

Supporting Information for

Copper complexes bearing NHC-calixarene unit: synthesis and application in click chemistry.

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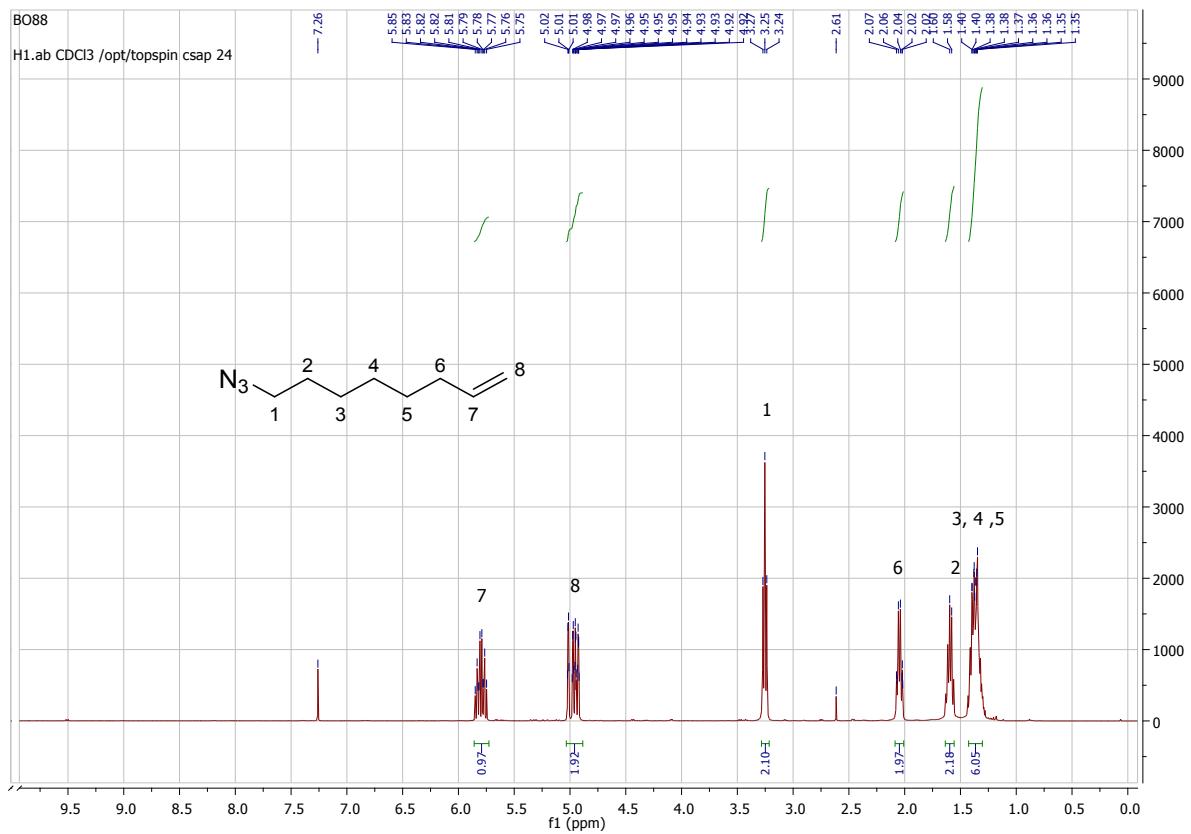


Figure 1: ^1H NMR spectrum of 8-azidoct-1-ene

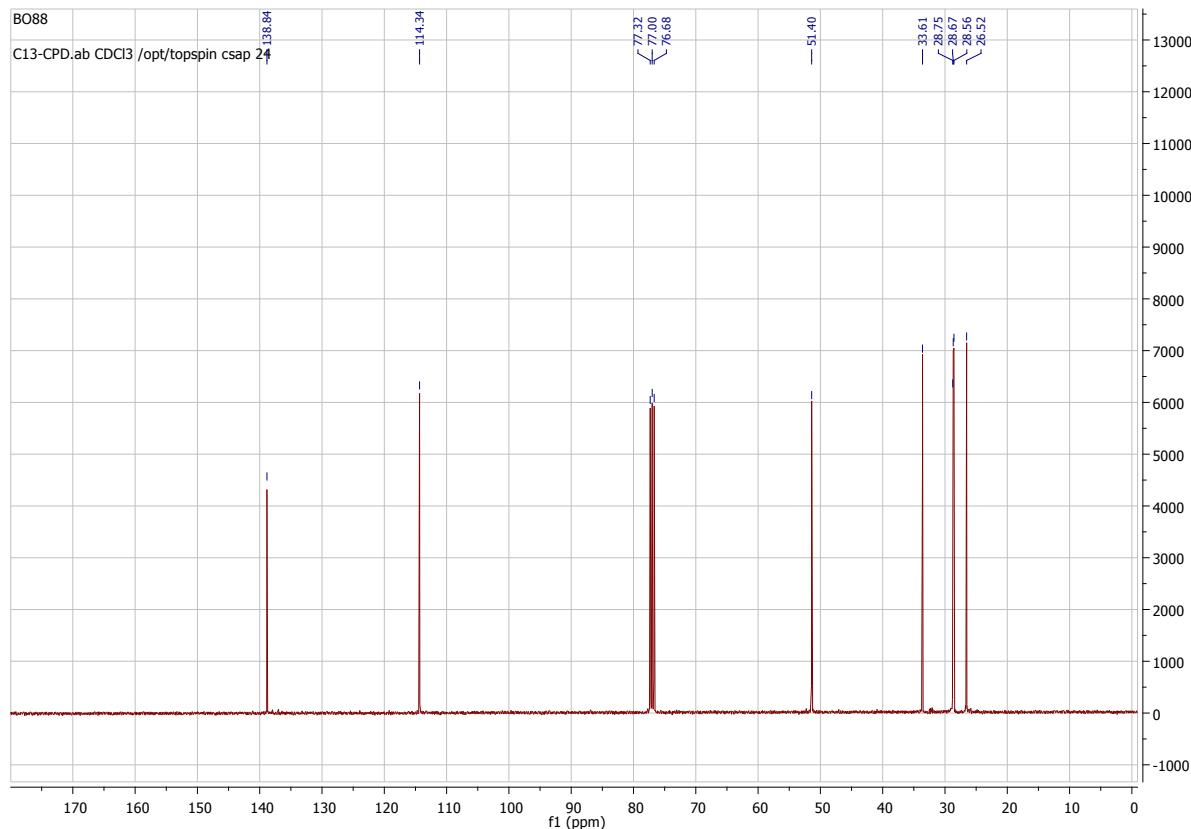


Figure 2: ^{13}C NMR spectrum of 8-azidoct-1-ene

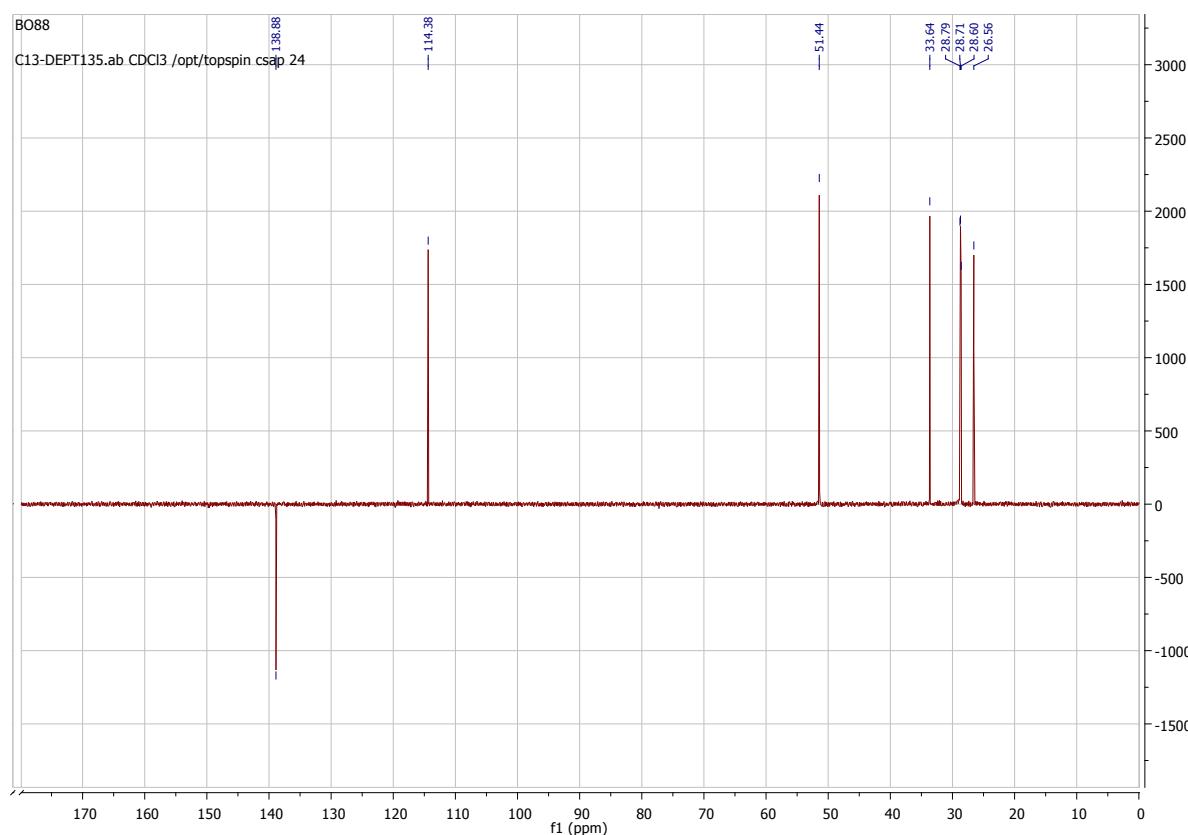


Figure 3: ¹³C DEPT NMR spectrum of 8-azidoct-1-ene

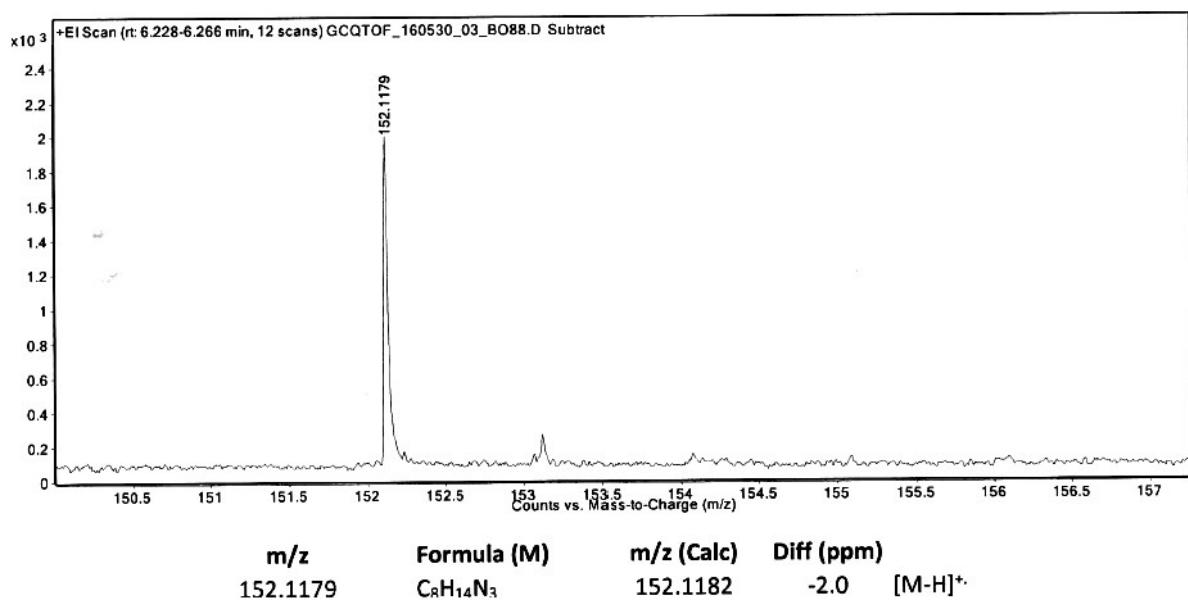


Figure 4: HRMS (GCMS-EI) spectrum of 8-azidoct-1-ene

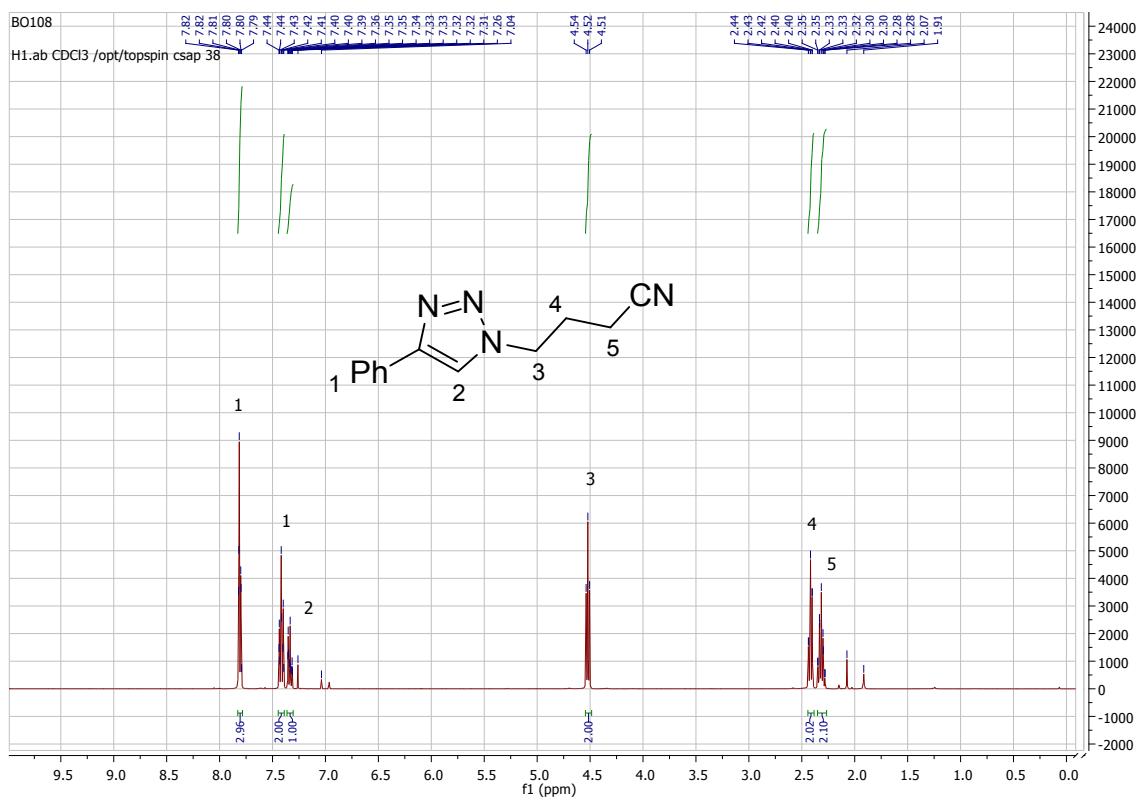


Figure 5: ¹H NMR spectrum of compound 4d

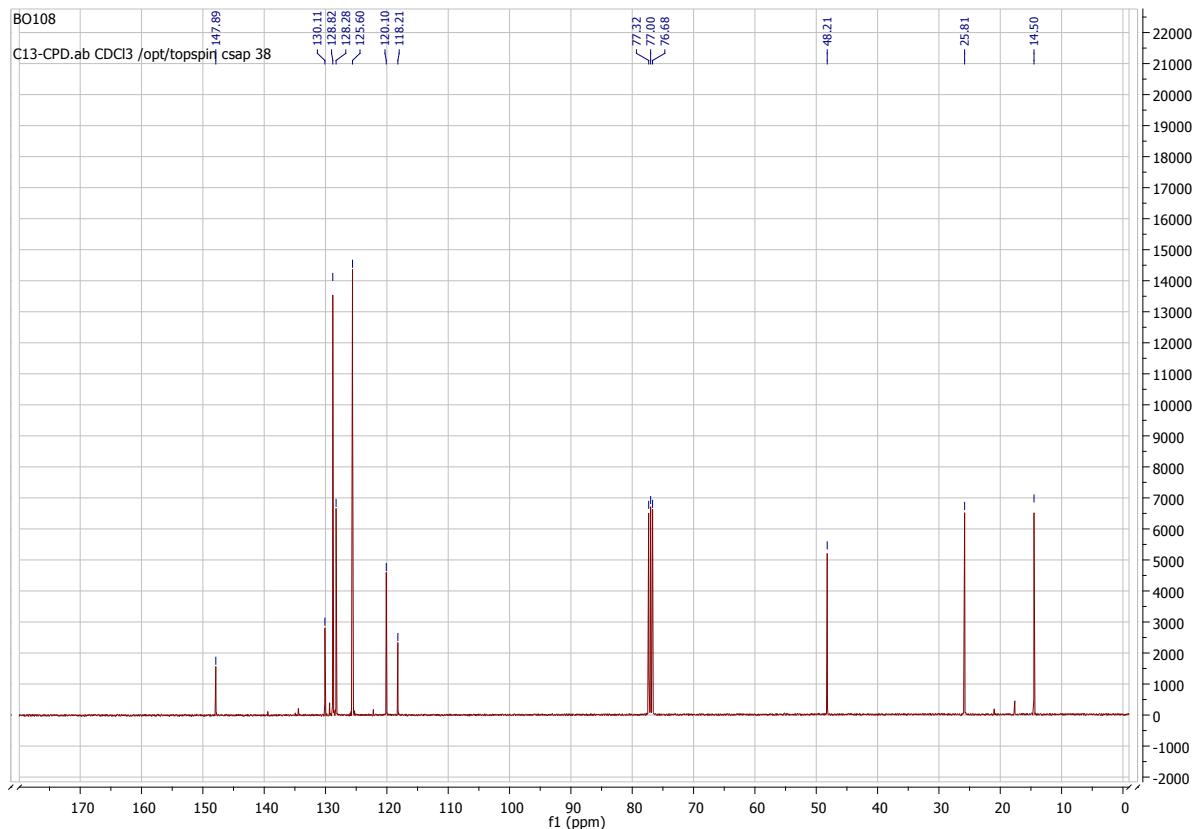


Figure 6: ¹³C NMR spectrum of compound 4d

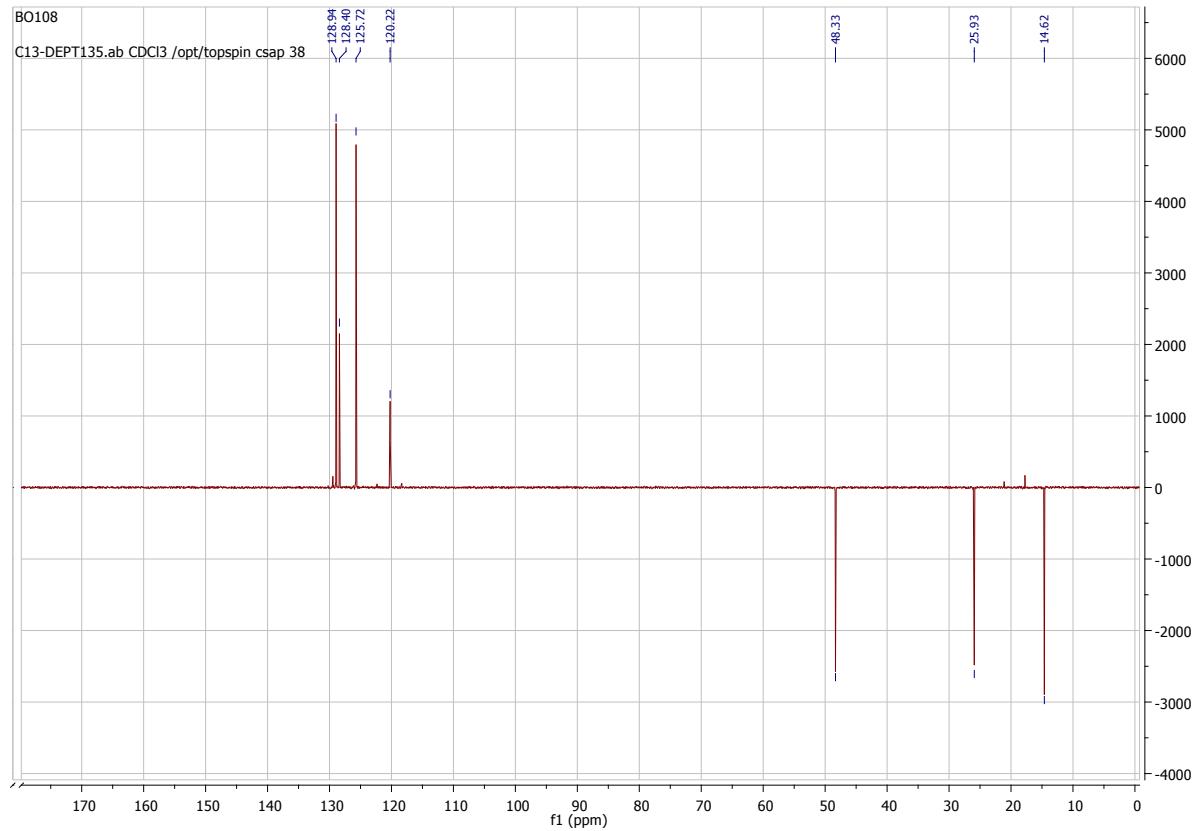


Figure 7: ^{13}C DEPT NMR spectrum of compound 4d

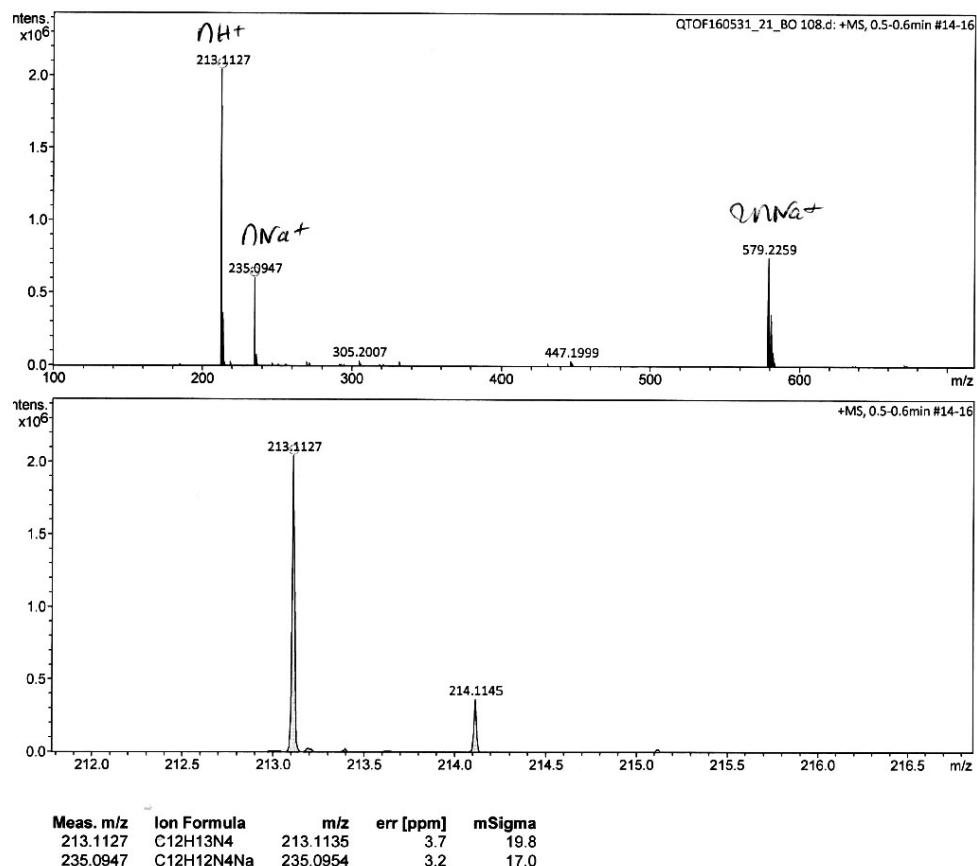


Figure 8: HRMS spectrum of compound 4d

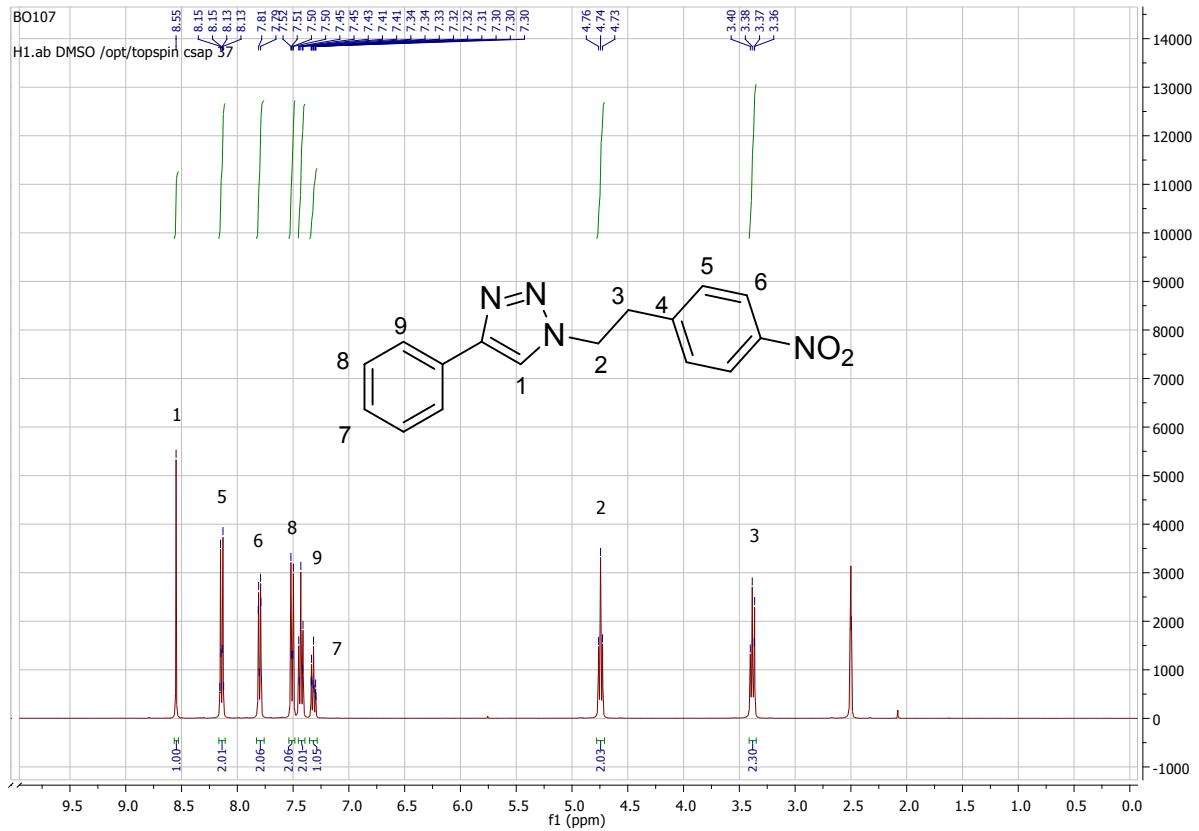


Figure 9: ¹H NMR spectrum of compound 4e

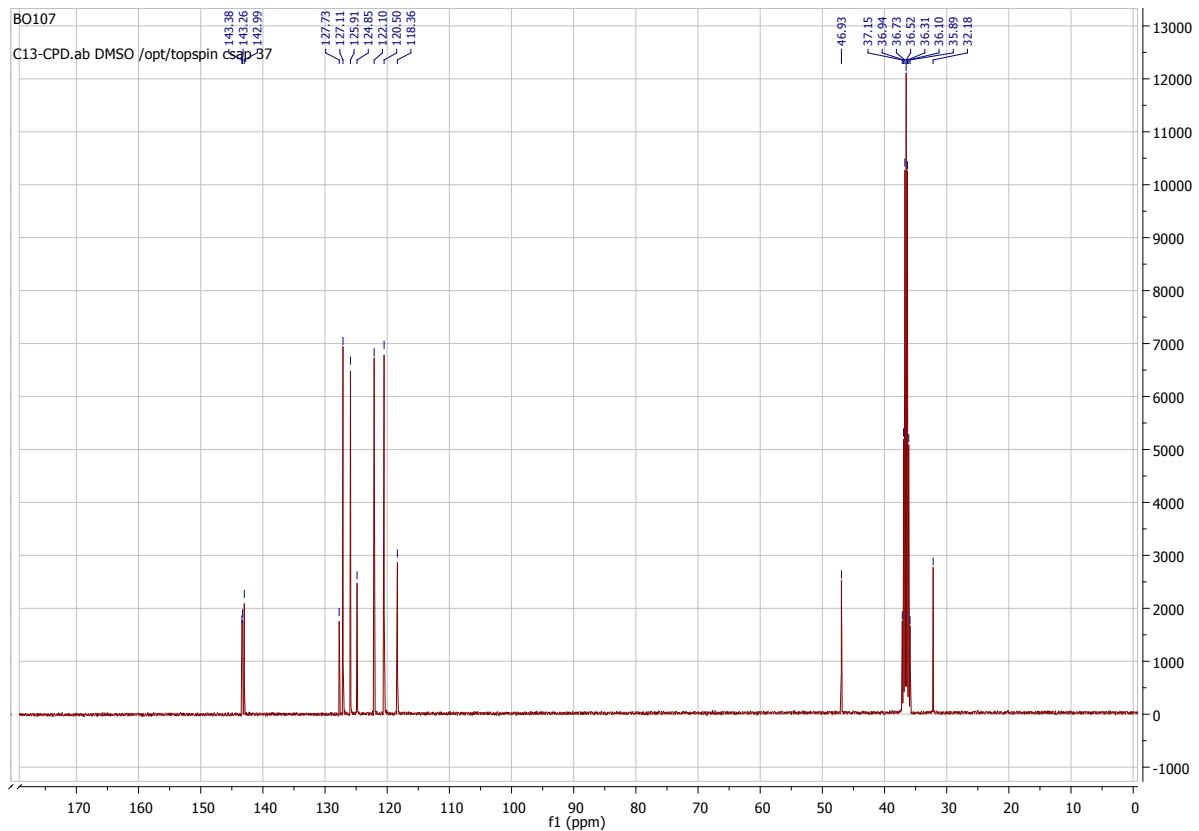


Figure 10: ¹³C NMR spectrum of compound 4e

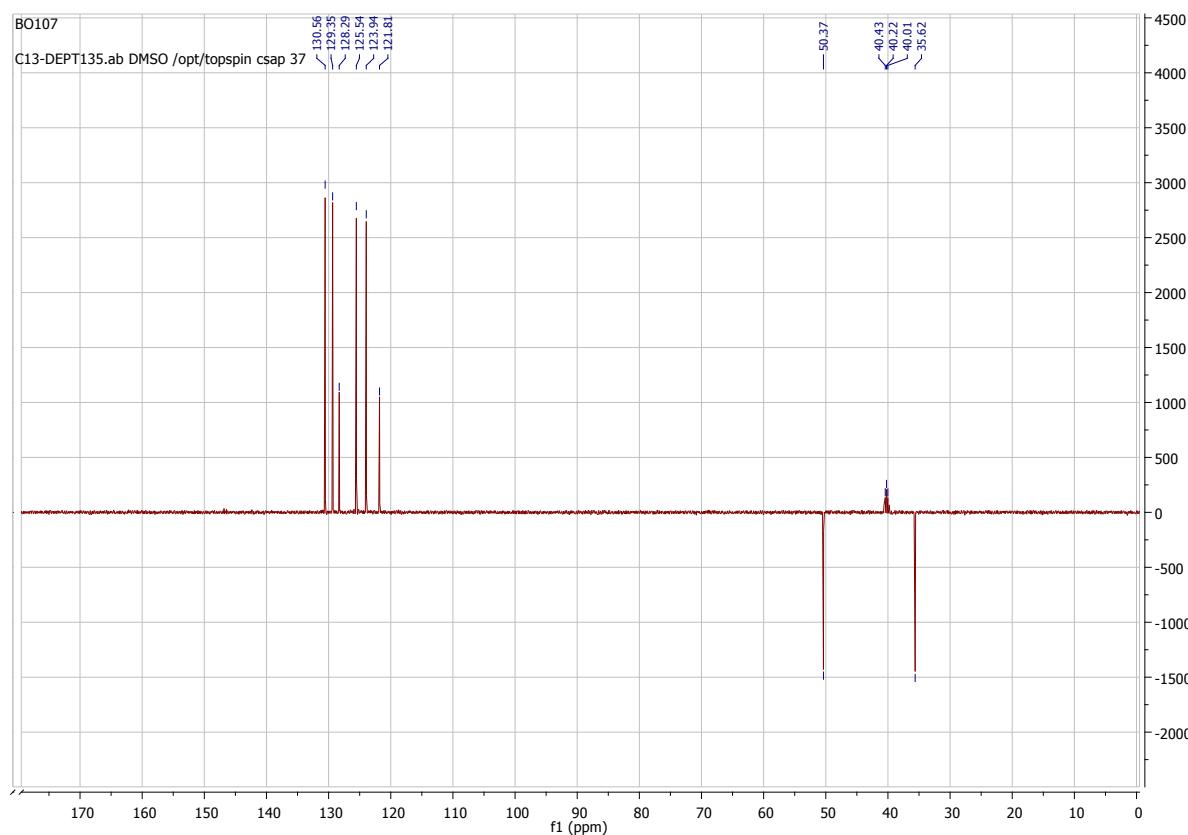


Figure 11: ^{13}C DEPT NMR spectrum of compound **4e**

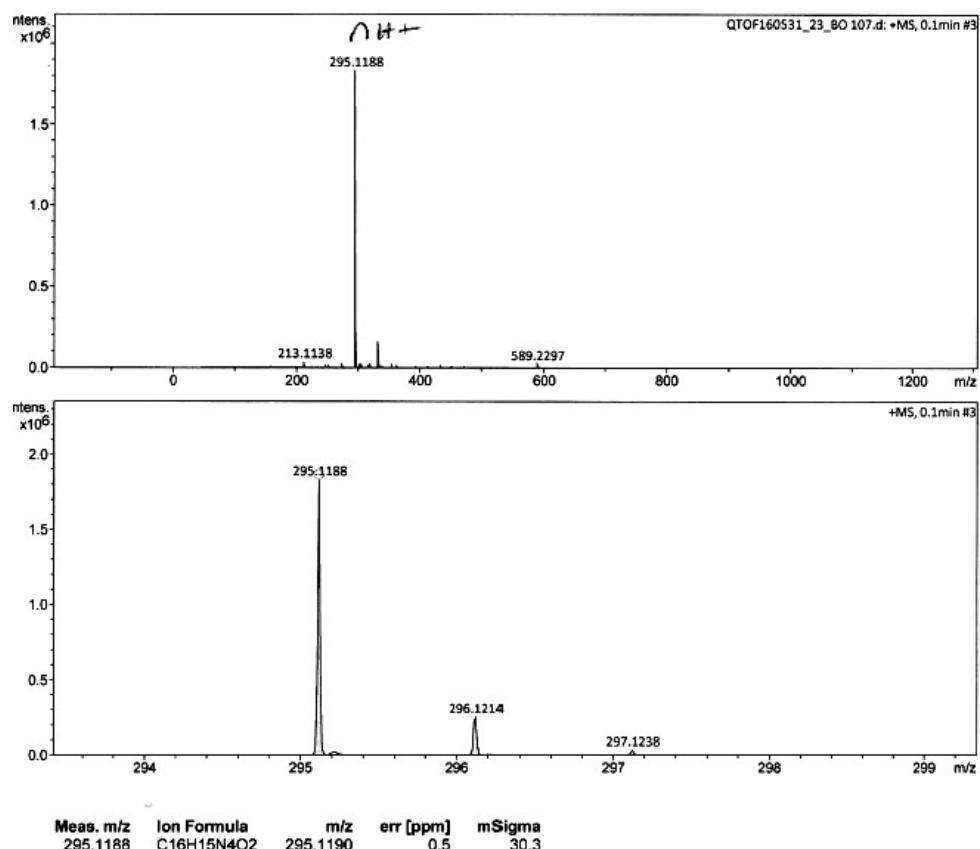


Figure 12: HRMS spectrum of compound **4e**

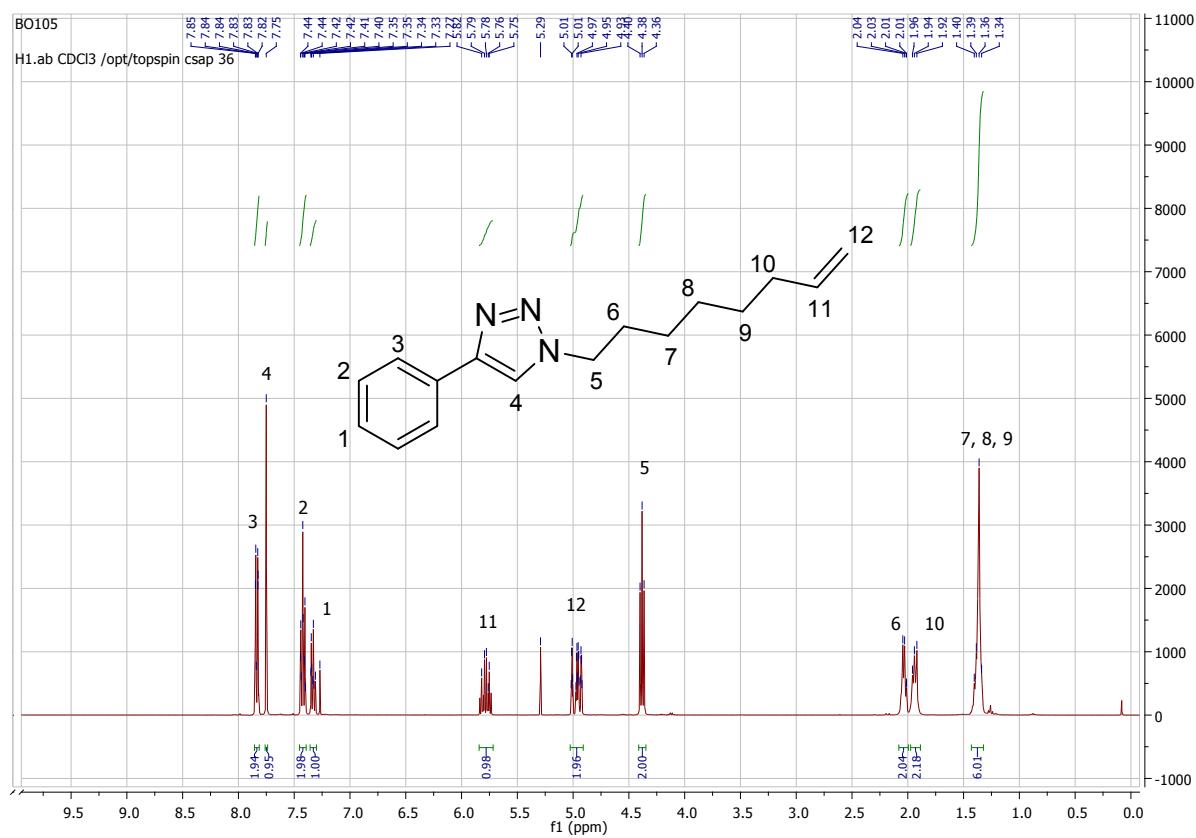


Figure 13: ¹H NMR spectrum of compound 4f

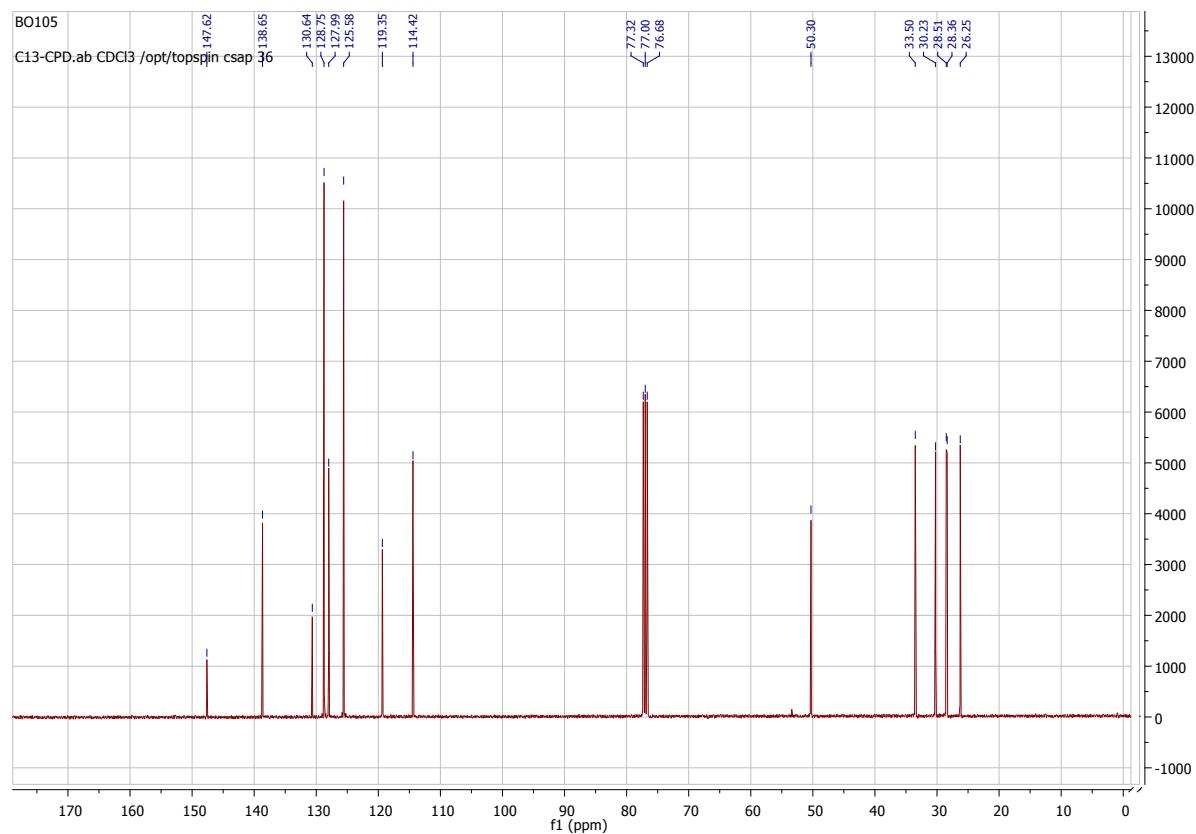


Figure 14: ¹³C NMR spectrum of compound 4f

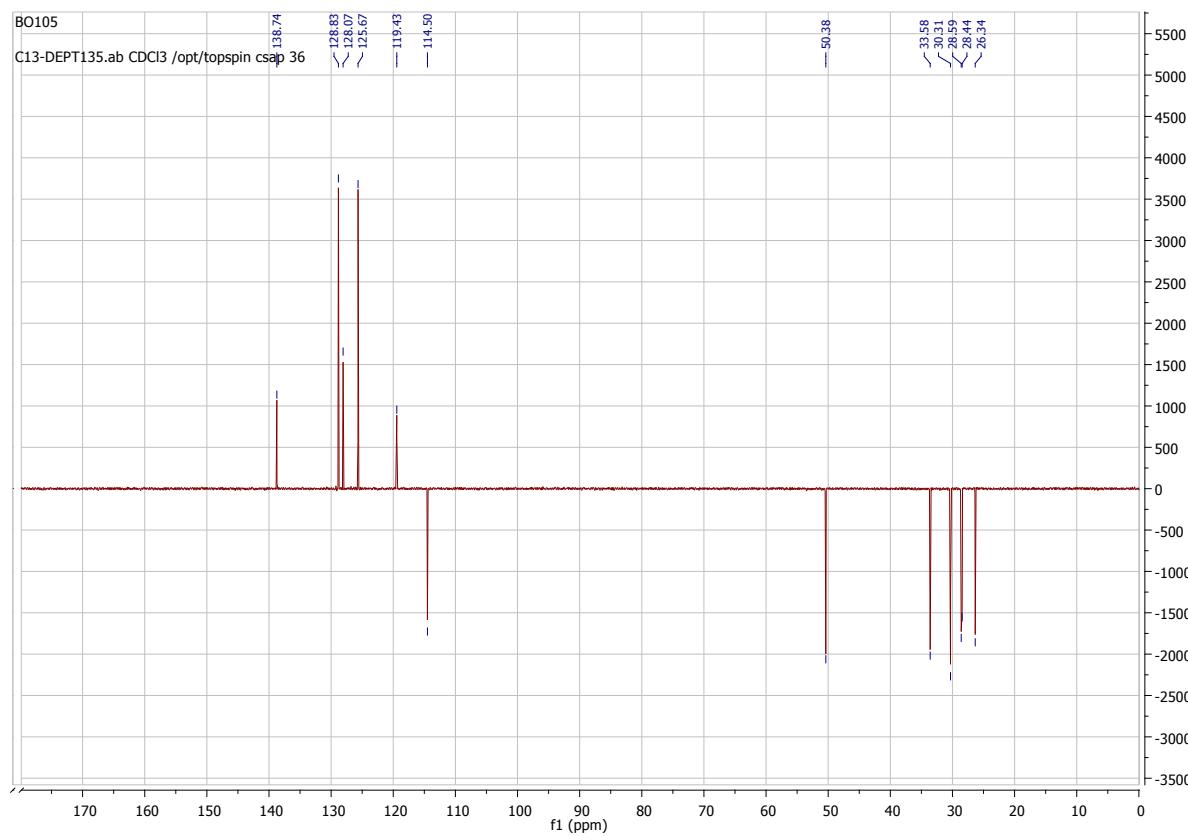


Figure 15: ¹³C DEPT NMR spectrum of compound **4f**

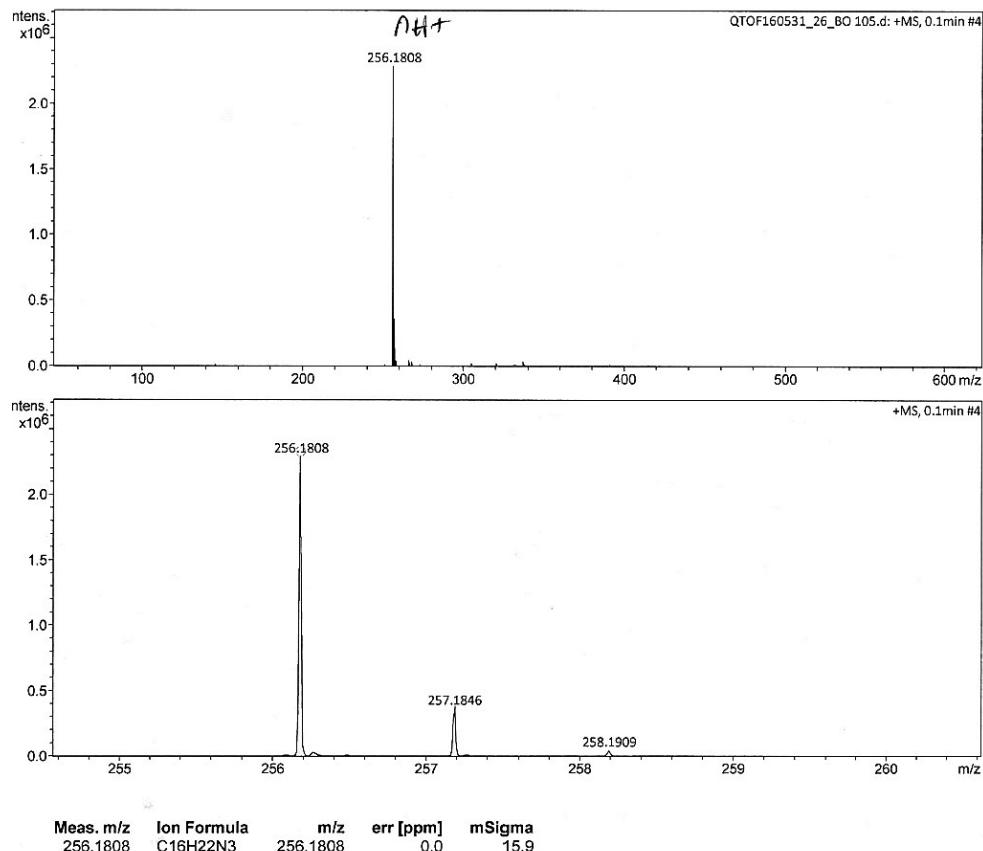


Figure 16: HMRS spectrum of compound **4f**

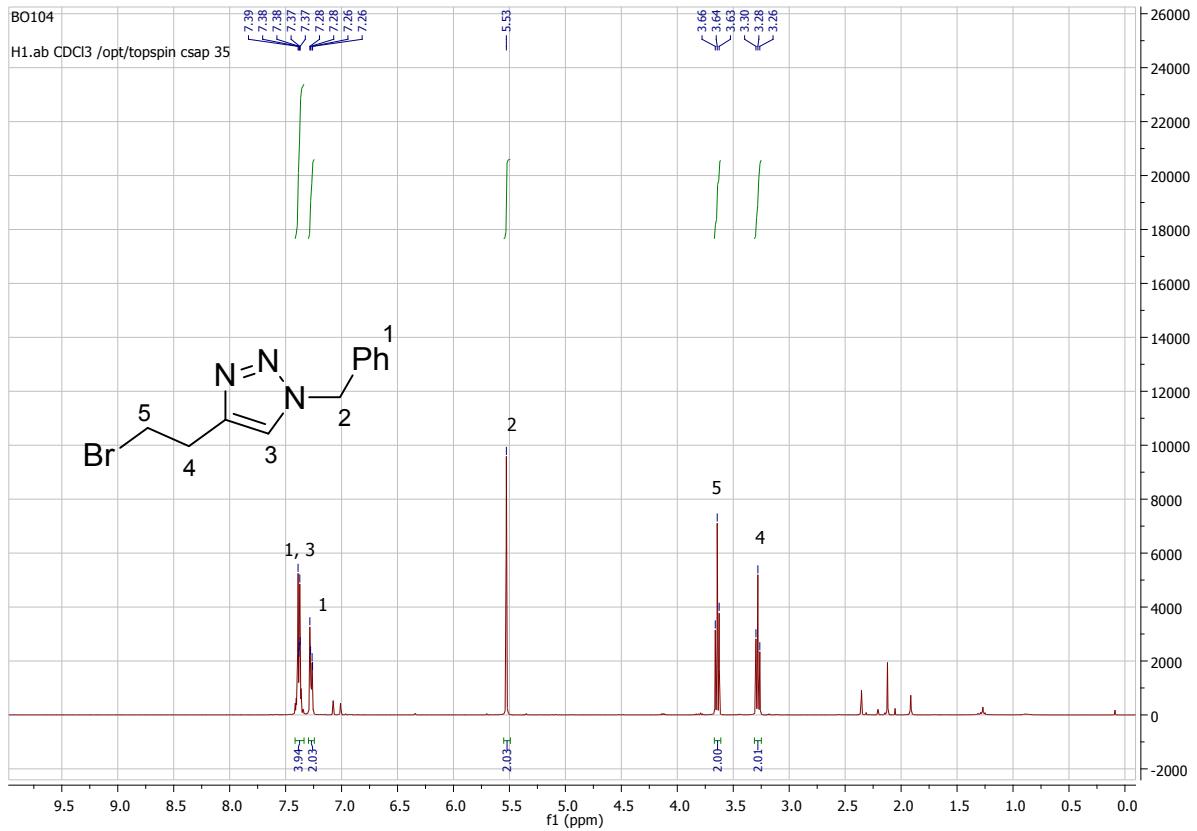


Figure 17: ¹H NMR spectrum of compound 4g

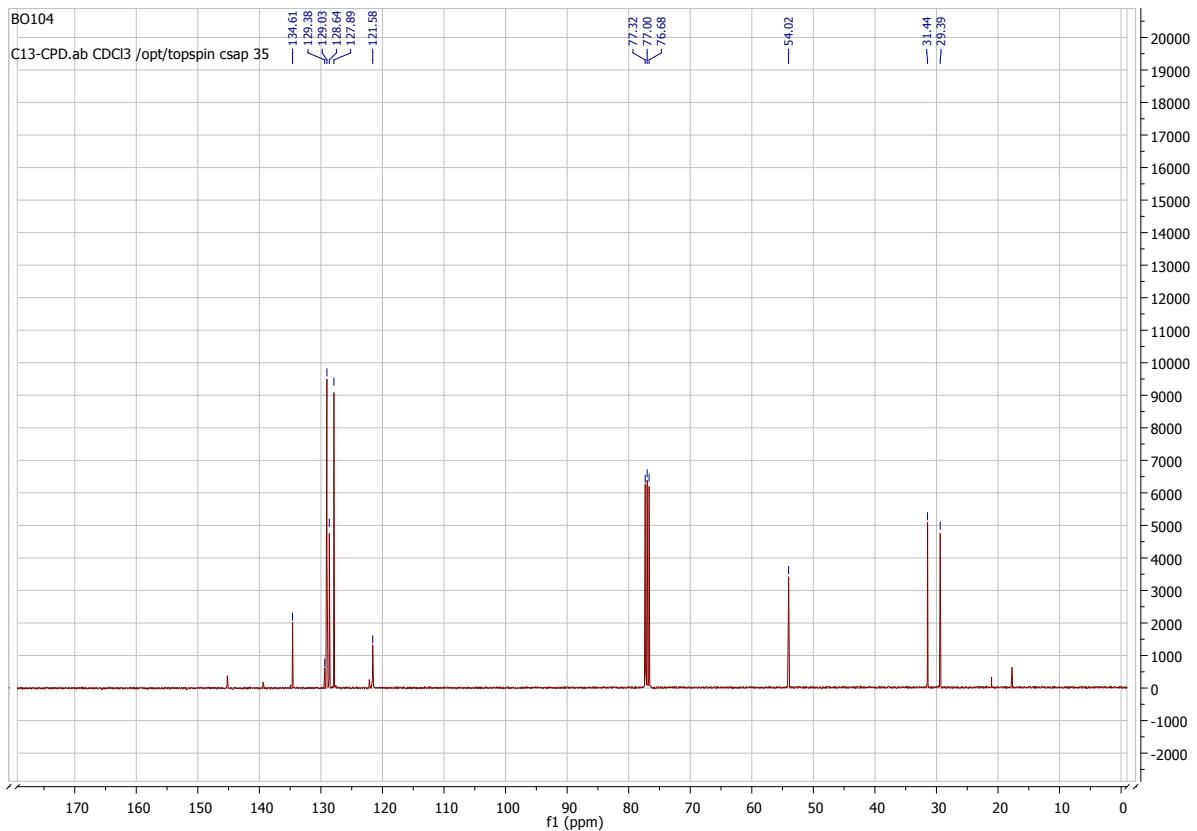


Figure 18: ¹³C NMR spectrum of compound 4g

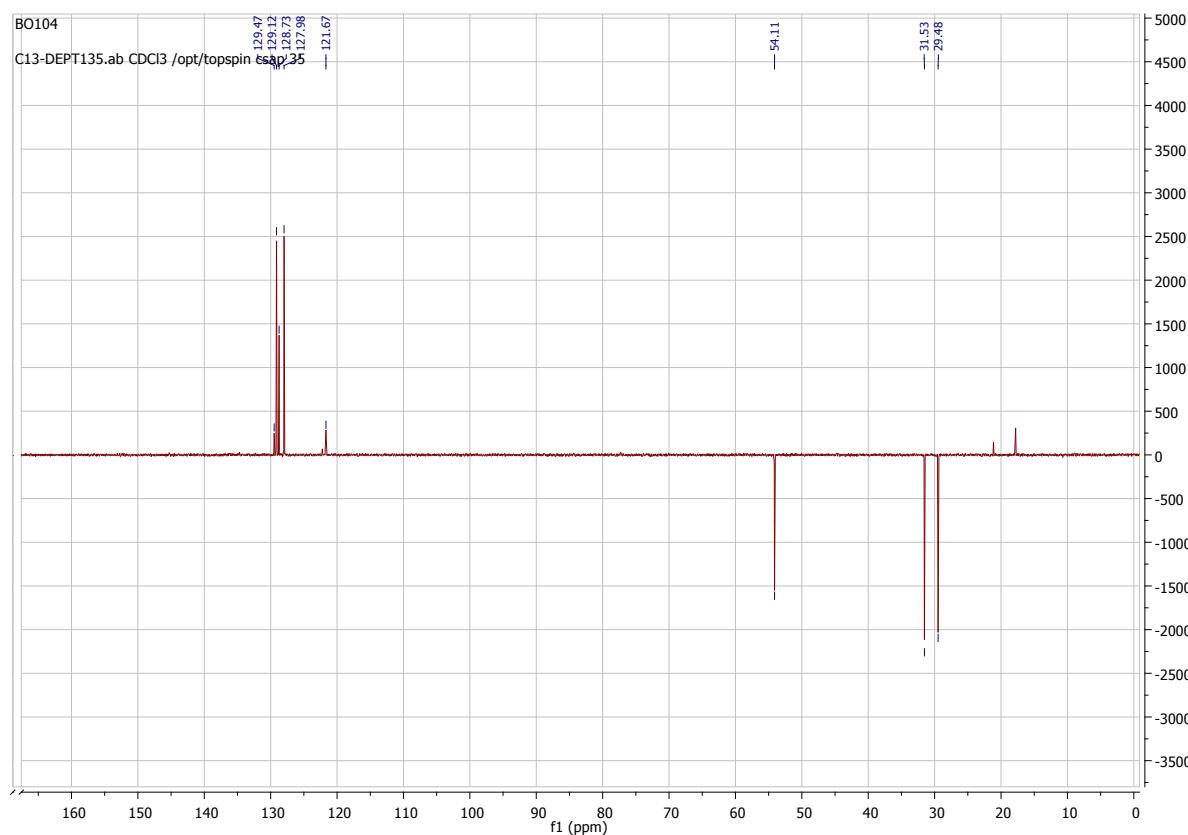


Figure 19: ^{13}C DEPT NMR spectrum of compound **4g**

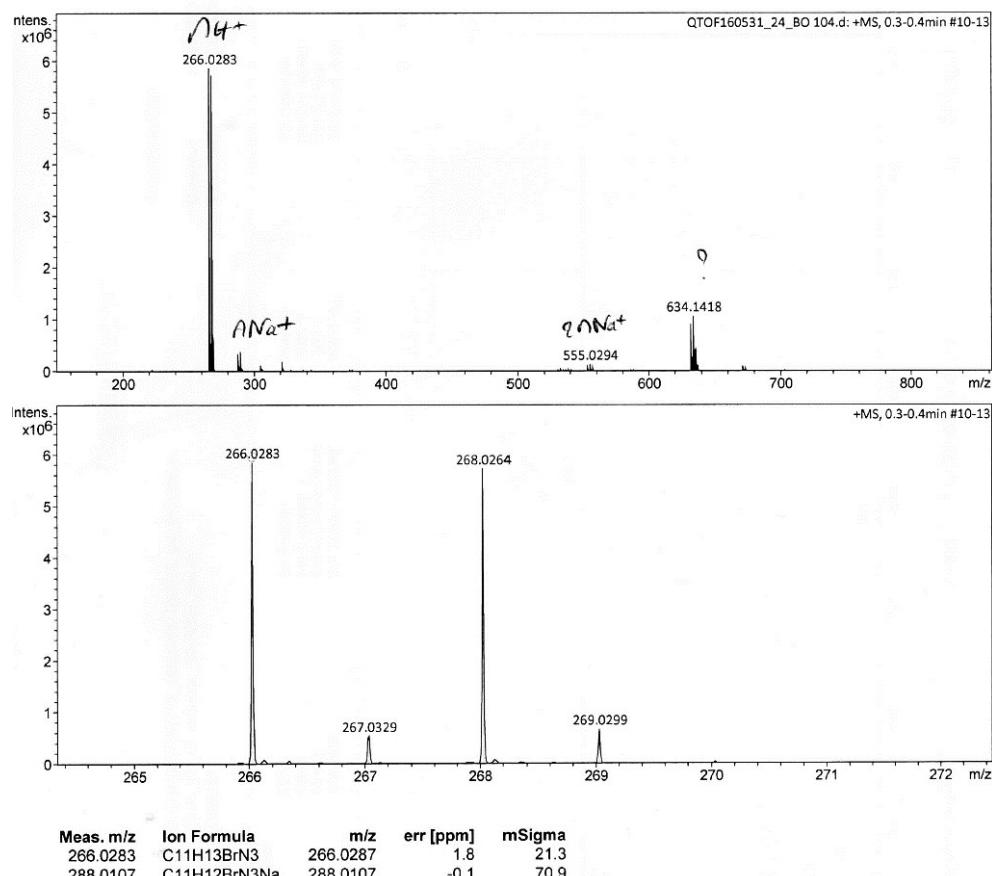


Figure 20: HRMS spectrum of compound **4g**

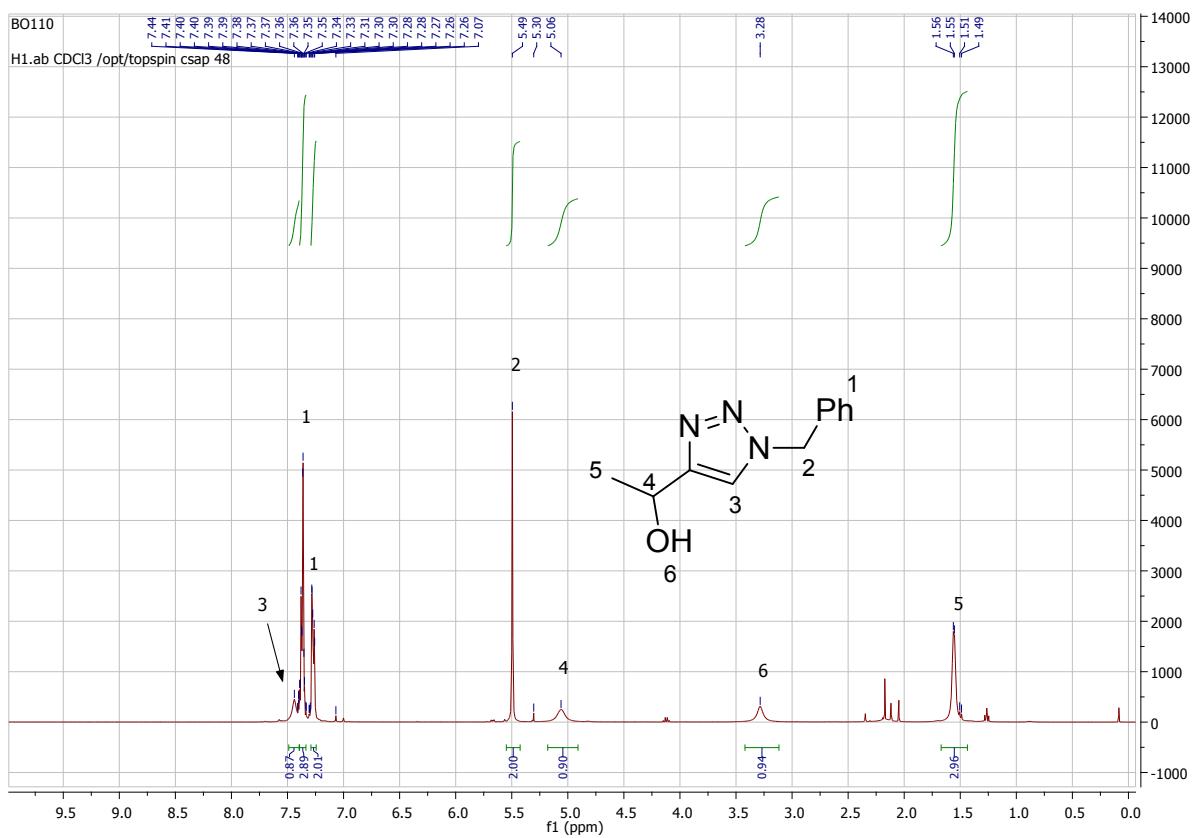


Figure 21: ¹H NMR spectrum of compound 4h

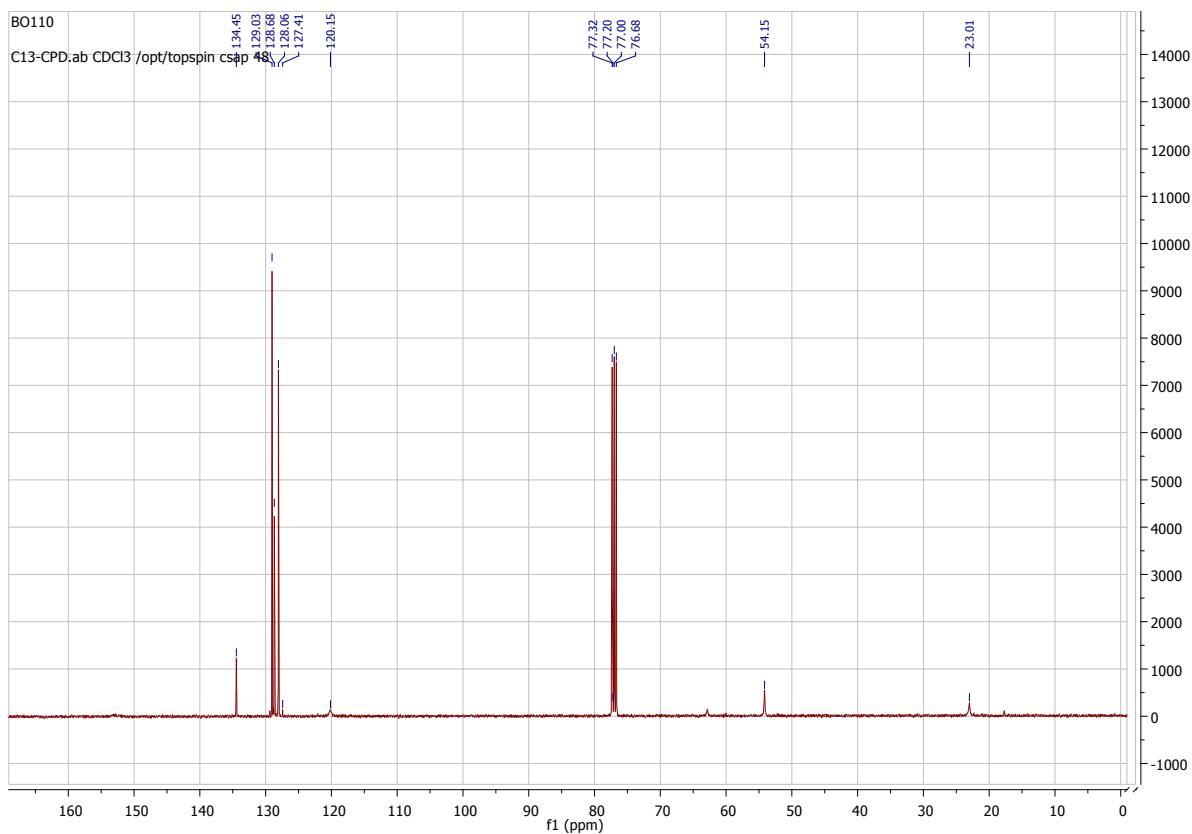


Figure 22: ¹³C NMR spectrum of compound 4h

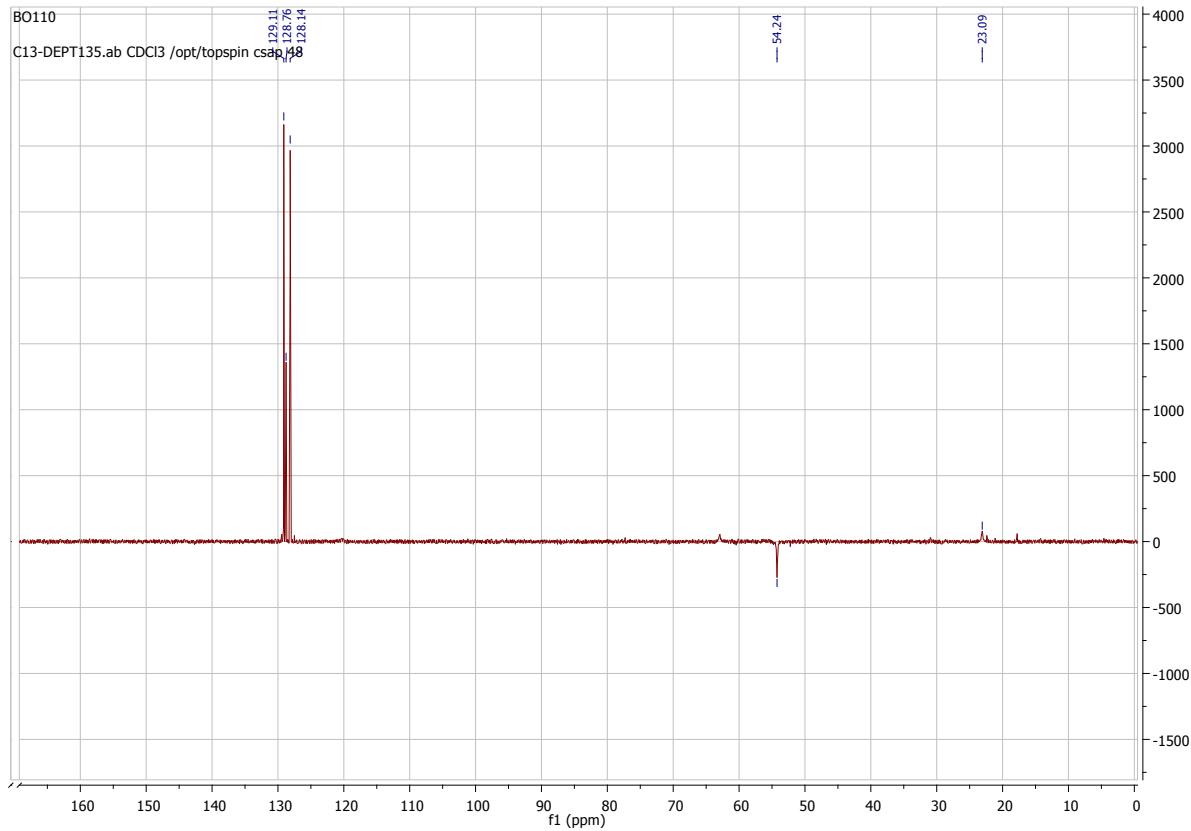
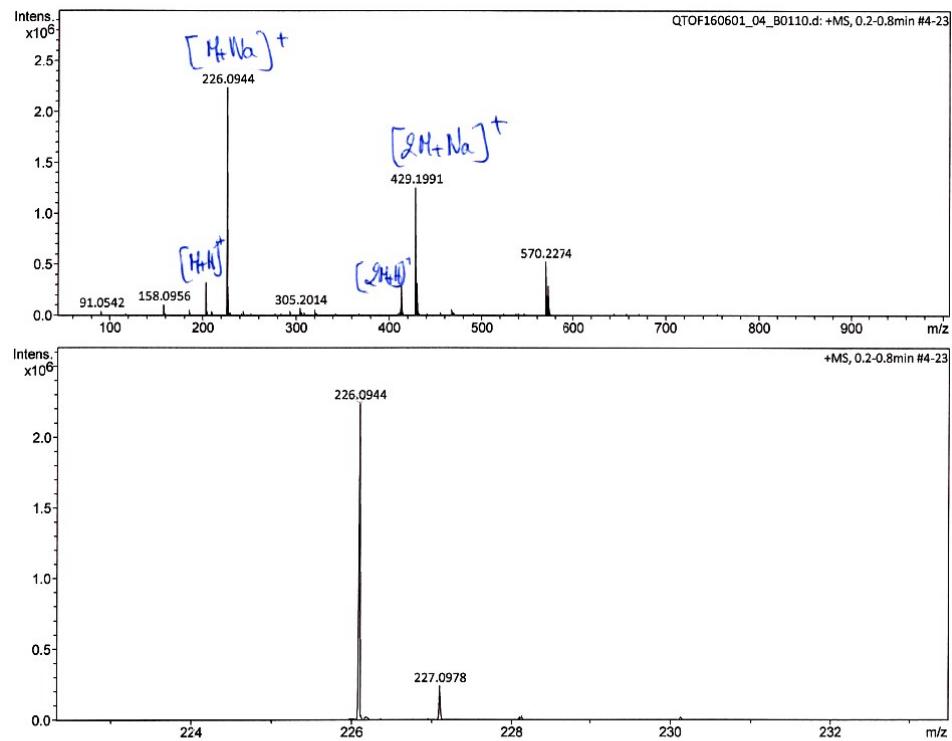


Figure 23: ^{13}C DEPT NMR spectrum of compound **4h**



Meas. m/z	Ion Formula	m/z	err [ppm]	mSigma
204.1124	C ₁₁ H ₁₄ N ₃ O	204.1131	3.5	1.4
226.0944	C ₁₁ H ₁₃ N ₃ NaO	226.0951	2.9	15.0

Figure 24: HRMS spectrum of compound **4h**

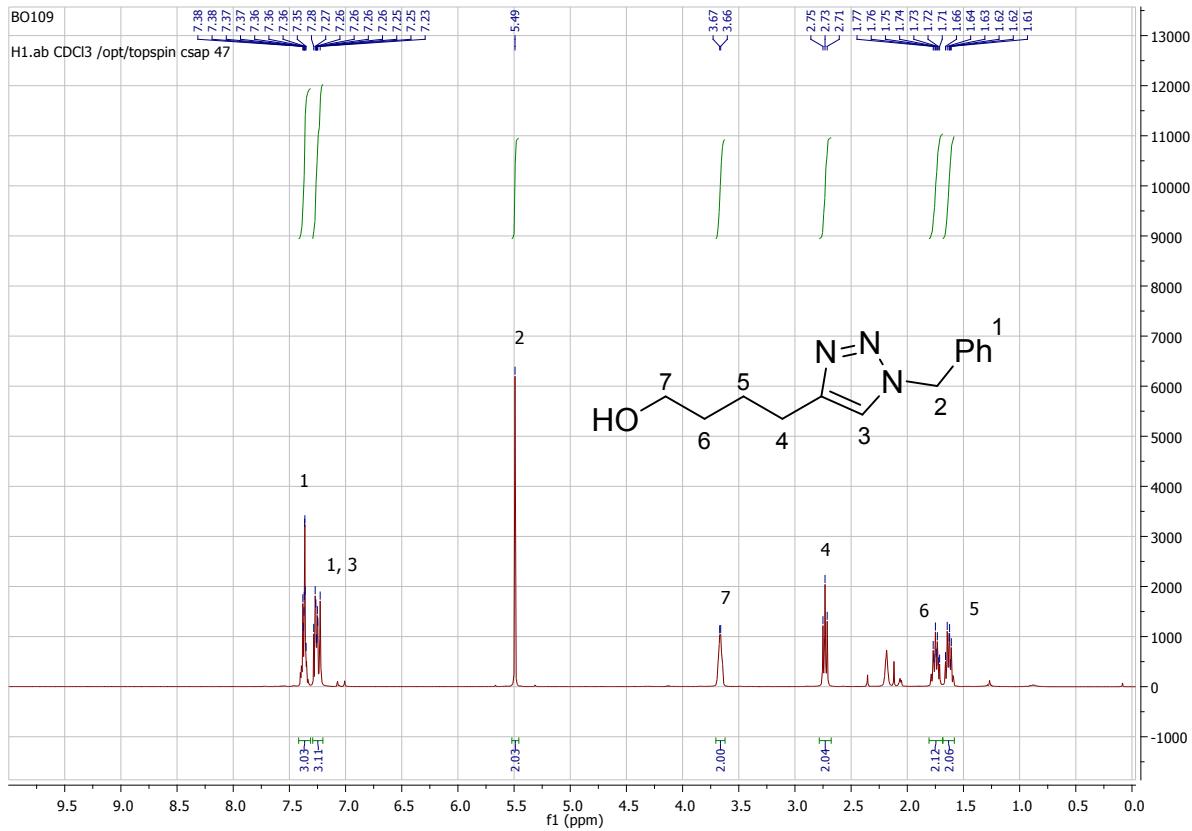


Figure 25: ¹H NMR spectrum of compound 4i

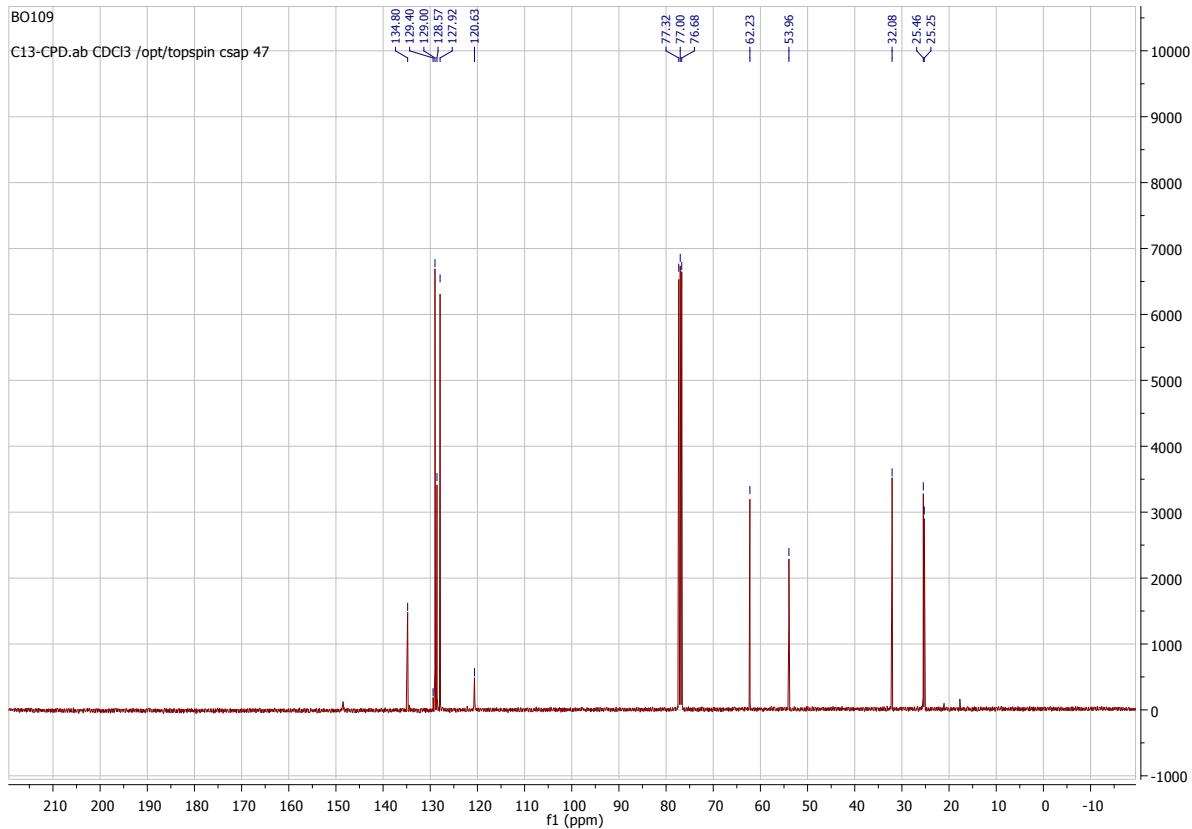


Figure 26: ¹³C NMR spectrum of compound 4i

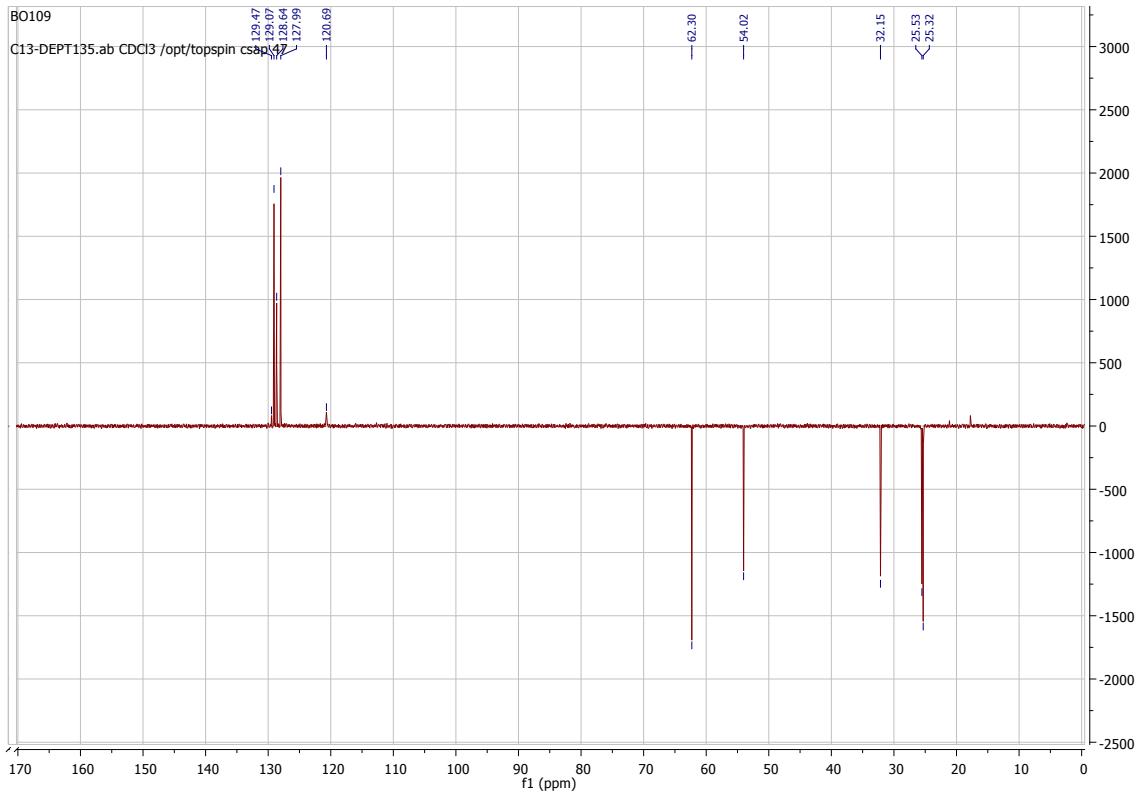


Figure 27: ^{13}C DEPT NMR spectrum of compound **4i**

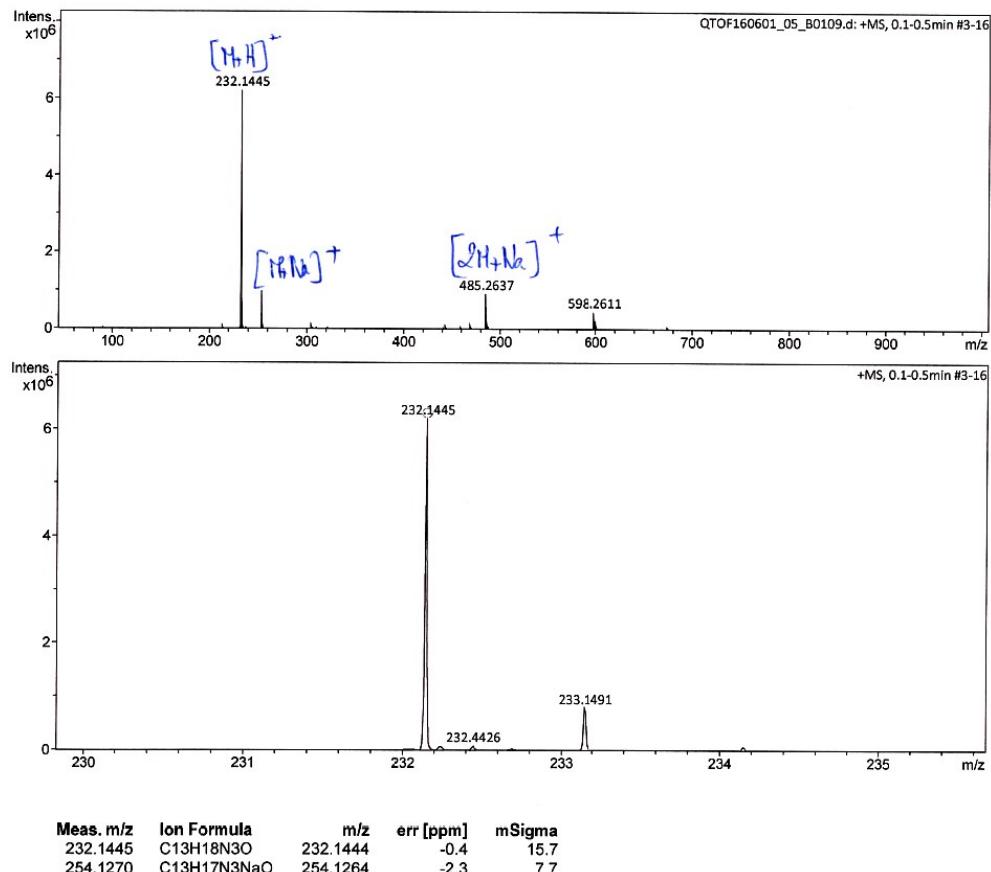


Figure 28: HRMS spectrum of compound **4i**

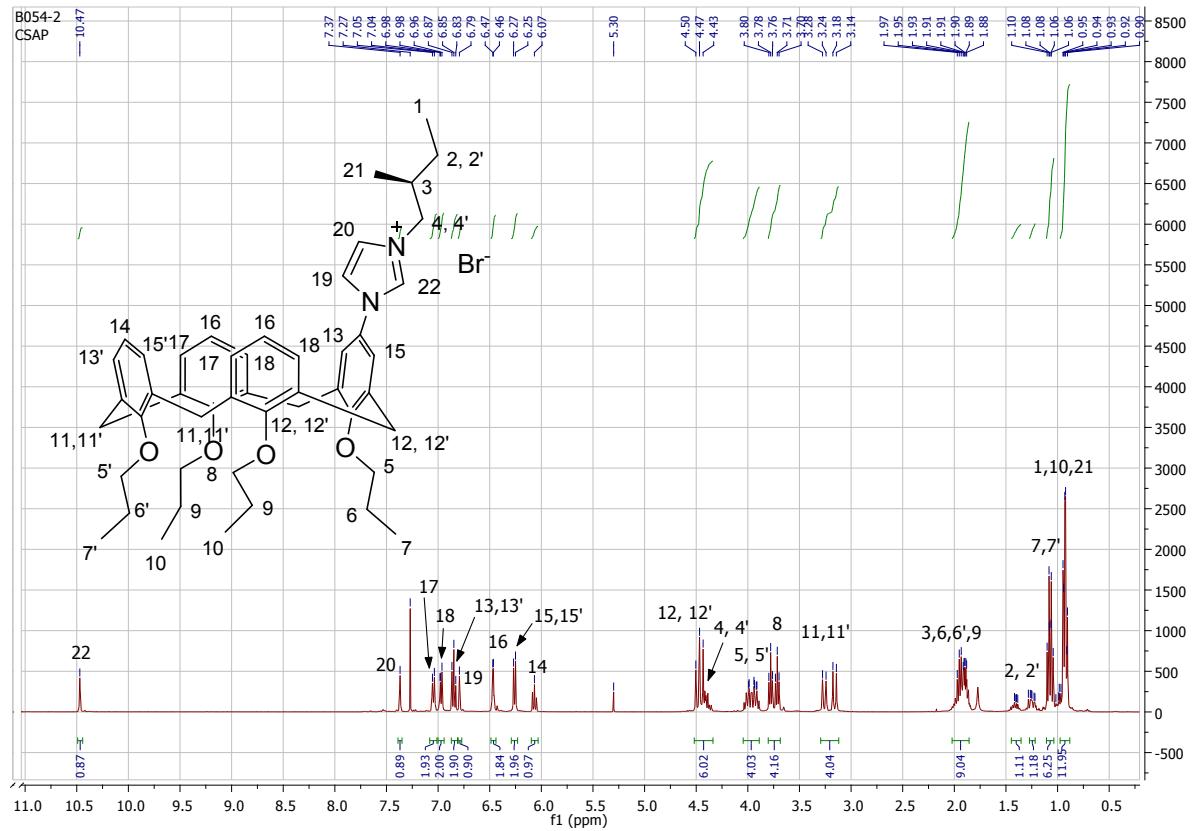


Figure 29: ¹H NMR spectrum of compound 2b

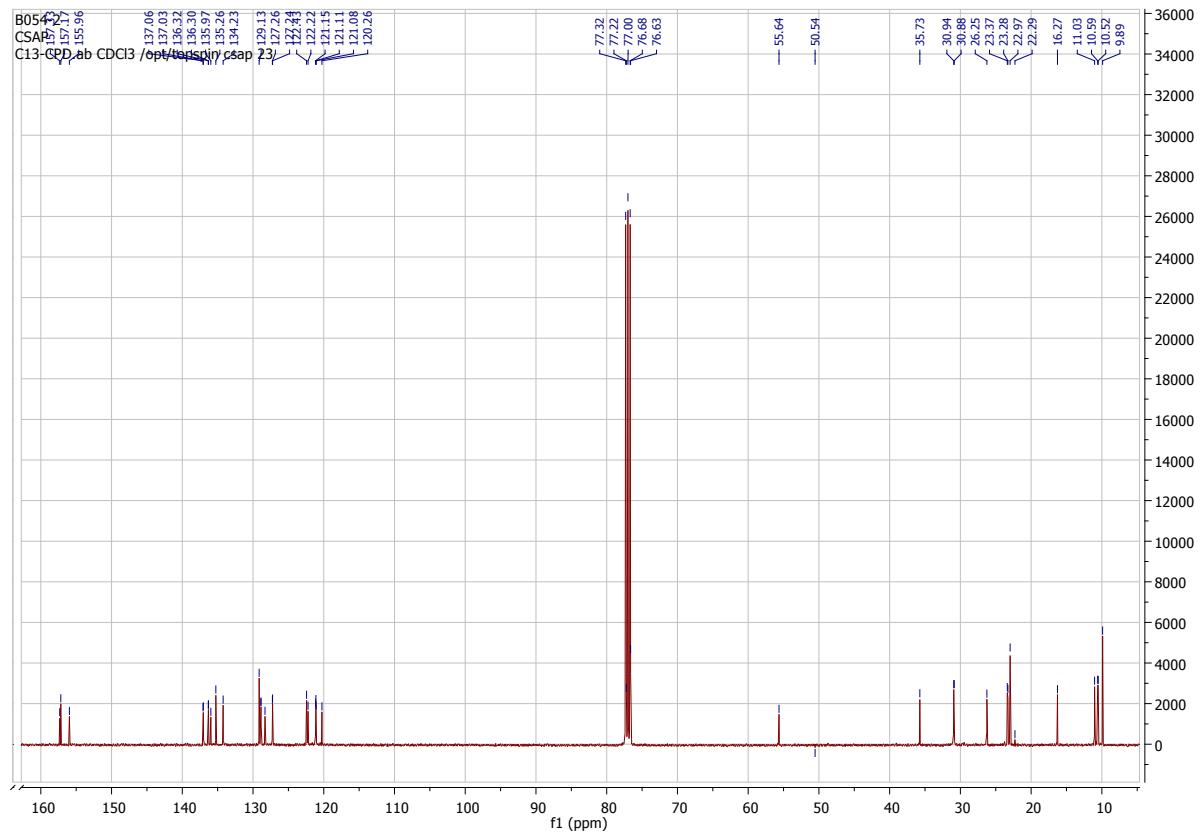


Figure 30: ¹³C NMR spectrum of compound 2b

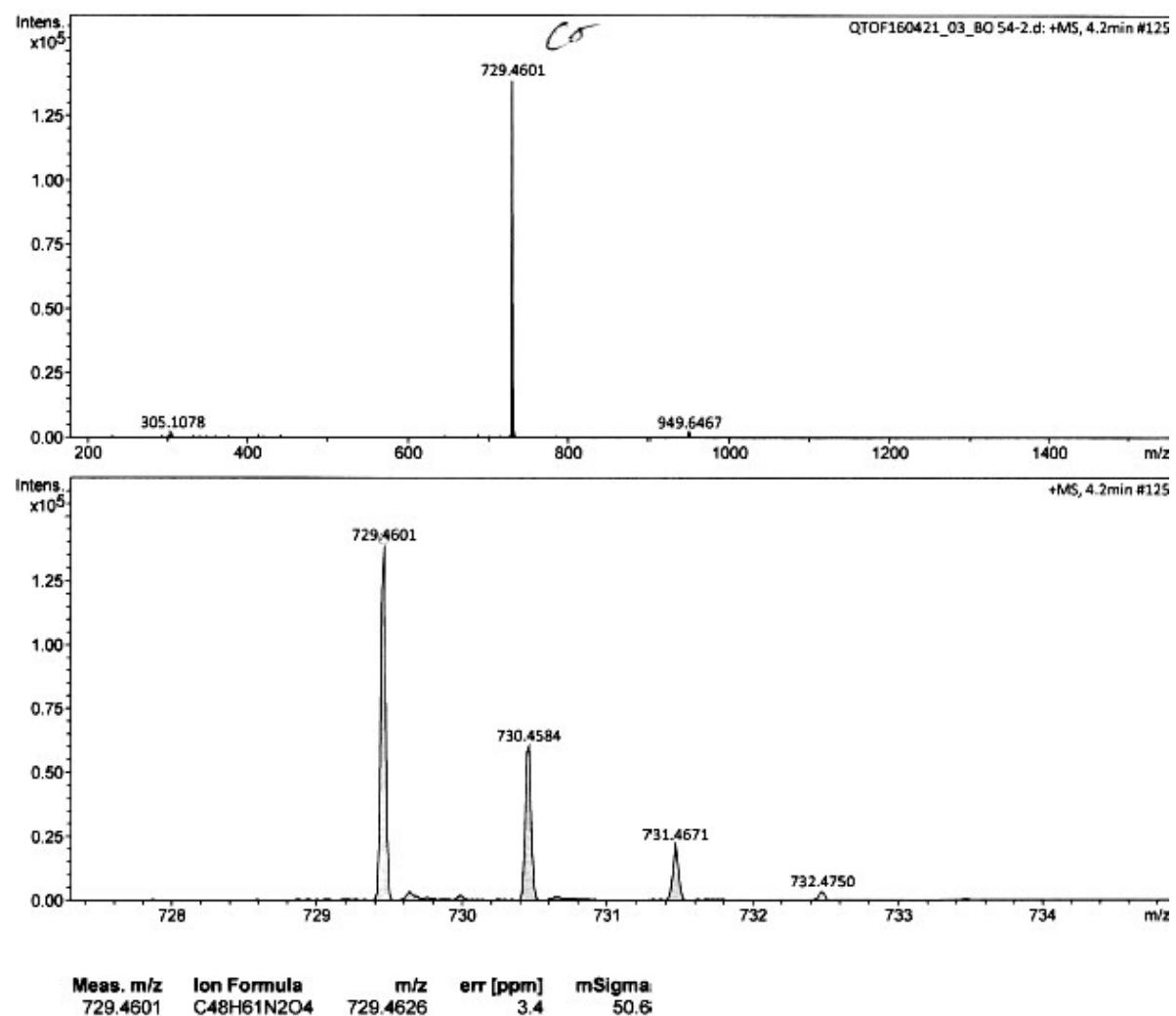


Figure 31: HRMS spectrum of compound **2b**

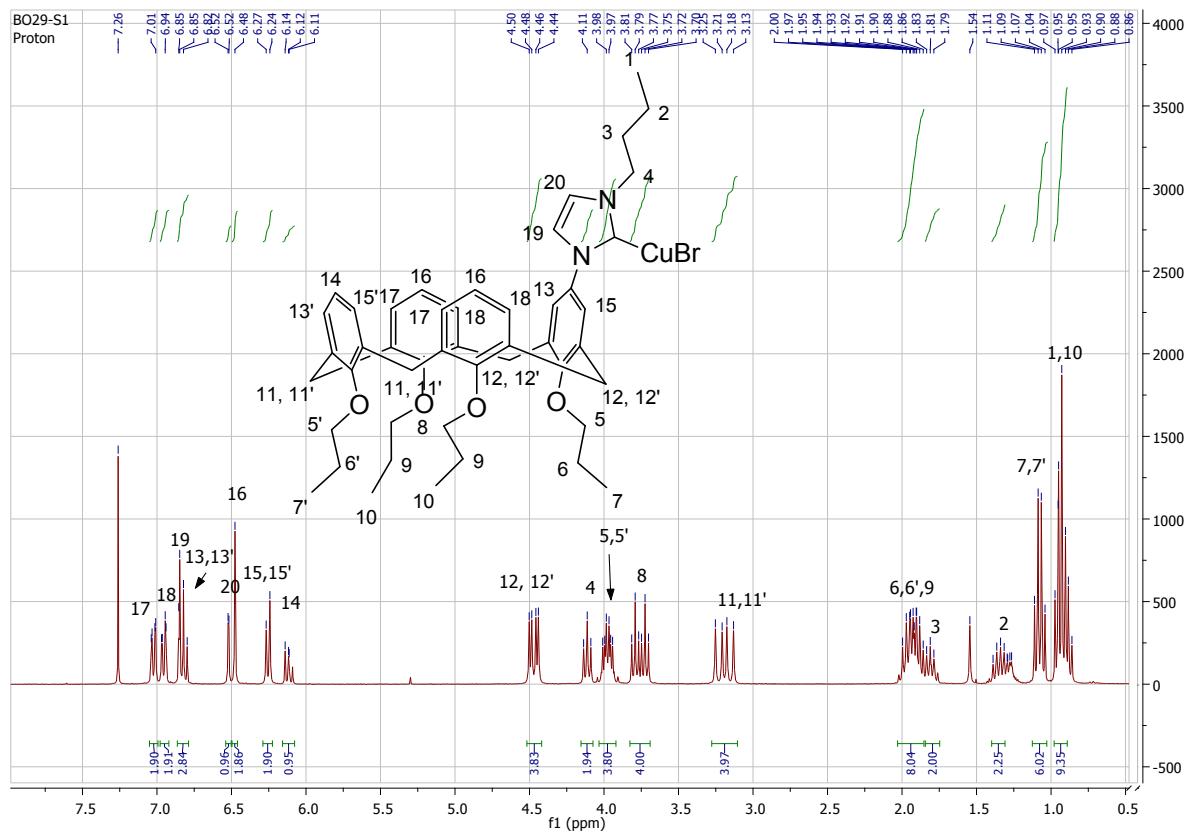


Figure 32: ^1H NMR spectrum of compound **3a**

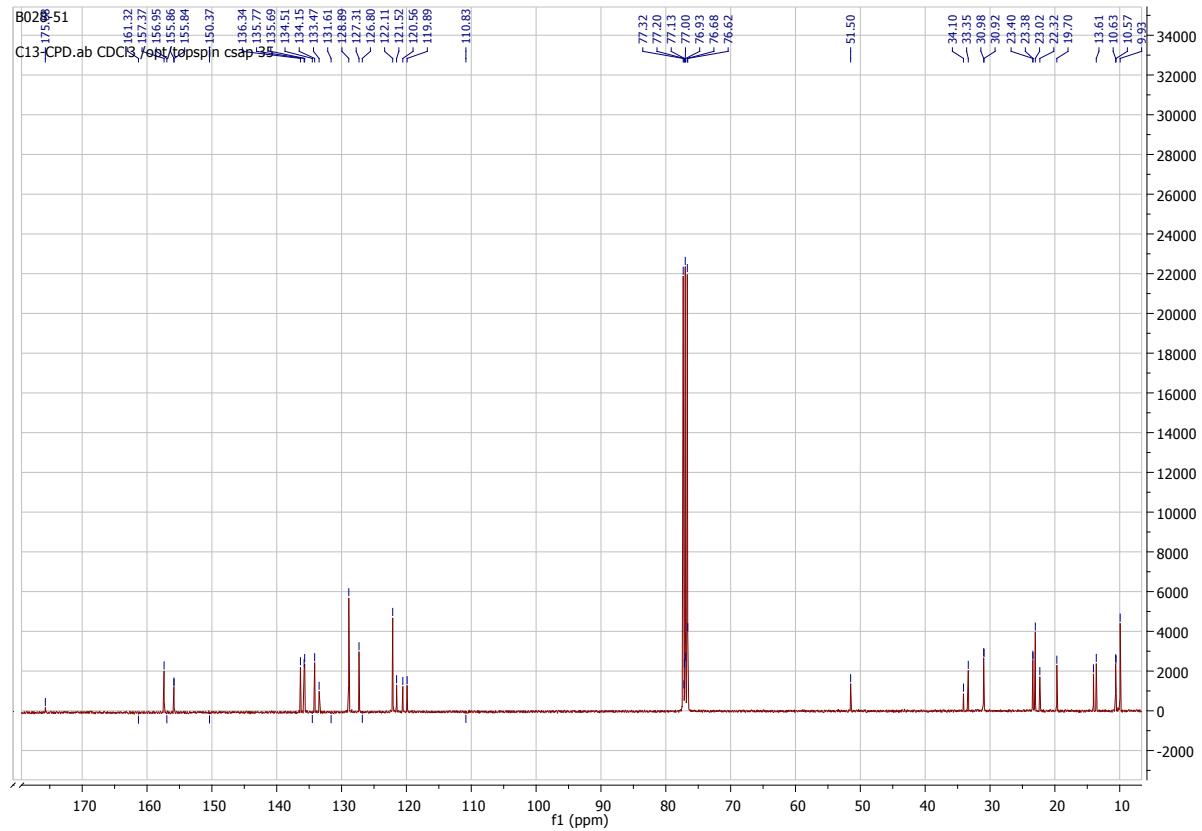


Figure 33: ¹³C NMR spectrum of compound 3a

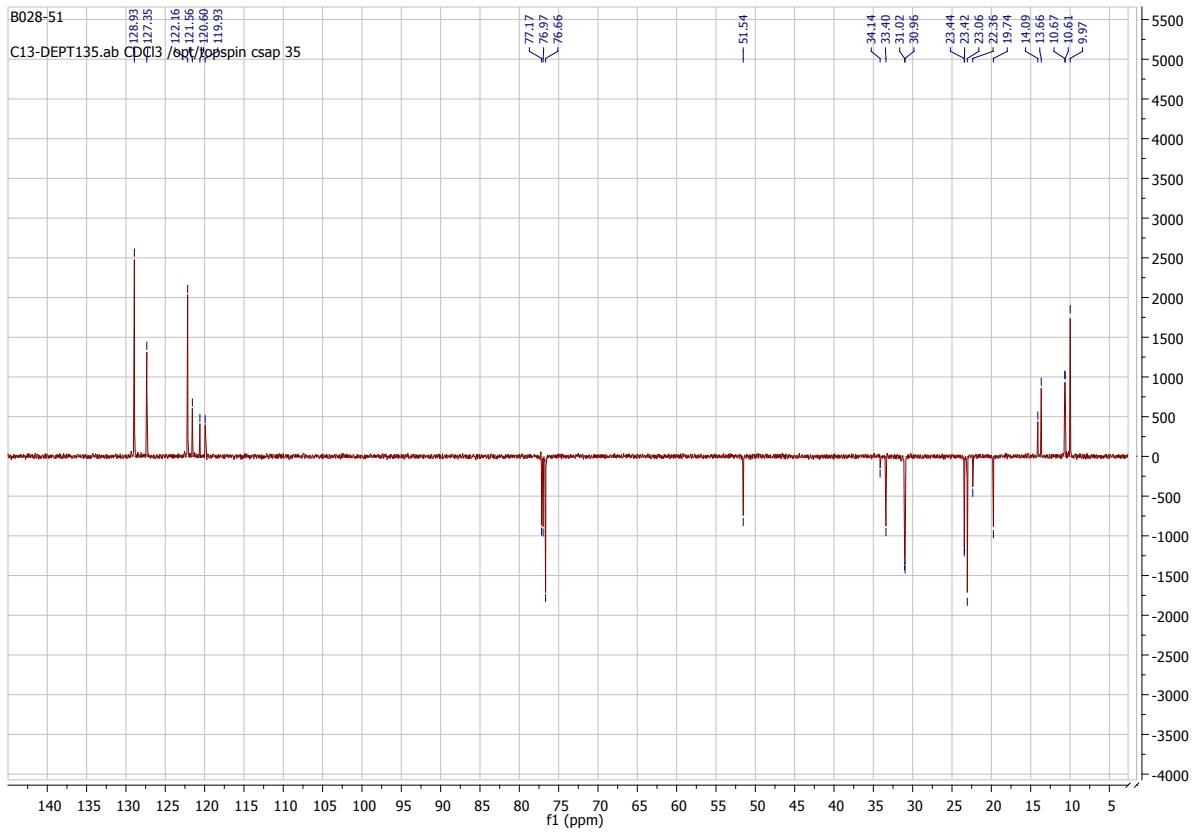


Figure 34: ¹³C DEPT NMR spectrum of compound 3a

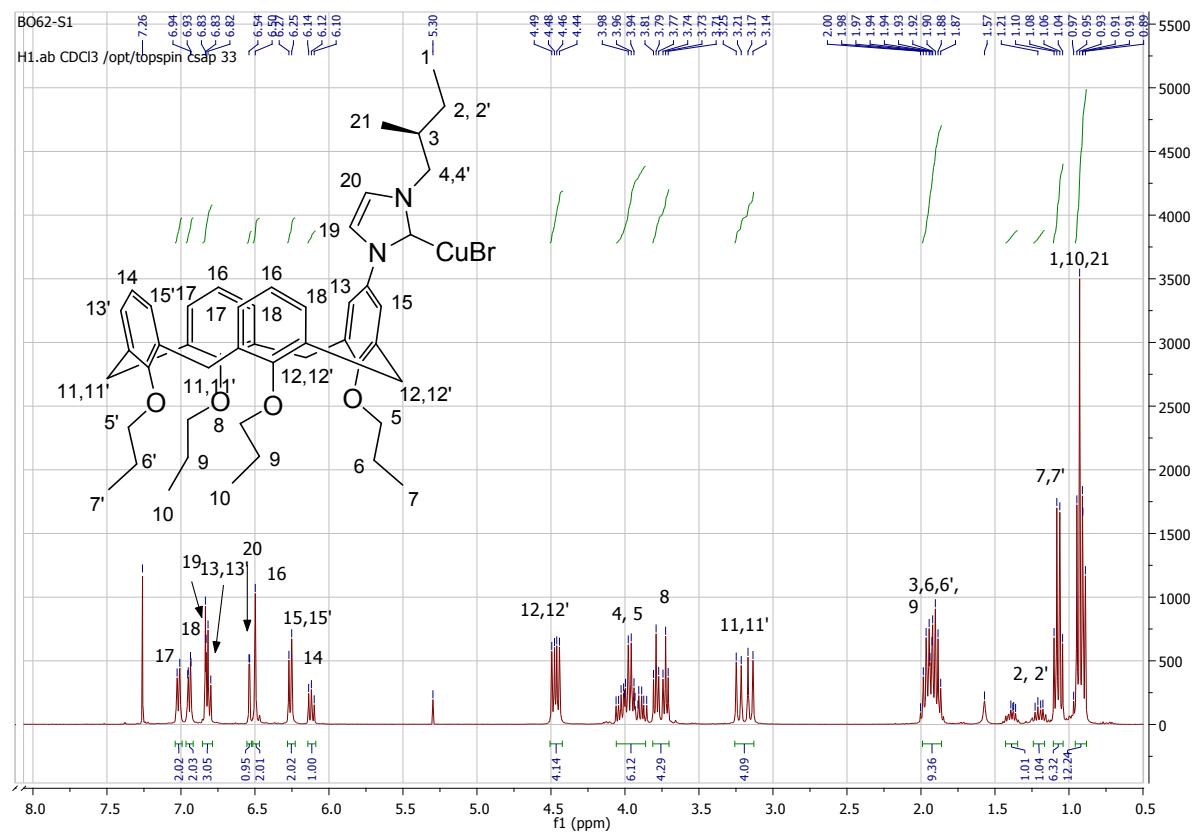


Figure 35: ^1H NMR spectrum of compound **3b**

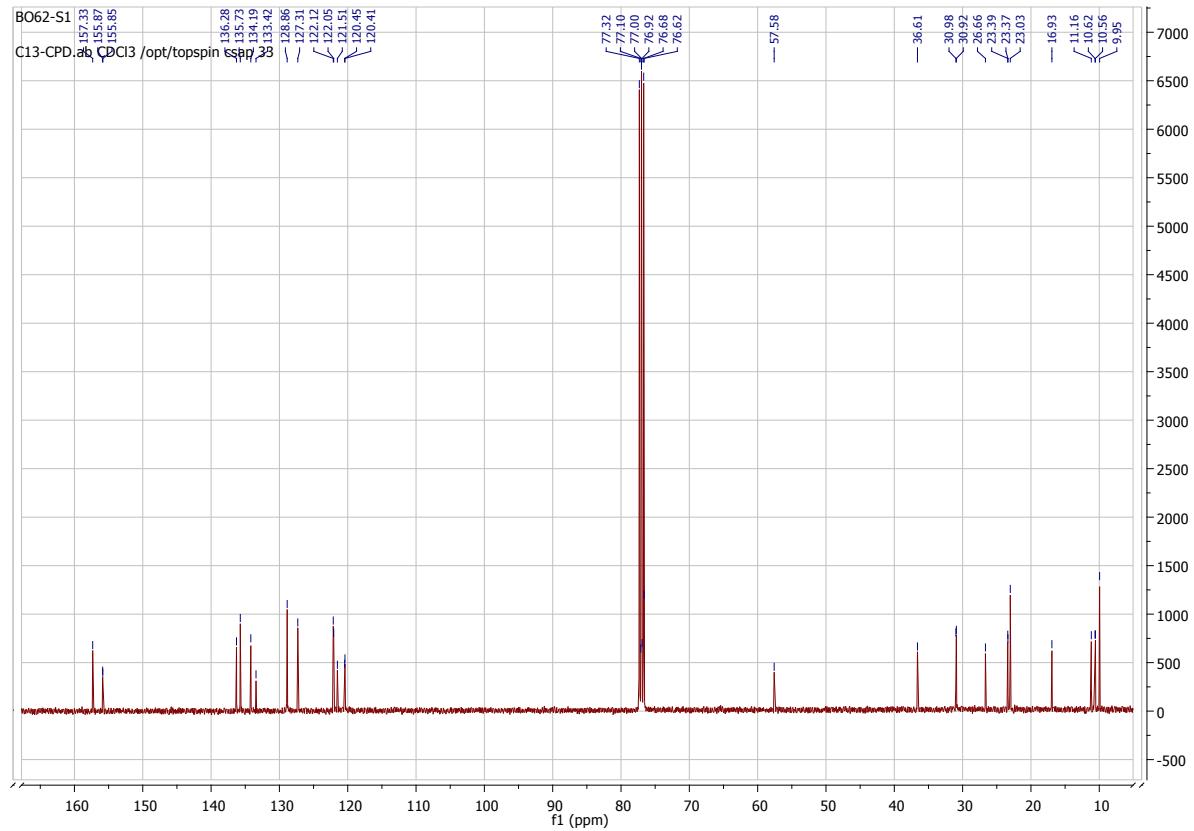


Figure 36: ¹³C NMR spectrum of compound 3b

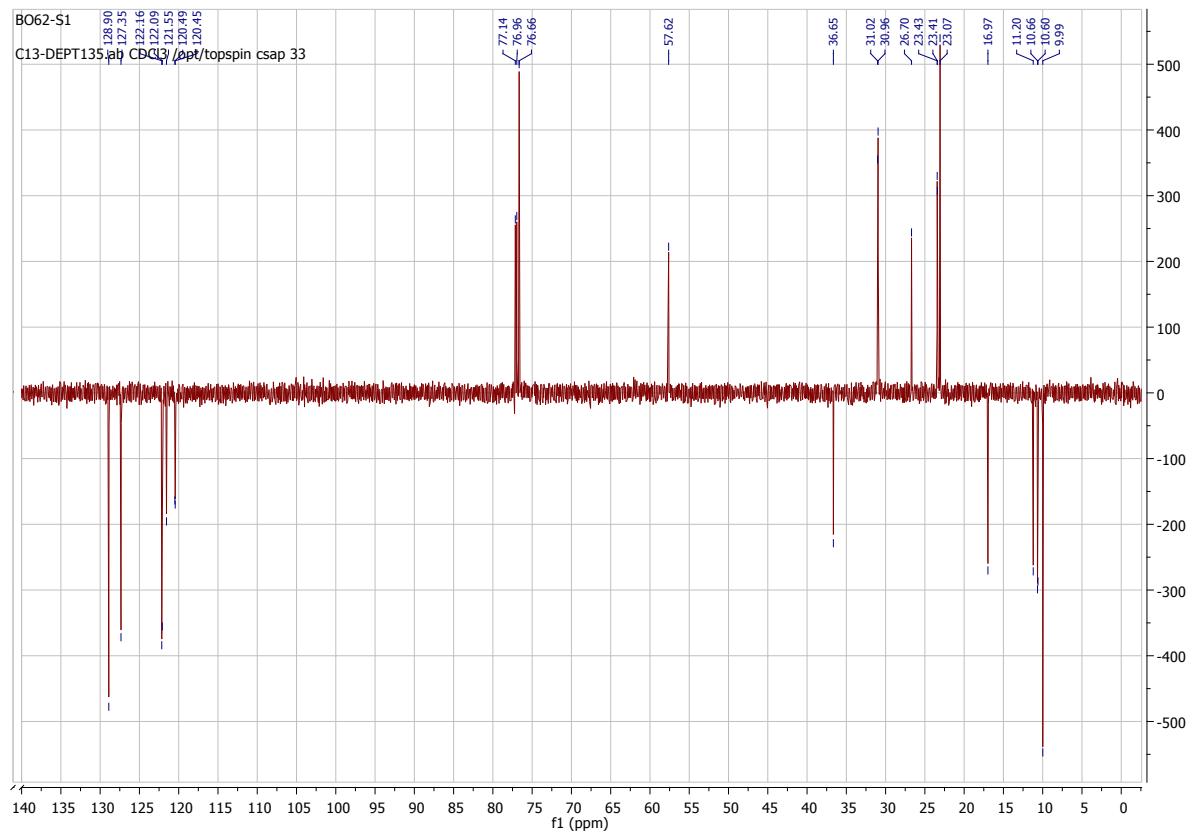


Figure 37: ^{13}C DEPT NMR spectrum of compound **3b**

V Free	V Buried	V Total	V Exact
133.182	46.353	179.535	179.594
%V_Free	%V_Bur	% Tot/Ex	
74.182	25.818	99.967	

Table 1: calculation result of SambVca for **3a** (Bondi radii scaled by 1.17 for the atoms, radius of the sphere R = 3.5 Å)

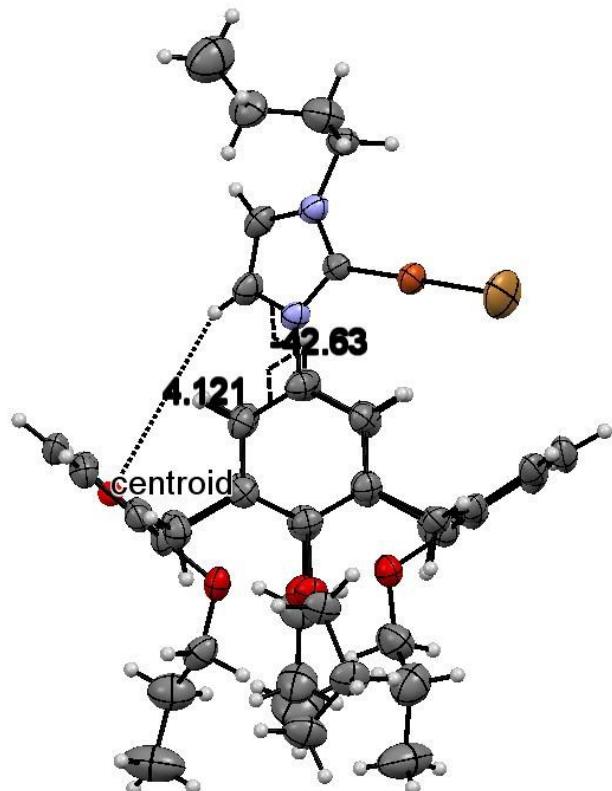


Figure 38: X-ray structures of **3a**: weak CH/π interaction