Supporting Information

Isocadiolides A-H: Polybrominated Aromatics from a *Synoicum* sp. Ascidian

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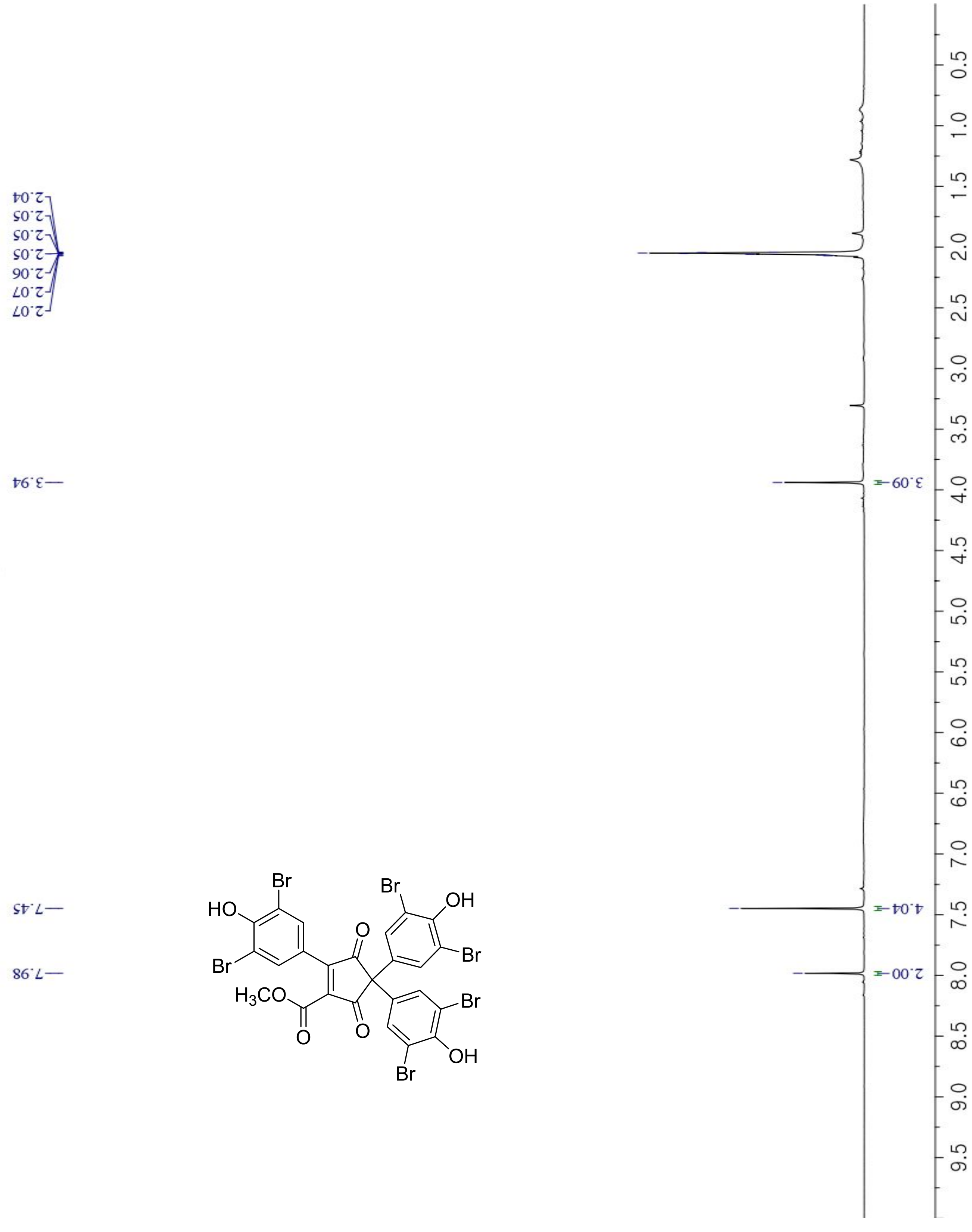


Figure S1. The ^{1}H NMR (800 MHz, acetone-d_6) spectrum of **1**

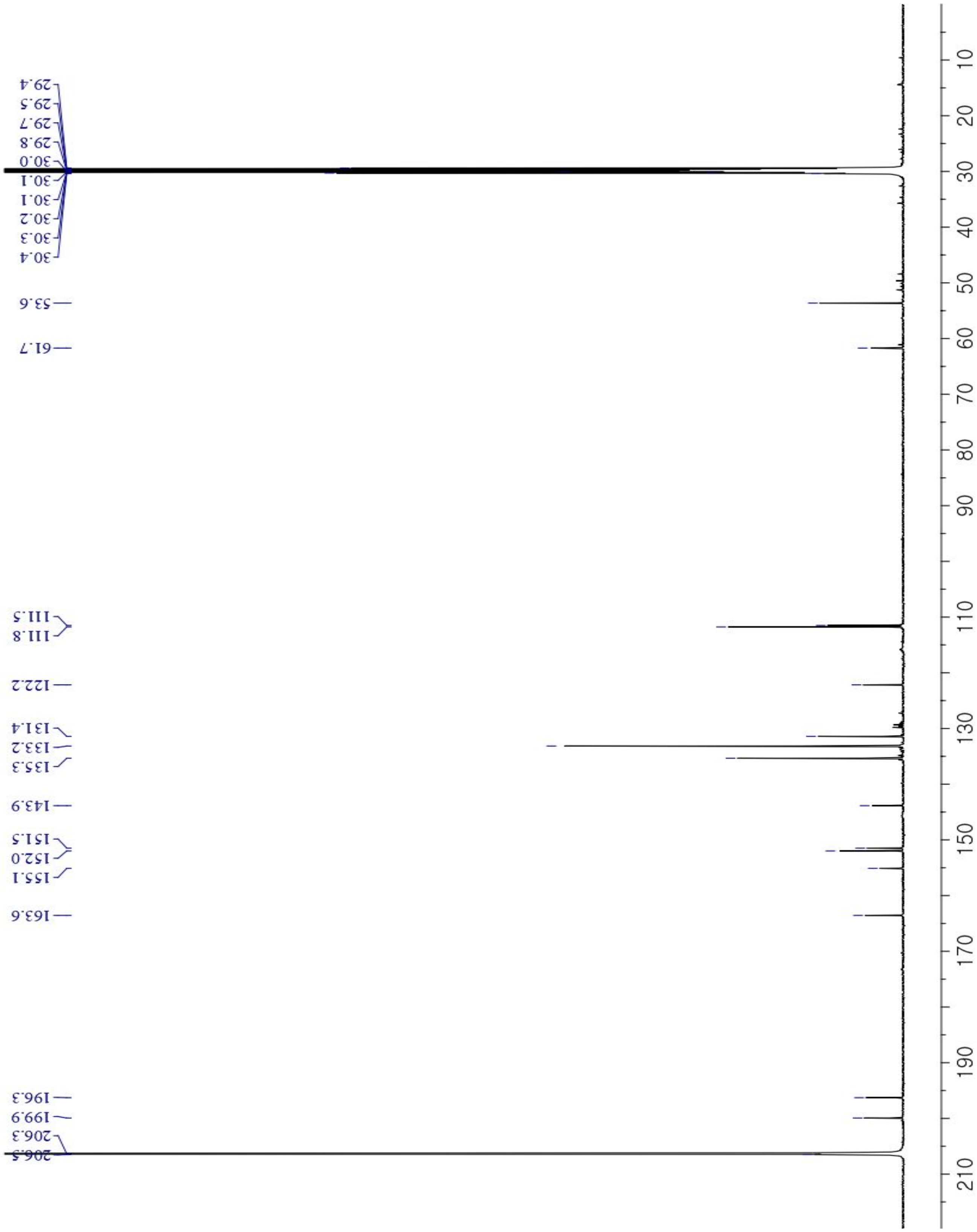


Figure S2. The ^{13}C NMR (200 MHz, acetone-d_6) spectrum of **1**

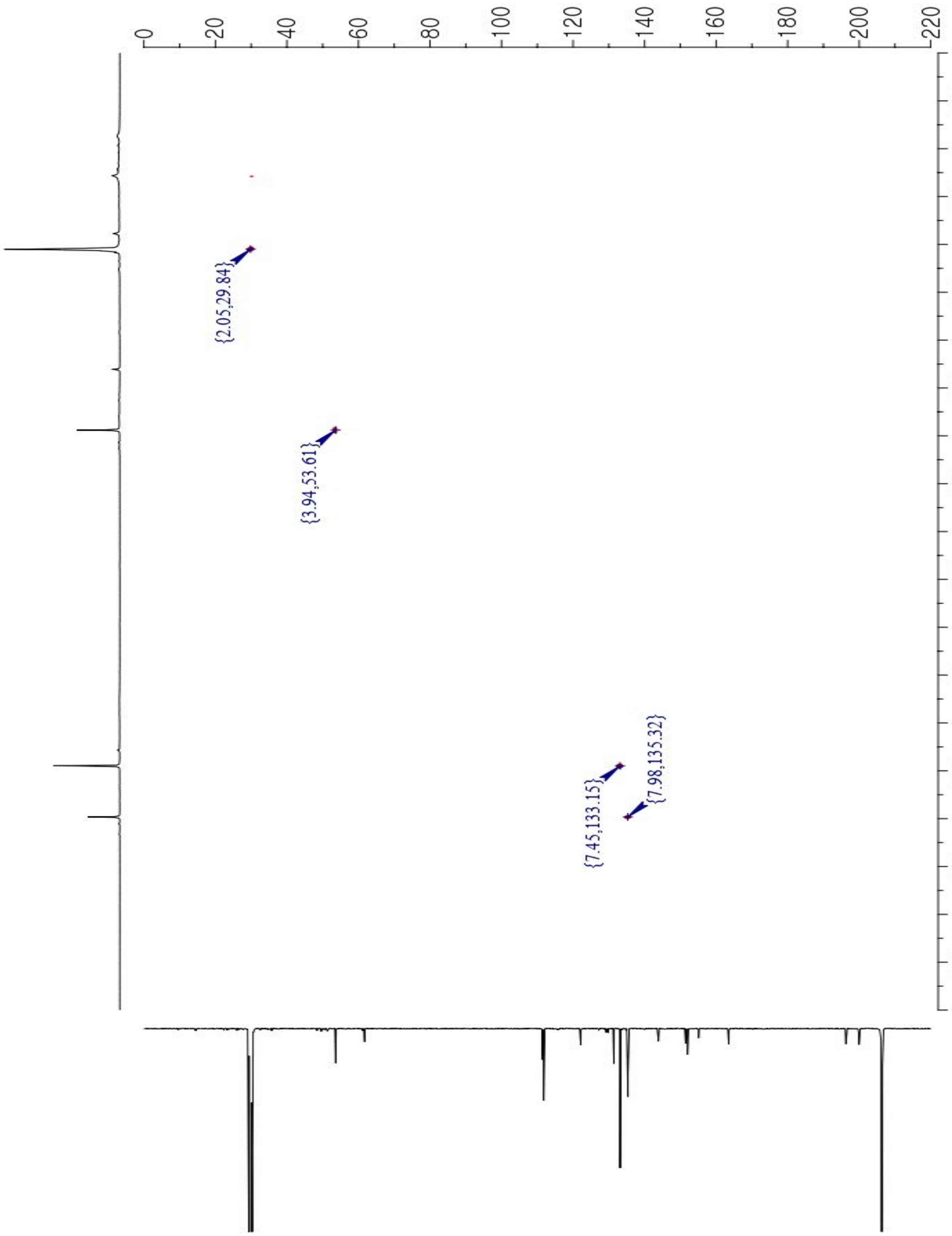


Figure S3. The HSQC (800 MHz, acetone-d_6) spectrum of **1**

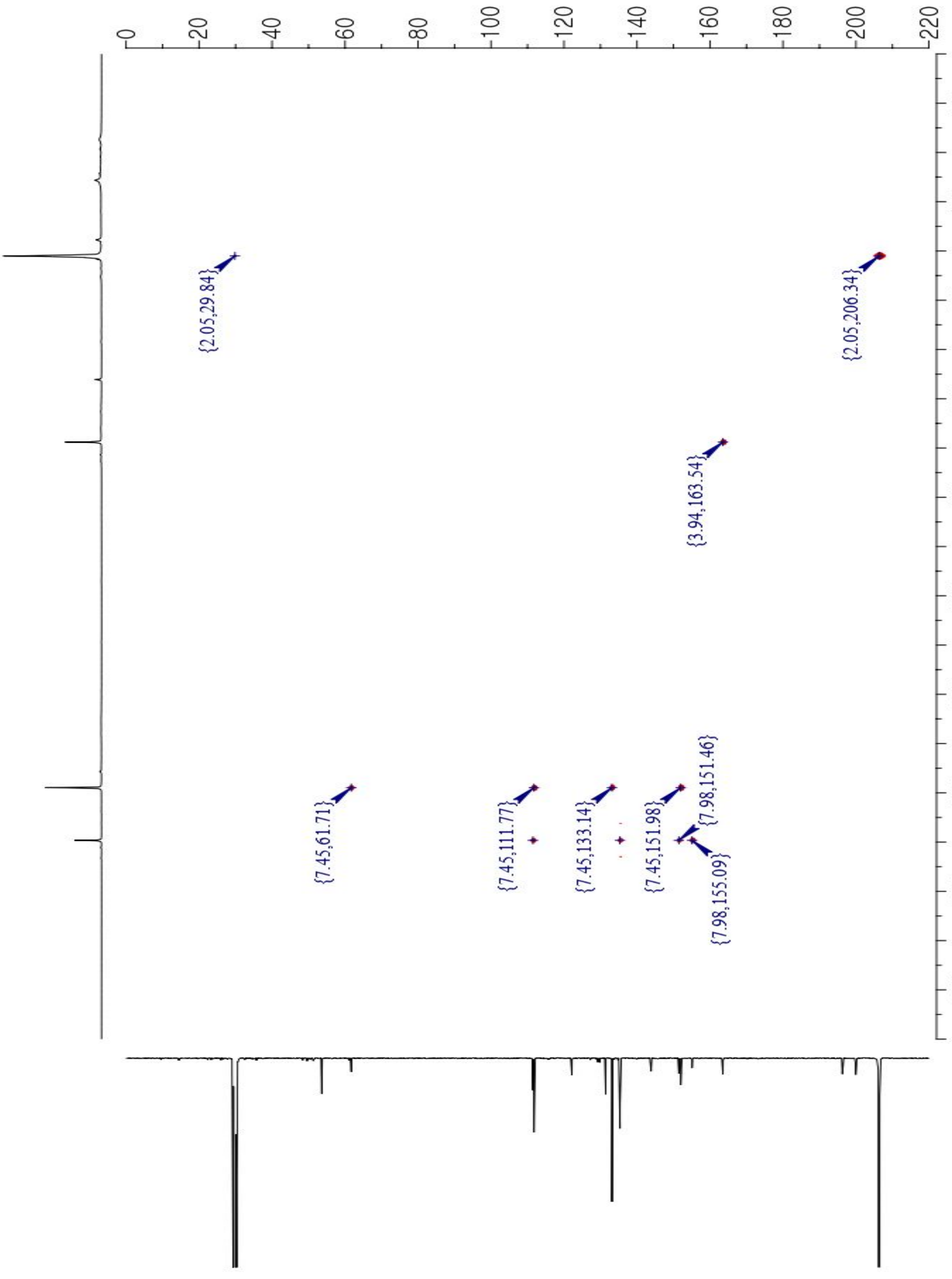


Figure S4. The HMBC (800 MHz, acetone-$d_{6,}$ J_{CH} = 8 Hz) spectrum of **1**

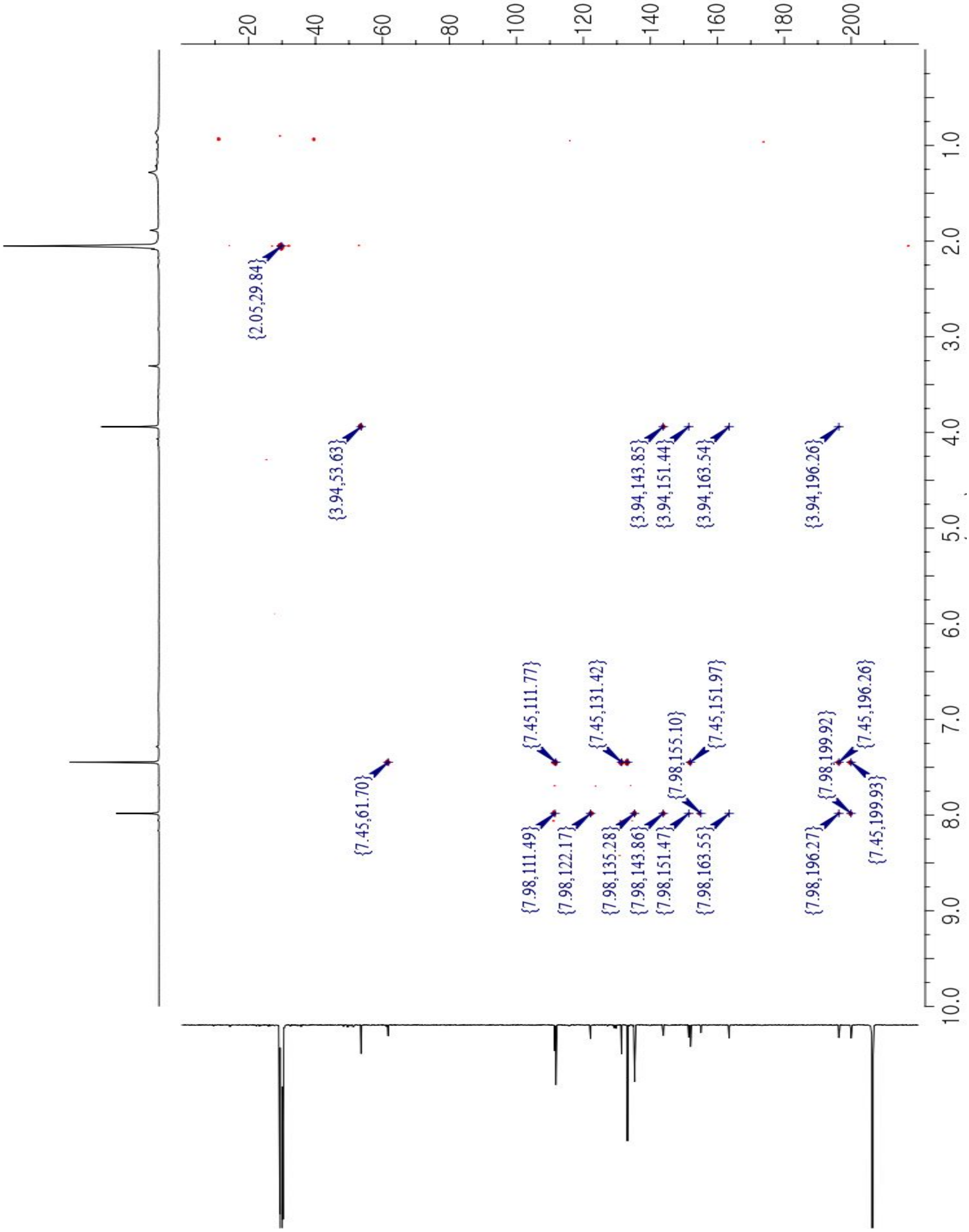


Figure S5. The D-HMBC (800 MHz, acetone-d_6, J_{CH} = 1 Hz) spectrum of **1**

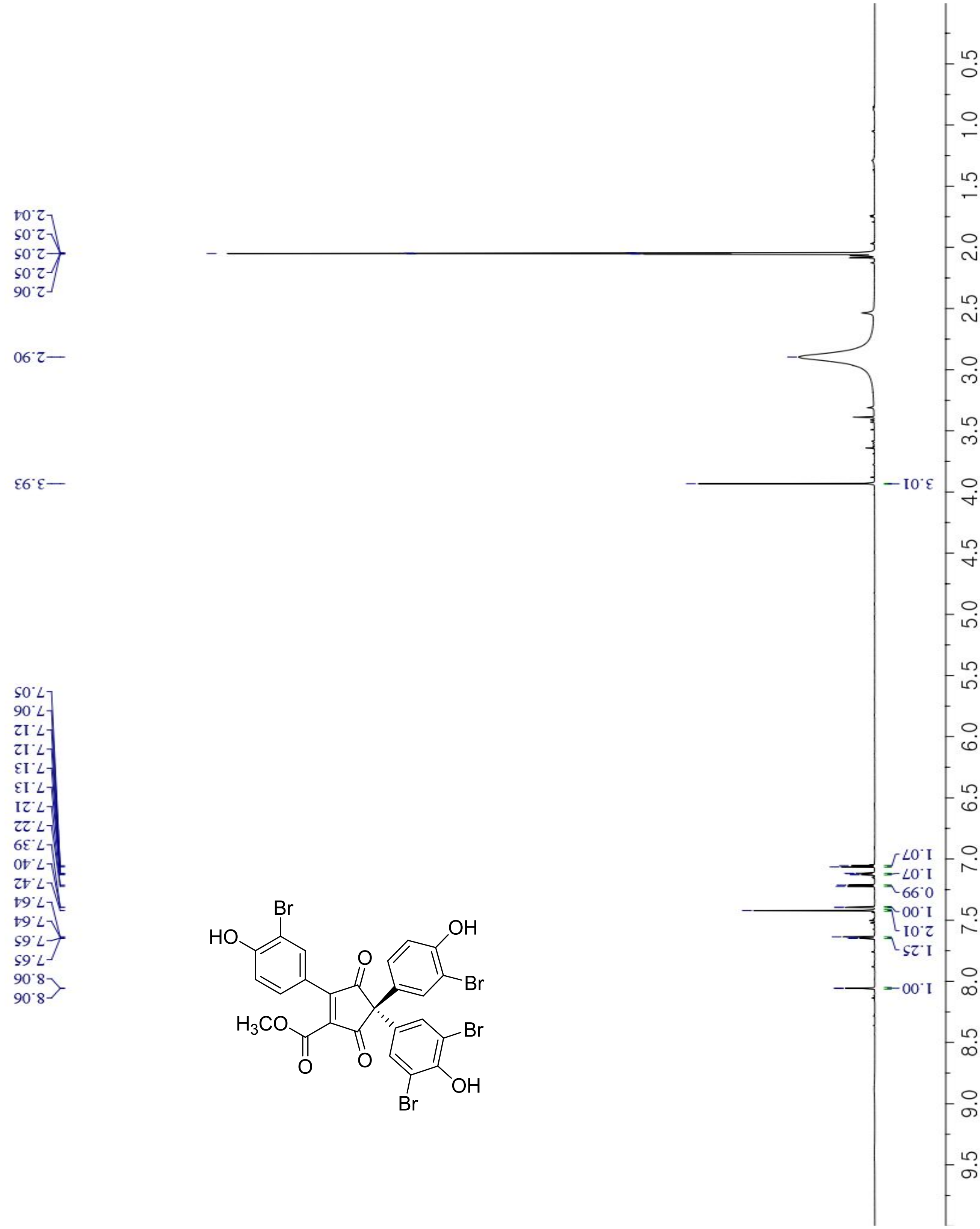


Figure S6. The [1]H NMR (800 MHz, acetone-d_6) spectrum of **2**

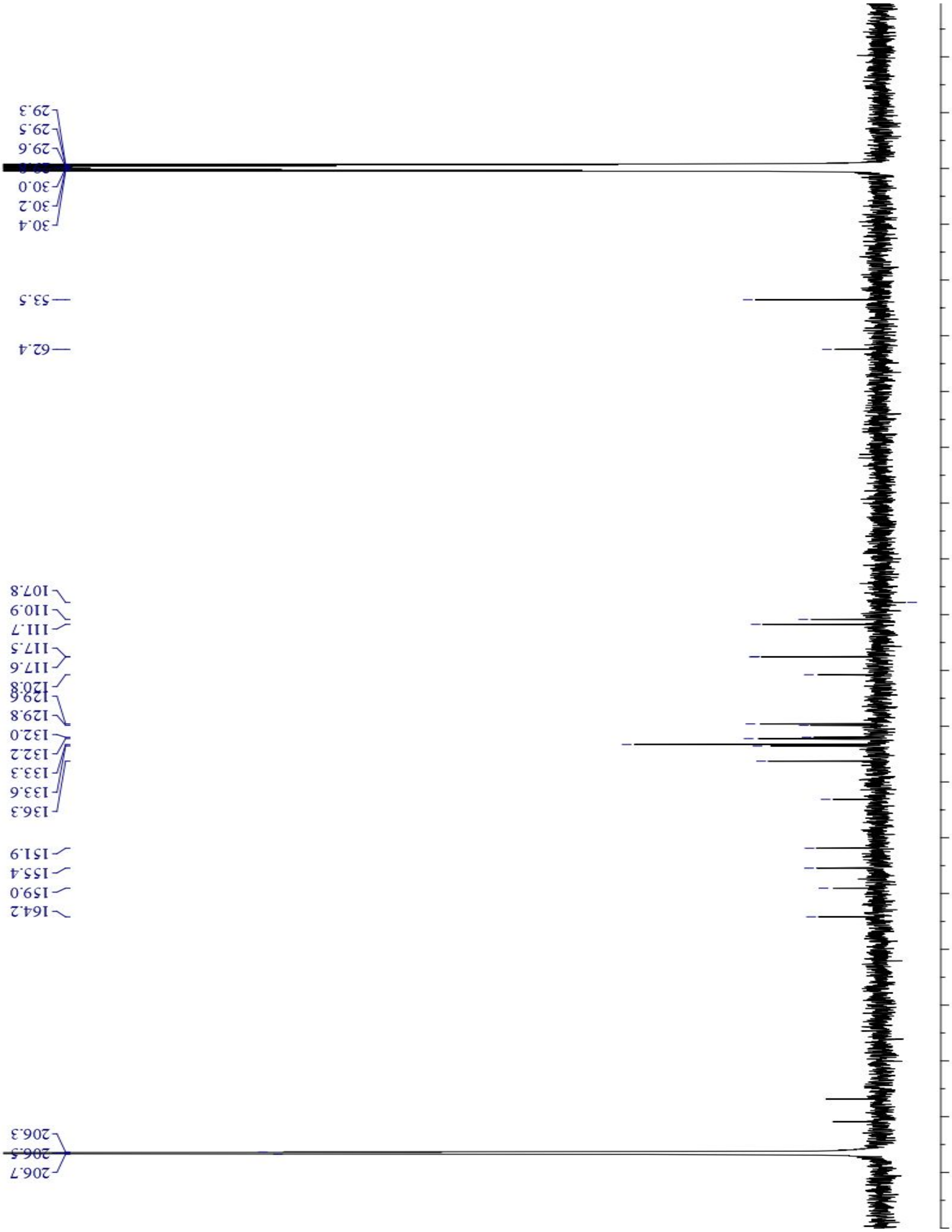


Figure S7. The ^{13}C NMR (200 MHz, acetone-d_6) spectrum of **2**

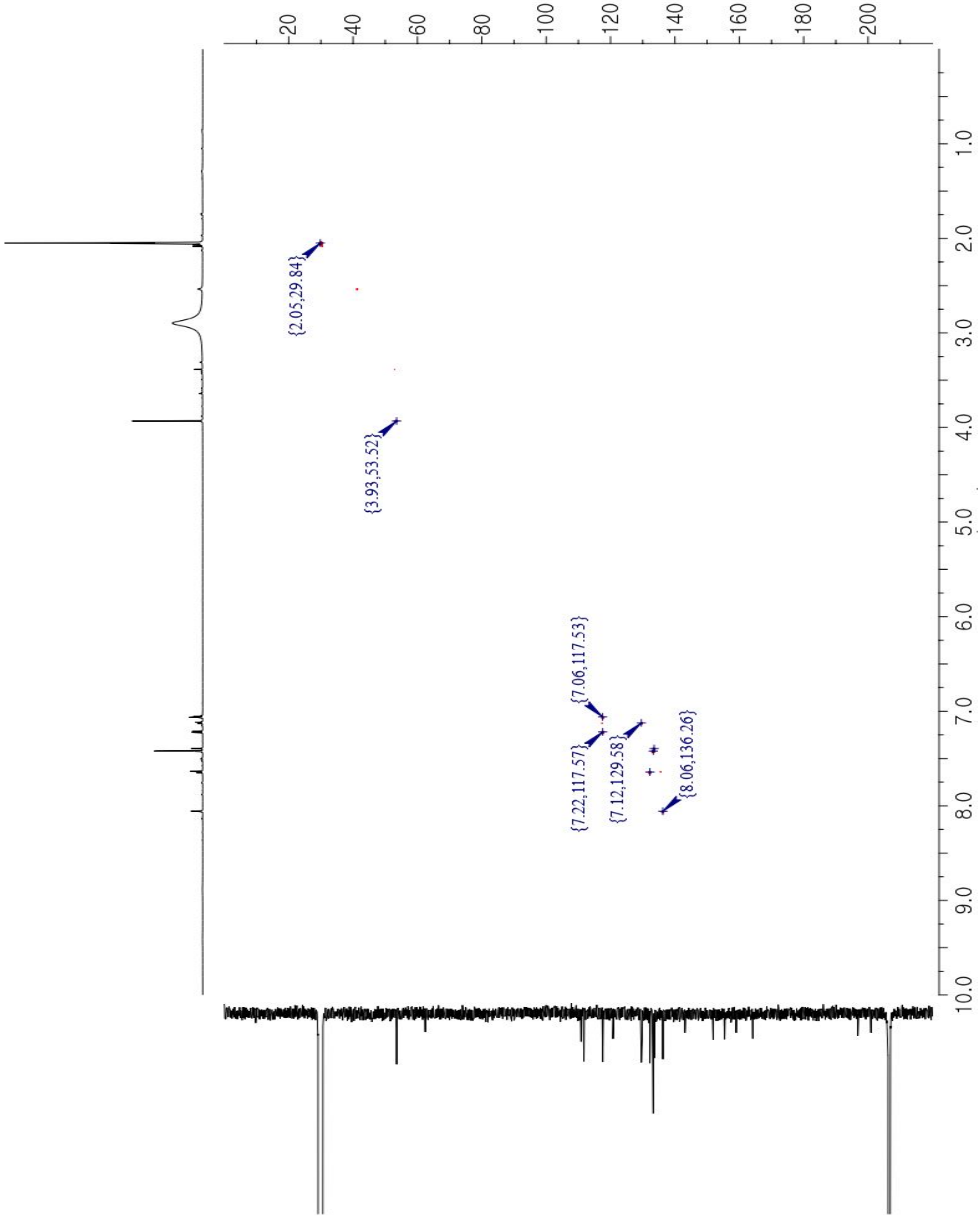


Figure S8. The HSQC (800 MHz, acetone-d_6) spectrum of **2**

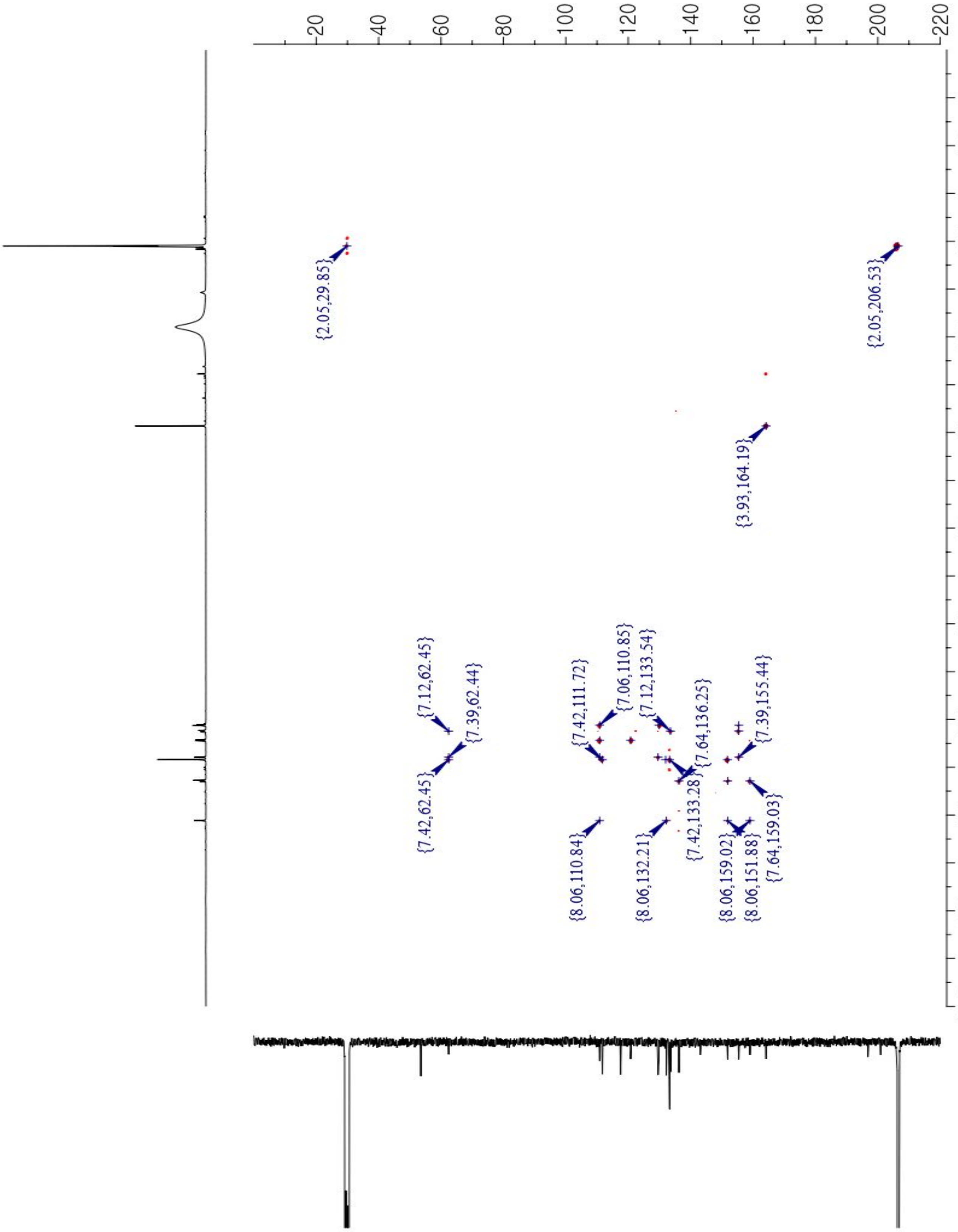


Figure S9. The HMBC (800 MHz, acetone-$d_{6,}$ J_{CH} = 8 Hz) spectrum of **2**

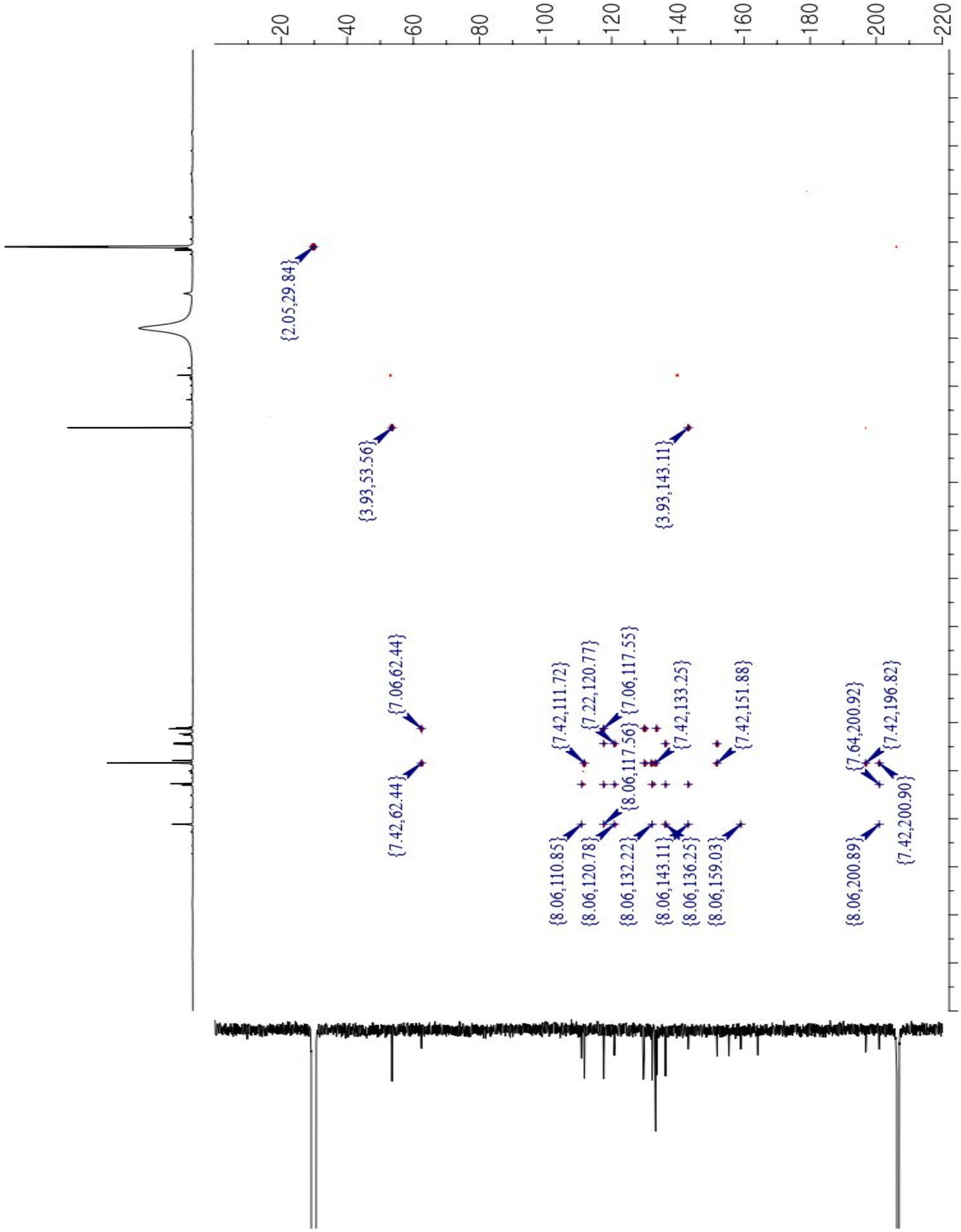


Figure S10. The D-HMBC (800 MHz, Acetone-$d_{6,}$ J_{CH} = 1 Hz) spectrum of **2**

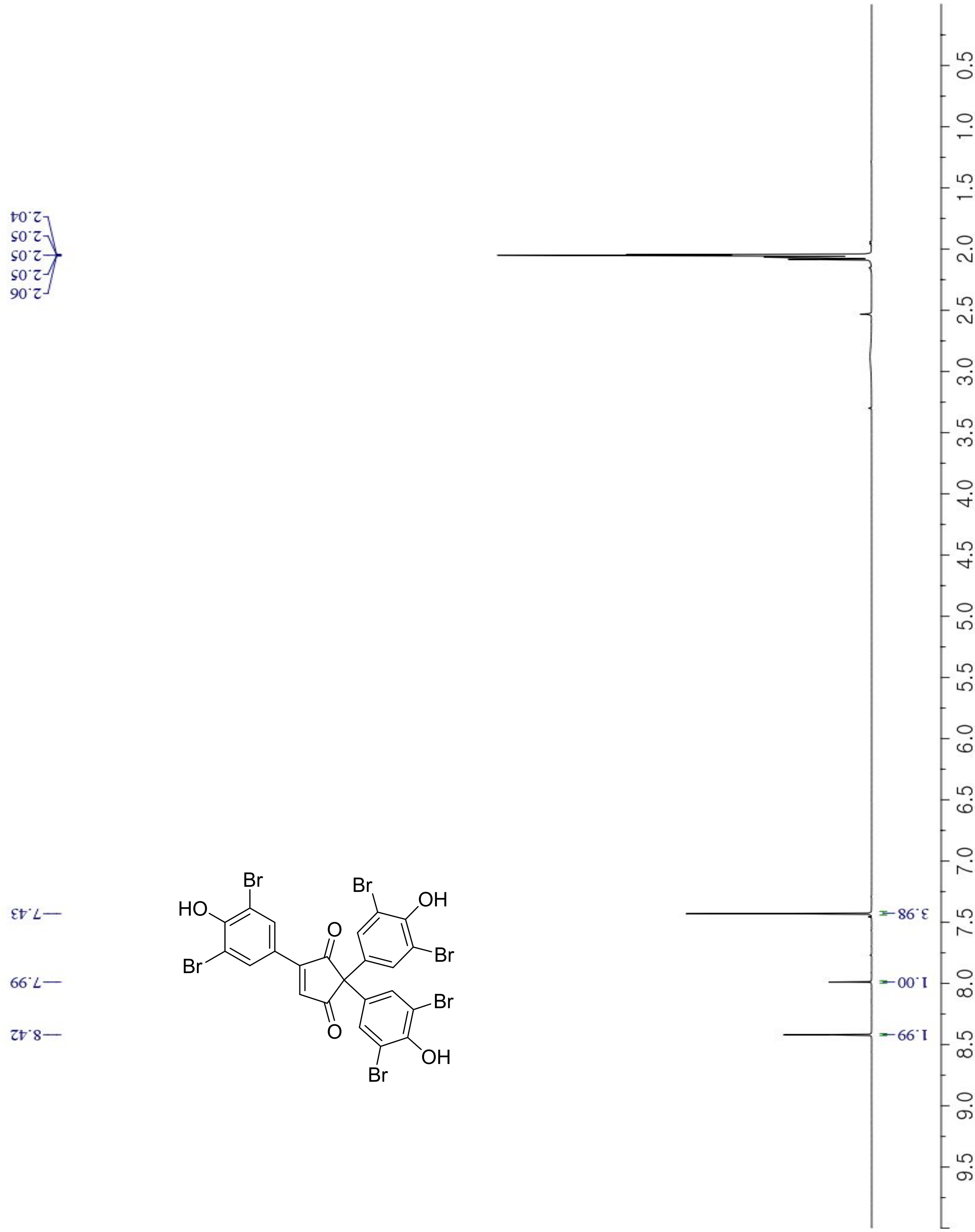


Figure S11. The ^{1}H NMR (800 MHz, acetone-d_6) spectrum of **3**

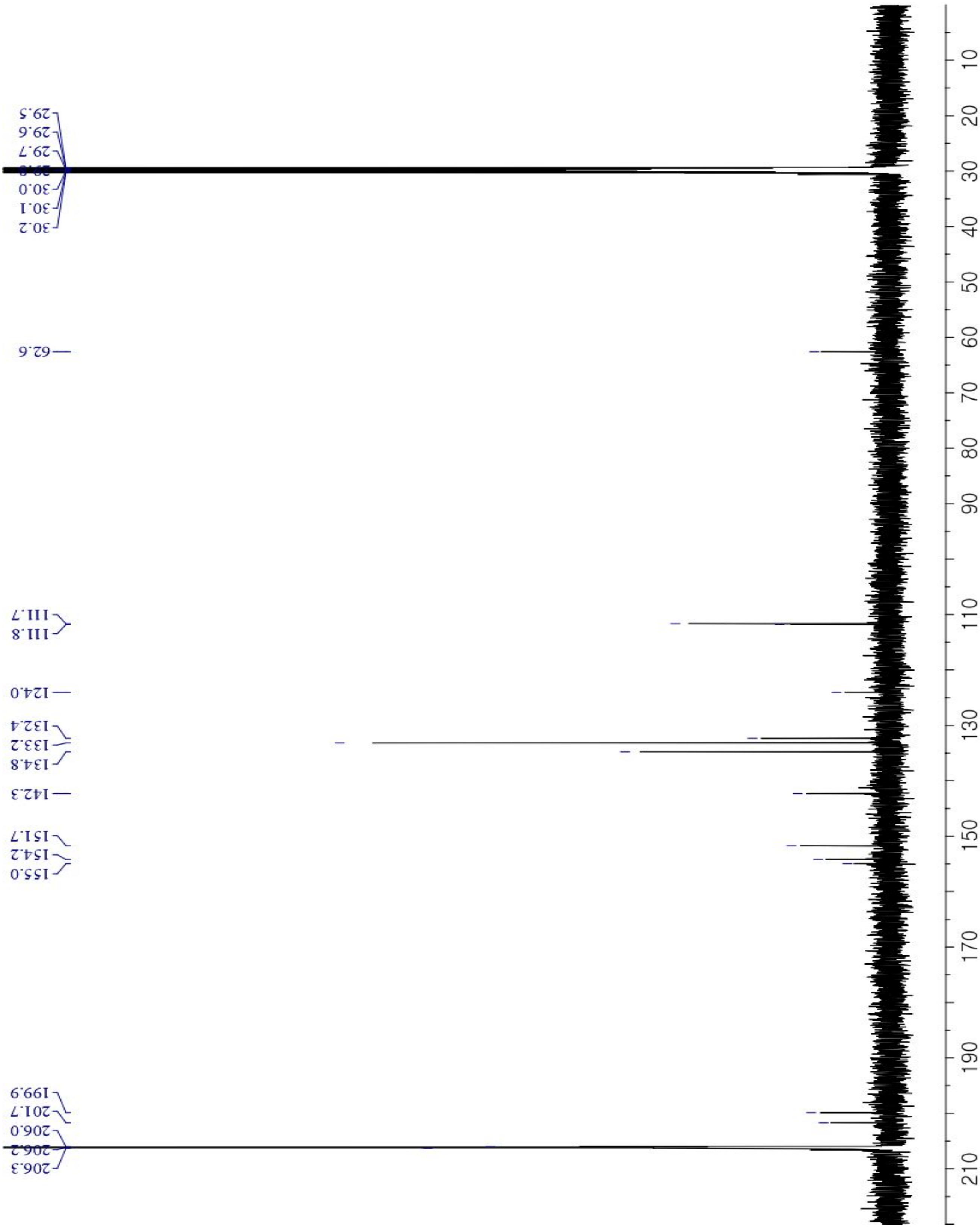


Figure S12. The ^{13}C NMR (200 MHz, acetone-d_6) spectrum of **3**

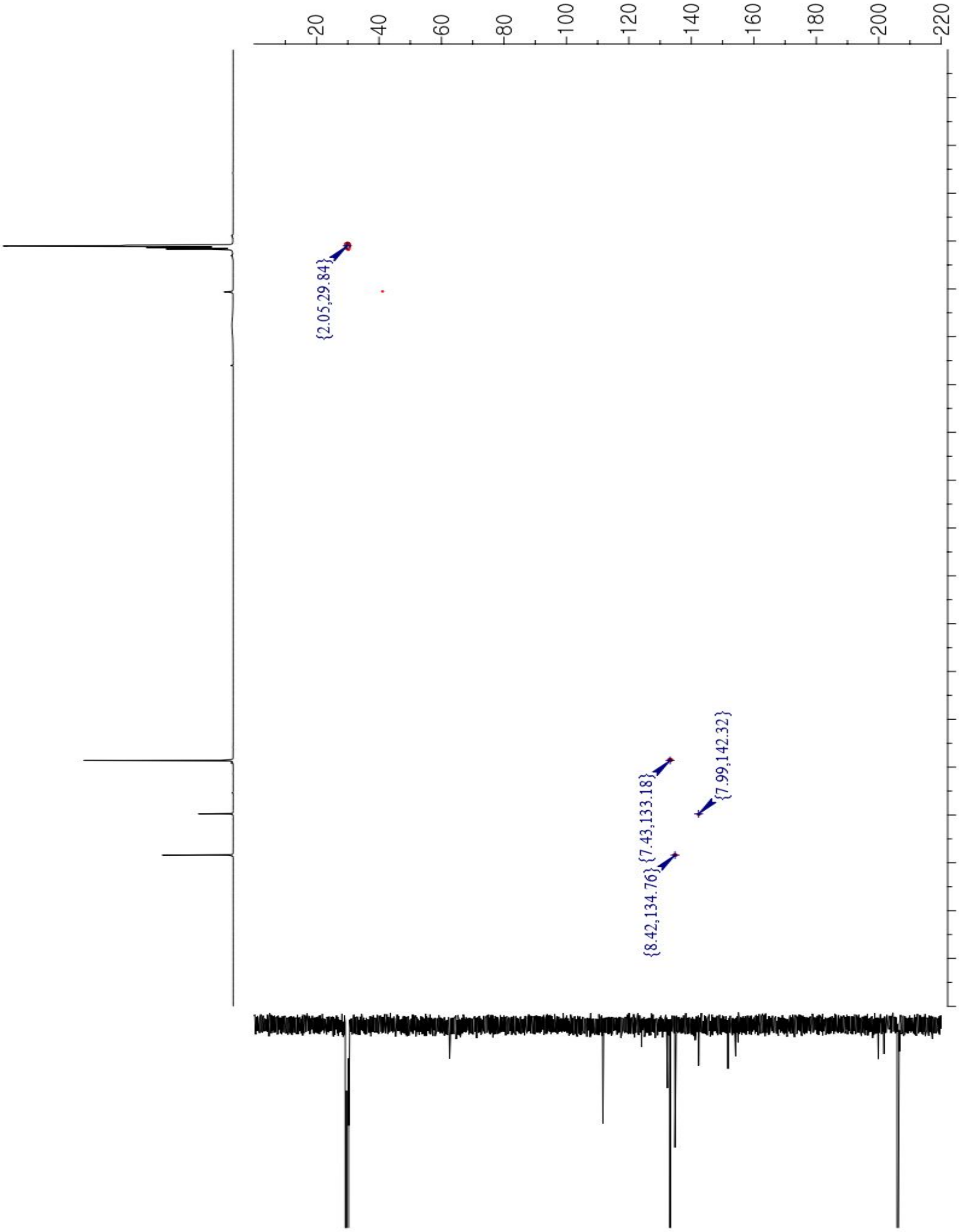


Figure S13. The HSQC (800 MHz, acetone-d_6) spectrum of **3**

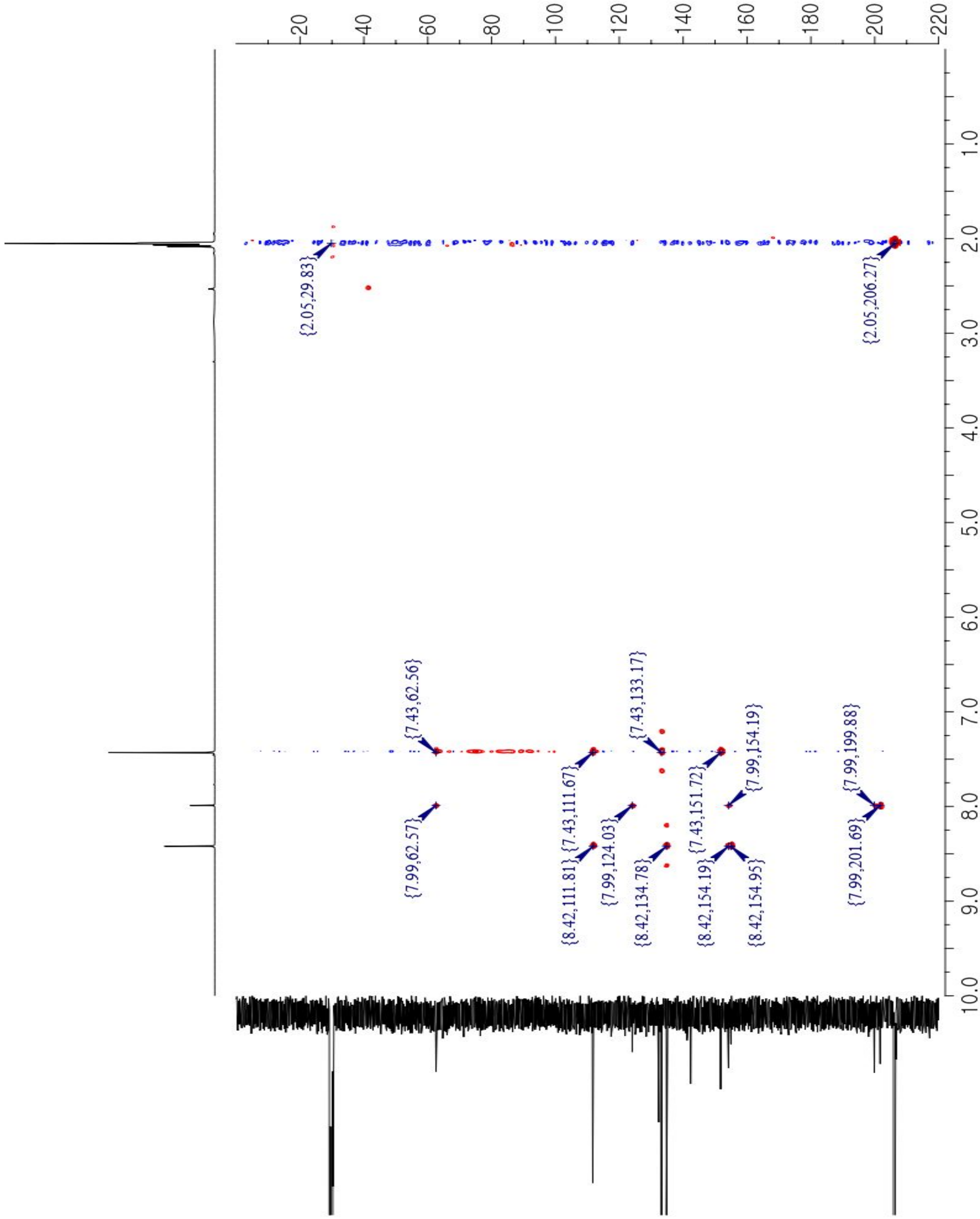


Figure S14. The HMBC (800 MHz, acetone-$d_{6,}$ J_{CH} = 8 Hz) spectrum of **3**

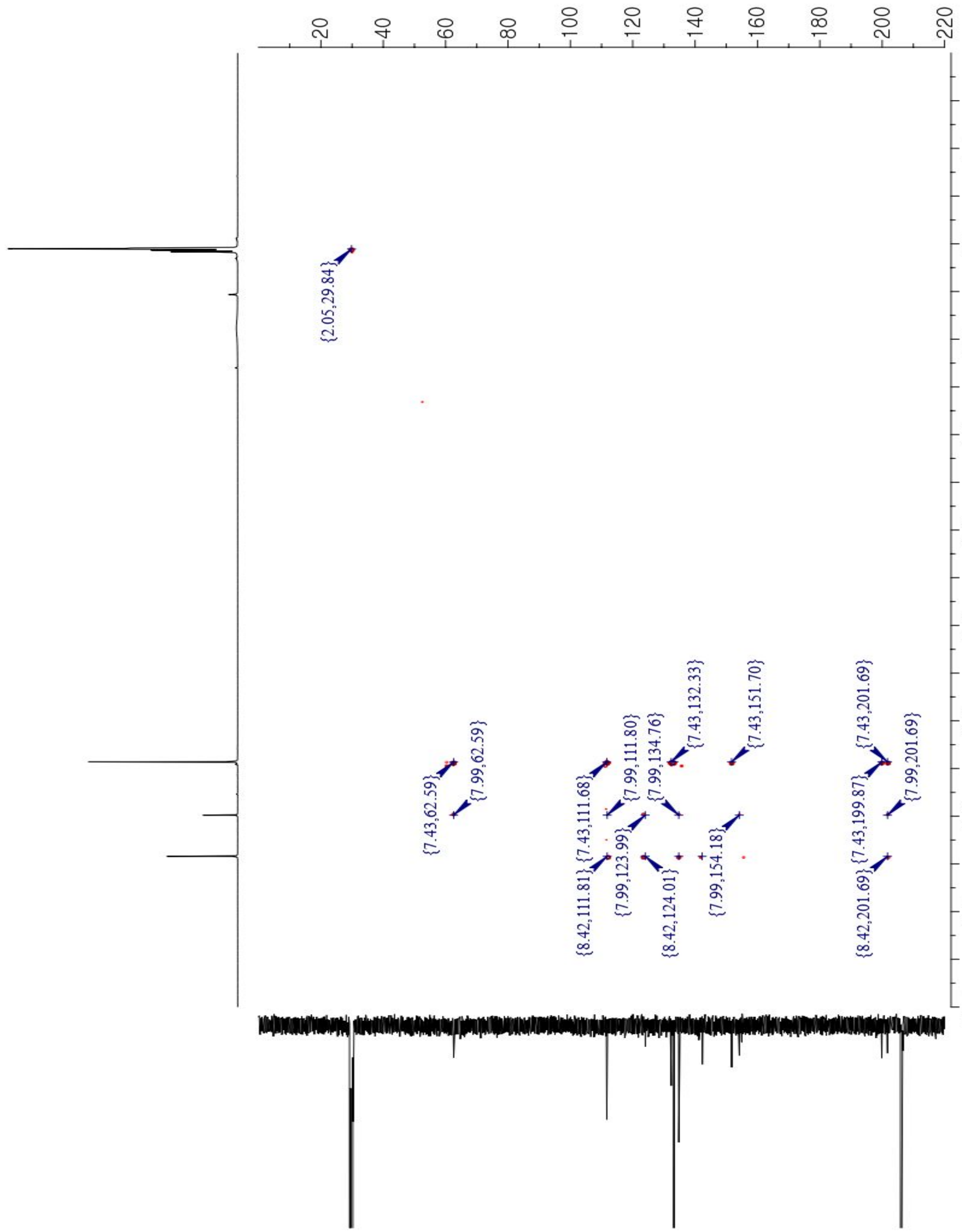


Figure S15. The D-HMBC (800 MHz, acetone-d_6, J_{CH} = 1 Hz) spectrum of **3**

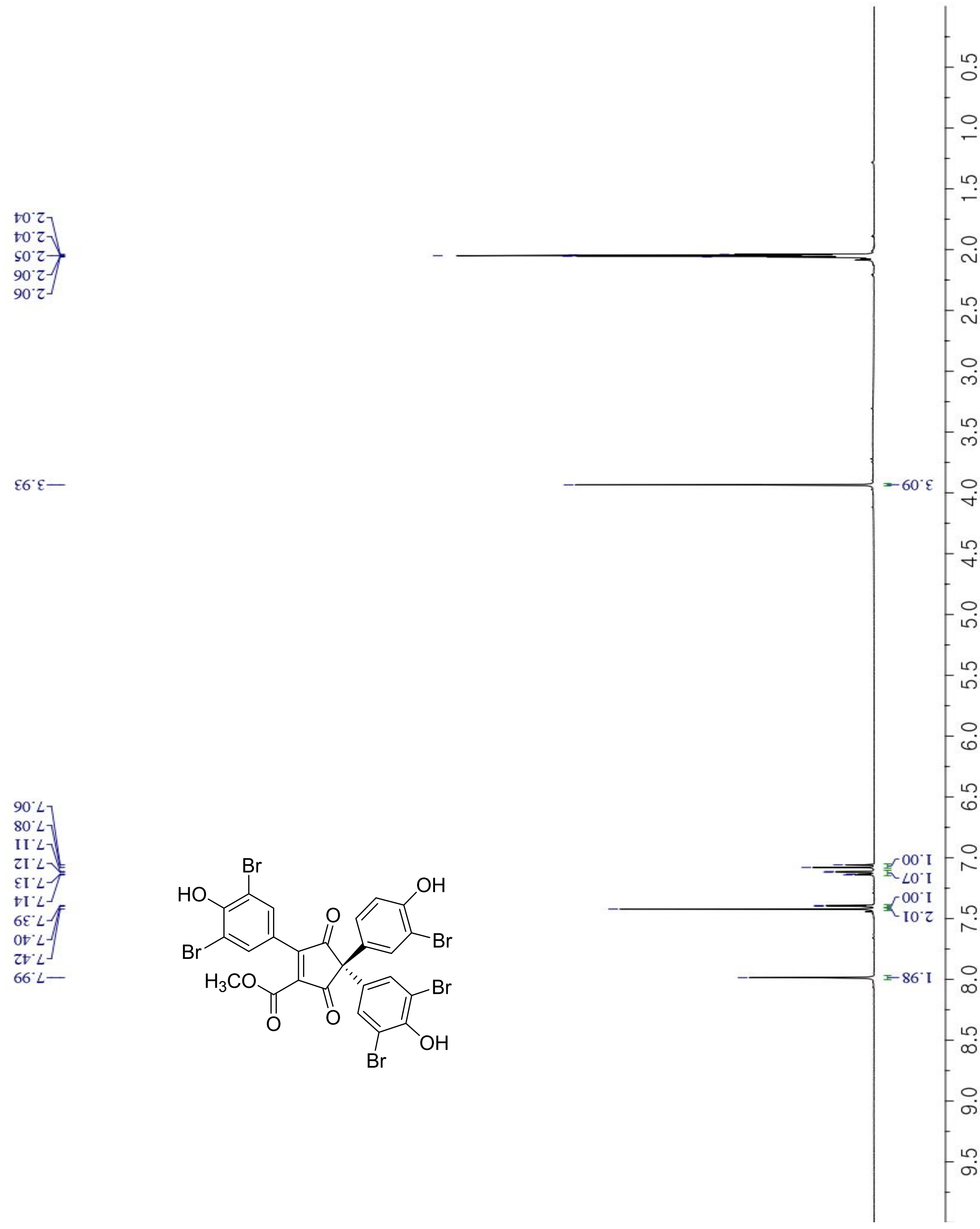


Figure S16. The ^{1}H NMR (600 MHz, acetone-d_6) spectrum of **4**

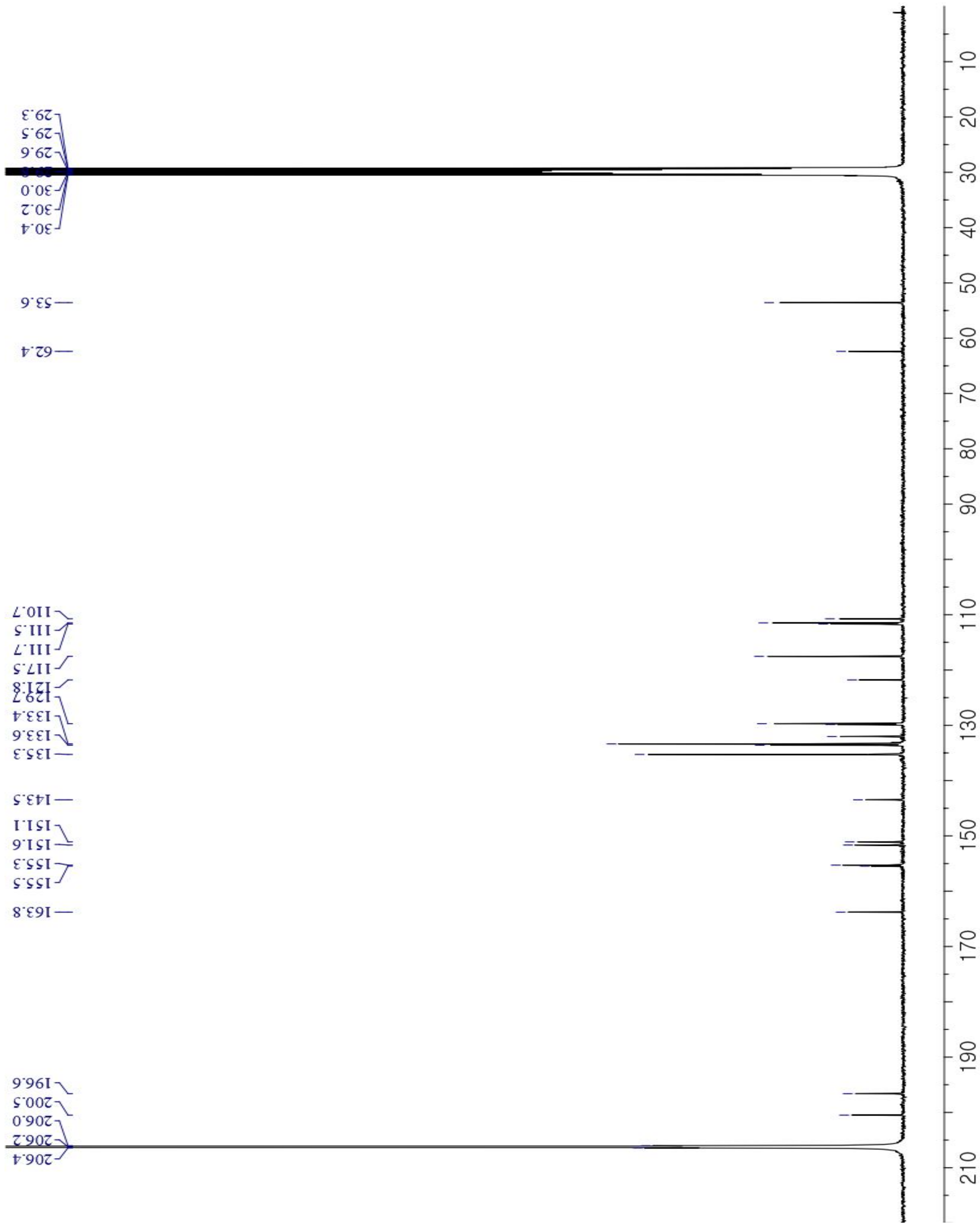


Figure S17. The ^{13}C NMR (150 MHz, acetone-d_6) spectrum of **4**

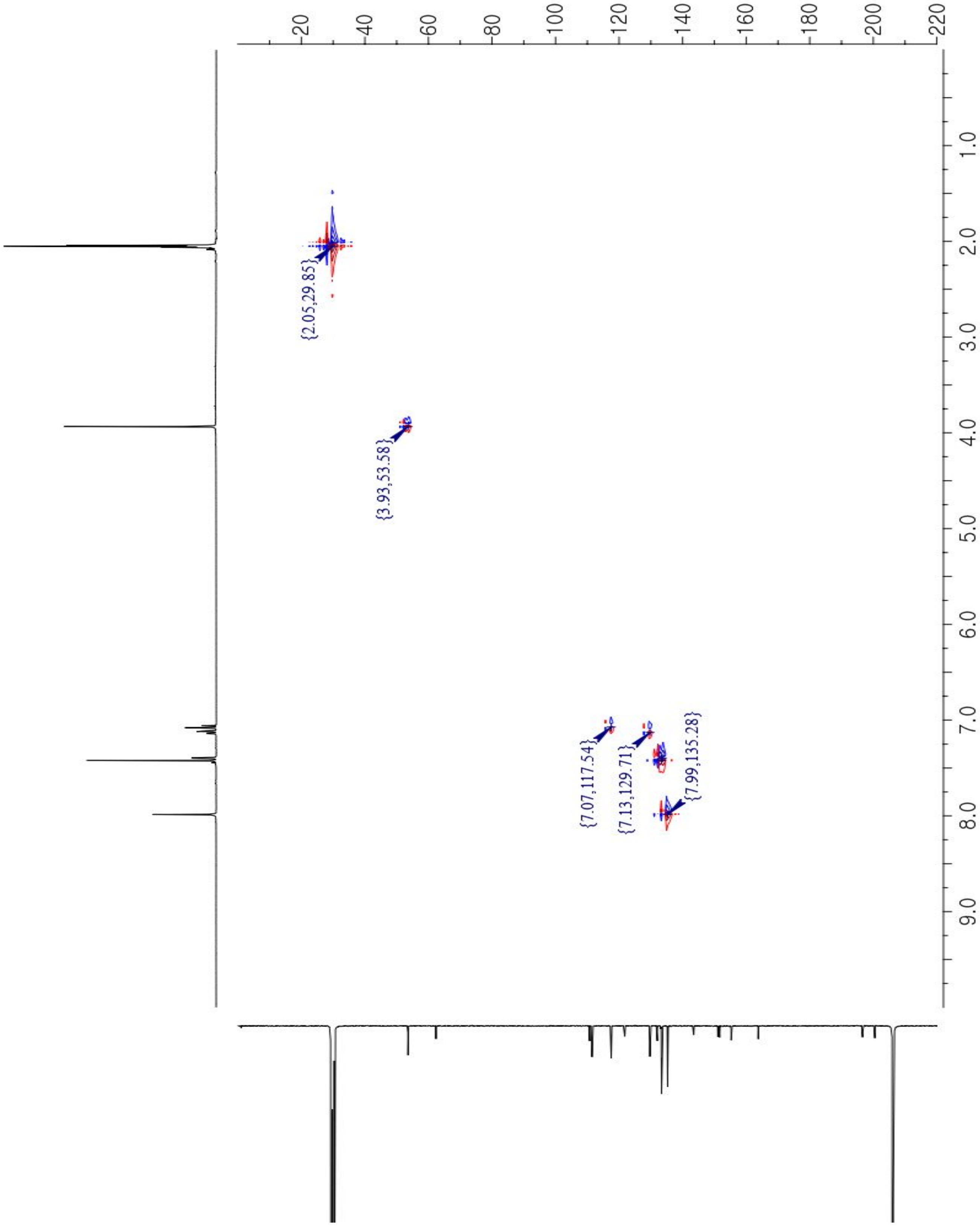


Figure S18. The HSQC (600 MHz, acetone-d_6) spectrum of **4**

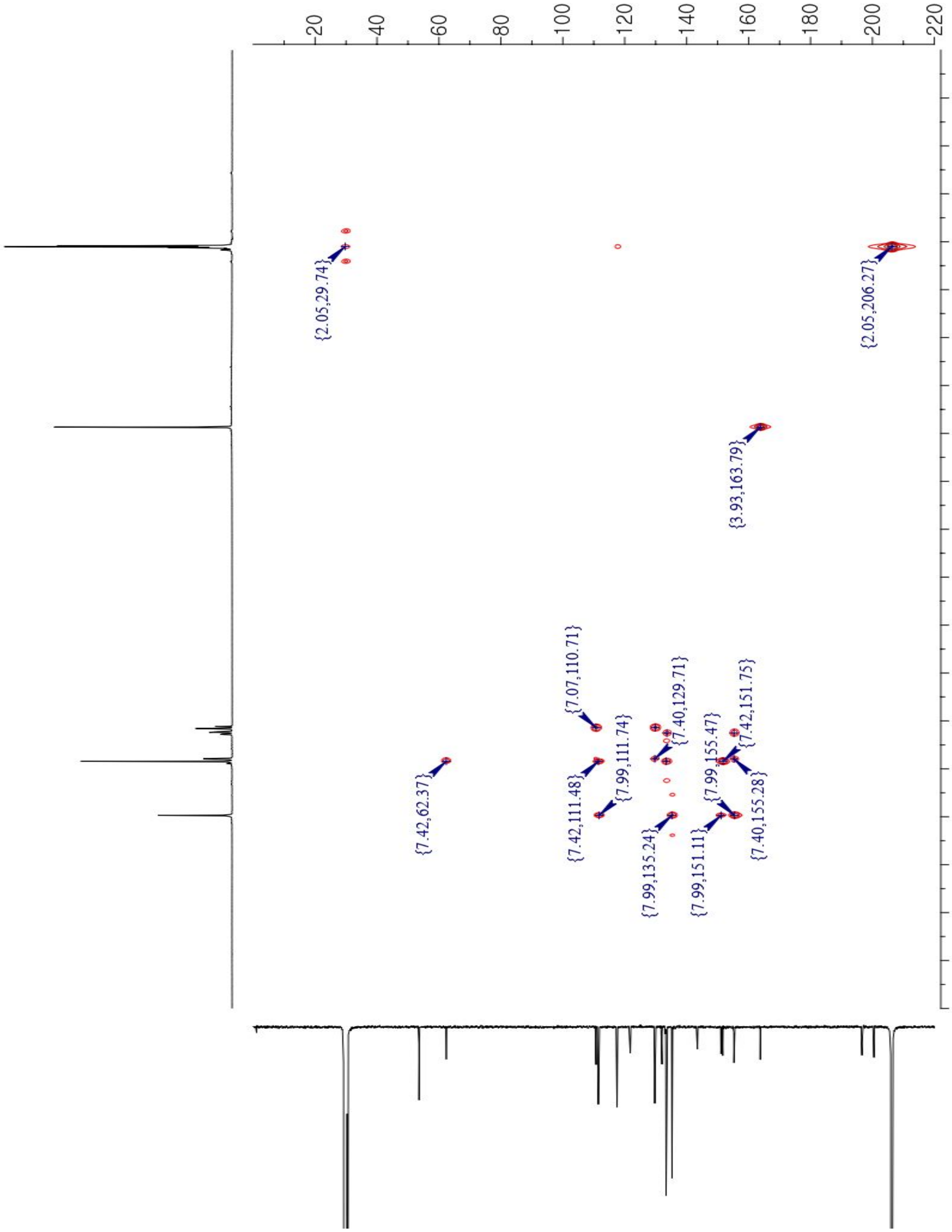


Figure S19. The HMBC (600 MHz, acetone-$d_{6,}$ J_{CH} = 8 Hz) spectrum of **4**

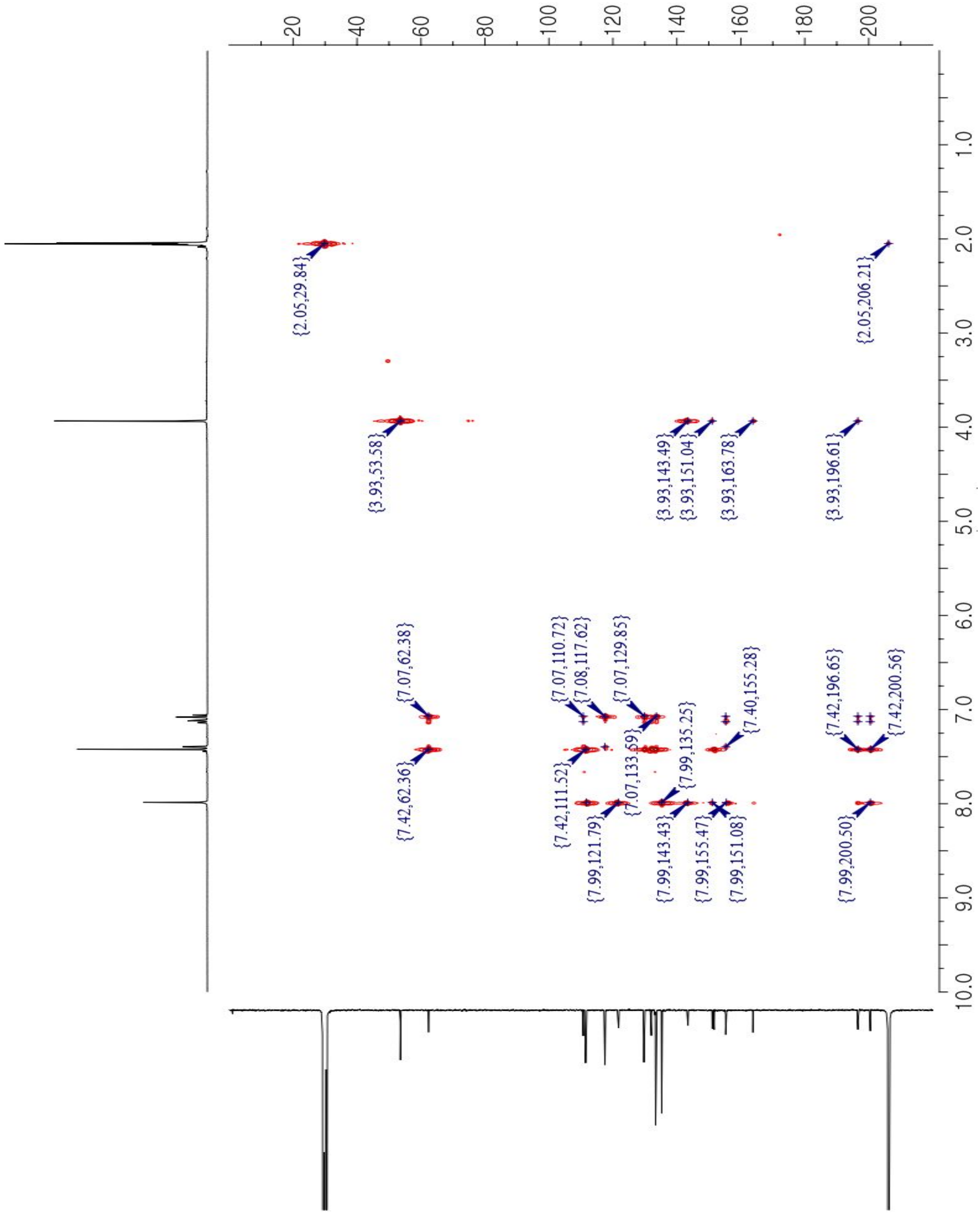


Figure S20. The D-HMBC (800 MHz, acetone-d_6, J_{CH} = 1 Hz) spectrum of **4**

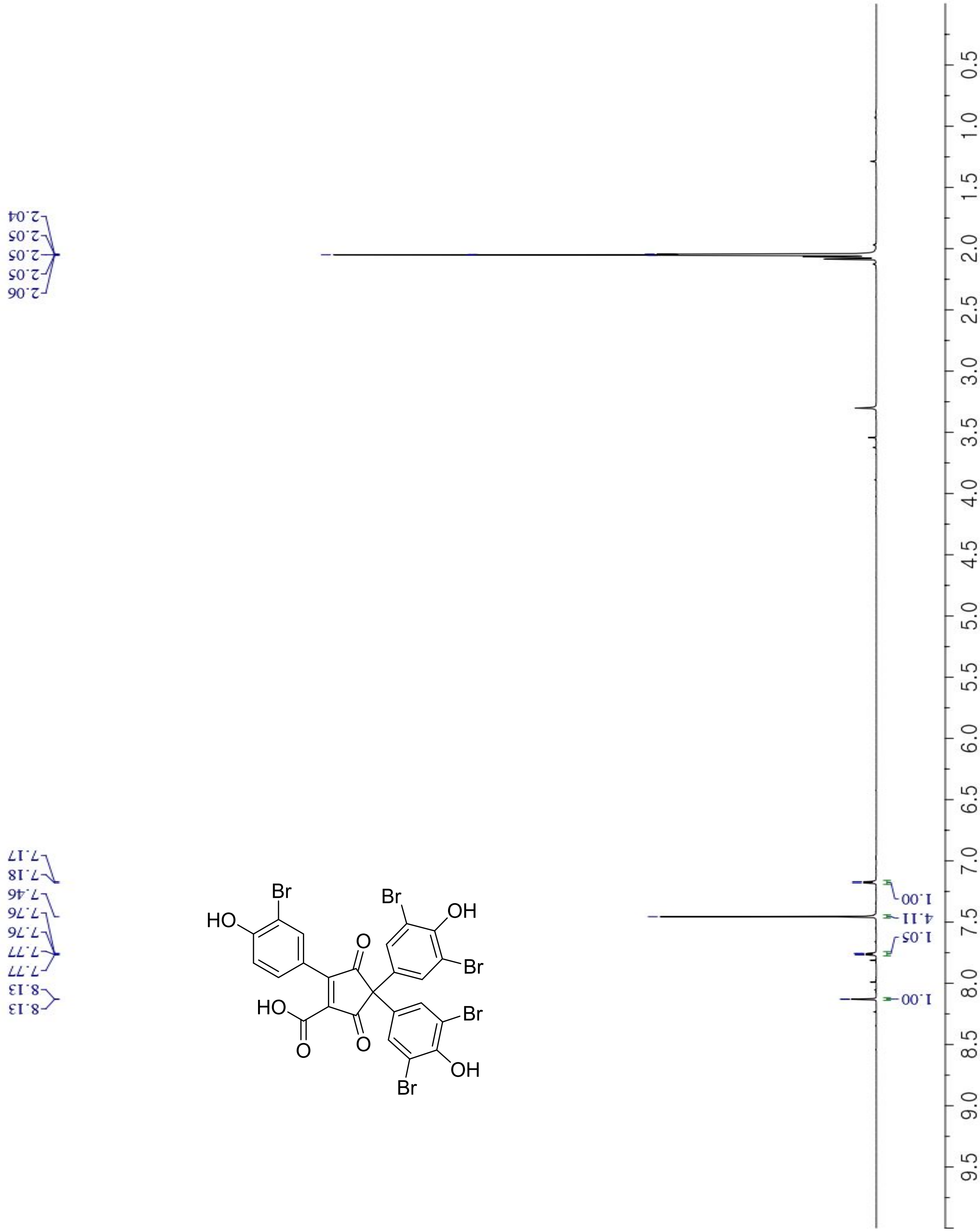


Figure S21. The ^{1}H NMR (800 MHz, acetone-d_6) spectrum of **5**

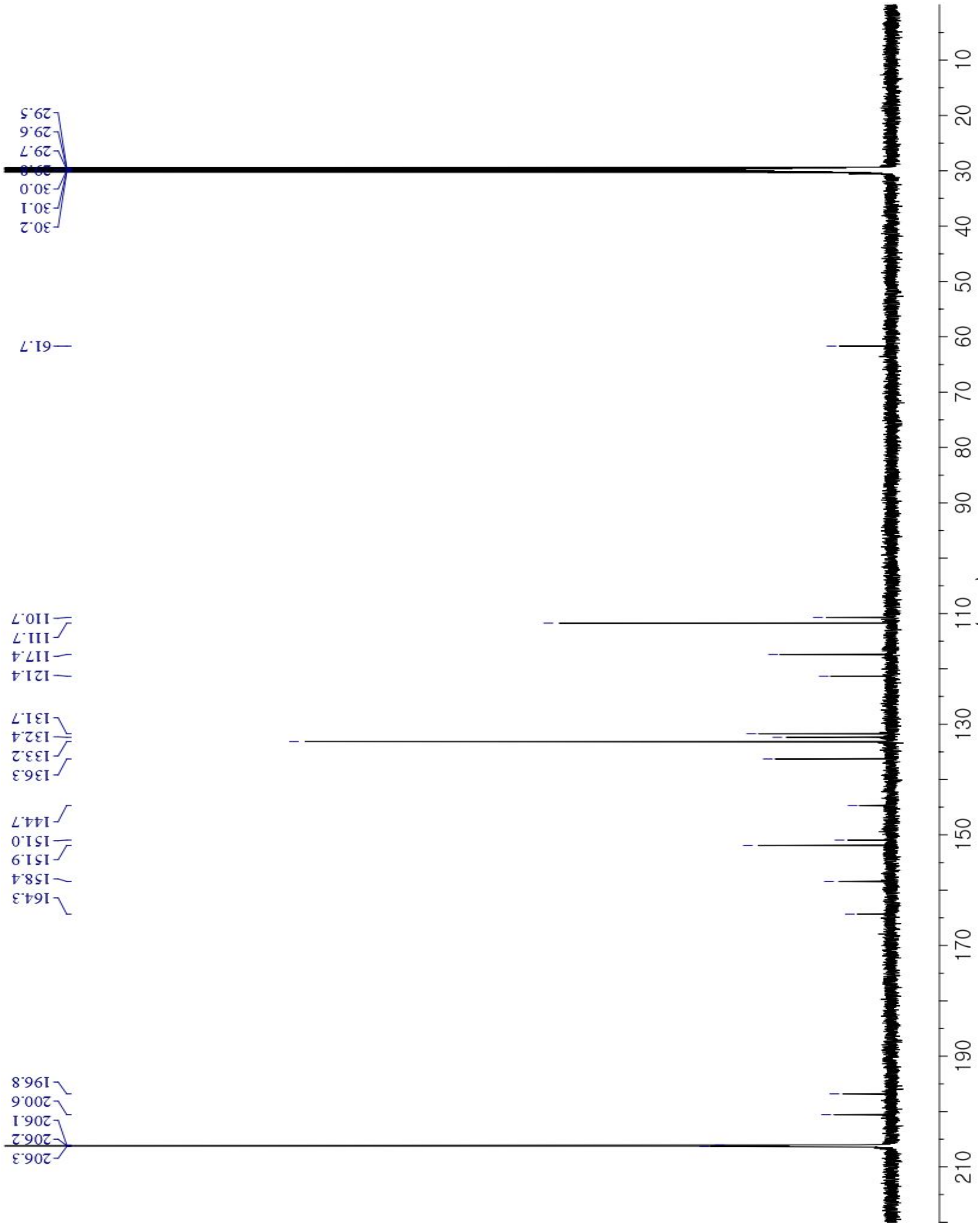


Figure S22. The ^{13}C NMR (200 MHz, acetone-d_6) spectrum of **5**

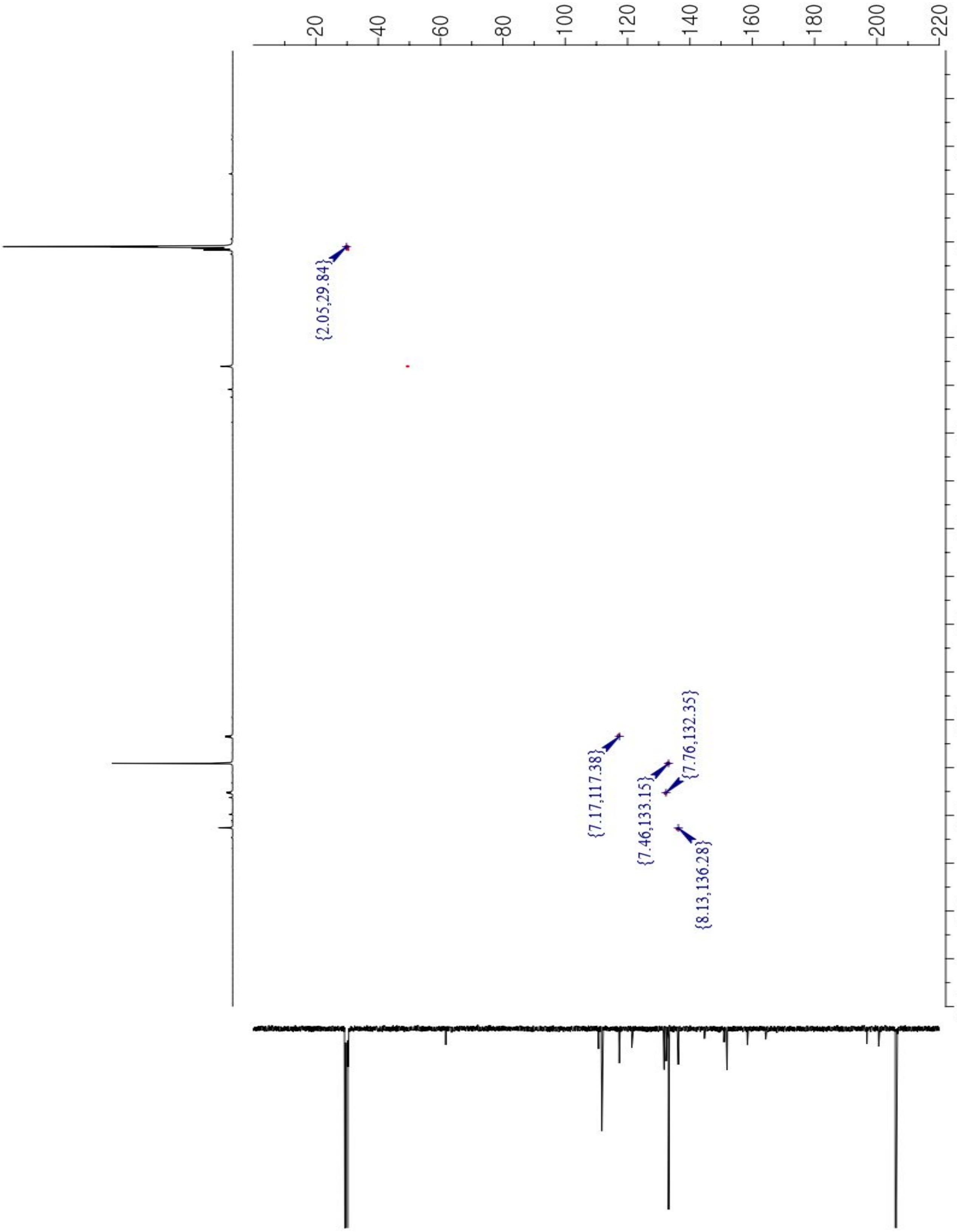


Figure S23. The HSQC (800 MHz, acetone-d_6) spectrum of **5**

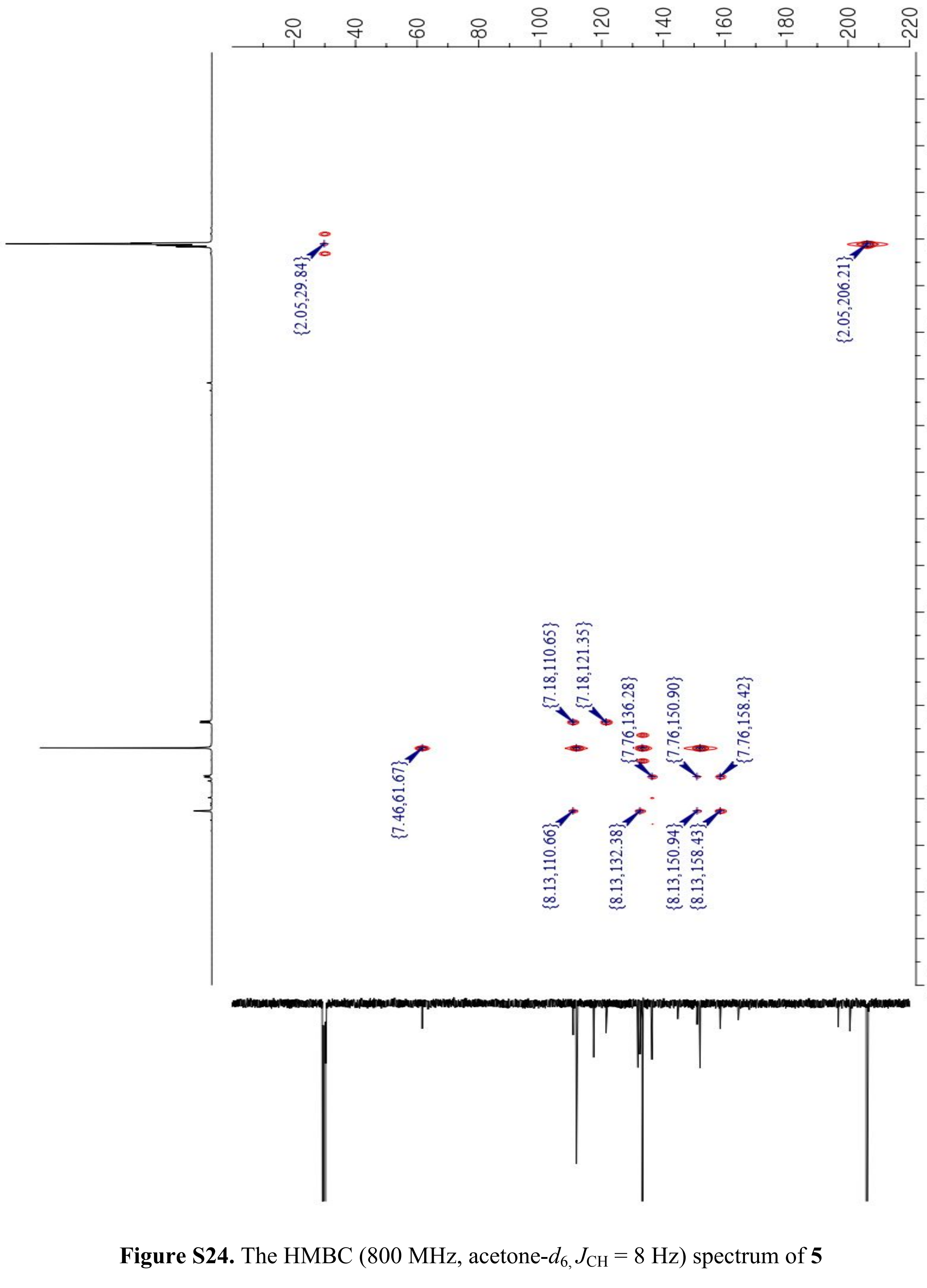


Figure S24. The HMBC (800 MHz, acetone-$d_{6,}$ J_{CH} = 8 Hz) spectrum of **5**

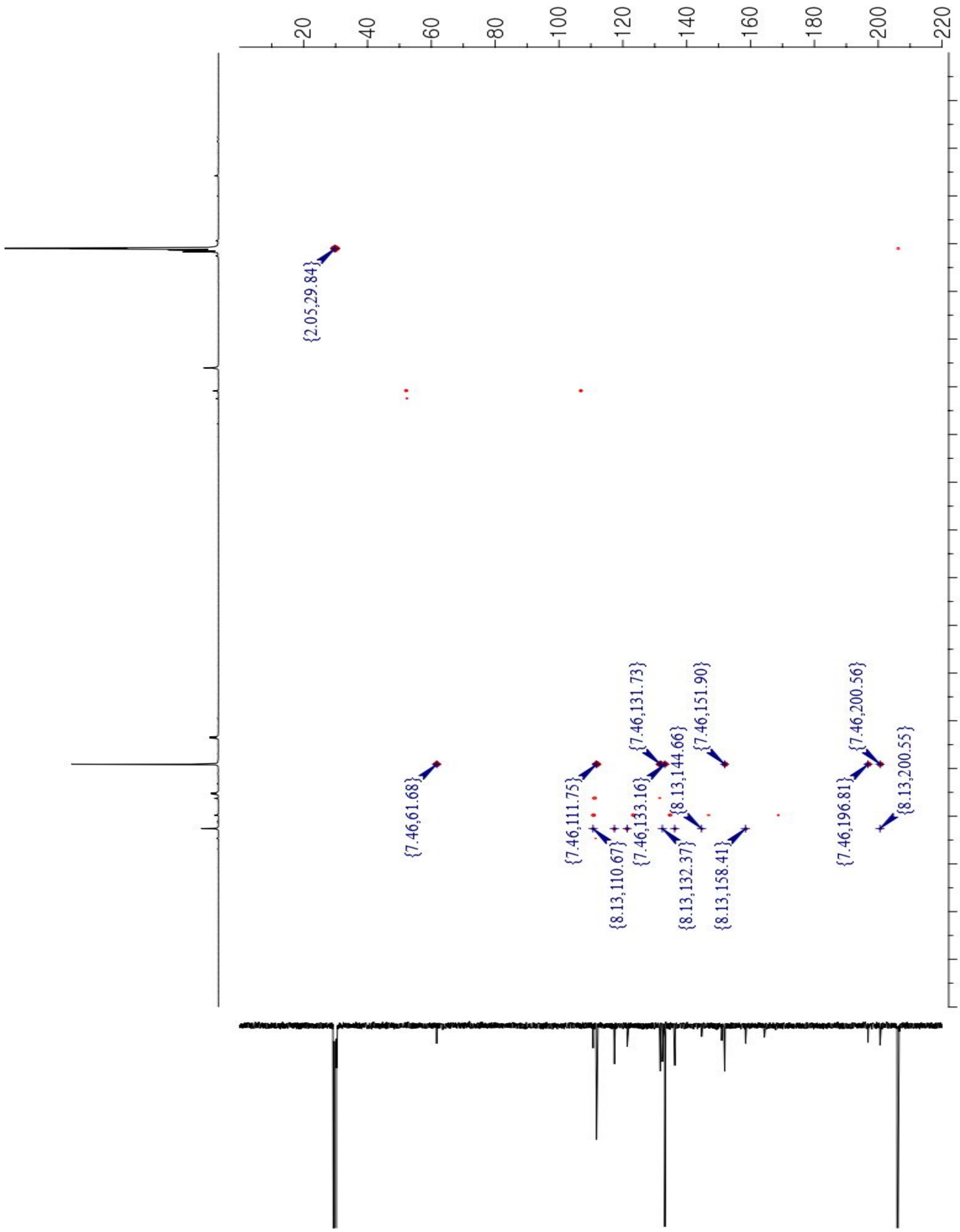


Figure S25. The D-HMBC (800 MHz, acetone-d_6, J_{CH} = 1 Hz) spectrum of **5**

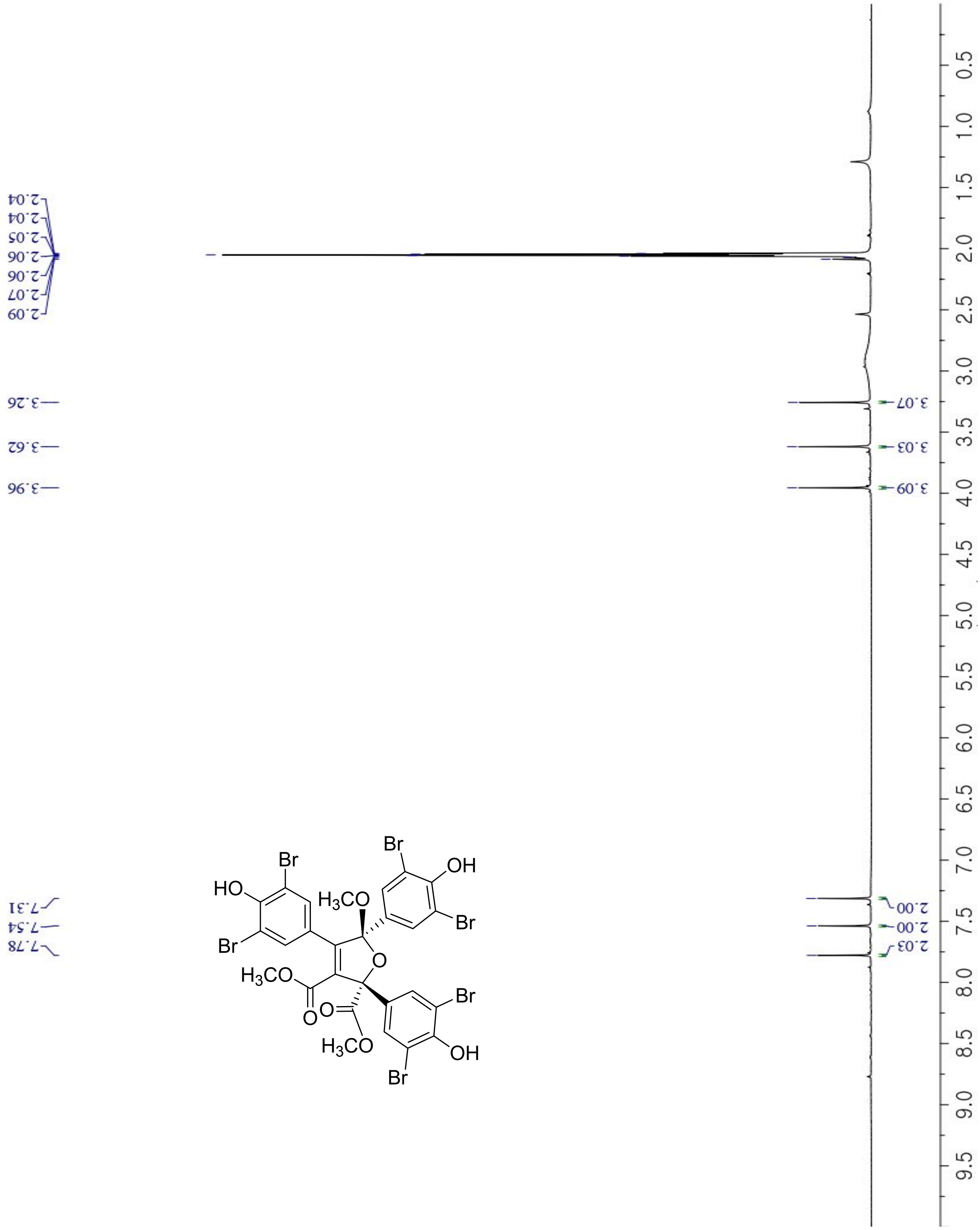


Figure S26. The ^{1}H NMR (600 MHz, acetone-d_6) spectrum of **6**

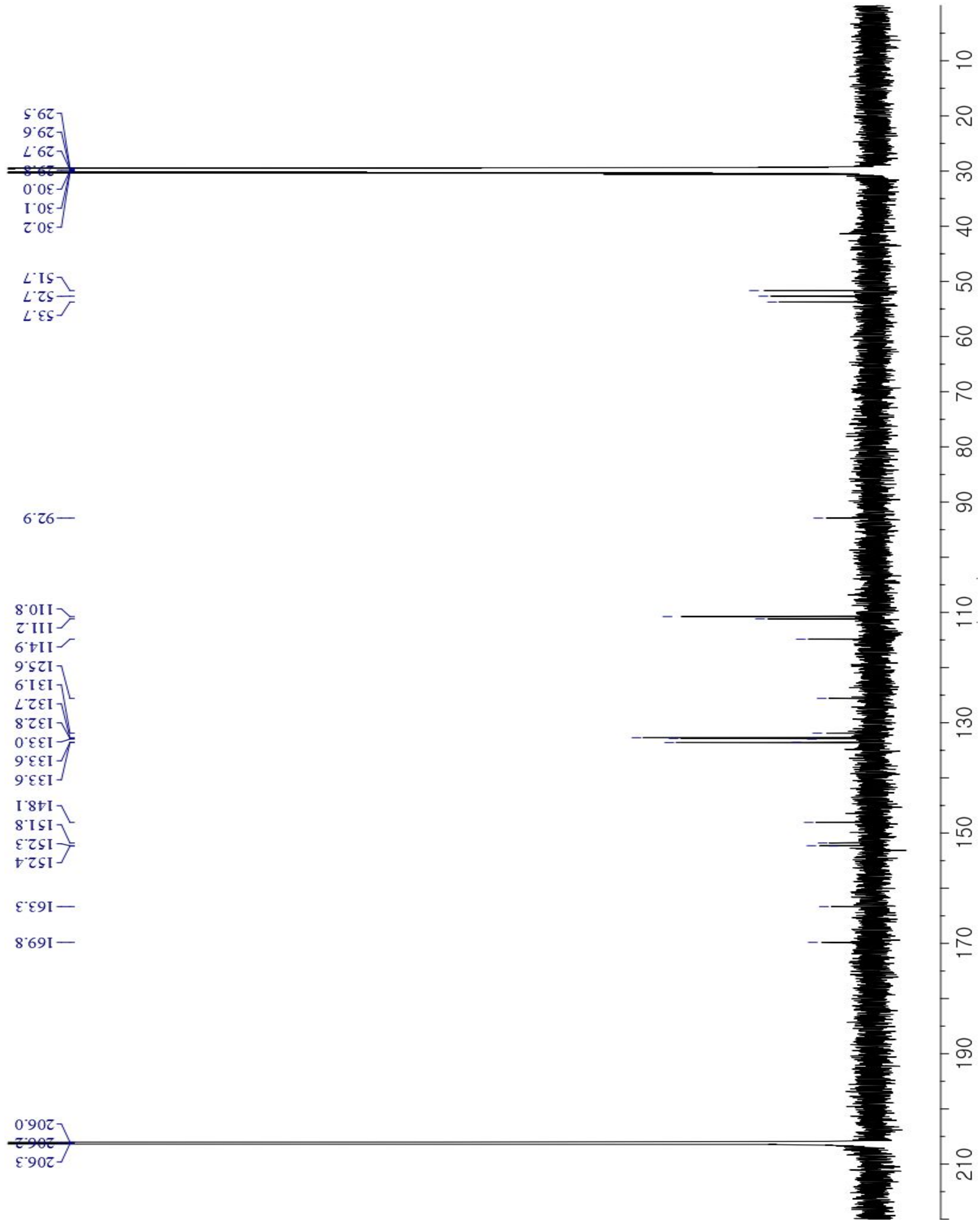


Figure S27. The ^{13}C NMR (150 MHz, acetone-d_6) spectrum of **6**

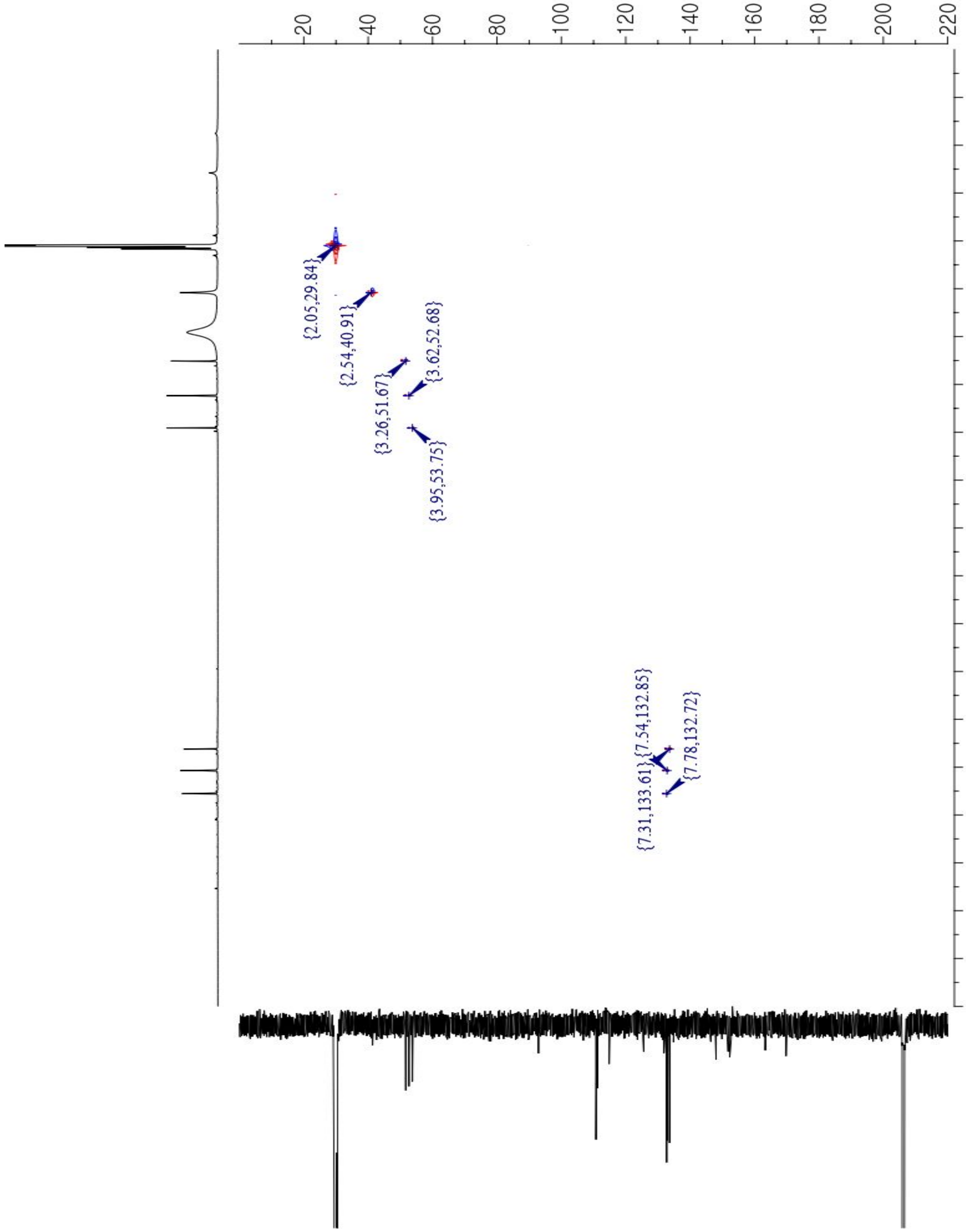


Figure S28. The HSQC (600 MHz, acetone-d_6) spectrum of **6**

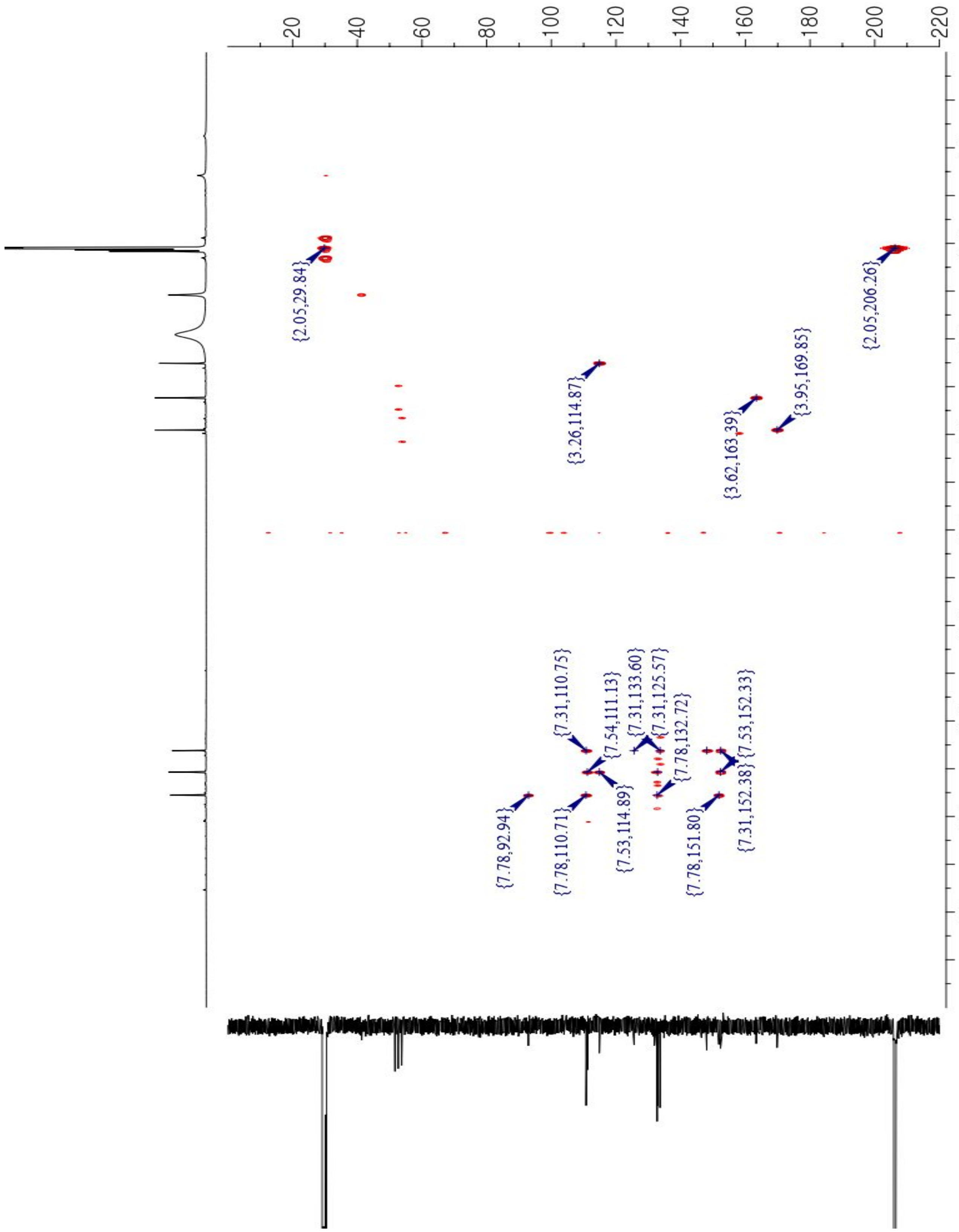


Figure S29. The HMBC (600 MHz, acetone-d_6, J_{CH} = 8 Hz) spectrum of **6**

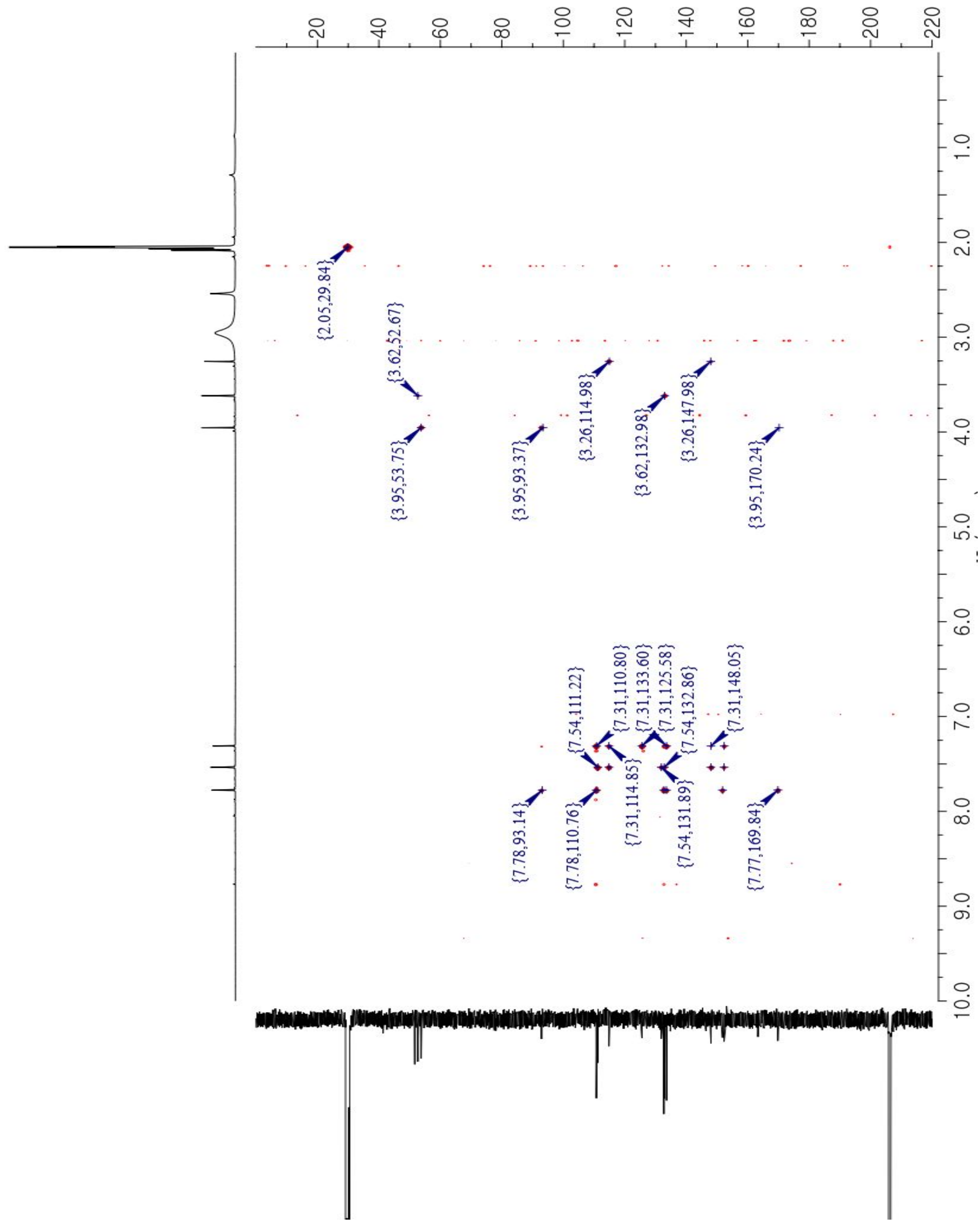


Figure S30. The D-HMBC (800 MHz, acetone-d_6, J_{CH} = 1 Hz) spectrum of **6**

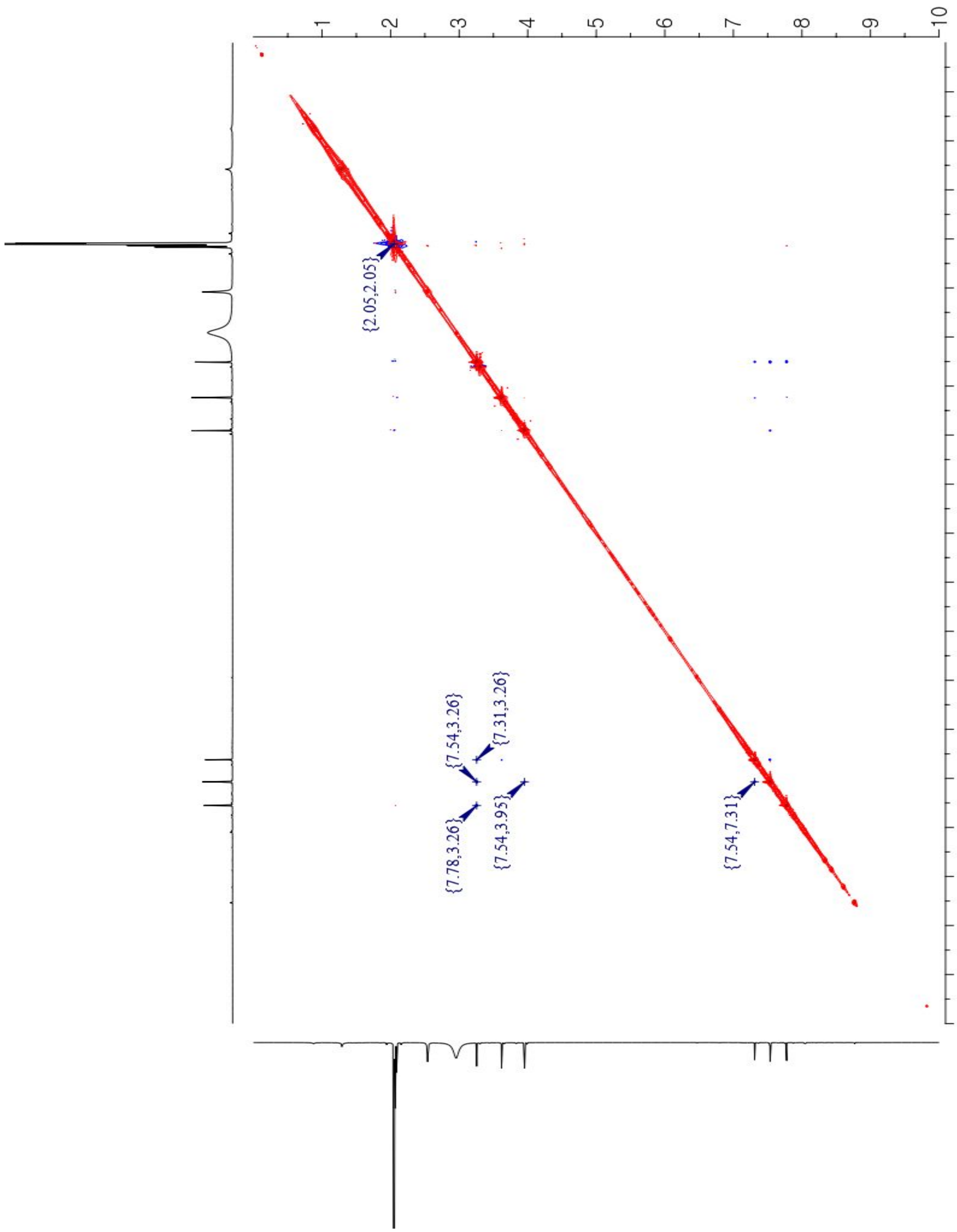


Figure S31. The NOESY (800 MHz, acetone-d_6) spectrum of **6**

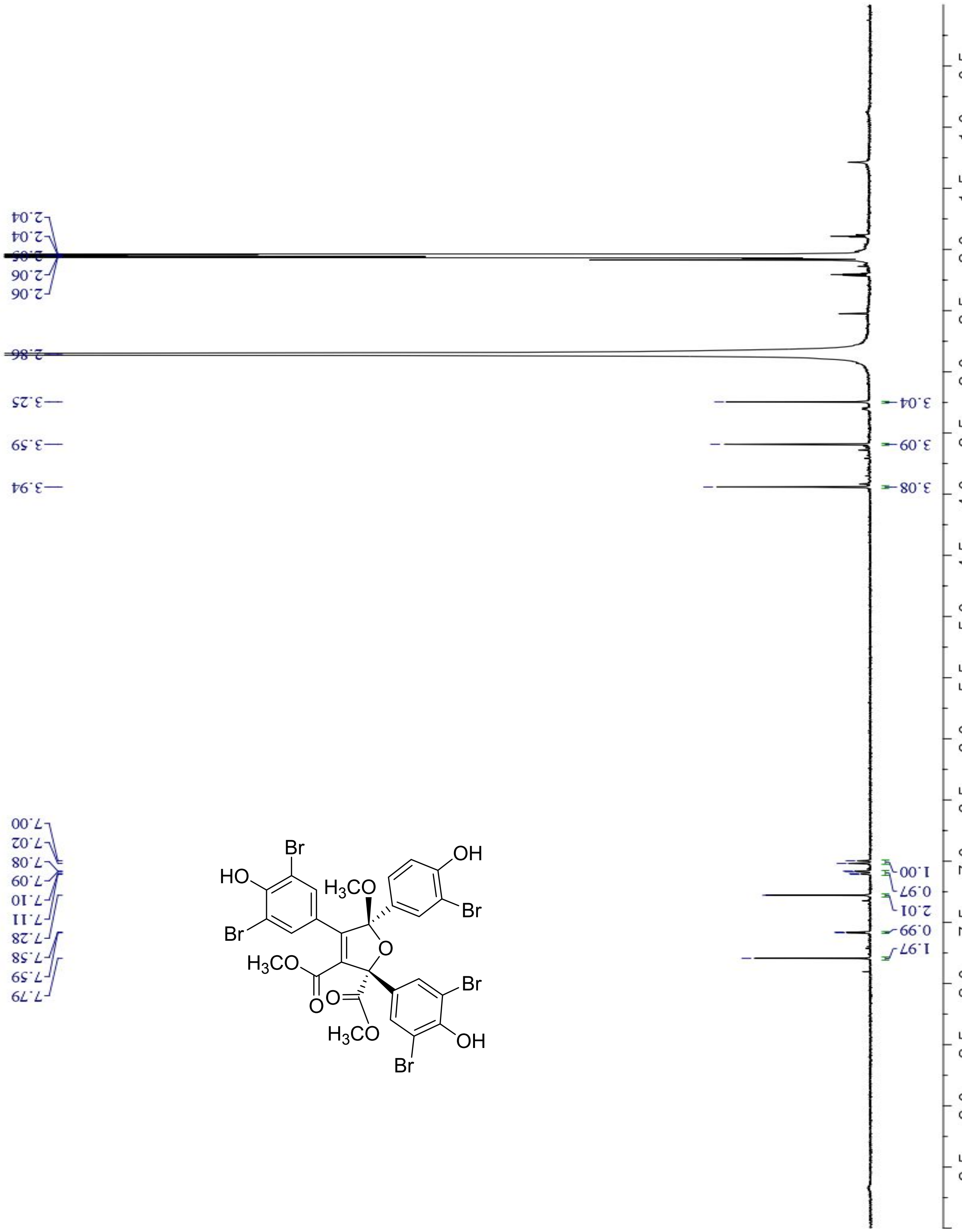


Figure S32. The [1]H NMR (400 MHz, acetone-d_6) spectrum of **7**

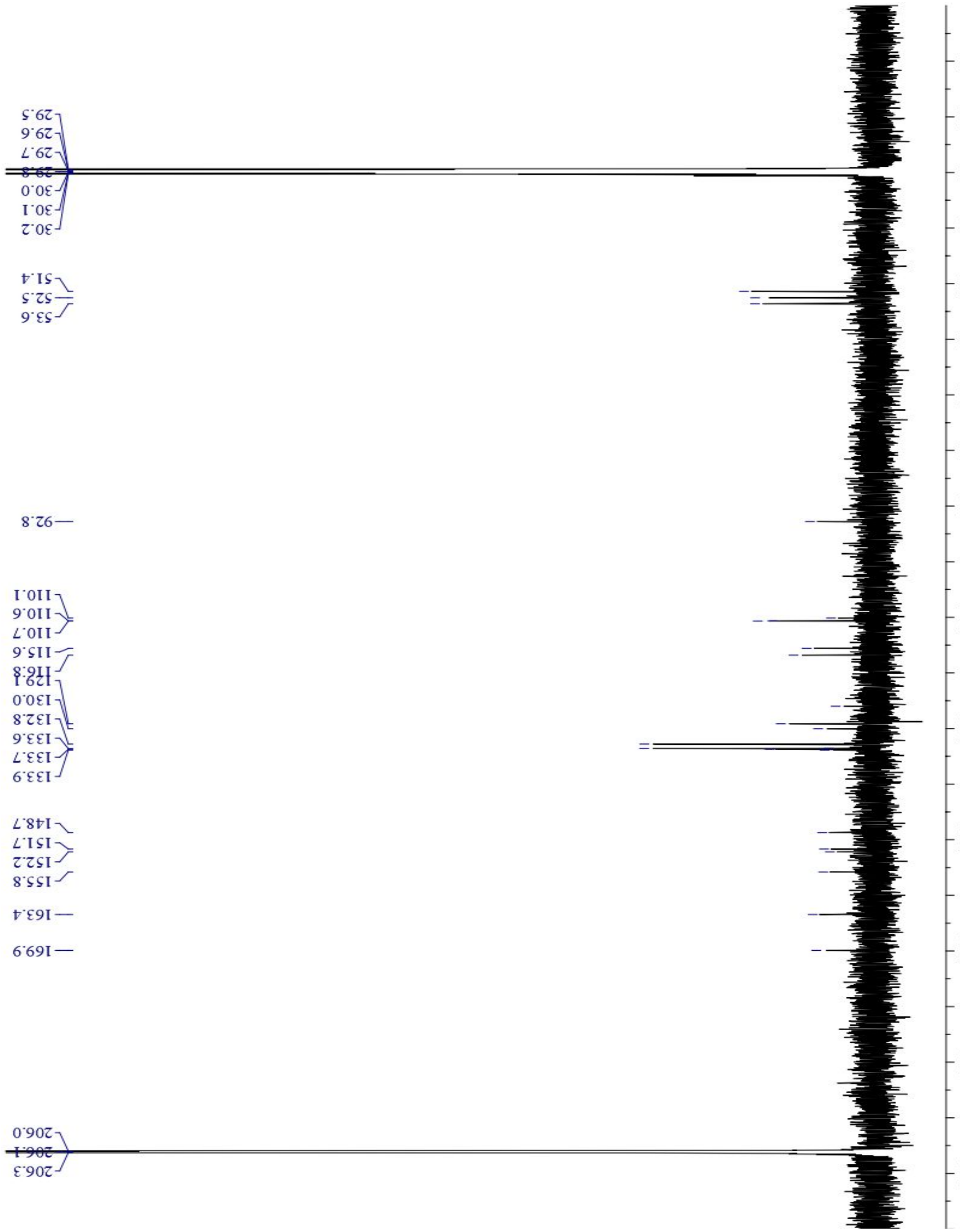


Figure S33. The ^{13}C NMR (100 MHz, acetone-d_6) spectrum of **7**

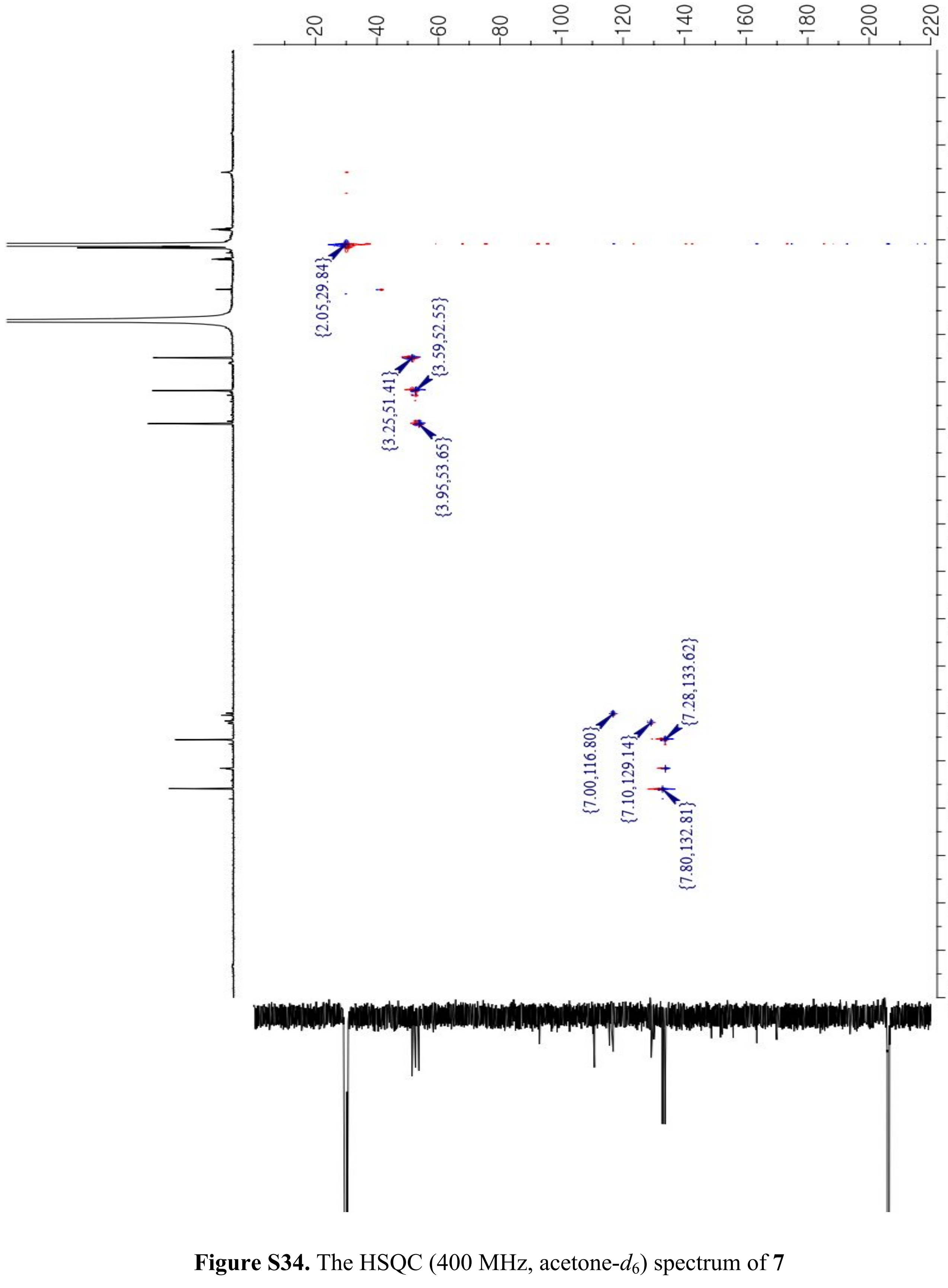


Figure S34. The HSQC (400 MHz, acetone-d_6) spectrum of **7**

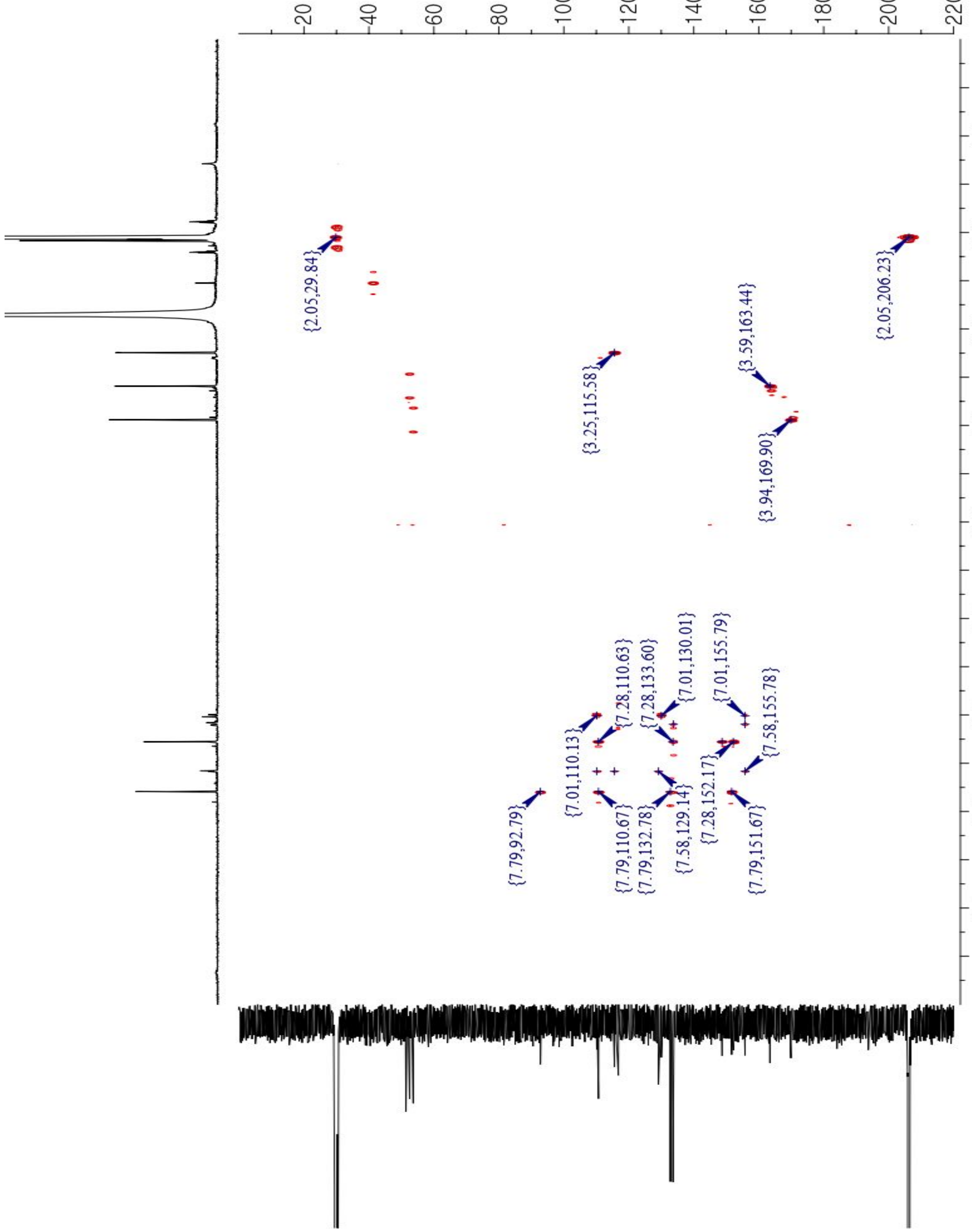


Figure S35. The HMBC (400 MHz, acetone-d_6, J_{CH} = 8 Hz) spectrum of **7**

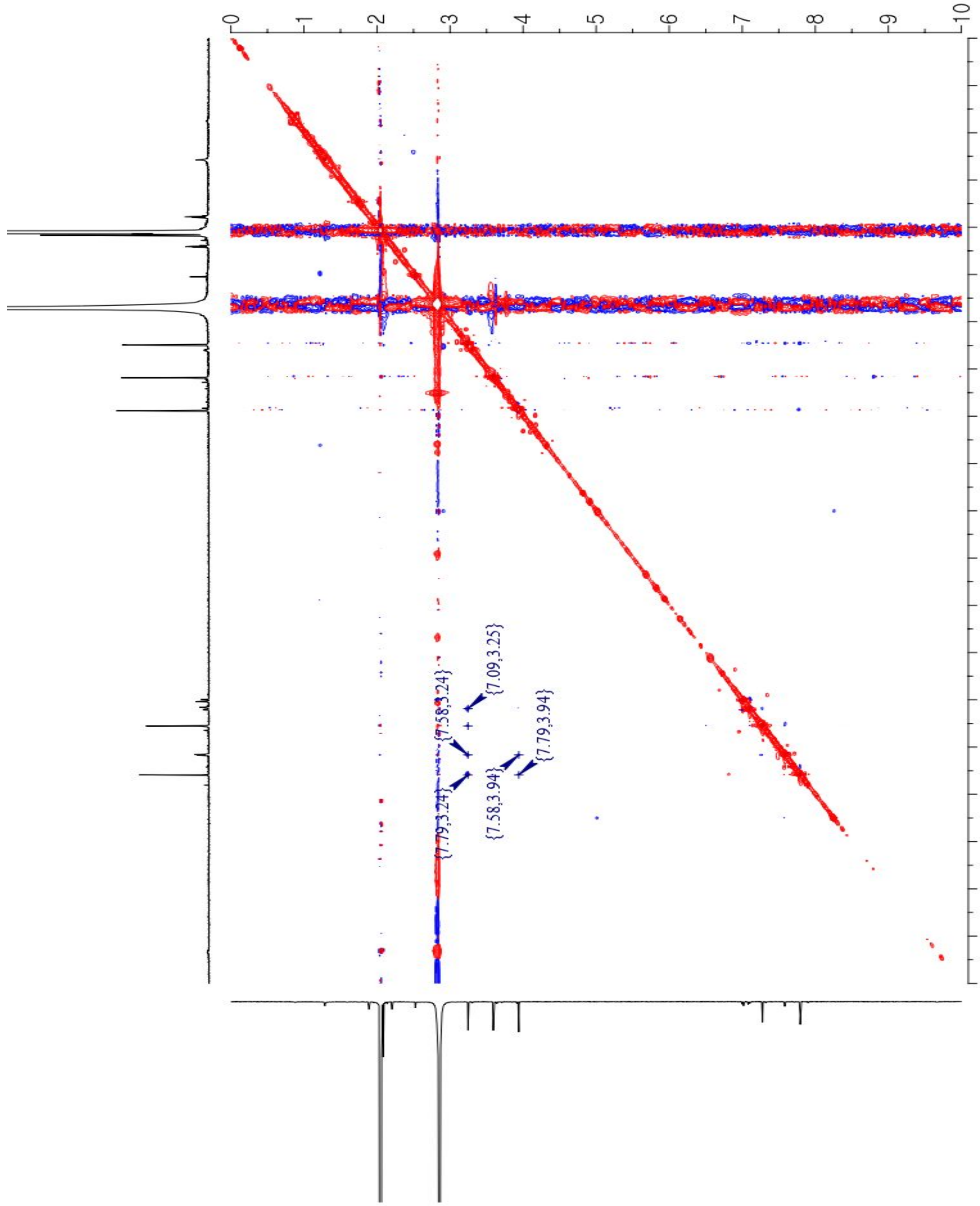


Figure S36. The NOESY (800 MHz, acetone-d_6) spectrum of **7**

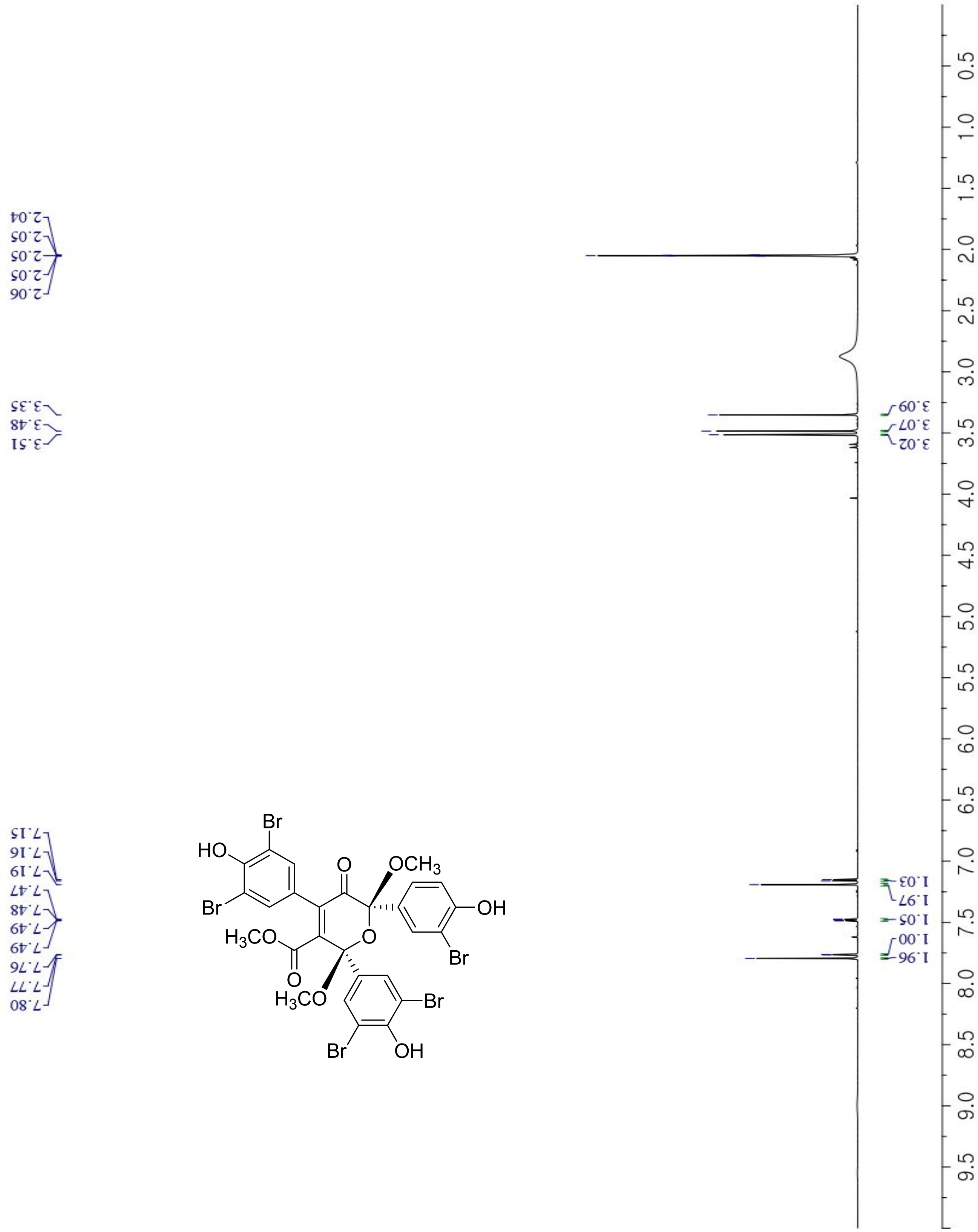


Figure S37. The [1]H NMR (800 MHz, acetone-d_6) spectrum of **8**

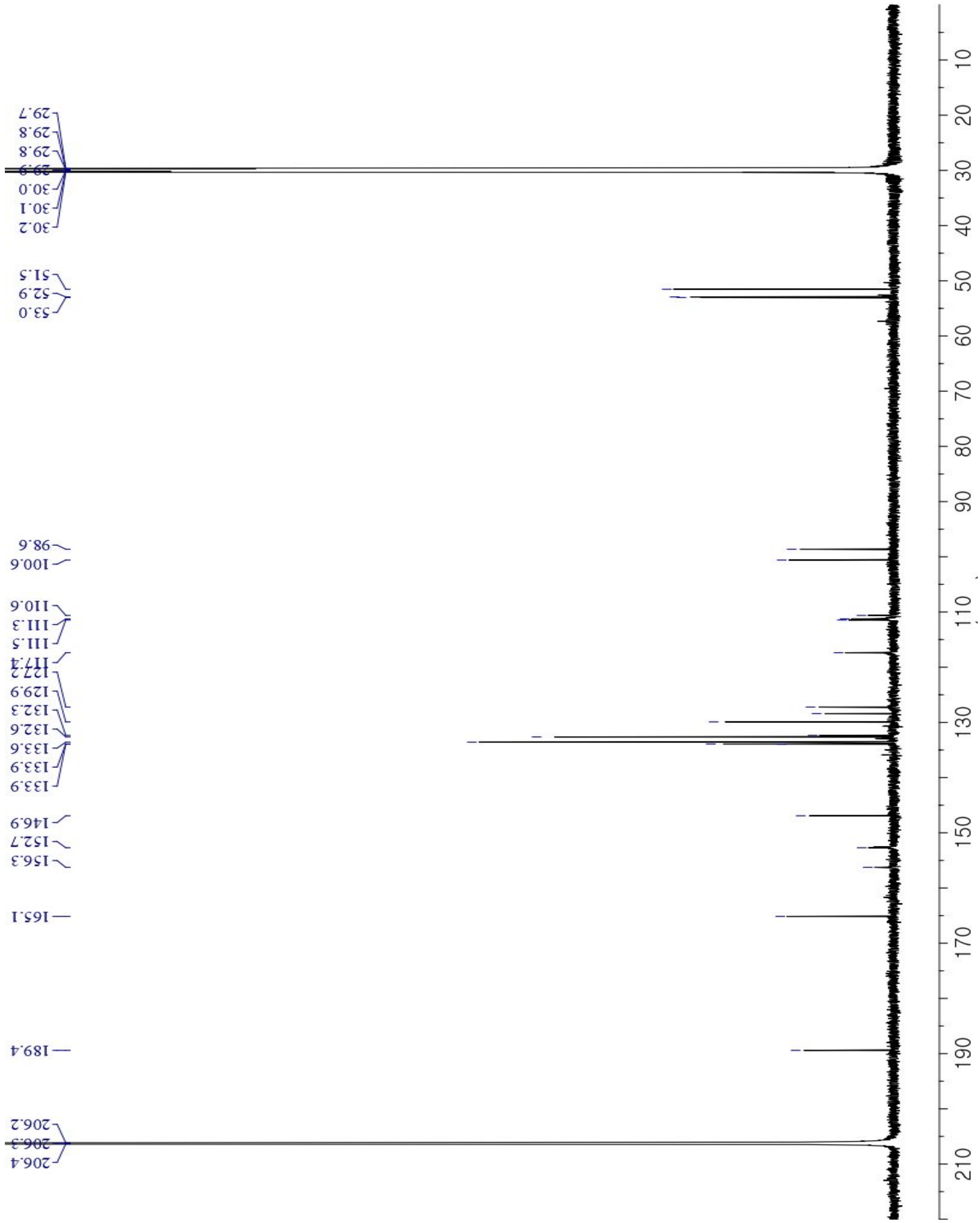


Figure S38. The ^{13}C NMR (200 MHz, acetone-d_6) spectrum of **8**

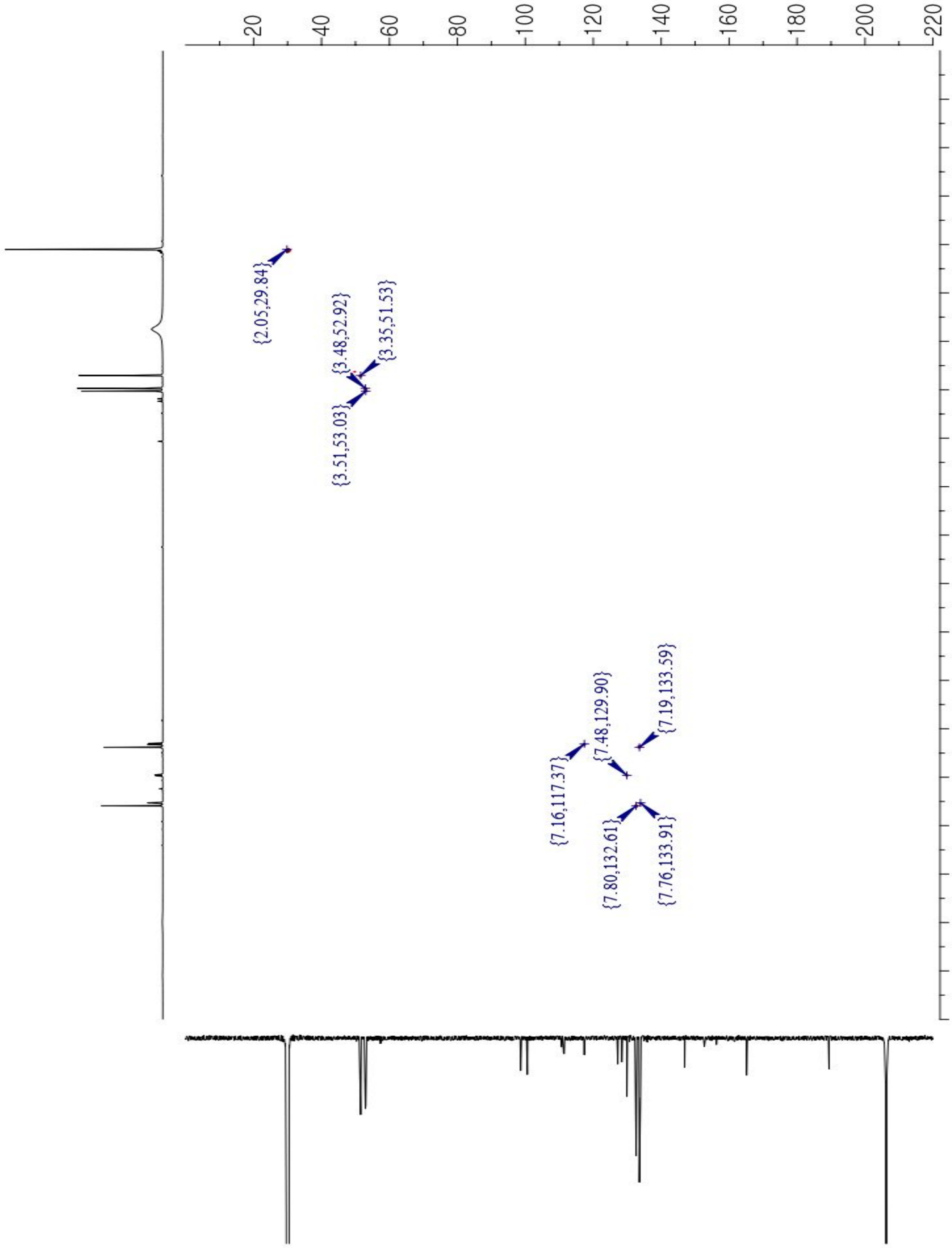


Figure S39. The HSQC (800 MHz, acetone-d_6) spectrum of **8**

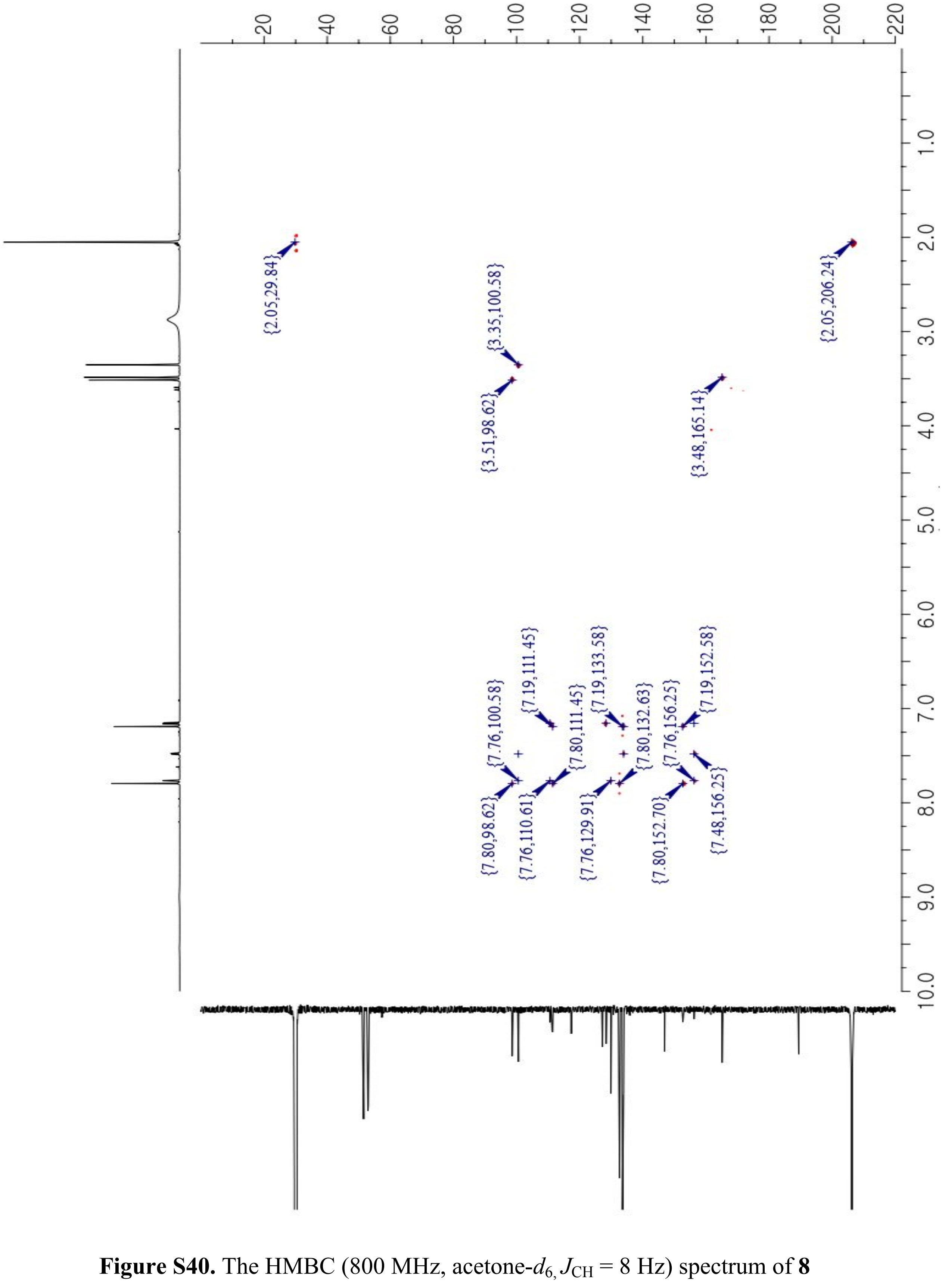


Figure S40. The HMBC (800 MHz, acetone-d_6, J_{CH} = 8 Hz) spectrum of **8**

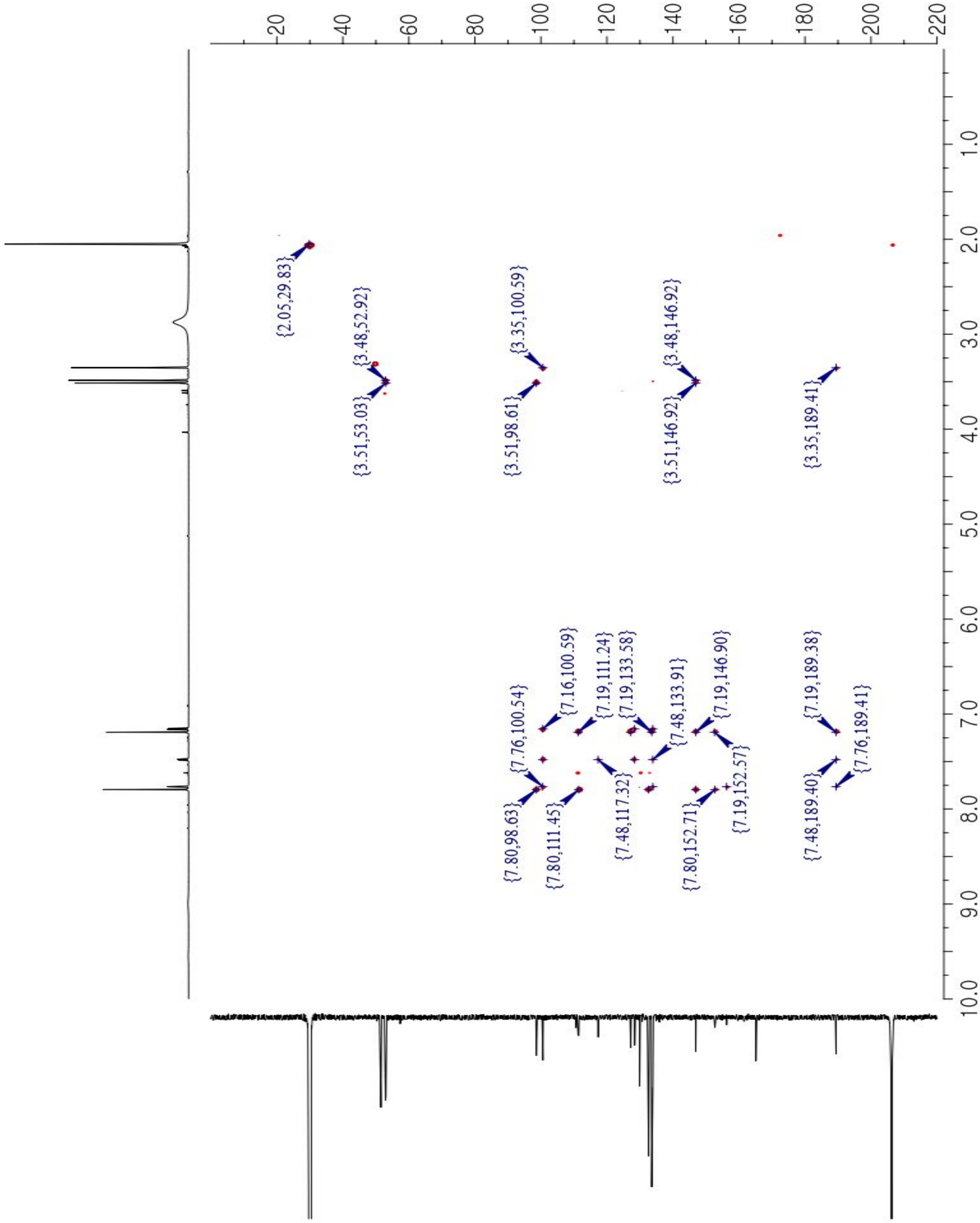


Figure S41. The D-HMBC (800 MHz, acetone-d_6, J_{CH} = 1 Hz) spectrum of **8**

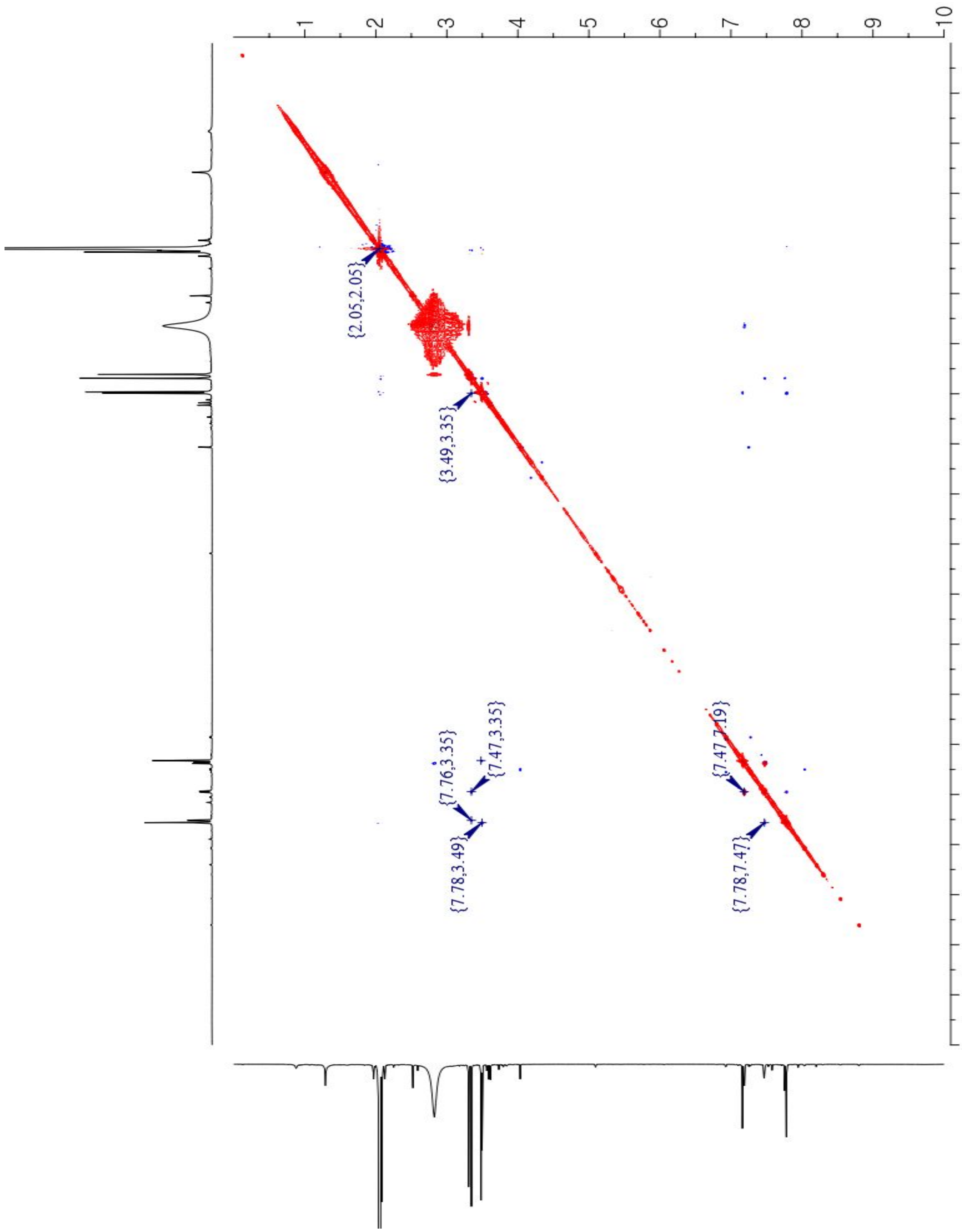


Figure S42. The NOESY (800 MHz, acetone-d_6) spectrum of **8**

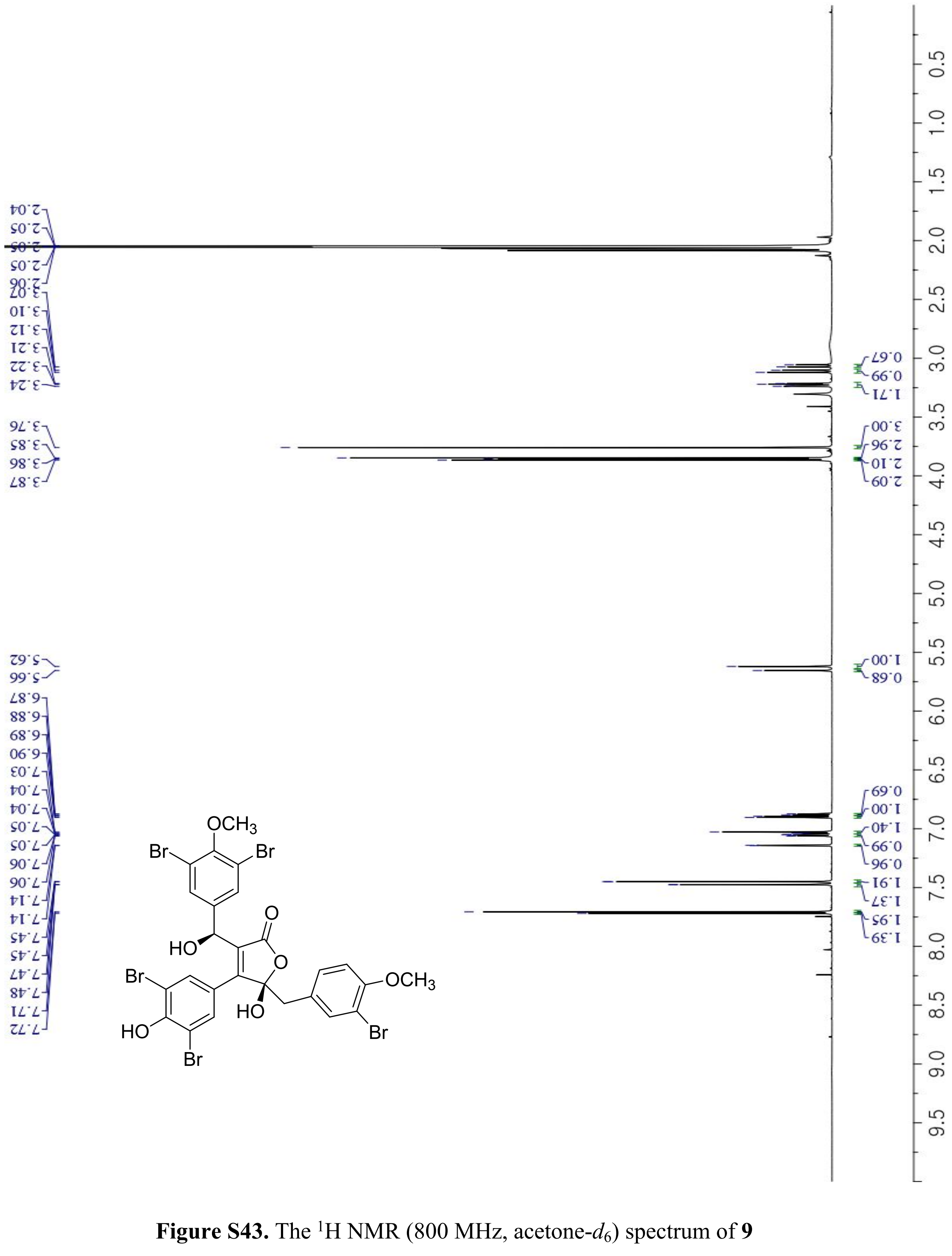


Figure S43. The ^{1}H NMR (800 MHz, acetone-d_6) spectrum of **9**

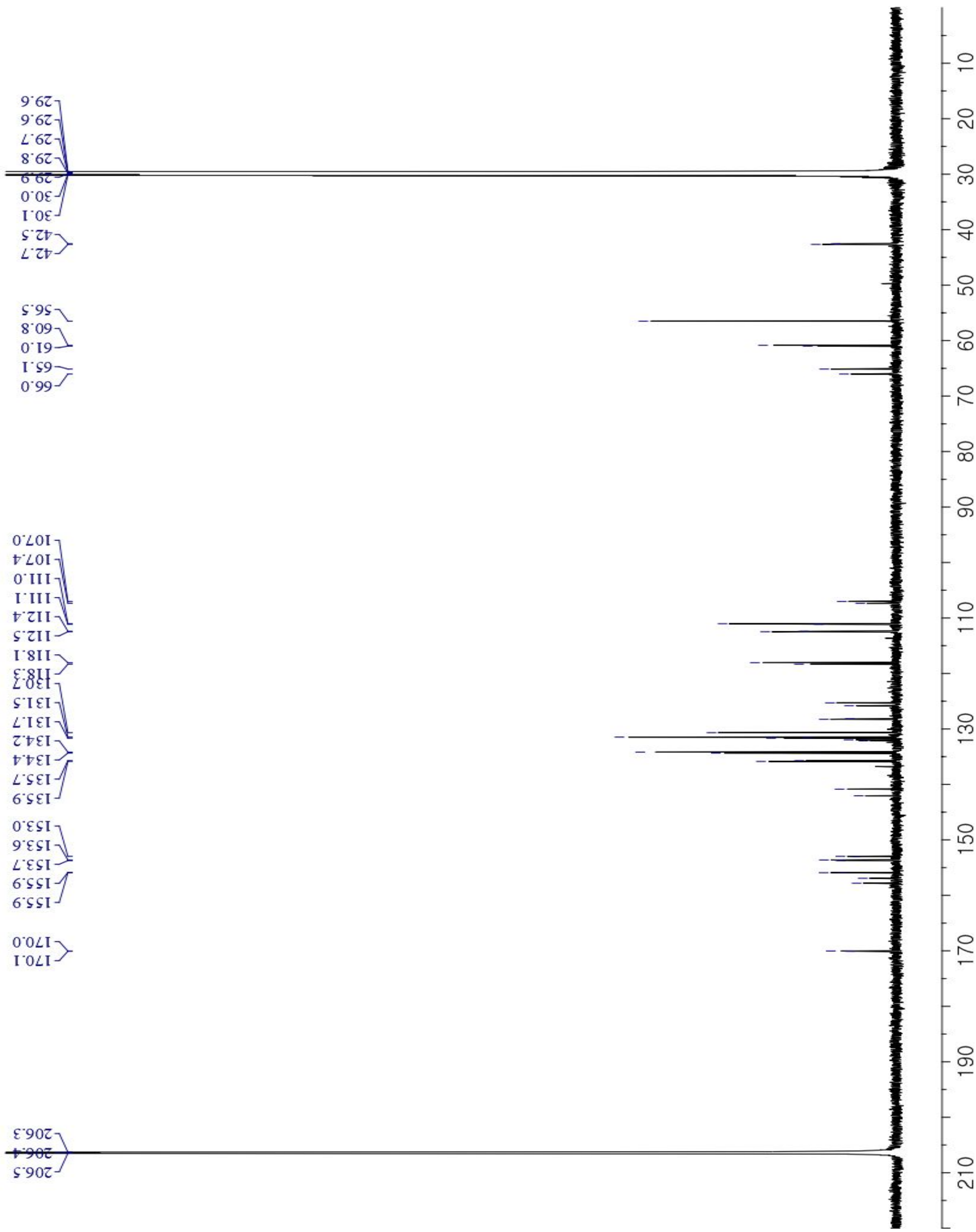


Figure S44. The ^{13}C NMR (200 MHz, acetone-d_6) spectrum of **9**

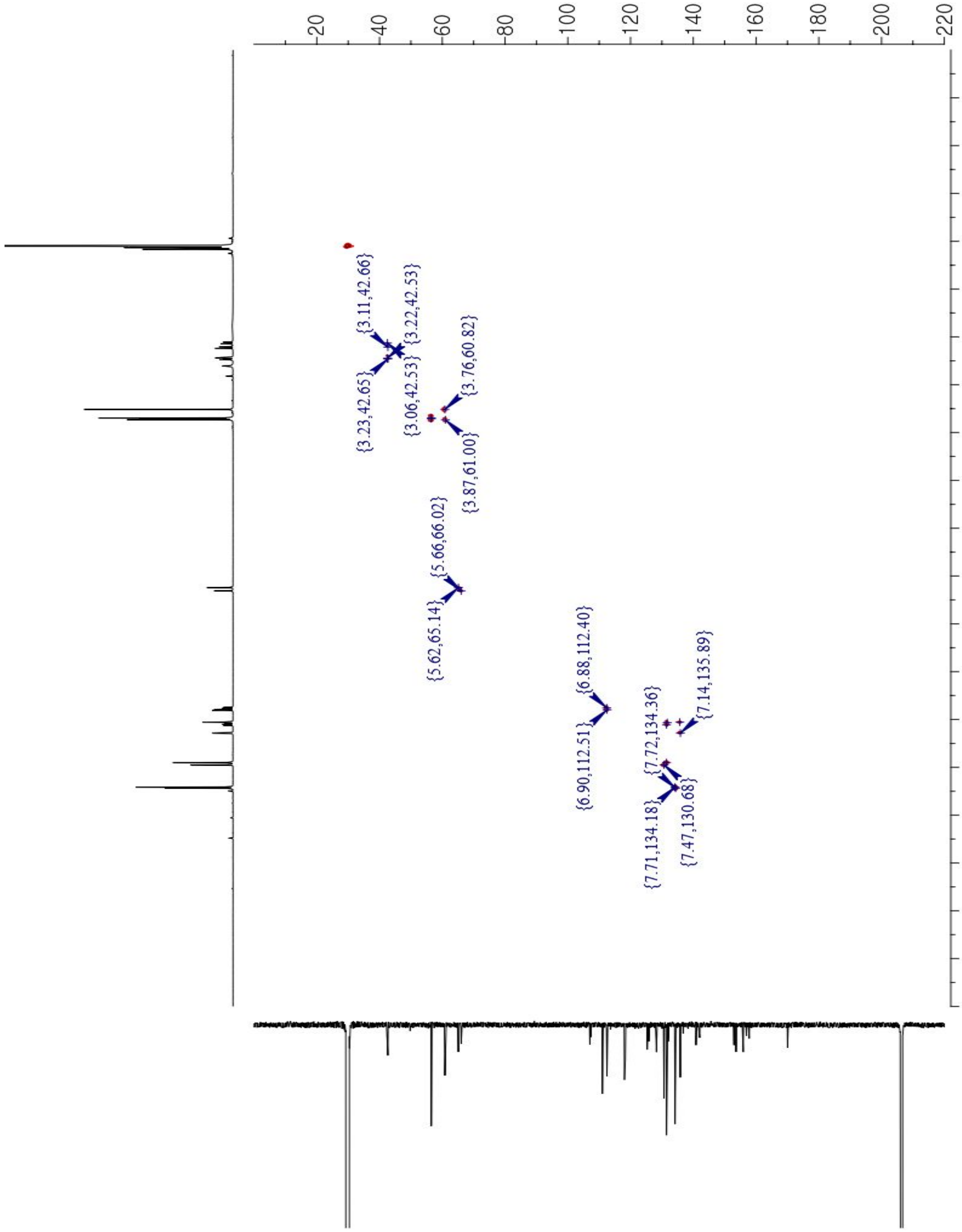


Figure S45. The HSQC (800 MHz, acetone-d_6) spectrum of **9**

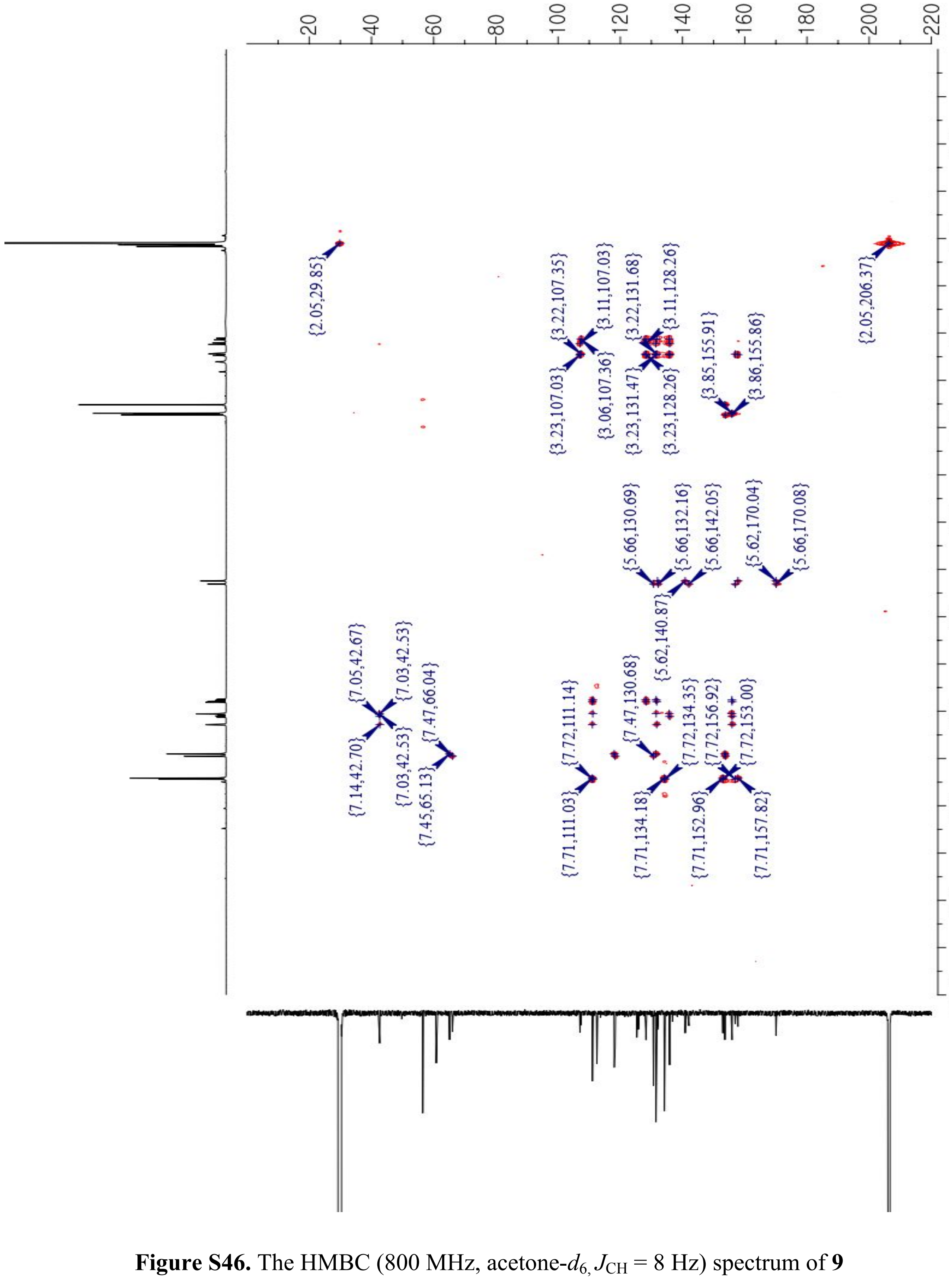


Figure S46. The HMBC (800 MHz, acetone-d_6, J_{CH} = 8 Hz) spectrum of **9**

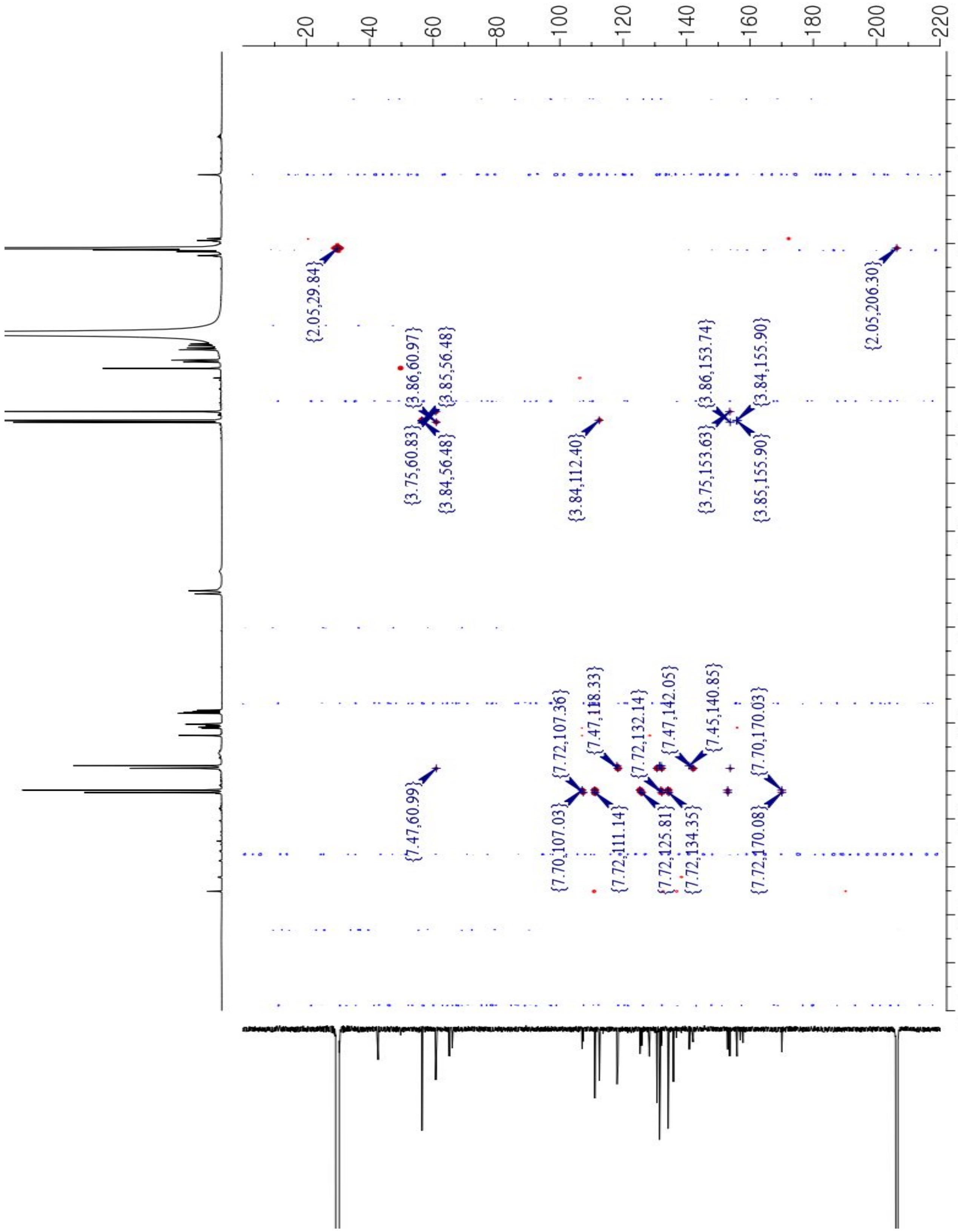


Figure S47. The D-HMBC (800 MHz, acetone-d_6, J_{CH} = 1 Hz) spectrum of **9**

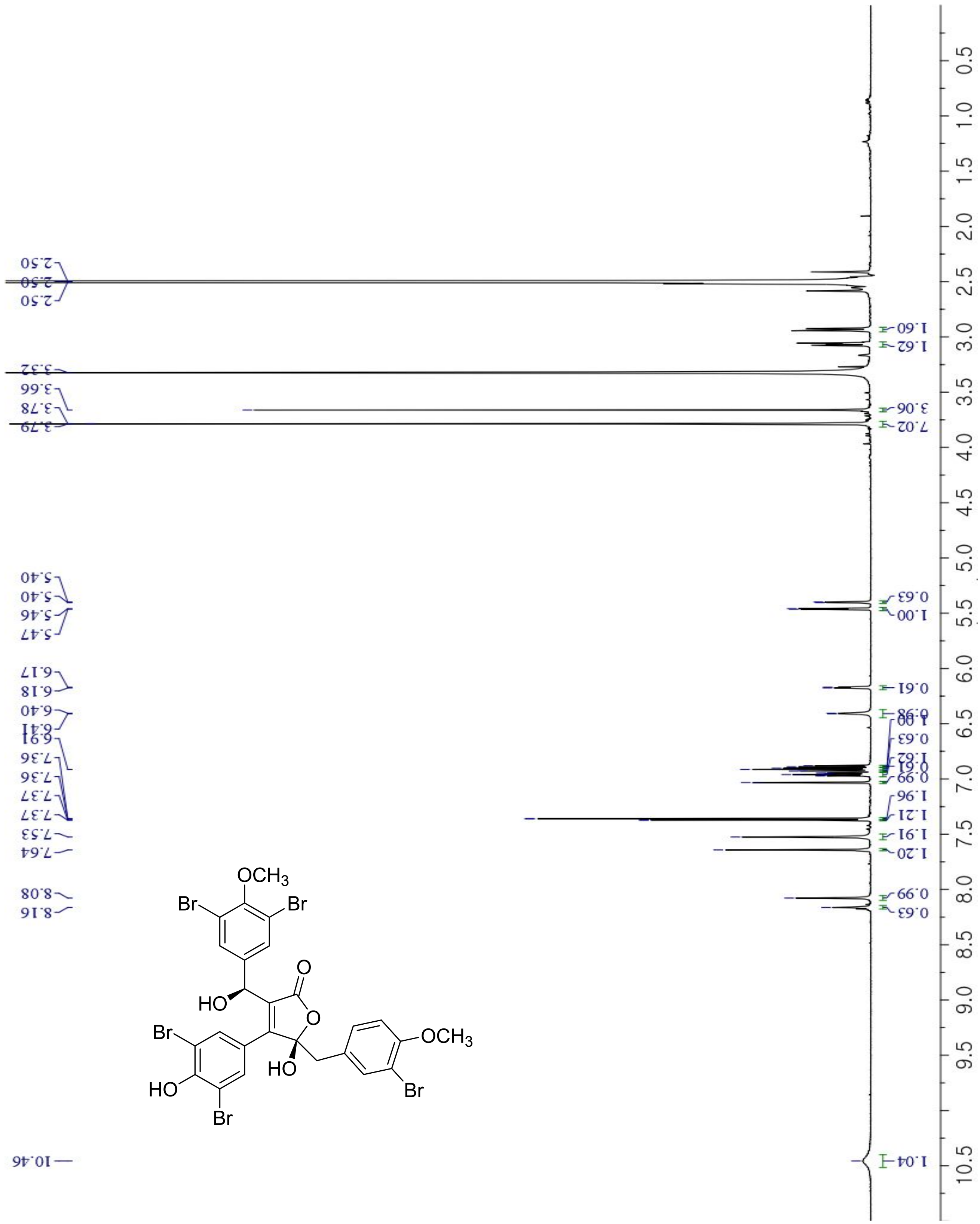


Figure S48. The ^{1}H NMR (800 MHz, DMSO-d_6) spectrum of **9**

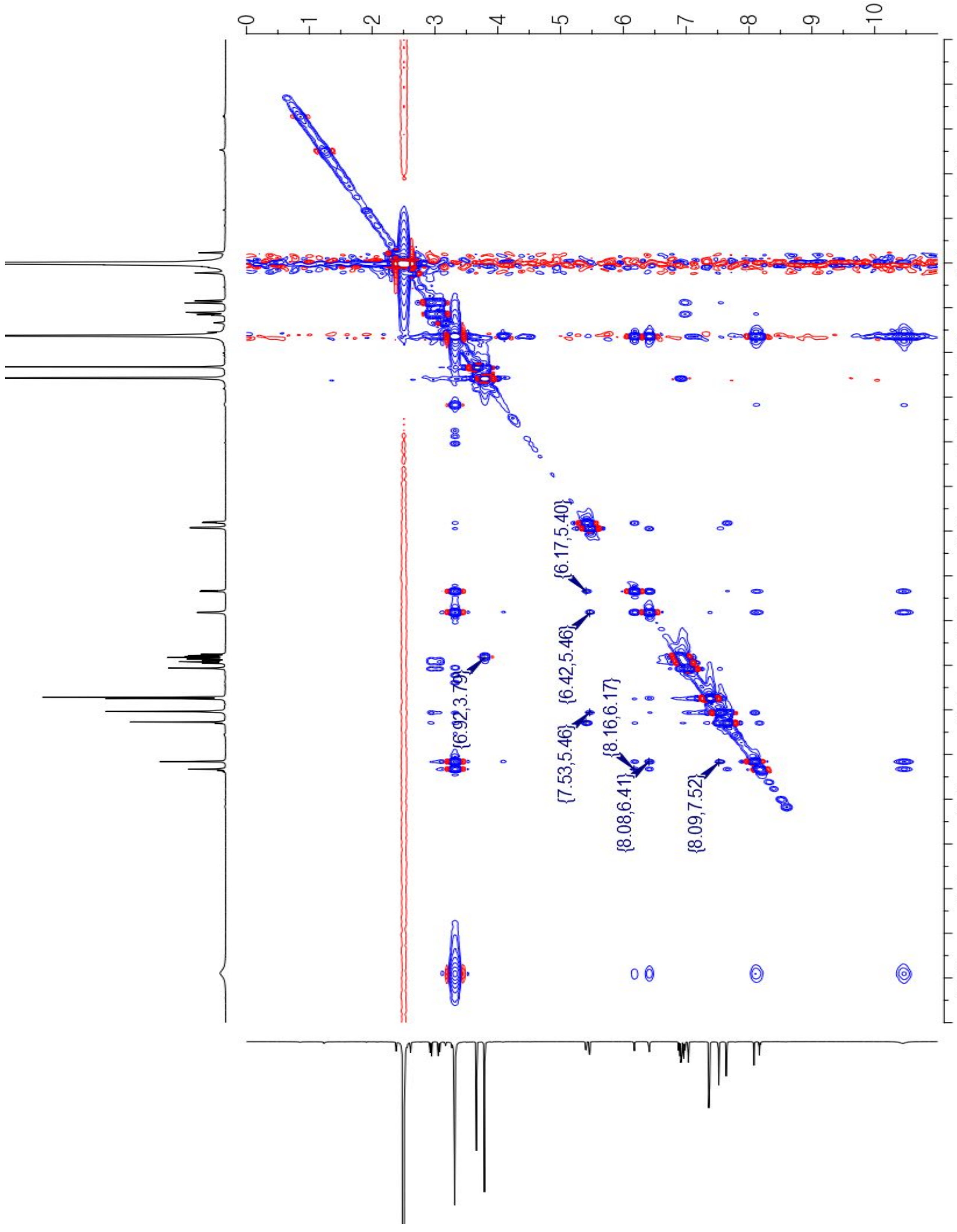


Figure S49. The NOESY (800 MHz, DMSO-d_6) spectrum of **9**

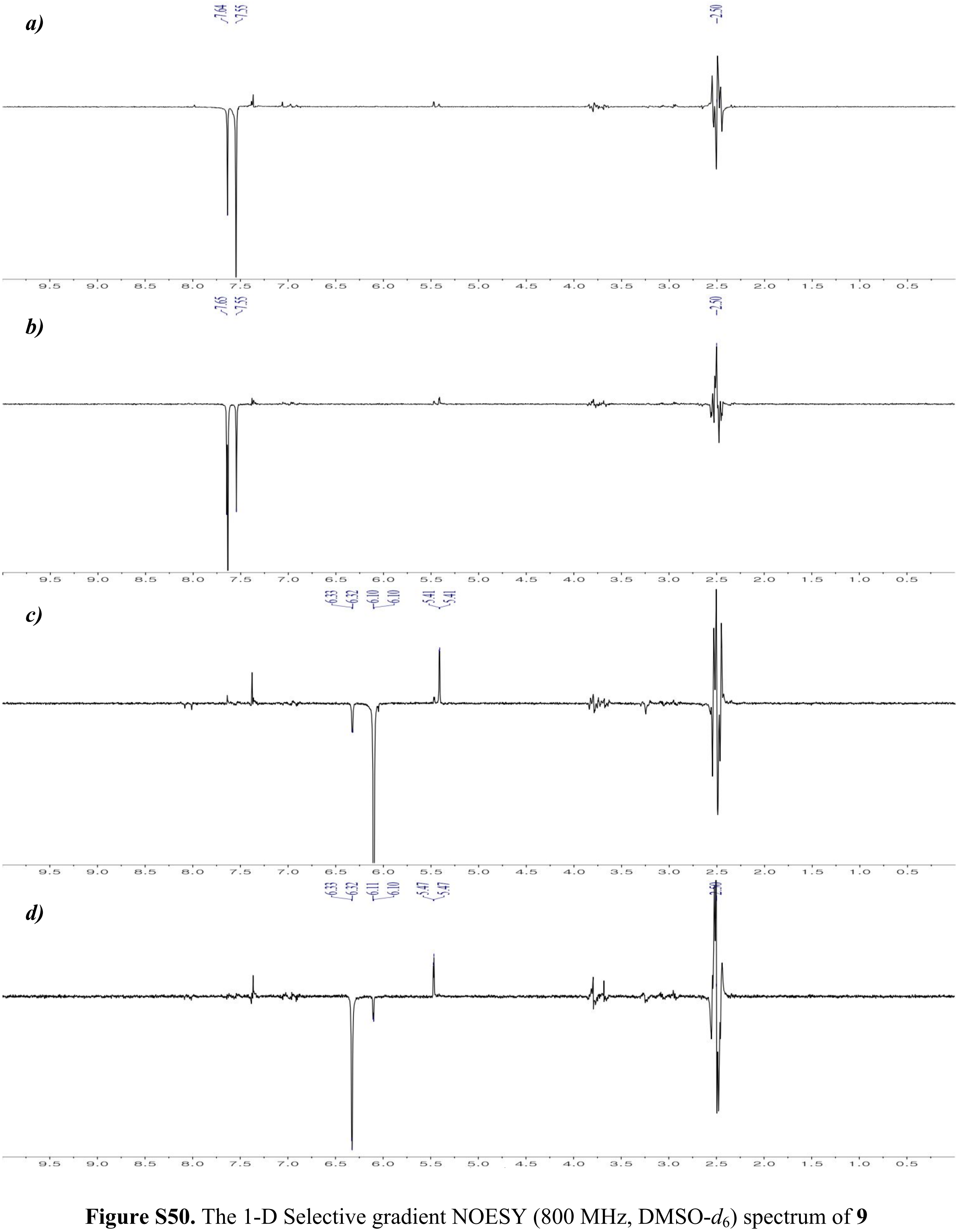
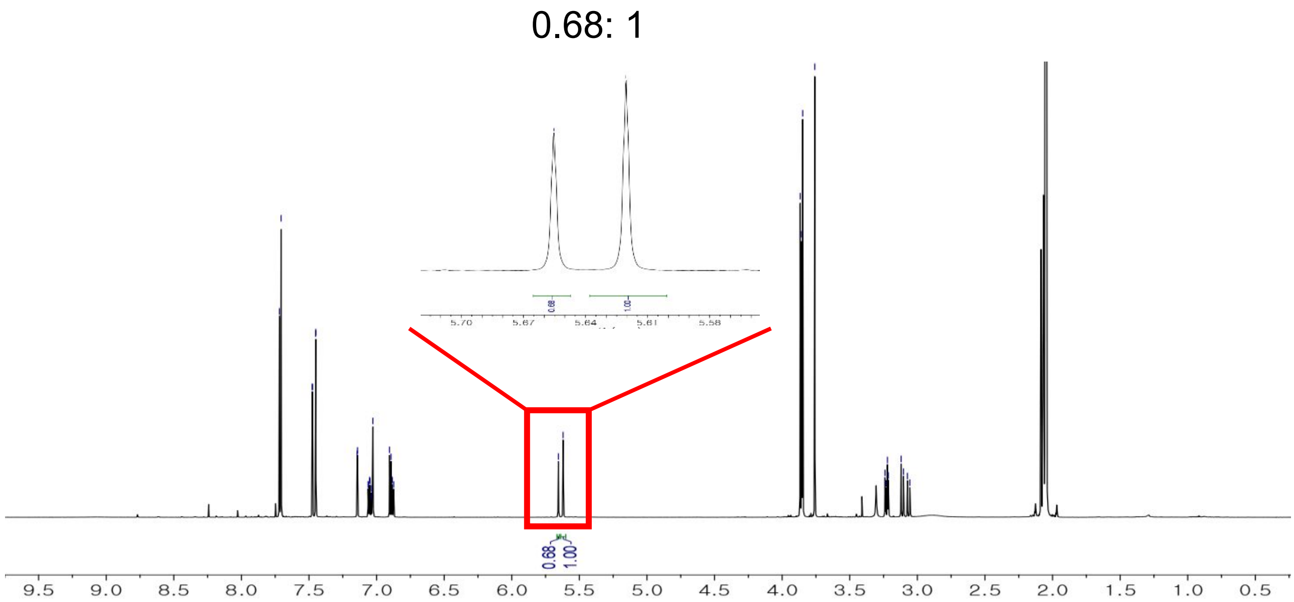
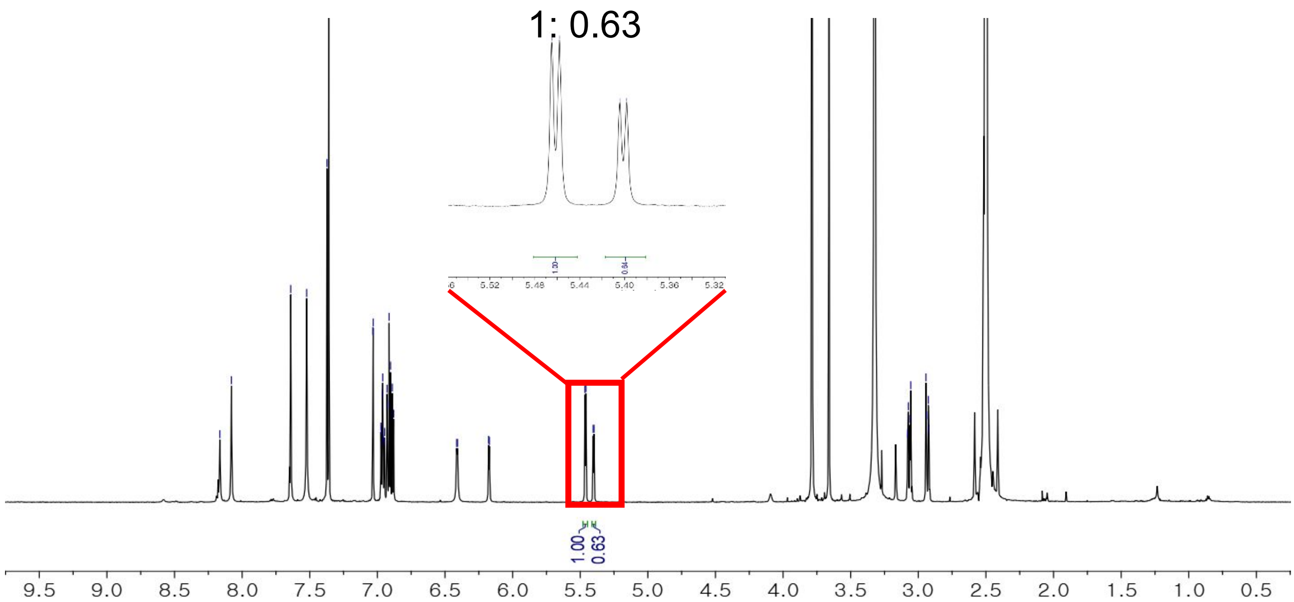


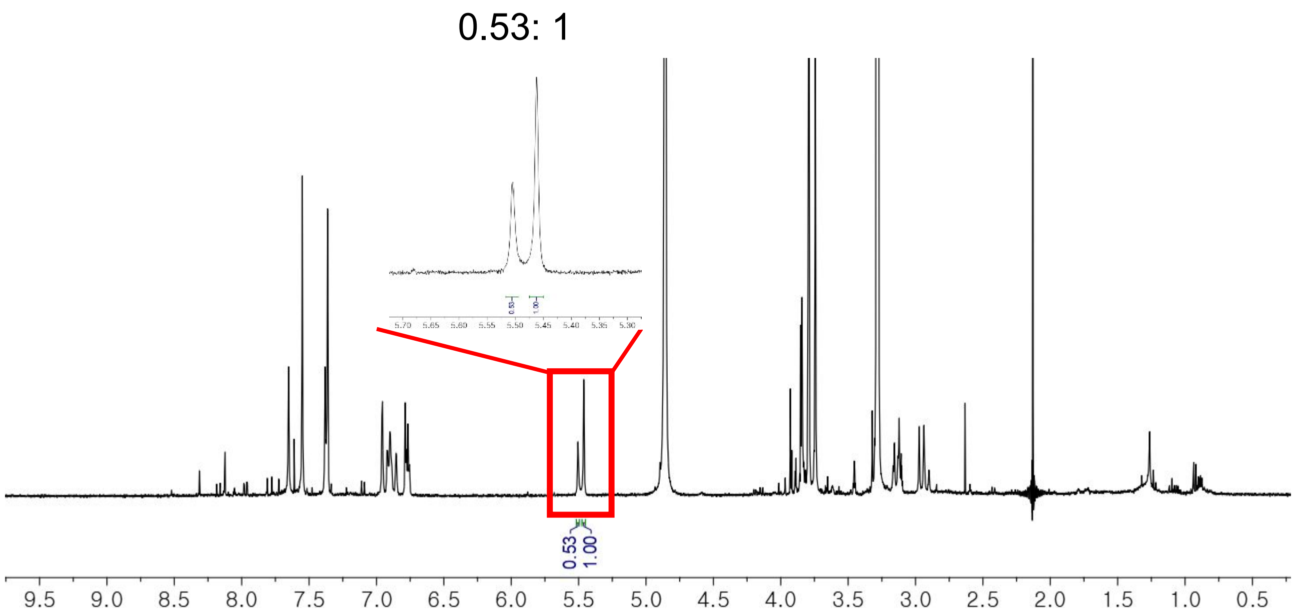
Figure S50. The 1-D Selective gradient NOESY (800 MHz, DMSO-d_6) spectrum of **9** (Irradiation at δ_H *a)* 7.55 (H-2'/6' of **9a**), *b)* 7.64 (H-2'/6' of **9b**), *c)* 6.10 (6-OH of **9b**), and *d)* 6.32 (6-OH of **9a**)



The [1]H NMR (400 MHz, acetone-d_6) spectrum of **9**



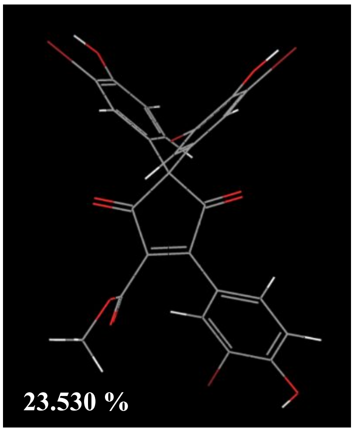
The [1]H NMR (800 MHz, DMSO-d_6) spectrum of **9**

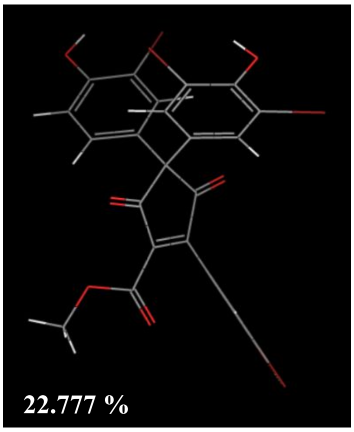


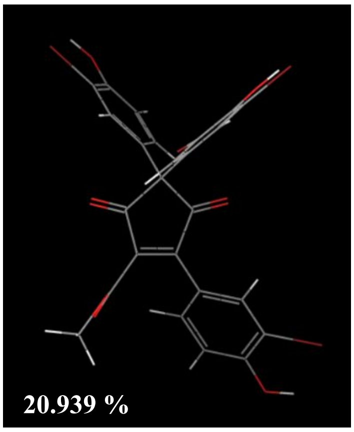
The ^1H NMR (400 MHz, methanol-d_4) spectrum of **9**

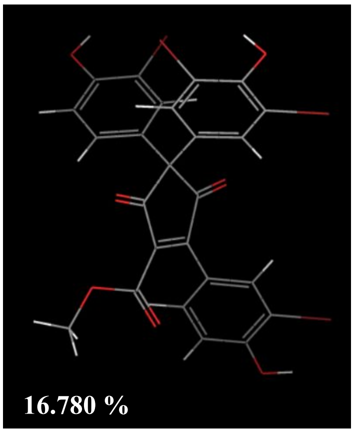
Figure S51. The varied ratios of **9a** and **9b** in diverse NMR solvents

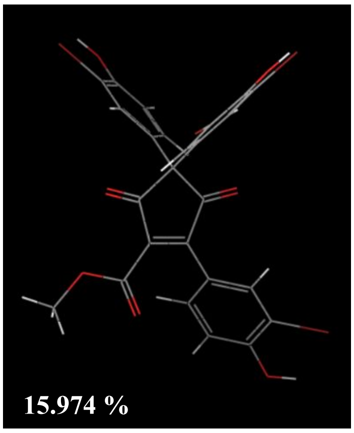
Parameters for calculating specific rotations
Functional: B3-LYP
Basis set: def-SVP
Gridsize: m3
Frequency: 0.7735713524617996E-01
Frequency / eV: 2.104995653760073
Frequency / nm: 589.0000000000000
Frequency / cm^ (-1): 16977.92869016530









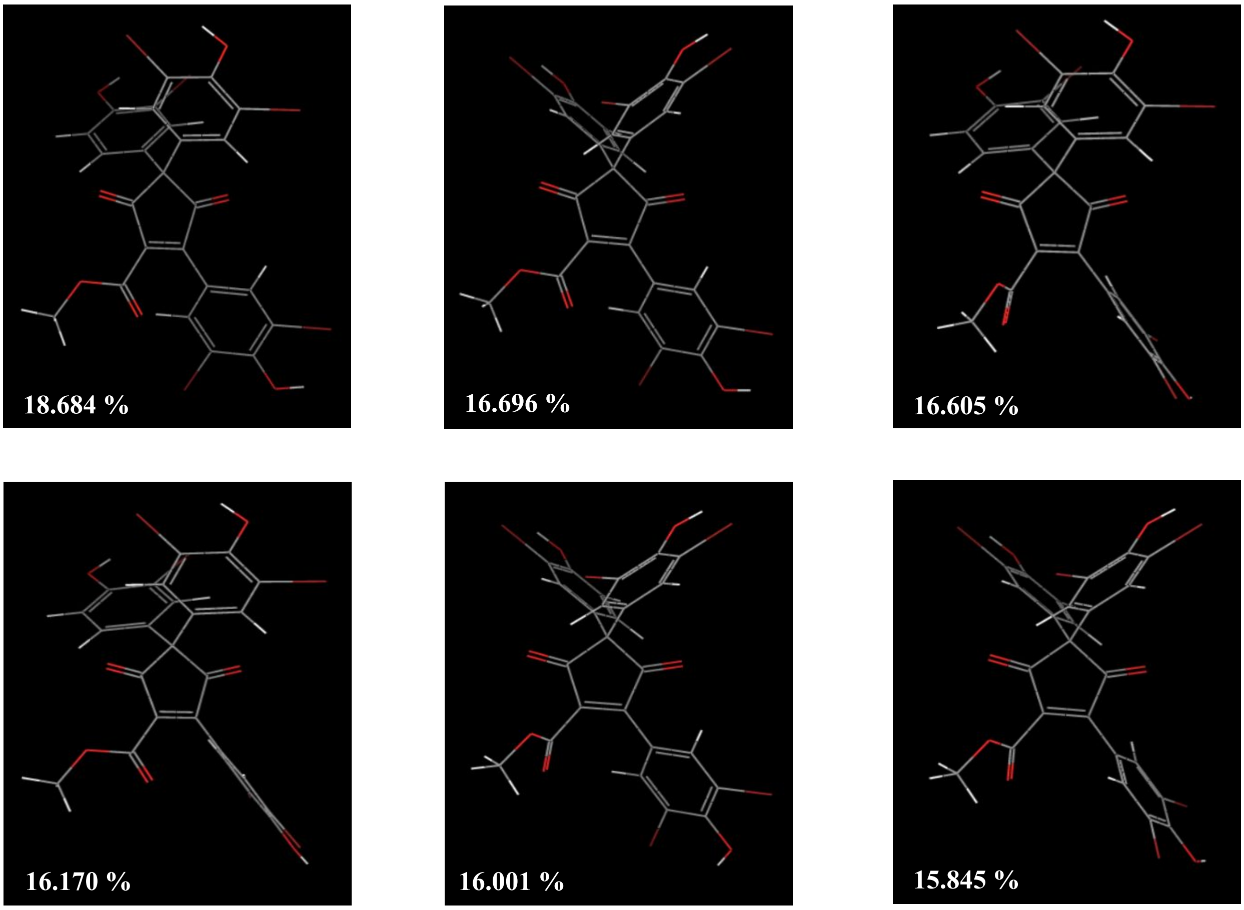


Five major conformers (> 15% population) under the relative energy of 1kJ/mol in calculated Boltzmann distribution

Compound **2**	1/3*trace (dipole polarizability)	1/3*trace (rotatory dispersion)	Specific rotation [α] in deg*[dm(g/cc)]^(-1)
23.530 %	397.0	9.9	+513.4
22.777 %	396.5	-10.4	-538.3
20.939 %	397.3	9.7	+501.5
16.780 %	400.8	-19.4	-1009.0
15.974 %	402.5	7.7	+397.5

Figure S52. Calculated optical rotations of major conformers of **2**

Parameters for calculating specific rotations
Functional: B3-LYP
Basis set: def-SVP
Gridsize: m3
Frequency: 0.7735713524617996E-01
Frequency / eV: 2.104995653760073
Frequency / nm: 589.0000000000000
Frequency / cm^ (-1): 16977.92869016530



Six major conformers (> 15% population) under the relative energy of 1kJ/mol in calculated Boltzmann distribution

Compound **4**	1/3*trace (dipole polarizability)	1/3*trace (rotatory dispersion)	Specific rotation [α] in deg*[dm(g/cc)]^(-1)
18.684 %	420.3	-19.5	-914.6
16.696 %	422.0	8.2	+386.4
16.605 %	421.0	-9.6	-451.2
16.170 %	416.0	-13.4	-627.2
16.001 %	416.6	11.9	+560.1
15.845 %	420.8	17.7	+831.1

Figure S53. Calculated optical rotations of major conformers of **4**