

Supporting Information

Design and Synthesis of a 4-Nitrobromobenzene Derivative bearing an Ethylene Glycol Tetraacetic acid Unit for a New Generation of Caged Calcium Compounds with Two-photon Absorption Properties in the Near-IR Region, and Their Application *In Vivo*

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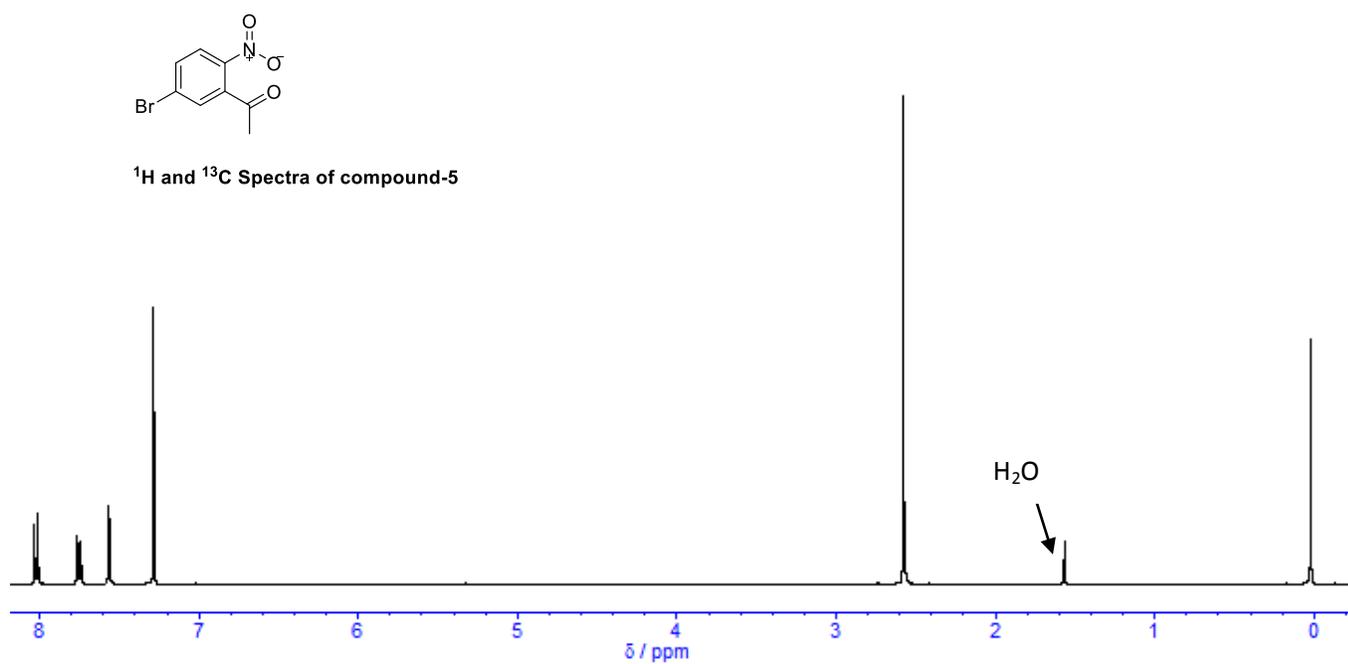


Figure S1: ¹H-NMR spectrum of compound **5** in CDCl₃.

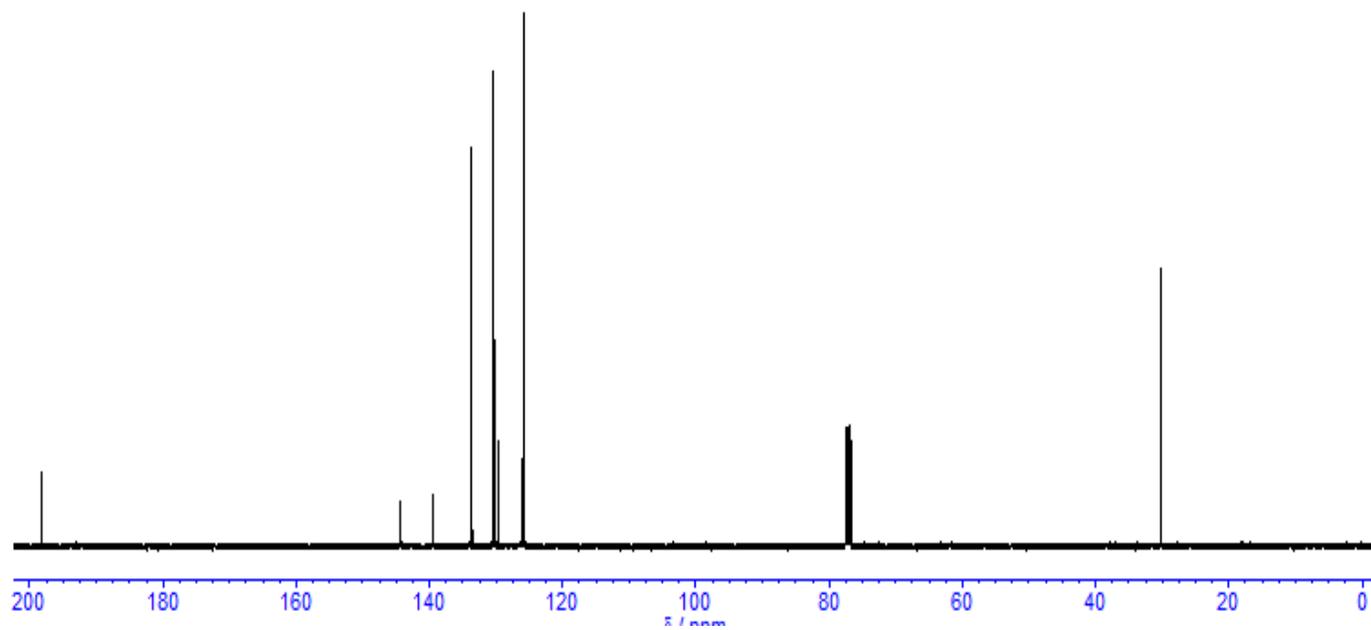


Figure S2: ¹³C-NMR spectrum of compound **5** in CDCl₃.

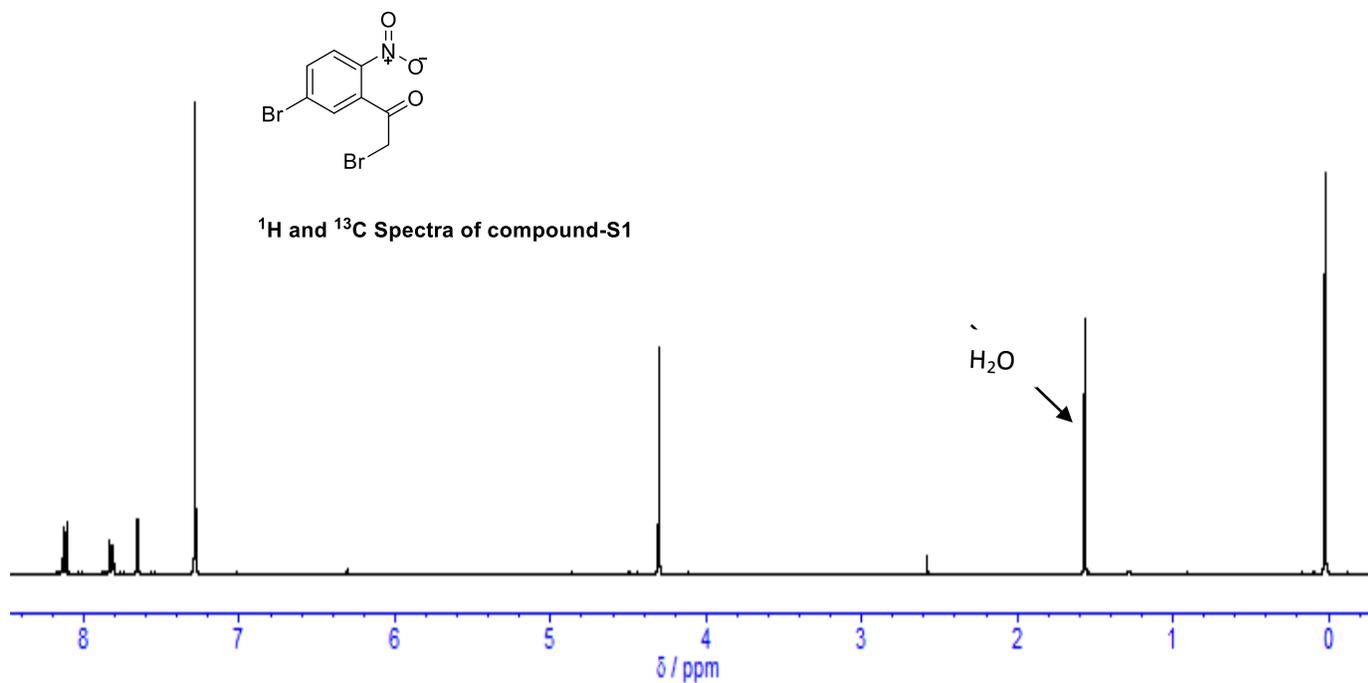


Figure S3: ¹H-NMR spectrum of compound **S1** in CDCl₃.

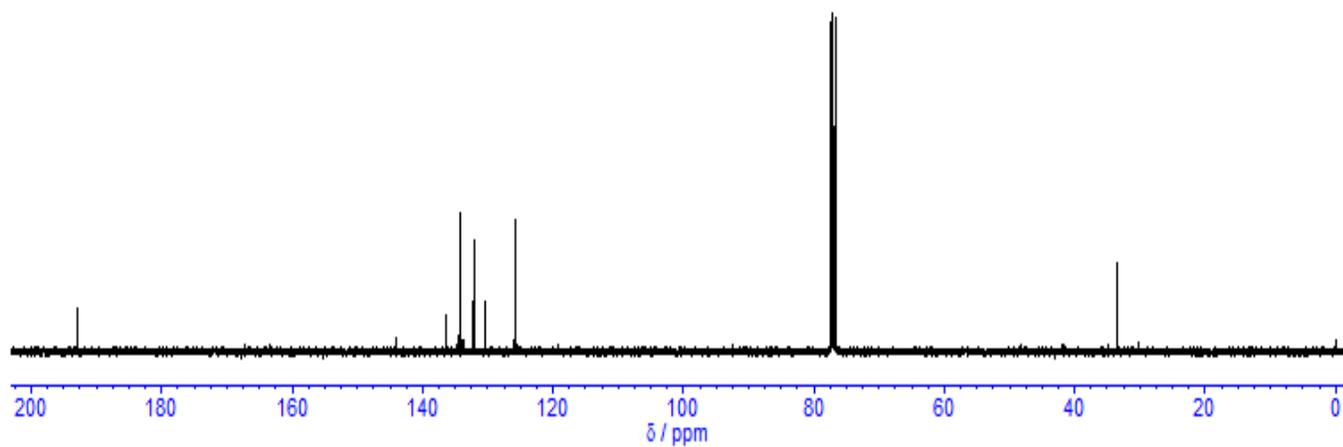


Figure S4: ¹³C-NMR spectrum of compound **S1** in CDCl₃.

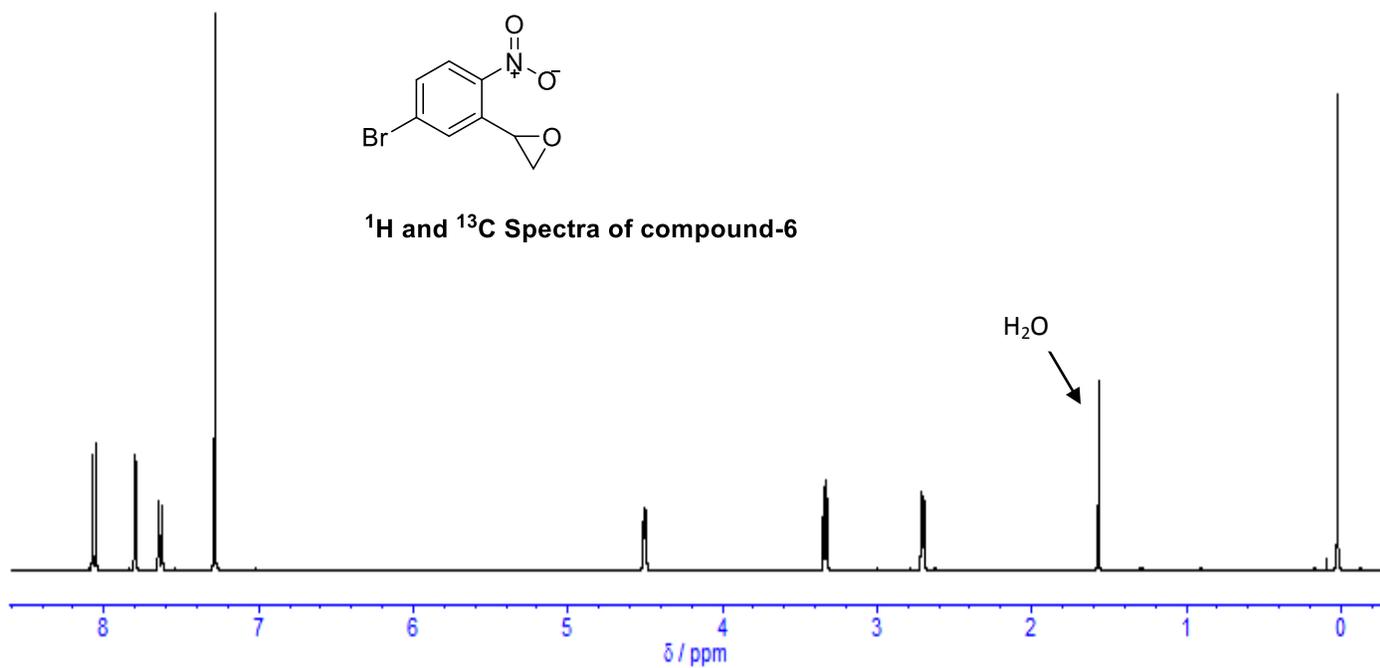


Figure S5: ¹H-NMR spectrum of compound **6** in CDCl₃.

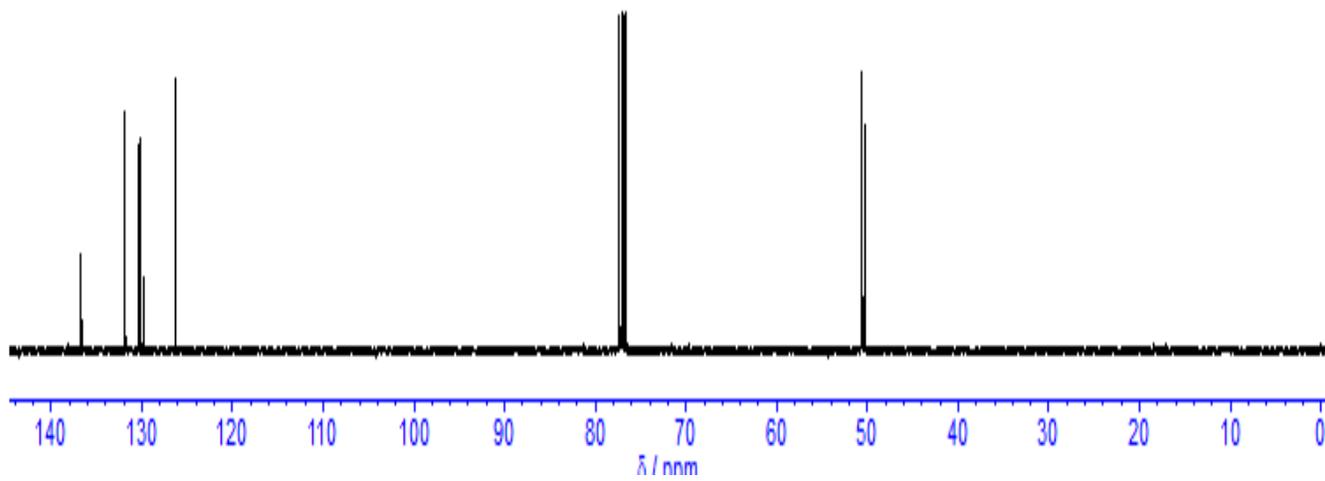


Figure S6: ¹³C-NMR spectrum of compound **6** in CDCl₃.

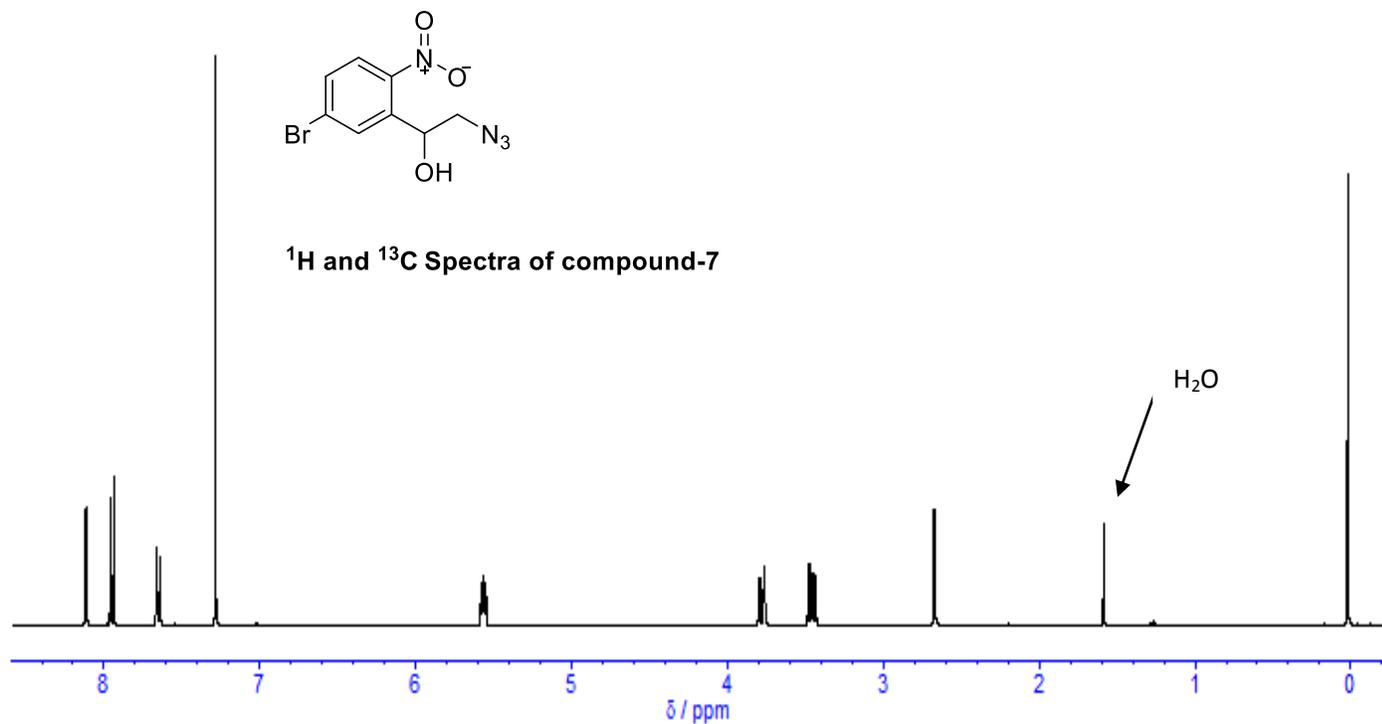


Figure S7: ¹H-NMR spectrum of compound **7** in CDCl₃.

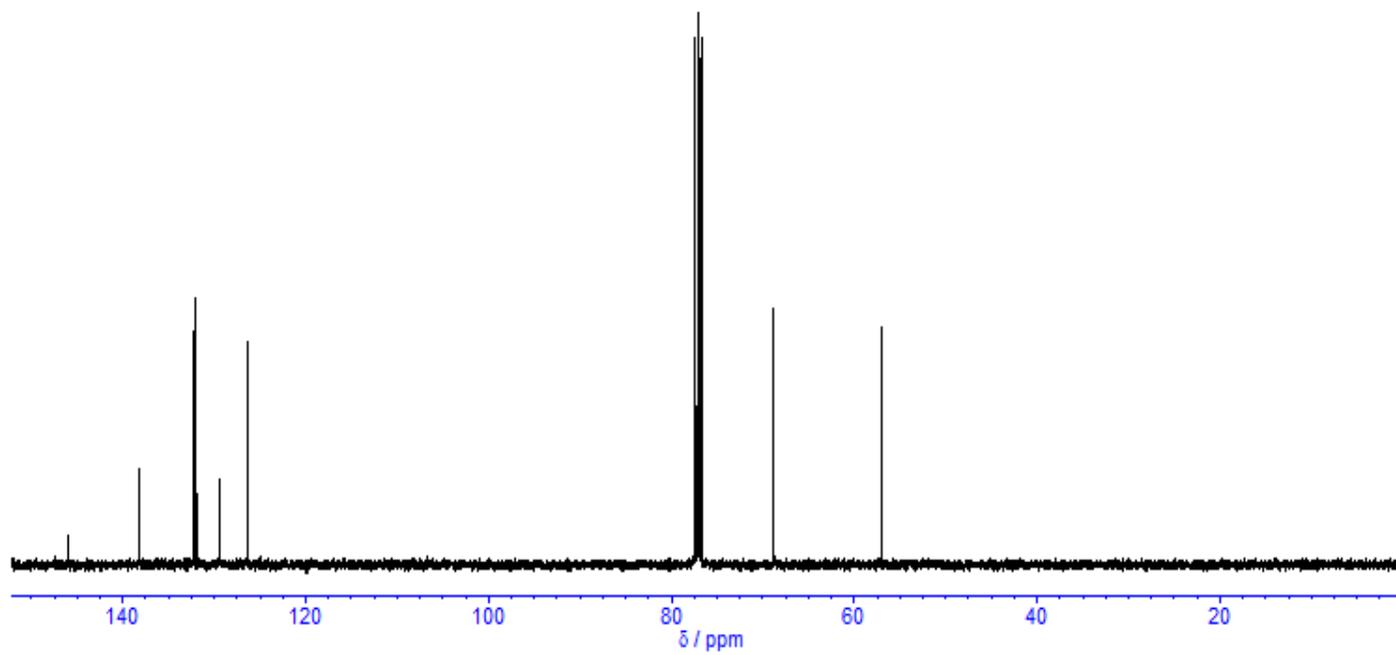


Figure S8: ¹³C-NMR spectrum of compound **7** in CDCl₃.

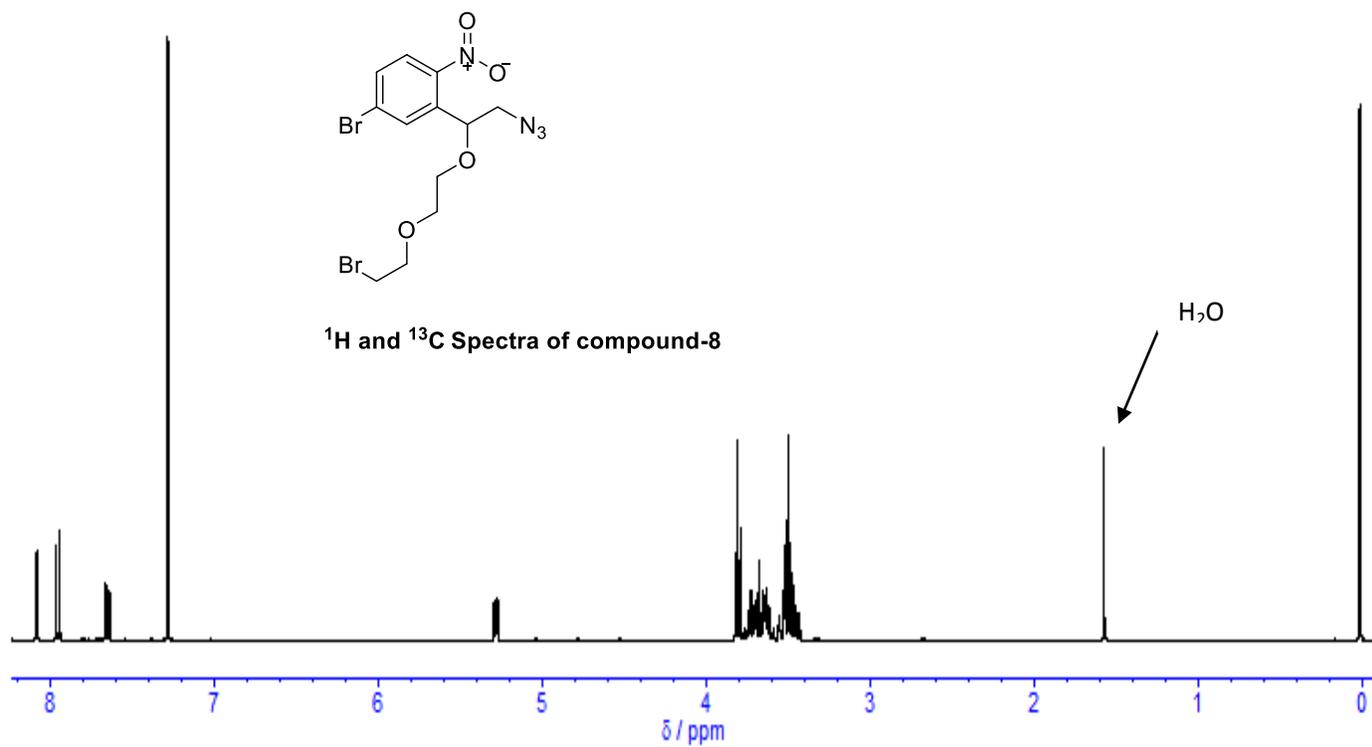


Figure S9: ¹H-NMR spectrum of compound **8** in CDCl₃.

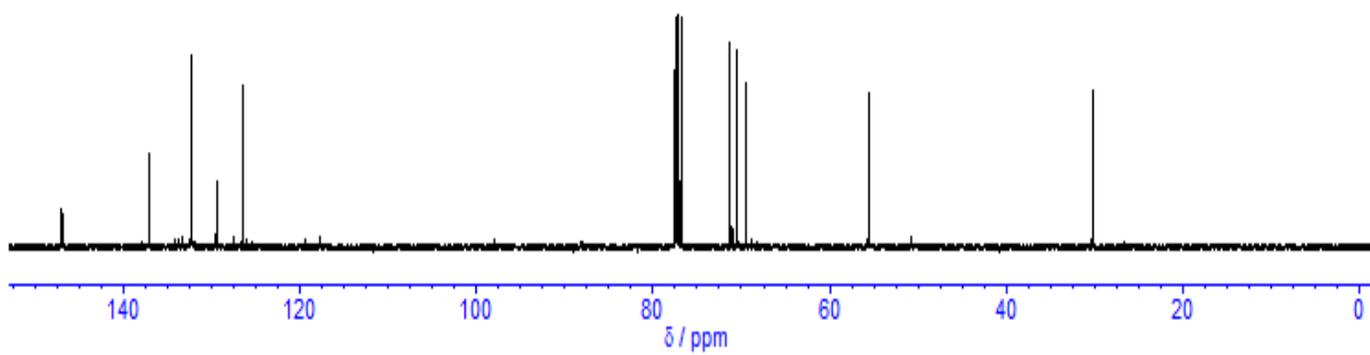


Figure S10: ¹³C-NMR spectrum of compound **8** in CDCl₃.

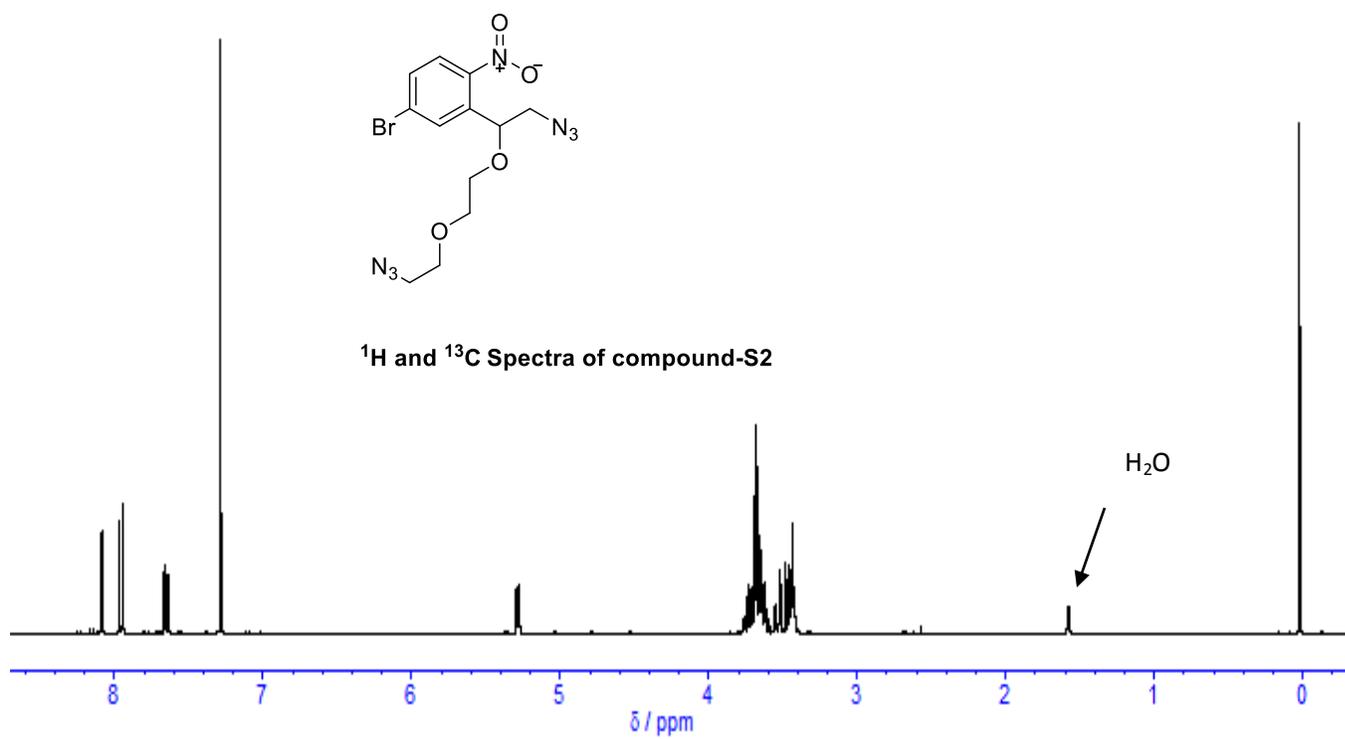


Figure S11: ¹H-NMR spectrum of compound S2 in CDCl₃.

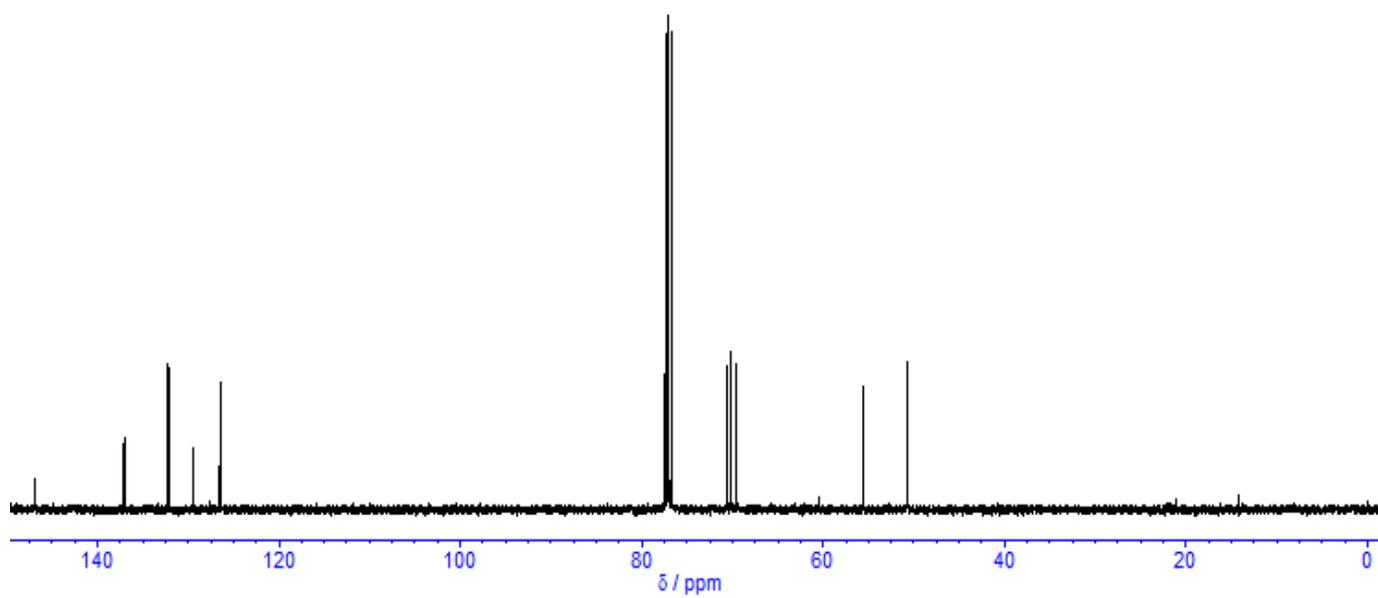


Figure S12: ¹³C-NMR spectrum of compound S2 in CDCl₃.

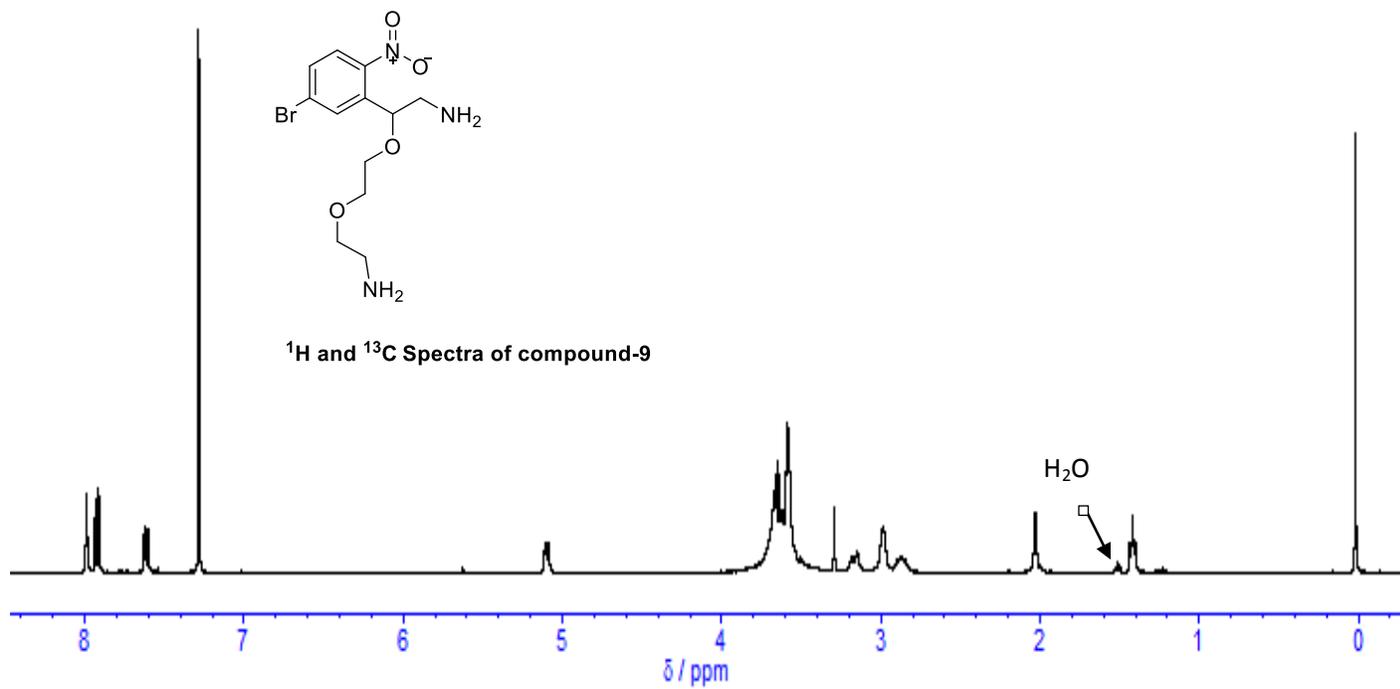


Figure S13: ¹H-NMR spectrum of compound **9** in CDCl₃.

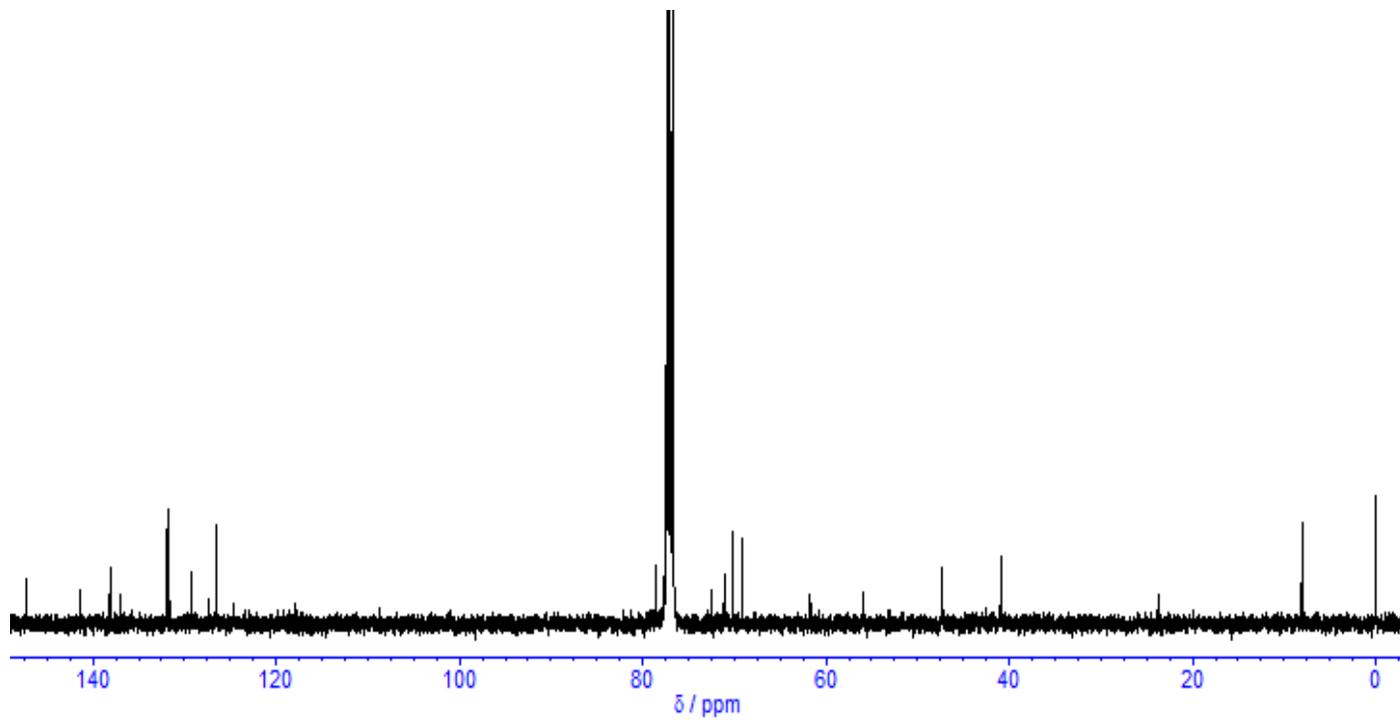


Figure S14: ¹³C-NMR spectrum of compound **9** in CDCl₃.

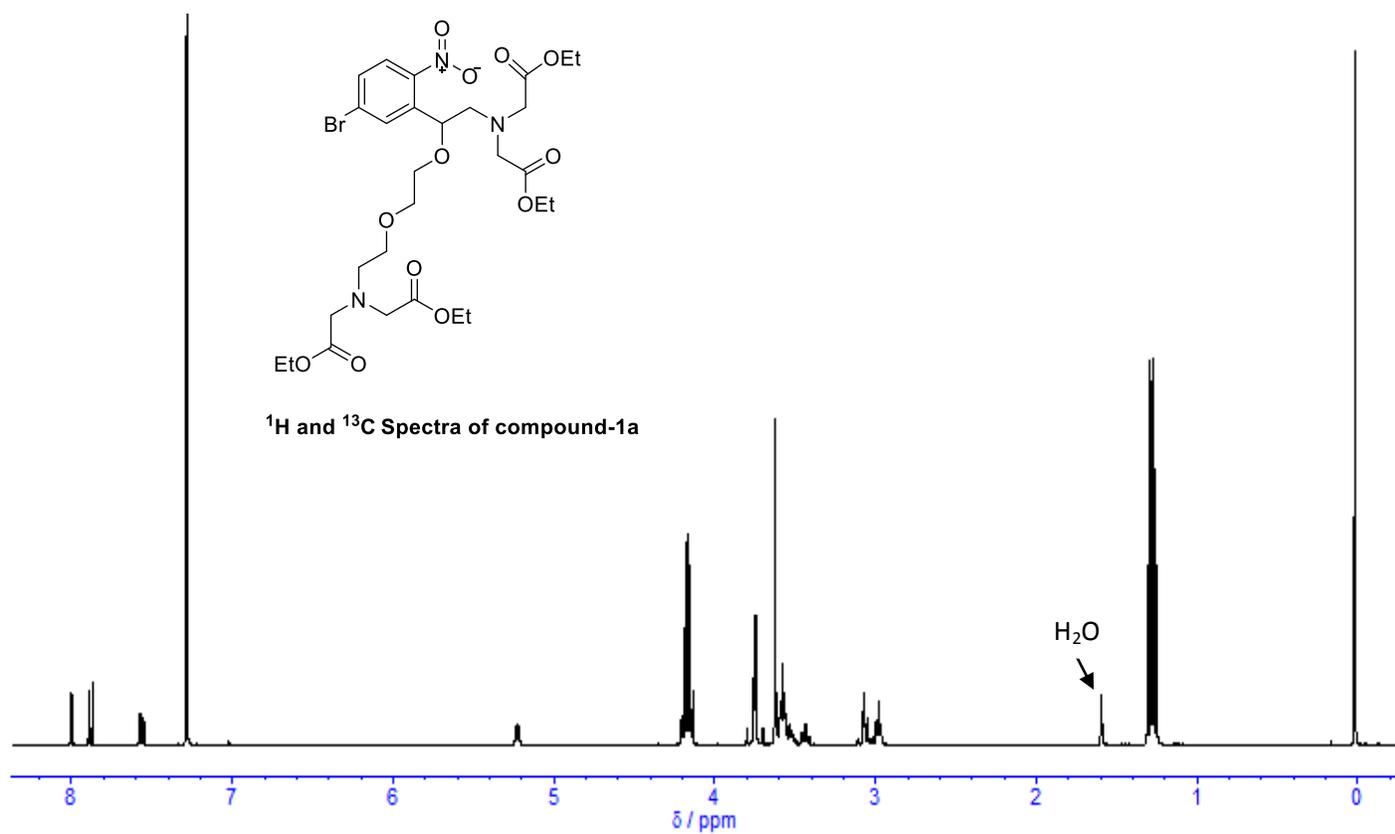


Figure S15: ¹H-NMR spectrum of compound **1a** in CDCl₃.

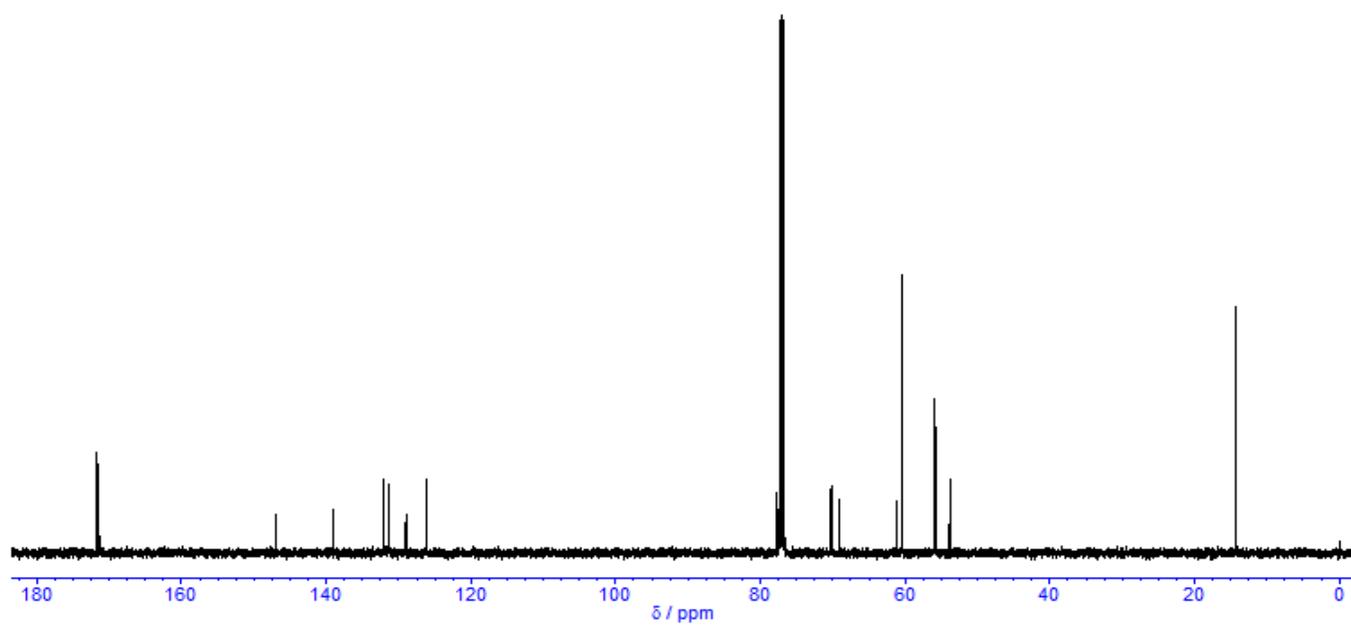


Figure S16: ¹³C-NMR spectrum of compound **1a** in CDCl₃.

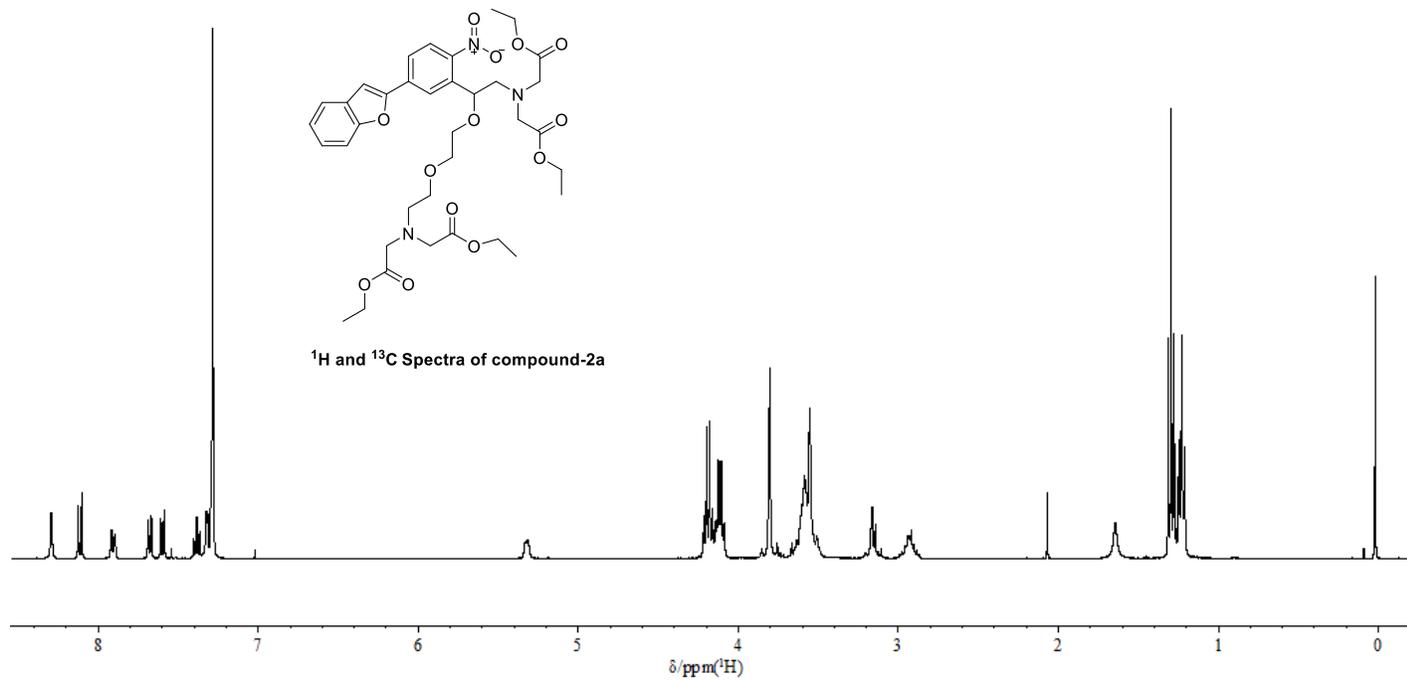


Figure S17: ¹H-NMR spectrum of compound 2a in CDCl₃.

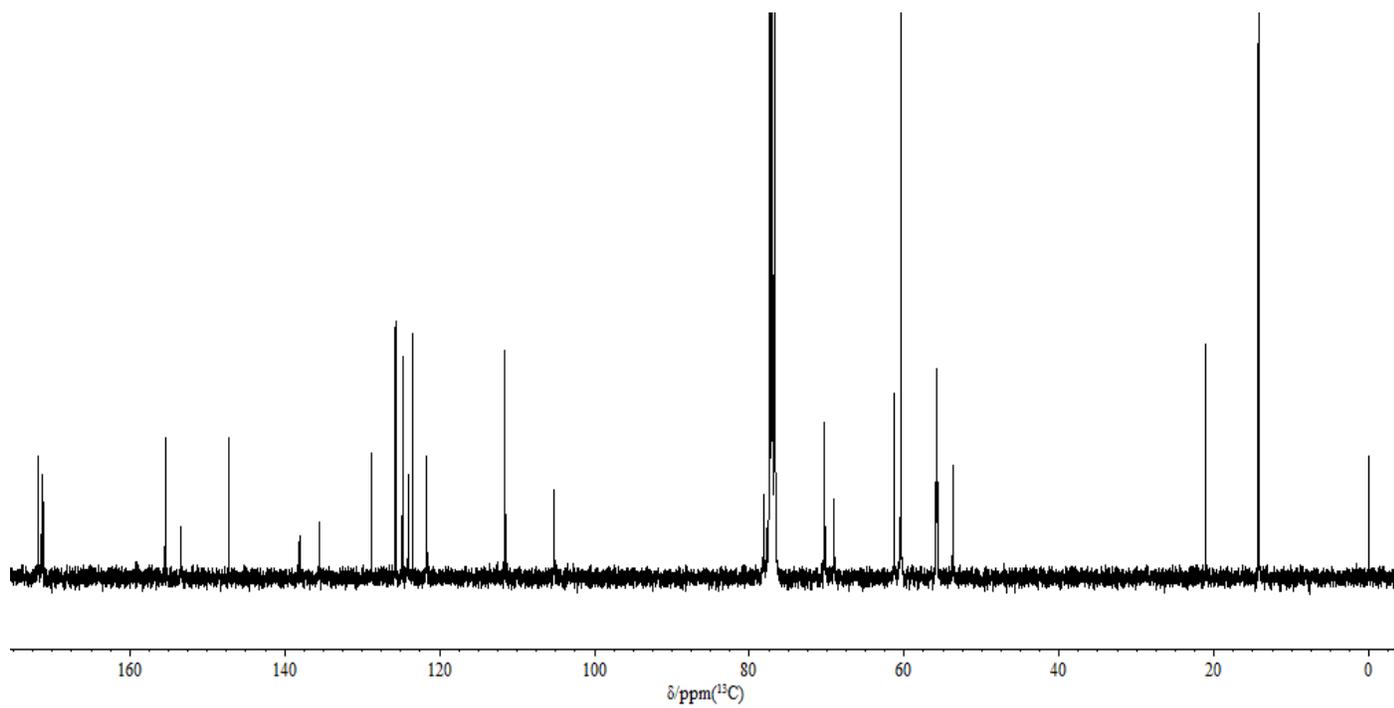


Figure S18: ¹³C-NMR spectrum of compound 2a in CDCl₃.

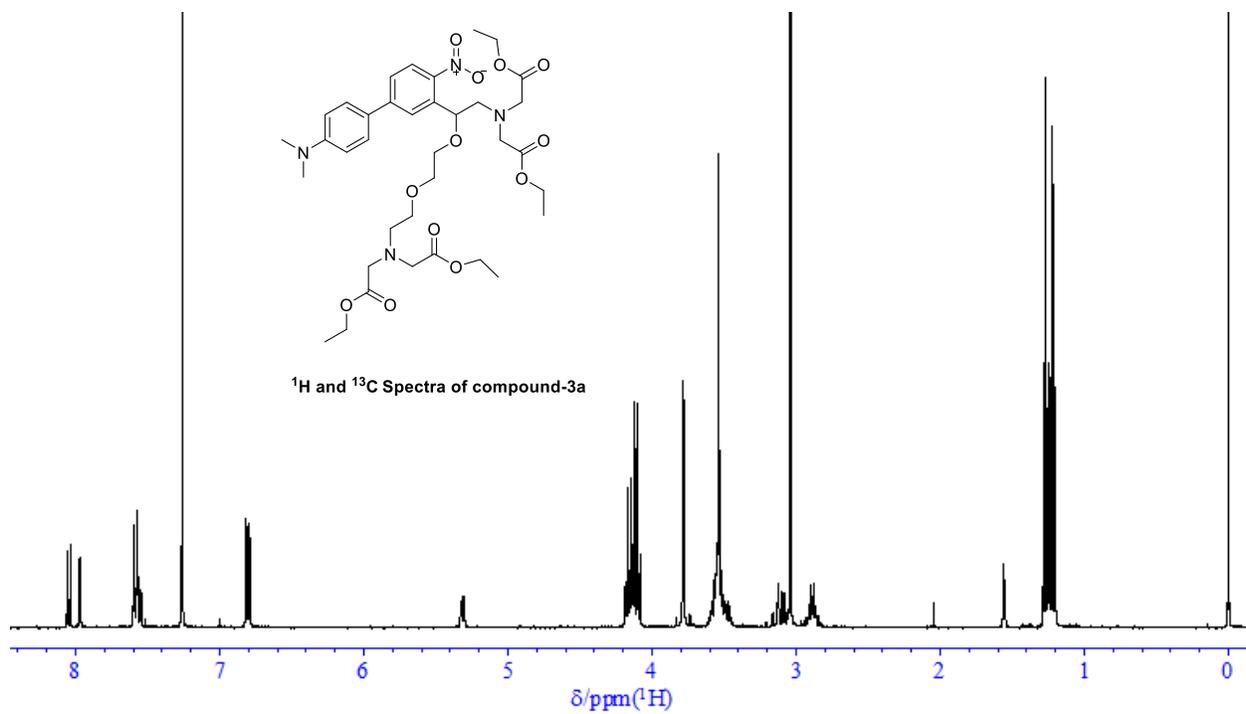


Figure S19: ¹H-NMR spectrum of compound **3a** in CDCl₃.

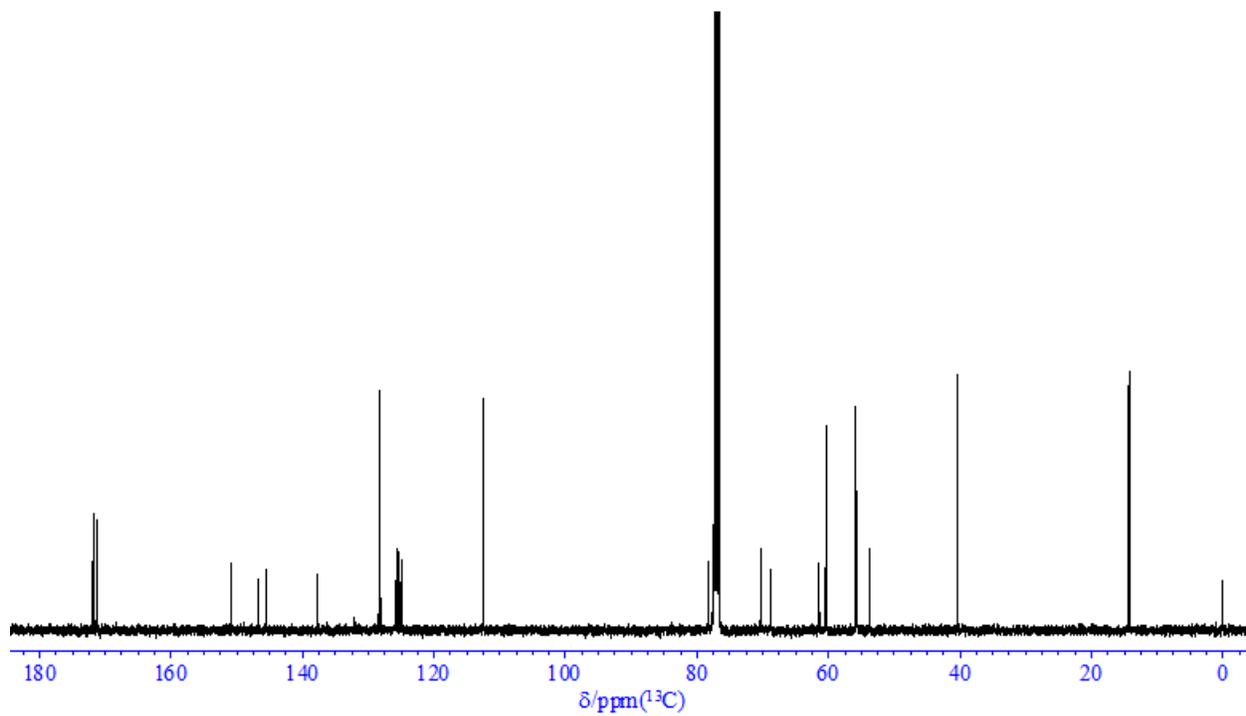


Figure S20: ¹³C-NMR spectrum of compound **3a** in CDCl₃.

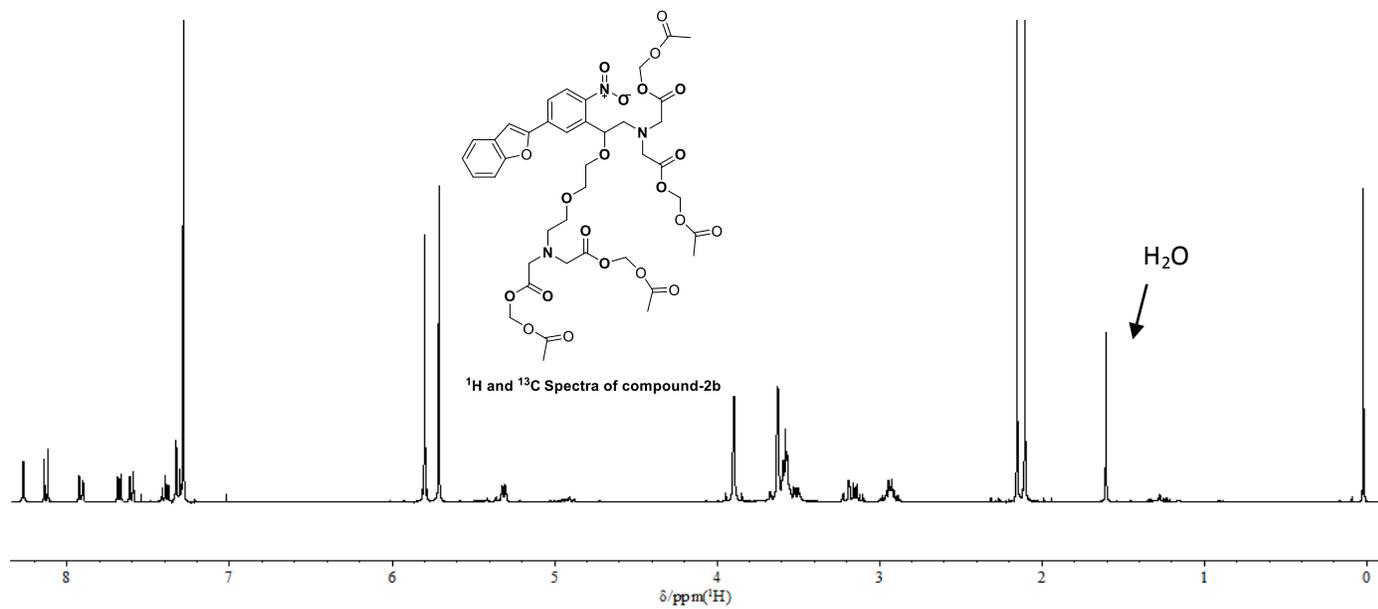


Figure S21: ¹H-NMR spectrum of compound **2b** in CDCl₃.

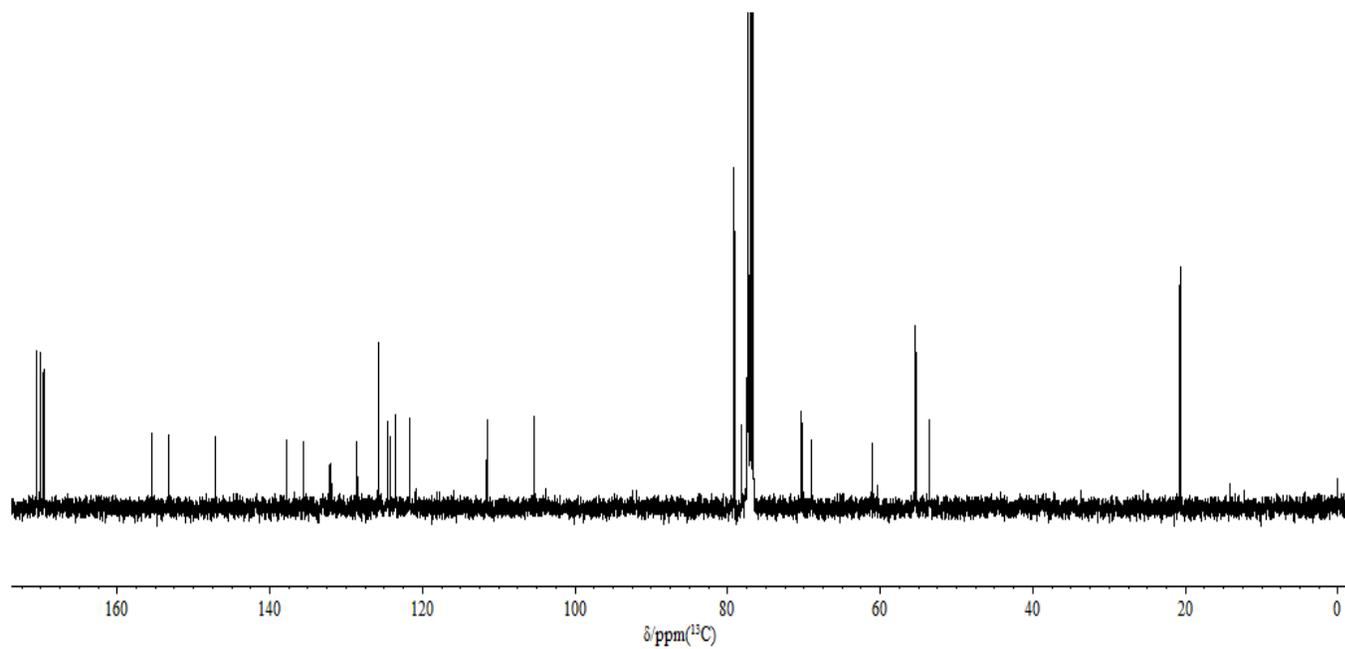


Figure S22: ¹³C-NMR spectrum of compound **2b** in CDCl₃.

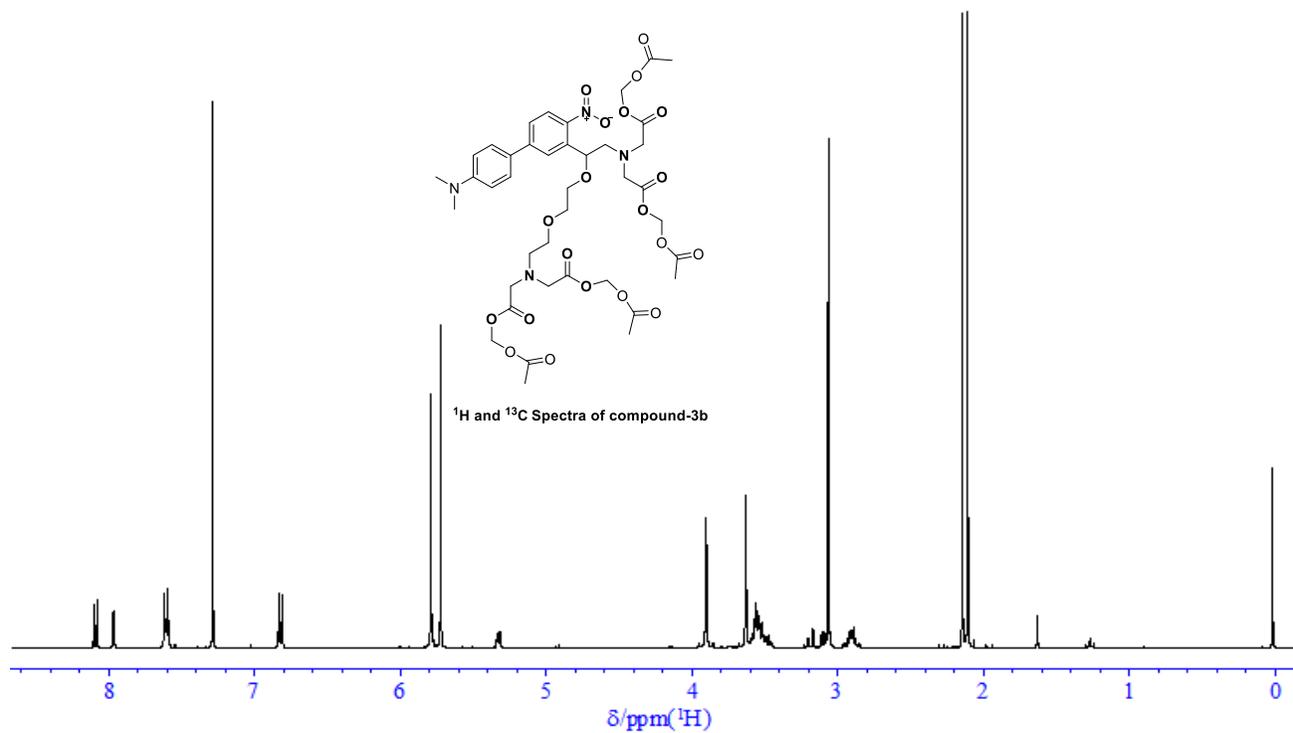


Figure S23: ¹H-NMR spectrum of compound **3b** in CDCl₃.

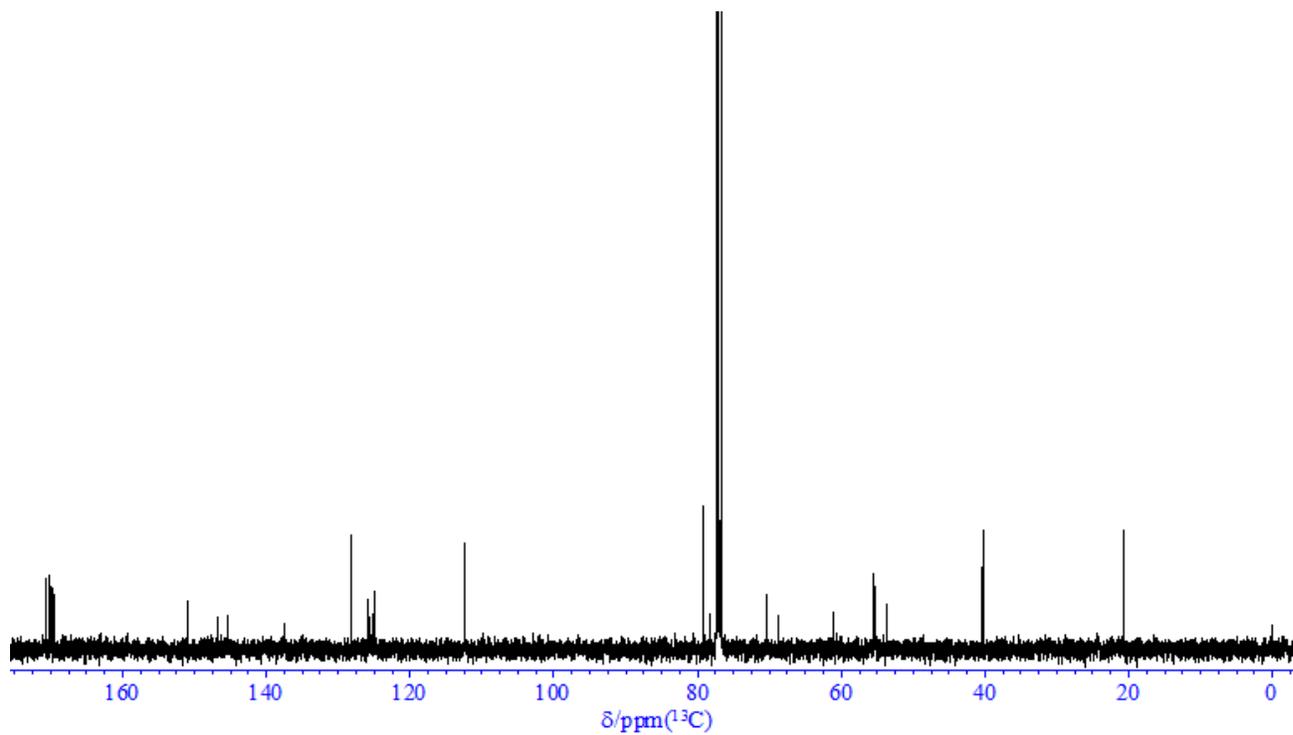


Figure S24: ¹³C-NMR spectrum of compound **3b** in CDCl₃.

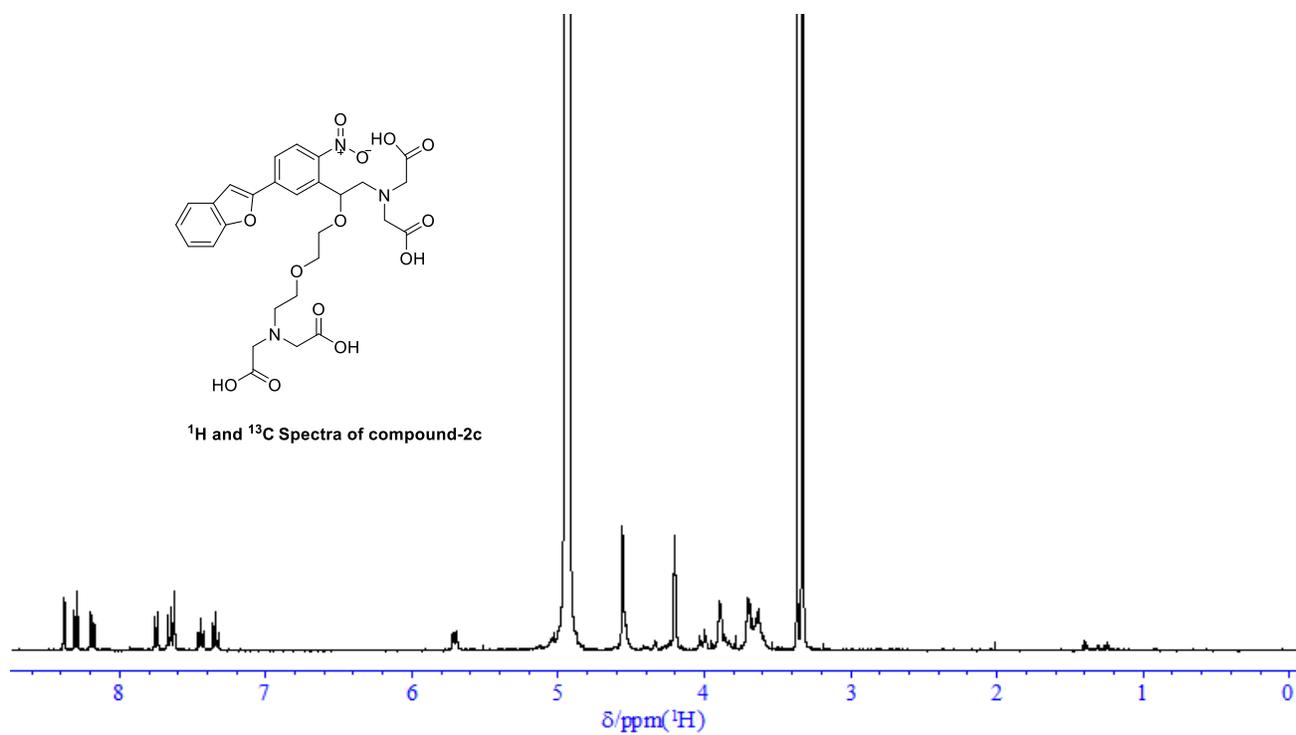


Figure S25: ¹H-NMR spectrum of compound **2c** in CD₃OD.

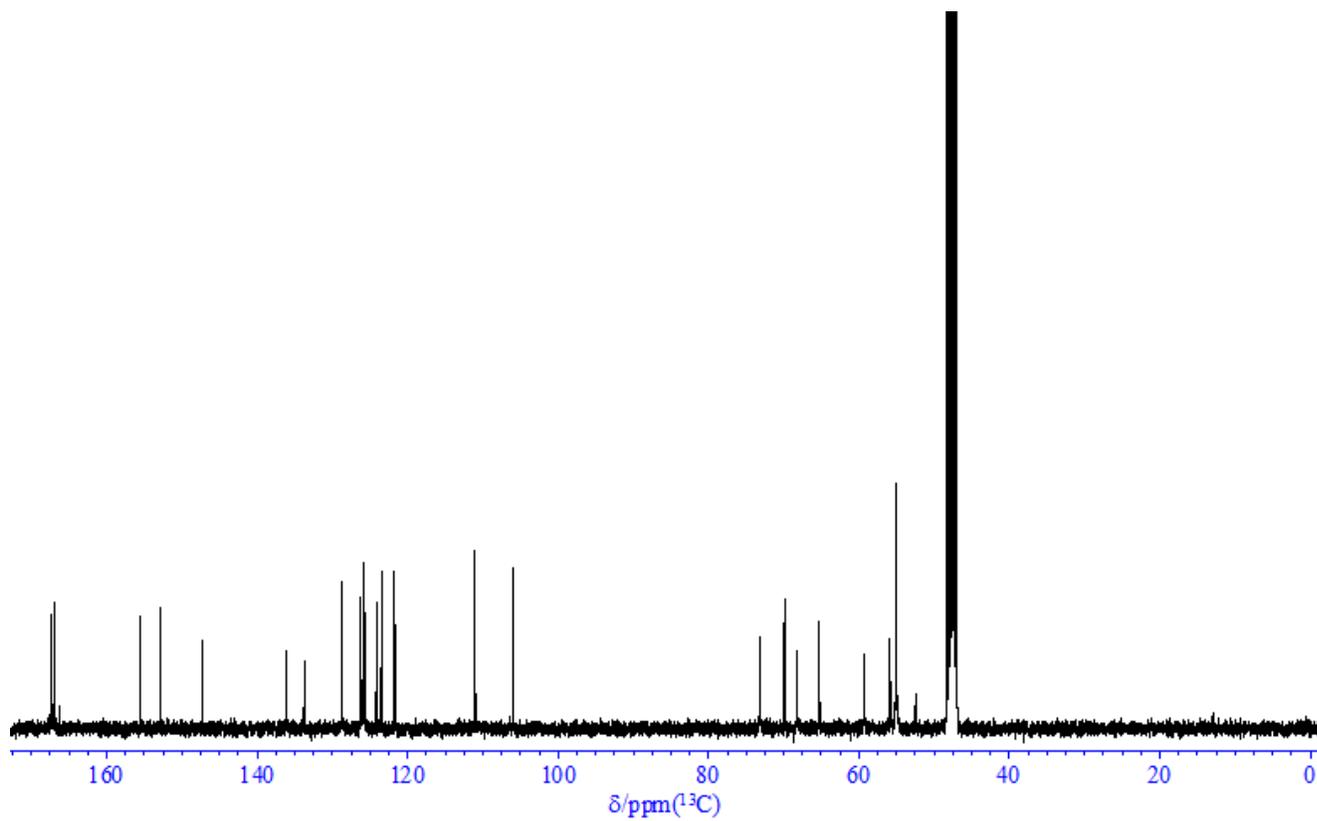


Figure S26: ¹³C-NMR spectrum of compound **2c** in CD₃OD.

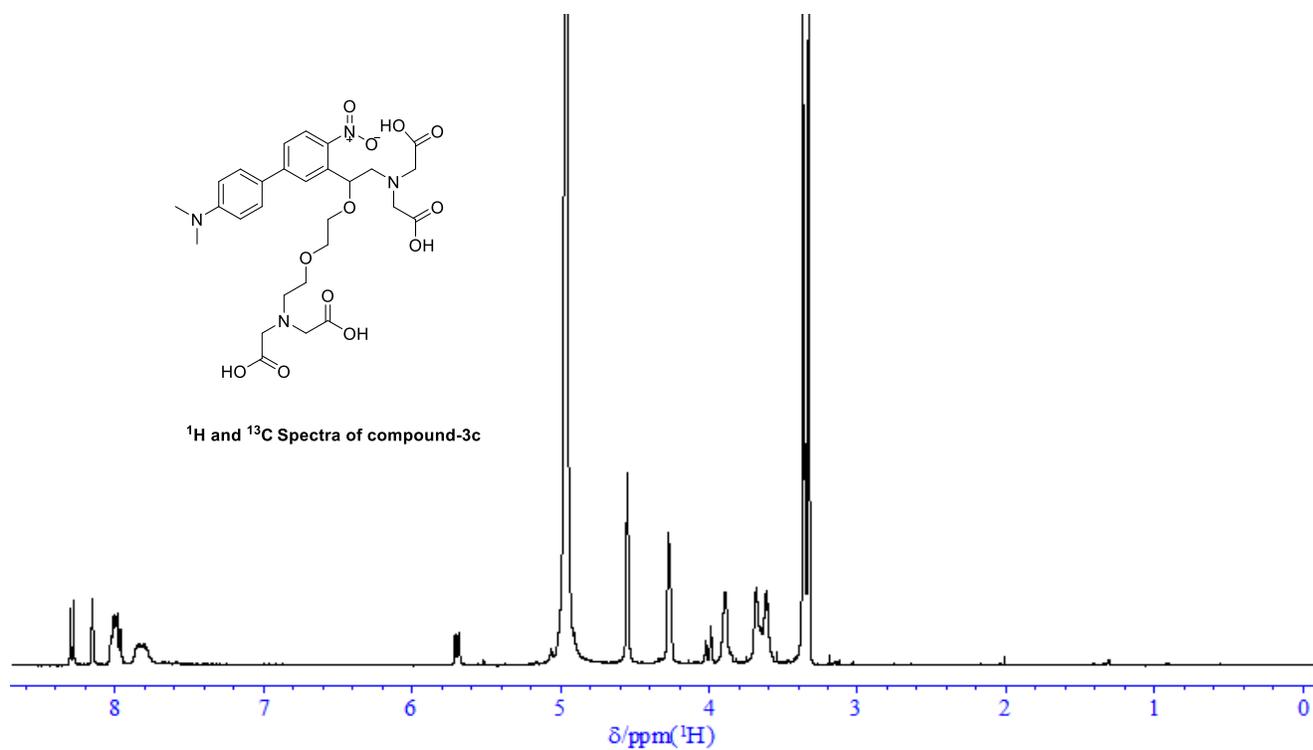


Figure S27: ¹H-NMR spectrum of compound 3c in CD₃OD.

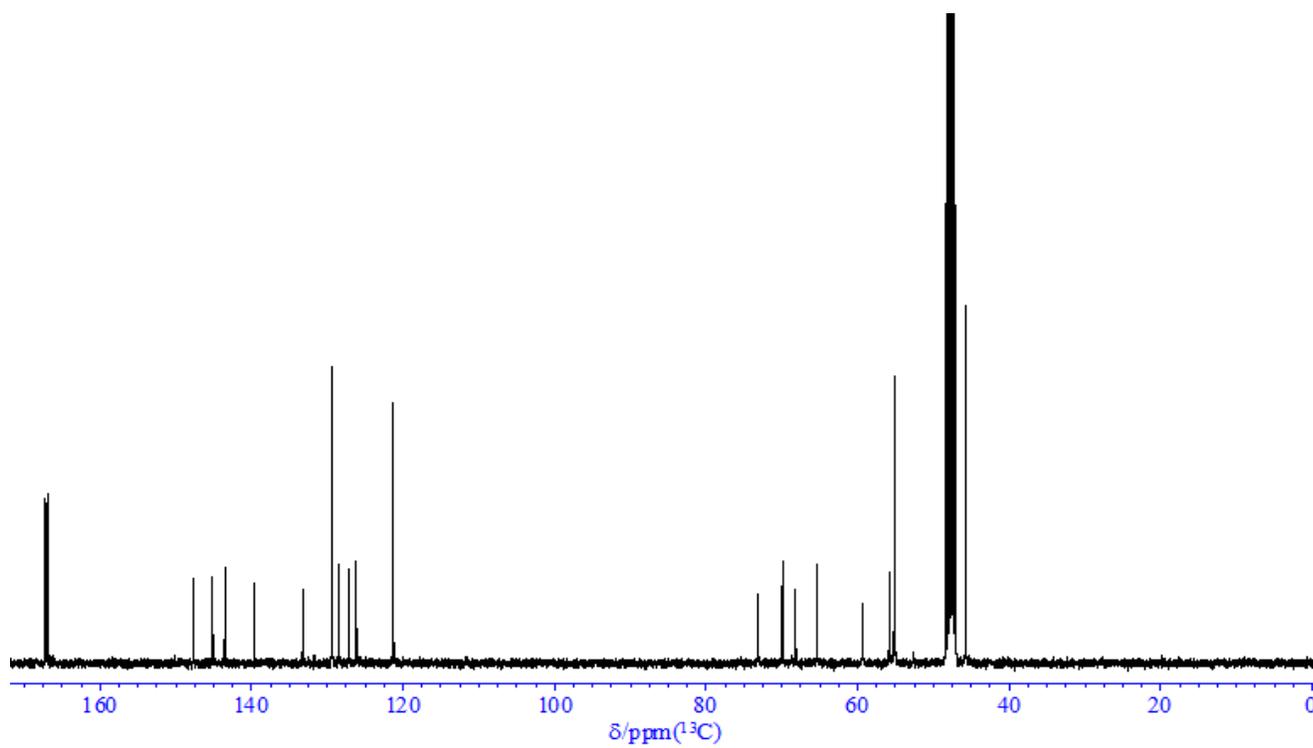


Figure S28: ¹³C-NMR spectrum of compound 3c in CD₃OD.