

Supplementary Materials to Oxidized resveratrol metabolites as potent antioxidants and xanthine oxidase inhibitors

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Figure S1. HPLC-PDA fingerprint of oxidized product mixture Ox1.

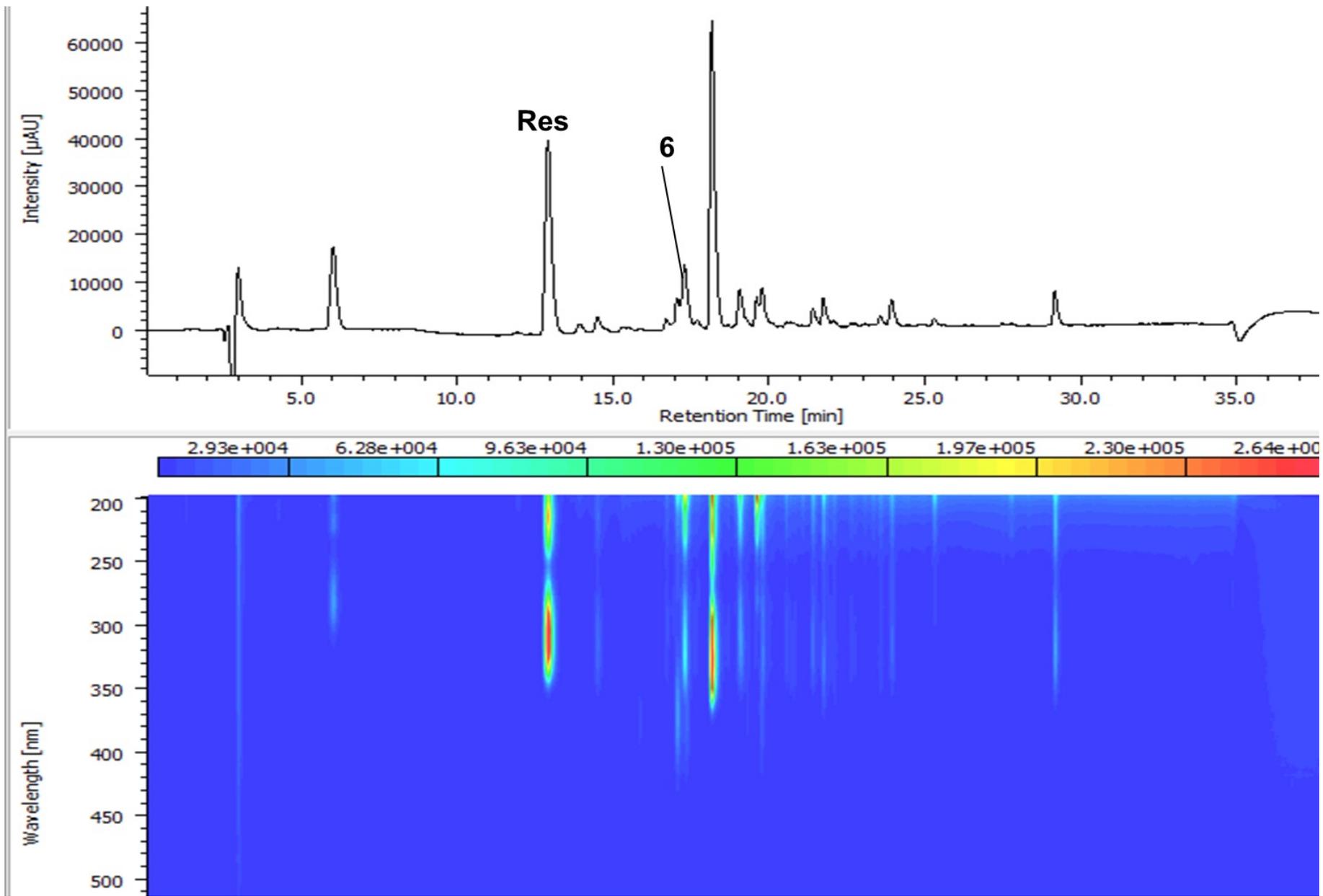


Figure S2. HPLC-PDA fingerprint of oxidized product mixture Ox2.

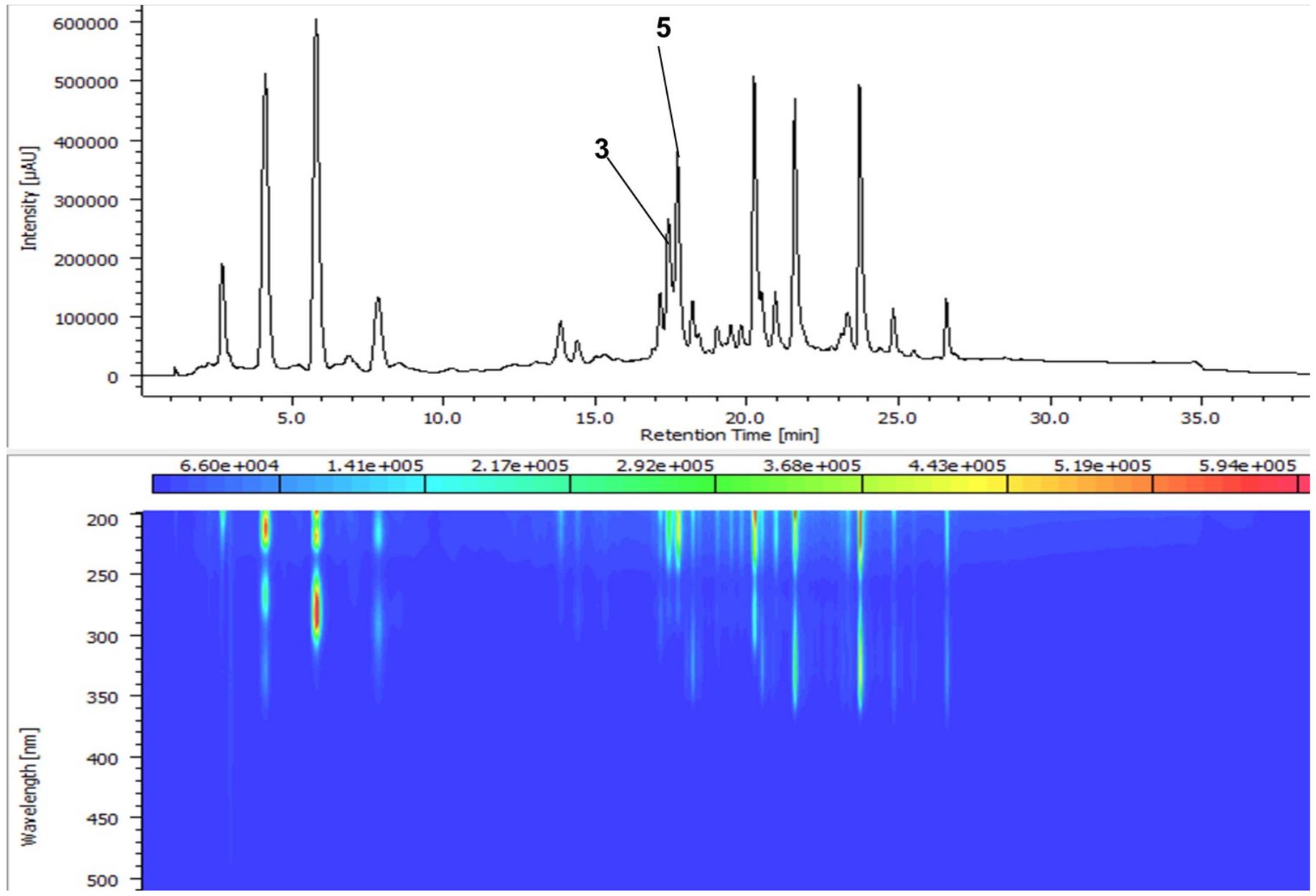


Figure S3. HPLC-PDA fingerprint of oxidized product mixture Ox3.

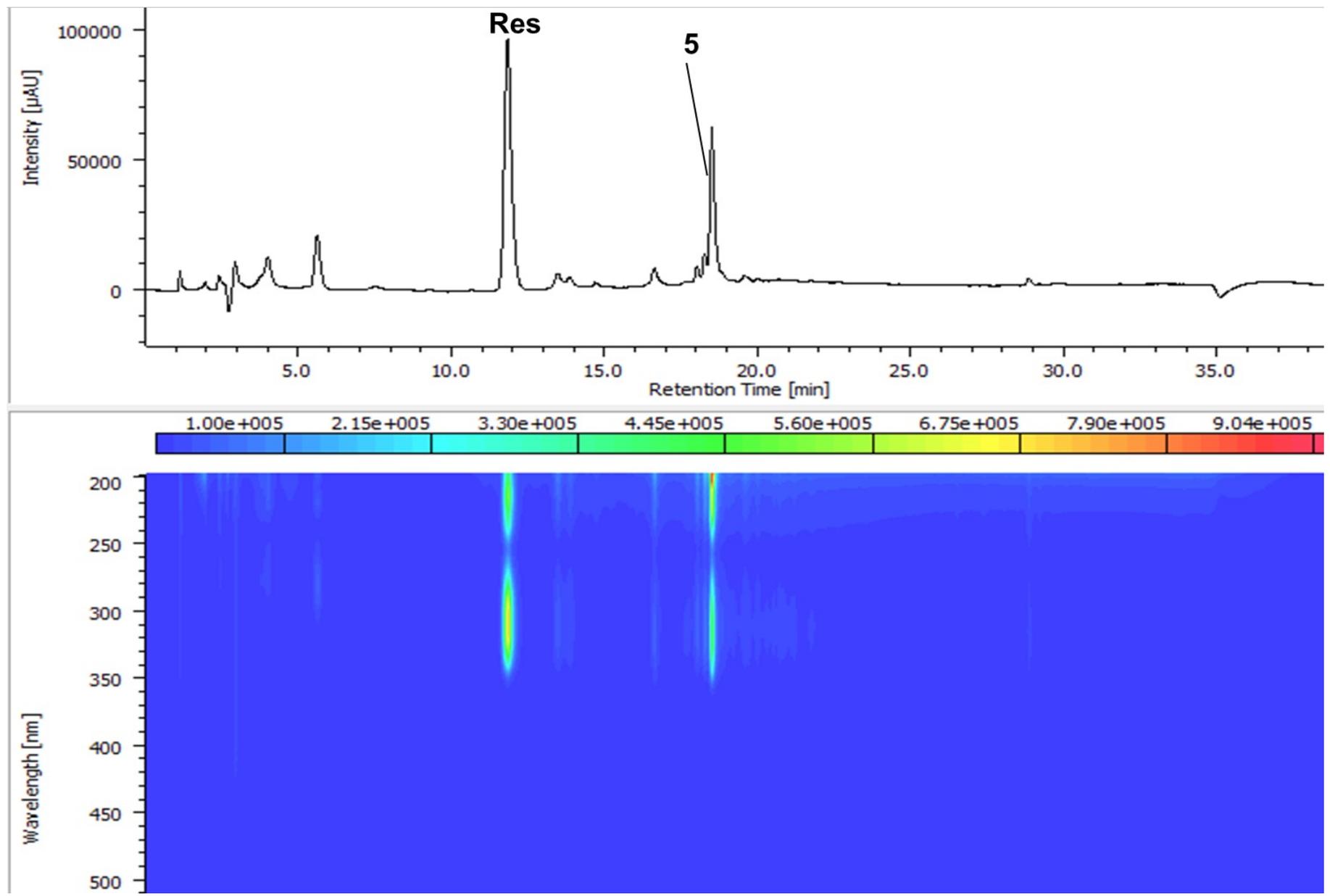


Figure S4. HPLC-PDA fingerprint of oxidized product mixture Ox4.

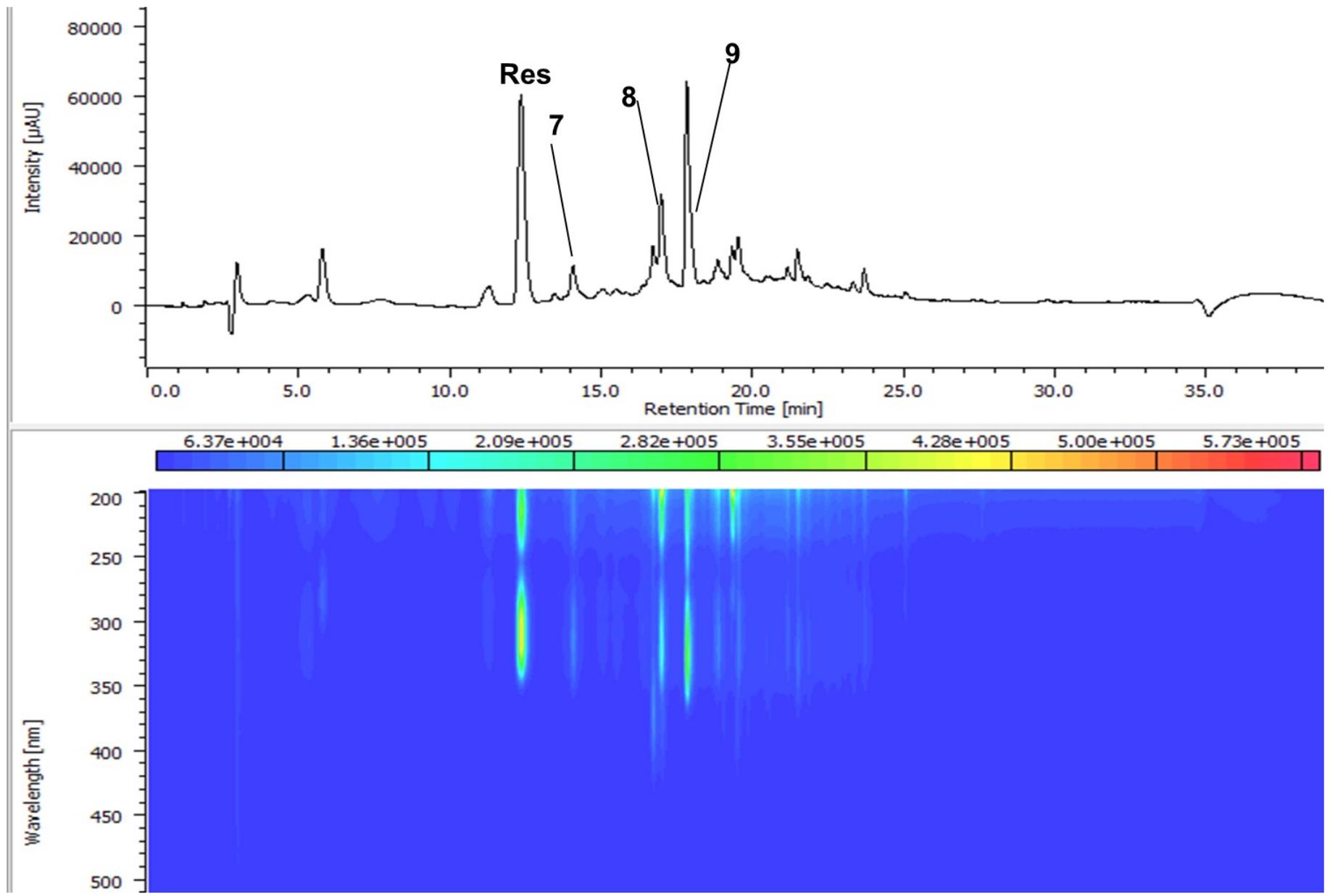


Figure S5. HPLC-PDA fingerprint of oxidized product mixture Ox5.

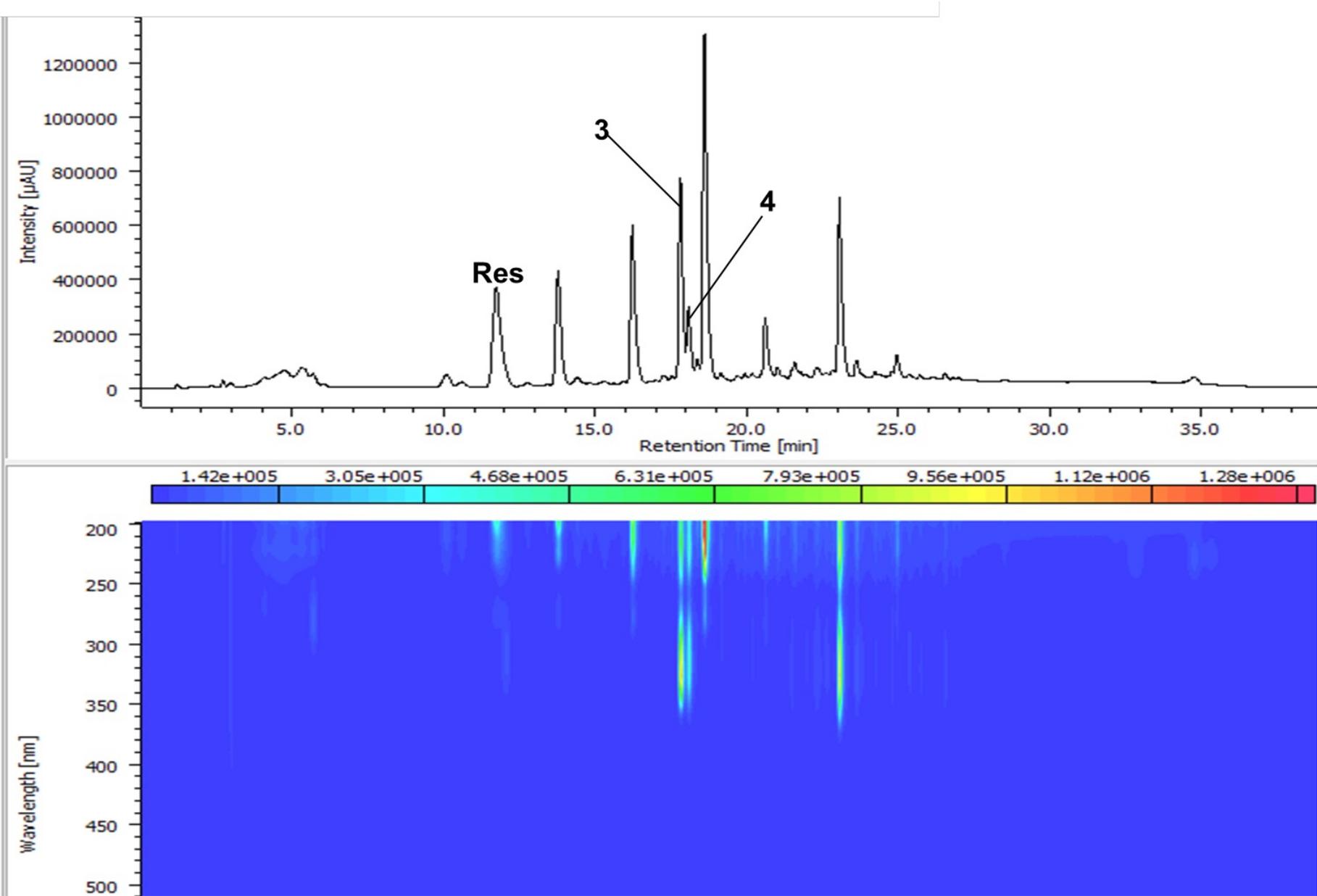


Figure S6. HPLC-PDA fingerprint of oxidized product mixture Ox6.

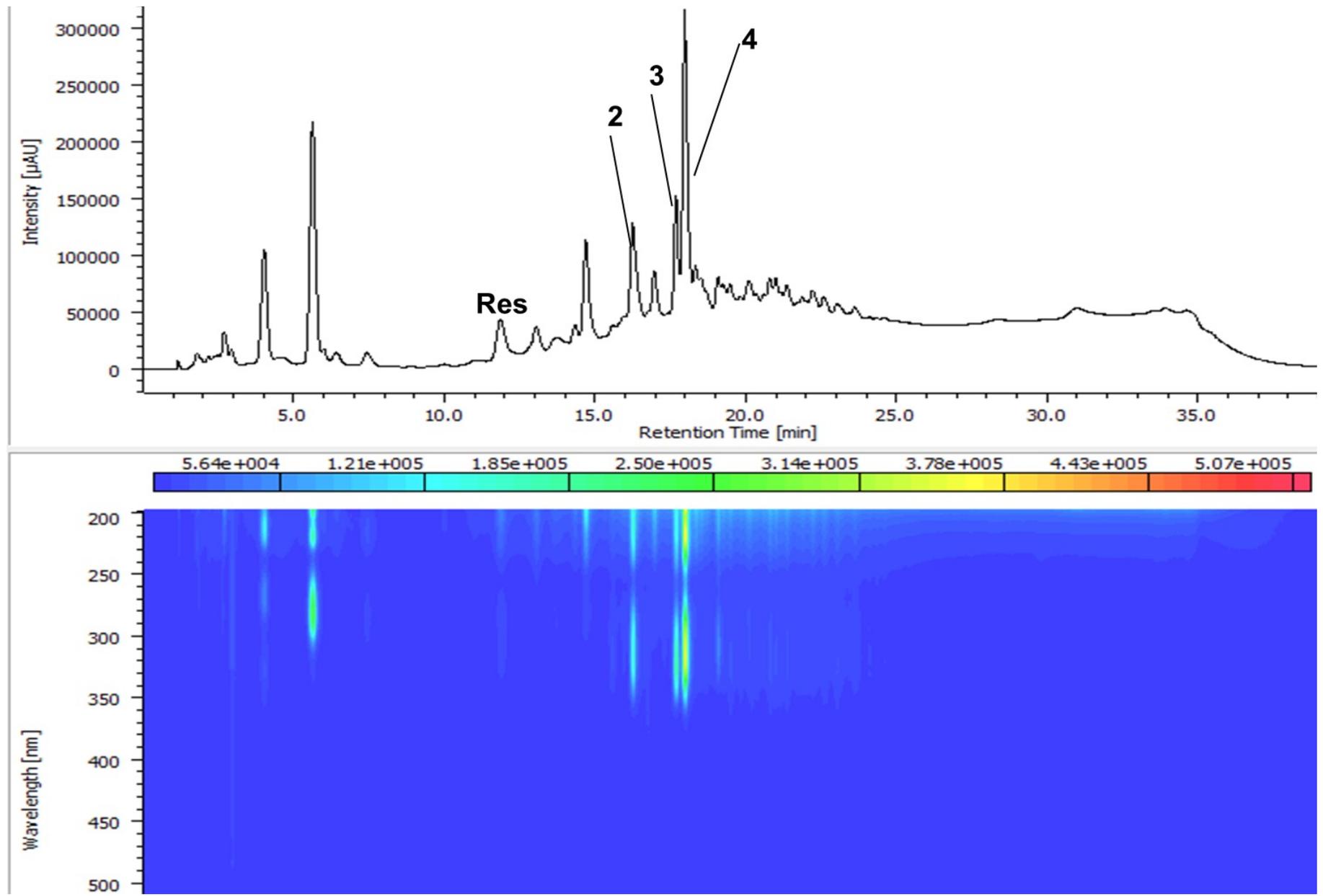


Figure S7. HPLC-PDA fingerprint of oxidized product mixture Ox7.

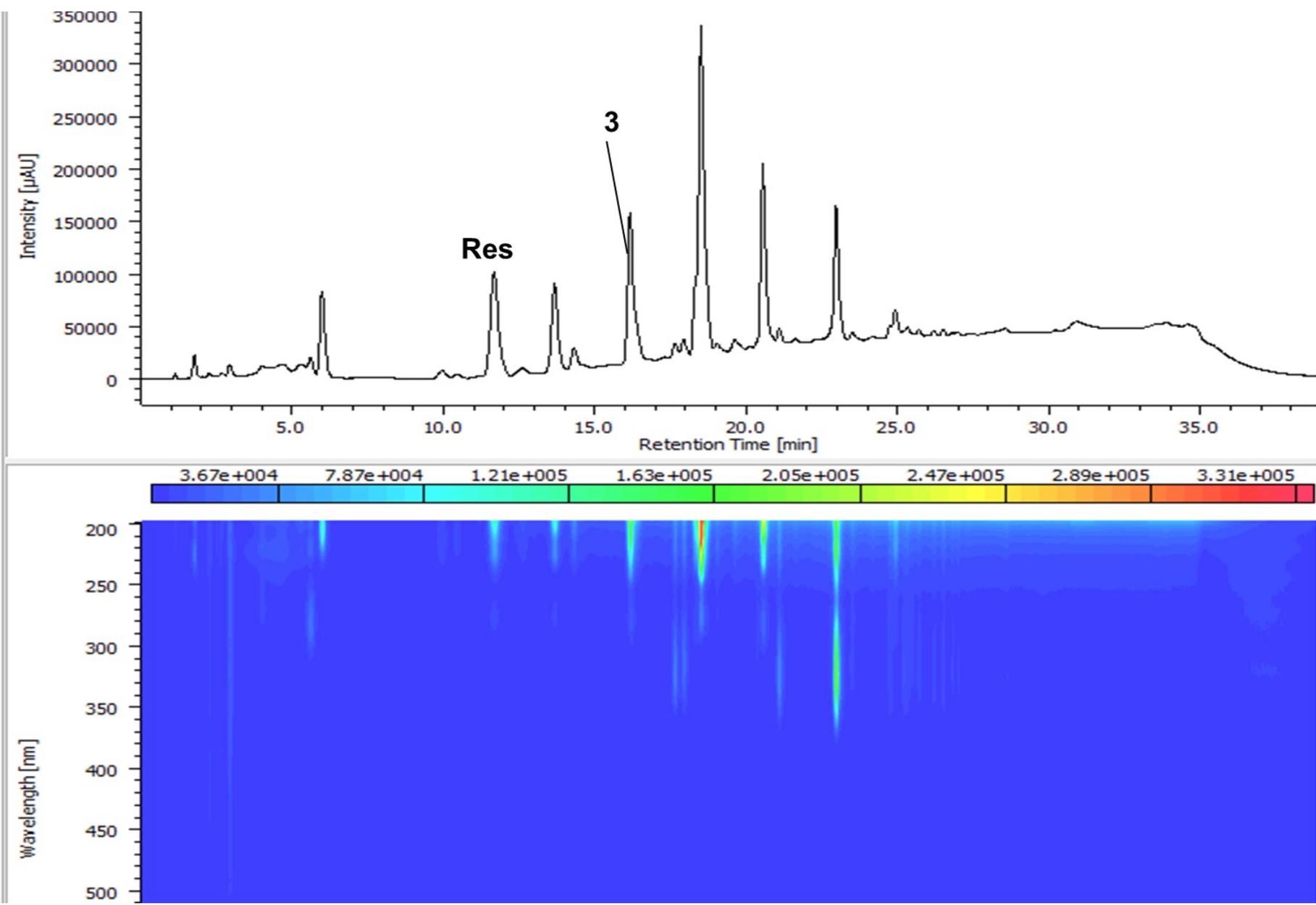
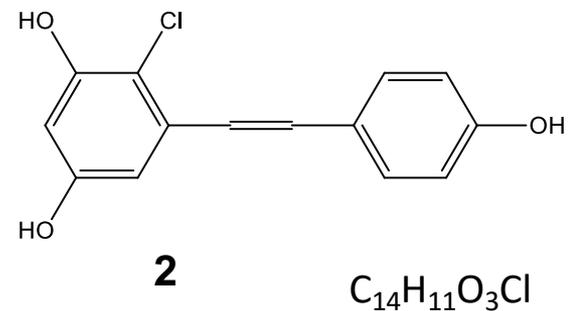
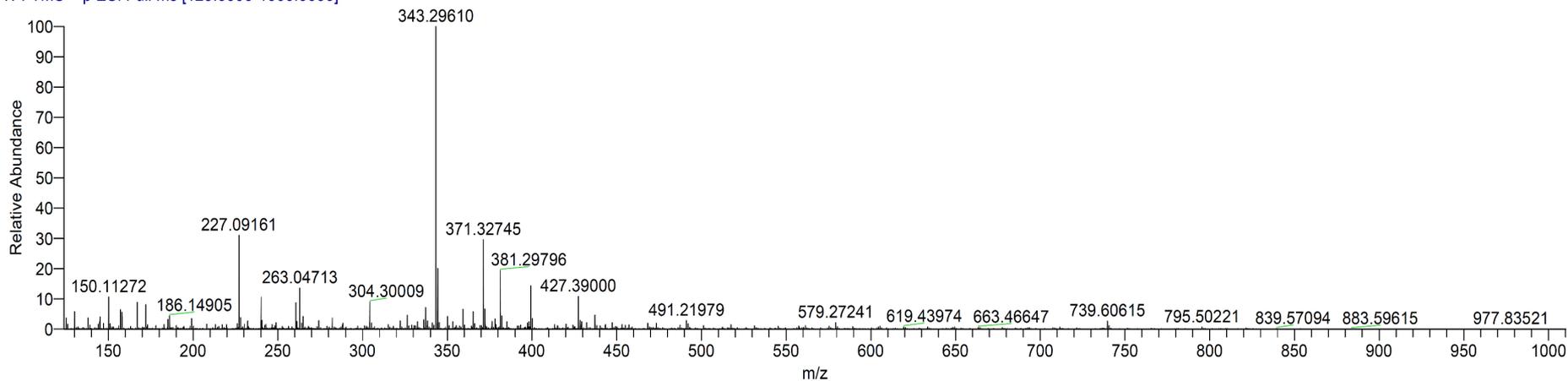


Figure S8. Compound **2**, HRMS (positive mode).



vm-20211012-pos-3 #2621-2637 RT: 14.00-14.08 AV: 17 NL: 6.21E7
T: FTMS + p ESI Full ms [125.0000-1000.0000]



vm-20211012-pos-3 #2621-2637 RT: 14.00-14.08 AV: 17 NL: 8.42E6
T: FTMS + p ESI Full ms [125.0000-1000.0000]

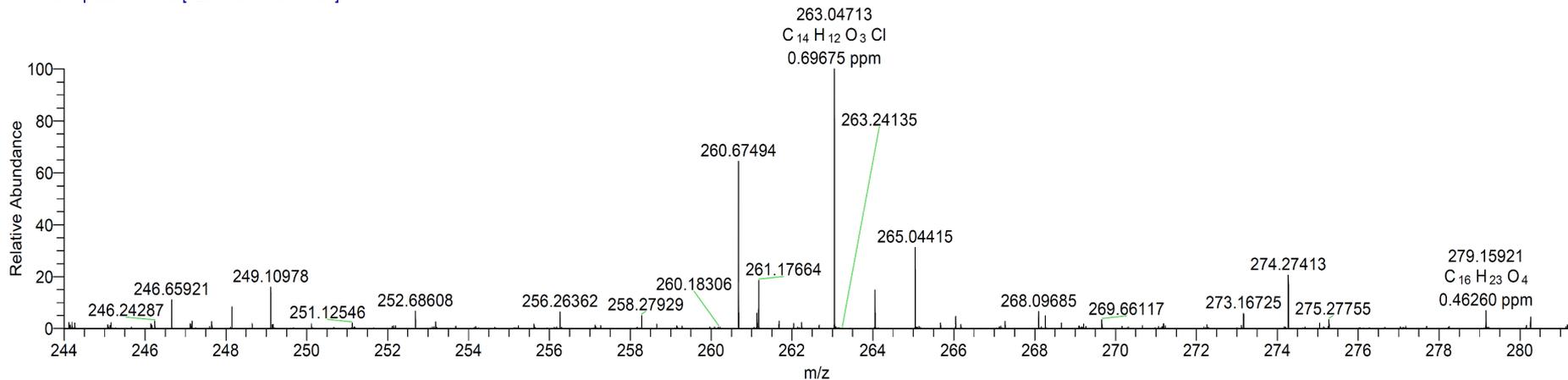
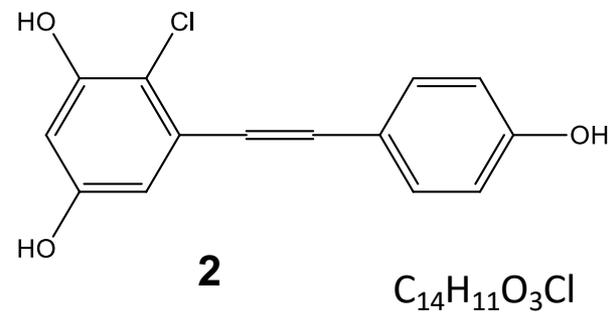
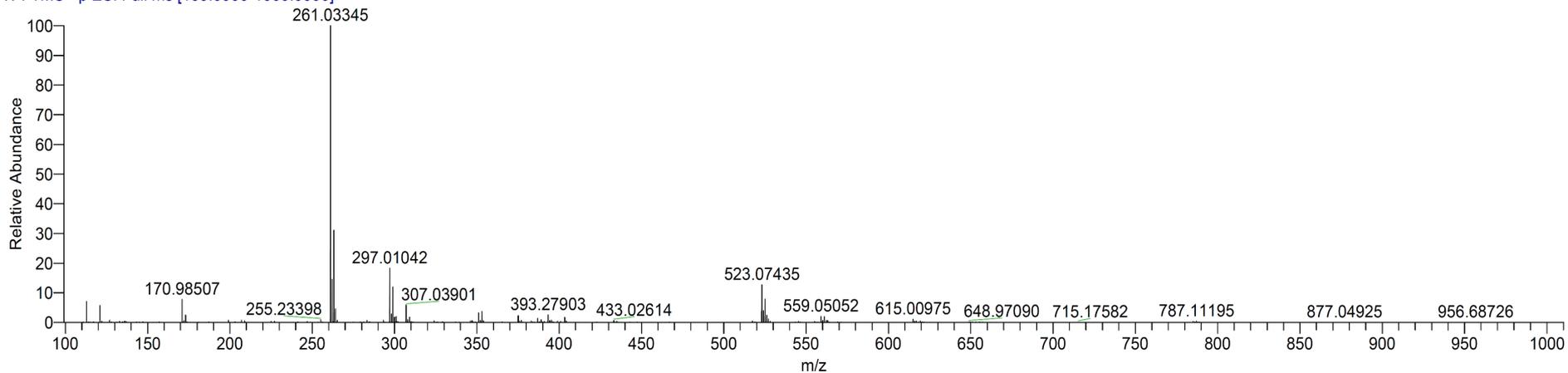


Figure S9. Compound **2**, HRMS (negative mode).



VM-20211012-NEG-2 #2438-2456 RT: 16.01-16.11 AV: 19 NL: 1.29E8
T: FTMS - p ESI Full ms [100.0000-1000.0000]



VM-20211012-NEG-2 #2438-2456 RT: 16.01-16.11 AV: 19 NL: 1.29E8
T: FTMS - p ESI Full ms [100.0000-1000.0000]

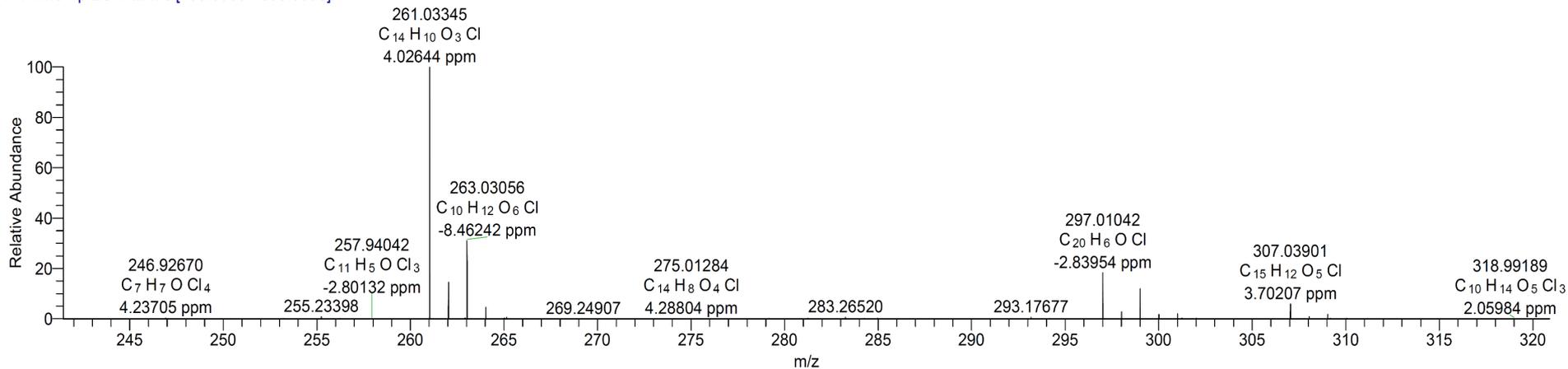


Figure S10. Compound **3**, HRMS (negative mode).

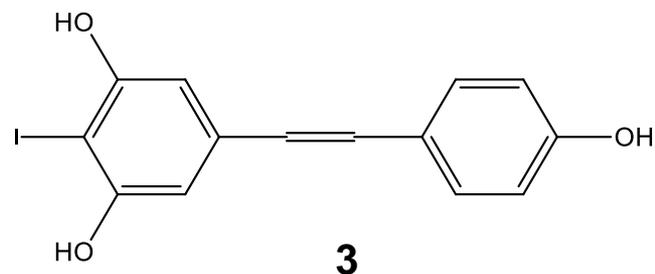
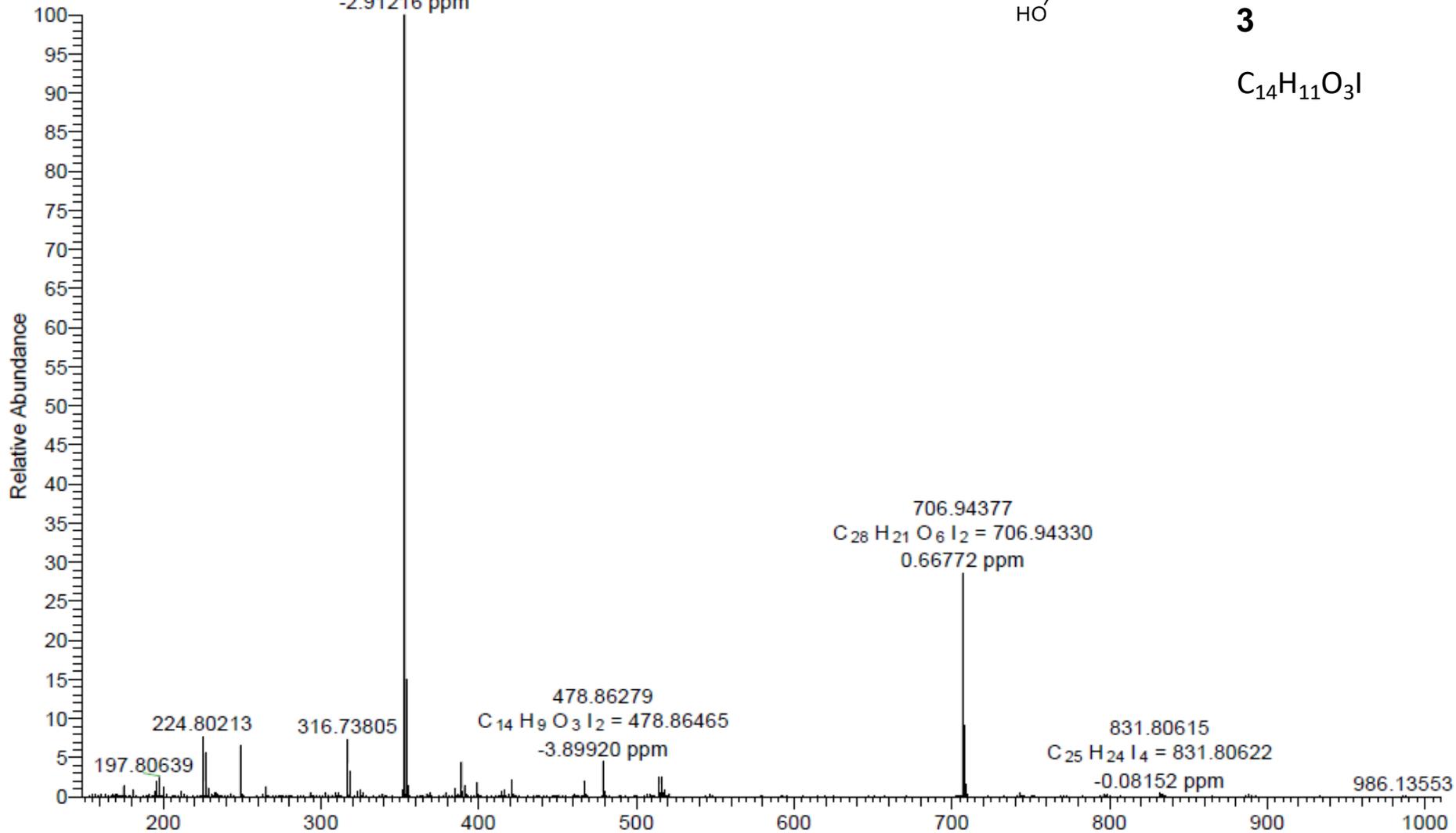
OA-220624-NEG #260-275 RT: 1.66-1.74 AV: 16 NL: 1.52E8

T: FTMS - p ESI Full ms [150.0000-1000.0000]

352.96698 [M-H]⁻

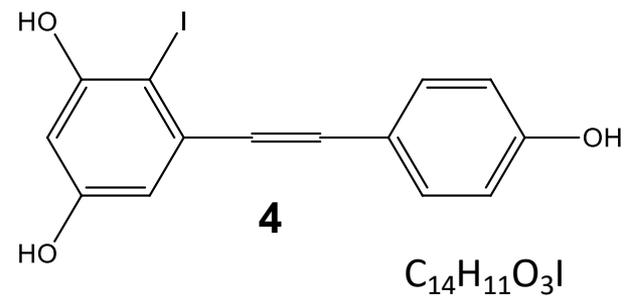
C₁₄H₁₀O₃I = 352.96801

-2.91216 ppm



C₁₄H₁₁O₃I

Figure S11. Compound **4**, HRMS (positive mode).



oa-20200930 #2070-2094 RT: 11.82-11.95 AV: 25 NL: 1.46E7
T: FTMS + p ESI Full lock ms [100.0000-1000.0000]

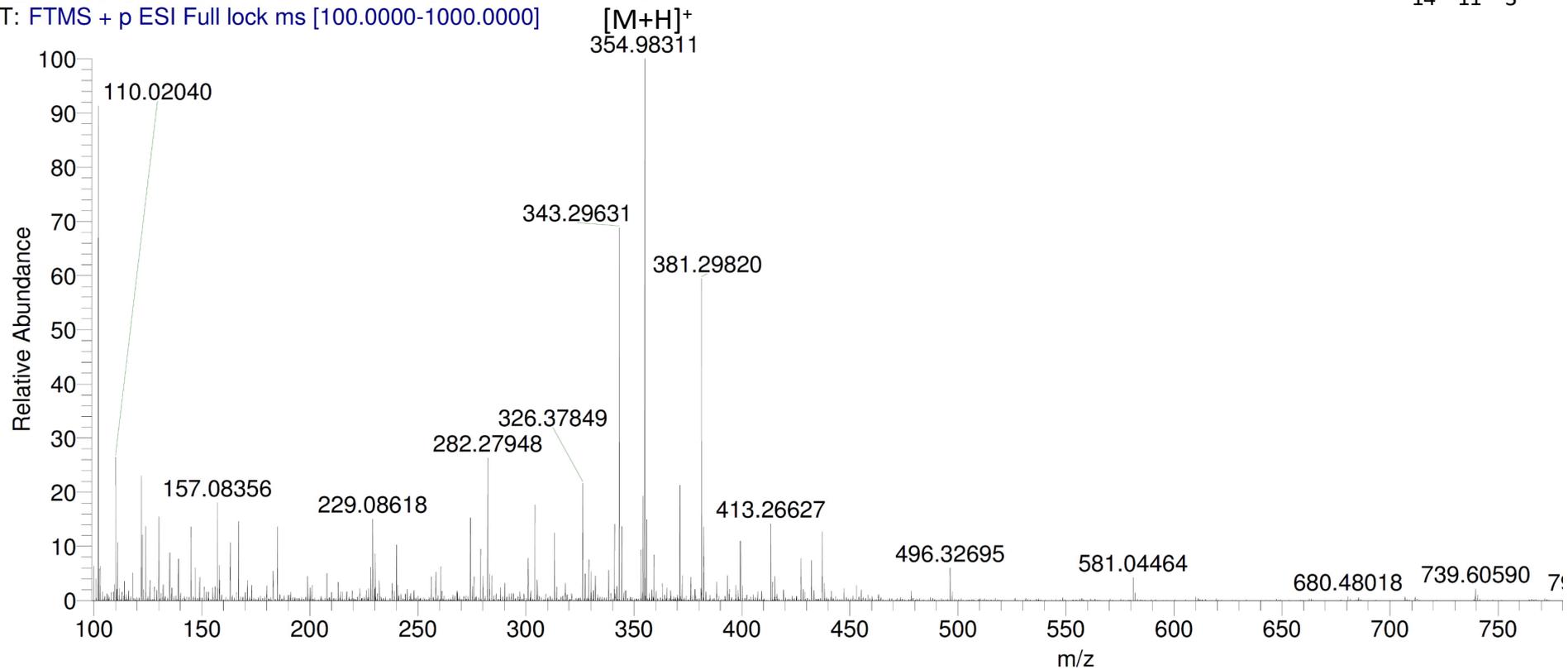
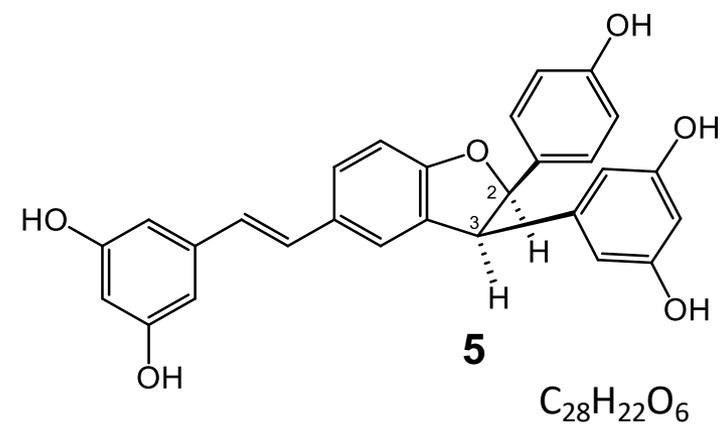


Figure S12. Compound **5**, HRMS (positive mode).



oa-20200930 #1405-1427 RT: 7.97-8.09 AV: 23 NL: 1.89E7
T: FTMS + p ESI Full lock ms [100.0000-1000.0000]

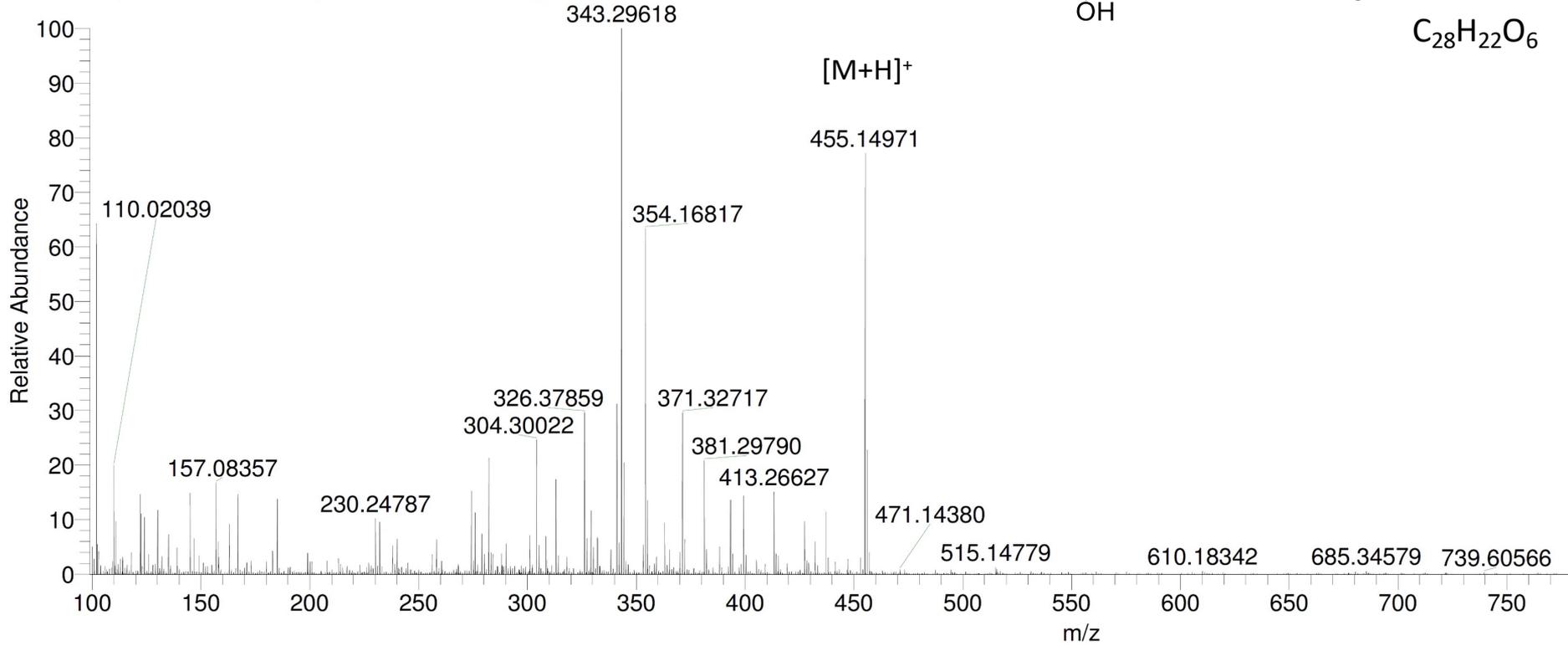


Figure S13. Compound **6**, HRMS (positive mode).

OA201027-pos #249-259 RT: 2.48-2.58 AV: 11 NL: 3.48E7
T: FTMS + p ESI Full lock ms [100.0000-1000.0000]

[M+H]⁺

455.14957

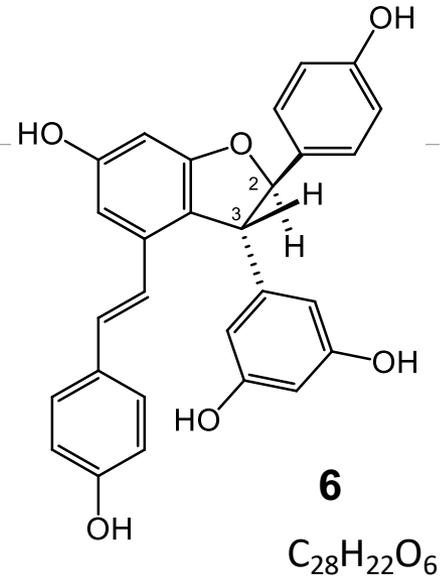
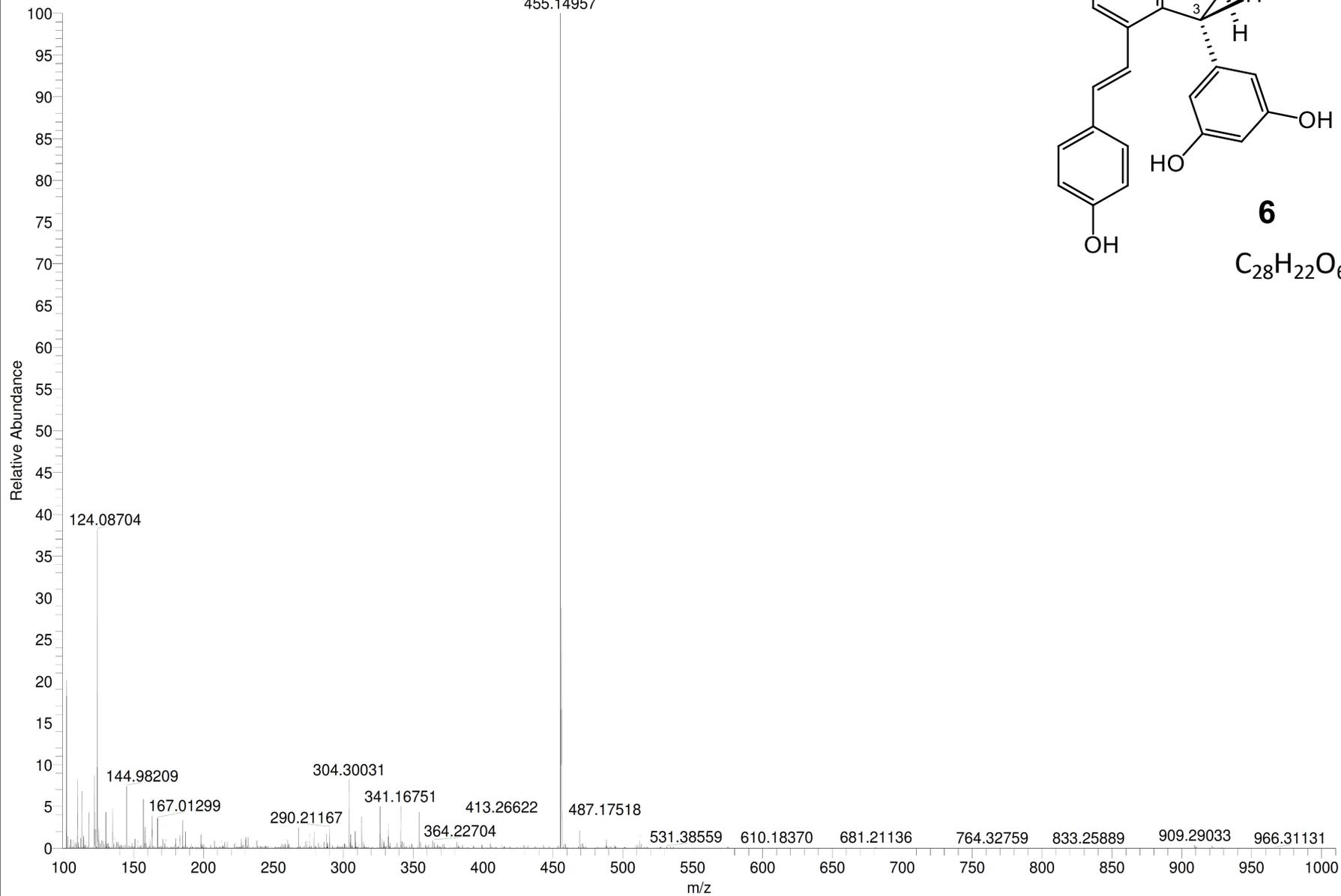
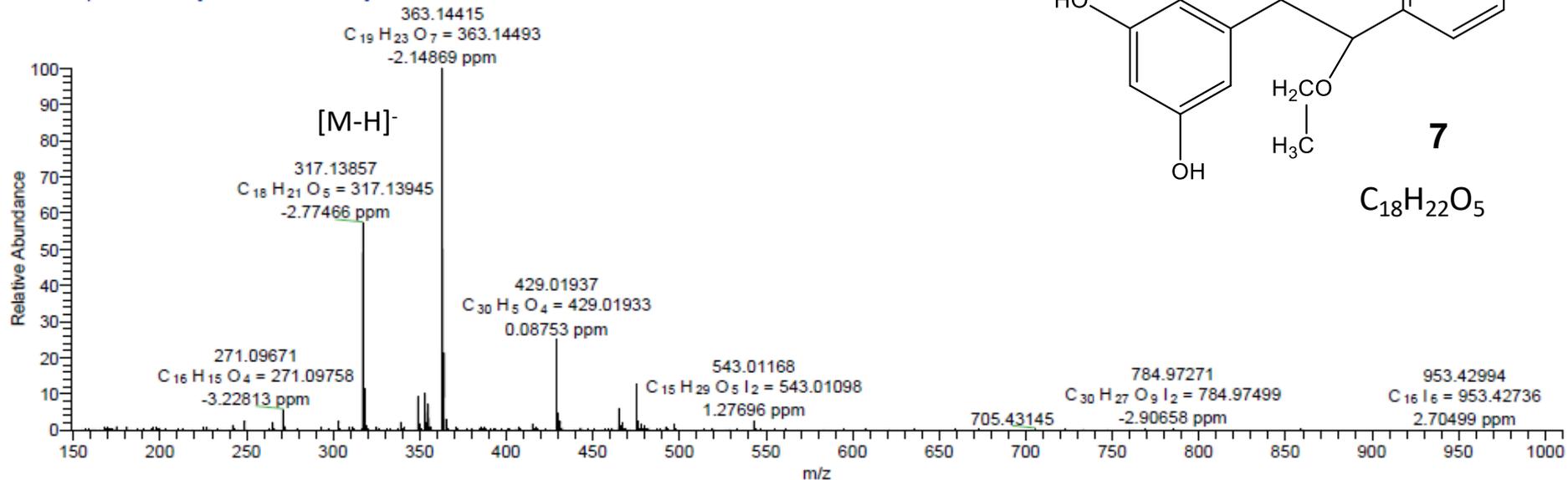
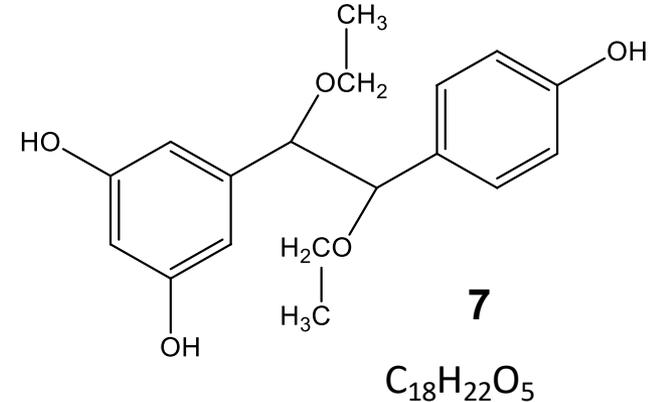


Figure S14. Compound **7**, HRMS (negative mode).

OA-220624-NEG #387-410 RT: 2.45-2.57 AV: 24 NL: 1.74E8
T: FTMS - p ESI Full ms [150.0000-1000.0000]



OA-220624-NEG #387-410 RT: 2.45-2.57 AV: 24 NL: 1.74E8
T: FTMS - p ESI Full ms [150.0000-1000.0000]

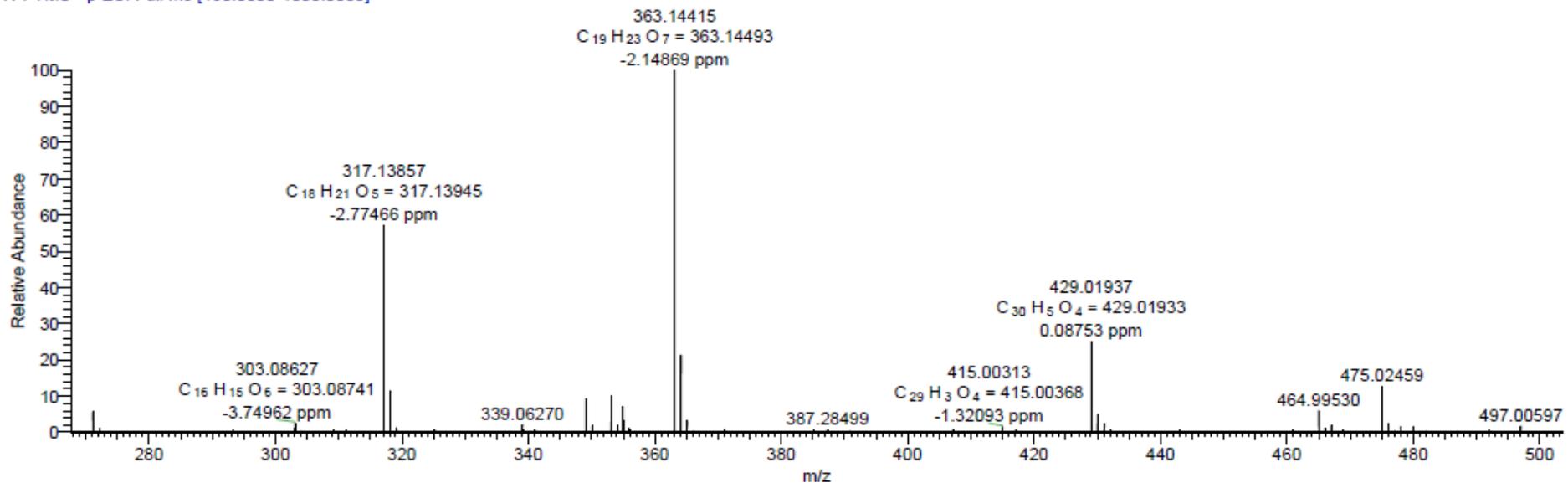
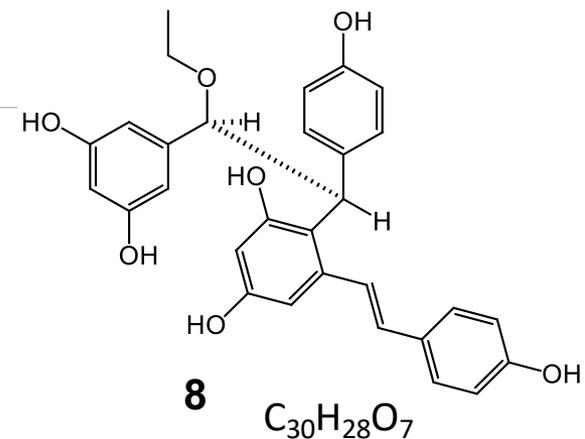
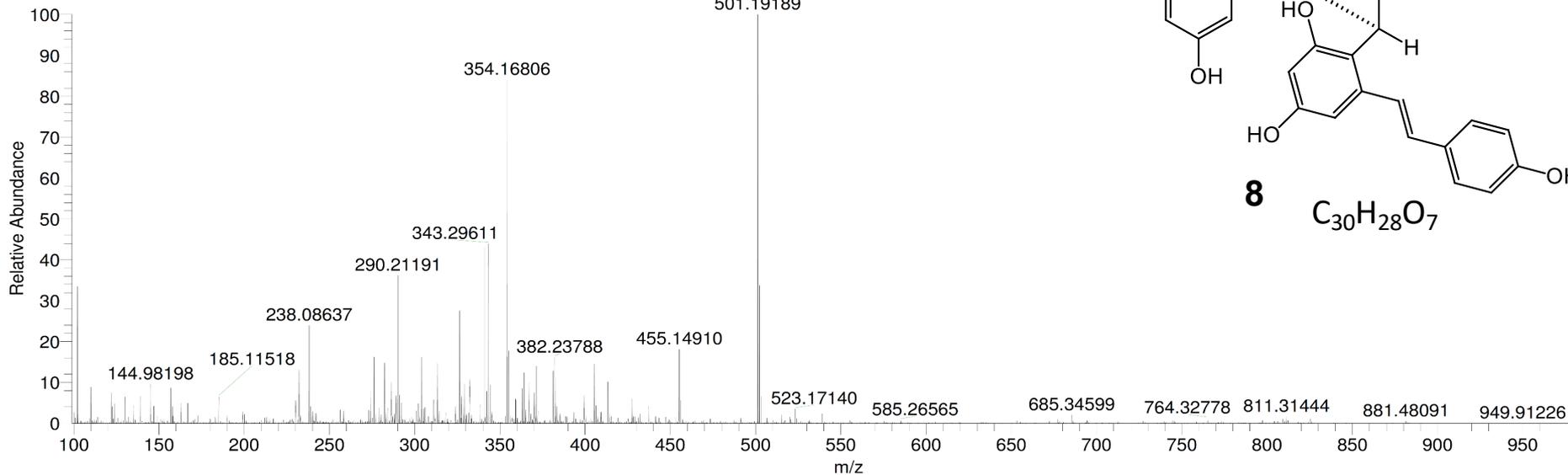


Figure S15. Compound 8, HRMS (positive mode).

oa-20200930 #742-760 RT: 4.17-4.26 AV: 19 NL: 3.14E7
T: FTMS + p ESI Full lock ms [100.0000-1000.0000]



oa-20200930 #742-760 RT: 4.17-4.26 AV: 19 NL: 3.14E7
T: FTMS + p ESI Full lock ms [100.0000-1000.0000]

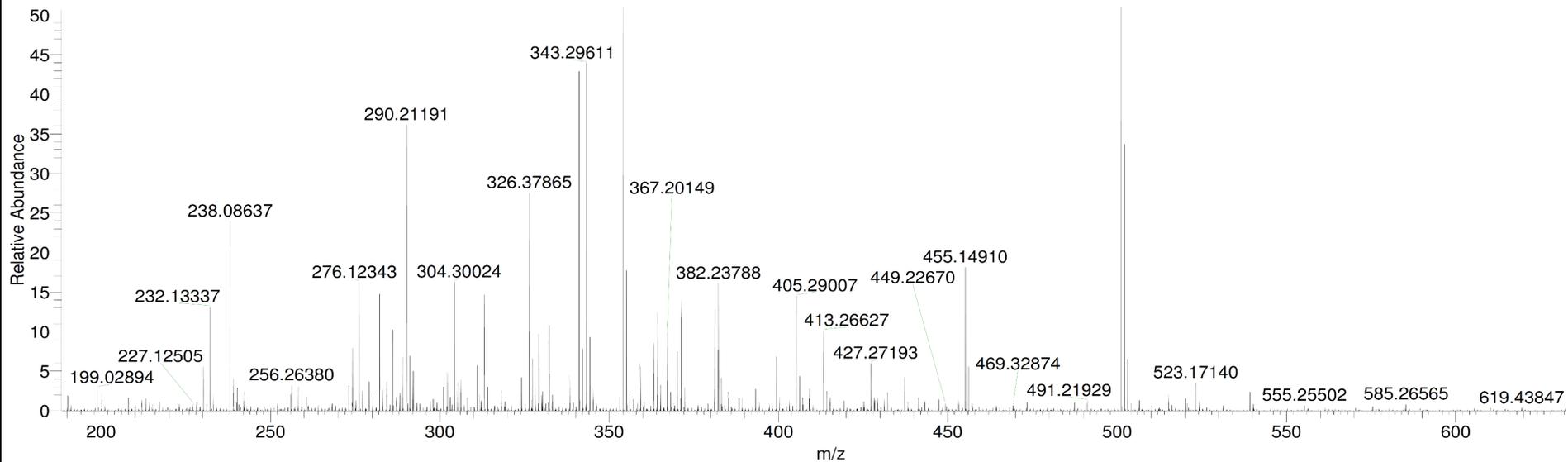


Figure S16. Compound 2, ^1H NMR spectrum.

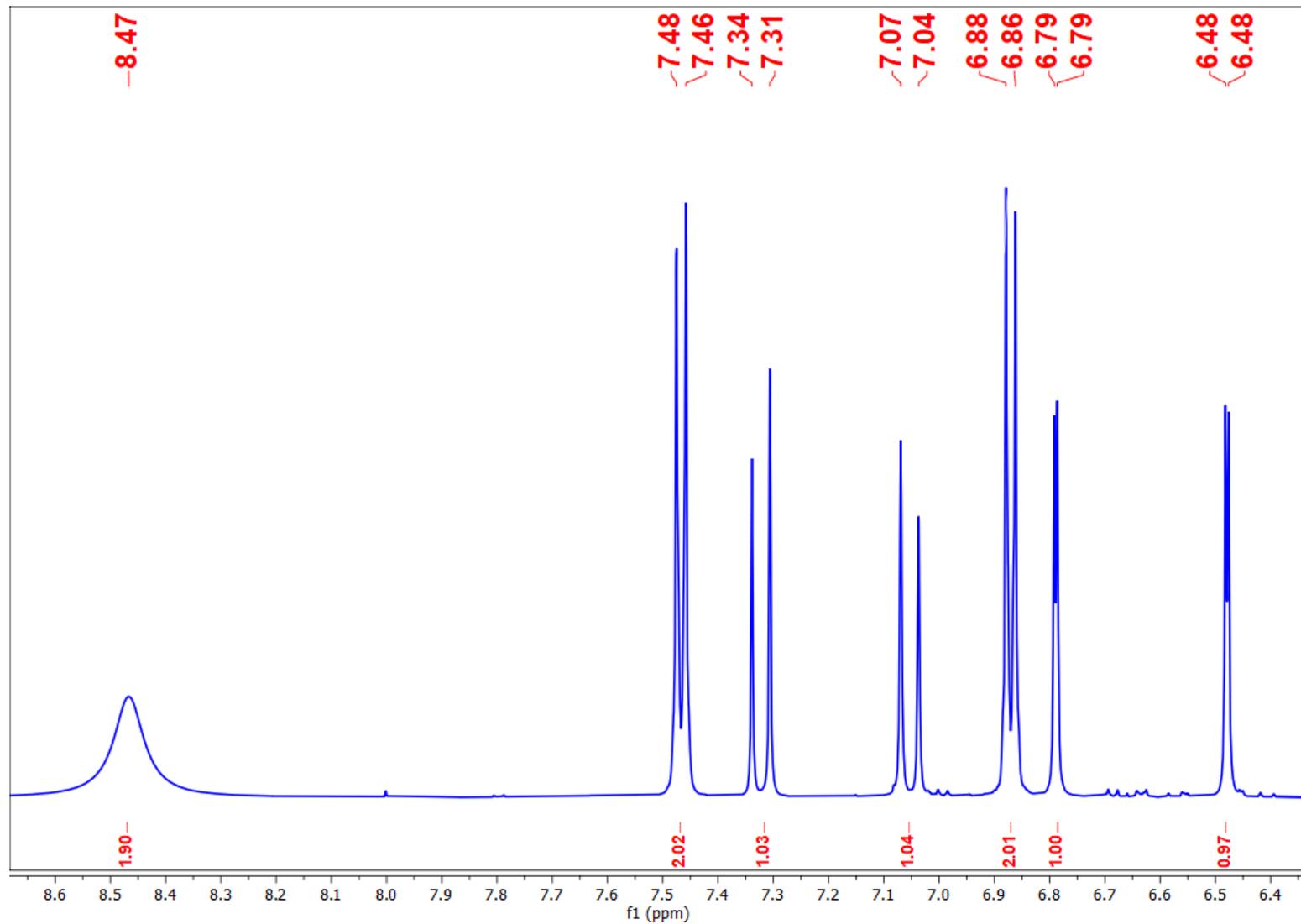
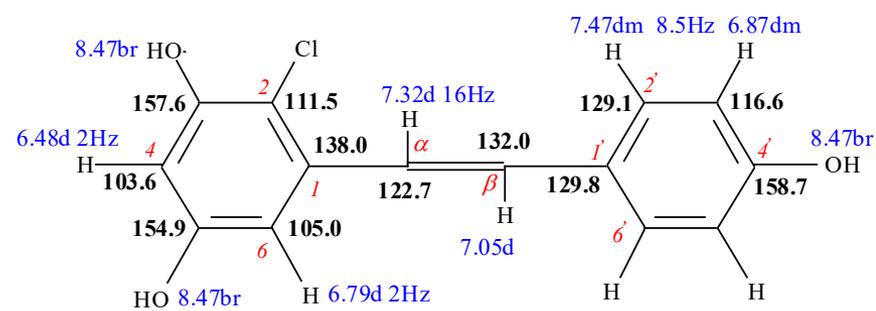


Figure S17. Compound 2, ^{13}C , APT NMR spectrum

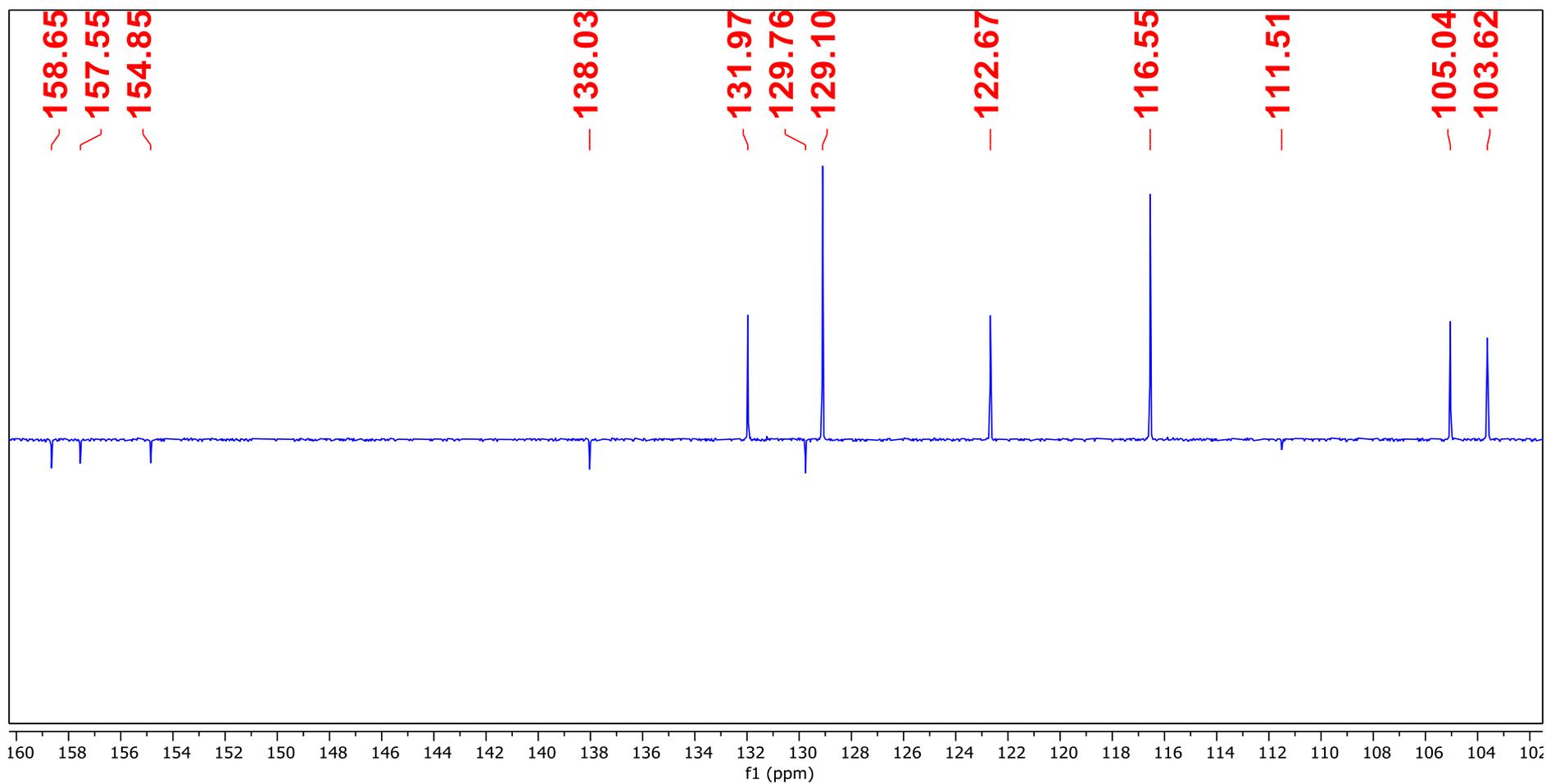
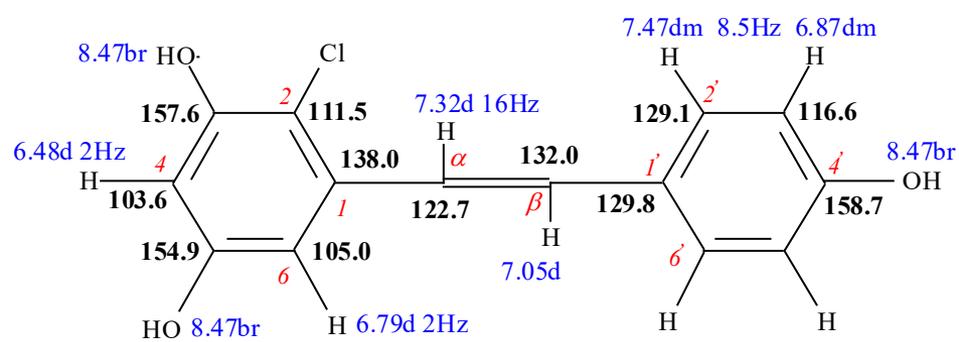


Figure S18. Compound 2, HSQC and HMBC spectra.

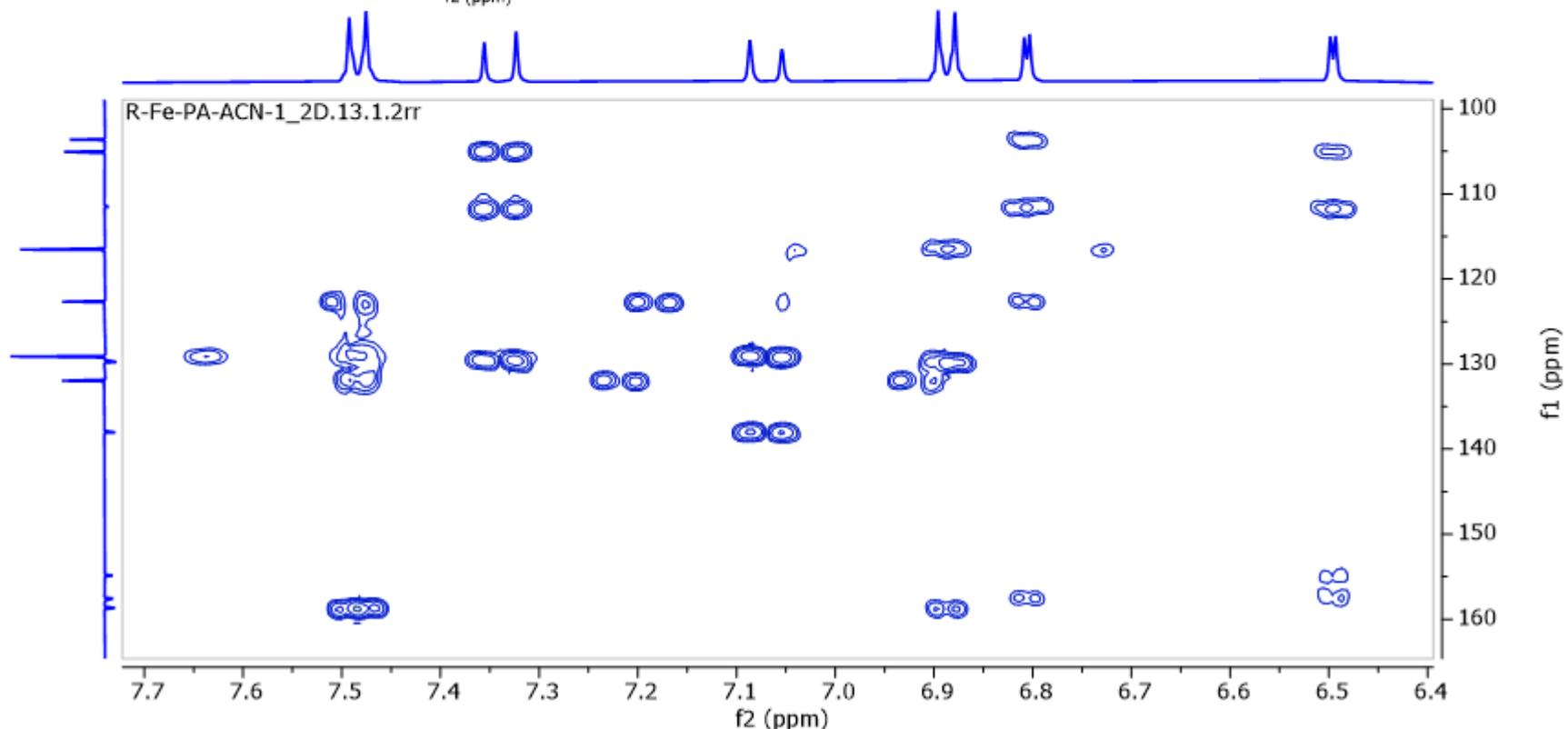
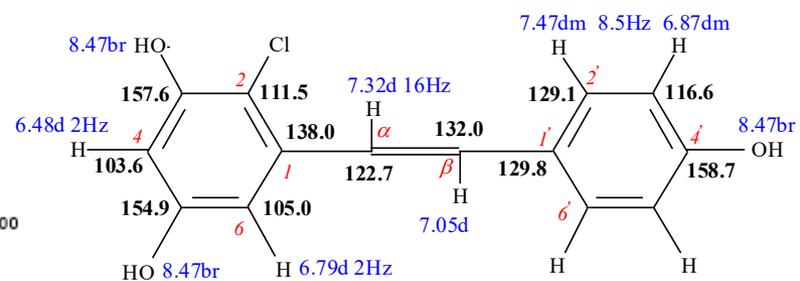
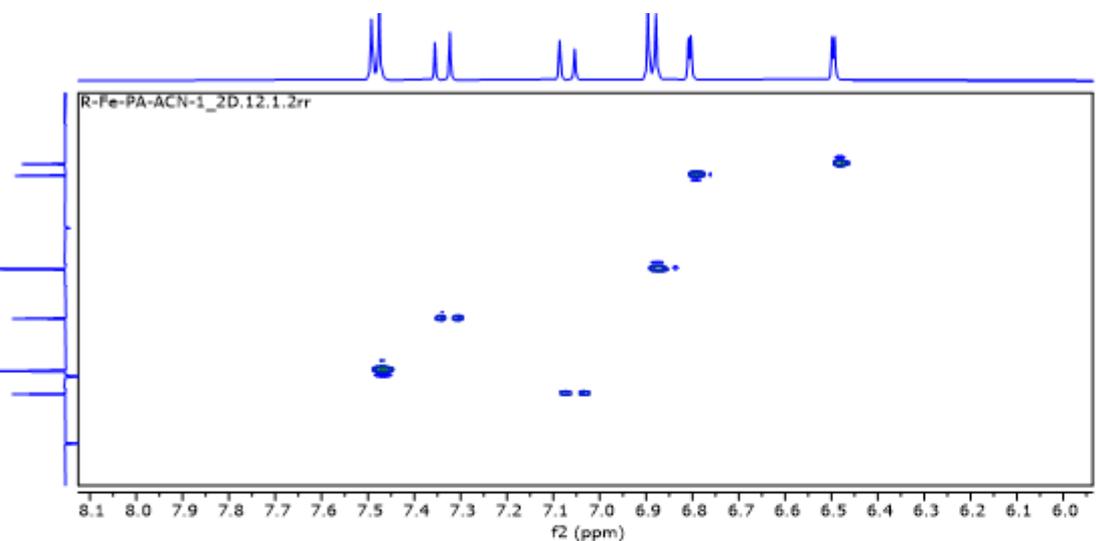


Figure S20. Compound **3**, ^1H NMR spectrum.

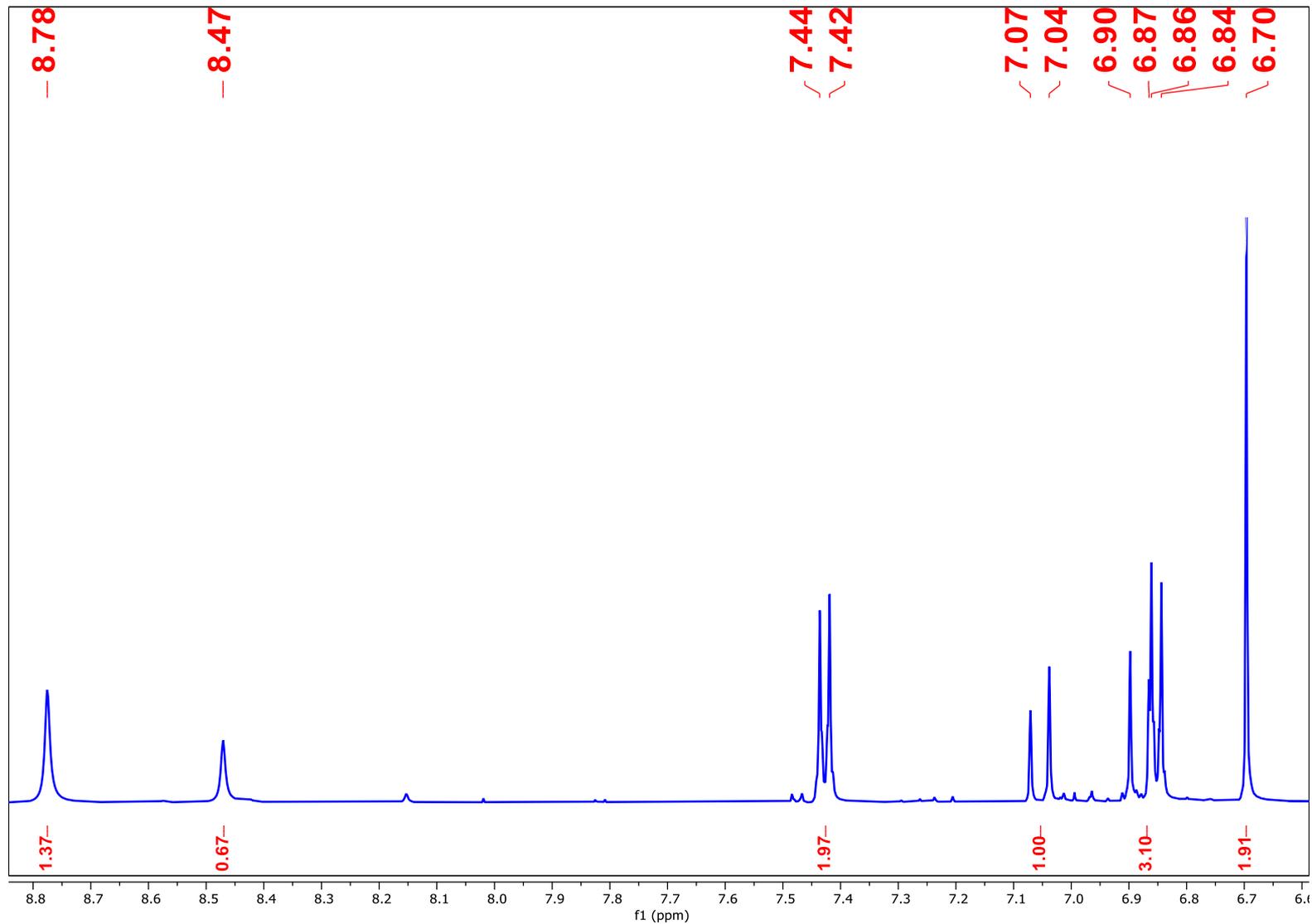
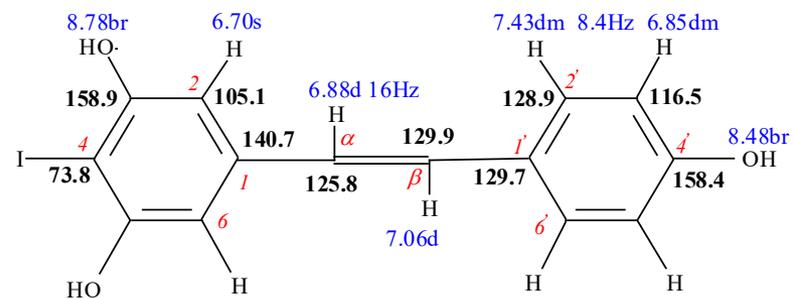


Figure S21. Compound **3**, ^{13}C , APT NMR spectrum.

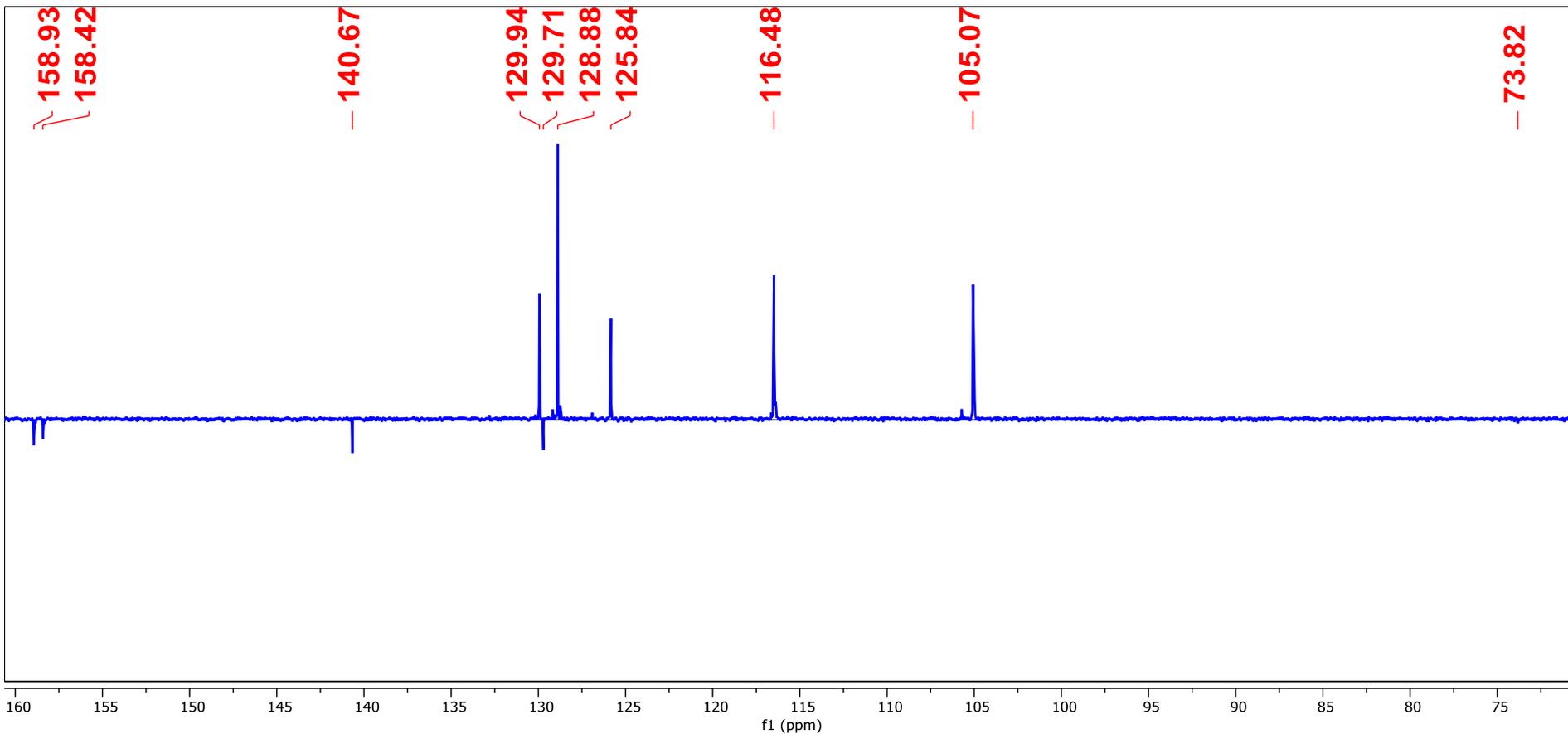
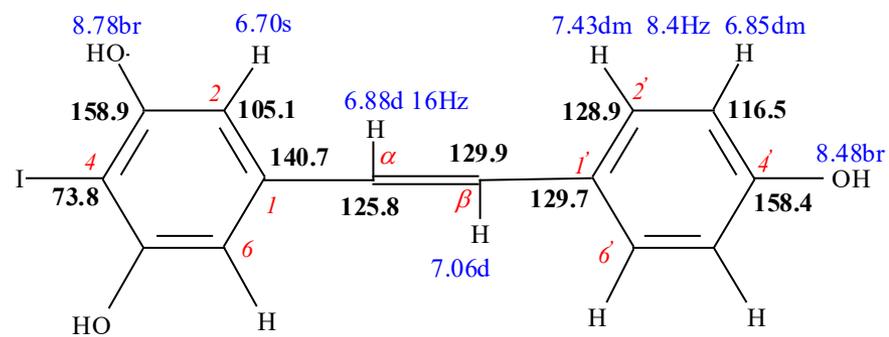


Figure S22. Compound **3**, HSQC and HMBCC spectra.

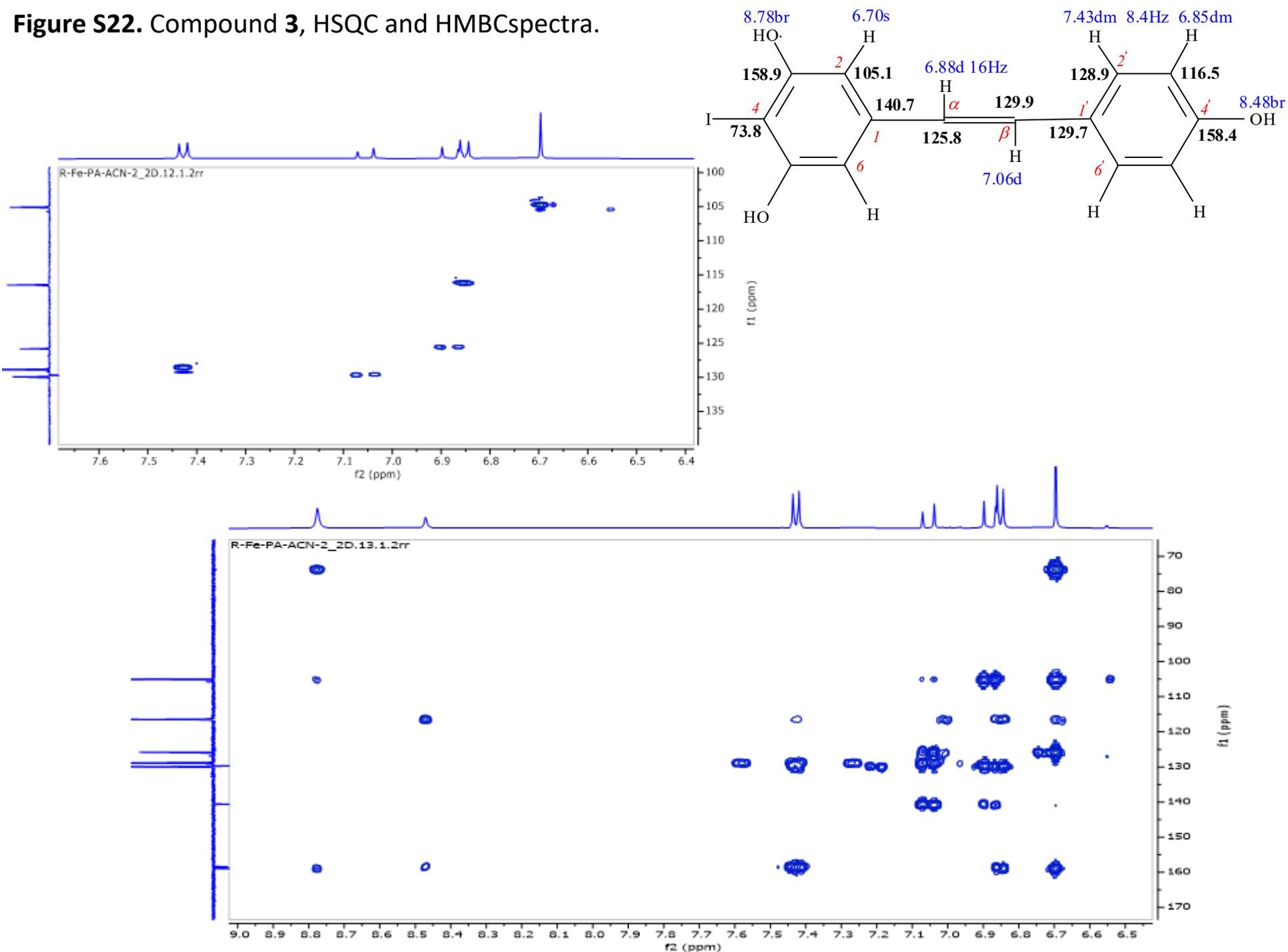


Figure S24. Compound **4**, ^1H NMR spectrum.

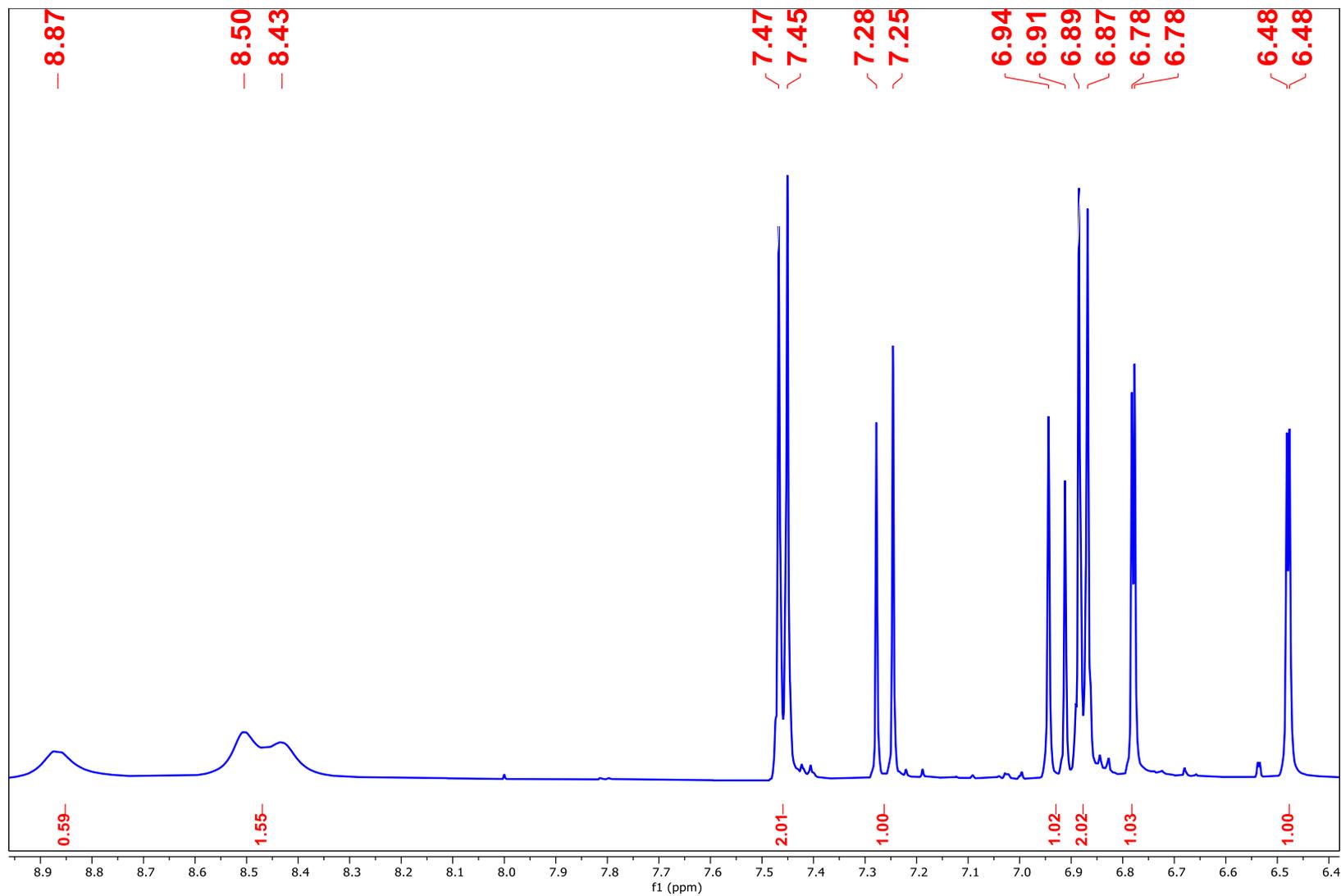
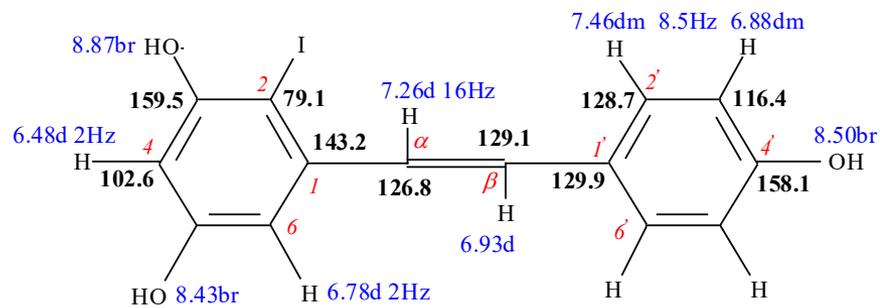


Figure S25. Compound 4, ^{13}C , APT NMR spectrum.

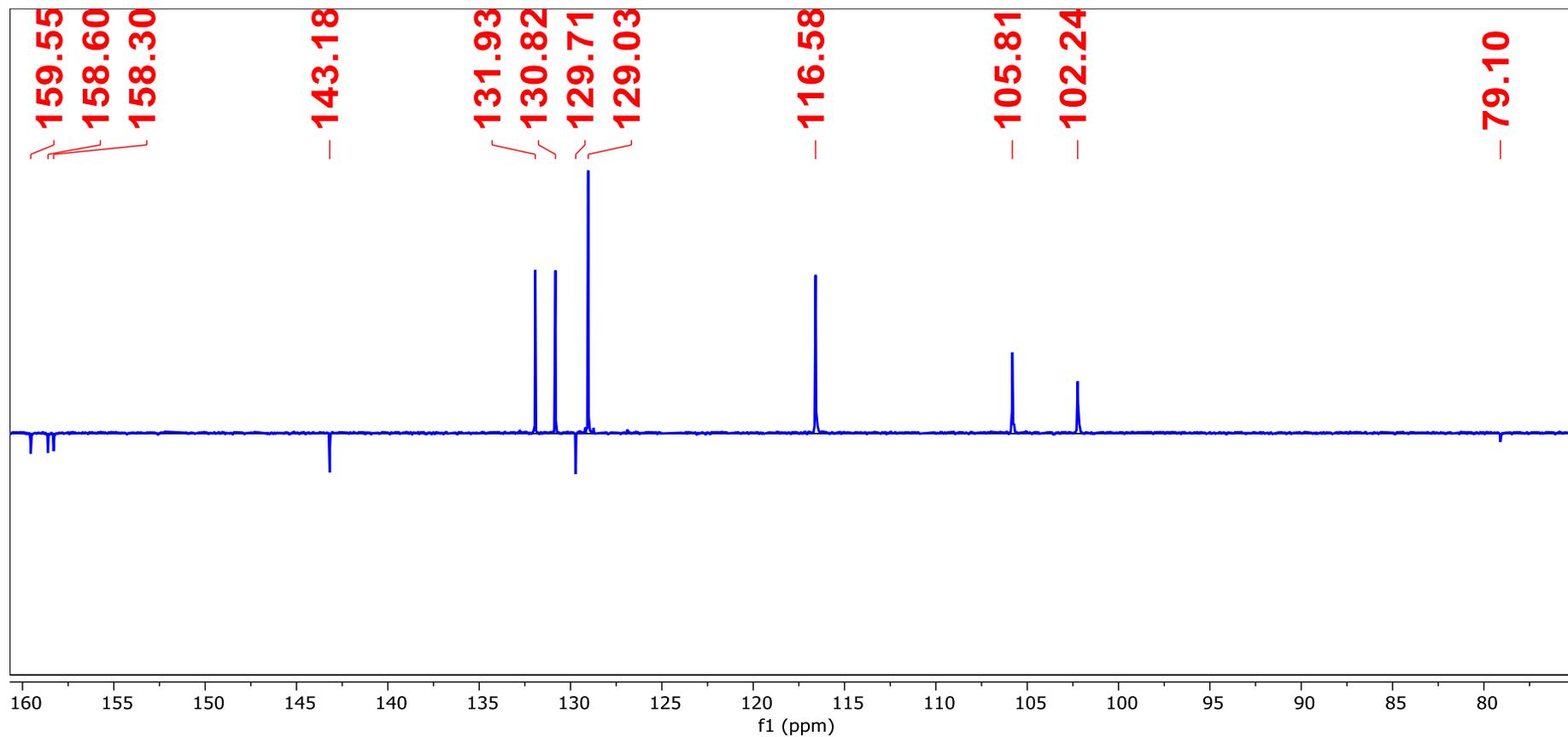
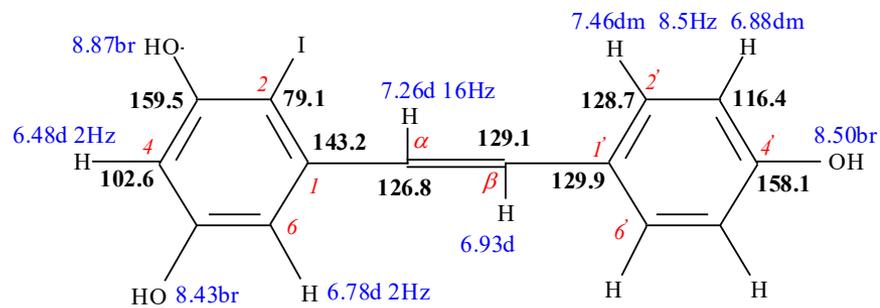


Figure S26. Compound **4**, HSQC and HMBC spectra.

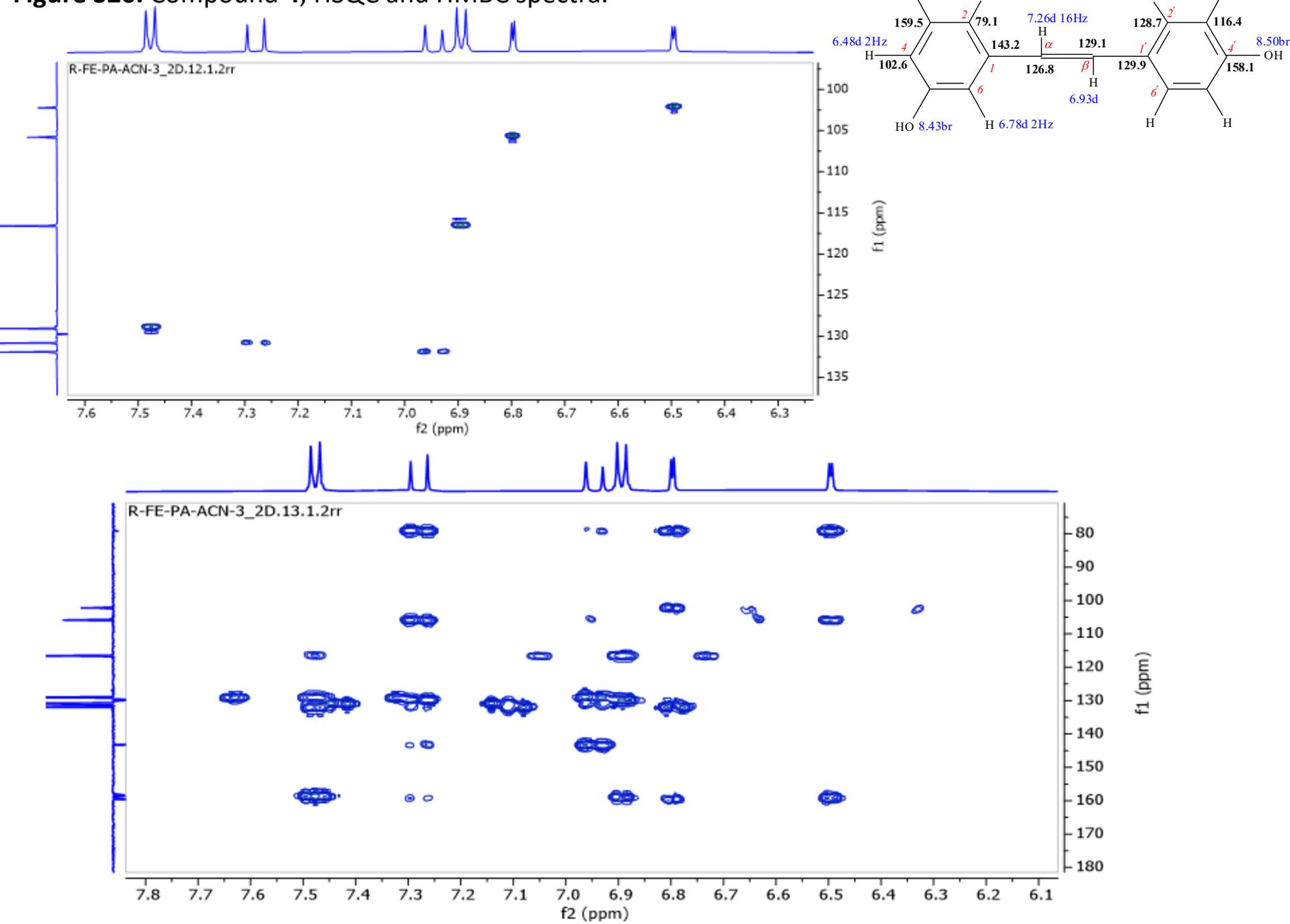


Figure S27. Compound 4, COSY spectrum.

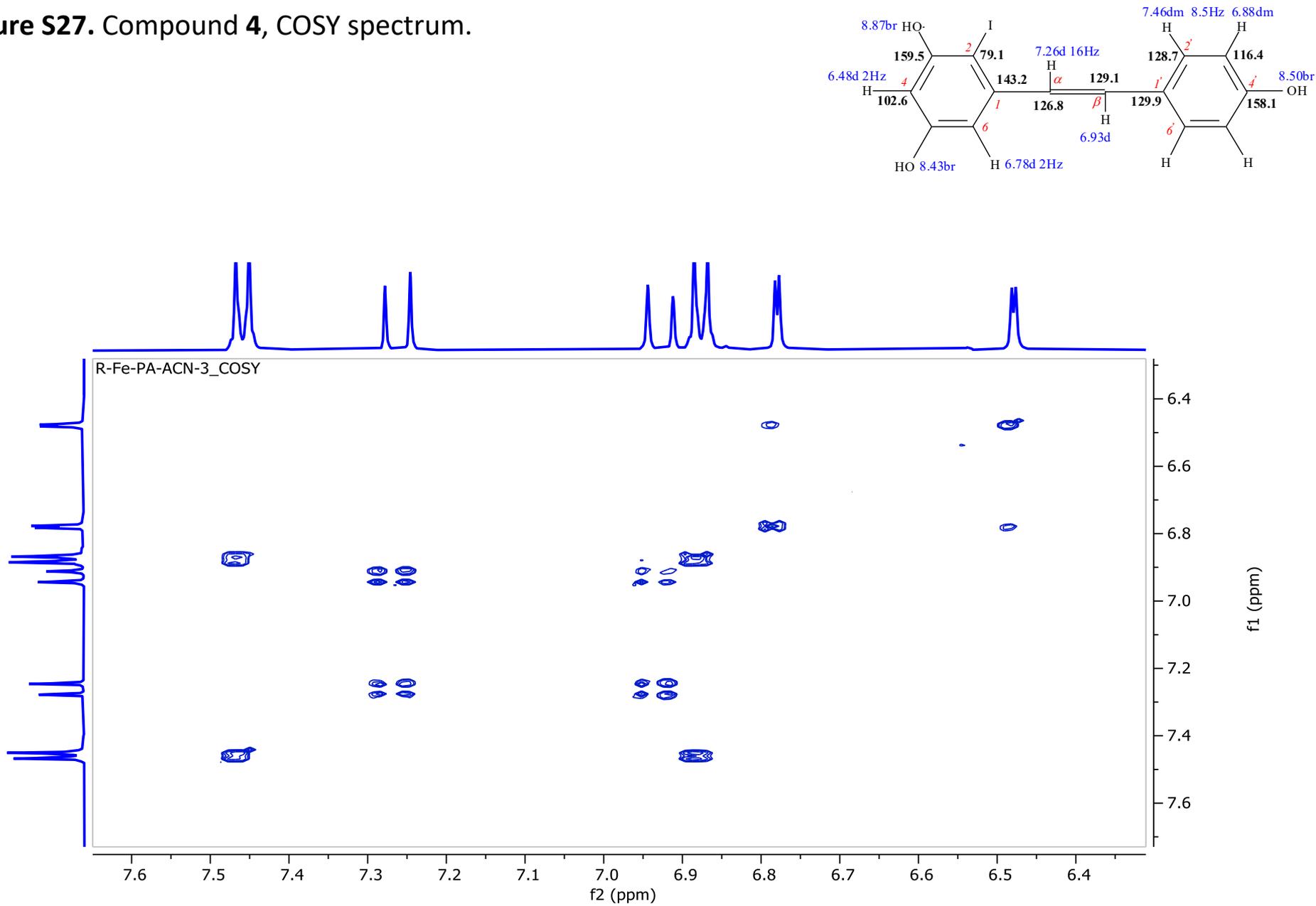


Figure S28. Compound **5**, ^1H NMR spectrum, and selROE on δ 4.47 and δ 5.45 ppm.

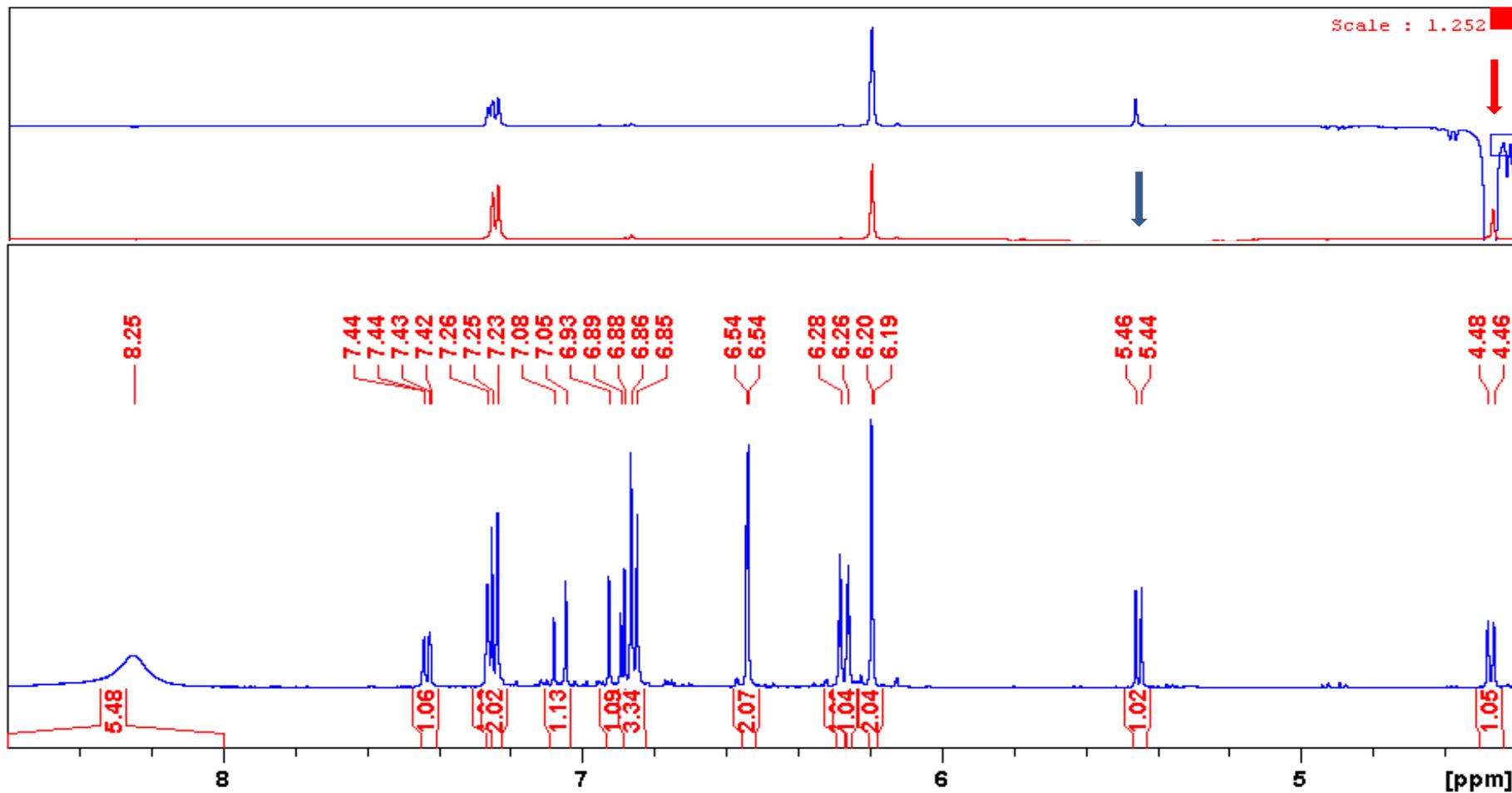
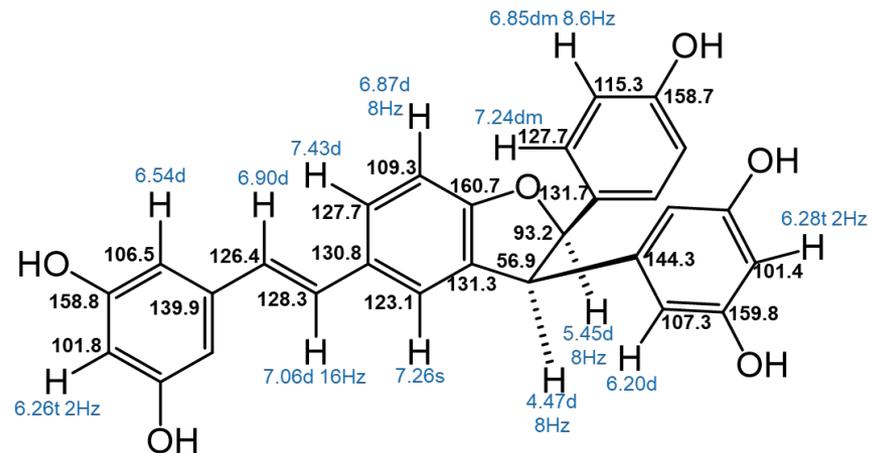


Figure S31. Compound 5, COSY spectrum.

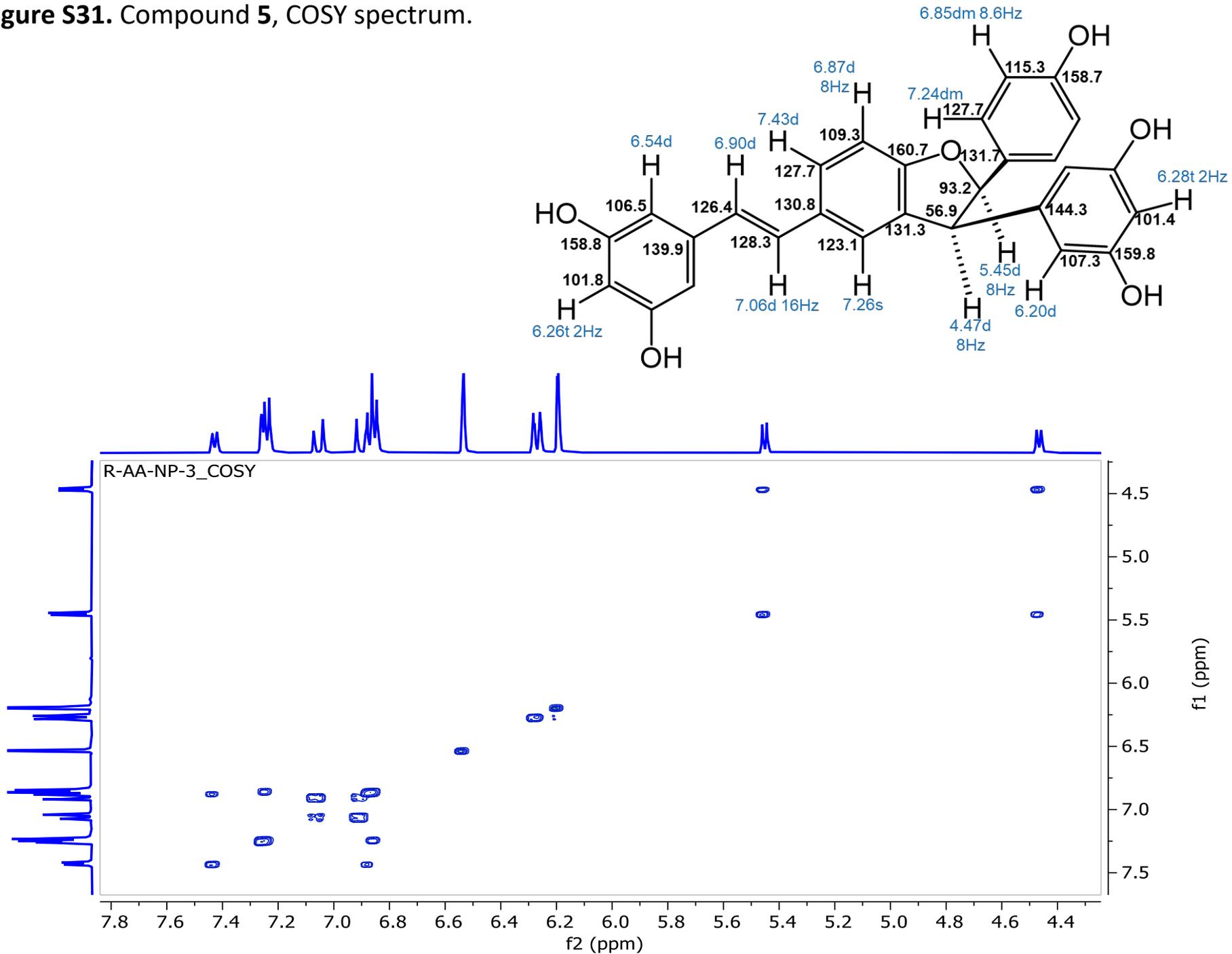


Figure S33. Compound 6, ¹H, selNOE on δ4.48 and δ5.42 ppm.

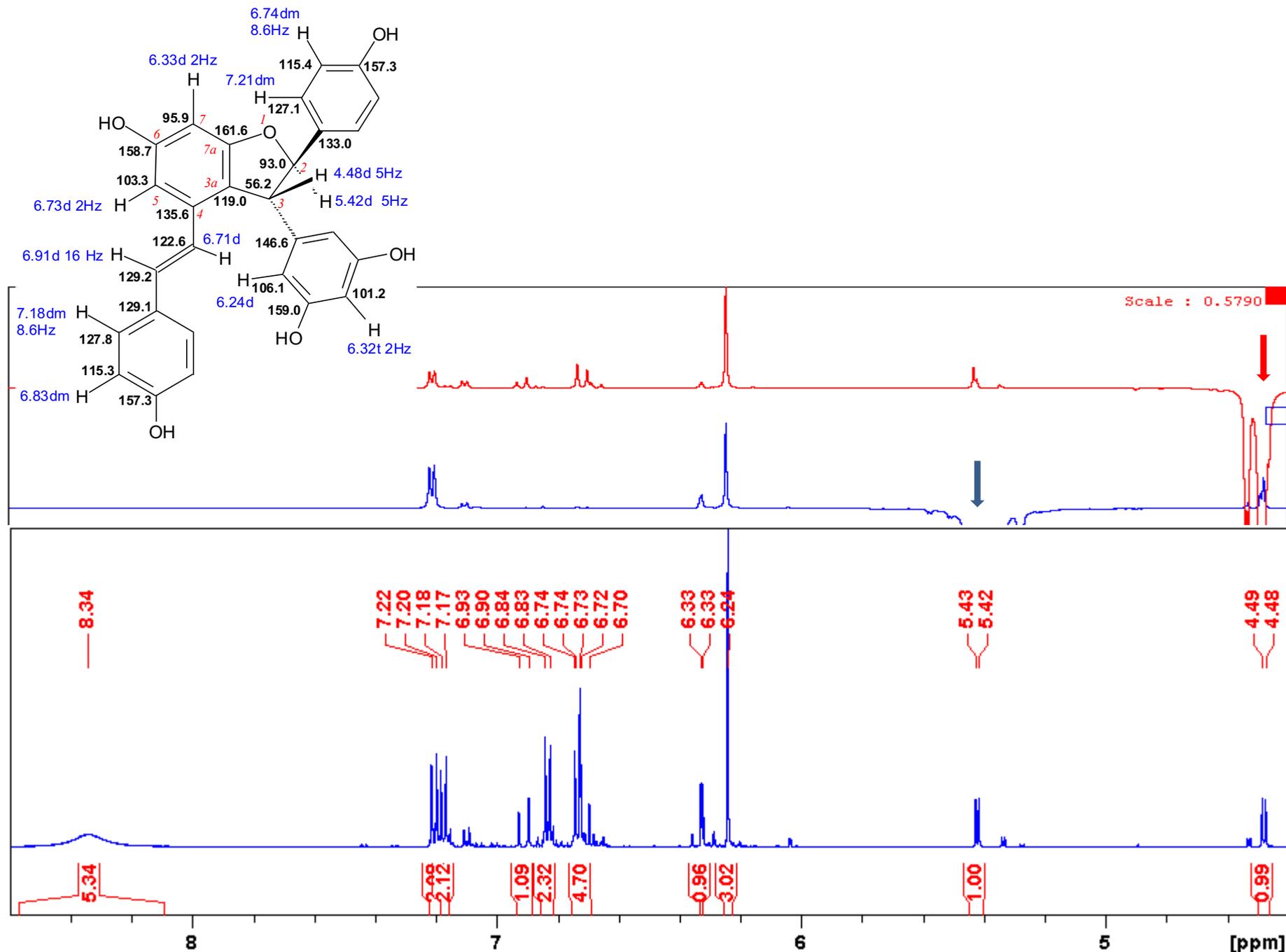


Figure S34. Compound 6, ^{13}C , APT NMR spectrum.

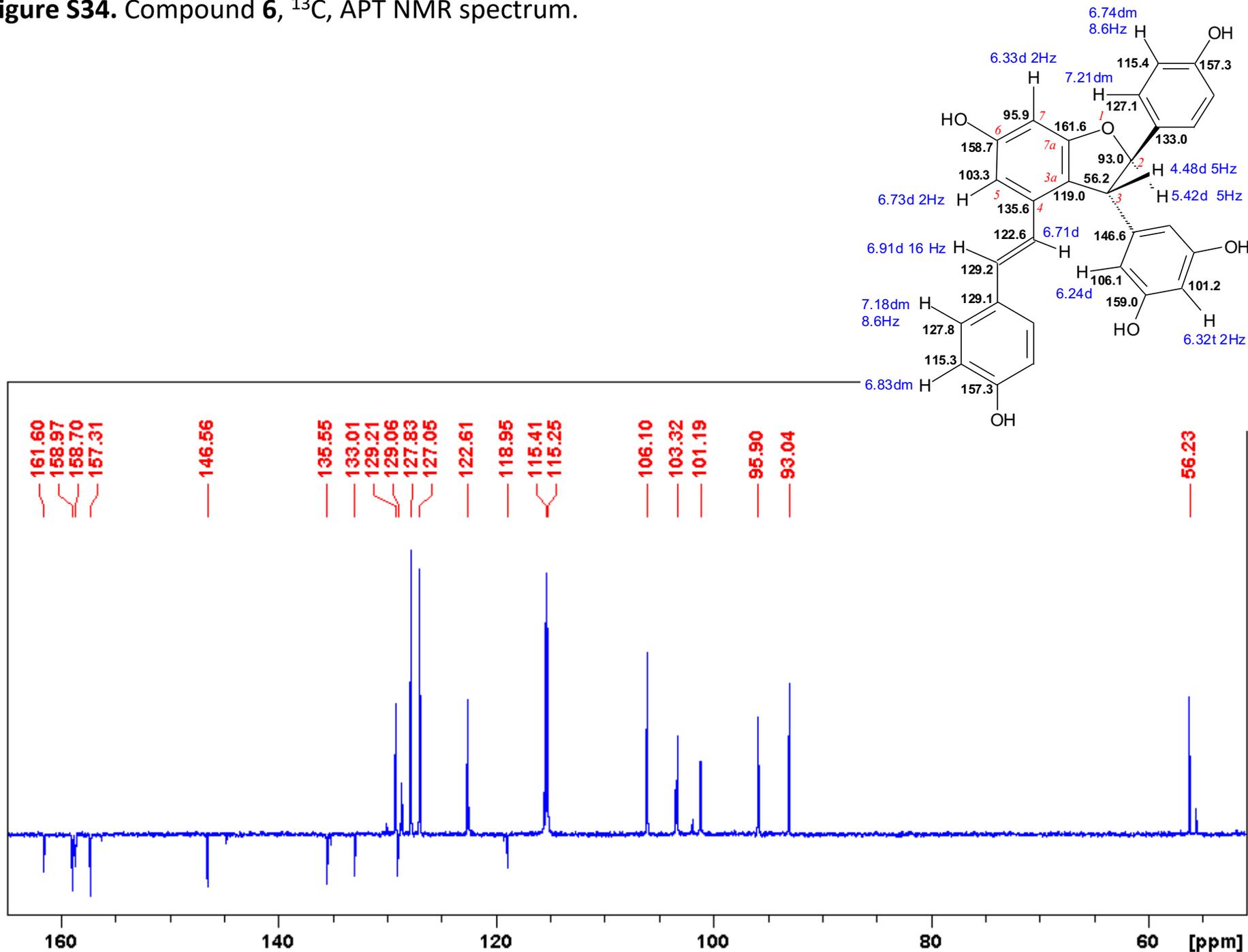


Figure S35. Compound 6, HSQC spectrum.

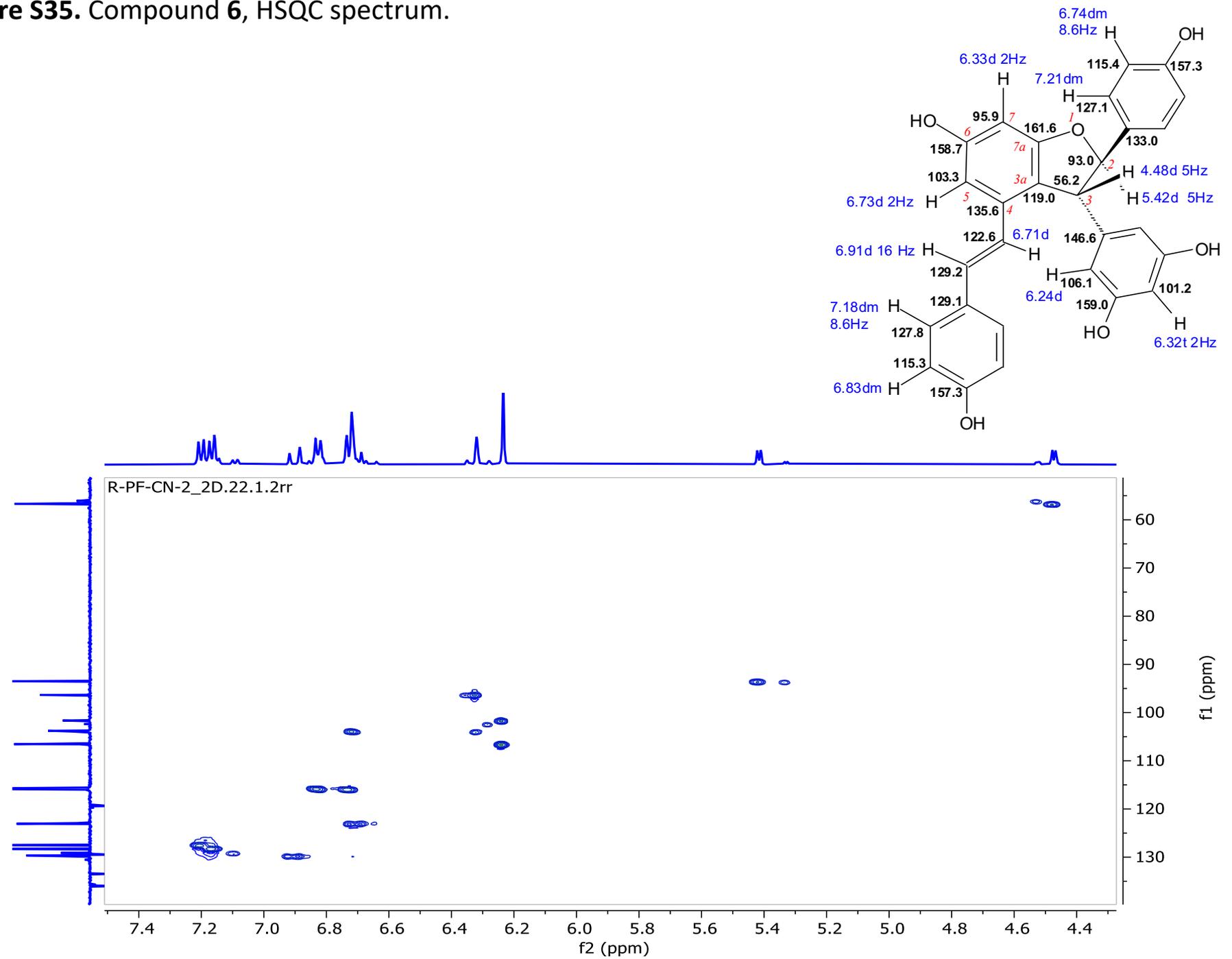


Figure S36. Compound 6, HMBC spectrum.

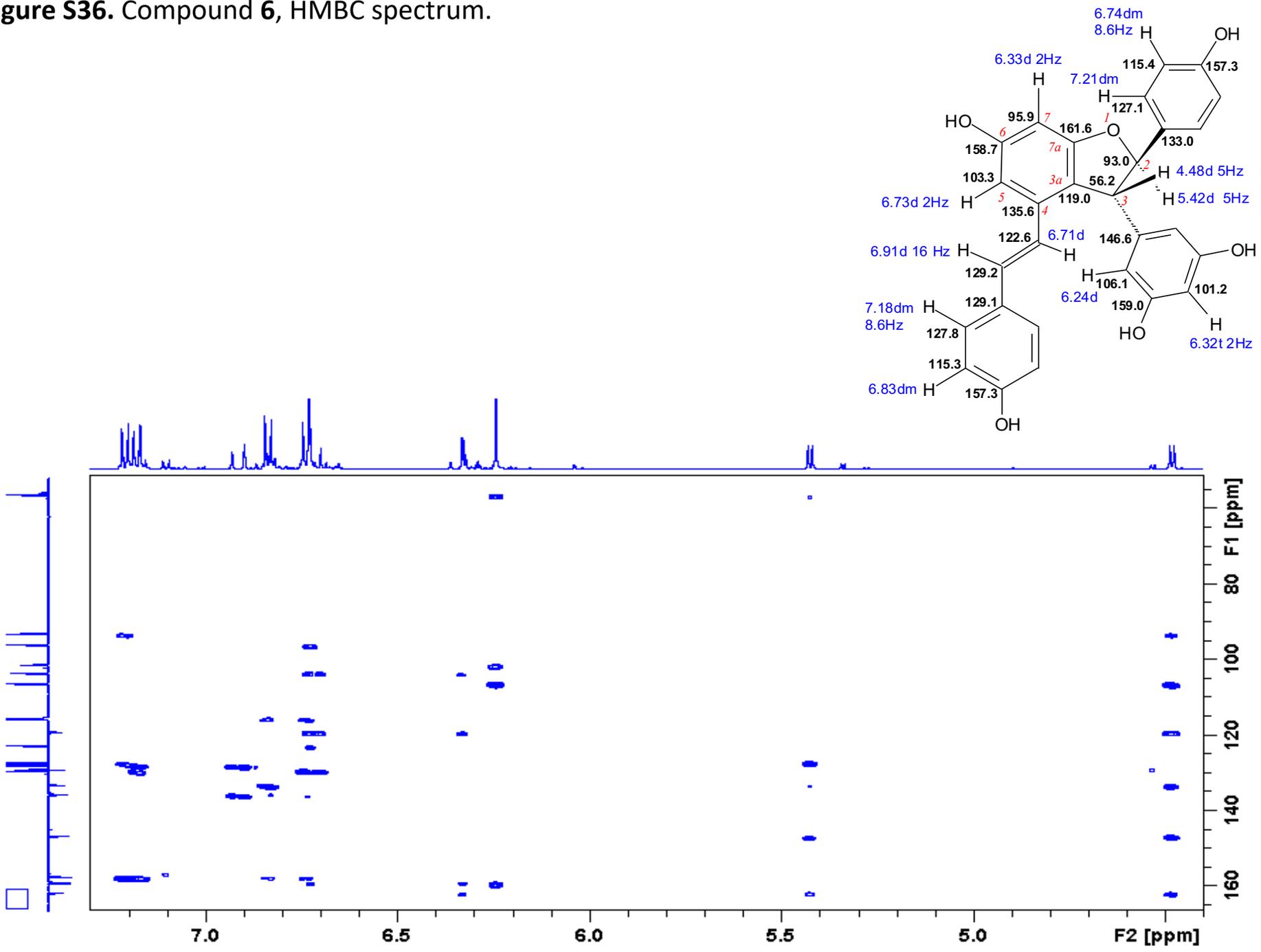


Figure S37. Compound 6, COSY and NOESY spectra.

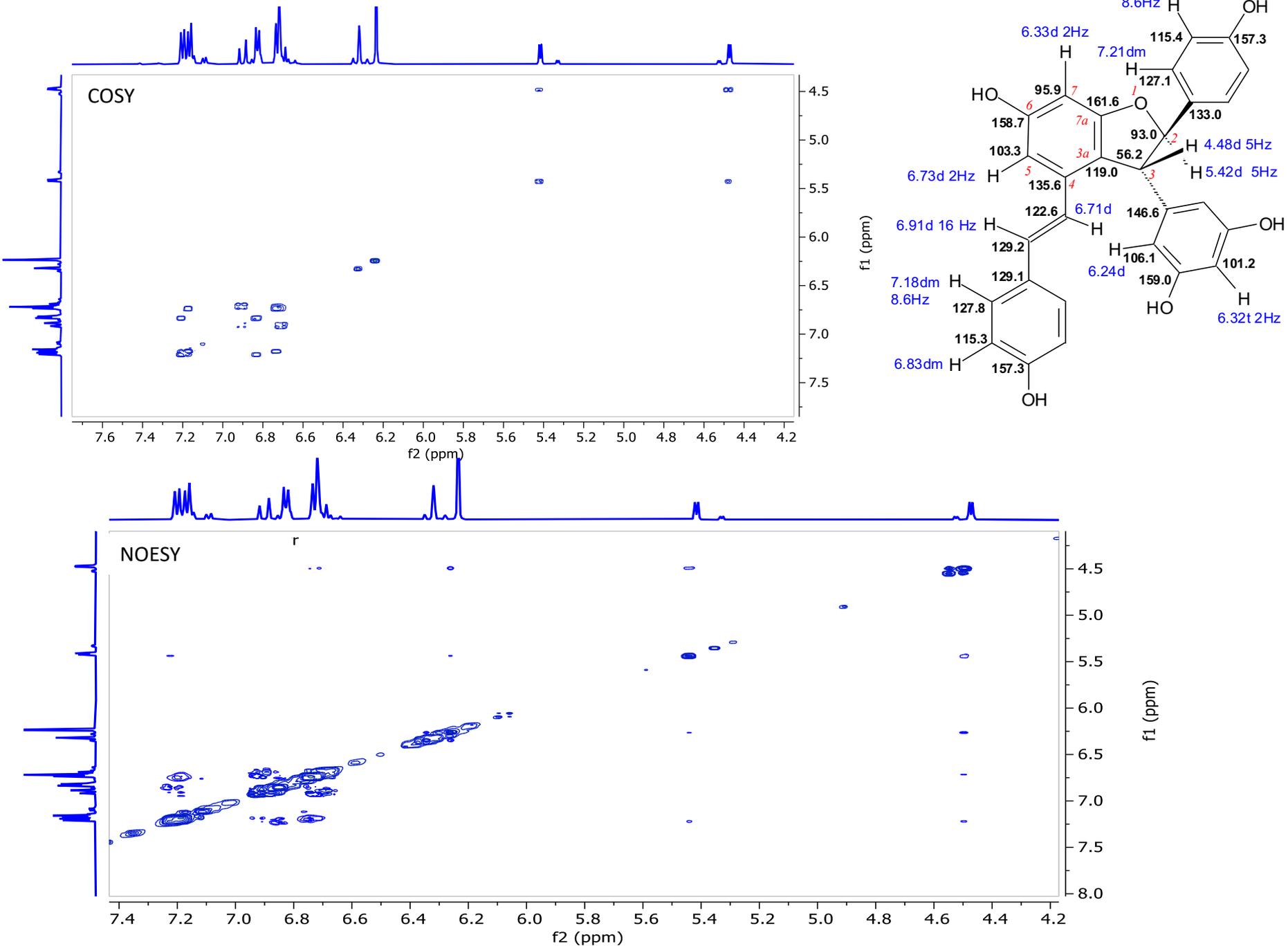


Figure S38. Compound 7, ^1H NMR spectrum.

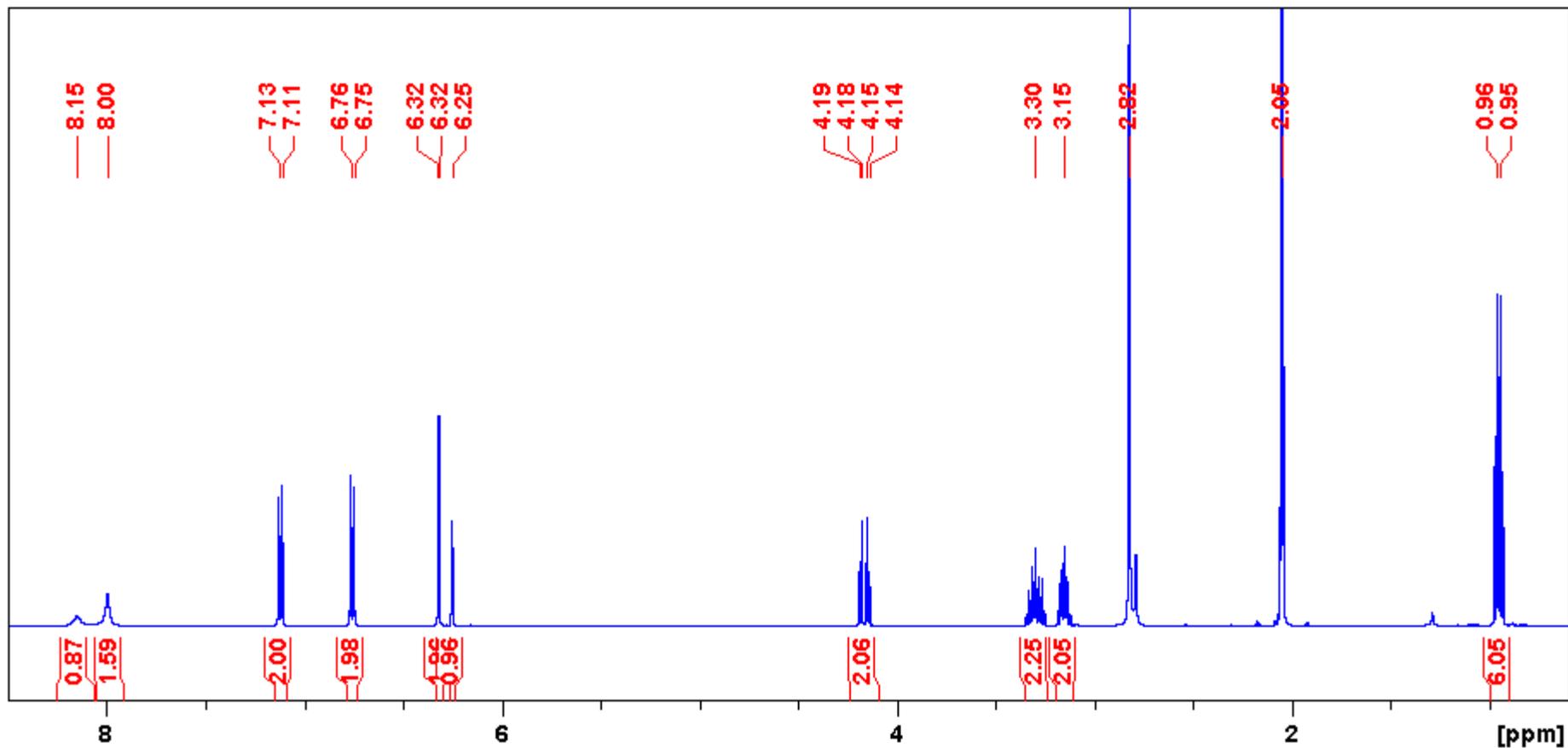
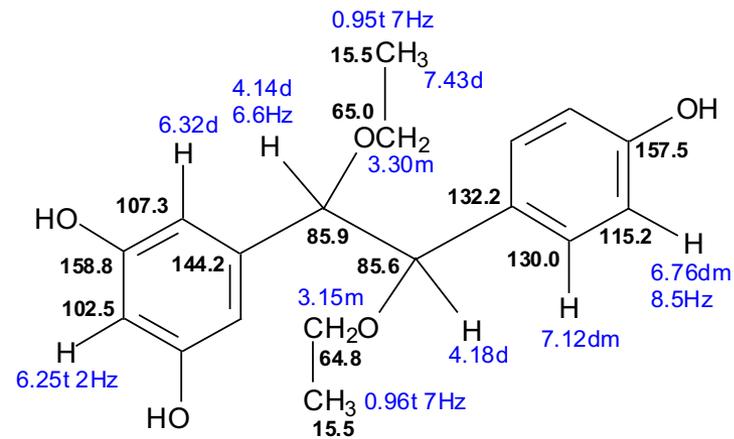


Figure S39. Compound 7, ^{13}C , APT NMR spectrum.

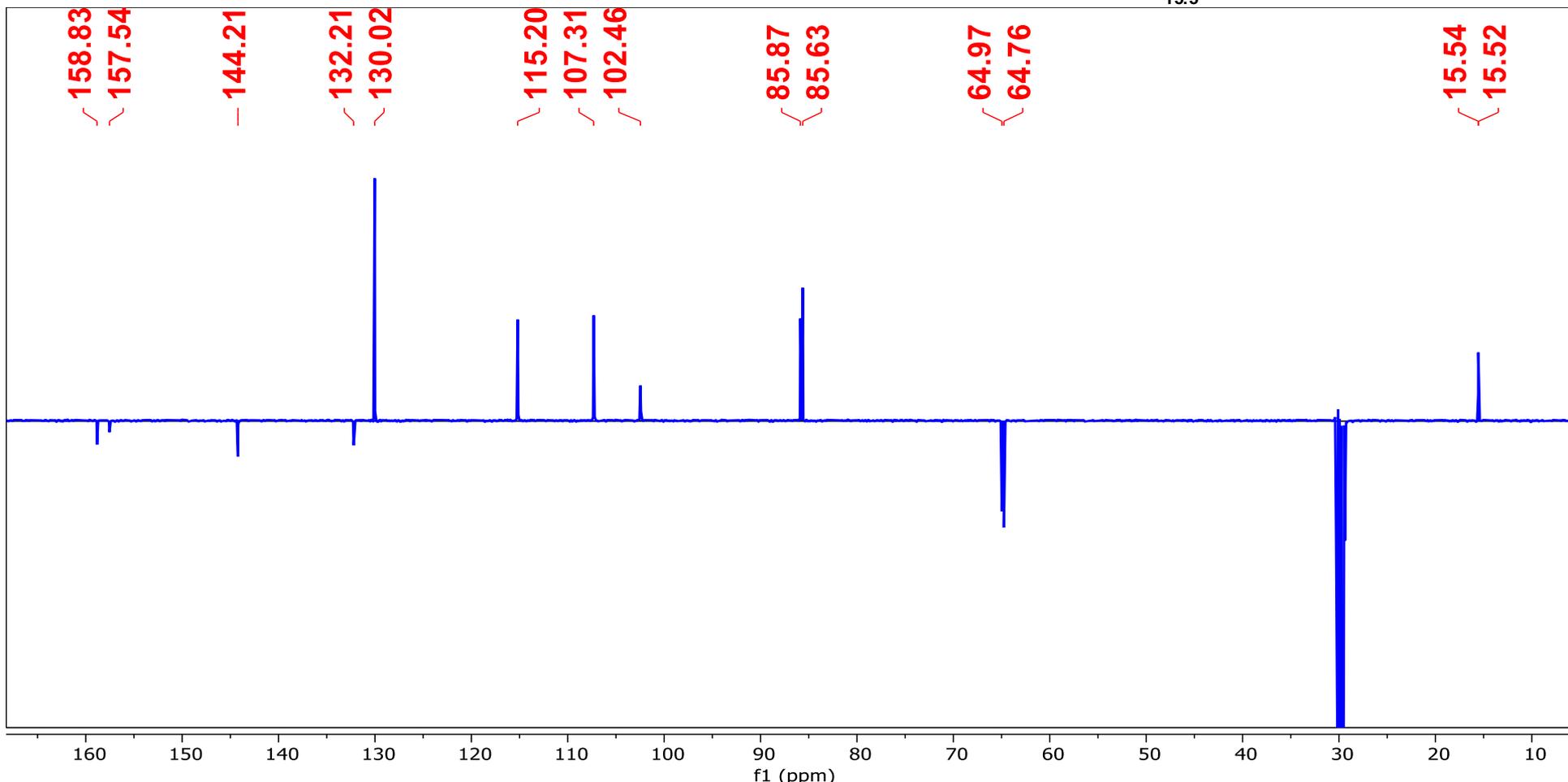
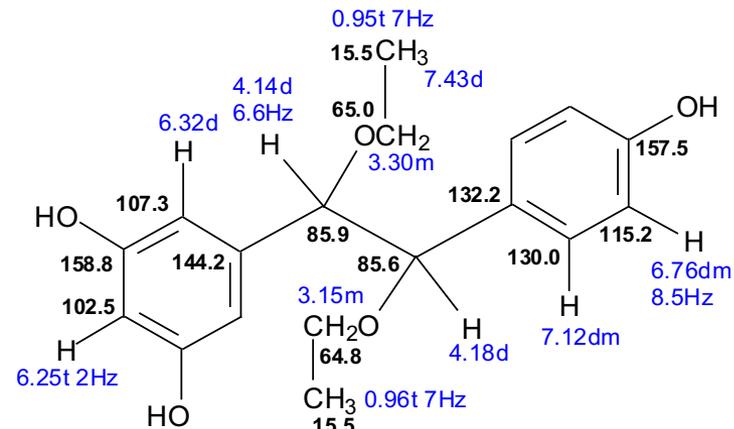


Figure S40. Compound 7, NOESY spectrum and NOESY section.

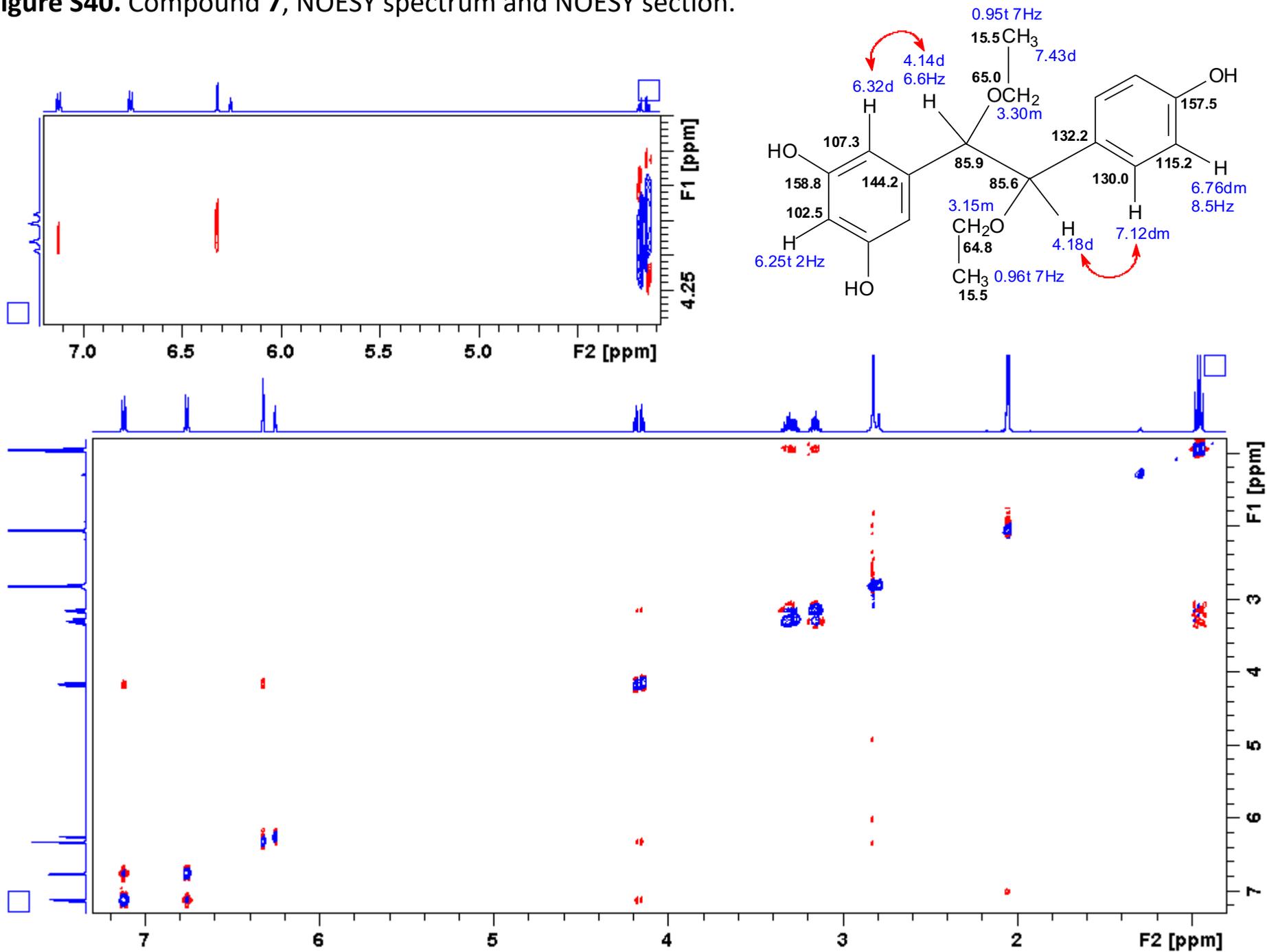


Figure S41. Compound 7, HSQC and HMBC spectra.

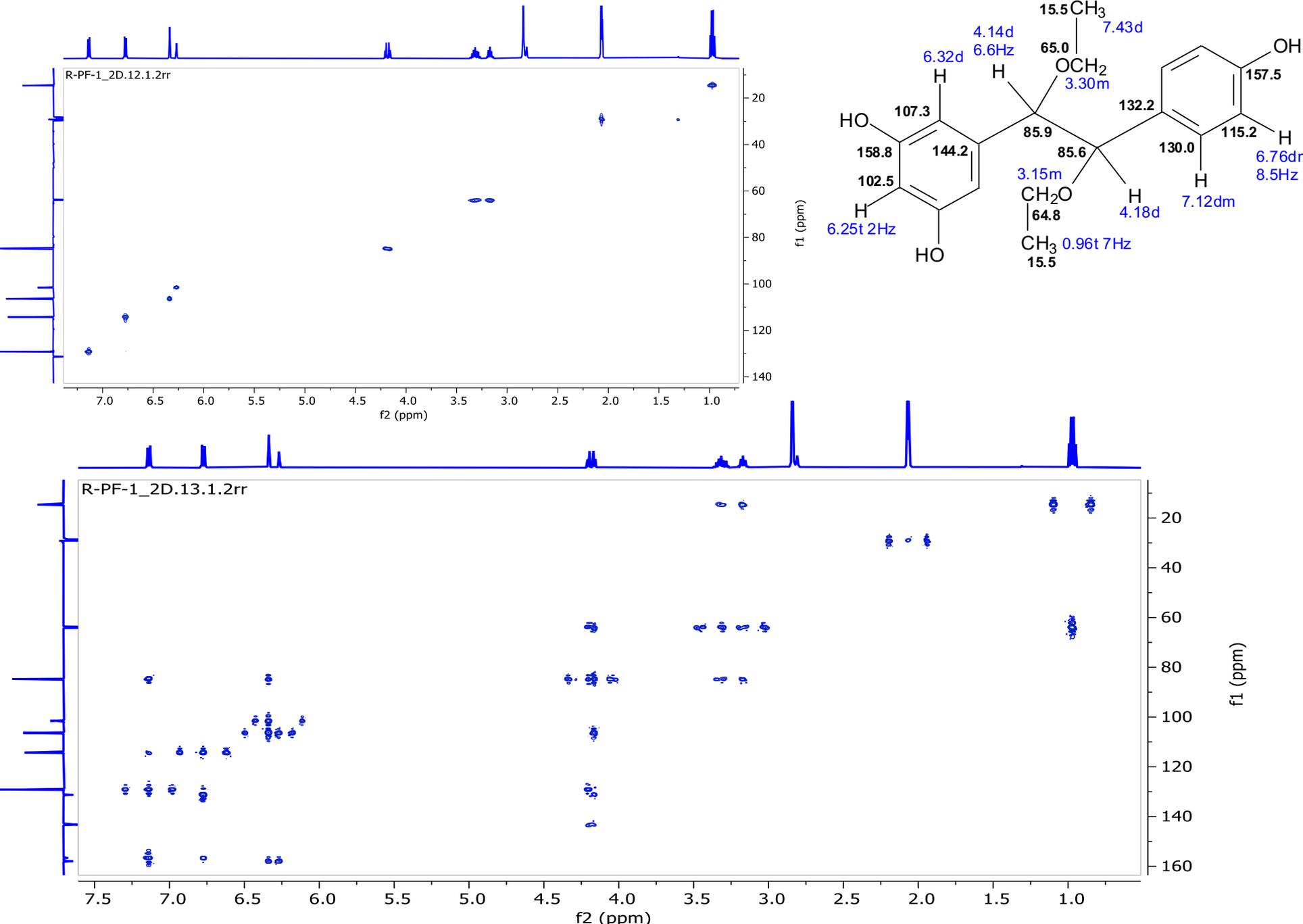


Figure S42. Compound 7, COSY spectrum.

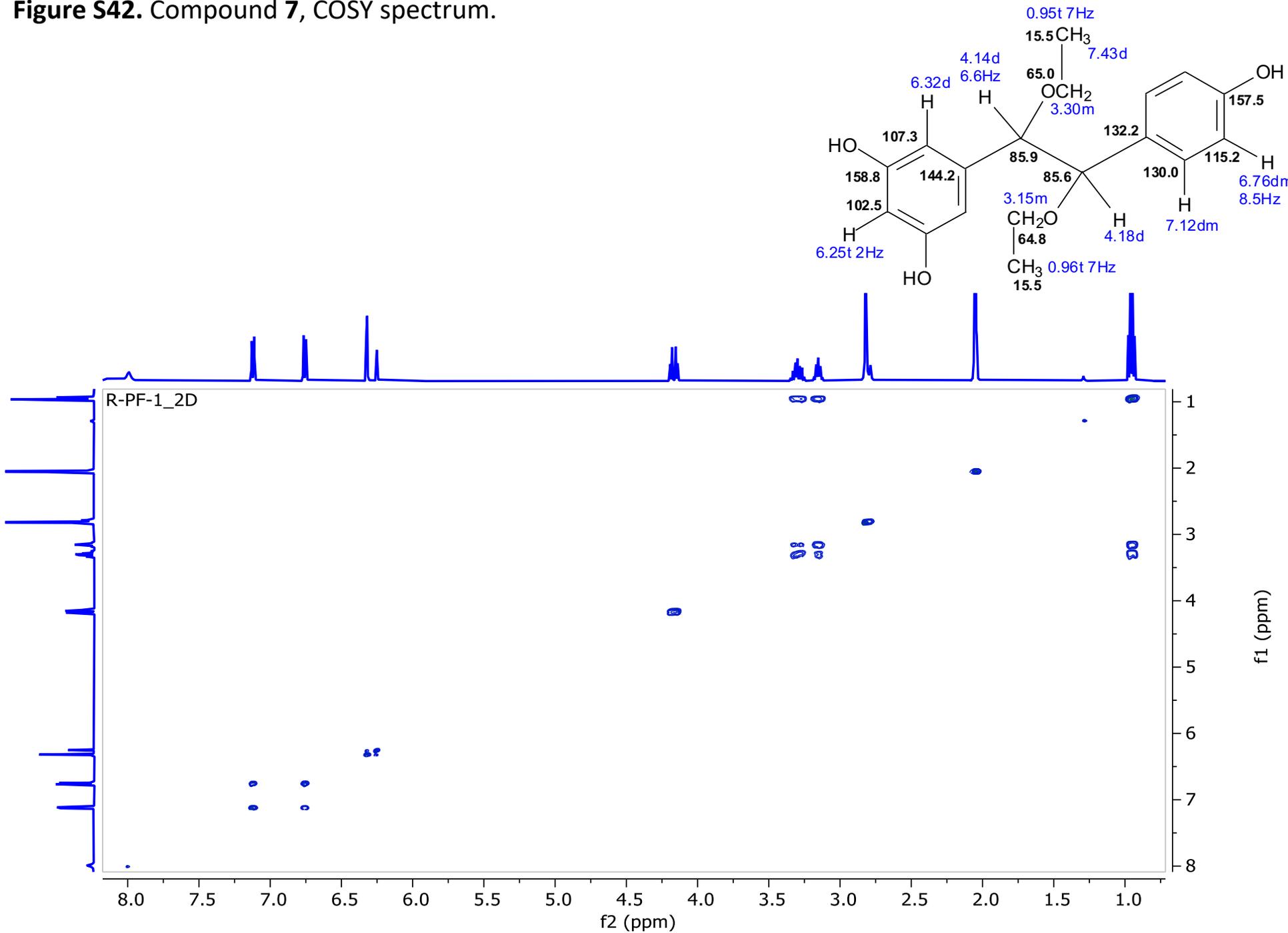


Figure S43. Compound **8**, ^1H NMR spectrum.

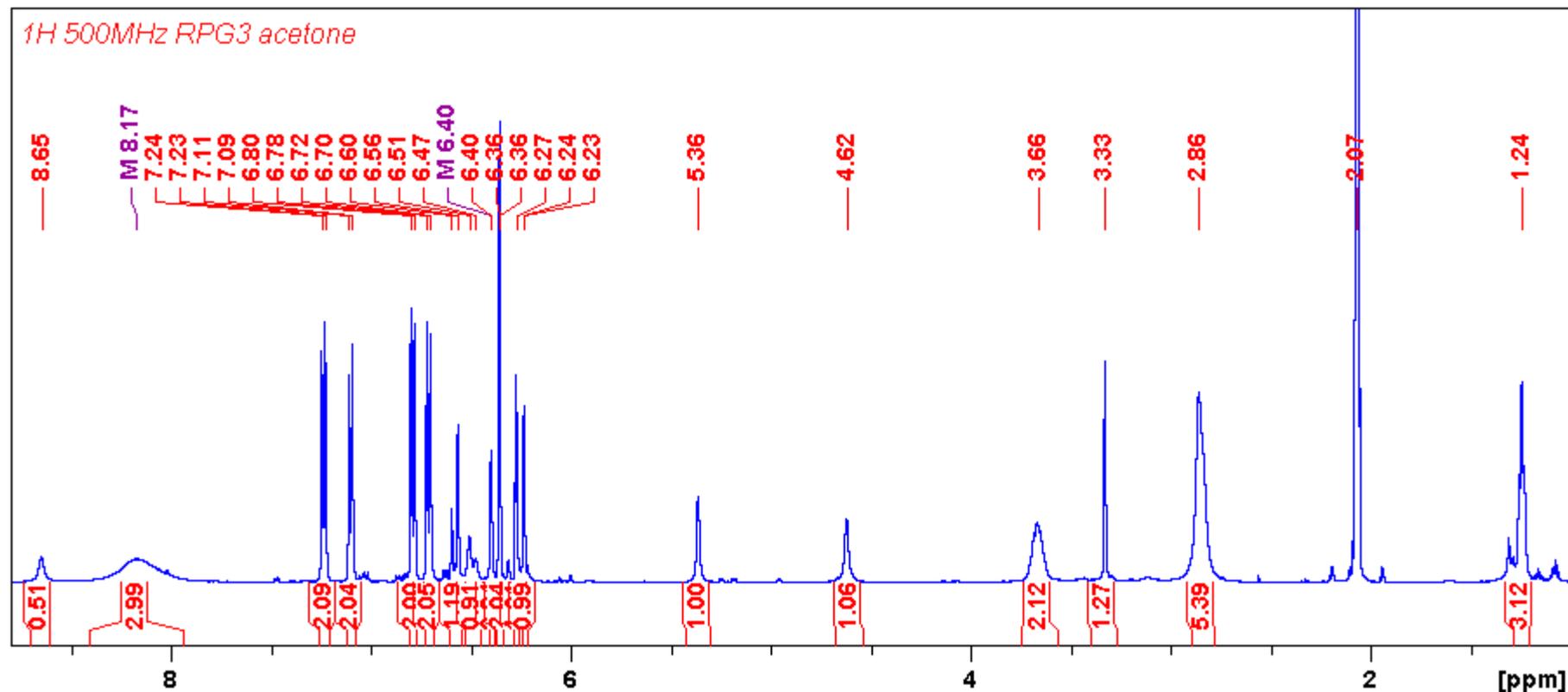
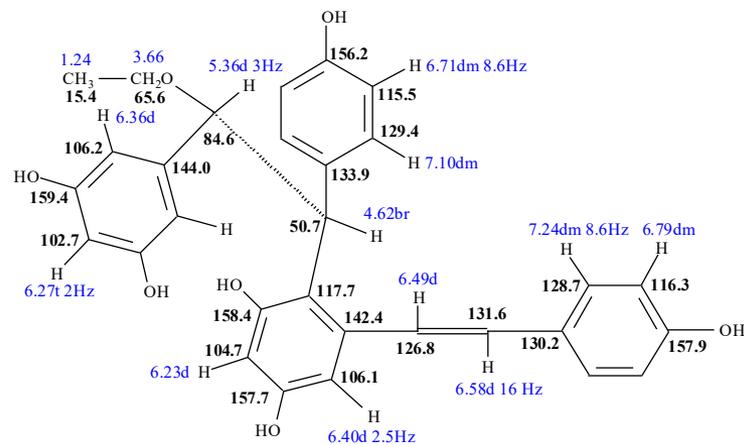
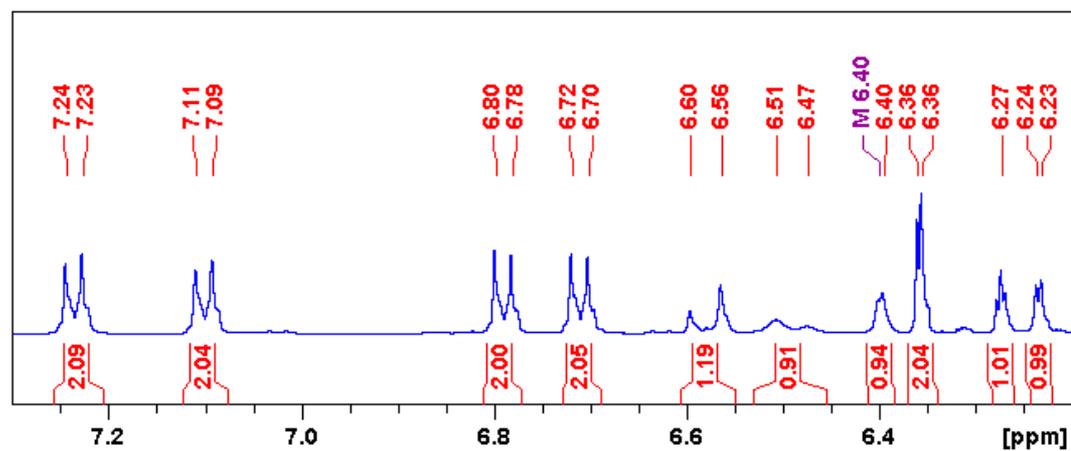


Figure S44. Compound **8**, ^{13}C , APT NMR spectrum.

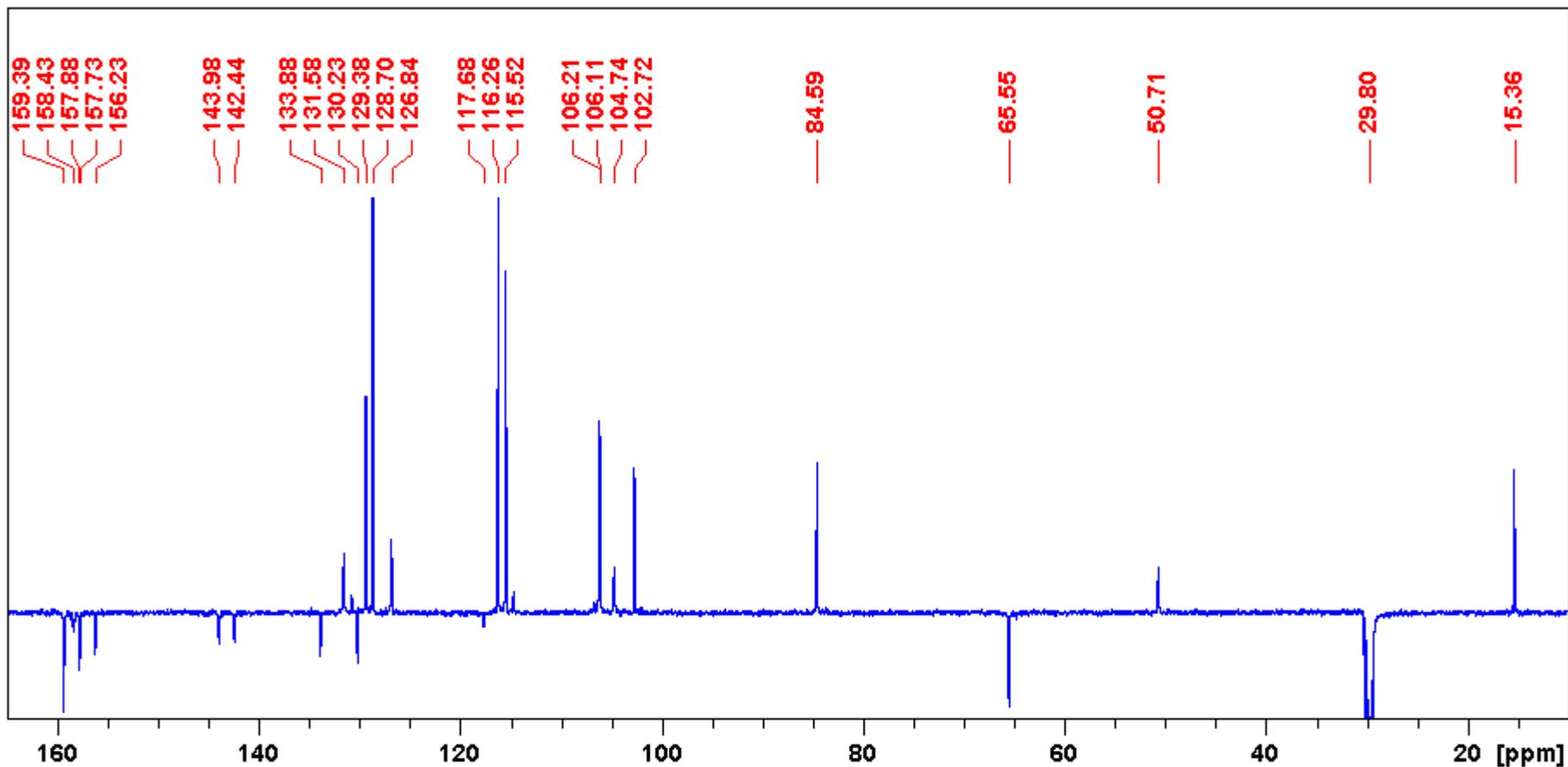
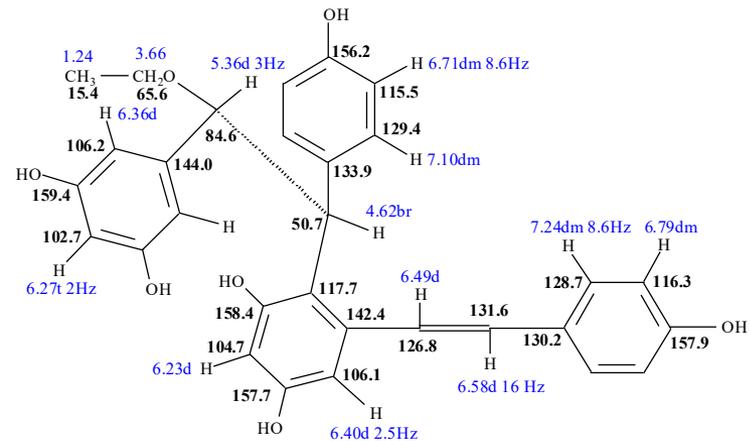


Figure S45. Compound **8**, HSQC spectrum and HSQC section.

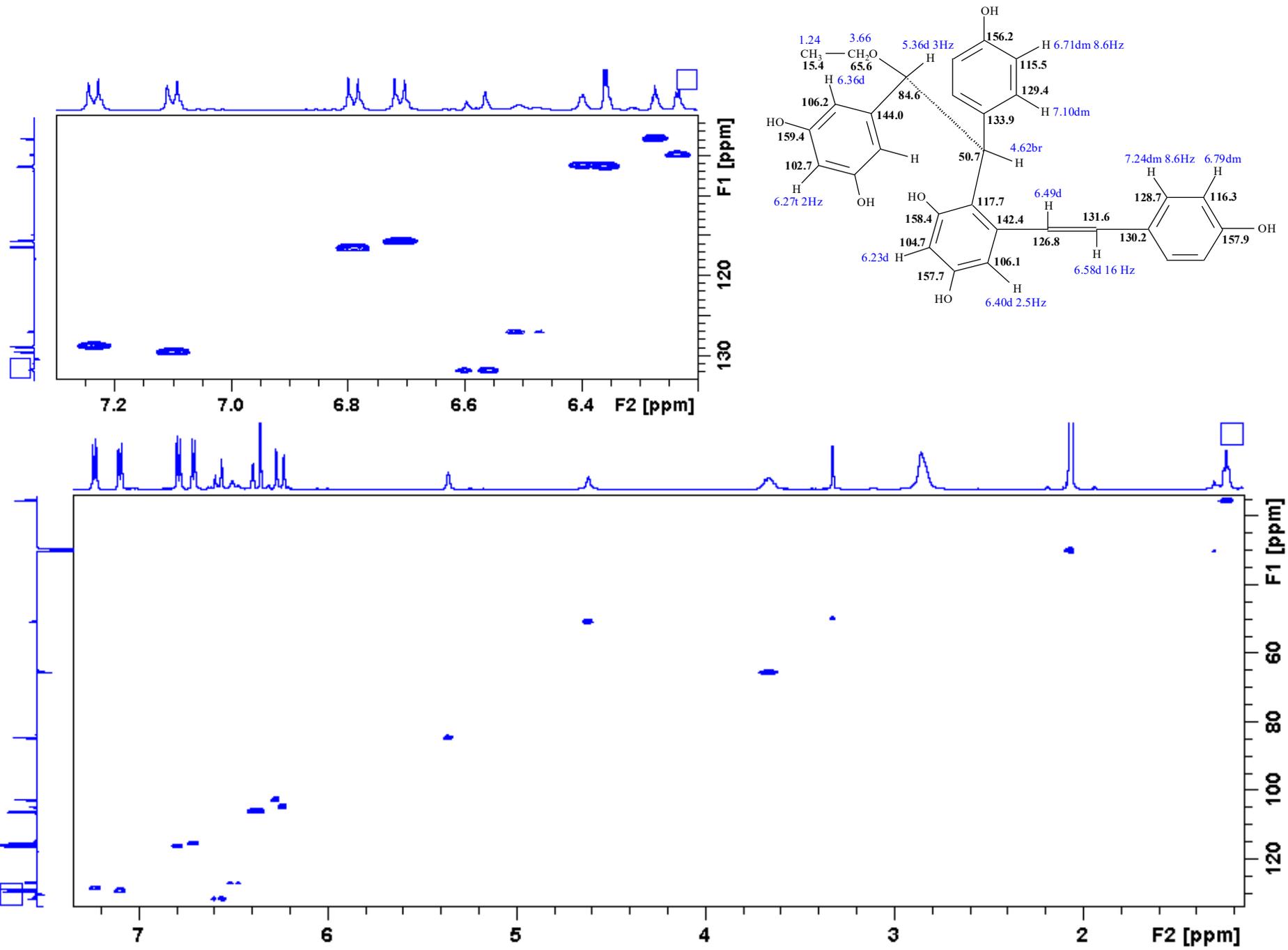


Figure S47. Compound **8**, COSY spectrum and COSY aromatic section.

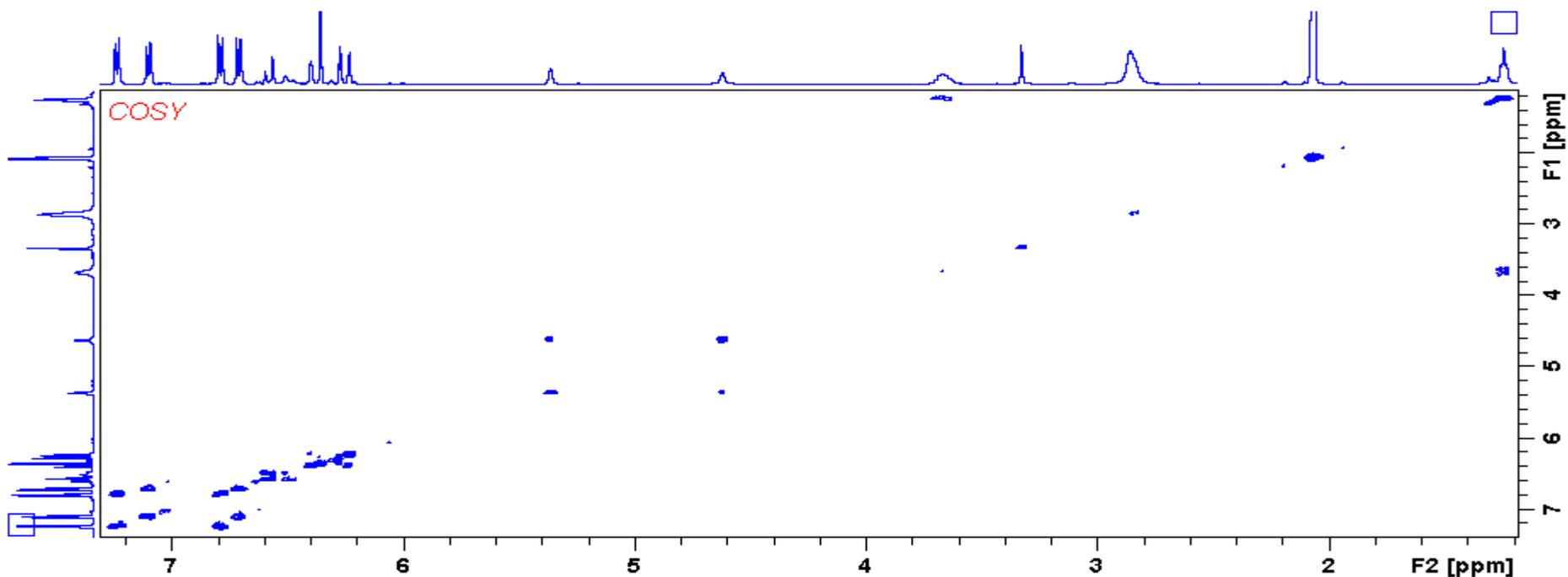
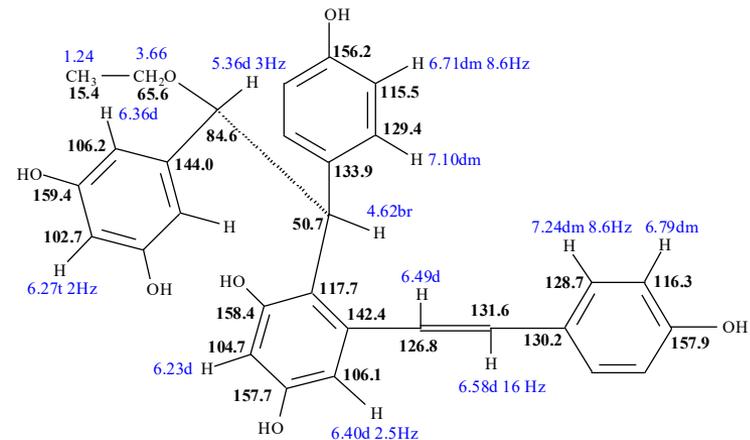
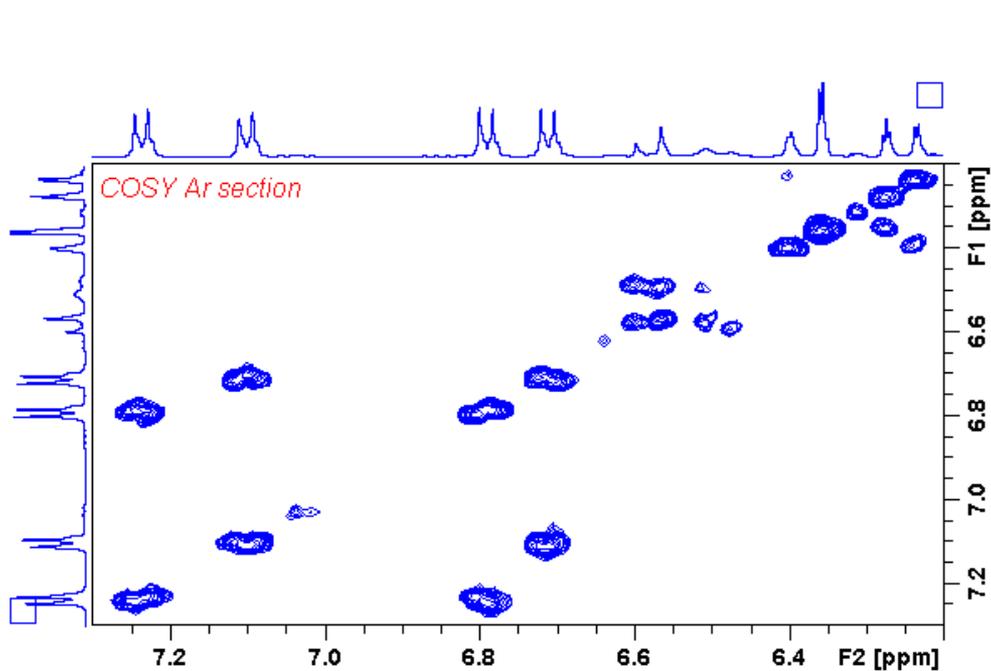


Figure S48. Compound **8**, NOESY; arrows indicate steric proximities, and assign configuration and the dominant conformer

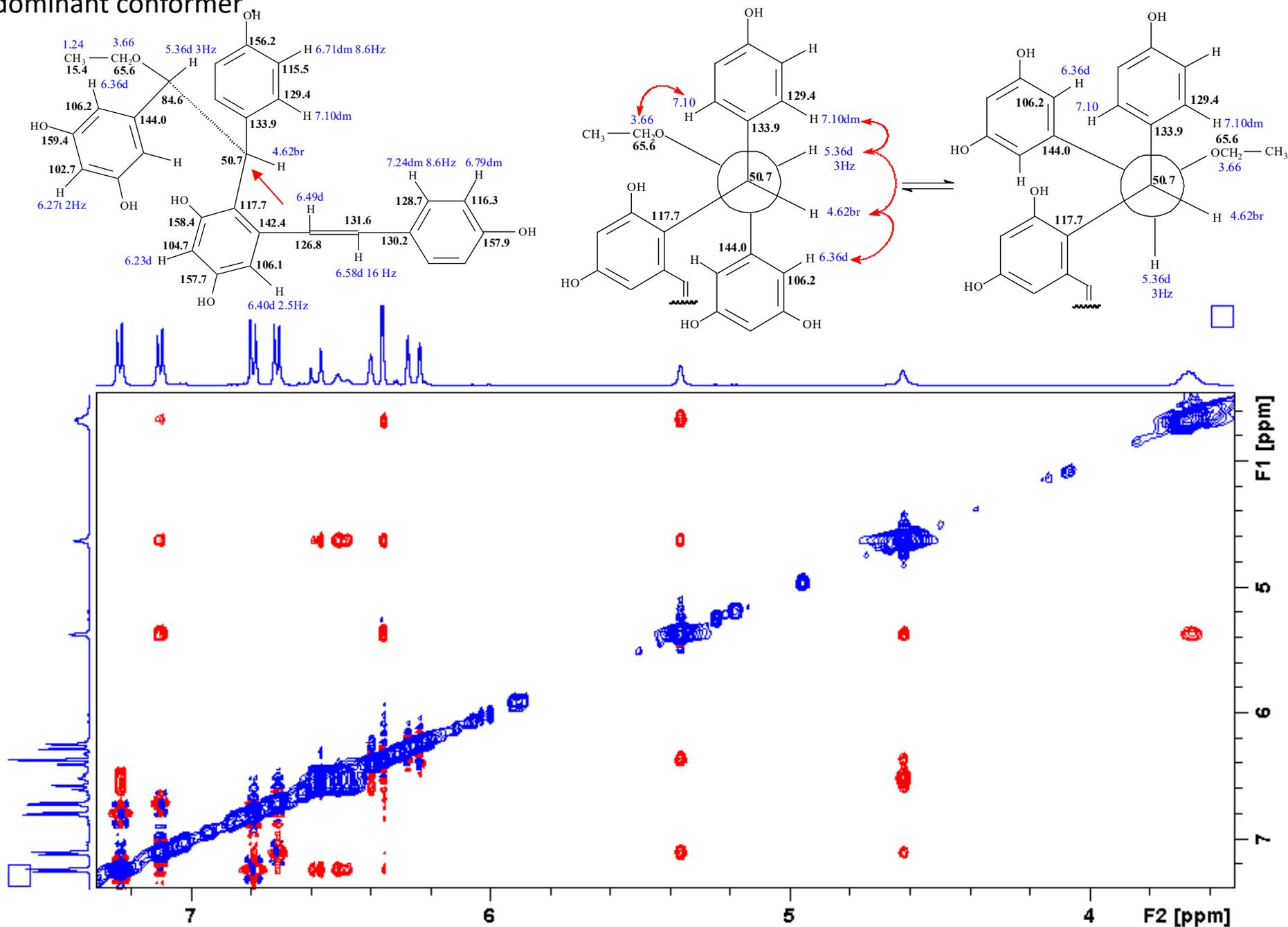


Figure S49. Compound **9**, ^1H NMR spectrum.

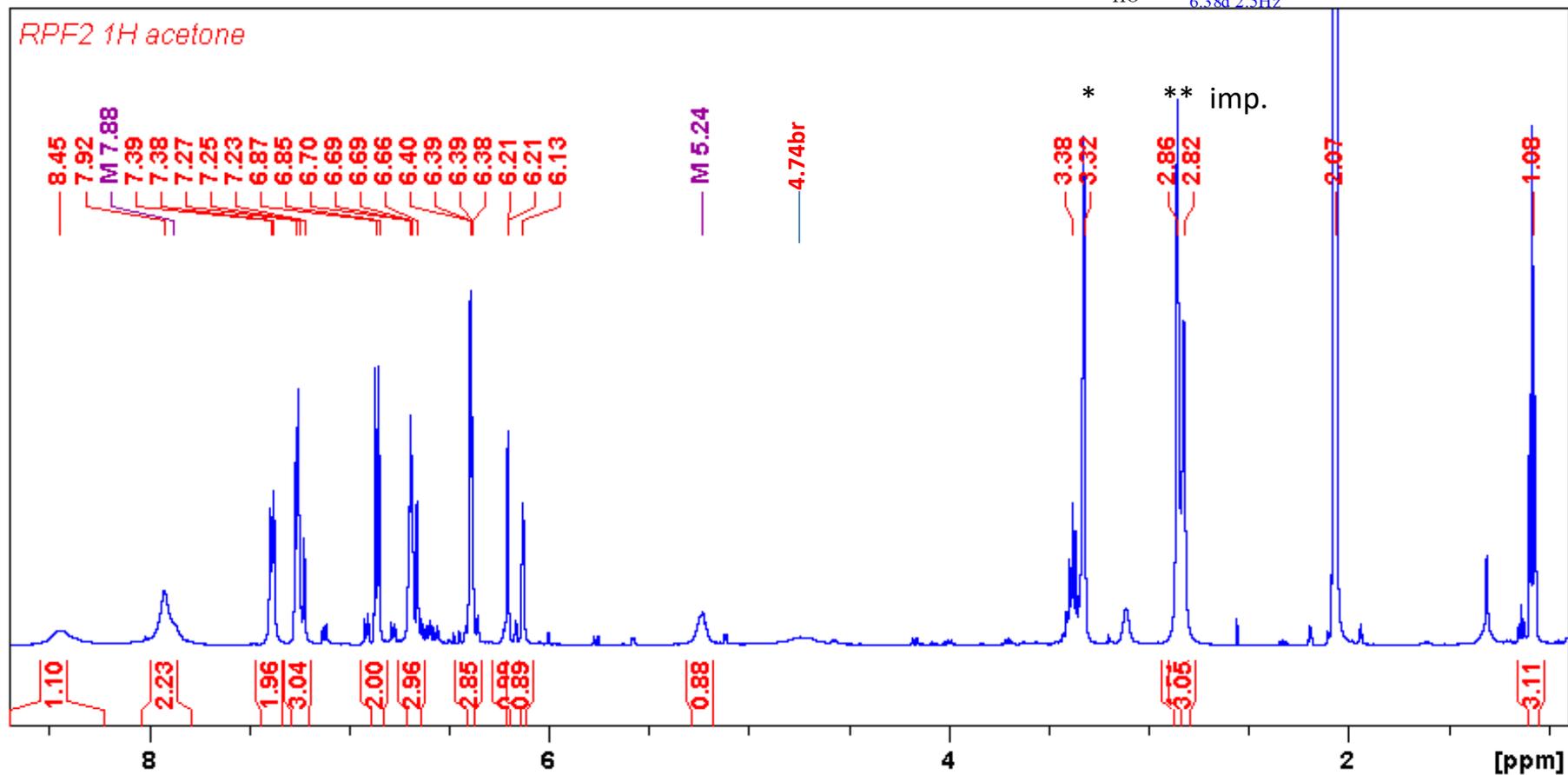
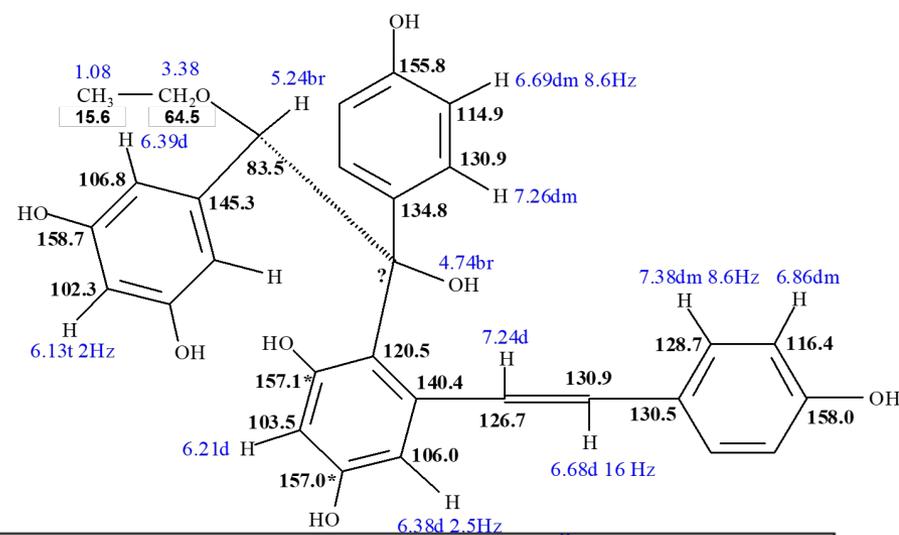


Figure S50. Compound **9**, ^{13}C , APT NMR spectrum.

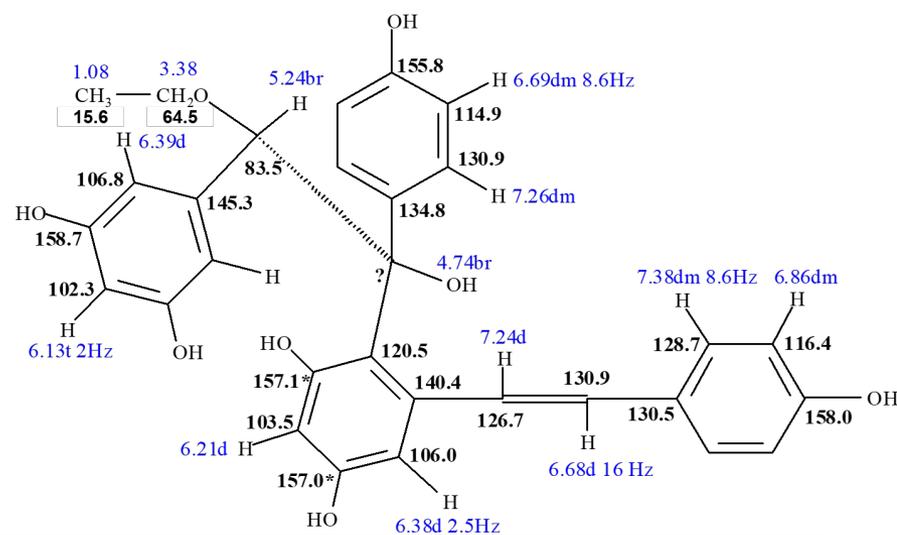
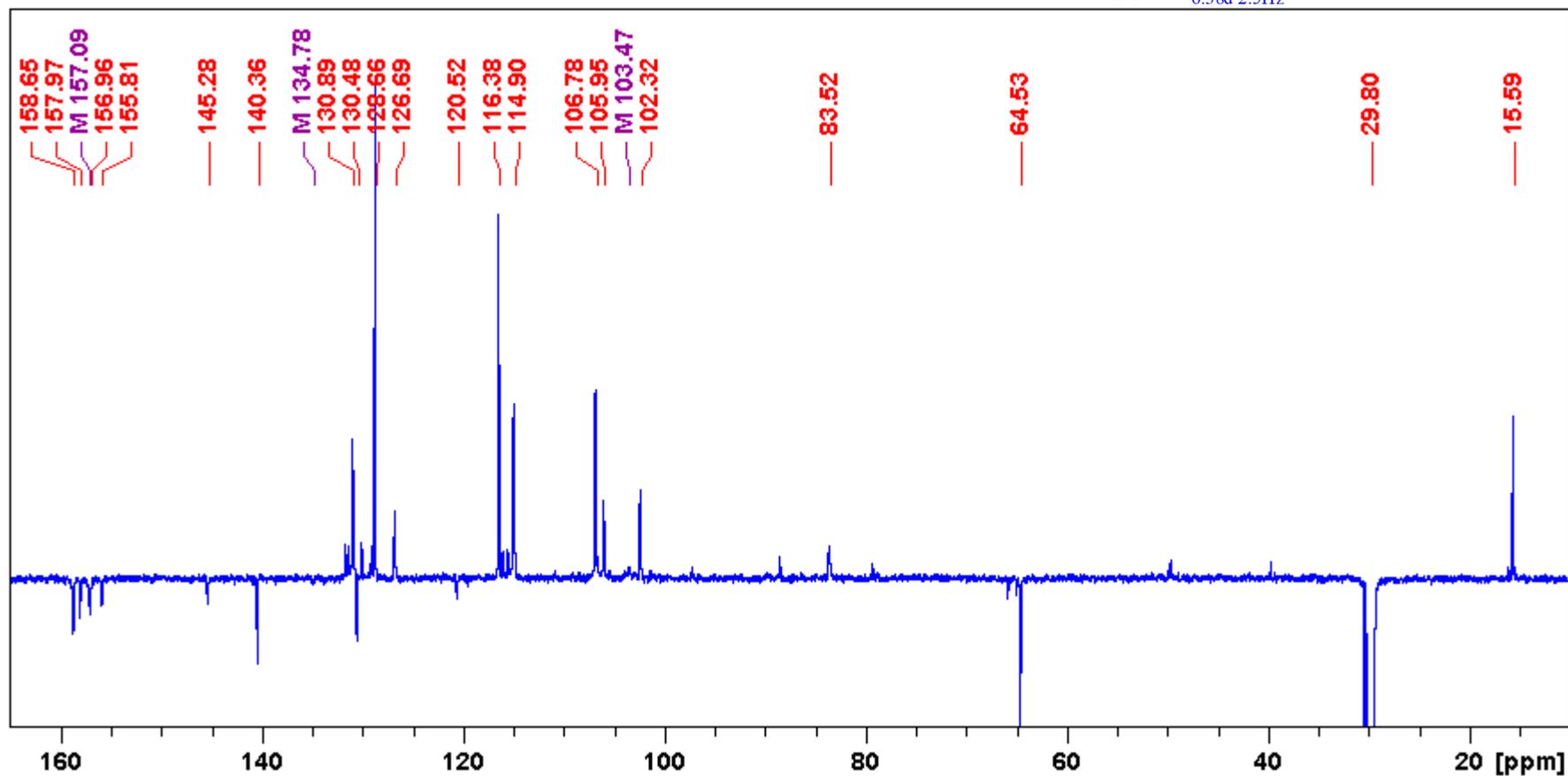


Figure S51. Compound 9, HSQC spectrum and HSQC section.

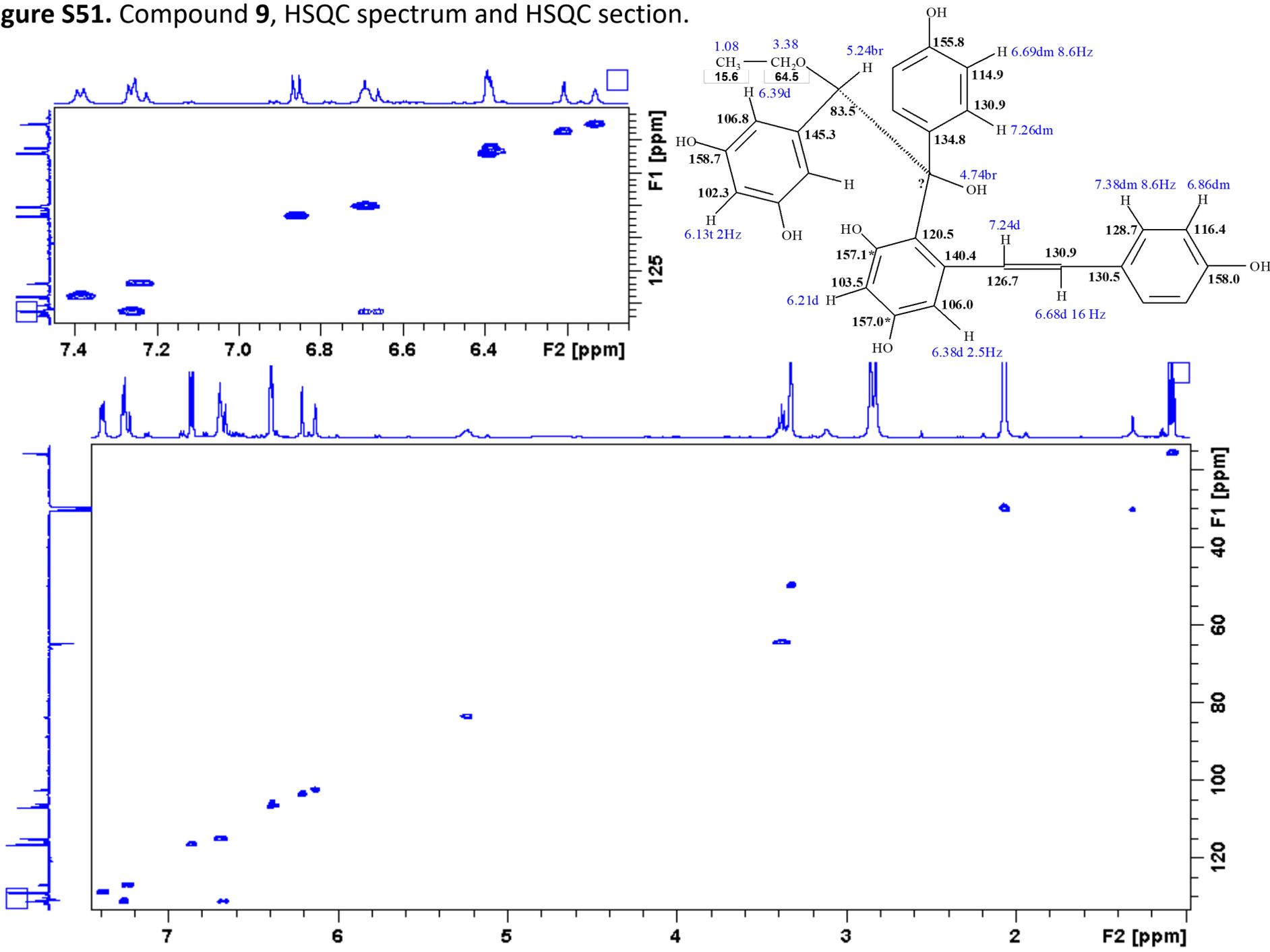


Figure S52. Compound 9, HMBC spectrum.

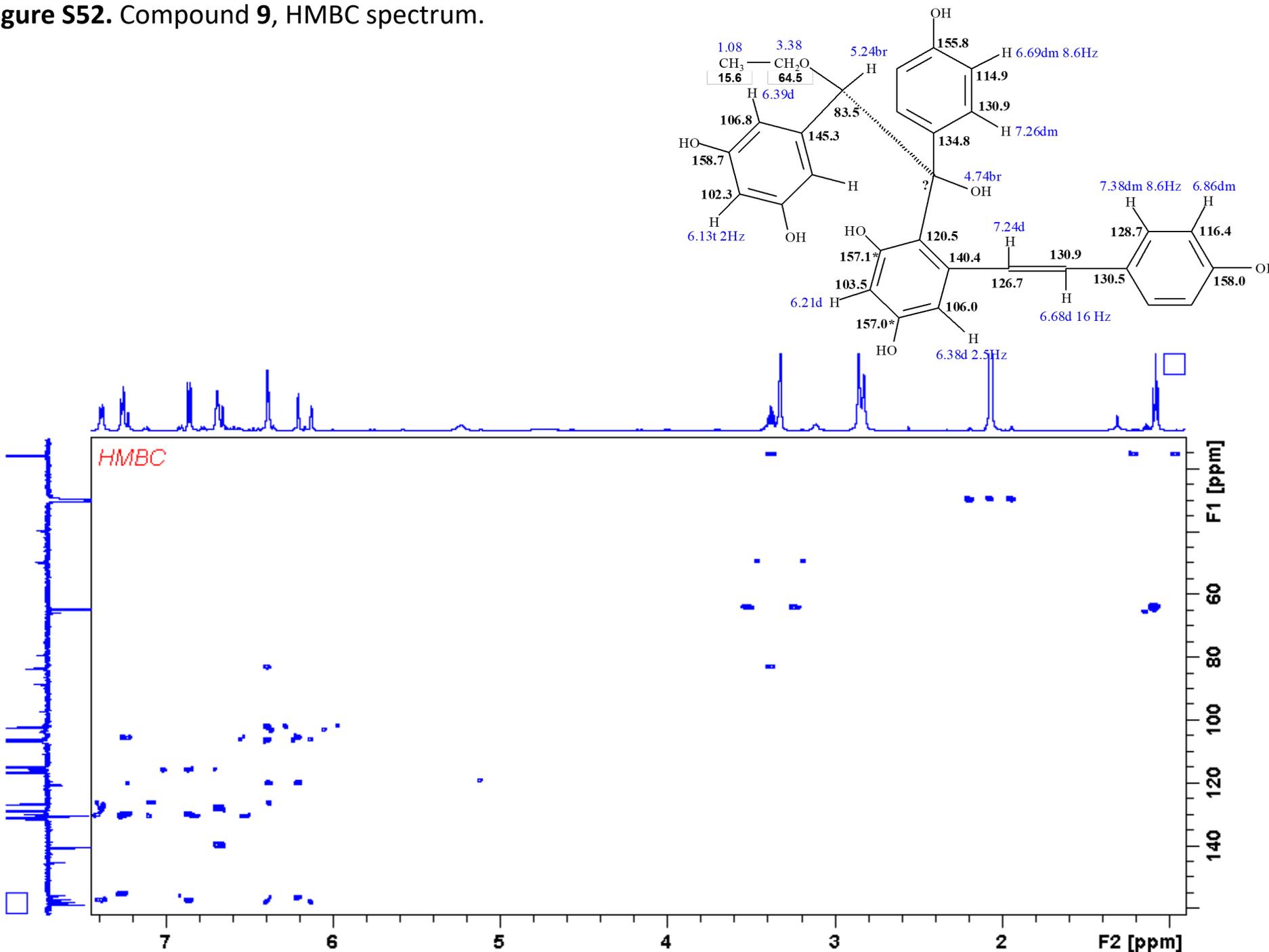


Figure S53. Compound 9, NOESY spectrum.

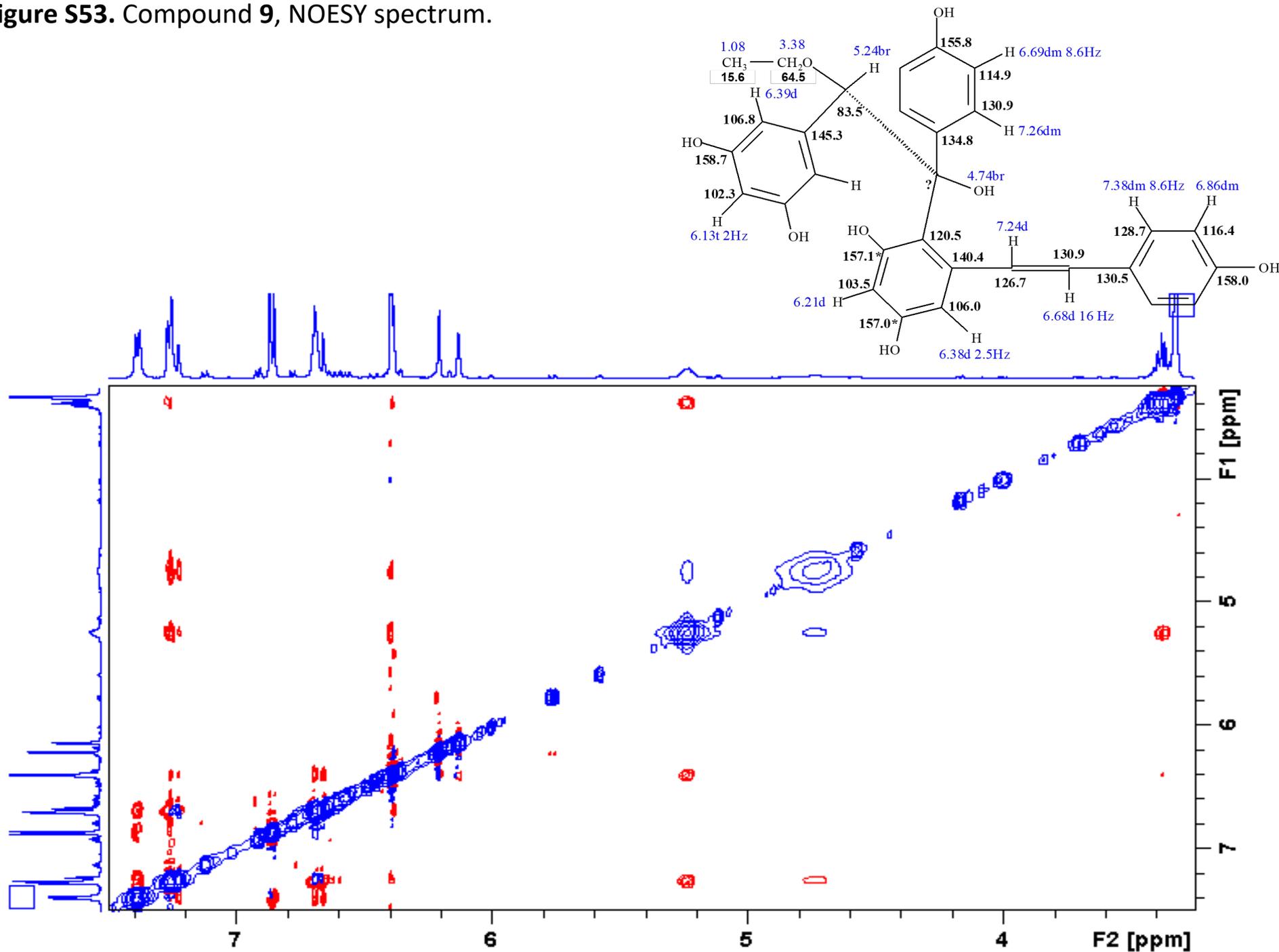


Figure S54. Compound **9**, HSQC spectrum and HSQC section, DMSO-d₆, T=80°C.

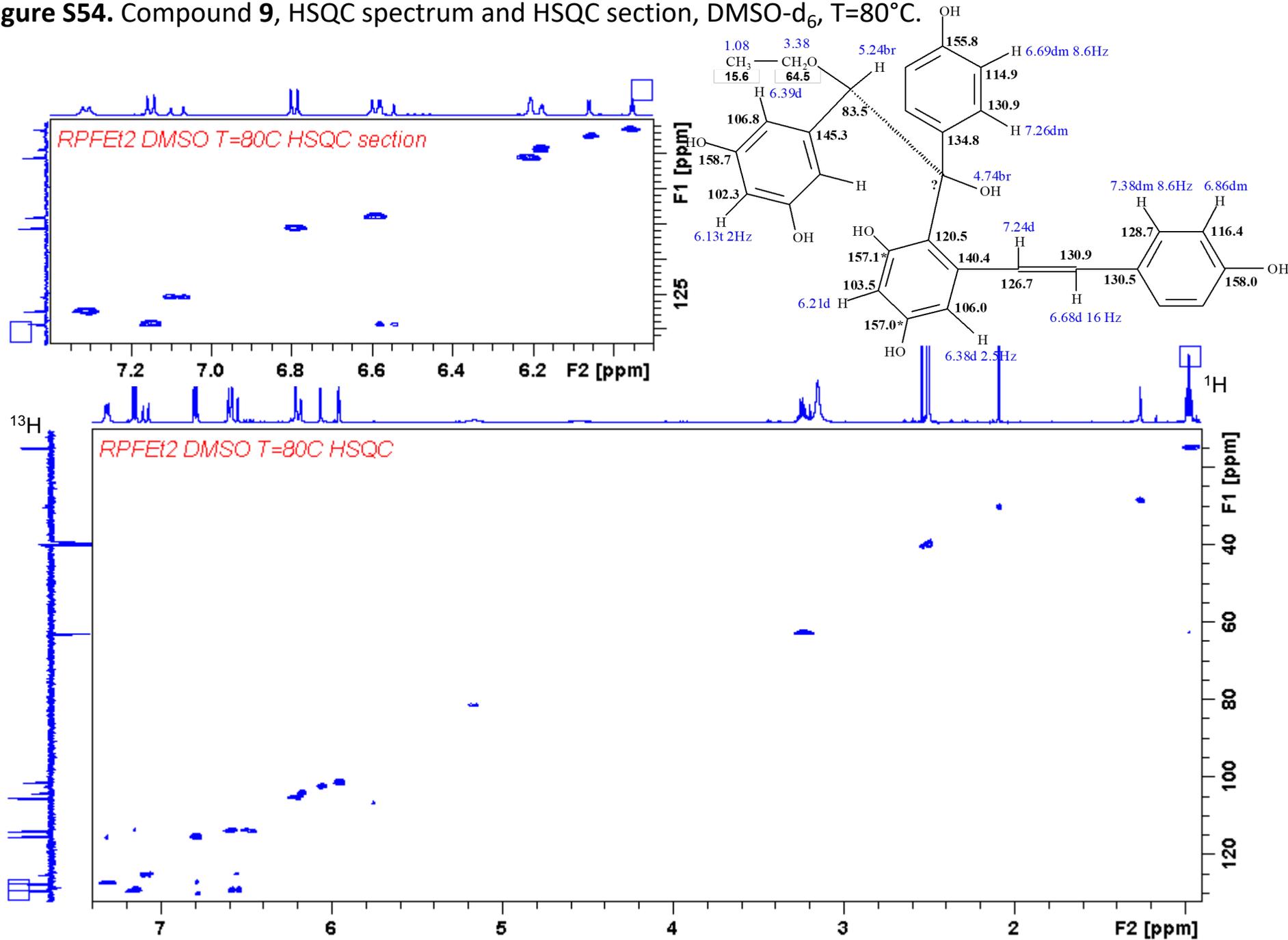


Figure S55. Compound **9**, ^{13}C , APT NMR spectrum, DMSO- d_6 , $T=80^\circ\text{C}$.

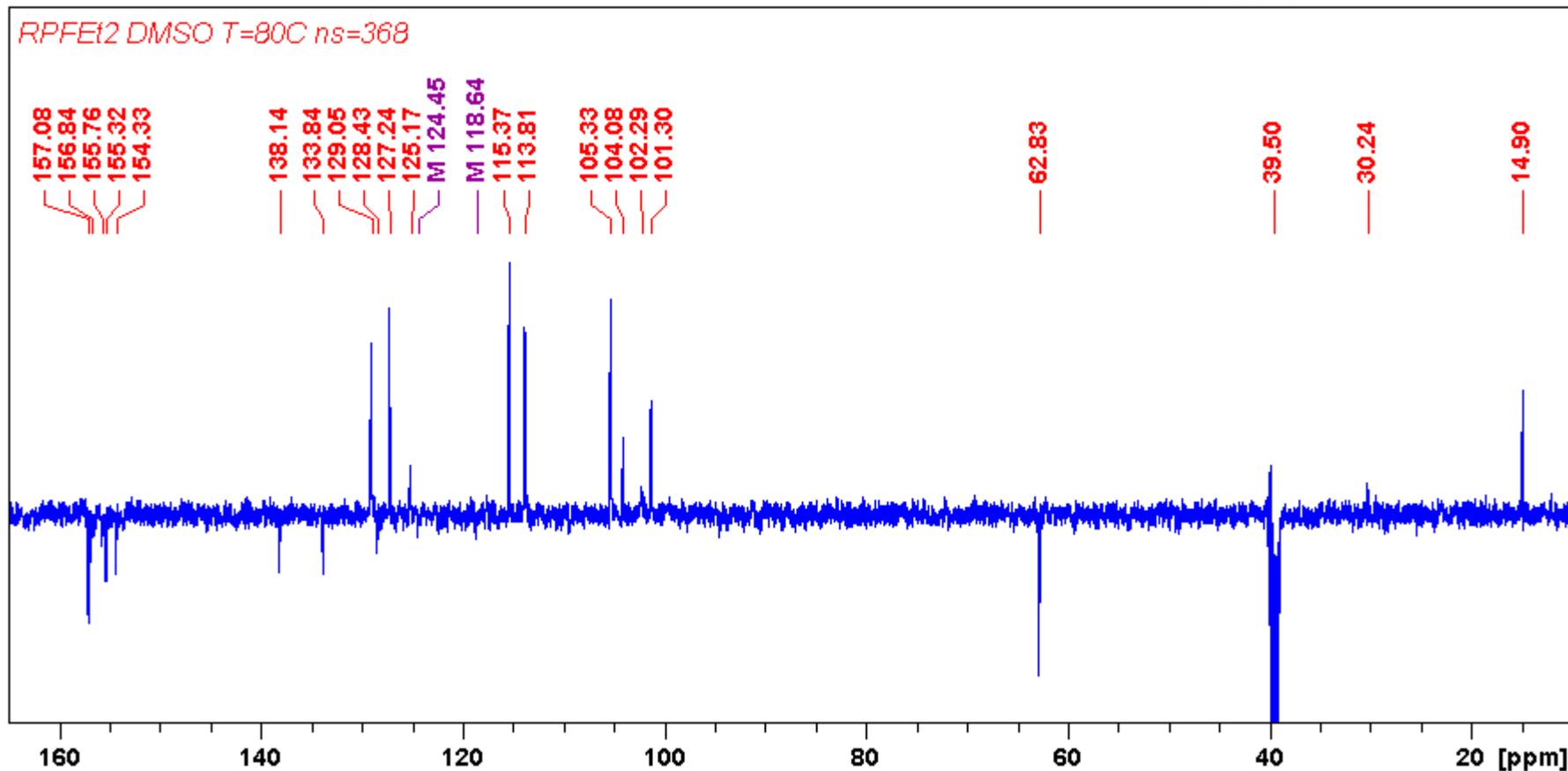
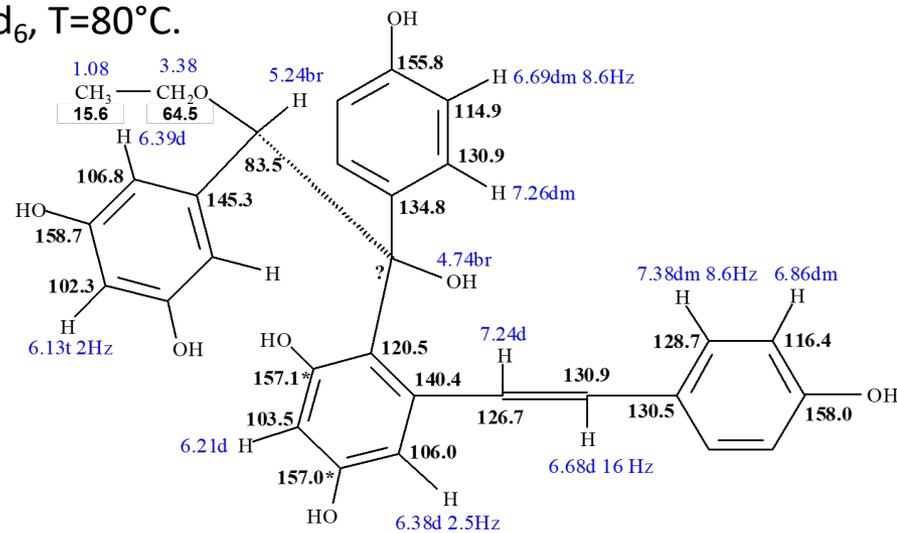
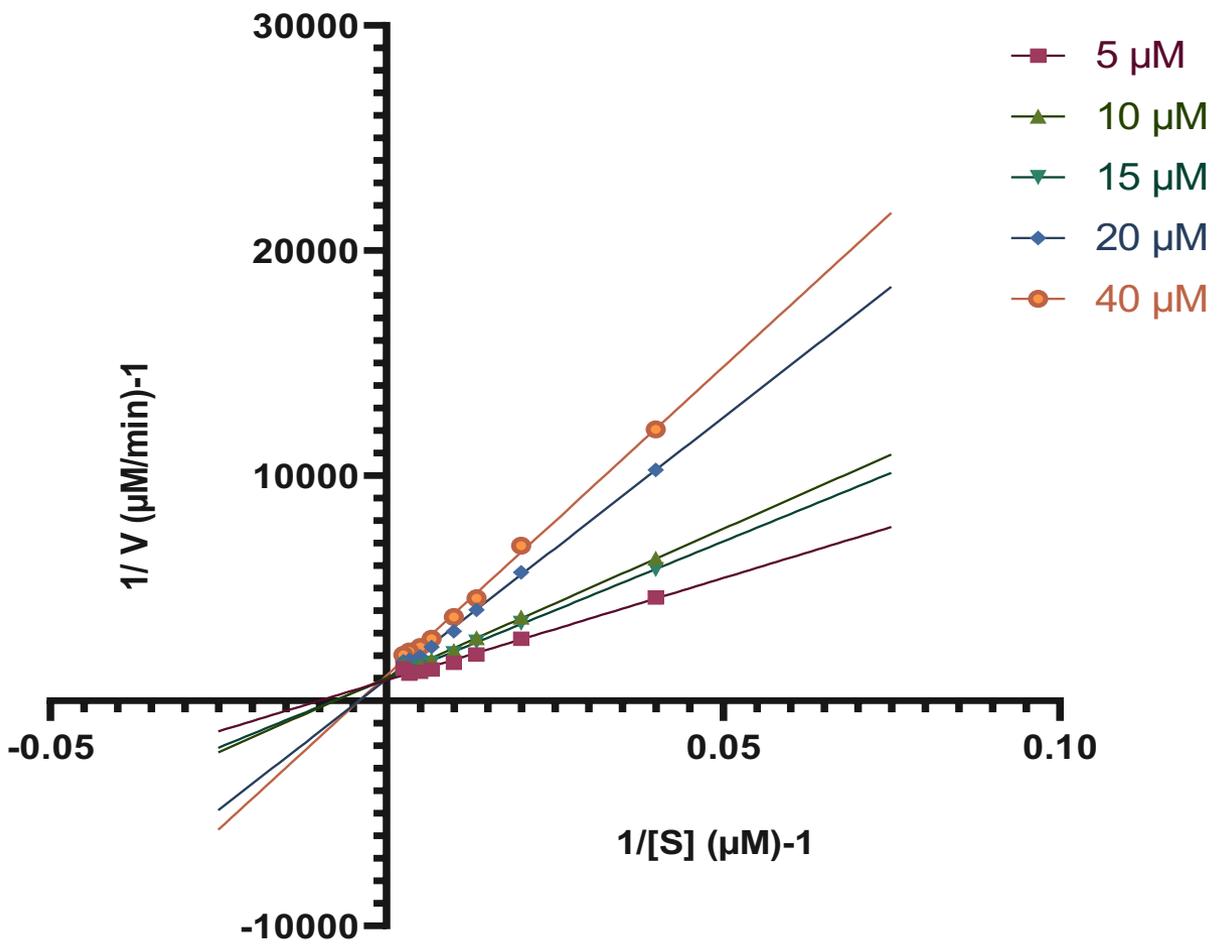
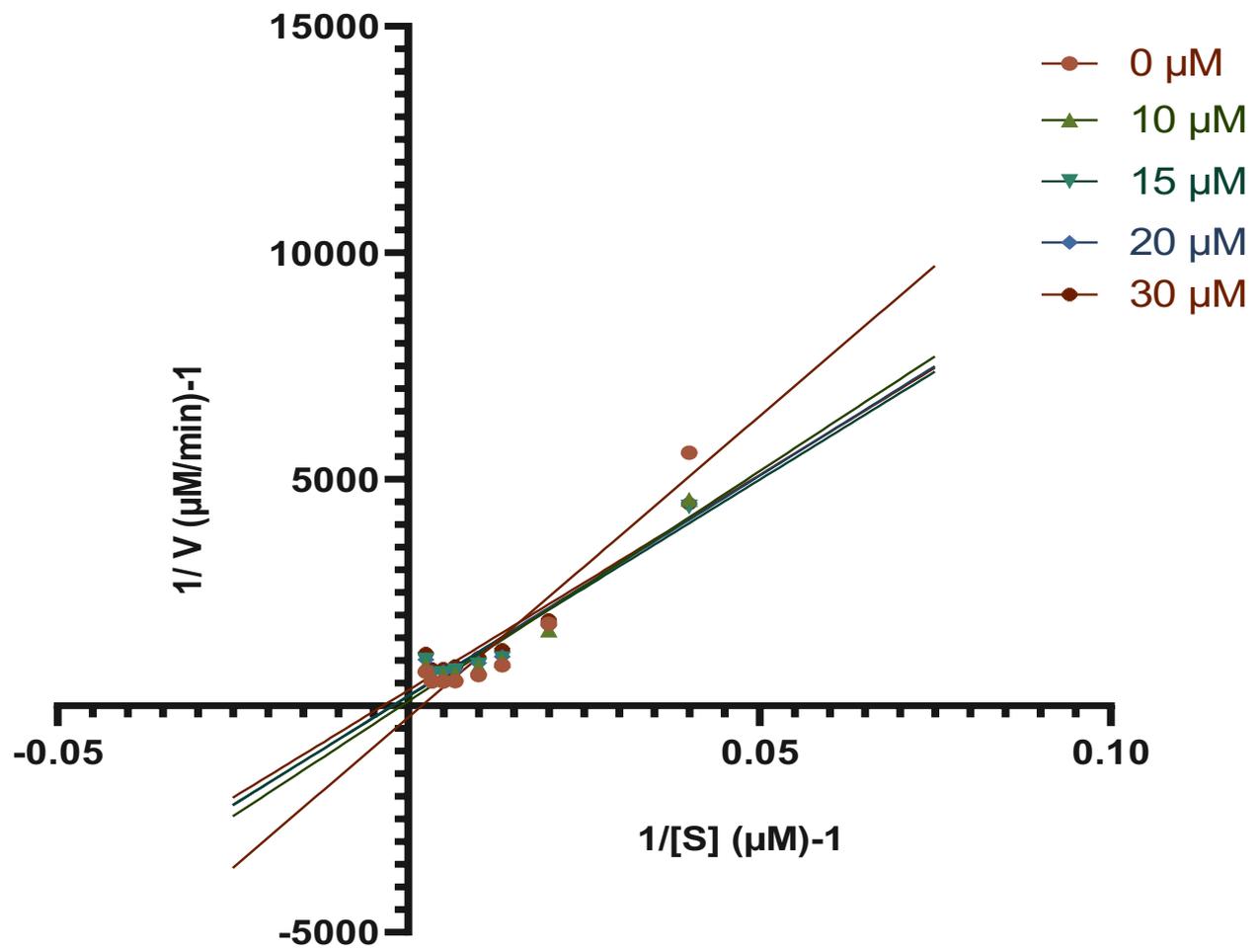


Figure S57 : Lineweaver-Burk Plot of compound 2



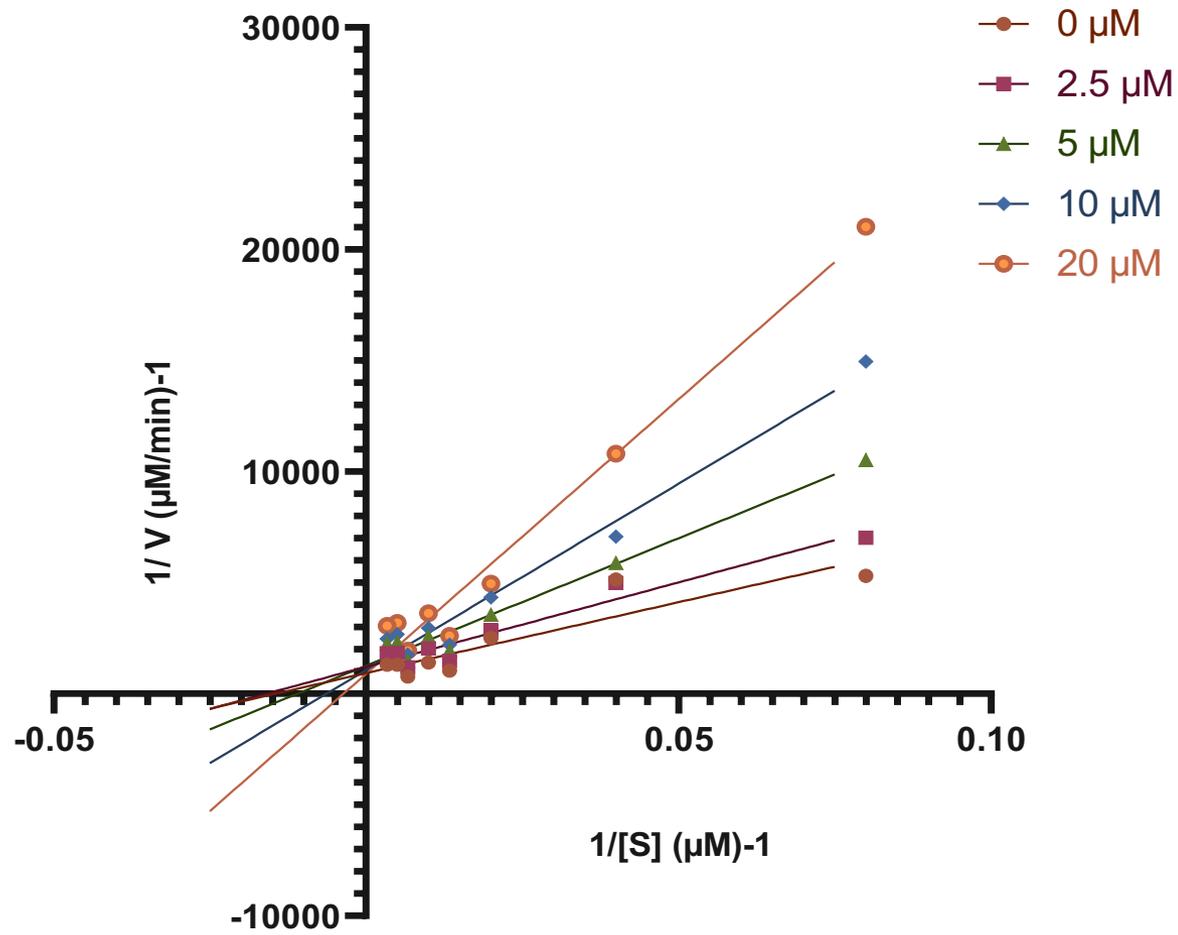
Concentration (μM)	Vmax ($\times 10^{-3}$ mM/min)	Km (μM)	Inhibition type
5	1.1	99.5	Competitive inhibition
10	0.98	129.7	
15	1.04	126.5	
20	1.05	244.0	
40	0.89	244.0	

Figure S58 : Lineweaver-Burk Plot of compound 3



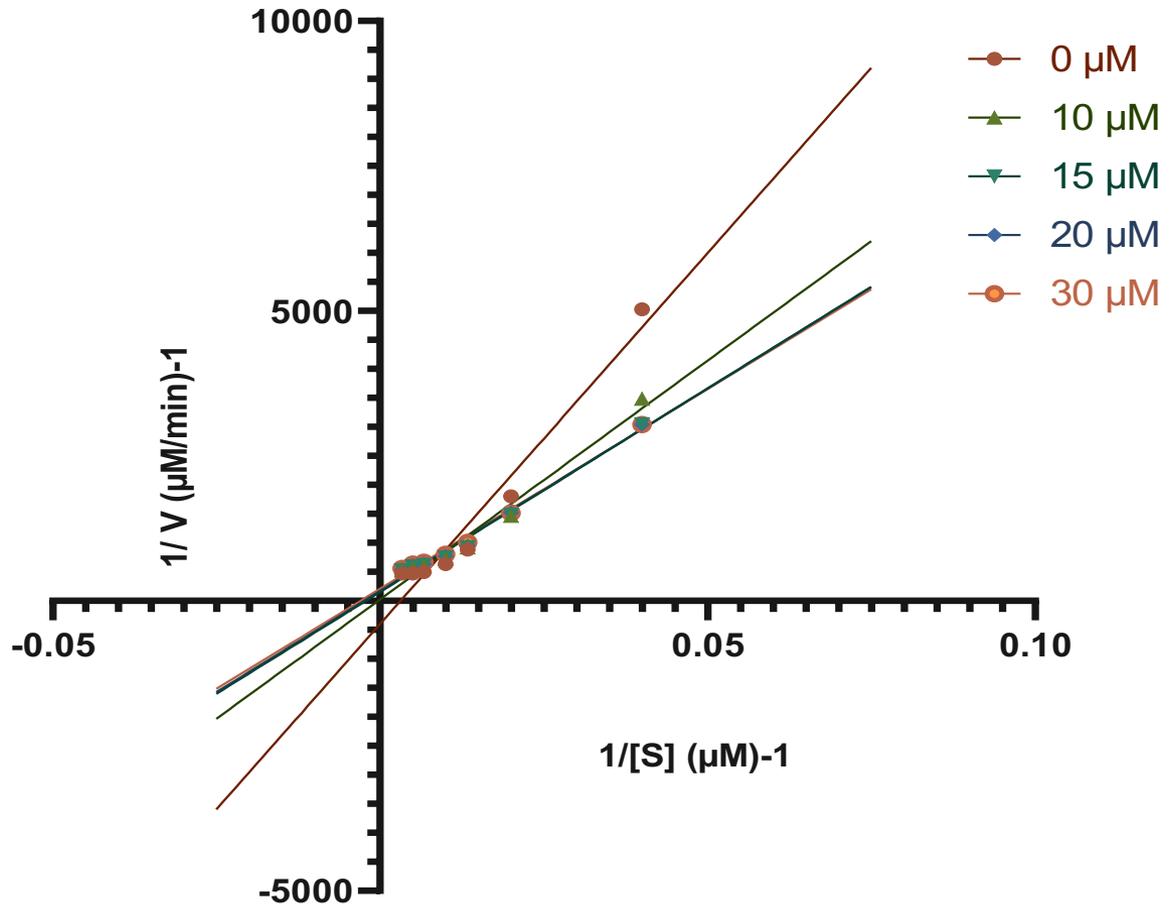
Concentration (μM)	Vmax ($\times 10^{-3}$ mM/min)	Km (μM)	Inhibition type
0	-3.9	-521.8	Mixed inhibition
10	10.1	1030.7	
15	4.8	463.1	
20	4.4	427.4	
30	2.9	275.4	

Figure S59 : Lineweaver-Burk Plot of compound 4



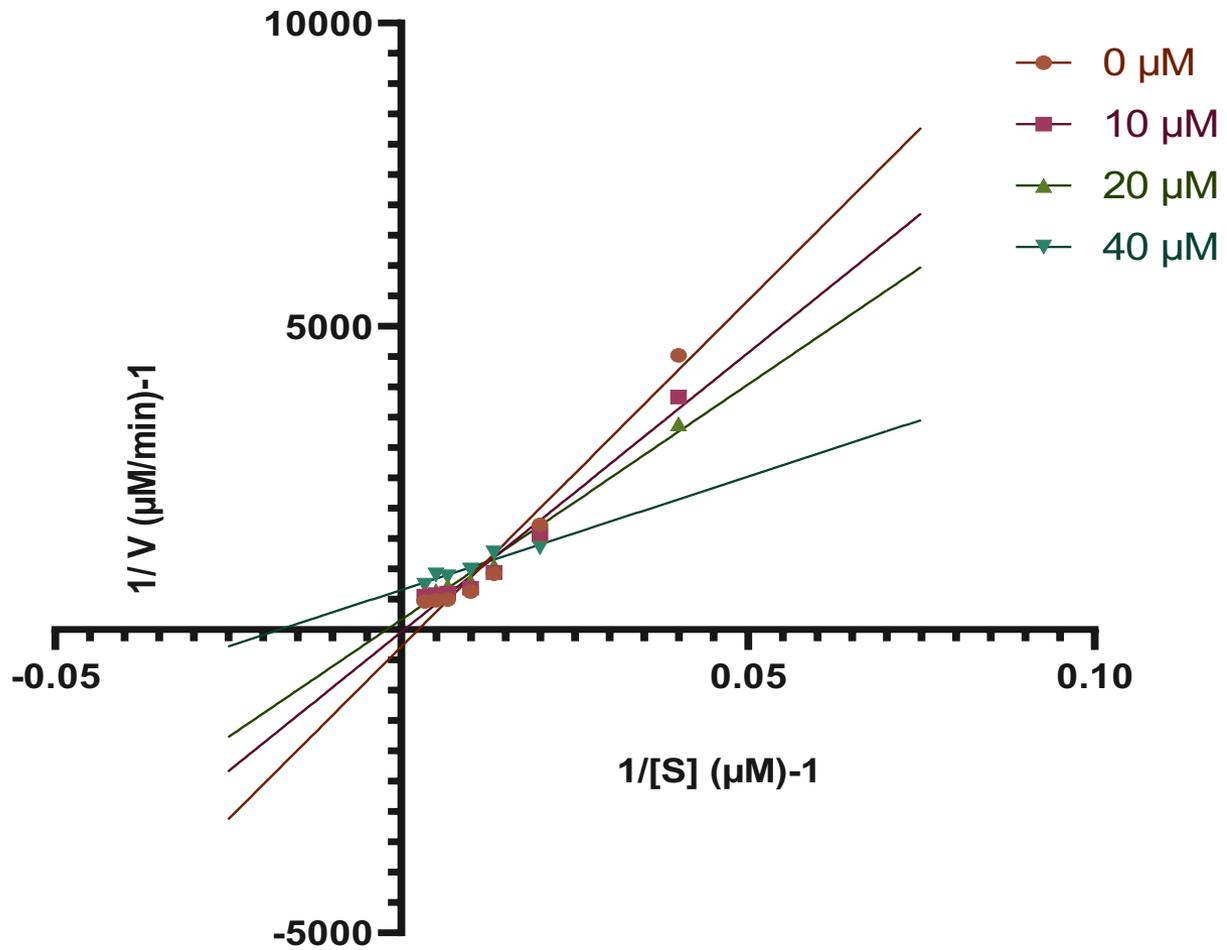
Concentration (μM)	V_{max} ($\times 10^{-3}$ mM/min)	K_m (μM)	Inhibition type
0	1.1	68.7	Competitive inhibition
2.5	0.8	62.5	
5	0.8	91.0	
10	0.9	157.1	
20	1.1	276.9	

Figure S60 : Lineweaver-Burk Plot of compound 5



Concentration (μM)	Vmax ($\times 10^{-3}$ mM/min)	Km (μM)	Inhibition type
0	-2.5	-320.5	Mixed inhibition
10	40.6	3342.3	
15	6.6	460.8	
20	5.8	406.2	
30	4.8	333.3	

Figure S61 : Lineweaver-Burk Plot of compound 6



Concentration (μM)	Vmax ($\times 10^{-3}$ mM/min)	Km (μM)	Inhibition type
0	-3.6	-407.4	Mixed inhibition
10	-25.8	-2373.9	
20	6.1	471.1	
40	1.5	57.0	