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.

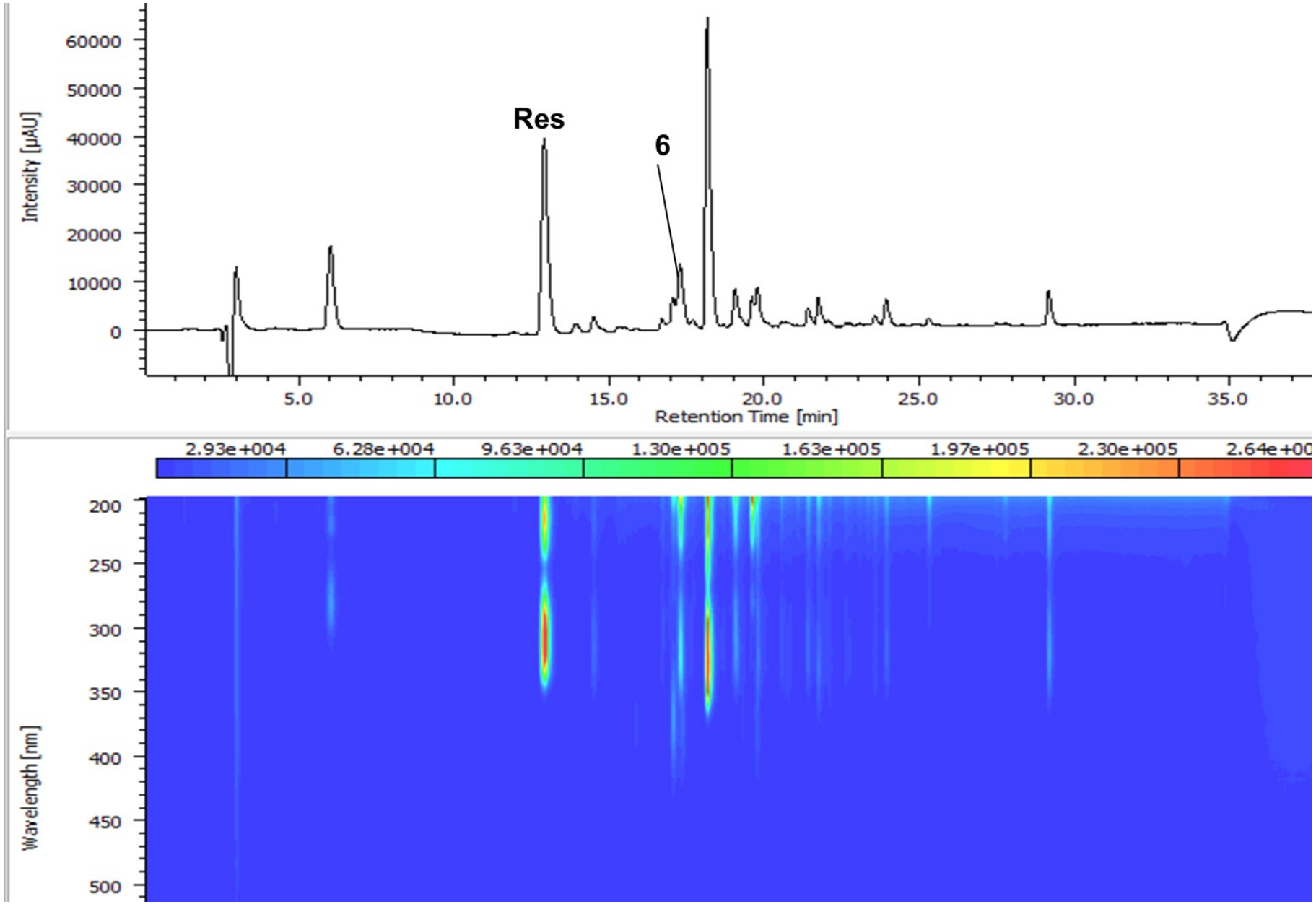


Figure S2. HPLC-PDA fingerprint of oxidized product mixture Ox2.

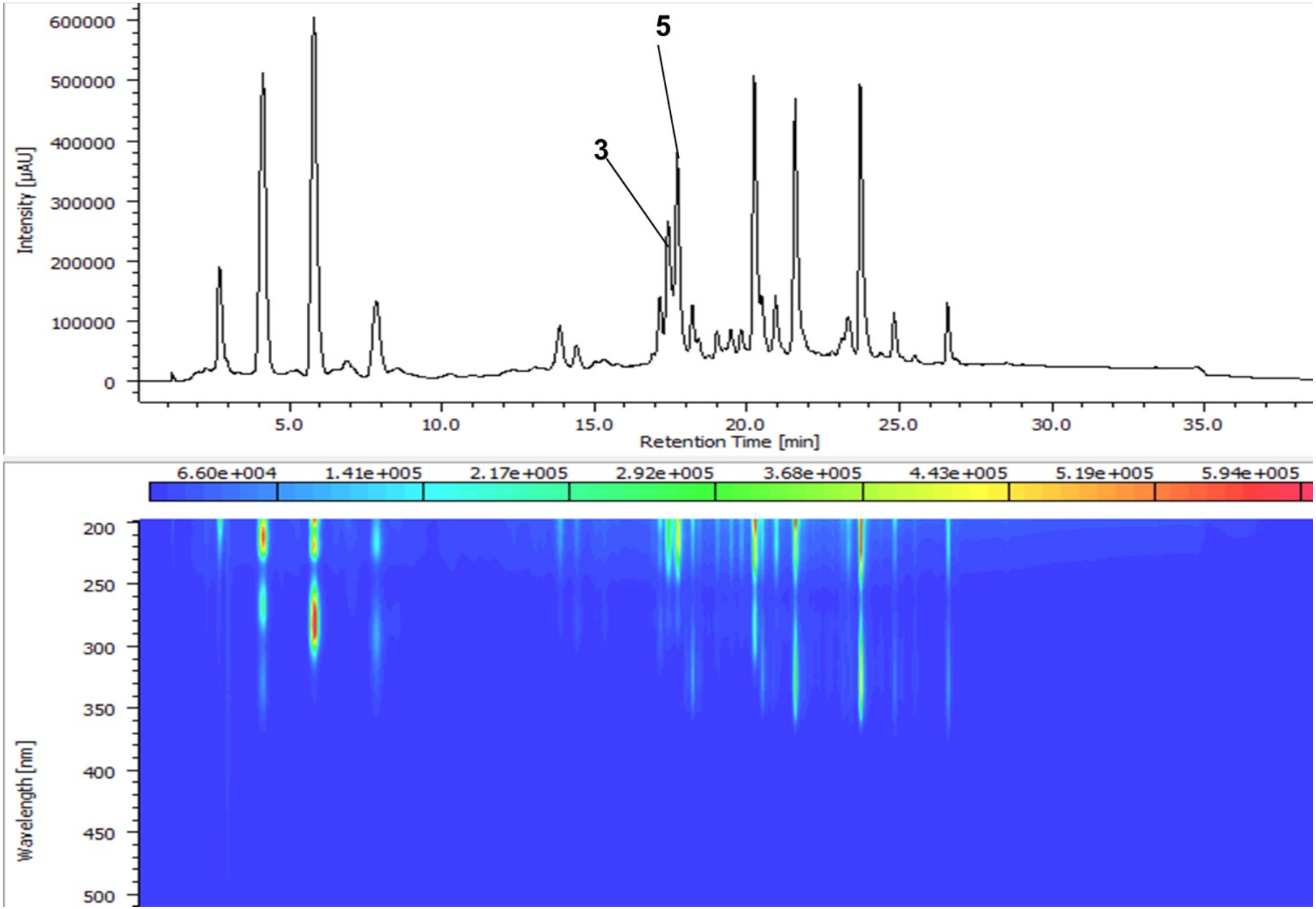


Figure S3. HPLC-PDA fingerprint of oxidized product mixture Ox3.

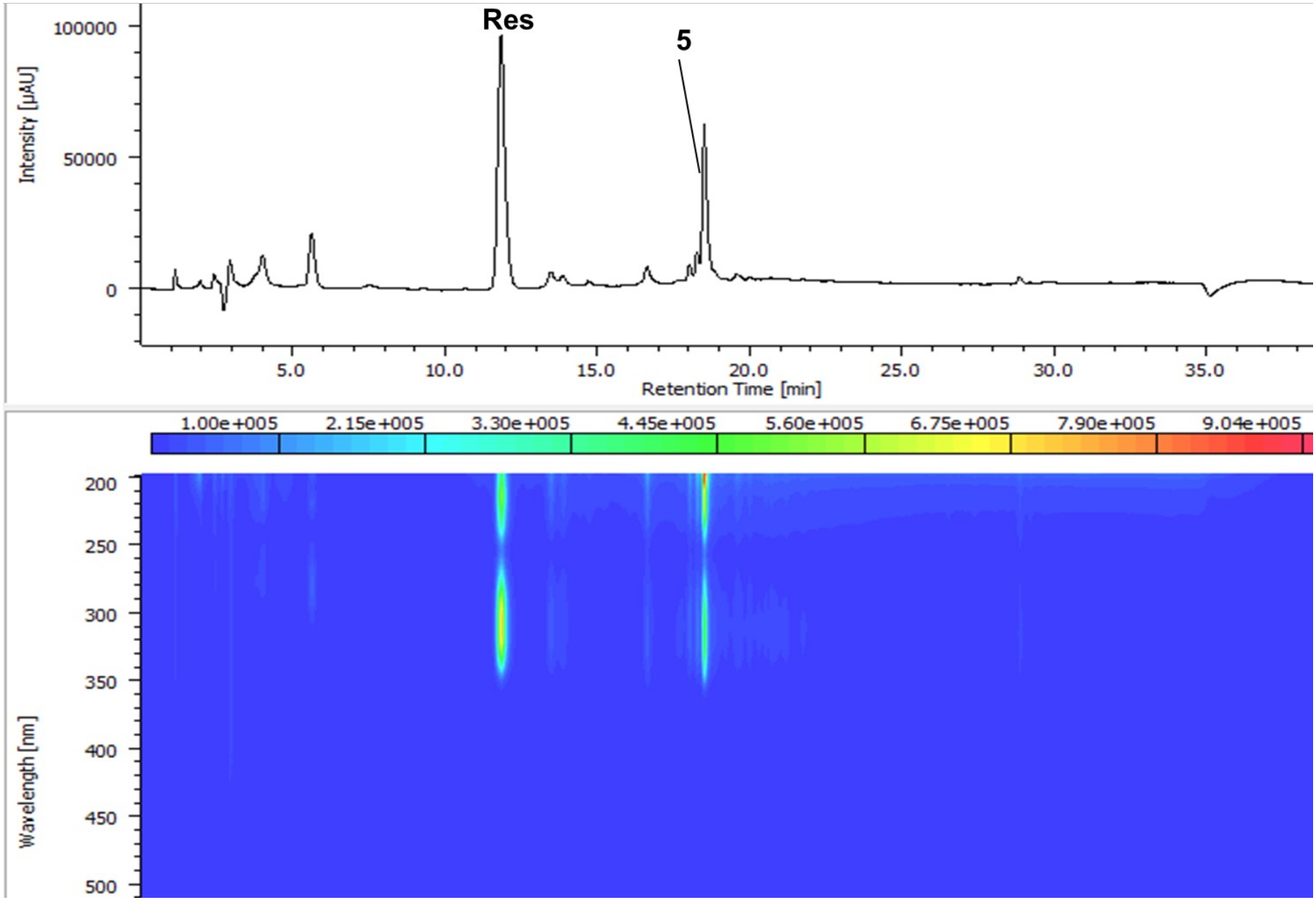


Figure S4. HPLC-PDA fingerprint of oxidized product mixture Ox4.

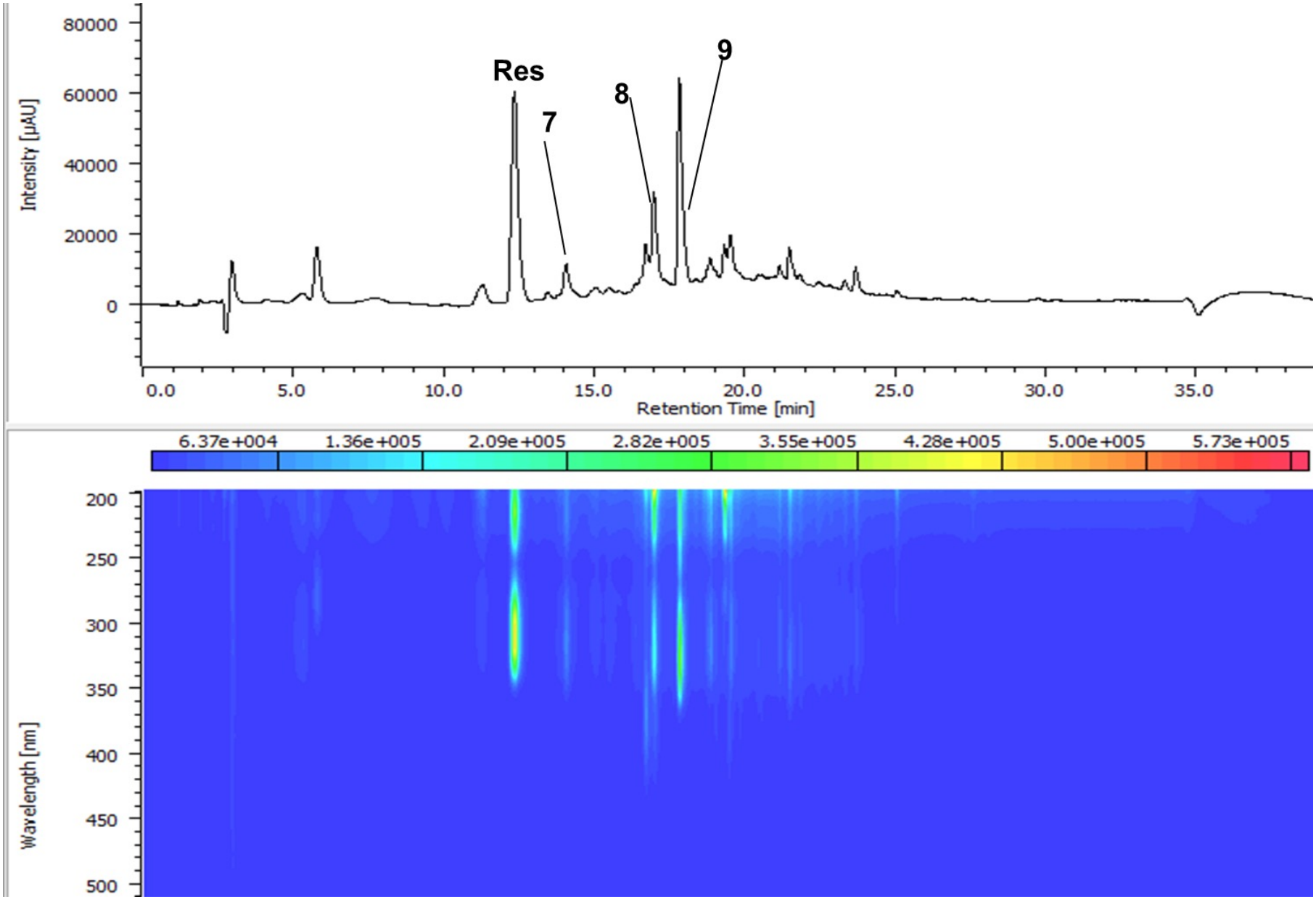


Figure S5. HPLC-PDA fingerprint of oxidized product mixture Ox5.

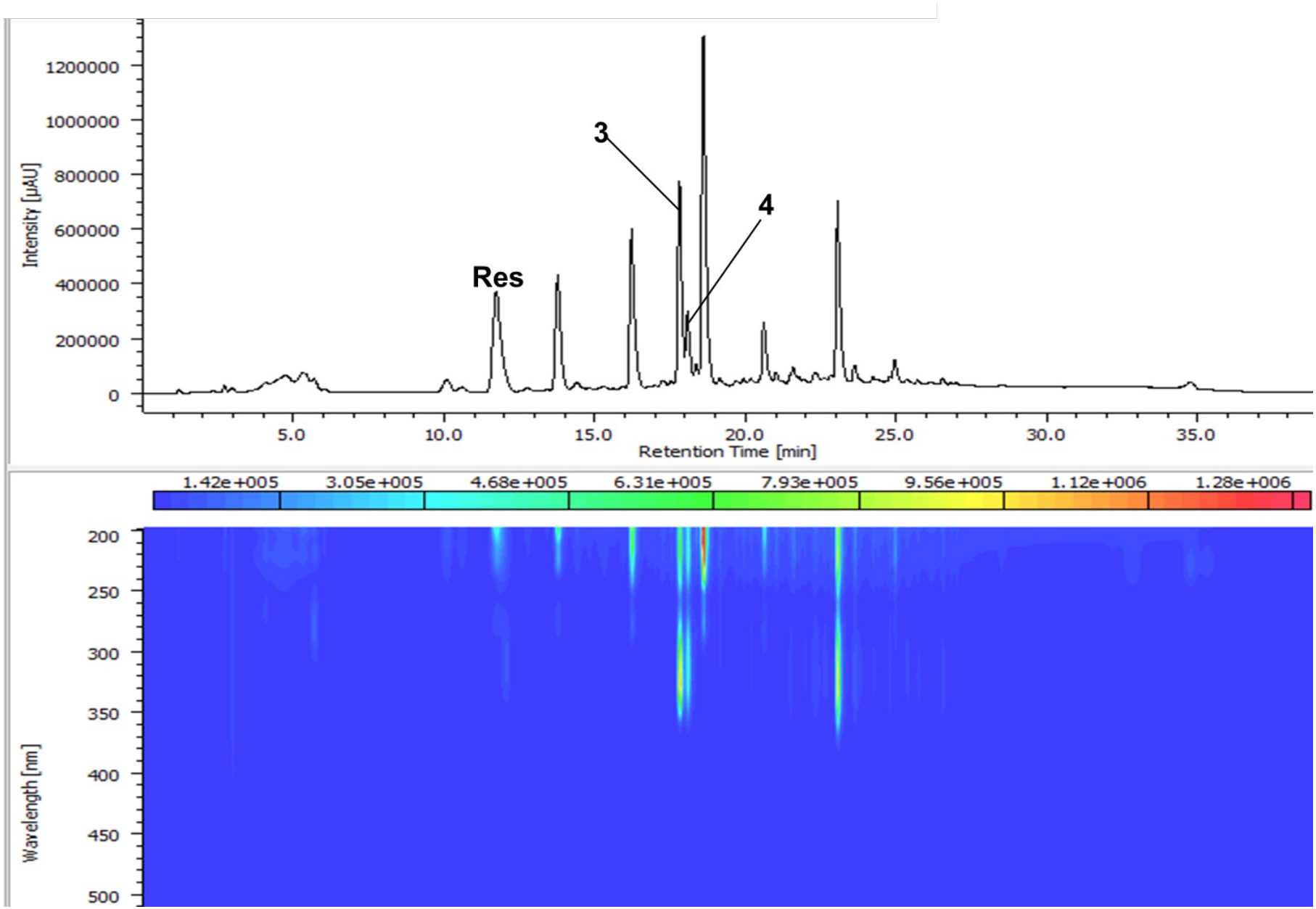


Figure S6. HPLC-PDA fingerprint of oxidized product mixture Ox6.

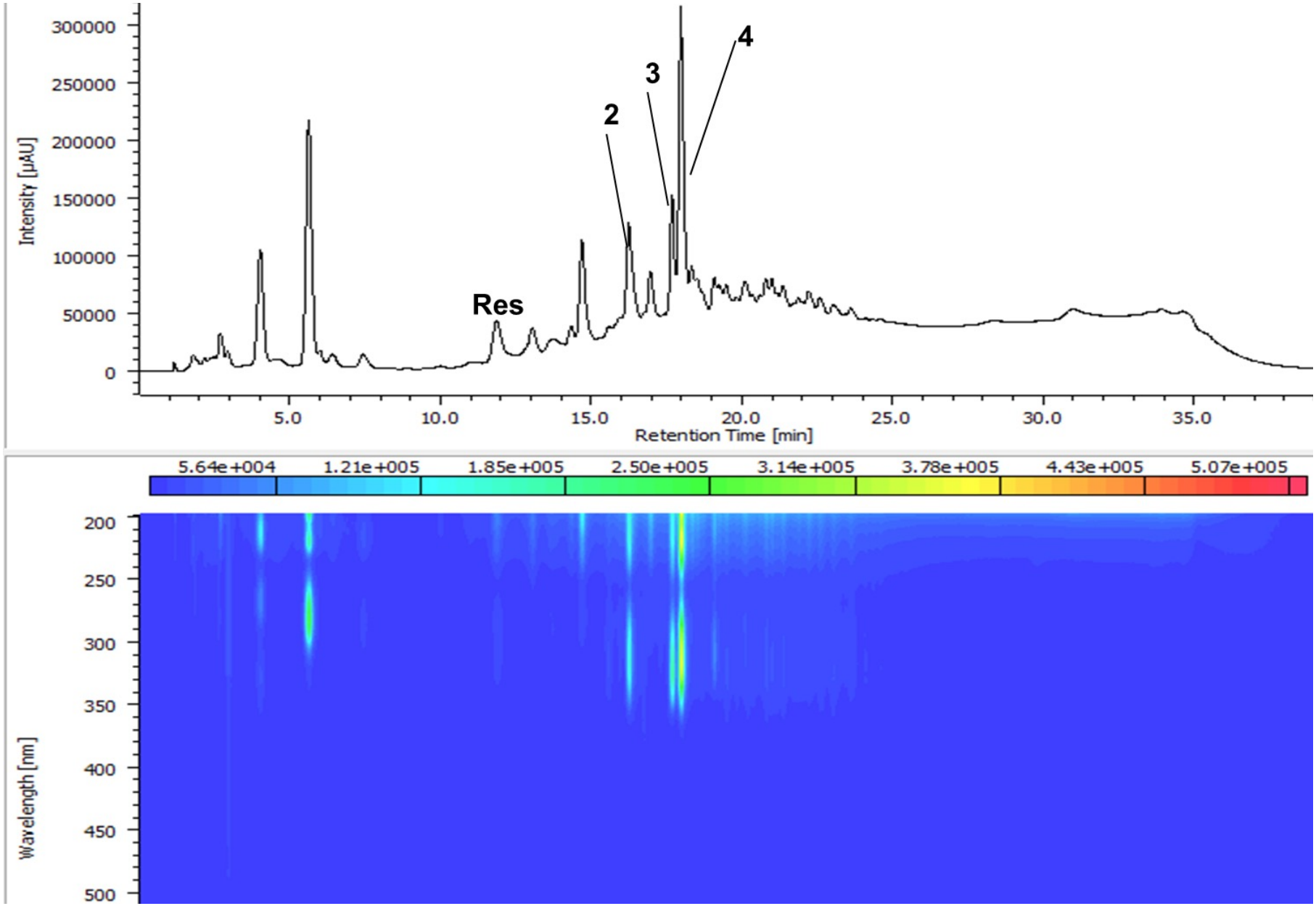


Figure S7. HPLC-PDA fingerprint of oxidized product mixture Ox7.

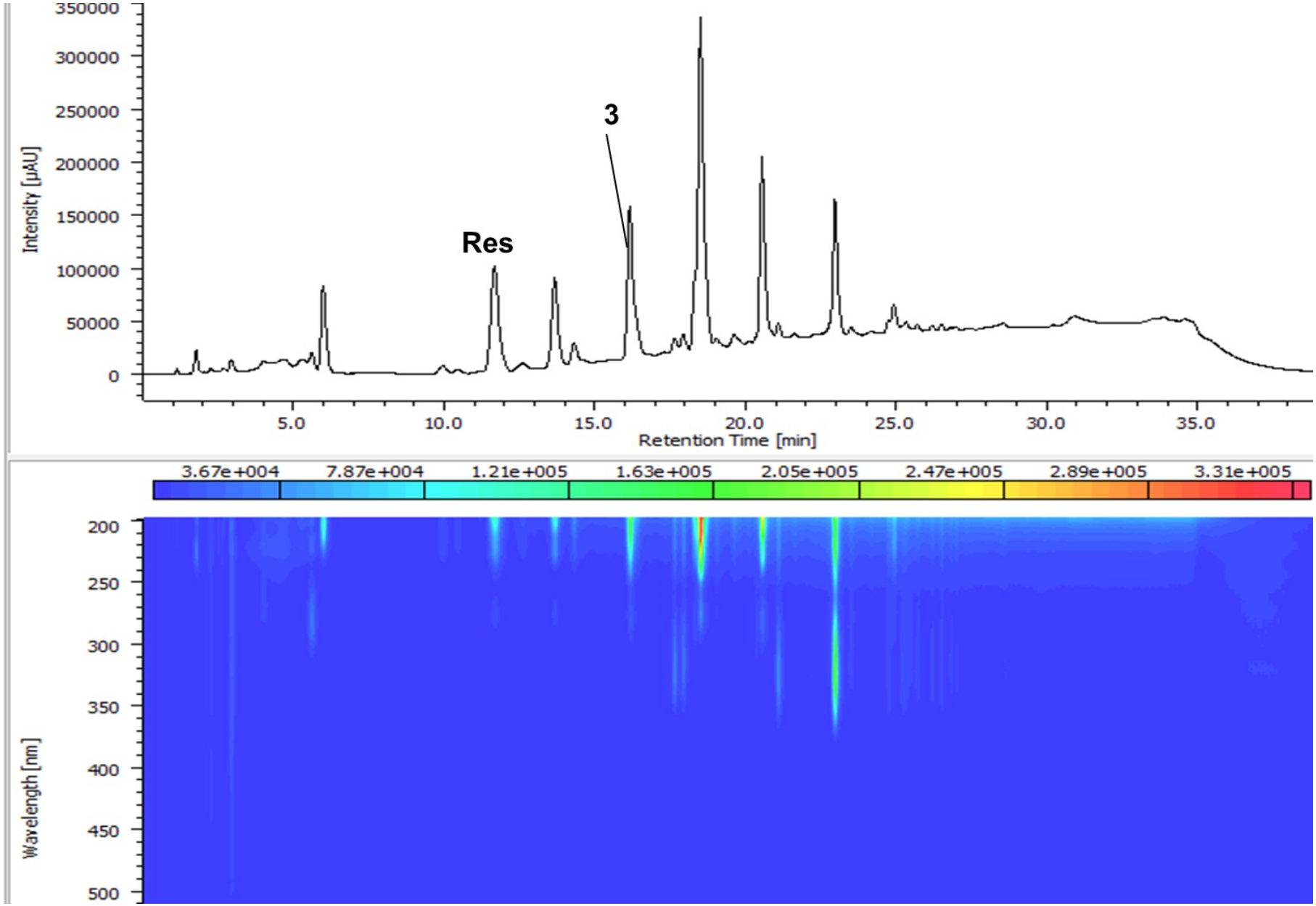
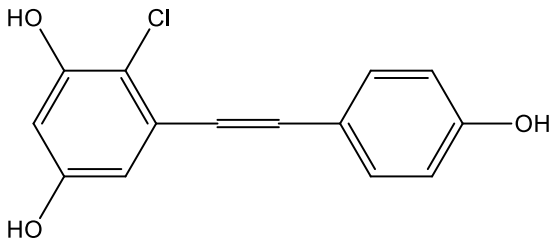
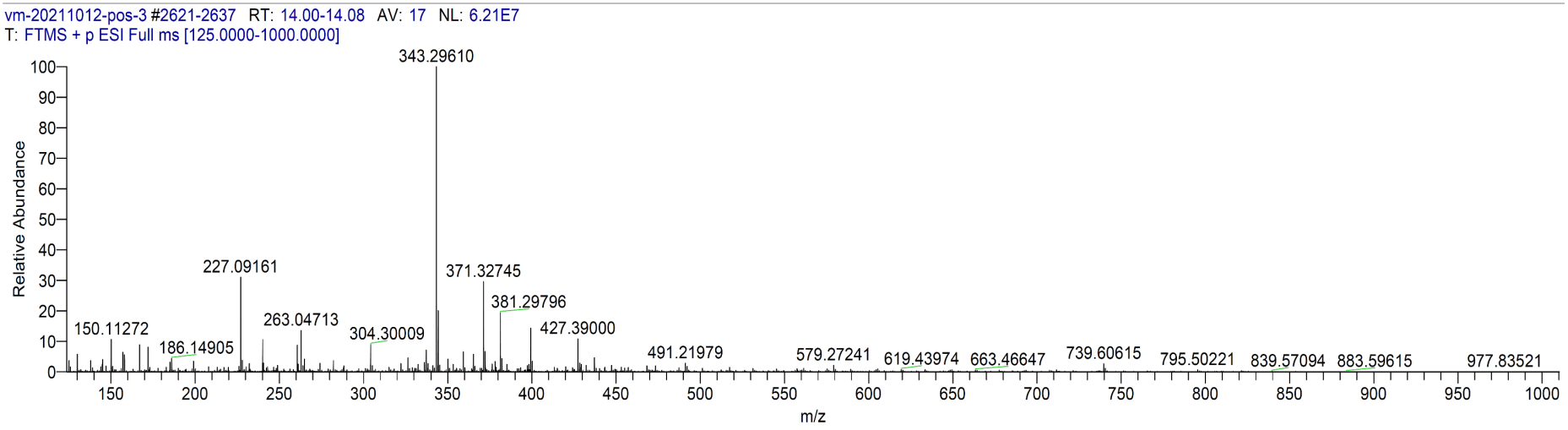


Figure S8. Compound **2**, HRMS (positive mode).



2

$C_{14}H_{11}O_3Cl$



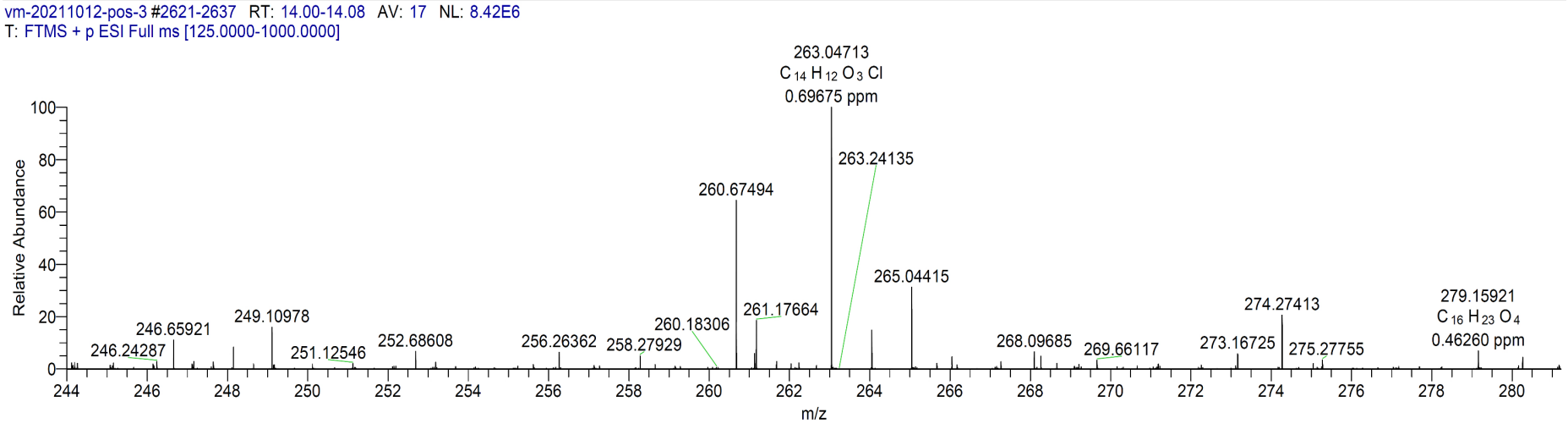
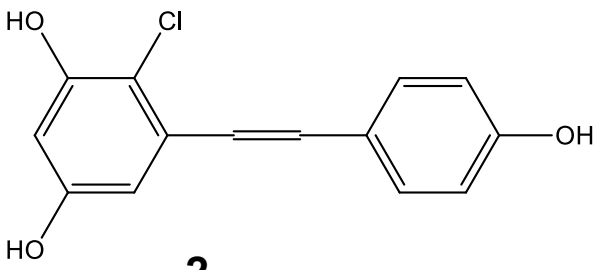


Figure S9. Compound **2**, HRMS (negative mode).



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$C_{14}H_{11}O_3Cl$

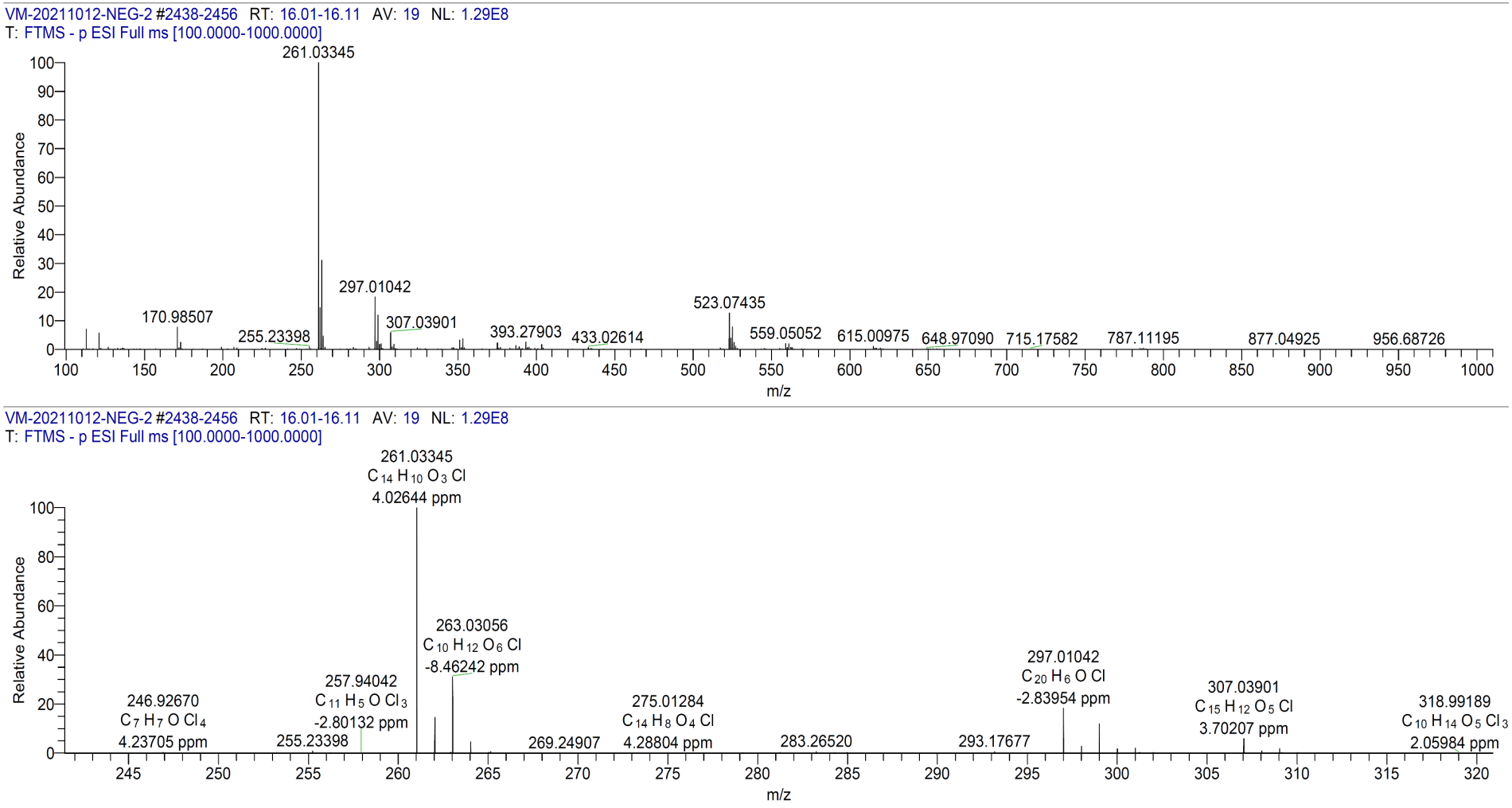
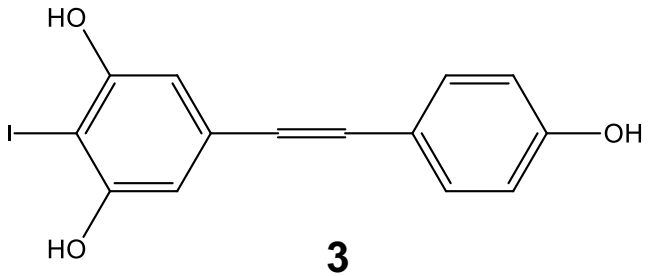


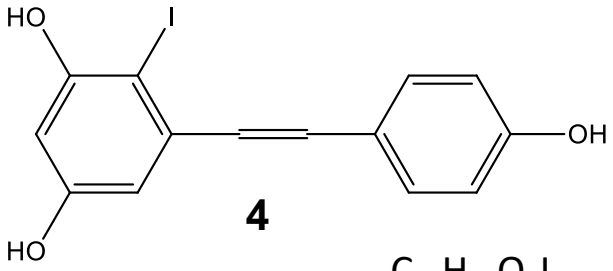
Figure S10. Compound **3**, HRMS (negative mode).



3

$C_{14}H_{11}O_3I$

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



4

$C_{14}H_{11}O_3I$

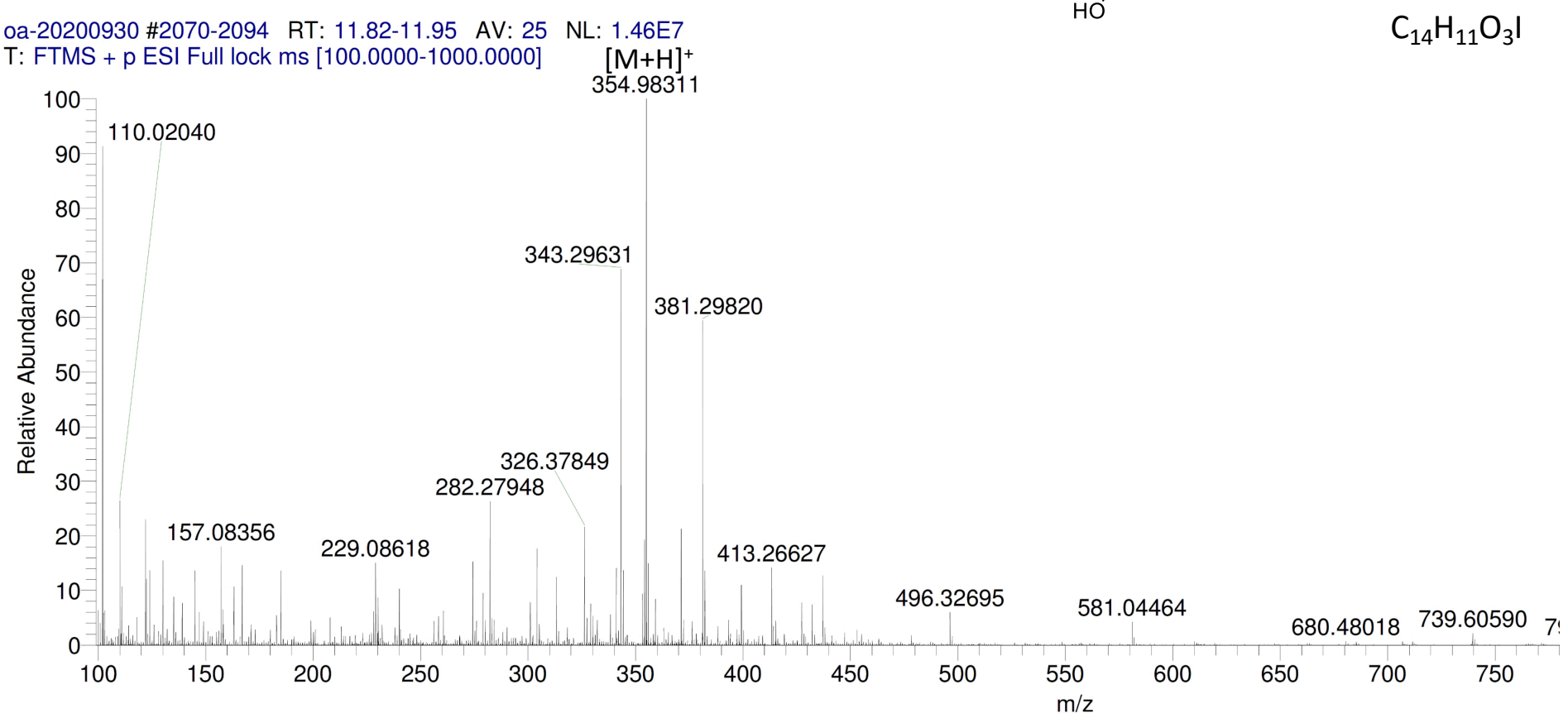
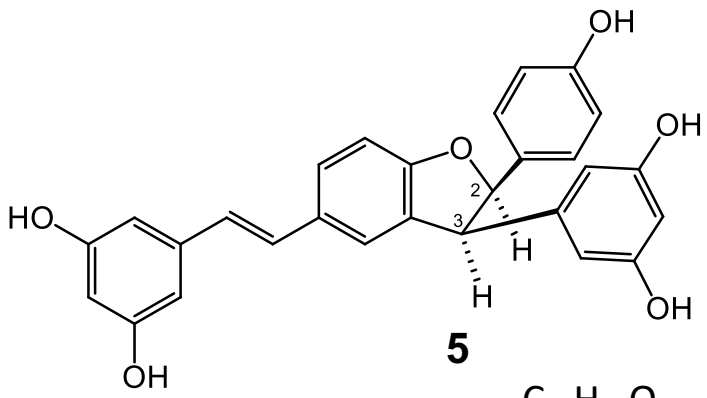


Figure S12. Compound **5**, HRMS (positive mode).



5

$C_{28}H_{22}O_6$

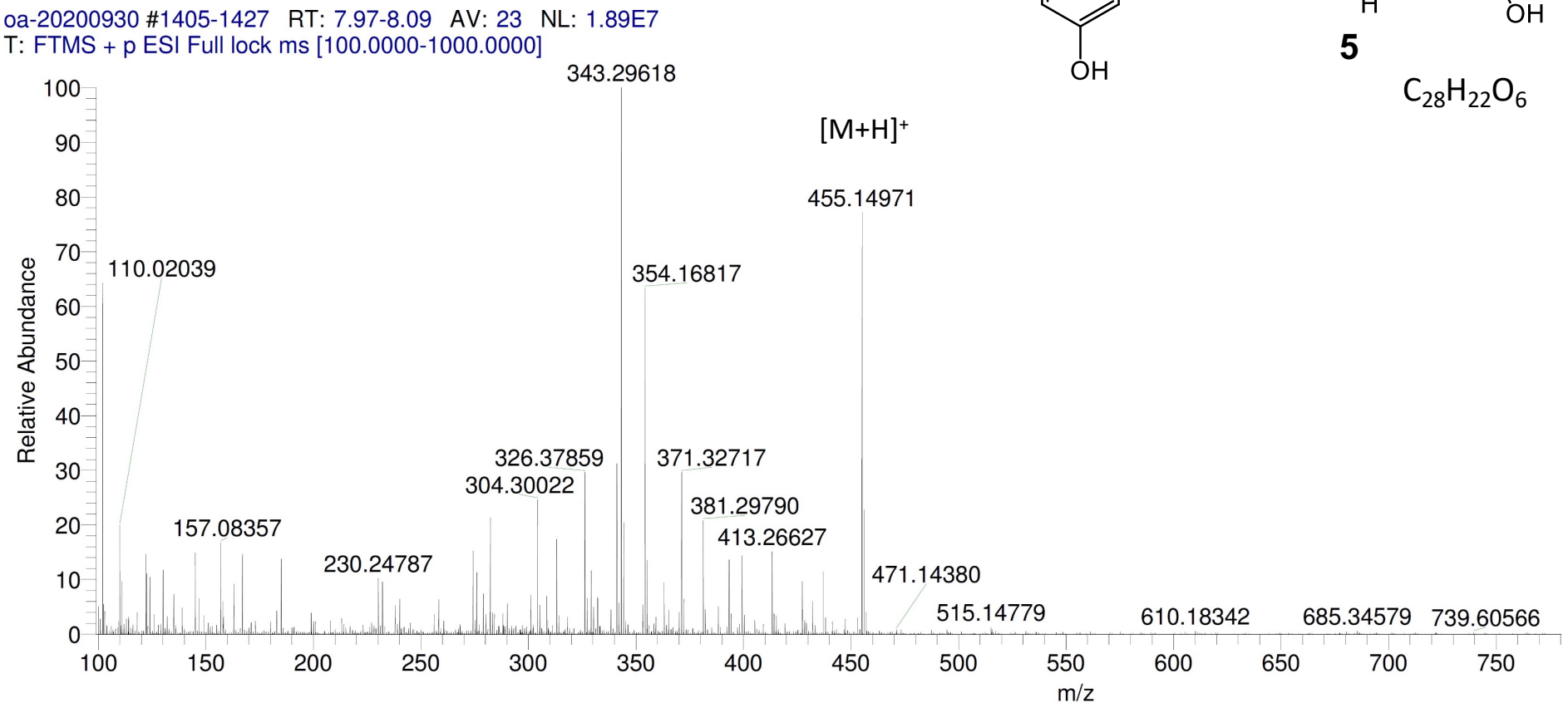


Figure S13. Compound **6**, HRMS (positive mode).

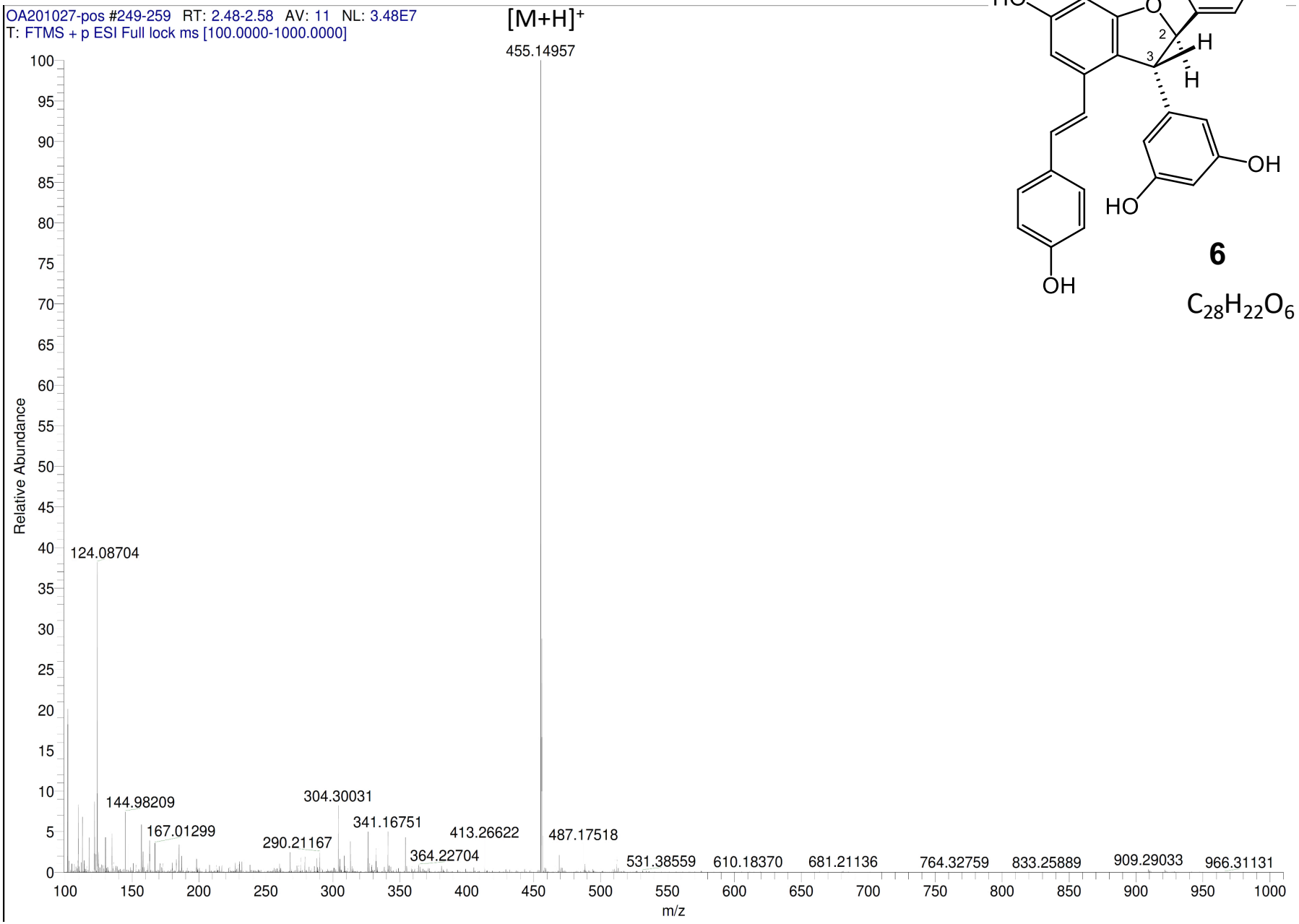


Figure S14. Compound **7**, HRMS (negative mode).

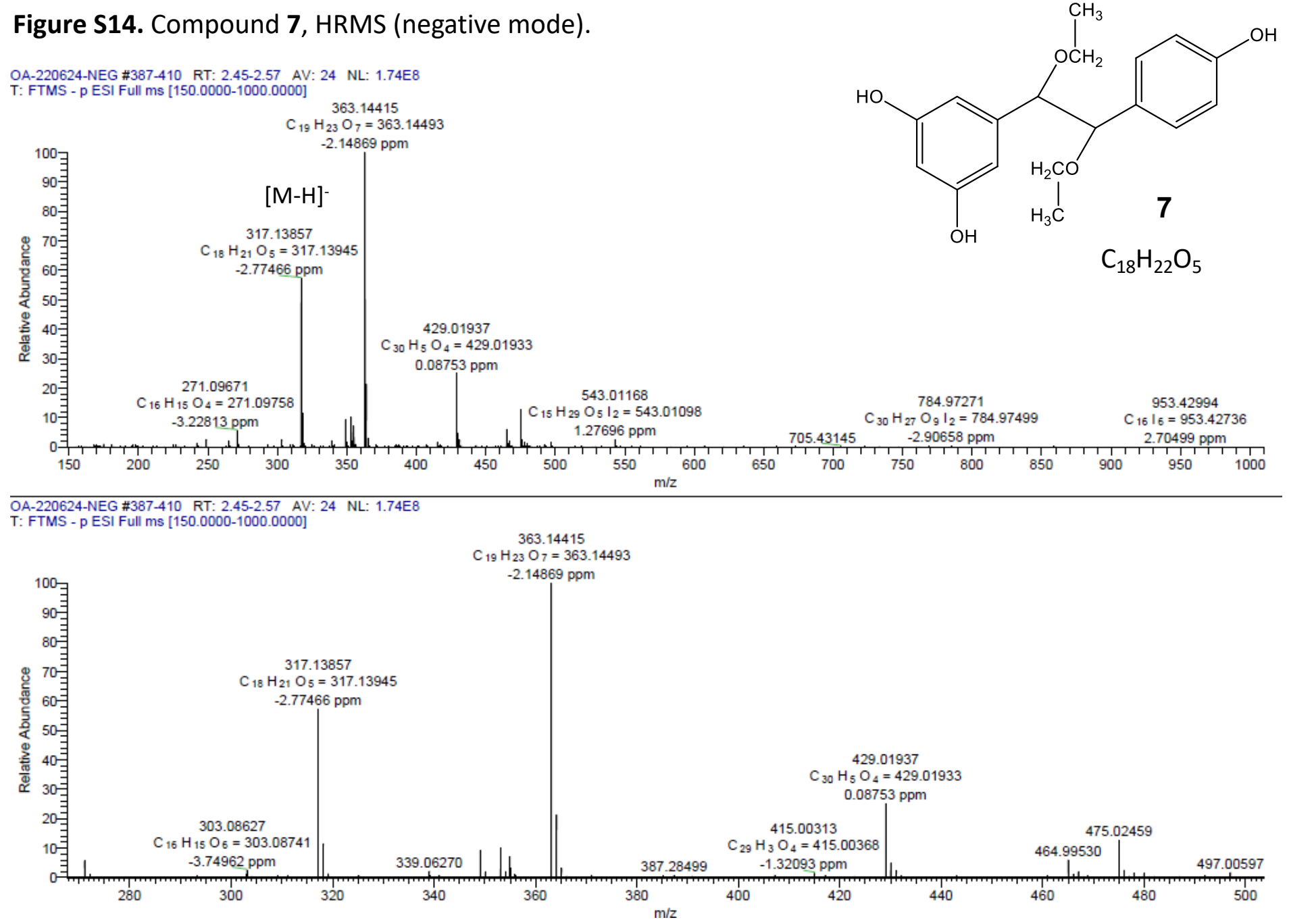
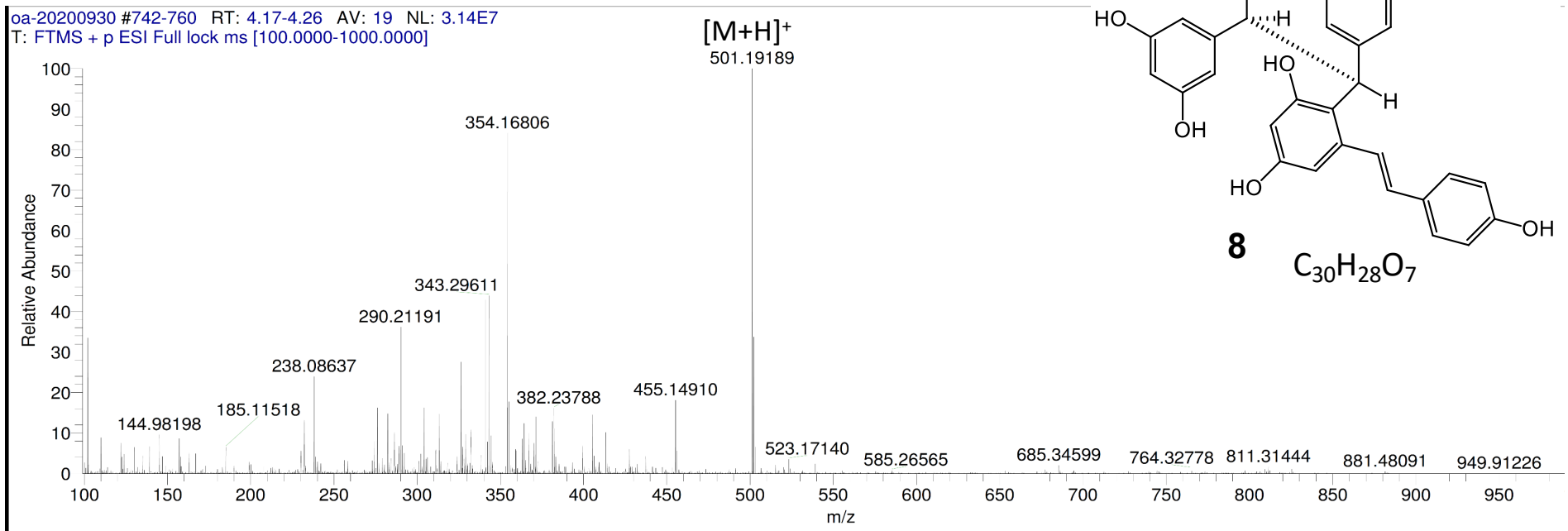


Figure S15. Compound **8**, HRMS (positive mode).



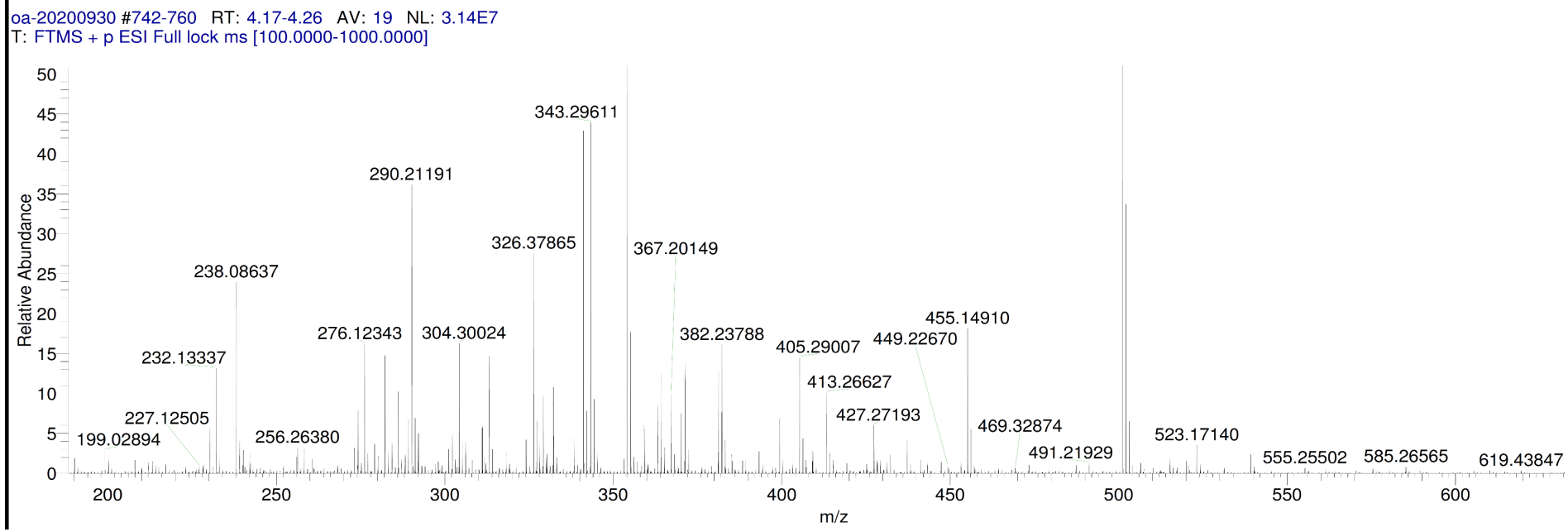
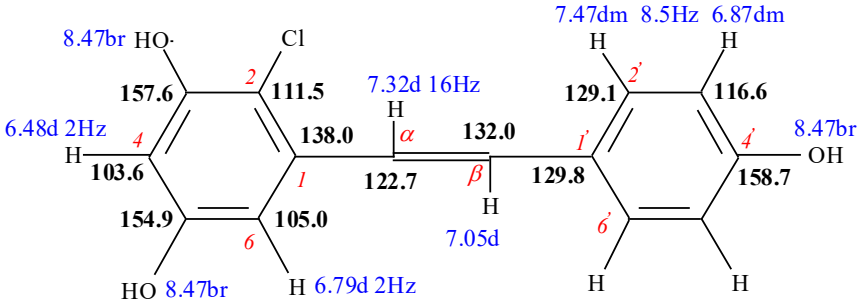


Figure S16. Compound **2**, ^{1}H NMR spectrum.



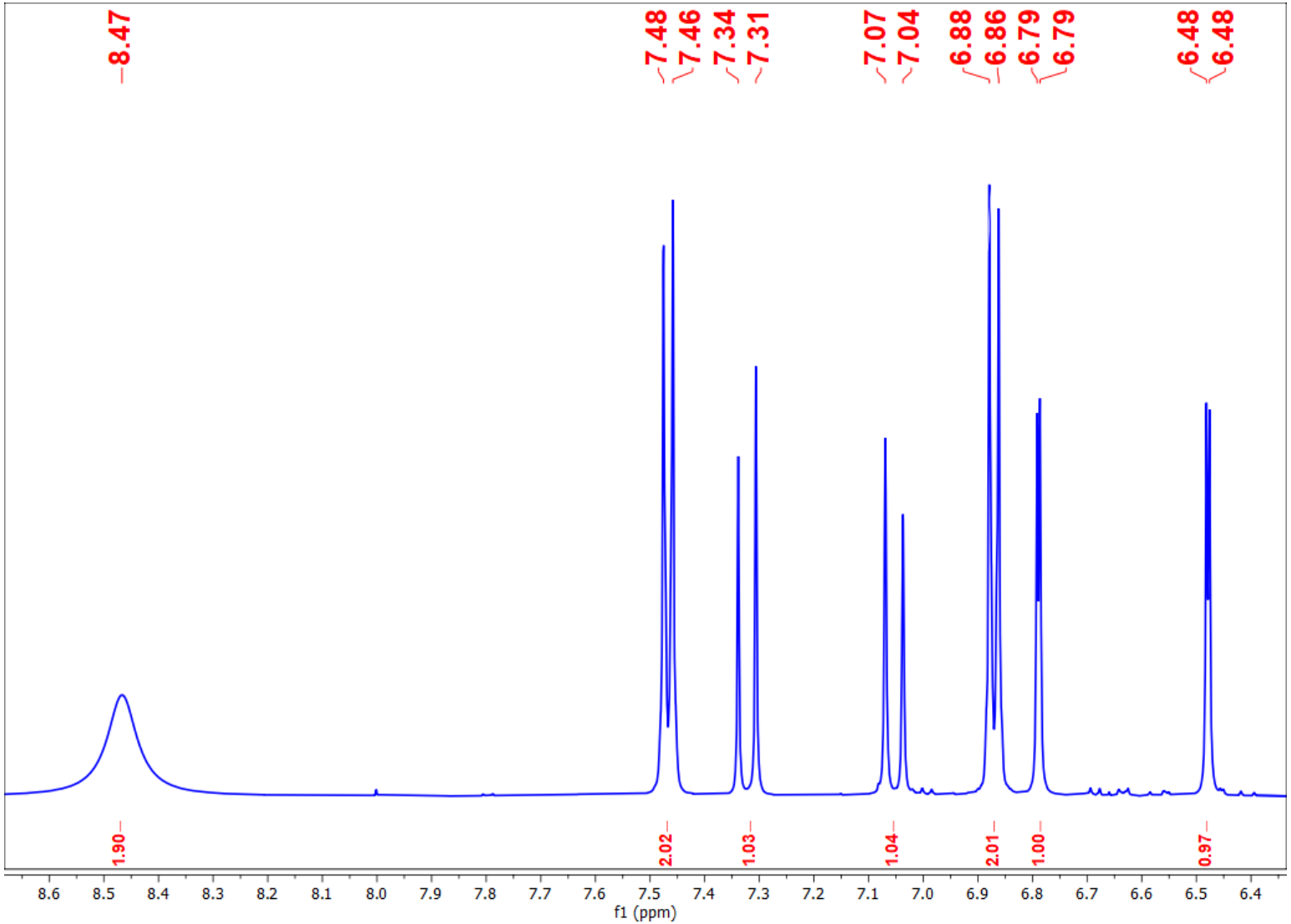
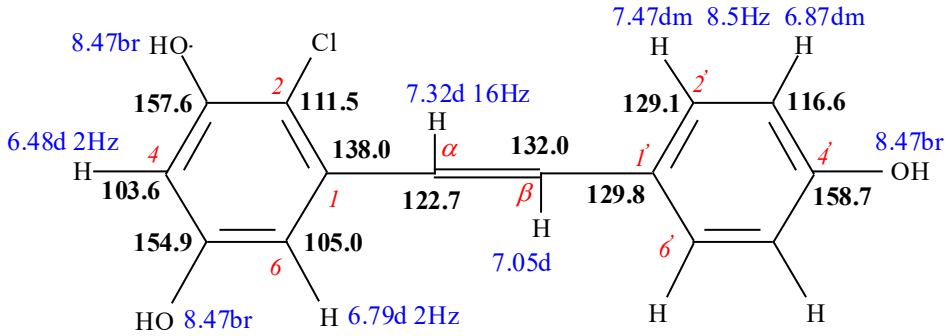


Figure S17. Compound **2**, ^{13}C, APT NMR spectrum



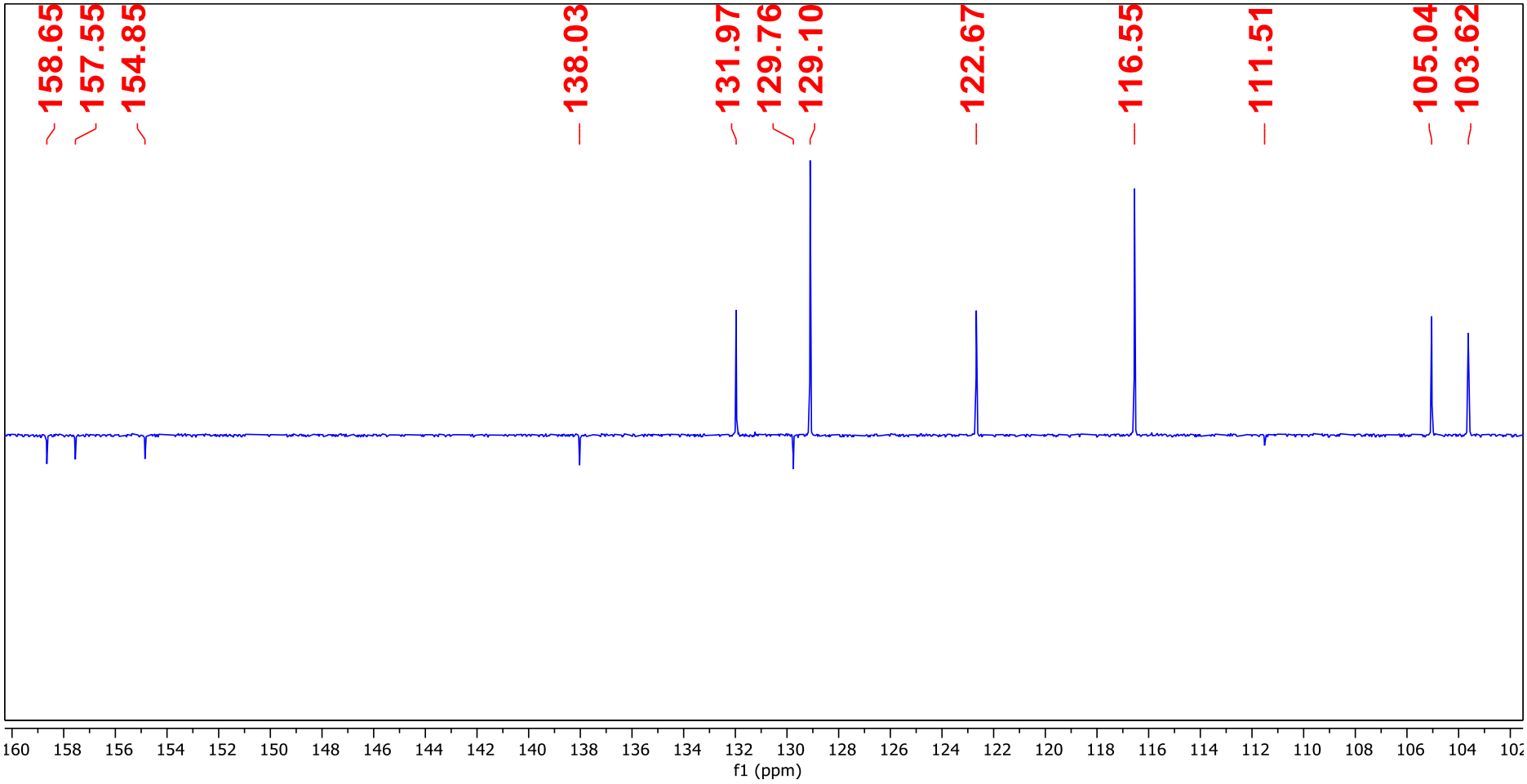


Figure S18. Compound **2**, HSQC and HMBC spectra.

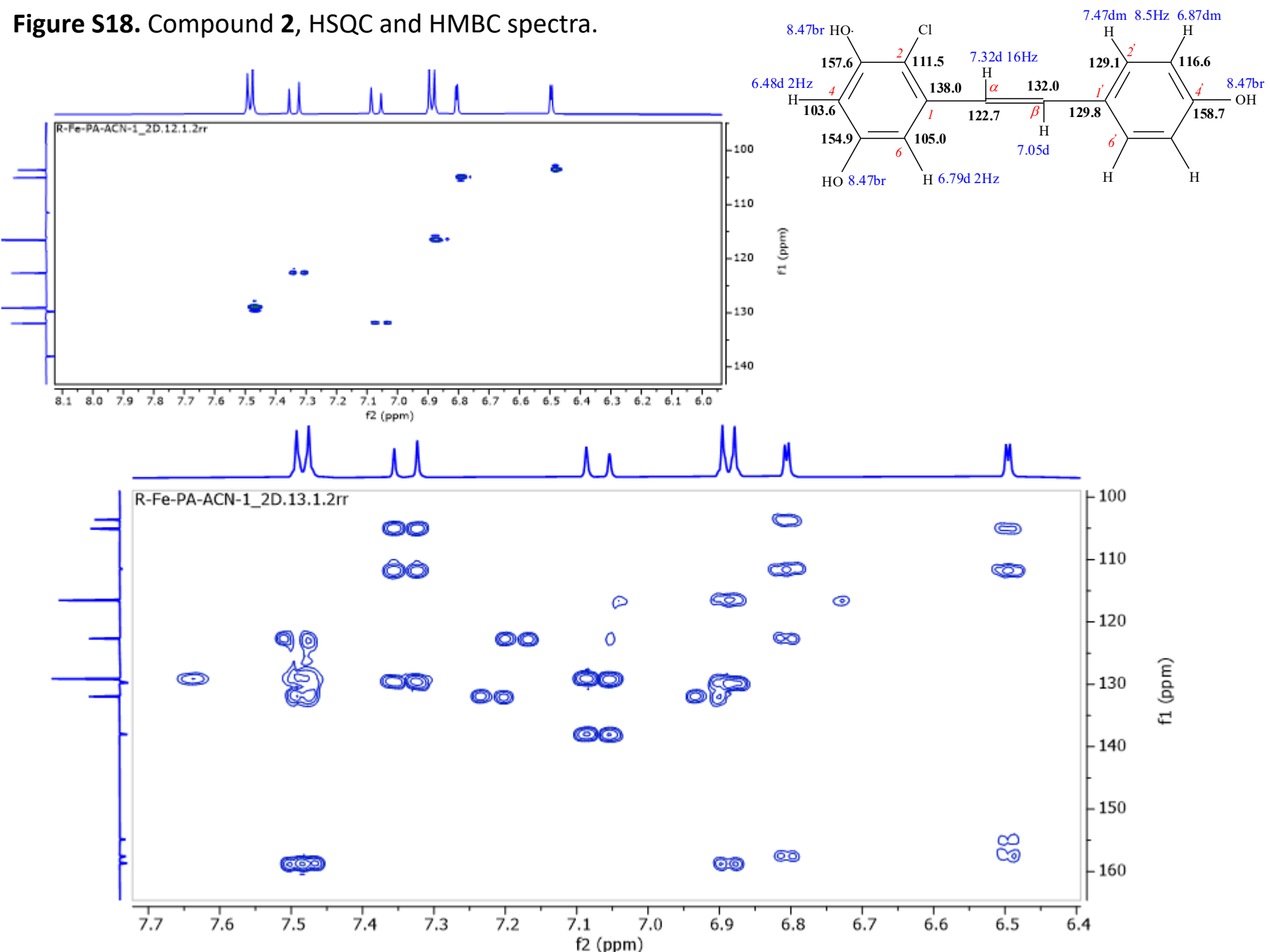
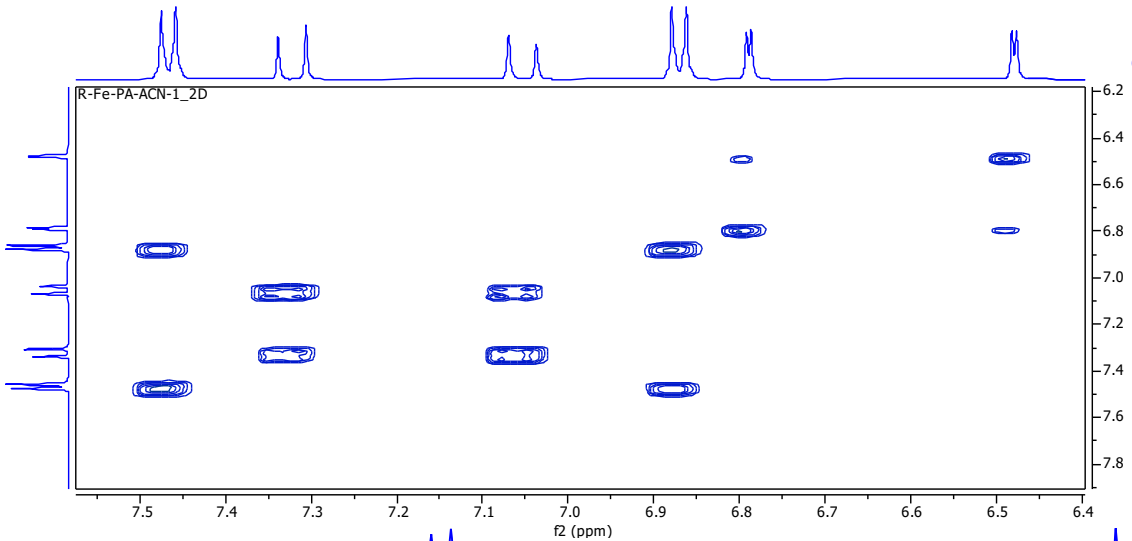
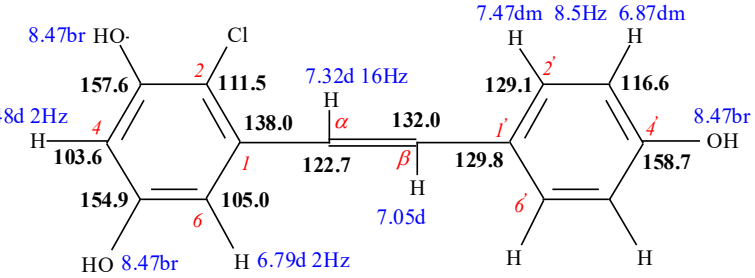


Figure S19. Compound **2**, COSY and NOESY spectra.





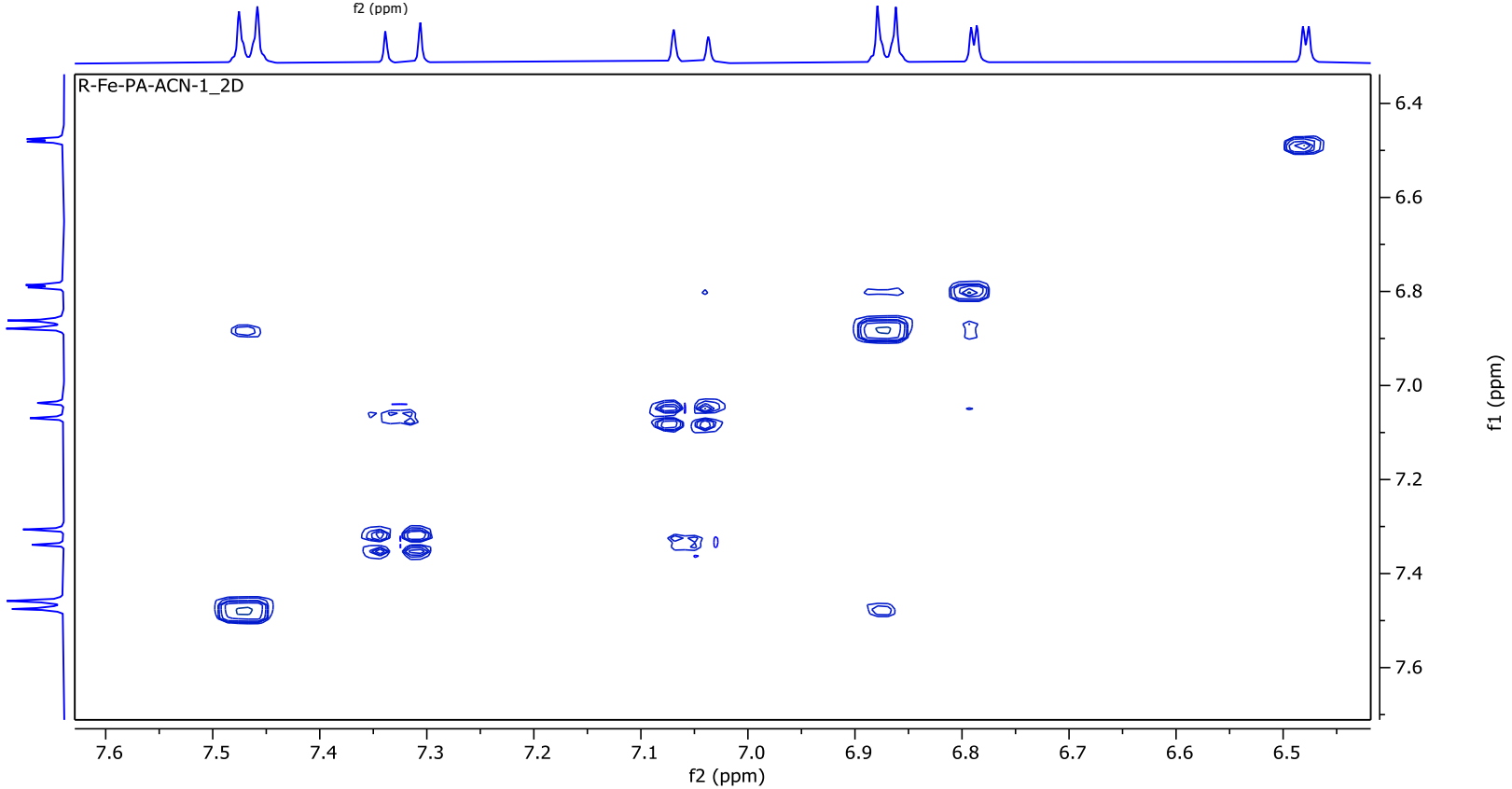
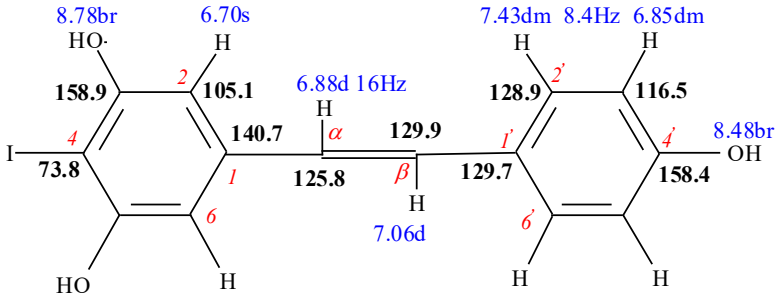


Figure S20. Compound **3**, ^{1}H NMR spectrum.



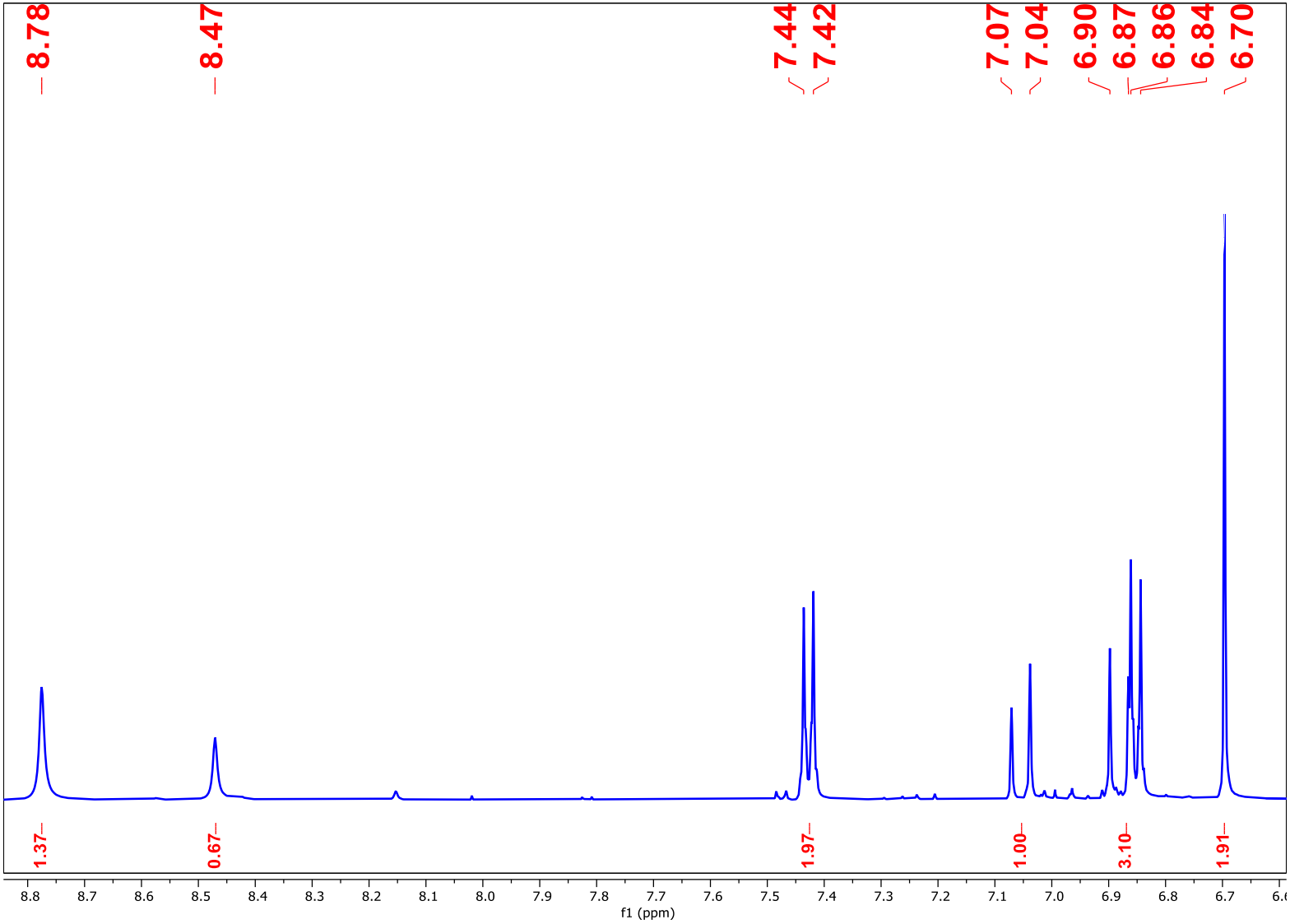
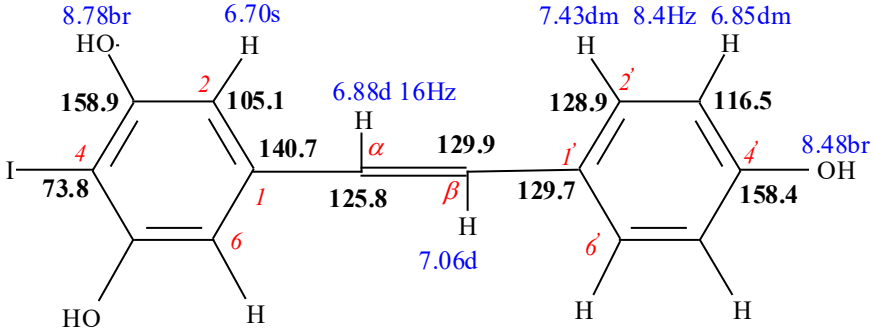


Figure S21. Compound **3**, ^{13}C, APT NMR spectrum.



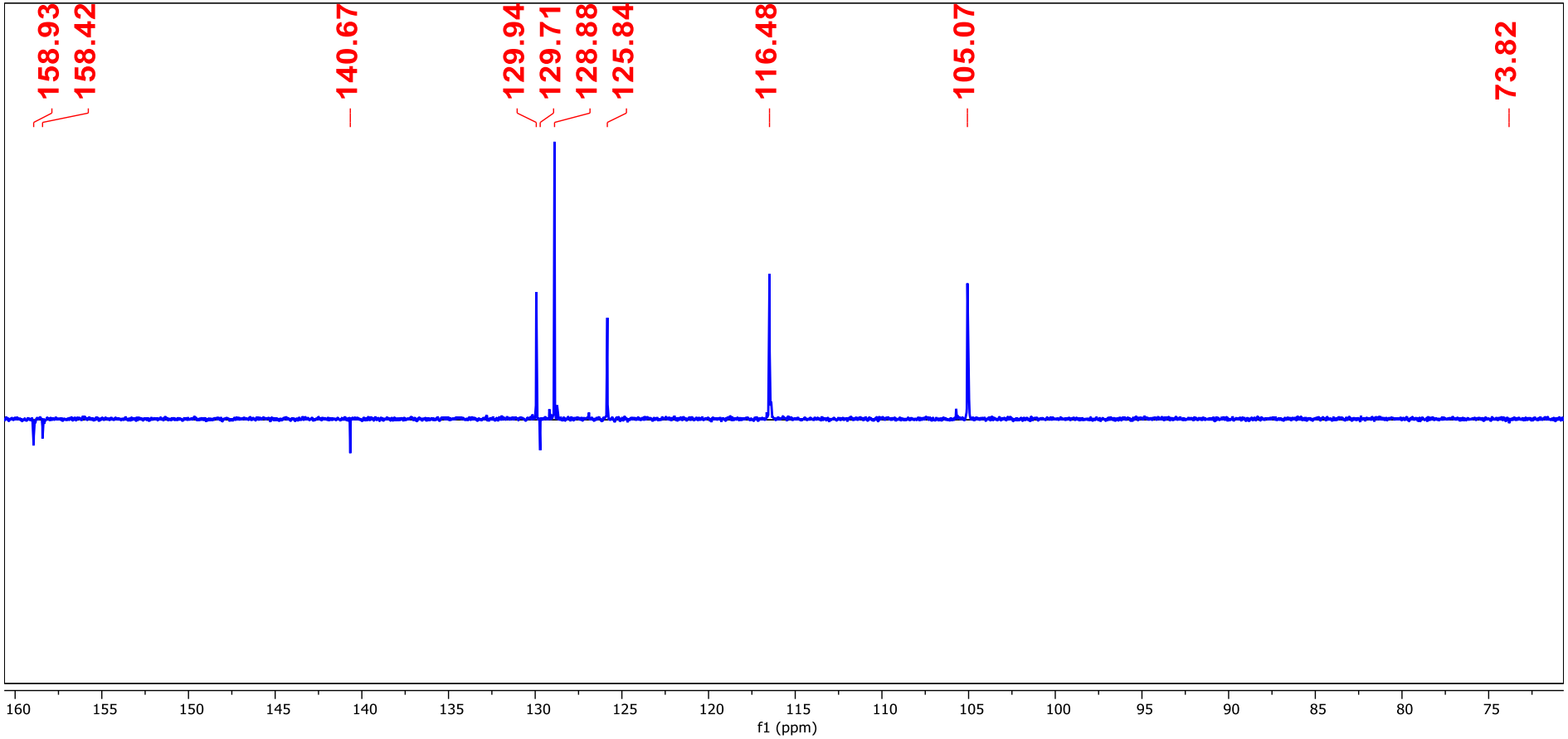


Figure S22. Compound **3**, HSQC and HMBCspectra.

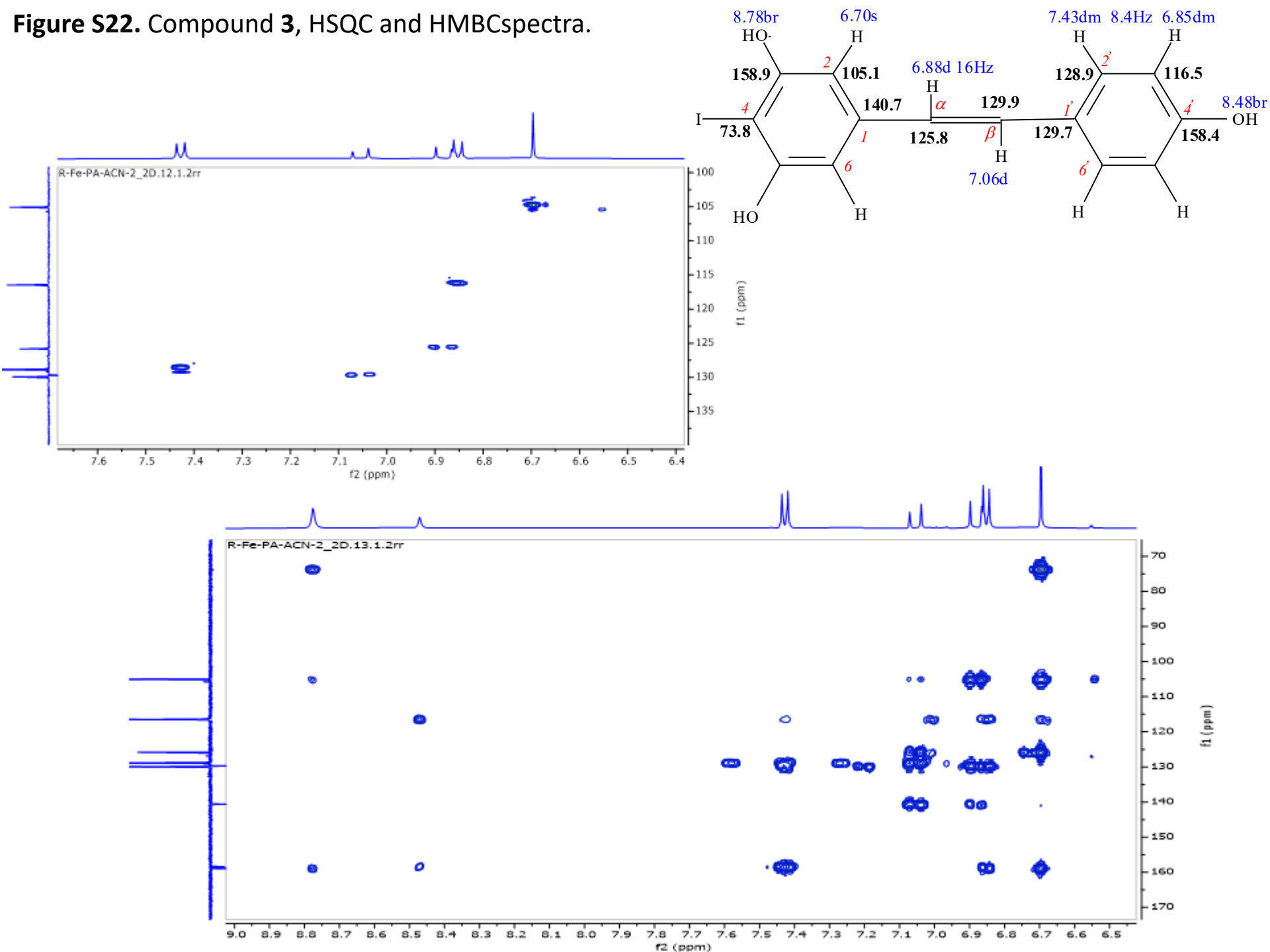
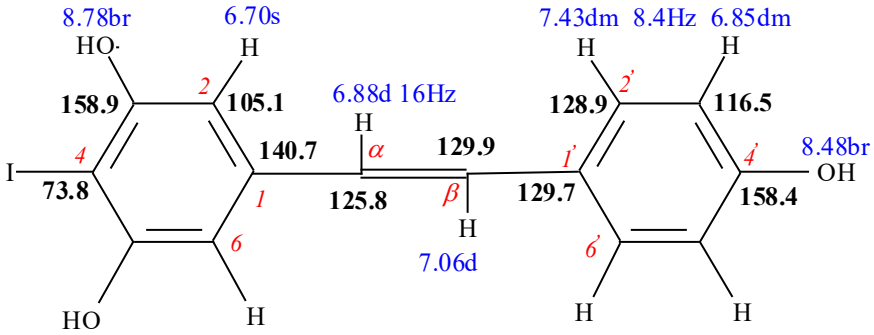


Figure S23. Compound **3**, COSY spectrum.



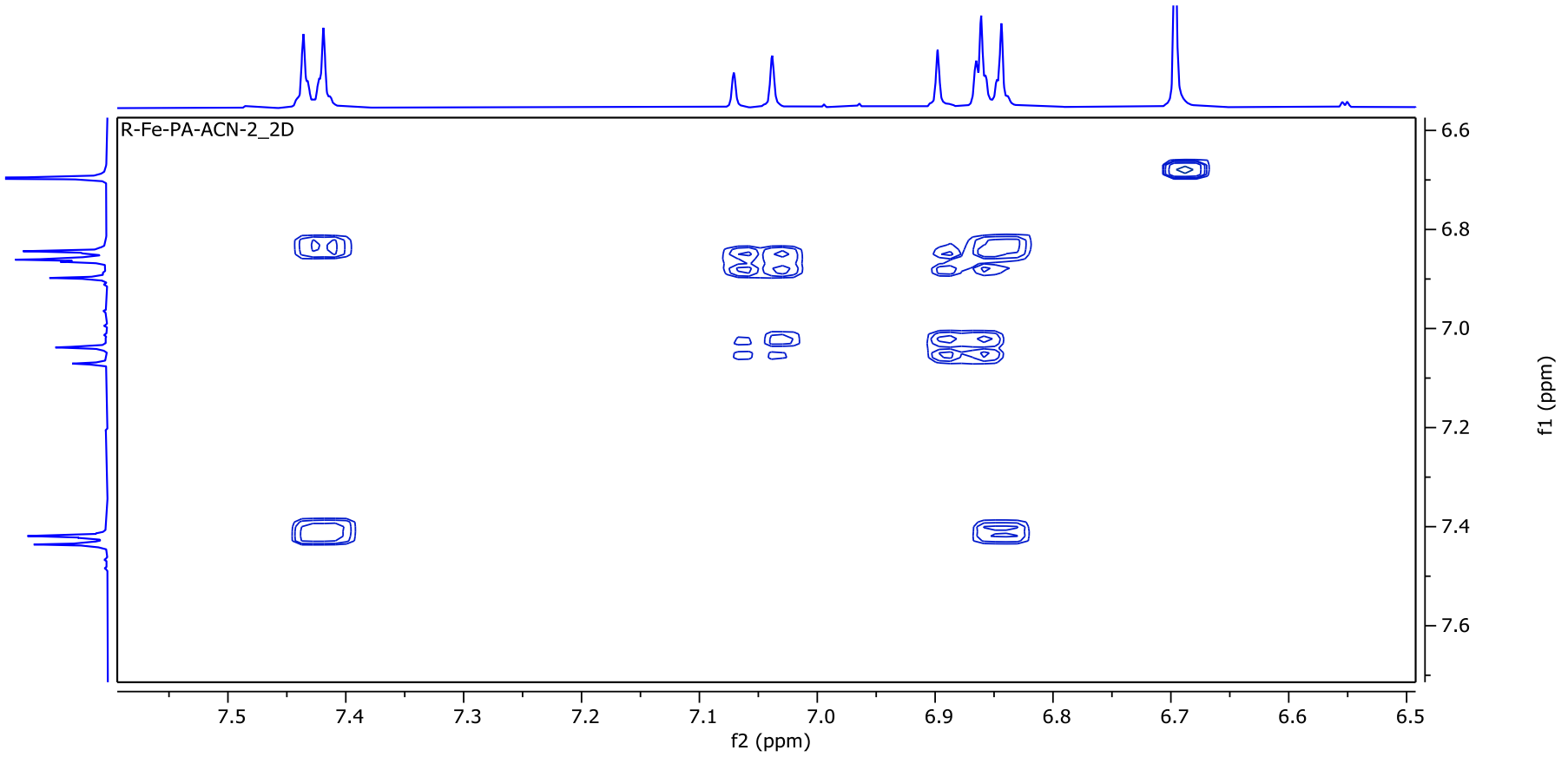
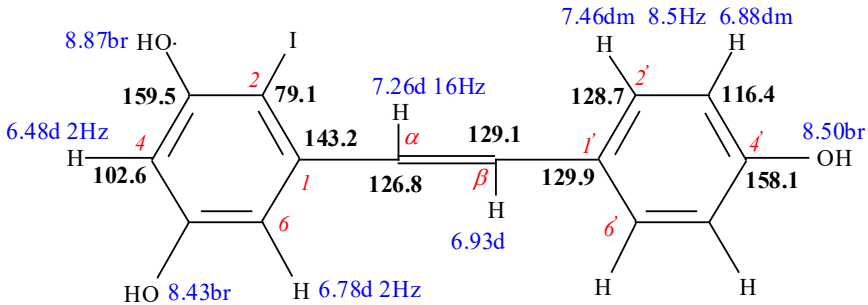


Figure S24. Compound **4**, ^{1}H NMR spectrum.



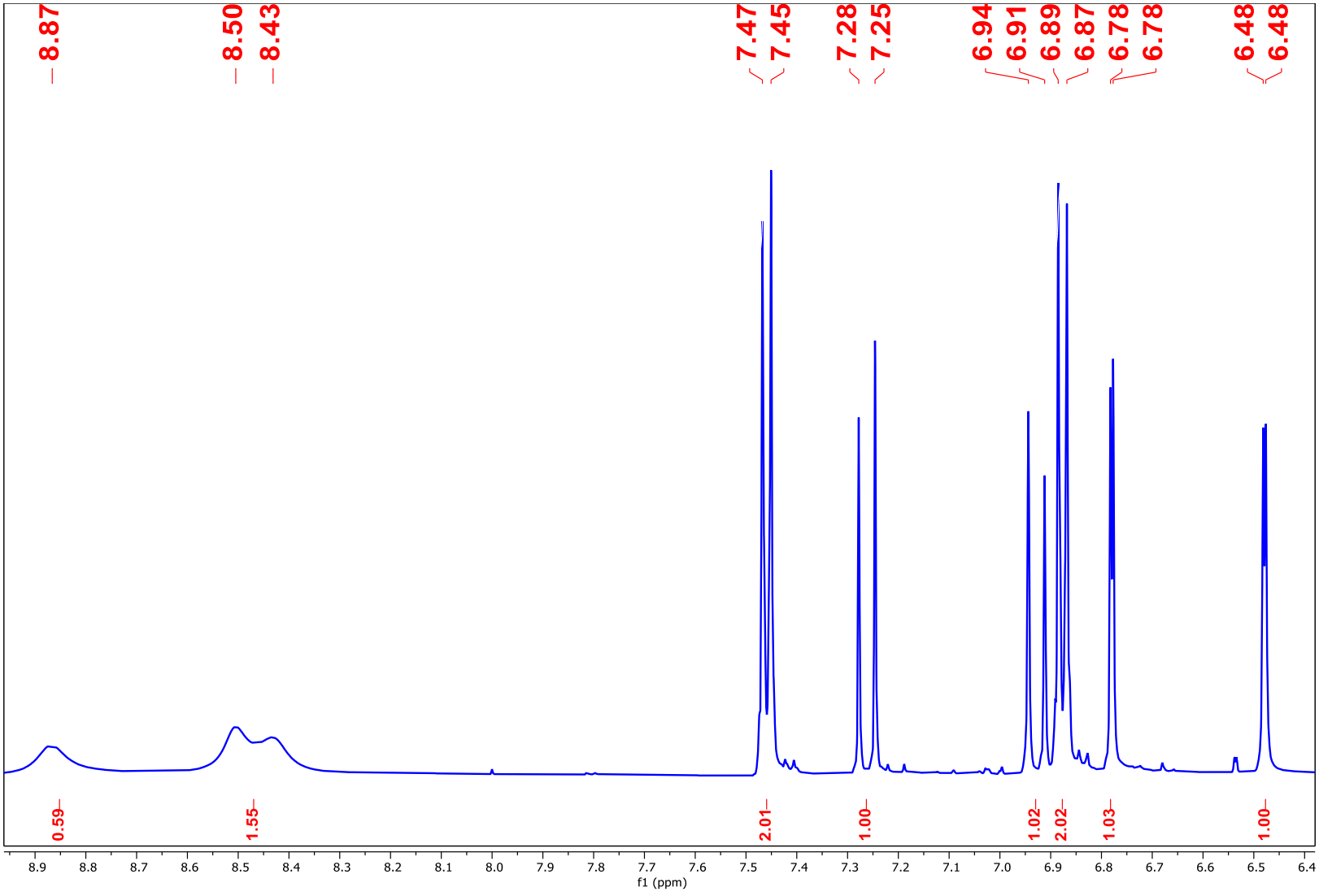
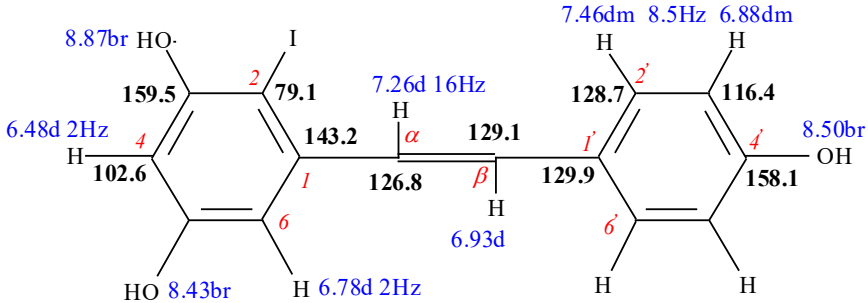


Figure S25. Compound **4**, ^{13}C, APT NMR spectrum.



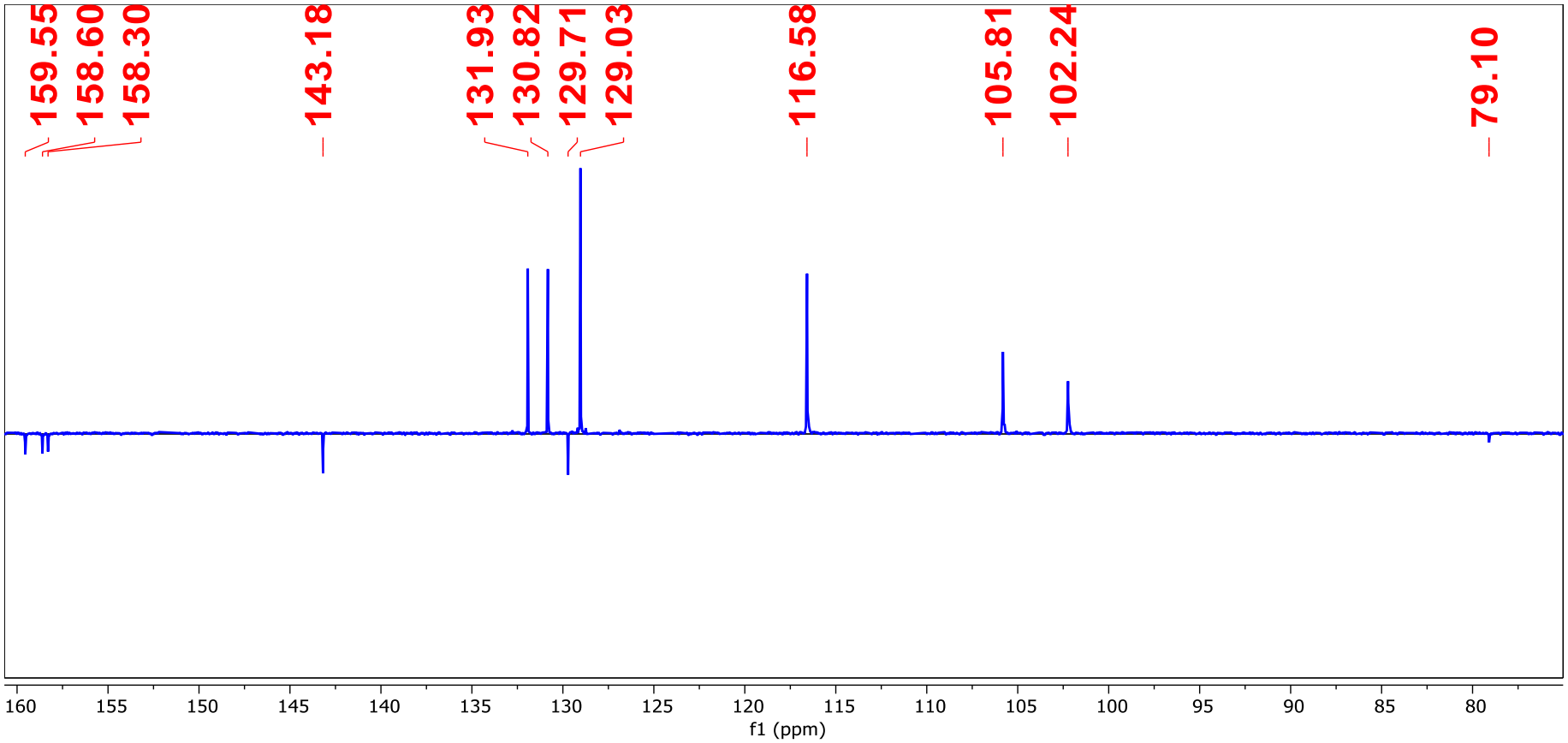
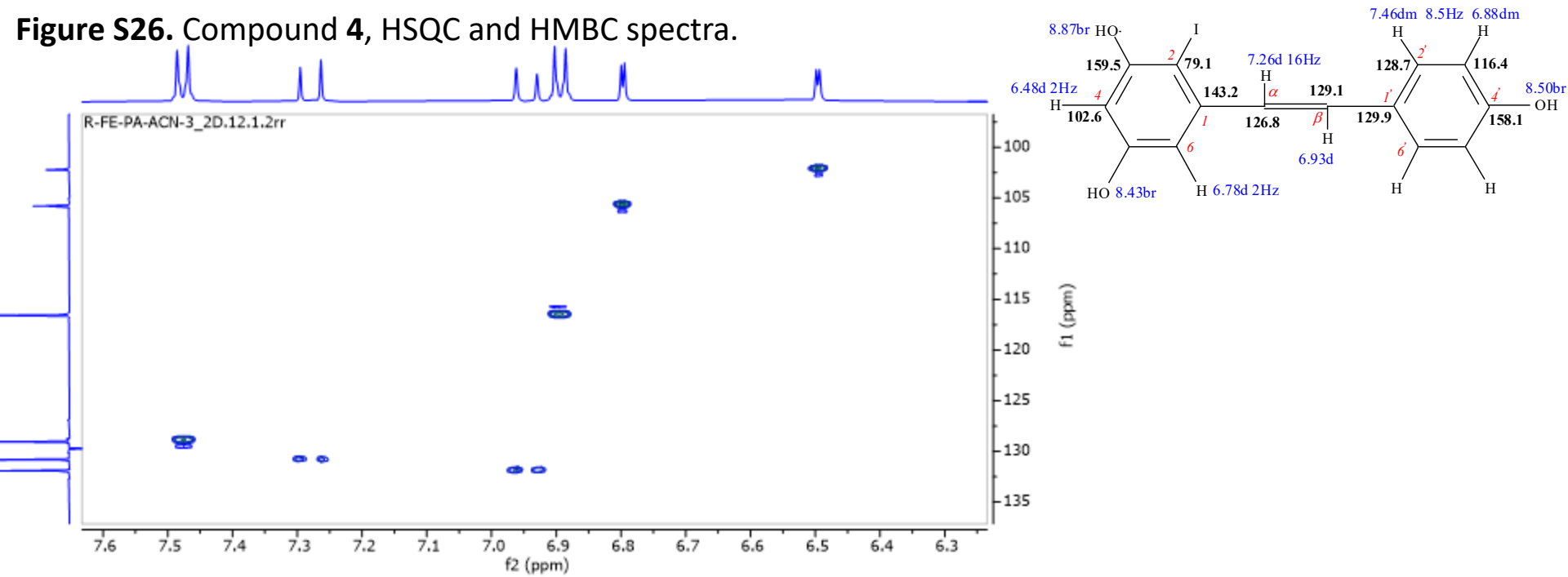


Figure S26. Compound **4**, HSQC and HMBC spectra.



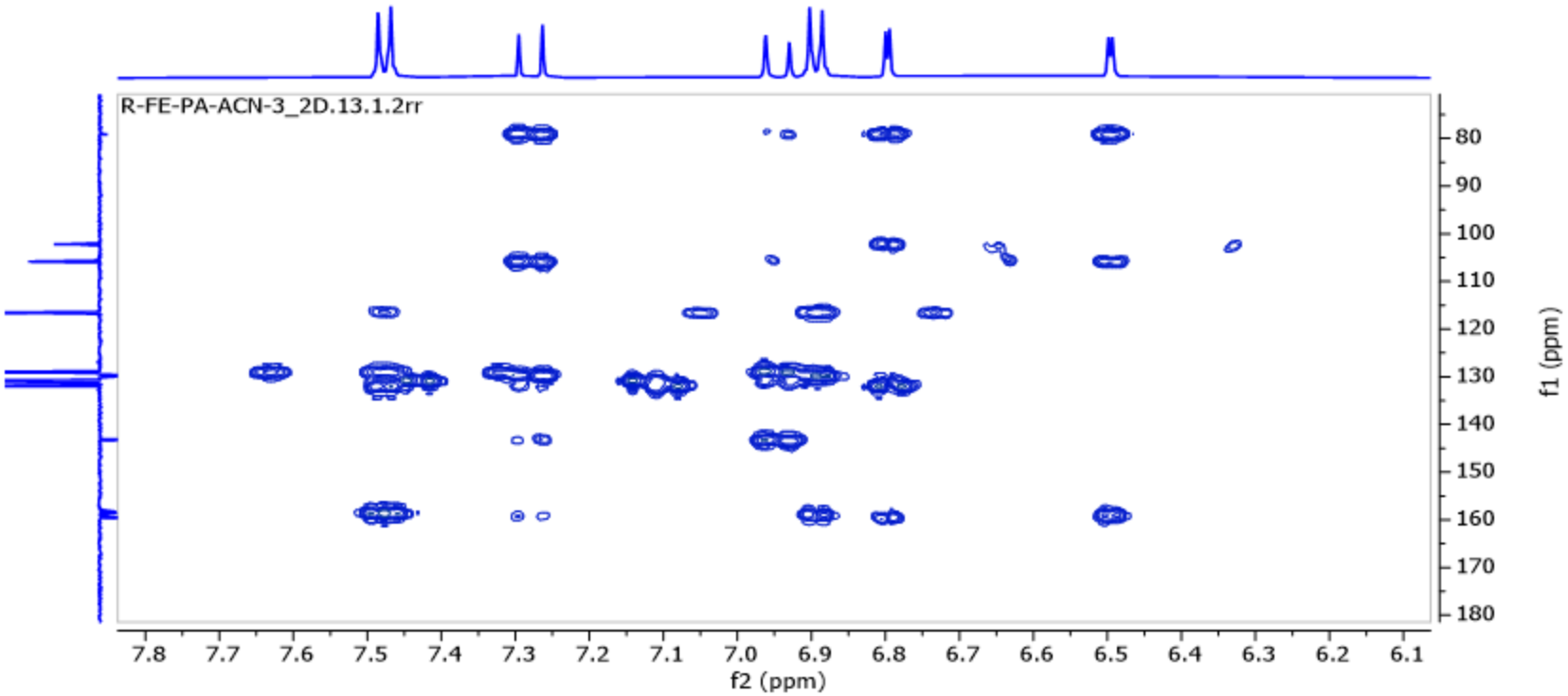
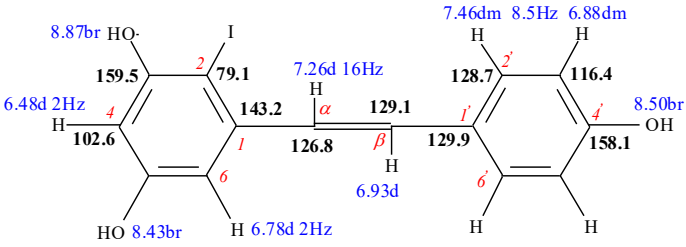


Figure S27. Compound **4**, COSY spectrum.



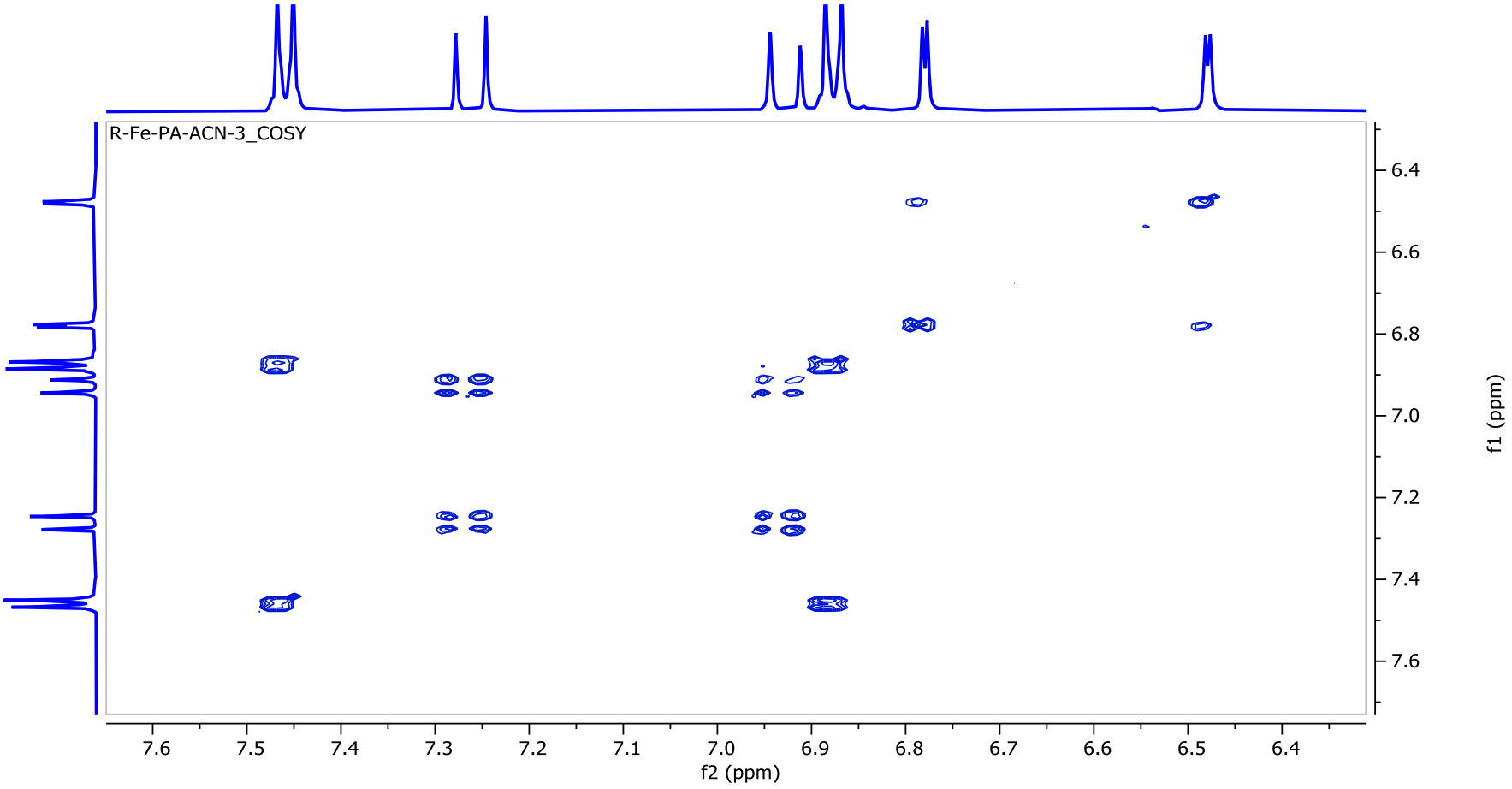
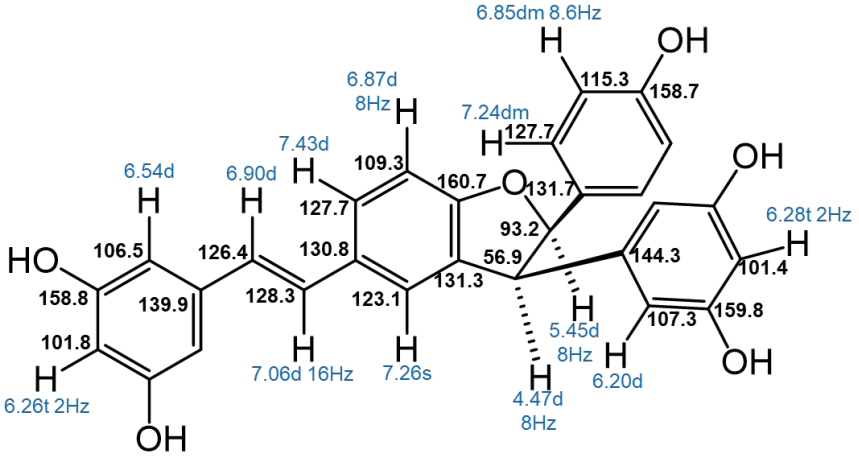


Figure S28. Compound **5**, ^{1}H NMR spectrum, and selROE on δ4.47 and δ5.45 ppm.



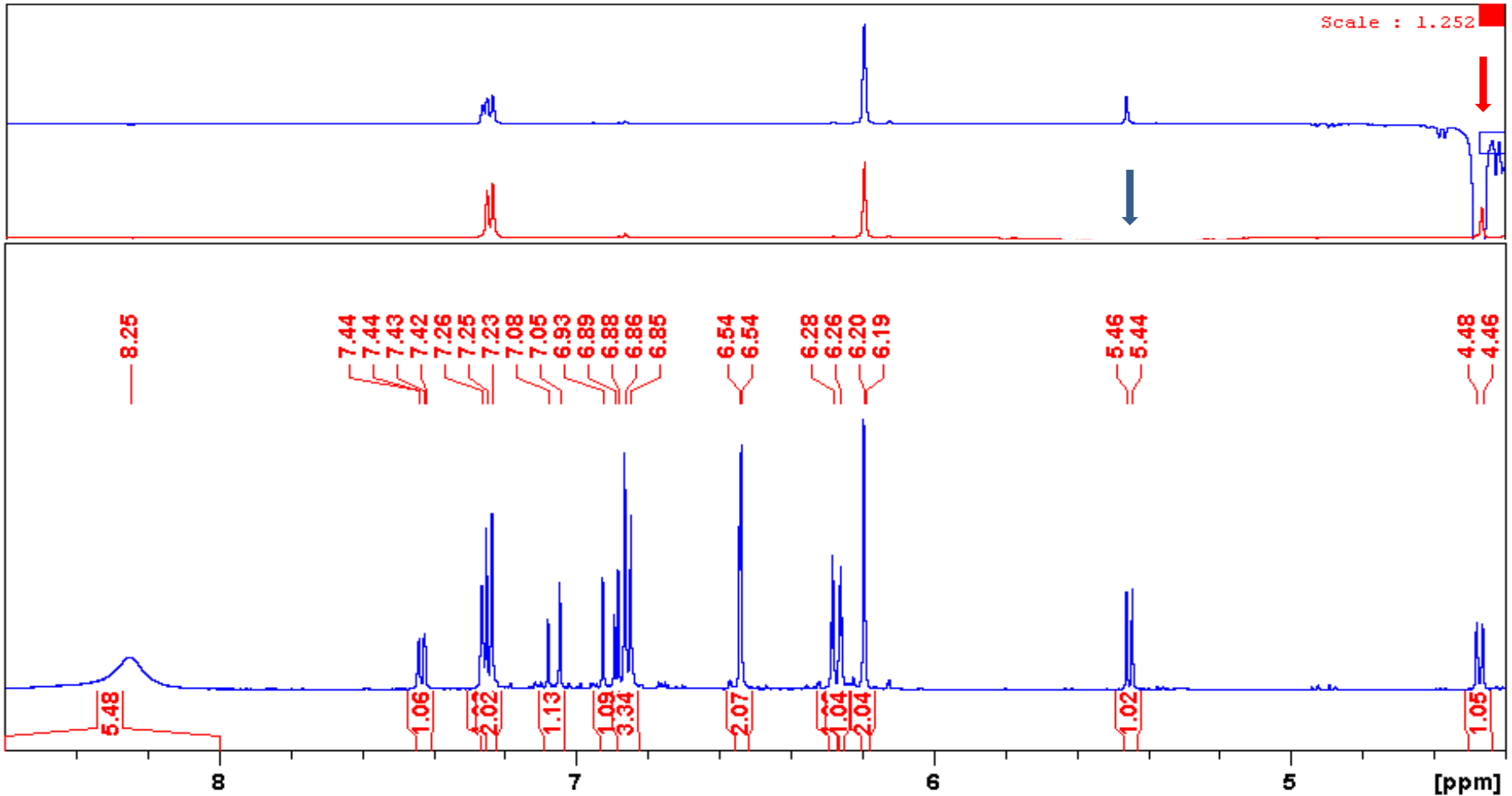
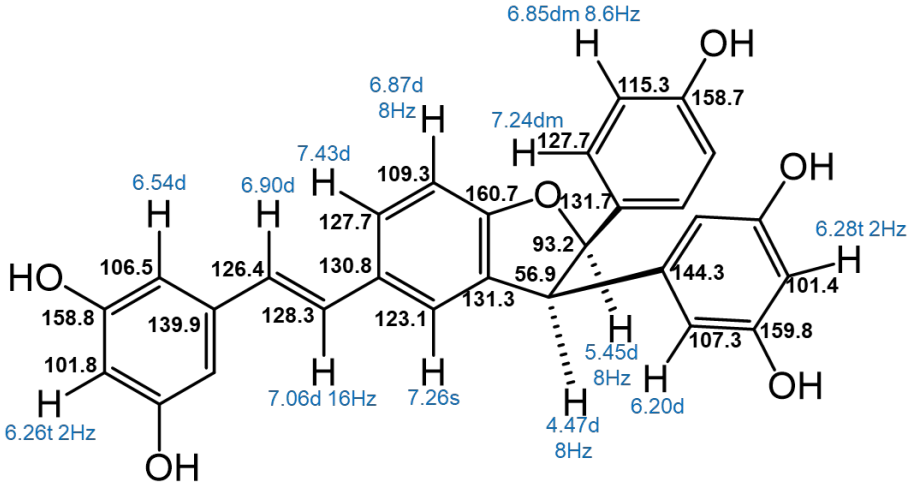


Figure S29. Compound **5**, ^{13}C, APT NMR spectrum.



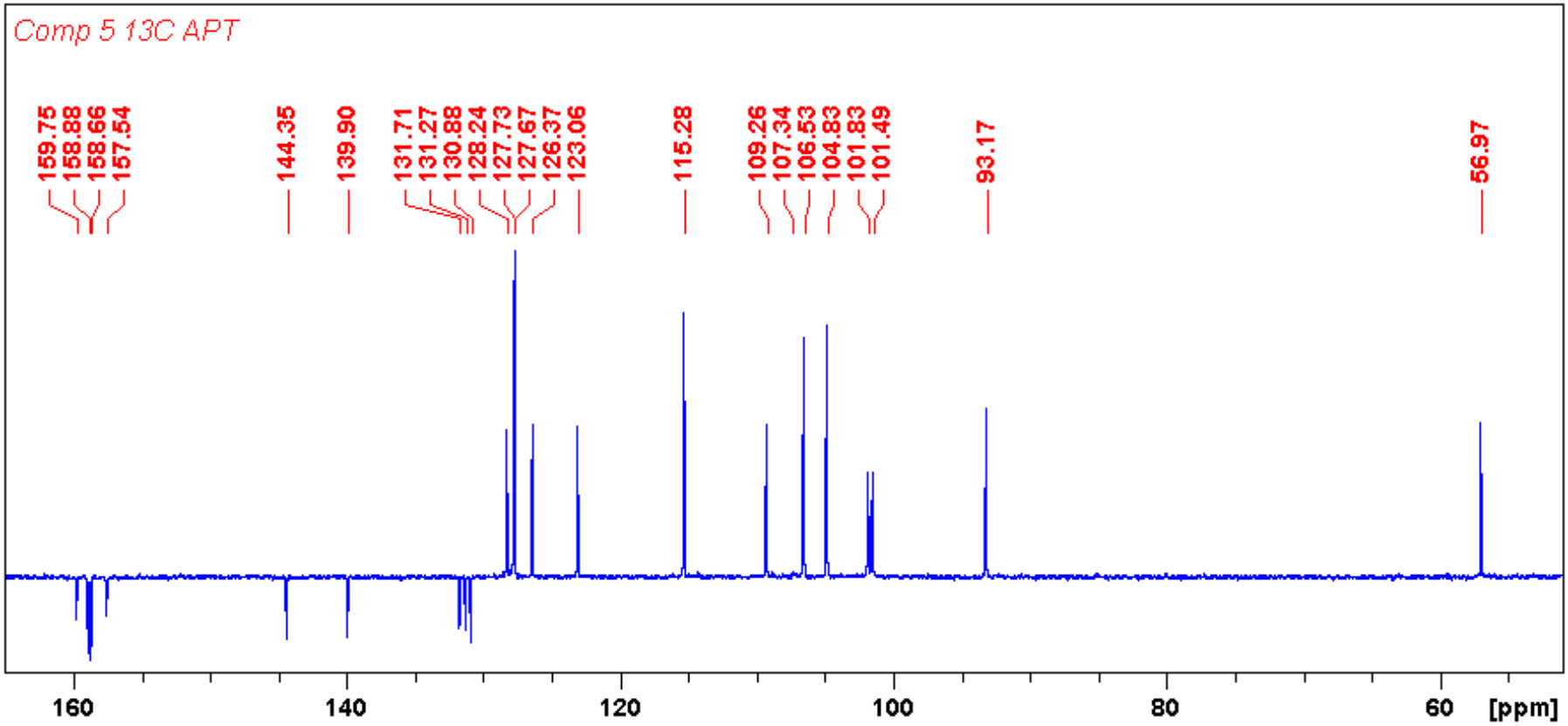


Figure S30. Compound **5**, HSQC spectrum and HSQC section.

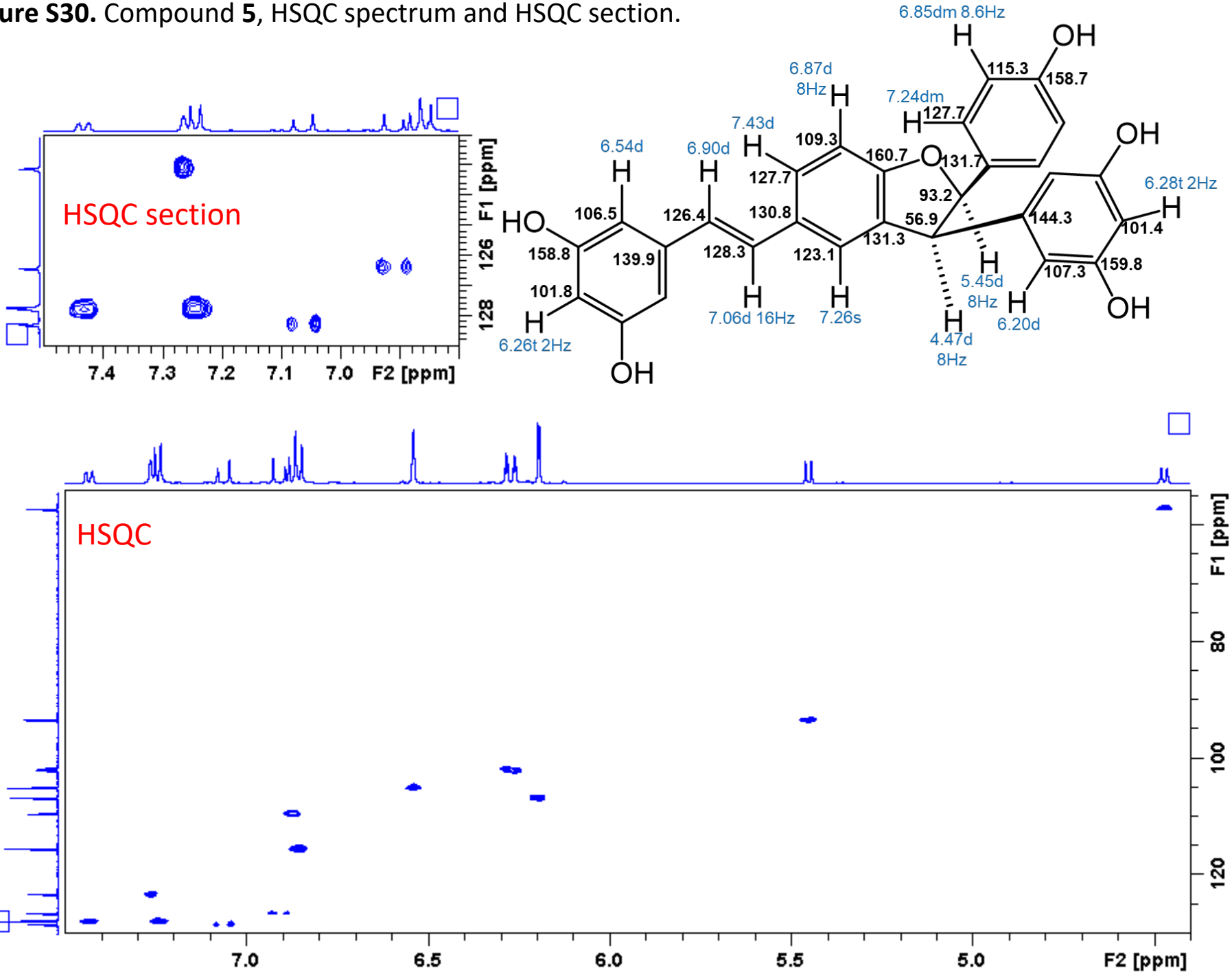


Figure S31. Compound **5**, COSY spectrum.

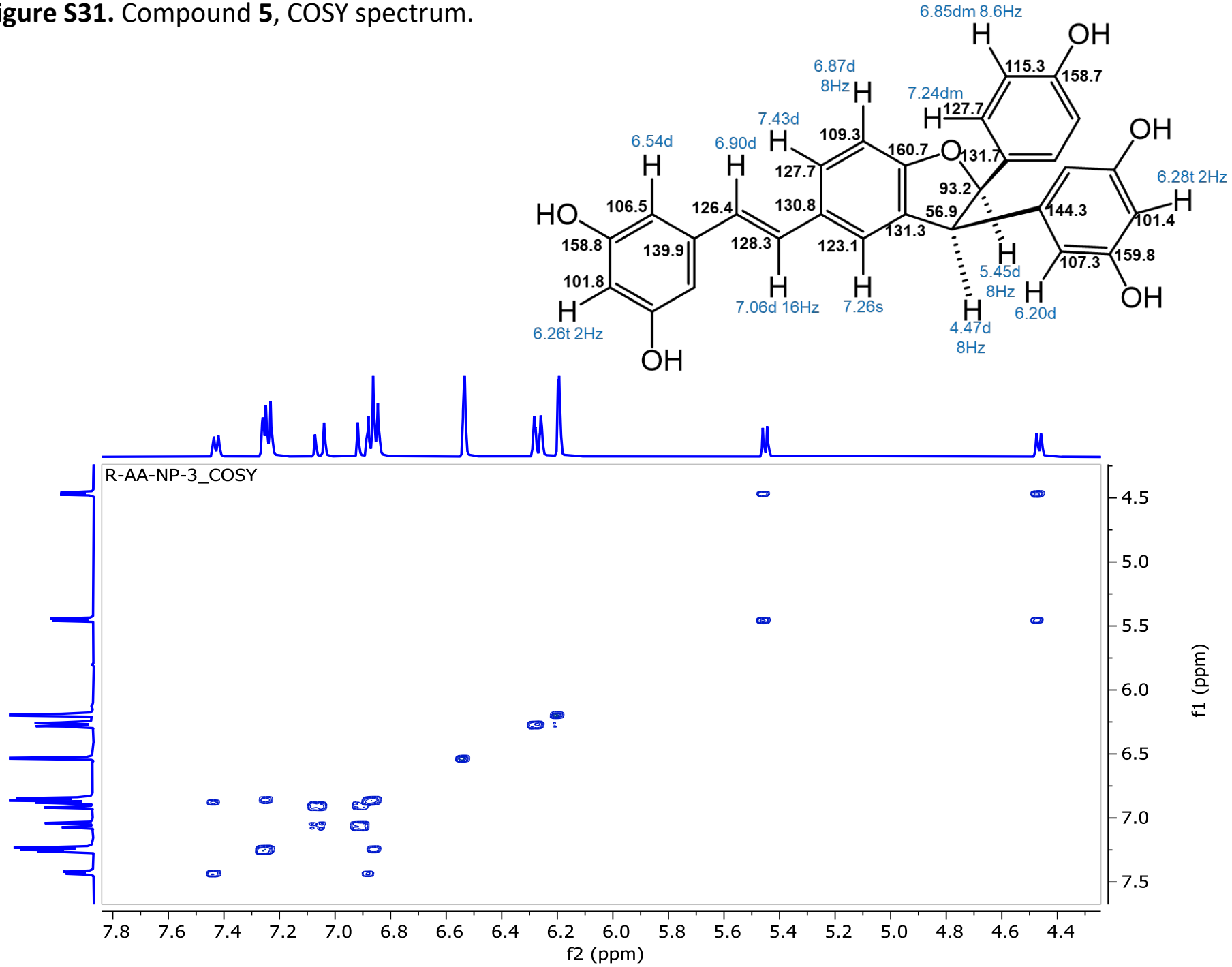
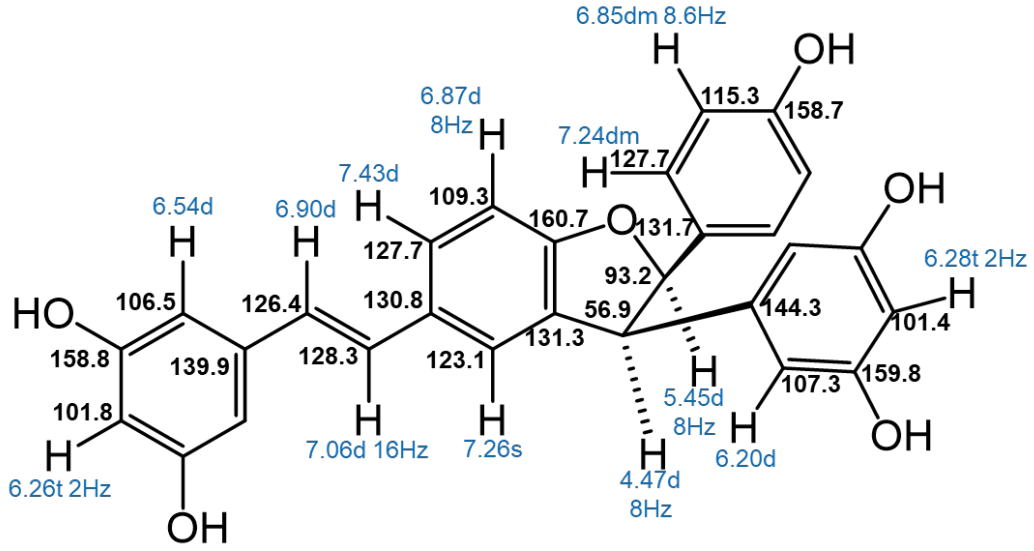


Figure S32. Compound **5**, HMBC spectrum.



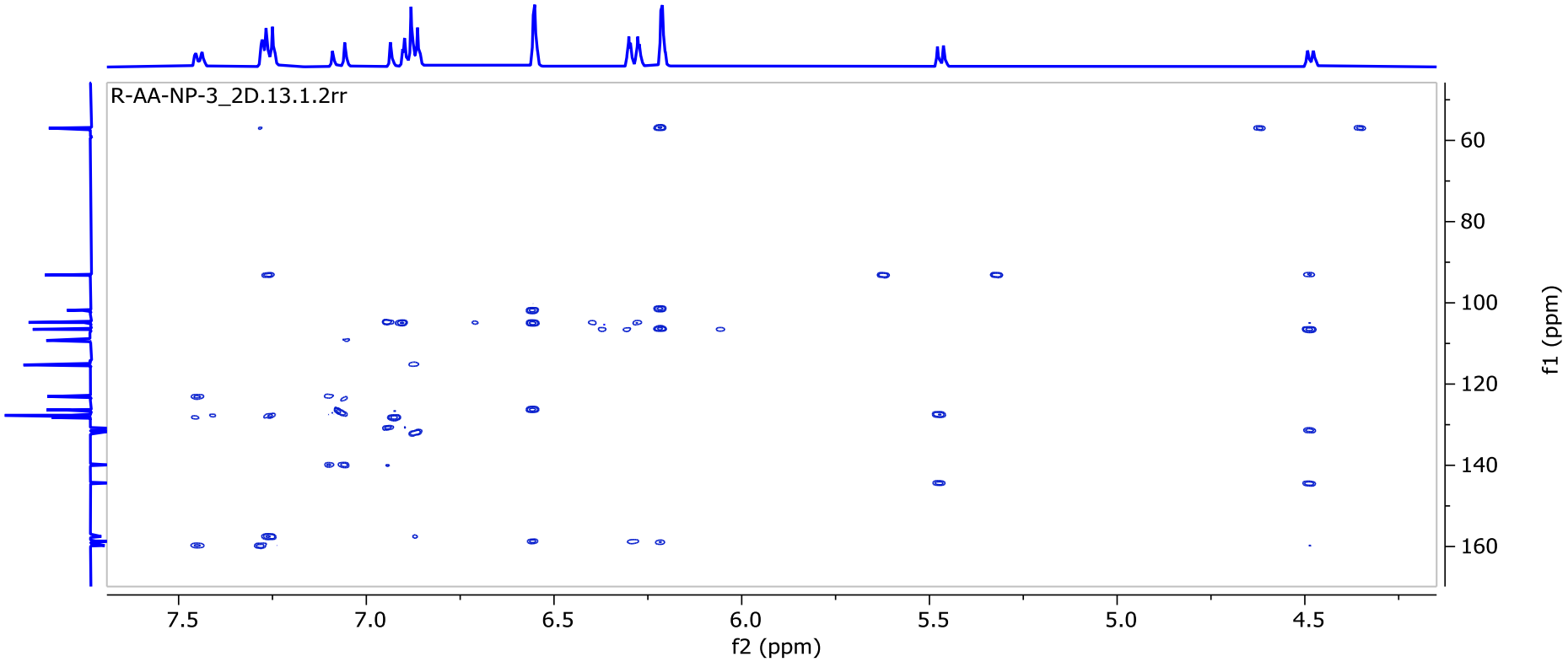


Figure S33. Compound **6**, ^{1}H, selNOE on δ4.48 and δ5.42 ppm.

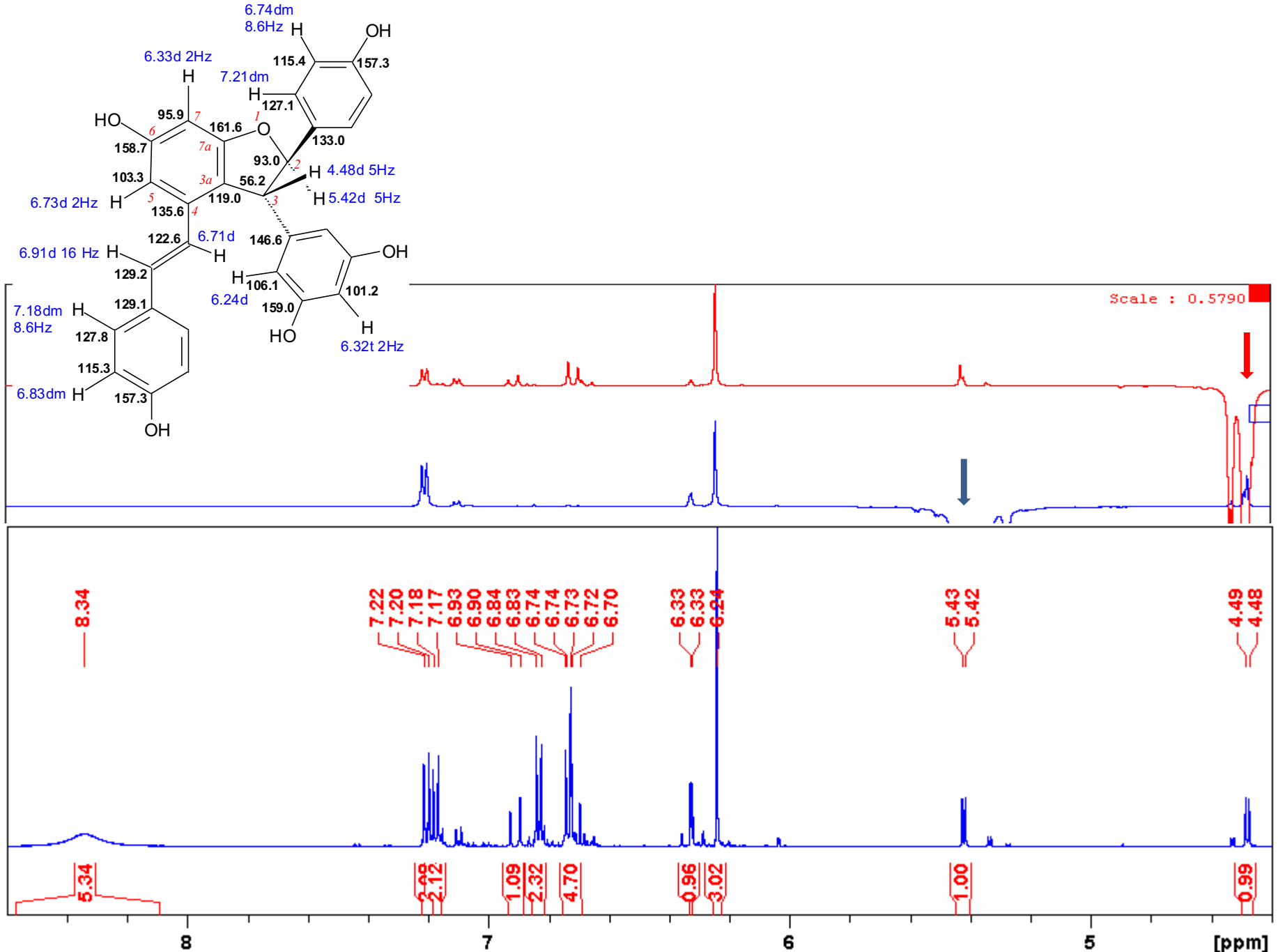
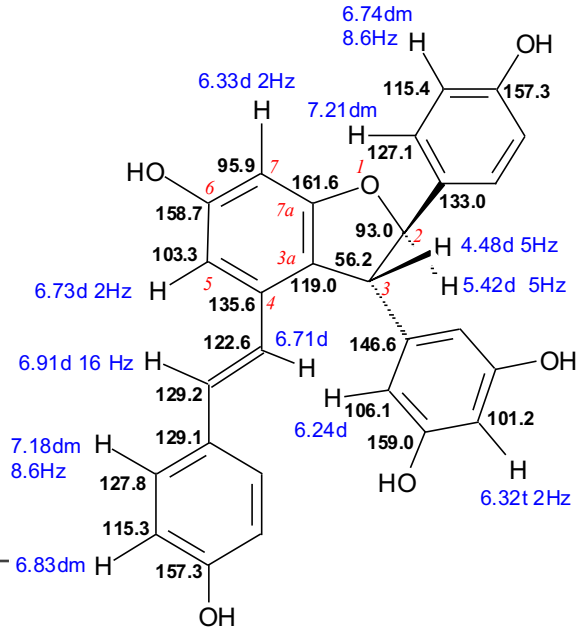


Figure S34. Compound **6**, ^{13}C, APT NMR spectrum.



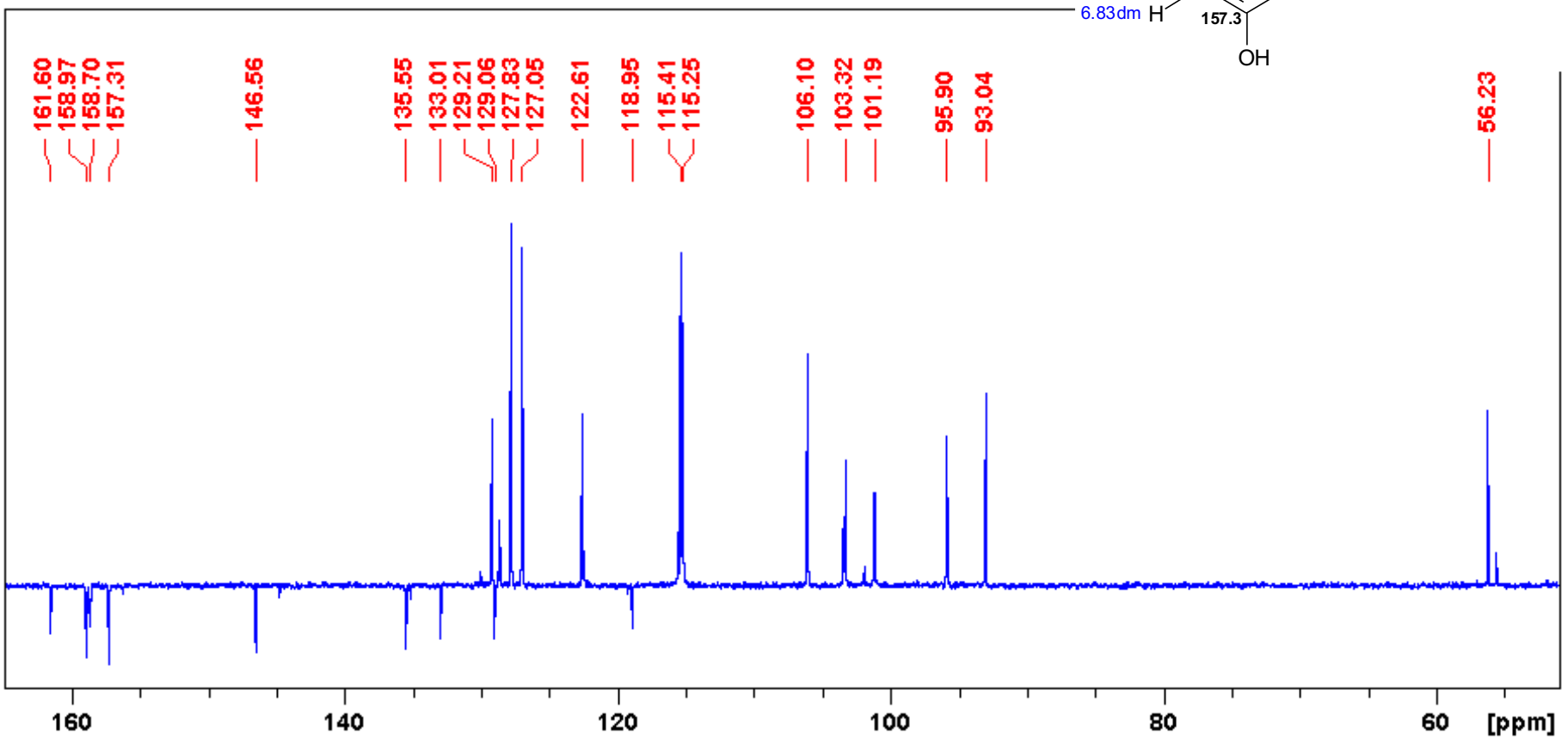


Figure S35. Compound **6**, HSQC spectrum.

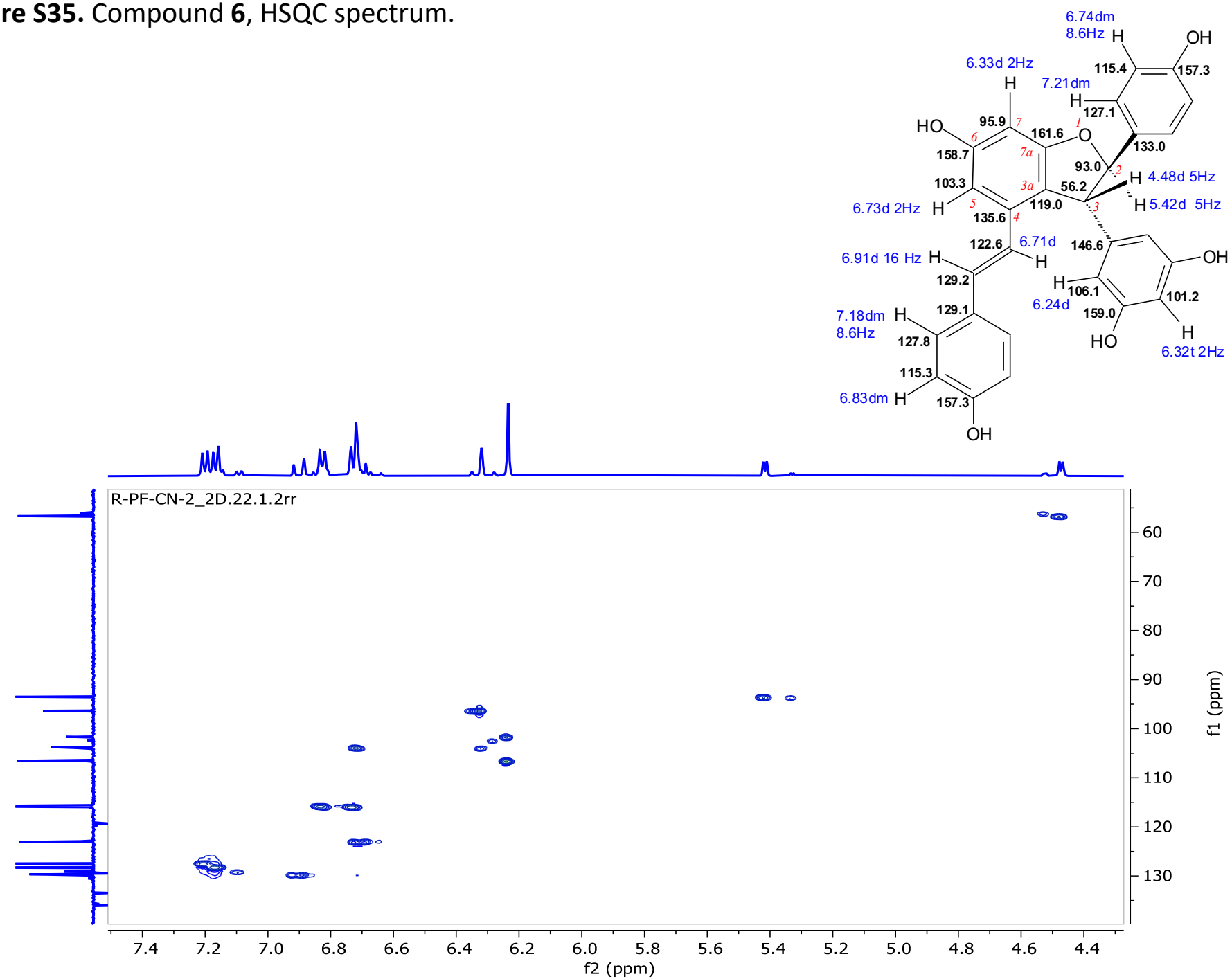
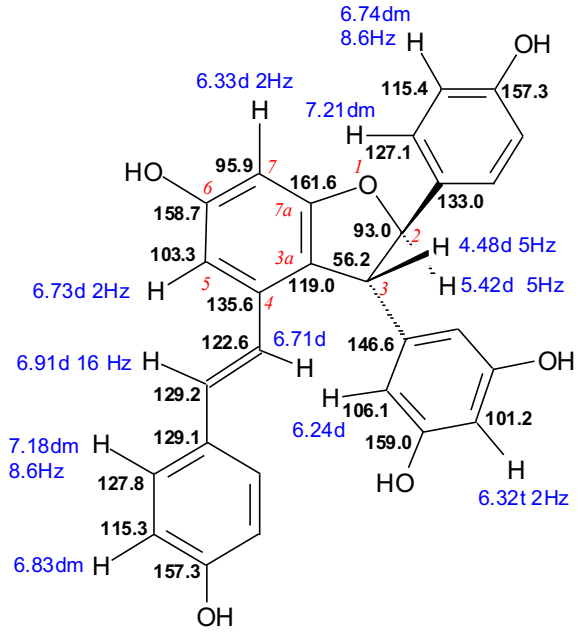


Figure S36. Compound **6**, HMBC spectrum.



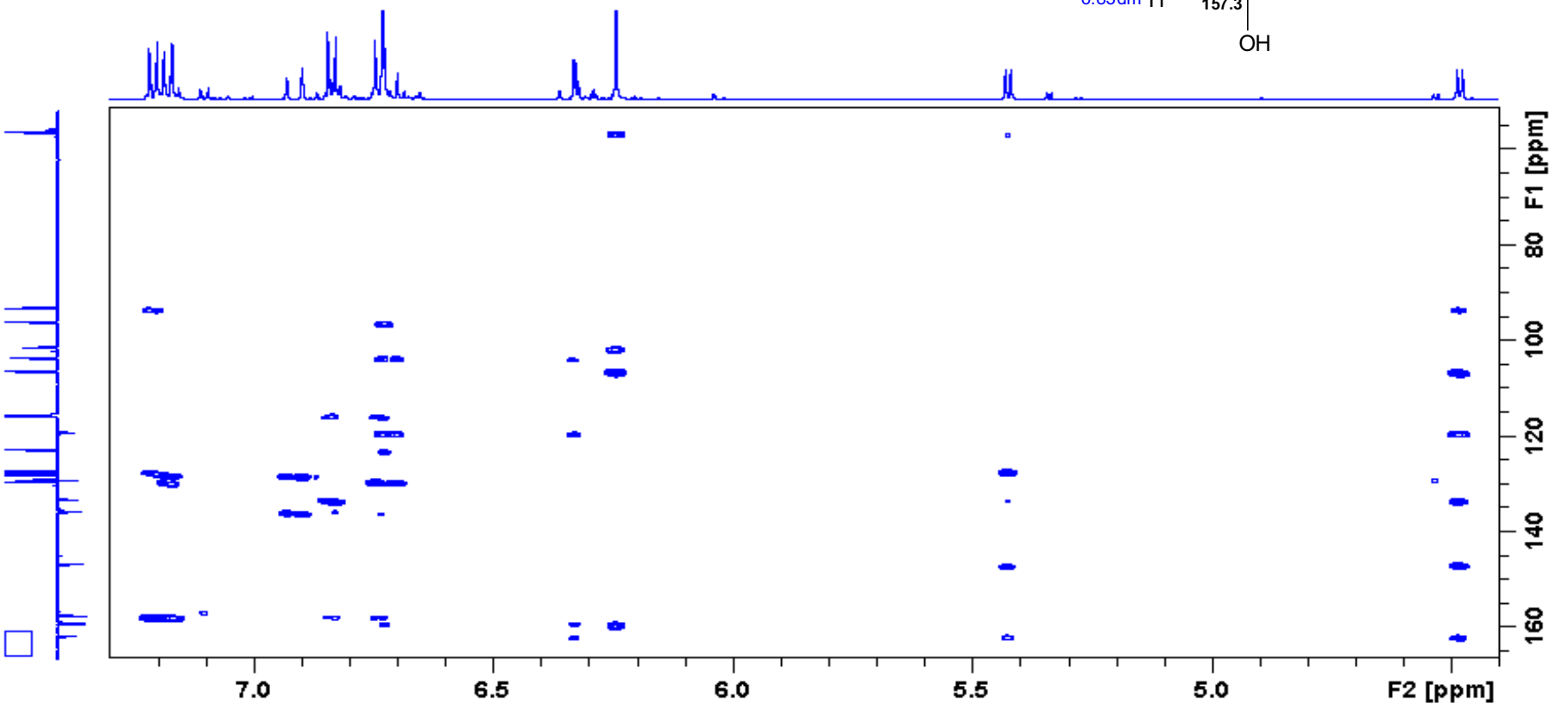
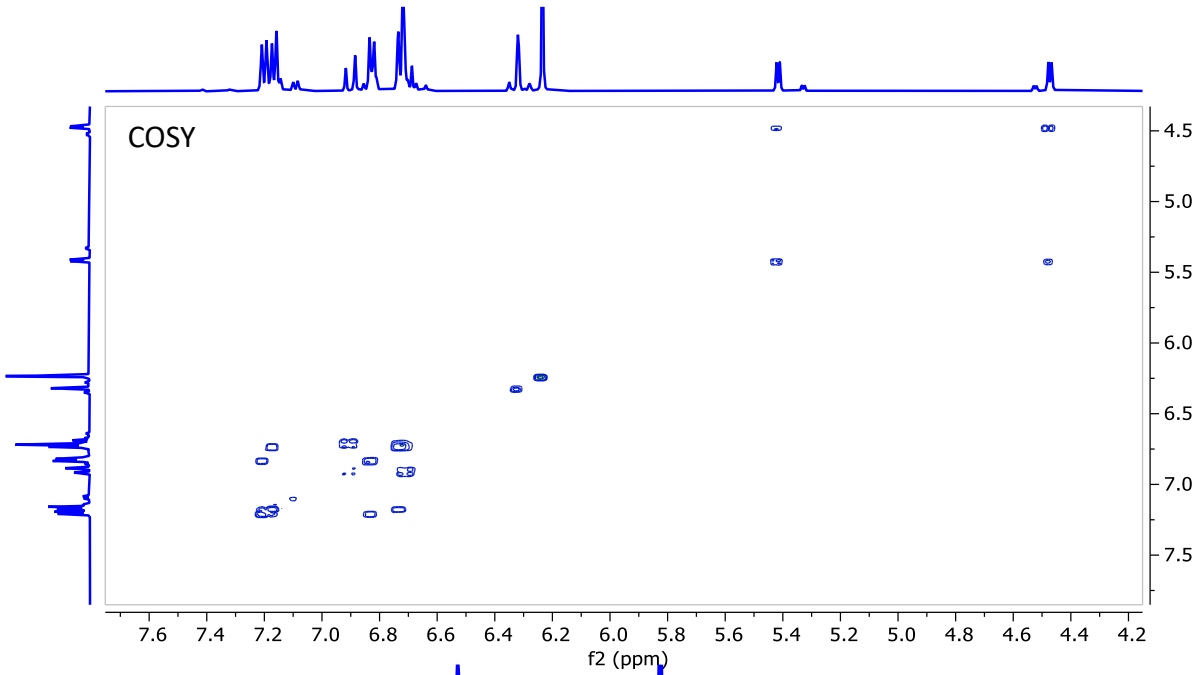
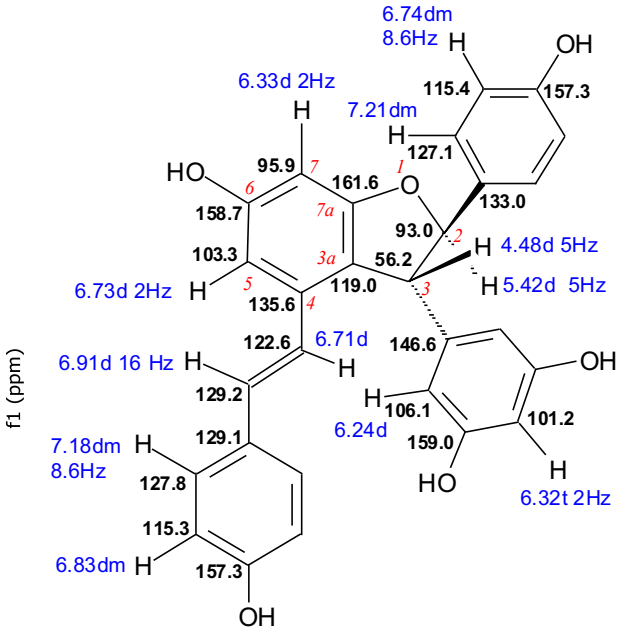


Figure S37. Compound **6**, COSY and NOESY spectra.





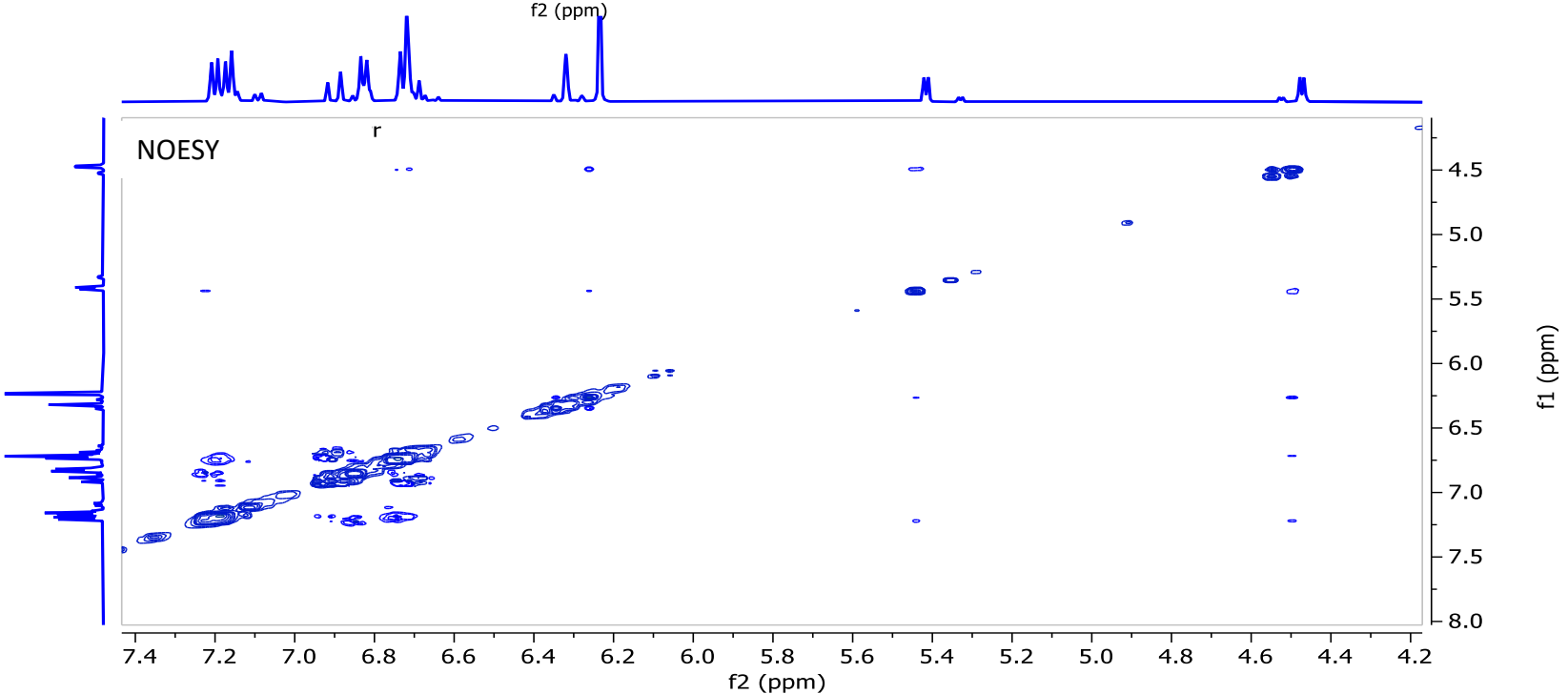
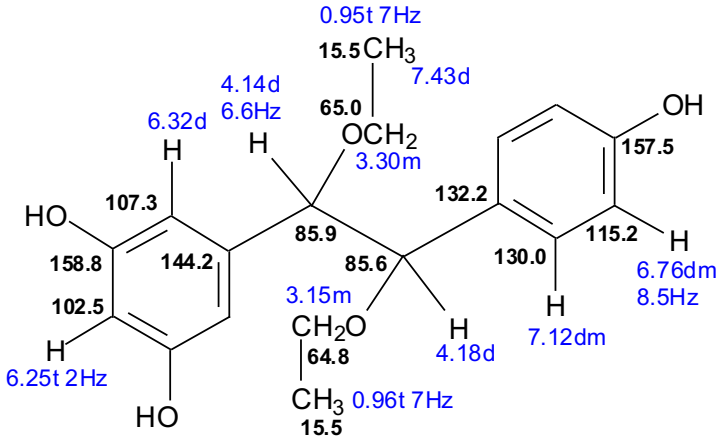


Figure S38. Compound **7**, ^{1}H NMR spectrum.



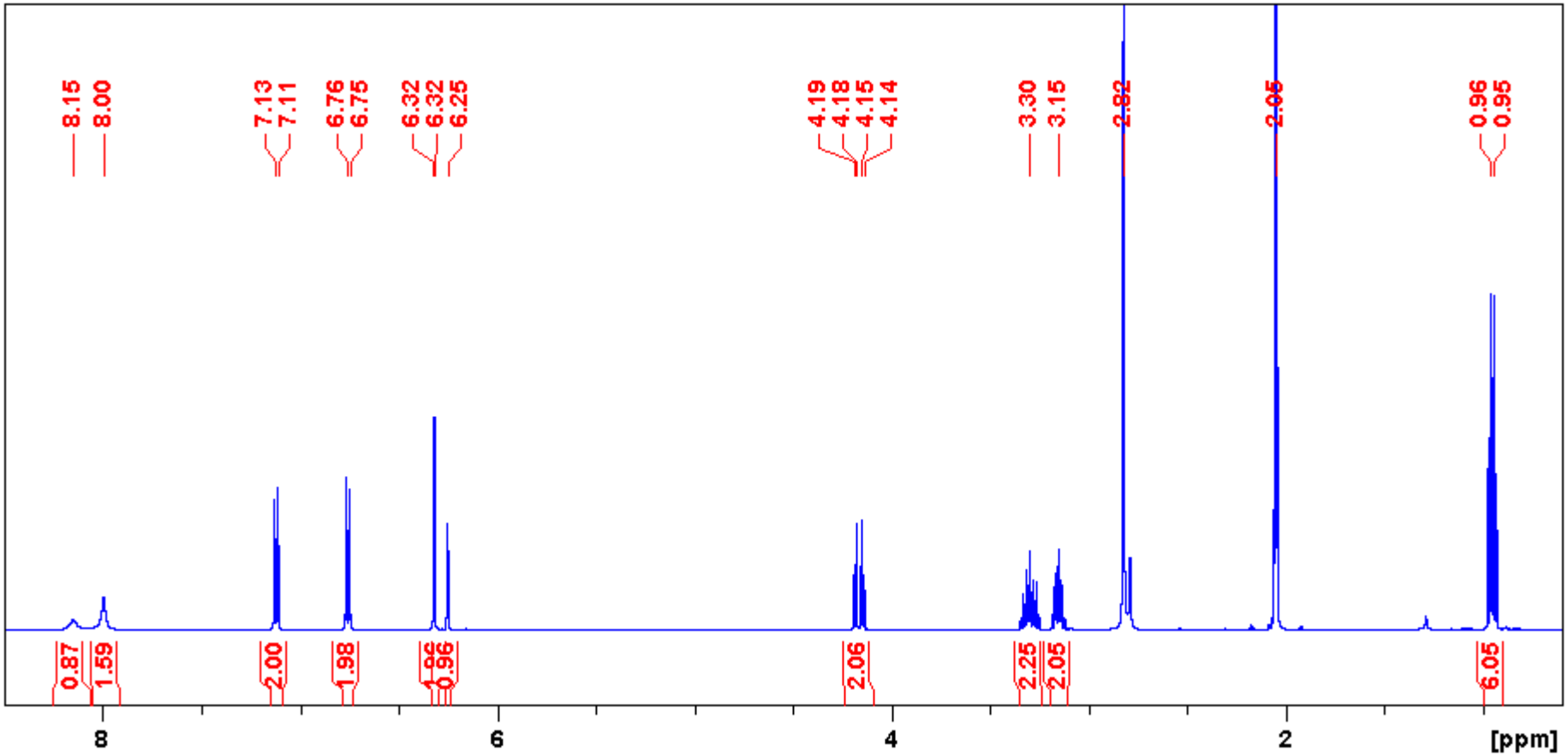
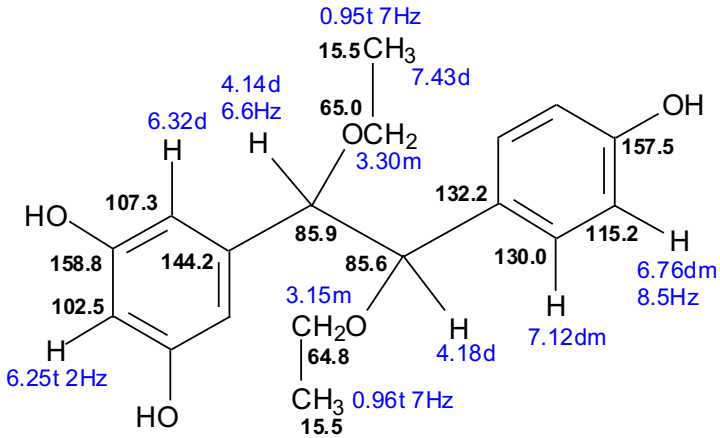


Figure S39. Compound **7**, ^{13}C, APT NMR spectrum.



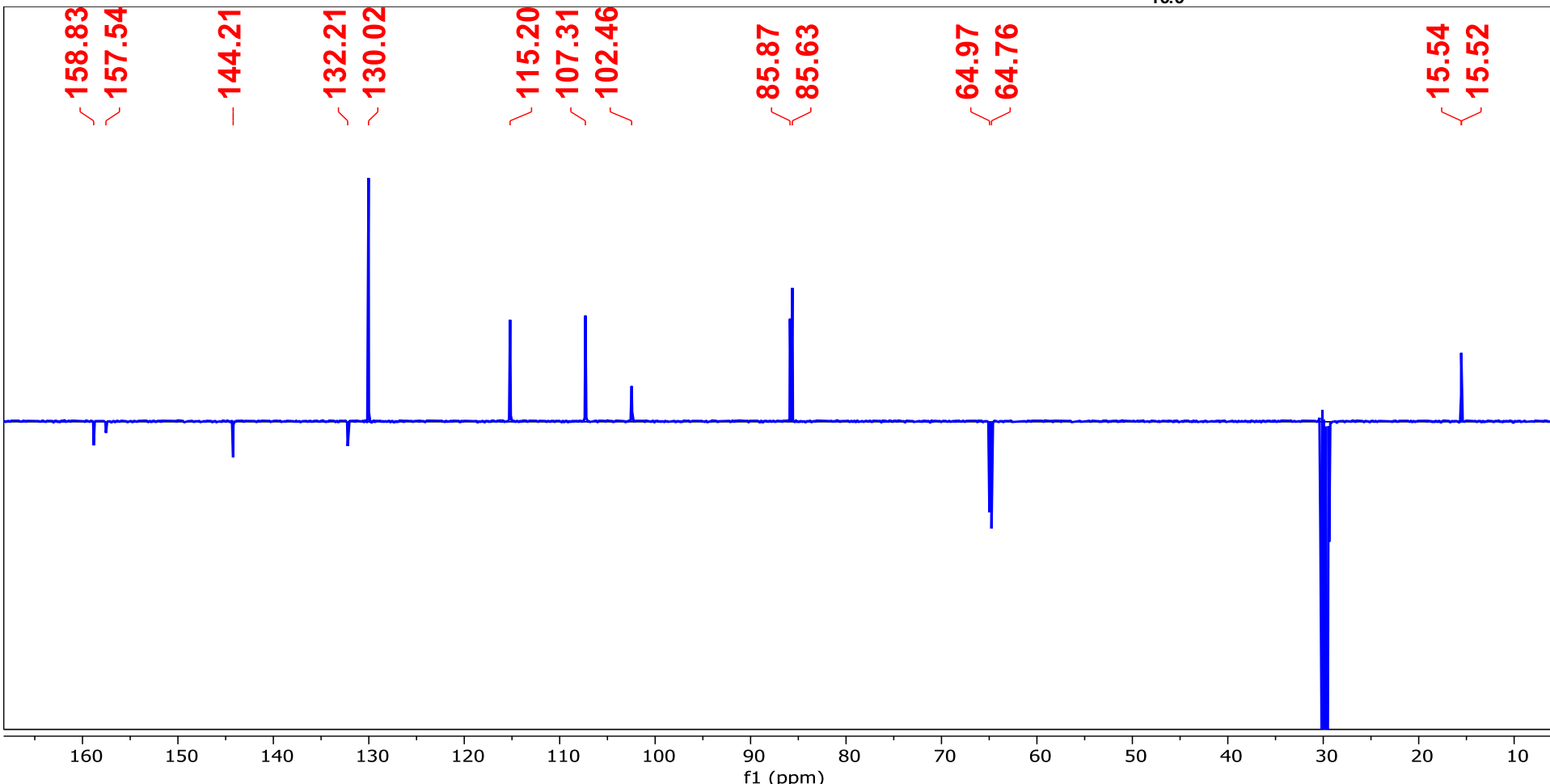


Figure S40. Compound **7**, NOESY spectrum and NOESY section.

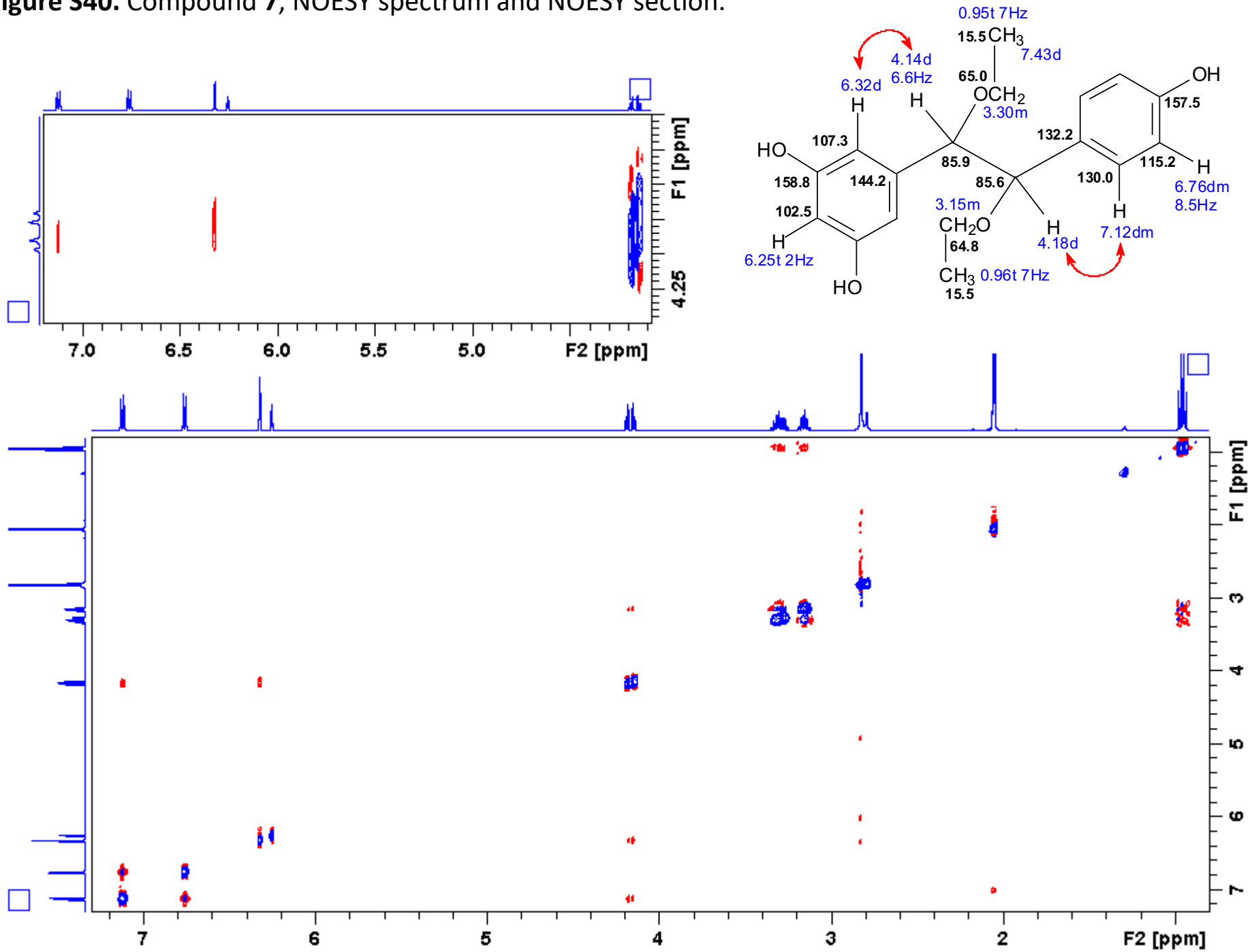
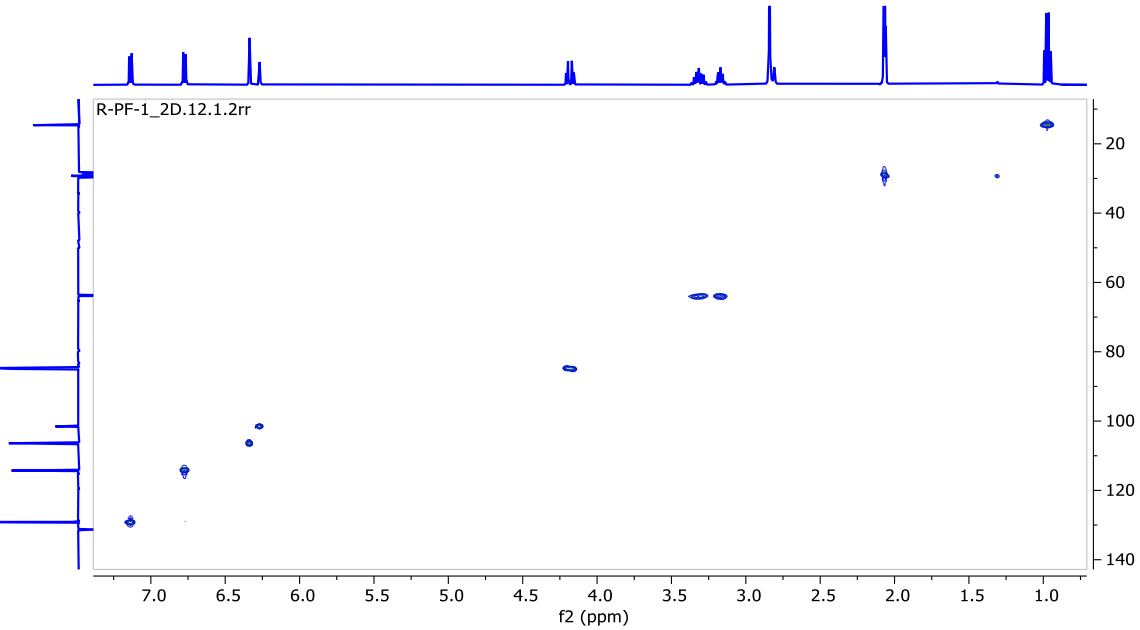
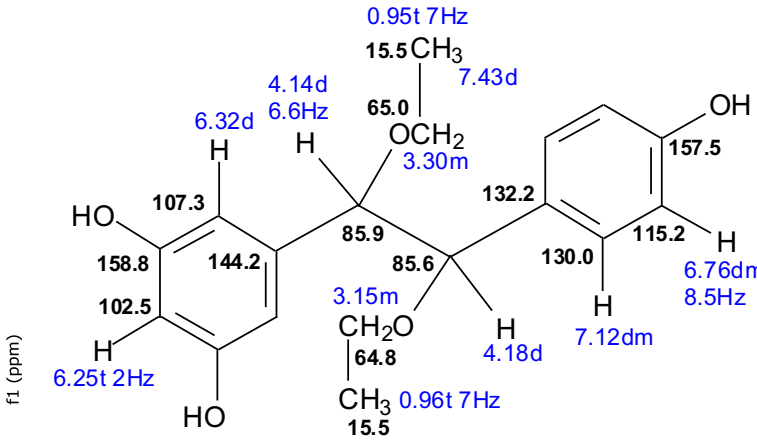


Figure S41. Compound **7**, HSQC and HMBC spectra.





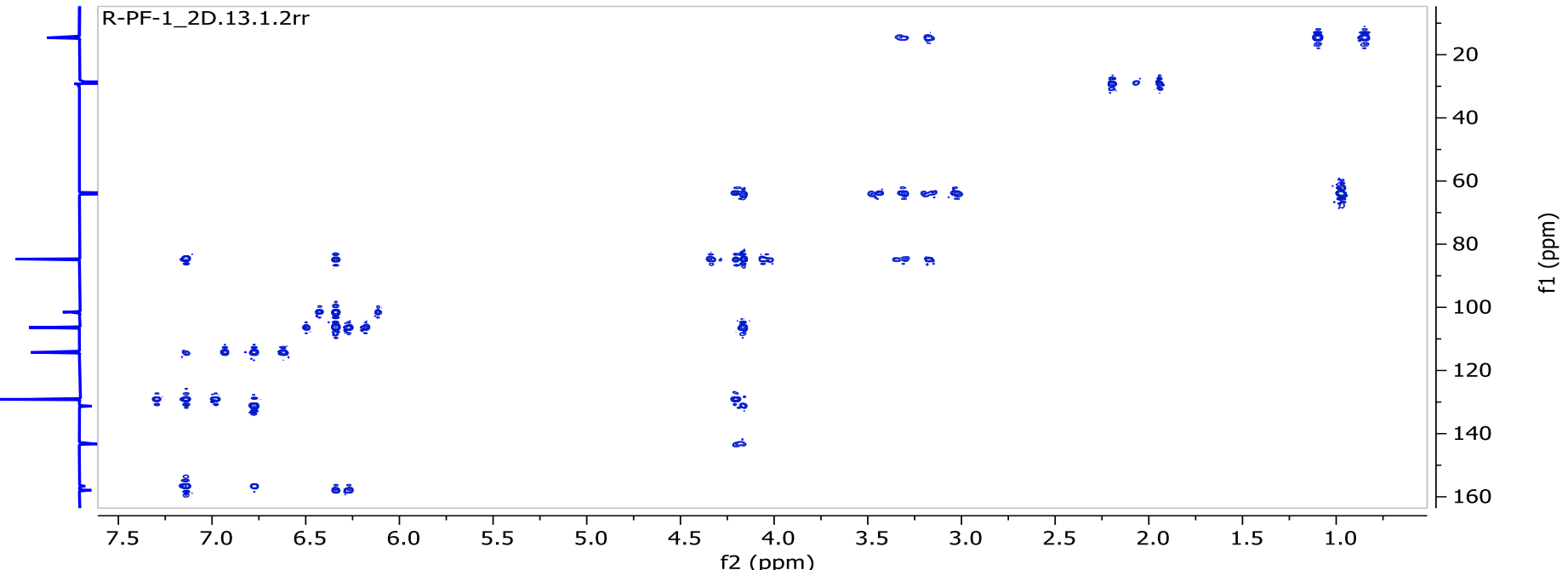


Figure S42. Compound **7**, COSY spectrum.

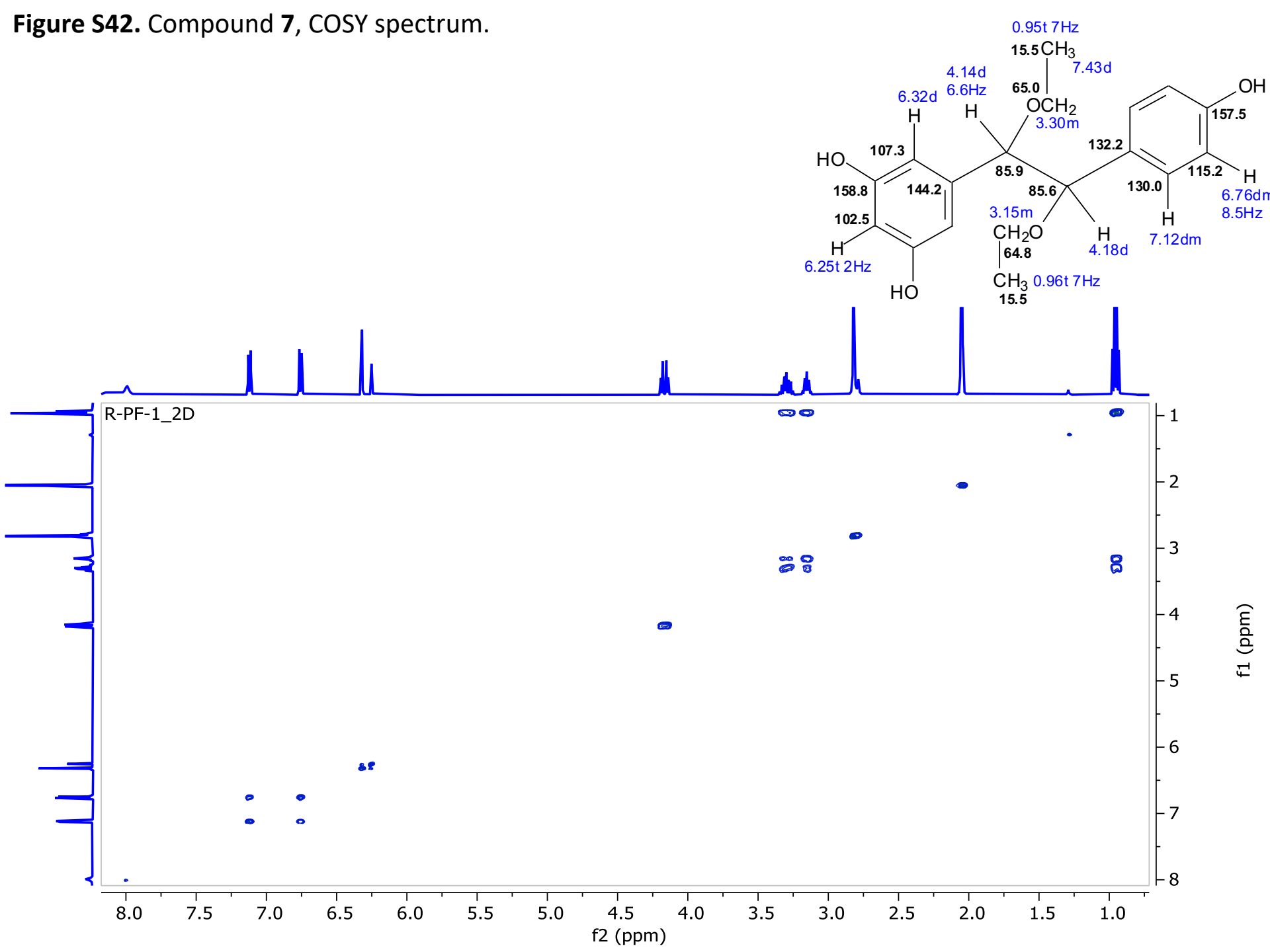
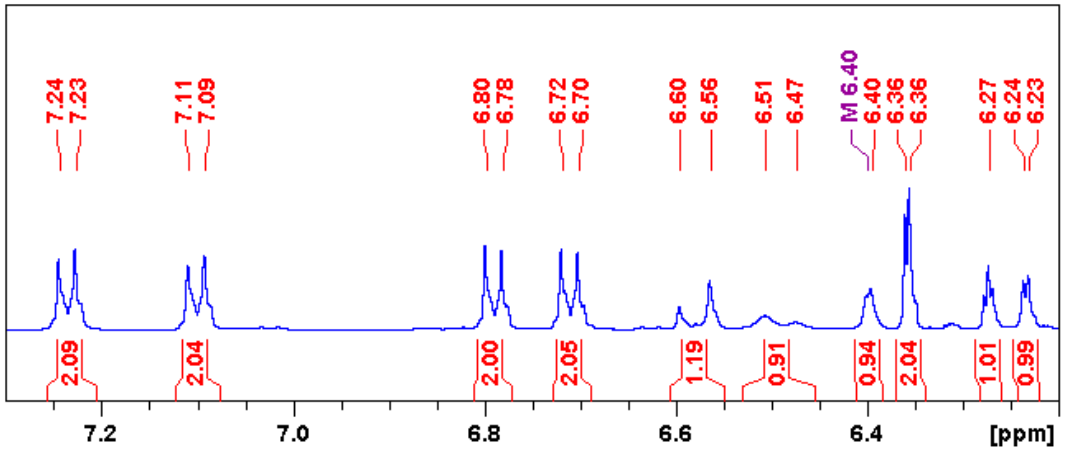
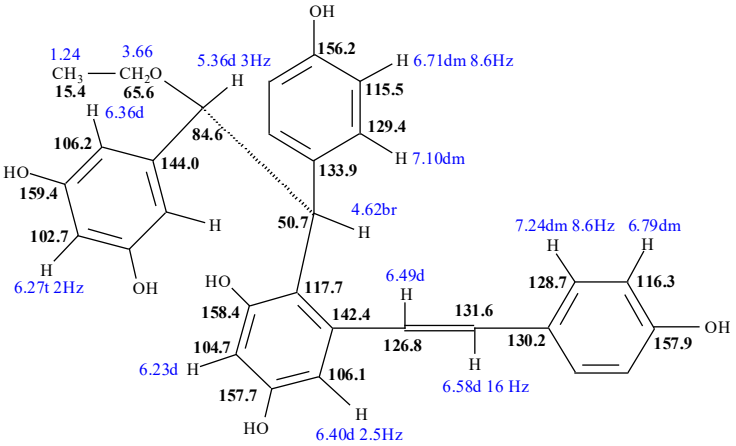


Figure S43. Compound **8**, ^{1}H NMR spectrum.





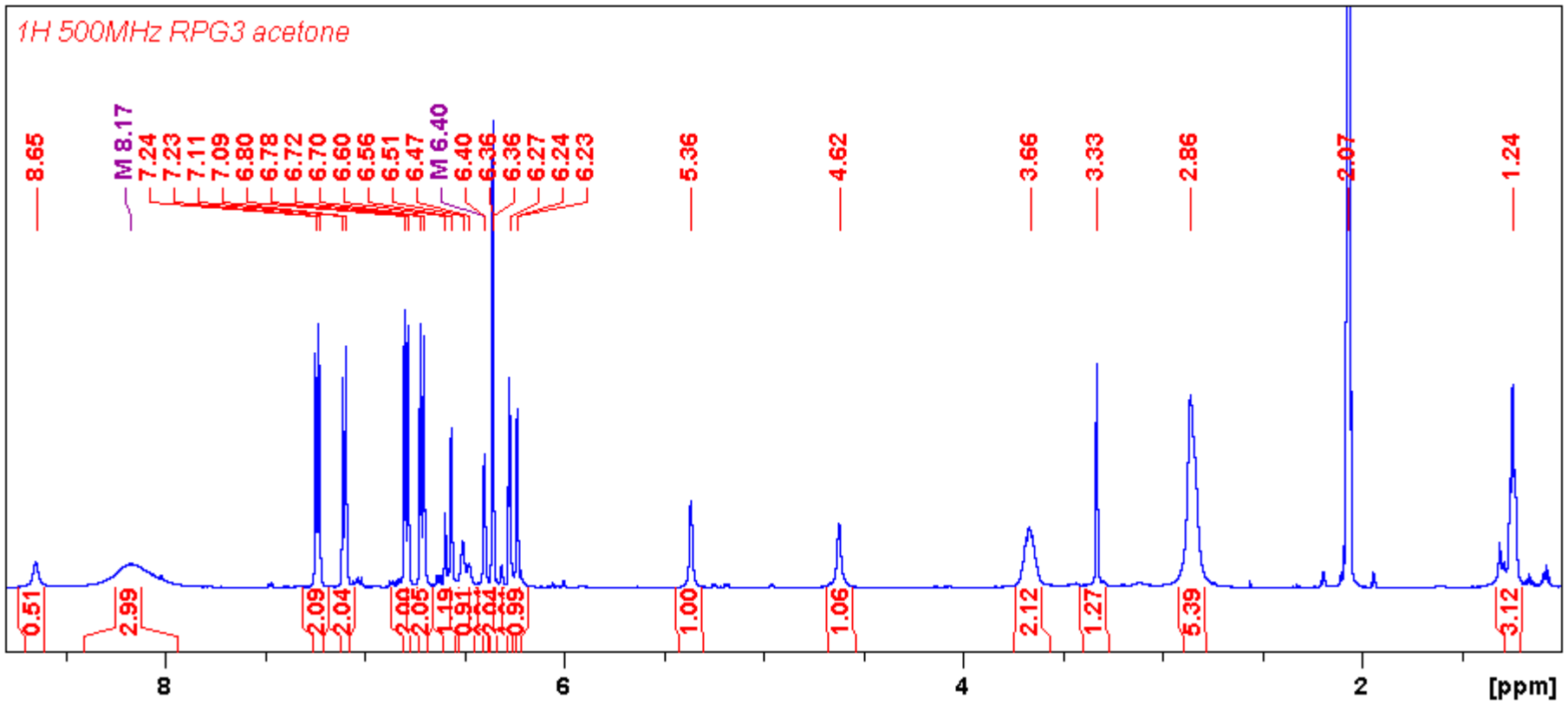
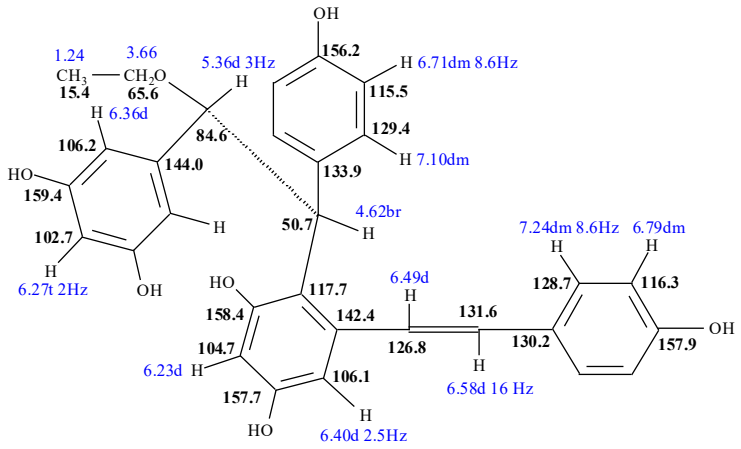


Figure S44. Compound **8**, ^{13}C, APT NMR spectrum.



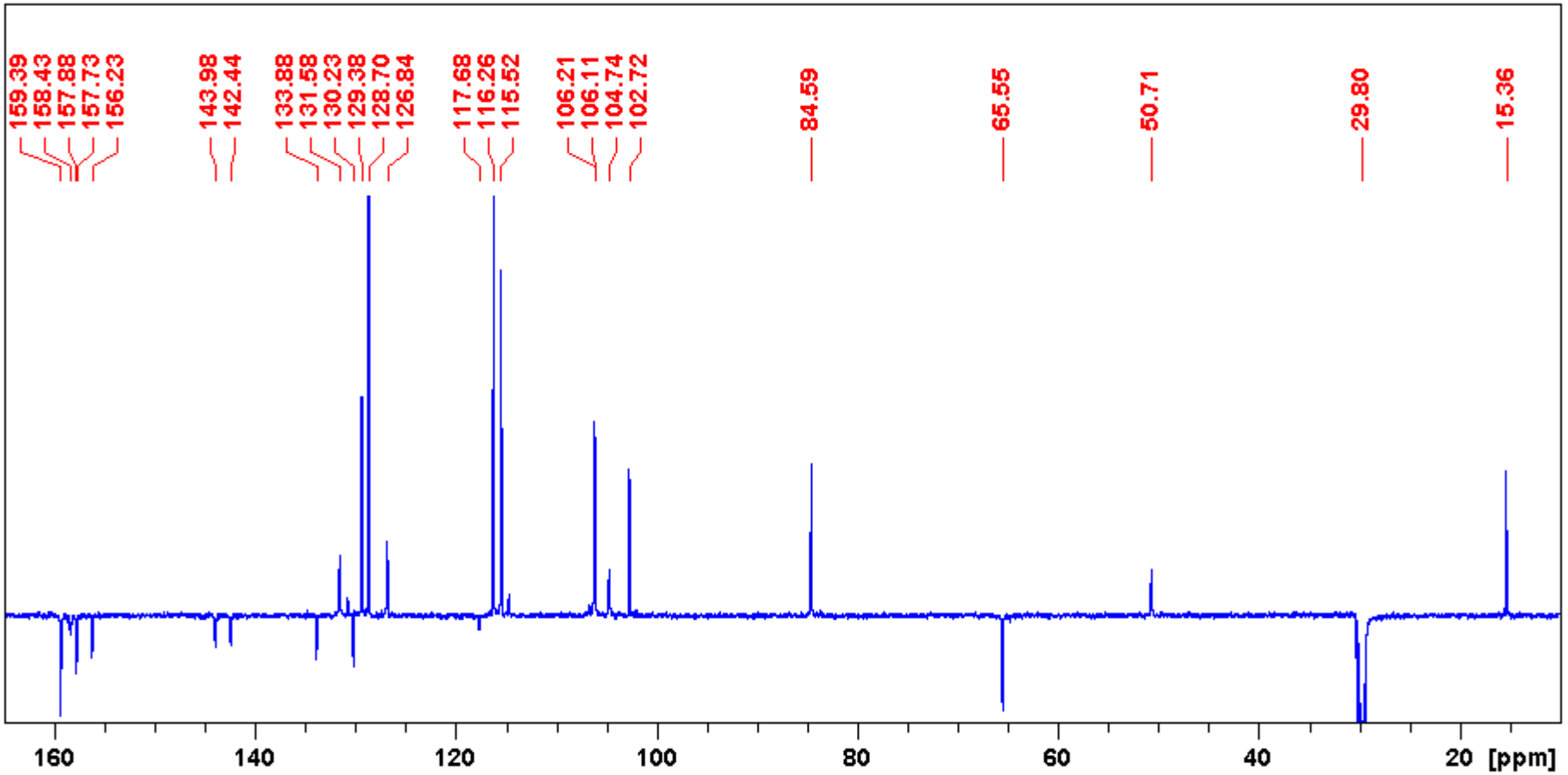


Figure S45. Compound **8**, HSQC spectrum and HSQC section.

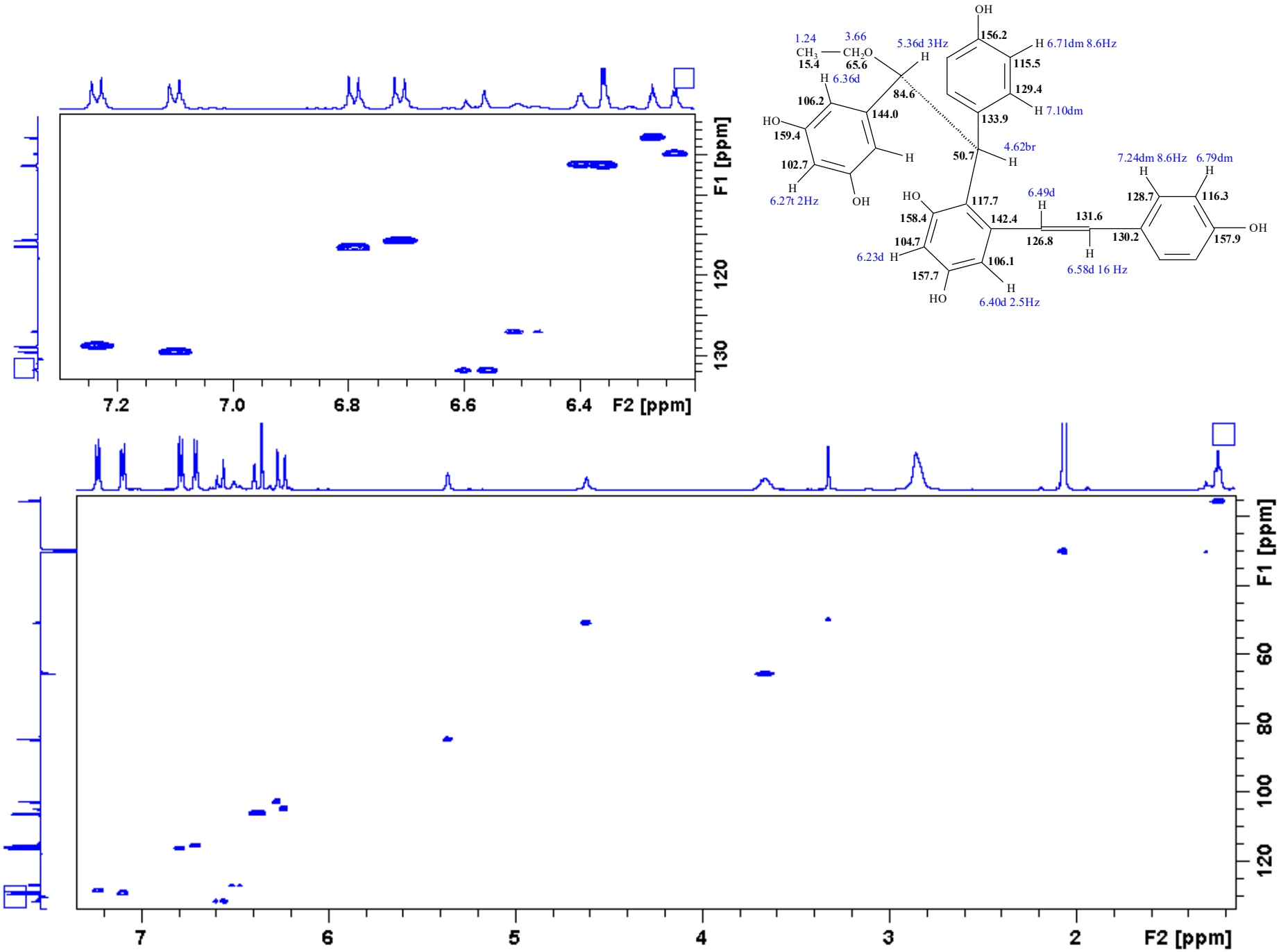


Figure S46. Compound **8**, HMBC spectrum and HMBC section; arrows indicate characteristic responses.

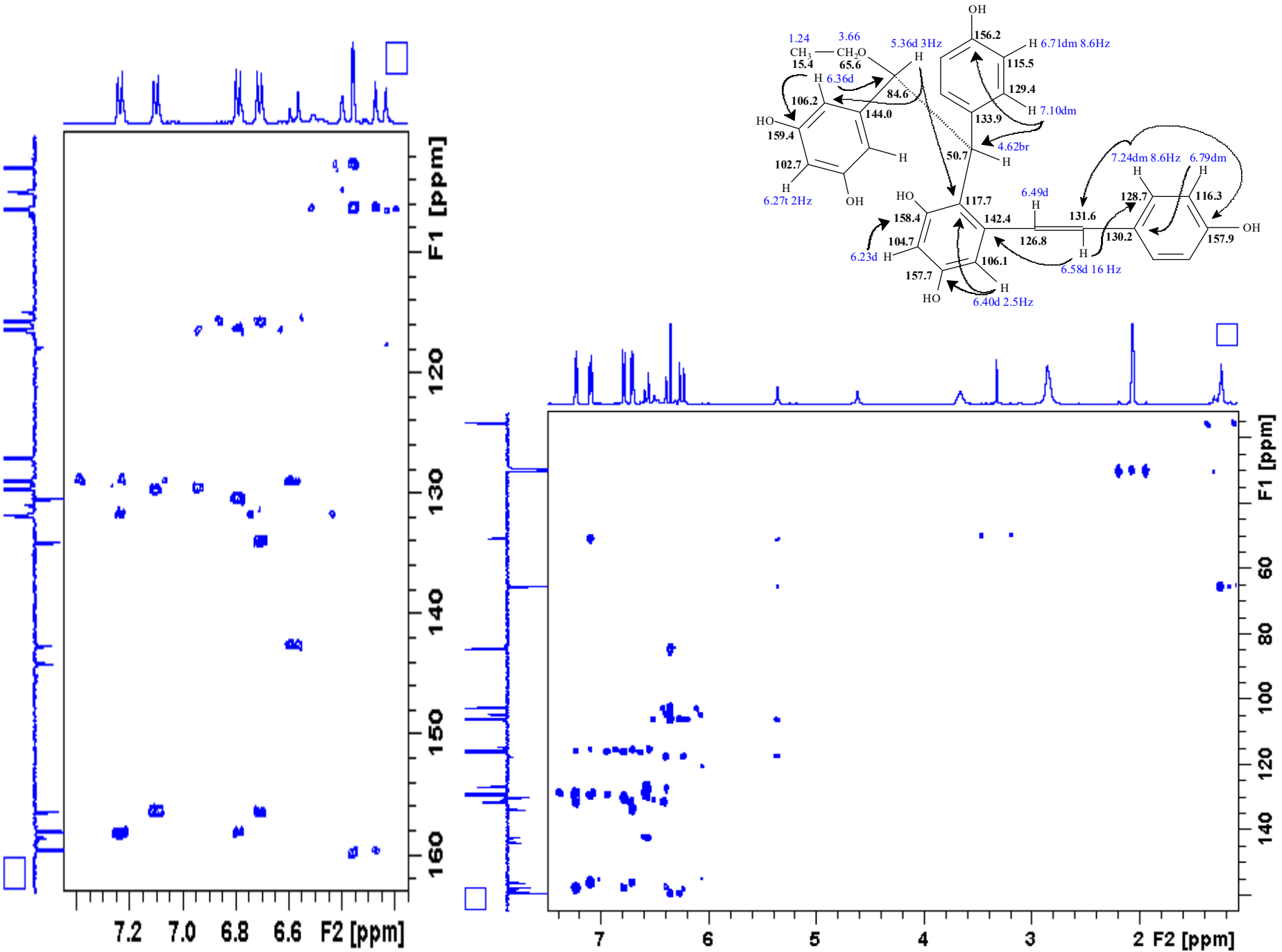
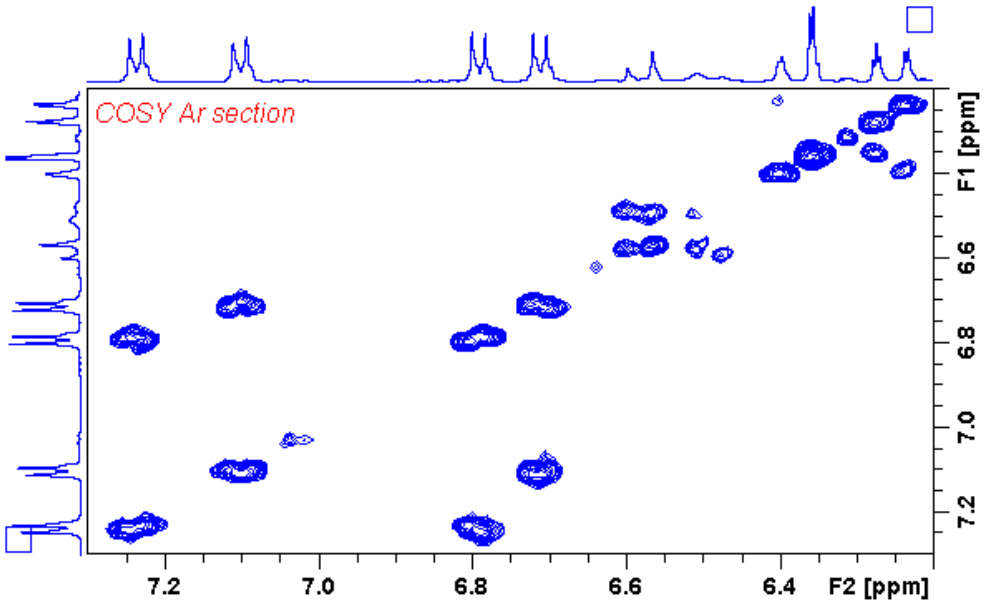
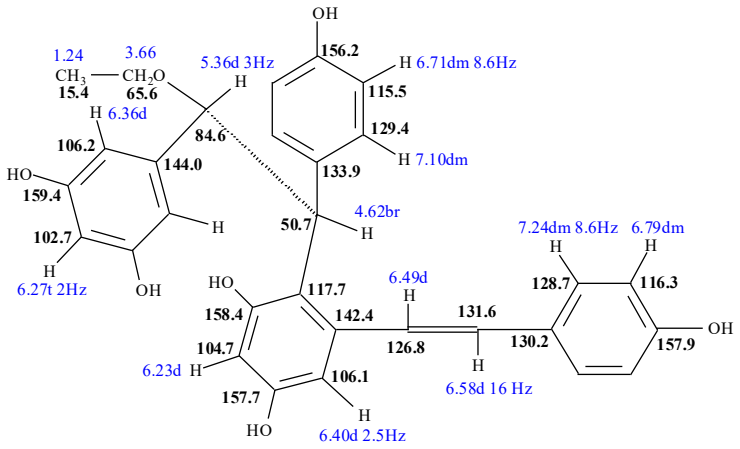


Figure S47. Compound **8**, COSY spectrum and COSY aromatic section.





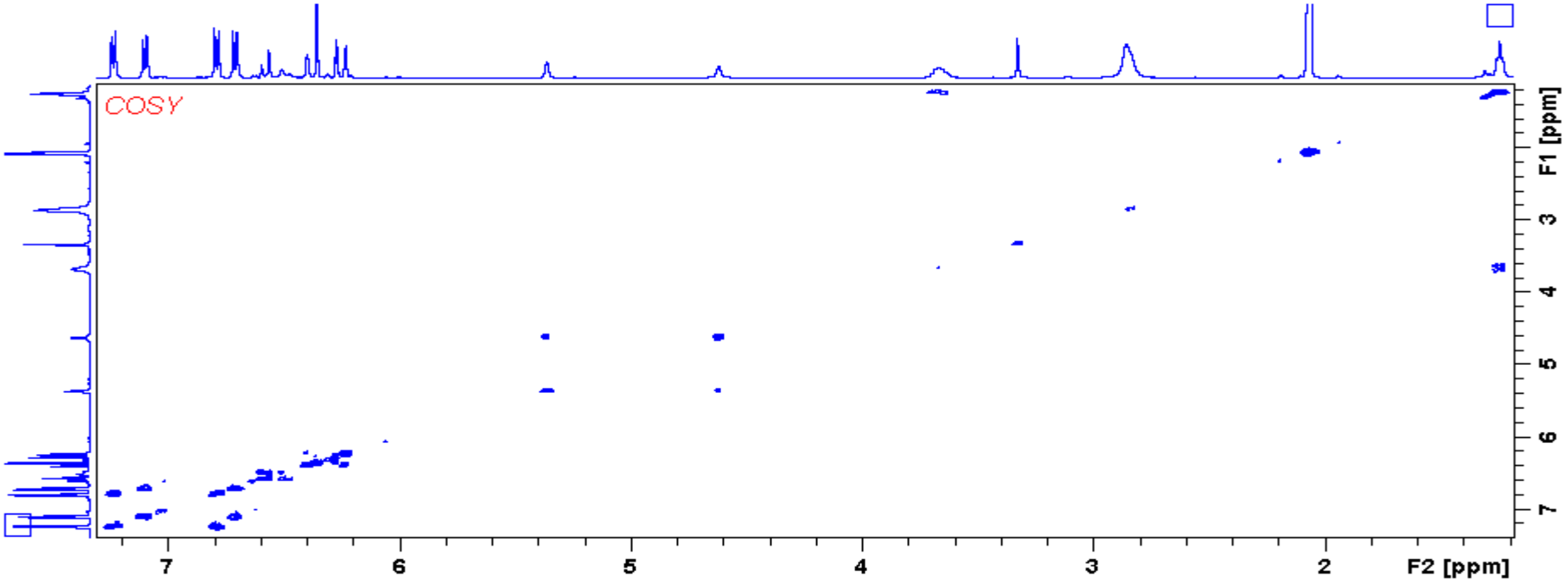


Figure S48. Compound **8**, NOESY; arrows indicate steric proximities, and assign configuration and the dominant conformer.

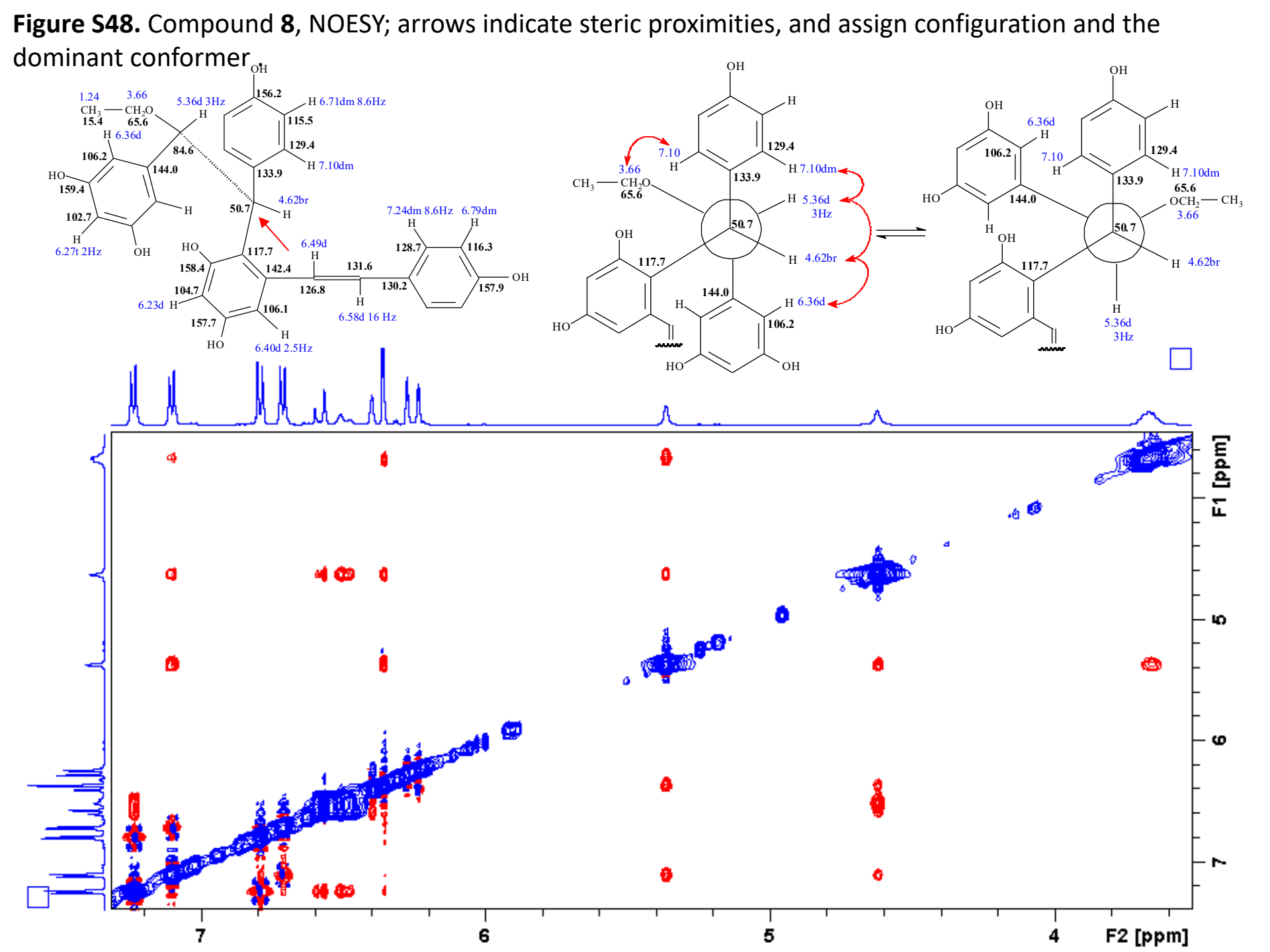
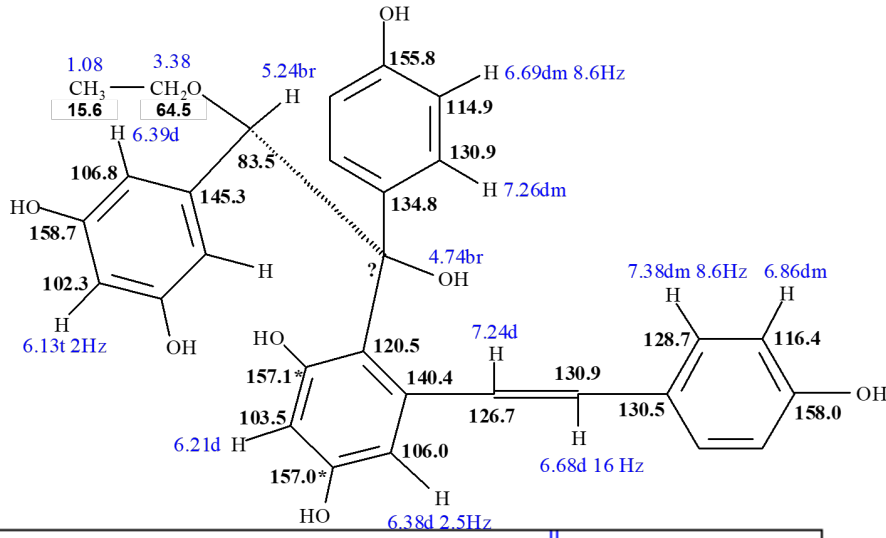


Figure S49. Compound **9**, ^{1}H NMR spectrum.



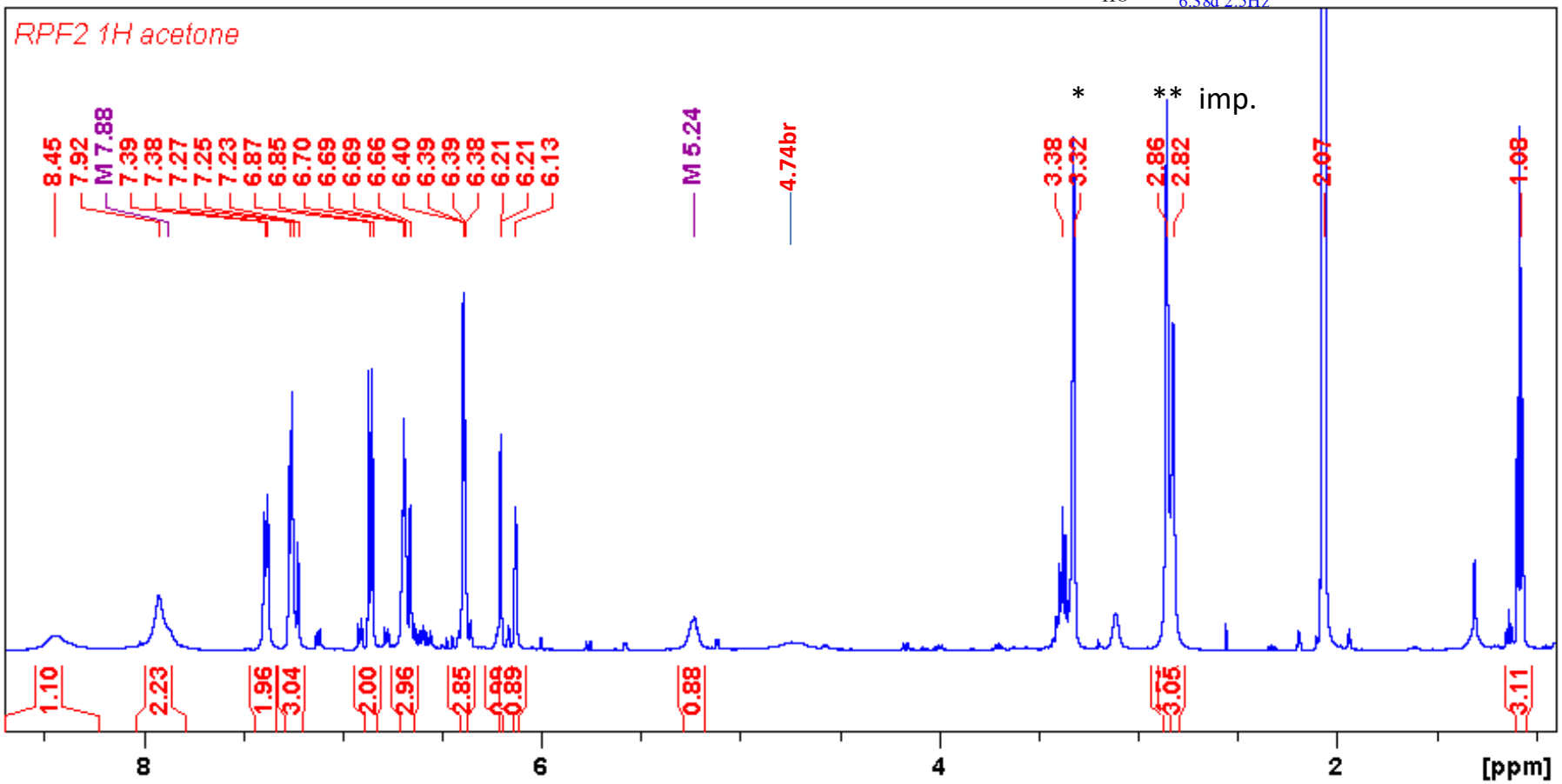
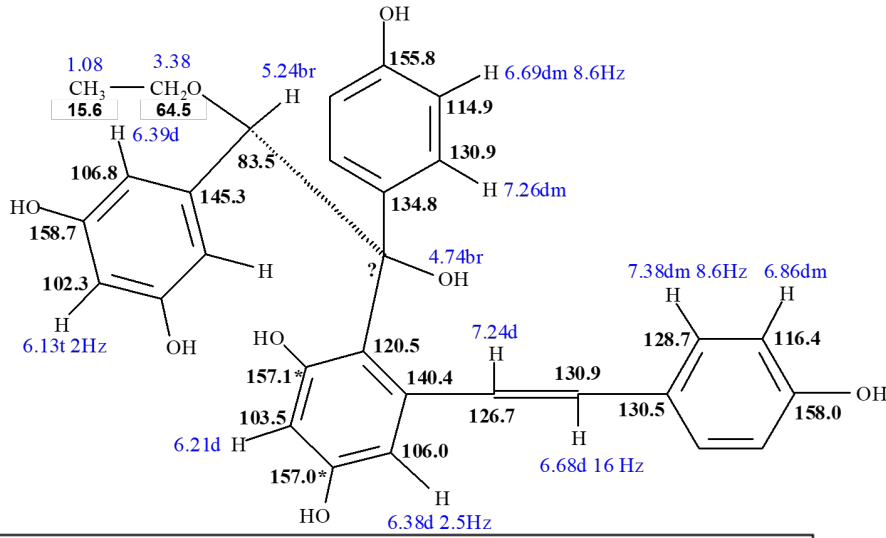


Figure S50. Compound **9**, ^{13}C, APT NMR spectrum.



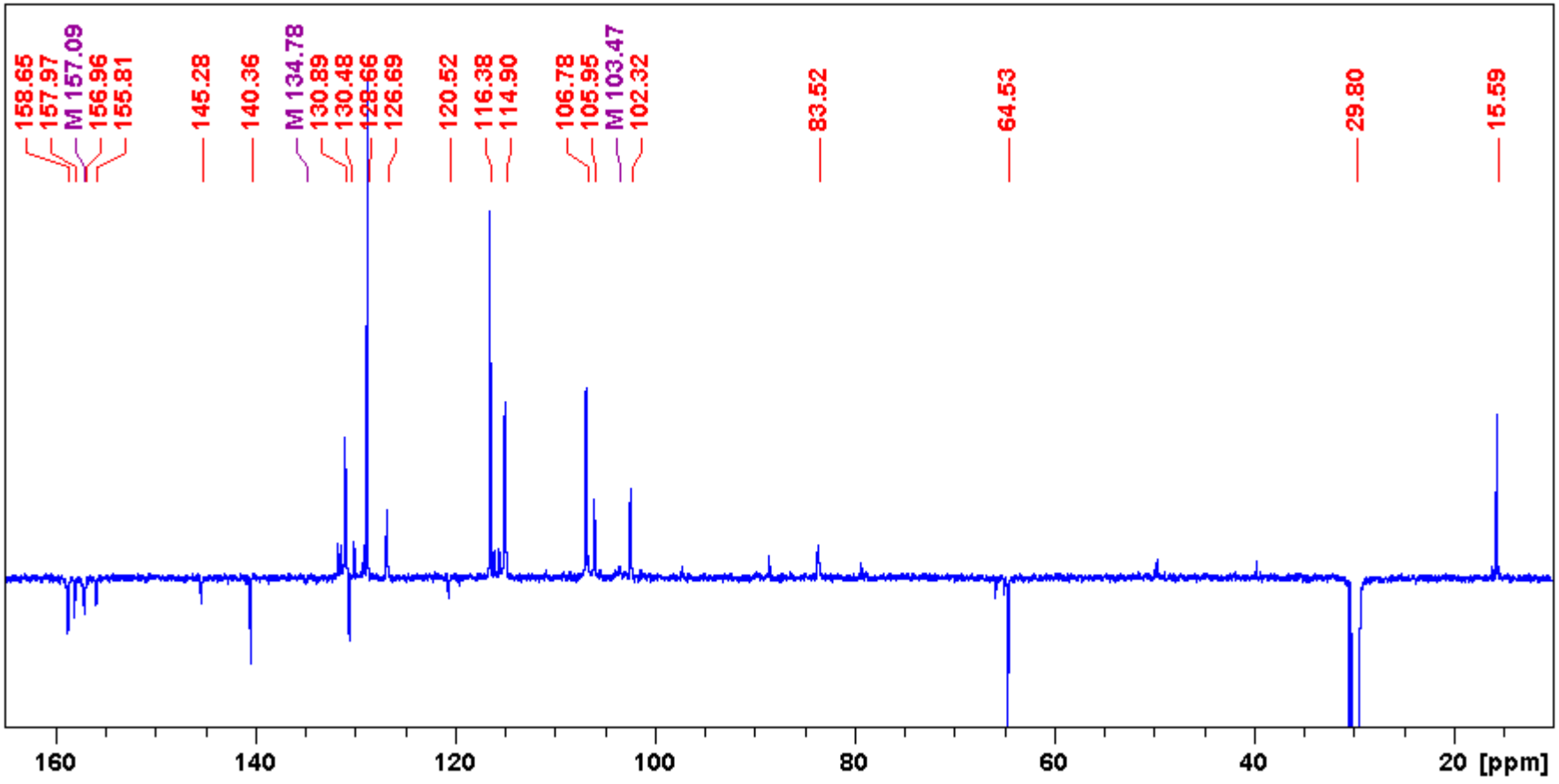
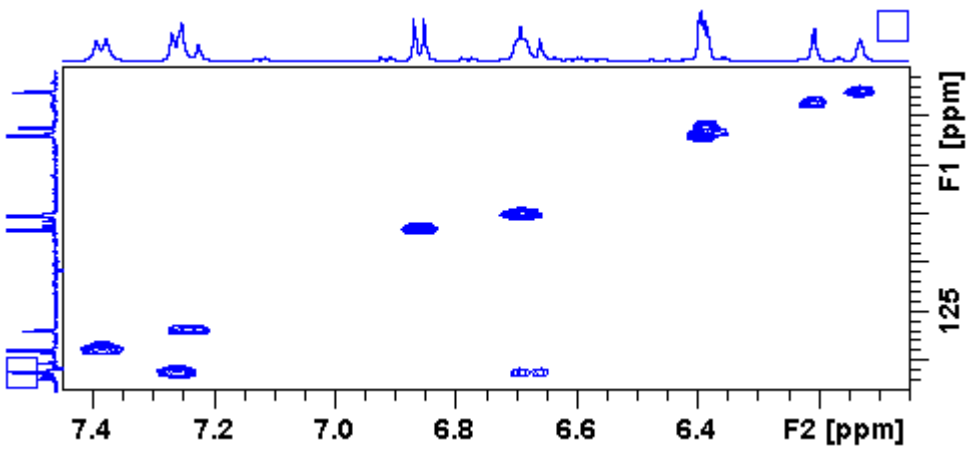
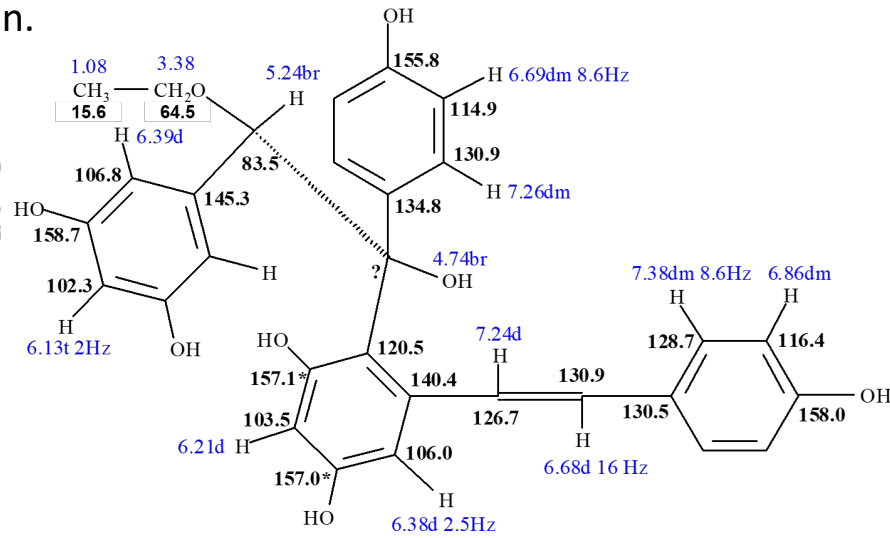


Figure S51. Compound **9**, HSQC spectrum and HSQC section.





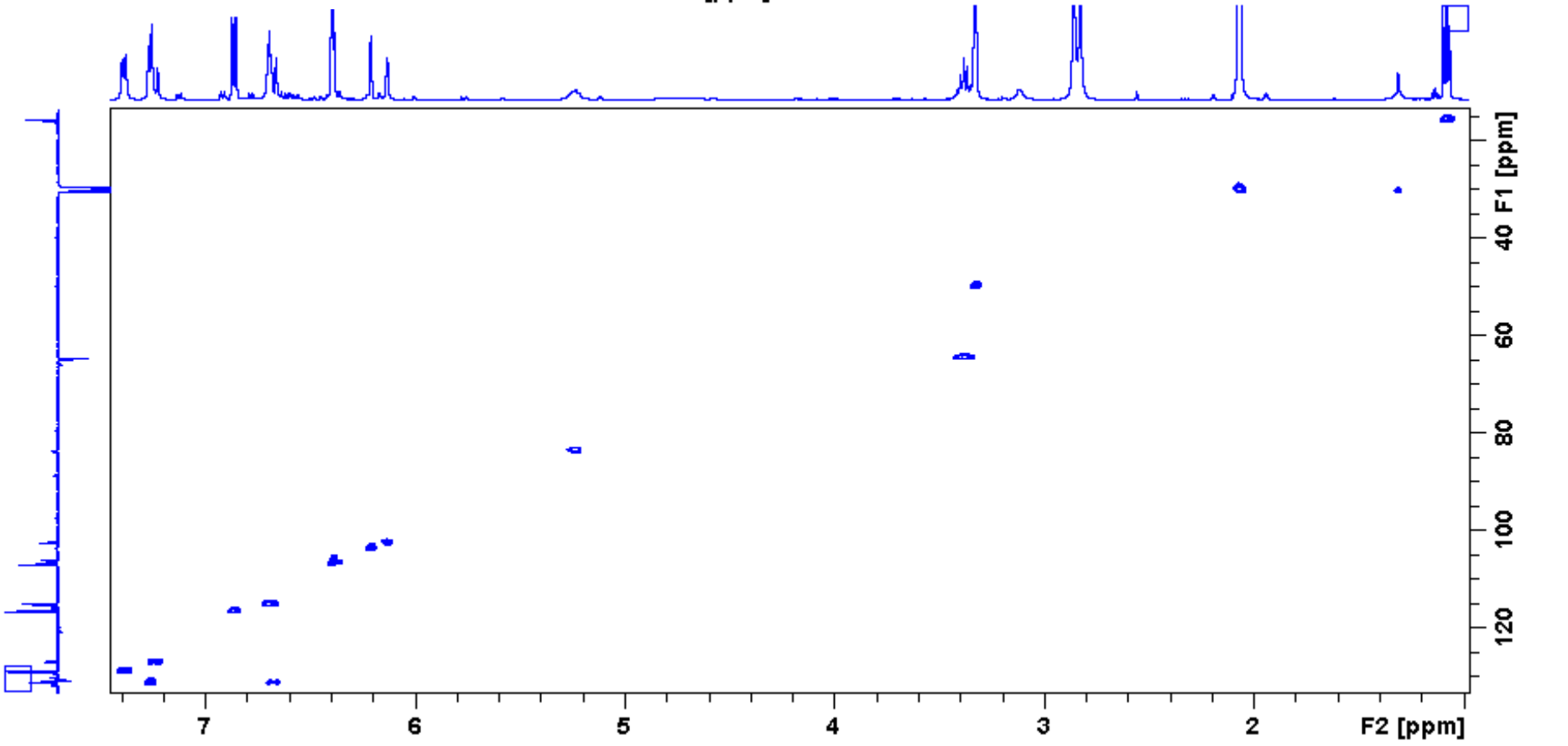


Figure S52. Compound **9**, HMBC spectrum.

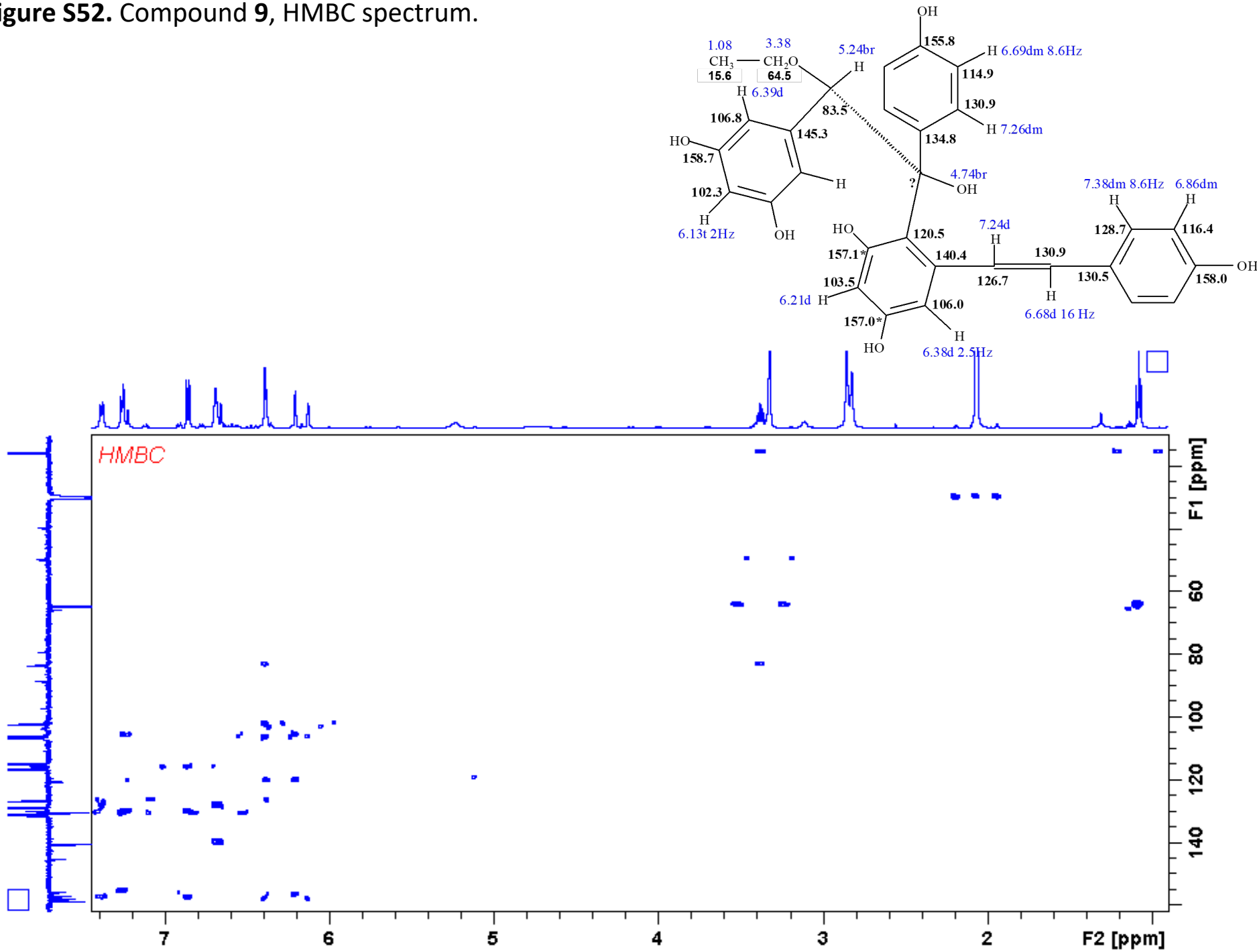


Figure S53. Compound **9**, NOESY spectrum.

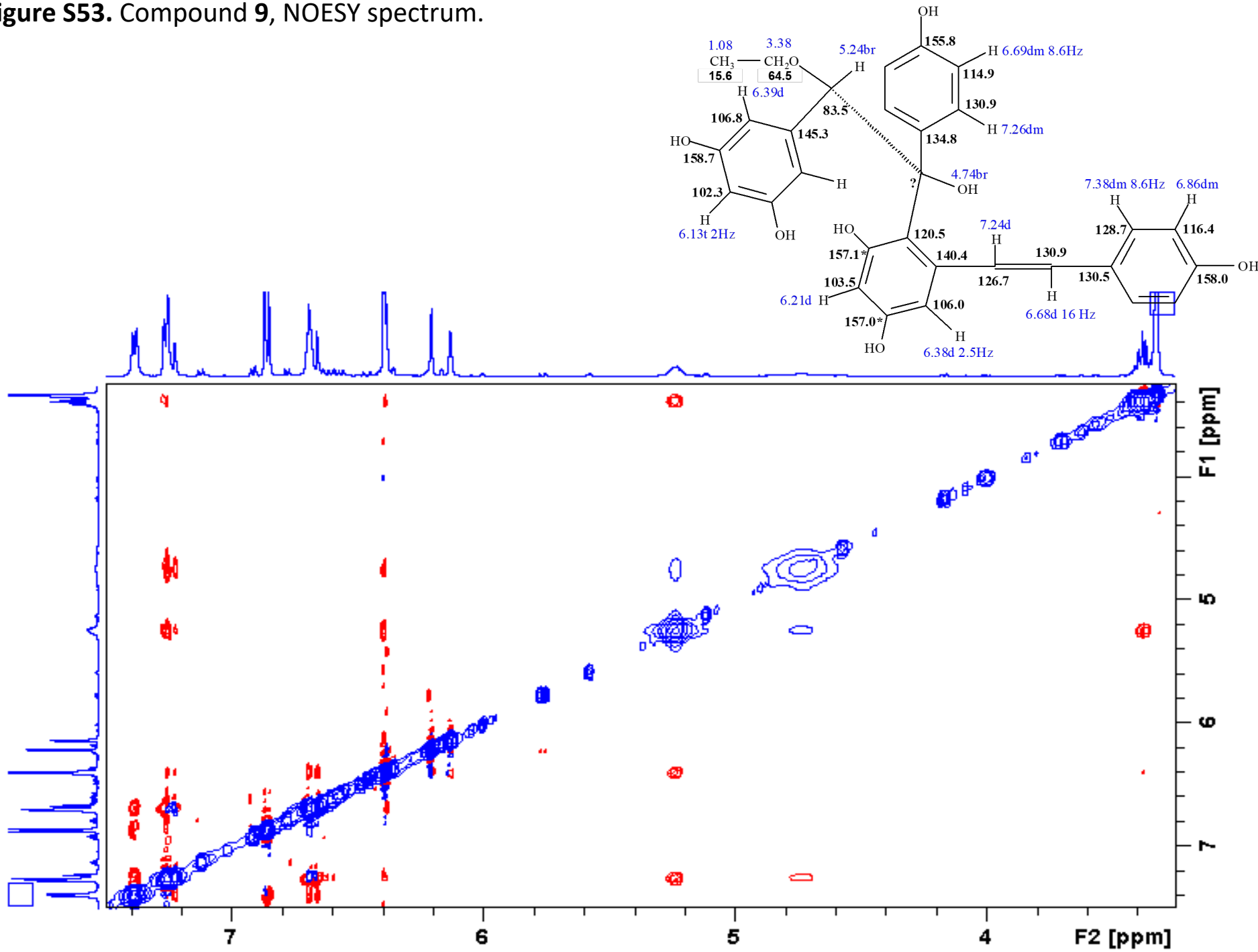


Figure S54. Compound **9**, HSQC spectrum and HSQC section, DMSO-d_6, T=80°C.

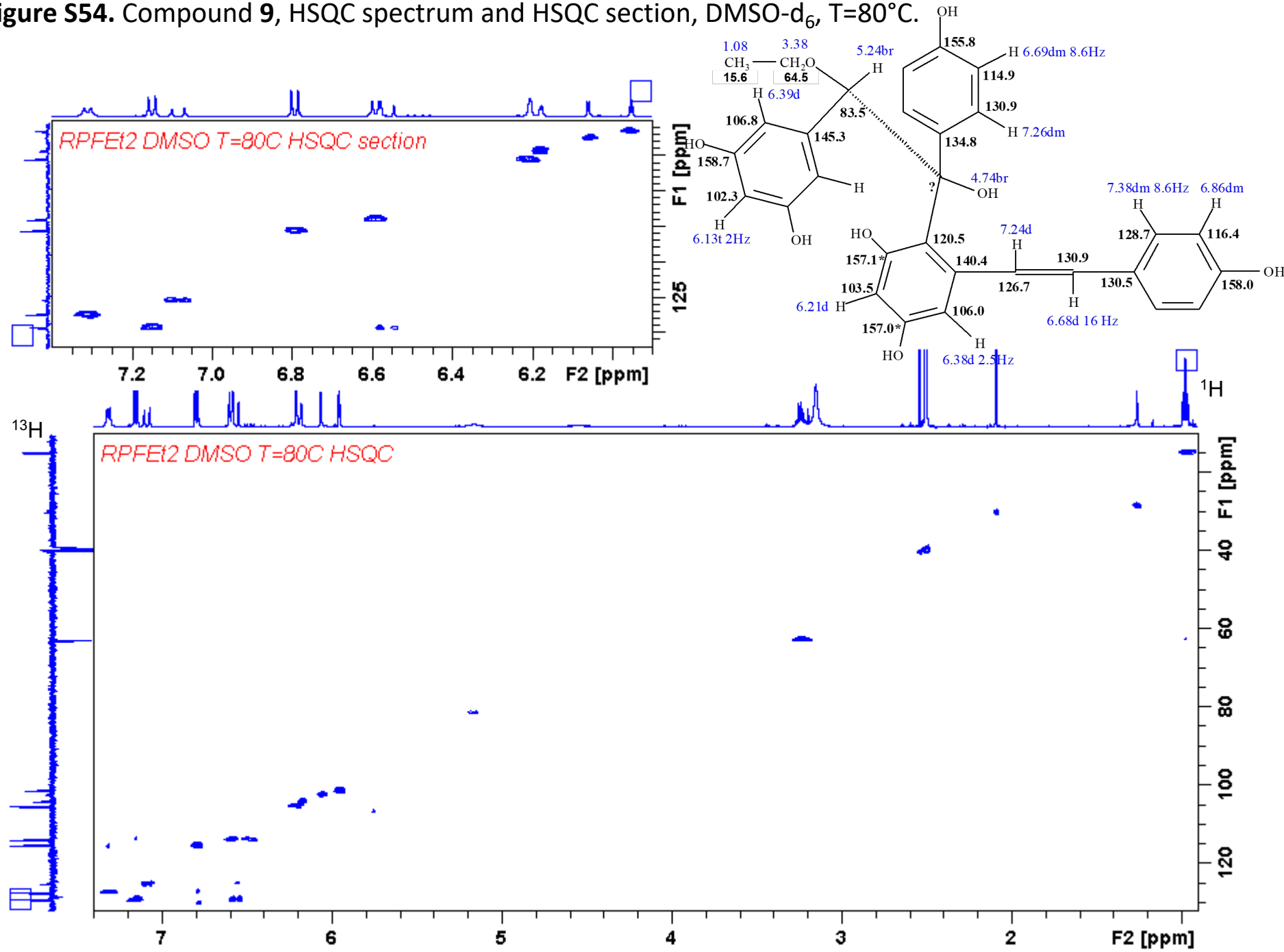
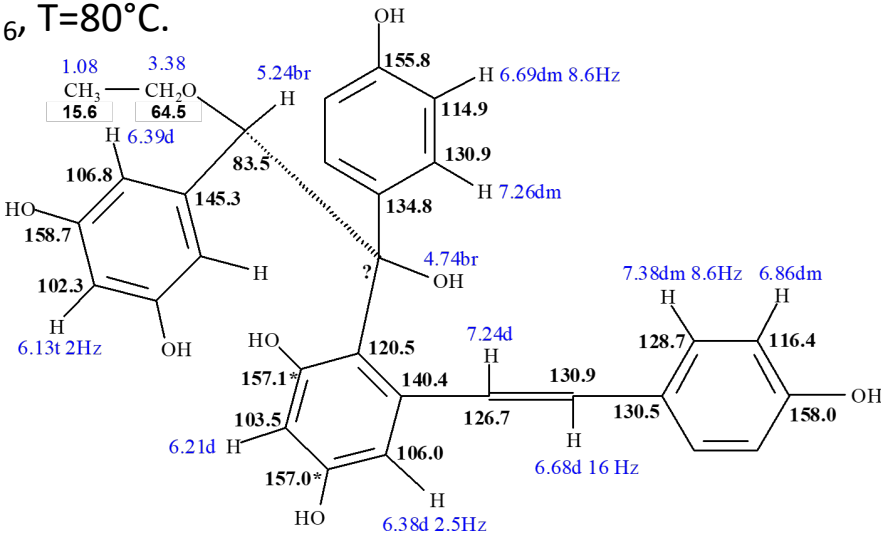


Figure S55. Compound **9**, ^{13}C, APT NMR spectrum, DMSO-d_6, T=80°C.



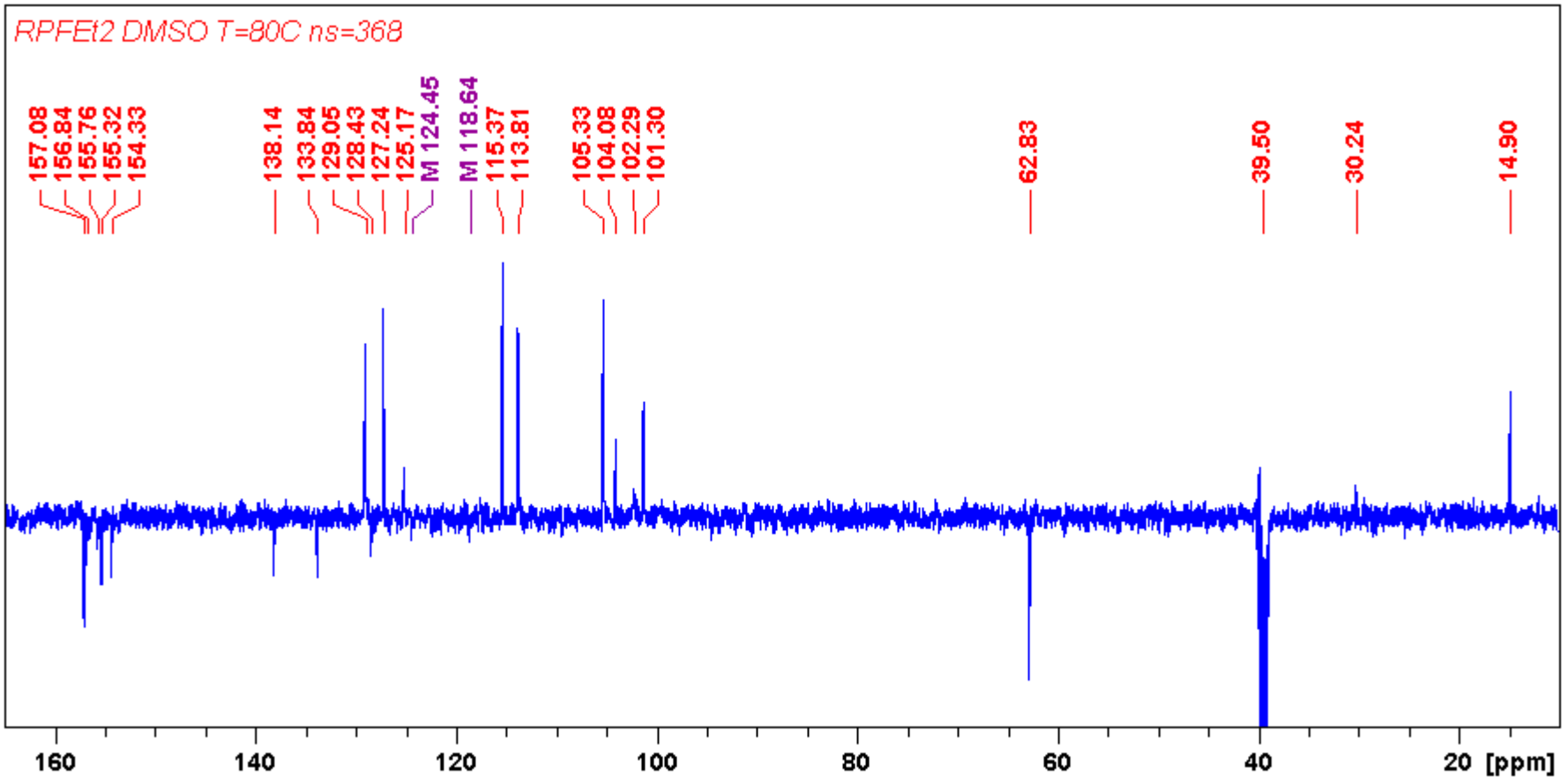


Figure S56. Compound **9**, selROE on CH (5.16 ppm) and OH (4.53 ppm) , DMSO-d_6, T=80°C.

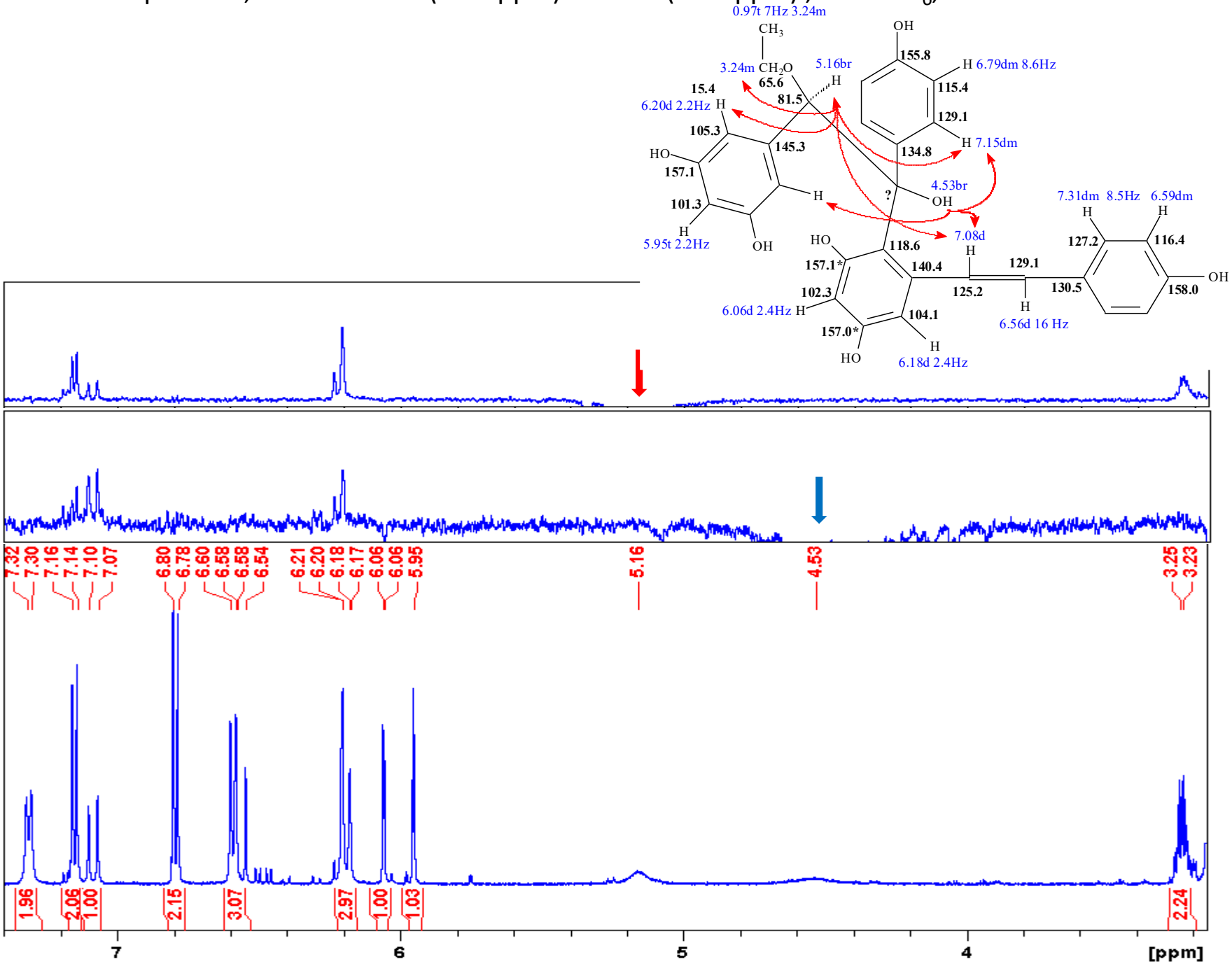
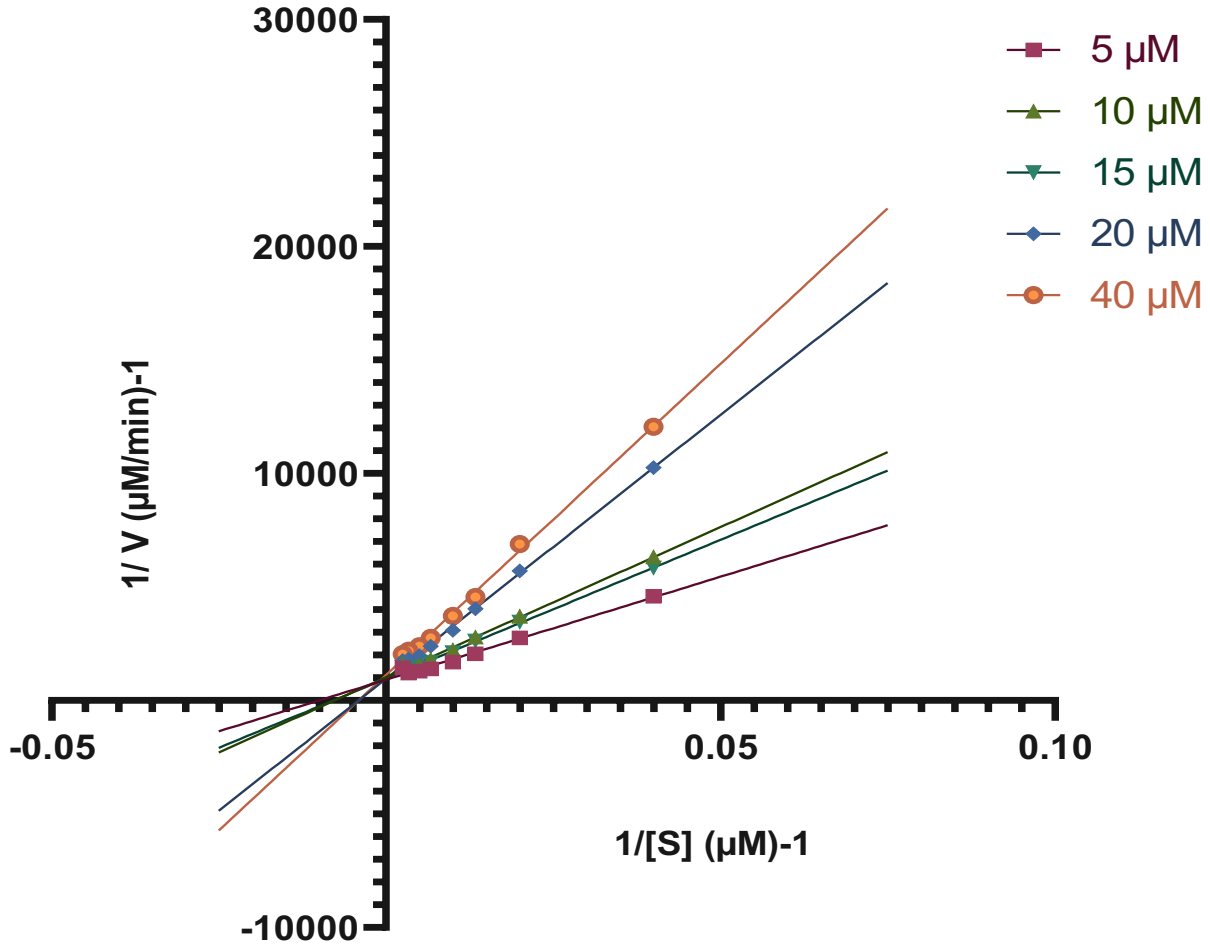
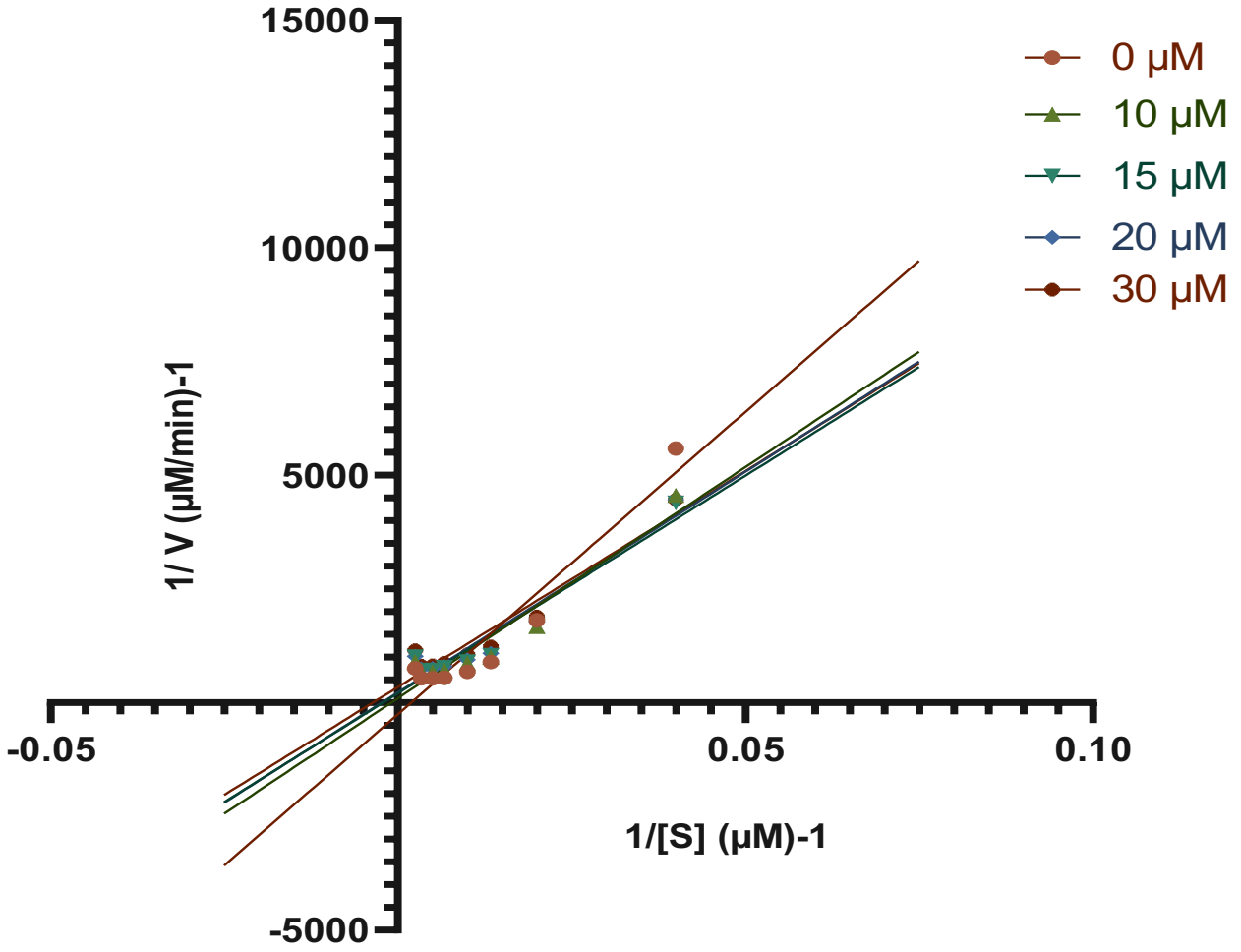


Figure S57 : Lineweaver-Burk Plot of compound 2



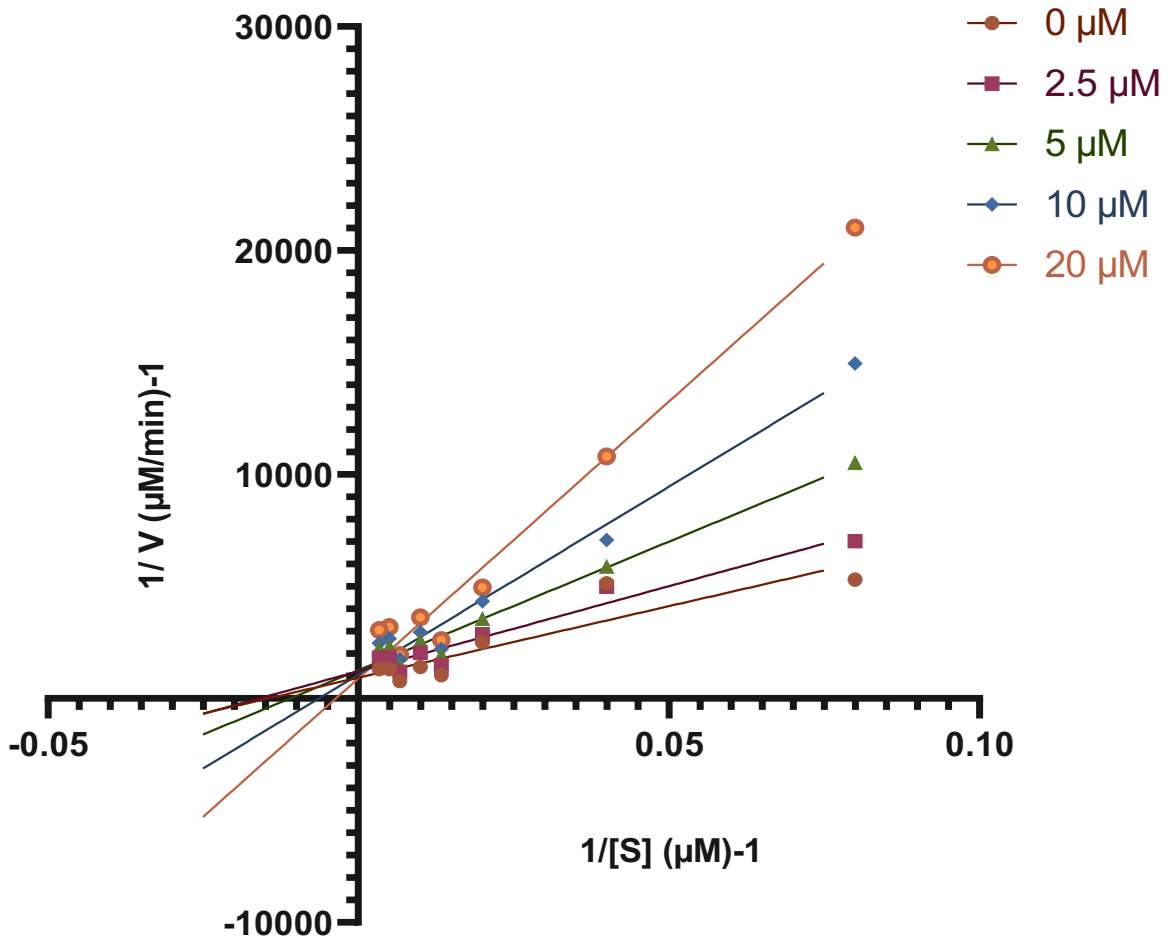
Concentration (µM)	Vmax (x 10^{-3} mM/min)	Km (µM)	Inhibition type
5	1.1	99.5	Competitive inhibition
10	0.98	129.7	
15	1.04	126.5	
20	1.05	244.0	
40	0.89	244.0	

Figure S58 : Lineweaver-Burk Plot of compound 3



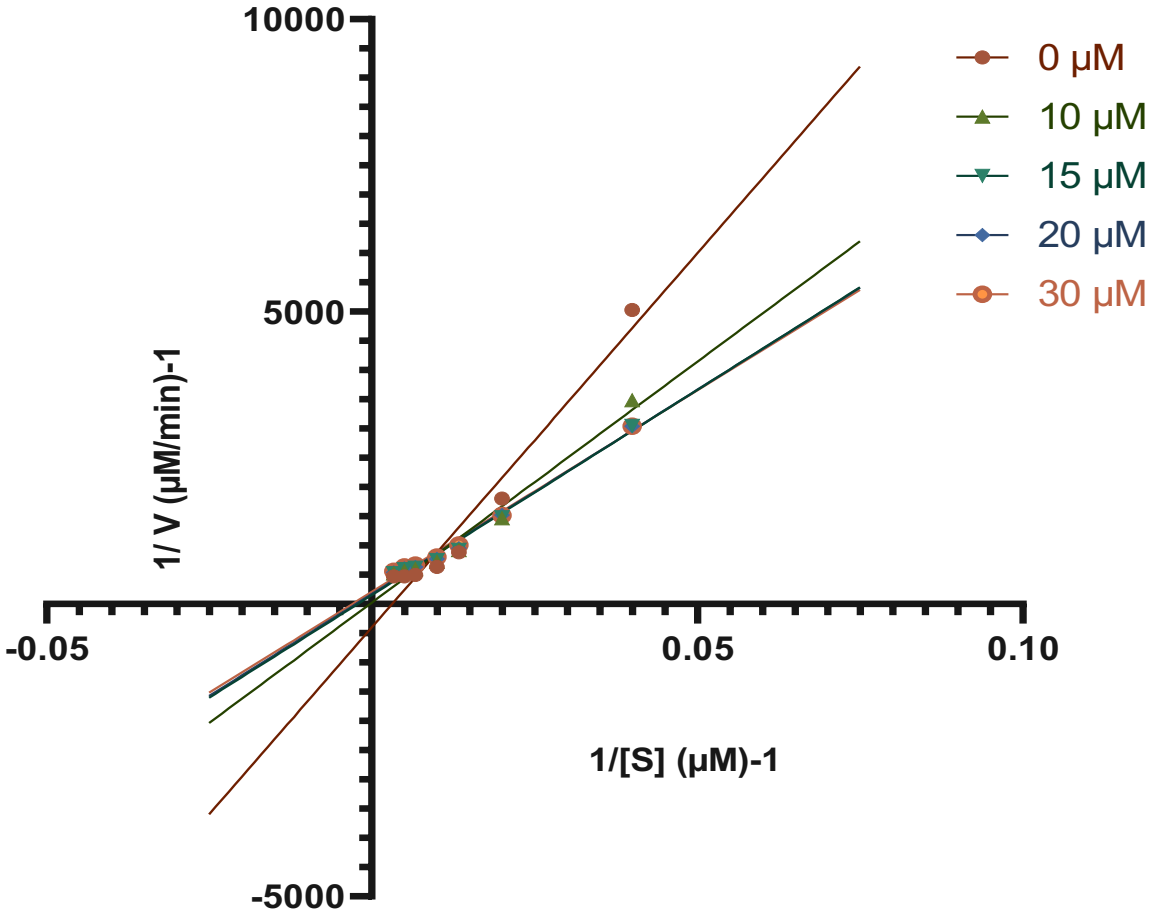
Concentration (µM)	Vmax (x 10^{-3} mM/min)	Km (µM)	Inhibition type
0	-3.9	-521.8	Mixed inhibition
10	10.1	1030.7	
15	4.8	463.1	
20	4.4	427.4	
30	2.9	275.4	

Figure S59 : Lineweaver-Burk Plot of compound 4



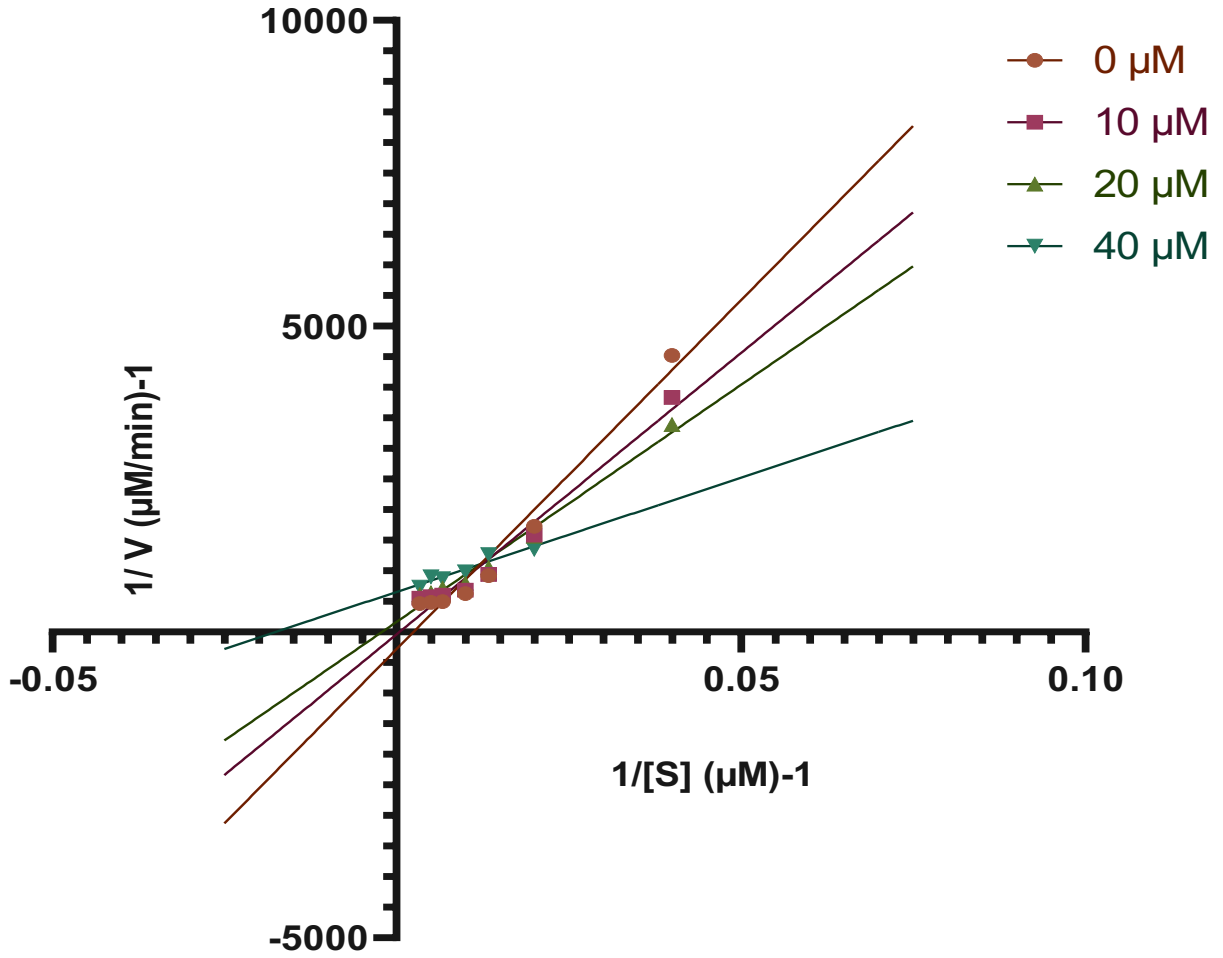
Concentration (µM)	Vmax (x 10^{-3} mM/min)	Km (µM)	Inhibition type
0	1.1	68.7	Competitive inhibition
2.5	0.8	62.5	
5	0.8	91.0	
10	0.9	157.1	
20	1.1	276.9	

Figure S60 : Lineweaver-Burk Plot of compound 5



Concentration (µM)	Vmax ($x\ 10^{-3}$ 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 (x 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	