

# Coumarinolignans with Reactive Oxygen Species (ROS) and NF- $\kappa$ B Inhibitory Activities from the Roots of *Waltheria indica*

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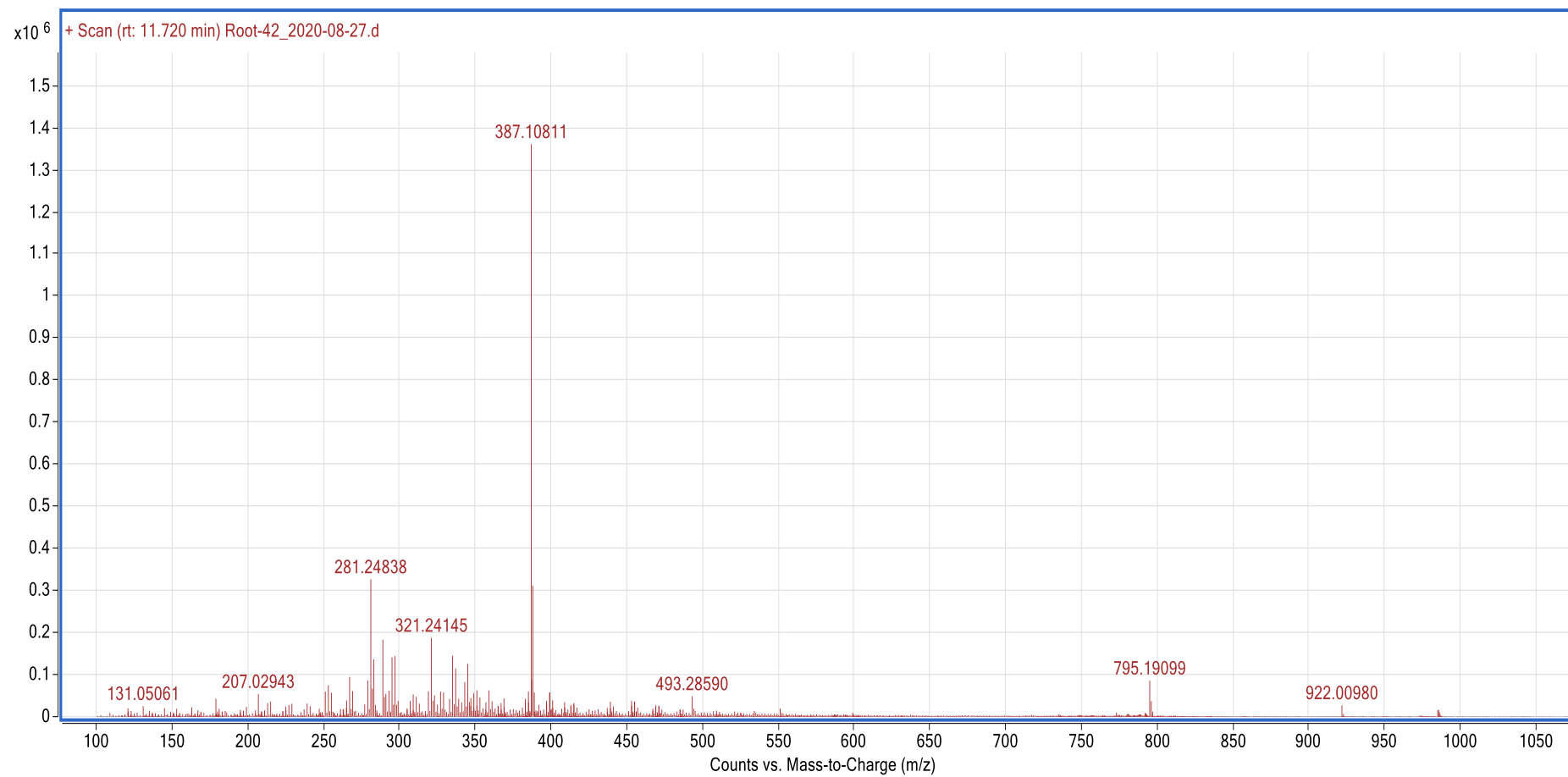
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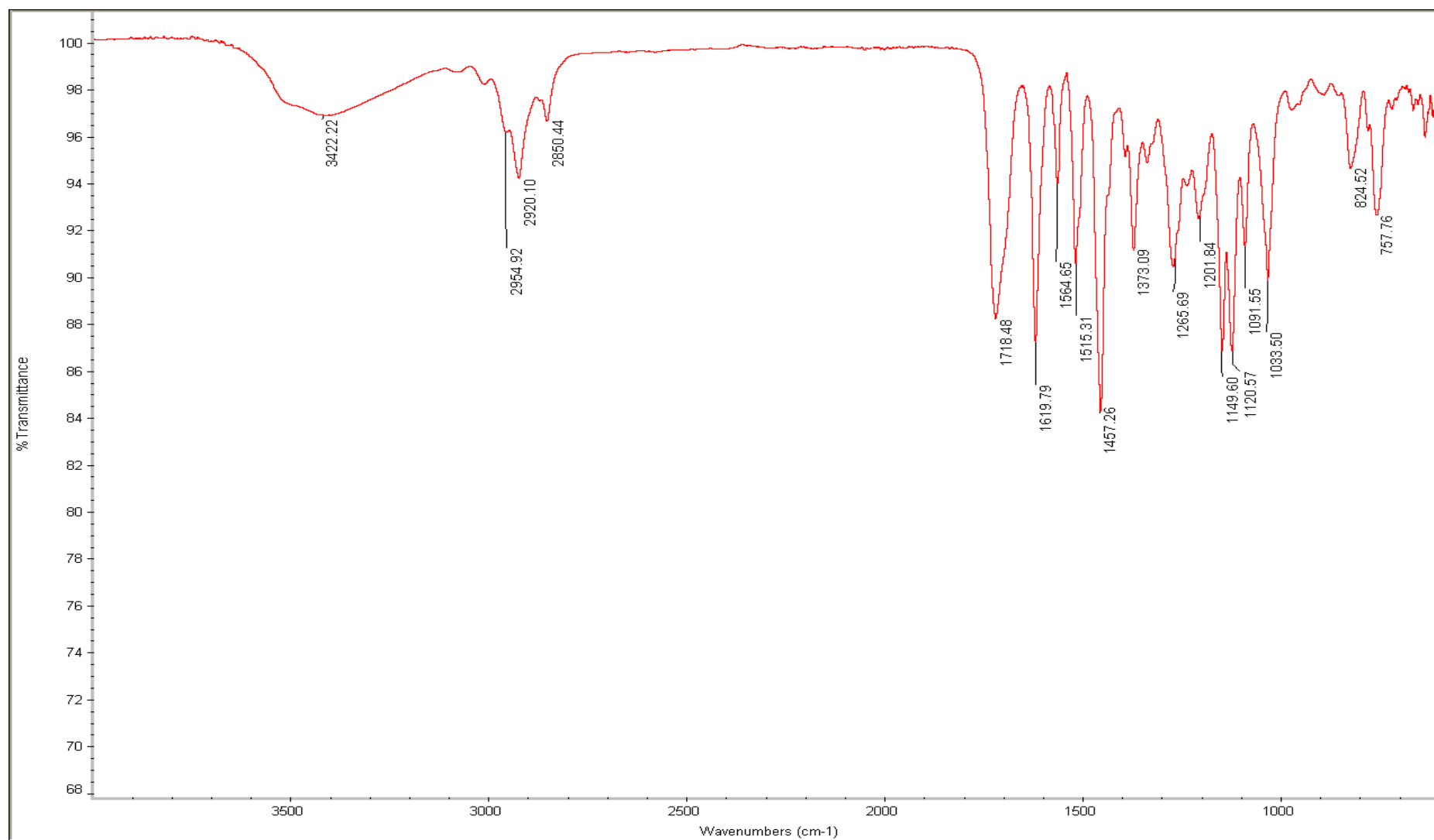
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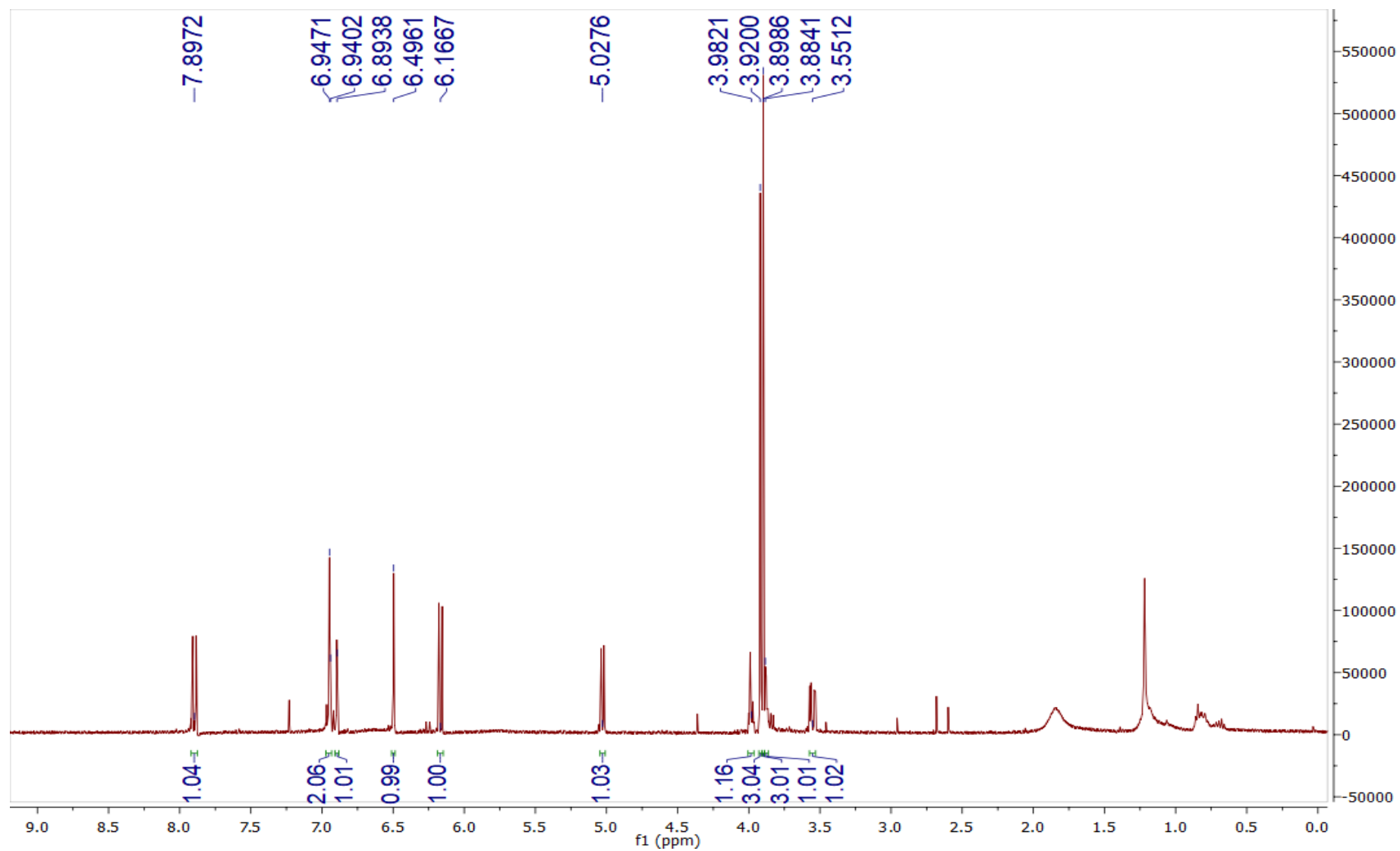
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**Figure S1.** HRESI-MS spectrum of the new compound **1a**

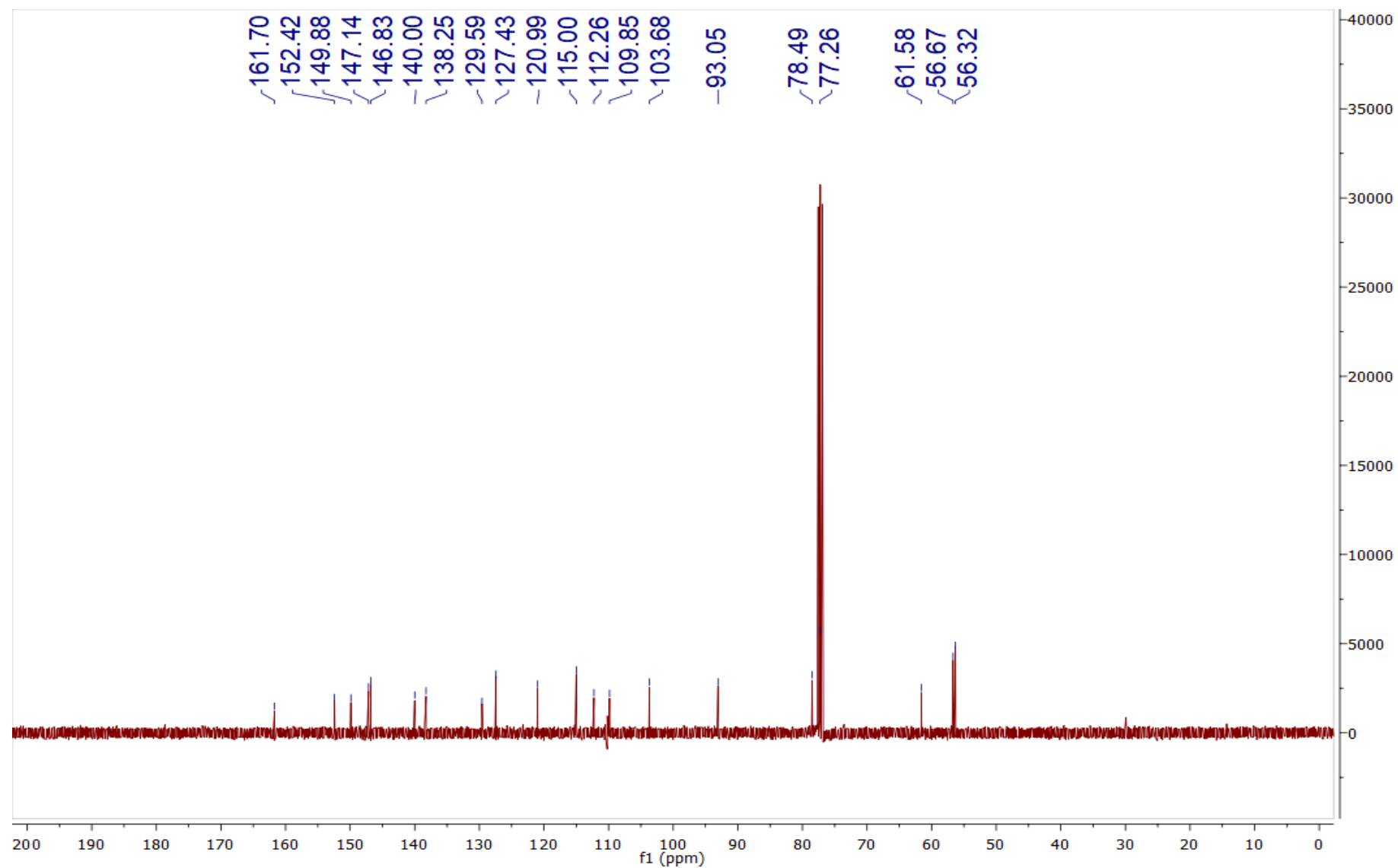


**Figure S2.** IR spectrum of the new compound **1a**

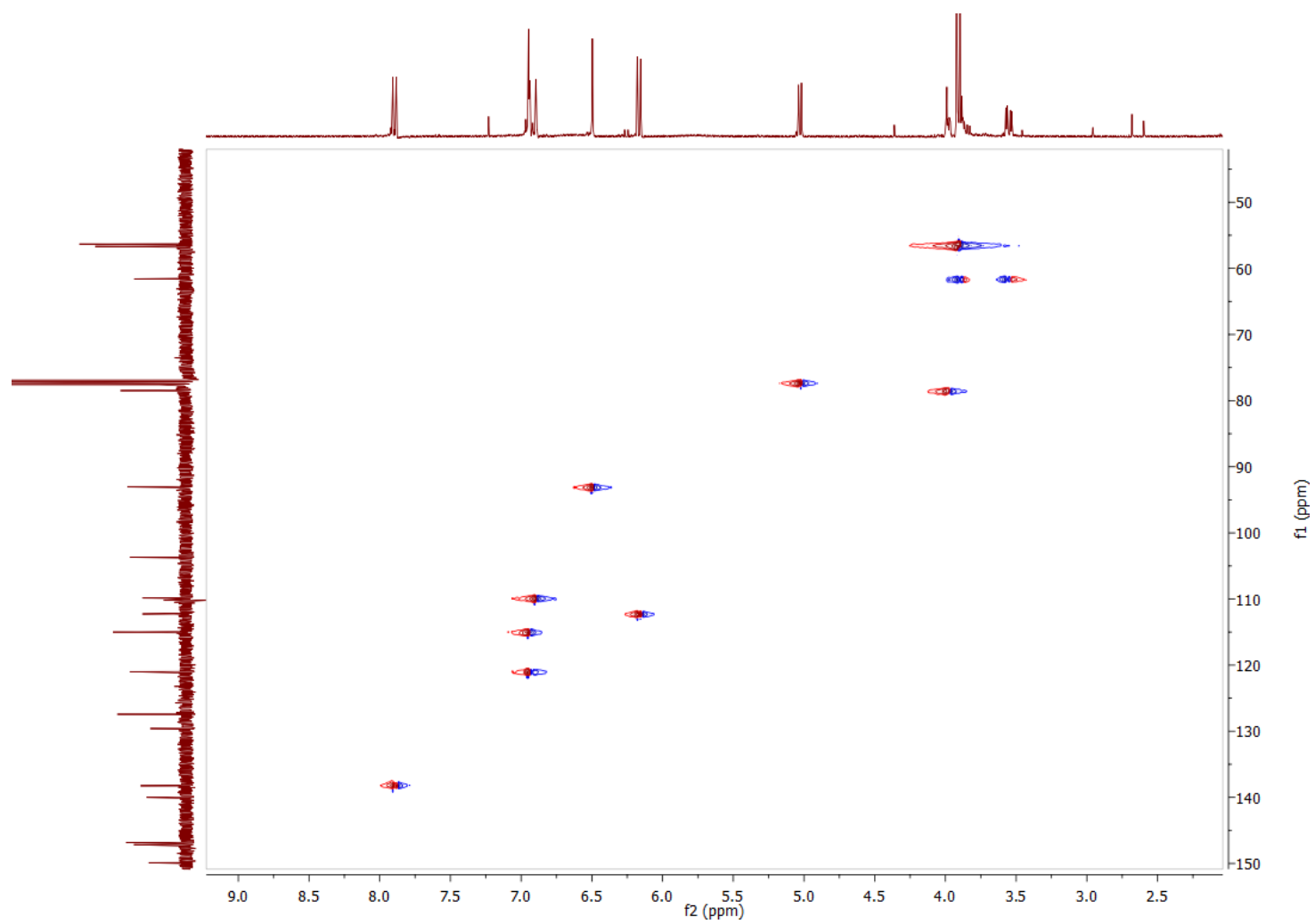


**Figure S3.**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectrum of the new compound **1a**

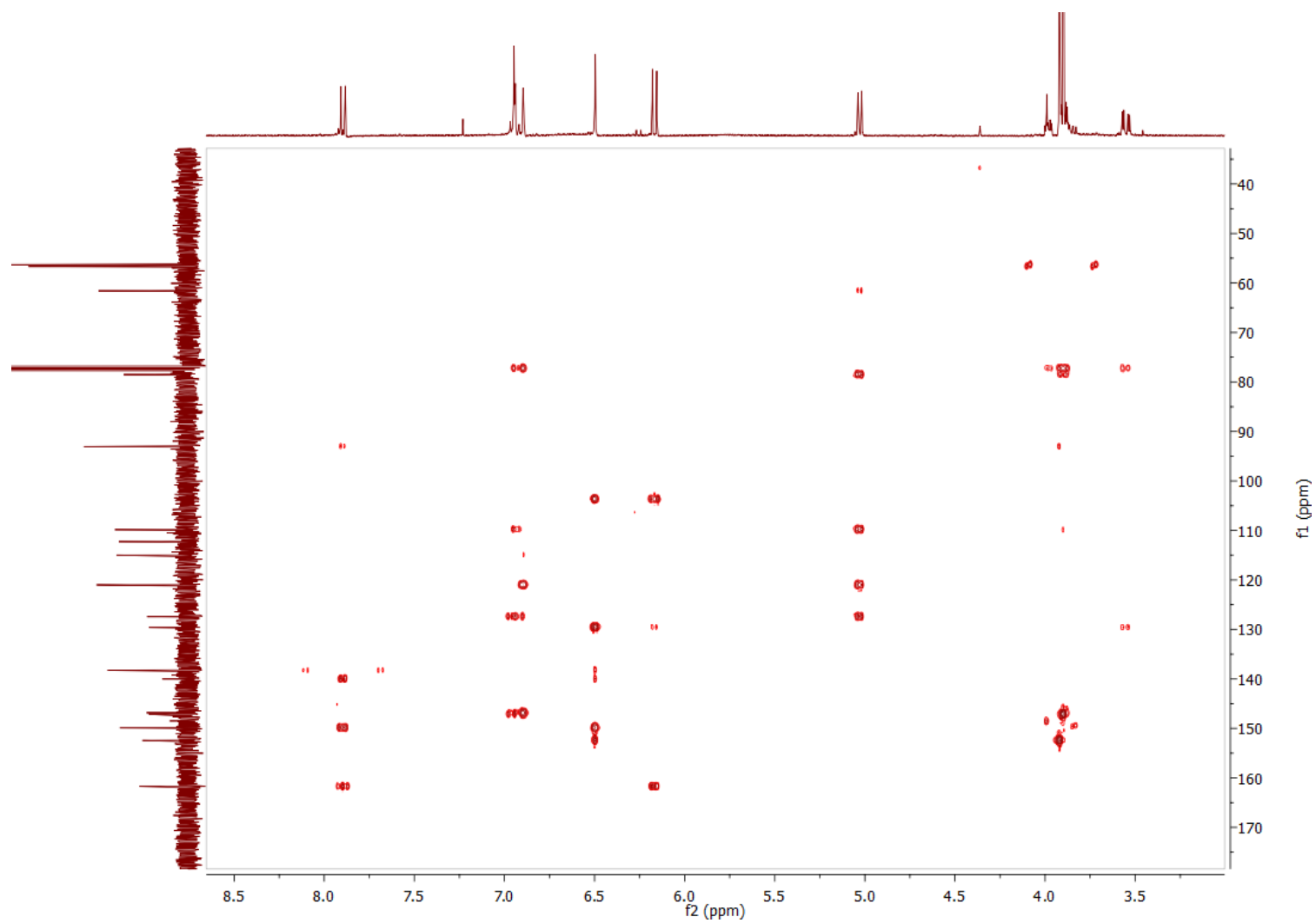




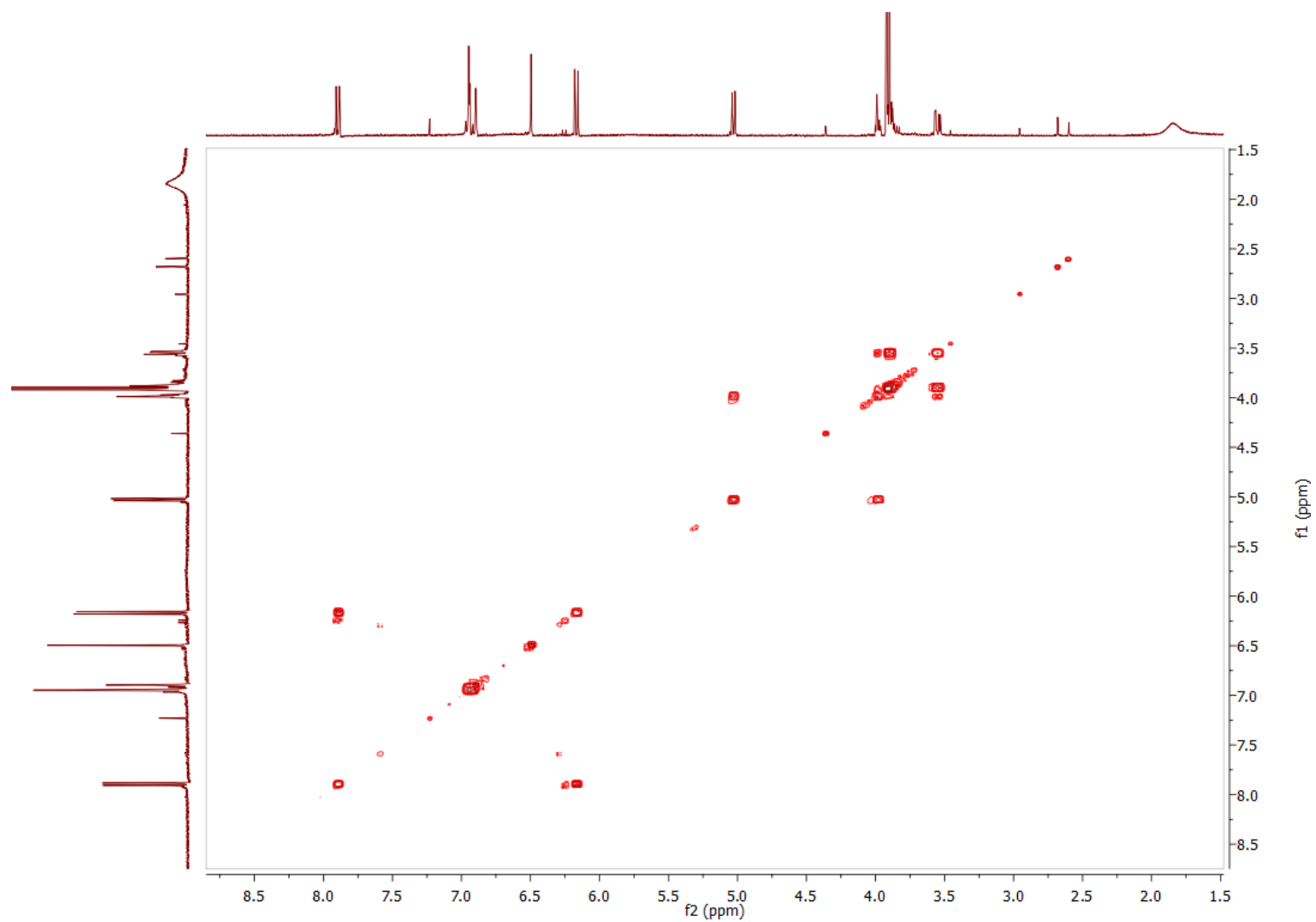
**Figure S4.**  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) spectrum of the new compound **1a**



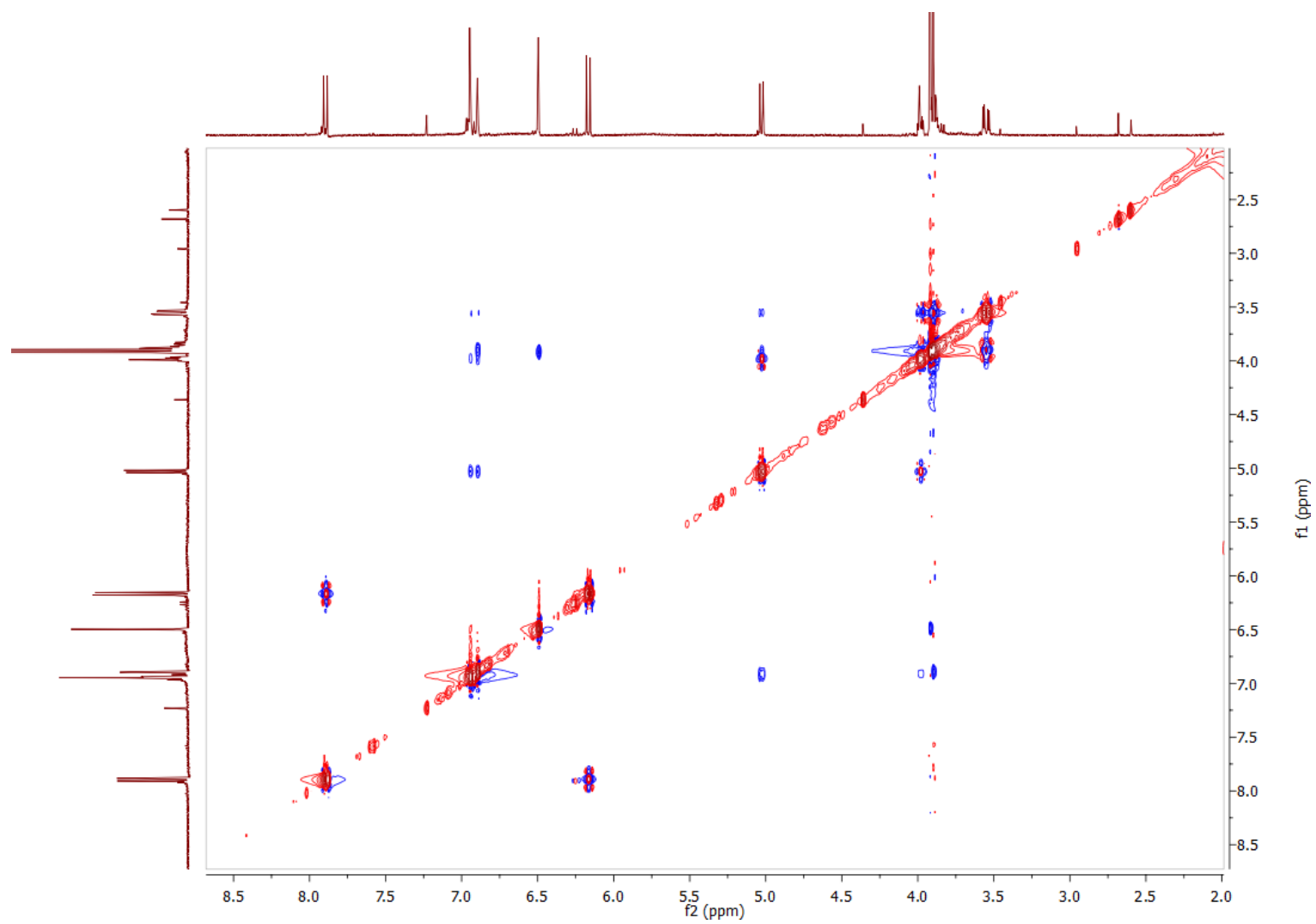
**Figure S5.** HSQC spectrum of the new compound **1a**



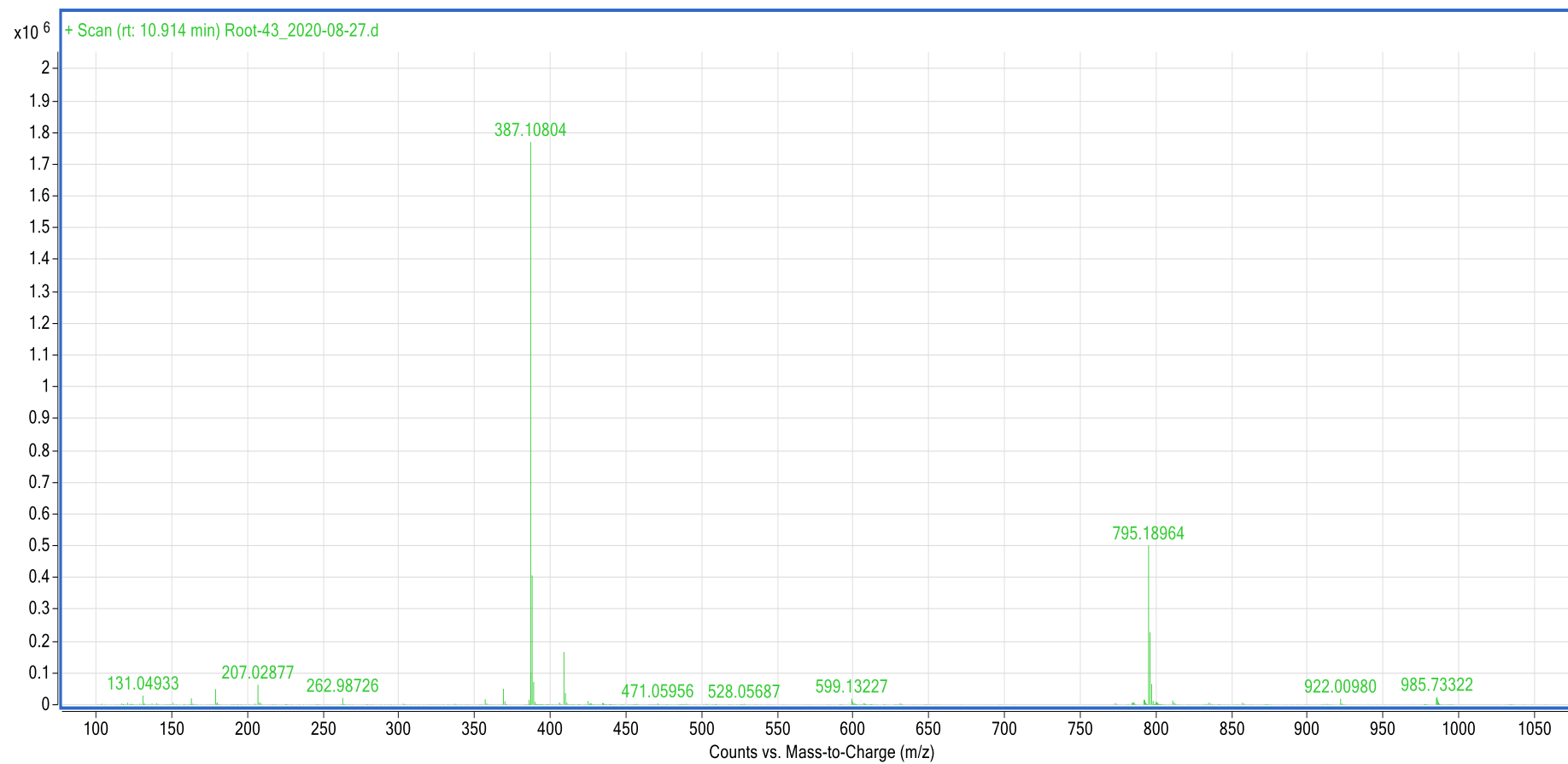
**Figure S6.** HMBC spectrum of the new compound **1a**



**Figure S7.** COSY spectrum of the new compound **1a**



**Figure S8.** NOESY spectrum of the new compound **1a**



**Figure S9.** HRESI-MS spectrum of the new compound **1b**

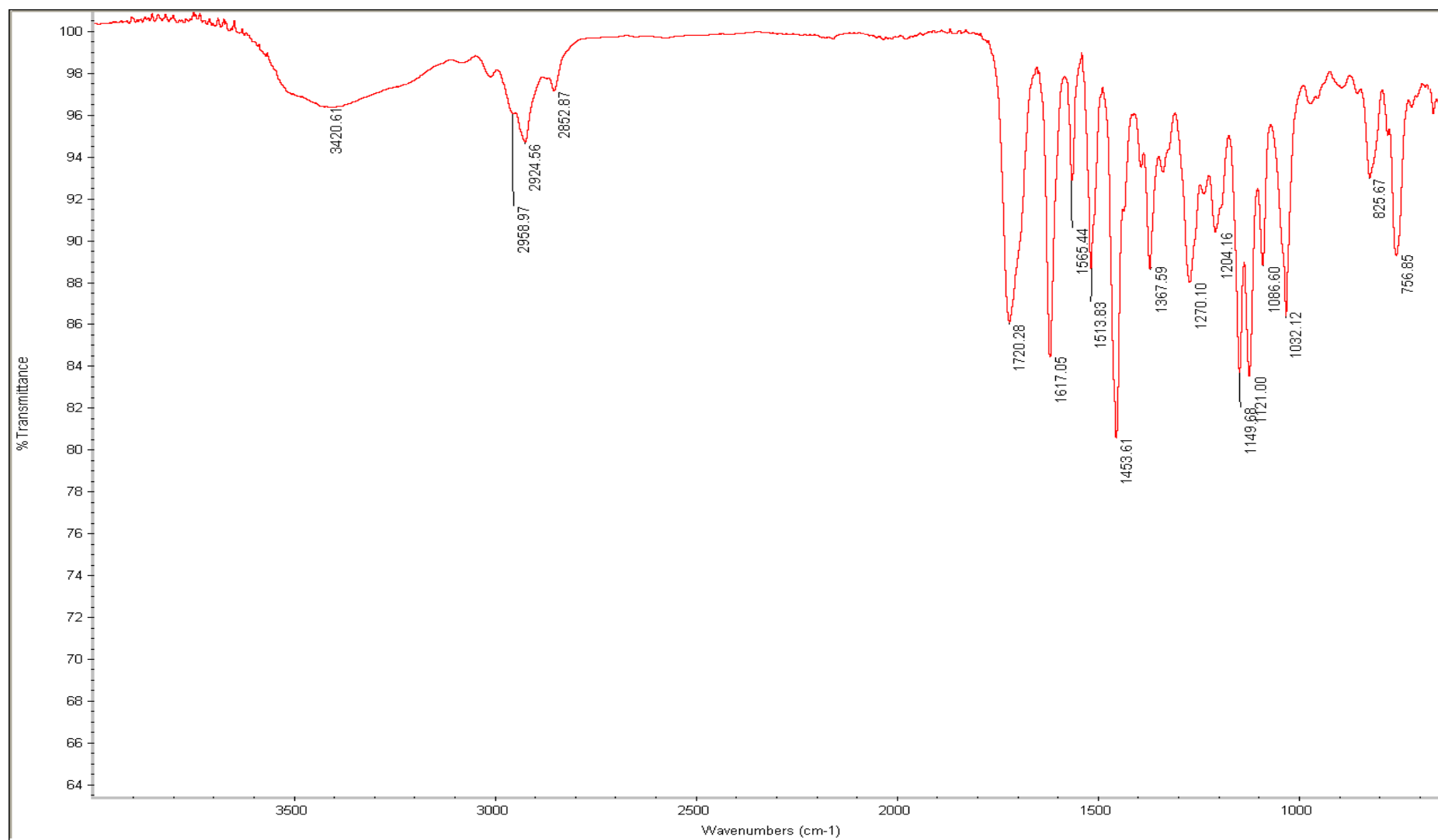


Figure S10. IR spectrum of the new compound **1b**

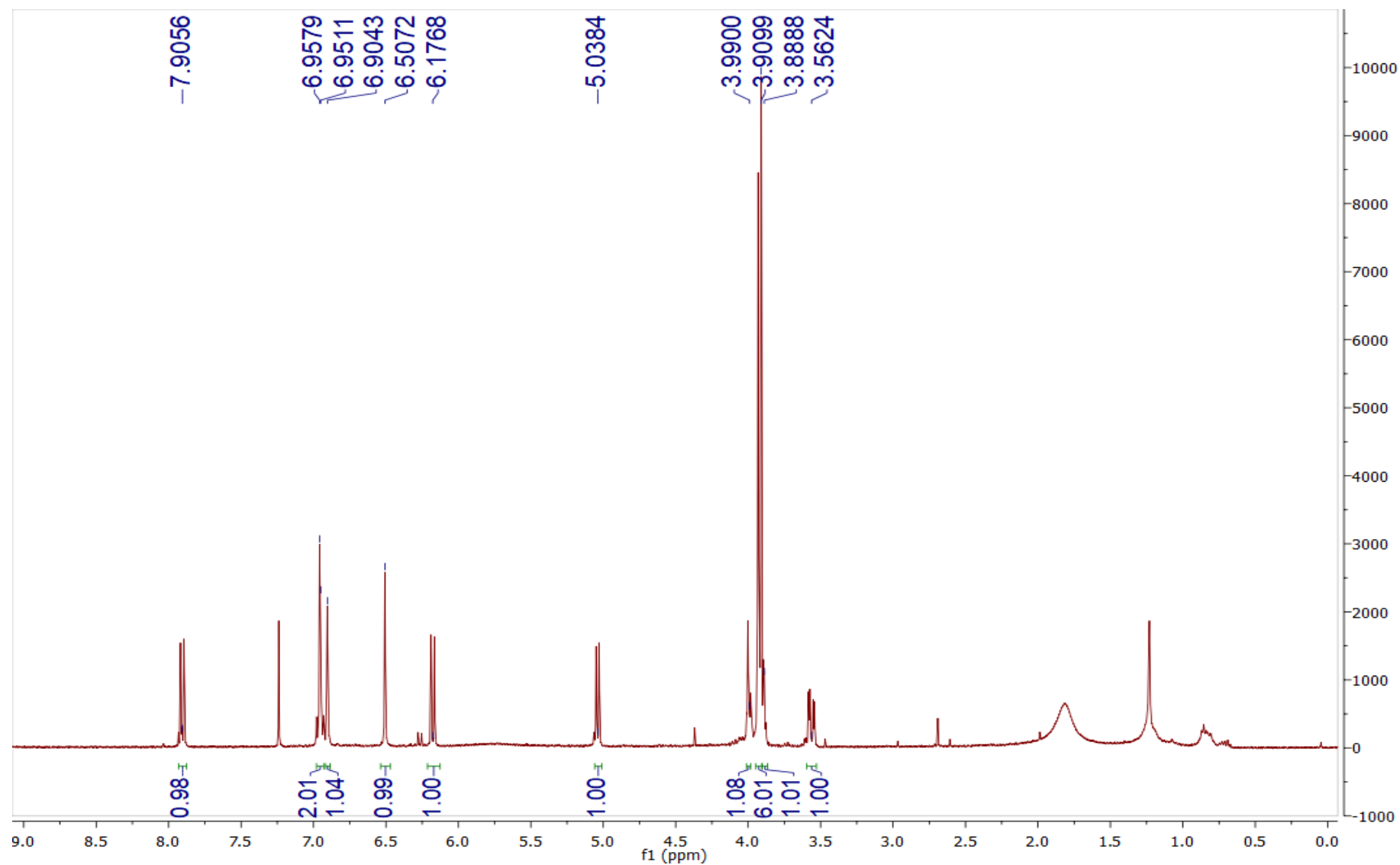


Figure S11.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectrum of the new compound **1b**



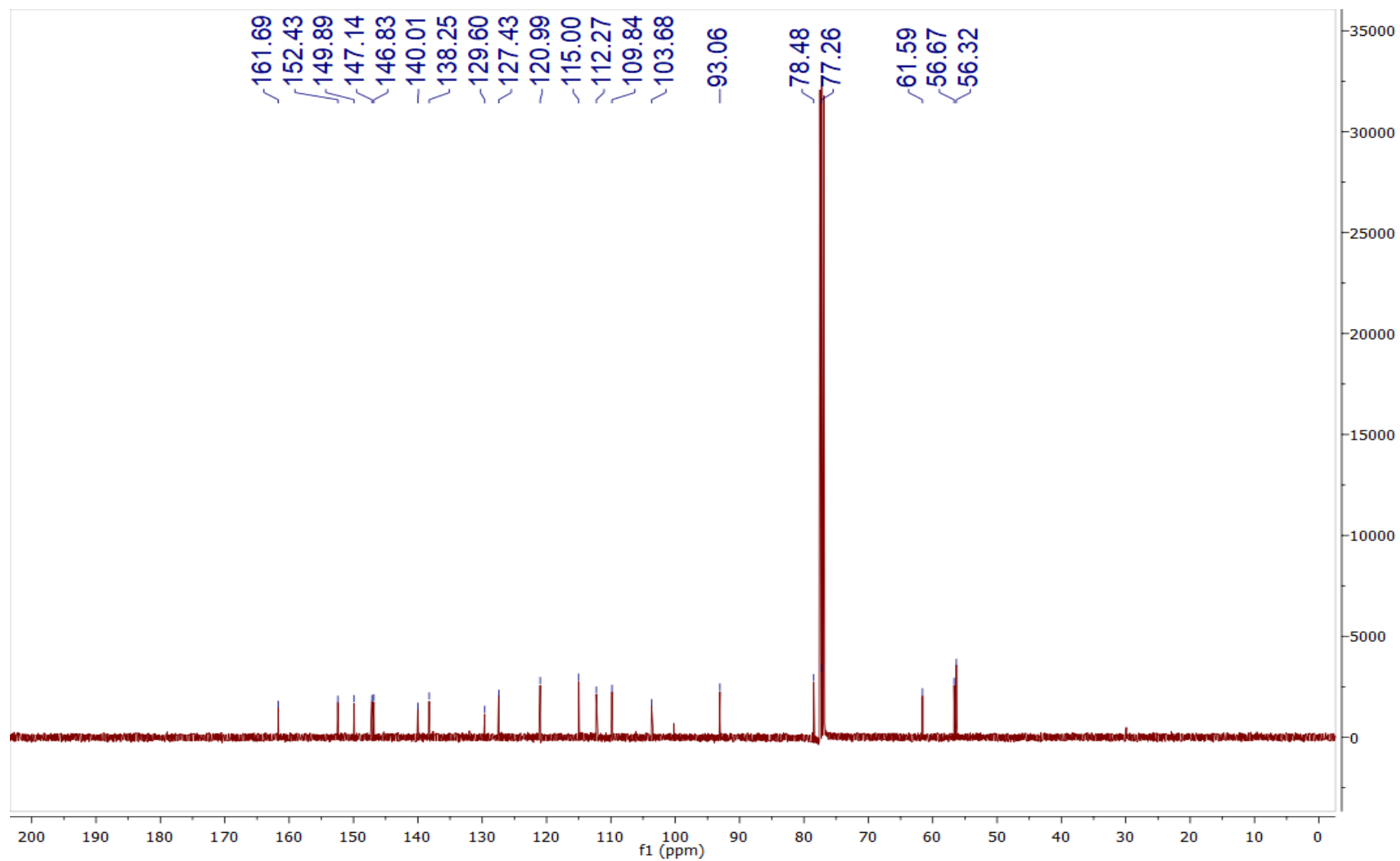


Figure S12. <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) spectrum of the new compound **1b**

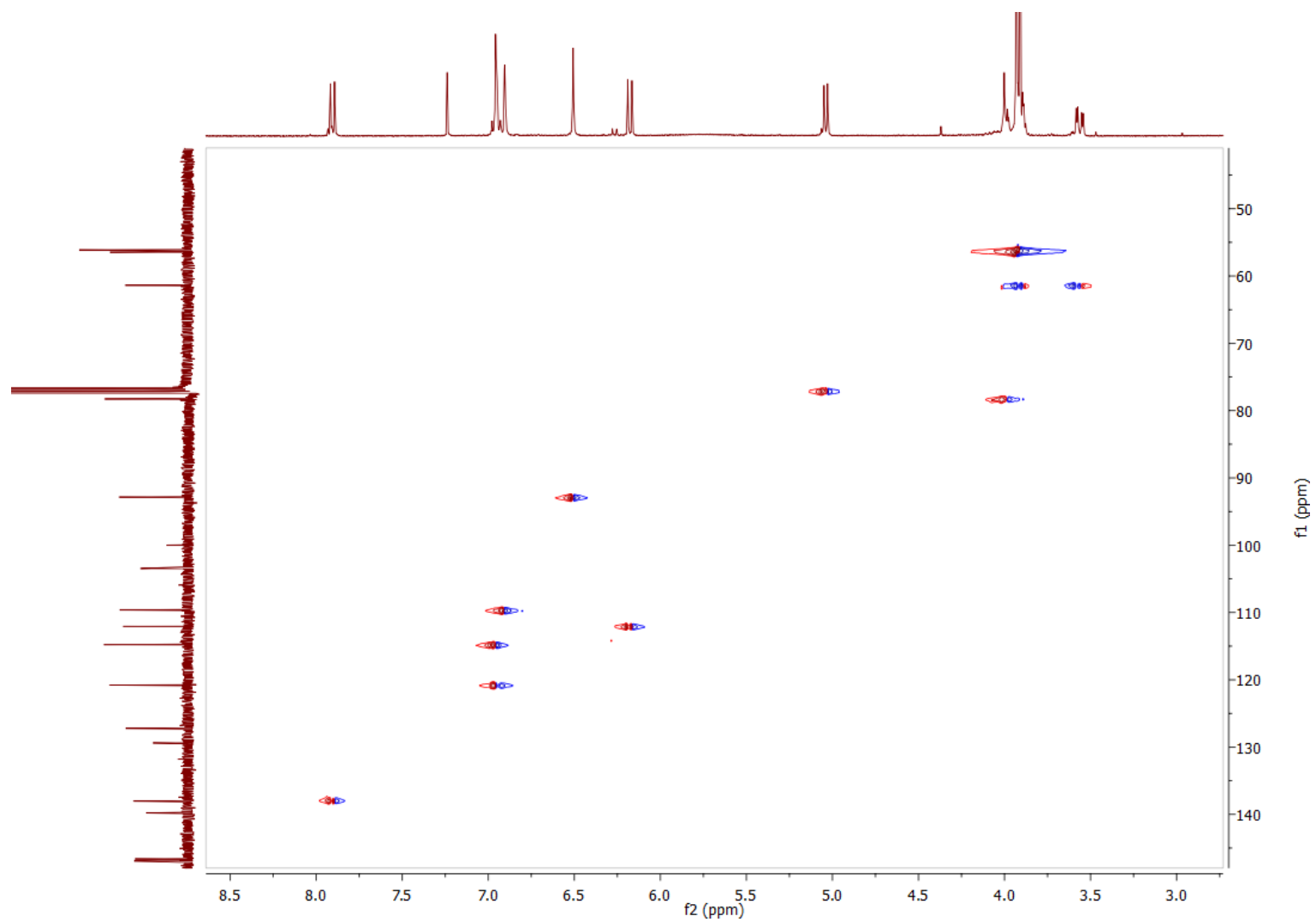


Figure S13. HSQC spectrum of the new compound **1b**

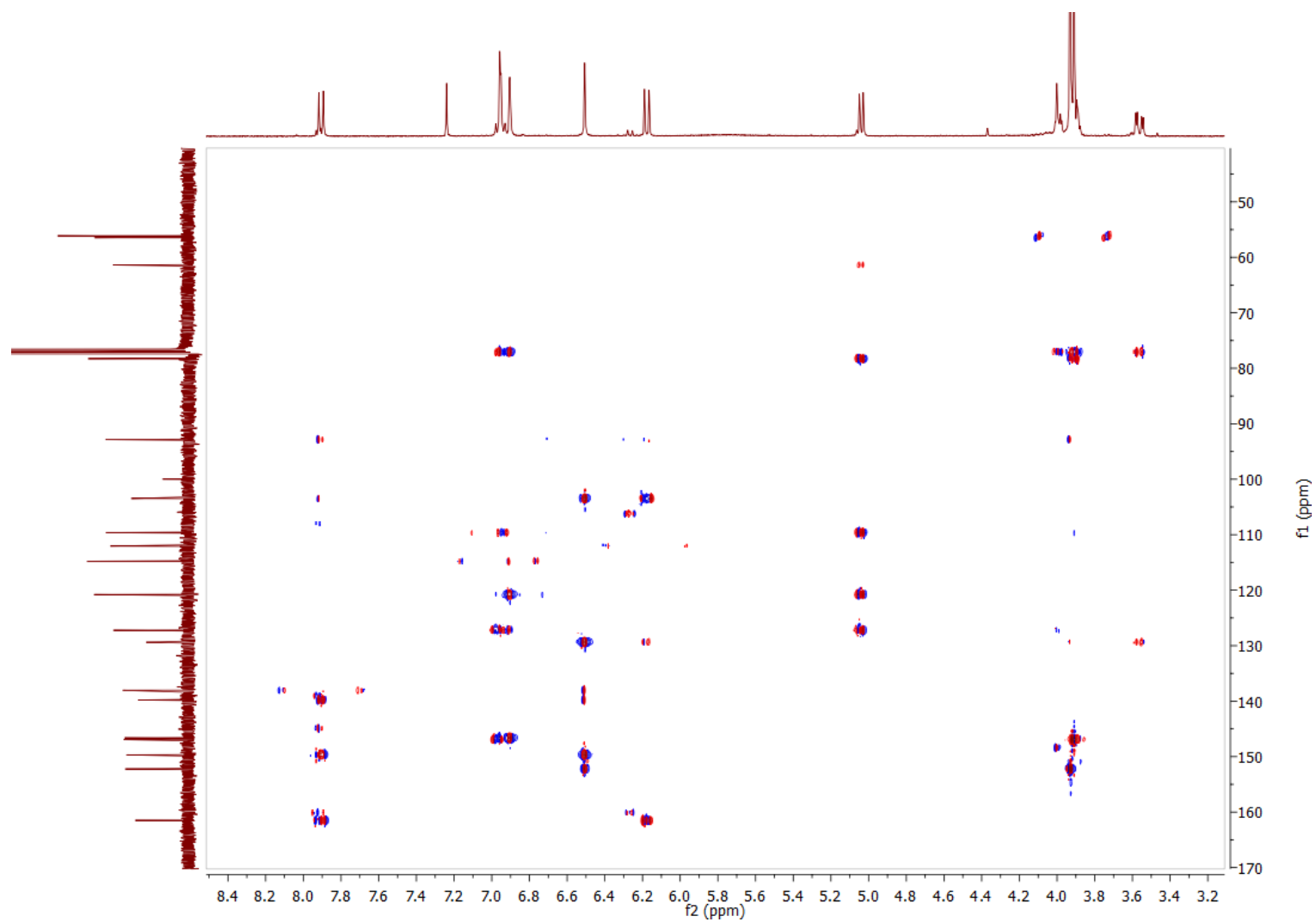
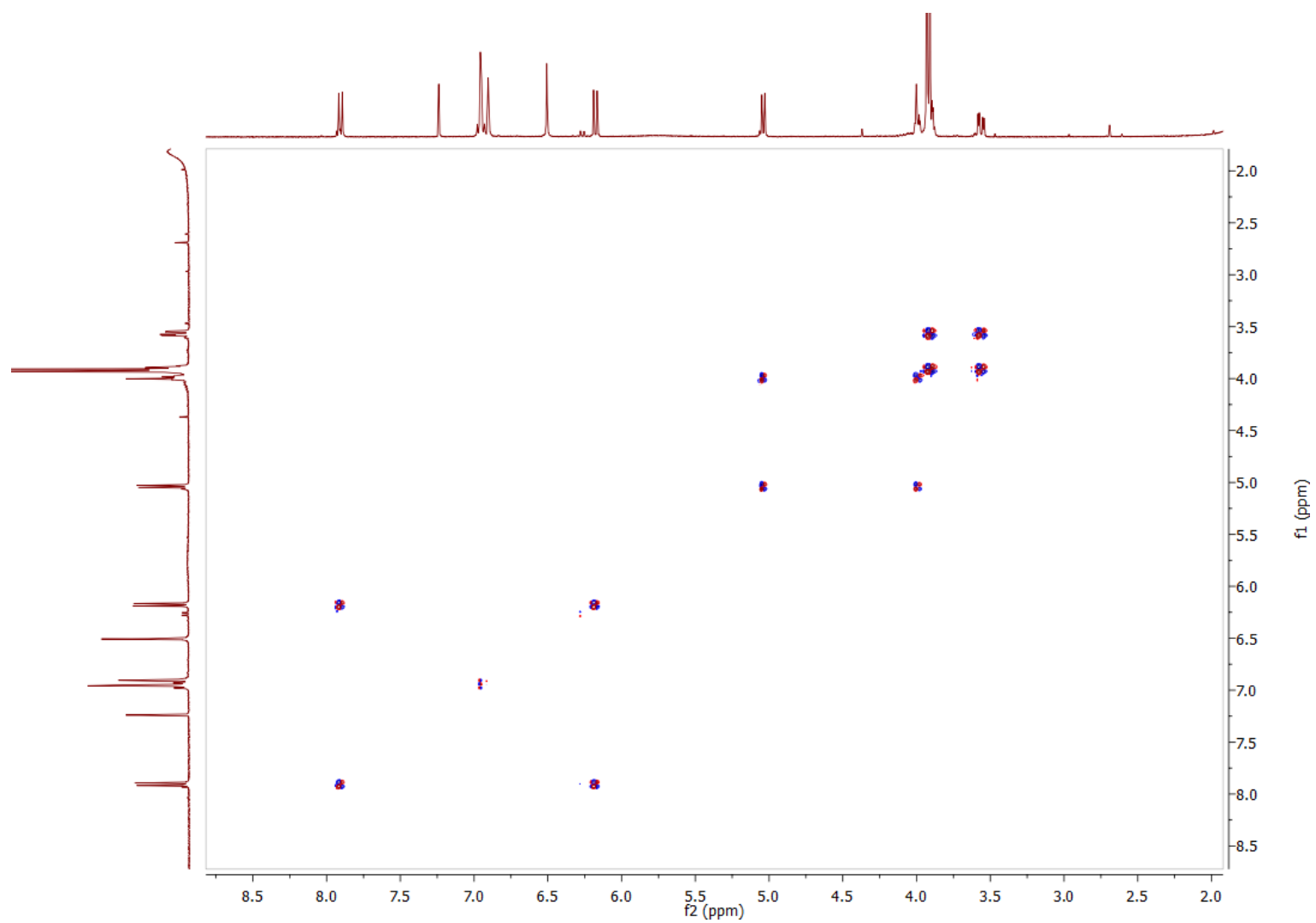


Figure S14. HMBC spectrum of the new compound **1b**



**Figure S15.** COSY spectrum of the new compound **1b**

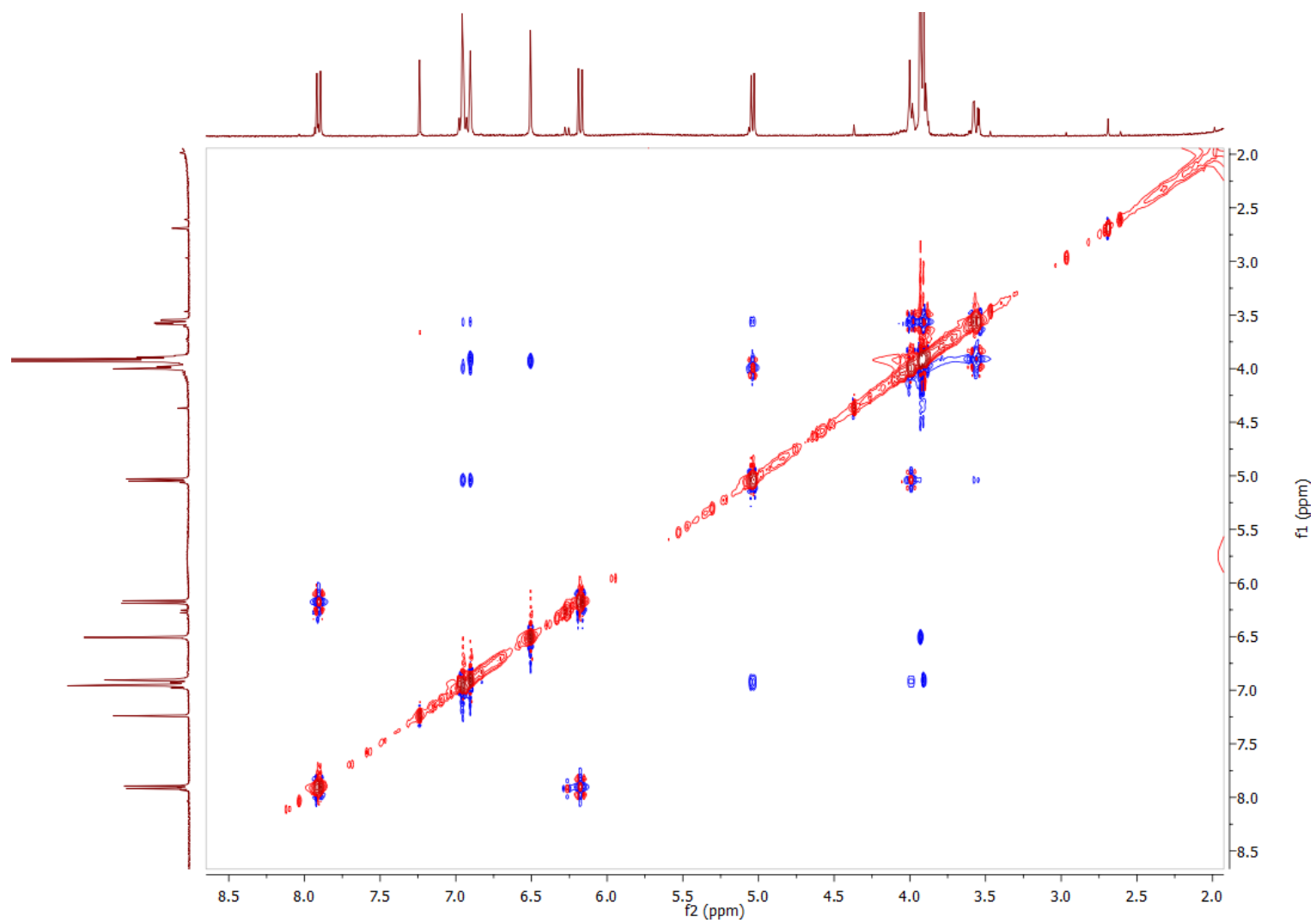
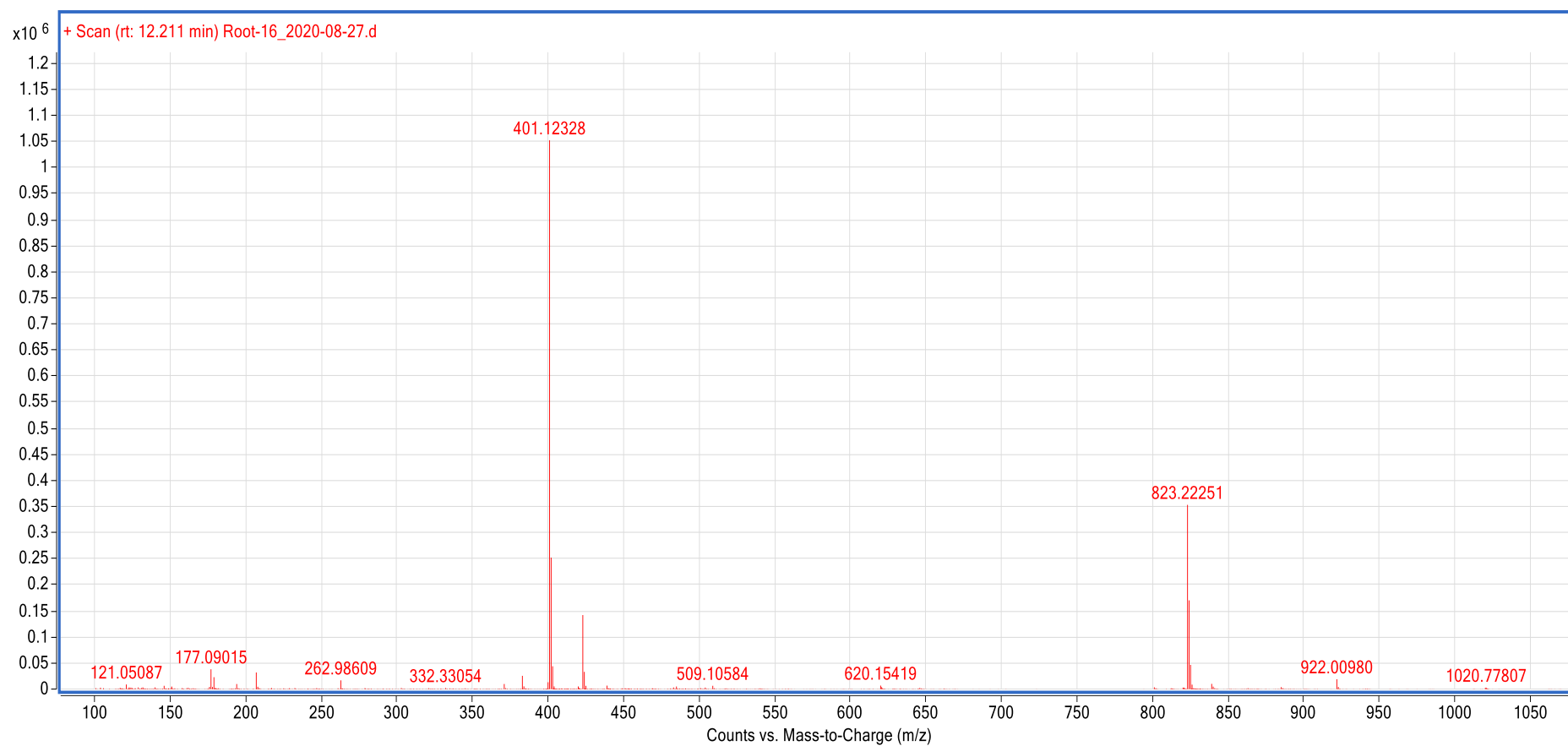
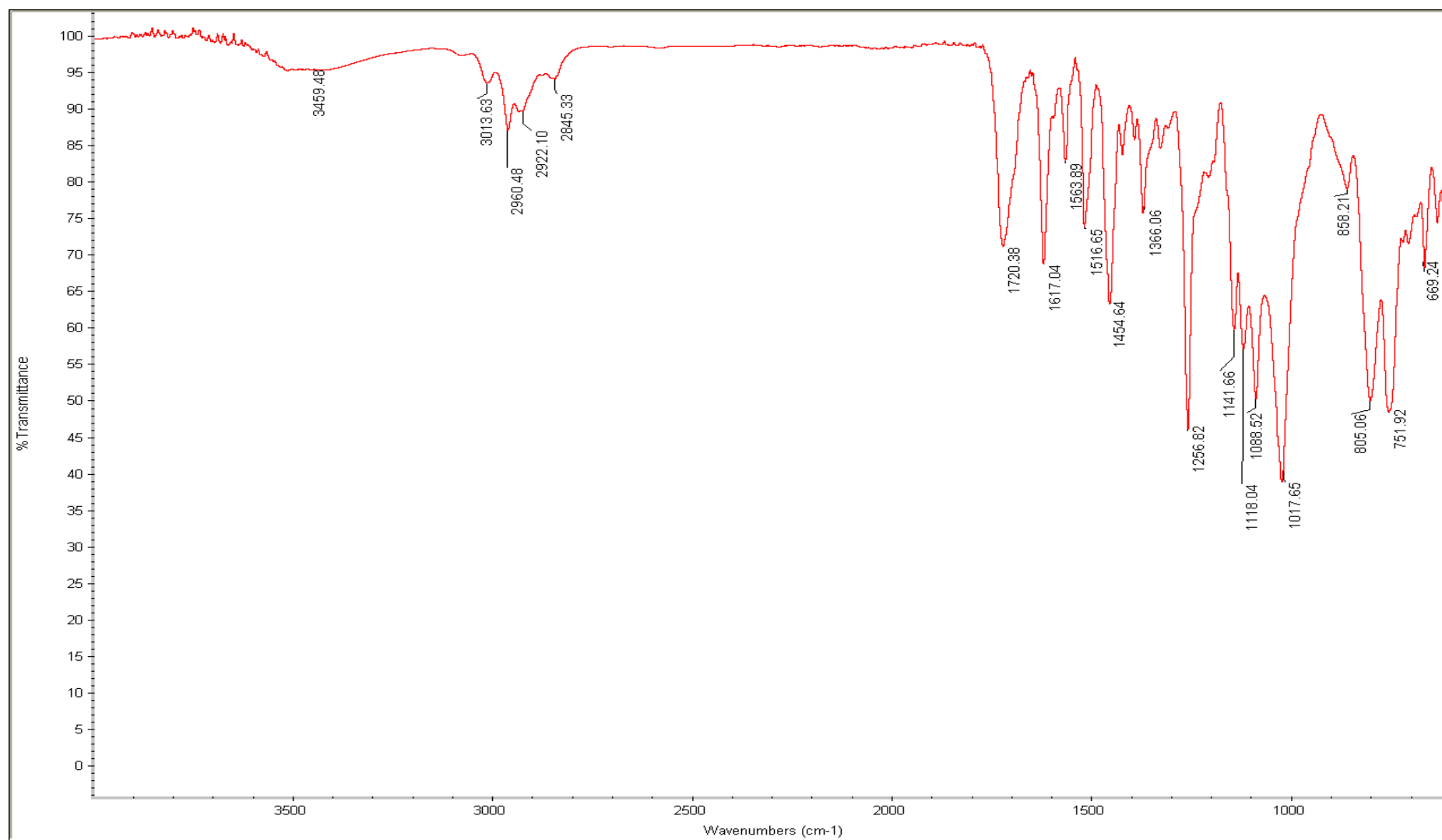


Figure S16. NOESY spectrum of the new compound **1b**



**Figure S17.** HRESI-MS spectrum of the new compound **2**



**Figure S18.** IR spectrum of the new compound **2**

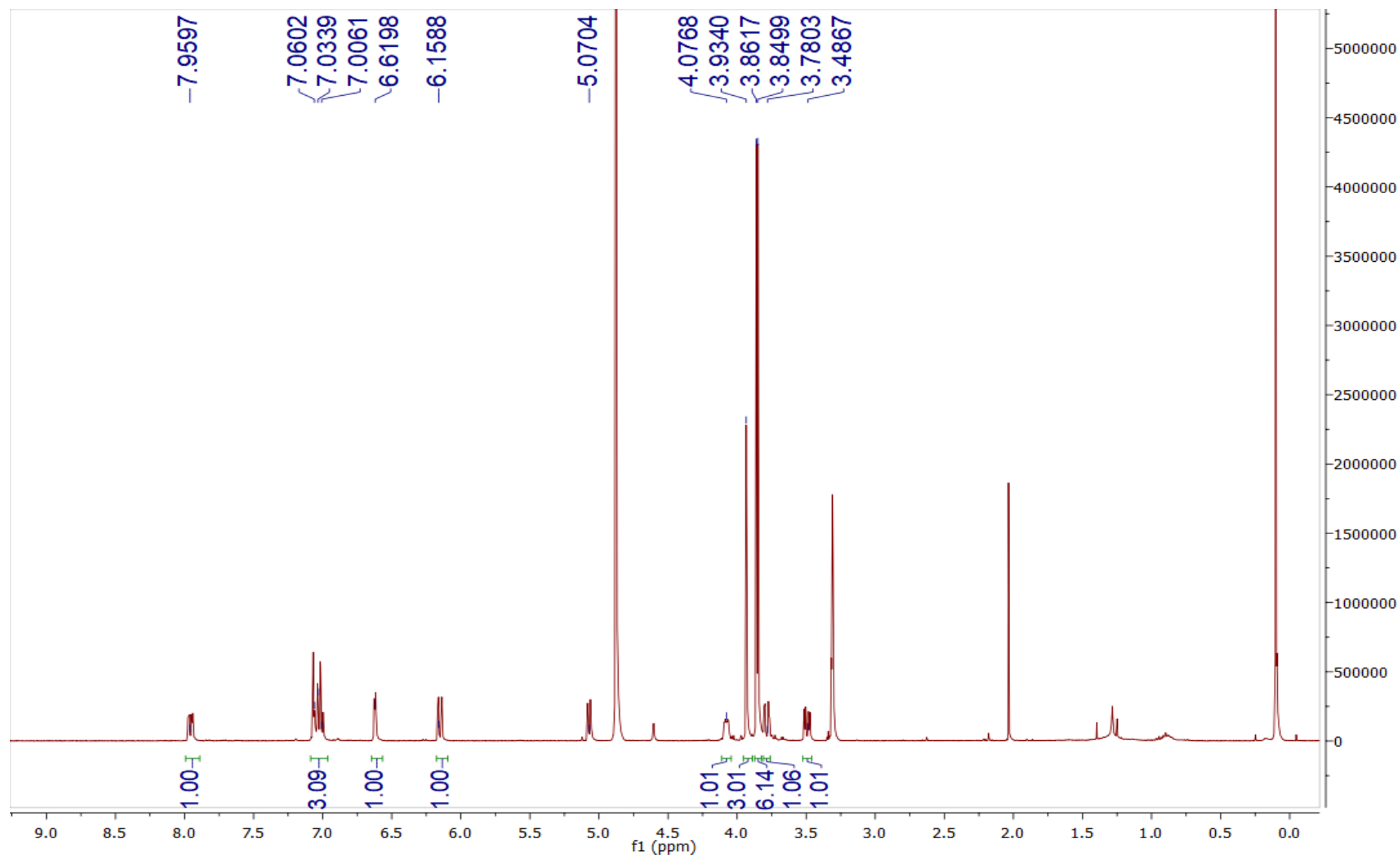


Figure S19. <sup>1</sup>H NMR (400 MHz, MeOD) spectrum of the new compound **2**



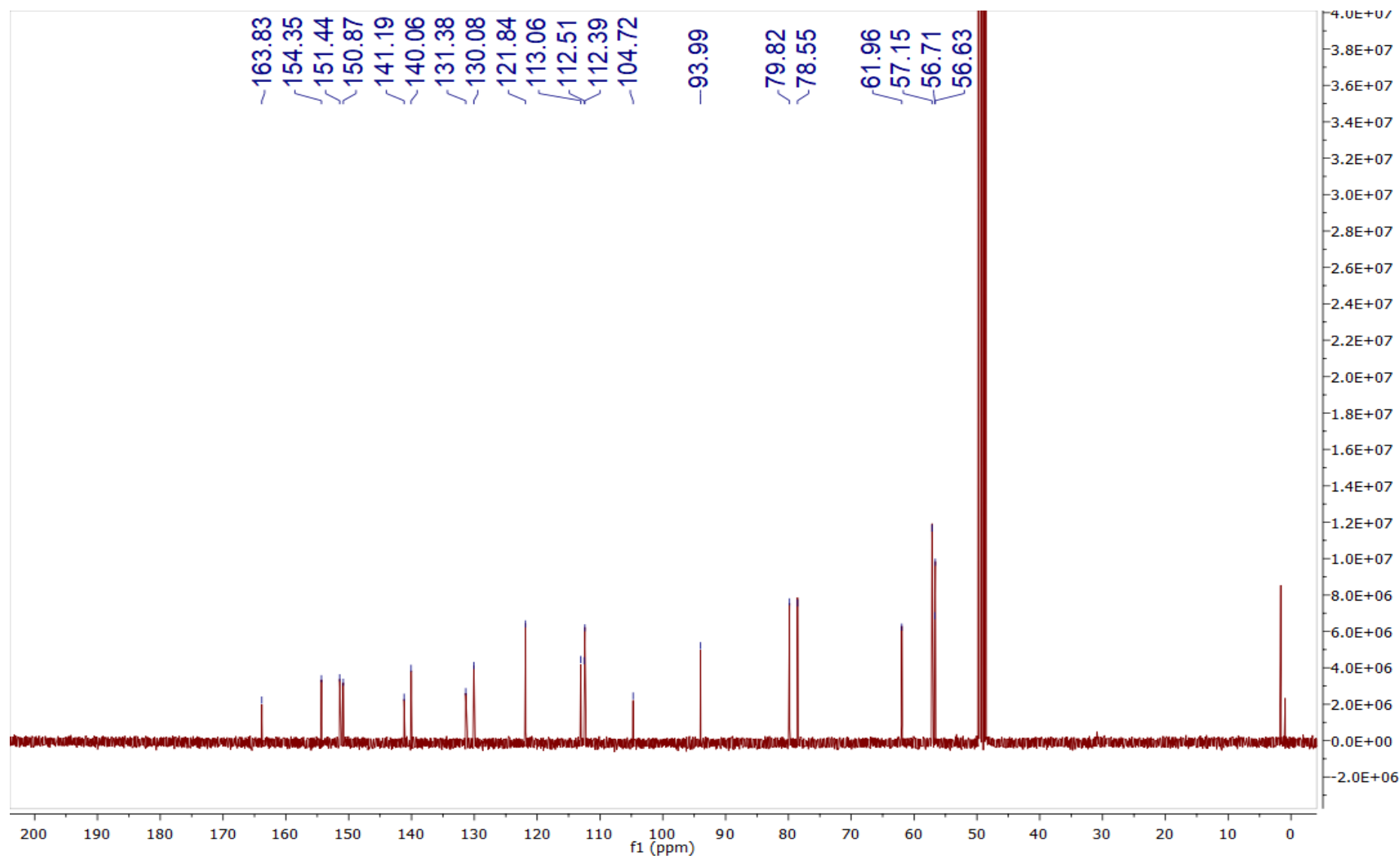


Figure S20.  $^{13}\text{C}$  NMR (100 MHz, MeOD) spectrum of the new compound **2**

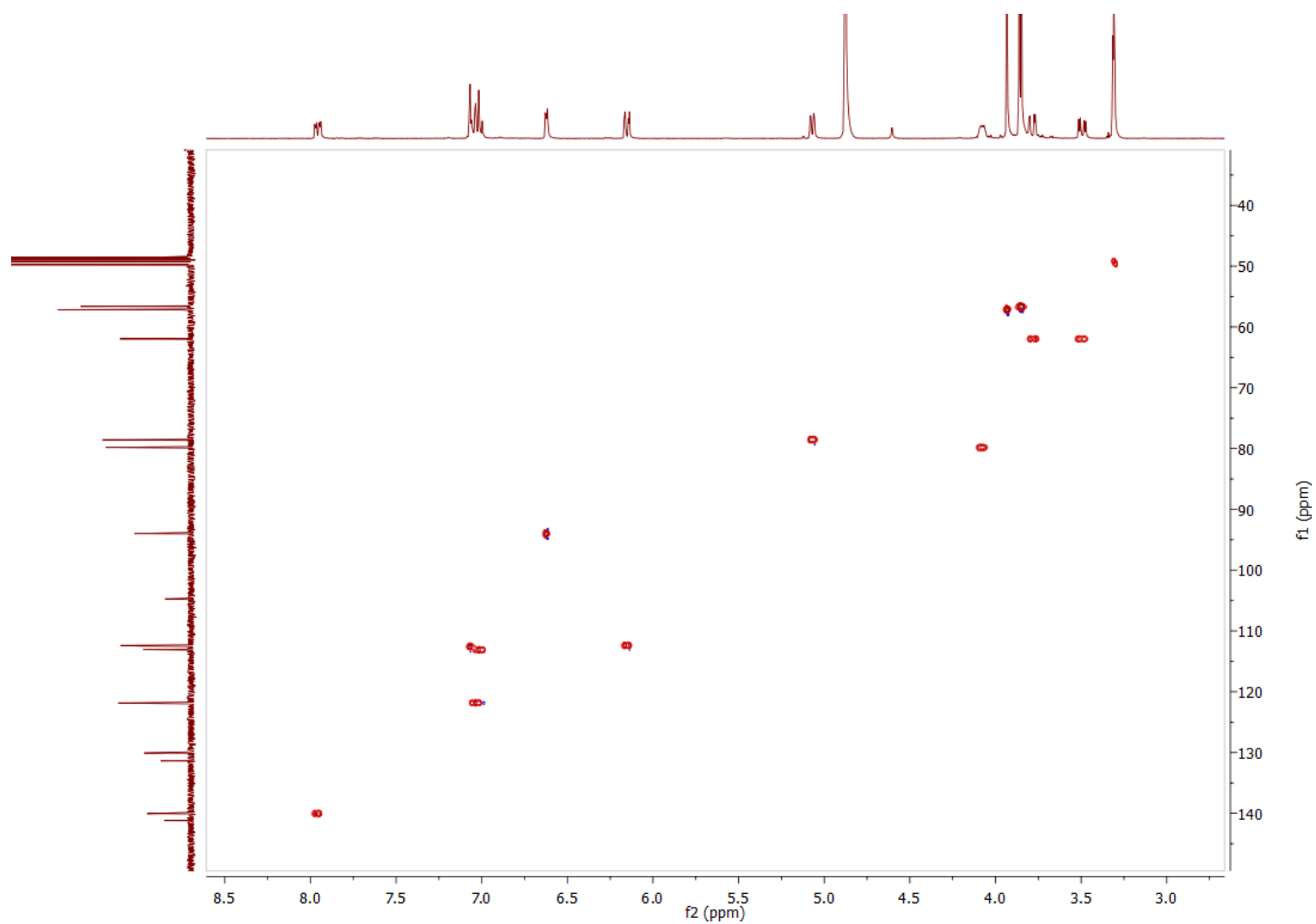
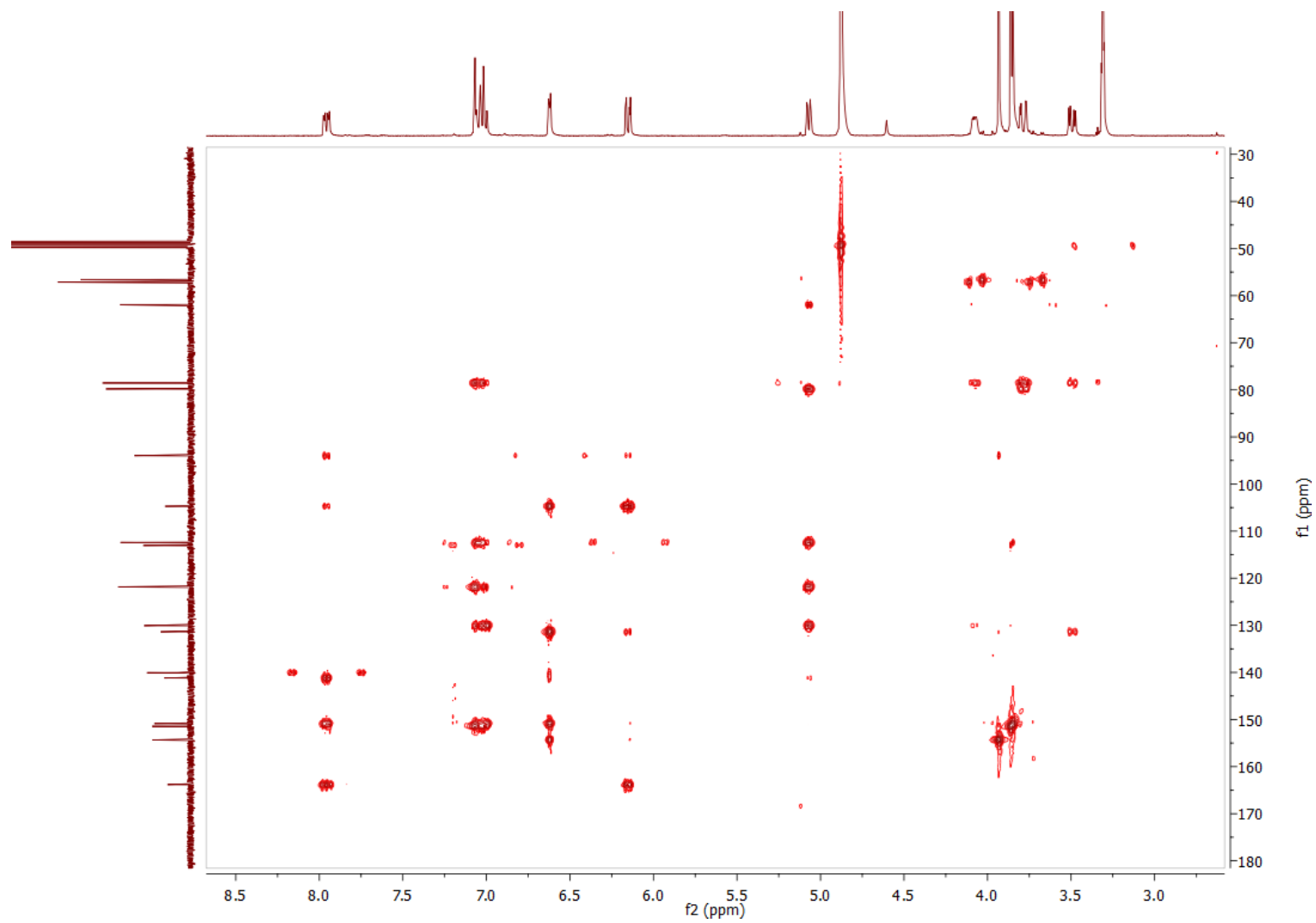
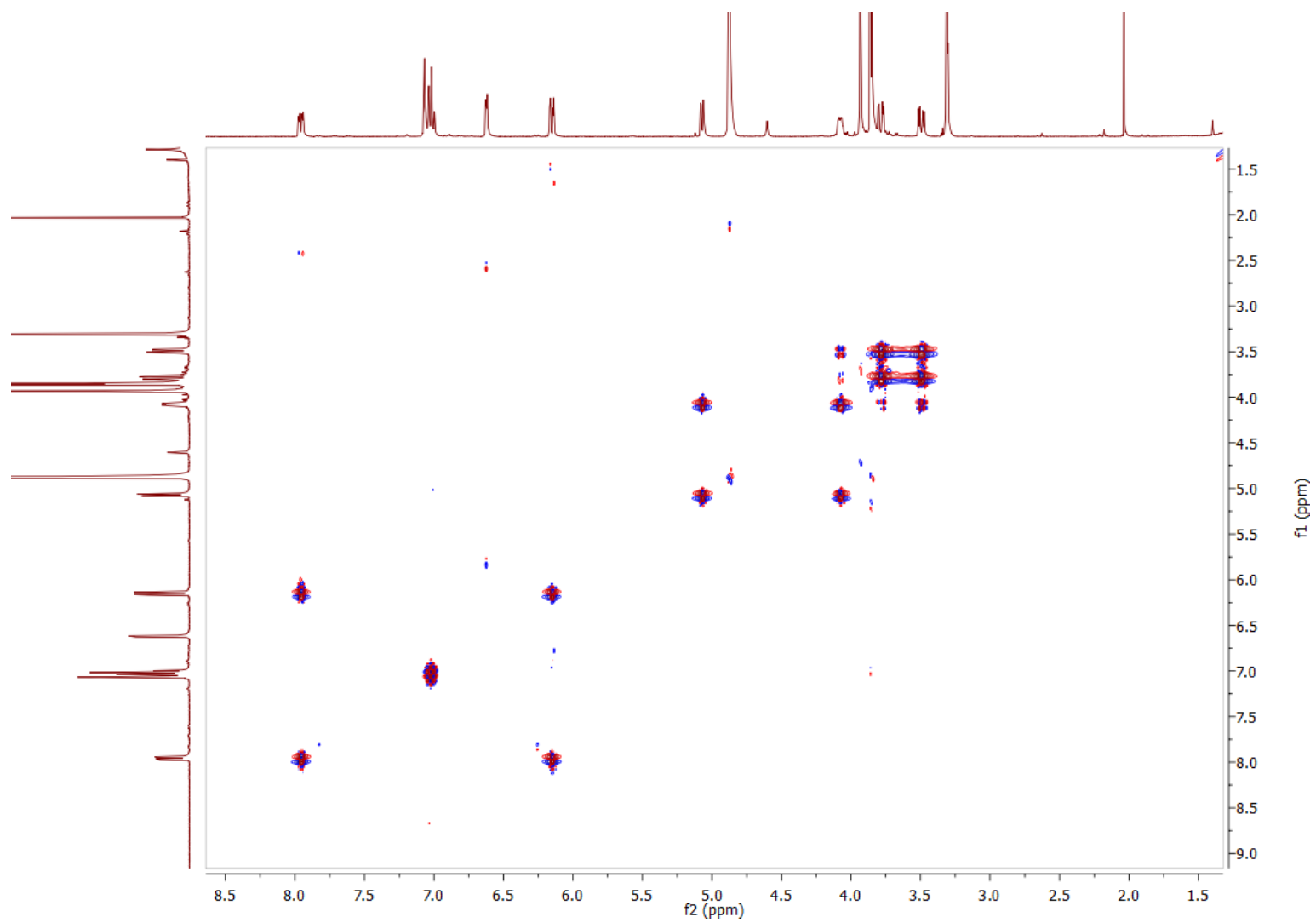


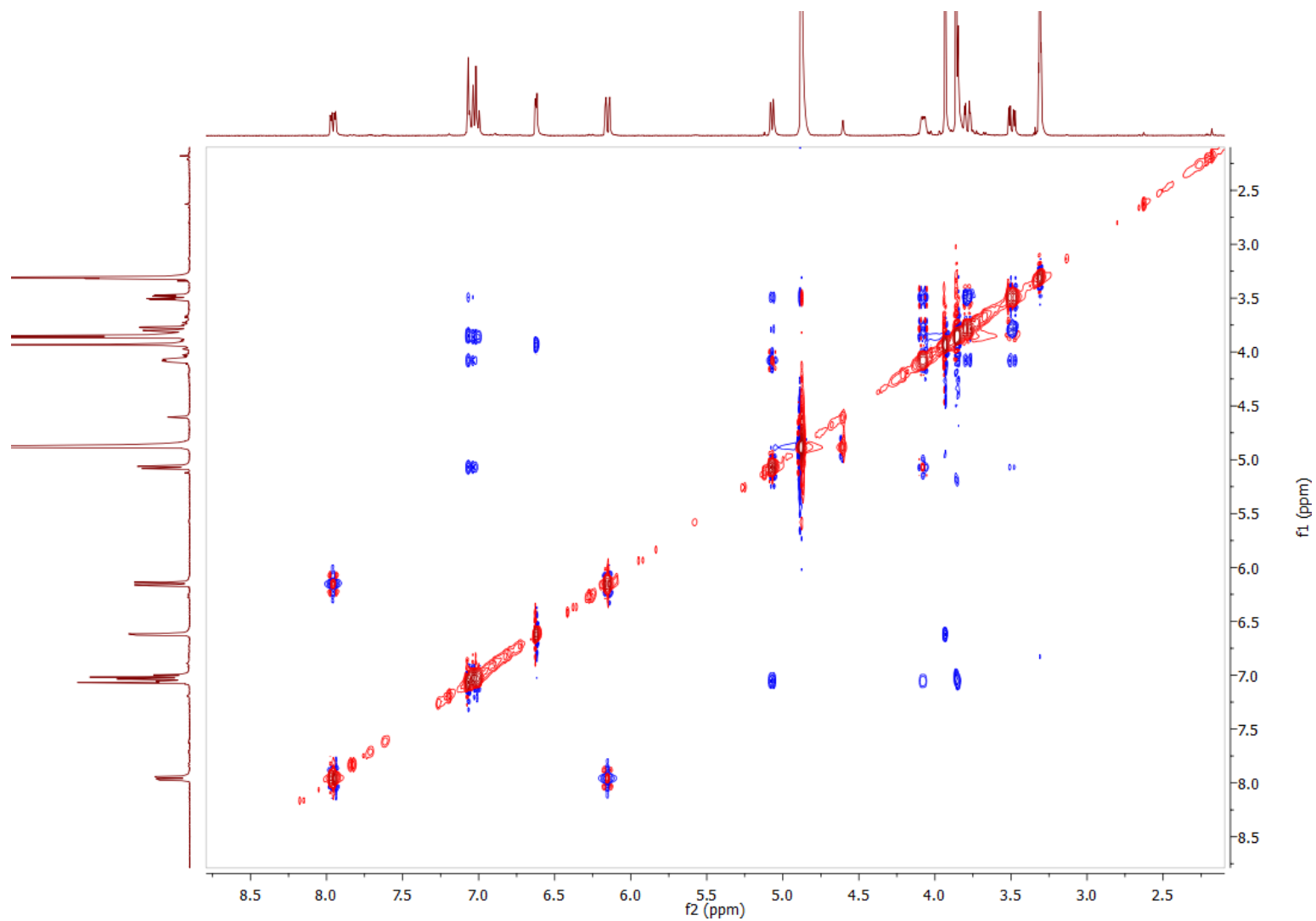
Figure S21. HSQC spectrum of the new compound **2**



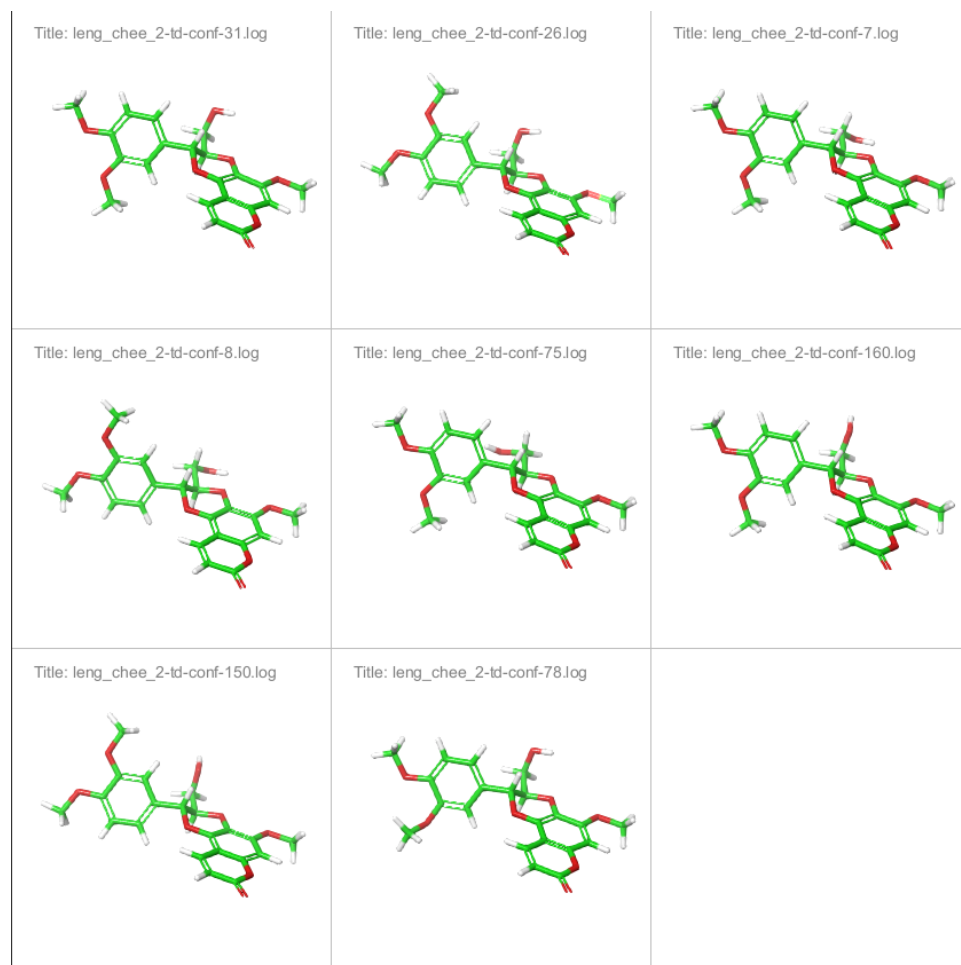
**Figure S22.** HMBC spectrum of the new compound **2**



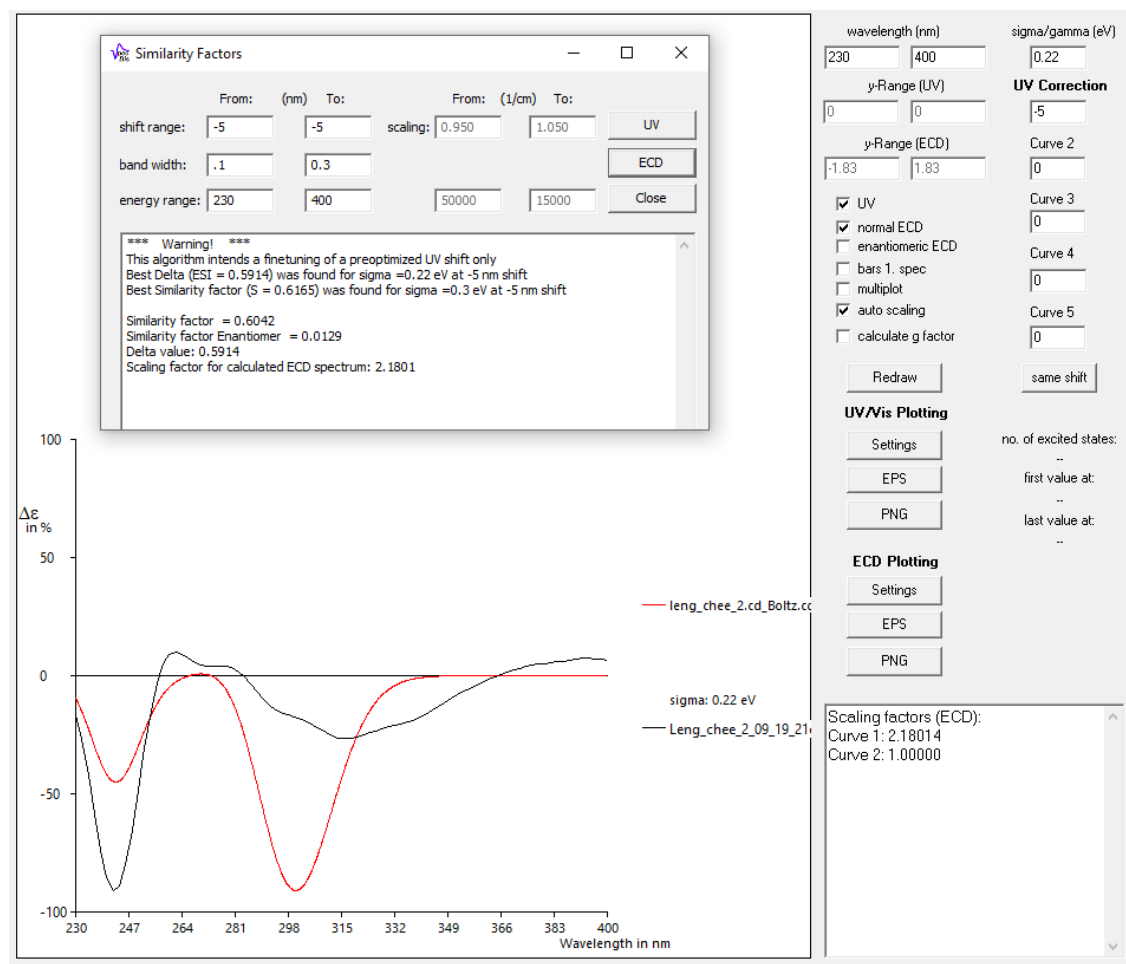
**Figure S23.** COSY spectrum of the new compound **2**



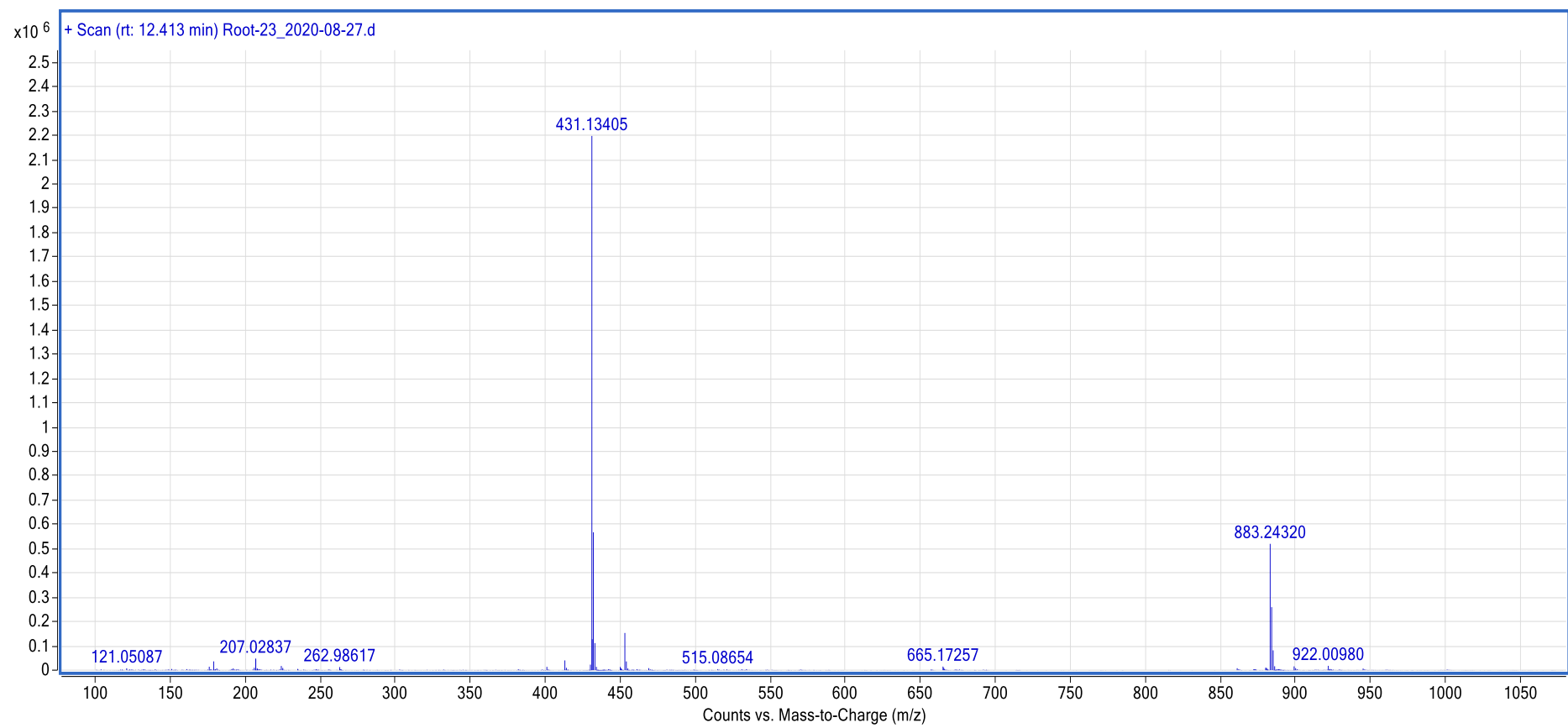
**Figure S24.** NOESY spectrum of the new compound **2**



**Figure S25.** Images of conformers (>1%) for the new compound **2**

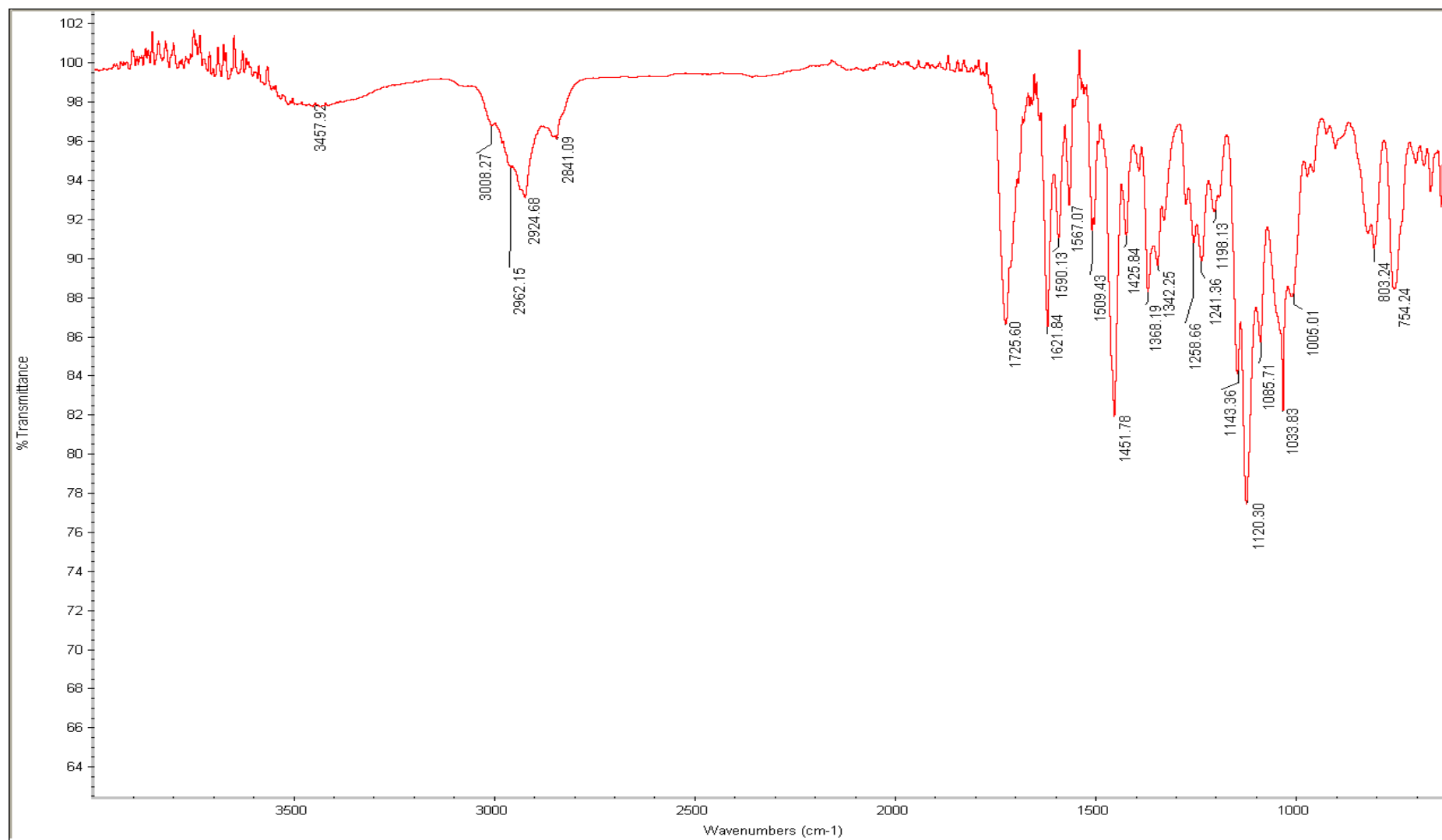


**Figure S26.** CD spectrum (experimental to calculated comparison by SpecDis) of the new compound **2**

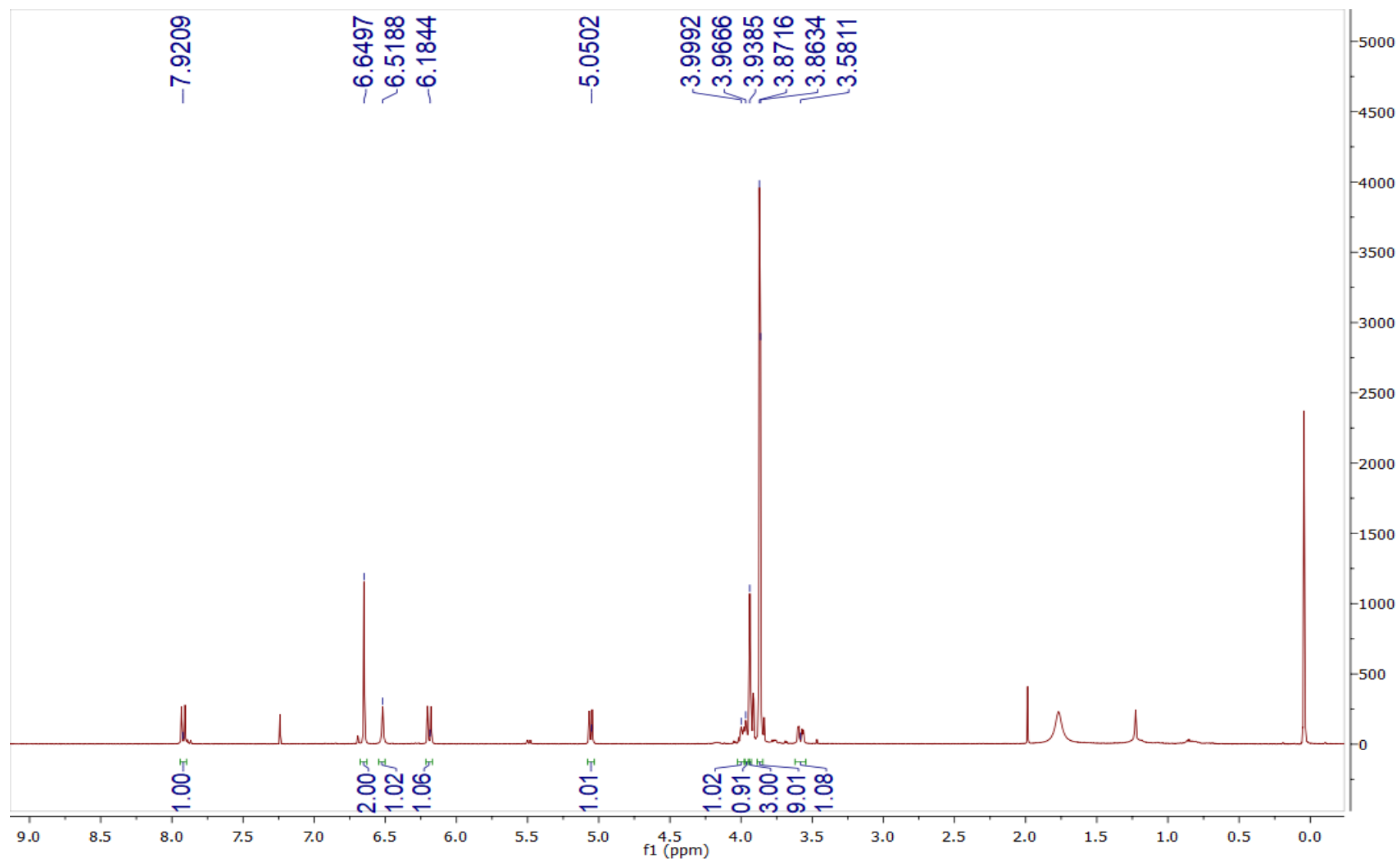


**Figure S27.** HRESI-MS spectrum of the new compound **3**





**Figure S28.** IR spectrum of the new compound **3**



**Figure S29.**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectrum of the new compound **3**

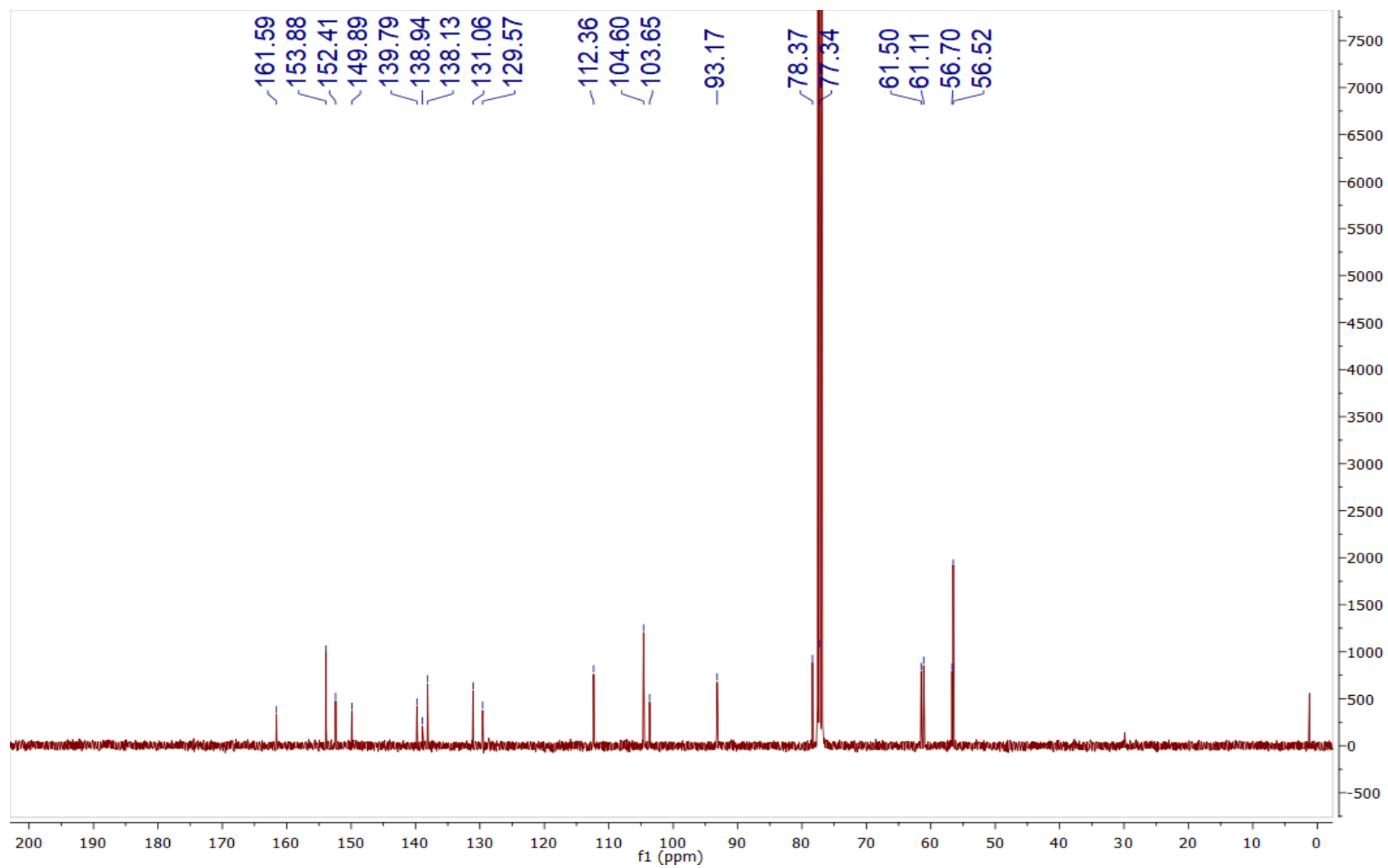


Figure S30. <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) spectrum of the new compound **3**

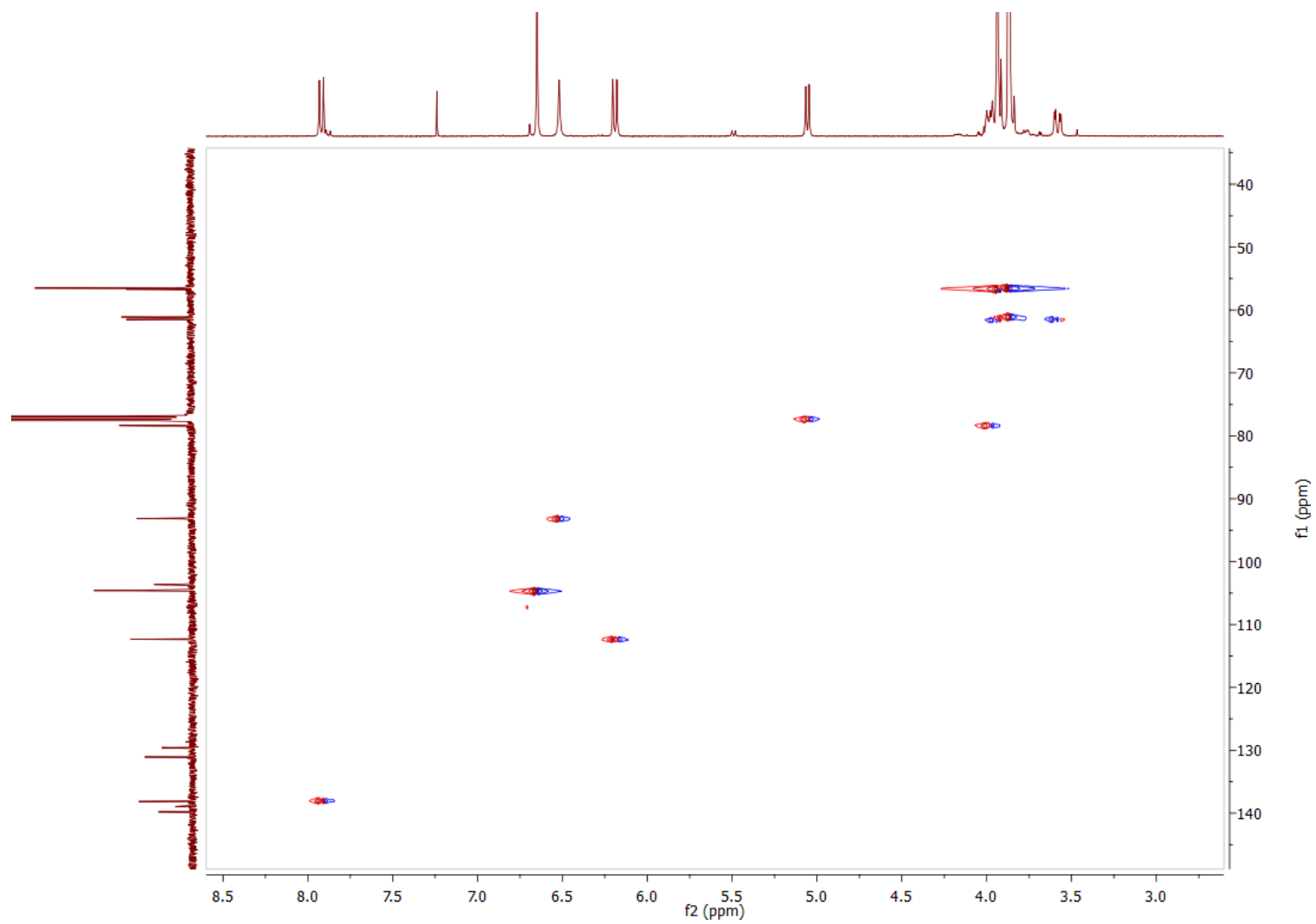
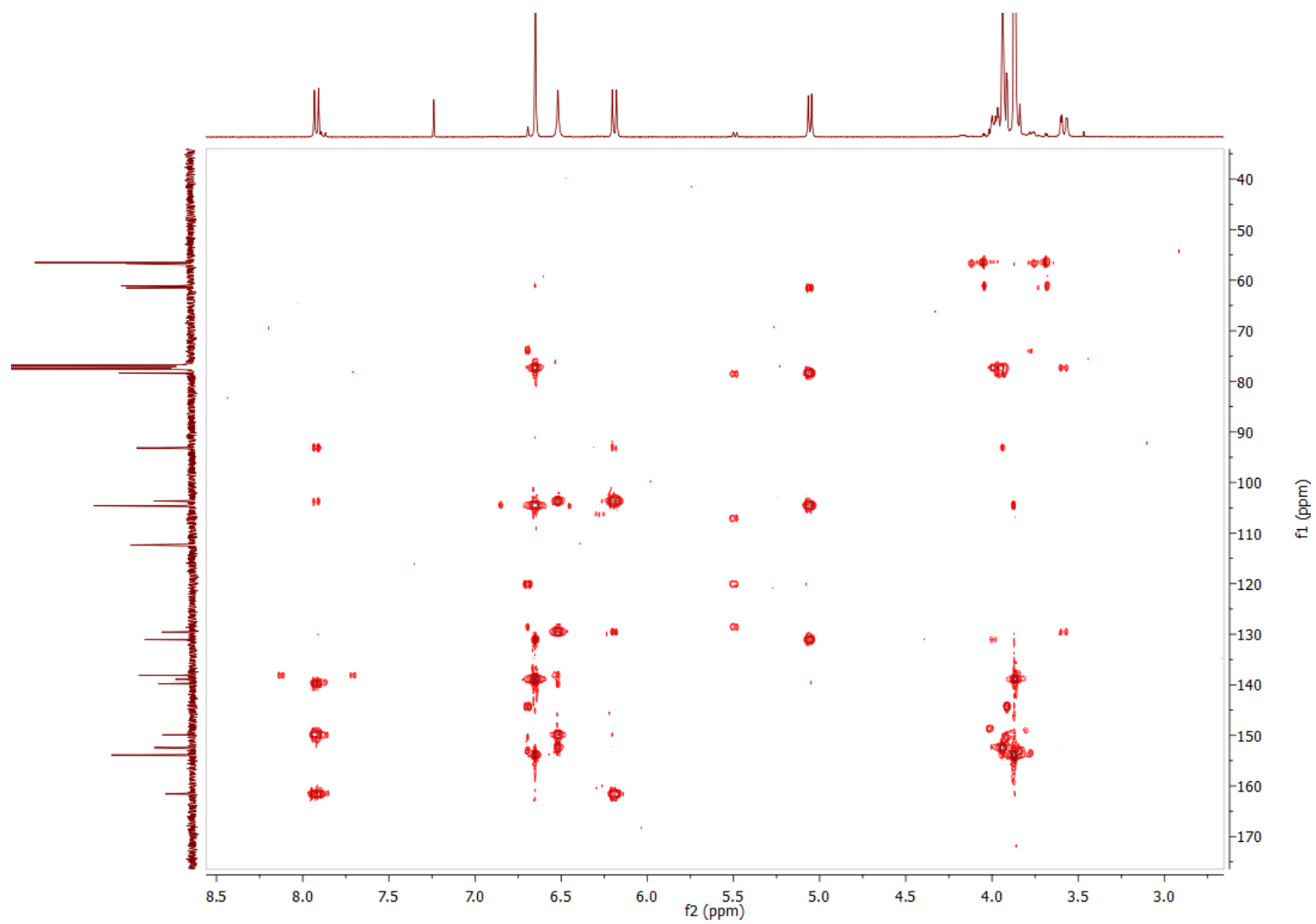
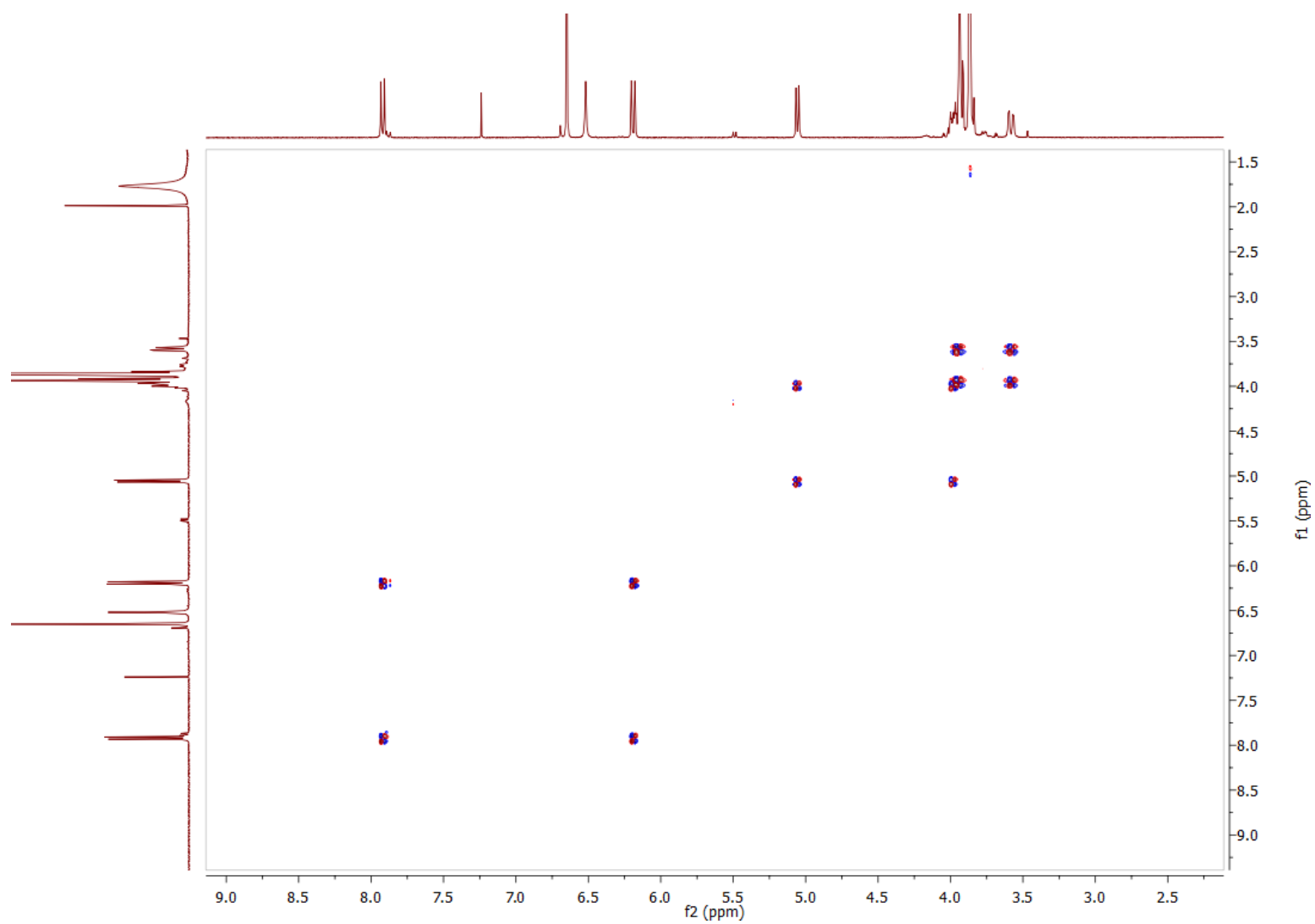


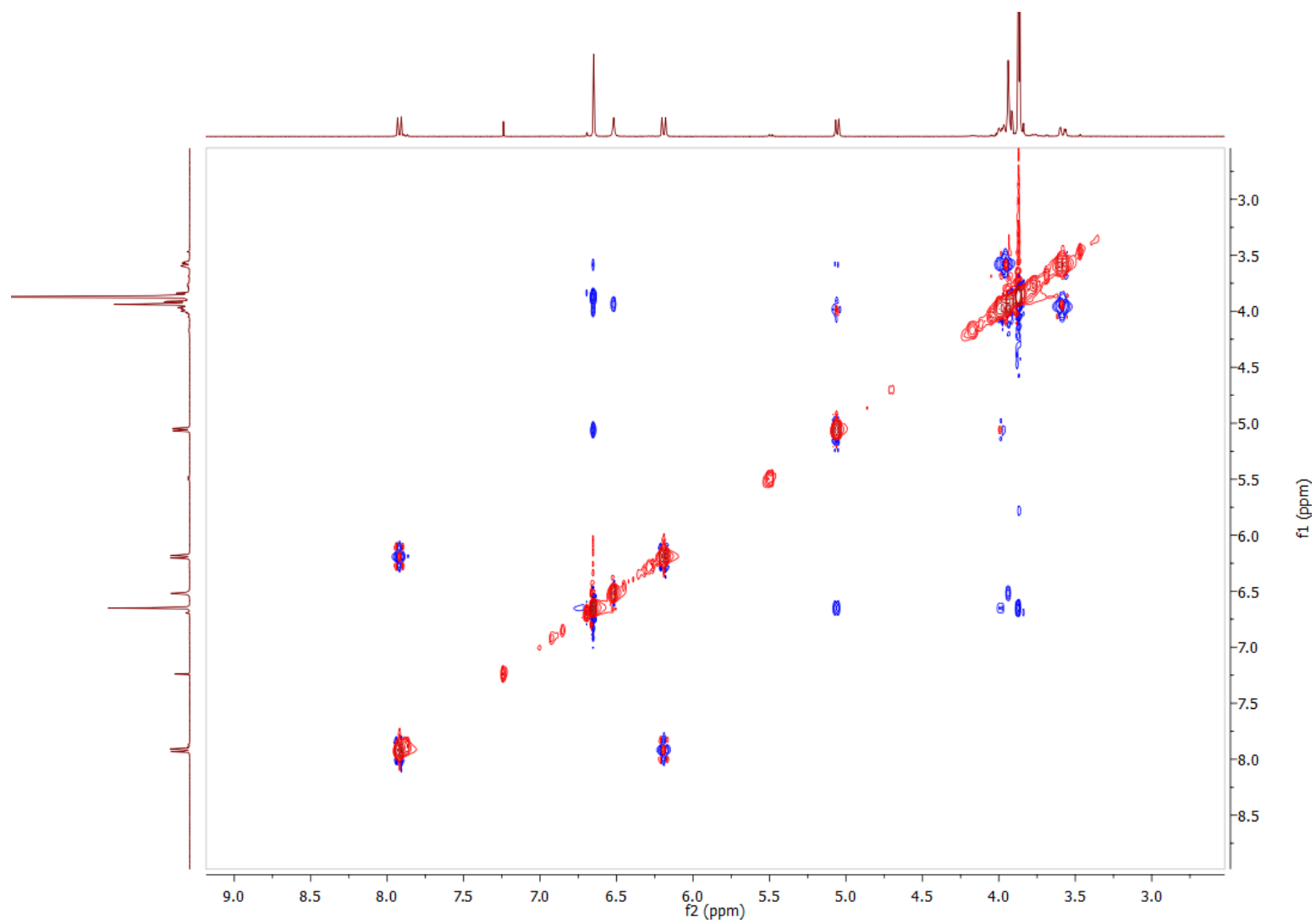
Figure S31. HSQC spectrum of the new compound **3**



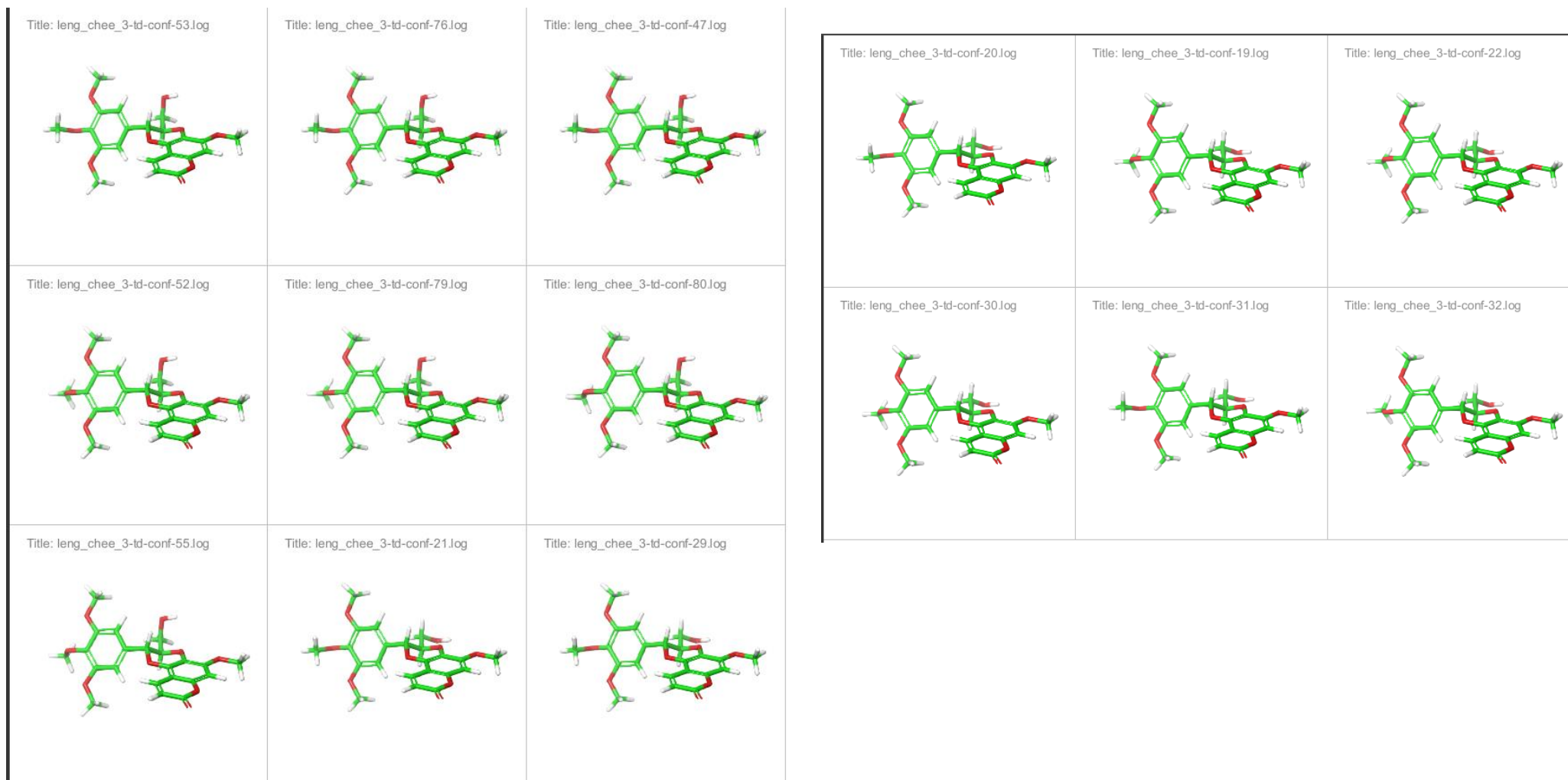
**Figure S32.** HMBC spectrum of the new compound **3**



**Figure S33.** COSY spectrum of the new compound **3**

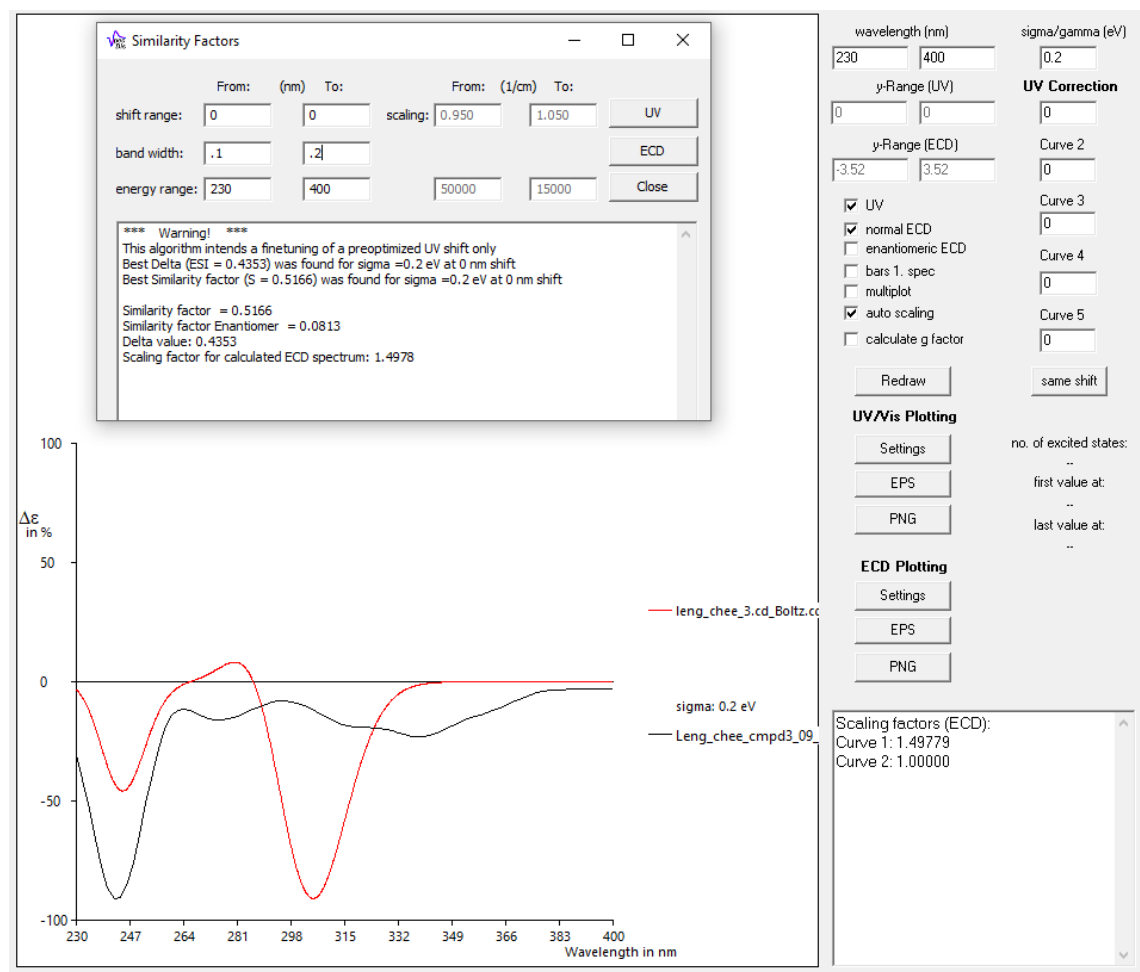


**Figure S34.** NOESY spectrum of the new compound **3**

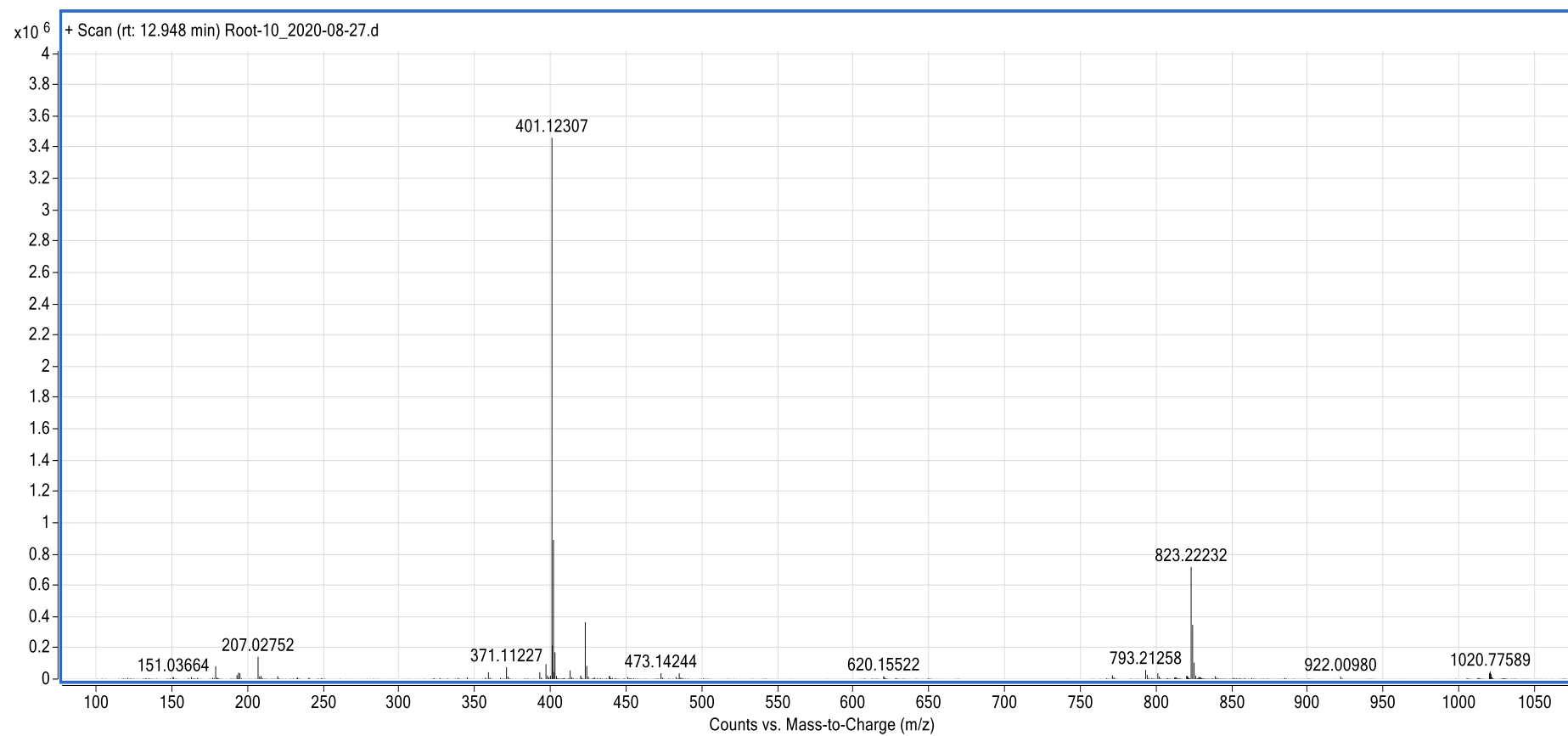


**Figure S35.** Images of Conformers (>1%) for the new compound **3**

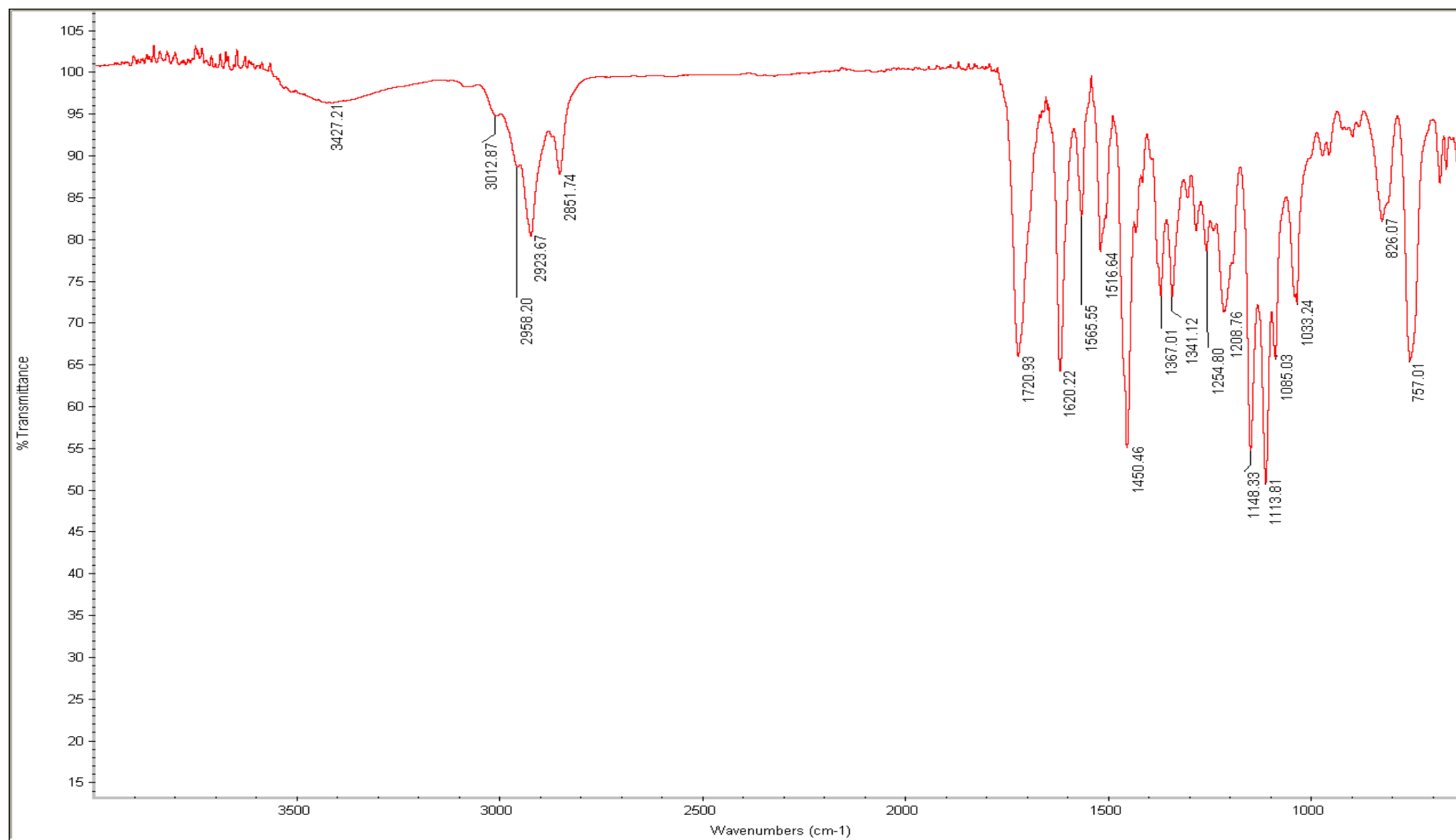




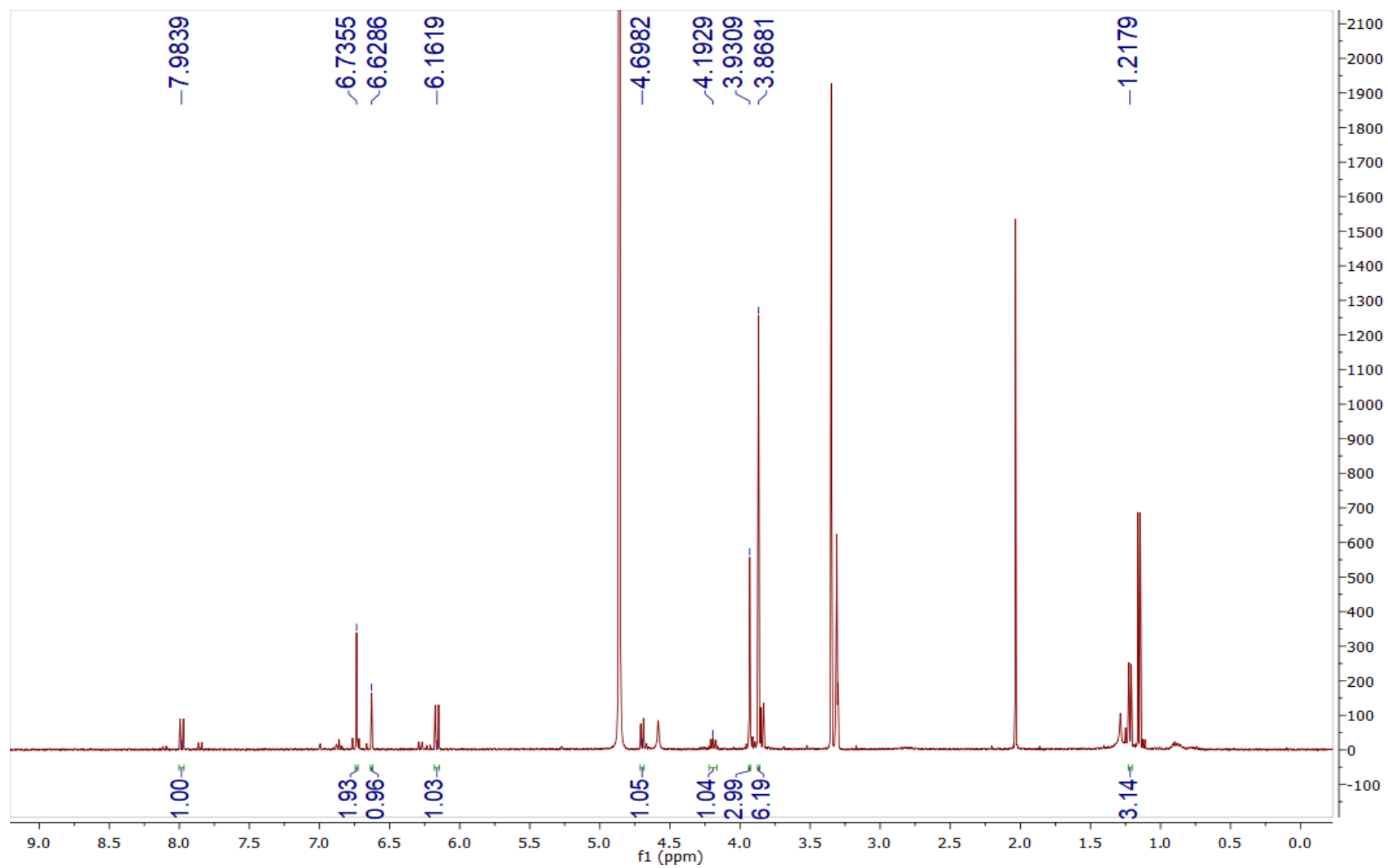
**Figure S36.** CD spectrum (experimental to calculated comparison by SpecDis) of the new compound **3**



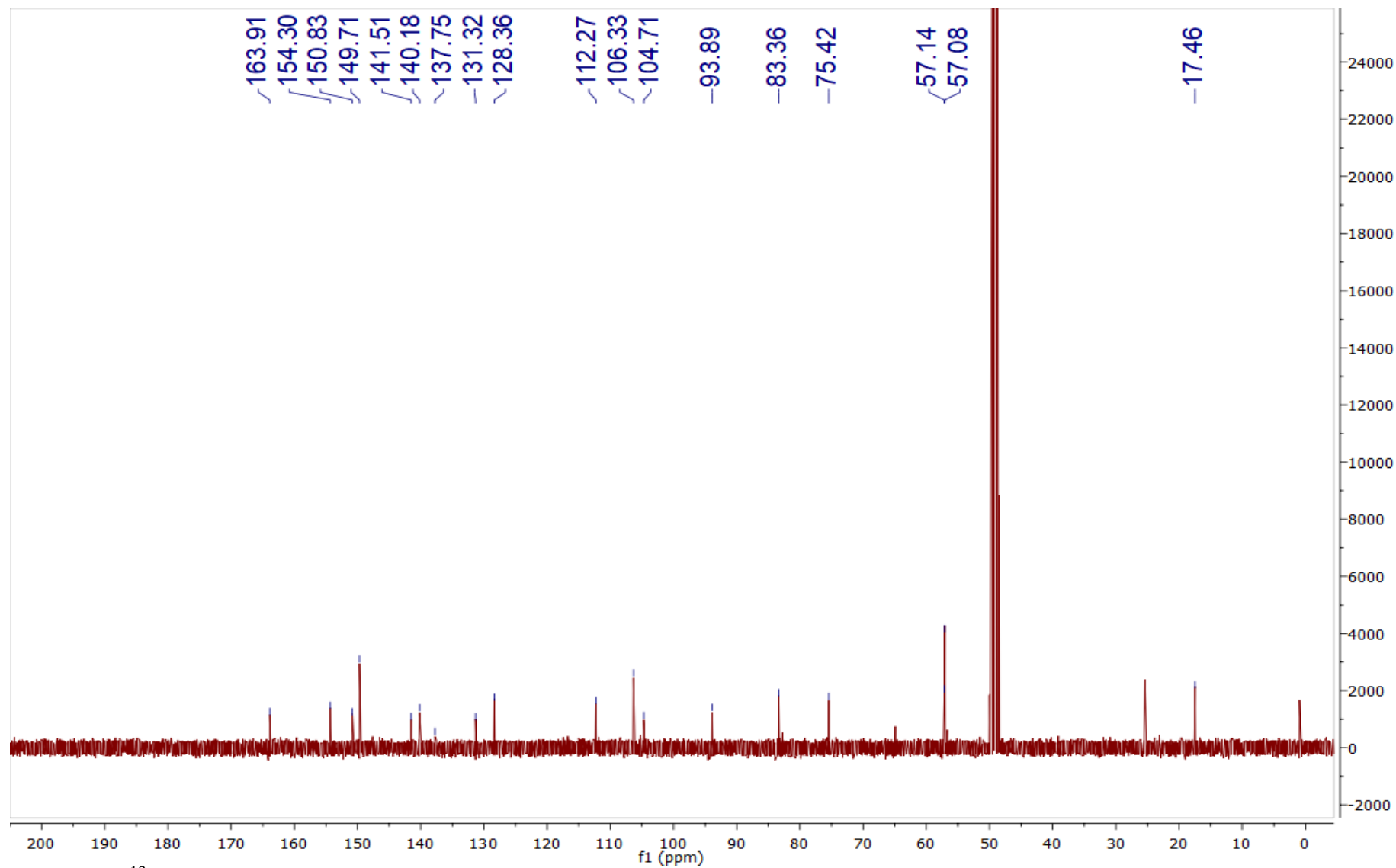
**Figure S37.** HRESI-MS spectrum of the new compound **4**



**Figure S38.** IR spectrum of the new compound **4**



**Figure S39.**  $^1\text{H}$  NMR (400 MHz, MeOD) spectrum of the new compound **4**



**Figure S40.** <sup>13</sup>C NMR (100 MHz, MeOD) spectrum of the new compound **4**

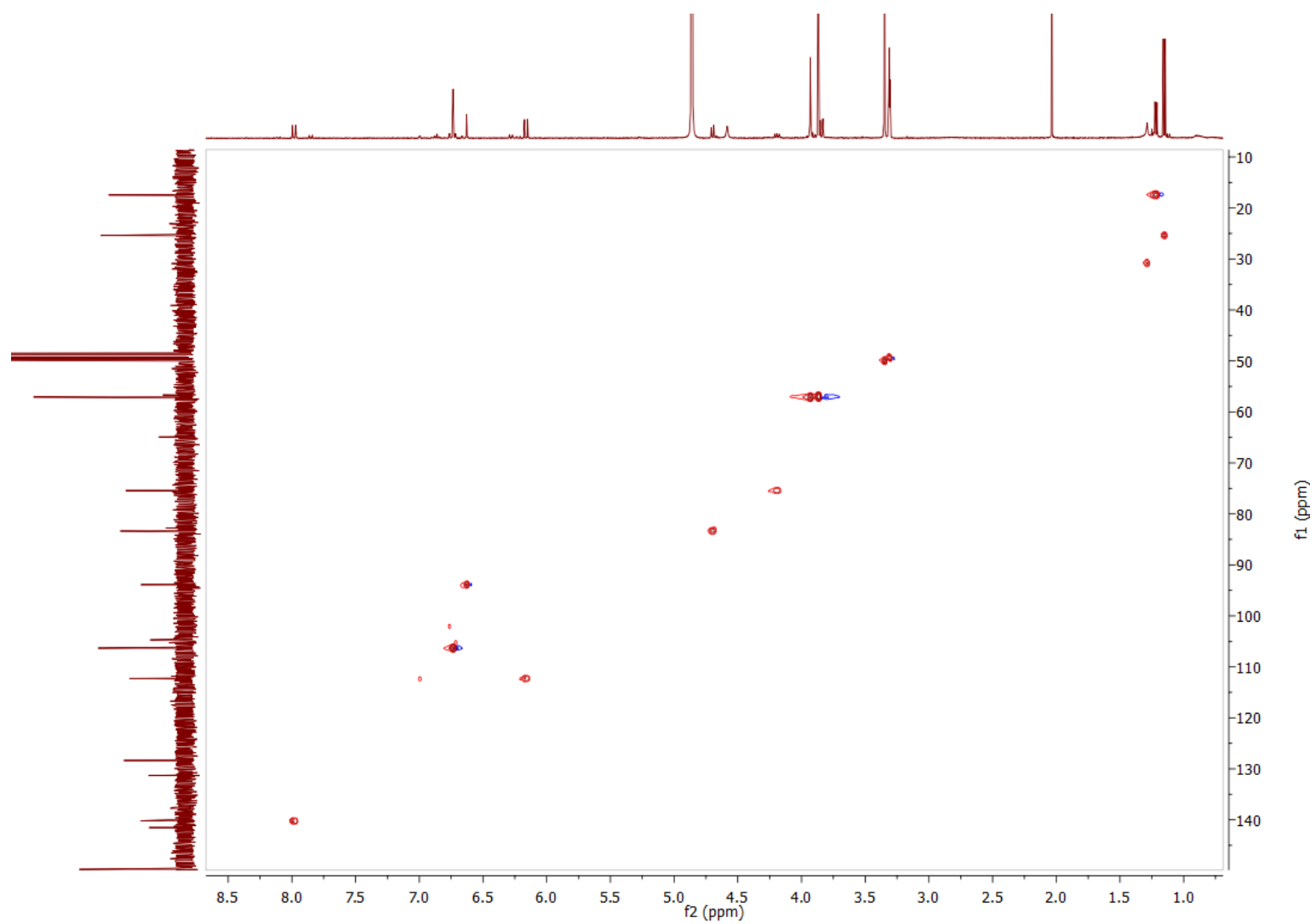


Figure S41. HSQC spectrum of the new compound **4**

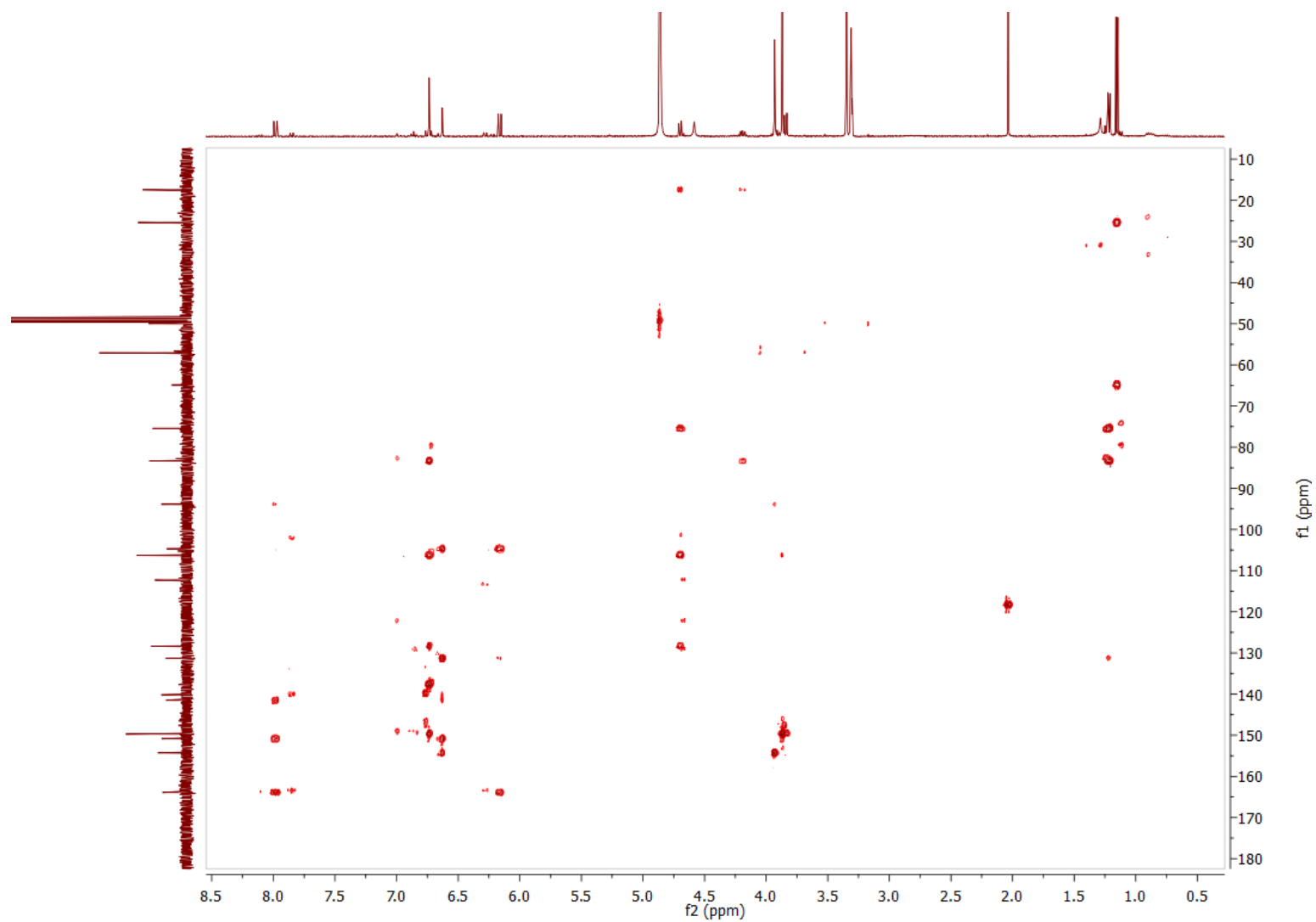


Figure S42. HMBC spectrum of the new compound **4**

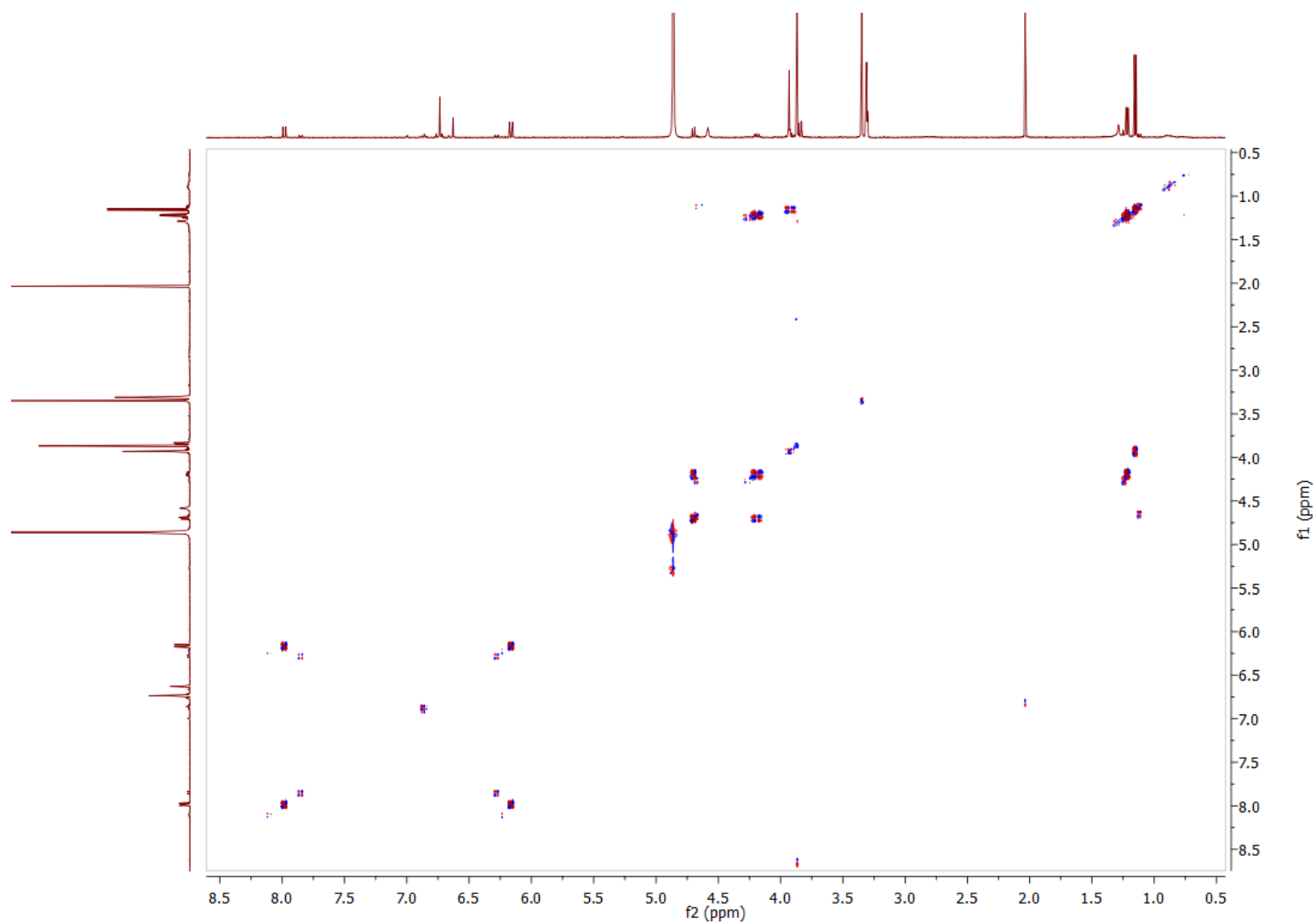
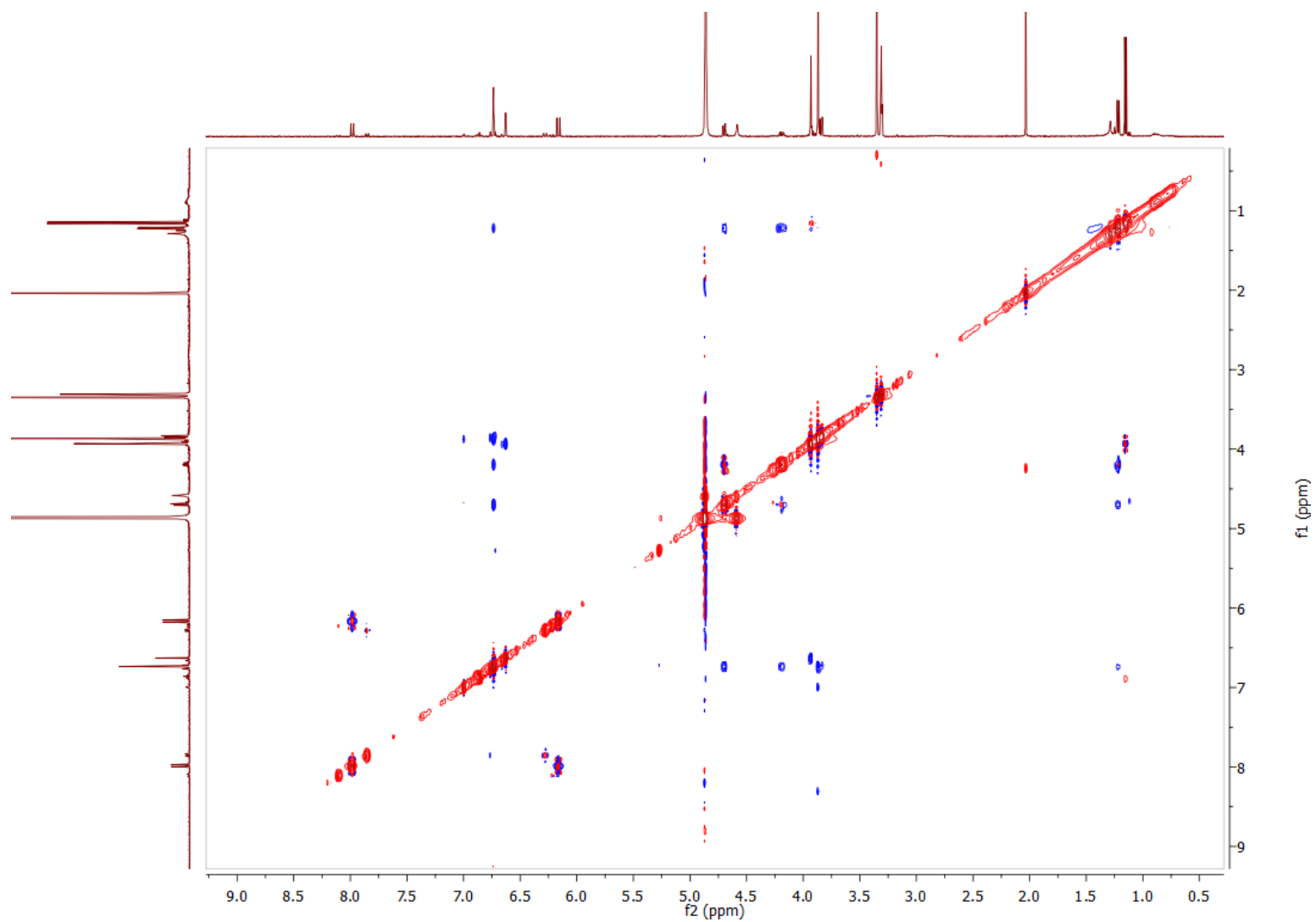
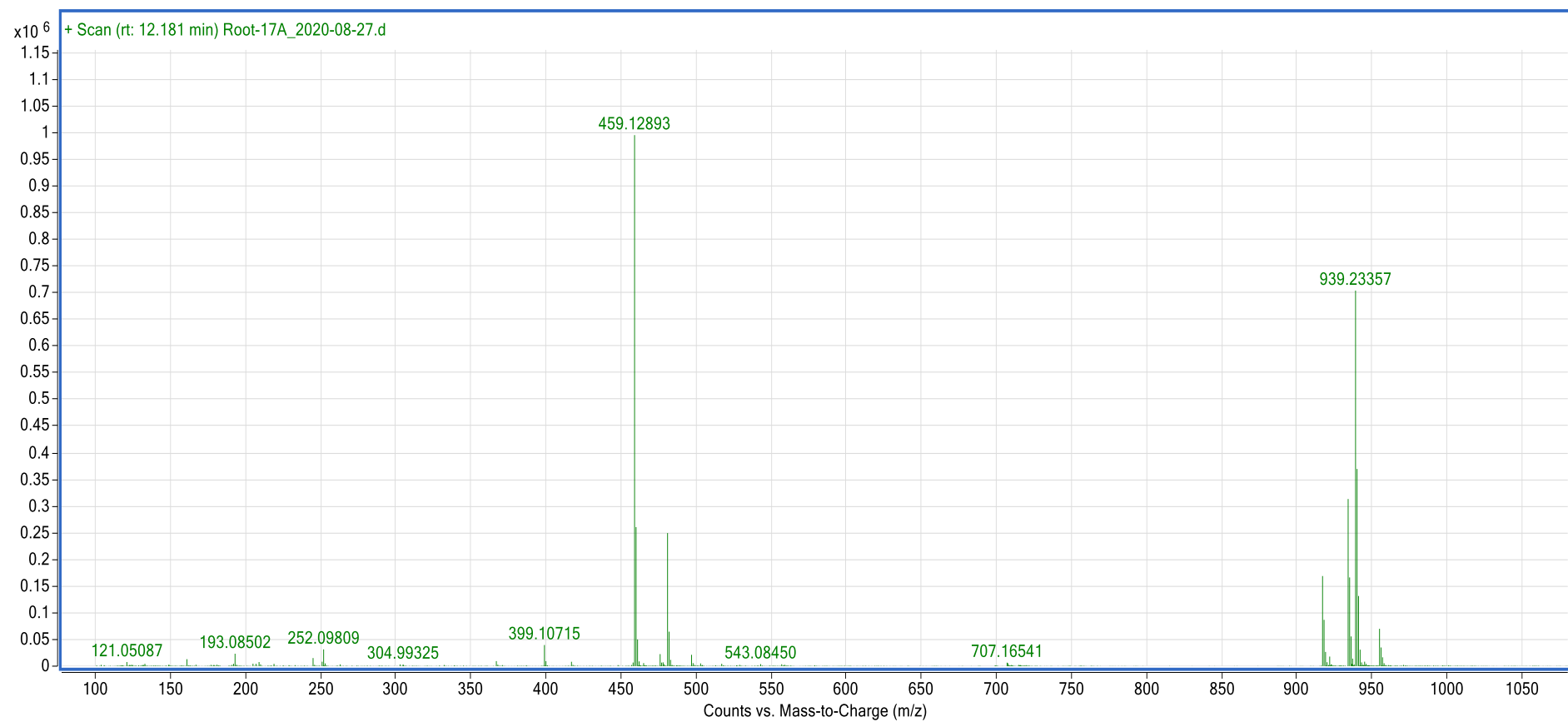


Figure S43. COSY spectrum of the new compound **4**





**Figure S44.** NOESY spectrum of the new compound **4**



**Figure S45.** HRESI-MS spectrum of the new compound **5**

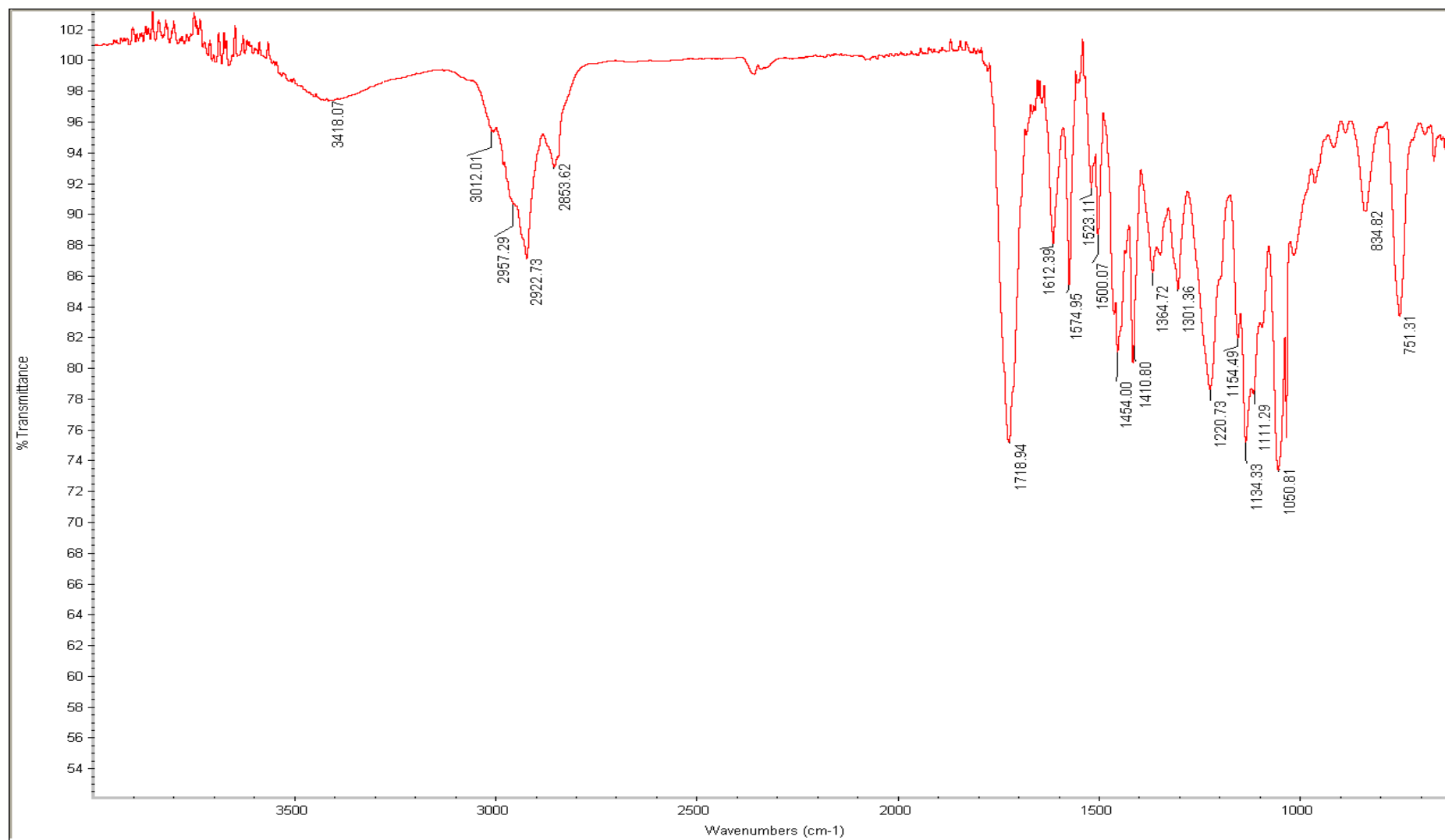
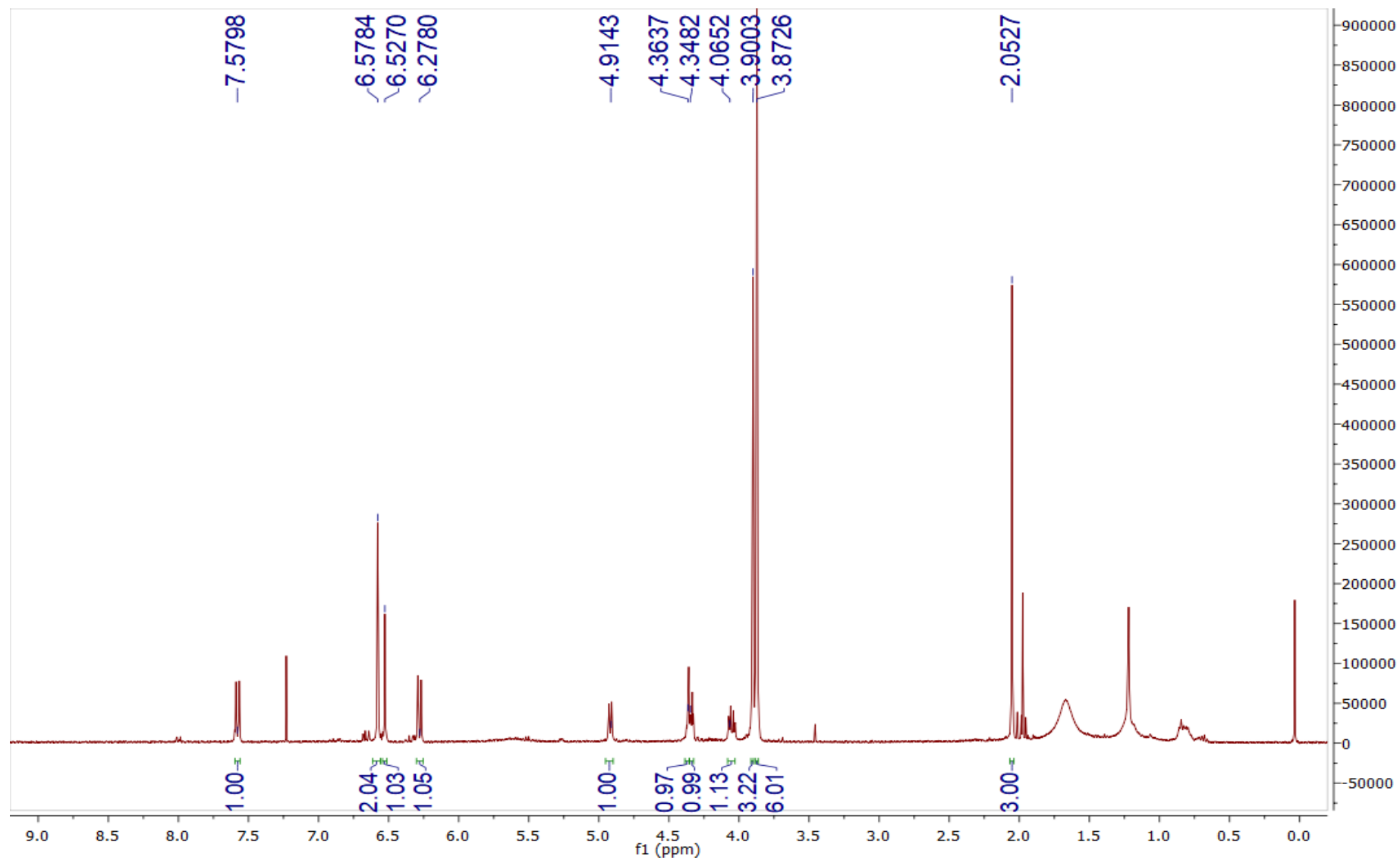


Figure S46. IR spectrum of the new compound **5**



**Figure S47.**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectrum of the new compound **5**

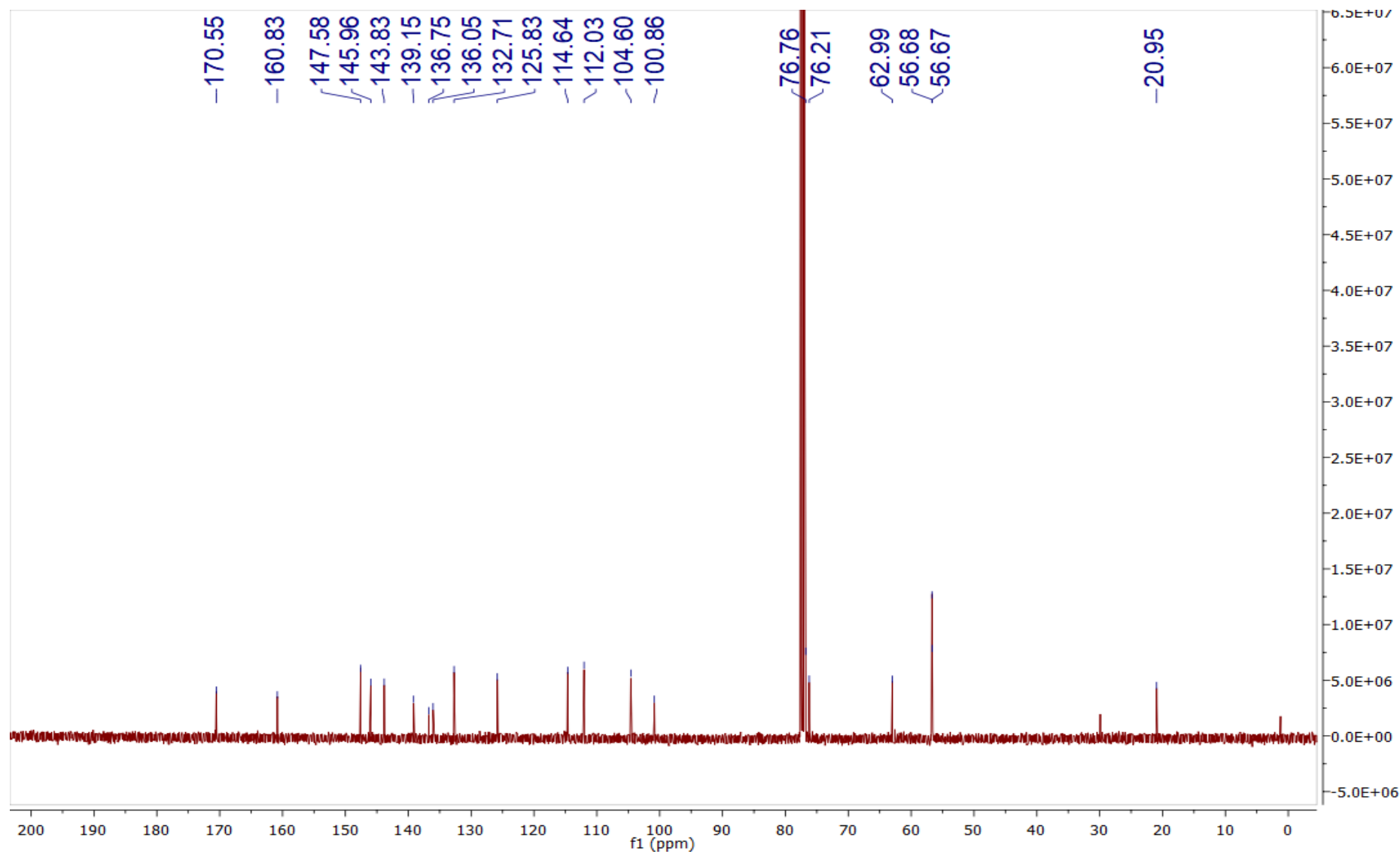


Figure S48. <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) spectrum of the new compound **5**

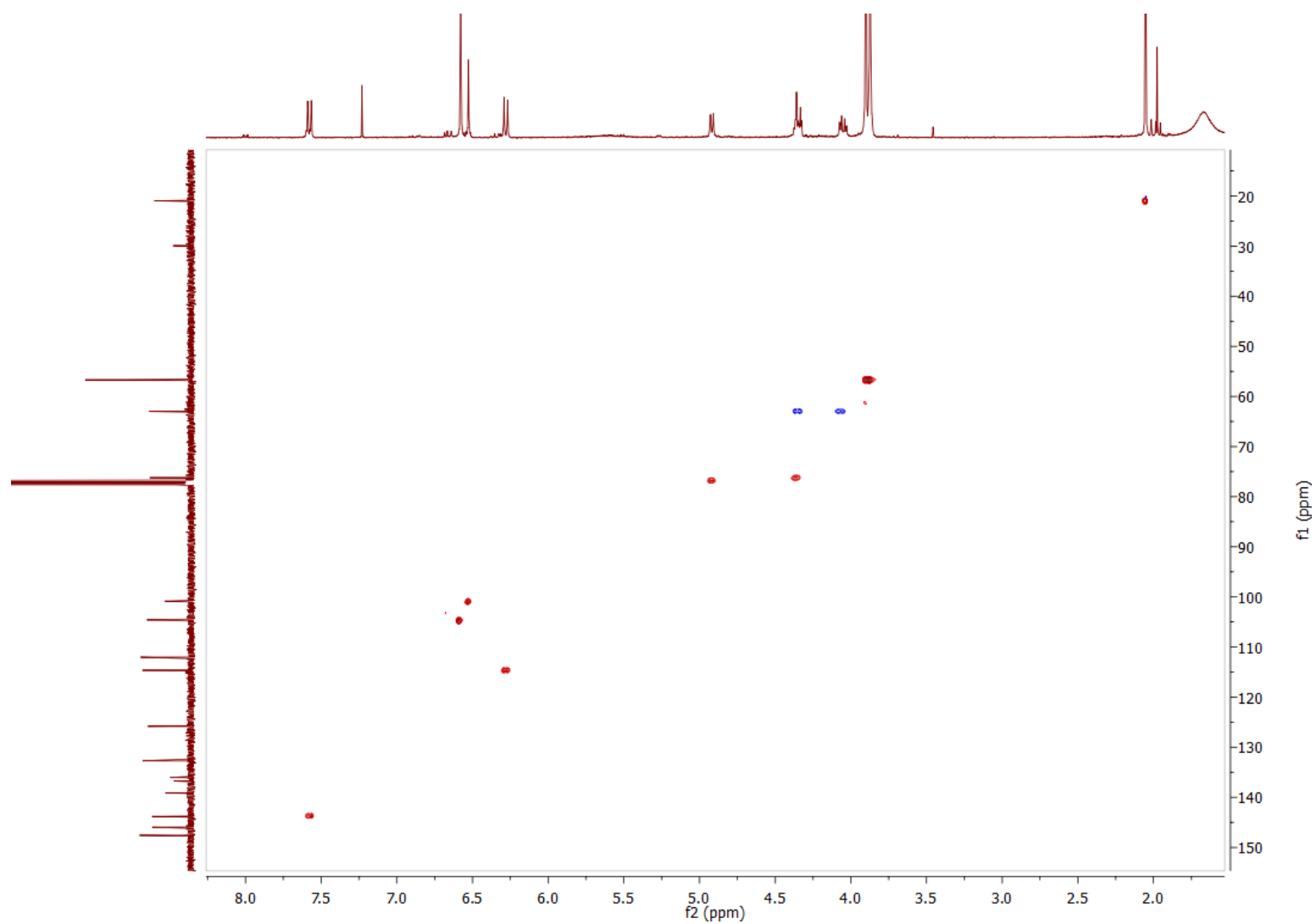


Figure S49. HSQC spectrum of the new compound **5**

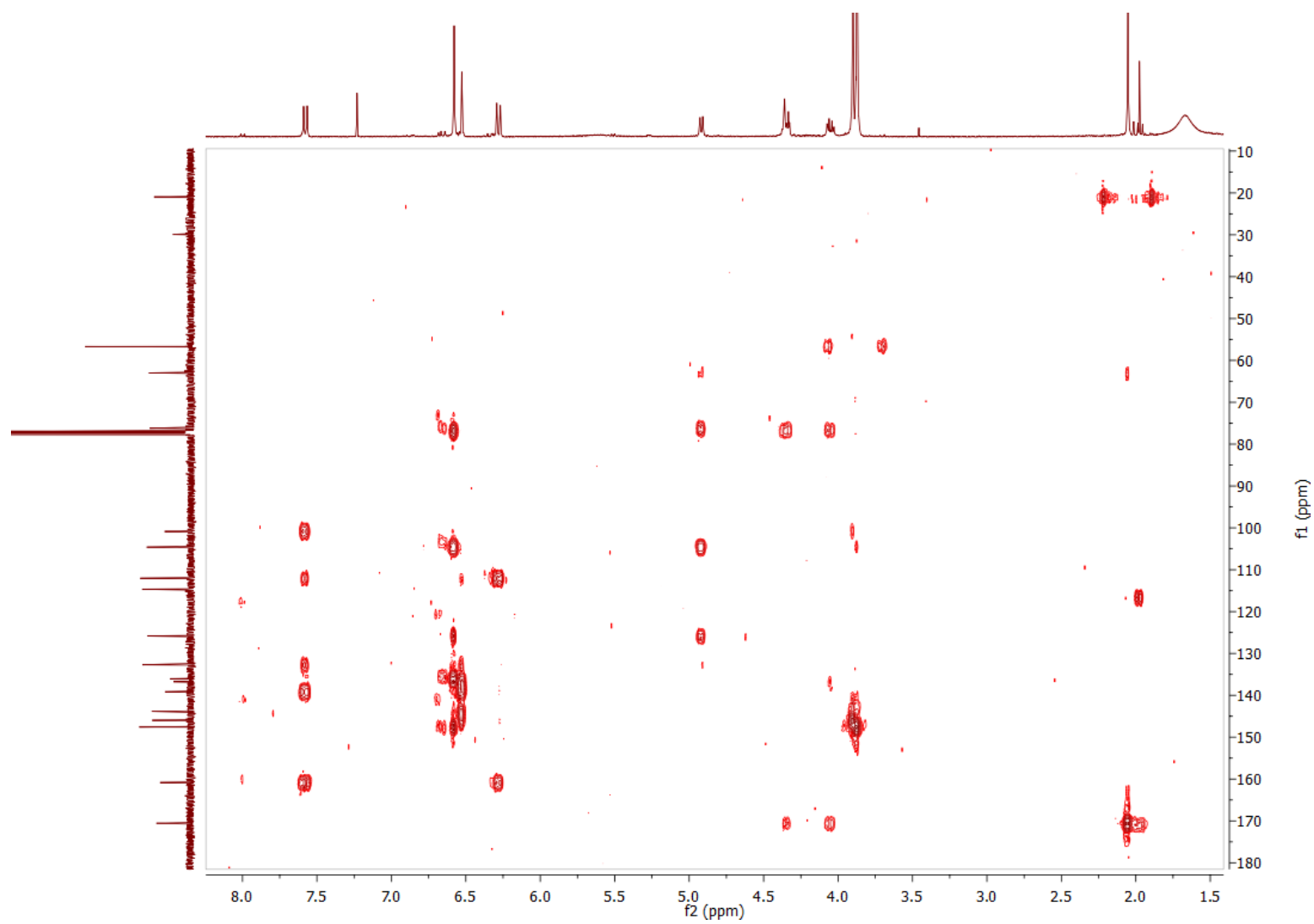
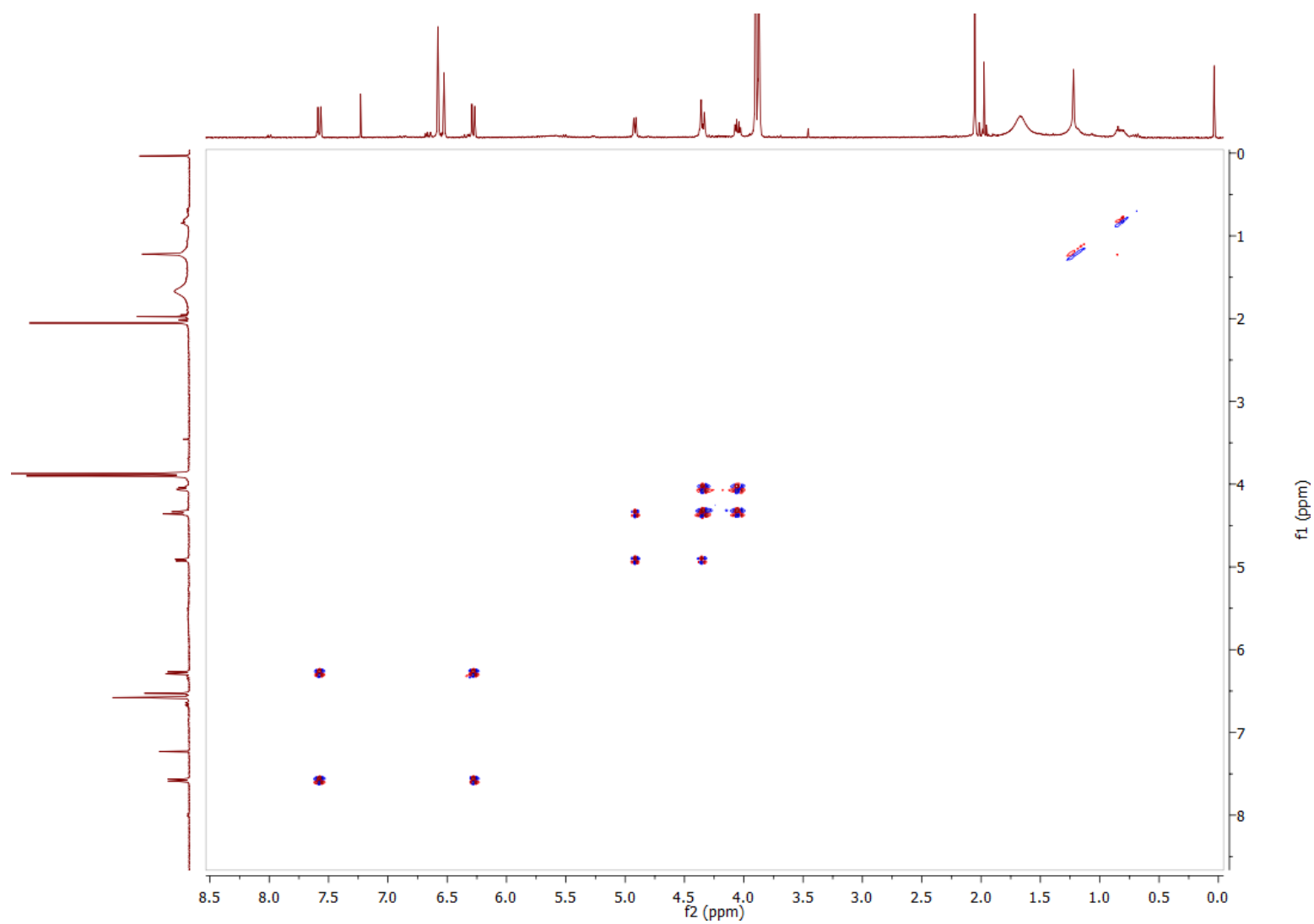
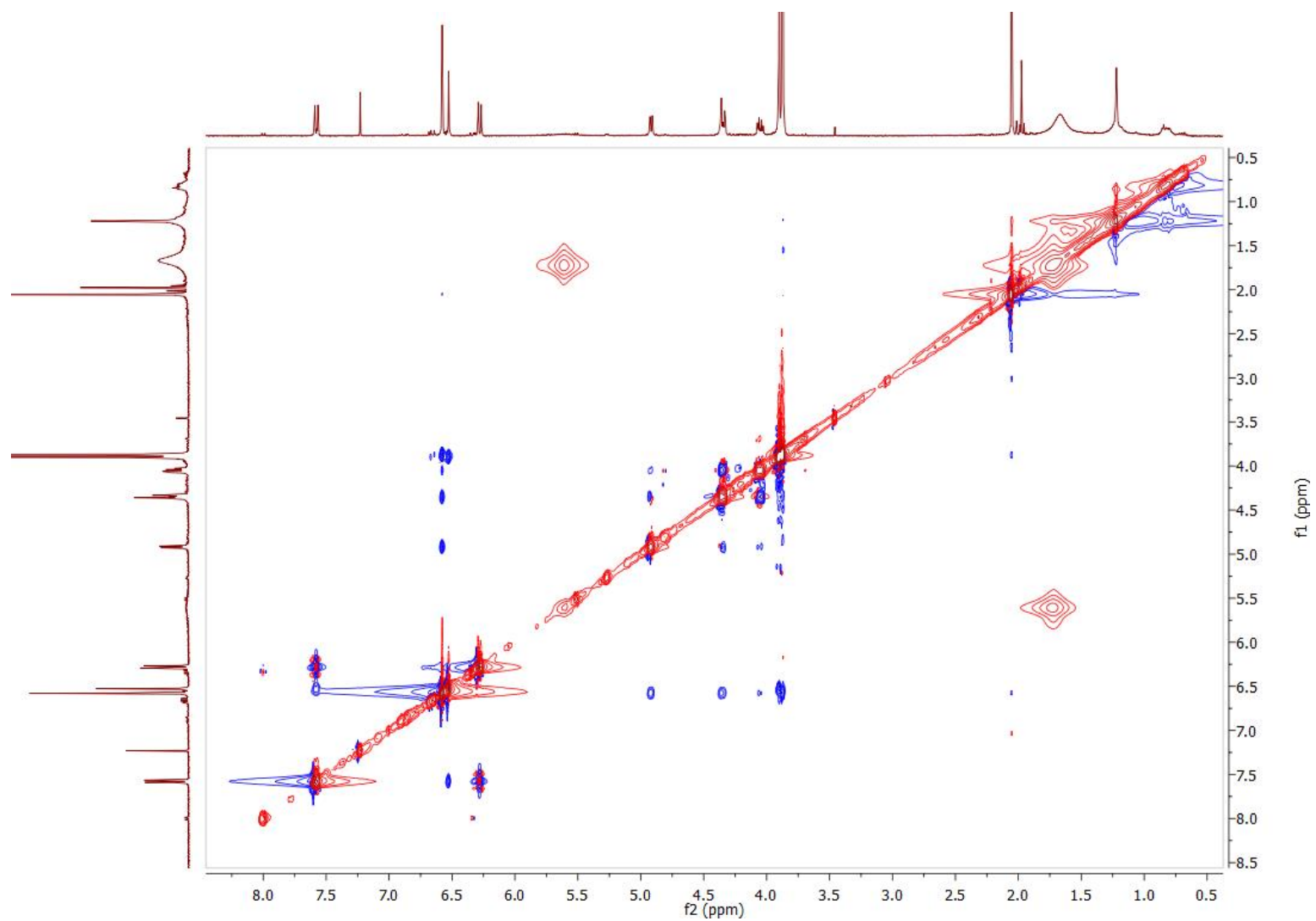


Figure S50. HMBC spectrum of the new compound **5**

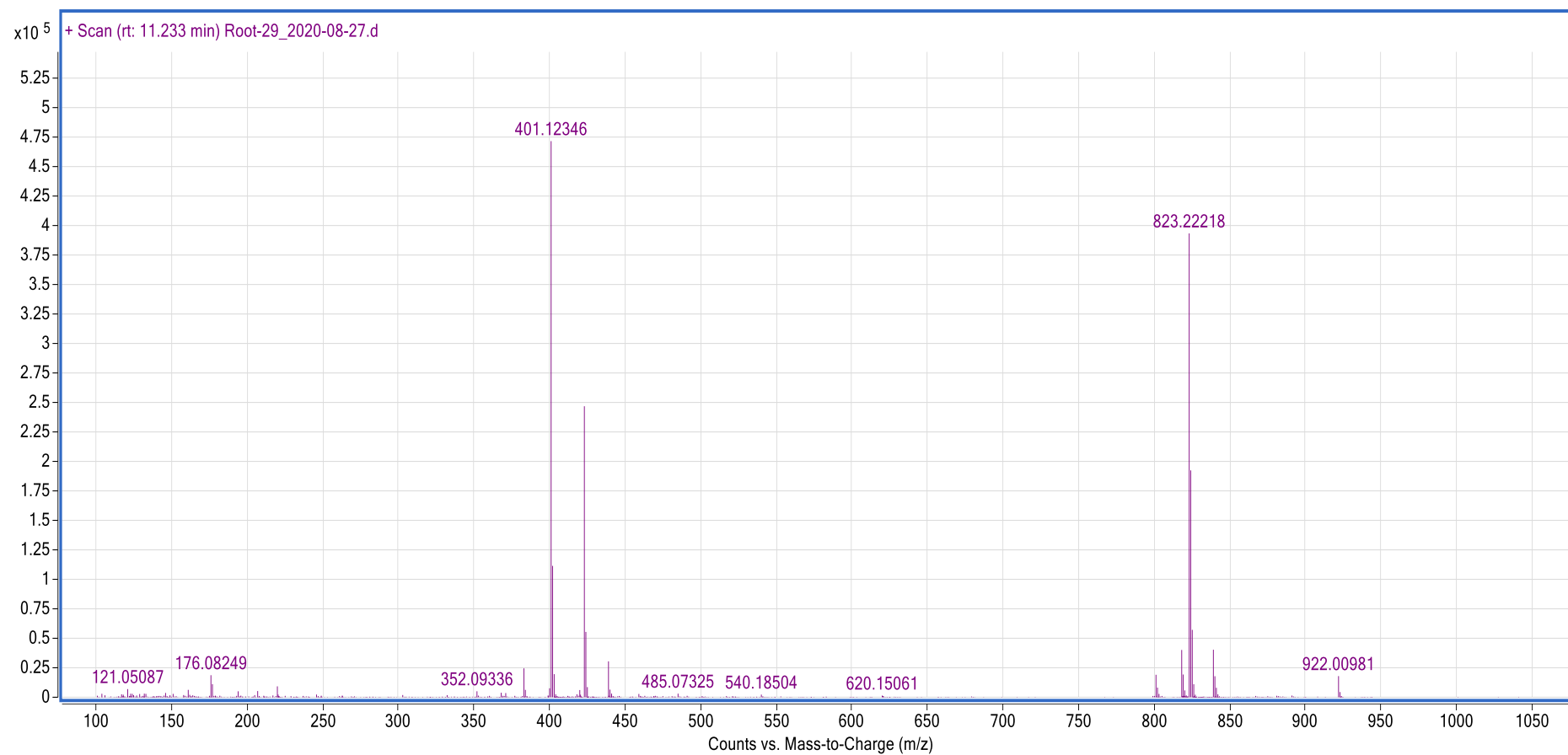


**Figure S51.** COSY spectrum of the new compound **5**





**Figure S52.** NOESY spectrum of the new compound **5**



**Figure S53.** HRESI-MS spectrum of the new compound **7**

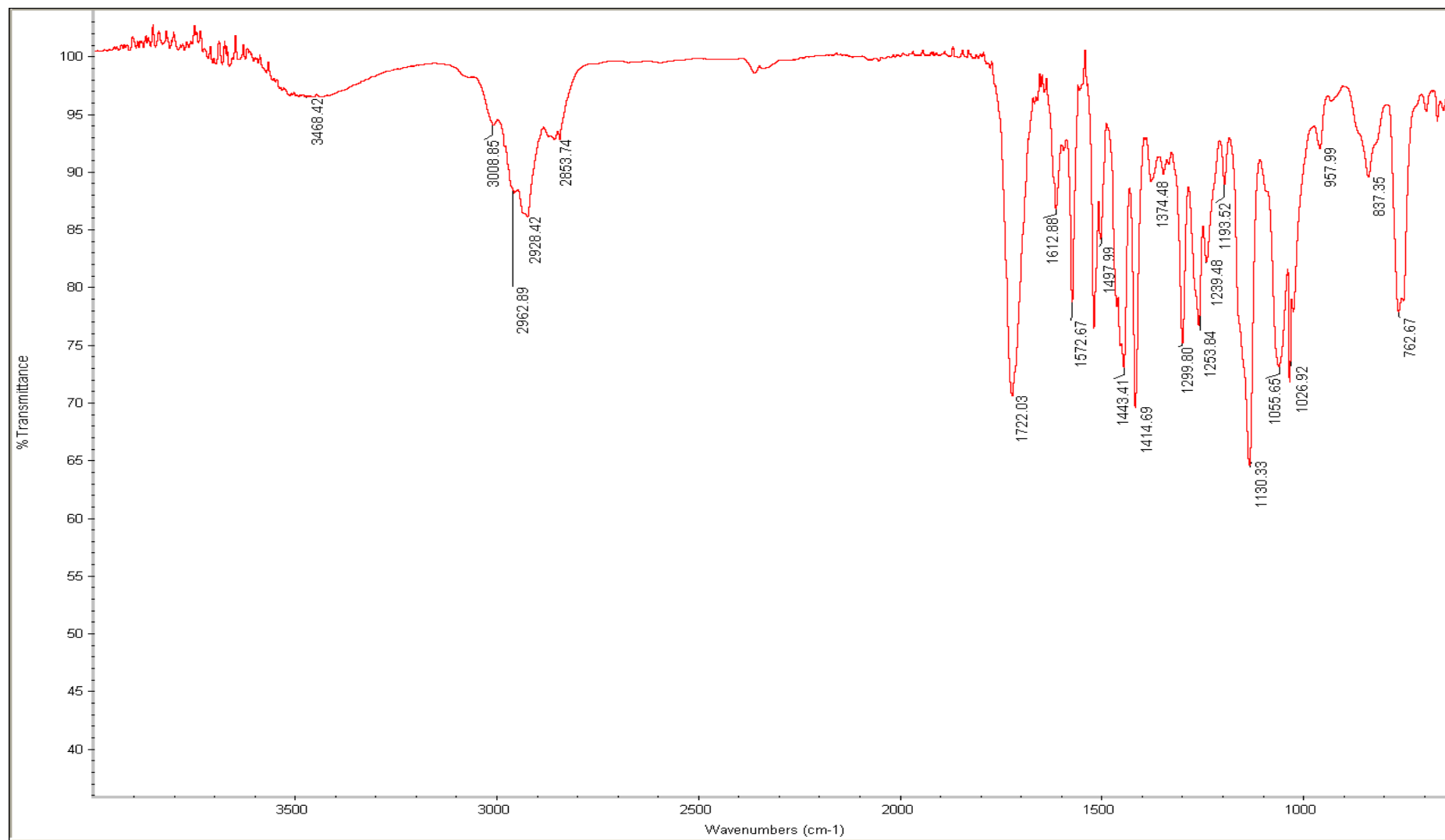
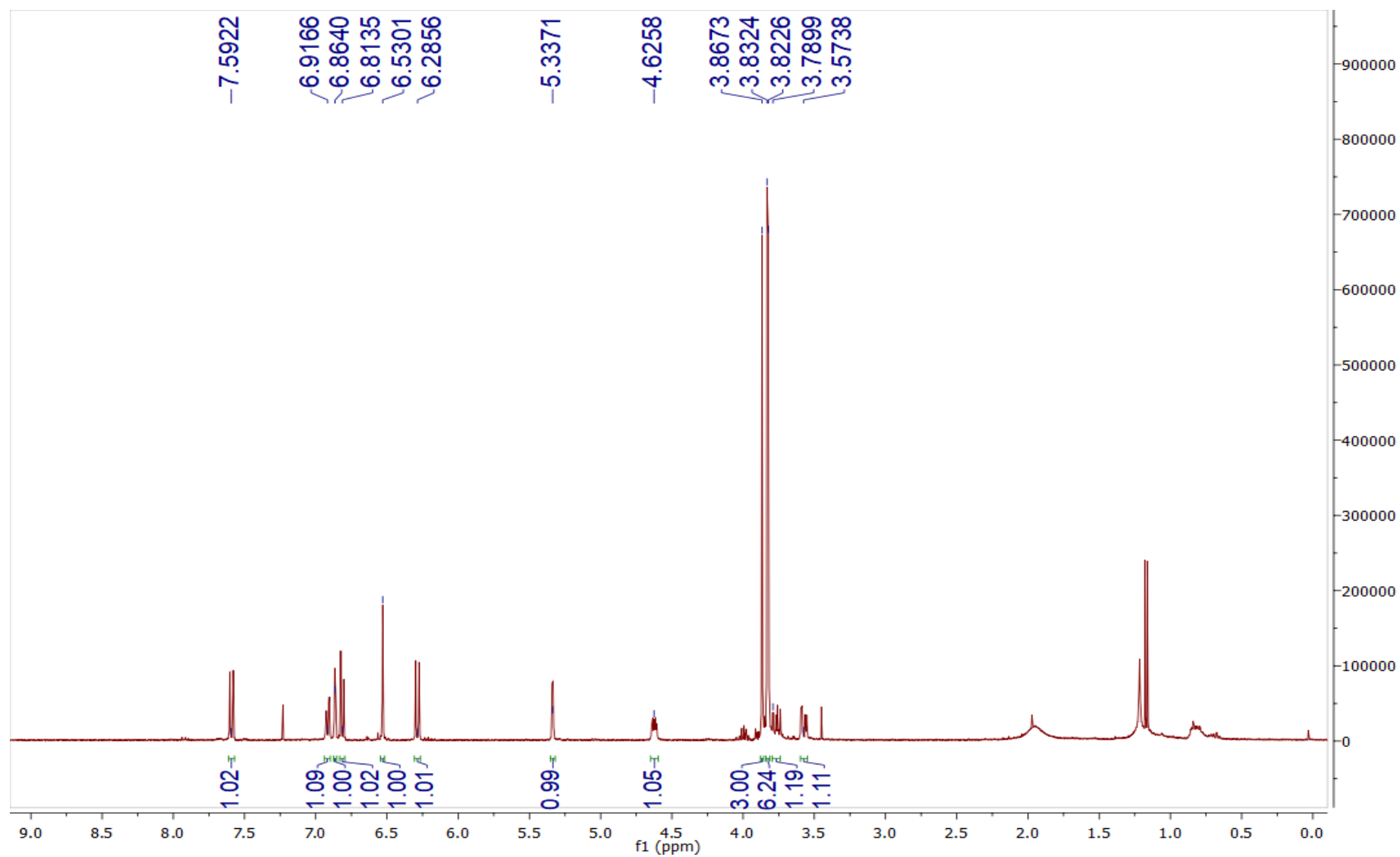
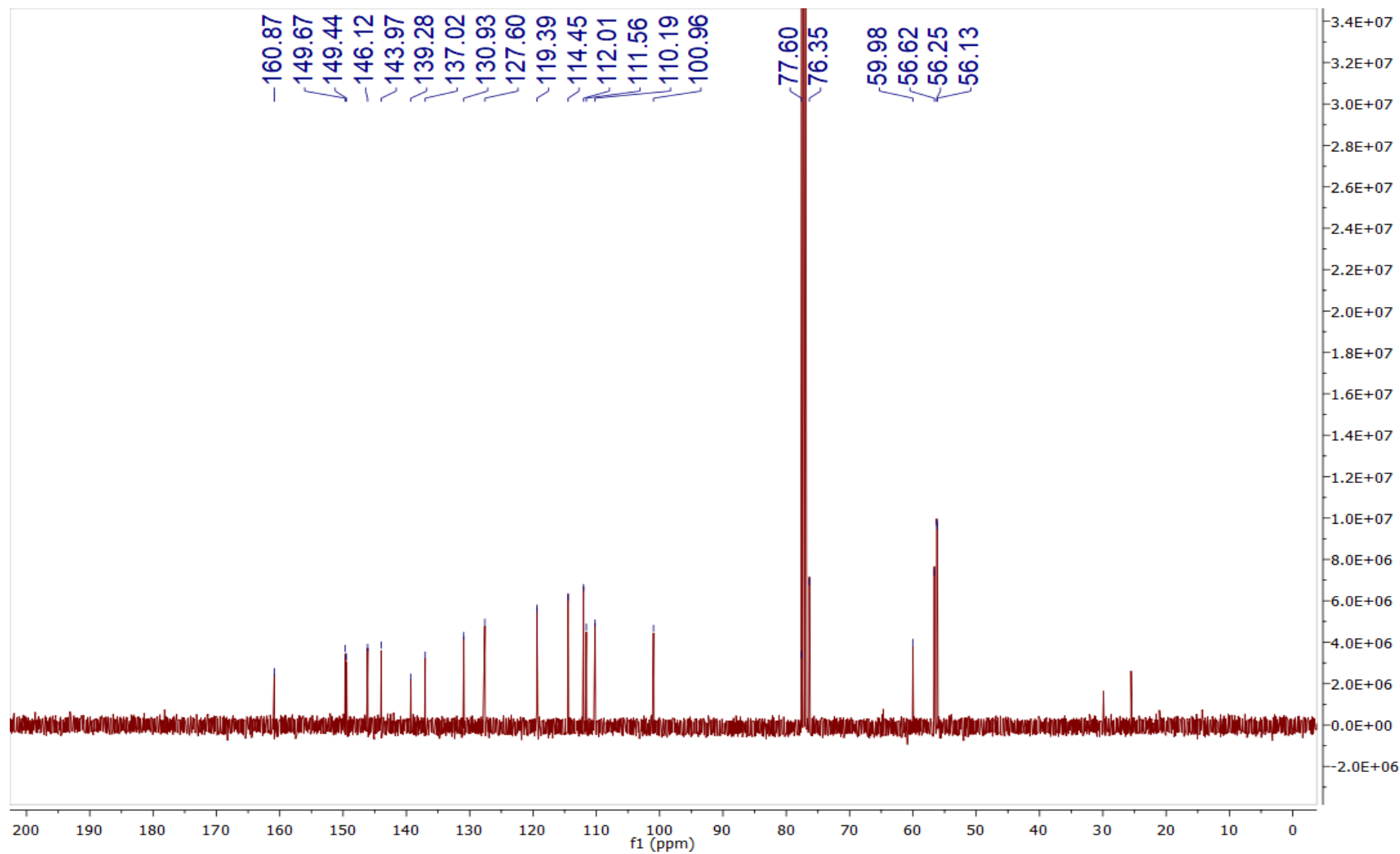


Figure S54. IR spectrum of the new compound **7**



**Figure S55.**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectrum of the new compound **7**



**Figure S56.** <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) spectrum of the new compound **7**

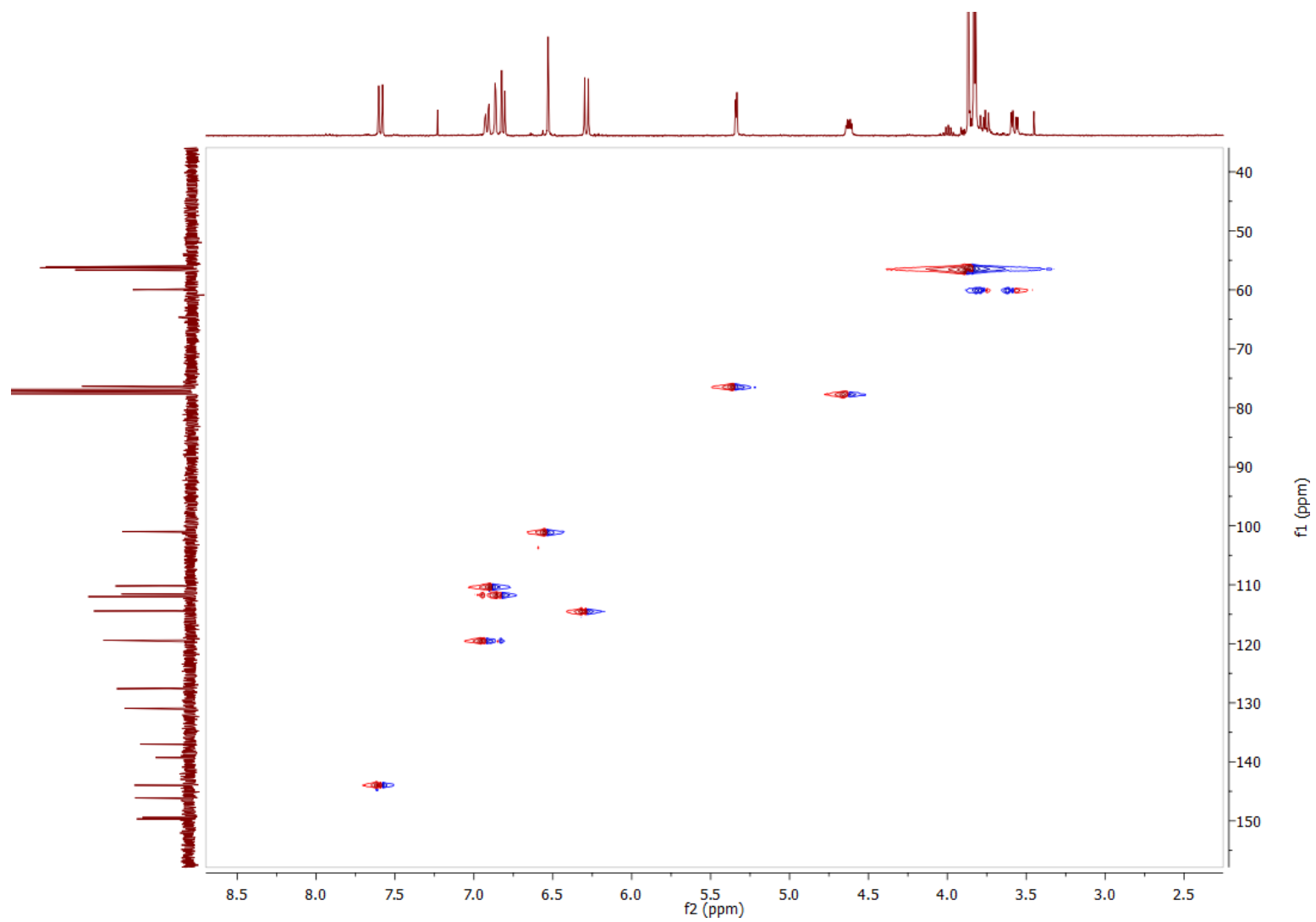


Figure S57. HSQC spectrum of the new compound **7**

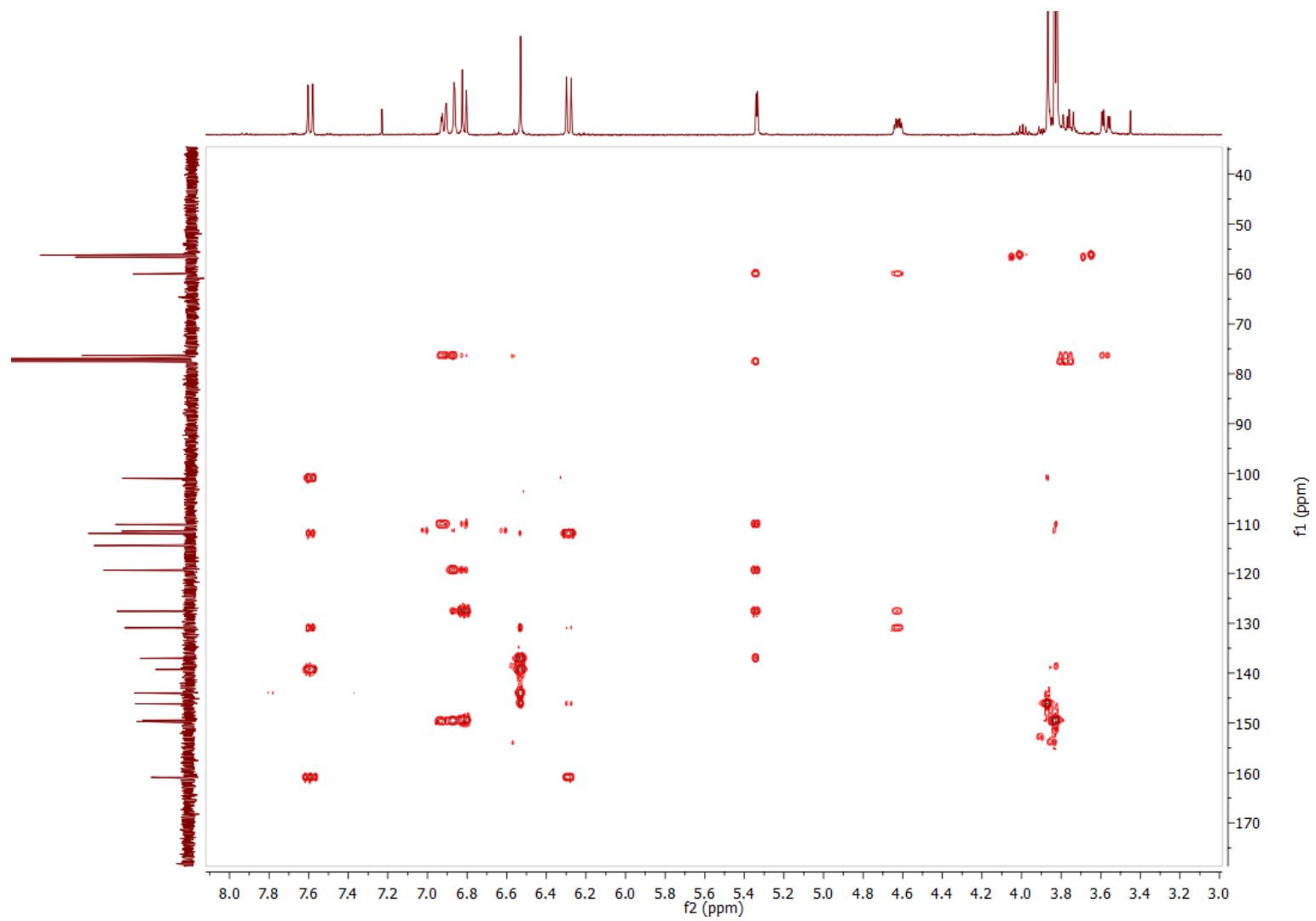


Figure S58. HMBC spectrum of the new compound **7**

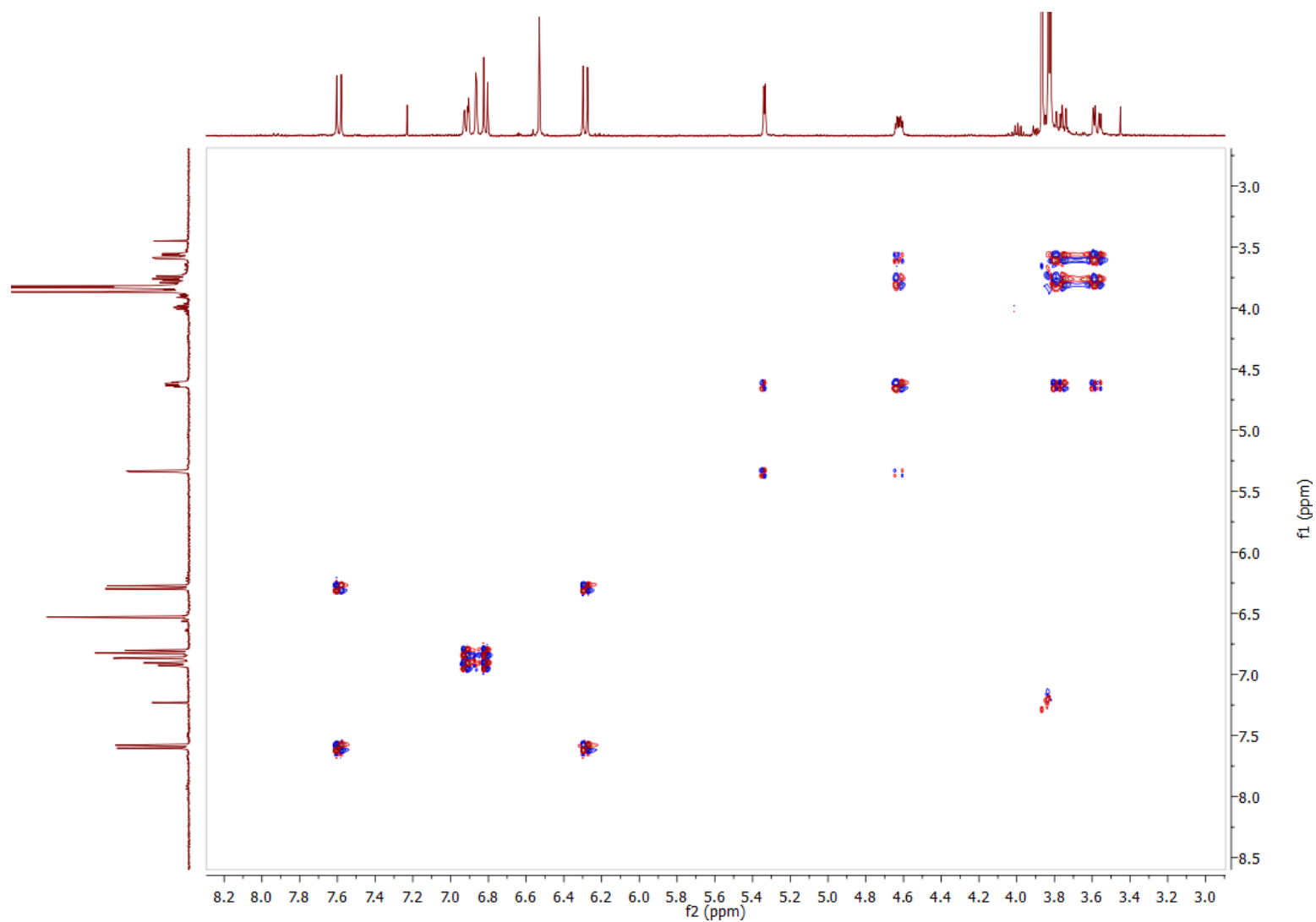
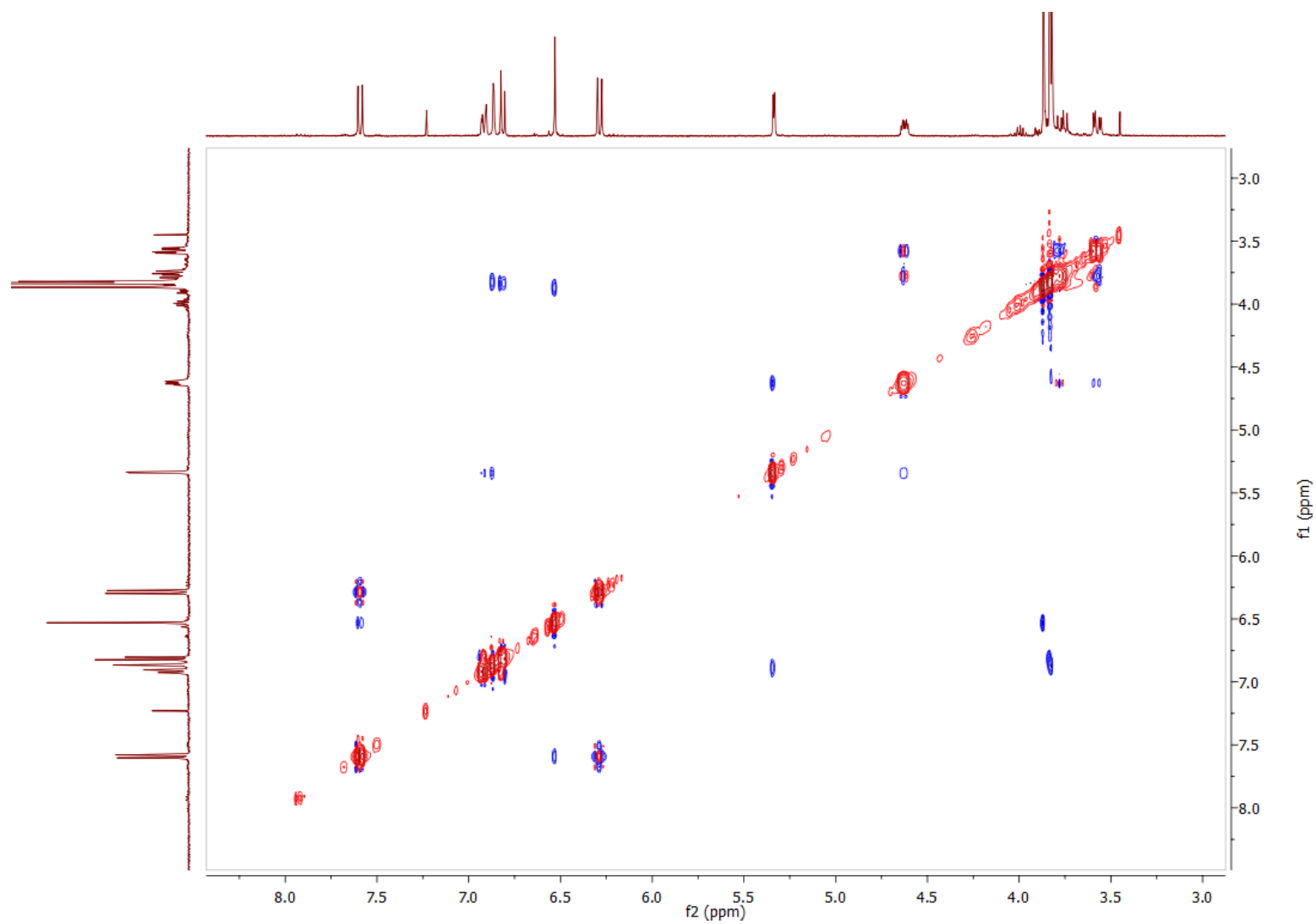
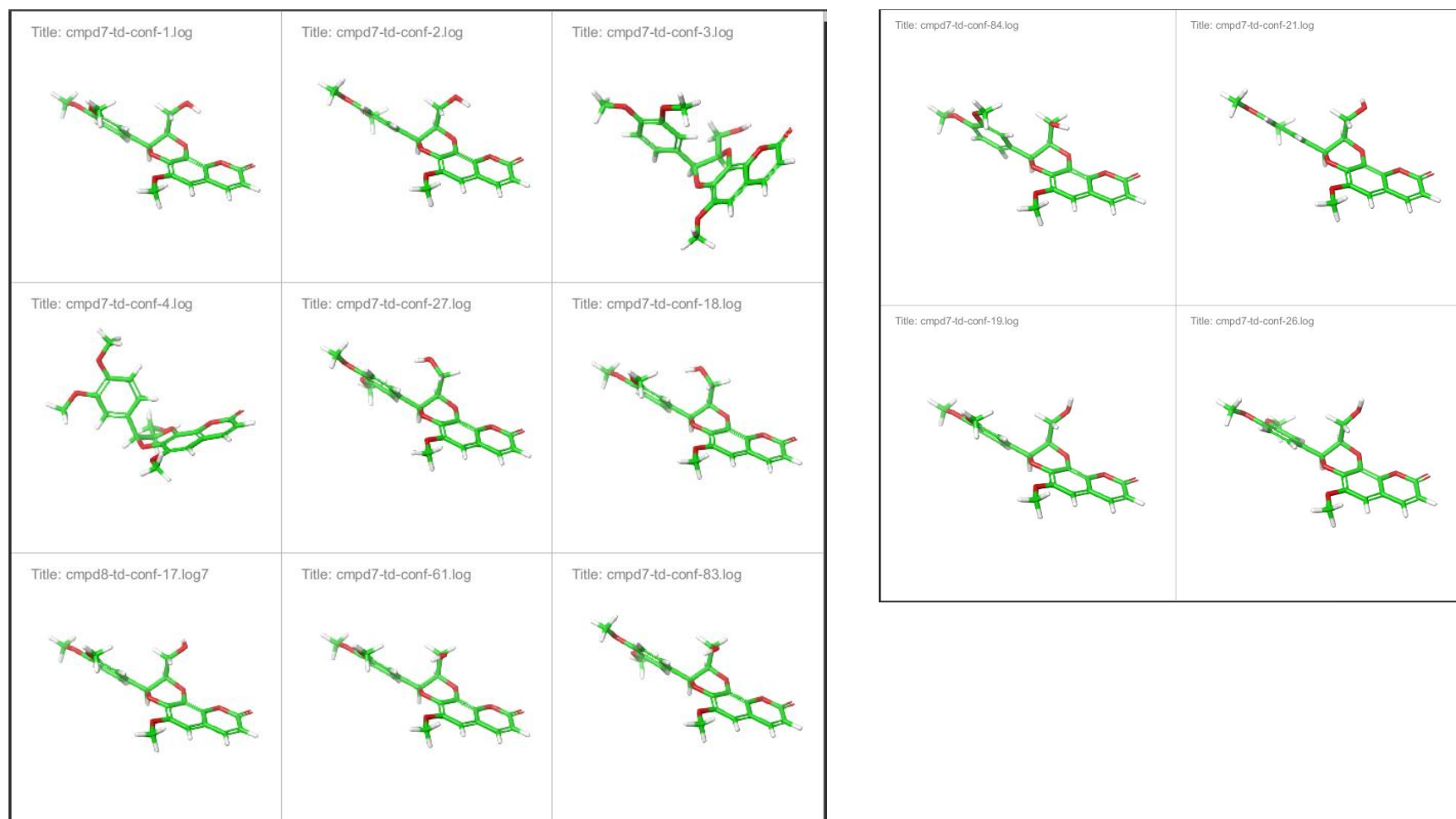


Figure S59. COSY spectrum of the new compound **7**





**Figure S60.** NOESY spectrum of the new compound **7**



**Figure S61.** Images of conformers (>1%) for the new compound **7**