

Supplementary Material

Synthesis and structure determination of diastereomeric carbapenems in the Ad_NE-reaction of (\pm)-4,4-dimethyl-3-mercaptodihydrofuran-2(3H)-one with chiral carbapenem enol phosphate

Zuleykhā Valiullina,^{*a} Adeliya Galeeva,^a Alexander Lobov,^a
Leonard Khalilov,^b and Mansur Miftakhov^a

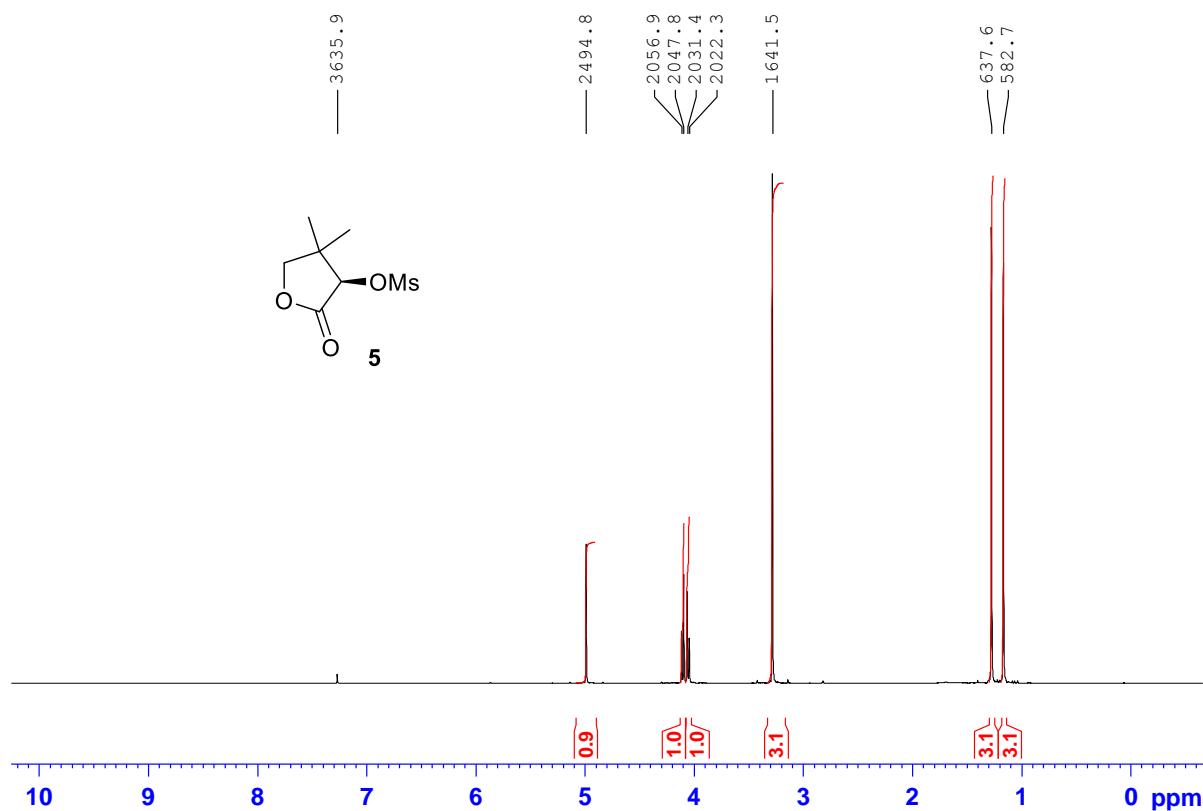
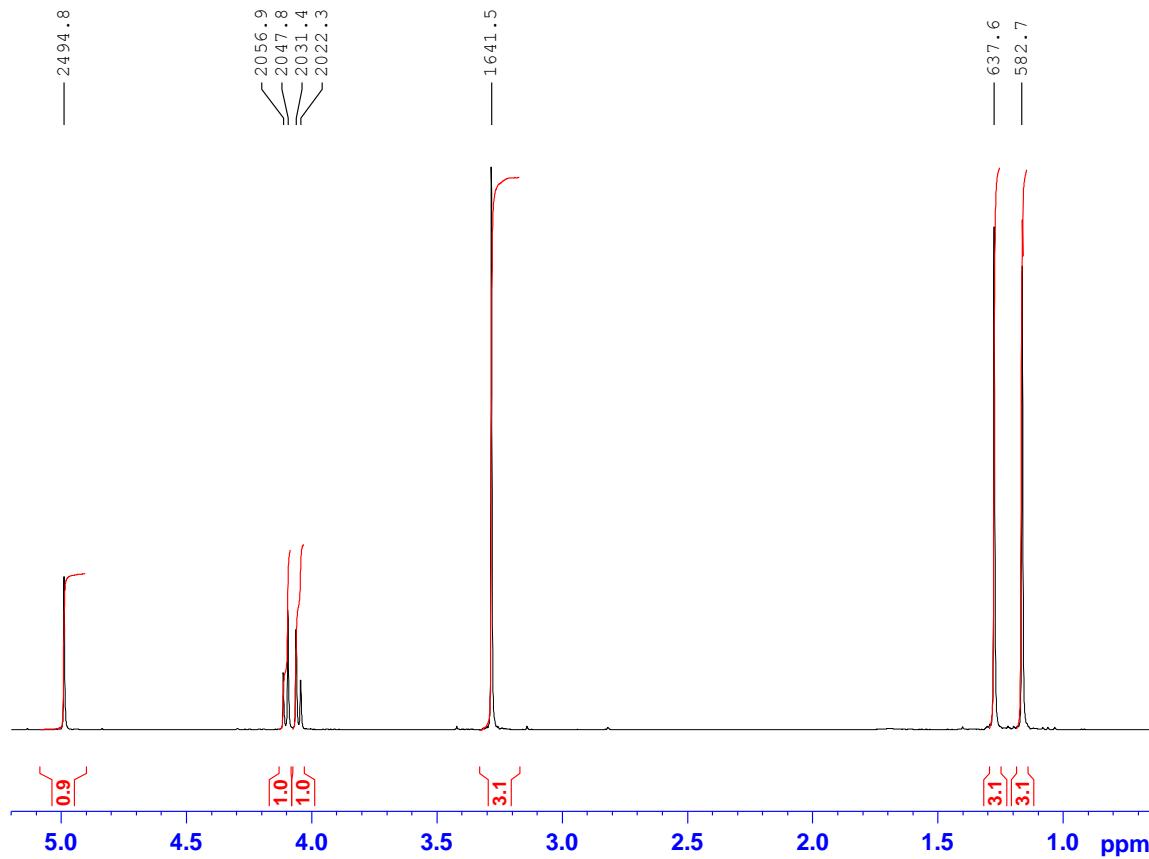
^a Ufa Institute of Chemistry, Ufa Federal Research Centre of the Russian Academy of Sciences, 450054 Ufa, Russian Federation

^b Institute of Petrochemistry and Catalysis, Ufa Federal Research Centre of the Russian Academy of Sciences, 450071 Ufa, Russian Federation

E-mail: bioreq@anrb.ru

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NMR data**Figure S1.** Complete ^1H NMR spectrum of compound **5** in CDCl_3 , 500 MHz.**Figure S2.** Expanded ^1H NMR spectrum of compound **5** in CDCl_3 , 500 MHz.

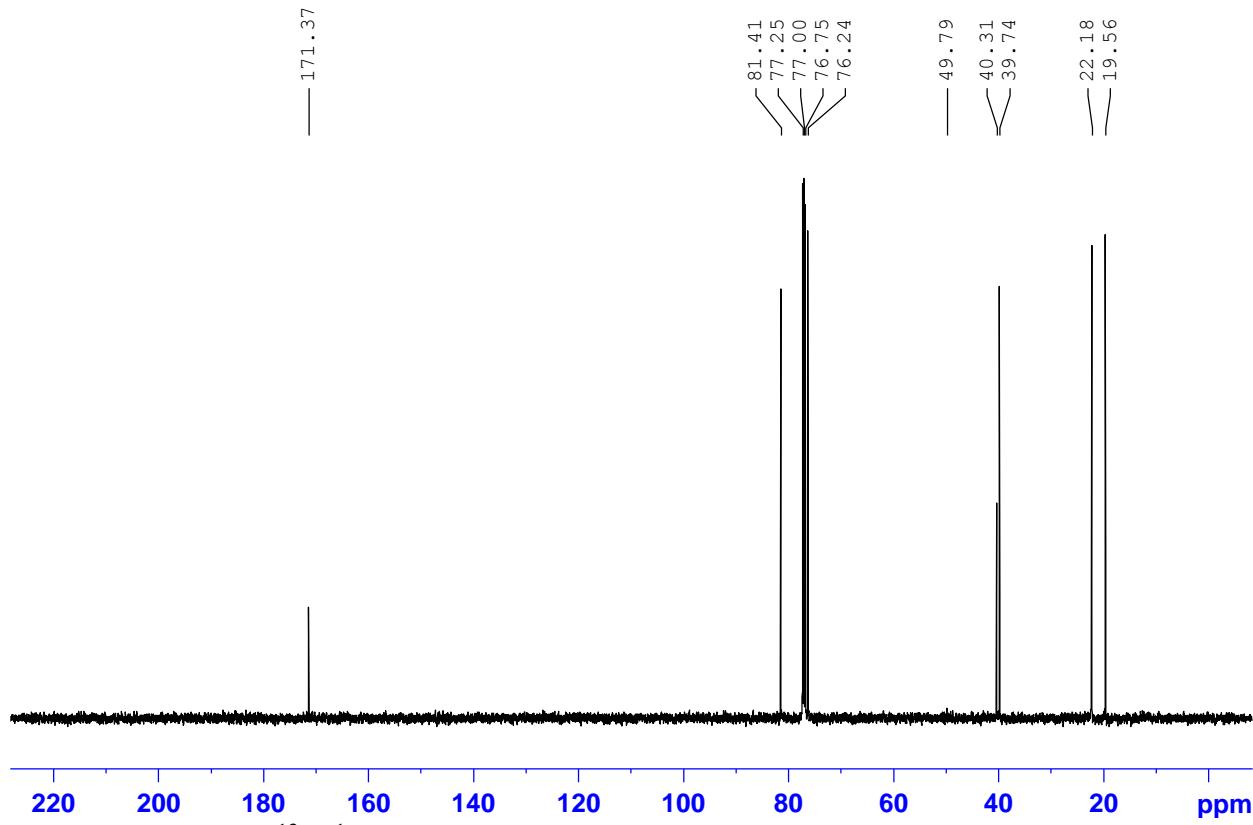


Figure S3. Complete $^{13}\text{C}\{\text{H}\}$ spectrum of compound 5 in CDCl_3 , 125 MHz.

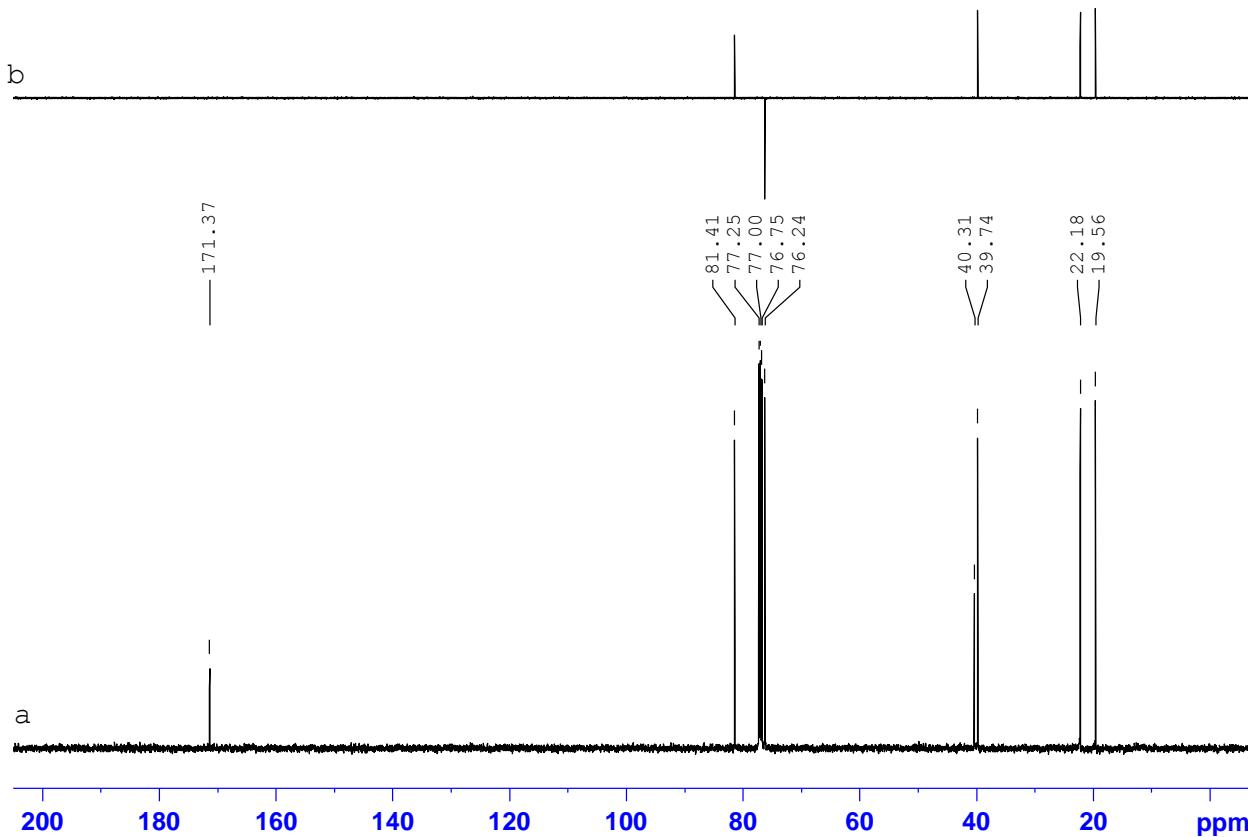


Figure S4. DEPT-135 editing $^{13}\text{C}\{\text{H}\}$ NMR spectrum of compound 5 in CDCl_3 , 125 MHz: a) $^{13}\text{C}\{\text{H}\}$ spectrum; b) DEPT-135.

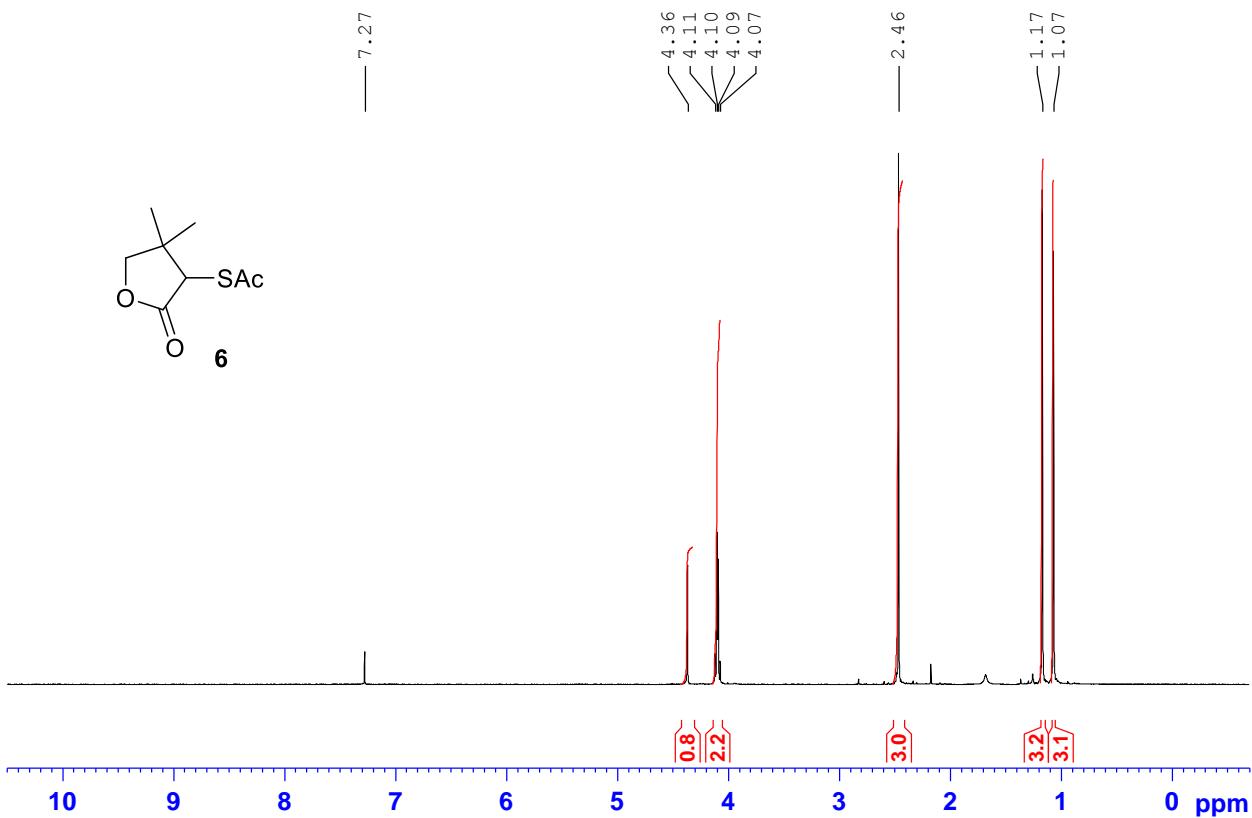


Figure S5. Complete ^1H NMR spectrum of compound **6** in CDCl_3 , 500 MHz.

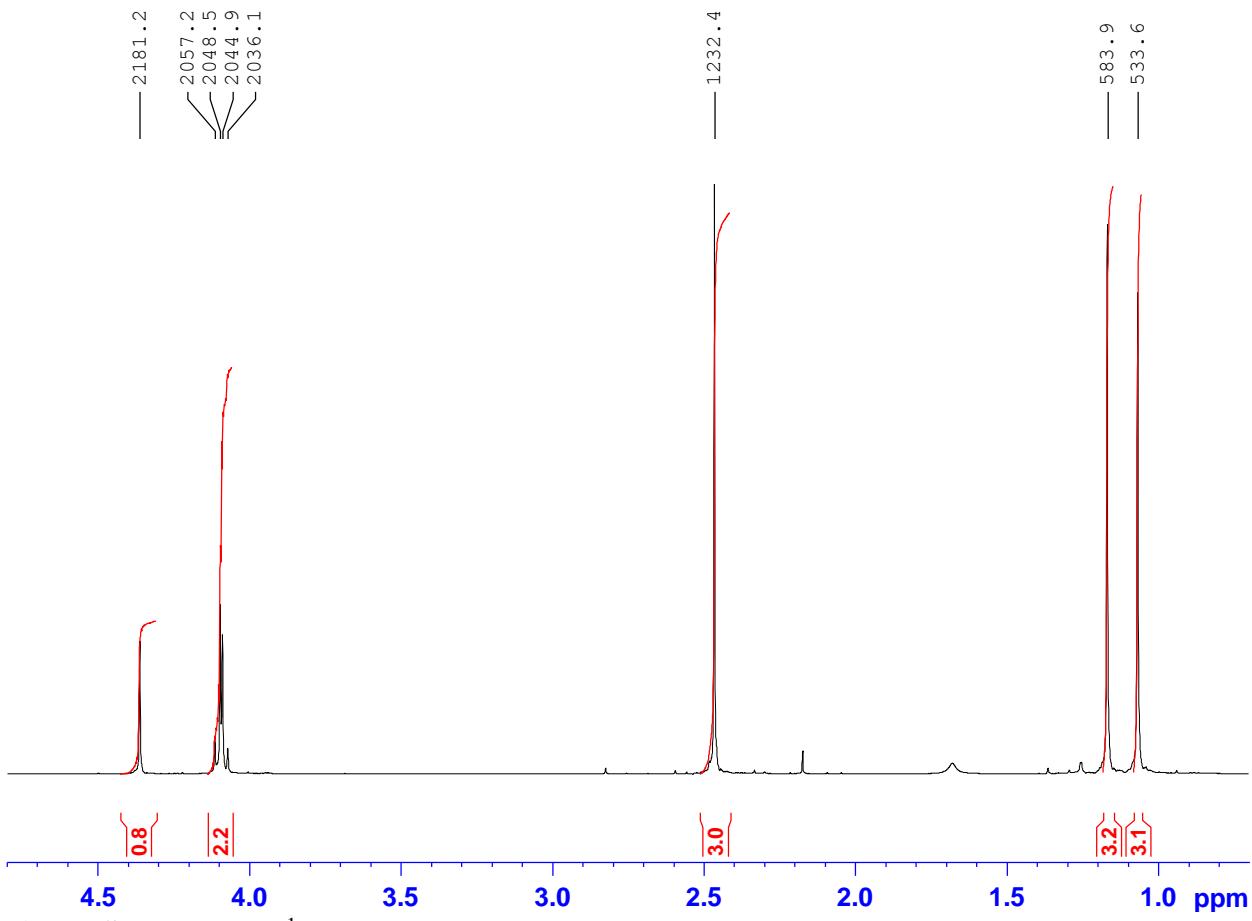


Figure S6. Expanded ^1H NMR spectrum of compound **6** in CDCl_3 , 500 MHz.

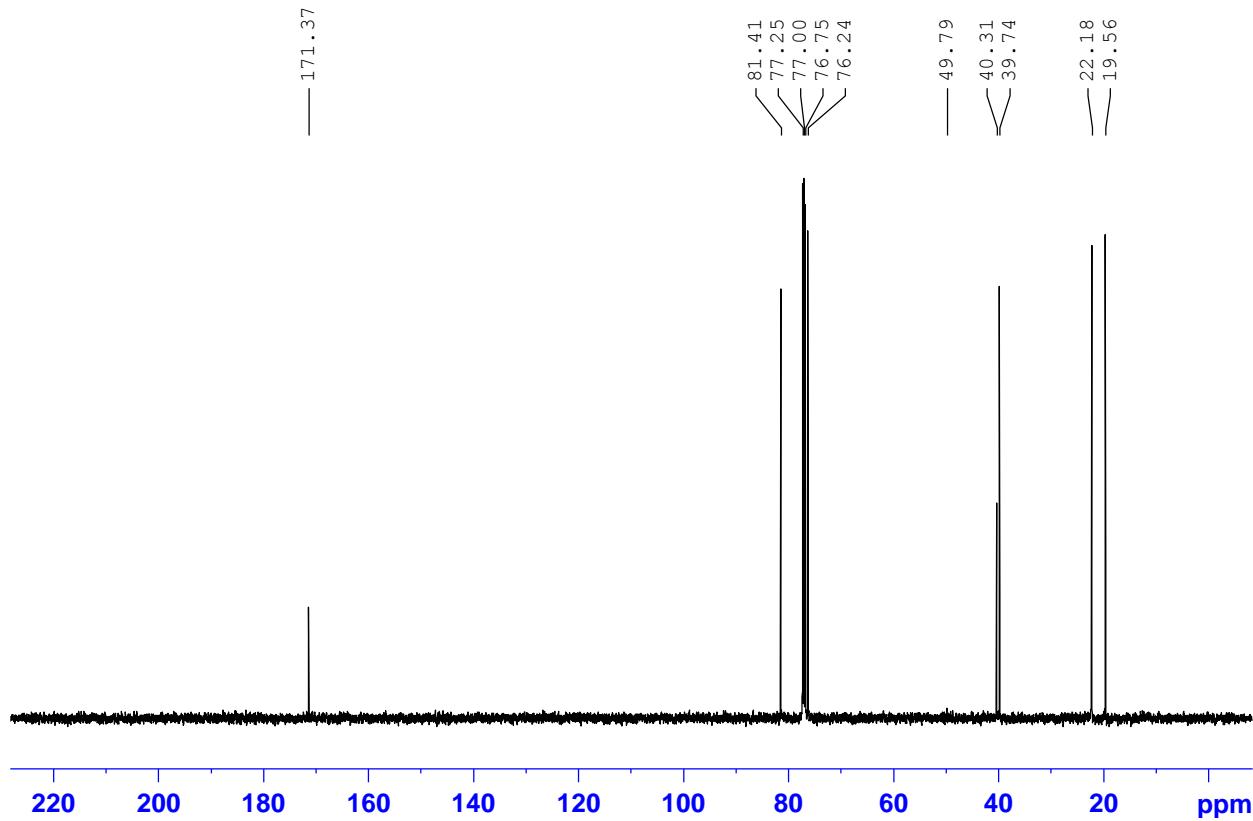


Figure S7. Complete $^{13}\text{C}\{^1\text{H}\}$ spectrum of compound 6 in CDCl_3 , 125 MHz.

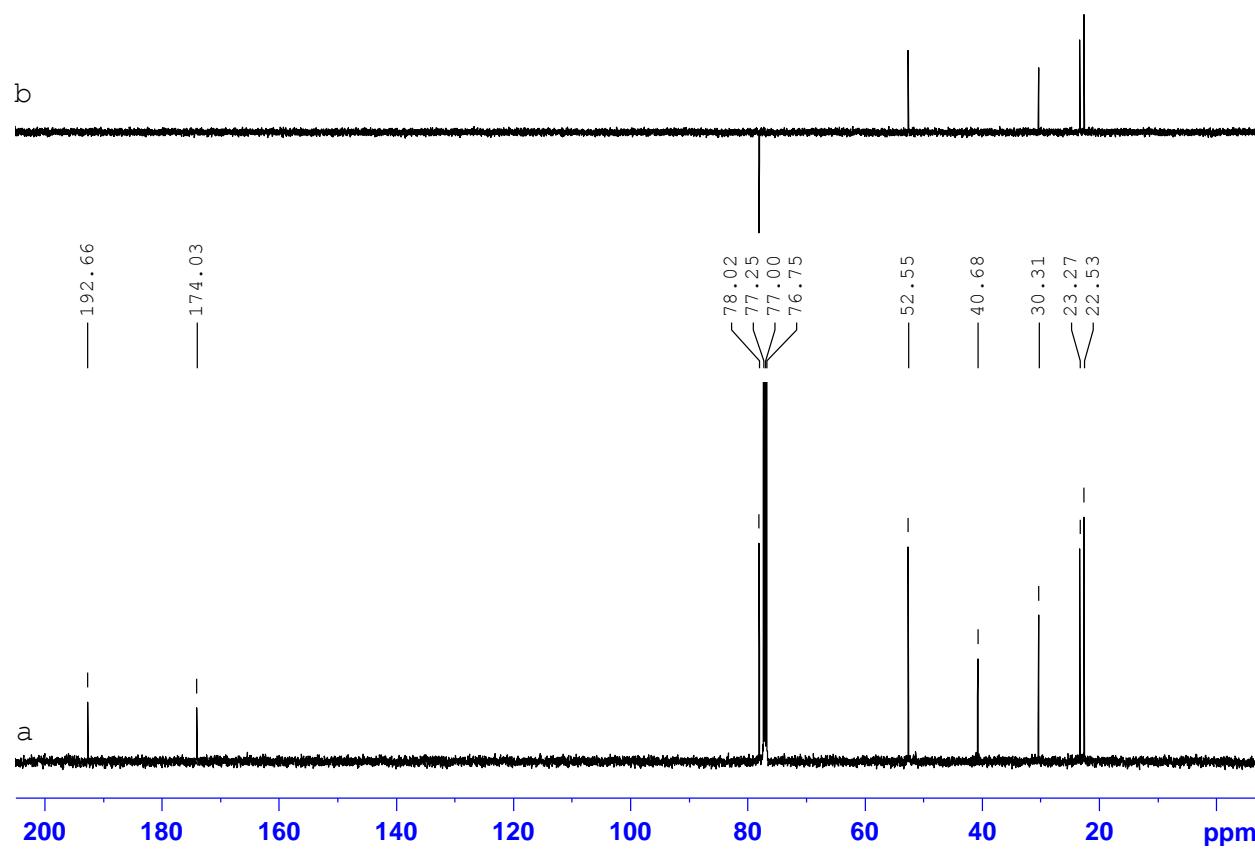


Figure S8. DEPT-135 editing $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound 6 in CDCl_3 , 125 MHz: a) $^{13}\text{C}\{^1\text{H}\}$ spectrum; b) DEPT-135.

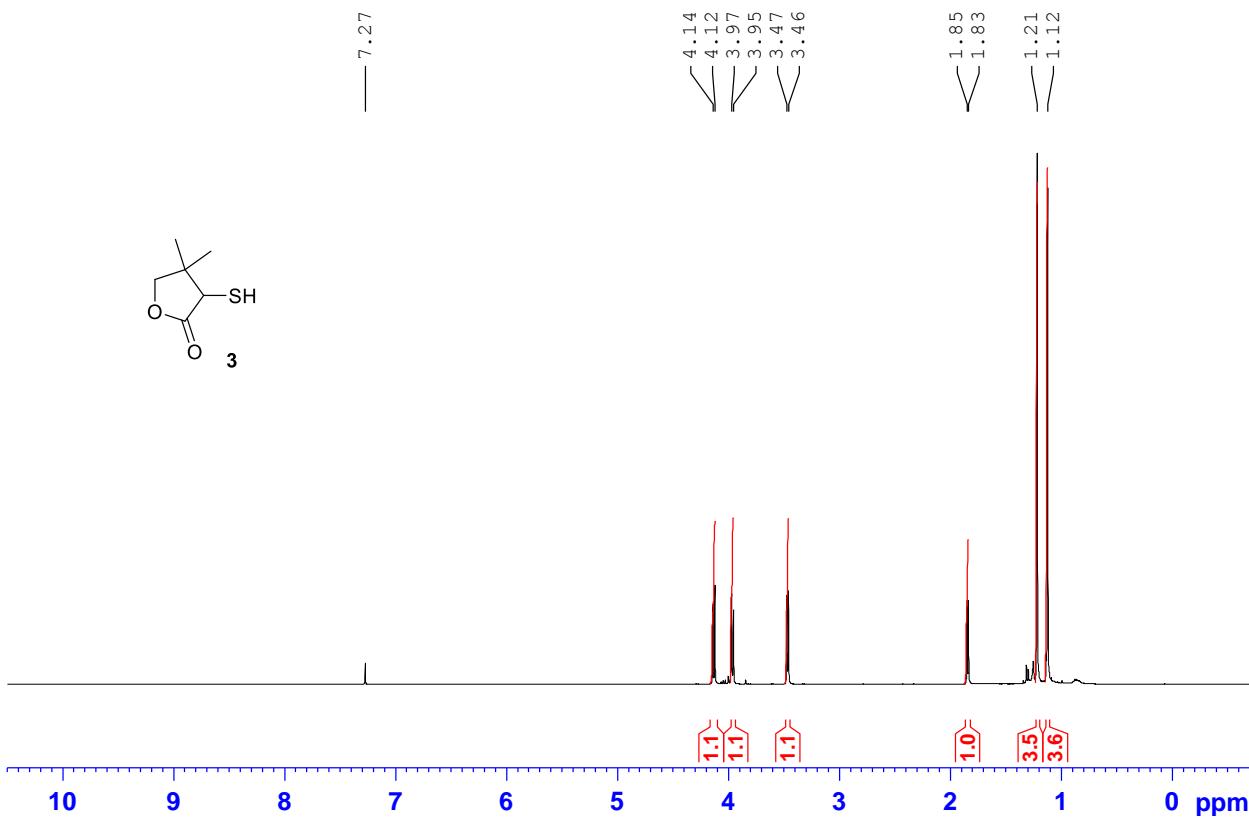


Figure S9. Complete ¹H NMR spectrum of compound 3 in CDCl₃, 500 MHz.

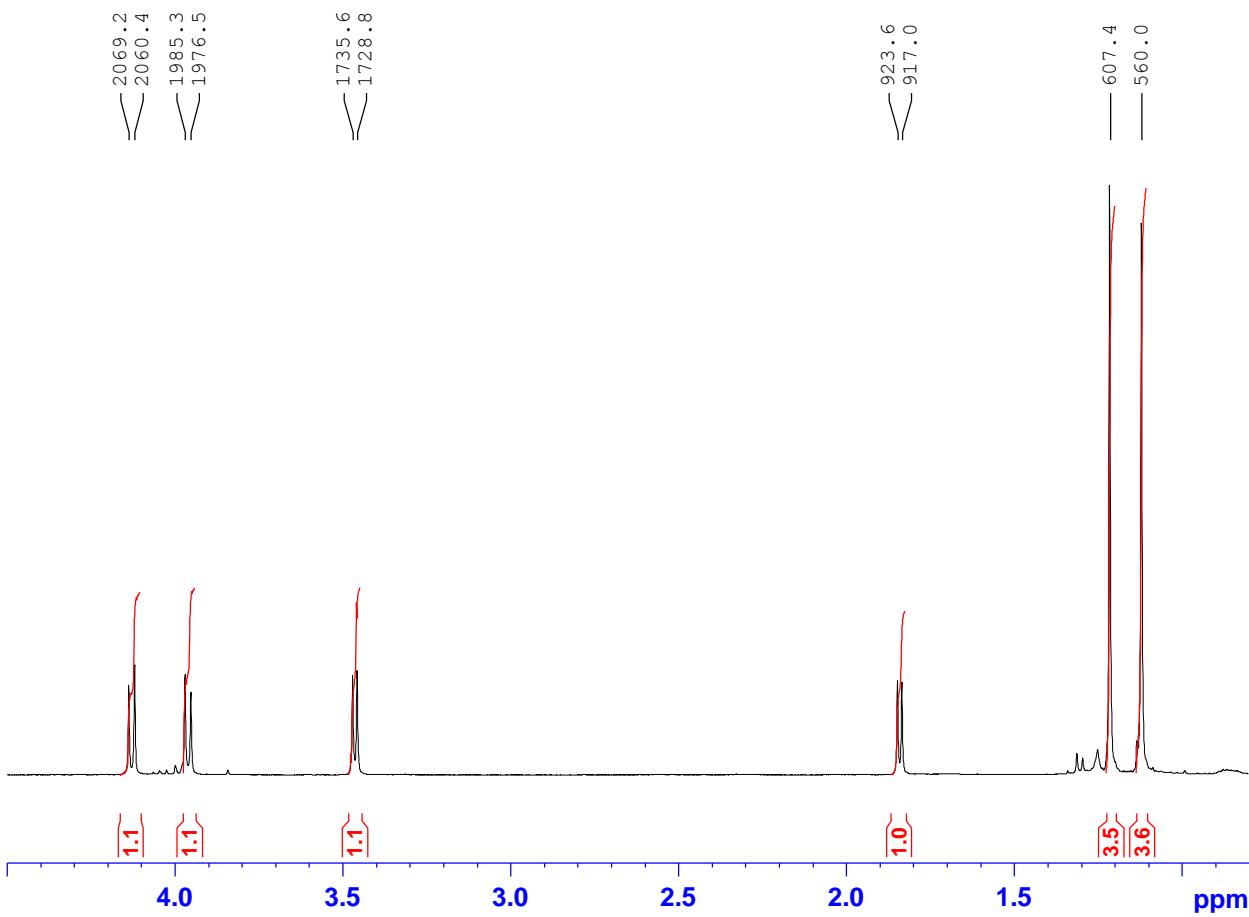


Figure S10. Expanded ¹H NMR spectrum of compound 3 in CDCl₃, 500 MHz.

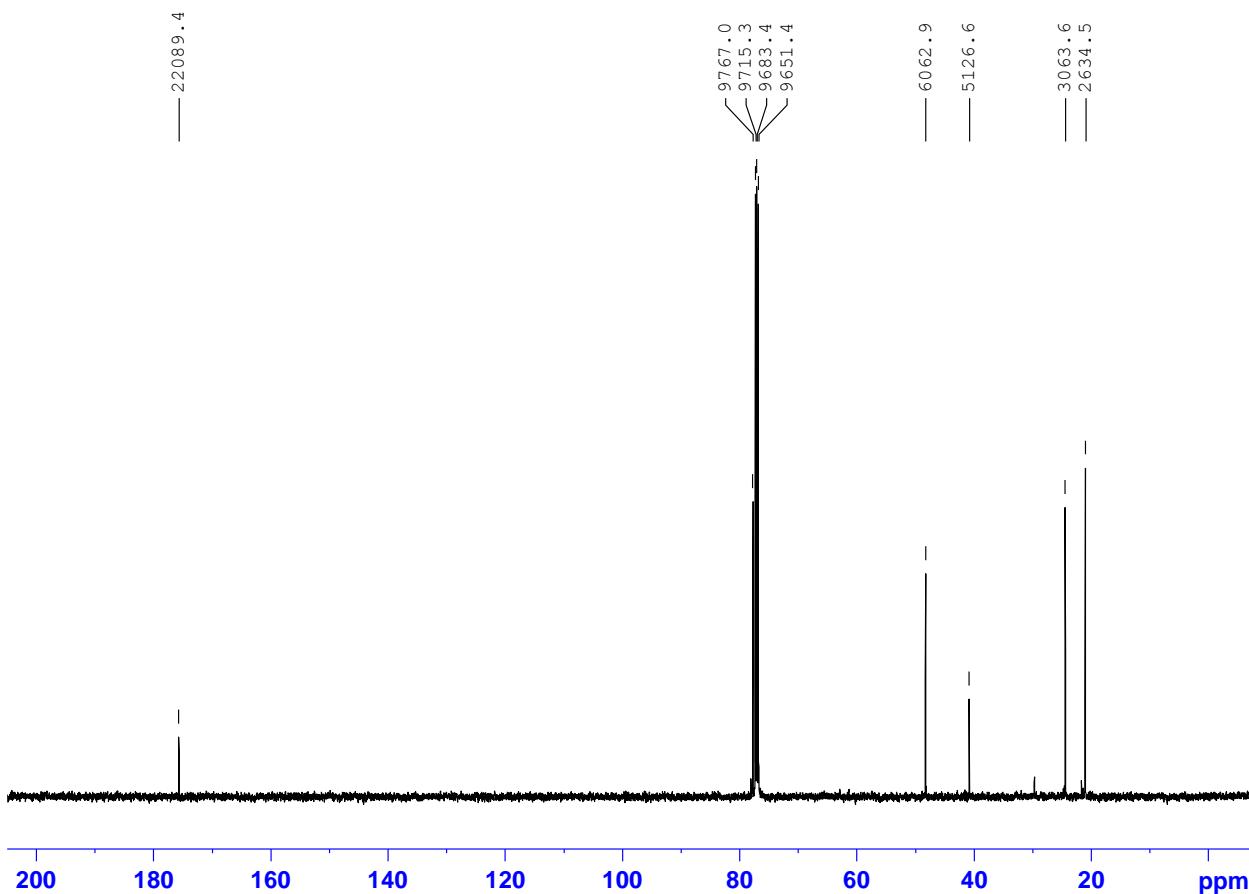


Figure S11. Complete $^{13}\text{C}\{^1\text{H}\}$ spectrum of compound 3 in CDCl_3 , 125 MHz.

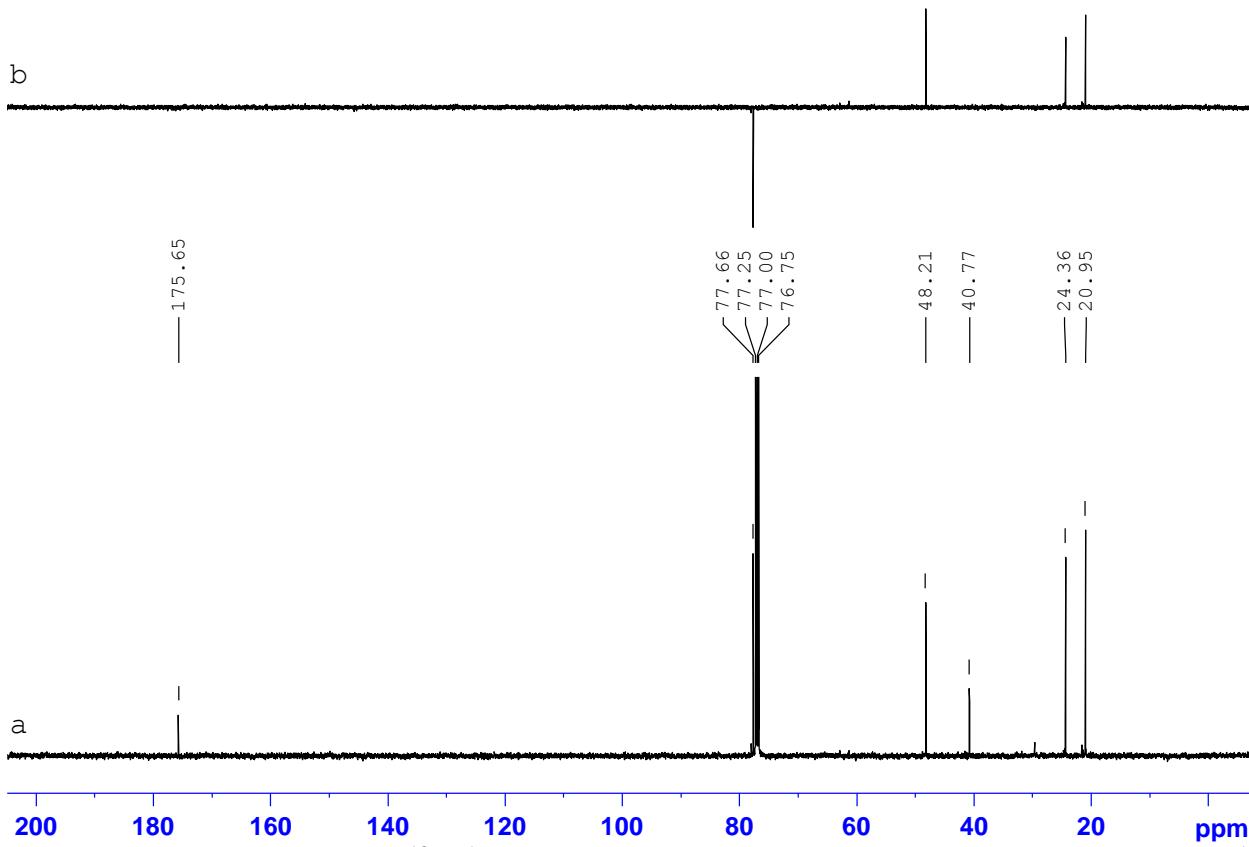


Figure S12. DEPT-135 editing $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound 3 in CDCl_3 , 125 MHz: a) $^{13}\text{C}\{^1\text{H}\}$ spectrum; b) DEPT-135.

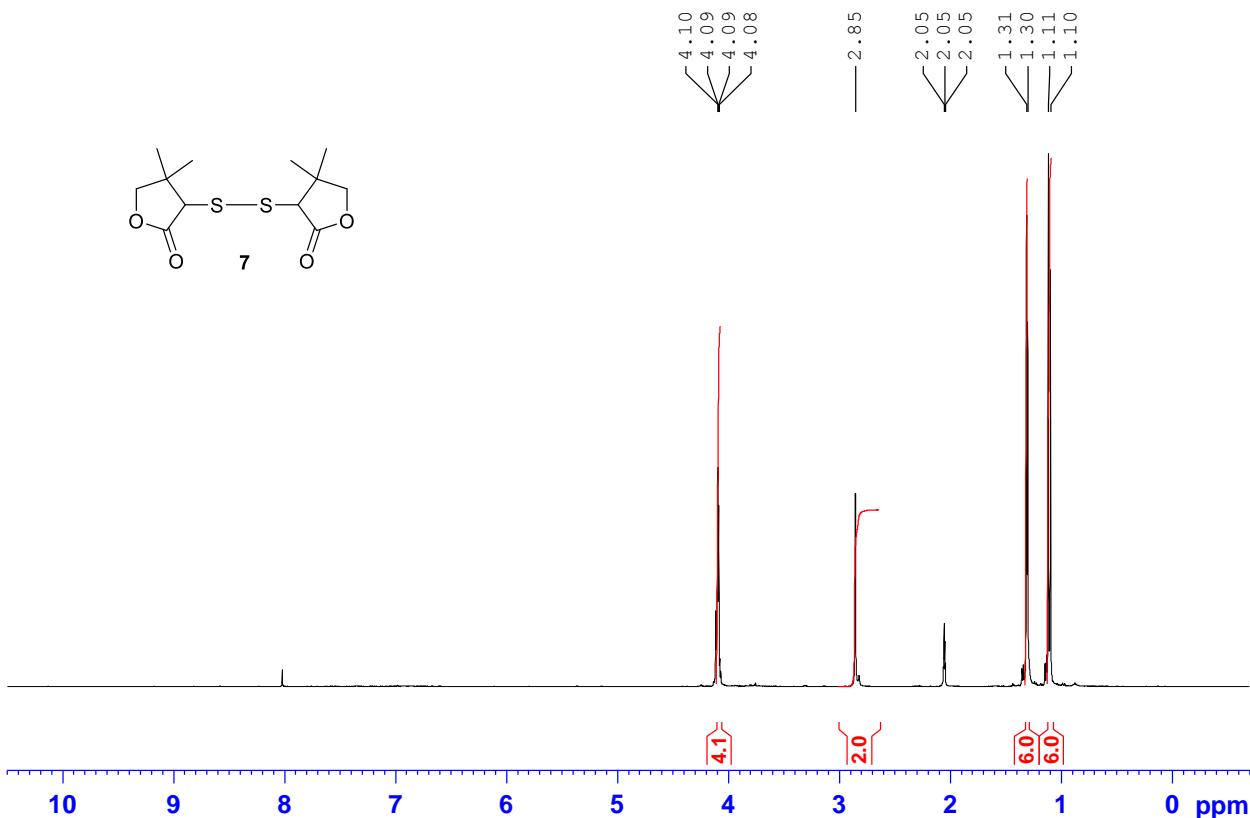


Figure S13. Complete ^1H NMR spectrum of compound 7 in Acetone- d_6 , 500 MHz.

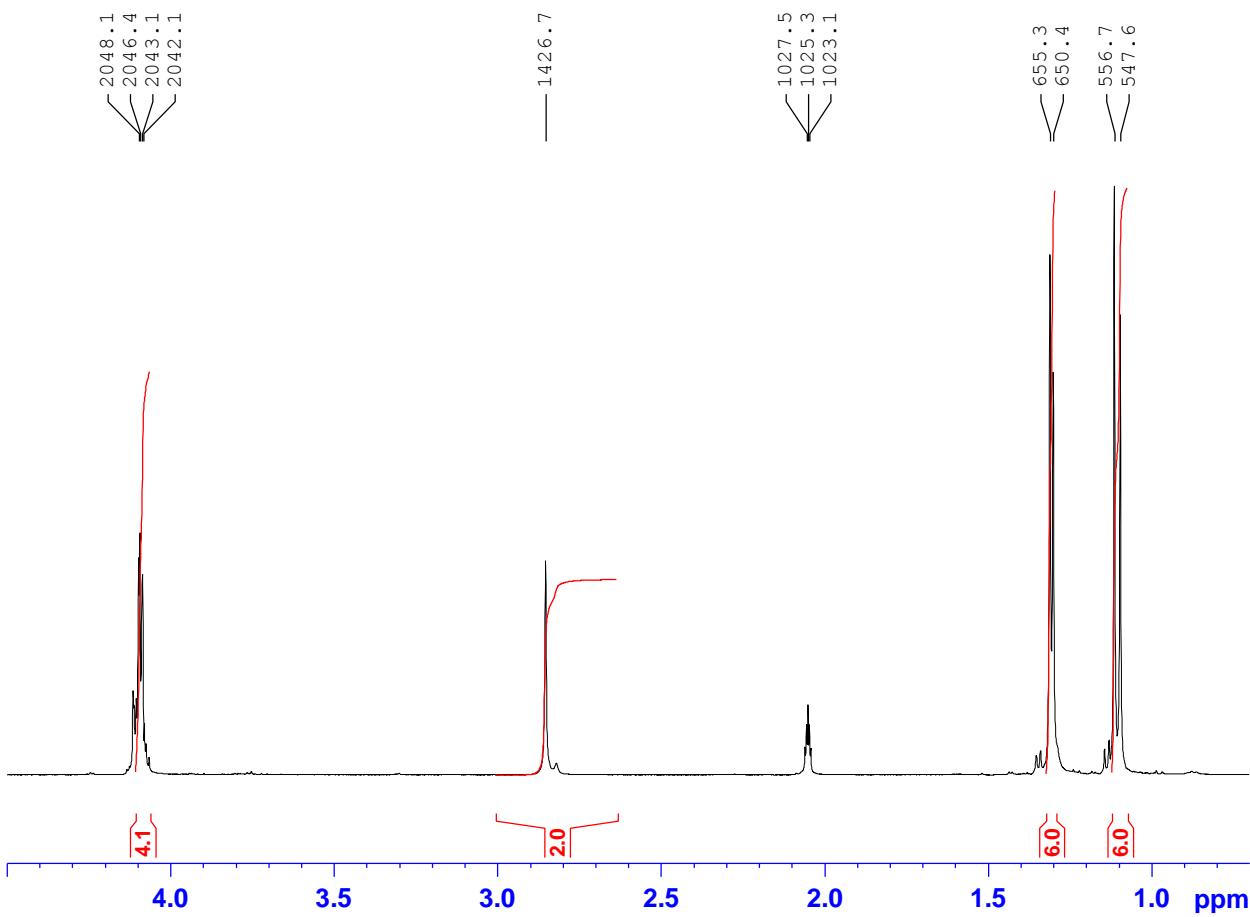


Figure S14. Expanded ^1H NMR spectrum of compound 7 in Acetone- d_6 , 500 MHz.

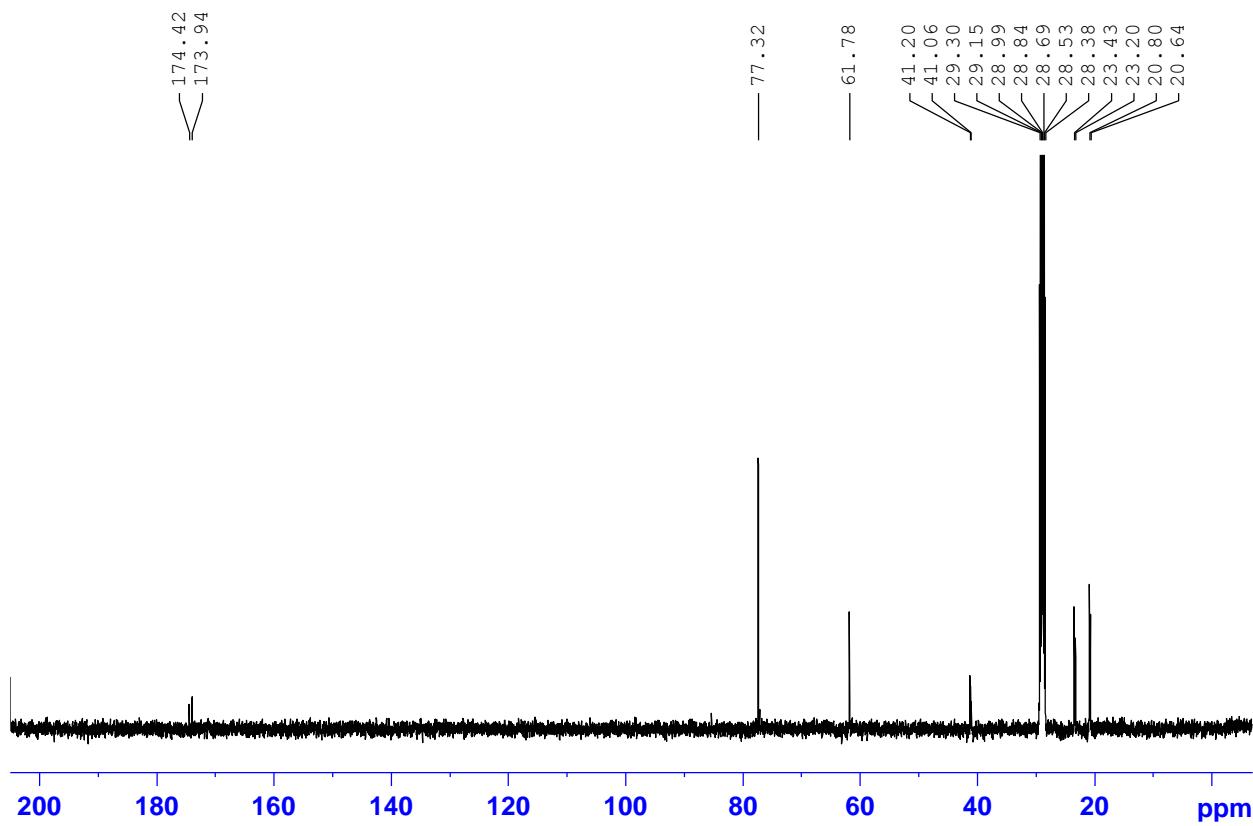


Figure S15. Complete $^{13}\text{C}\{^1\text{H}\}$ spectrum of compound 7 in Acetone- d_6 , 125 MHz.

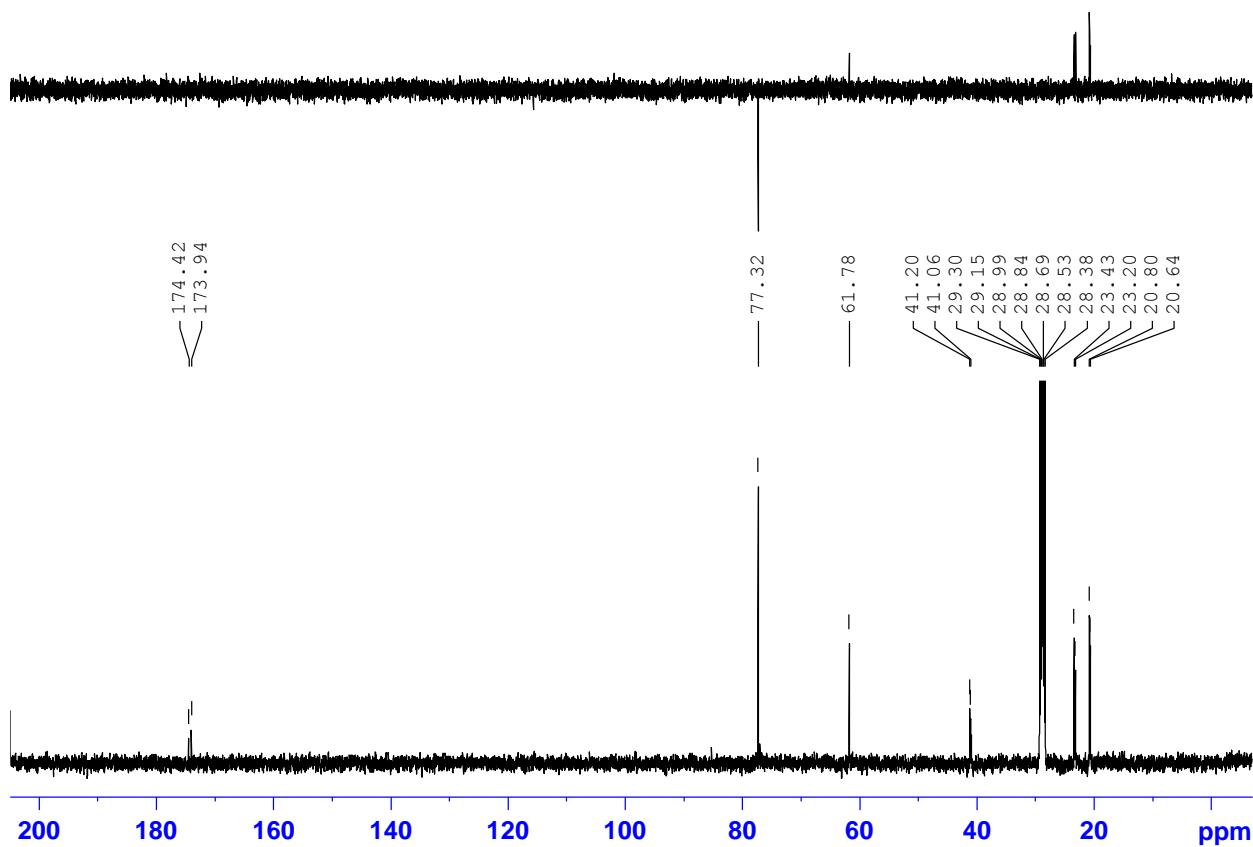


Figure S16. DEPT-135 editing $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound 7 in Acetone- d_6 , 125 MHz: a) $^{13}\text{C}\{^1\text{H}\}$ spectrum; b) DEPT-135.

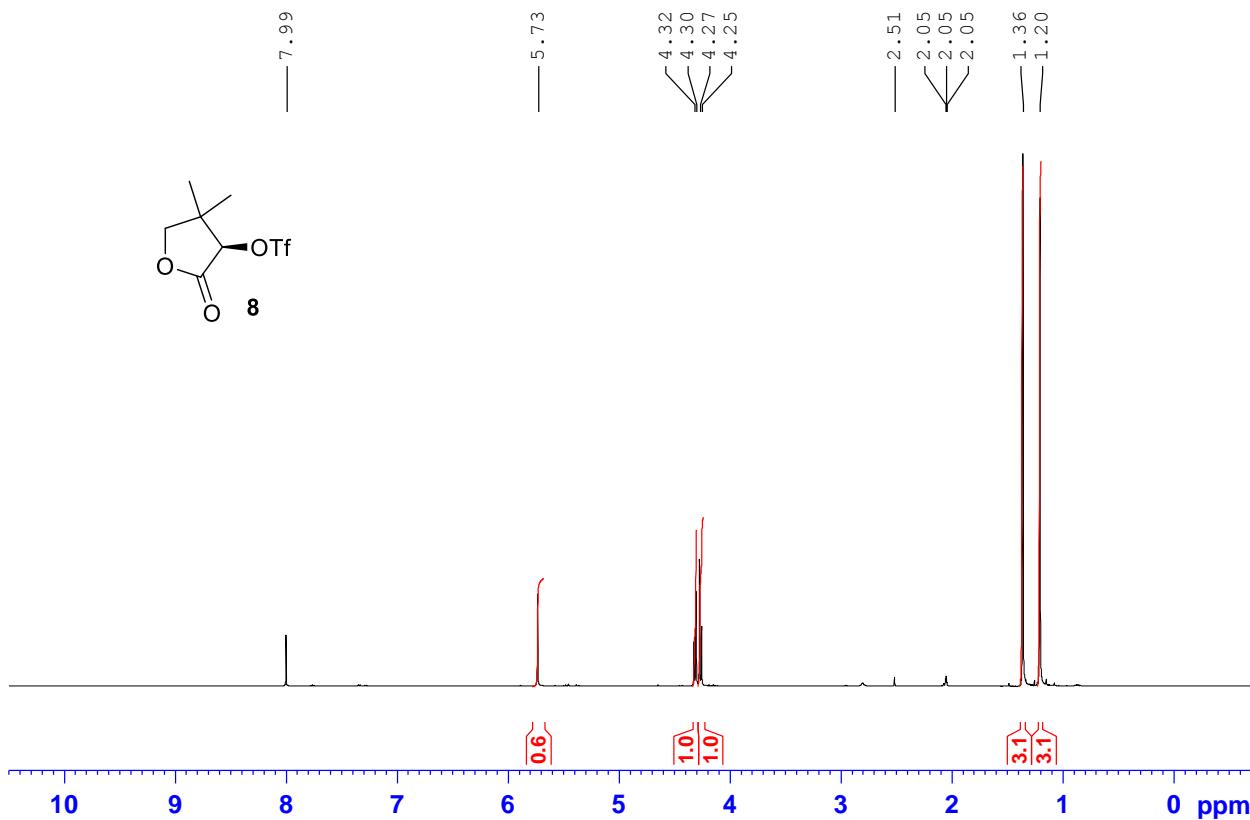


Figure S17. Complete ^1H NMR spectrum of compound **8** in Acetone- d_6 , 500 MHz.

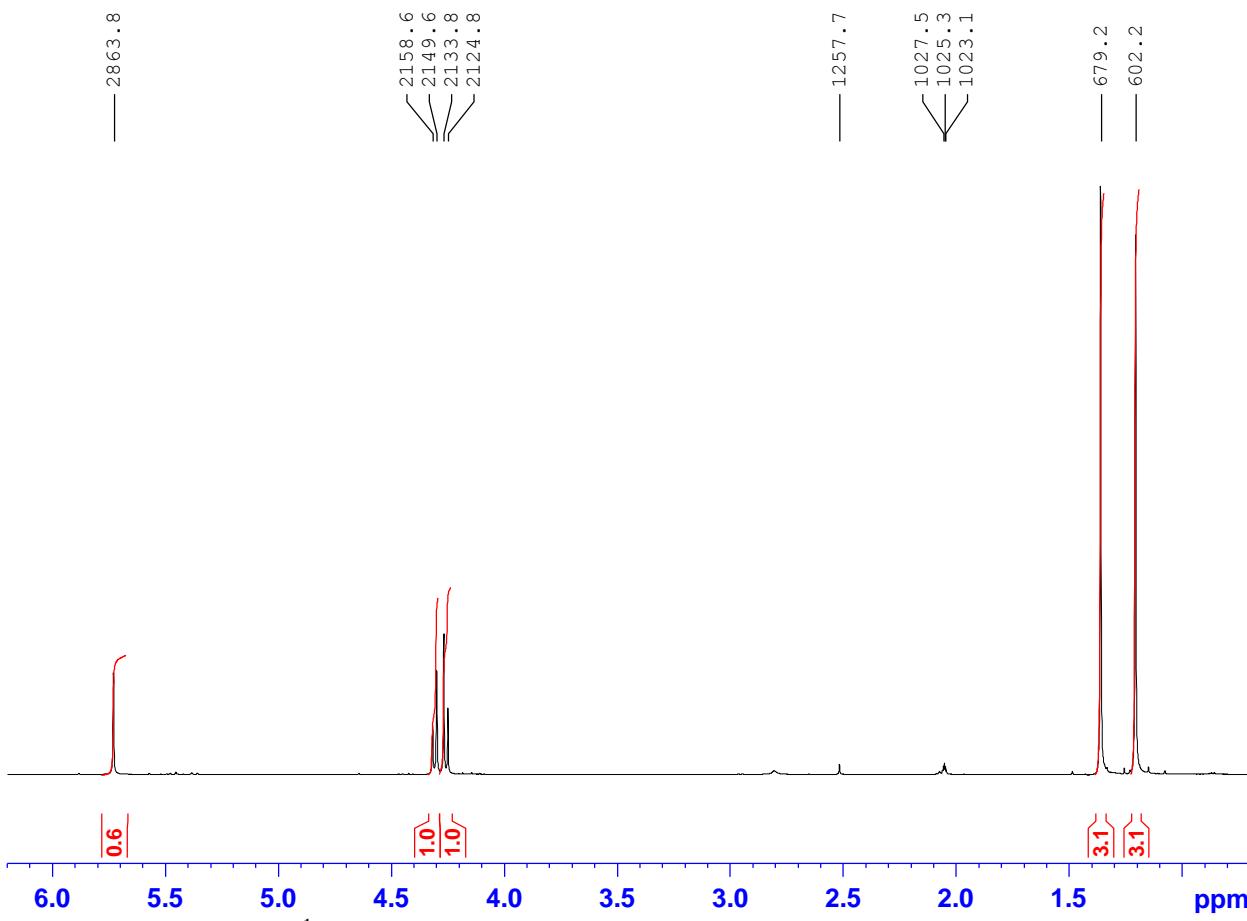


Figure S18. Expanded ^1H NMR spectrum of compound **8** in Acetone- d_6 , 500 MHz.

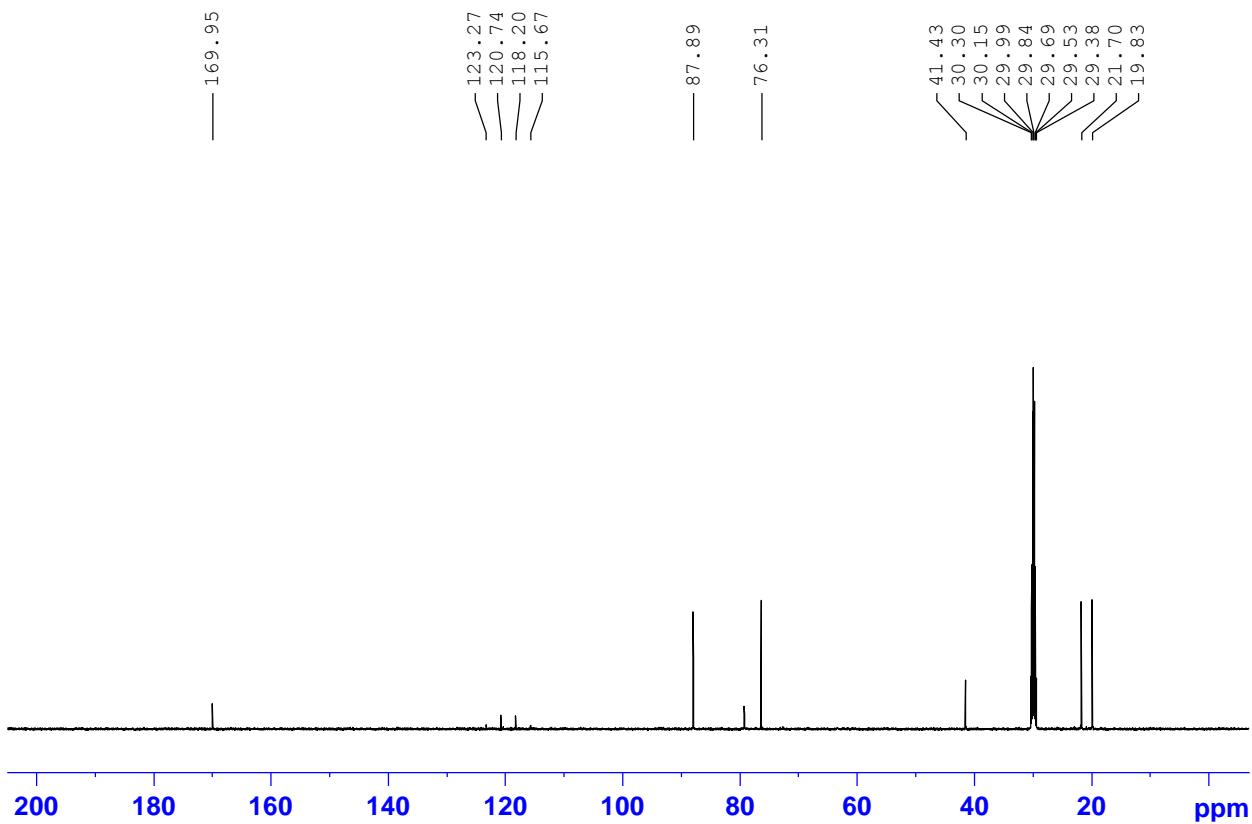


Figure S19. Complete $^{13}\text{C}\{^1\text{H}\}$ spectrum of compound **8** in Acetone- d_6 , 125 MHz.

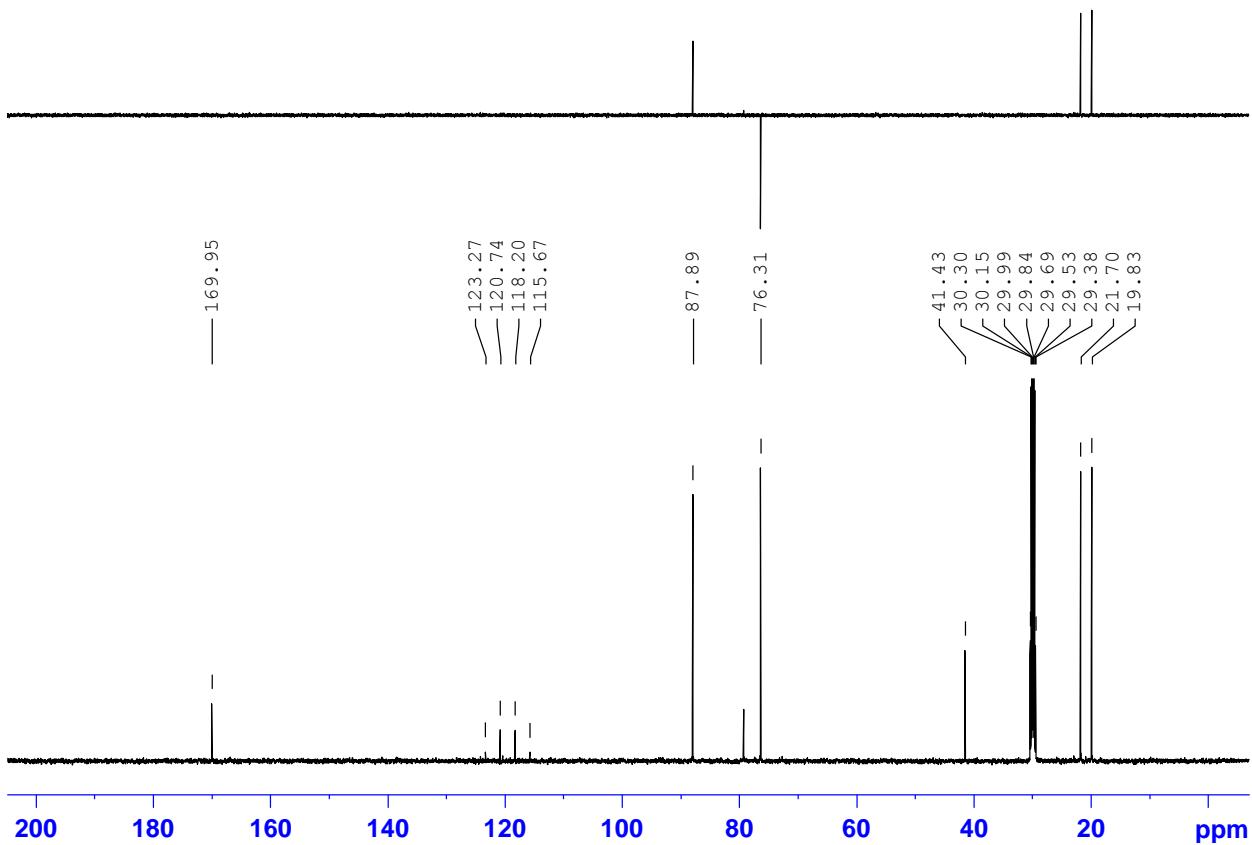
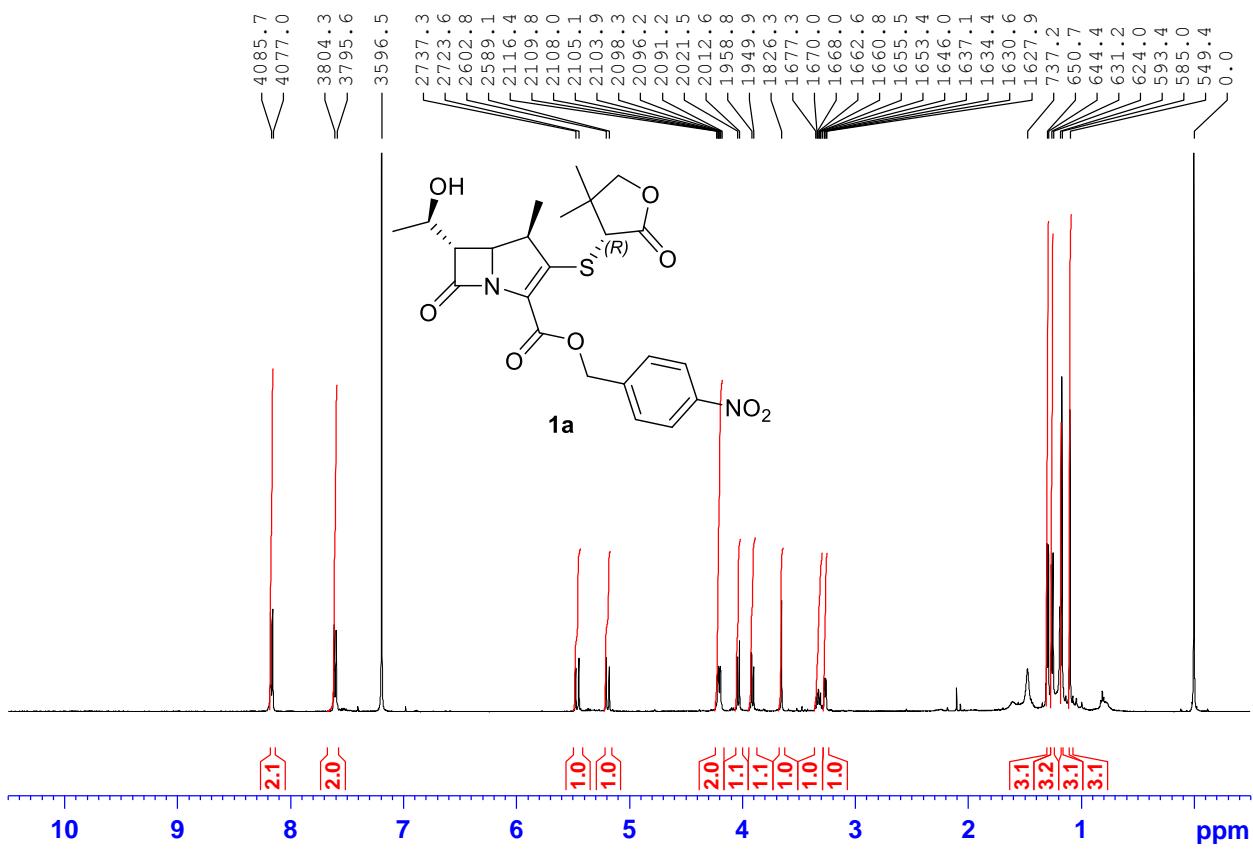
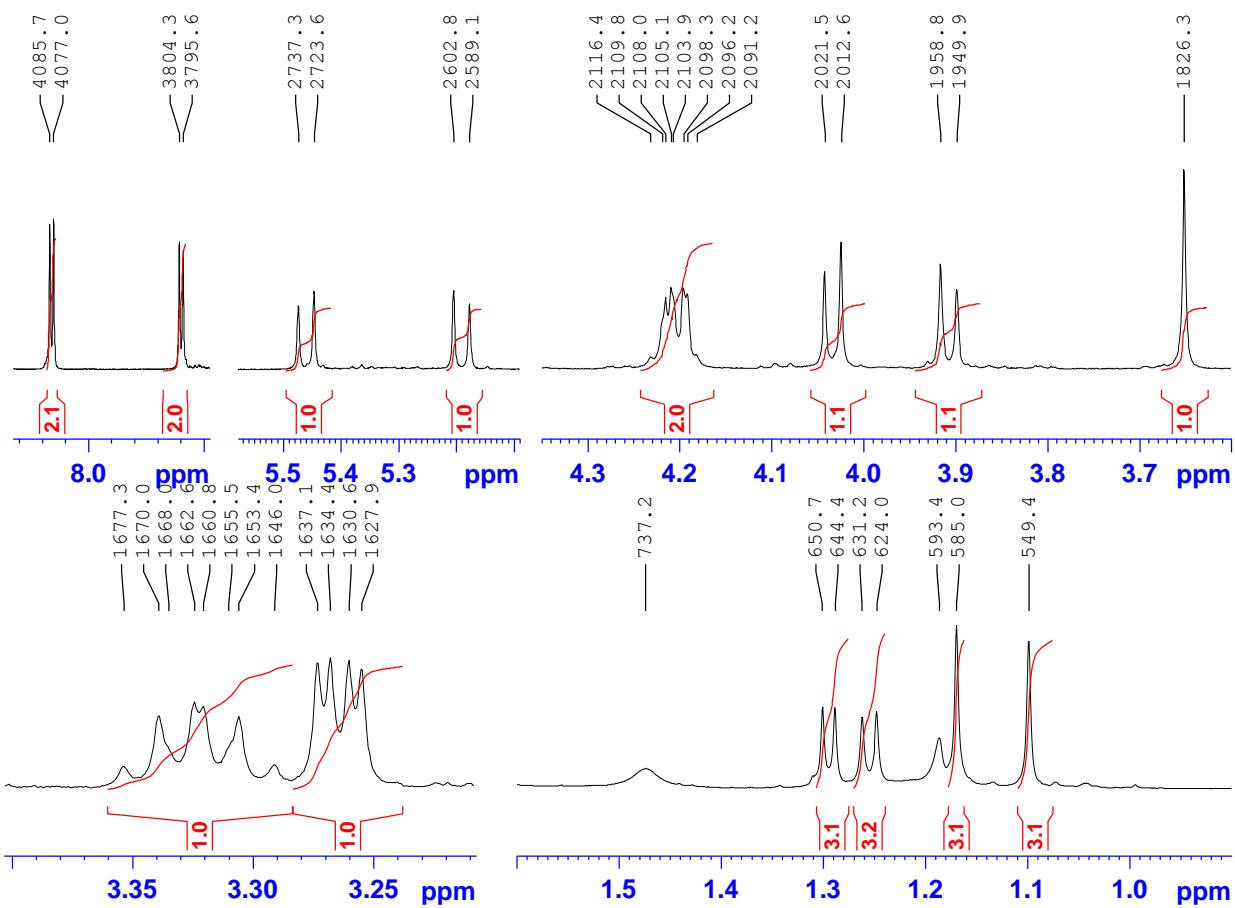


Figure S20. DEPT-135 editing $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **8** in Acetone- d_6 , 125 MHz: a) $^{13}\text{C}\{^1\text{H}\}$ spectrum; b) DEPT-135.

Figure S21. Complete ^1H NMR spectrum of compound **1a** in CDCl_3 , 500 MHz.Figure S22. Expanded ^1H NMR spectrum of compound **1a** in CDCl_3 , 500 MHz.

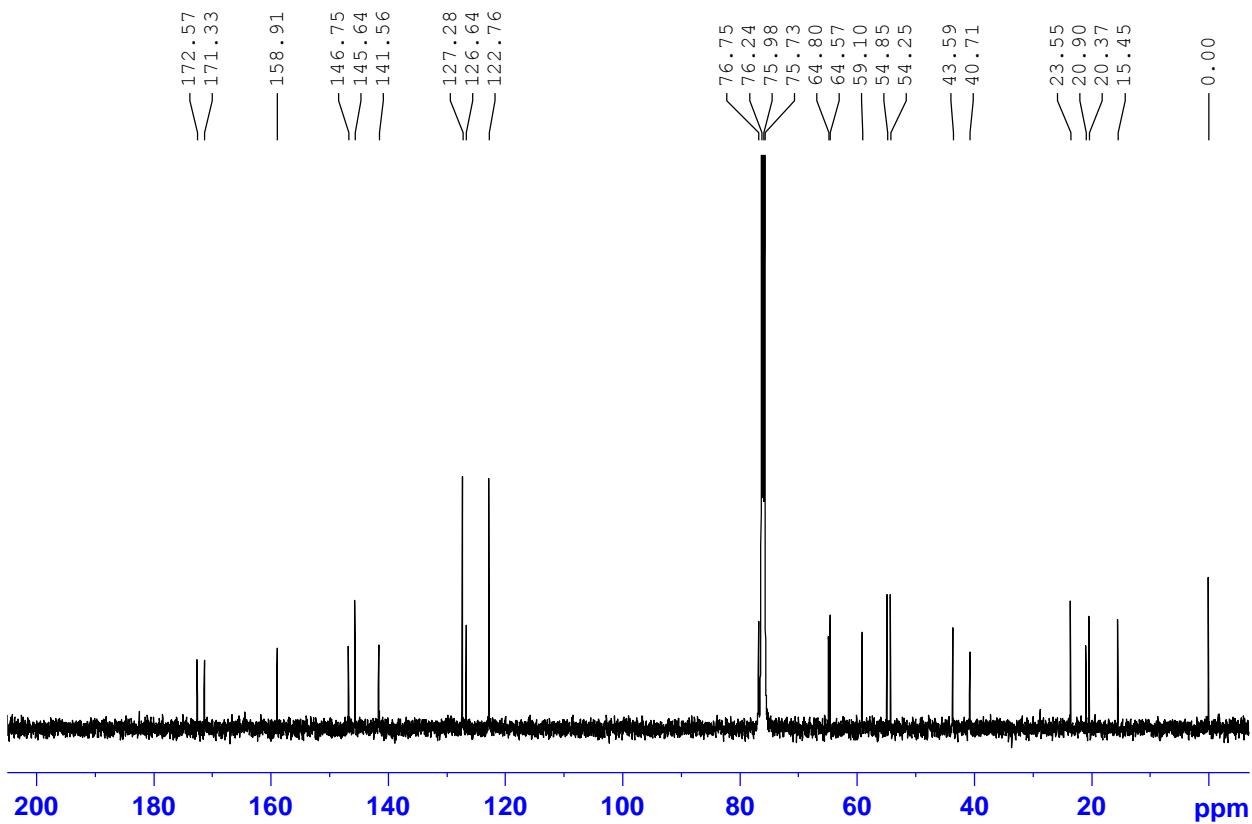


Figure S23. Complete $^{13}\text{C}\{\text{H}\}$ spectrum of compound **1a** in CDCl_3 , 125 MHz.

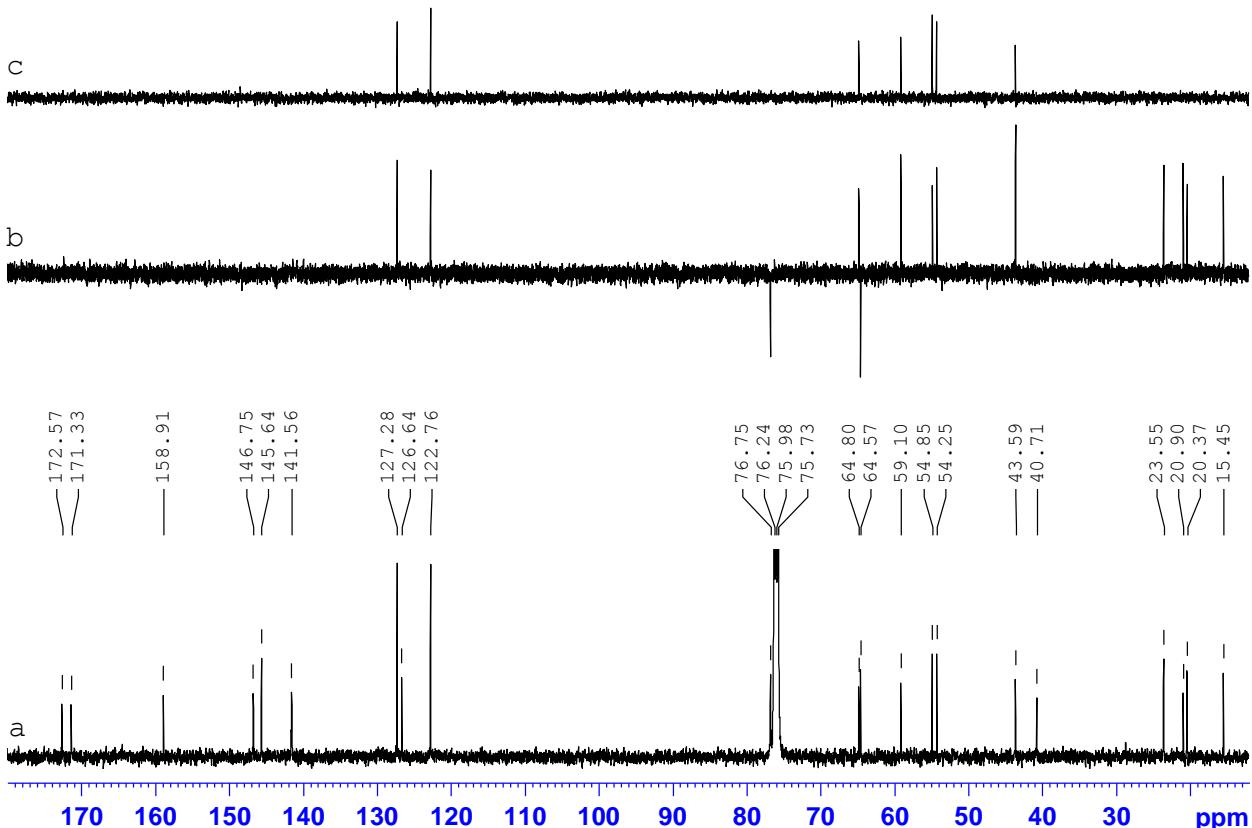


Figure S24. DEPT editing $^{13}\text{C}\{\text{H}\}$ NMR spectrum of compound **1a** in CDCl_3 , 125 MHz: a) $^{13}\text{C}\{\text{H}\}$ spectrum; b) DEPT-135; c) DEPT-90.

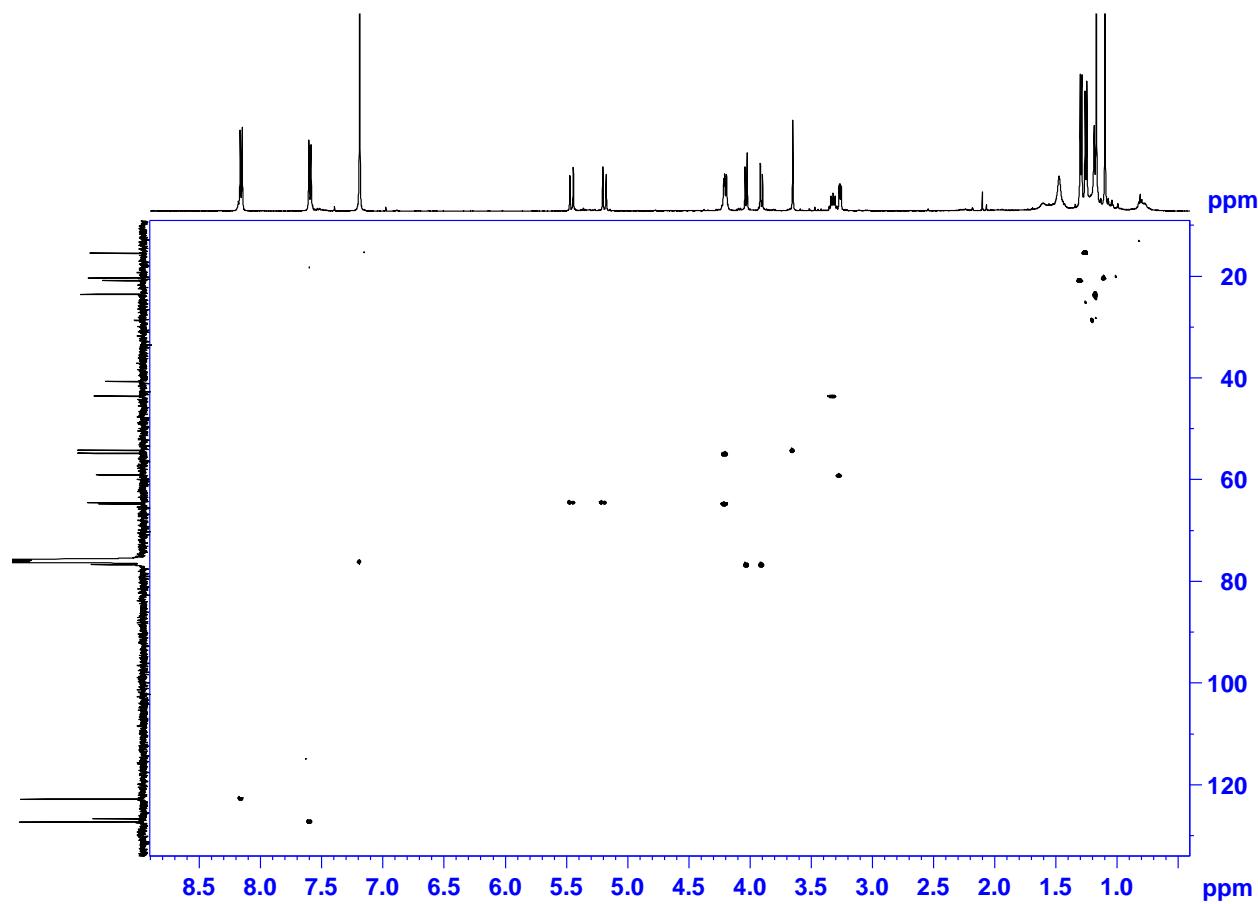


Figure S25. $\{^1\text{H}, ^{13}\text{C}\}$ HSQC NMR spectrum of compound **1a** in CDCl_3 , 500 MHz.

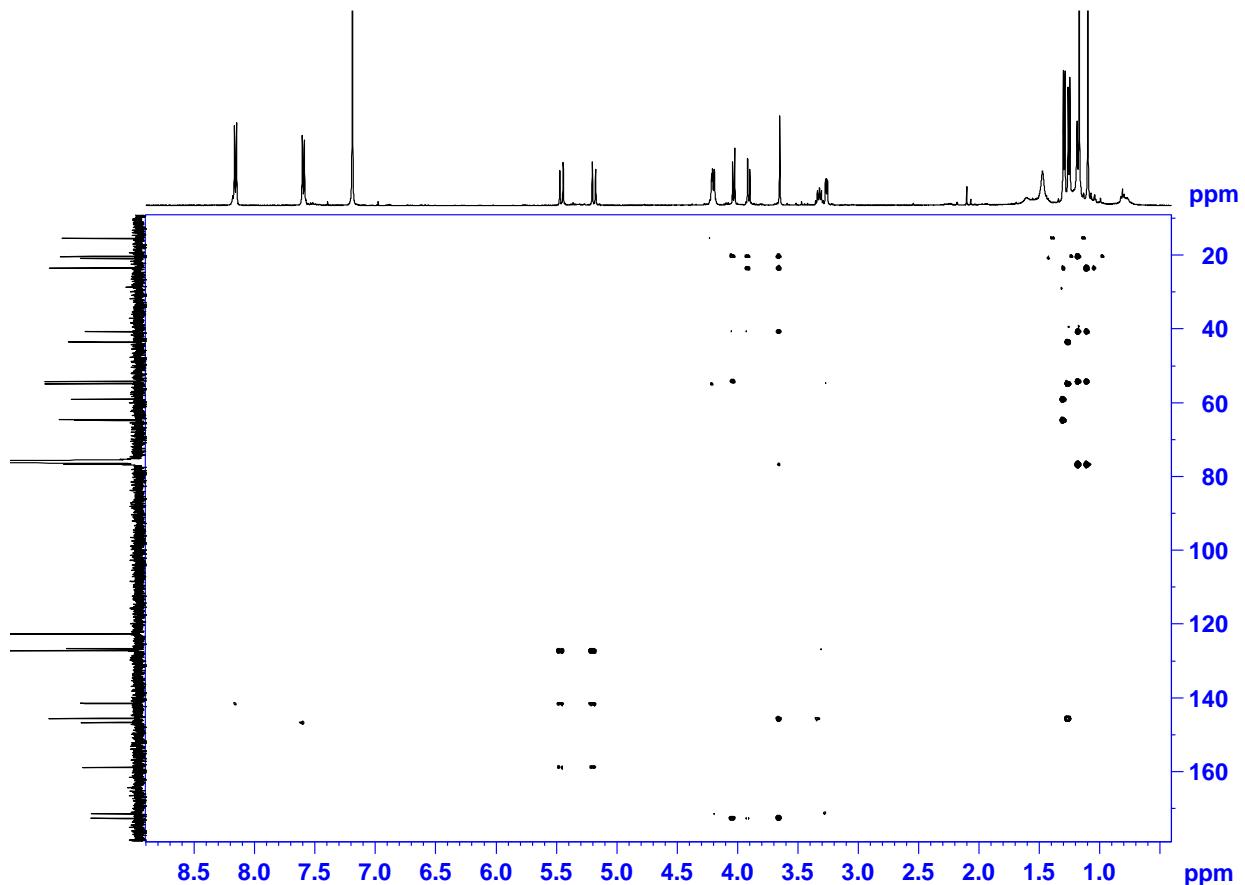


Figure S26. $\{^1\text{H}, ^{13}\text{C}\}$ HMBC NMR spectrum of compound **1a** in CDCl_3 , 500 MHz.

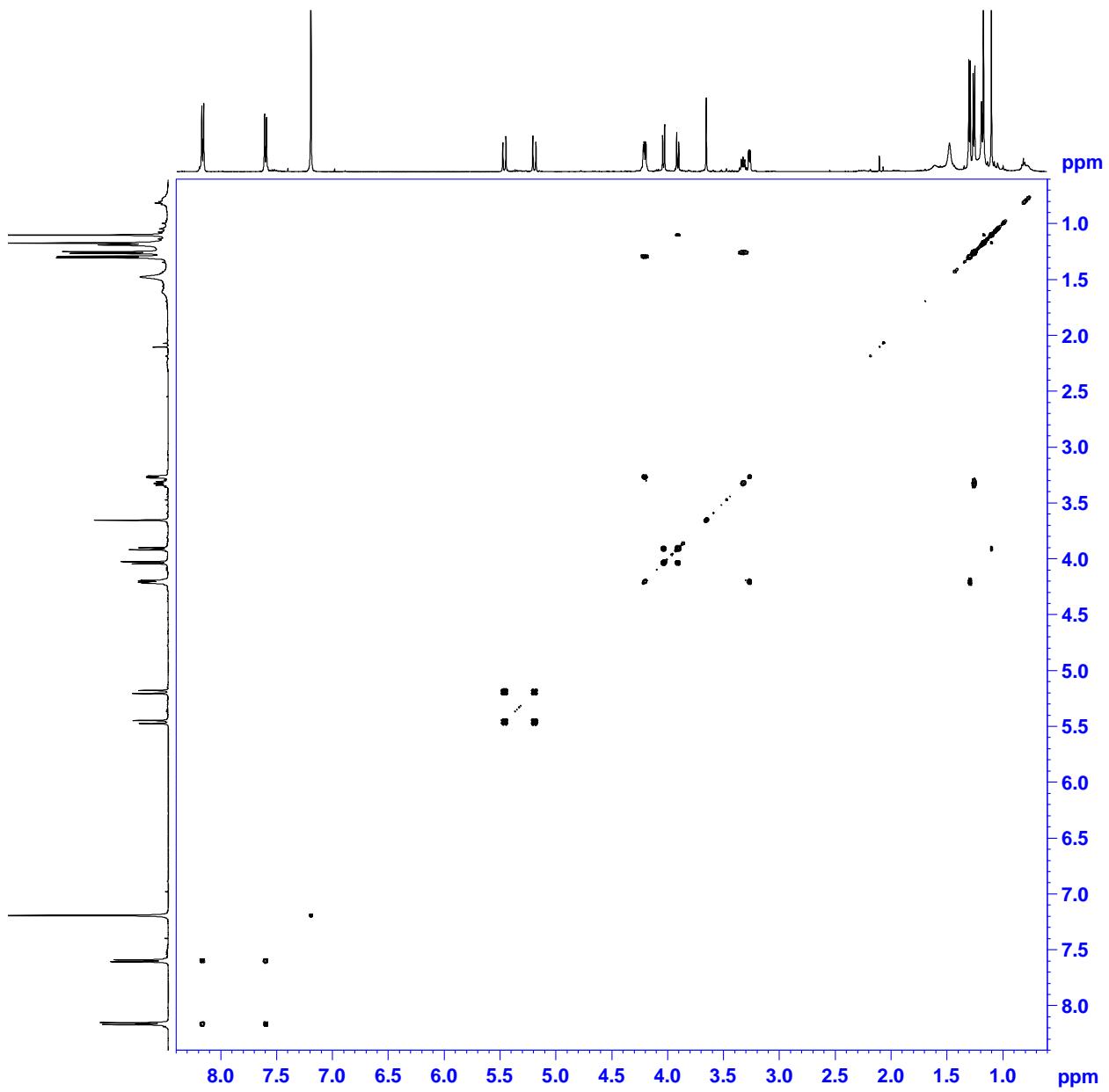


Figure S27. $\{^1\text{H}, ^1\text{H}\}$ COSY NMR spectrum of compound **1a** in CDCl_3 , 500 MHz.

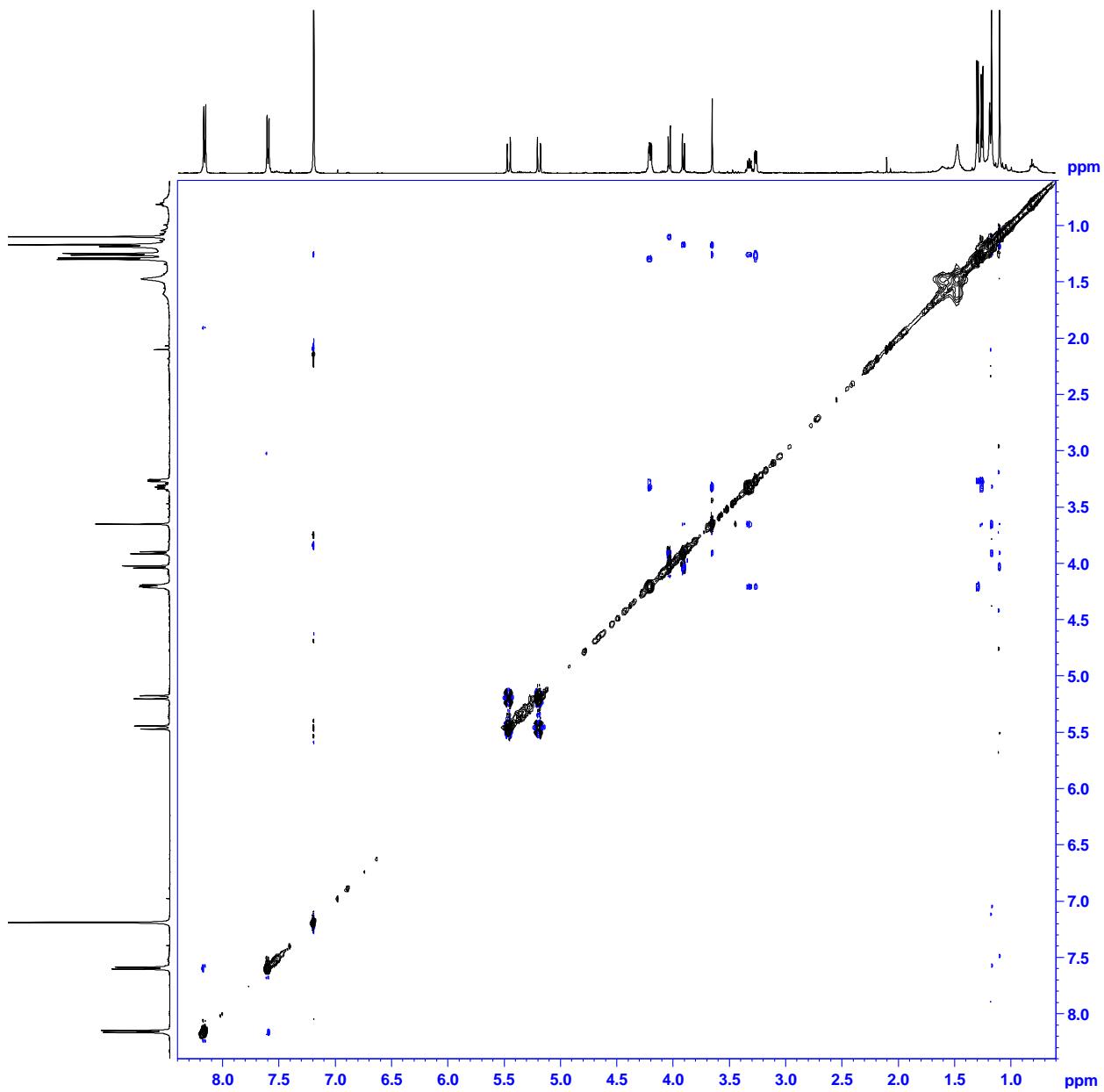


Figure S28. $\{^1\text{H}, ^1\text{H}\}$ NOESY NMR spectrum of compound **1a** in CDCl_3 , 500 MHz.

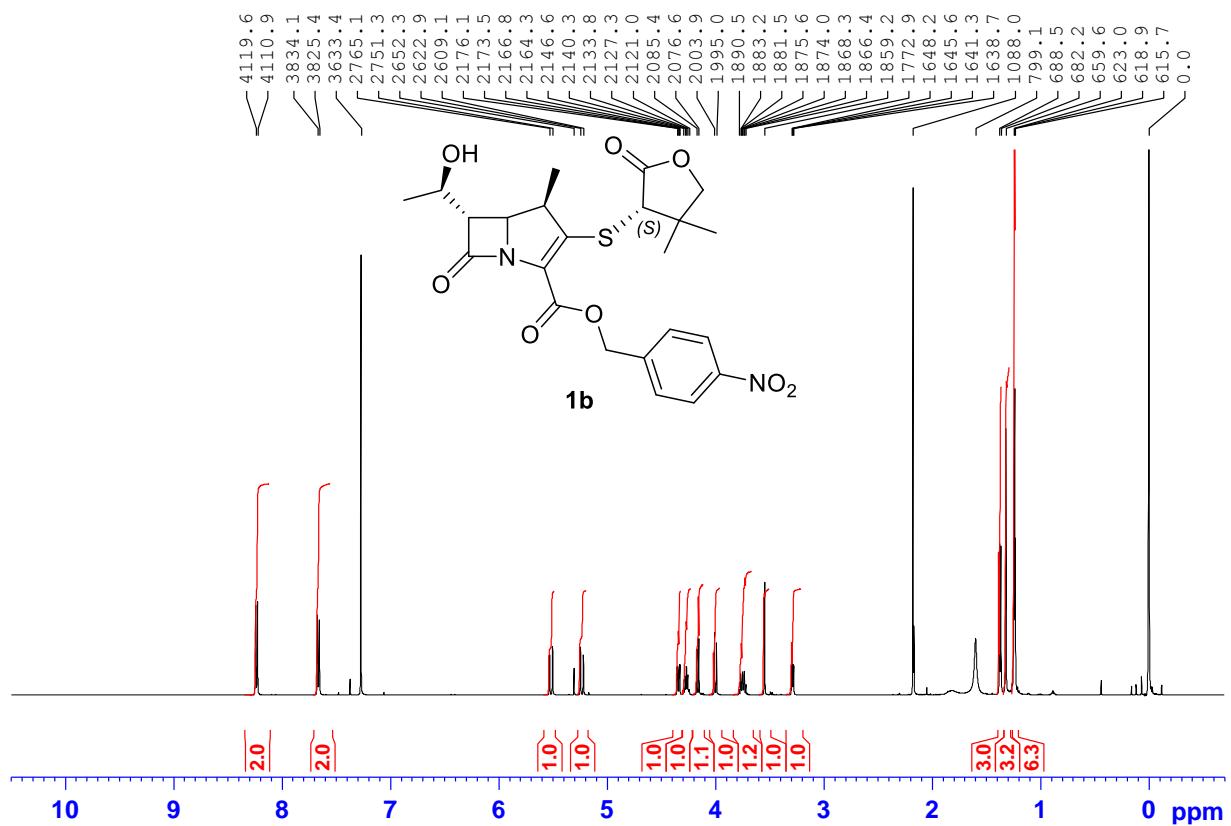


Figure S29. Complete ^1H NMR spectrum of compound **1b** in CDCl_3 , 500 MHz.

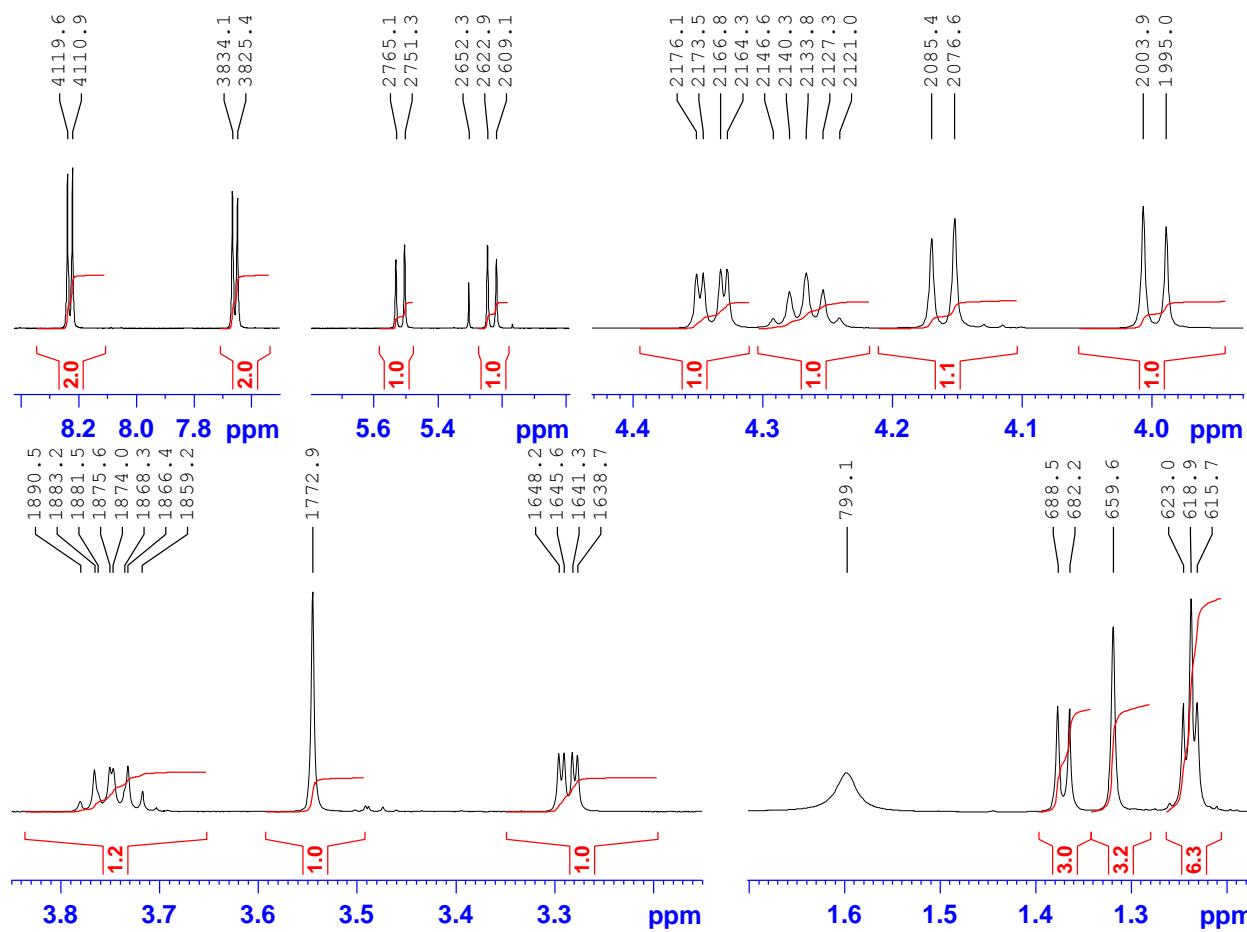


Figure S30. Expanded ^1H NMR spectrum of compound **1b** in CDCl_3 , 500 MHz.

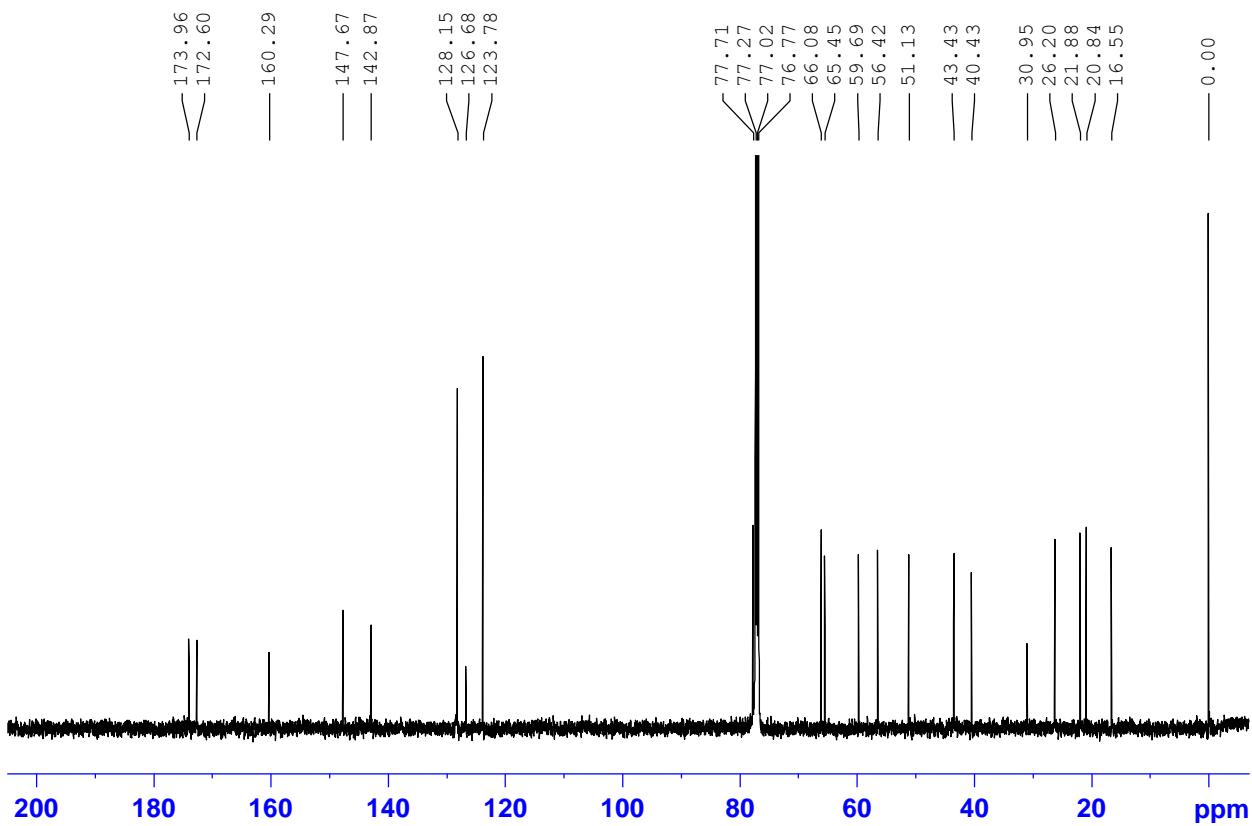


Figure S31. Complete $^{13}\text{C}\{\text{H}\}$ spectrum of compound **1b** in CDCl_3 , 125 MHz.

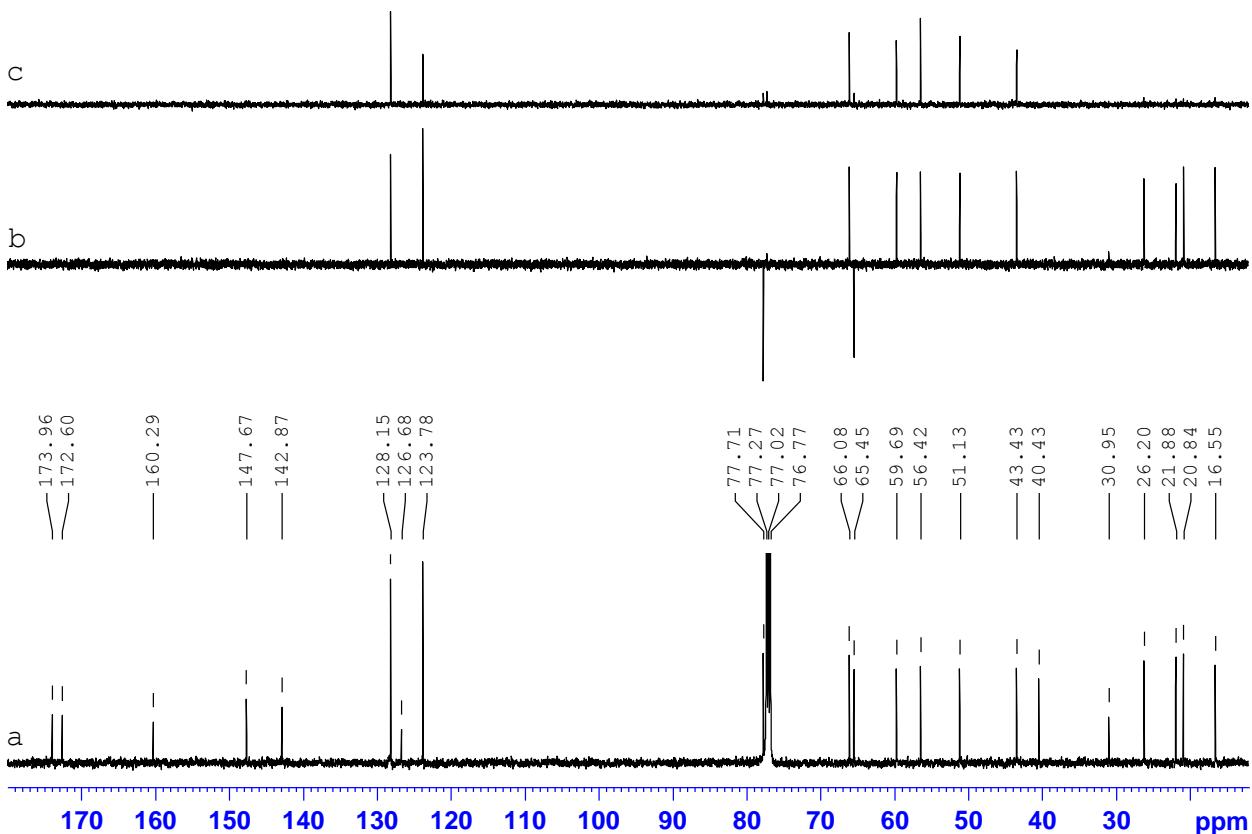


Figure S32. DEPT editing $^{13}\text{C}\{\text{H}\}$ NMR spectrum of compound **1b** in CDCl_3 , 125 MHz: a) $^{13}\text{C}\{\text{H}\}$ spectrum; b) DEPT-135; c) DEPT-90.

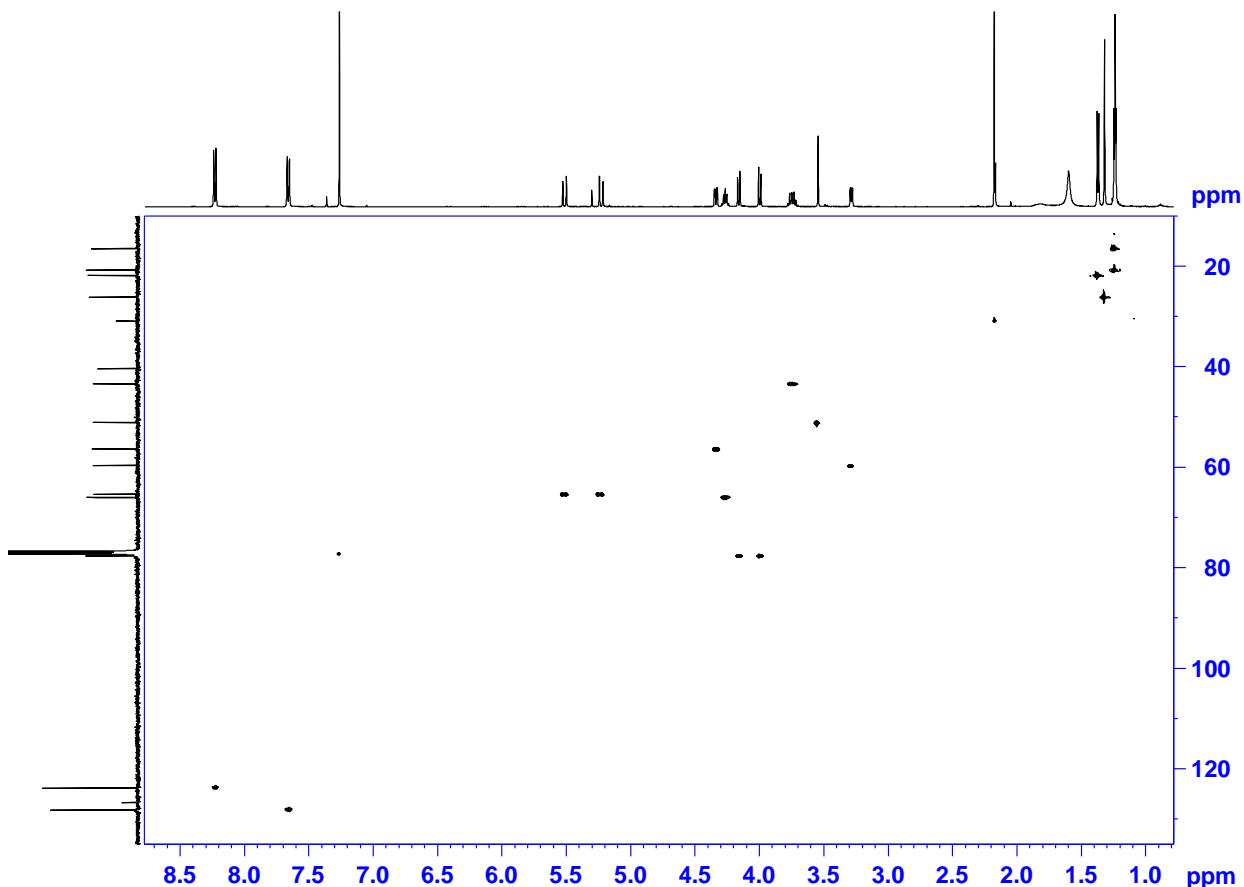


Figure S33. {¹H, ¹³C} HSQC NMR spectrum of compound **1b** in CDCl₃, 500 MHz.

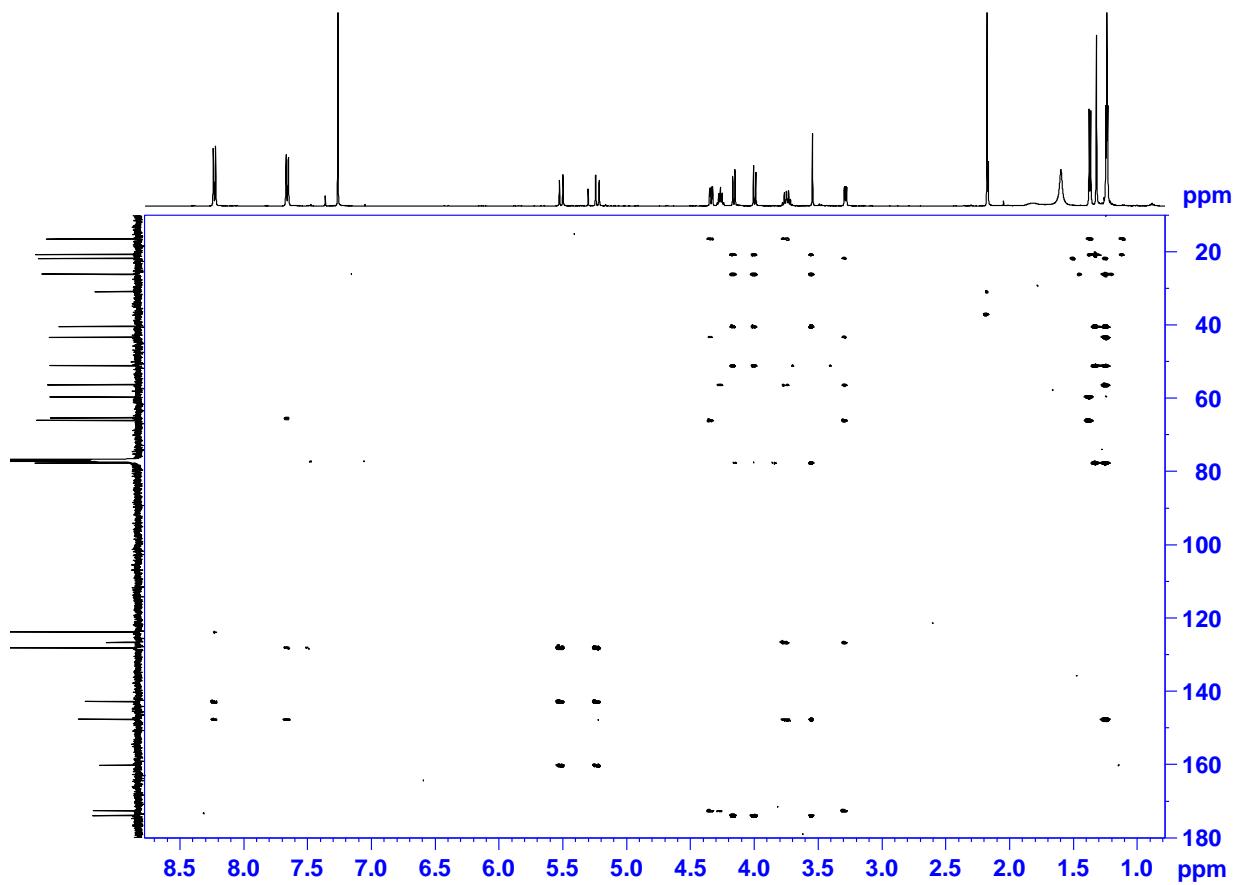


Figure S34. {¹H, ¹³C} HMBC NMR spectrum of compound **1b** in CDCl₃, 500 MHz.

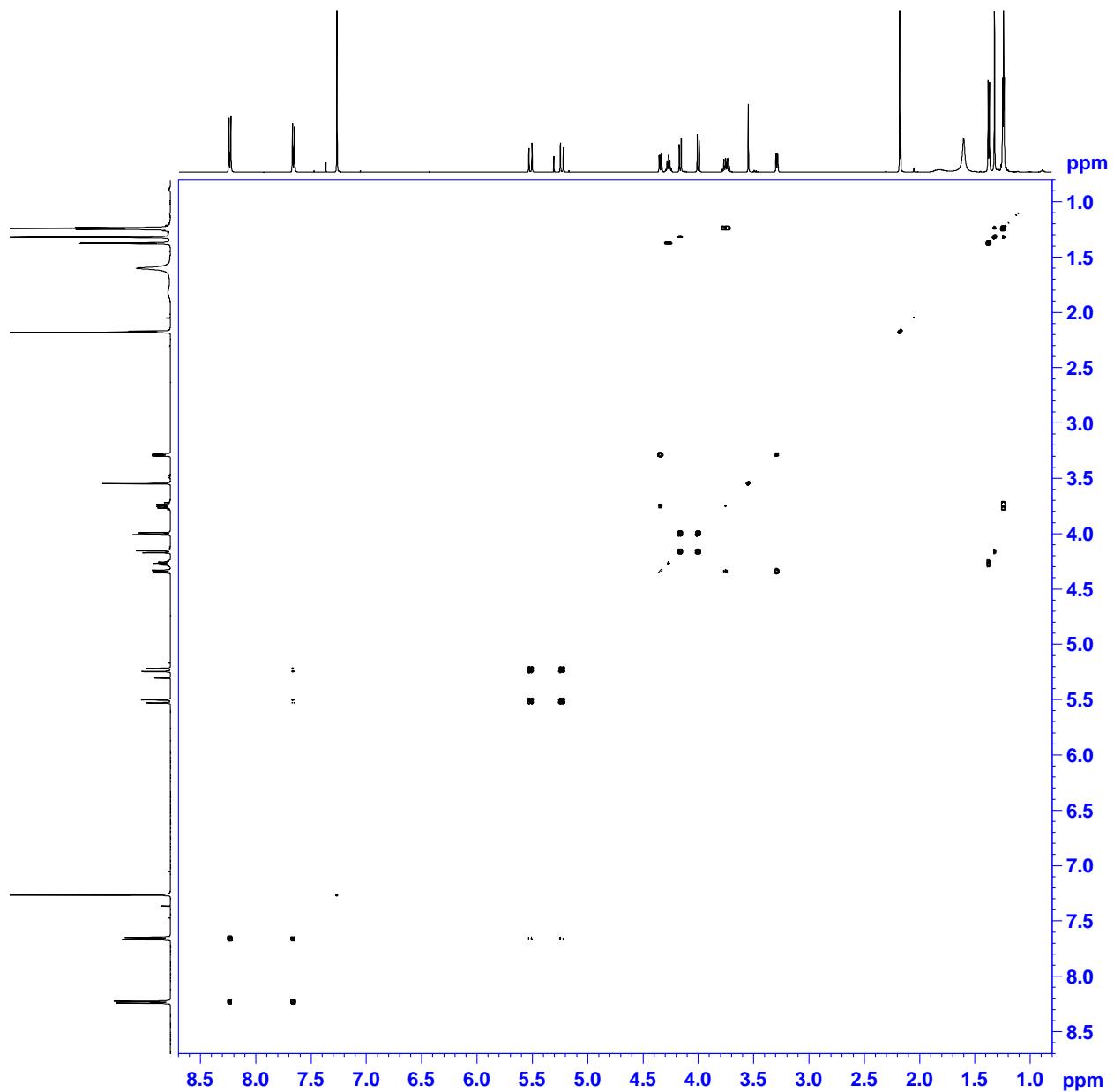


Figure S35. $\{^1\text{H}, ^1\text{H}\}$ COSY NMR spectrum of compound **1b** in CDCl_3 , 500 MHz.

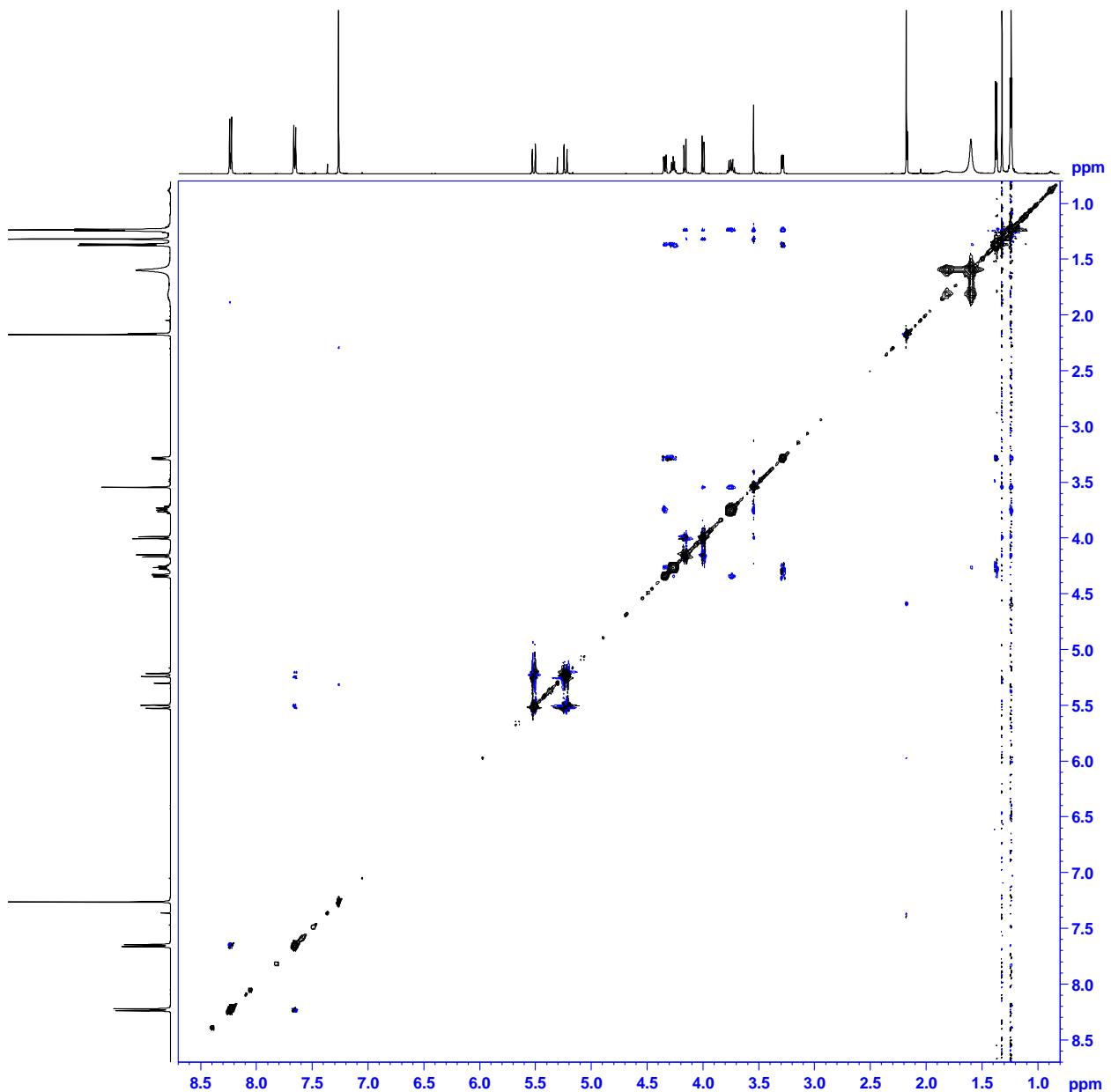


Figure S36. $\{^1\text{H}, ^1\text{H}\}$ NOESY NMR spectrum of compound **1b** in CDCl_3 , 500 MHz.

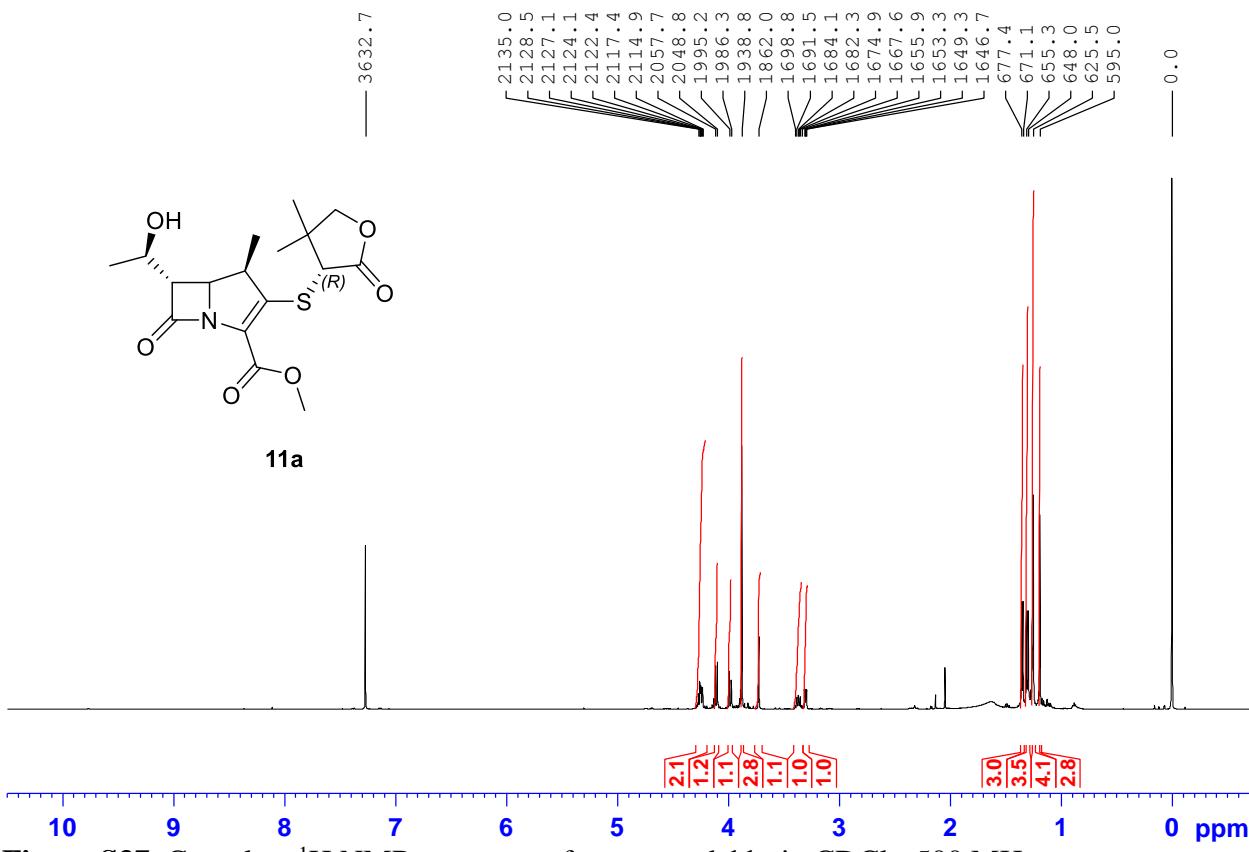


Figure S37. Complete ^1H NMR spectrum of compound **11a** in CDCl_3 , 500 MHz.

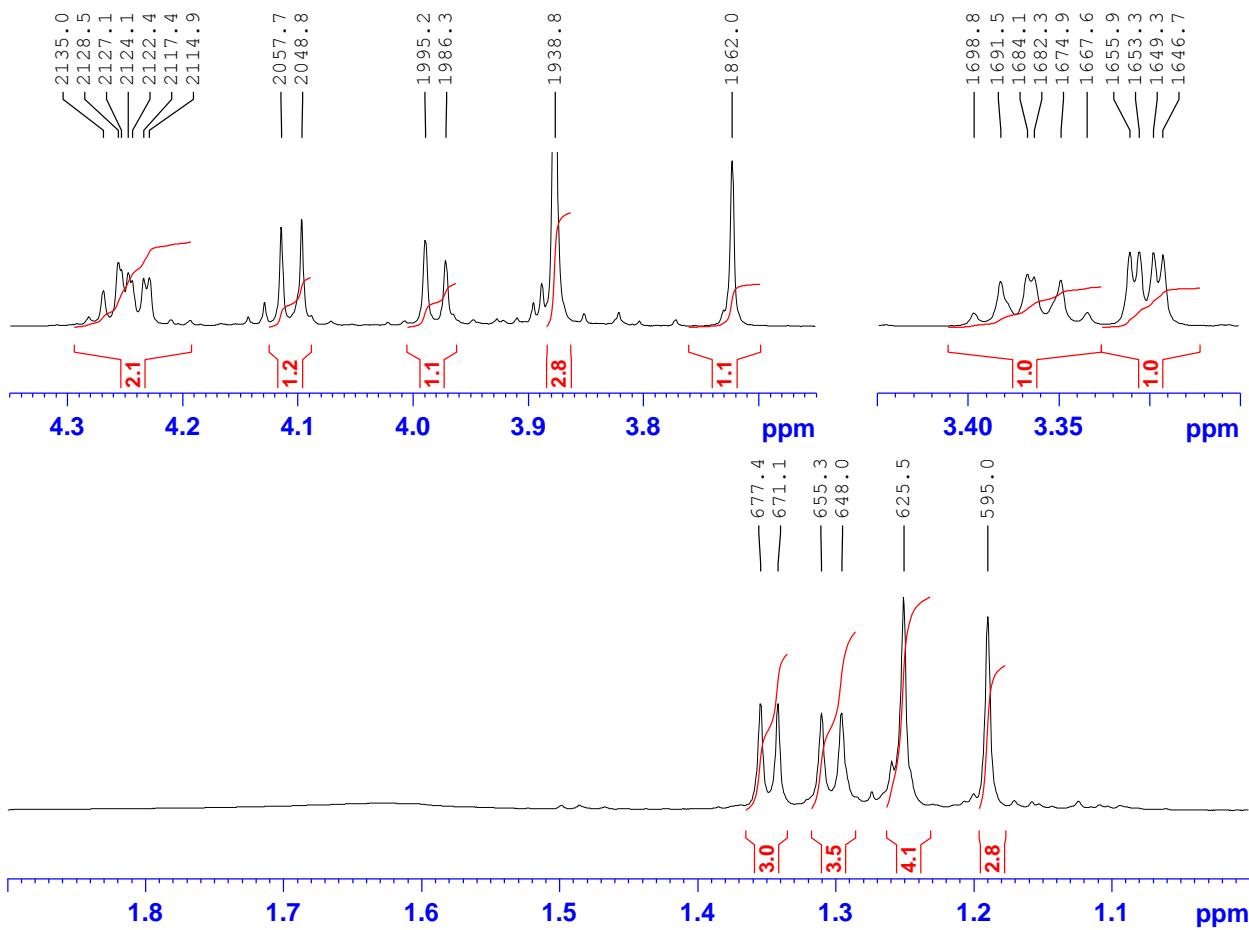


Figure S38. Expanded ^1H NMR spectrum of compound **11a** in CDCl_3 , 500 MHz.

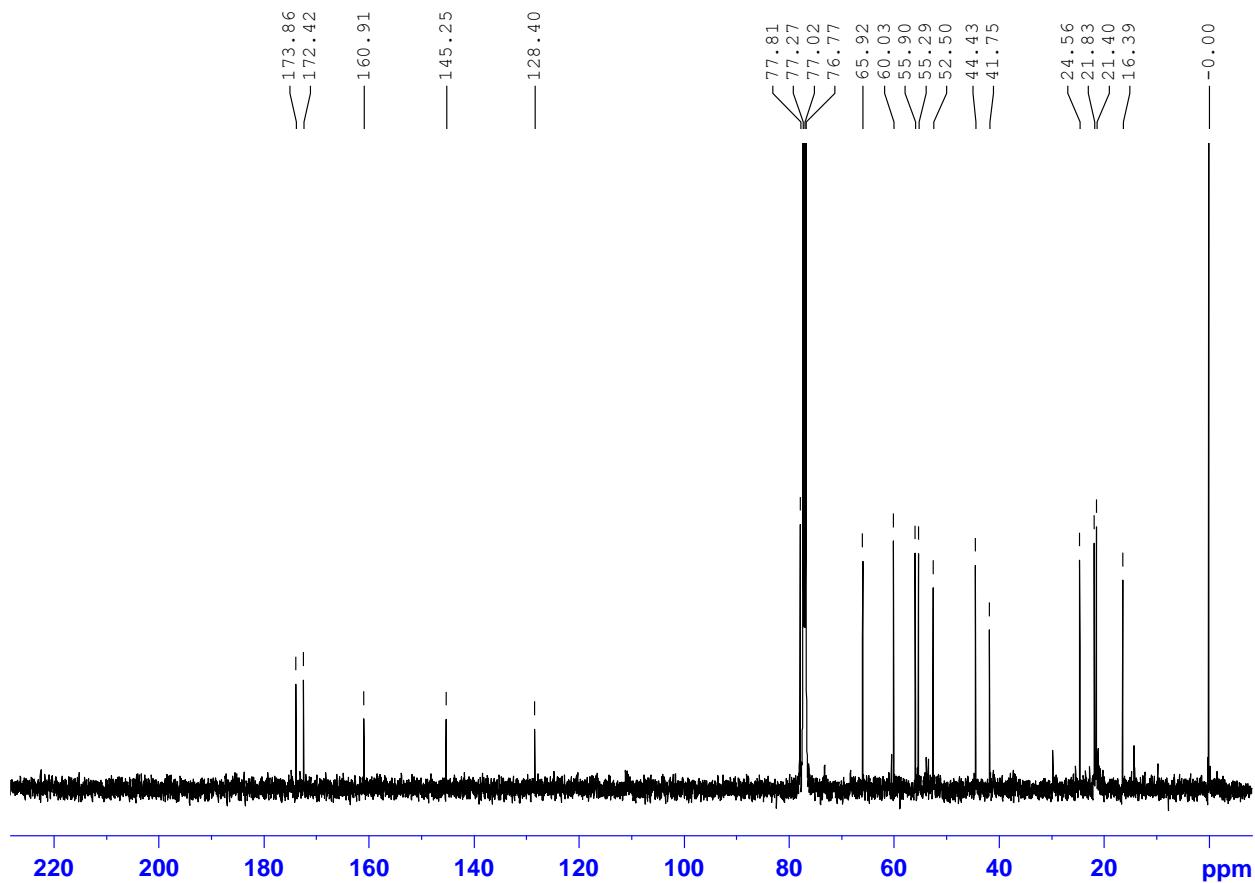


Figure S39. Complete $^{13}\text{C}\{^1\text{H}\}$ spectrum of compound **11a** in CDCl_3 , 125 MHz.

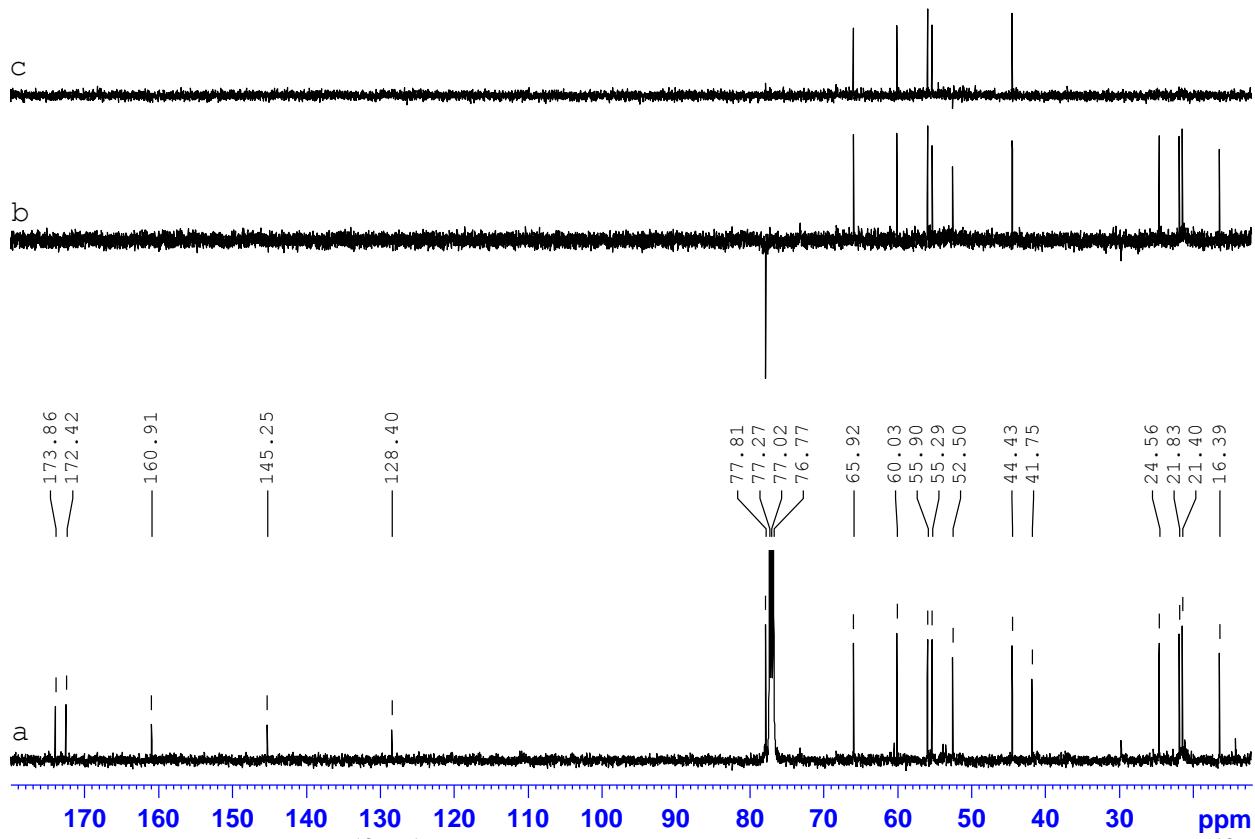


Figure S40. DEPT editing $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **11a** in CDCl_3 , 125 MHz: a) $^{13}\text{C}\{^1\text{H}\}$ spectrum; b) DEPT-135; c) DEPT-90.

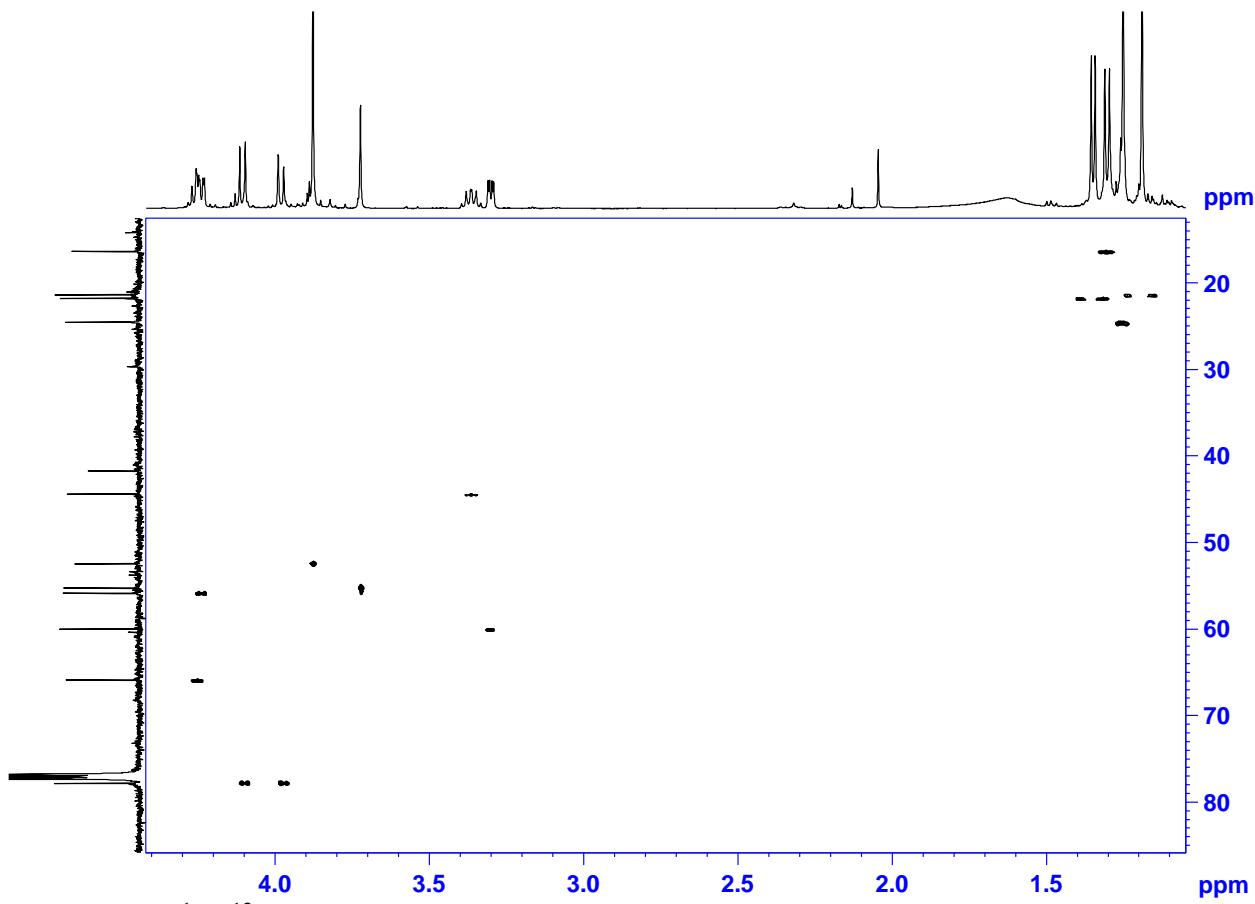


Figure S41. $\{^1\text{H}, ^{13}\text{C}\}$ HSQC NMR spectrum of compound **11a** in CDCl_3 , 500 MHz.

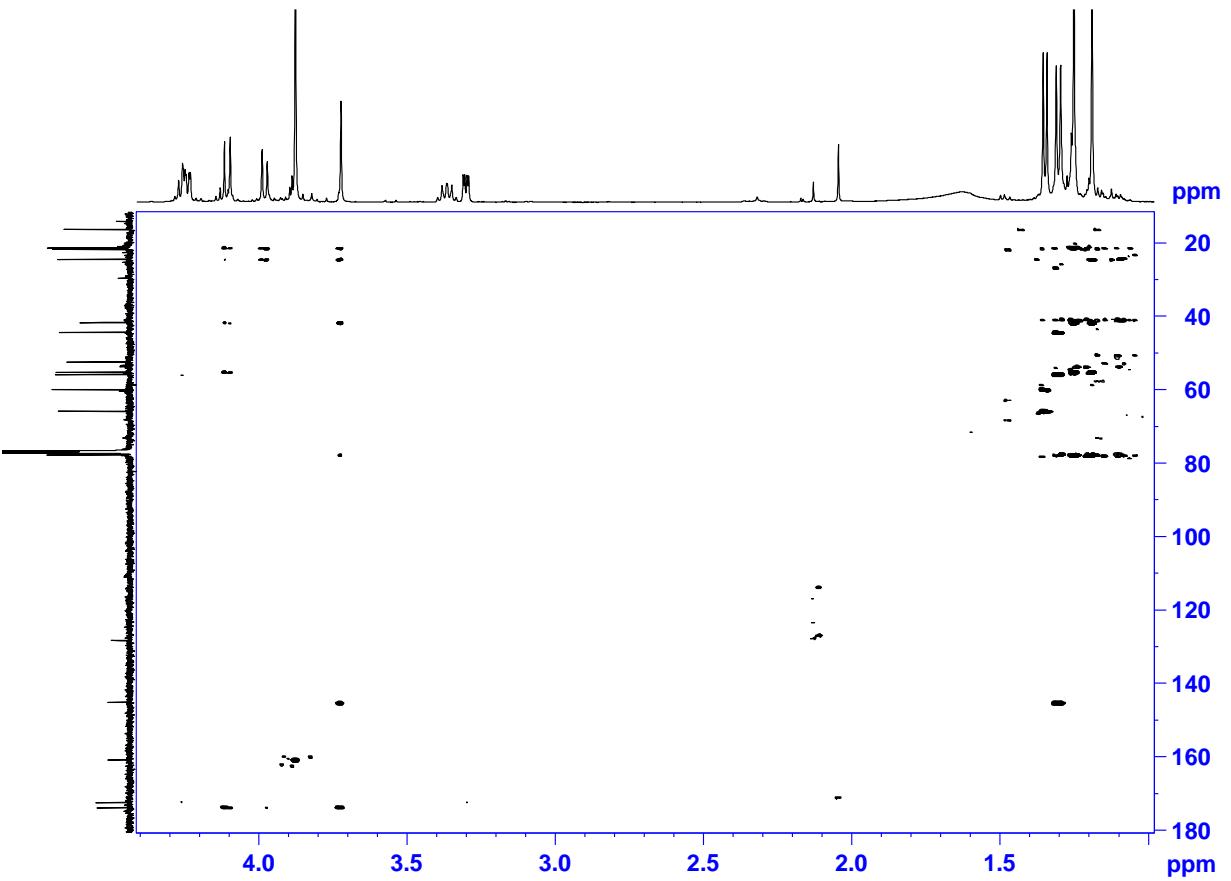


Figure S42. $\{^1\text{H}, ^{13}\text{C}\}$ HMBC NMR spectrum of compound **11a** in CDCl_3 , 500 MHz.

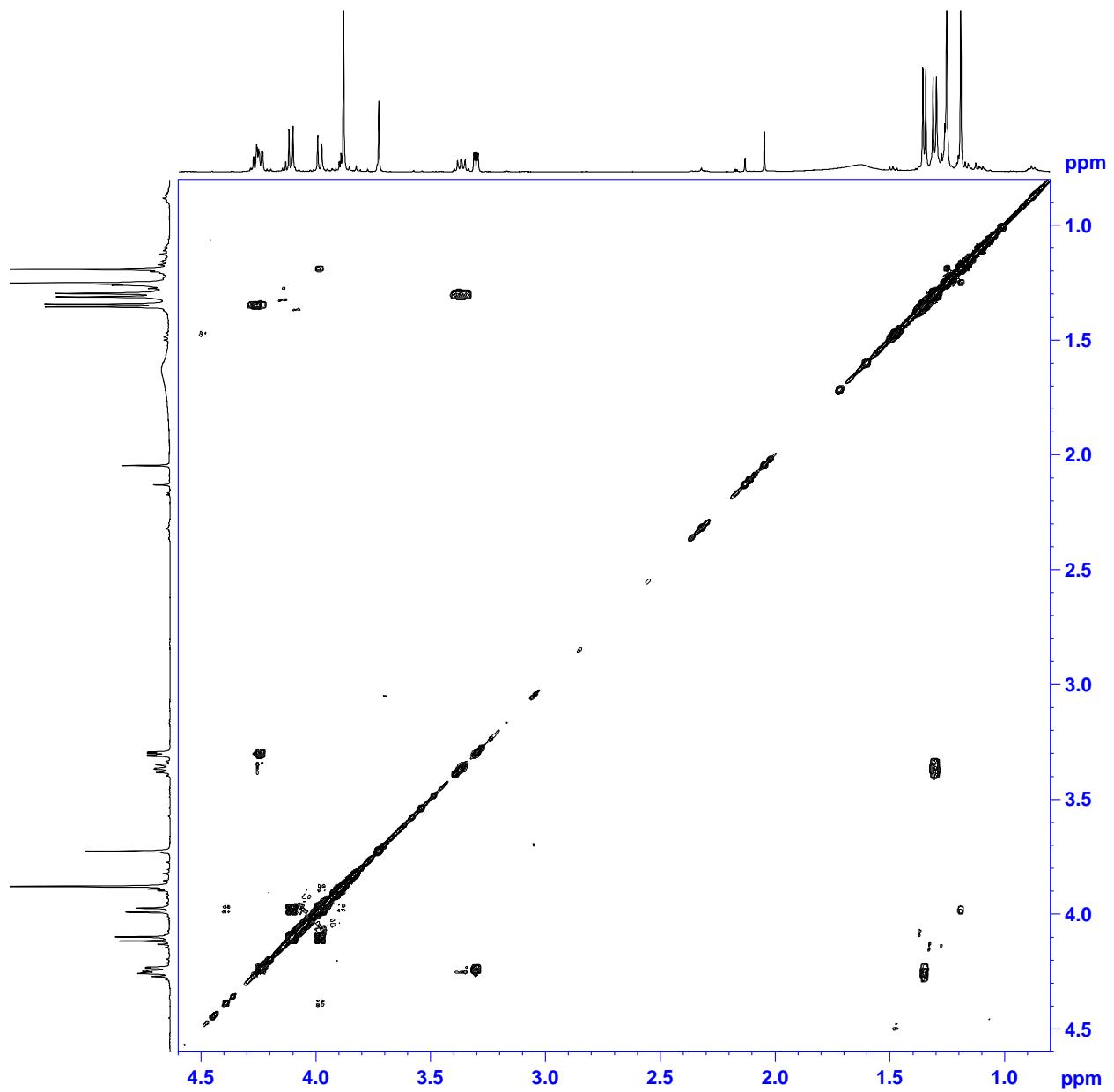


Figure S43. $\{^1\text{H}, ^1\text{H}\}$ COSY NMR spectrum of compound **11a** in CDCl_3 , 500 MHz.

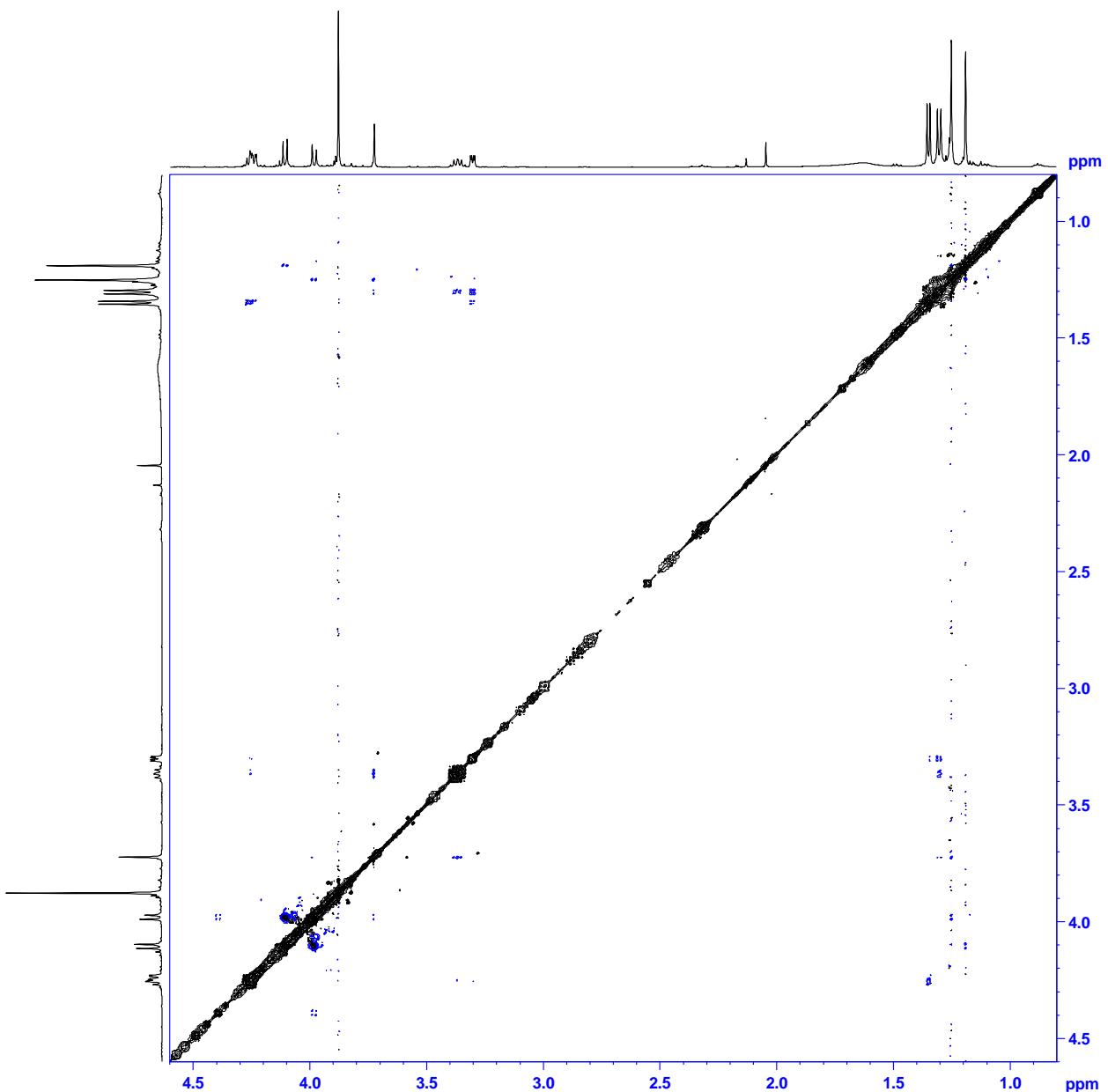


Figure S44. $\{^1\text{H}, ^1\text{H}\}$ NOESY NMR spectrum of compound **11a** in CDCl_3 , 500 MHz.

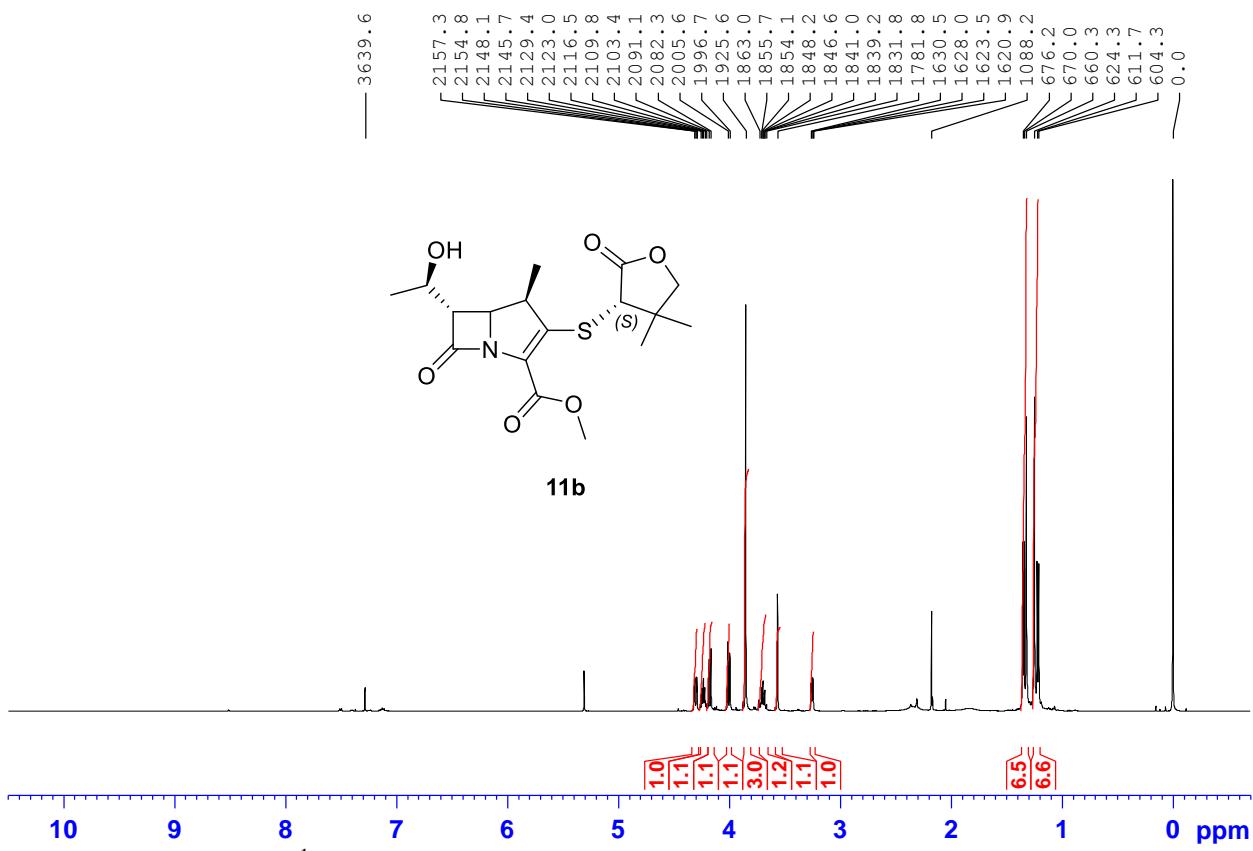


Figure S45. Complete ^1H NMR spectrum of compound **11b** in CDCl_3 , 500 MHz.

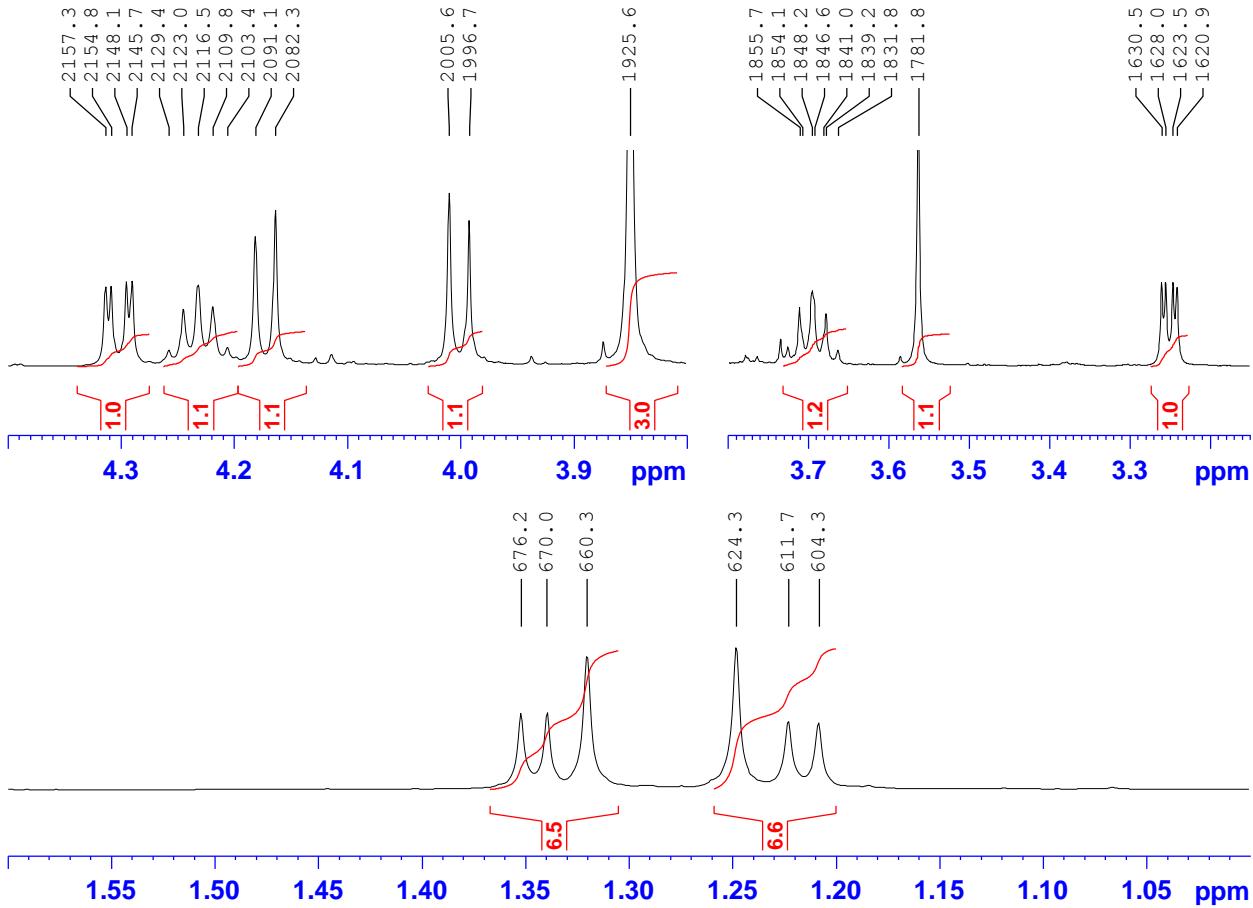


Figure S46. Expanded ^1H NMR spectrum of compound **11b** in CDCl_3 , 500 MHz.

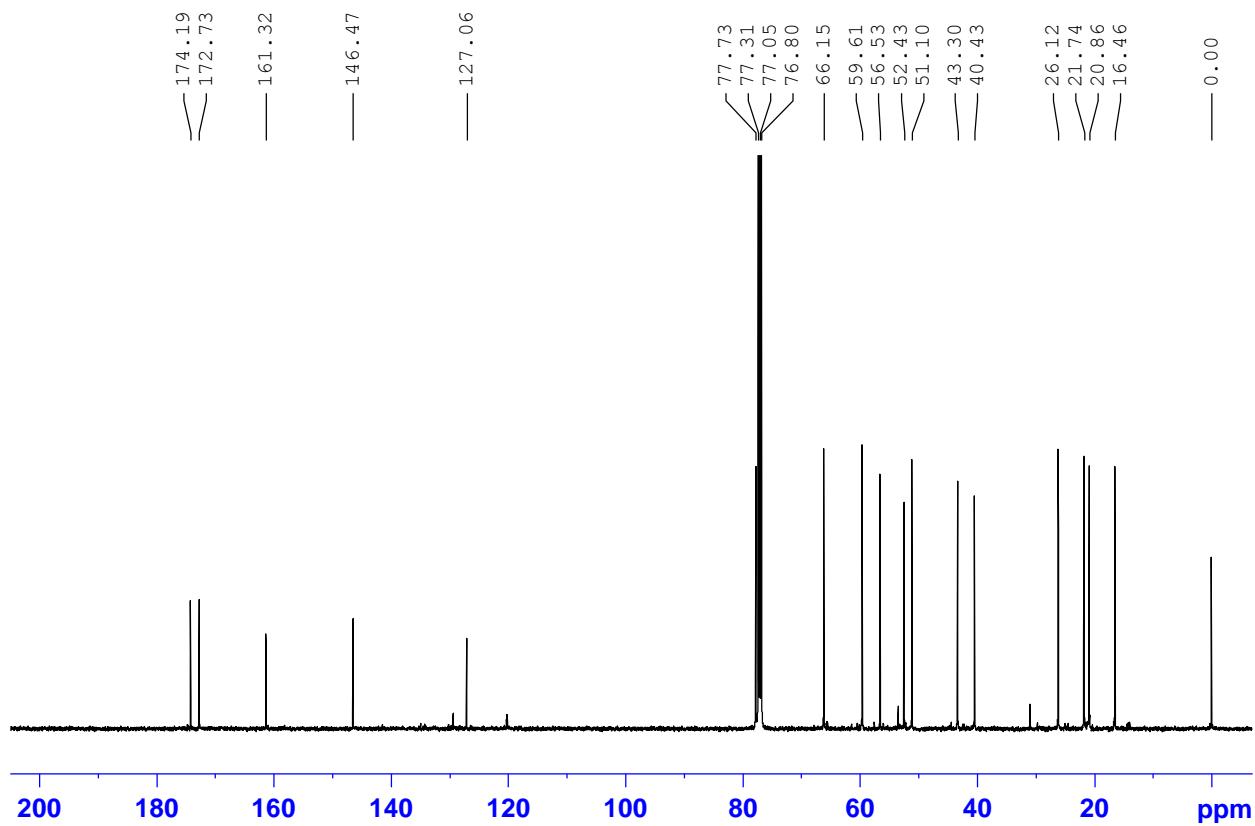


Figure S47. Complete $^{13}\text{C}\{\text{H}\}$ spectrum of compound **11b** in CDCl_3 , 125 MHz.

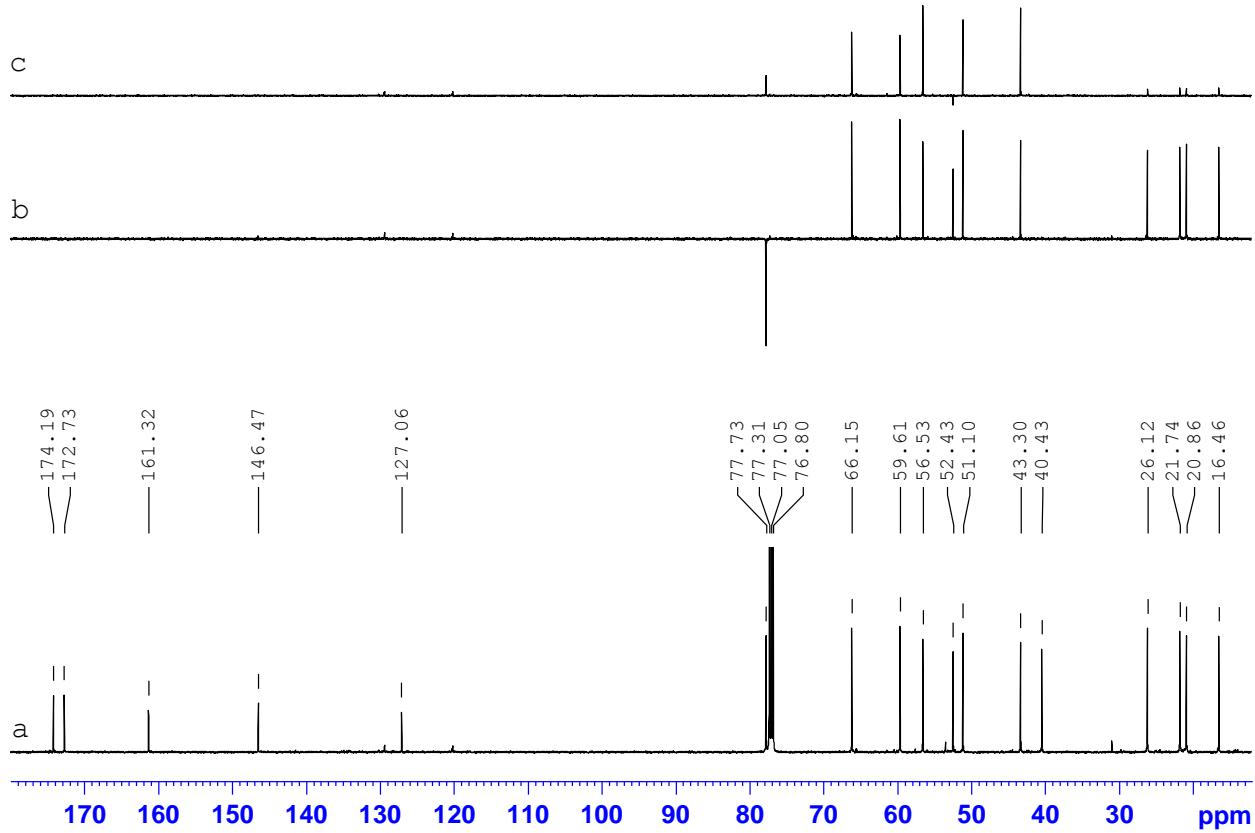


Figure S48. DEPT editing $^{13}\text{C}\{\text{H}\}$ NMR spectrum of compound **11b** in CDCl_3 , 125 MHz: a) $^{13}\text{C}\{\text{H}\}$ spectrum; b) DEPT-135; c) DEPT-90.

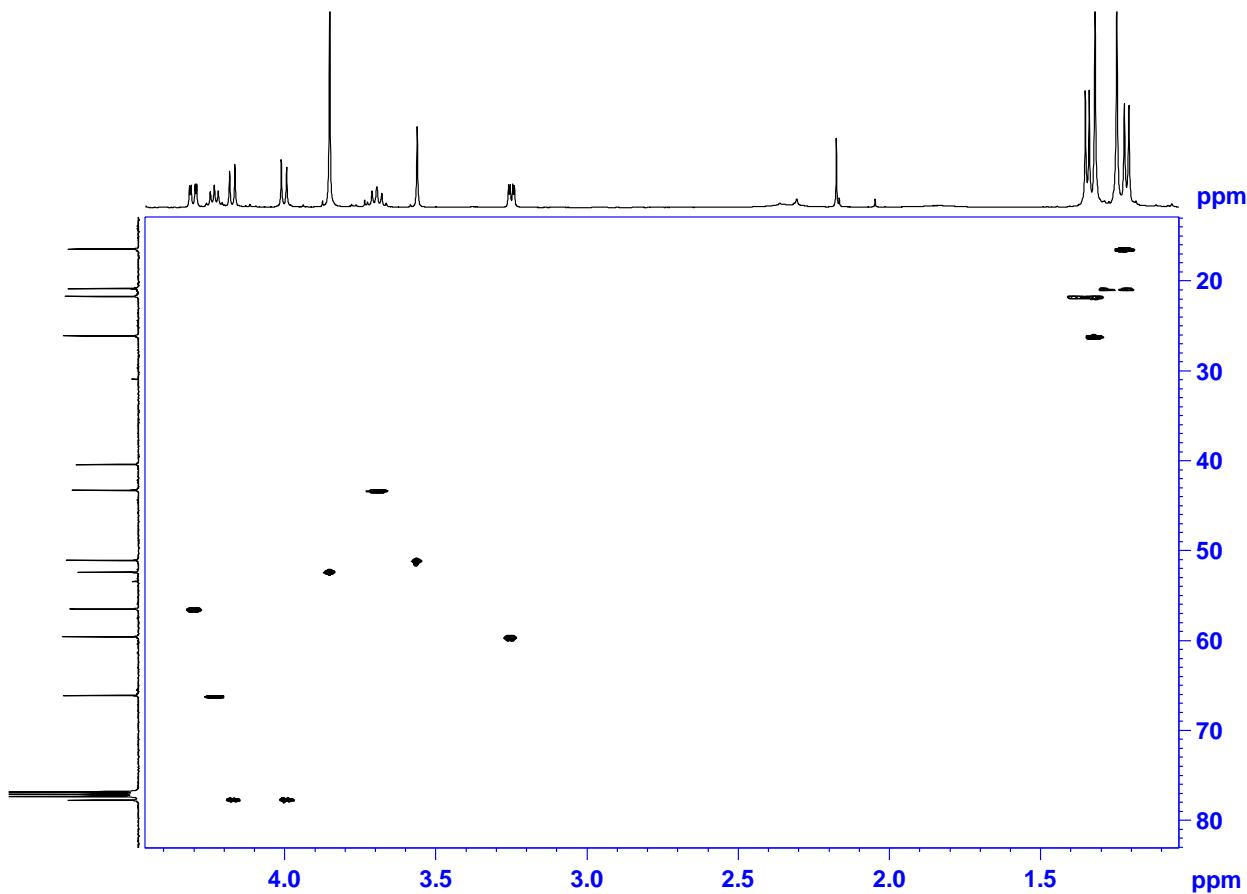


Figure S49. $\{^1\text{H}, ^{13}\text{C}\}$ HSQC NMR spectrum of compound **11b** in CDCl_3 , 500 MHz.

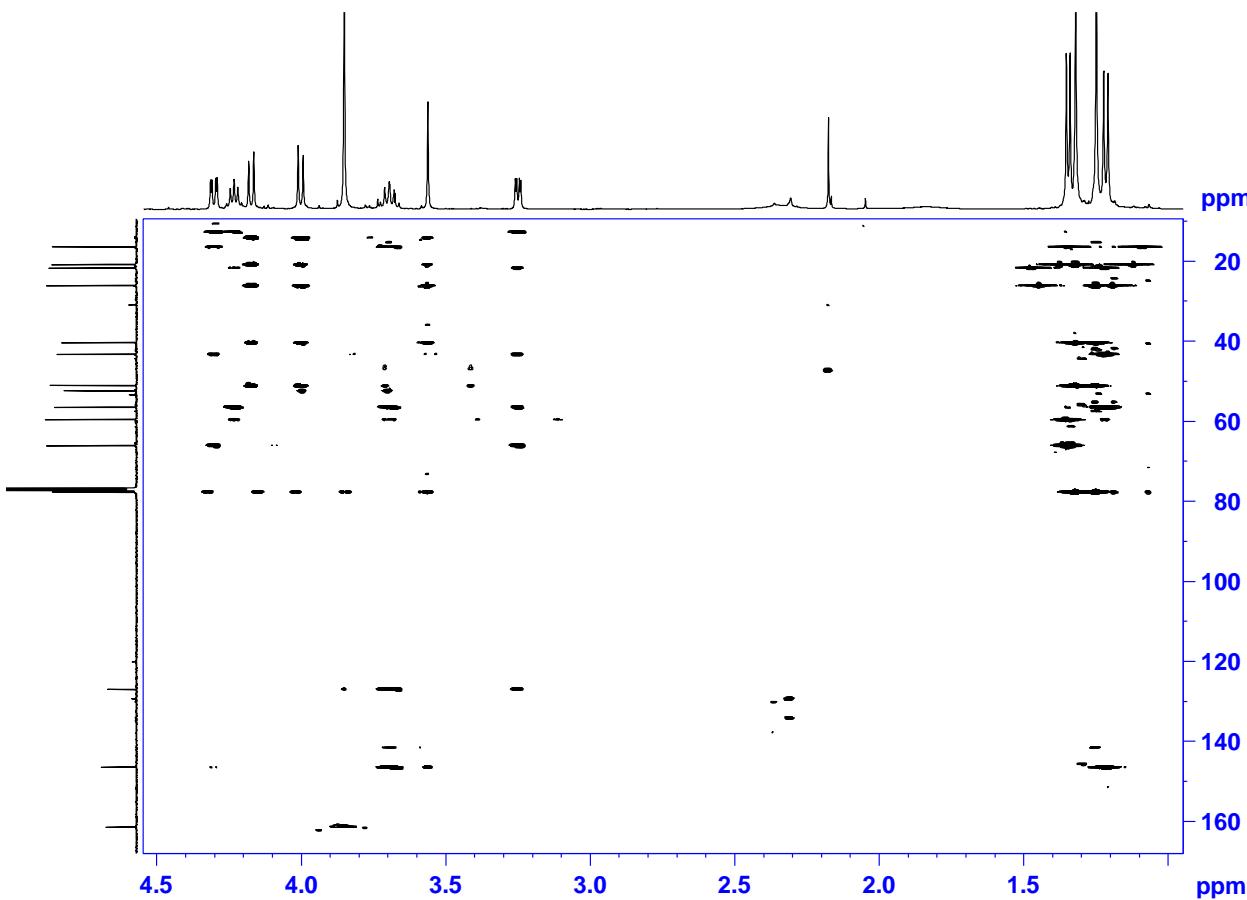


Figure S50. $\{^1\text{H}, ^{13}\text{C}\}$ HMBC NMR spectrum of compound **11b** in CDCl_3 , 500 MHz.

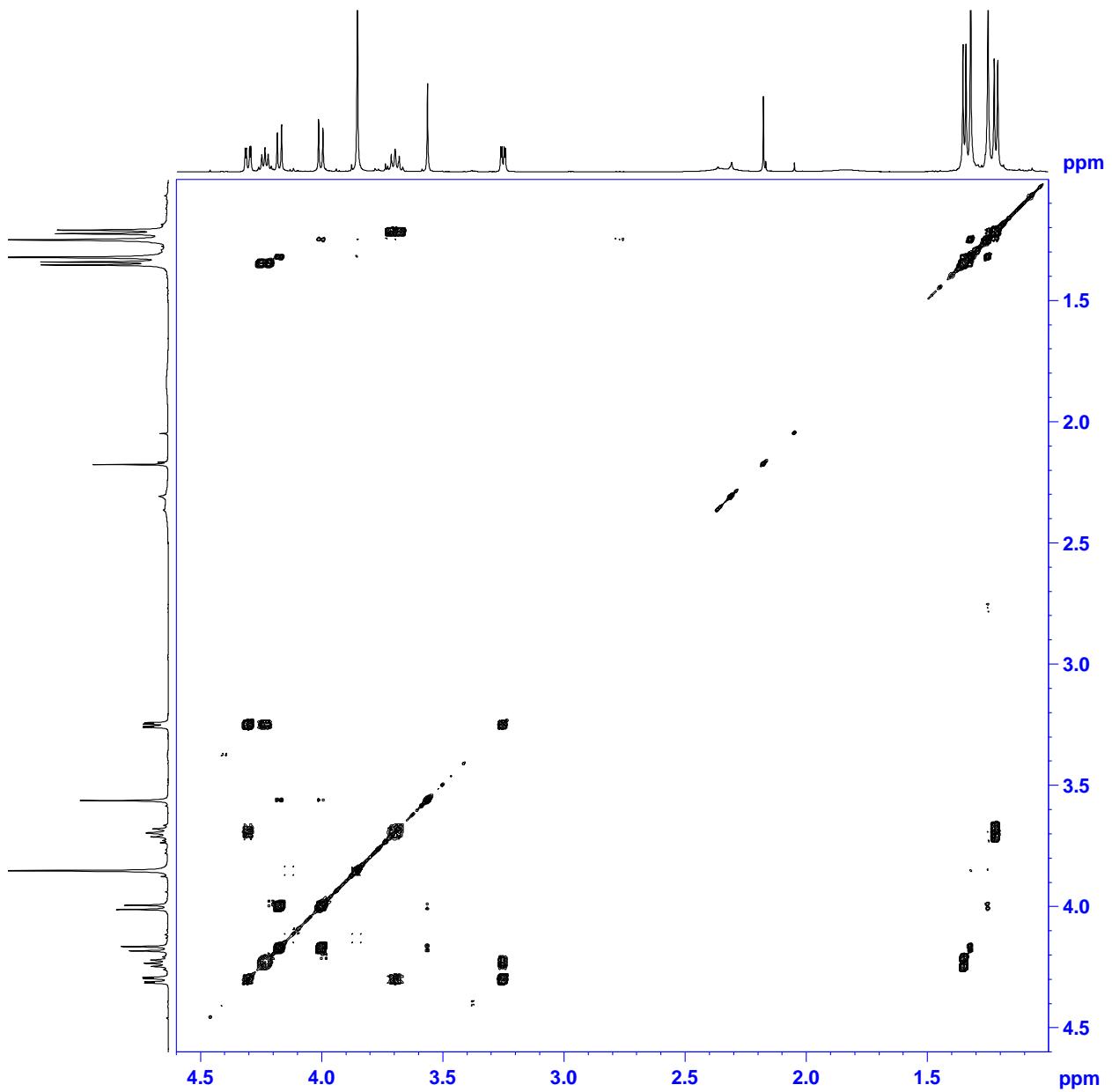


Figure S51. $\{^1\text{H}, ^1\text{H}\}$ COSY NMR spectrum of compound **11b** in CDCl_3 , 500 MHz.

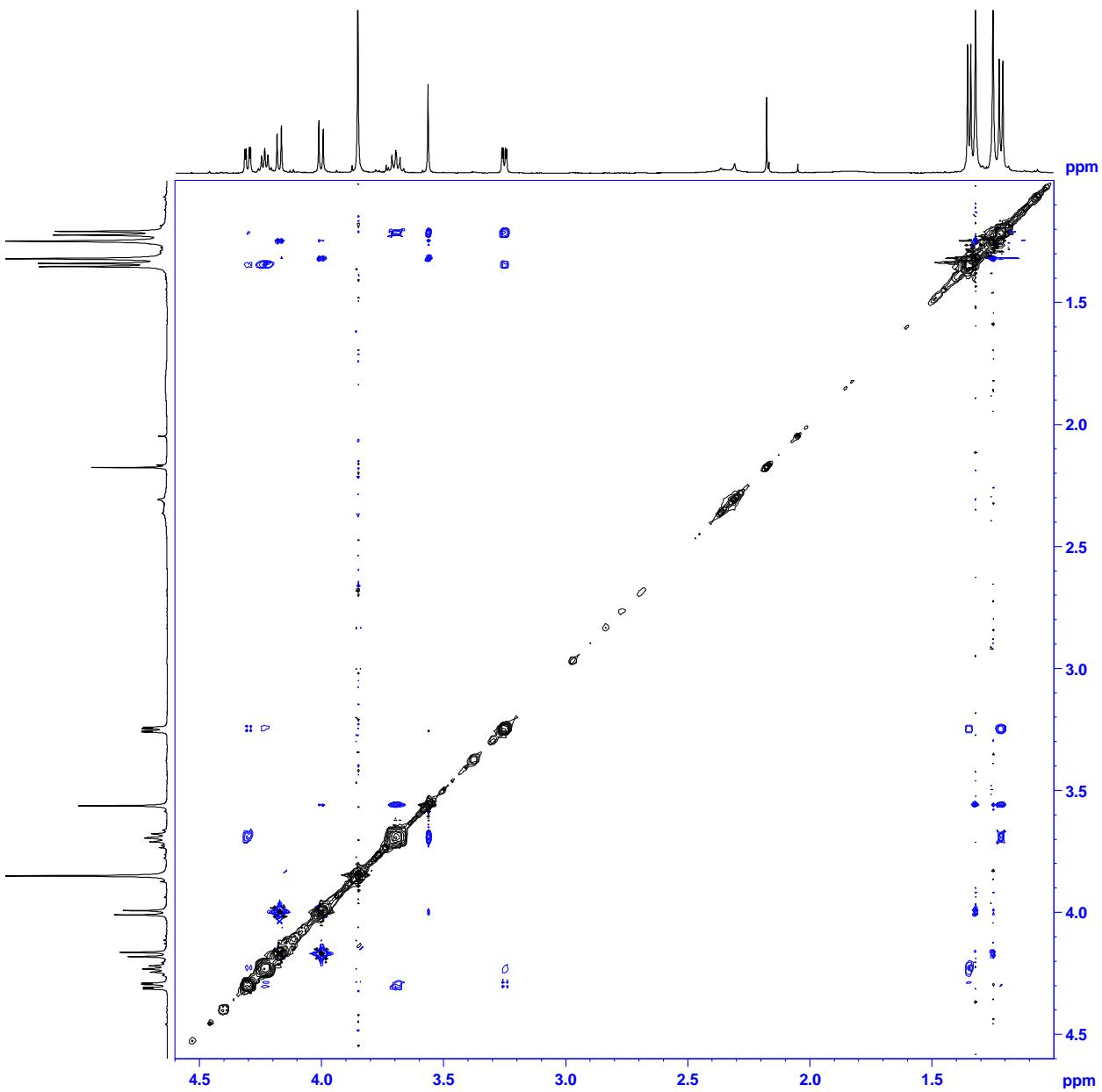


Figure S52. $\{^1\text{H}, ^1\text{H}\}$ NOESY NMR spectrum of compound **11b** in CDCl_3 , 500 MHz.

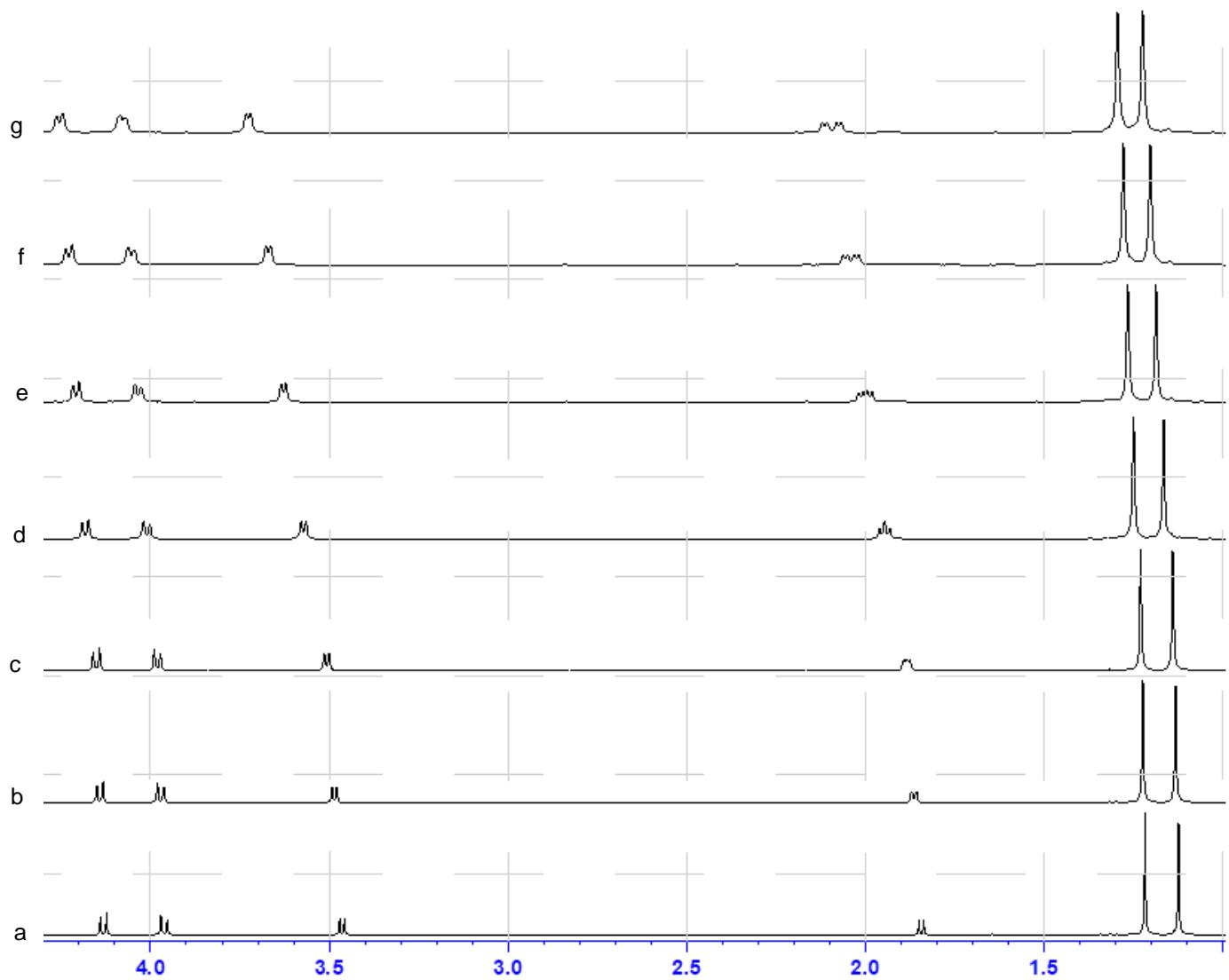


Figure S53. Spectrum (\pm) -3 (a) and spectra (\pm) -3 after each addition of (-)-Eu(hfc)₃ (b-g).

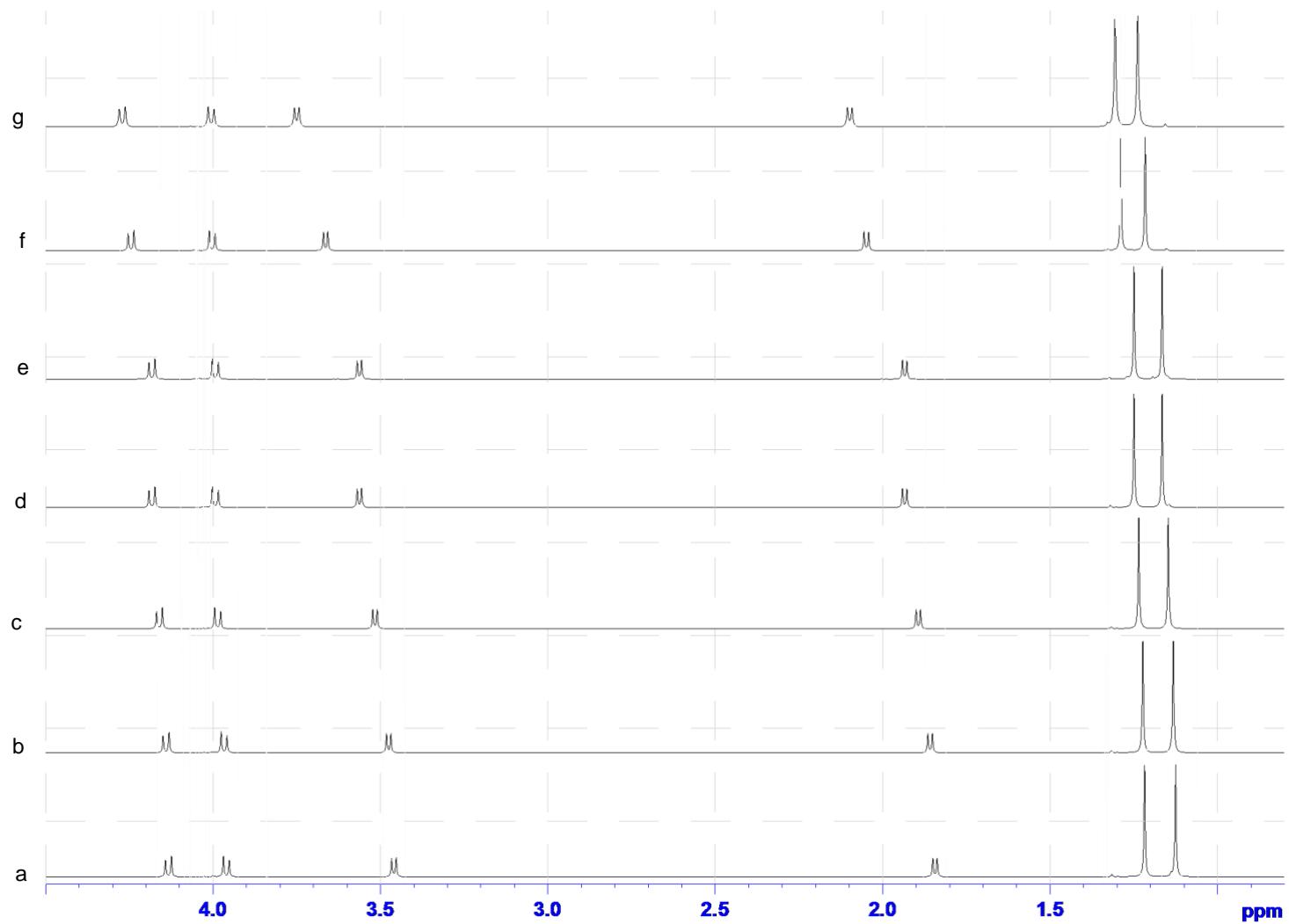


Figure S54. Spectrum S-3 (a) and spectra S-3 after each addition of (-)-Eu(hfc)₃ (b-g).

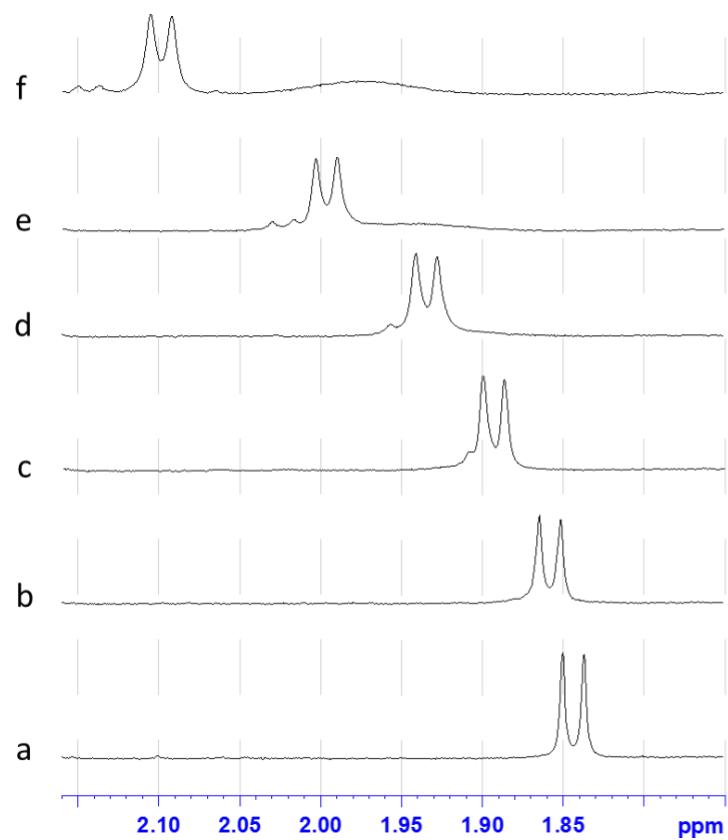


Figure S55. SH signal in the spectrum of *S*-**3** (a) and spectra of *S*-**3** after each addition of (-)-Eu(hfc)₃ (b-f).

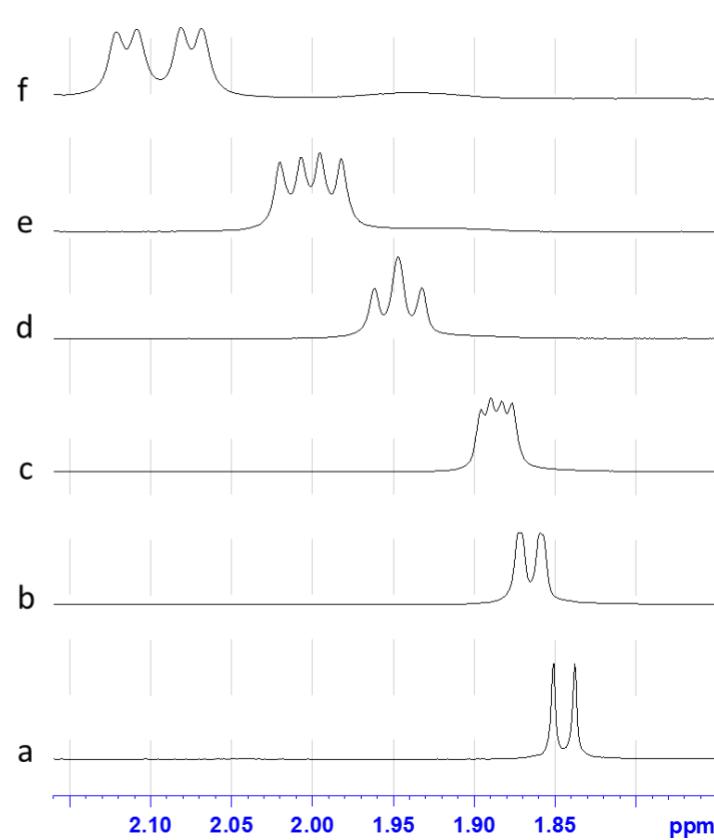


Figure S56. SH signal in the spectrum of (\pm)-**3** (a) and spectra of (\pm)-**3** after each addition of (-)-Eu(hfc)₃ (b-f).

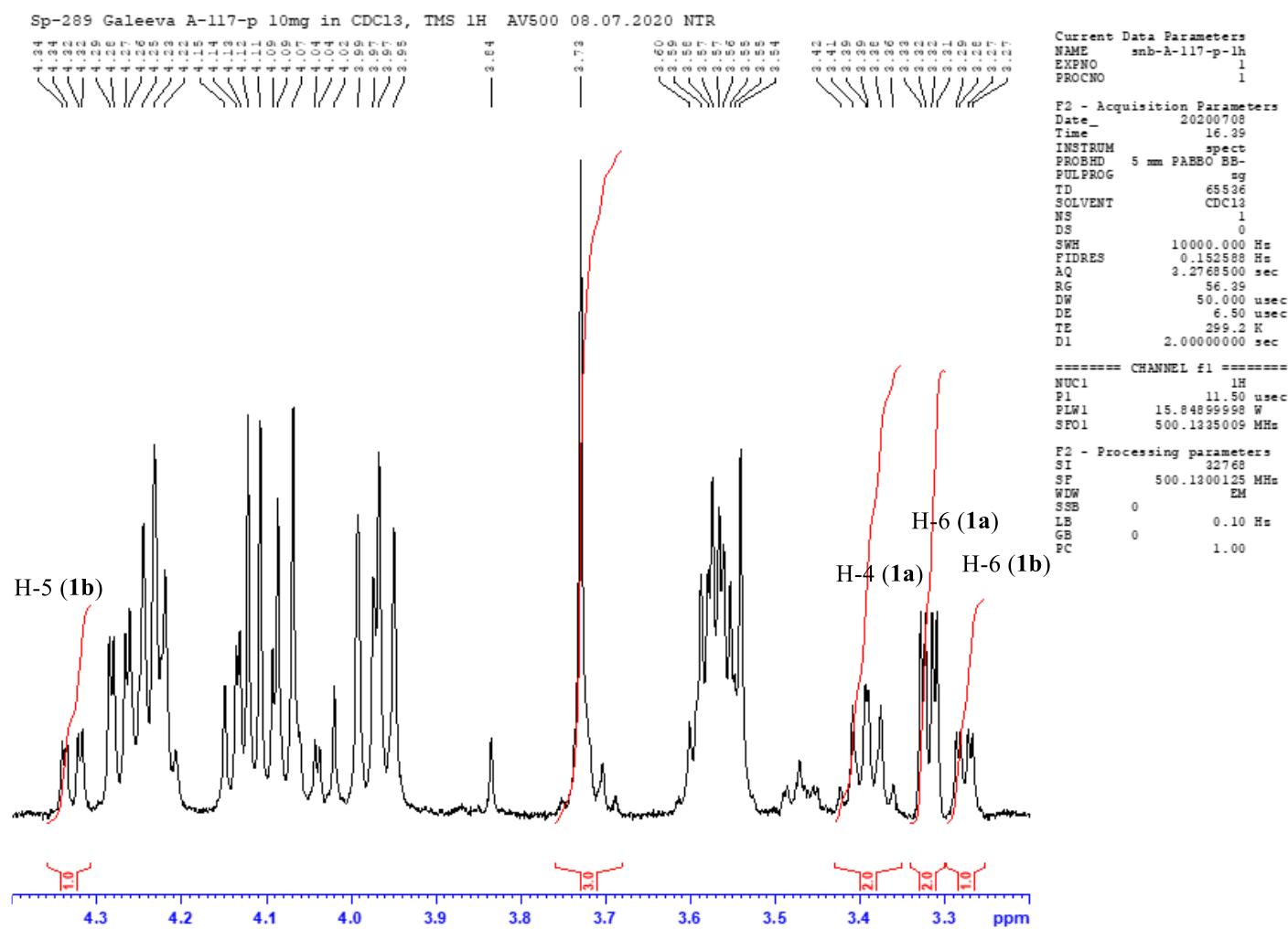


Figure S57. Part of ¹H NMR spectrum of reaction mixture after reaction **2** and **3**, before column chromatography (**1a:1b** = 2:1, by integrated intensity of signals H-6)

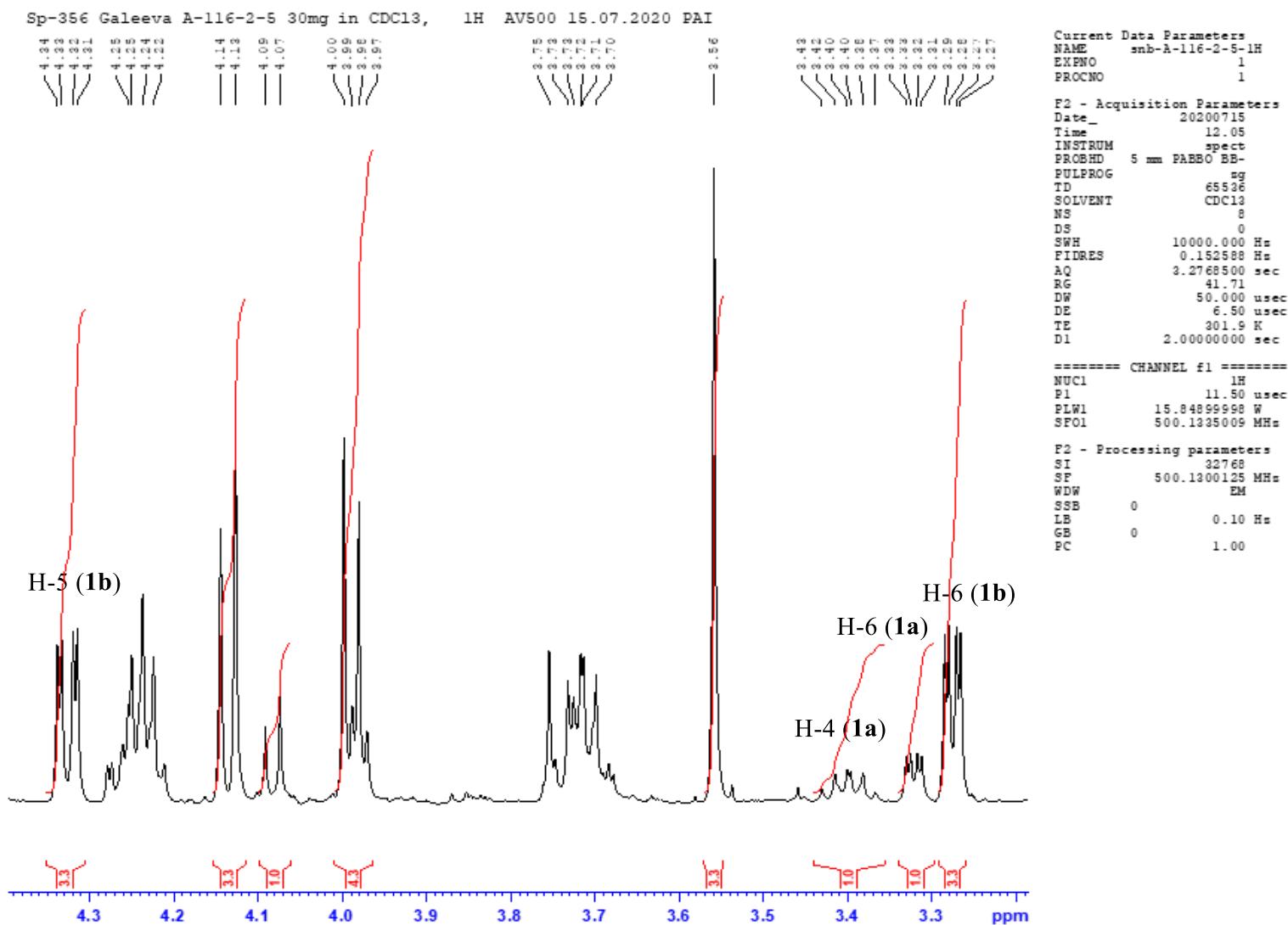


Figure S58. Part of ¹H NMR spectrum of mixture **1a**, **1b** after column chromatography on SiO₂ with CHCl₃-MeOH-Et₃N (**1a**:**1b** = 1:3.3).

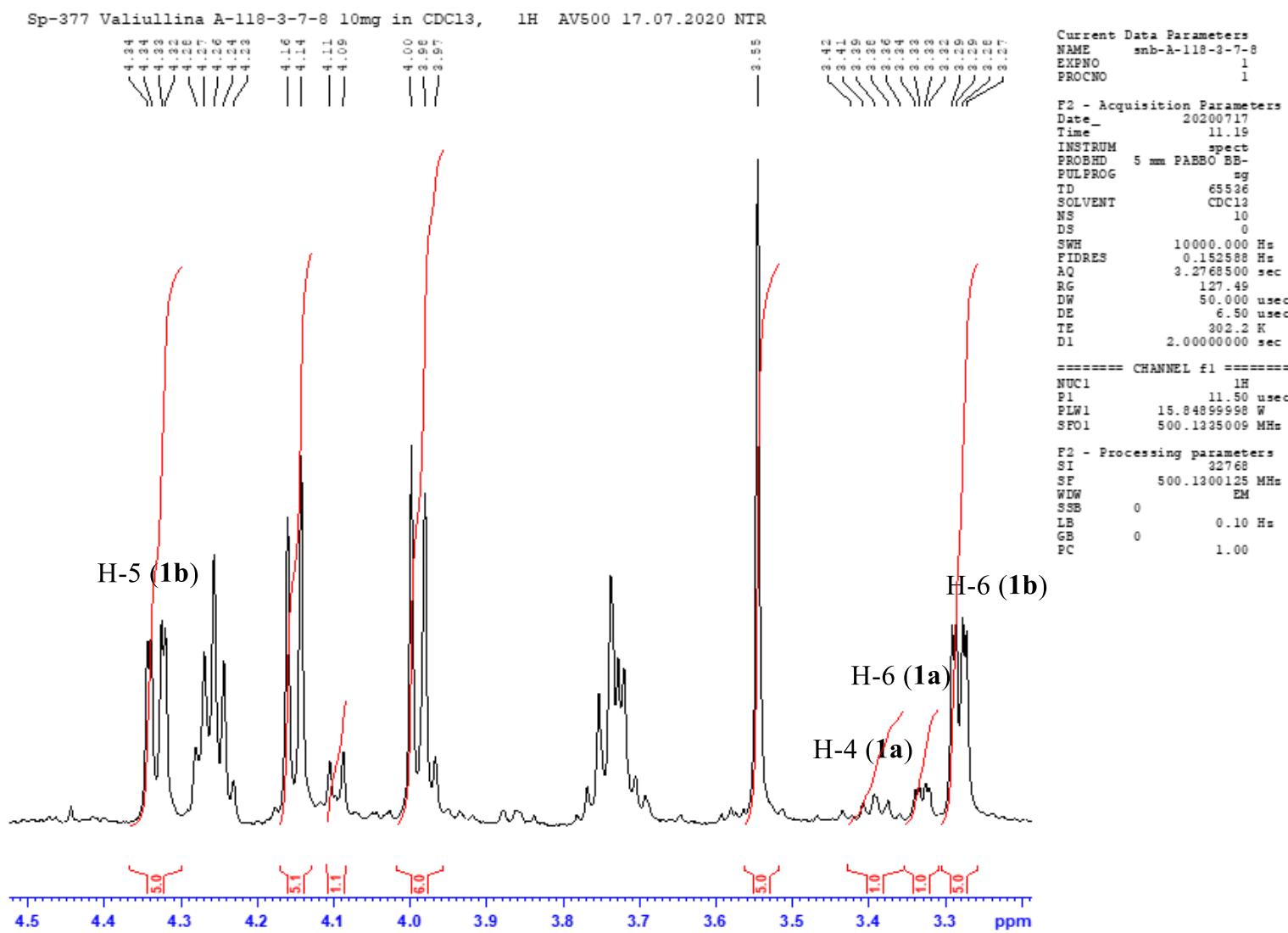


Figure S59. Part of ¹H NMR spectrum of mixture **1a**, **1b** after column chromatography **1a** on SiO₂ with CHCl₃-MeOH-Et₃N (**1a**:**1b** = 1:5).