

Supporting Information

Preparation and Evaluation of Carborane-Derived Inhibitors of Prostate Specific Membrane

Antigen (PSMA).

Mohamed E. El-Zaria,^{†‡} Afaf R. Genady,^{†‡} Nancy Janzen,[†] Christina I. Petlura,[†] Denis R. Beckford Vera,[†] and John F. Valliant^{†,*}

[†]Department of Chemistry and Chemical Biology, McMaster University, 1280 Main St. West, Hamilton, Ont. Canada L8S 4M1.

[‡]Department of Chemistry, Faculty of Science, Tanta University, 31527 Tanta, Egypt.

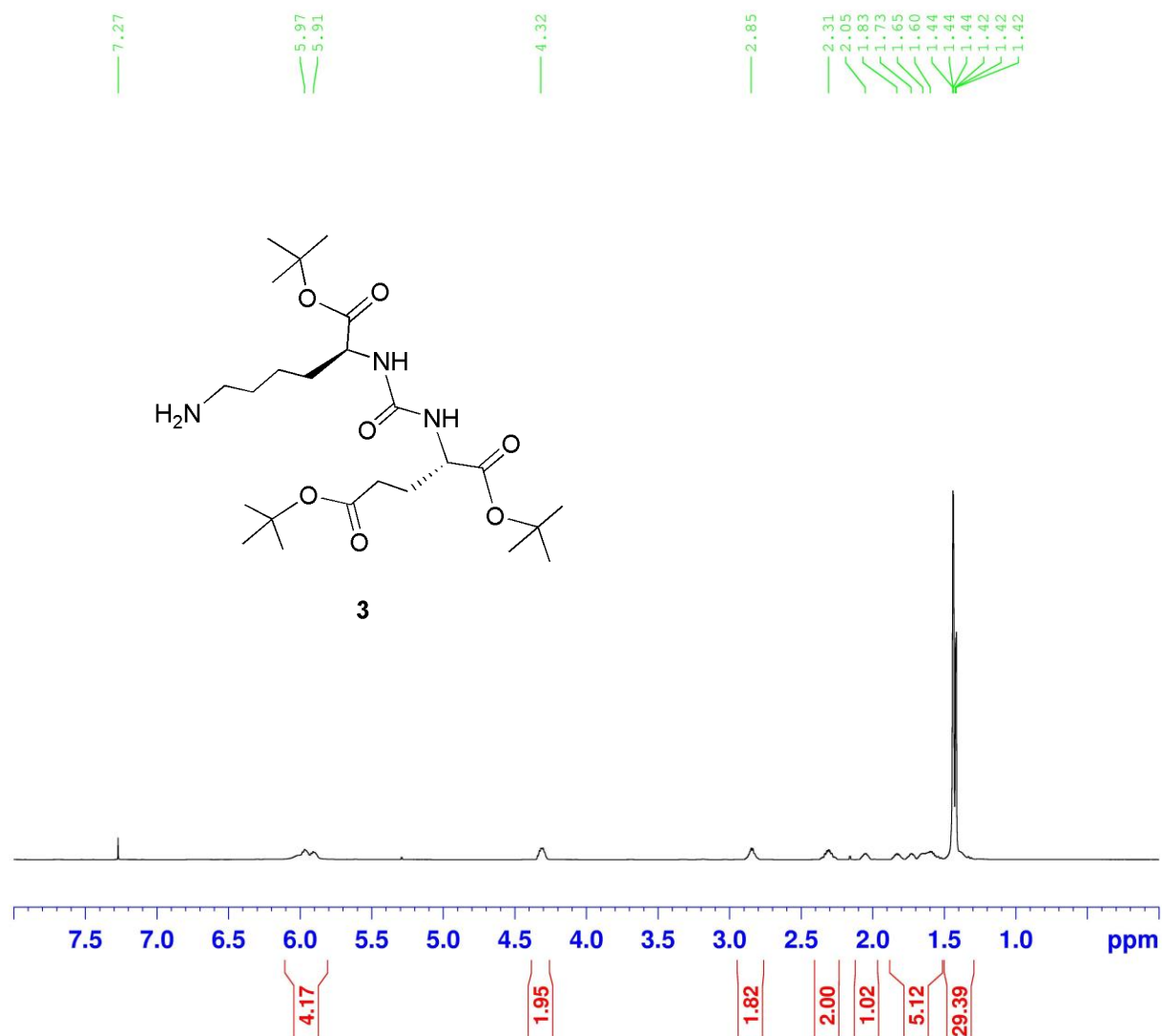


Figure S1. ^1H NMR spectrum of compound **3** (CDCl₃, 600 MHz).

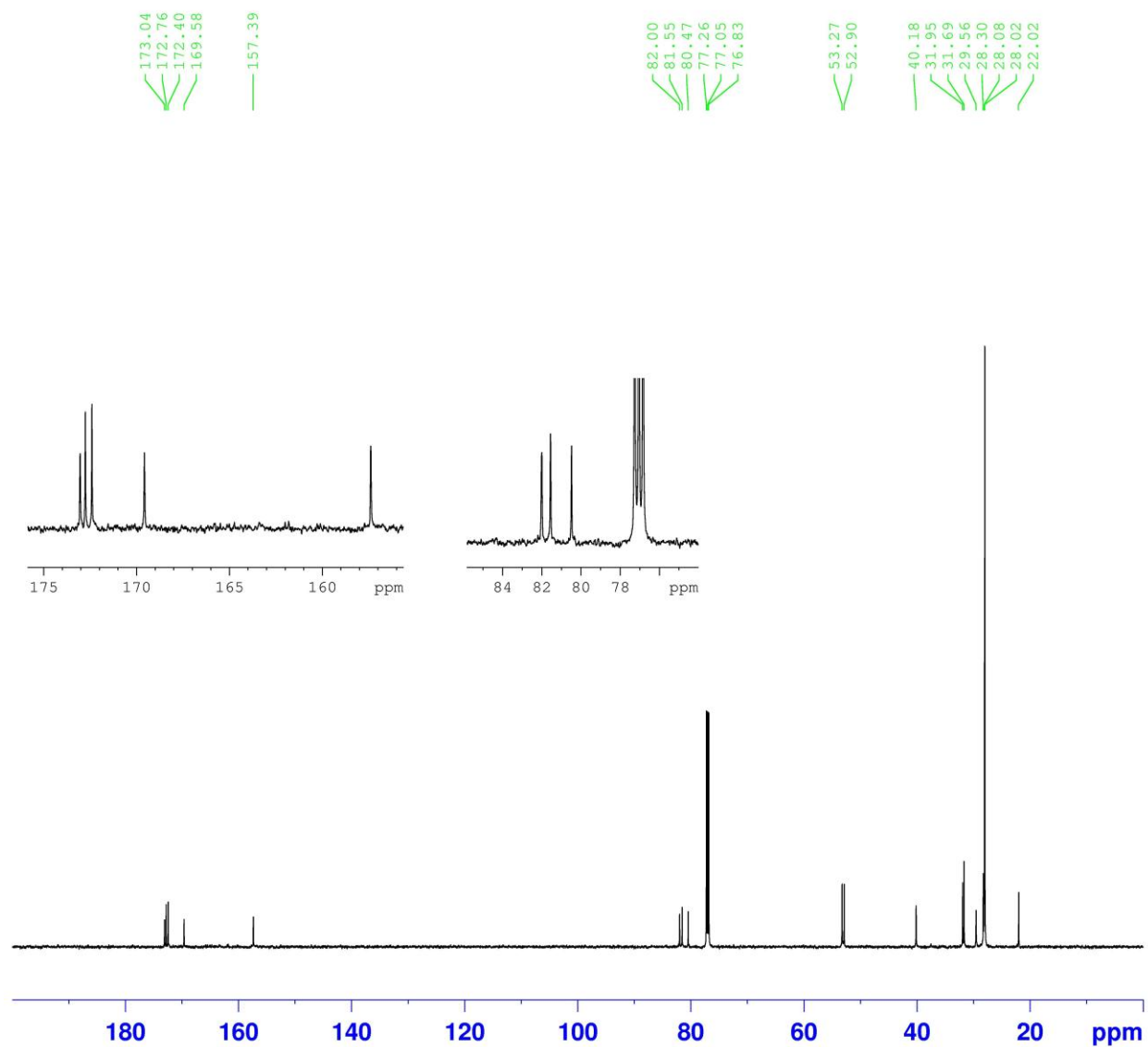


Figure S2. ^{13}C NMR spectrum of compound **3** (CDCl_3 , 150 MHz).

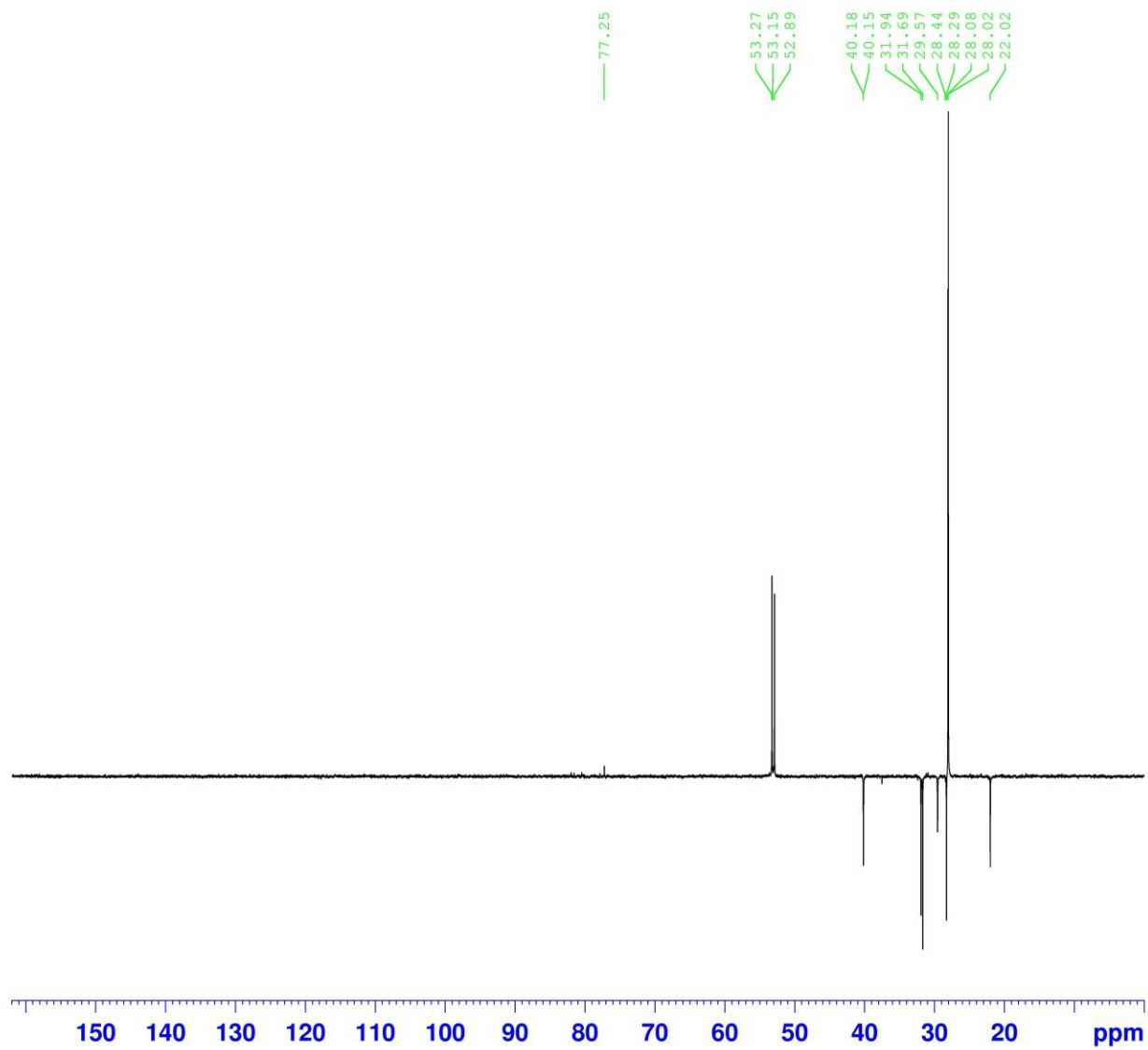


Figure S3. ^{13}C NMR (dept 135 $^\circ$) spectrum of compound **3** (CDCl_3 , 150 MHz).

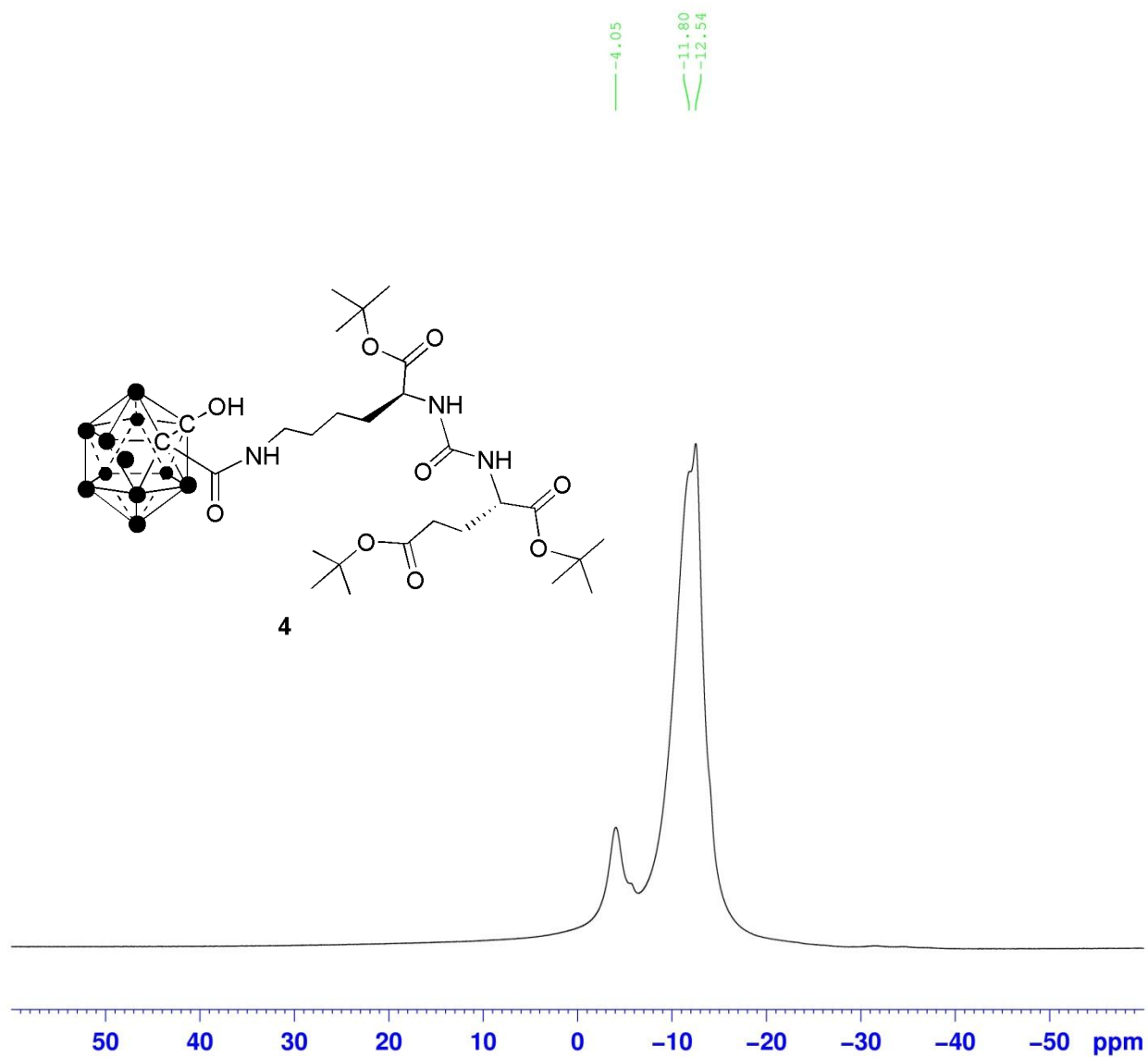


Figure S4. ^{11}B NMR spectrum of compound **4** (CDCl_3 , 192 MHz).

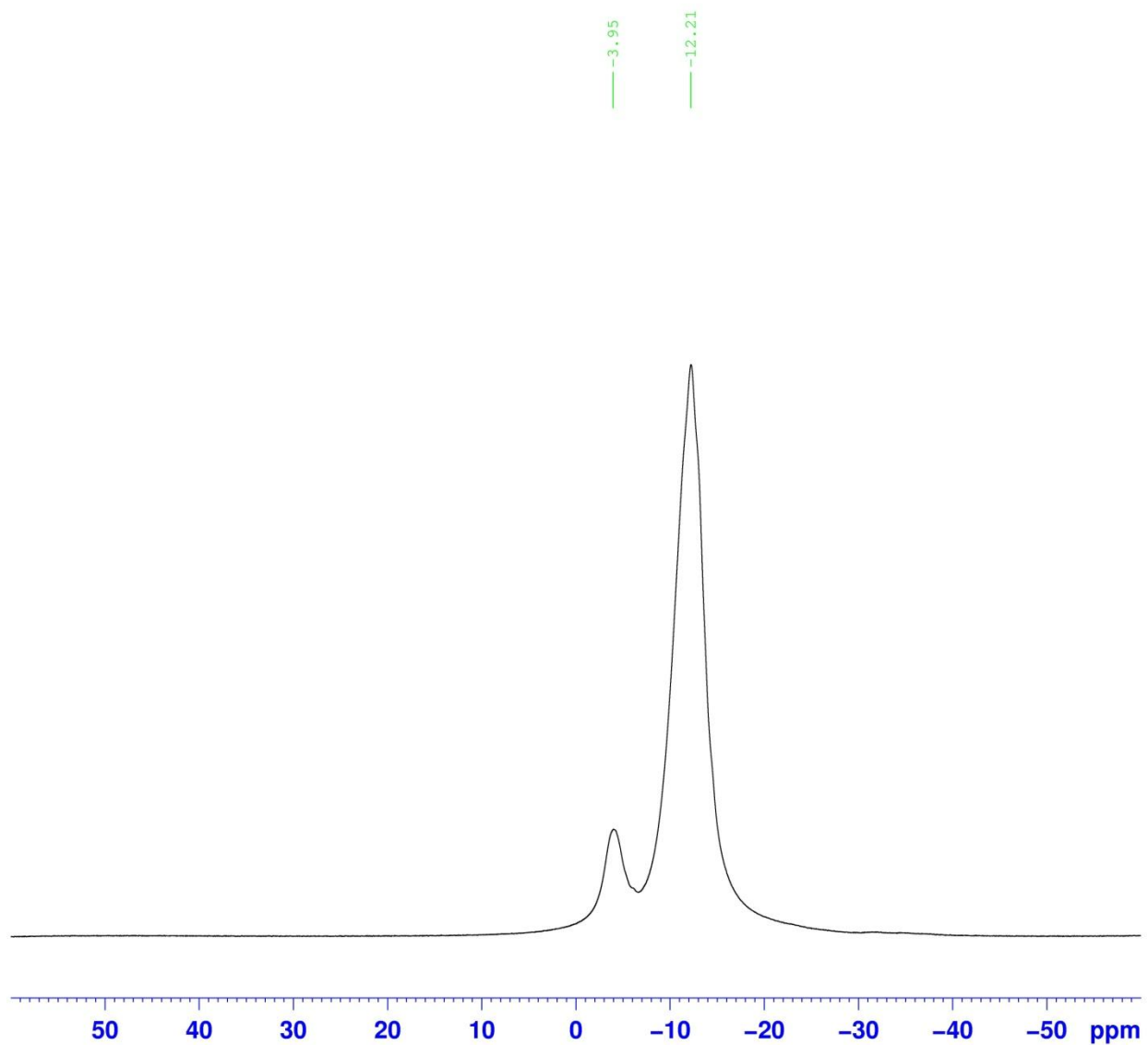


Figure S5. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of compound **4** (CDCl_3 , 192 MHz).

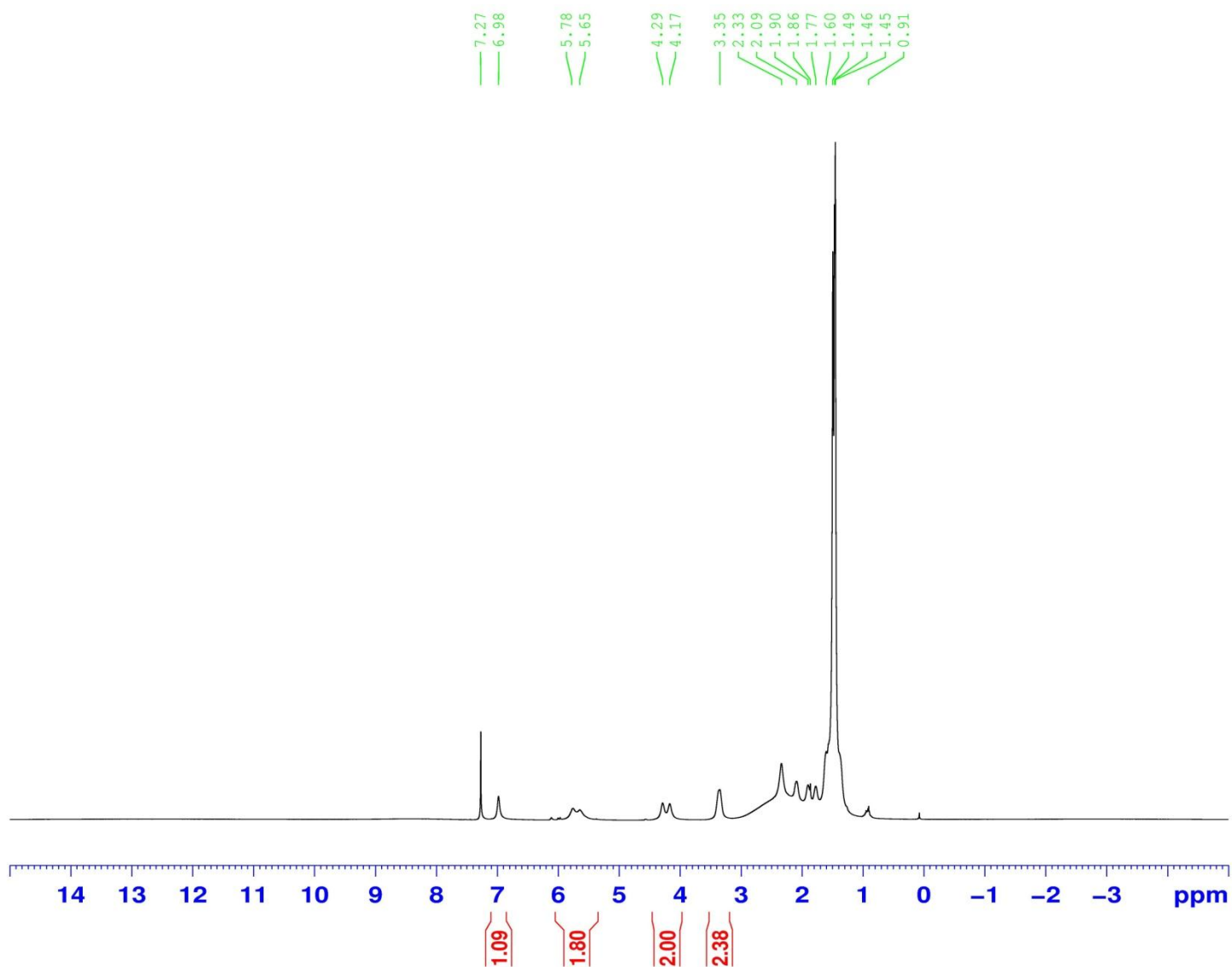


Figure S6. ^1H NMR spectrum of compound **4** (CDCl_3 , 600 MHz).

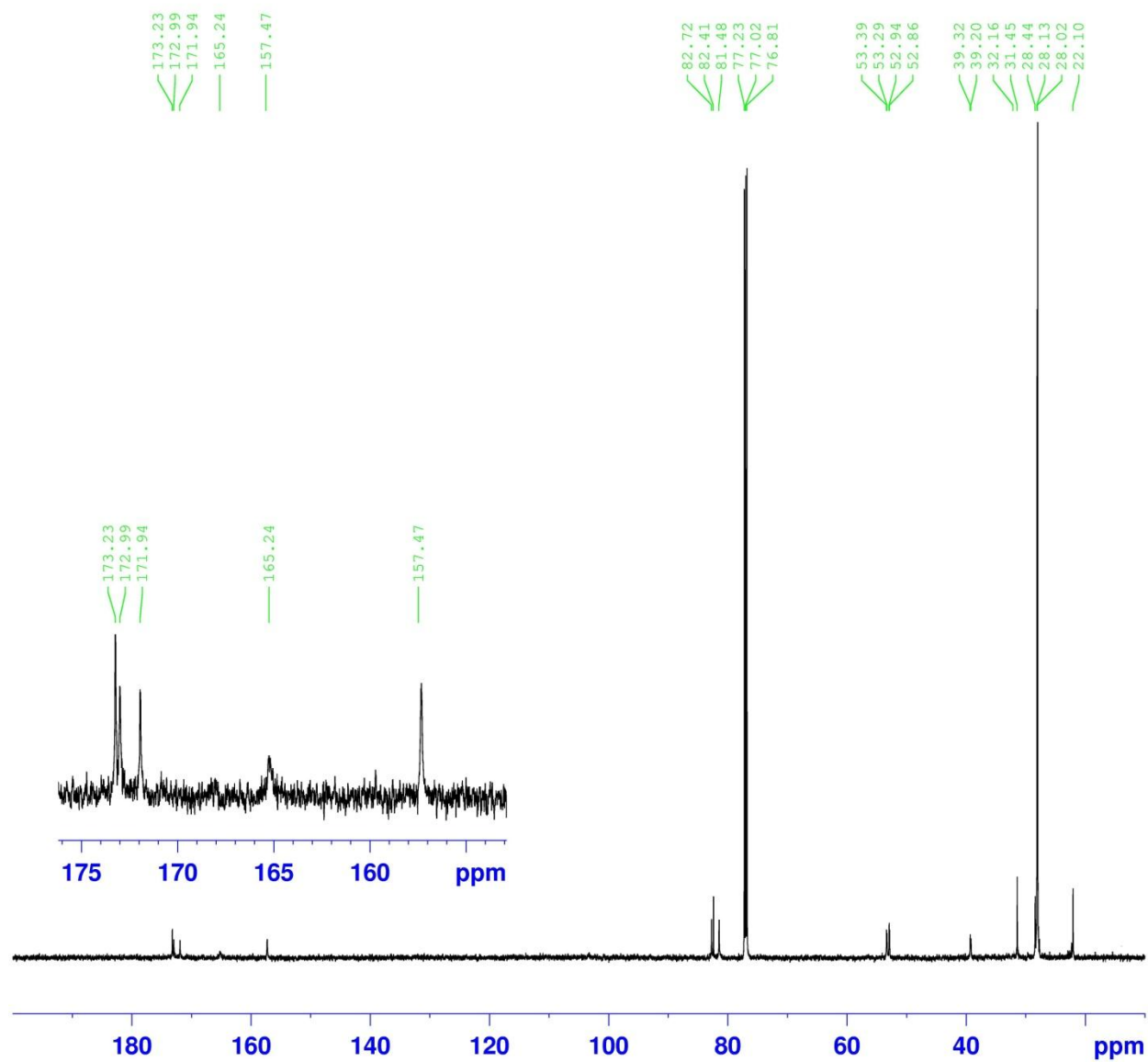


Figure S7. ^{13}C NMR spectrum of compound **4** (CDCl_3 , 150 MHz).

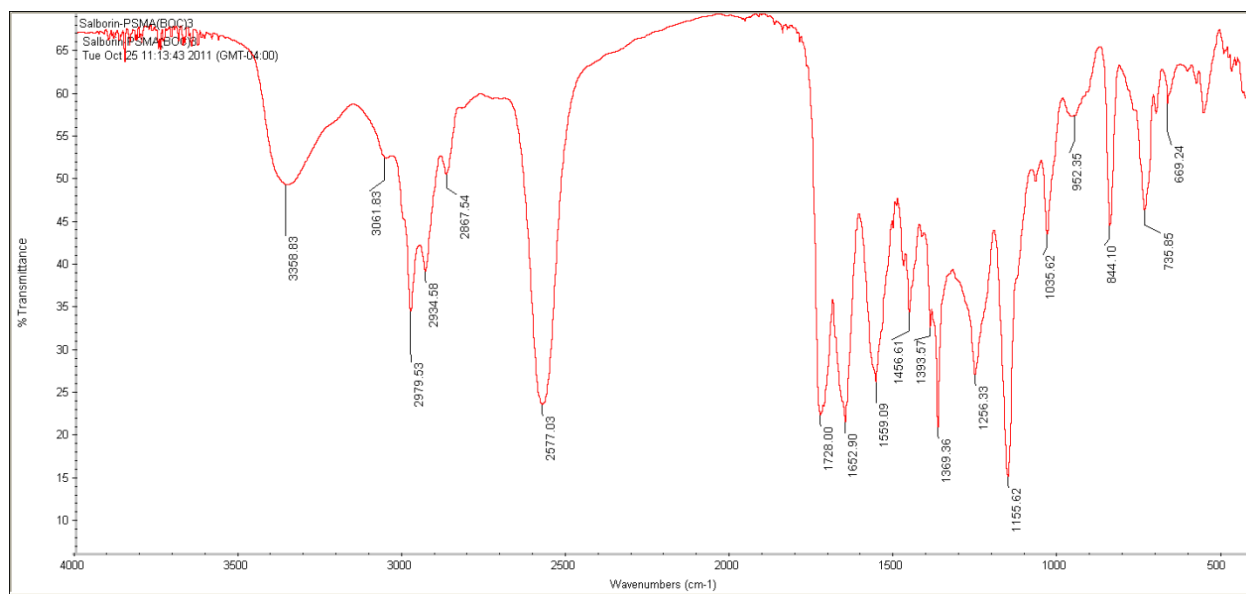


Figure S8. IR spectrum of compound **4**.

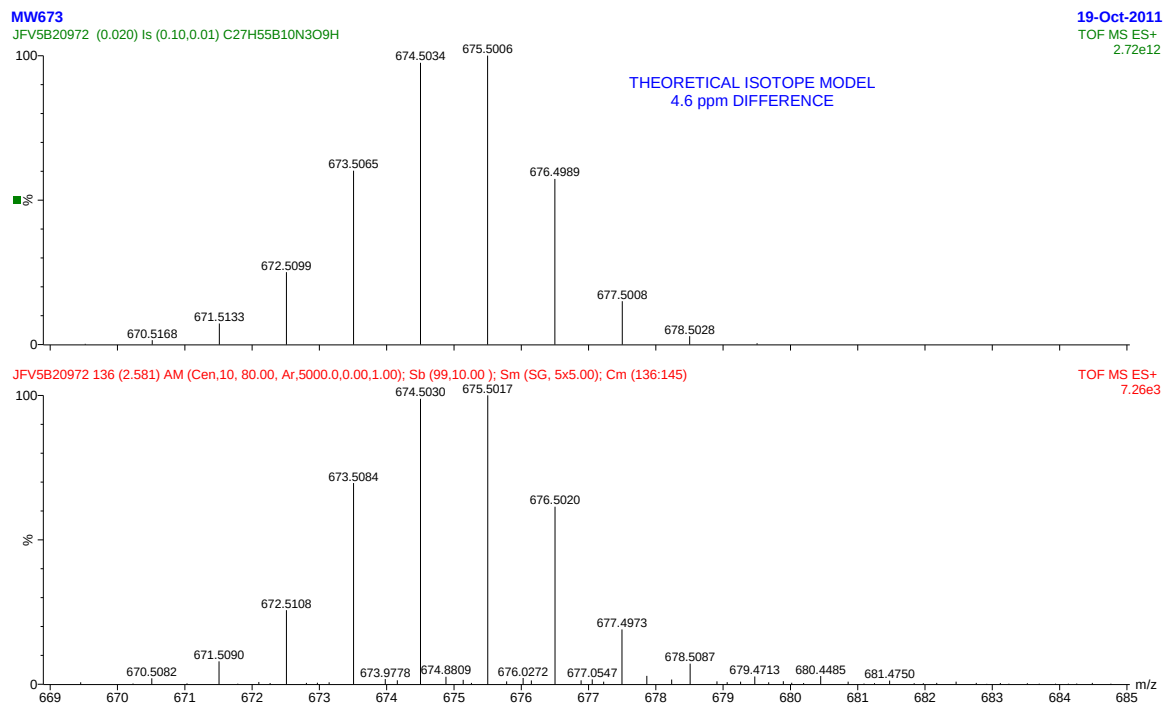


Figure S9. HRMS-ESI spectrum of compound **4**.

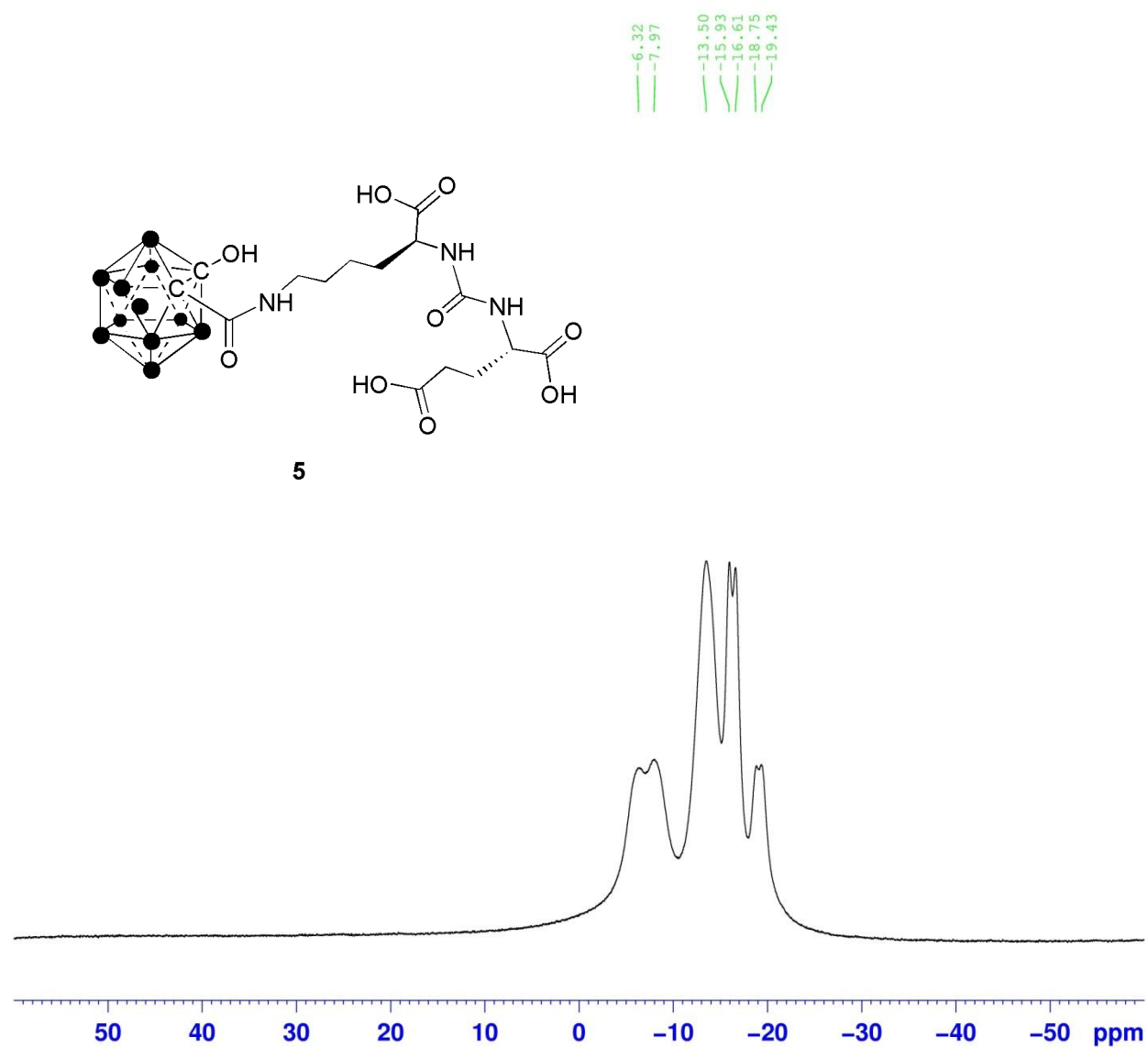


Figure S10. ^{11}B NMR spectrum of compound 5 (DMSO-*d*₆, 192 MHz).

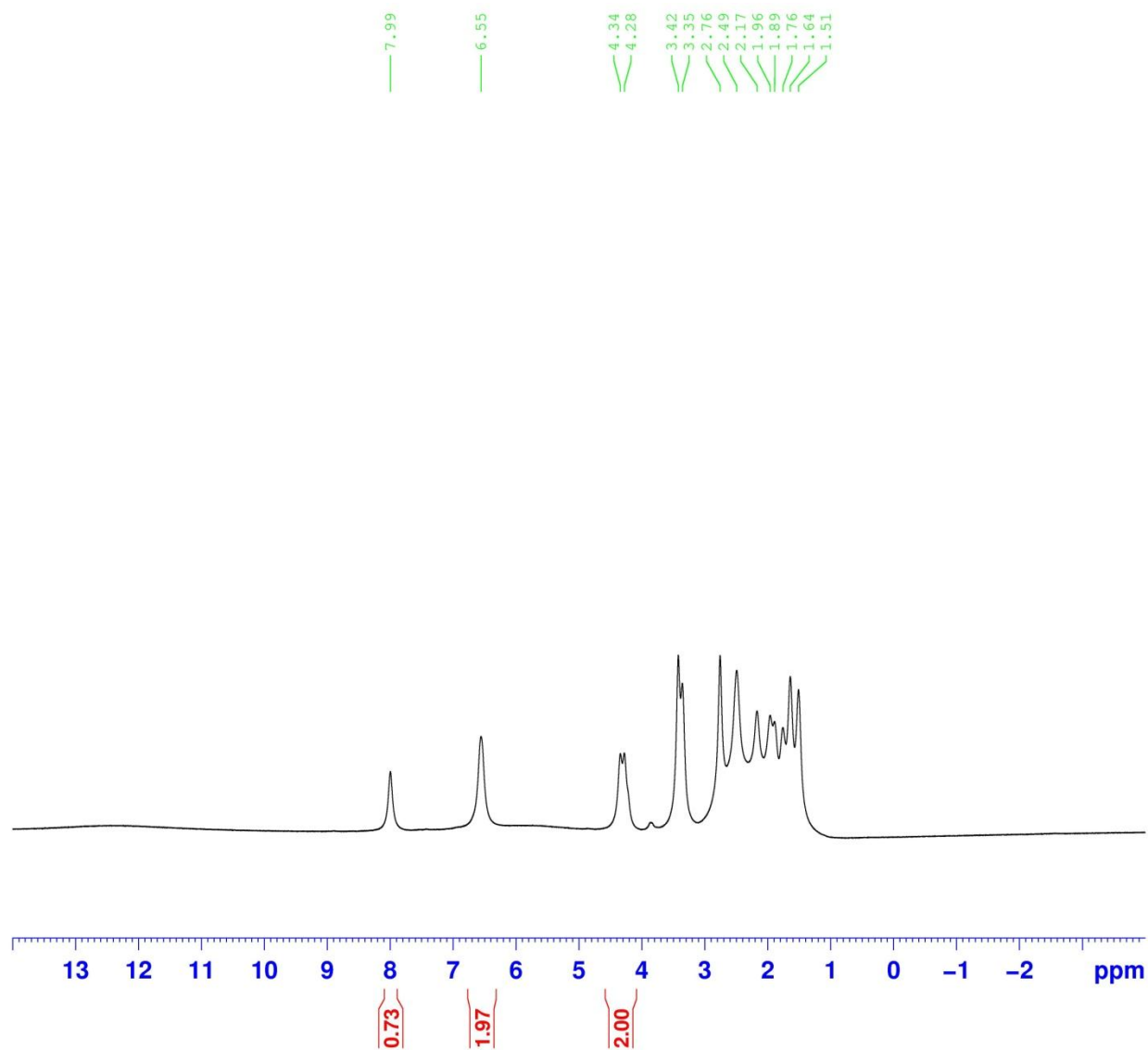


Figure S11. ^1H NMR spectrum of compound 5 ($\text{DMSO-}d_6$, 600 MHz).

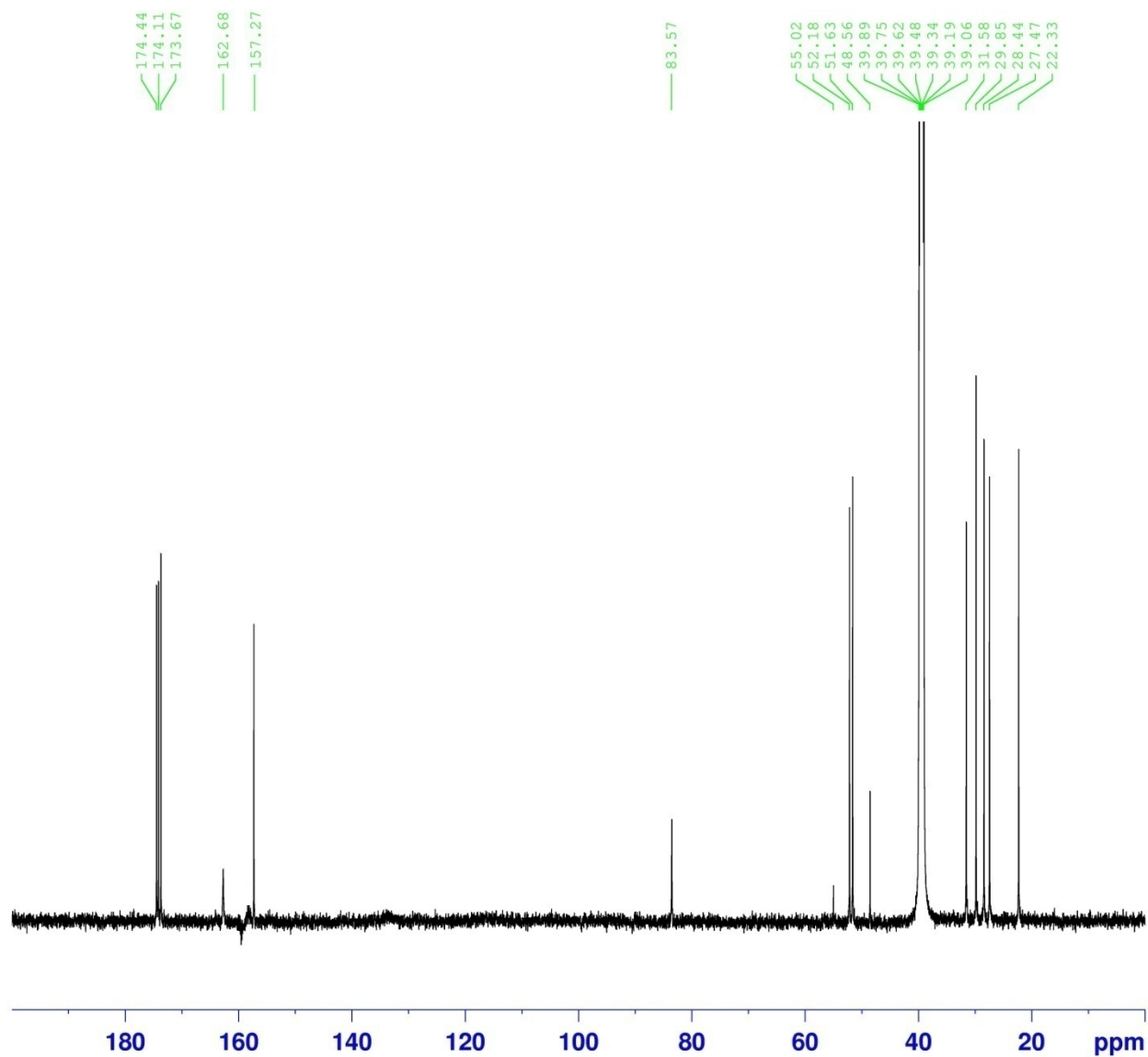


Figure S12. ^{13}C NMR spectrum of compound 5 ($\text{DMSO-}d_6$, 150 MHz).

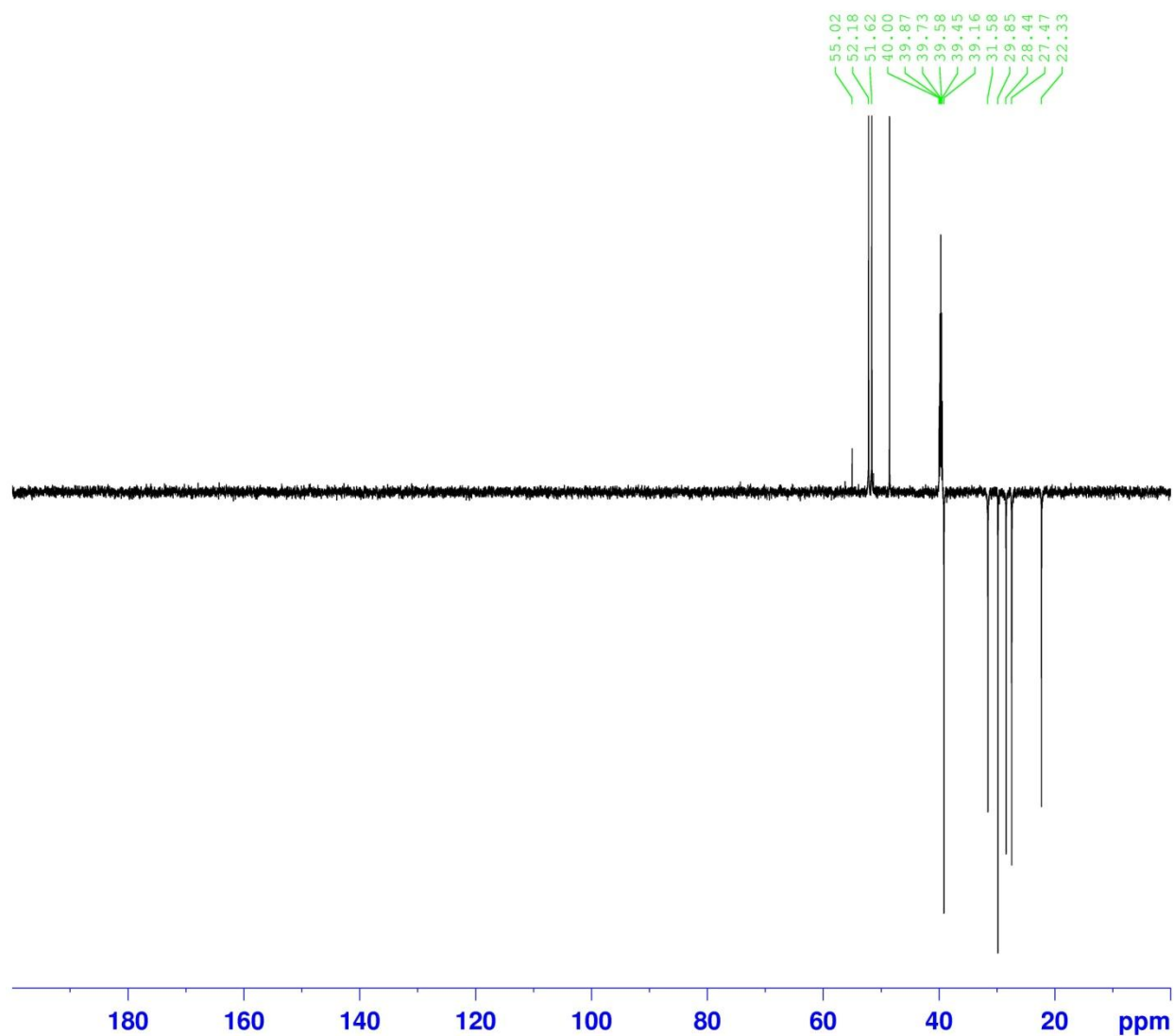


Figure S13. ^{13}C NMR (dept 135 °) spectrum of compound 5 (DMSO- d_6 , 150 MHz).

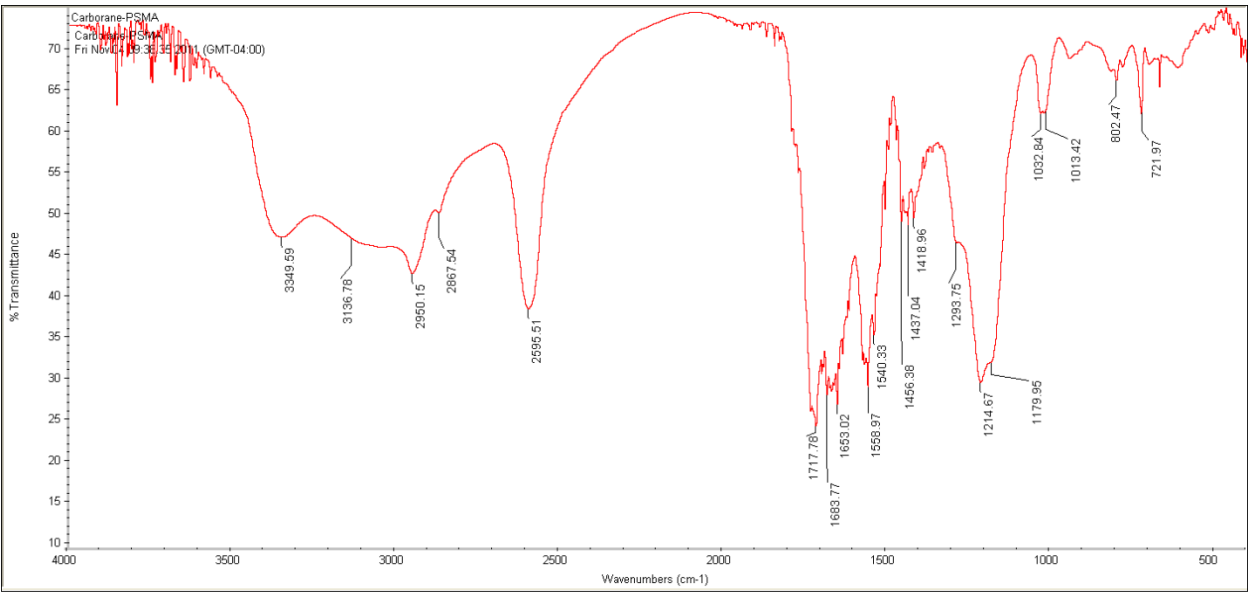


Figure S14. IR spectrum of compound 5.

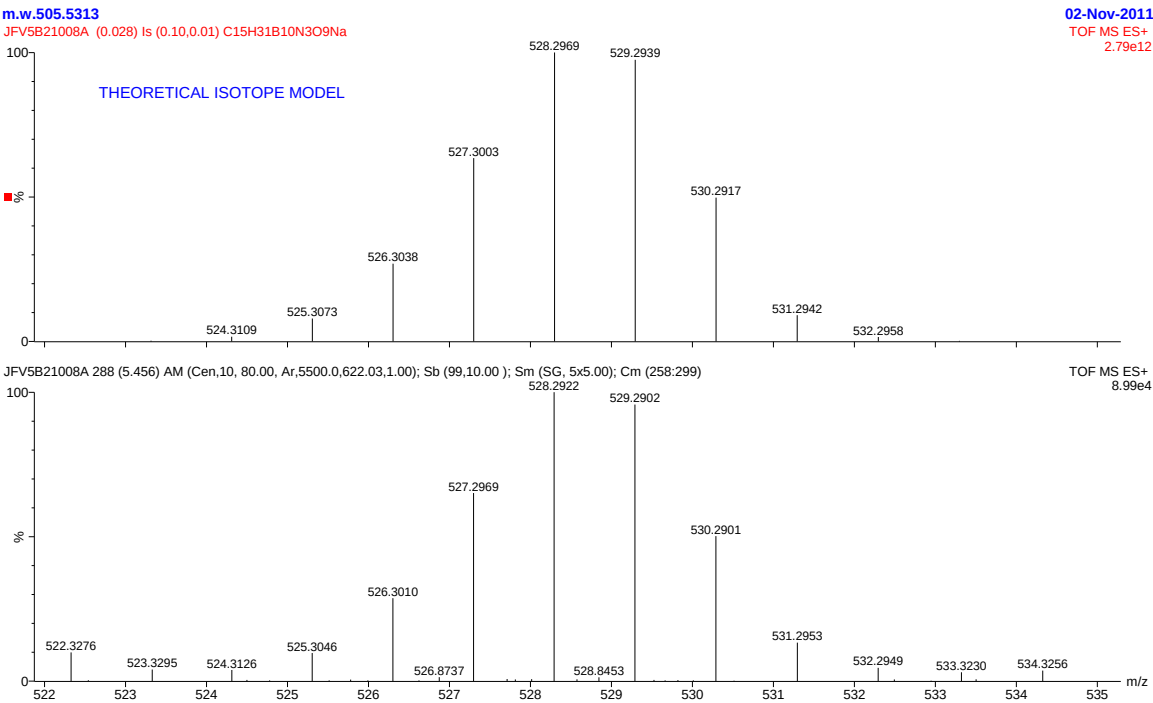


Figure S15. HRMS-ESI spectrum of compound 5.

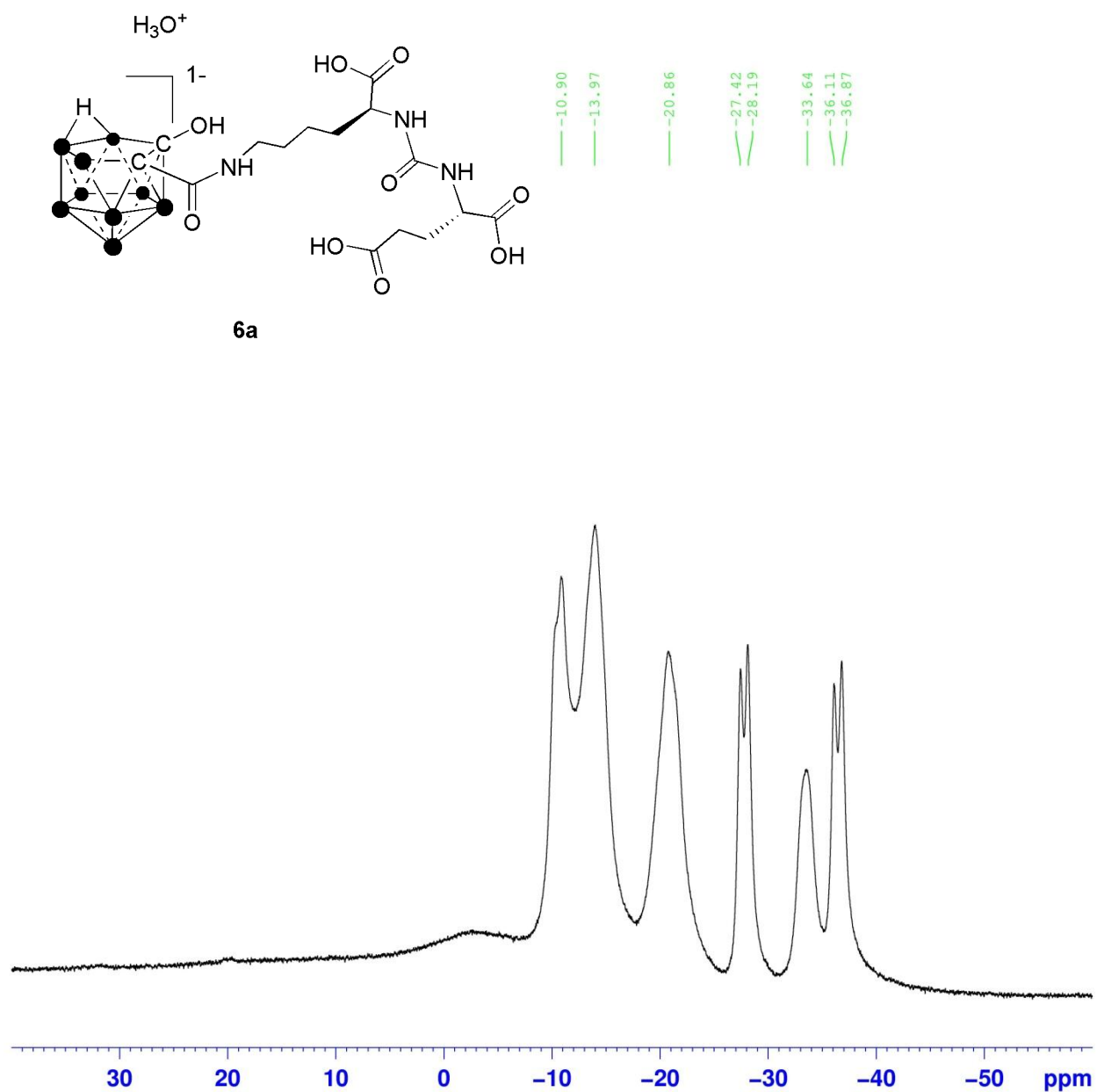


Figure S16. ^{11}B NMR spectrum of compound **6a** (DMSO- d_6 , 192 MHz).

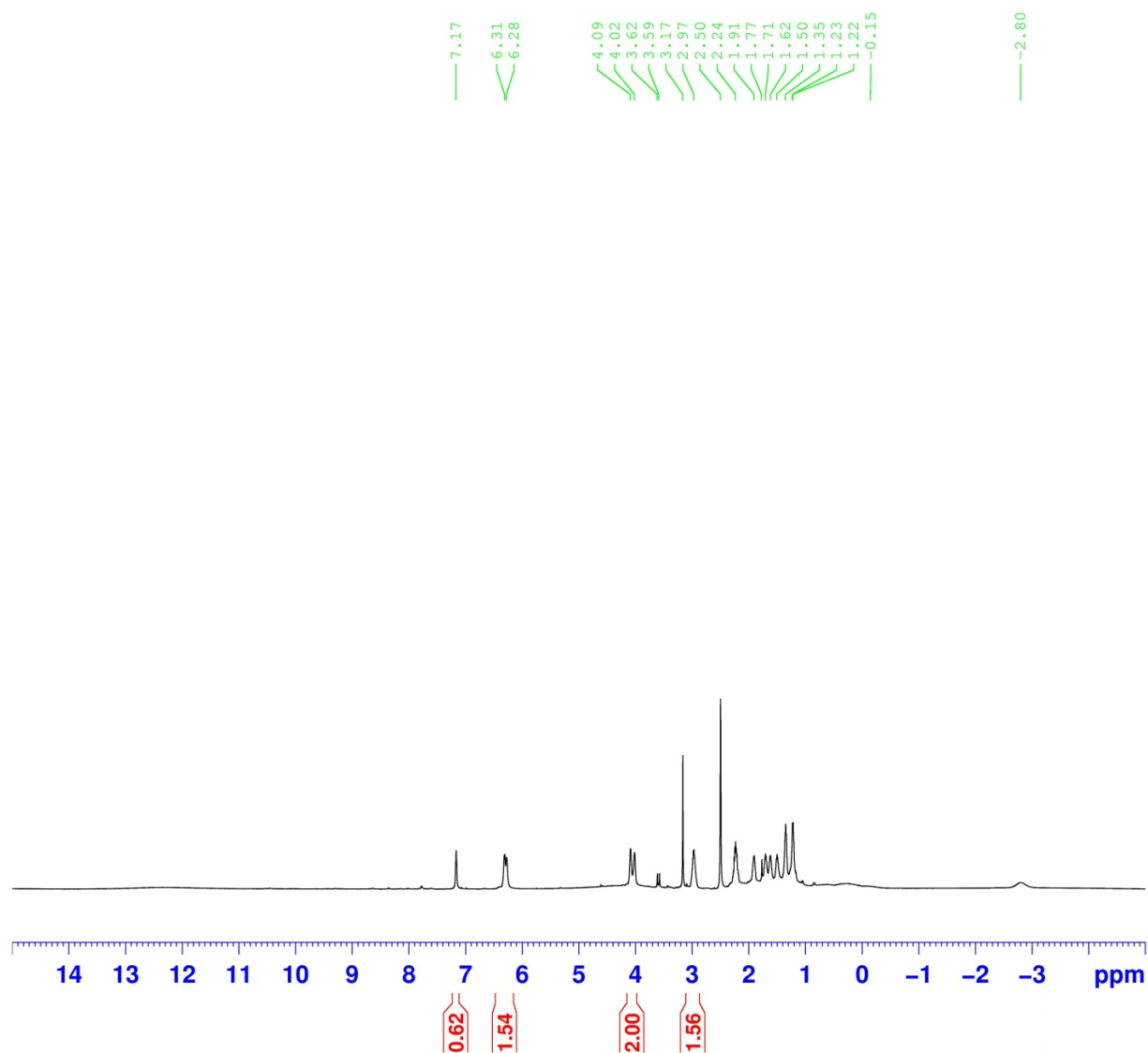


Figure S17. ^1H NMR spectrum of compound **6a** ($\text{DMSO-}d_6$, 600 MHz).

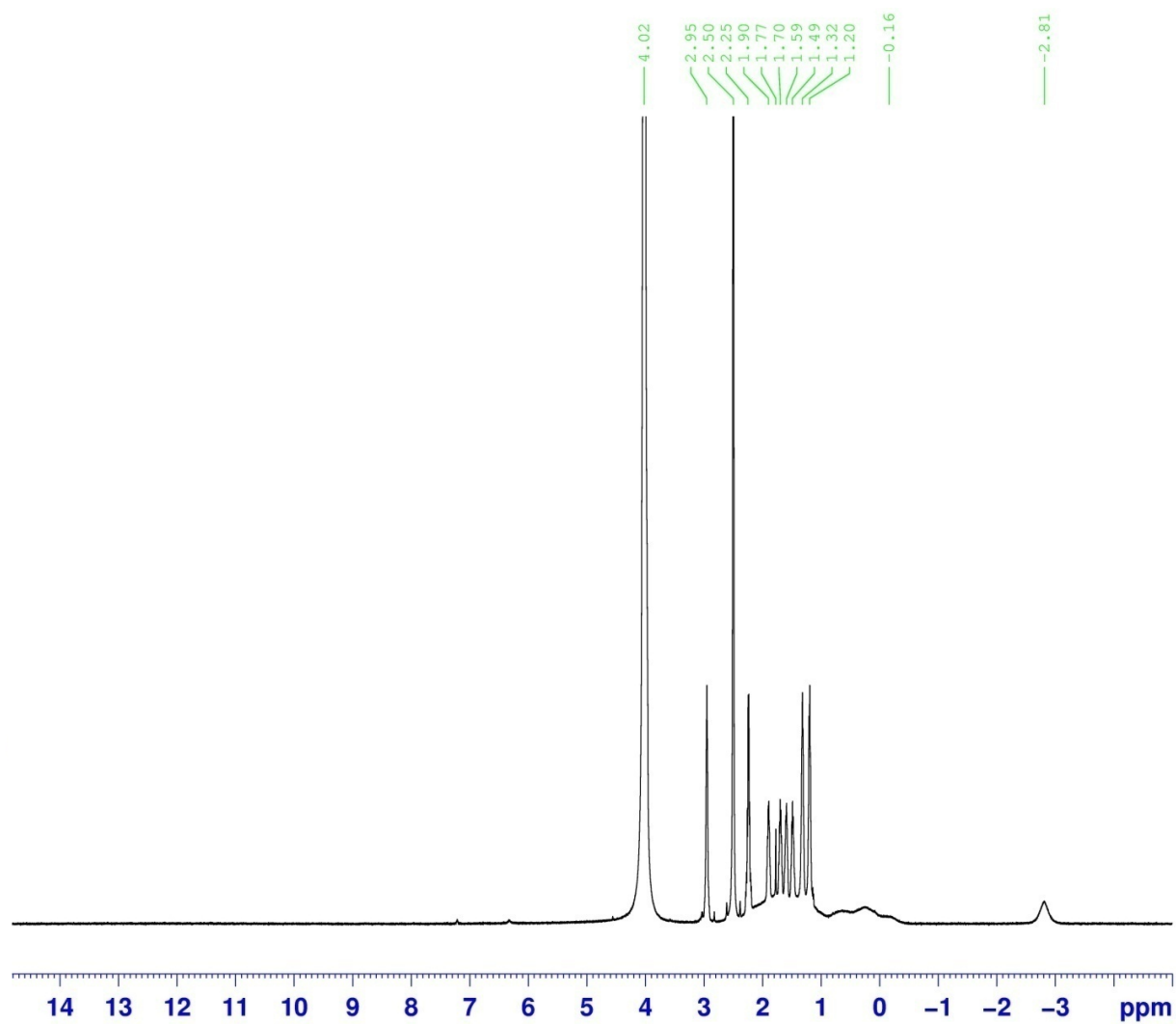


Figure S18. ^1H NMR spectrum of compound **6a** after D_2O exchange ($\text{DMSO}-d_6$, 600 MHz).

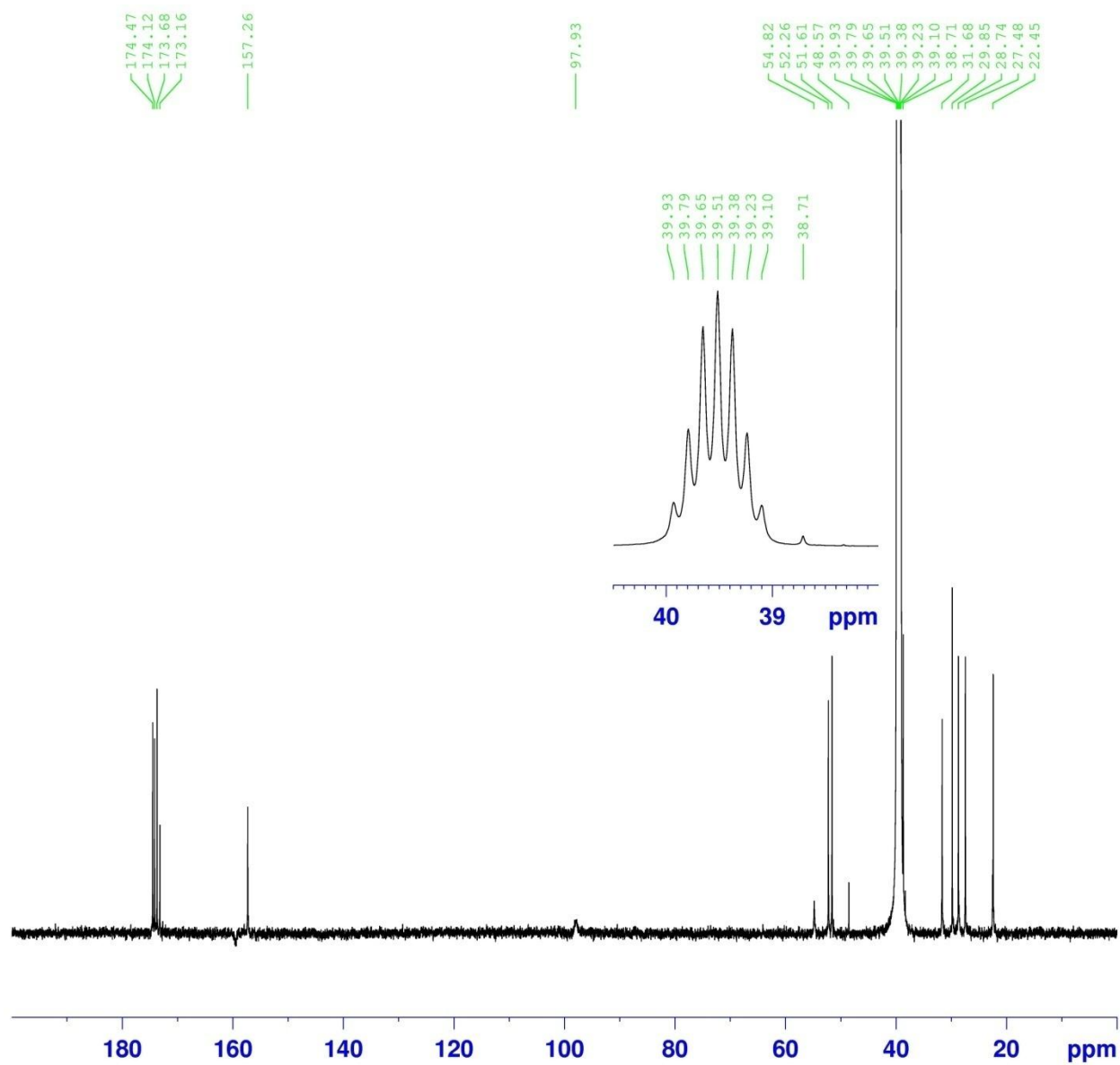


Figure S19. ^{13}C NMR spectrum of compound **6a** ($\text{DMSO-}d_6$, 150 MHz).

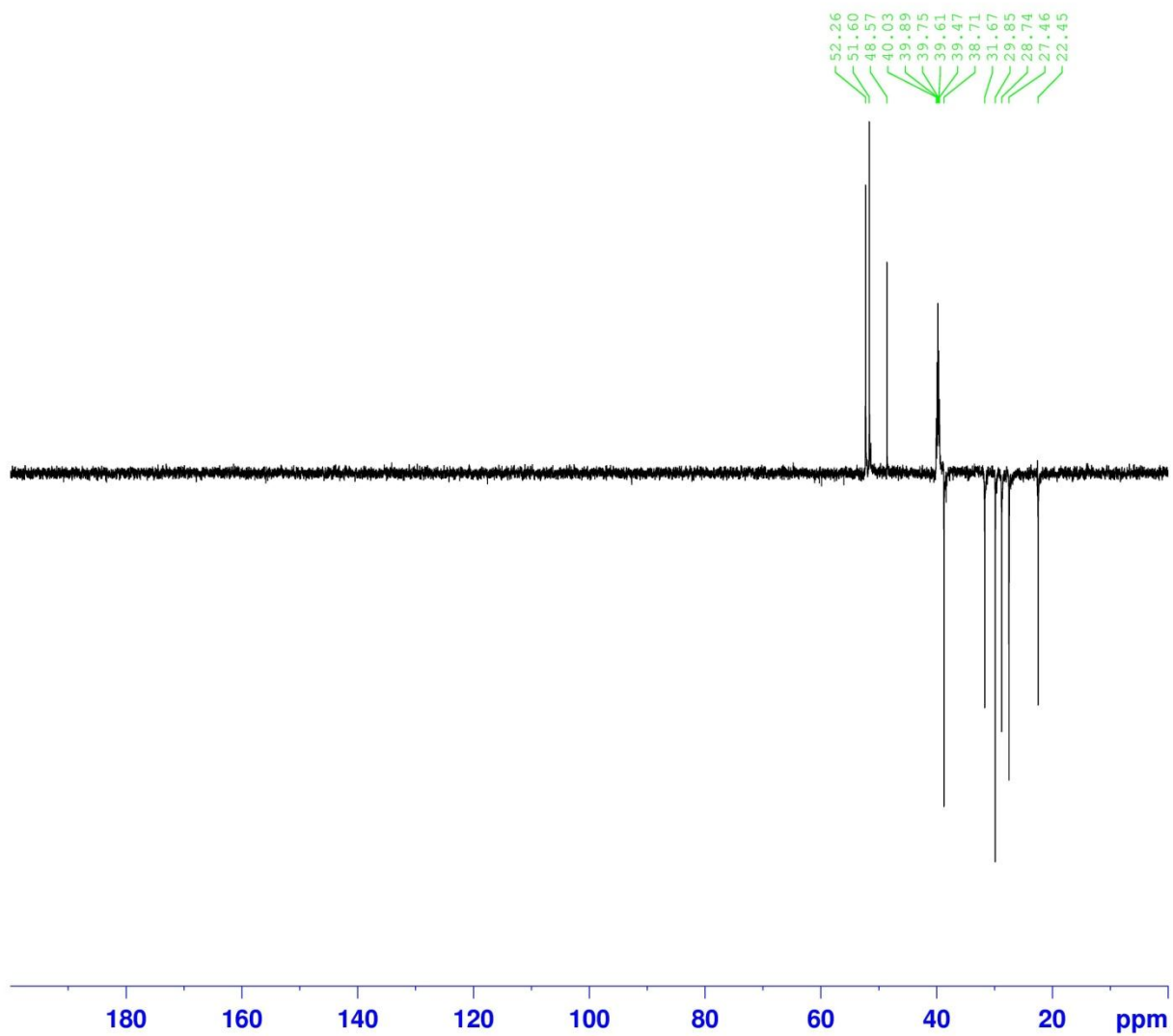


Figure S20. ^{13}C NMR (dept 135 $^{\circ}$) spectrum of compound **6a** ($\text{DMSO-}d_6$, 150 MHz).

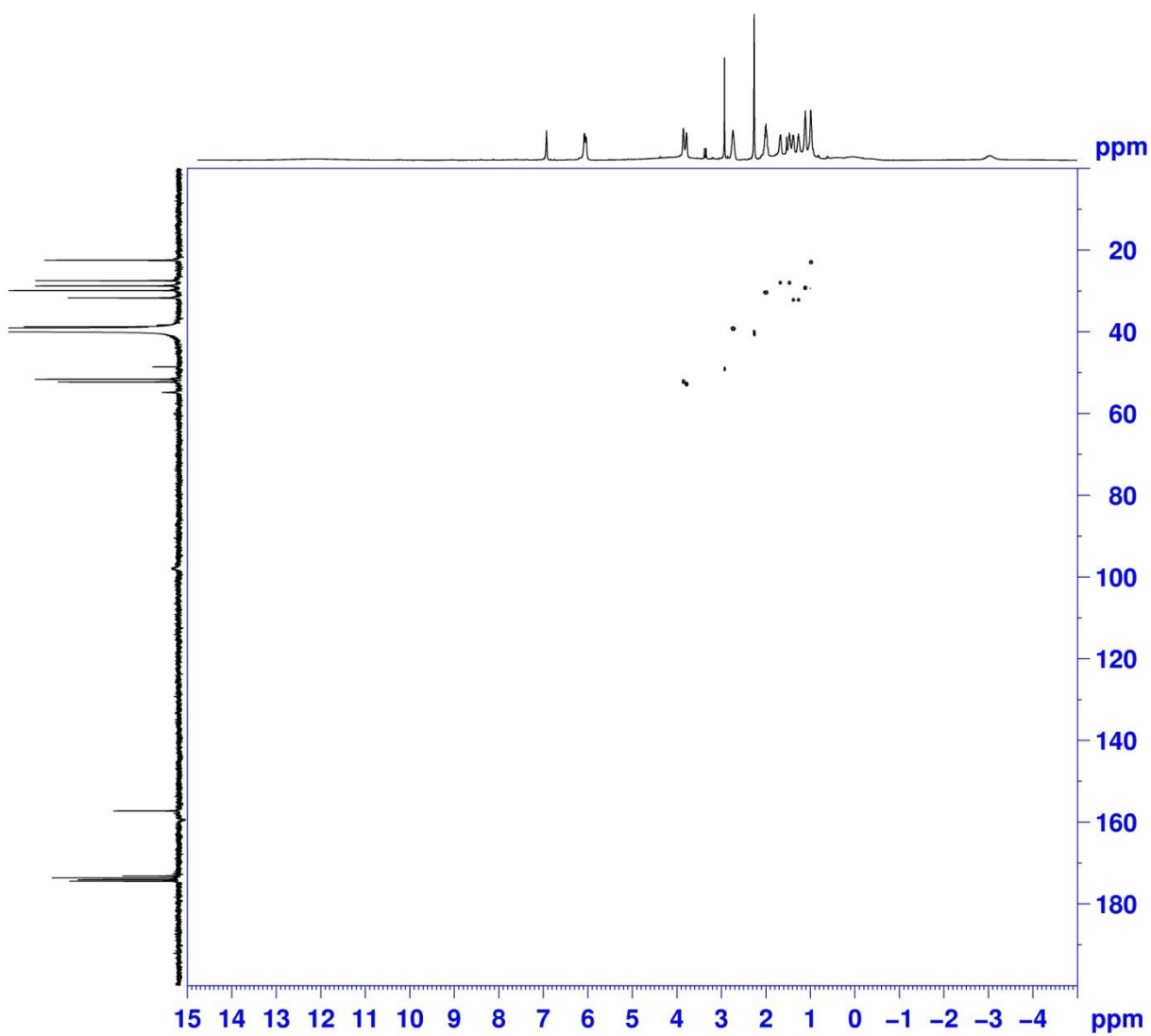


Figure S21. HSQC of compound **6a**.

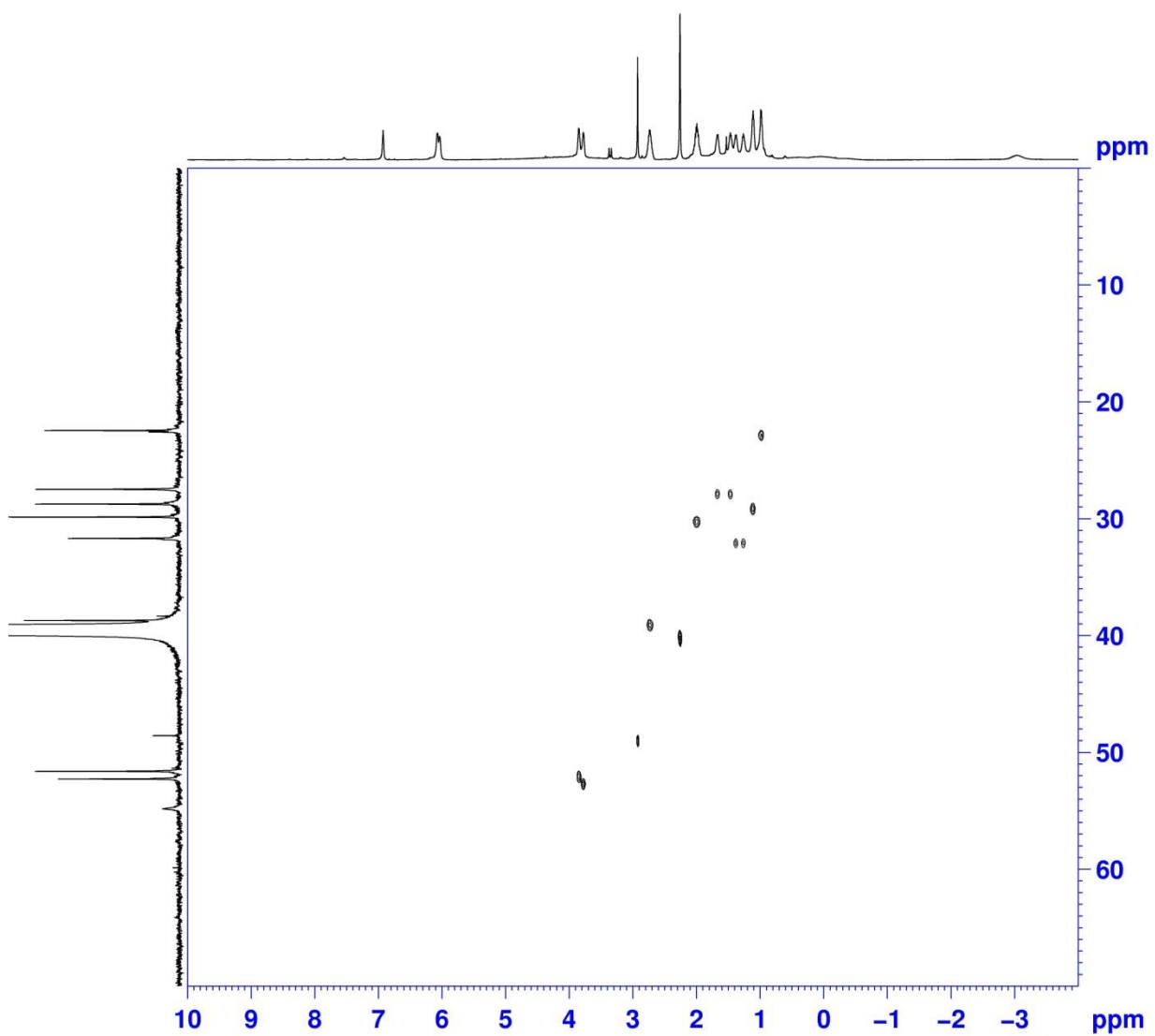


Figure S22. HMBC of compound **6a**.

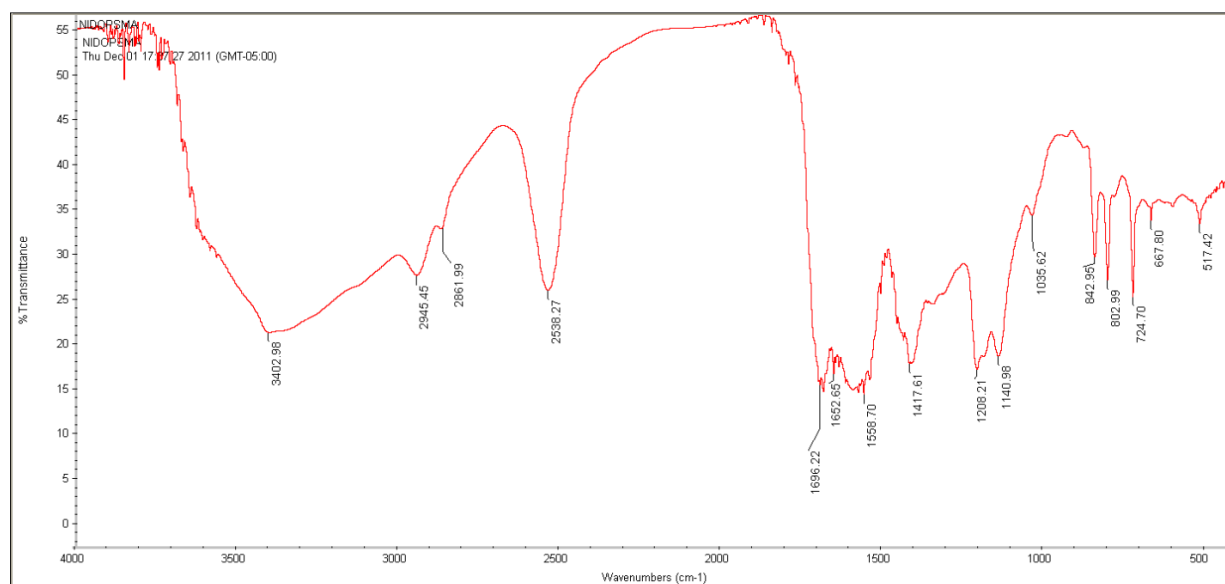


Figure S23. IR spectrum of compound **6a**.

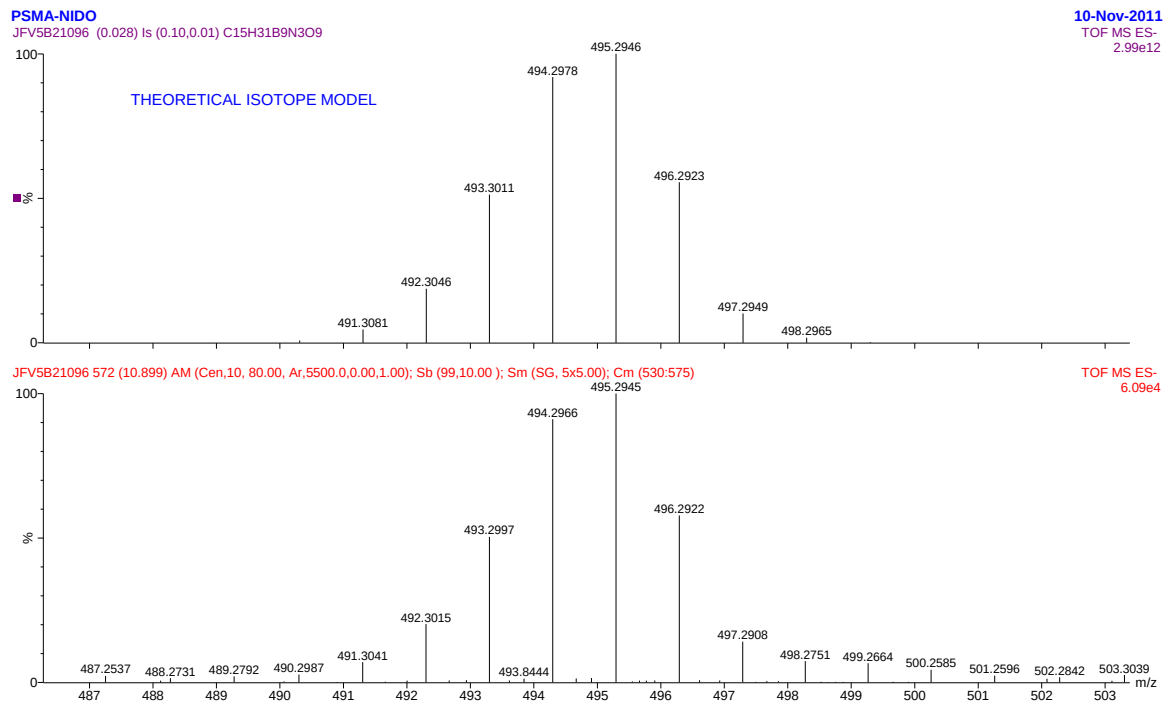


Figure S24. HRMS-ESI spectrum of compound **6a**.

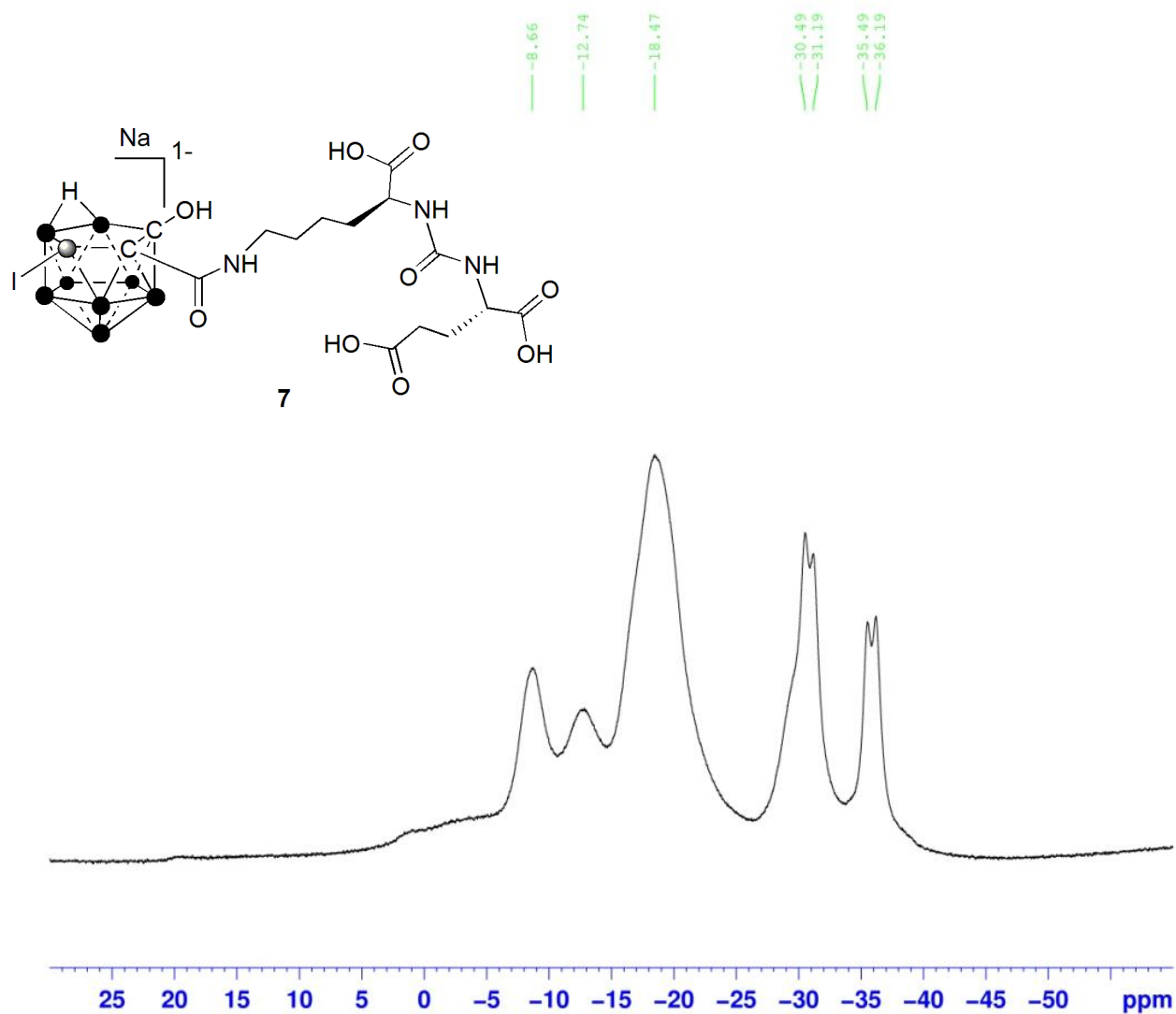


Figure S25. ^{11}B NMR spectrum of compound 7 (DMSO- d_6 , 192 MHz).

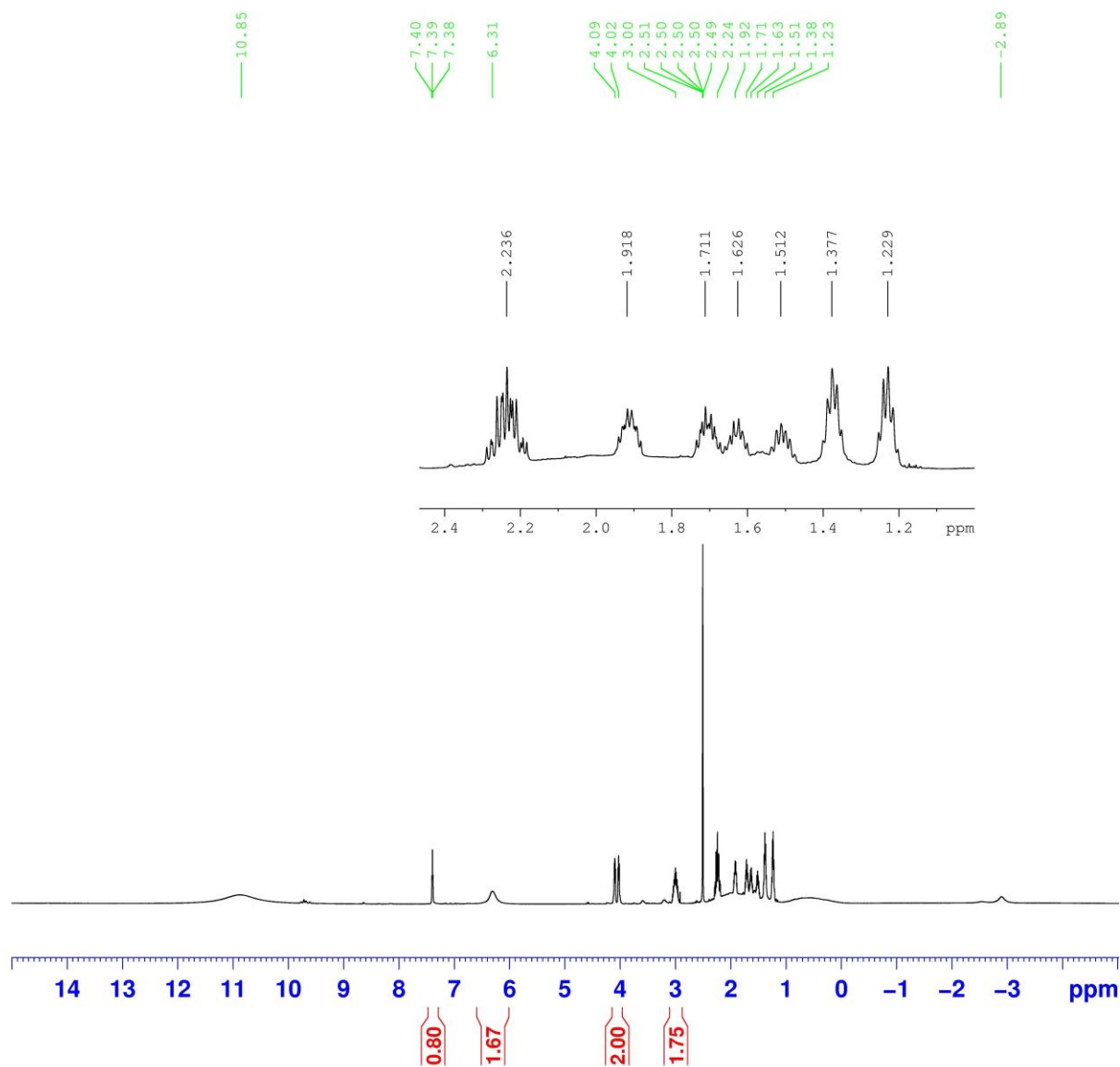


Figure S26. ^1H NMR spectrum of compound 7 (DMSO- d_6 , 600 MHz).

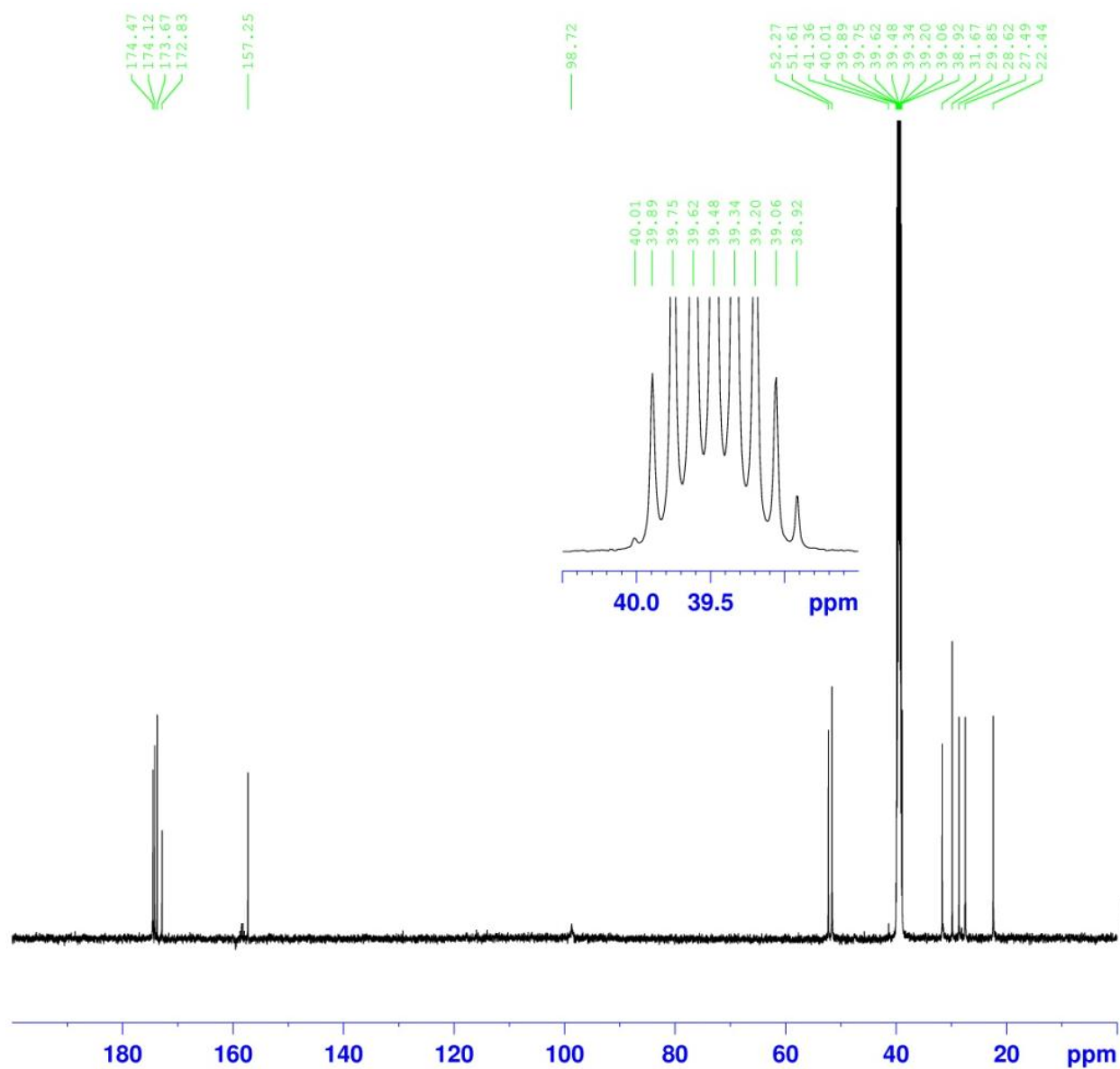


Figure 27. ^{13}C NMR spectrum of compound 7 (DMSO- d_6 , 150 MHz).

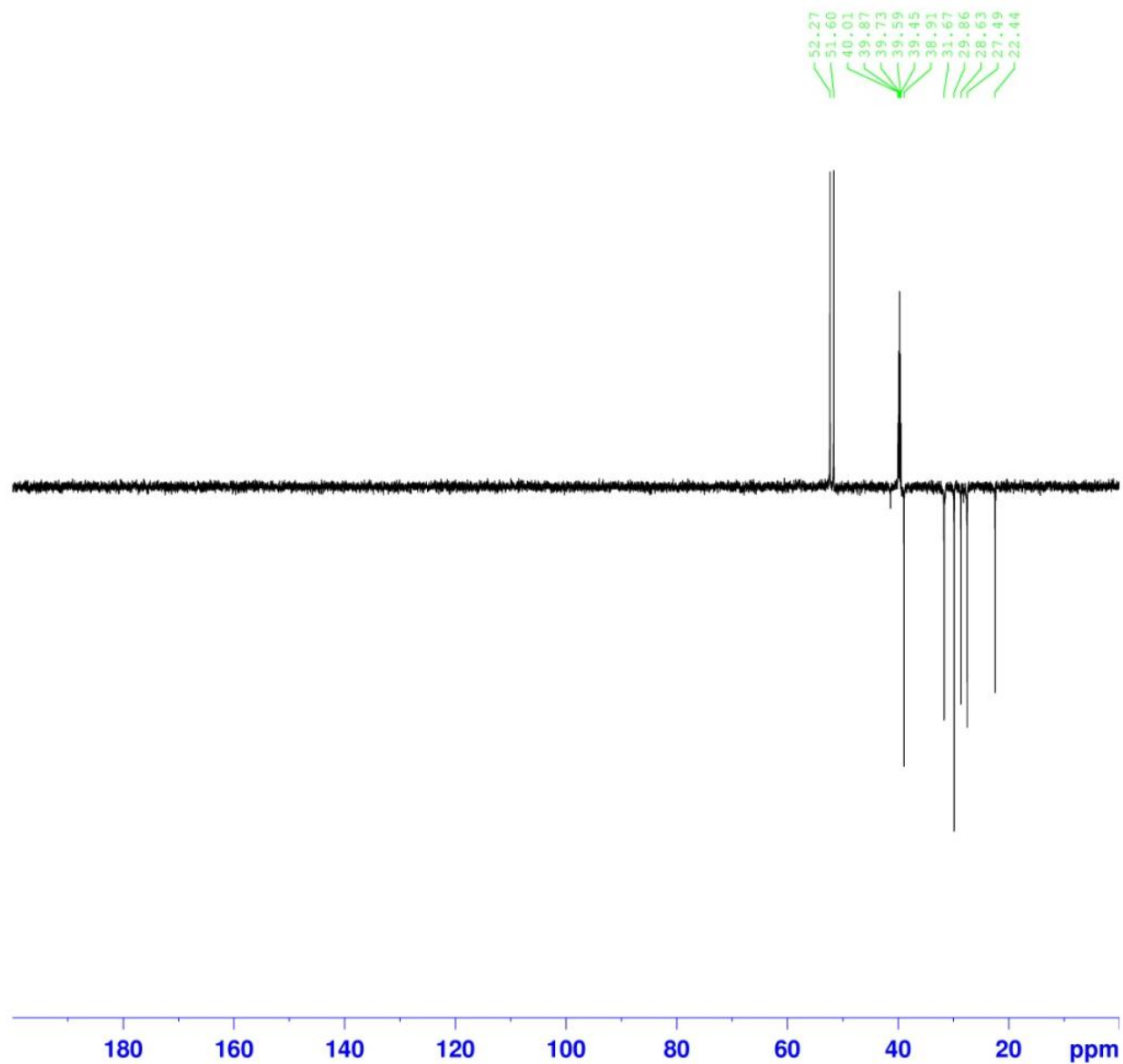


Figure S28. ^{13}C NMR (dept 135 °) spectrum of compound 7 ($\text{DMSO-}d_6$, 192 MHz).

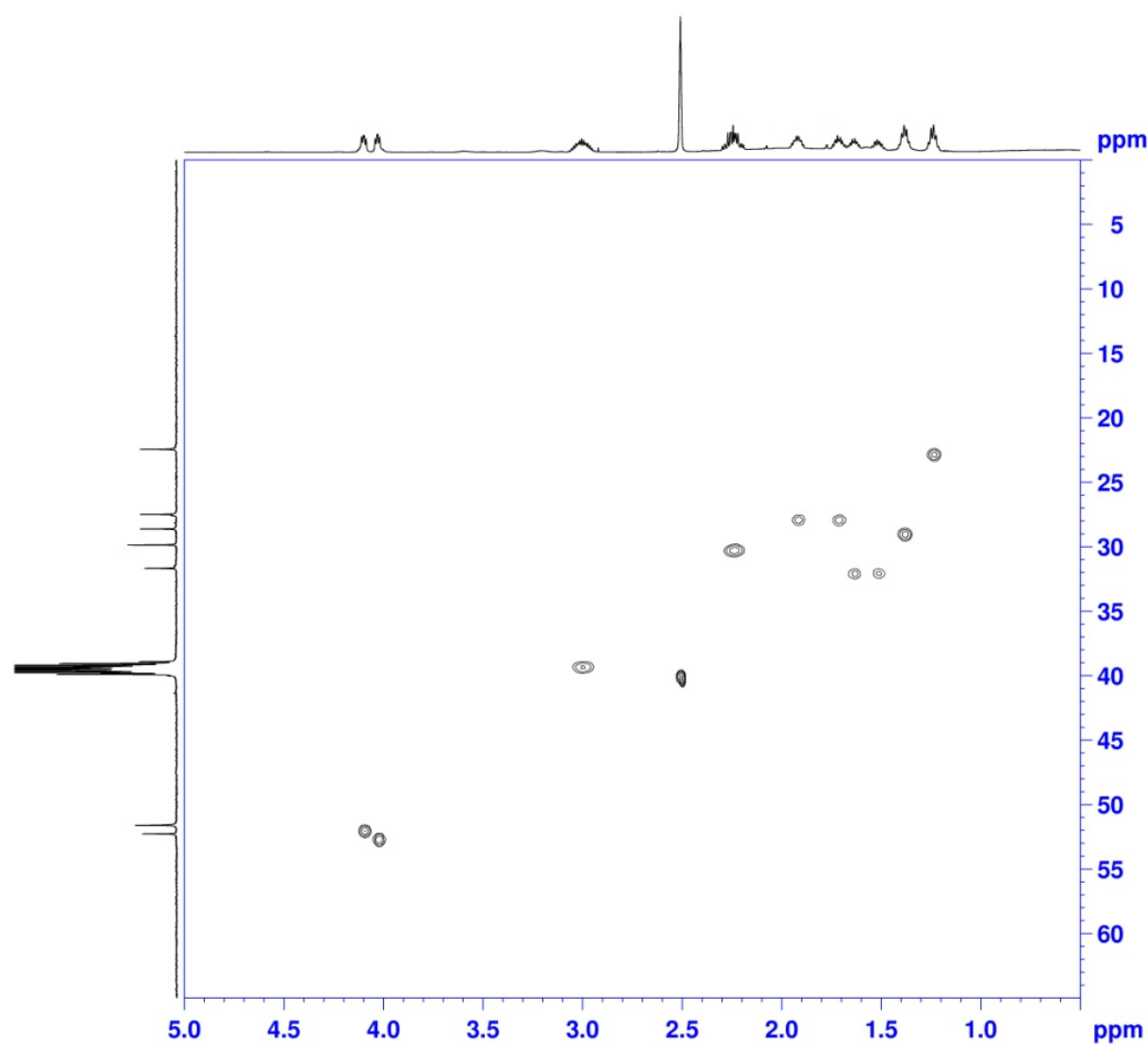


Figure S29. HSQC of compound 7.

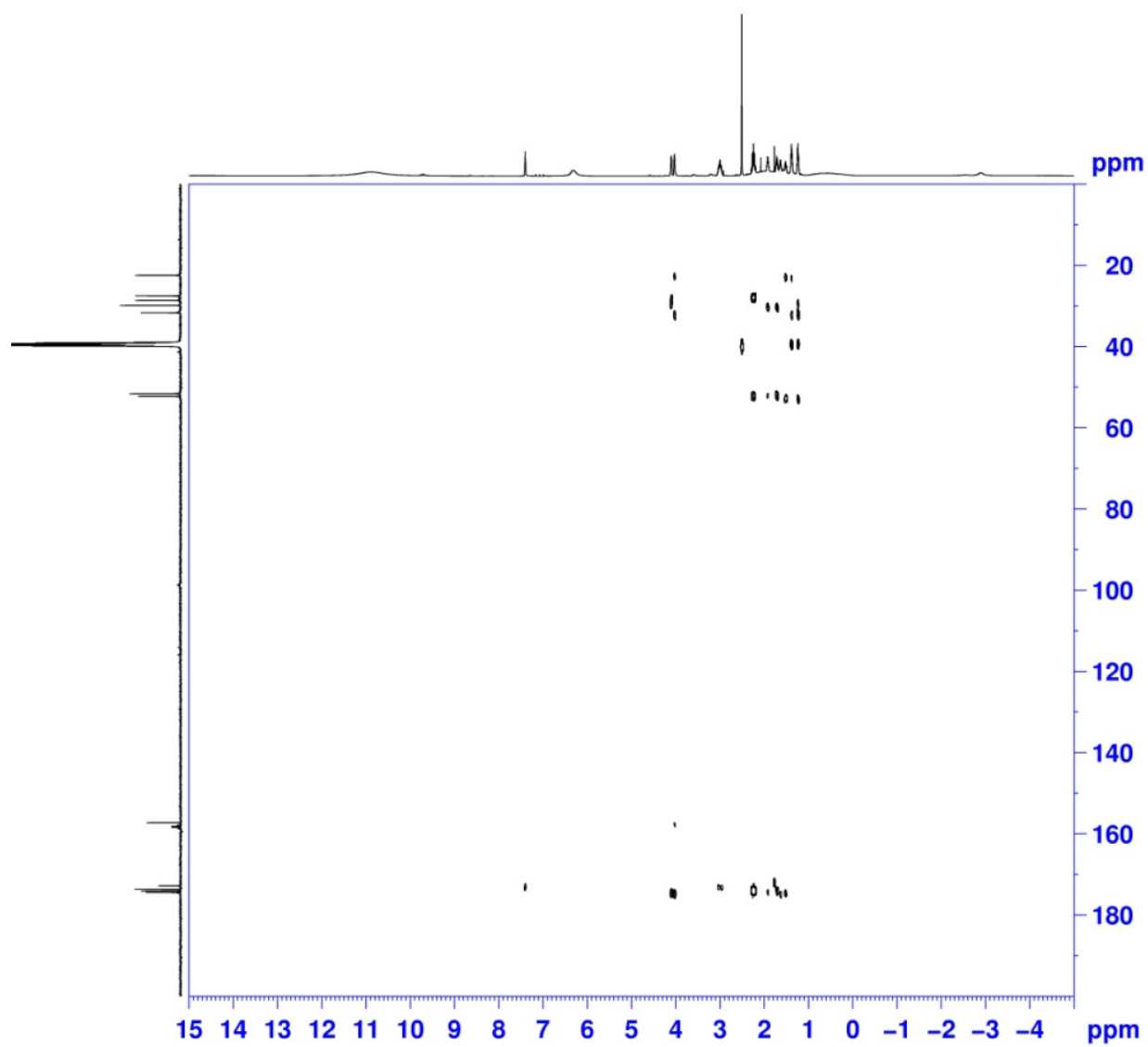


Figure S30. HMBC of compound 7.

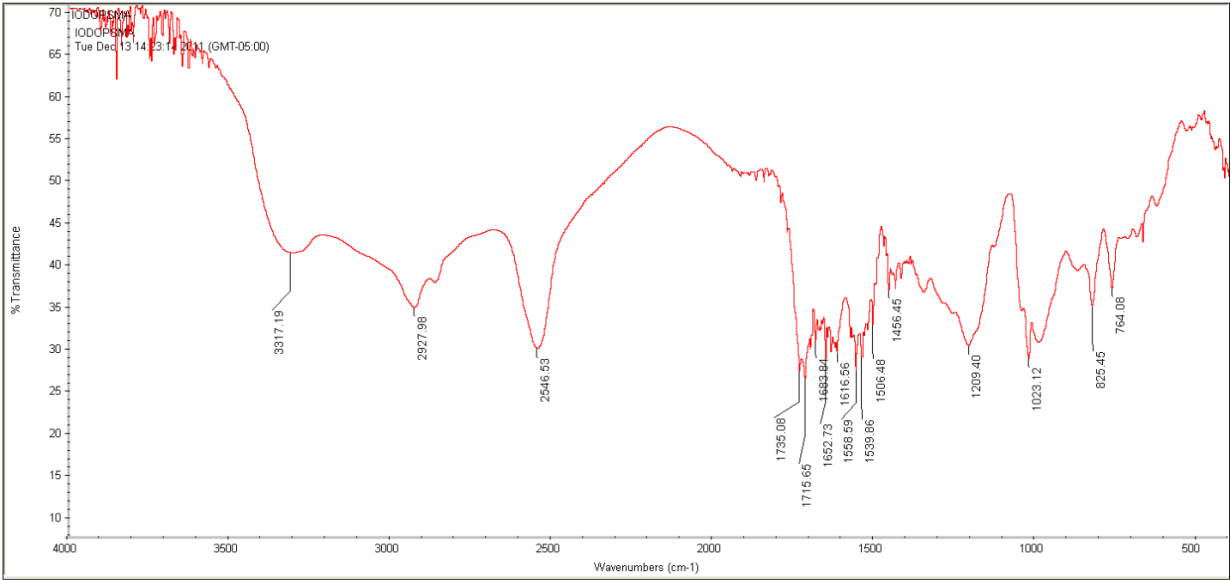


Figure S31. IR spectrum of compound 7.

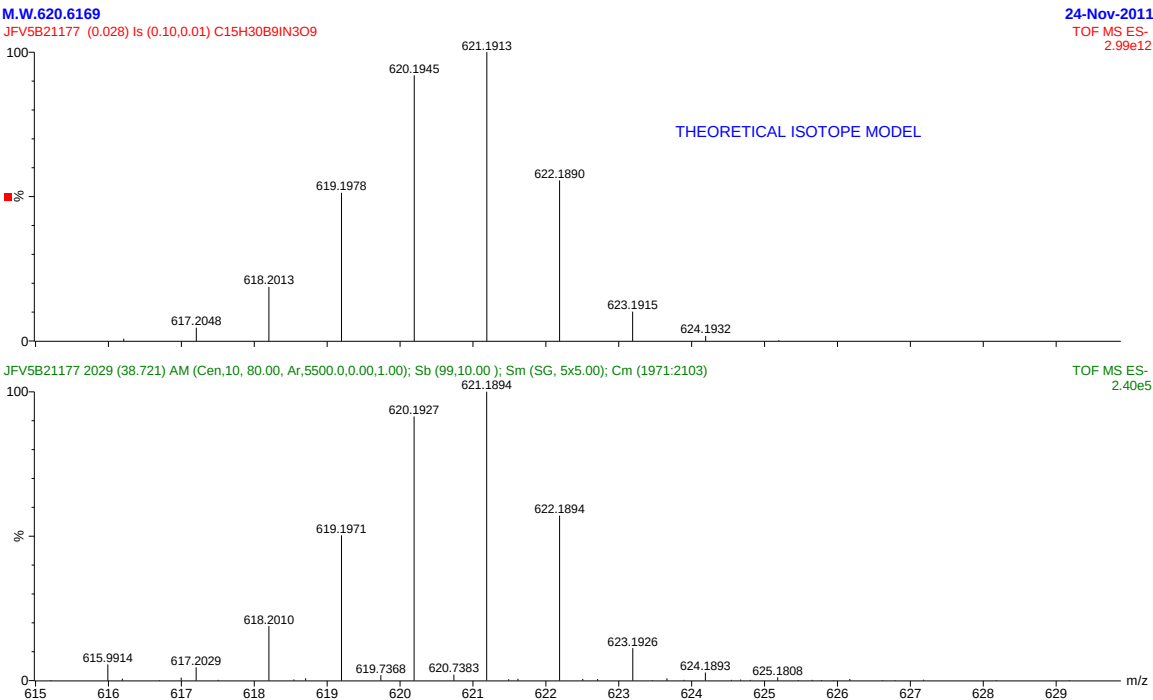


Figure S32. HRMS-ESI spectrum of compound 7.

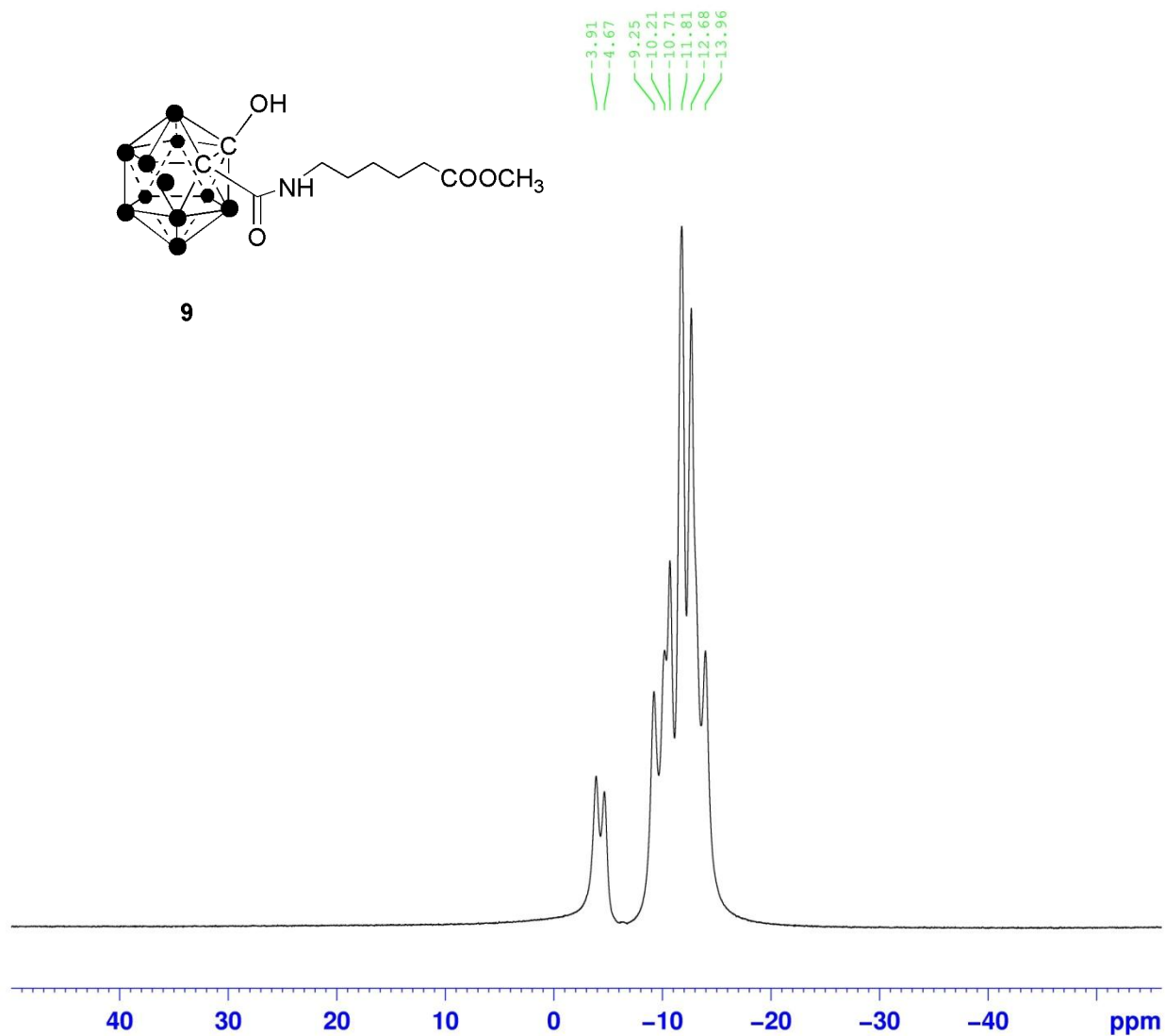


Figure S33. ^{11}B NMR spectrum of compound **9** (CDCl₃, 192 MHz).

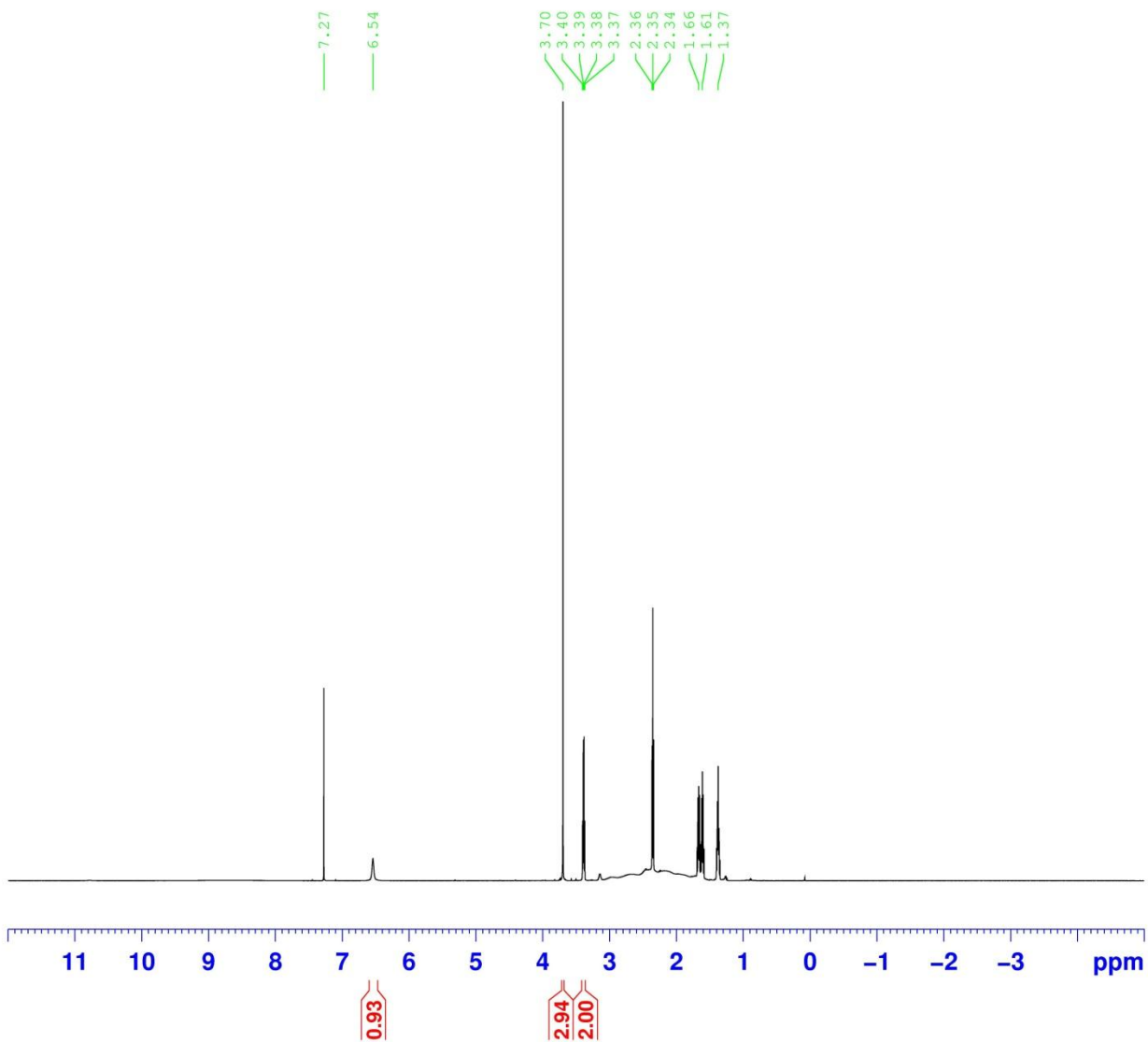


Figure S34. ^1H NMR spectrum of compound **9** (CDCl_3 , 600 MHz).

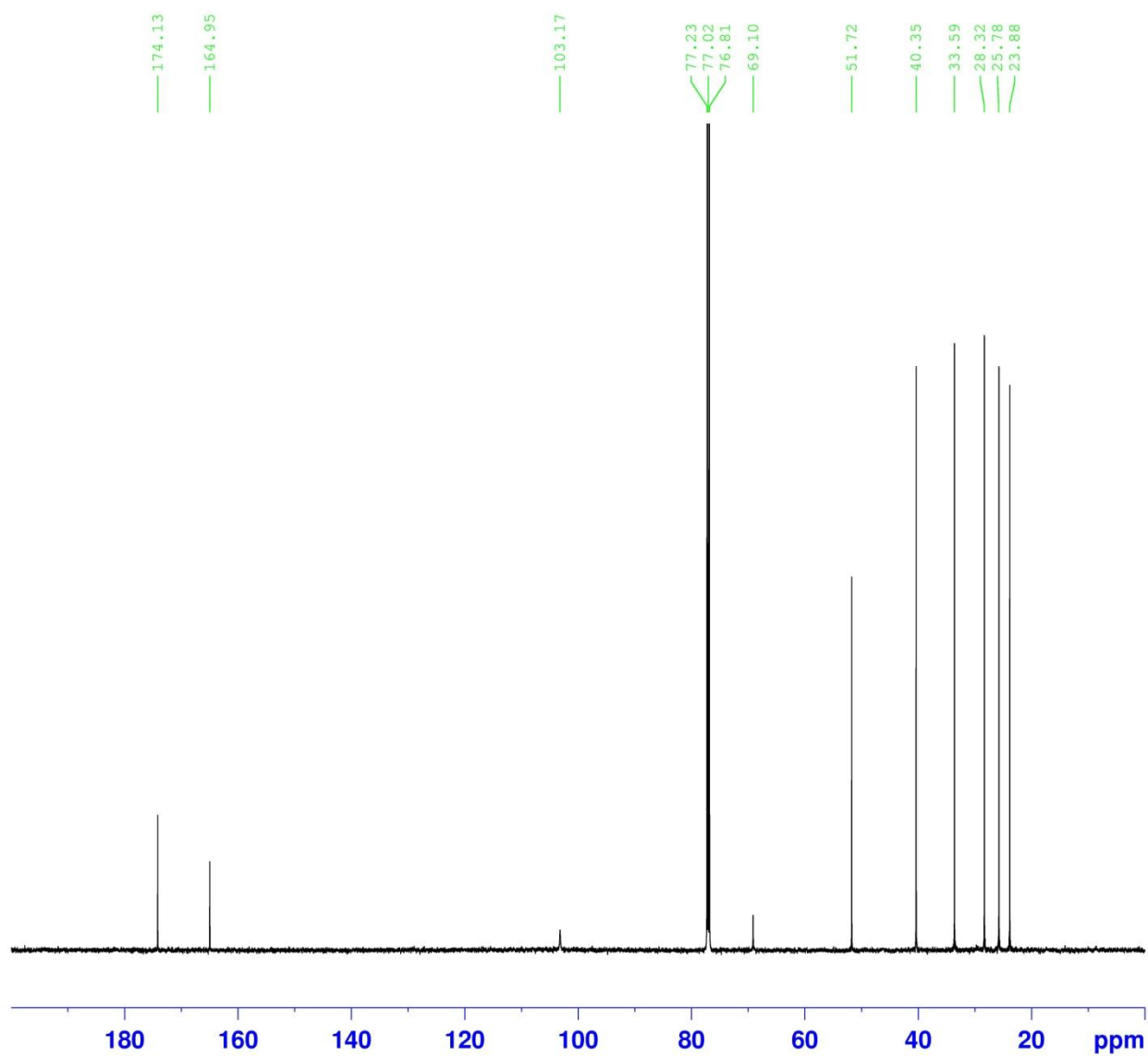


Figure S35. ^{13}C NMR spectrum of compound **9** (CDCl_3 , 150 MHz).

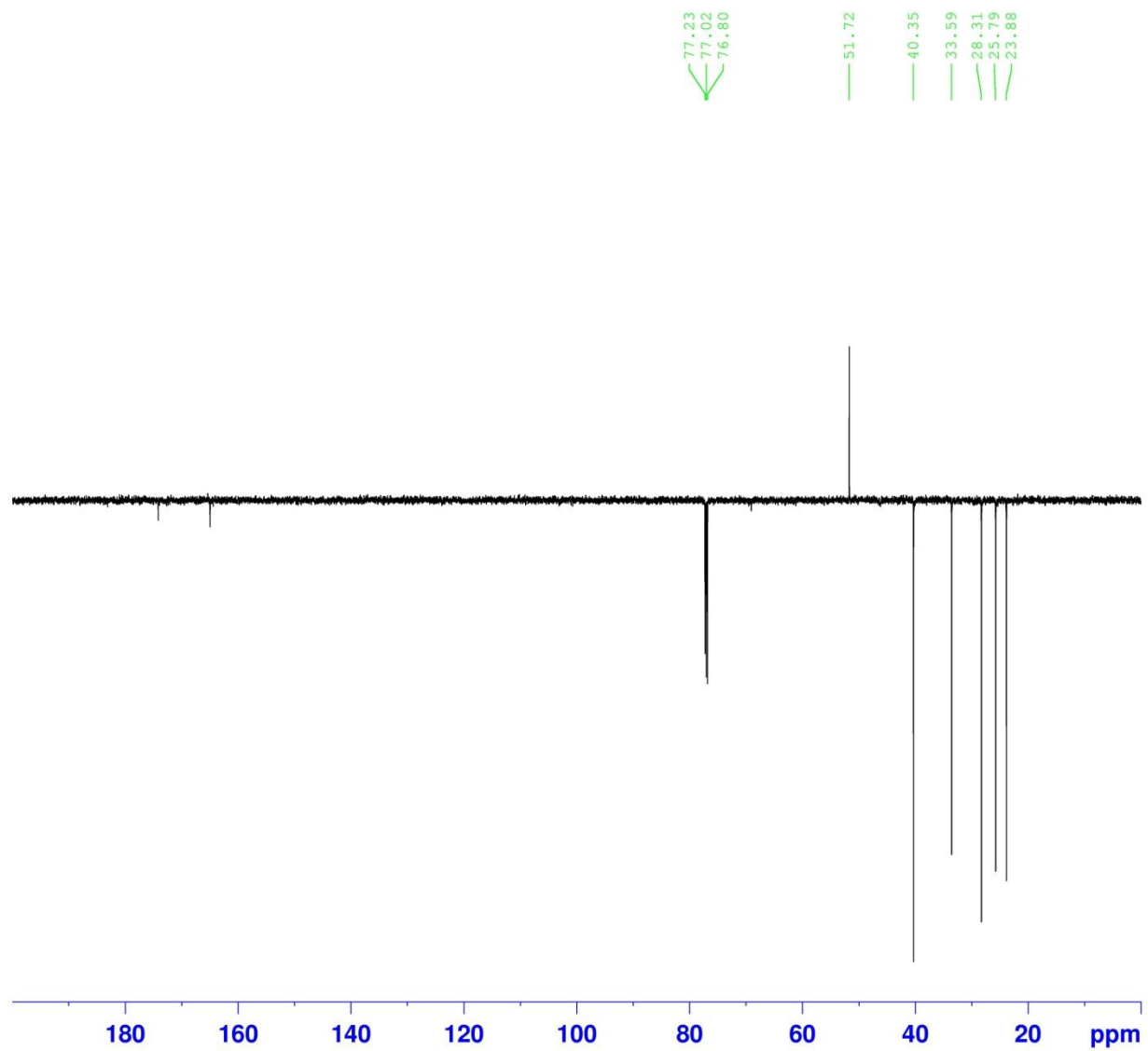


Figure S36. ^{13}C NMR (dept 135 °) spectrum of compound **9** (CDCl_3 , 150 MHz).

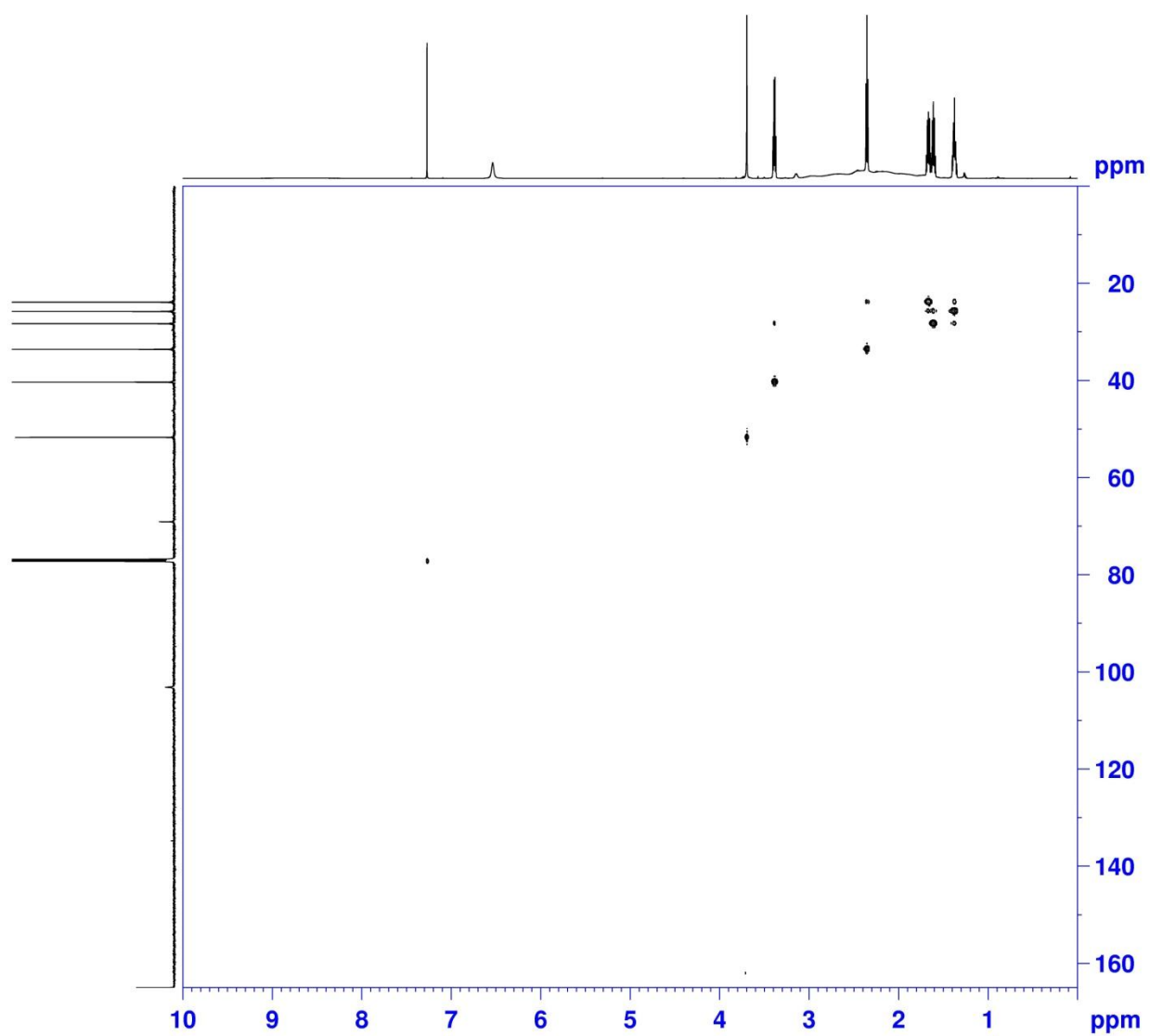


Figure S37. HSQC of compound 9.

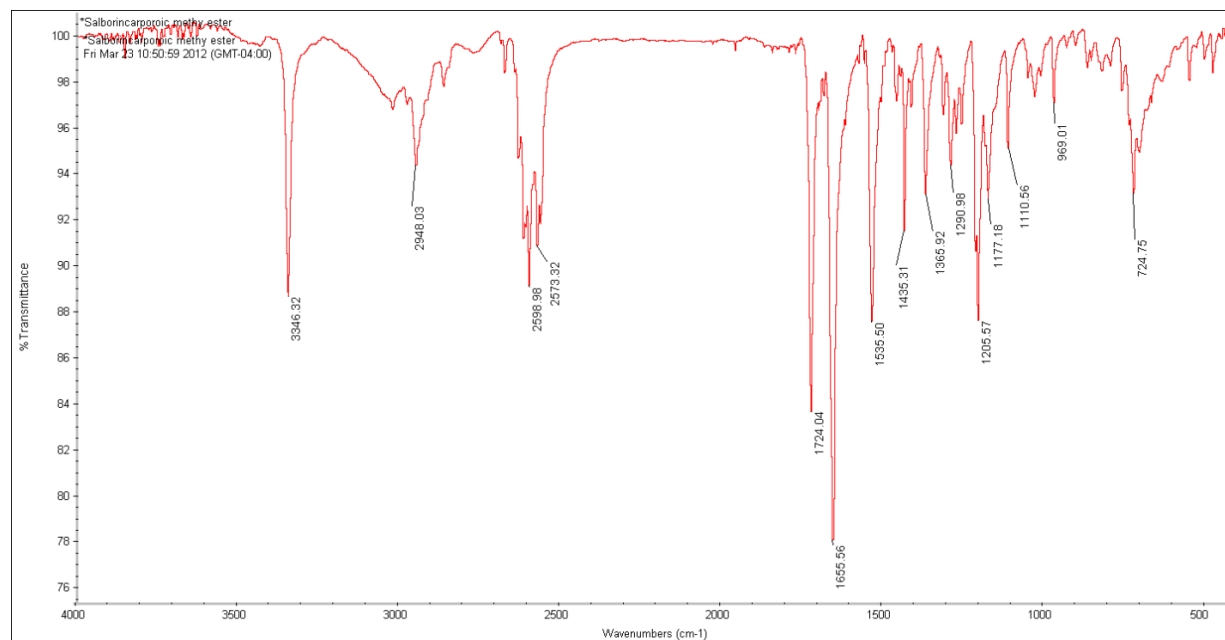


Figure S38. IR spectrum of compound **9**.

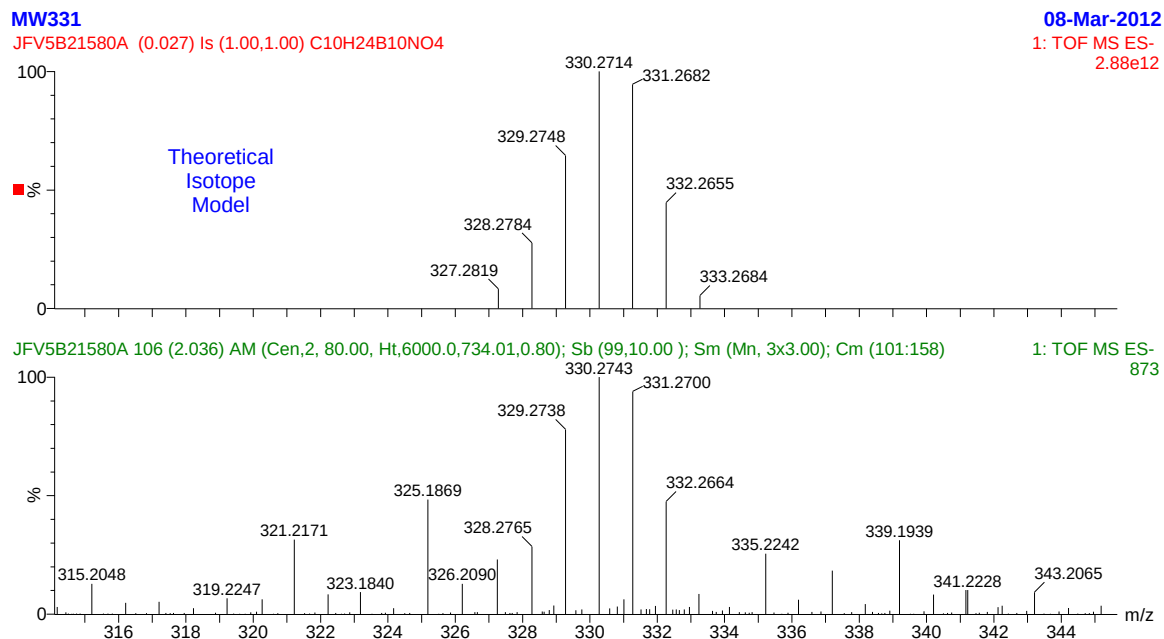


Figure S39. HRMS-ESI spectrum of compound **9**.

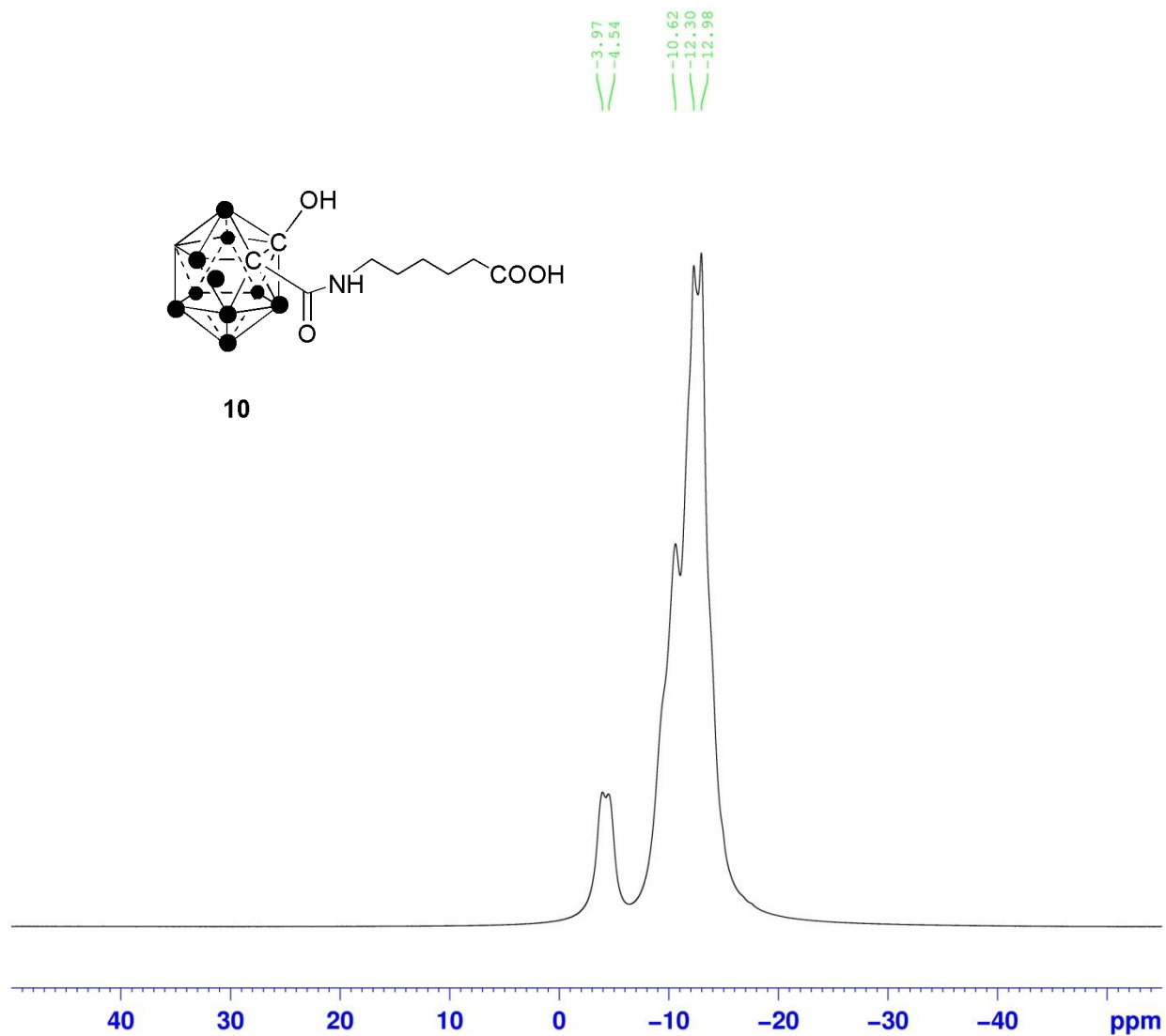


Figure S40. ¹¹B NMR spectrum of compound **10** (CD₂Cl₂, 192 MHz).

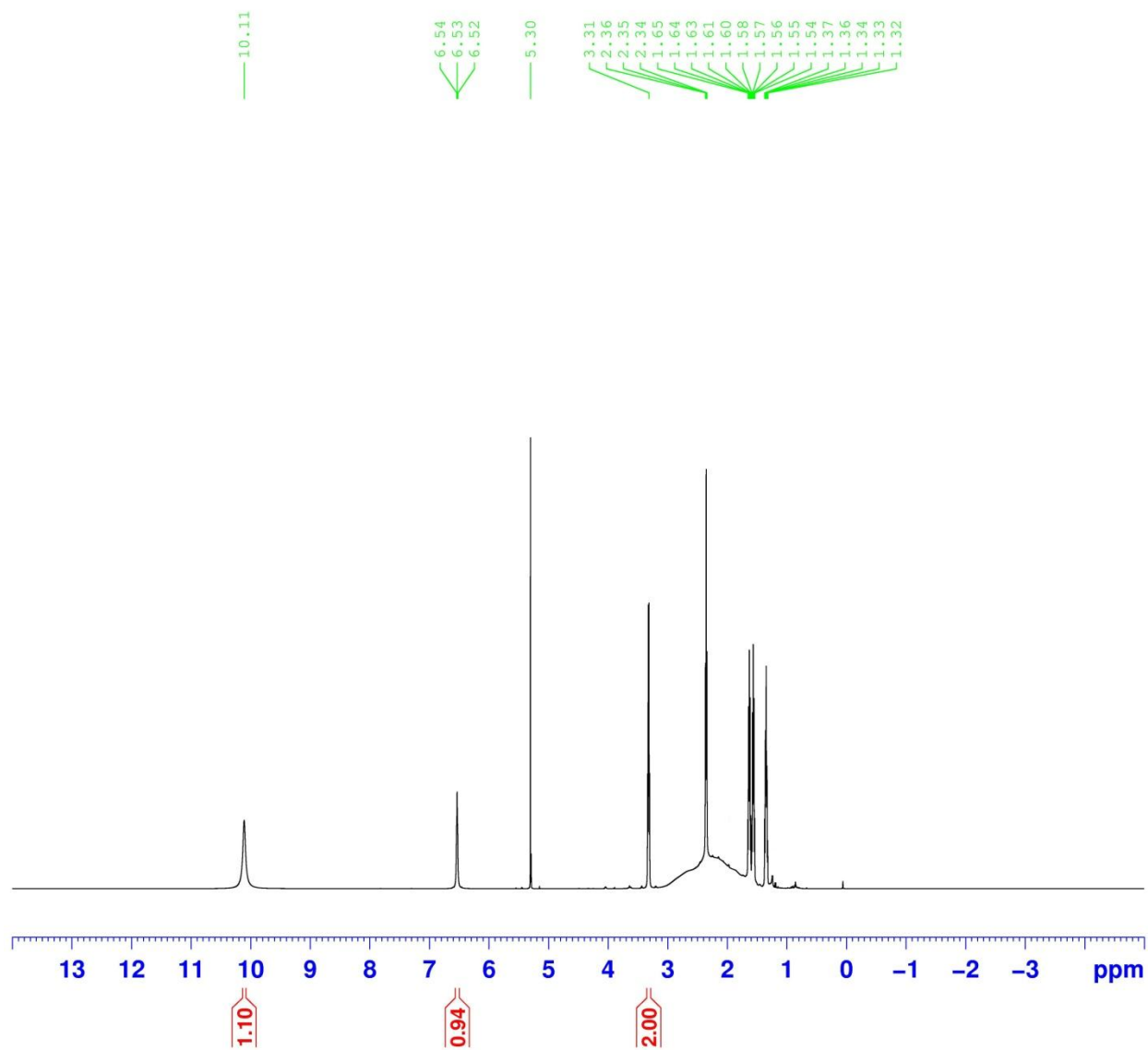


Figure S41. ^1H NMR spectrum of compound **10** (CD_2Cl_2 , 600 MHz).

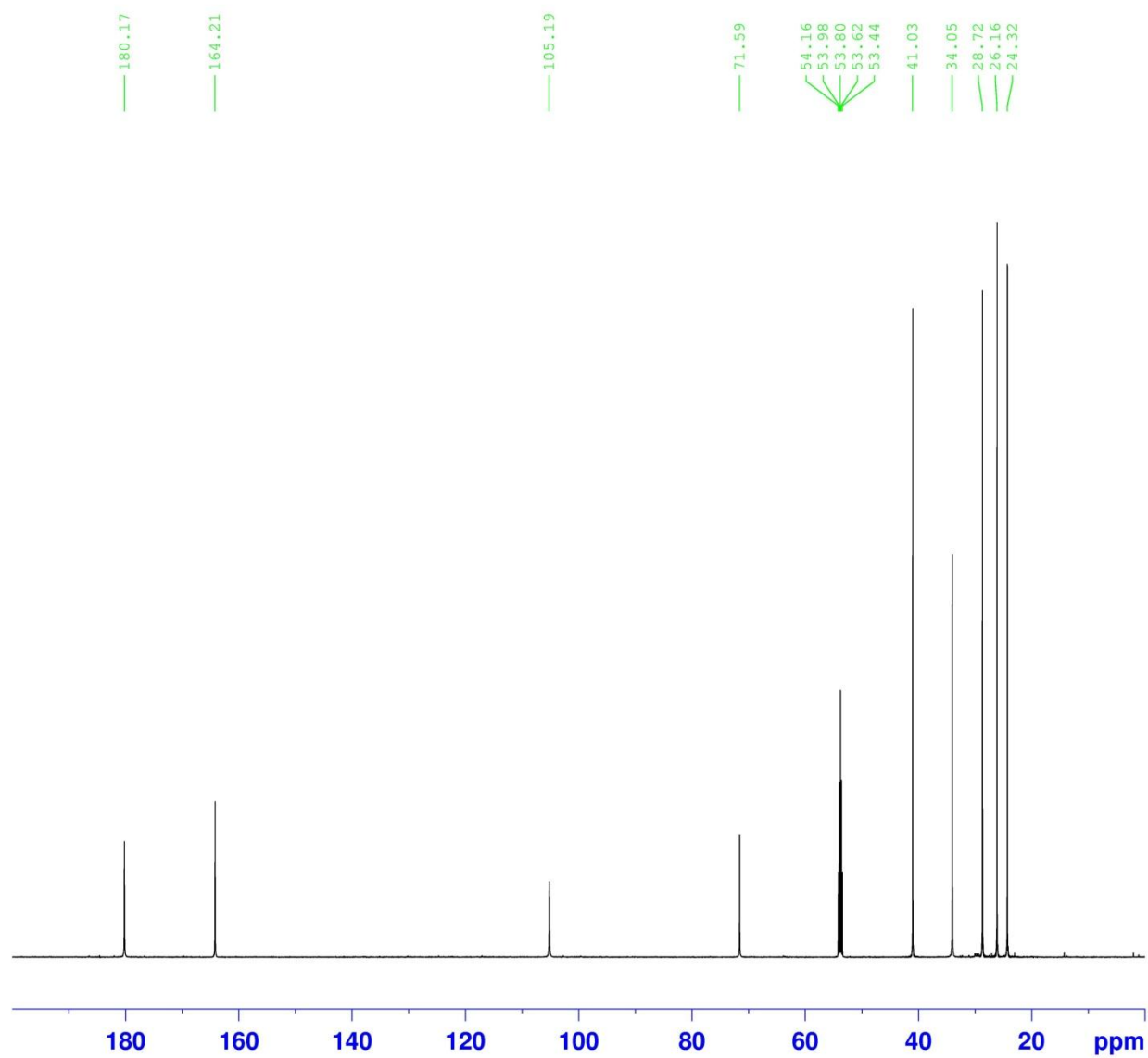


Figure S42. ^{13}C NMR spectrum of compound **10** (CD_2Cl_2 , 150 MHz).

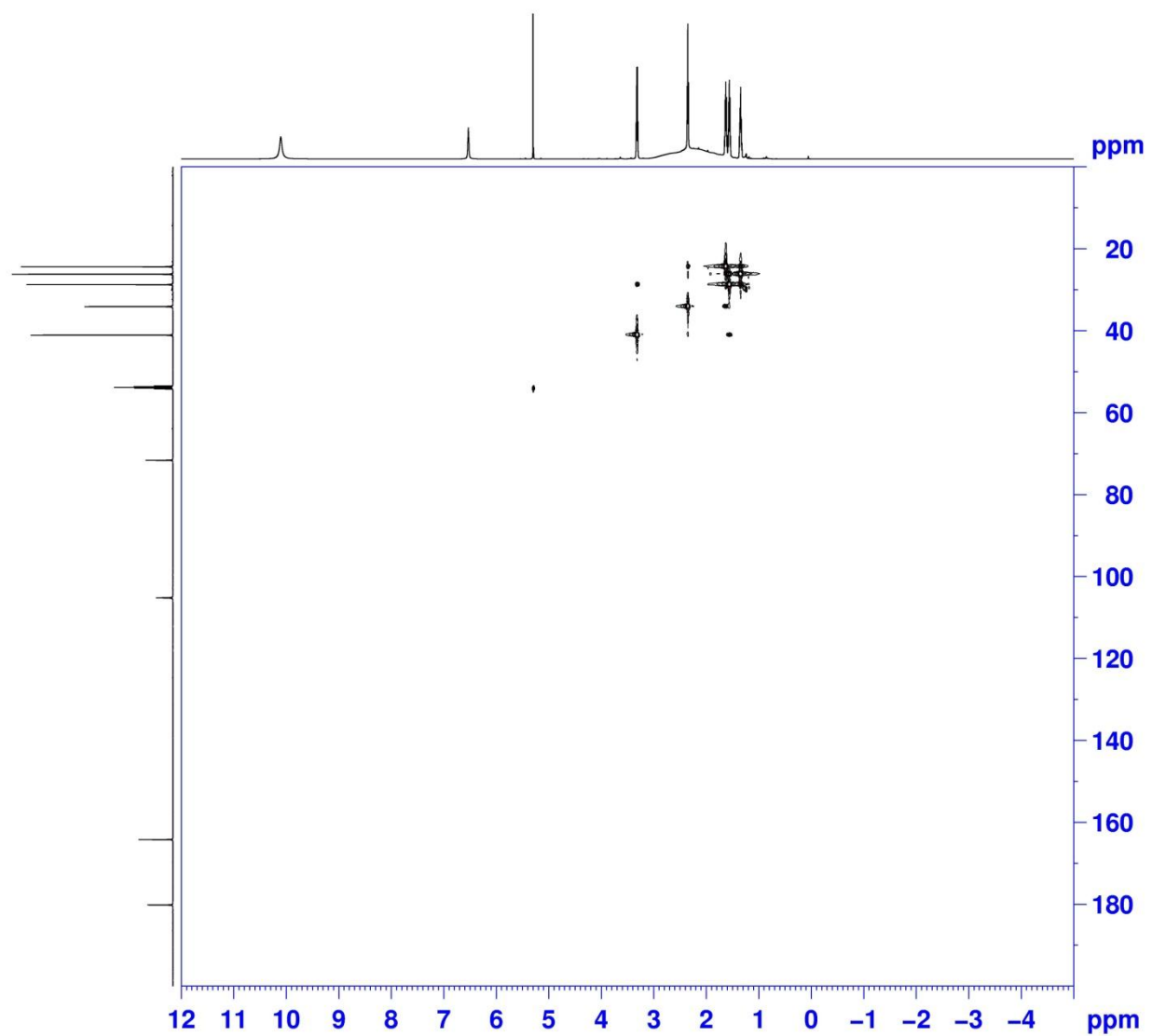


Figure S43. HSQC of compound **10**.

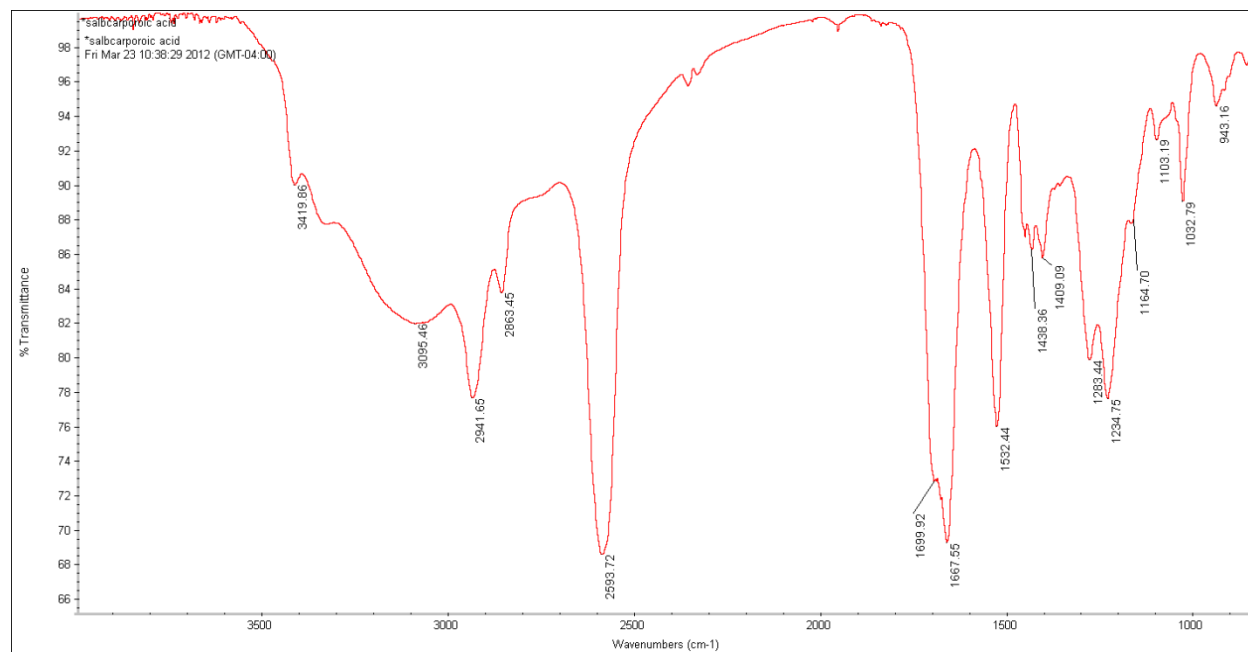


Figure S44. IR spectrum of compound **10**.

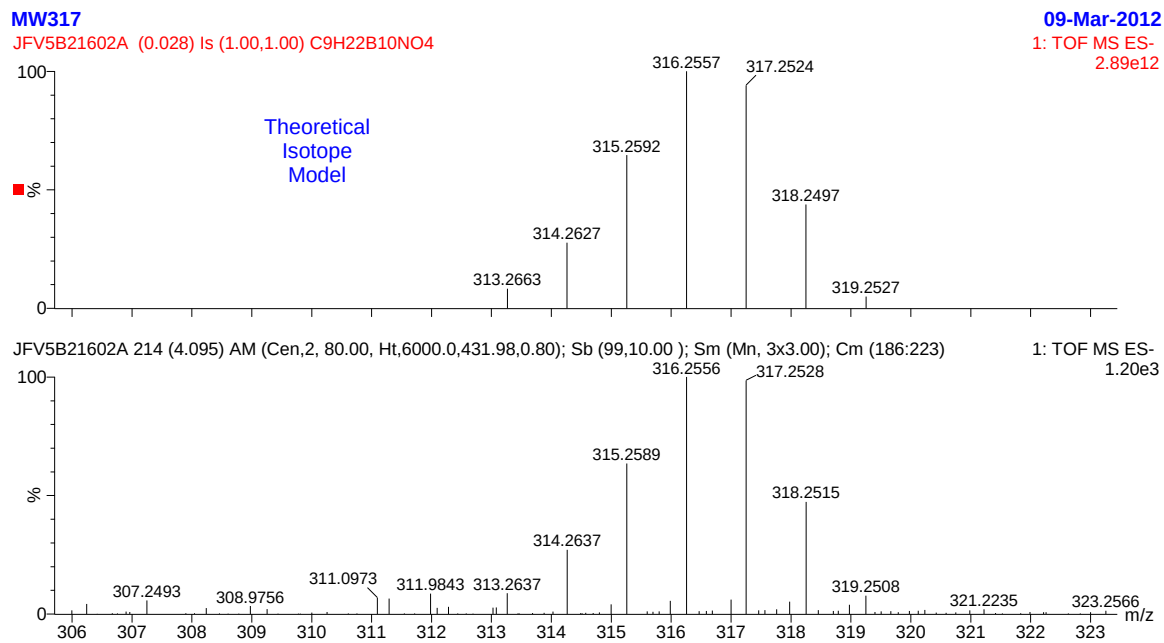


Figure S45. HRMS-ESI spectrum of compound **10**.

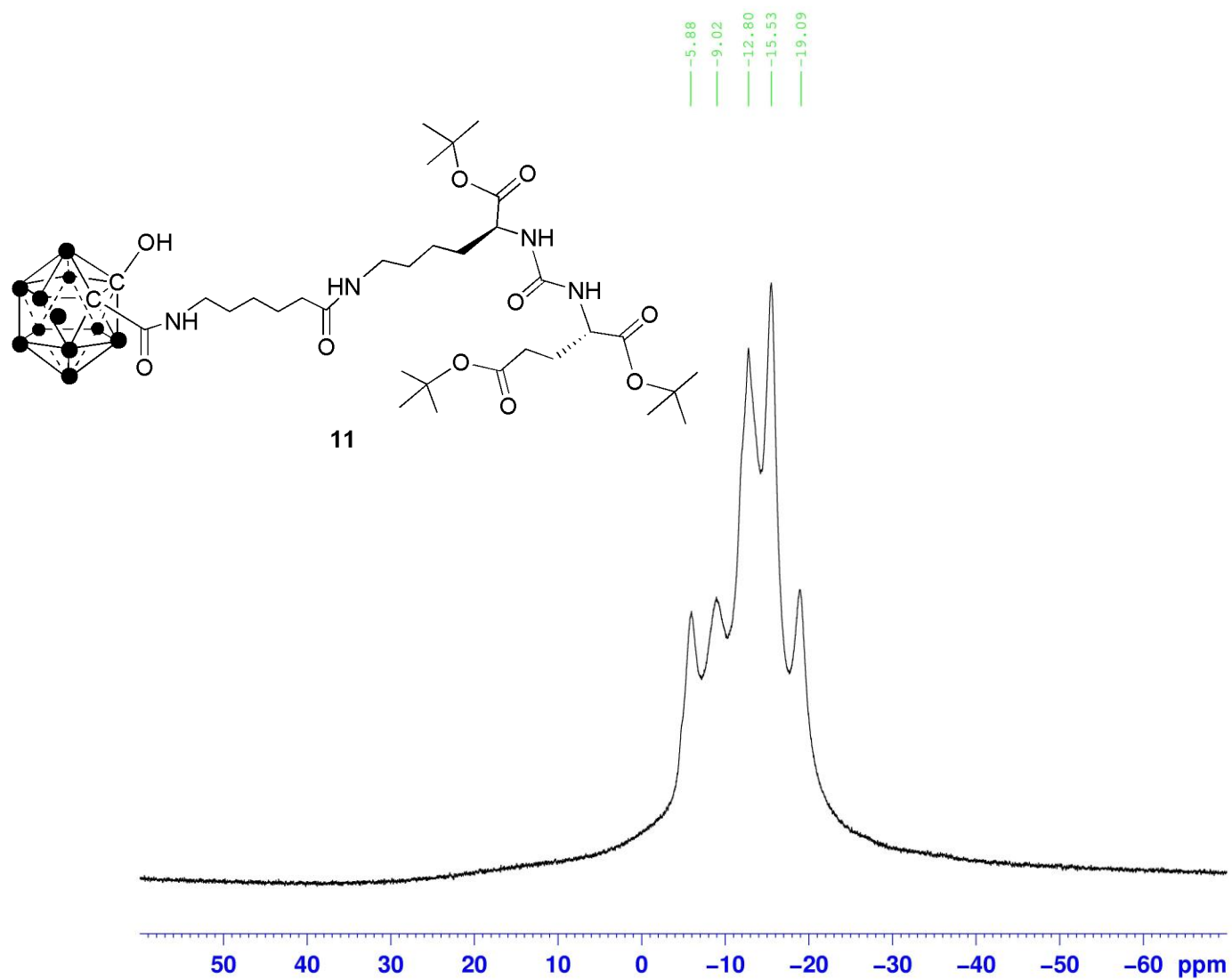


Figure S46. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of compound **11** (CD_2Cl_2 , 192 MHz).

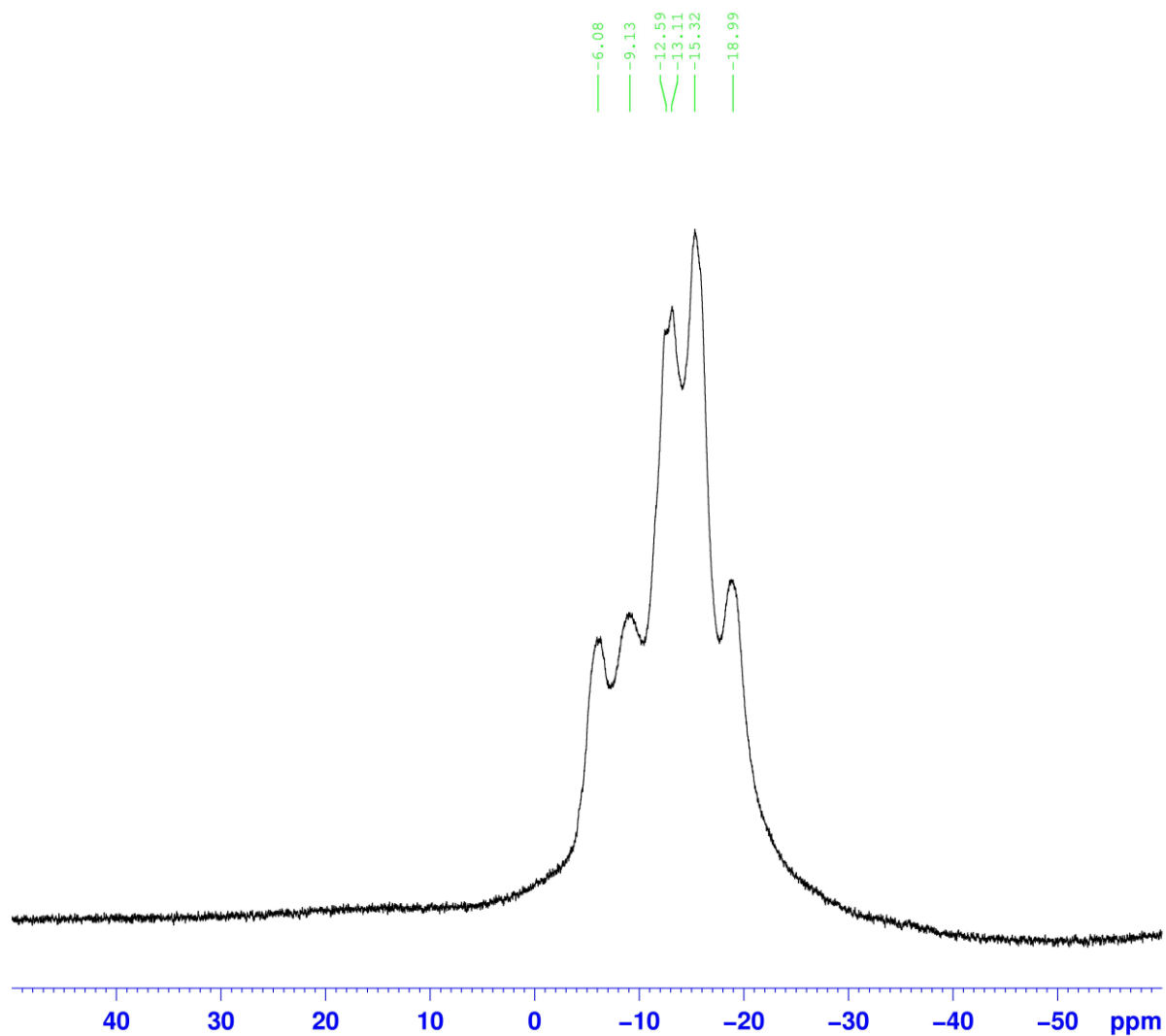


Figure S47. ^{11}B NMR spectrum of compound **11** (CD_2Cl_2 , 192 MHz).

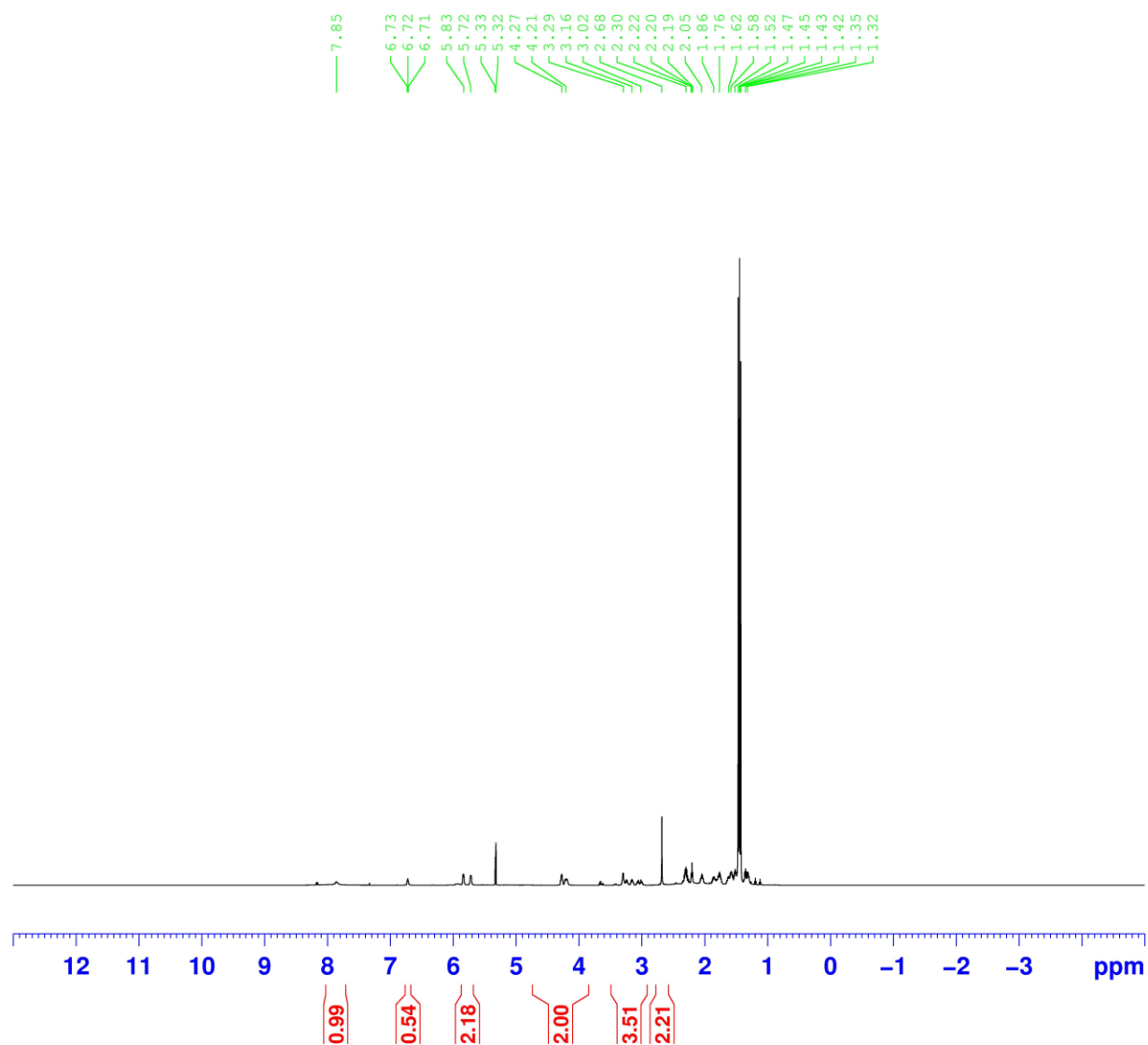


Figure S48. ^1H NMR spectrum of compound **11** (CD_2Cl_2 , 600 MHz).

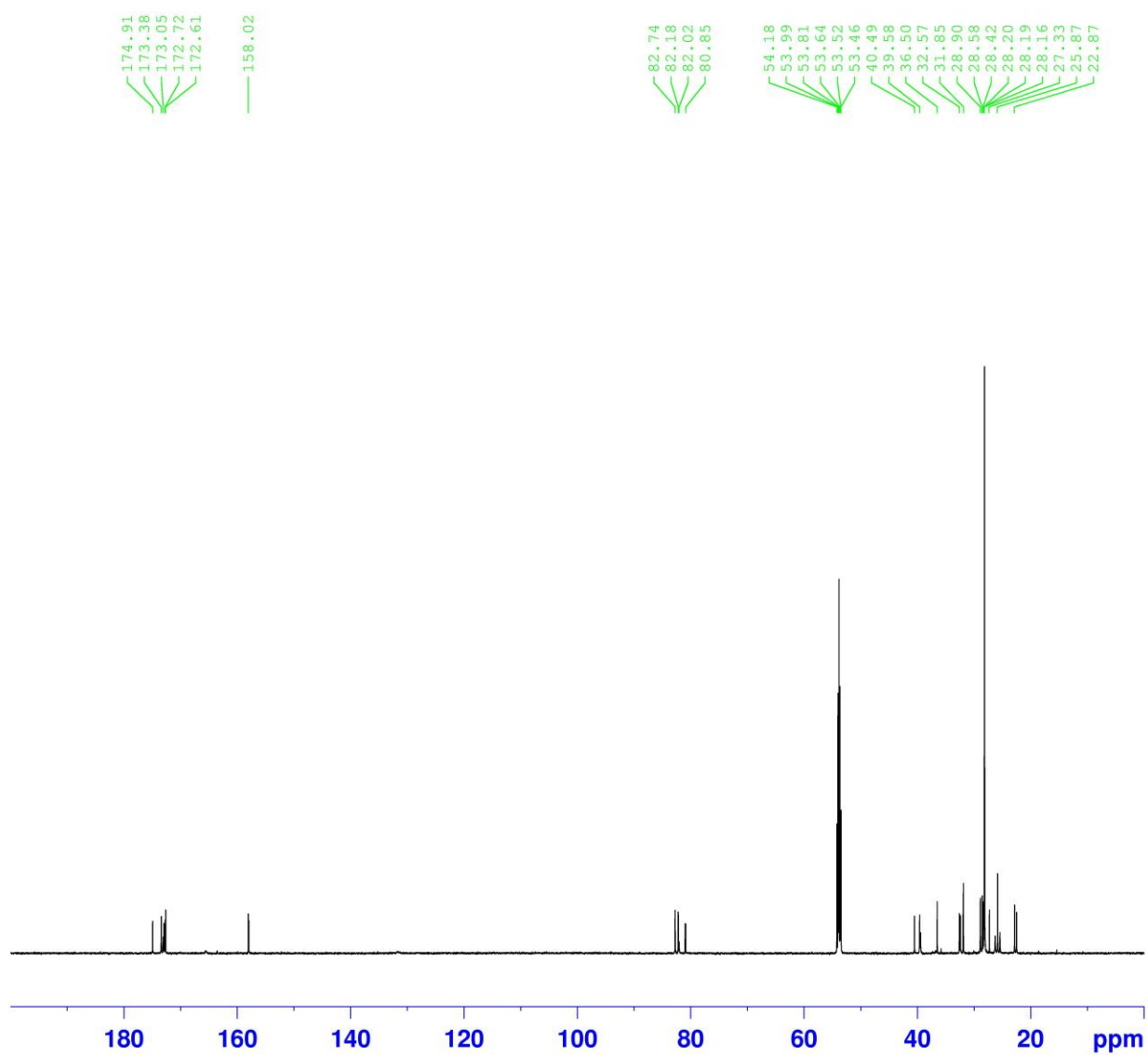


Figure S49. ^{13}C NMR spectrum of compound **11** (CD_2Cl_2 , 150 MHz).

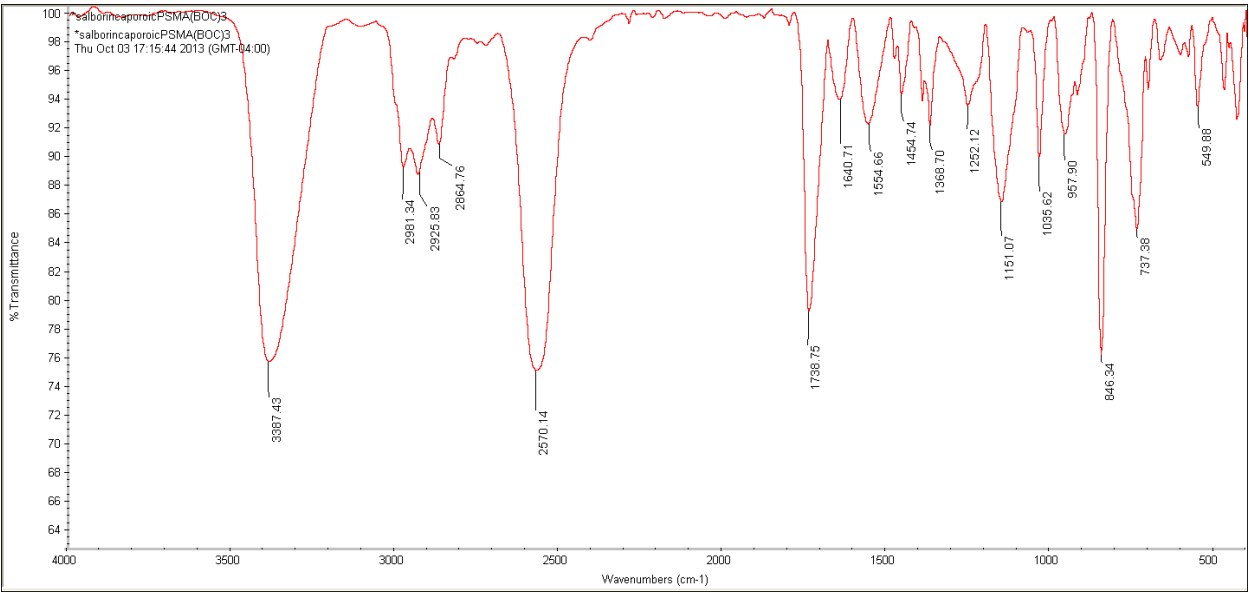


Figure S50. IR spectrum of compound 10.

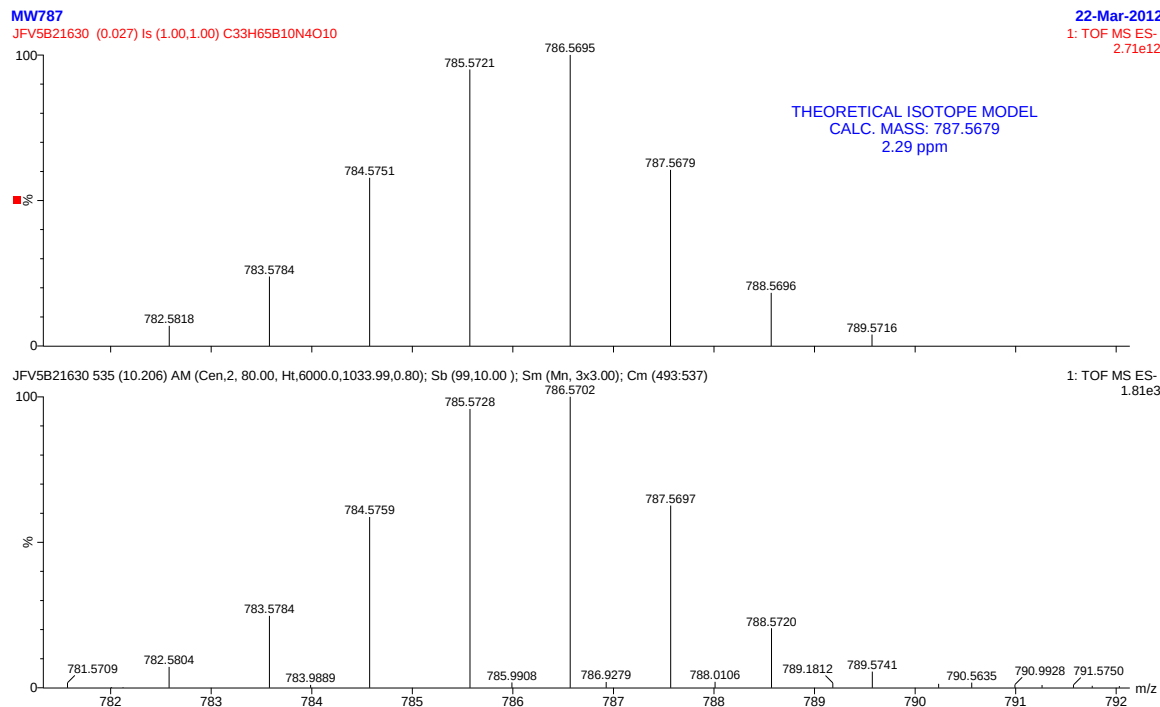


Figure S51. HRMS-ESI spectrum of compound 11.

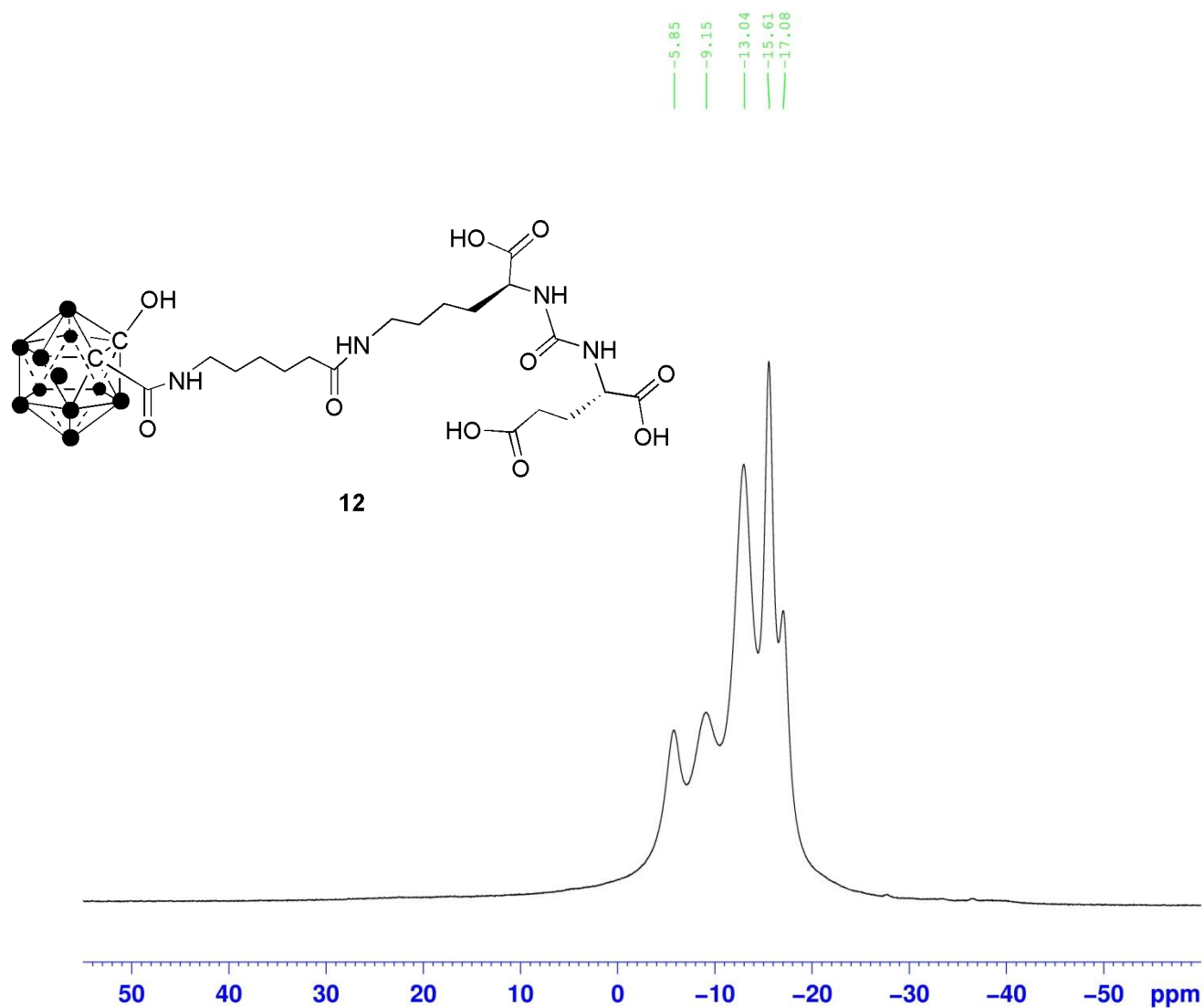


Figure S52. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of compound 12 (DMSO- d_6 , 192 MHz).

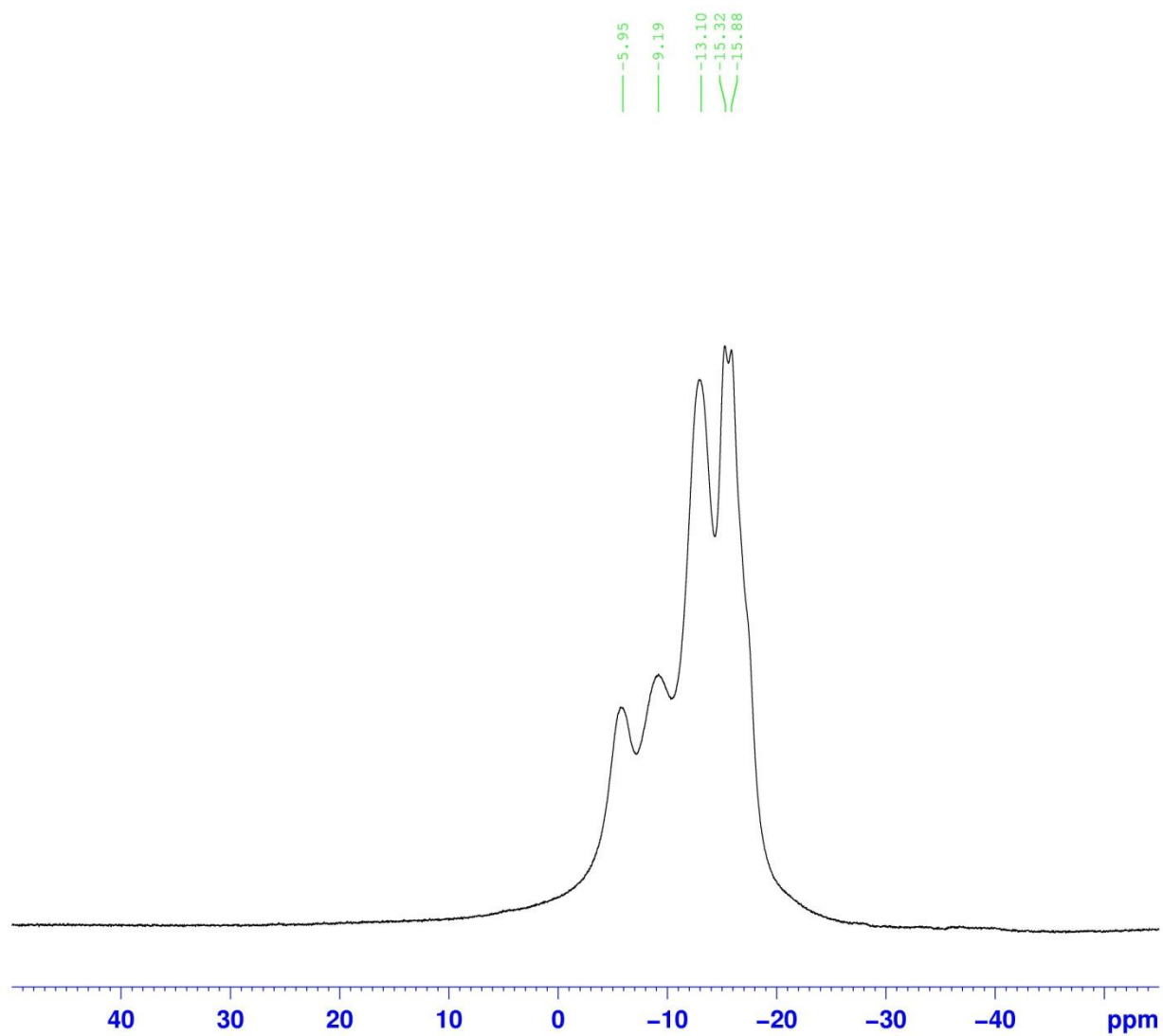


Figure S53. ^{11}B NMR spectrum of compound **12** ($\text{DMSO-}d_6$, 192 MHz).

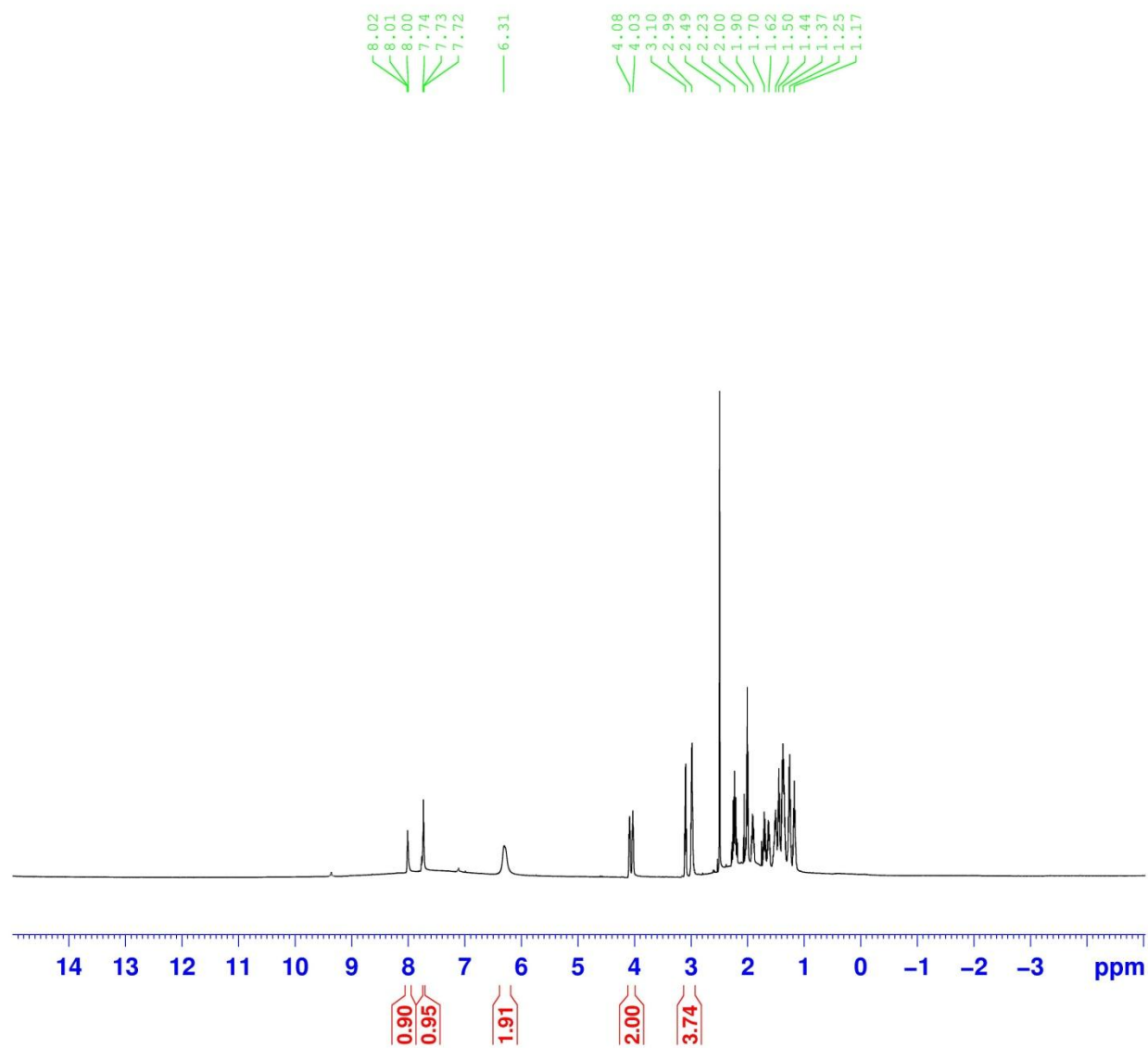


Figure S54. ¹H NMR spectrum of compound **12** (DMSO-*d*₆, 600 MHz).

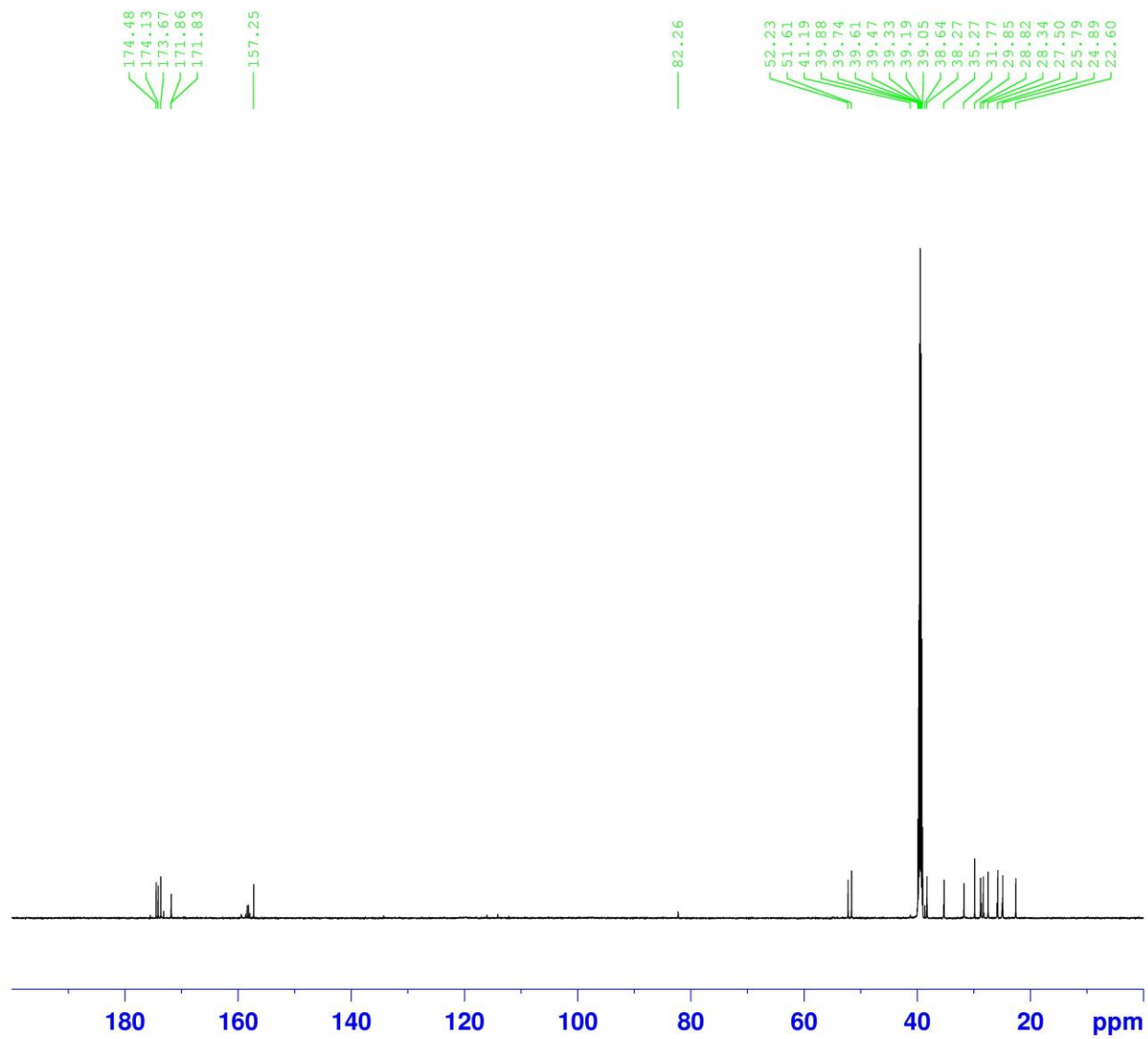


Figure S55. ^{13}C NMR spectrum of compound **12** ($\text{DMSO-}d_6$, 150 MHz).

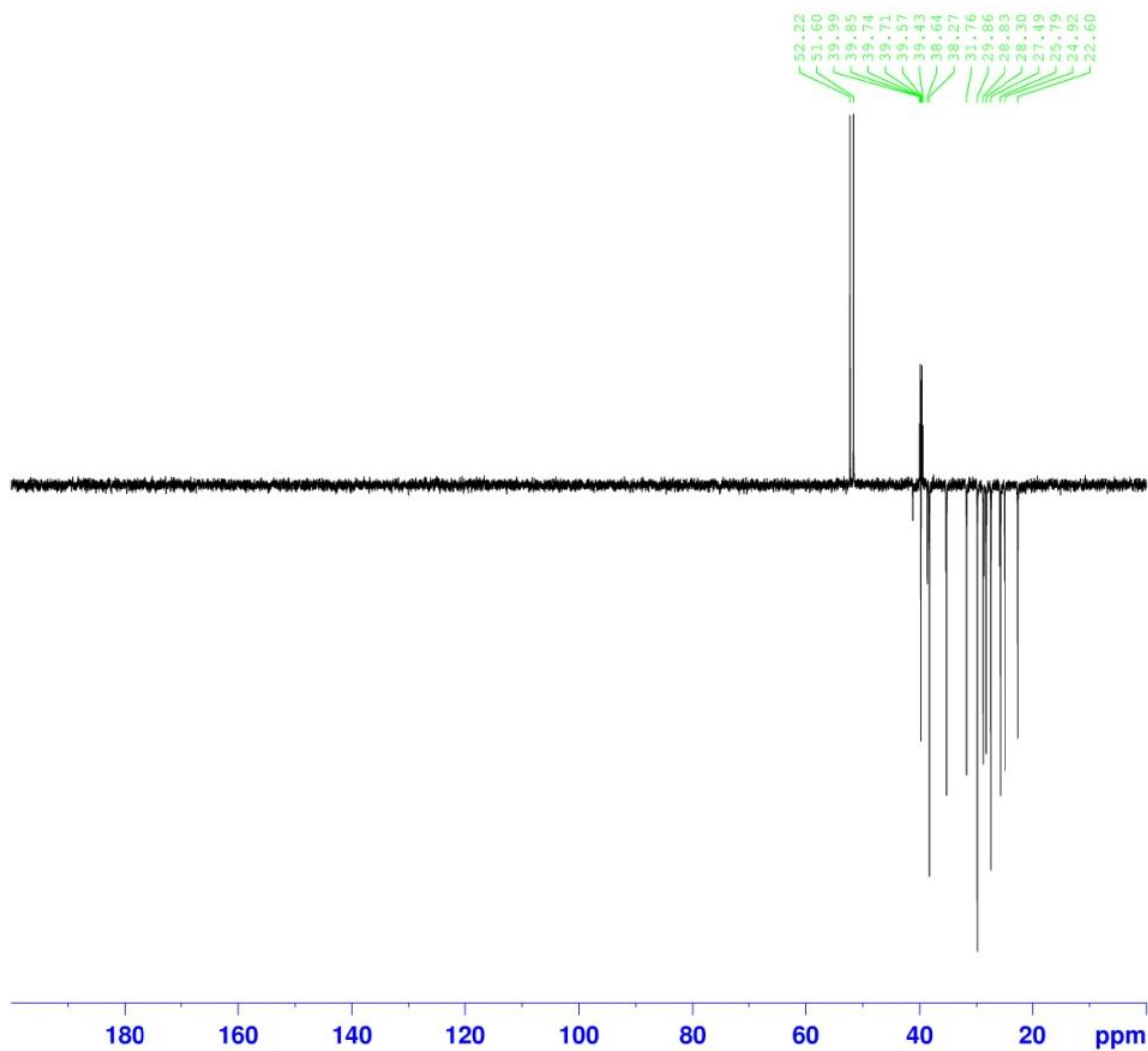


Figure S56. ^{13}C NMR (dept 135°) spectrum of compound **12** ($\text{DMSO}-d_6$, 150 MHz).

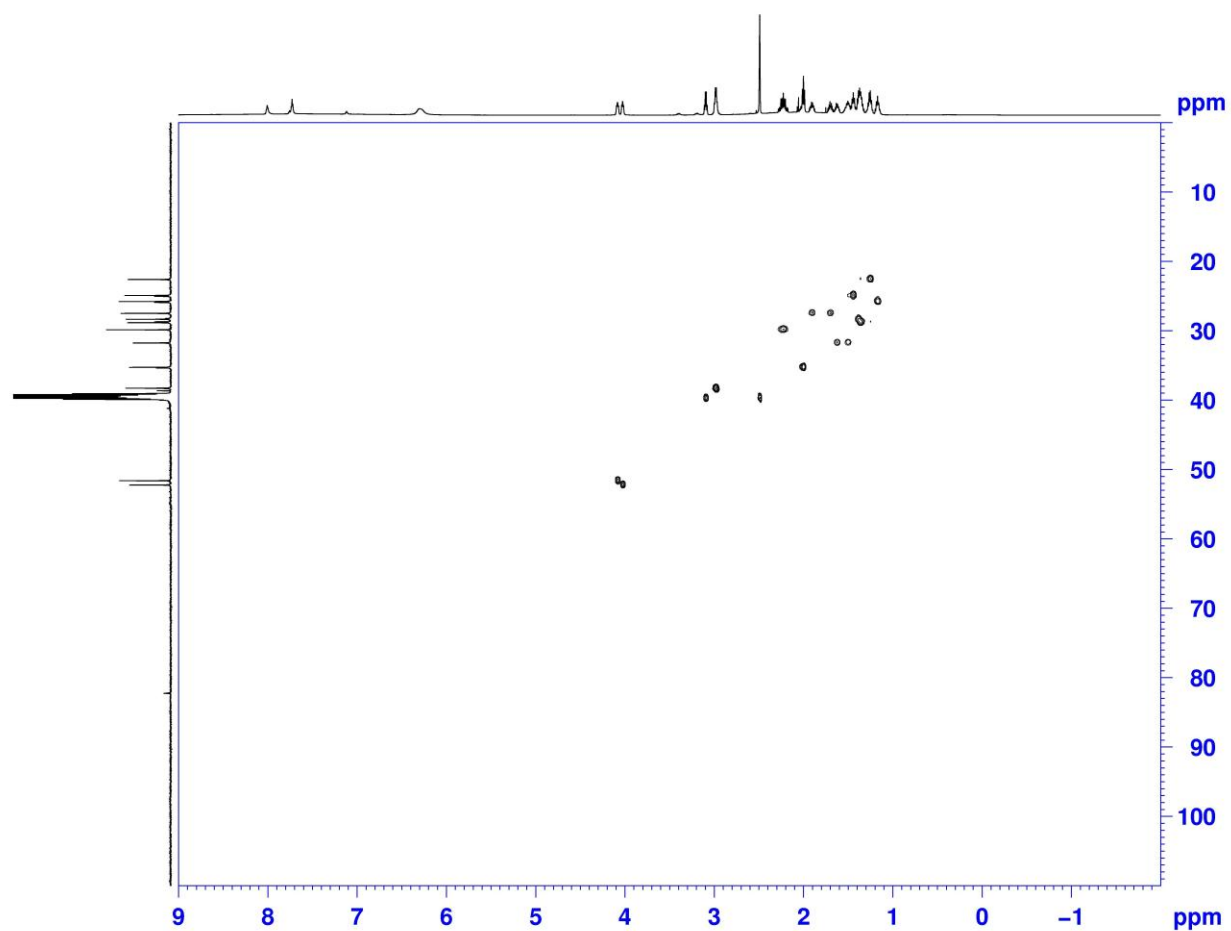


Figure S57. HSQC of compound **12**.



Figure S58. IR spectrum of compound 12.

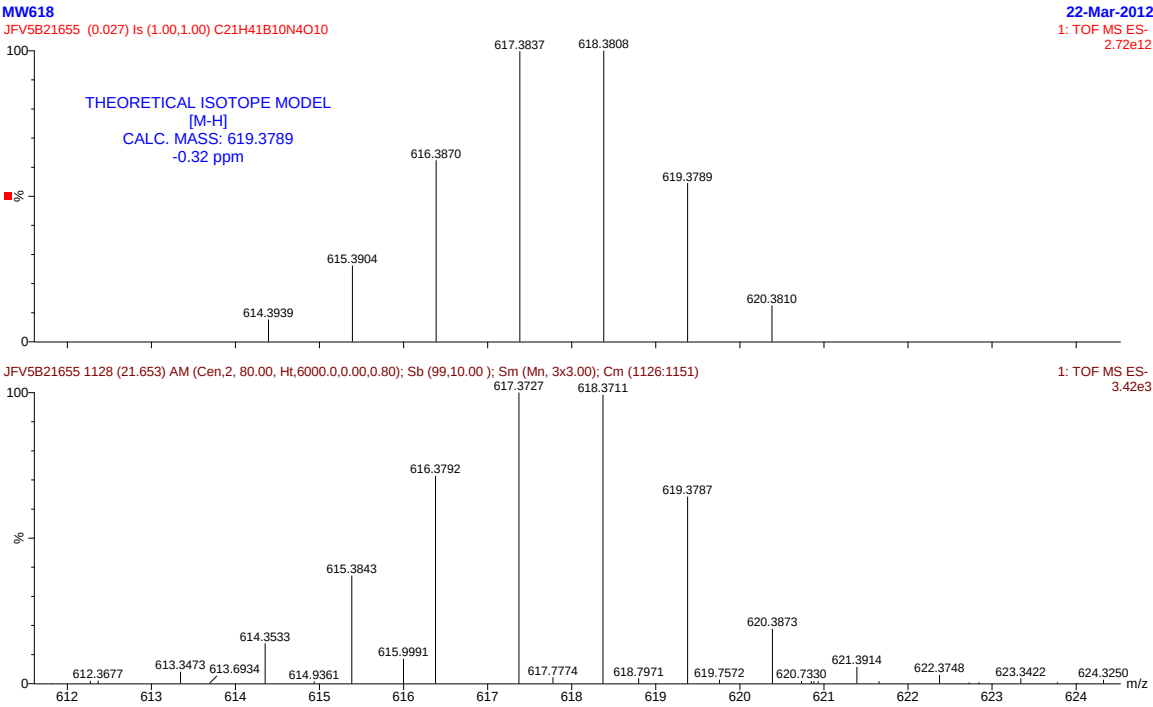


Figure S59. HRMS-ESI spectrum of compound 12.

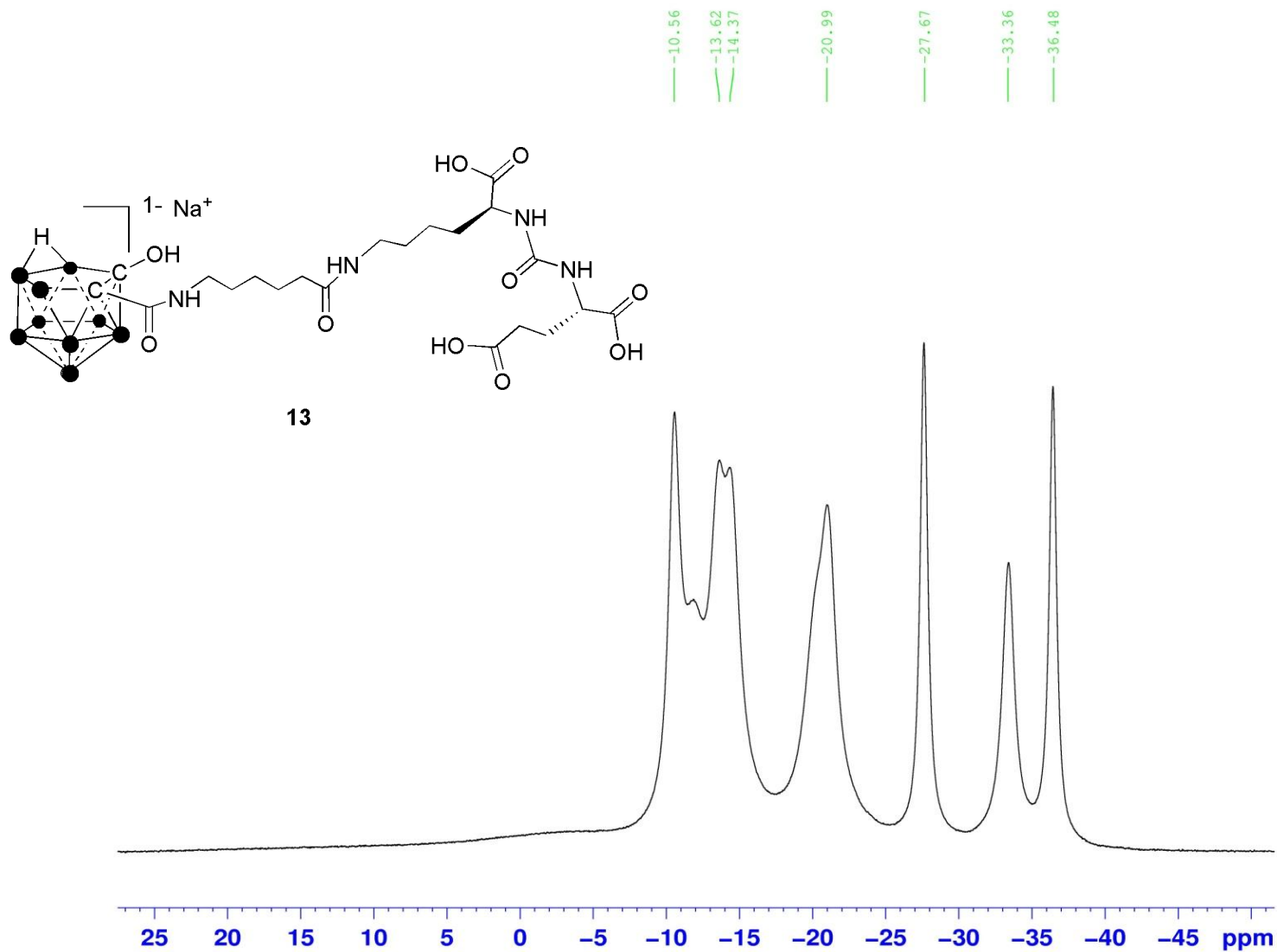


Figure S60. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of compound **13** (DMSO- d_6 , 192 MHz).

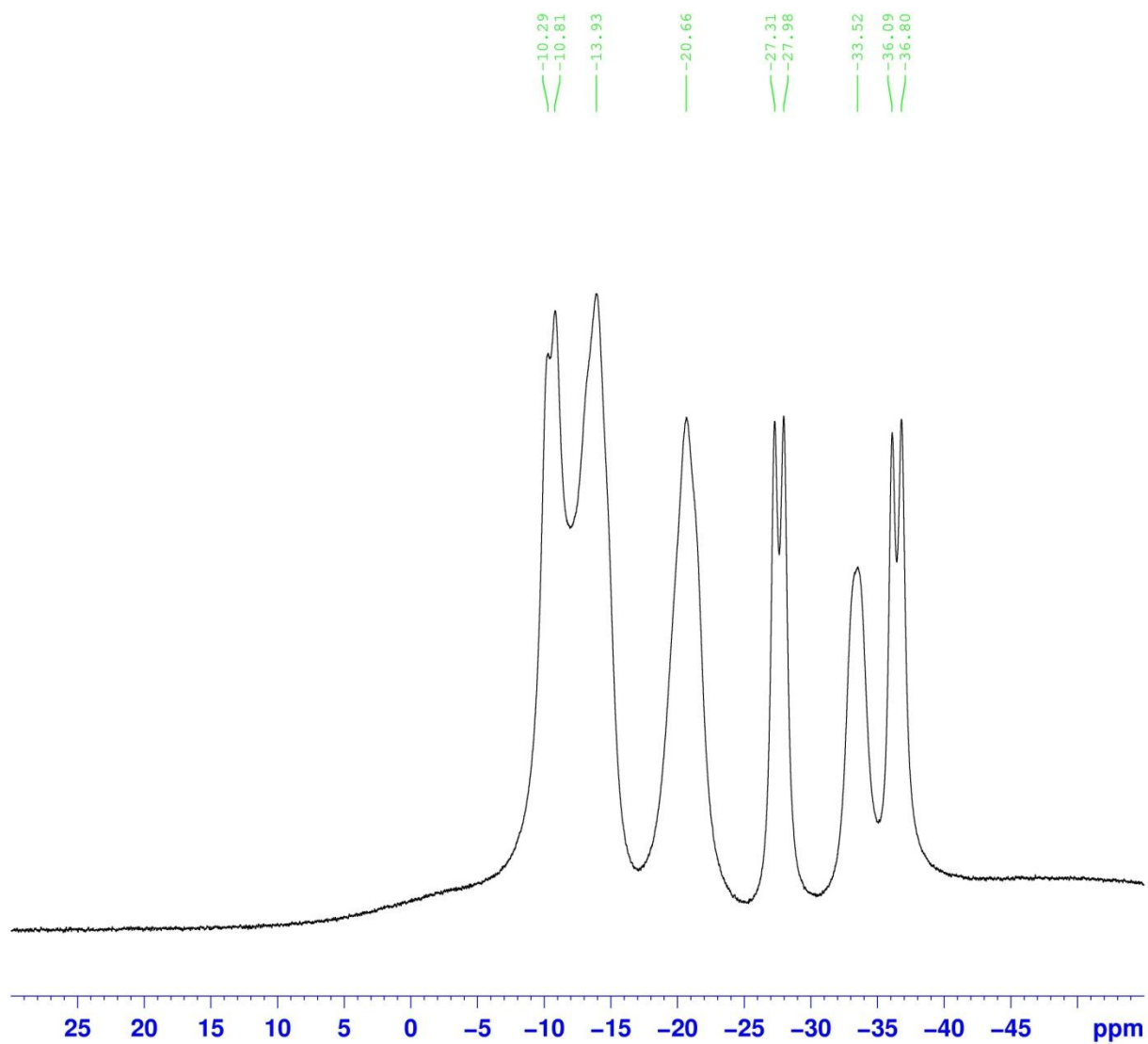


Figure S61. ^{11}B NMR spectrum of compound **13** ($\text{DMSO-}d_6$, 192 MHz).

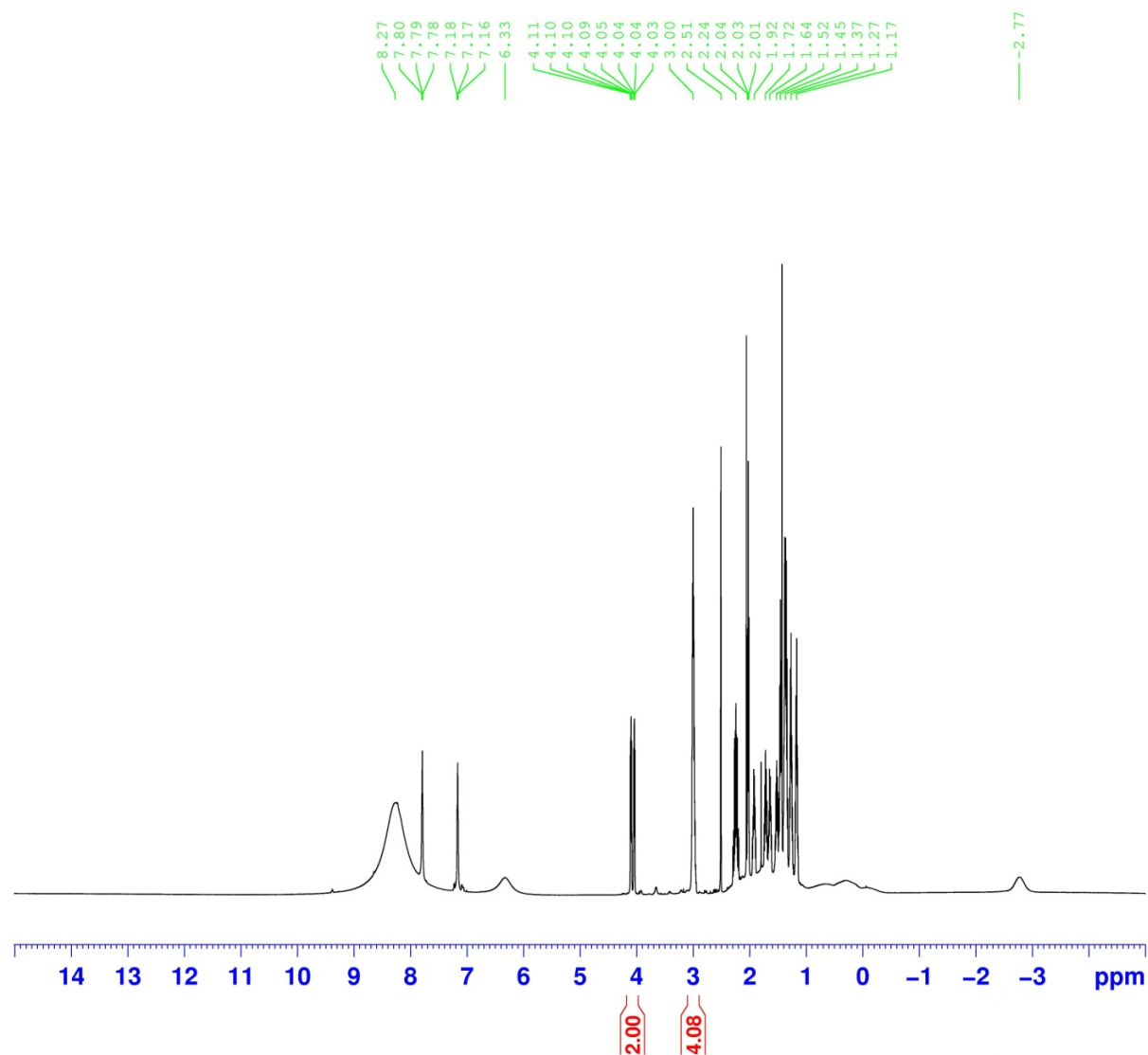


Figure S62. ¹H NMR spectrum of compound **13** (DMSO-*d*₆, 600 MHz).

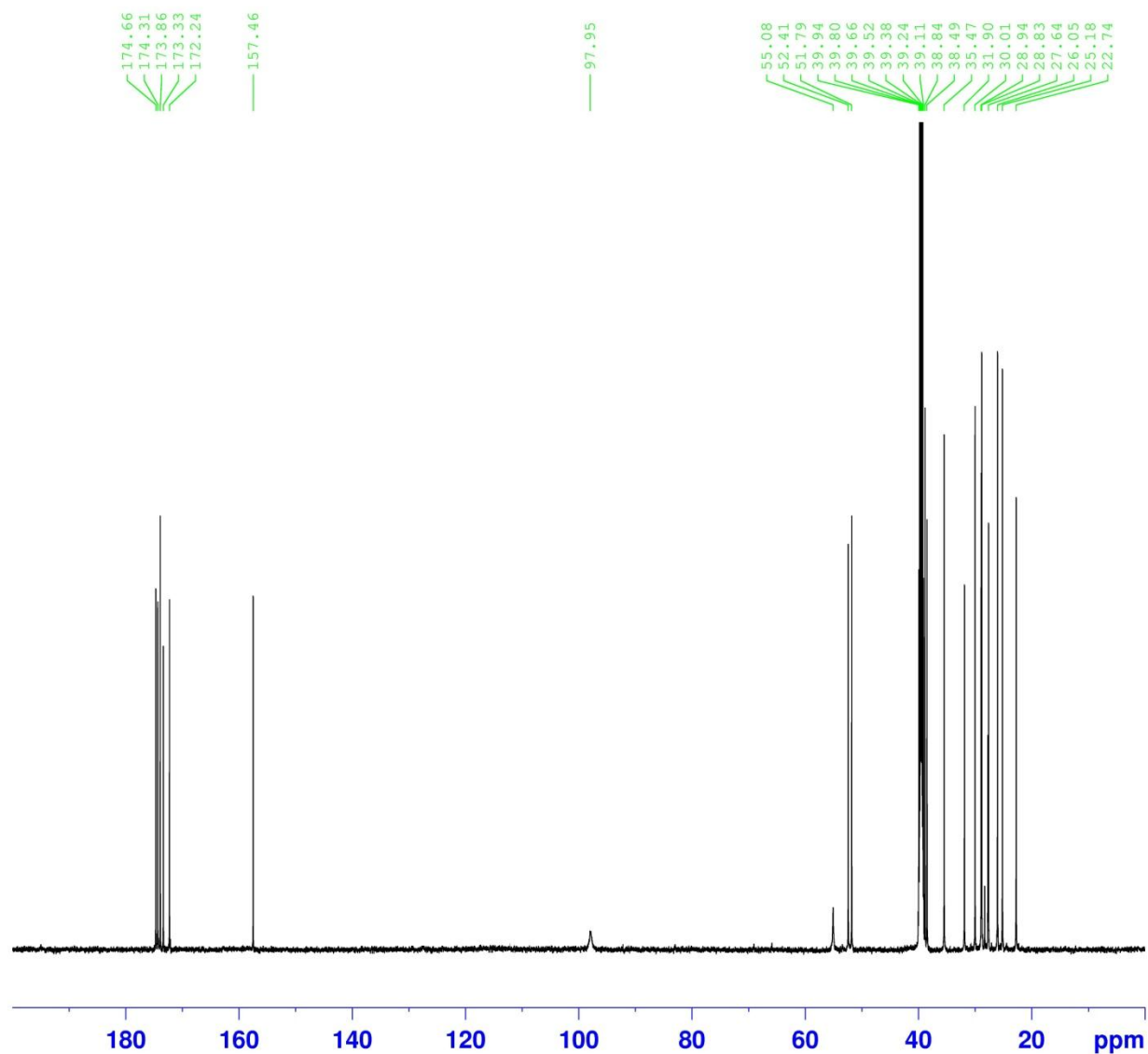


Figure S63. ¹³C NMR spectrum of compound **13** (DMSO-*d*₆, 150 MHz).

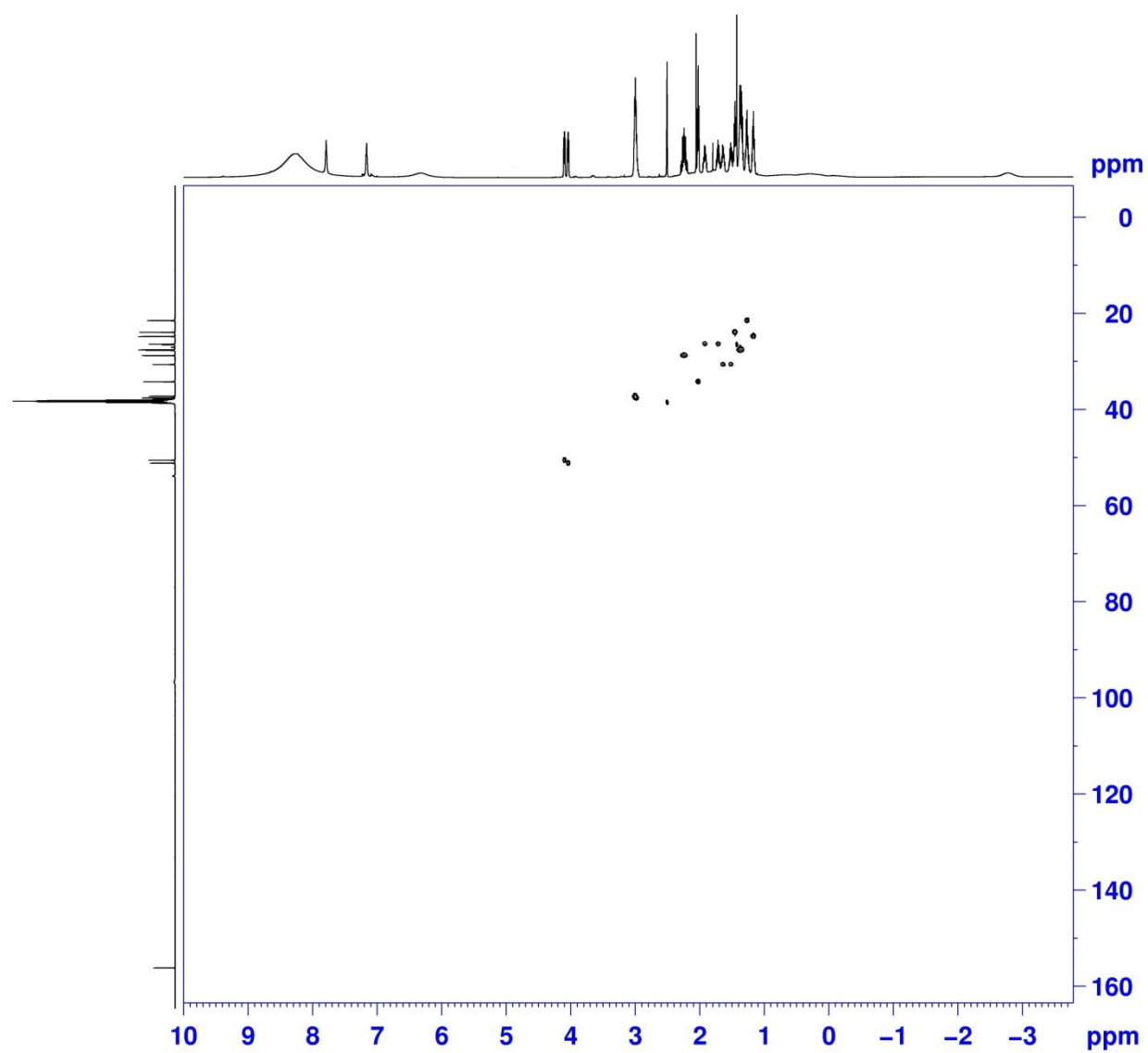


Figure S64. HSQC of compound **13**.

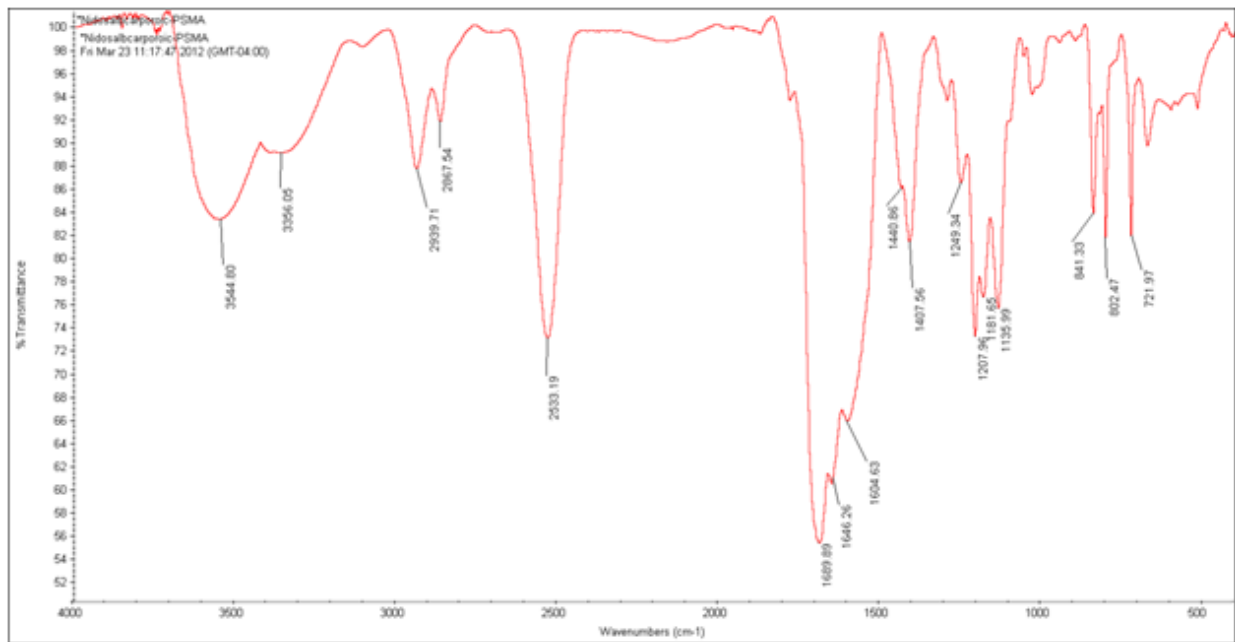


Figure S65. IR spectrum of compound **13**.

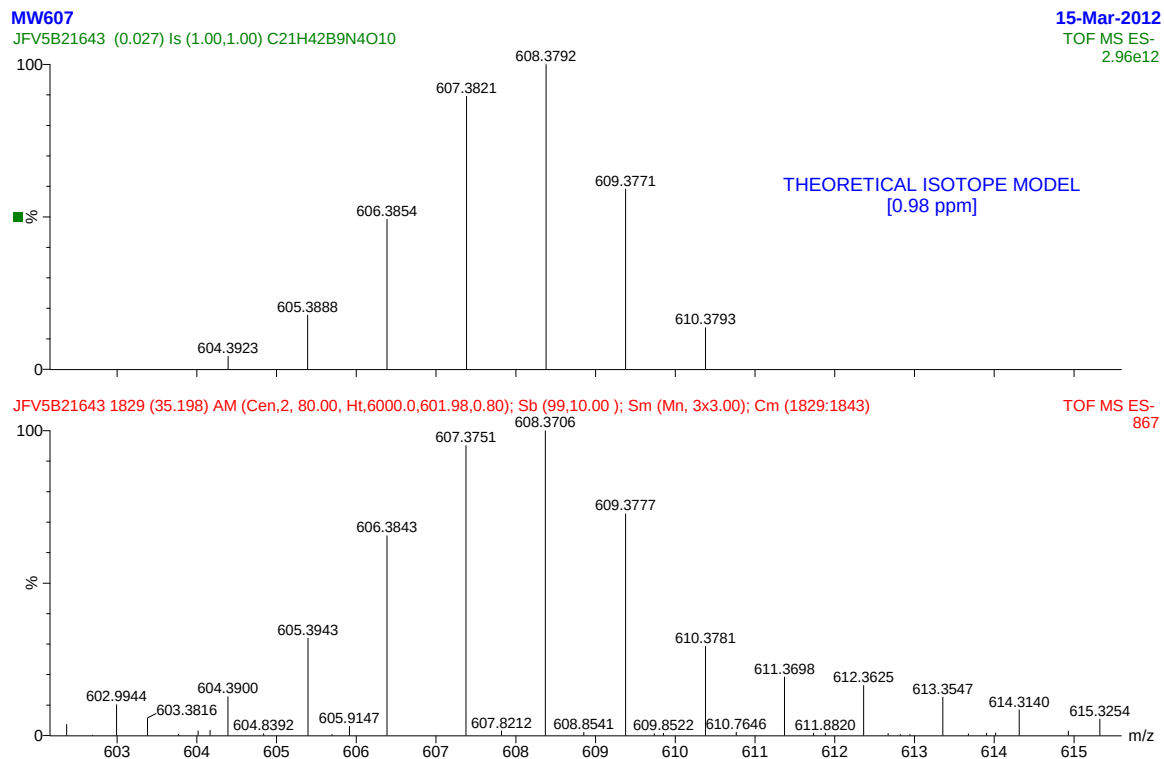


Figure S66. HRMS-ESI spectrum of compound **13**.

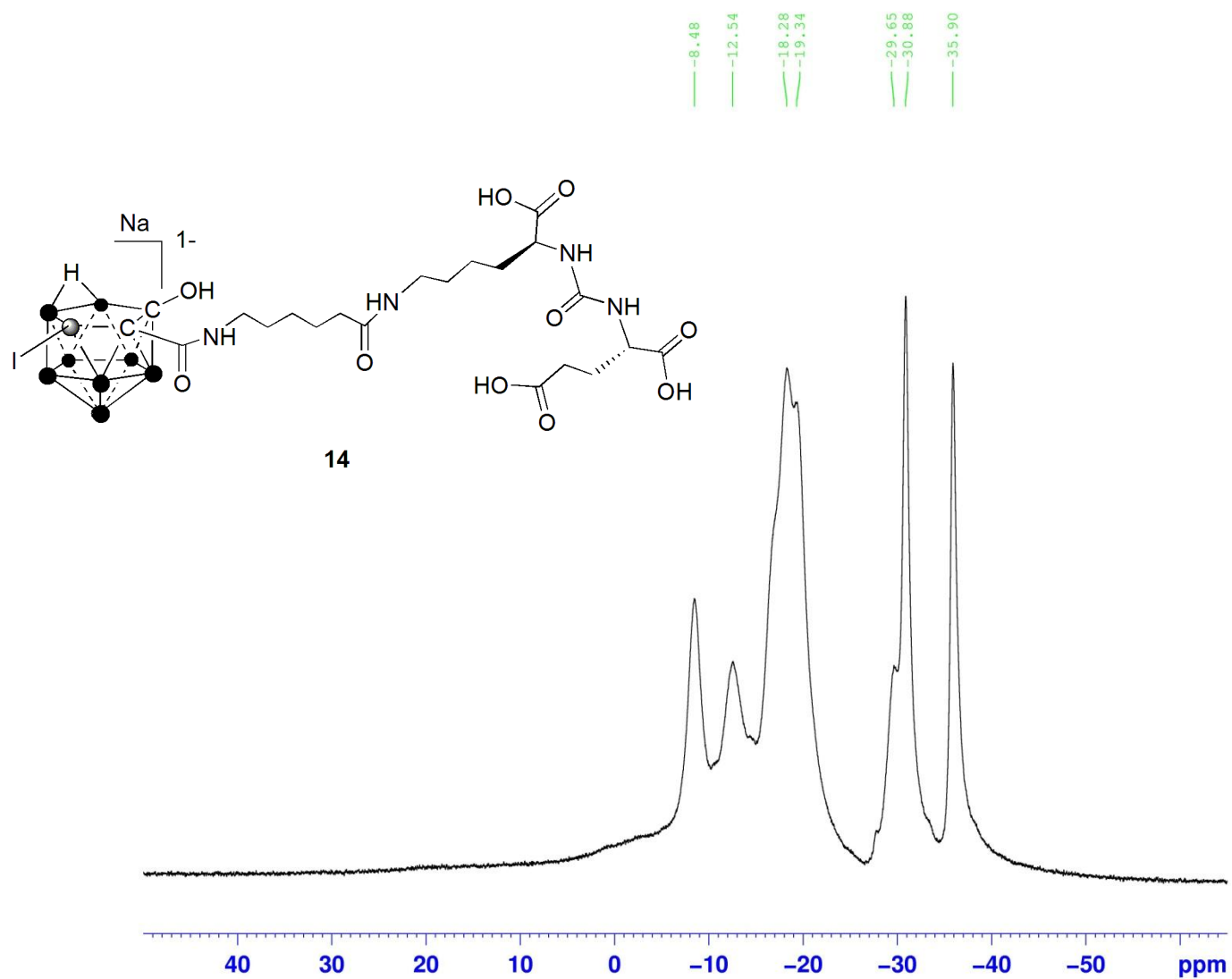


Figure S67. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of compound **14** (DMSO- d_6 , 192 MHz).

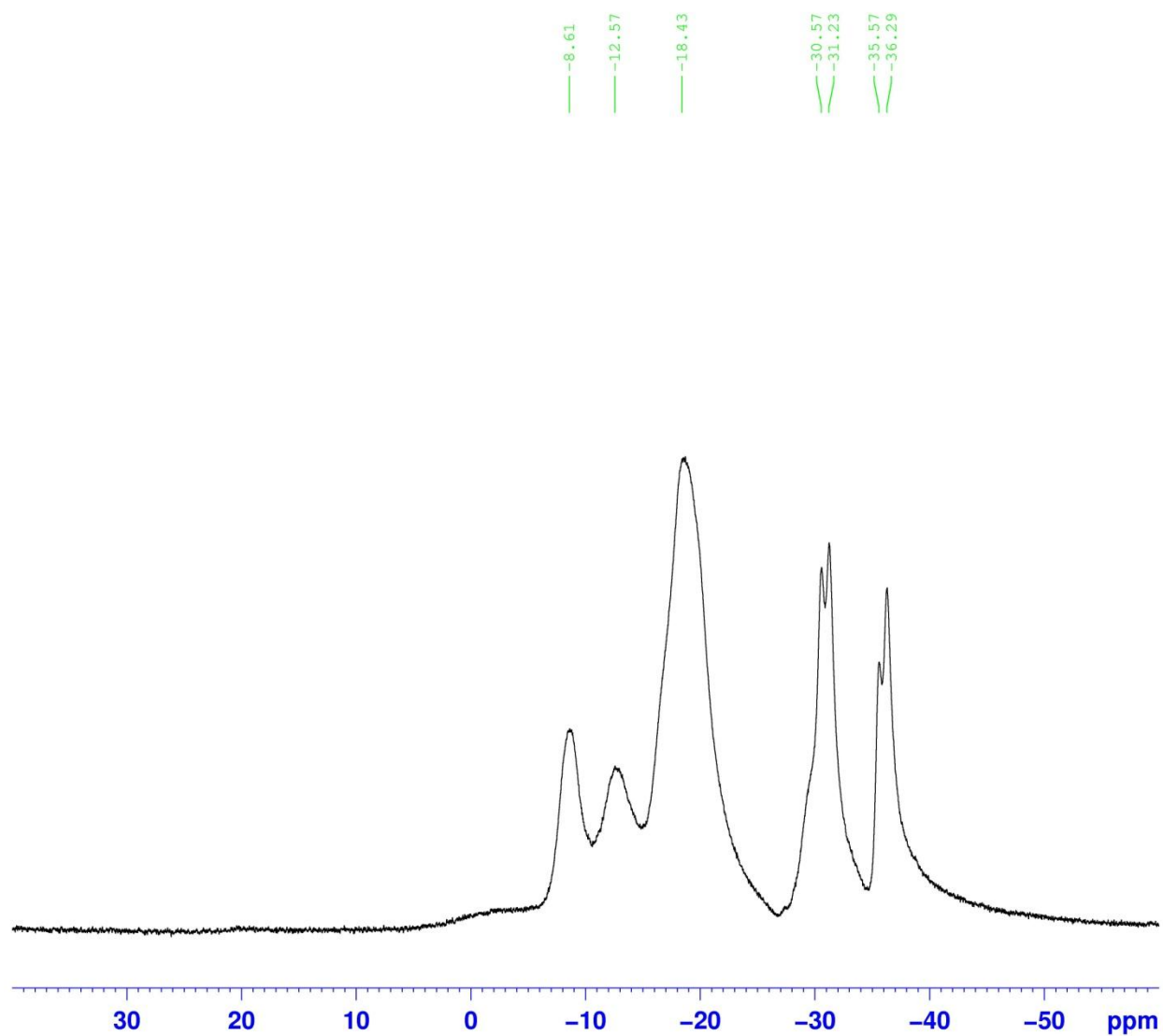


Figure S68. ^{11}B NMR spectrum of compound **14** ($\text{DMSO-}d_6$, 192 MHz).

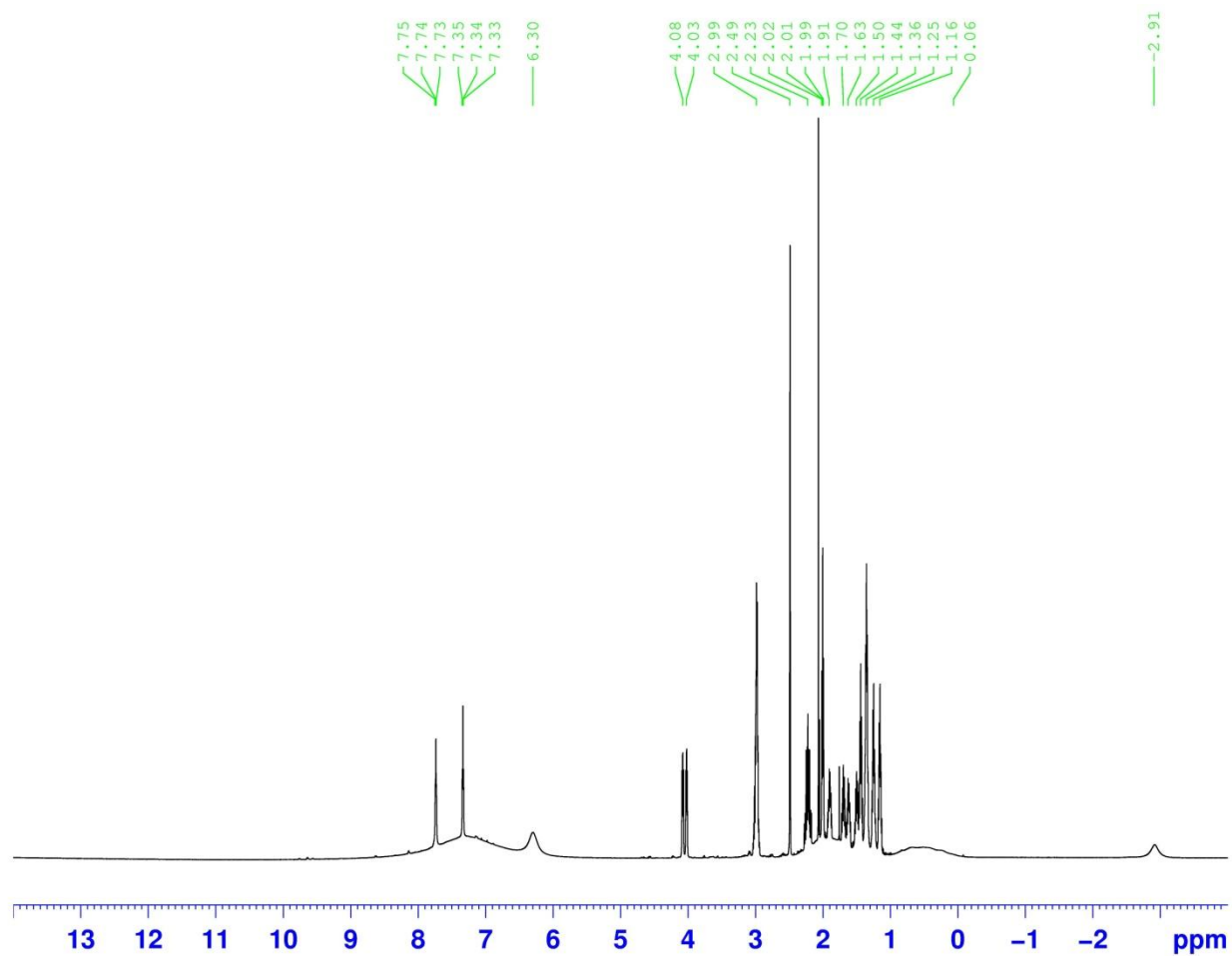


Figure S69. ¹H NMR spectrum of compound **14** (DMSO-*d*₆, 600 MHz).

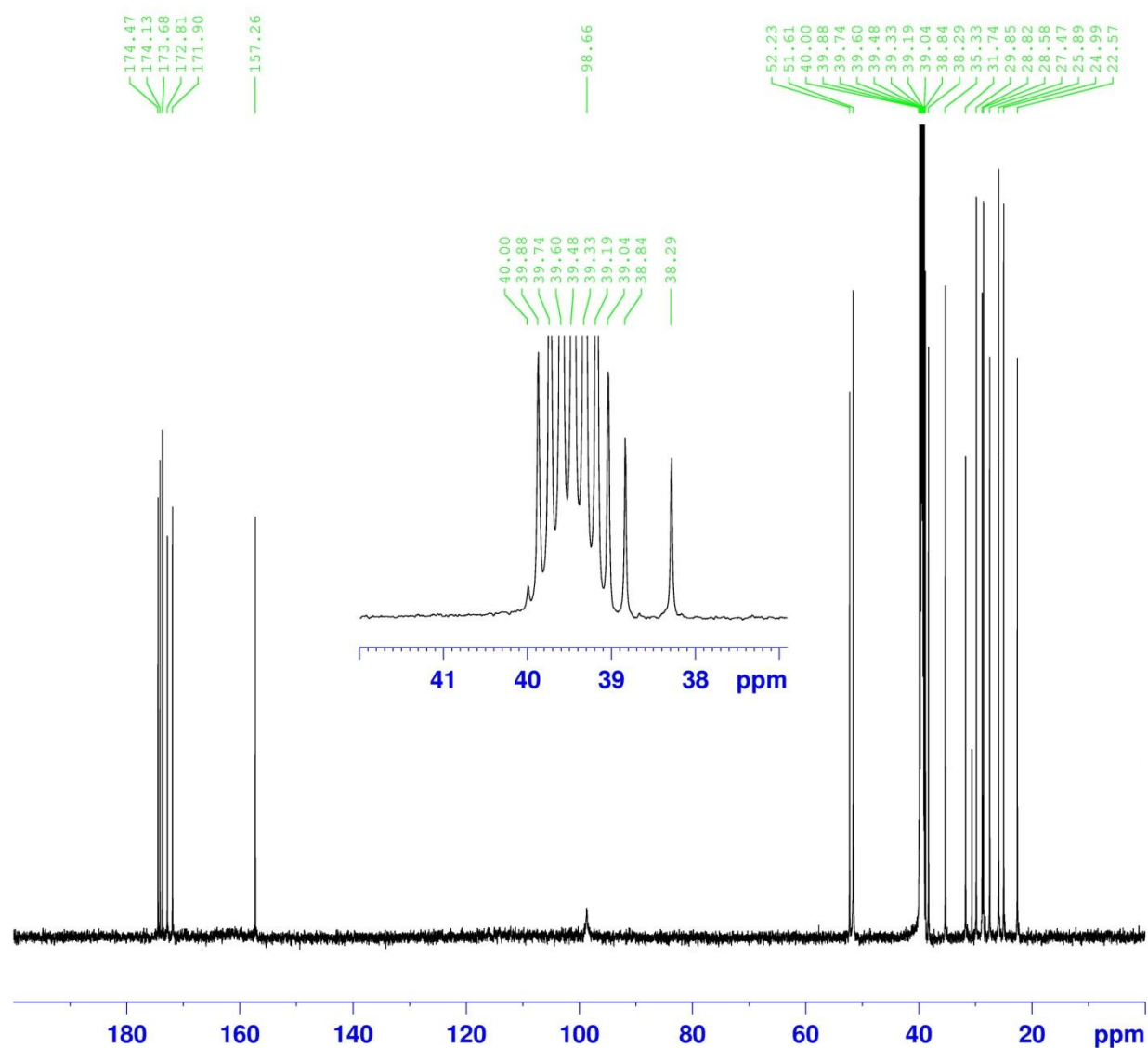


Figure S70. ^{13}C NMR spectrum of compound **14** ($\text{DMSO-}d_6$, 150 MHz).

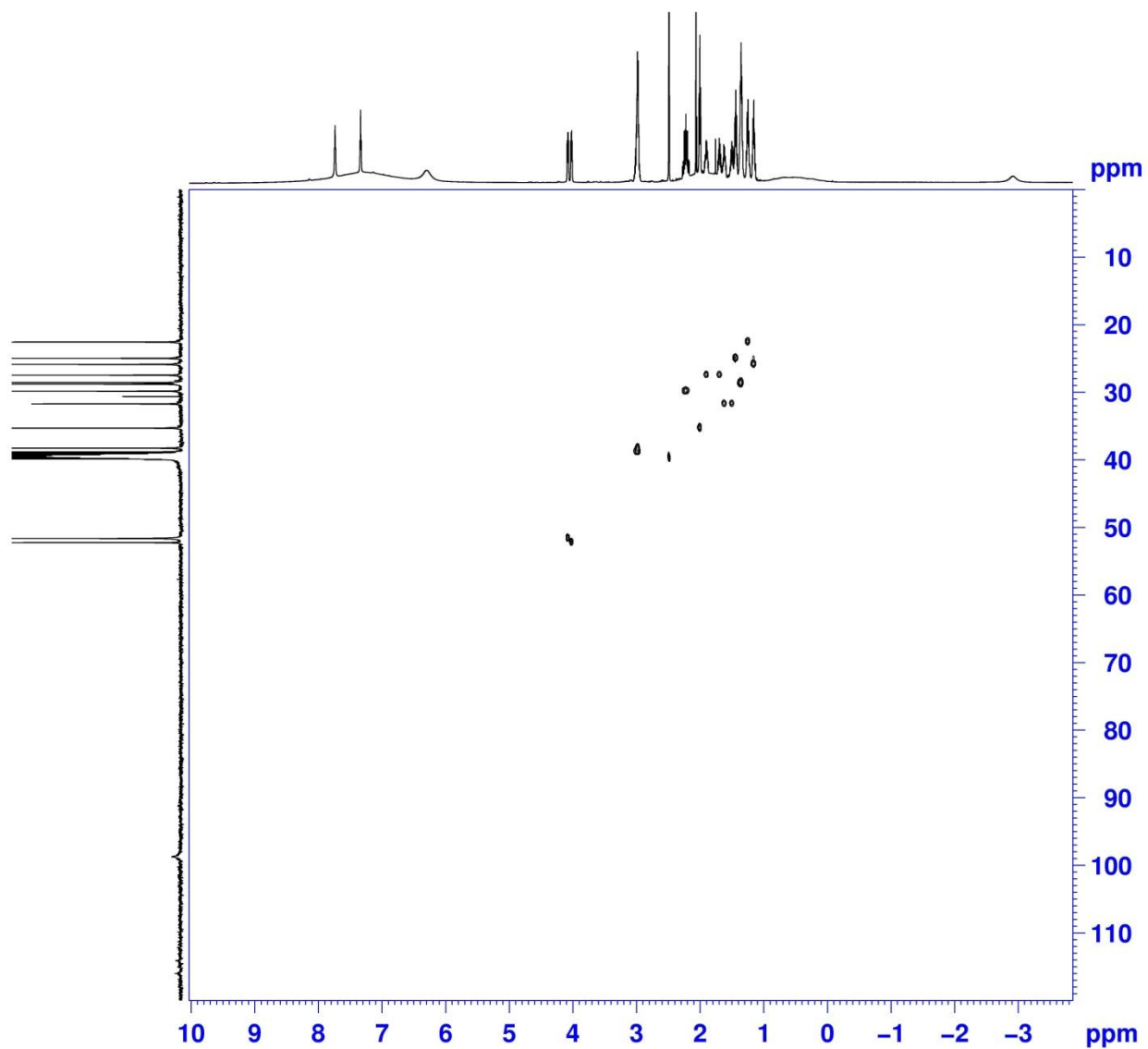


Figure S71. HSQC of compound **14**.

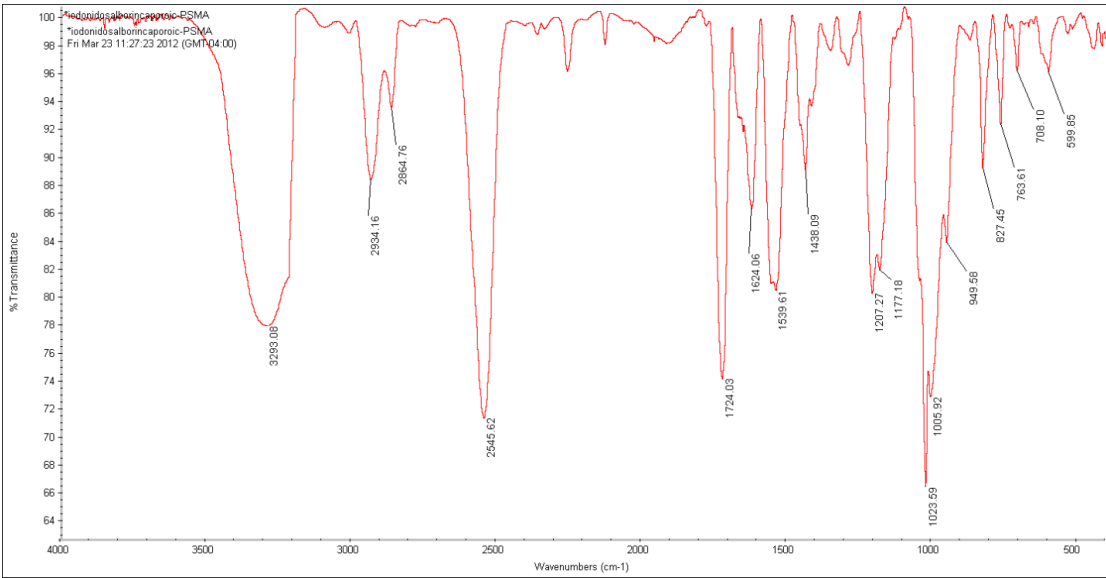


Figure S72. IR spectrum of compound **14**.

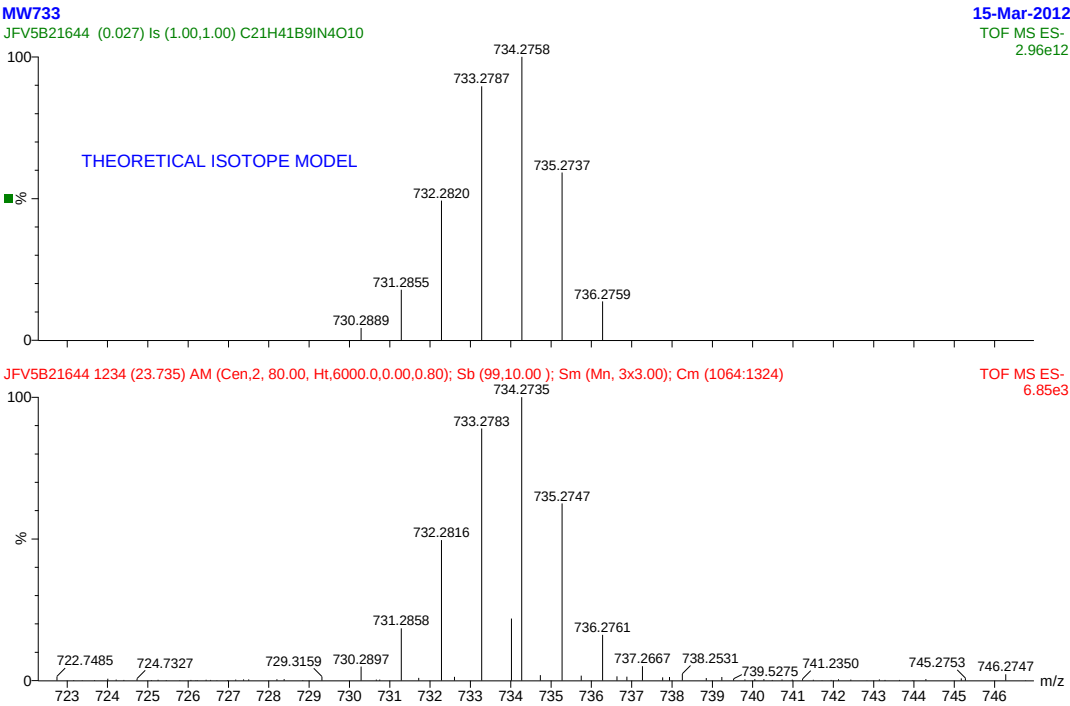


Figure S73. HRMS-ESI spectrum of compound **14**.

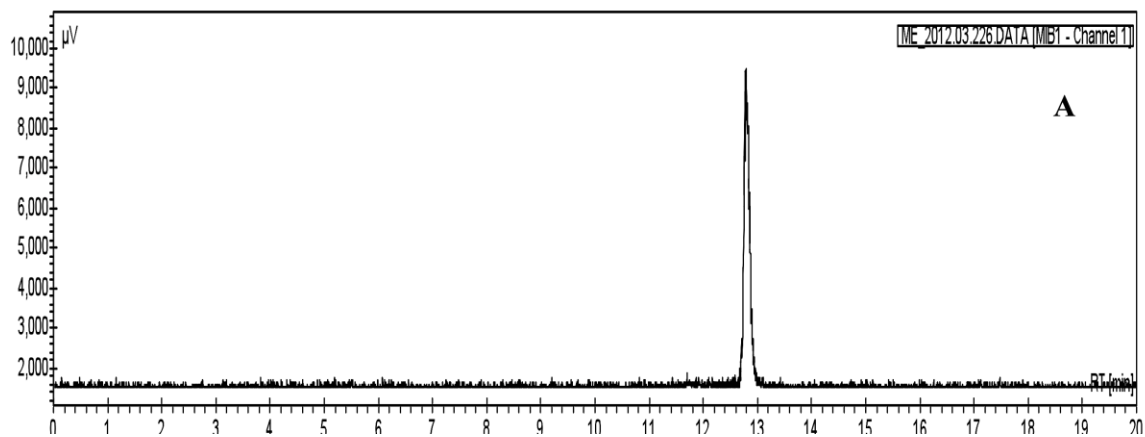


Figure S74. γ -HPLC- trace of **15b**.

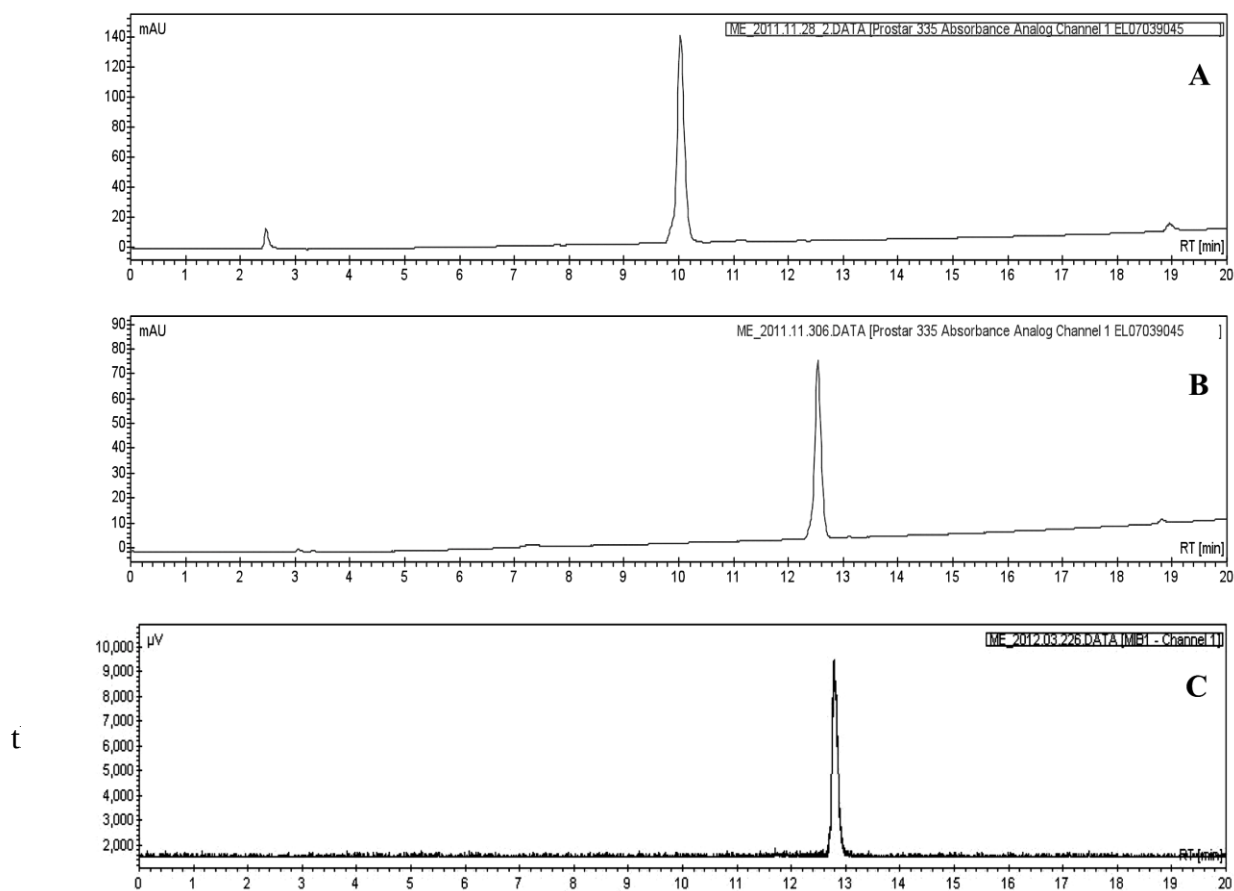


Figure S75. A) UV-HPLC chromatogram of **6b**; (B) UV-HPLC chromatogram of **7**; (C) γ -HPLC-chromatogram of **15**. Note that the UV and γ -detectors are connected in series.

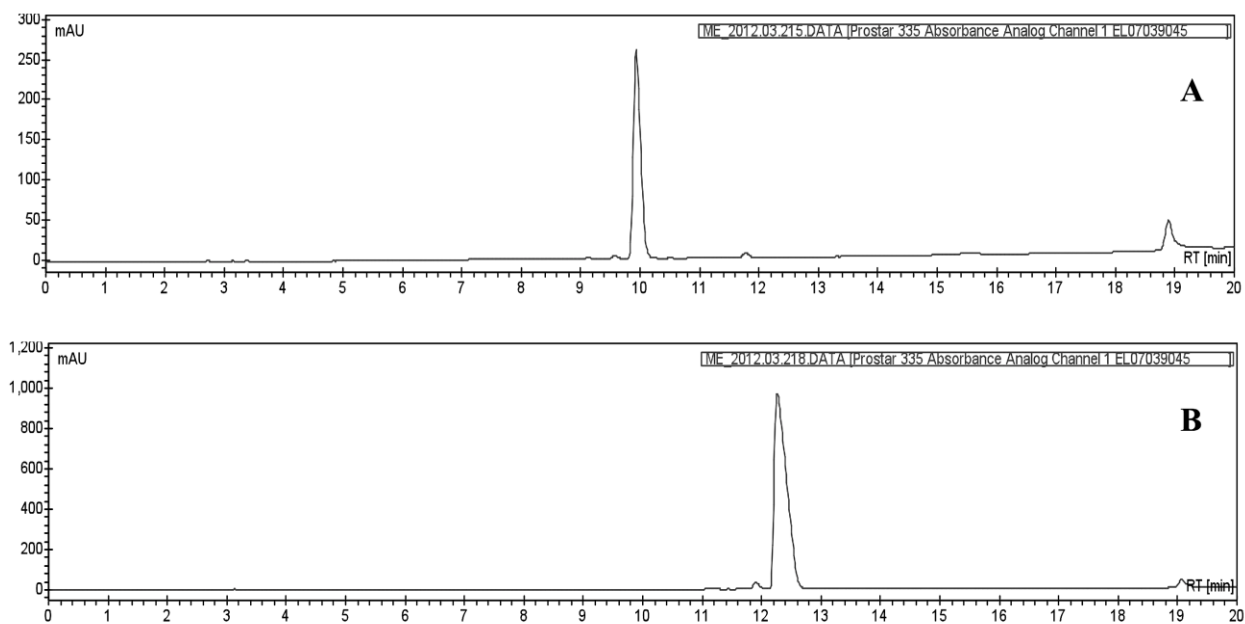


Figure S76. (A) UV-HPLC chromatogram of **13**; (B) UV-HPLC chromatogram of **14**.