

Supporting Information for

**Coordination chemistry of a calix[4]arene-based NHC ligand: Dinuclear
complexes and comparison to $\text{I}^{\ddagger}\text{Pr}_2\text{Me}_2$**

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1. ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of new compounds

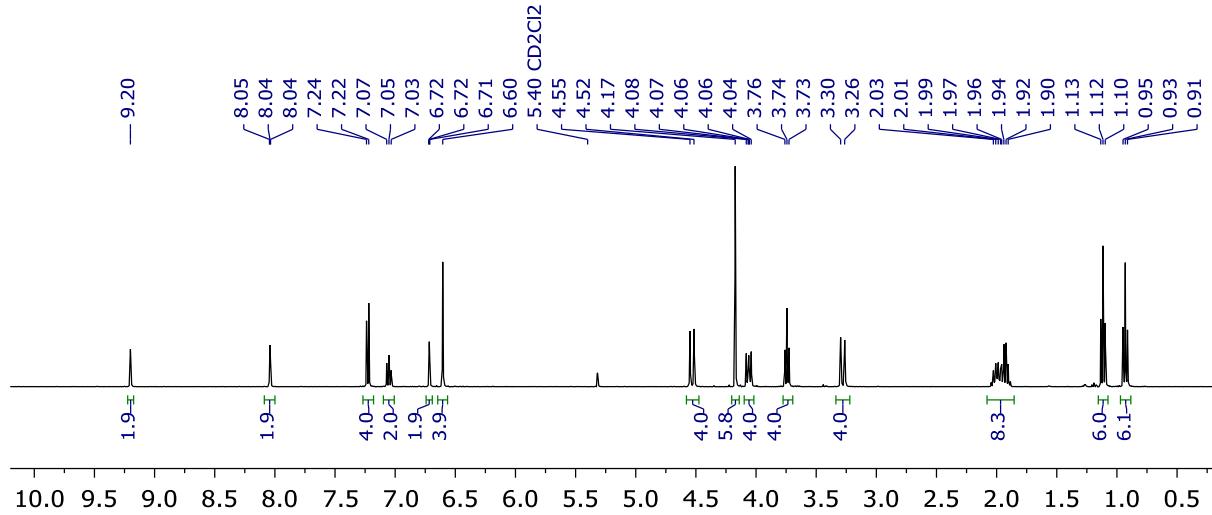


Figure SI-1: ^1H NMR spectrum of **1.2HI** (CD_2Cl_2 , 400 MHz)

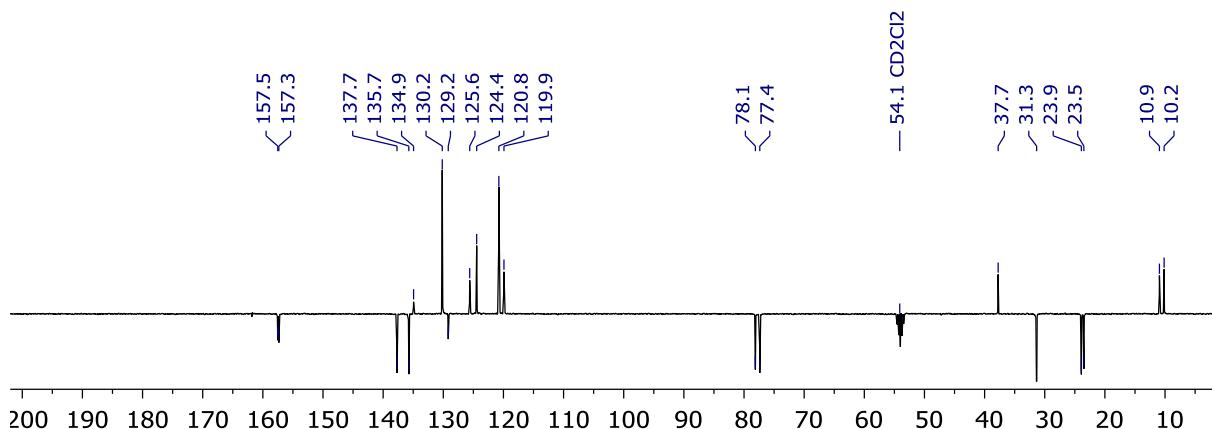


Figure SI-2: $^{13}\text{C}\{^1\text{H}\}$ PENDANT NMR spectrum of **1.2HI** (CD_2Cl_2 , 101 MHz)

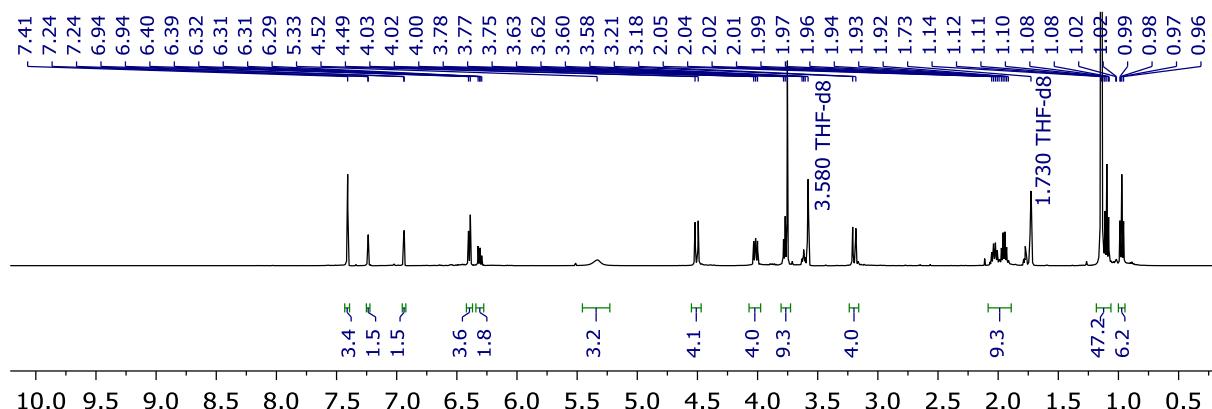


Figure SI-3: ^1H NMR spectrum of **1** ($\text{d}_8\text{-THF}$, 500 MHz)

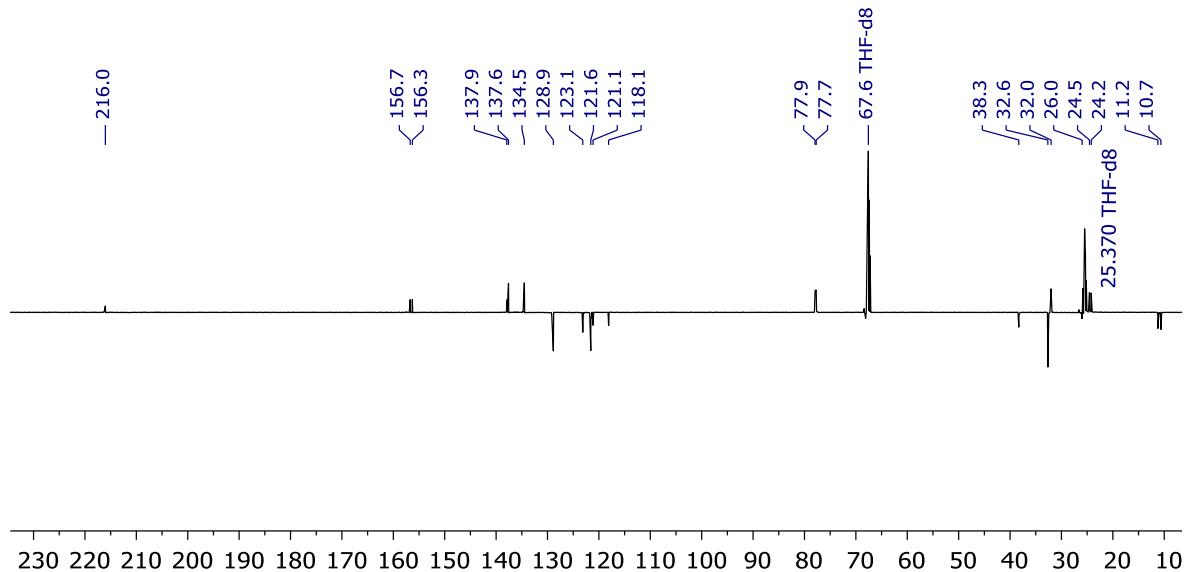


Figure SI-4: $^{13}\text{C}\{^1\text{H}\}$ APT NMR spectrum of **1** ($\text{d}_8\text{-THF}$, 126 MHz)

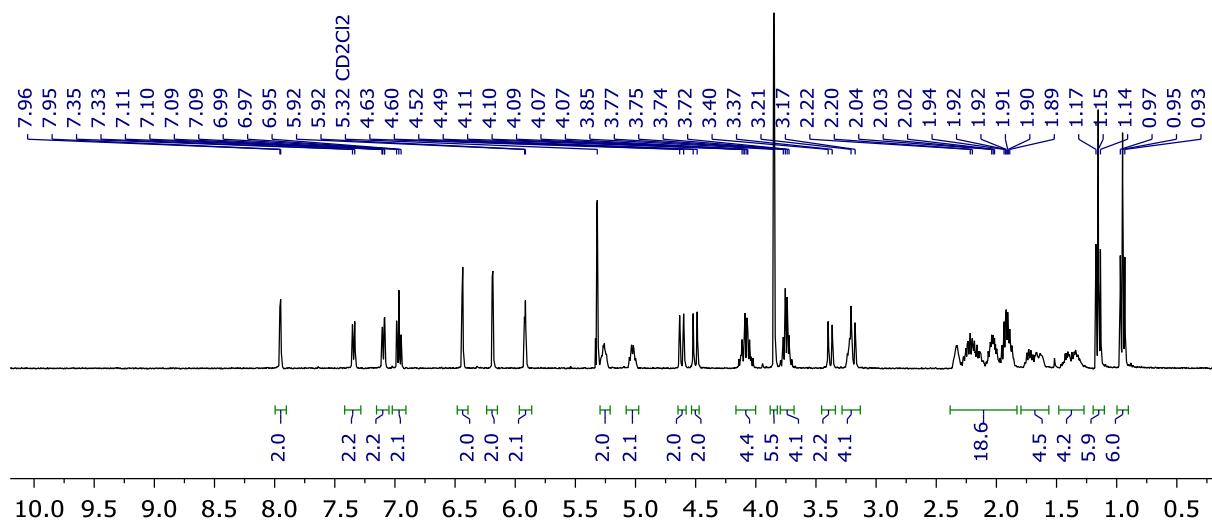


Figure SI-5: ^1H NMR spectrum of **2a** (CD_2Cl_2 , 400 MHz)

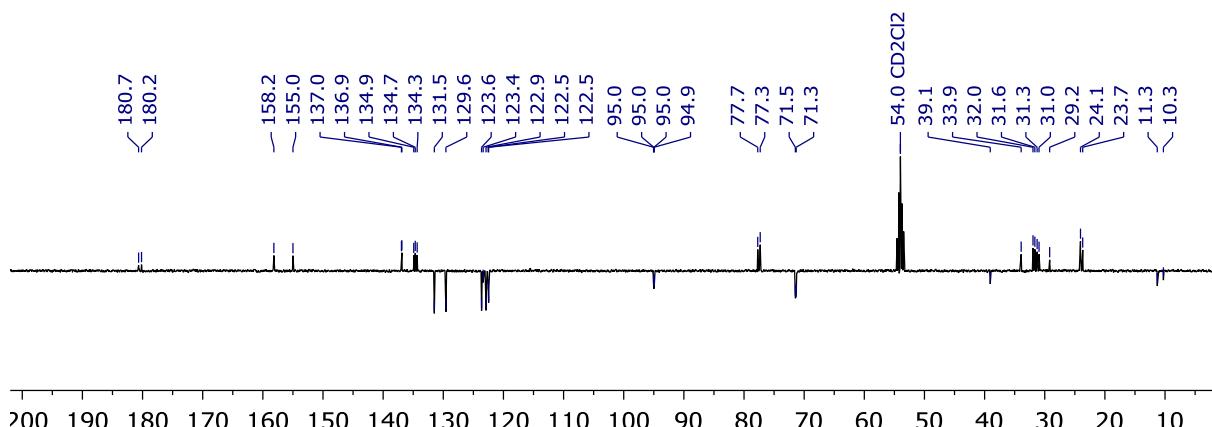


Figure SI-6: $^{13}\text{C}\{^1\text{H}\}$ PENDANT NMR spectrum of **2a** (CD_2Cl_2 , 101 MHz)

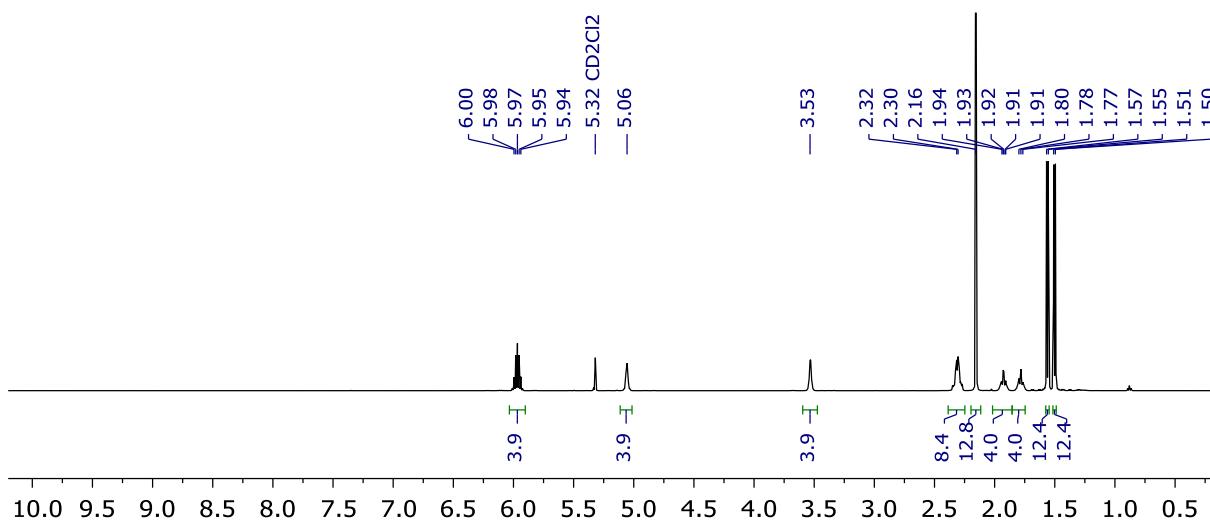


Figure SI-7: ^1H NMR spectrum of **2b** (CD_2Cl_2 , 500 MHz)

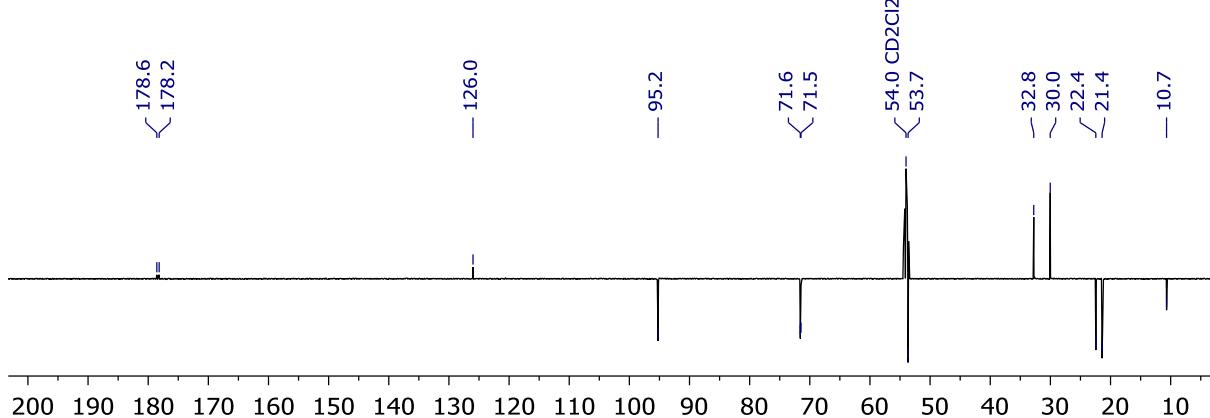


Figure SI-8: $^{13}\text{C}\{^1\text{H}\}$ APT NMR spectrum of **2b** (CD_2Cl_2 , 126 MHz)

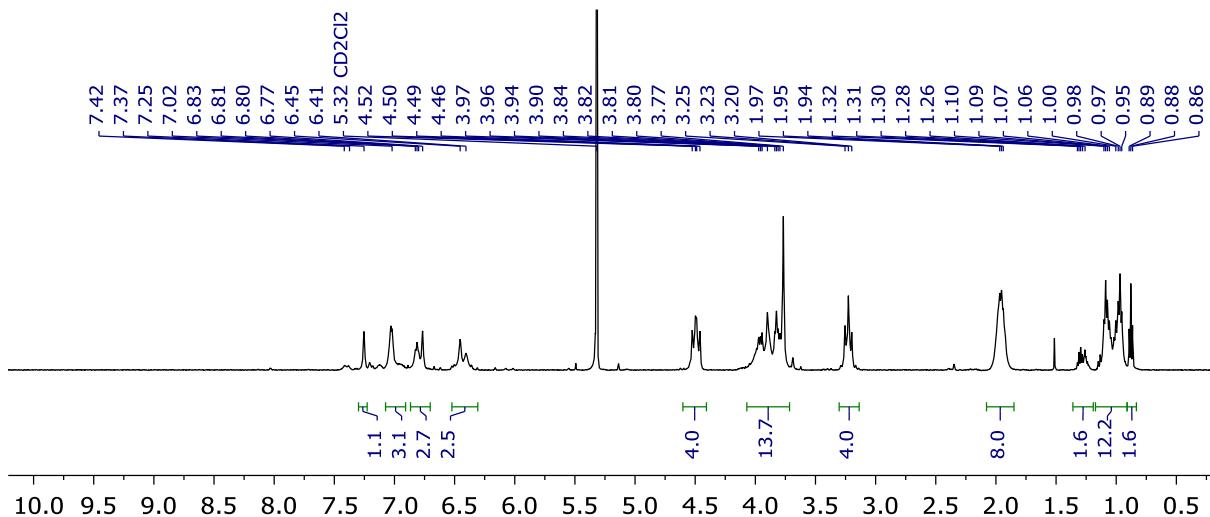


Figure SI-9: ^1H NMR spectrum **3a** (CD_2Cl_2 , 500 MHz)

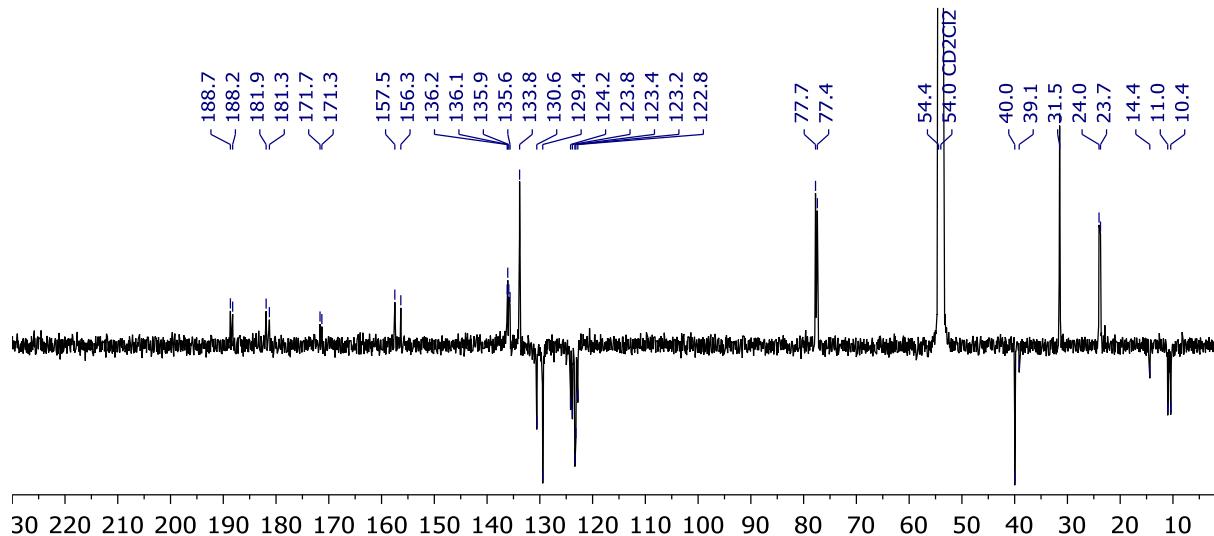


Figure SI-10: $^{13}\text{C}\{^1\text{H}\}$ APT NMR spectrum of **3a** (CD_2Cl_2 , 126 MHz)

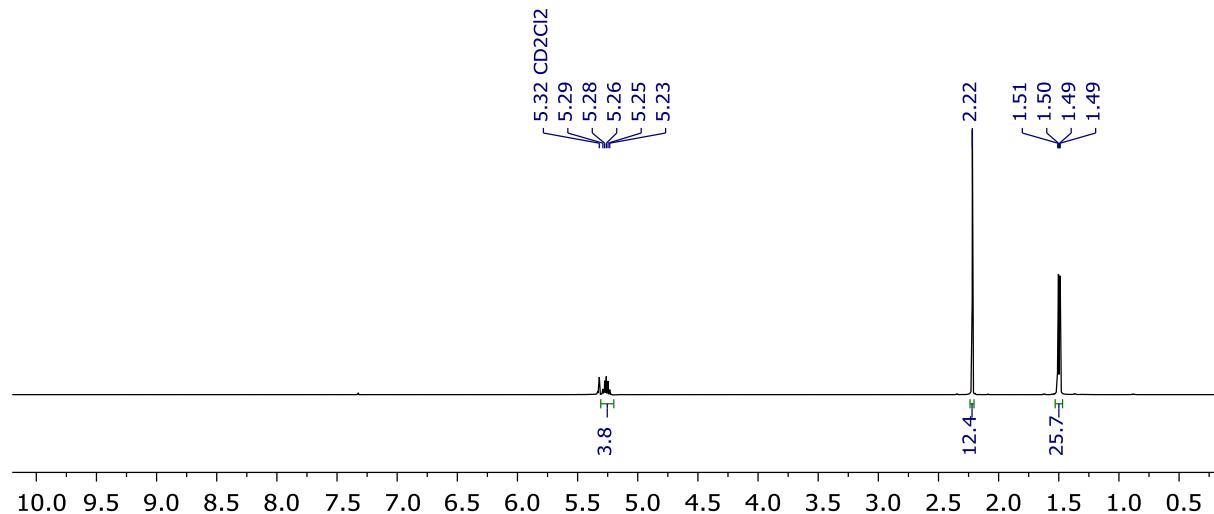


Figure SI-11: ^1H NMR spectrum of **3b** (CD_2Cl_2 , 500 MHz)

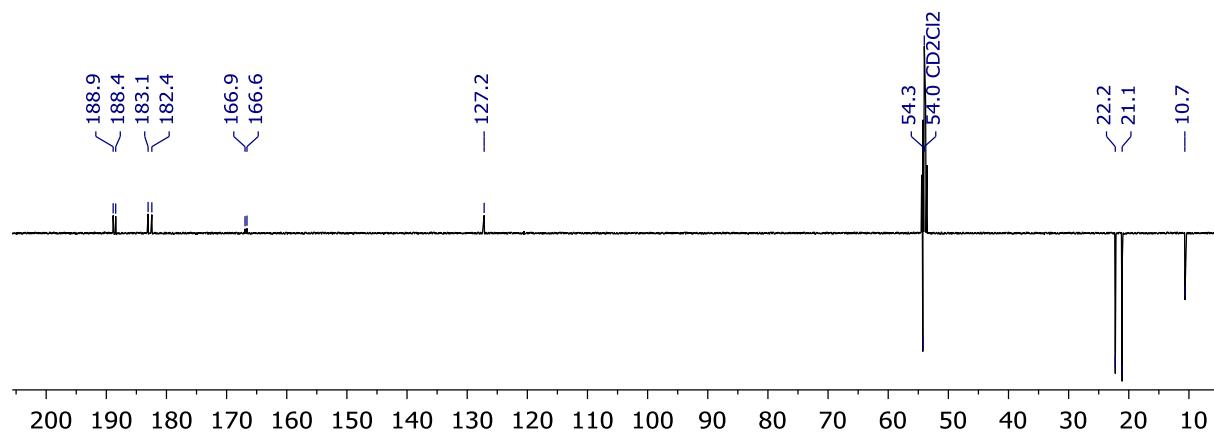


Figure SI-12: $^{13}\text{C}\{^1\text{H}\}$ APT NMR spectrum of **3b** (CD_2Cl_2 , 126 MHz)

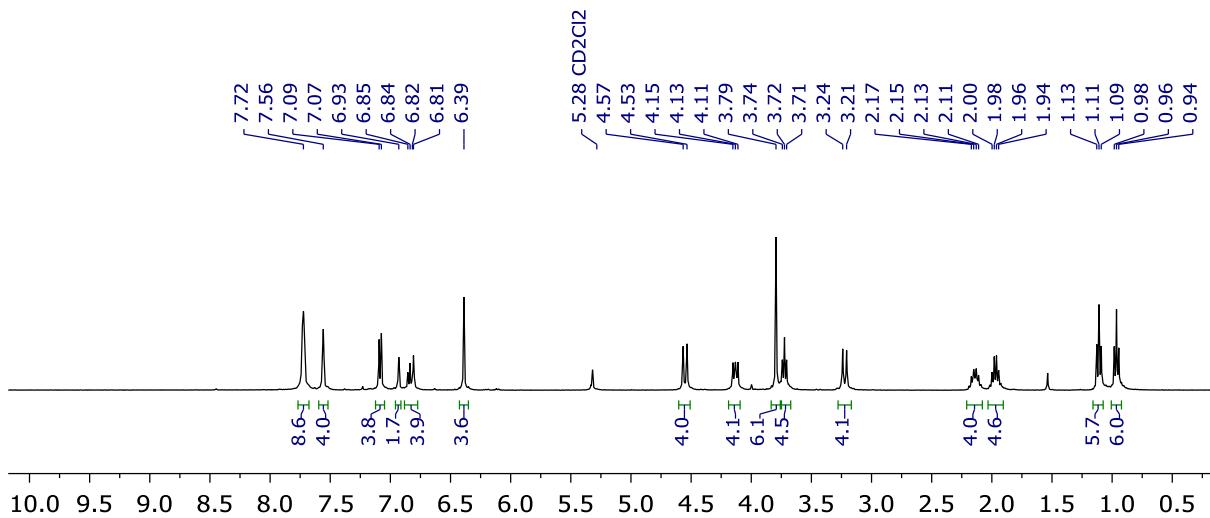


Figure SI-13: ^1H NMR spectrum of **4a** (CD_2Cl_2 , 400 MHz)

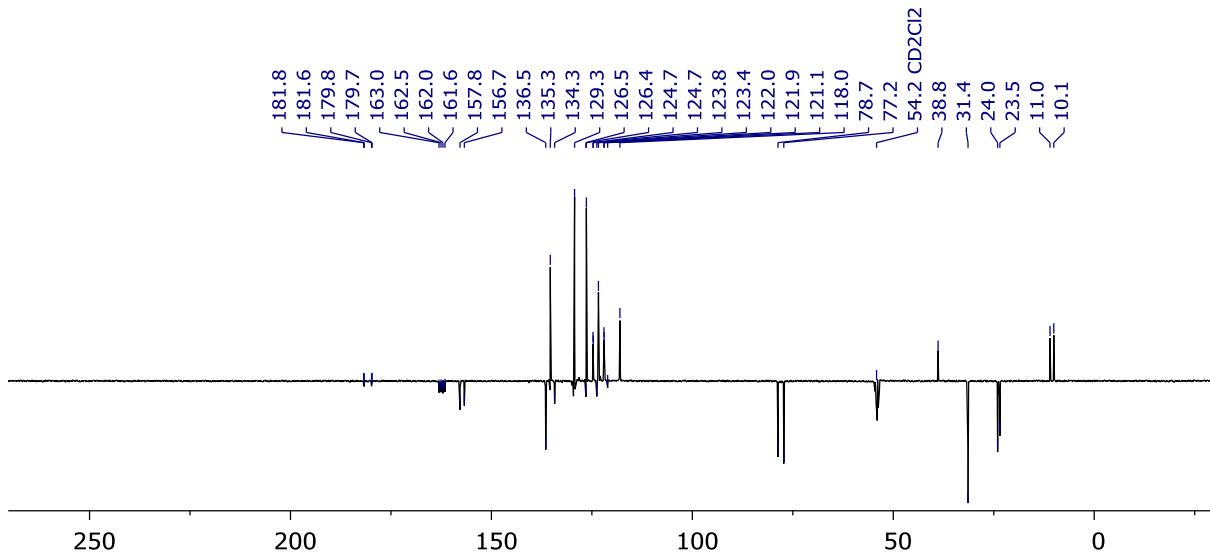


Figure SI-14: $^{13}\text{C}\{^1\text{H}\}$ PENDANT NMR spectrum of **4a** (CD_2Cl_2 , 101 MHz)

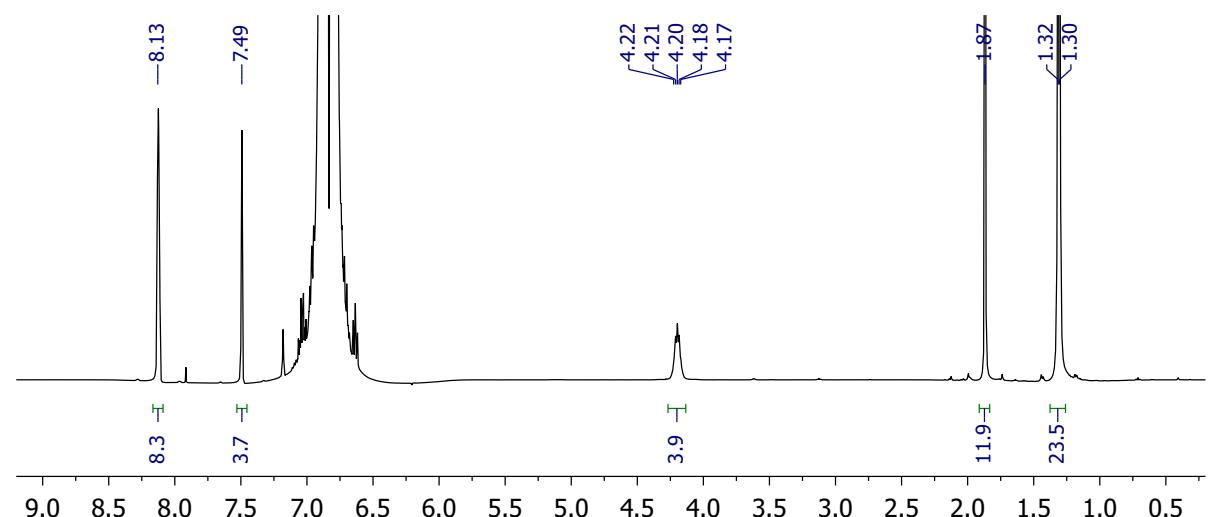


Figure SI-15: ^1H NMR spectrum of **4b** ($1,2\text{-C}_6\text{H}_4\text{F}_2$, 500 MHz)

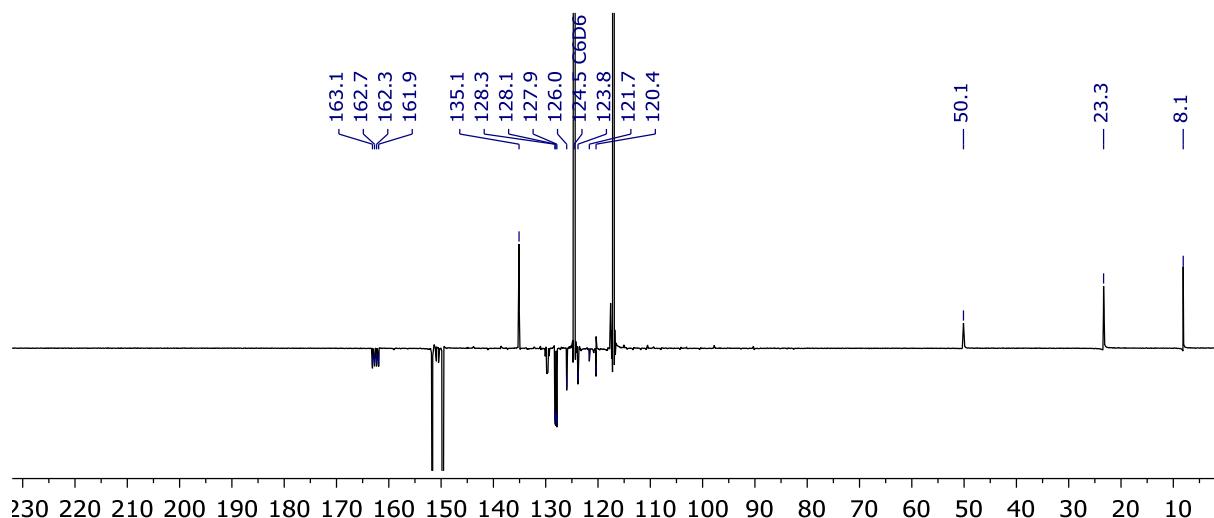


Figure SI-16: $^{13}\text{C}\{\text{H}\}$ APT NMR spectrum of **4b** ($1,2\text{-C}_6\text{H}_4\text{F}_2$, 126 MHz)

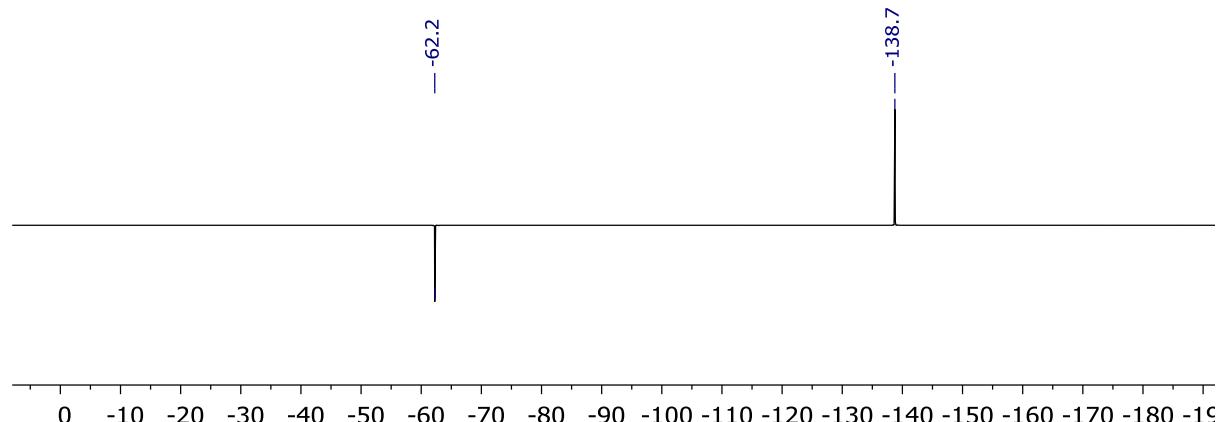


Figure SI-17: $^{19}\text{F}\{\text{H}\}$ NMR spectrum of **4b** ($1,2\text{-C}_6\text{H}_4\text{F}_2$, 282 MHz)

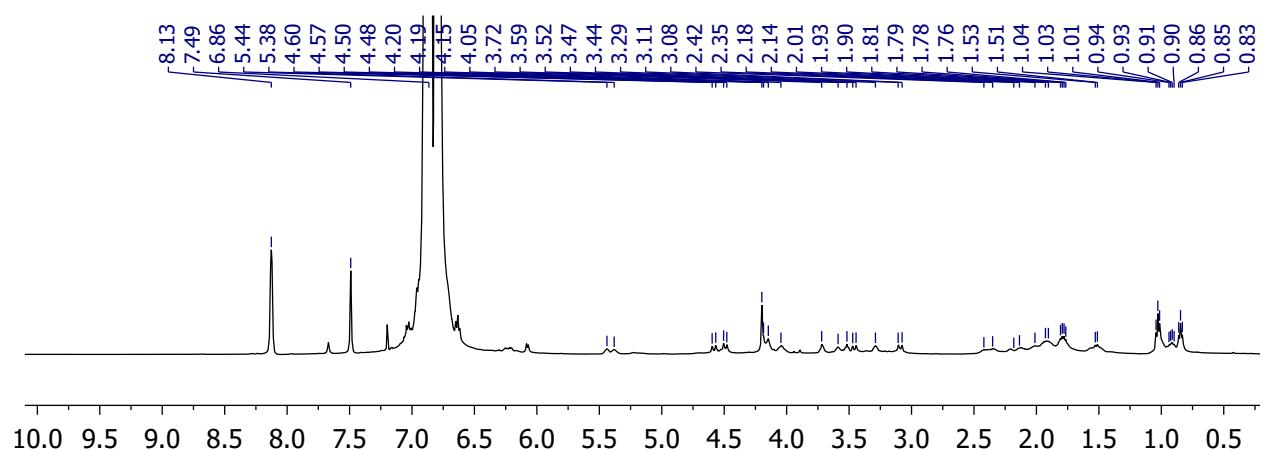


Figure SI-18: ^1H NMR spectrum of crude **5a** ($1,2\text{-C}_6\text{H}_4\text{F}_2$, 500 MHz)

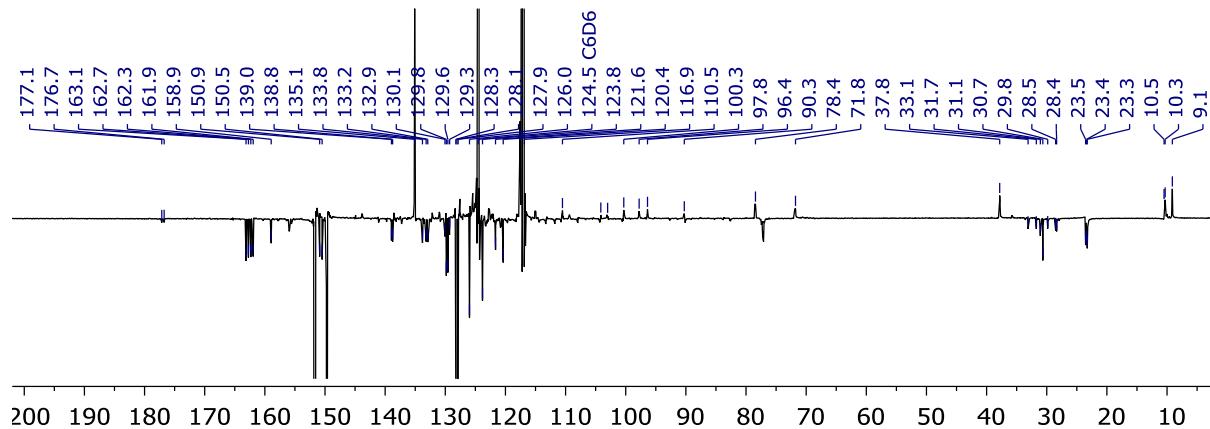


Figure SI-19: $^{13}\text{C}\{\text{H}\}$ APT NMR of crude **5a** ($1,2\text{-C}_6\text{H}_4\text{F}_2$, 126 MHz)

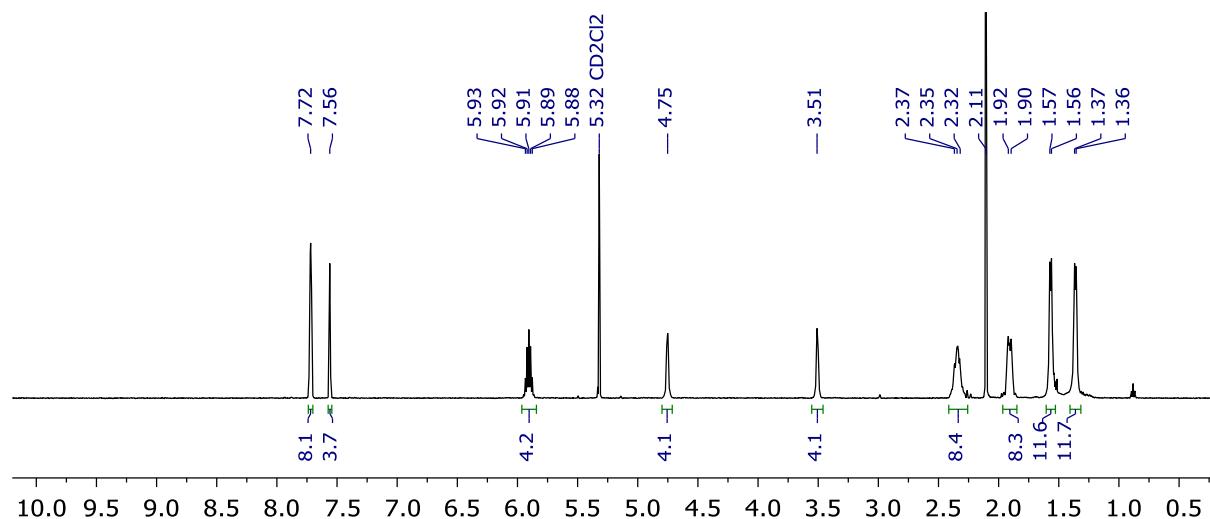


Figure SI-20: ^1H NMR spectrum of **5b** (CD_2Cl_2 , 500 MHz)

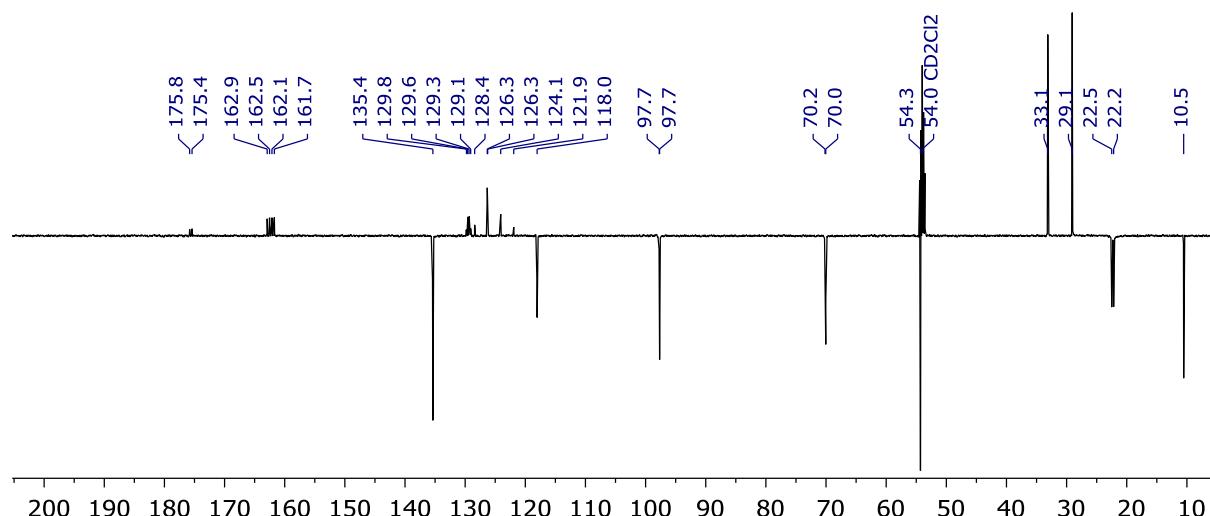


Figure SI-21: $^{13}\text{C}\{\text{H}\}$ APT NMR spectrum of **5b** (CD_2Cl_2 , 126 MHz)

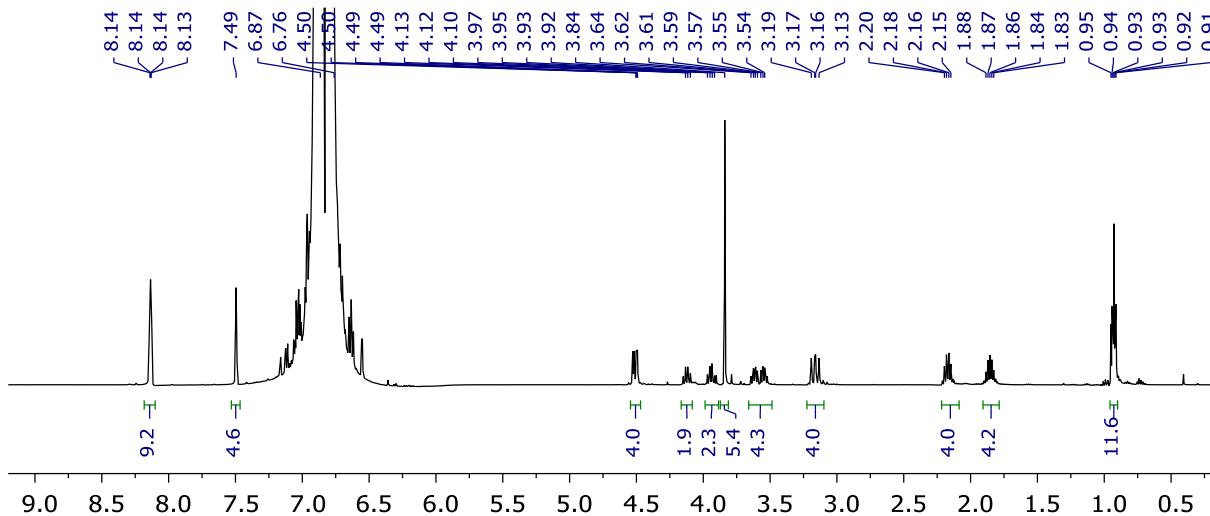


Figure SI-22: ^1H NMR spectrum of crude **6a** ($1,2\text{-C}_6\text{H}_4\text{F}_2$, 500 MHz)

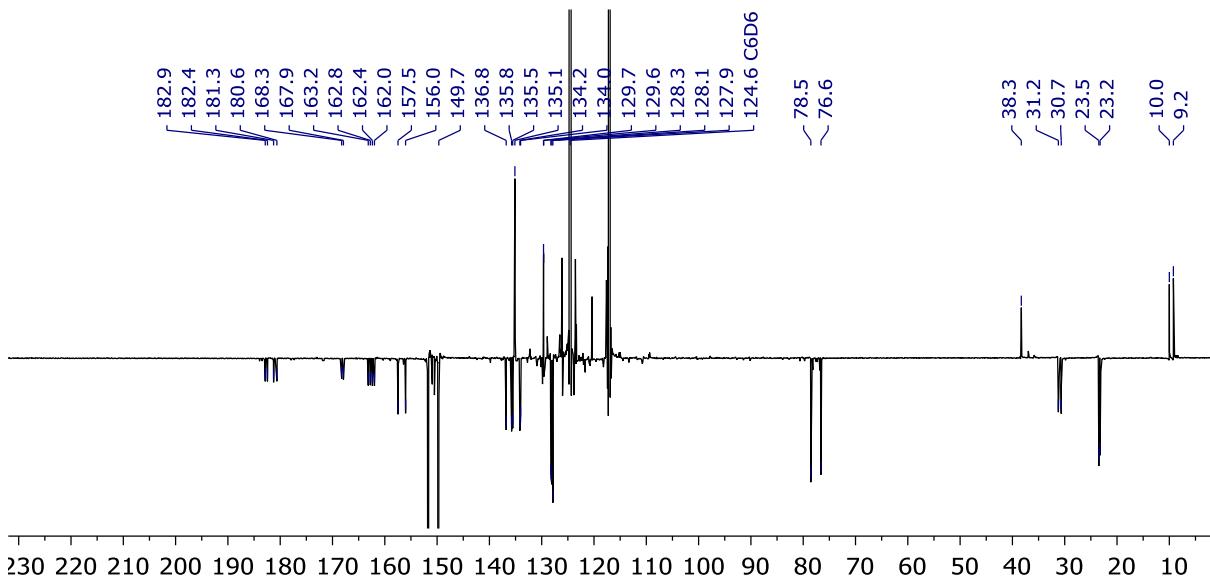


Figure SI-23: $^{13}\text{C}\{^1\text{H}\}$ APT NMR spectrum of crude **6a** ($1,2\text{-C}_6\text{H}_4\text{F}_2$, 126 MHz)

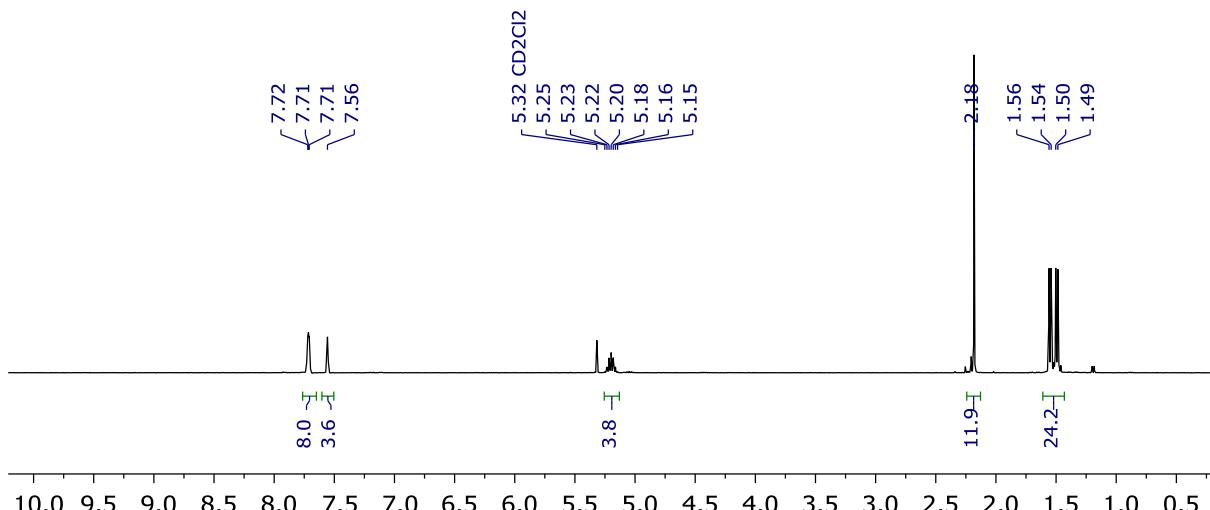


Figure SI-24: ^1H NMR spectrum of **6b** (CD_2Cl_2 , 400 MHz)

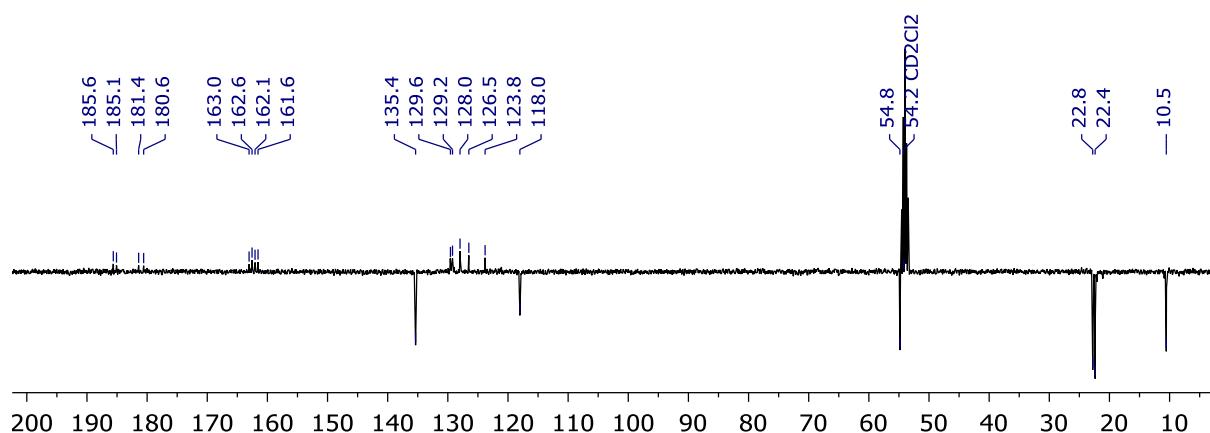


Figure SI-25: $^{13}\text{C}\{^1\text{H}\}$ PENDANT NMR spectrum **6b** (CD_2Cl_2 , 101 MHz)

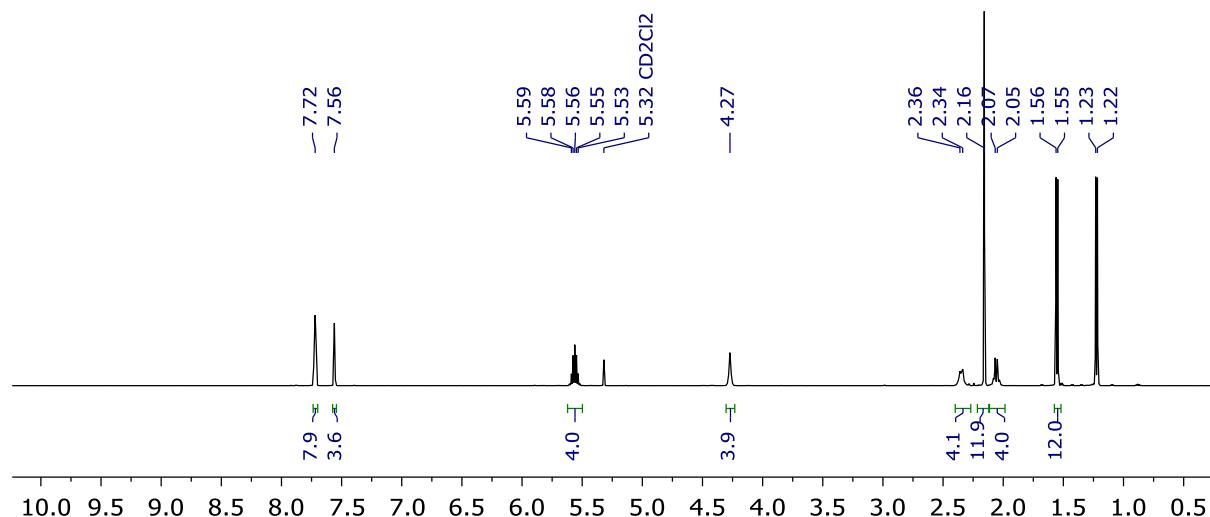


Figure S1-26: ^1H NMR spectrum of **7** (CD_2Cl_2 , 500 MHz)

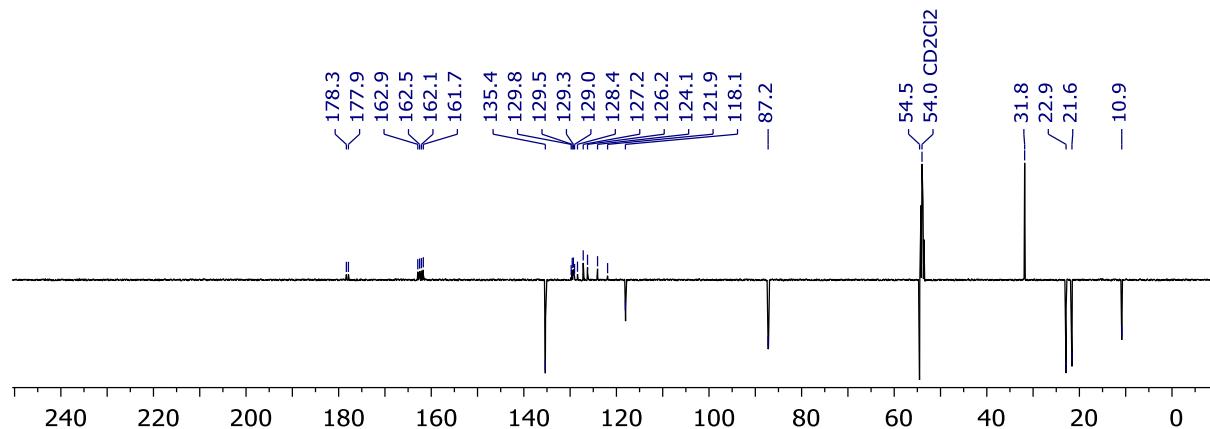


Figure SI-27: $^{13}\text{C}\{^1\text{H}\}$ APT NMR spectrum of **7** (CD_2Cl_2 , 126 MHz)

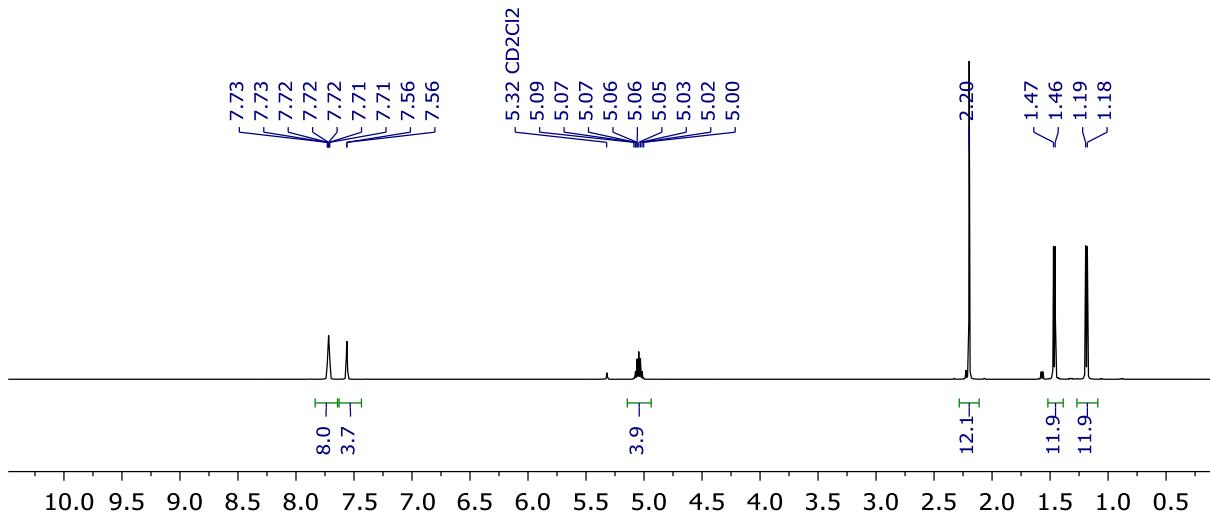


Figure SI-28: ^1H NMR spectrum of **8** (CD_2Cl_2 , 500 MHz)

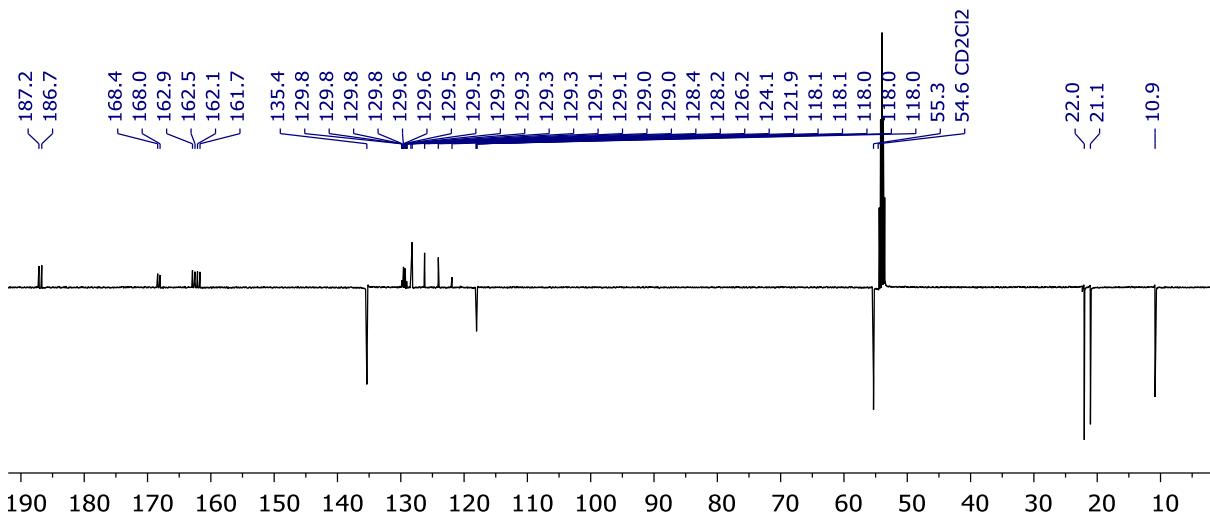


Figure SI-29: $^{13}\text{C}\{^1\text{H}\}$ APT NMR spectrum of **8** (CD_2Cl_2 , 126 MHz)

2. IR spectra of new carbonyl complexes

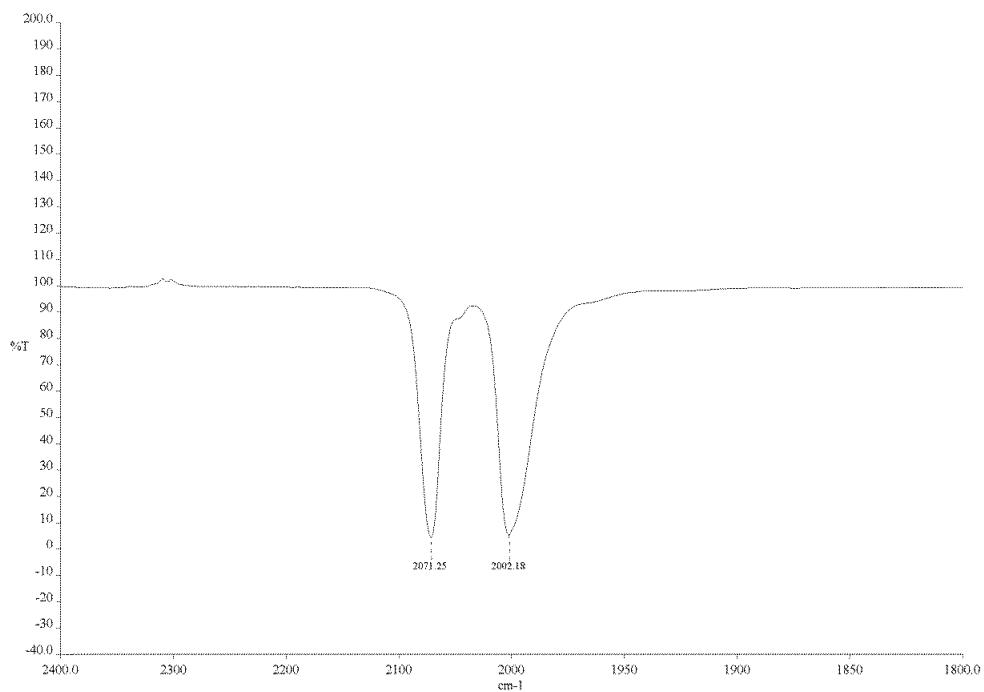


Figure SI-30: IR spectrum of **3a** (CH_2Cl_2)

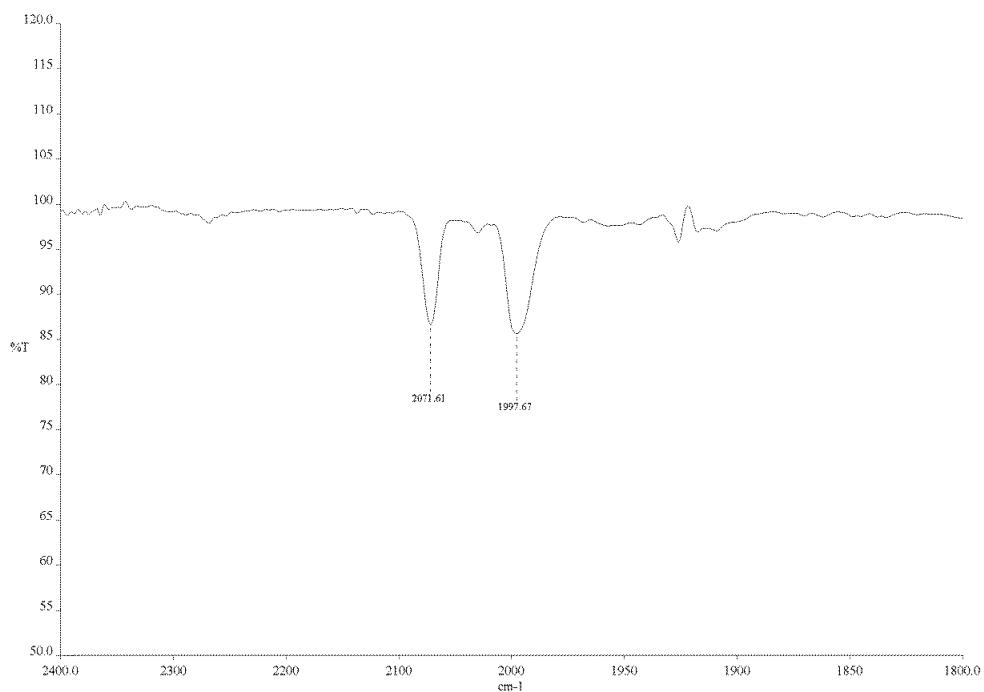


Figure SI-31: IR spectrum of **3b** (CH_2Cl_2)

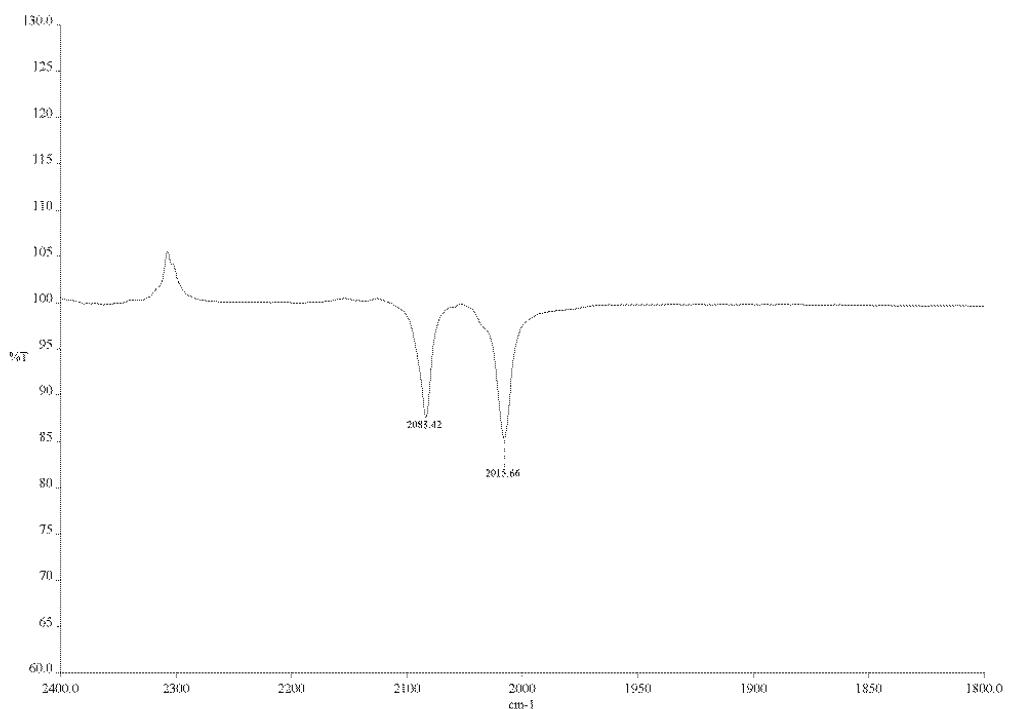


Figure SI-32: IR spectrum of **6a** (CH_2Cl_2)

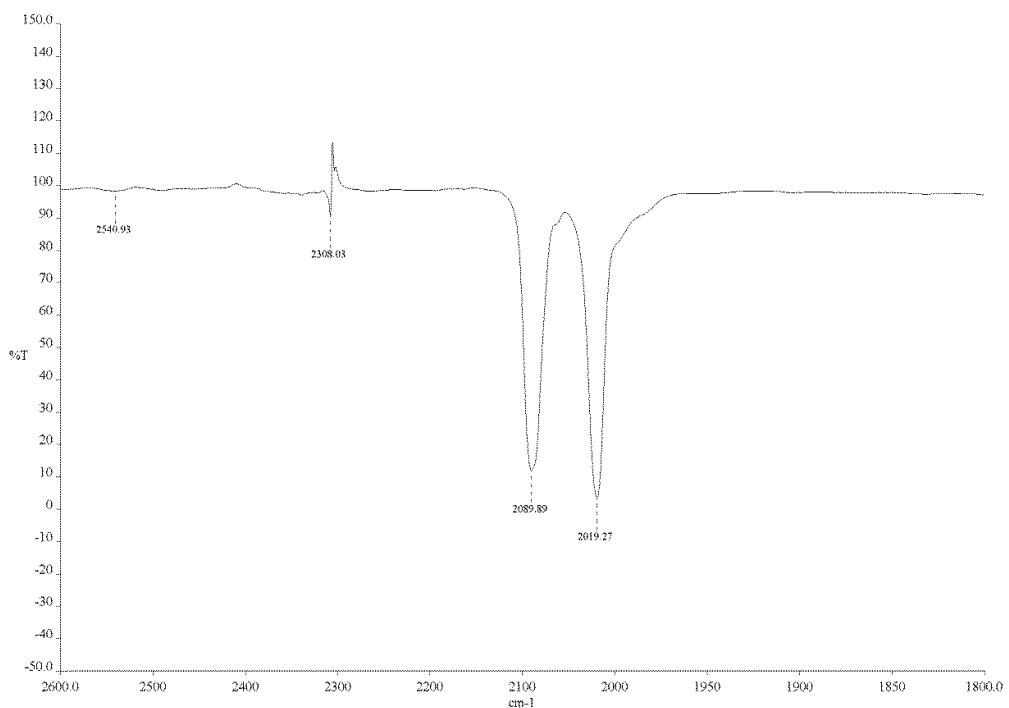


Figure SI-33: IR spectrum of **6b** (CH_2Cl_2)

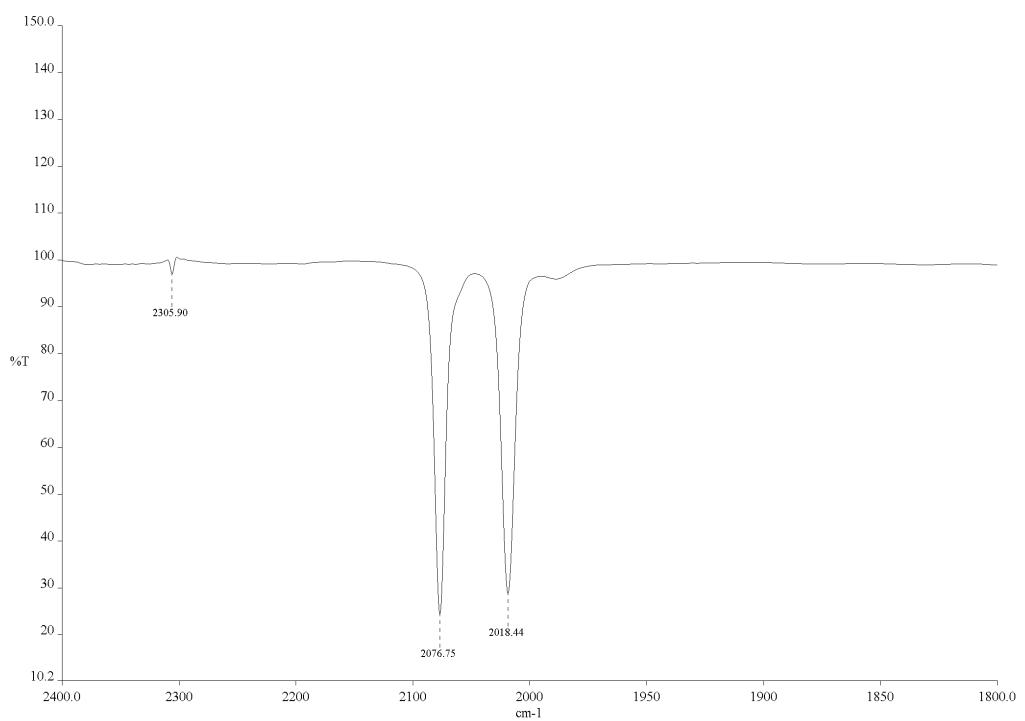


Figure SI-34: IR spectrum of **8** (CH_2Cl_2)

3. ESI-MS of new cationic compounds

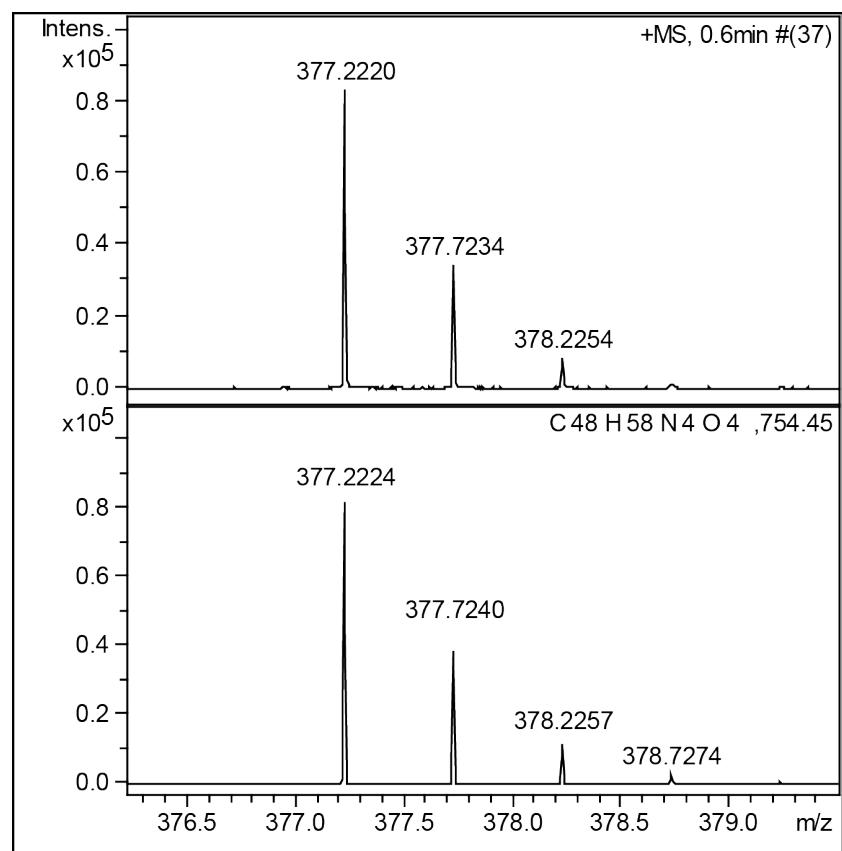


Figure SI-35: ESI-MS of **1.2HI**

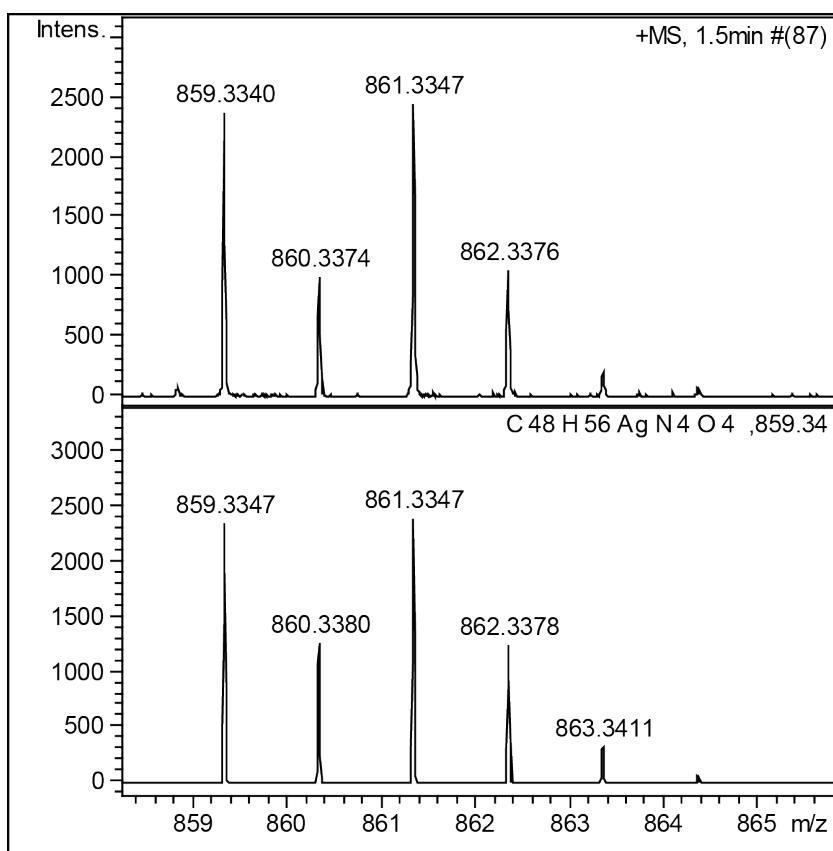


Figure SI-36: ESI-MS of **4a**

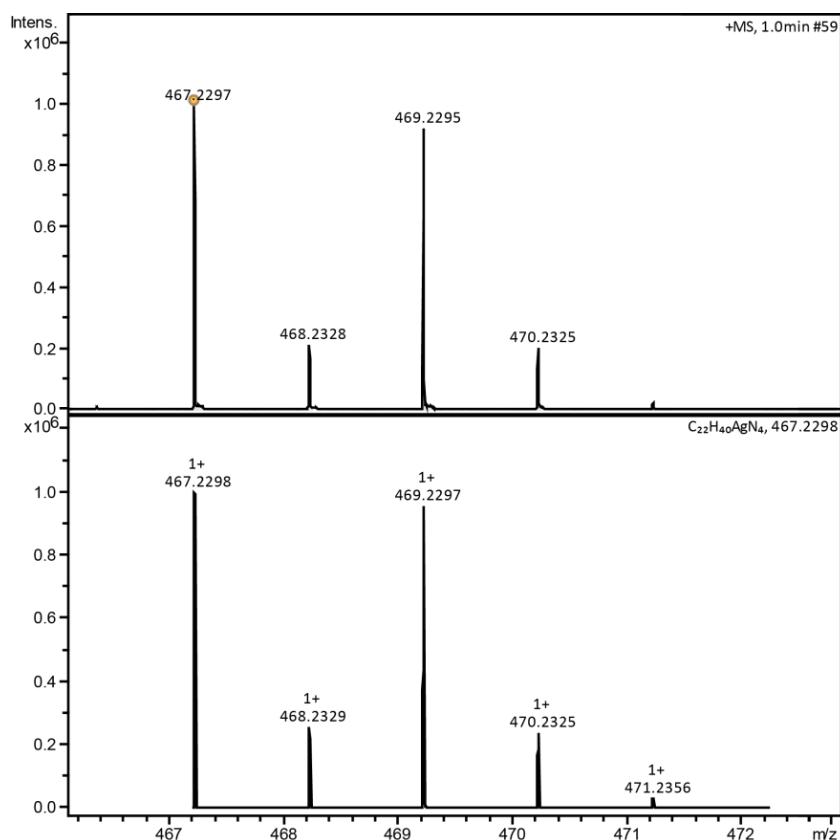


Figure SI-37: ESI-MS of **4b**

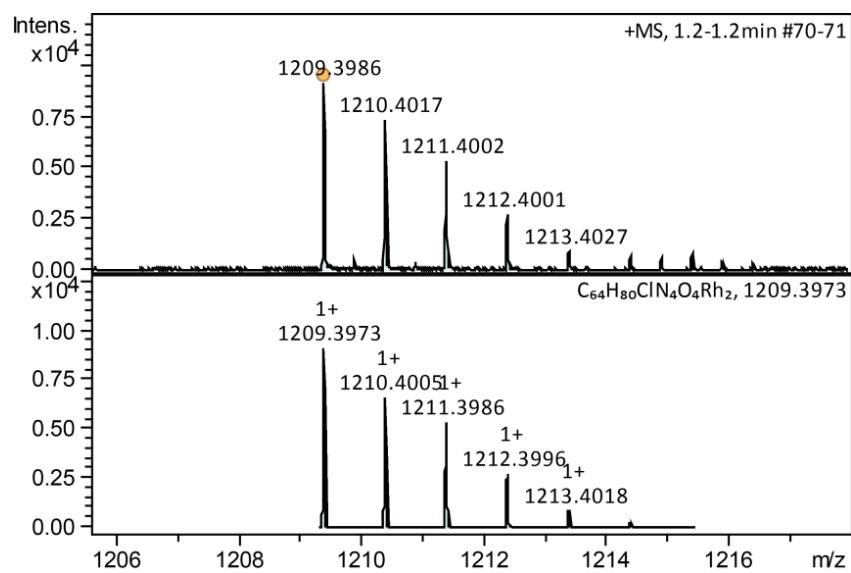


Figure SI-38: ESI-MS of **5a**

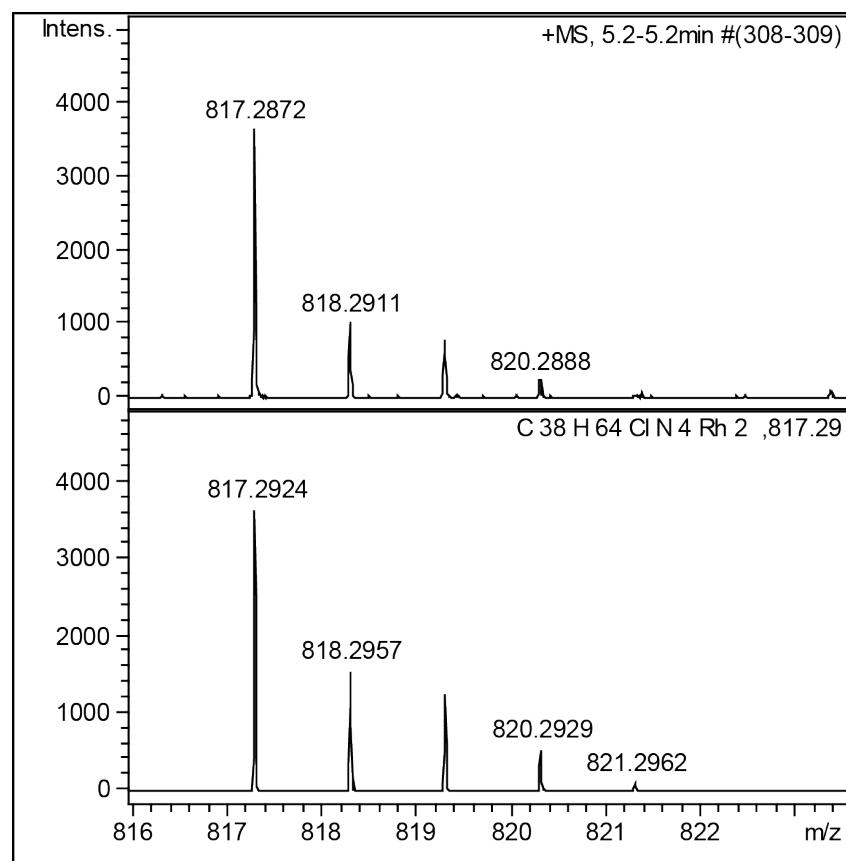


Figure SI-39: ESI-MS of **5b**

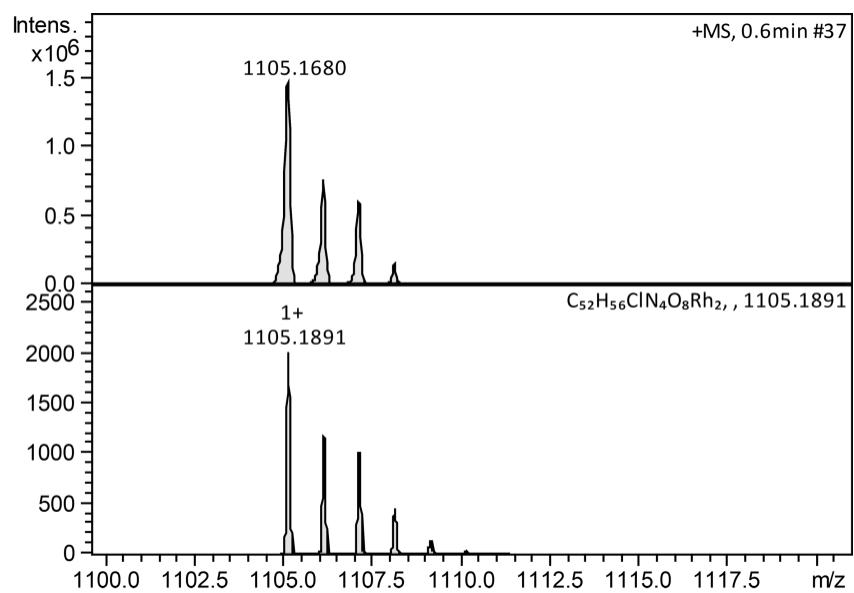


Figure SI-40: ESI-MS of **6a**

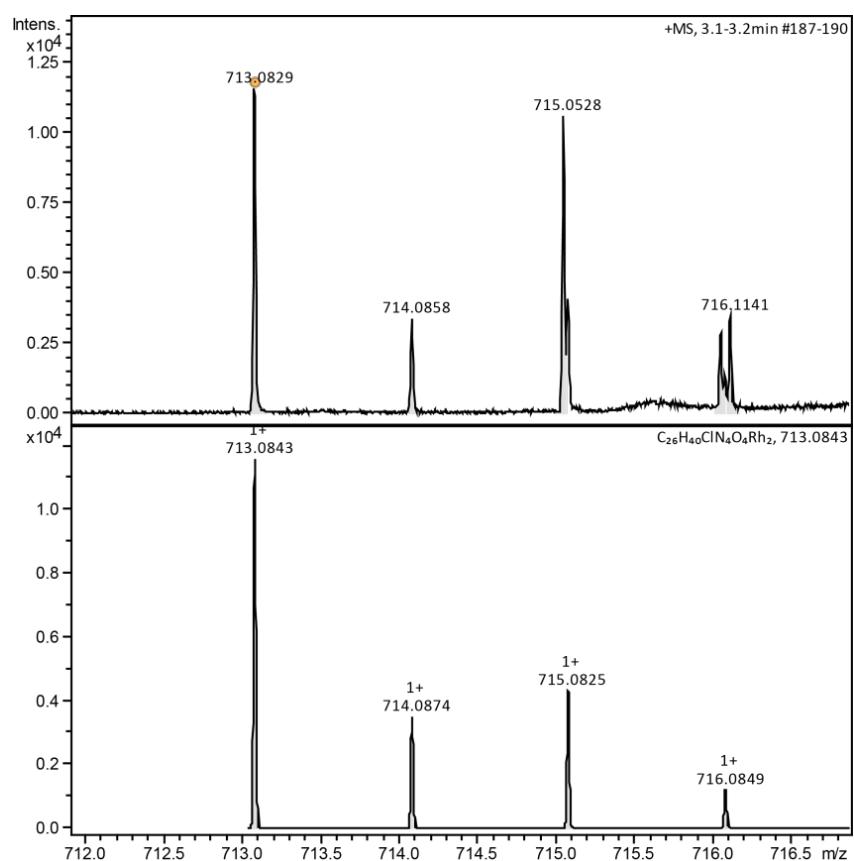


Figure SI-41: ESI-MS of **6b**

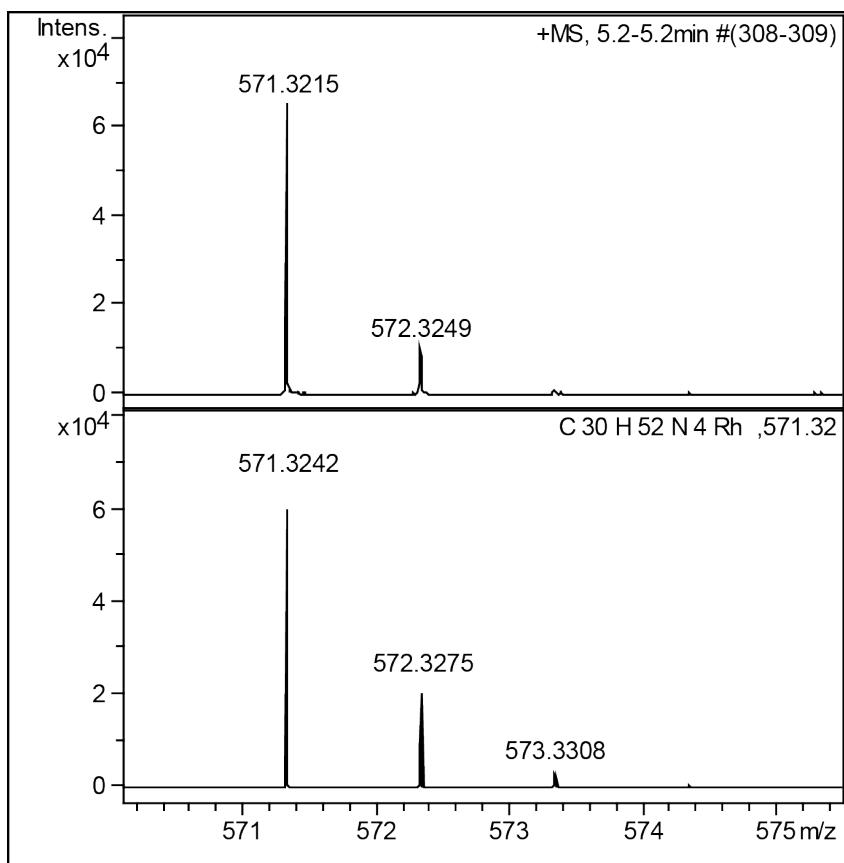


Figure SI-42: ESI-MS of **7**

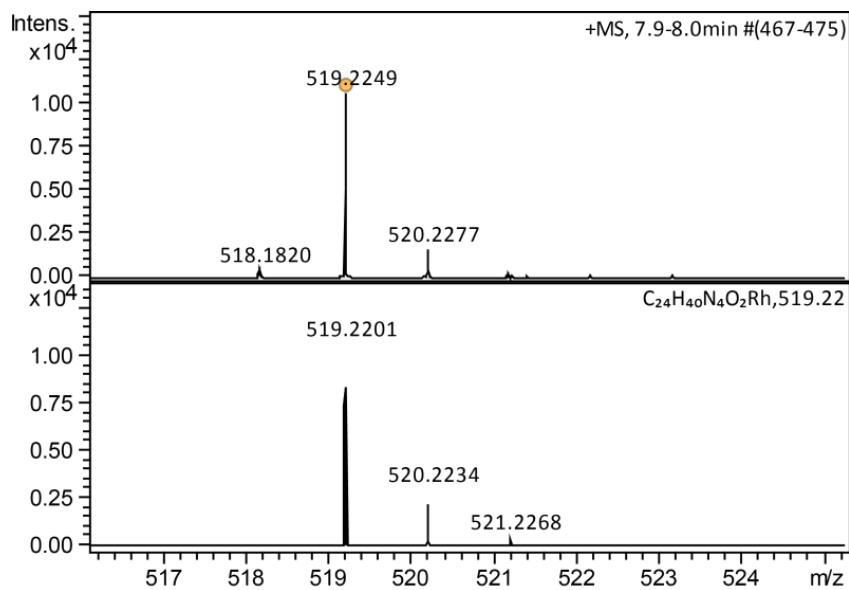


Figure SI-43: ESI-MS of **8**