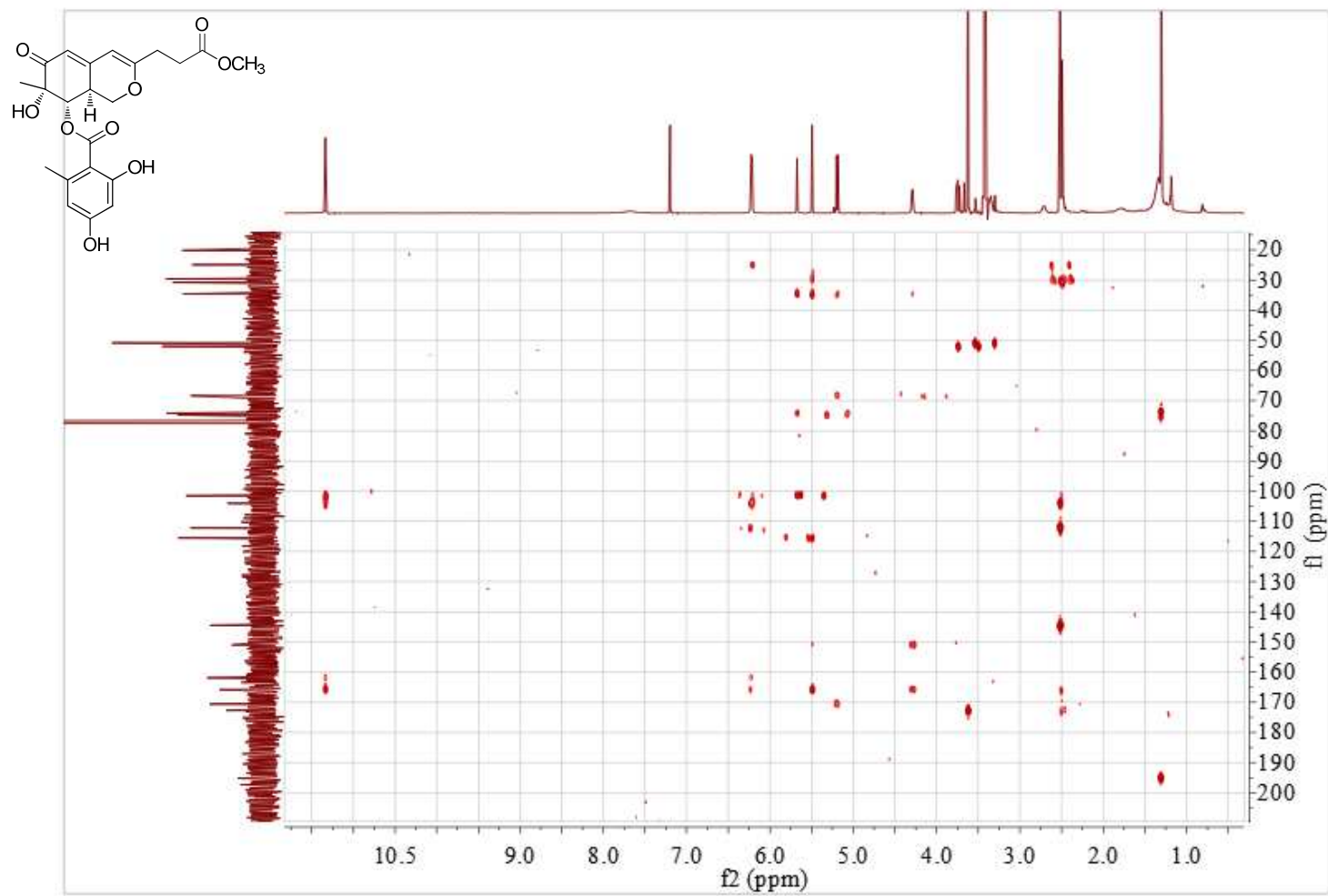
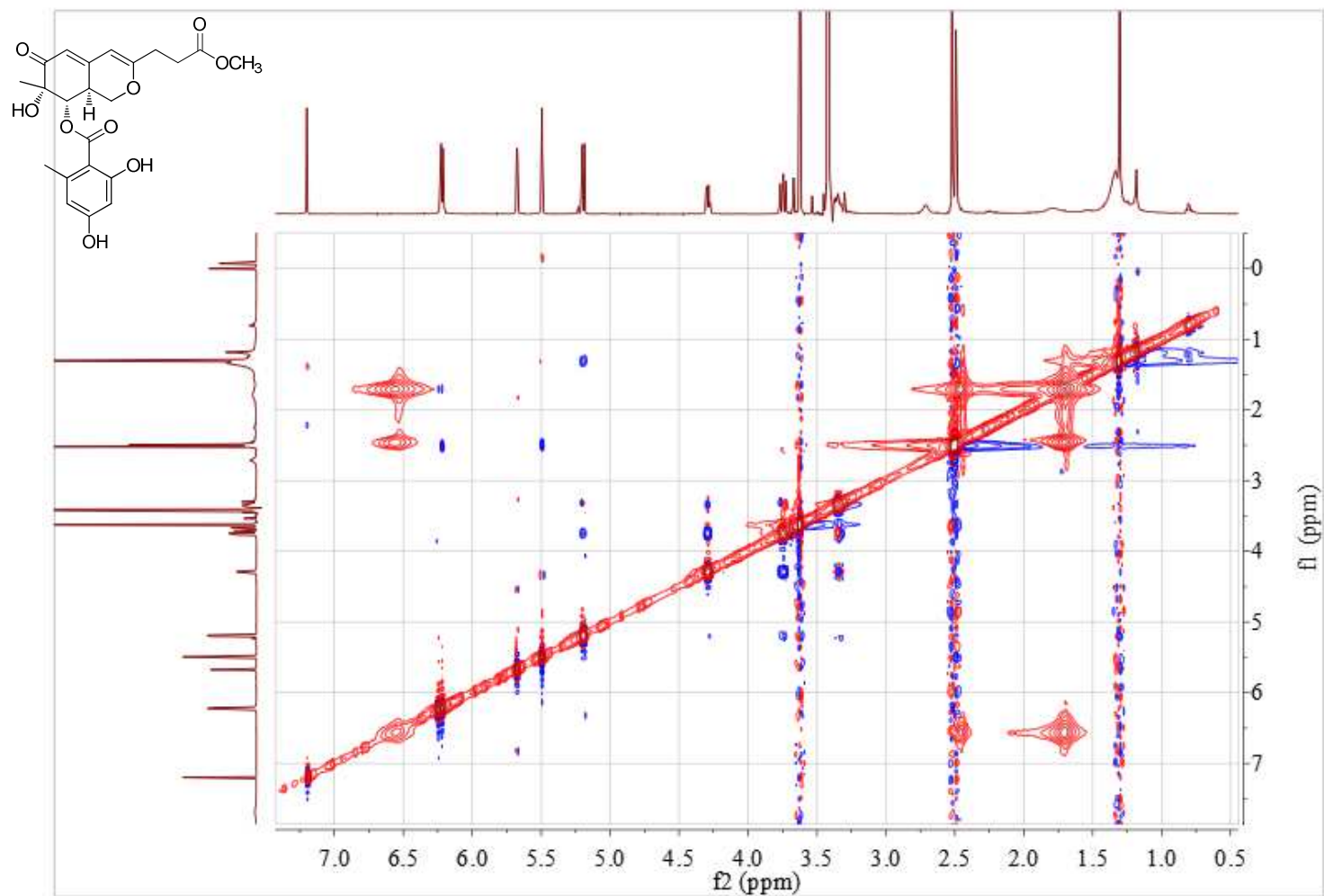


Figure S22. HMBC (CDCl₃) spectrum of compound **3**



20151029-DS-11_151027192708 #102 RT: 0.88 AV: 1 NL: 7.13E6

T: FTMS + p ESI Full ms [100.00-2000.00]

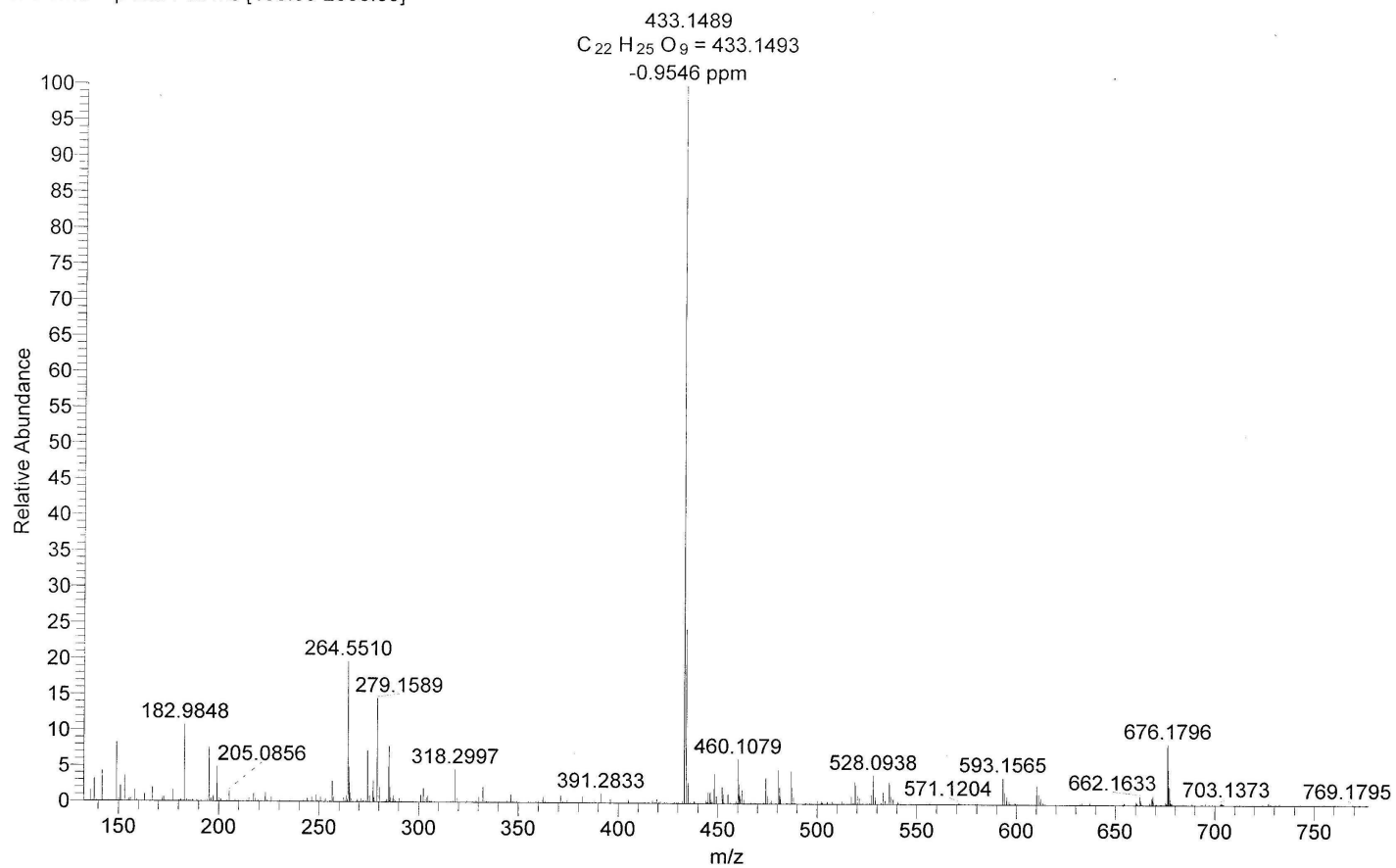


Figure S24. HRESIMS spectrum of compound 3

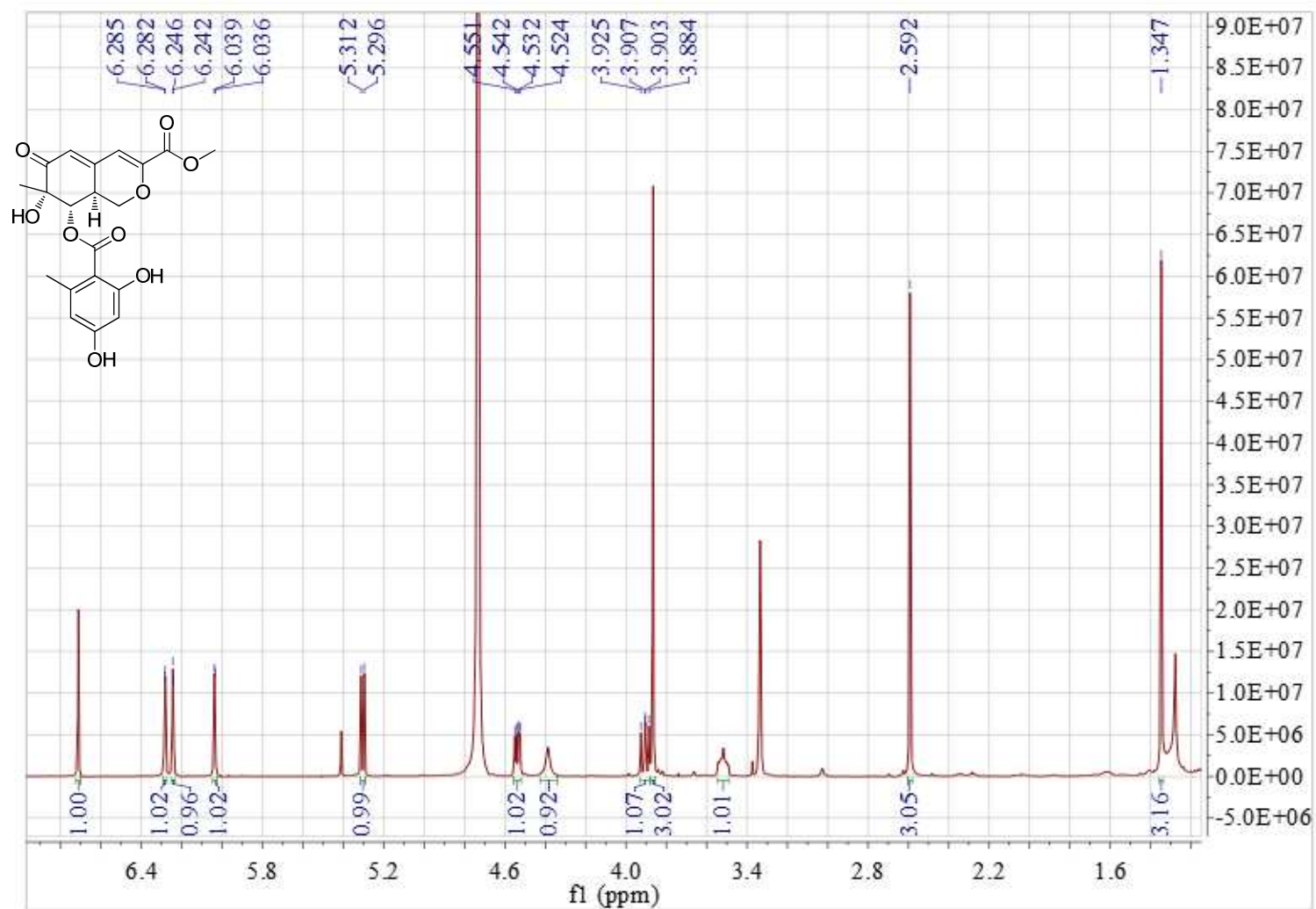


Figure S25. ¹H NMR (600 MHz, CD₃OD) spectrum of compound 4

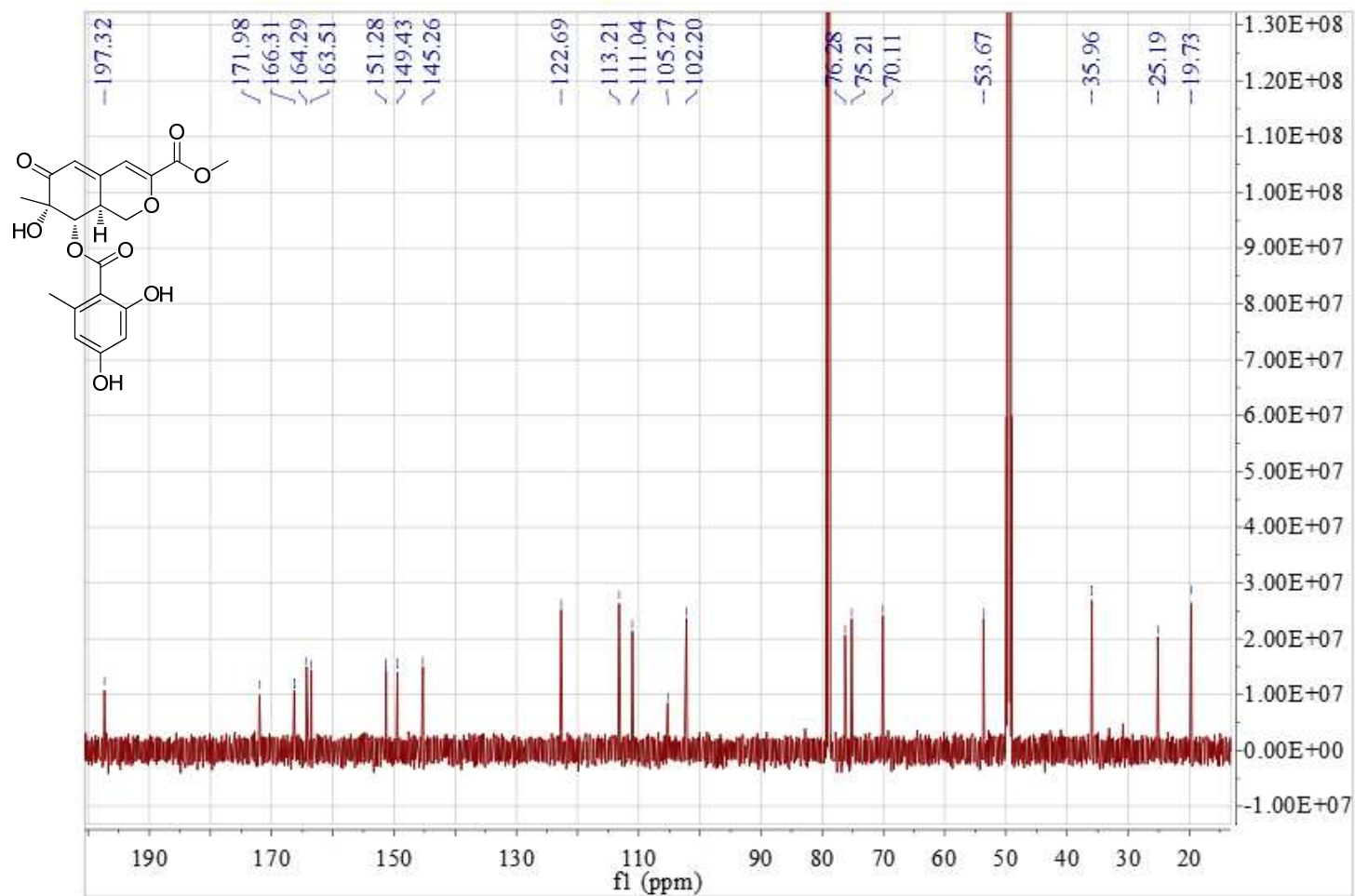


Figure S26. ¹³C NMR (150MHz, CD₃OD) spectrum of compound 4

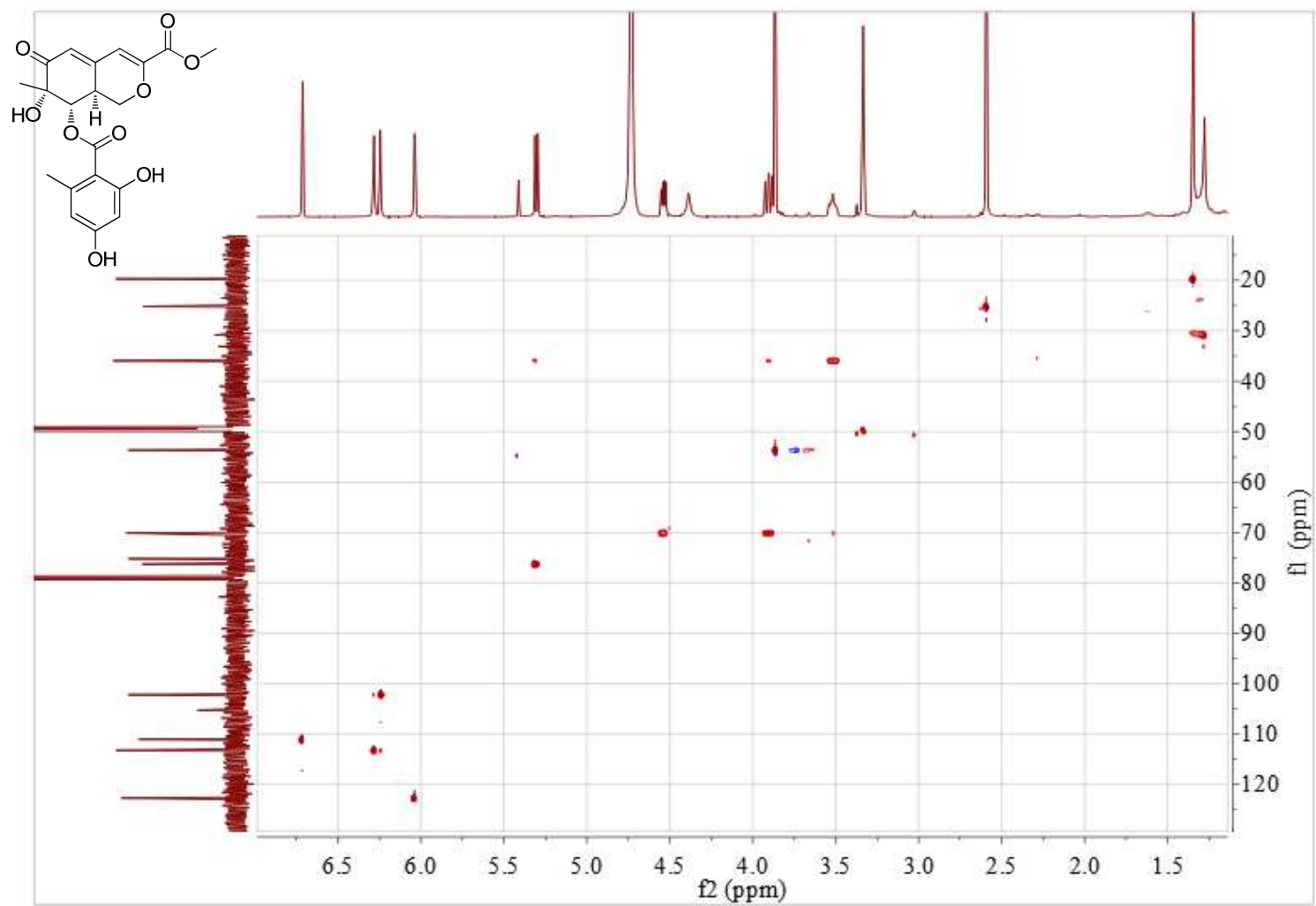


Figure S27. HSQC (CD₃OD) spectrum of compound 4

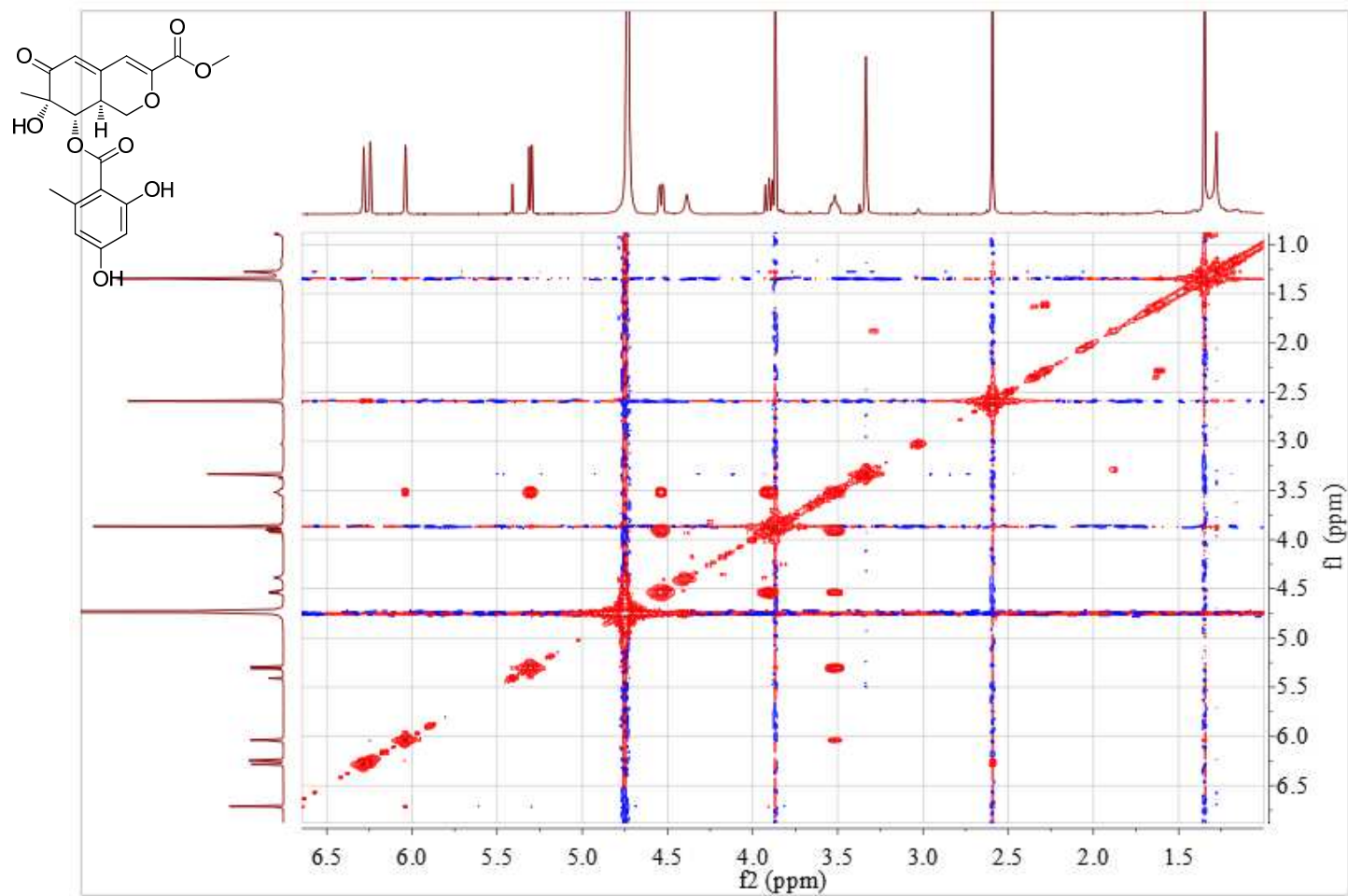


Figure S28. ^1H - ^1H COSY (CD_3OD) spectrum of compound 4

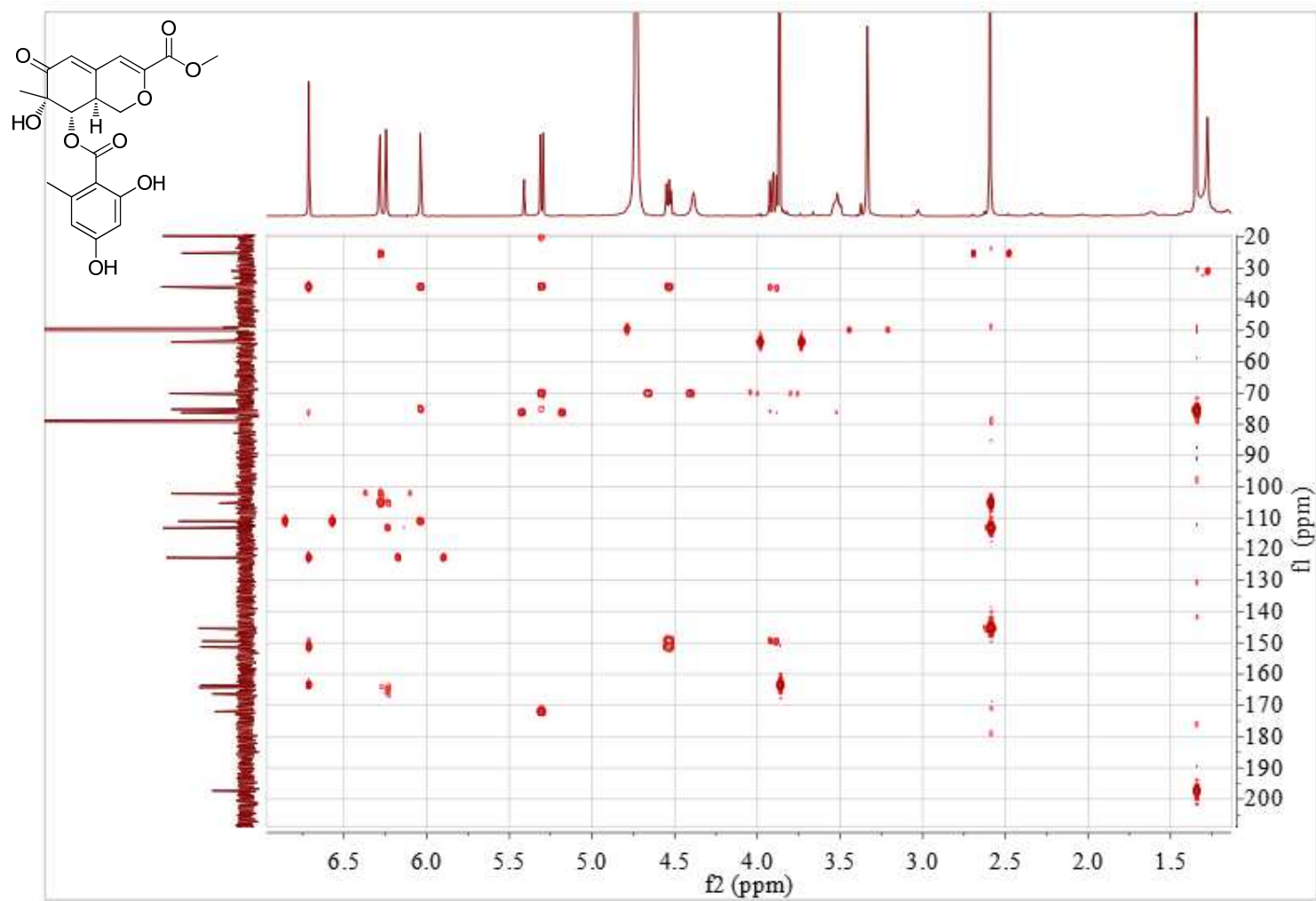


Figure S29. HMBC (CD₃OD) spectrum of compound 4

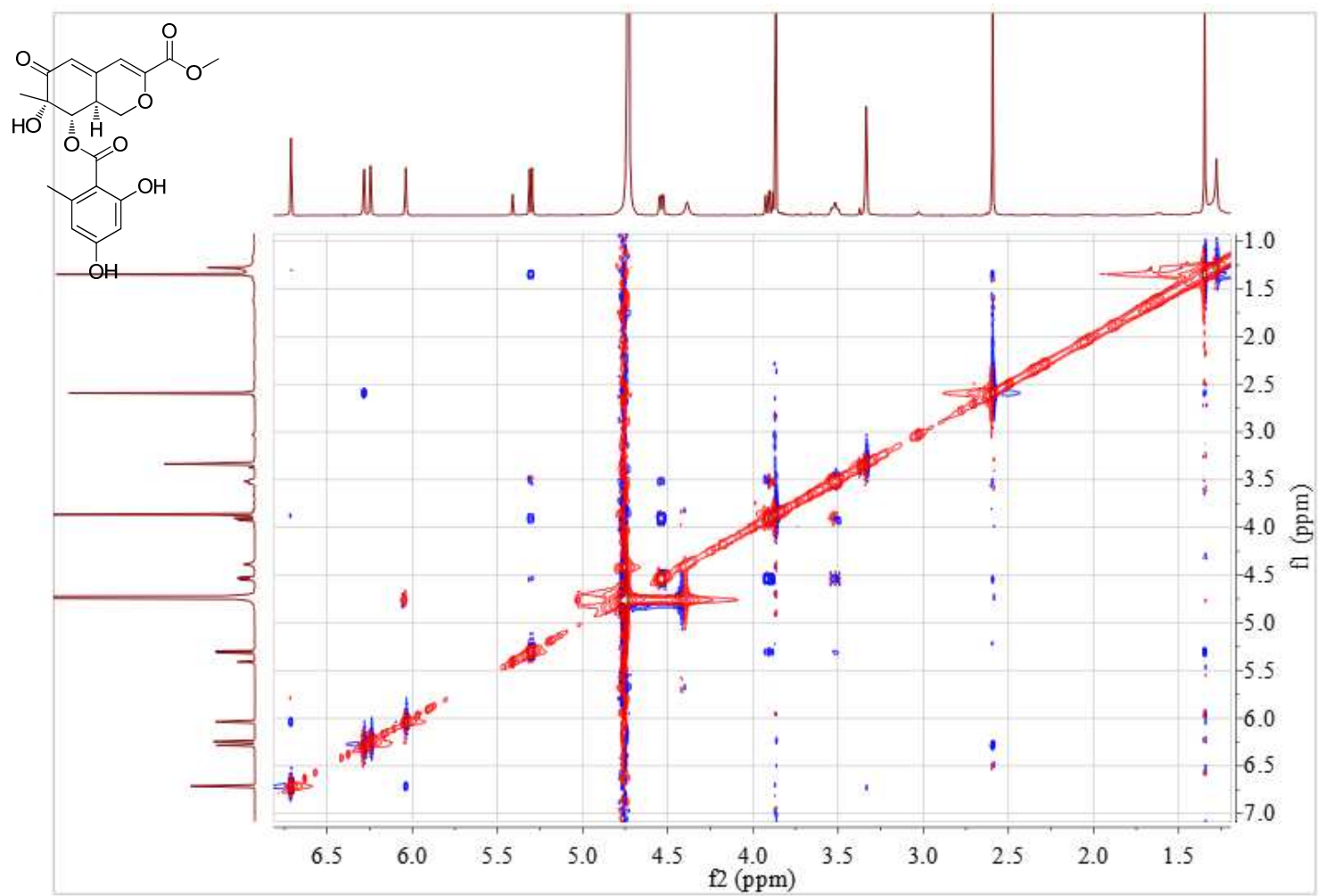


Figure S30. ROESY (CD₃OD) spectrum of compound 4

20151029-DS-17_151027192708 #95 RT: 1.06 AV: 1 NL: 6.67E5
T: FTMS + p ESI Full ms [100.00-2000.00]

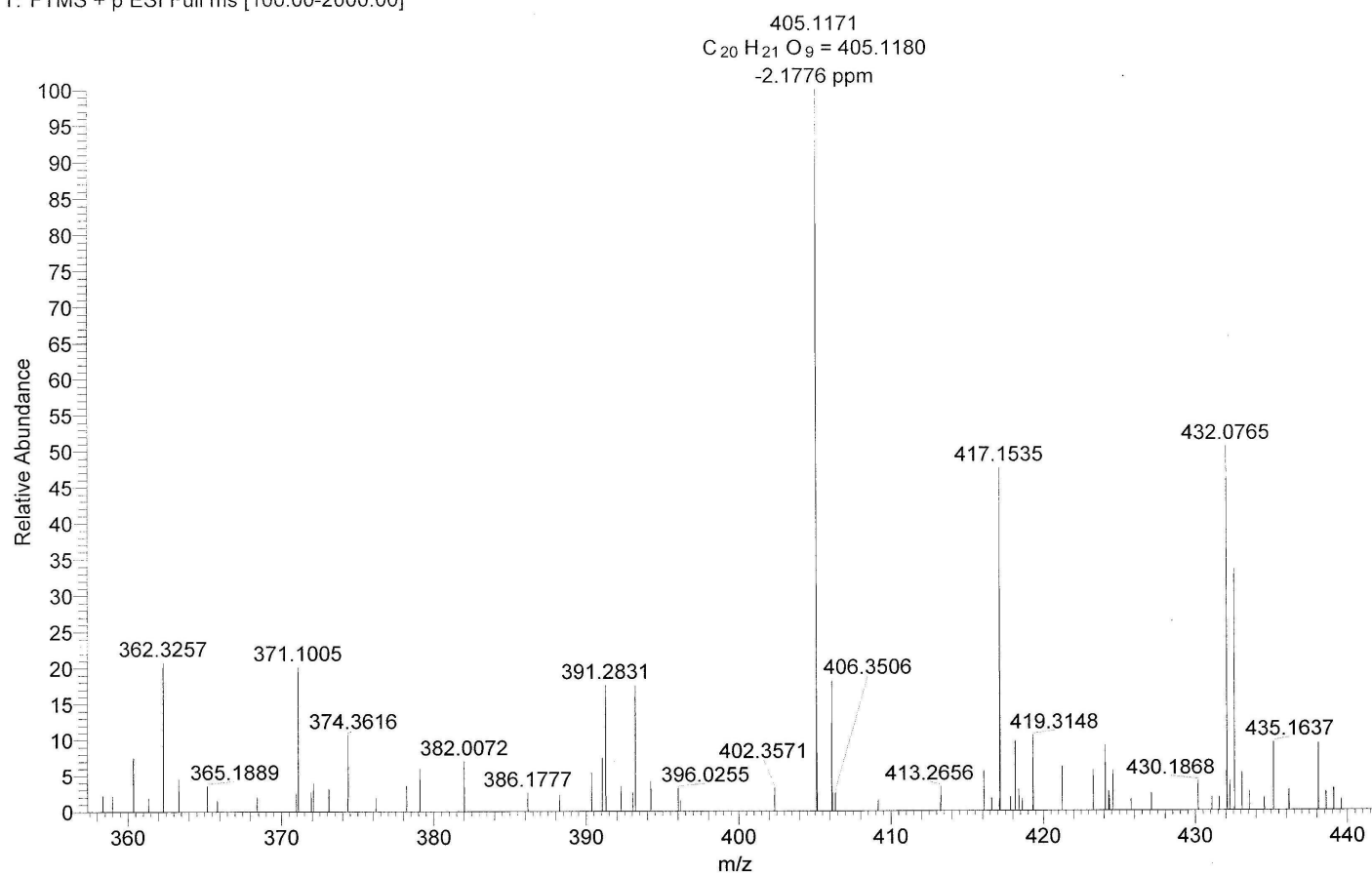


Figure S31. HRESIMS spectrum of compound 4

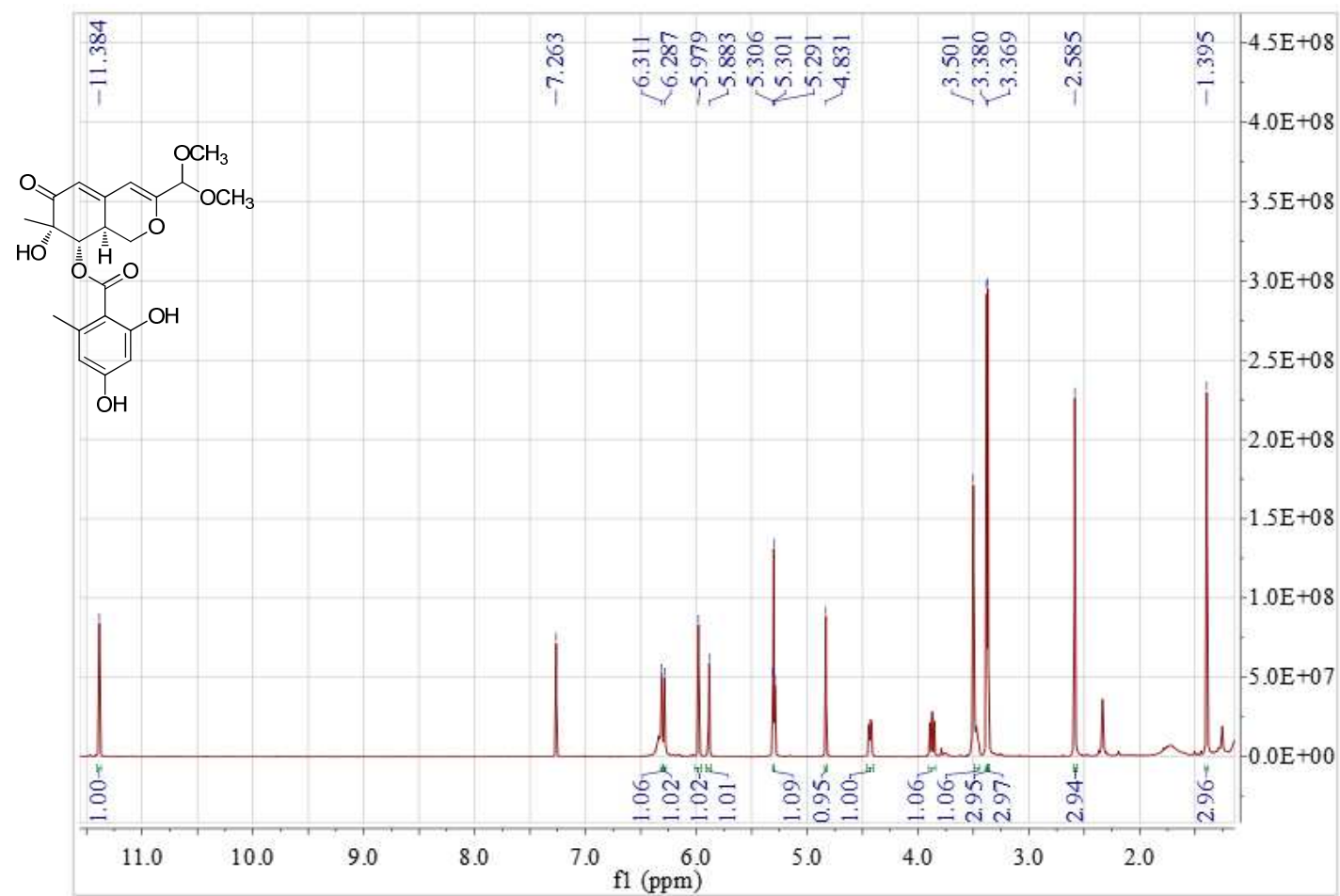


Figure S32. ¹H NMR (600 MHz, CDCl₃) spectrum of compound 5

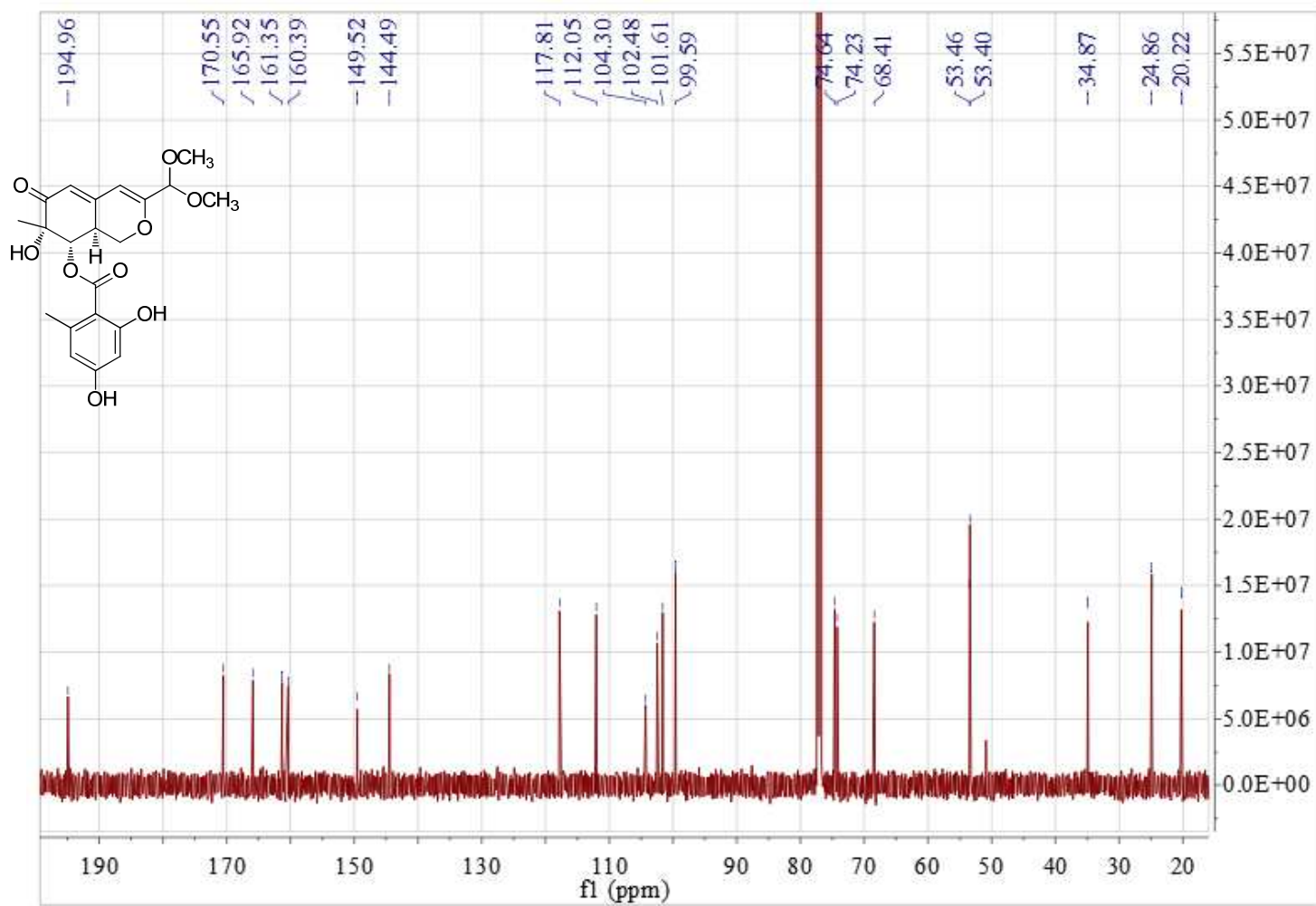


Figure S33. ^{13}C NMR (150MHz, CDCl_3) spectrum of compound 5

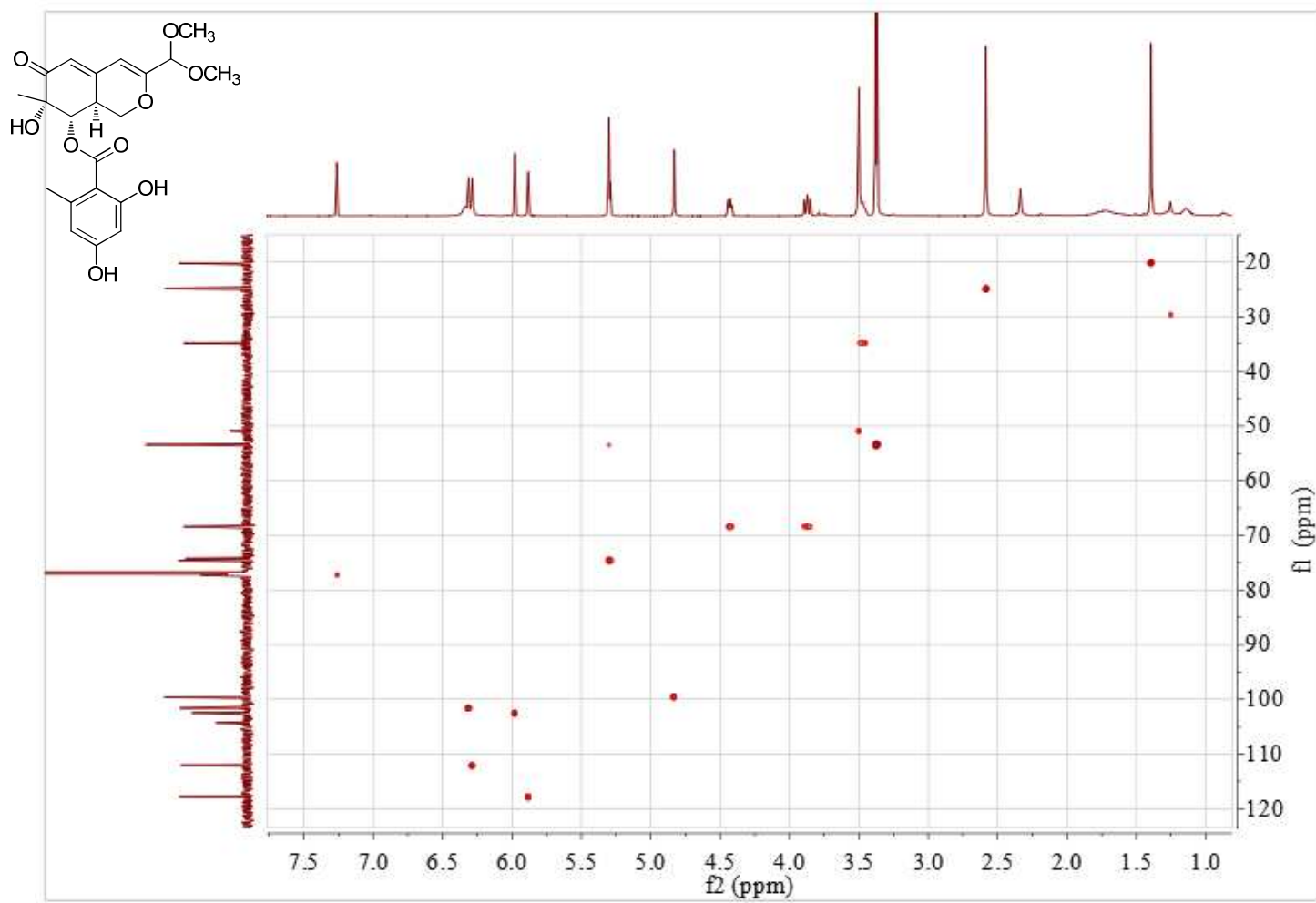


Figure S34. HSQC (CDCl₃) spectrum of compound 5

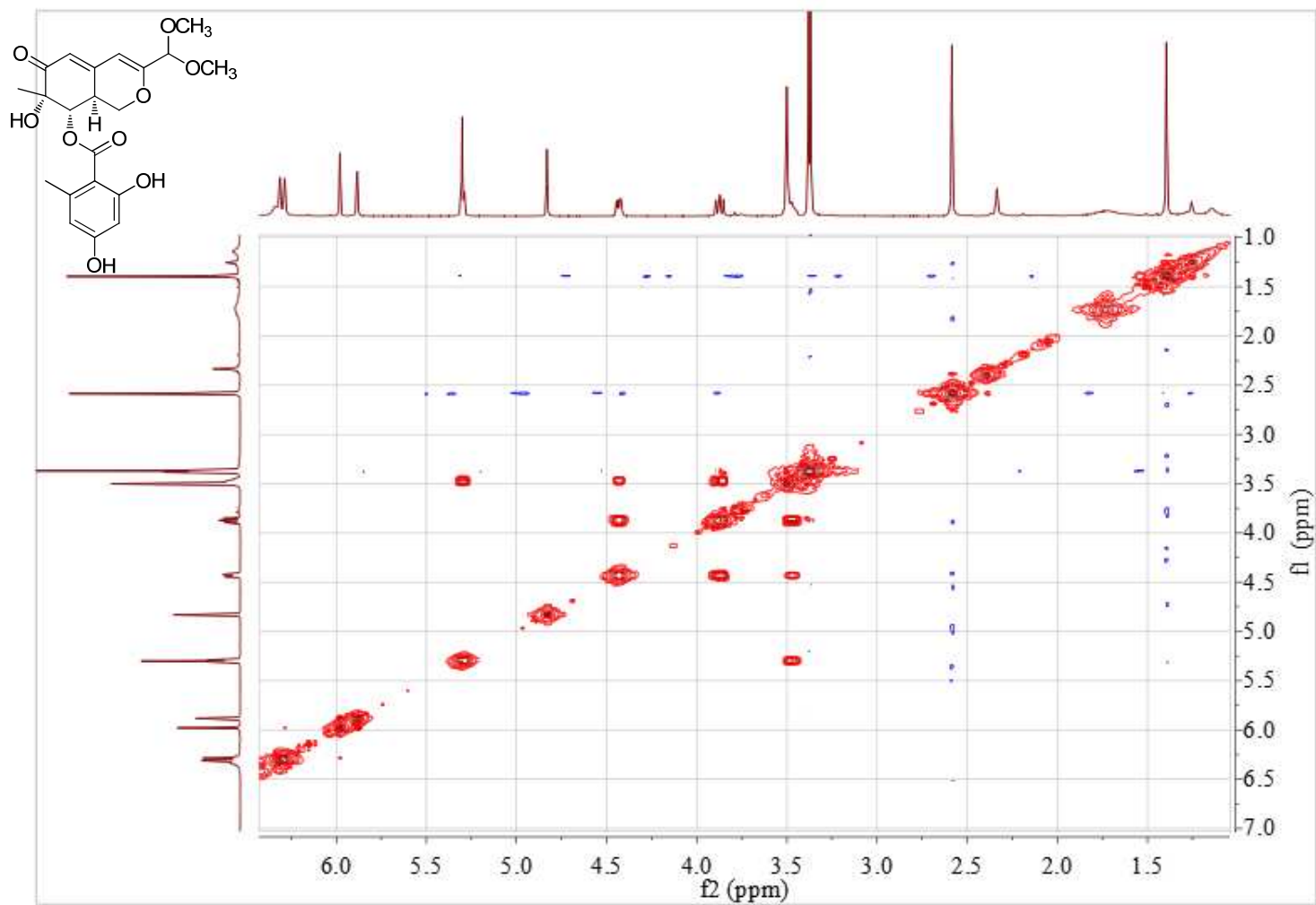


Figure S35. ^1H - ^1H COSY (CDCl_3) spectrum of compound **5**

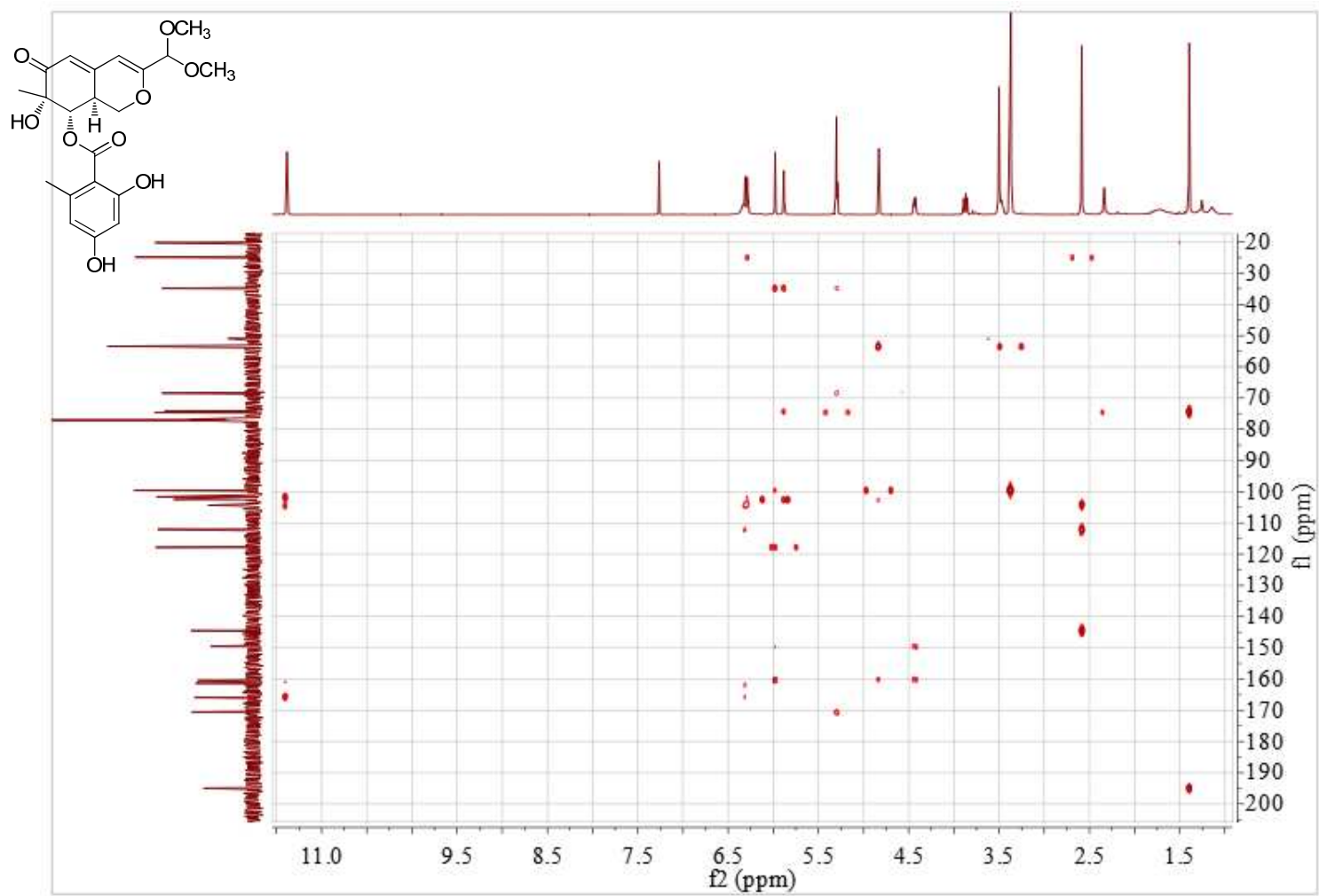


Figure S36. HMBC (CDCl_3) spectrum of compound **5**

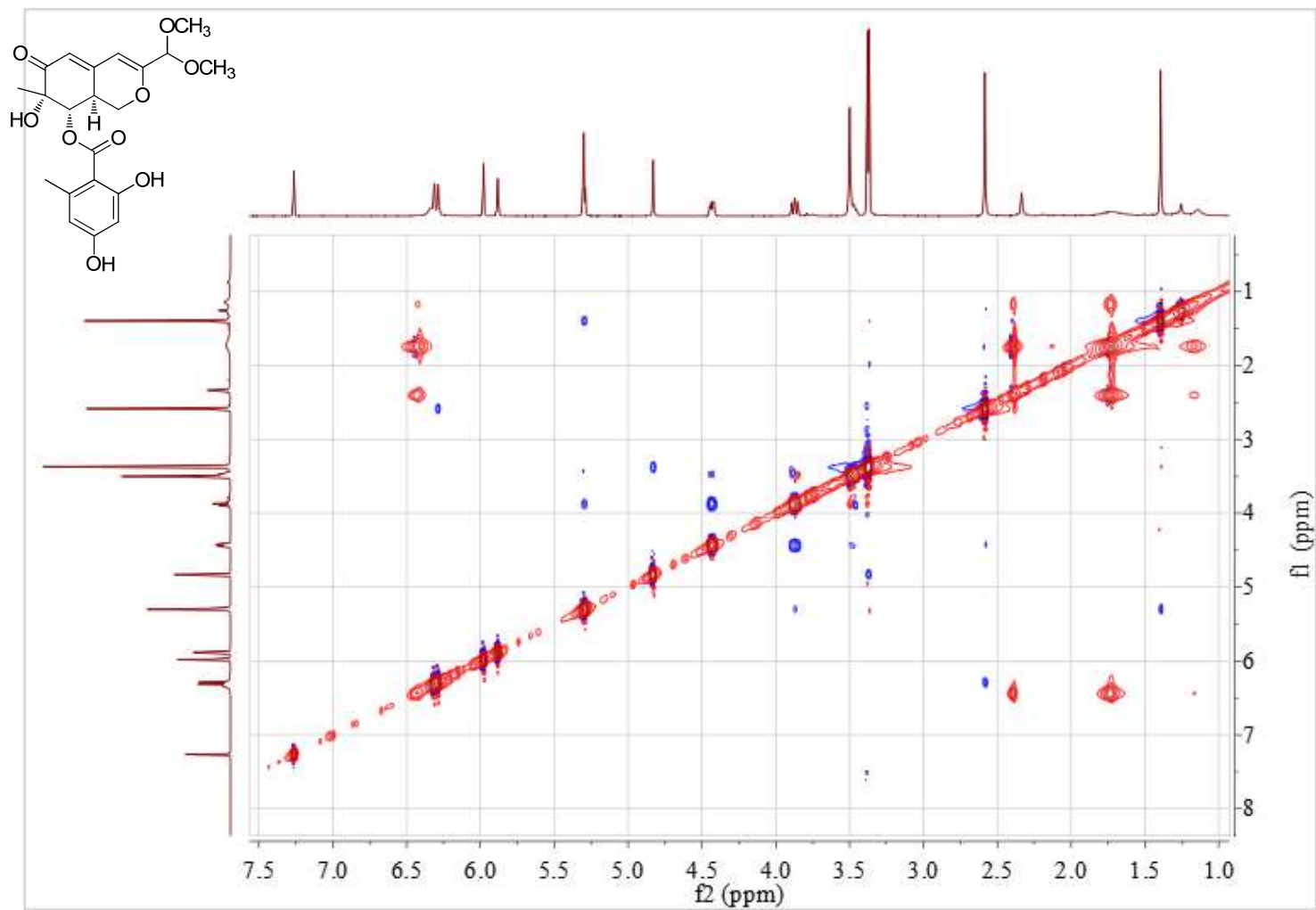


Figure S37. ROESY (CDCl₃) spectrum of compound5

151029-DS-14_151027192708 #104 RT: 0.88 AV: 1 NL: 1.55E7
FTMS + p ESI Full ms [100.00-2000.00]

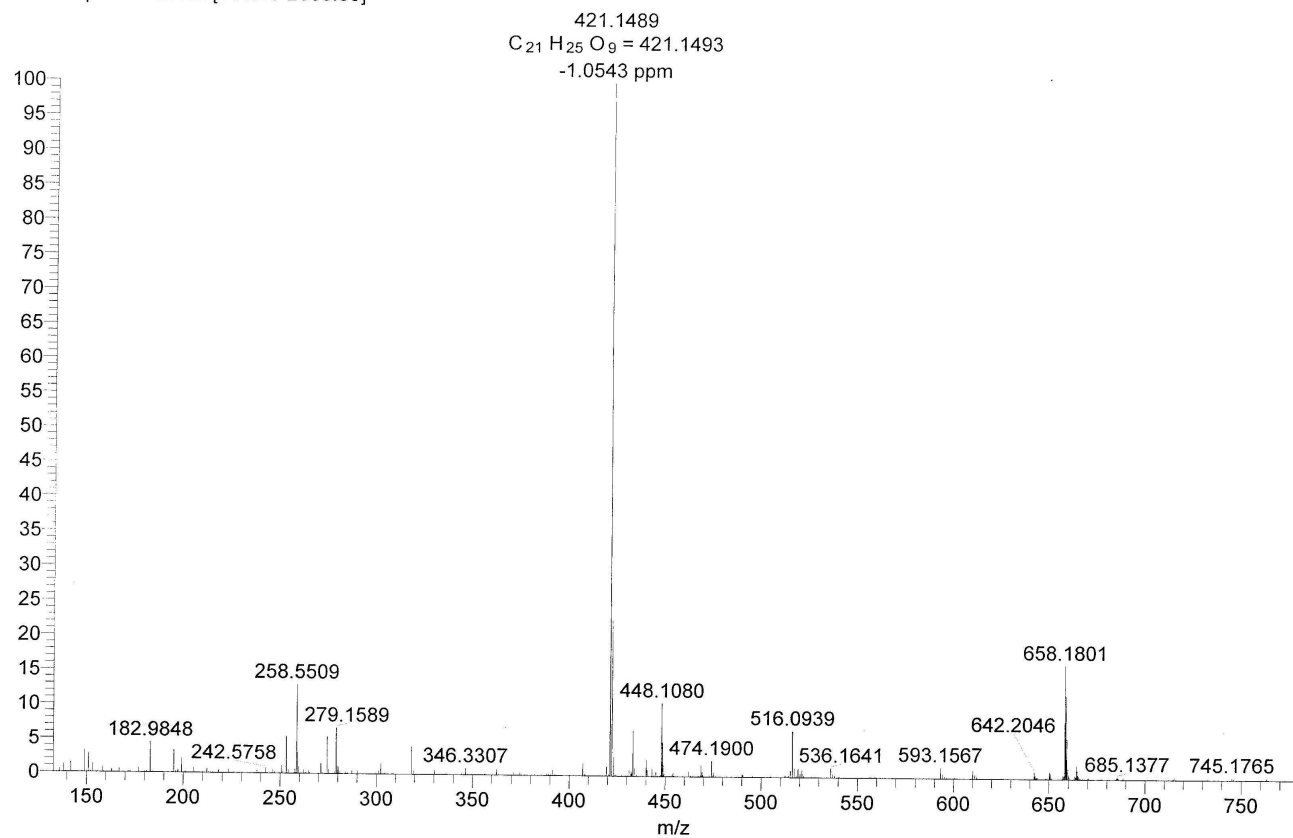


Figure S38. HRESIMS spectrum of compound 5

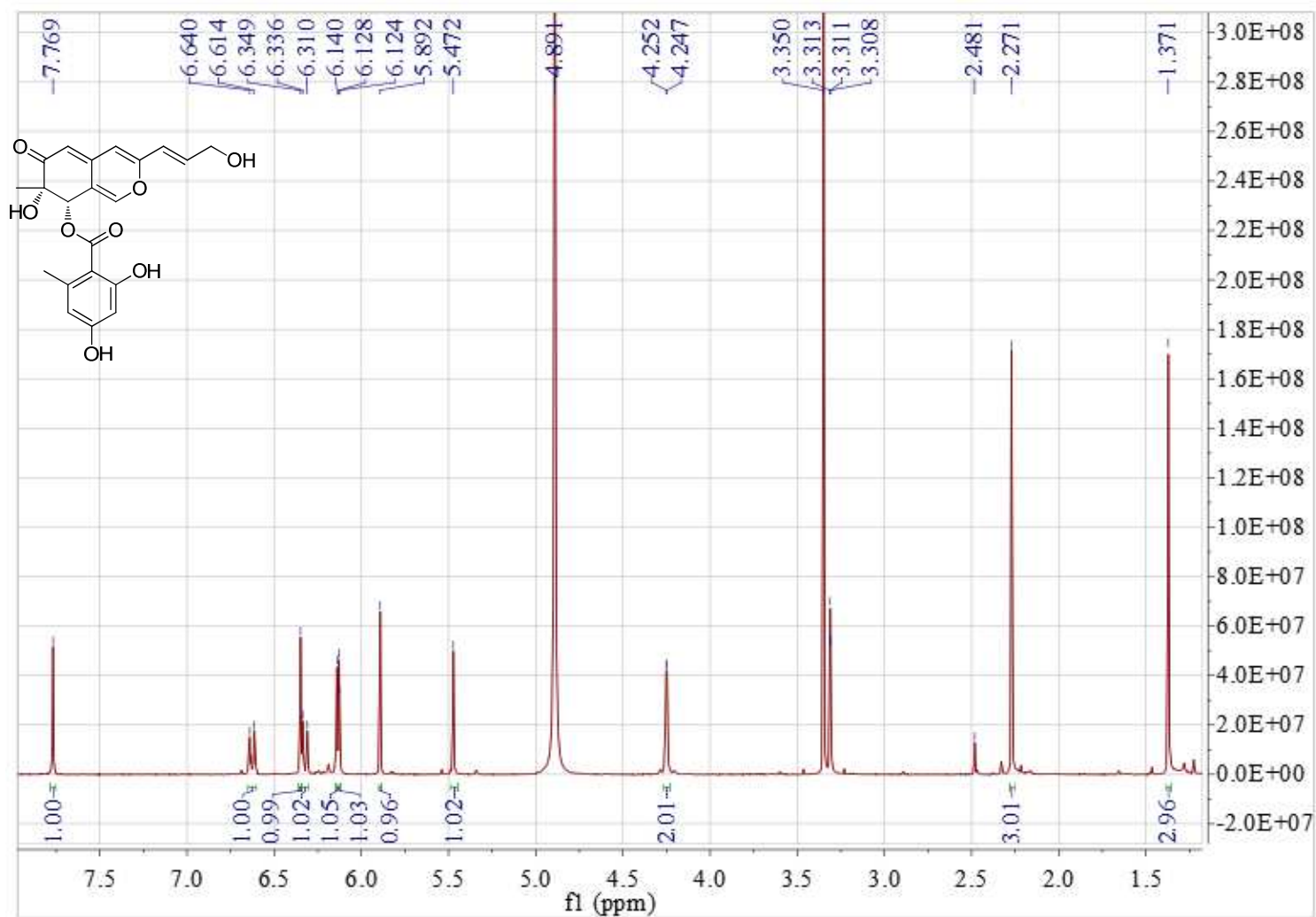


Figure S39. ^1H NMR (600 MHz, CD_3OD) spectrum of compound 6

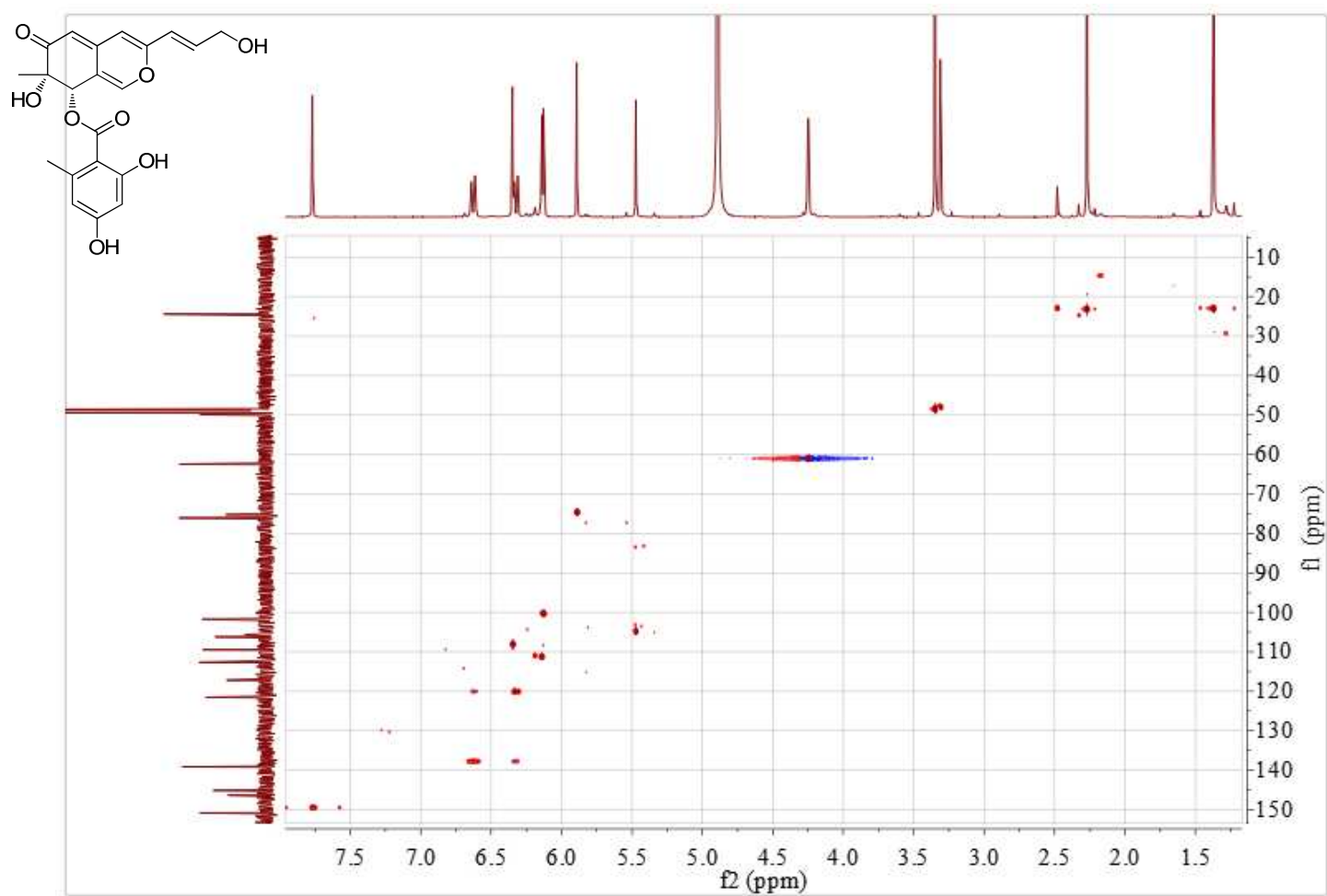


Figure S41. HSQC (CD₃OD) spectrum of compound 6

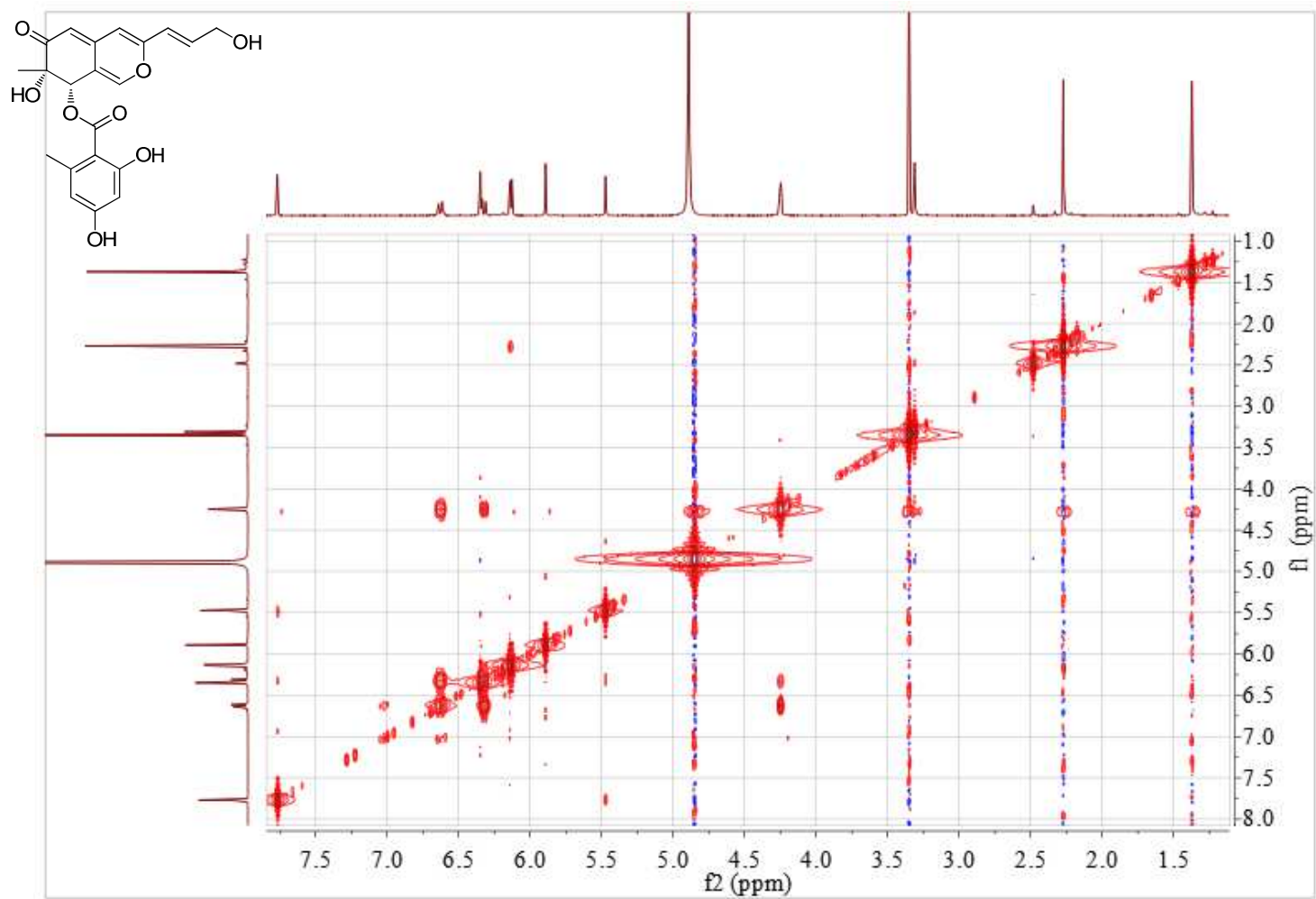


Figure S42. ^1H - ^1H COSY (CD_3OD) spectrum of compound 6

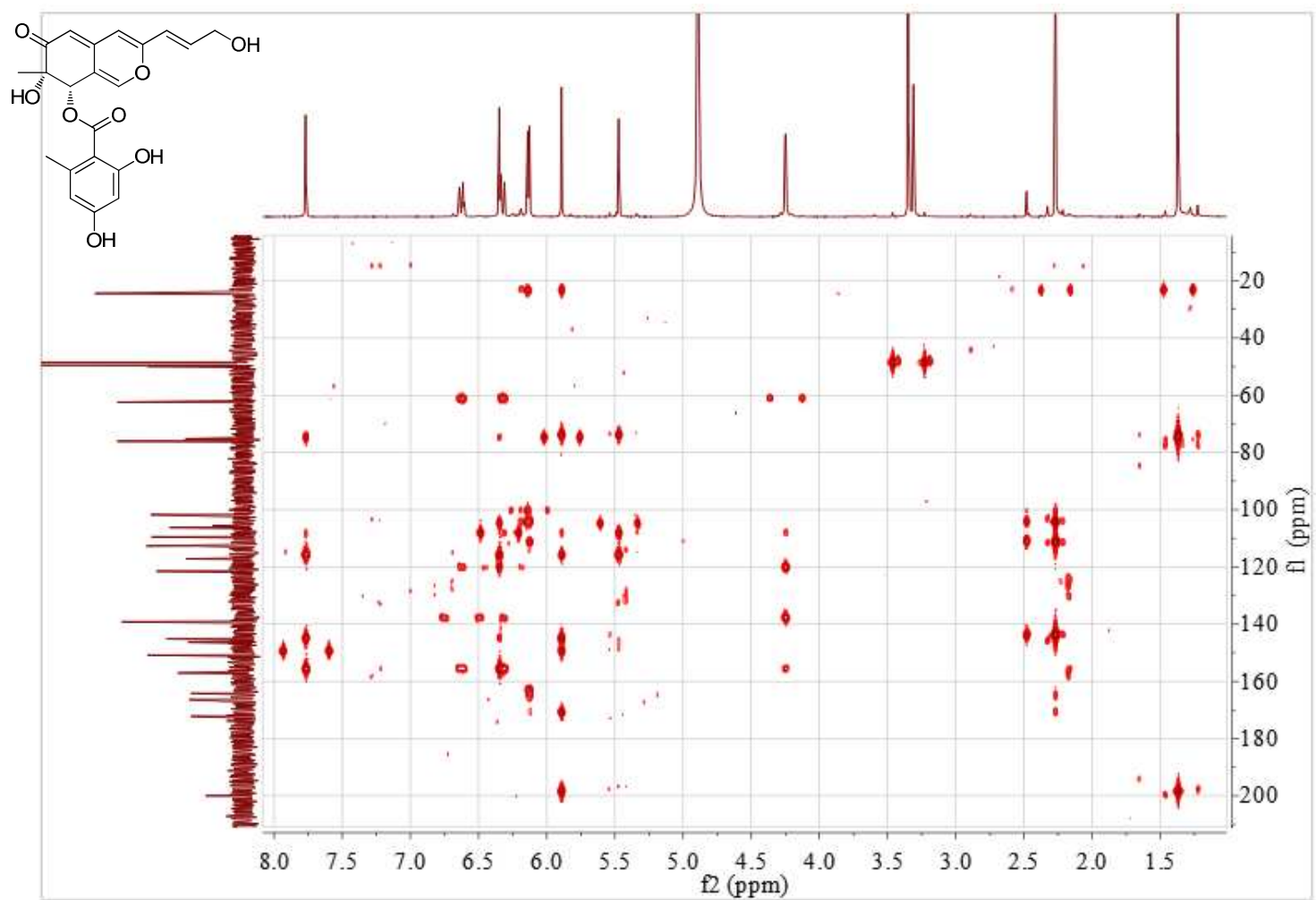


Figure S43 HMBC (CD₃OD) spectrum of compound6

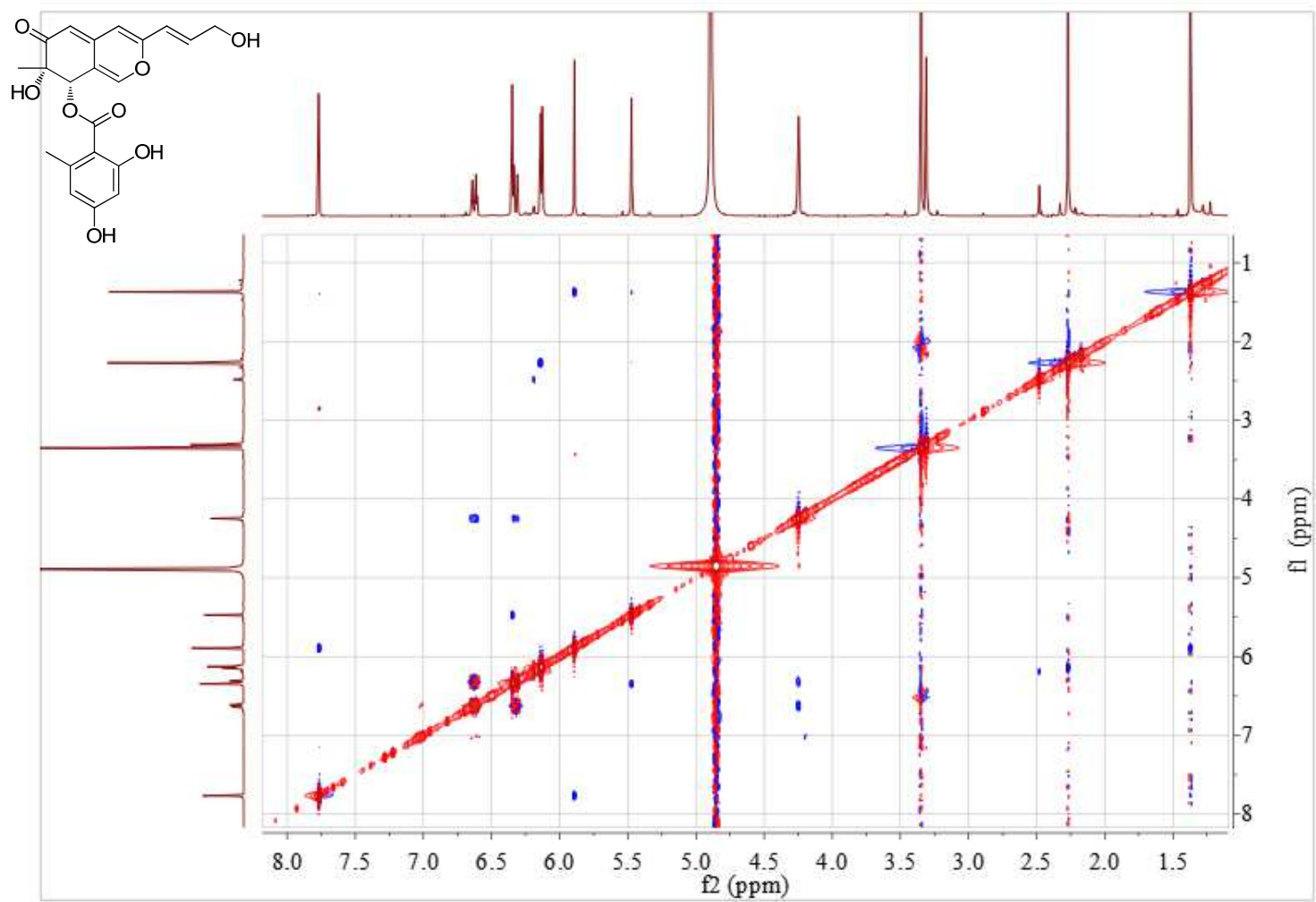


Figure S44. ROESY (CD₃OD) spectrum of compound 6

20160120-DS-02_160120112604 #98 RT: 0.79 AV: 1 NL: 9.32E6

T: FTMS + c ESI Full ms [150.00-1000.00]

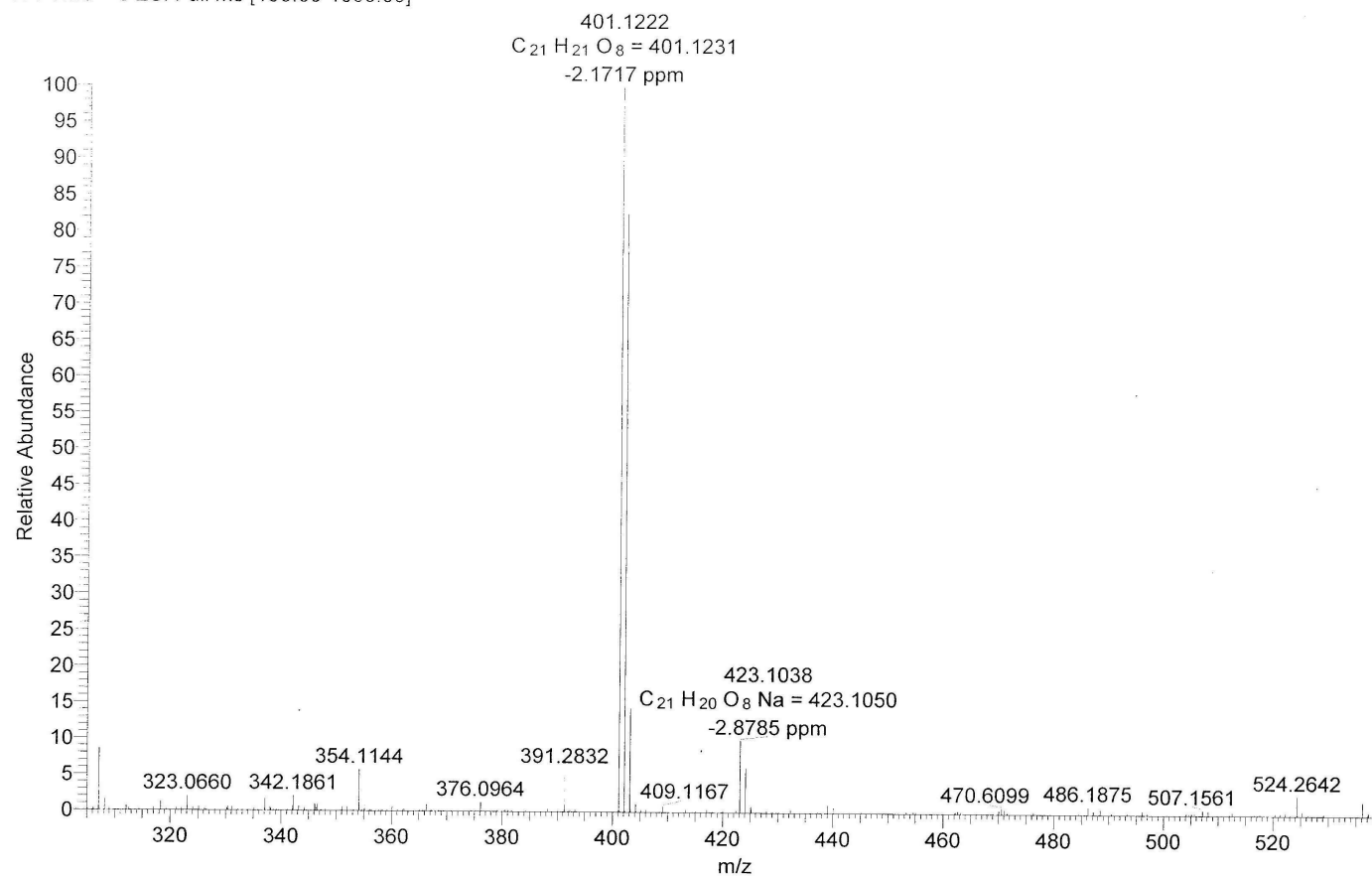


Figure S45. HRESIMS spectrum of compound 6

Table S1. Simulated ECD spectrum date of 7S,8S,8aS,12S-1

Wavenumber	ECD	Wavenumber	ECD	Wavenumber	ECD	Wavenumber	ECD	Wavenumber	ECD
400.5	1.83	375.5	5.05	350.5	6.76	325.5	1.27	300.5	-4.15
400	1.88	375	5.12	350	6.73	325	1.10	300	-4.15
399.5	1.92	374.5	5.19	349.5	6.69	324.5	0.94	299.5	-4.15
399	1.97	374	5.26	349	6.65	324	0.78	299	-4.14
398.5	2.02	373.5	5.33	348.5	6.61	323.5	0.61	298.5	-4.12
398	2.08	373	5.40	348	6.56	323	0.45	298	-4.10
397.5	2.13	372.5	5.47	347.5	6.51	322.5	0.29	297.5	-4.08
397	2.18	372	5.54	347	6.46	322	0.13	297	-4.05
396.5	2.24	371.5	5.60	346.5	6.41	321.5	-0.03	296.5	-4.01
396	2.29	371	5.67	346	6.34	321	-0.19	296	-3.97
395.5	2.35	370.5	5.73	345.5	6.28	320.5	-0.35	295.5	-3.93
395	2.40	370	5.80	345	6.21	320	-0.51	295	-3.88
394.5	2.46	369.5	5.86	344.5	6.14	319.5	-0.67	294.5	-3.83
394	2.52	369	5.92	344	6.07	319	-0.82	294	-3.77
393.5	2.58	368.5	5.98	343.5	5.99	318.5	-0.97	293.5	-3.71
393	2.64	368	6.04	343	5.91	318	-1.12	293	-3.64
392.5	2.70	367.5	6.10	342.5	5.82	317.5	-1.27	292.5	-3.57
392	2.76	367	6.15	342	5.73	317	-1.42	292	-3.50
391.5	2.82	366.5	6.21	341.5	5.64	316.5	-1.56	291.5	-3.43
391	2.88	366	6.26	341	5.55	316	-1.71	291	-3.35
390.5	2.95	365.5	6.31	340.5	5.45	315.5	-1.85	290.5	-3.26
390	3.01	365	6.36	340	5.35	315	-1.98	290	-3.18
389.5	3.07	364.5	6.41	339.5	5.24	314.5	-2.12	289.5	-3.09
389	3.14	364	6.46	339	5.13	314	-2.25	289	-3.00
388.5	3.21	363.5	6.50	338.5	5.02	313.5	-2.37	288.5	-2.91
388	3.27	363	6.54	338	4.91	313	-2.50	288	-2.81
387.5	3.34	362.5	6.58	337.5	4.79	312.5	-2.62	287.5	-2.71
387	3.41	362	6.62	337	4.67	312	-2.73	287	-2.62
386.5	3.48	361.5	6.66	336.5	4.54	311.5	-2.84	286.5	-2.52
386	3.54	361	6.69	336	4.42	311	-2.95	286	-2.41
385.5	3.61	360.5	6.72	335.5	4.29	310.5	-3.06	285.5	-2.31
385	3.68	360	6.75	335	4.15	310	-3.16	285	-2.21
384.5	3.75	359.5	6.78	334.5	4.02	309.5	-3.25	284.5	-2.11
384	3.82	359	6.80	334	3.88	309	-3.35	284	-2.00
383.5	3.90	358.5	6.82	333.5	3.74	308.5	-3.43	283.5	-1.90
383	3.97	358	6.84	333	3.60	308	-3.52	283	-1.80
382.5	4.04	357.5	6.86	332.5	3.45	307.5	-3.59	282.5	-1.69
382	4.11	357	6.87	332	3.31	307	-3.67	282	-1.59
381.5	4.18	356.5	6.88	331.5	3.16	306.5	-3.73	281.5	-1.49
381	4.25	356	6.89	331	3.01	306	-3.80	281	-1.39
380.5	4.33	355.5	6.89	330.5	2.86	305.5	-3.86	280.5	-1.29
380	4.40	355	6.89	330	2.70	305	-3.91	280	-1.20
379.5	4.47	354.5	6.89	329.5	2.55	304.5	-3.96	279.5	-1.10
379	4.54	354	6.89	329	2.39	304	-4.00	279	-1.01
378.5	4.62	353.5	6.88	328.5	2.23	303.5	-4.04	278.5	-0.91
378	4.69	353	6.87	328	2.07	303	-4.07	278	-0.83
377.5	4.76	352.5	6.85	327.5	1.91	302.5	-4.10	277.5	-0.74
377	4.83	352	6.83	327	1.75	302	-4.12	277	-0.65
376.5	4.91	351.5	6.81	326.5	1.59	301.5	-4.13	276.5	-0.57
276	-0.49	260	0.58	244	0.86	228	-0.30	212	-0.87
275.5	-0.42	259.5	0.59	243.5	0.86	227.5	-0.37	211.5	-0.82
275	-0.34	259	0.59	243	0.86	227	-0.44	211	-0.77
274.5	-0.27	258.5	0.59	242.5	0.86	226.5	-0.51	210.5	-0.72
274	-0.20	258	0.60	242	0.86	226	-0.57	210	-0.66
273.5	-0.14	257.5	0.60	241.5	0.86	225.5	-0.64	209.5	-0.61
273	-0.08	257	0.61	241	0.85	225	-0.70	209	-0.55
272.5	-0.02	256.5	0.61	240.5	0.84	224.5	-0.76	208.5	-0.50
272	0.03	256	0.62	240	0.83	224	-0.82	208	-0.45
271.5	0.09	255.5	0.63	239.5	0.81	223.5	-0.87	207.5	-0.40
271	0.13	255	0.63	239	0.80	223	-0.92	207	-0.35

270.5	0.18	254.5	0.64	238.5	0.78	222.5	-0.97	206.5	-0.30
270	0.22	254	0.65	238	0.75	222	-1.01	206	-0.25
269.5	0.26	253.5	0.66	237.5	0.72	221.5	-1.05	205.5	-0.21
269	0.30	253	0.67	237	0.69	221	-1.09	205	-0.17
268.5	0.33	252.5	0.68	236.5	0.66	220.5	-1.12	204.5	-0.13
268	0.36	252	0.69	236	0.62	220	-1.14	204	-0.10
267.5	0.39	251.5	0.70	235.5	0.58	219.5	-1.16	203.5	-0.07
267	0.41	251	0.71	235	0.54	219	-1.18	203	-0.04
266.5	0.44	250.5	0.72	234.5	0.50	218.5	-1.18	202.5	-0.01
266	0.46	250	0.74	234	0.45	218	-1.19	202	0.01
265.5	0.48	249.5	0.75	233.5	0.40	217.5	-1.19	201.5	0.03
265	0.49	249	0.76	233	0.34	217	-1.18	201	0.05
264.5	0.51	248.5	0.77	232.5	0.28	216.5	-1.17	200.5	0.06
264	0.52	248	0.79	232	0.23	216	-1.15	200	0.07
263.5	0.53	247.5	0.80	231.5	0.16	215.5	-1.13		
263	0.54	247	0.81	231	0.10	215	-1.10		
262.5	0.55	246.5	0.82	230.5	0.04	214.5	-1.07		
262	0.56	246	0.83	230	-0.03	214	-1.04		
261.5	0.56	245.5	0.84	229.5	-0.10	213.5	-1.00		
261	0.57	245	0.85	229	-0.17	213	-0.96		
260.5	0.58	244.5	0.85	228.5	-0.24	212.5	-0.92		

Table S2. Simulated ECD spectrum date of 7*S*,8*S*,8*aS*,12*R*-1

Wavenumber	ECD	Wavenumber	ECD	Wavenumber	ECD	Wavenumber	ECD	Wavenumber	ECD
401	0.51	360	3.44	319	2.40	278	-4.53	237	-3.54
400	0.53	359	3.52	318	2.20	277	-4.58	236	-3.29
399	0.56	358	3.62	317	1.98	276	-4.64	235	-3.05
398	0.60	357	3.71	316	1.78	275	-4.70	234	-2.82
397	0.64	356	3.79	315	1.57	274	-4.76	233	-2.62
396	0.68	355	3.88	314	1.34	273	-4.82	232	-2.44
395	0.72	354	3.96	313	1.12	272	-4.88	231	-2.28
394	0.77	353	4.04	312	0.89	271	-4.95	230	-2.15
393	0.82	352	4.11	311	0.65	270	-5.03	229	-2.04
392	0.87	351	4.18	310	0.42	269	-5.11	228	-1.96
391	0.92	350	4.24	309	0.20	268	-5.19	227	-1.91
390	0.98	349	4.30	308	-0.03	267	-5.28	226	-1.88
389	1.03	348	4.35	307	-0.29	266	-5.38	225	-1.86
388	1.09	347	4.40	306	-0.52	265	-5.47	224	-1.87
387	1.15	346	4.45	305	-0.74	264	-5.58	223	-1.90
386	1.21	345	4.48	304	-0.96	263	-5.68	222	-1.94
385	1.28	344	4.51	303	-1.20	262	-5.78	221	-1.99
384	1.34	343	4.53	302	-1.41	261	-5.88	220	-2.04
383	1.40	342	4.55	301	-1.64	260	-5.98	219	-2.10
382	1.48	341	4.56	300	-1.84	259	-6.06	218	-2.17
381	1.55	340	4.56	299	-2.04	258	-6.15	217	-2.23
380	1.63	339	4.55	298	-2.24	257	-6.22	216	-2.29
379	1.71	338	4.53	297	-2.44	256	-6.28	215	-2.35
378	1.78	337	4.50	296	-2.62	255	-6.32	214	-2.40
377	1.87	336	4.46	295	-2.79	254	-6.34	213	-2.45
376	1.95	335	4.42	294	-2.95	253	-6.35	212	-2.49
375	2.03	334	4.36	293	-3.12	252	-6.33	211	-2.52
374	2.12	333	4.30	292	-3.26	251	-6.29	210	-2.55
373	2.21	332	4.23	291	-3.41	250	-6.23	209	-2.57
372	2.30	331	4.14	290	-3.53	249	-6.14	208	-2.58
371	2.39	330	4.05	289	-3.66	248	-6.02	207	-2.58
370	2.49	329	3.94	288	-3.77	247	-5.88	206	-2.57
369	2.58	328	3.83	287	-3.88	246	-5.72	205	-2.55
368	2.67	327	3.71	286	-3.97	245	-5.53	204	-2.51
367	2.77	326	3.57	285	-4.06	244	-5.32	203	-2.46
366	2.86	325	3.42	284	-4.14	243	-5.09	202	-2.38
365	2.96	324	3.28	283	-4.22	242	-4.85	201	-2.28
364	3.06	323	3.12	282	-4.29	241	-4.60	200	-2.16
363	3.15	322	2.95	281	-4.35	240	-4.33		
362	3.25	321	2.77	280	-4.41	239	-4.07		
361	3.34	320	2.59	279	-4.47	238	-3.80		

Table S3. Simulated ECD spectrum date of 7S,8S-6.

Wavenumber	ECD	Wavenumber	ECD	Wavenumber	ECD	Wavenumber	ECD	Wavenumber	ECD
400	12.57	375.5	25.95	351	13.20	326.5	-6.75	302	-7.03
399.5	12.86	375	26.07	350.5	12.61	326	-6.77	301.5	-7.43
399	13.16	374.5	26.17	350	12.02	325.5	-6.77	301	-7.86
398.5	13.45	374	26.26	349.5	11.42	325	-6.76	300.5	-8.32
398	13.75	373.5	26.33	349	10.82	324.5	-6.74	300	-8.82
397.5	14.05	373	26.39	348.5	10.22	324	-6.70	299.5	-9.33
397	14.36	372.5	26.44	348	9.62	323.5	-6.65	299	-9.88
396.5	14.67	372	26.47	347.5	9.01	323	-6.59	298.5	-10.46
396	14.98	371.5	26.48	347	8.41	322.5	-6.52	298	-11.06
395.5	15.29	371	26.48	346.5	7.81	322	-6.44	297.5	-11.70
395	15.60	370.5	26.47	346	7.21	321.5	-6.35	297	-12.35
394.5	15.92	370	26.44	345.5	6.61	321	-6.25	296.5	-13.04
394	16.23	369.5	26.39	345	6.02	320.5	-6.14	296	-13.75
393.5	16.55	369	26.32	344.5	5.44	320	-6.03	295.5	-14.48
393	16.87	368.5	26.24	344	4.86	319.5	-5.91	295	-15.24
392.5	17.18	368	26.14	343.5	4.28	319	-5.79	294.5	-16.02
392	17.50	367.5	26.03	343	3.72	318.5	-5.66	294	-16.82
391.5	17.82	367	25.90	342.5	3.16	318	-5.54	293.5	-17.64
391	18.14	366.5	25.75	342	2.61	317.5	-5.41	293	-18.48
390.5	18.46	366	25.58	341.5	2.07	317	-5.28	292.5	-19.33
390	18.78	365.5	25.39	341	1.55	316.5	-5.15	292	-20.20
389.5	19.09	365	25.19	340.5	1.03	316	-5.02	291.5	-21.08
389	19.41	364.5	24.97	340	0.53	315.5	-4.90	291	-21.97
388.5	19.72	364	24.73	339.5	0.04	315	-4.79	290.5	-22.87
388	20.03	363.5	24.48	339	-0.44	314.5	-4.67	290	-23.78
387.5	20.34	363	24.20	338.5	-0.90	314	-4.57	289.5	-24.69
387	20.64	362.5	23.91	338	-1.35	313.5	-4.48	289	-25.61
386.5	20.94	362	23.61	337.5	-1.78	313	-4.39	288.5	-26.52
386	21.24	361.5	23.28	337	-2.19	312.5	-4.31	288	-27.43
385.5	21.53	361	22.94	336.5	-2.59	312	-4.25	287.5	-28.33
385	21.82	360.5	22.58	336	-2.97	311.5	-4.20	287	-29.23
384.5	22.11	360	22.21	335.5	-3.34	311	-4.16	286.5	-30.11
384	22.39	359.5	21.82	335	-3.68	310.5	-4.14	286	-30.98
383.5	22.66	359	21.42	334.5	-4.01	310	-4.13	285.5	-31.84
383	22.93	358.5	20.99	334	-4.32	309.5	-4.15	285	-32.67
382.5	23.19	358	20.56	333.5	-4.61	309	-4.18	284.5	-33.48
382	23.45	357.5	20.11	333	-4.89	308.5	-4.23	284	-34.27
381.5	23.70	357	19.65	332.5	-5.14	308	-4.30	283.5	-35.03
381	23.94	356.5	19.17	332	-5.38	307.5	-4.39	283	-35.76
380.5	24.17	356	18.68	331.5	-5.59	307	-4.50	282.5	-36.45
380	24.39	355.5	18.18	331	-5.79	306.5	-4.64	282	-37.11
379.5	24.61	355	17.66	330.5	-5.97	306	-4.80	281.5	-37.73
379	24.81	354.5	17.14	330	-6.13	305.5	-4.98	281	-38.31
378.5	25.01	354	16.60	329.5	-6.27	305	-5.19	280.5	-38.84
378	25.19	353.5	16.06	329	-6.39	304.5	-5.43	280	-39.33
377.5	25.37	353	15.50	328.5	-6.50	304	-5.69	279.5	-39.76
377	25.53	352.5	14.94	328	-6.59	303.5	-5.99	279	-40.14
376.5	25.68	352	14.37	327.5	-6.66	303	-6.30	278.5	-40.47
376	25.82	351.5	13.79	327	-6.71	302.5	-6.65	278	-40.75
277.5	-40.96	261.5	-15.57	245.5	12.00	229.5	0.99	213.5	15.18
277	-41.11	261	-14.10	245	11.87	229	0.90	213	15.96
276.5	-41.20	260.5	-12.63	244.5	11.70	228.5	0.83	212.5	16.70
276	-41.23	260	-11.17	244	11.47	228	0.80	212	17.42
275.5	-41.20	259.5	-9.71	243.5	11.21	227.5	0.80	211.5	18.09
275	-41.09	259	-8.27	243	10.90	227	0.84	211	18.72
274.5	-40.93	258.5	-6.85	242.5	10.56	226.5	0.91	210.5	19.29
274	-40.69	258	-5.45	242	10.19	226	1.01	210	19.80
273.5	-40.38	257.5	-4.08	241.5	9.79	225.5	1.16	209.5	20.24
273	-40.01	257	-2.75	241	9.37	225	1.33	209	20.62

272.5	-39.57	256.5	-1.45	240.5	8.93	224.5	1.55	208.5	20.93
272	-39.06	256	-0.20	240	8.47	224	1.81	208	21.16
271.5	-38.48	255.5	1.01	239.5	8.01	223.5	2.10	207.5	21.31
271	-37.84	255	2.17	239	7.54	223	2.44	207	21.39
270.5	-37.13	254.5	3.28	238.5	7.06	222.5	2.81	206.5	21.39
270	-36.35	254	4.32	238	6.59	222	3.23	206	21.32
269.5	-35.51	253.5	5.31	237.5	6.12	221.5	3.68	205.5	21.17
269	-34.61	253	6.24	237	5.65	221	4.18	205	20.95
268.5	-33.65	252.5	7.10	236.5	5.20	220.5	4.72	204.5	20.66
268	-32.63	252	7.90	236	4.75	220	5.30	204	20.31
267.5	-31.56	251.5	8.62	235.5	4.33	219.5	5.92	203.5	19.90
267	-30.44	251	9.28	235	3.92	219	6.57	203	19.44
266.5	-29.26	250.5	9.87	234.5	3.53	218.5	7.26	202.5	18.93
266	-28.04	250	10.39	234	3.16	218	7.98	202	18.38
265.5	-26.77	249.5	10.84	233.5	2.81	217.5	8.73	201.5	17.79
265	-25.47	249	11.21	233	2.49	217	9.50	201	17.18
264.5	-24.13	248.5	11.52	232.5	2.19	216.5	10.29	200.5	16.54
264	-22.76	248	11.76	232	1.92	216	11.10	200	15.88
263.5	-21.36	247.5	11.93	231.5	1.68	215.5	11.92		
263	-19.93	247	12.04	231	1.46	215	12.74		
262.5	-18.49	246.5	12.08	230.5	1.27	214.5	13.56		
262	-17.04	246	12.07	230	1.12	214	14.38		