

## Supporting Information

# Effect of Dimerization on Nucleic Acid Binding and Sensing of a Styrylquinolinium Molecular Rotor: Spectroscopic Insights to Aggregation

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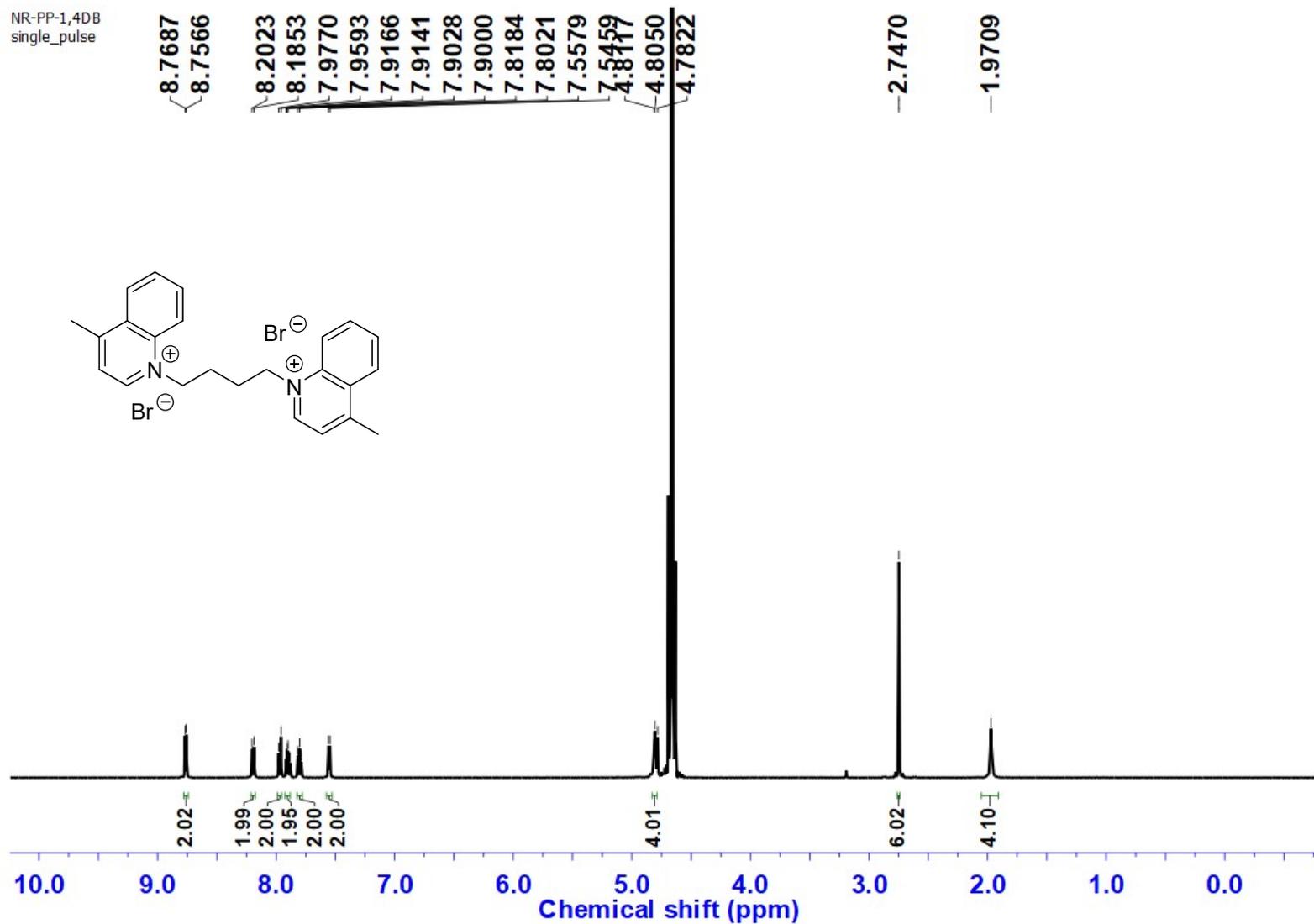


Figure S1.  $^1\text{H}$  NMR spectrum of compound 4a

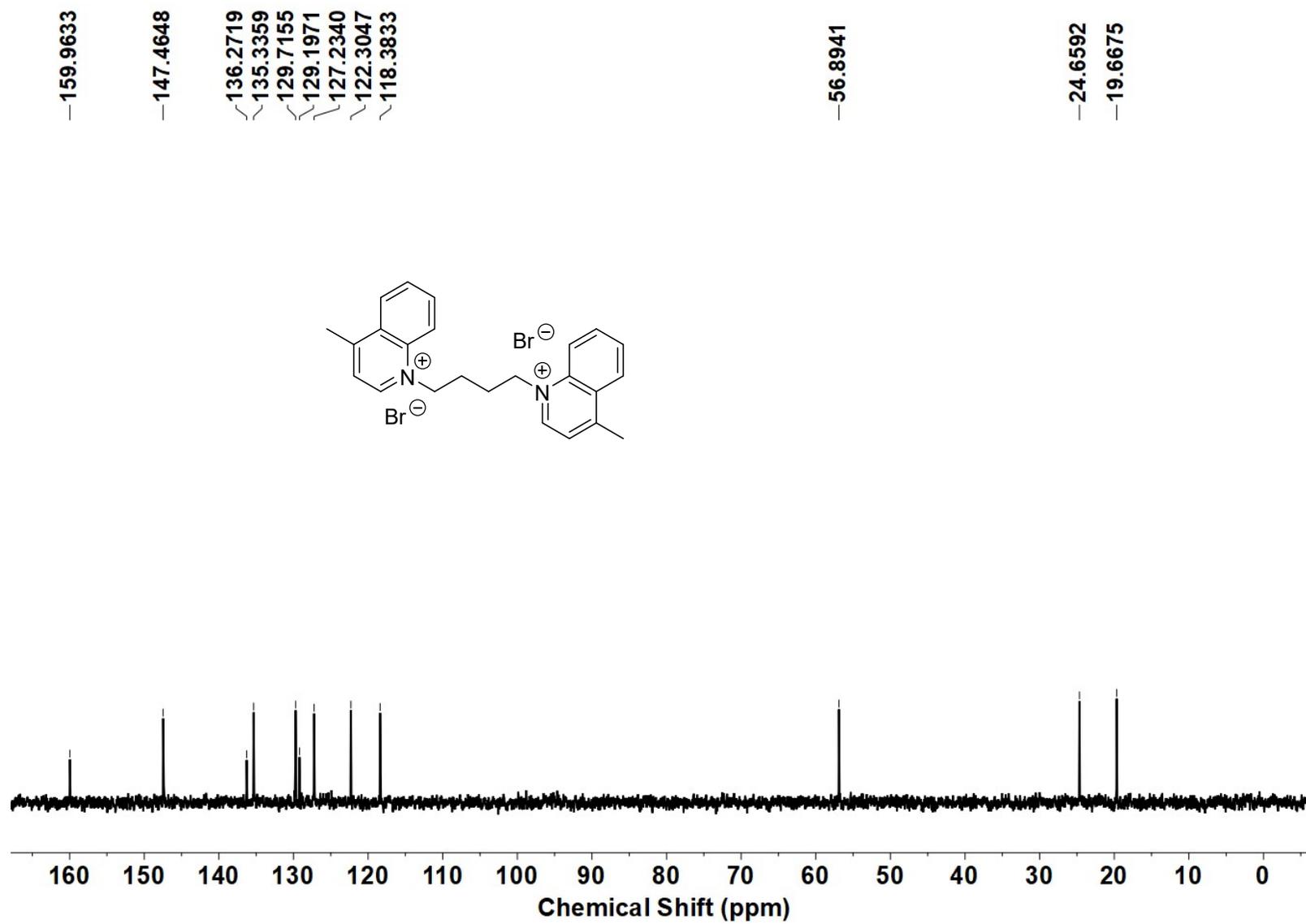
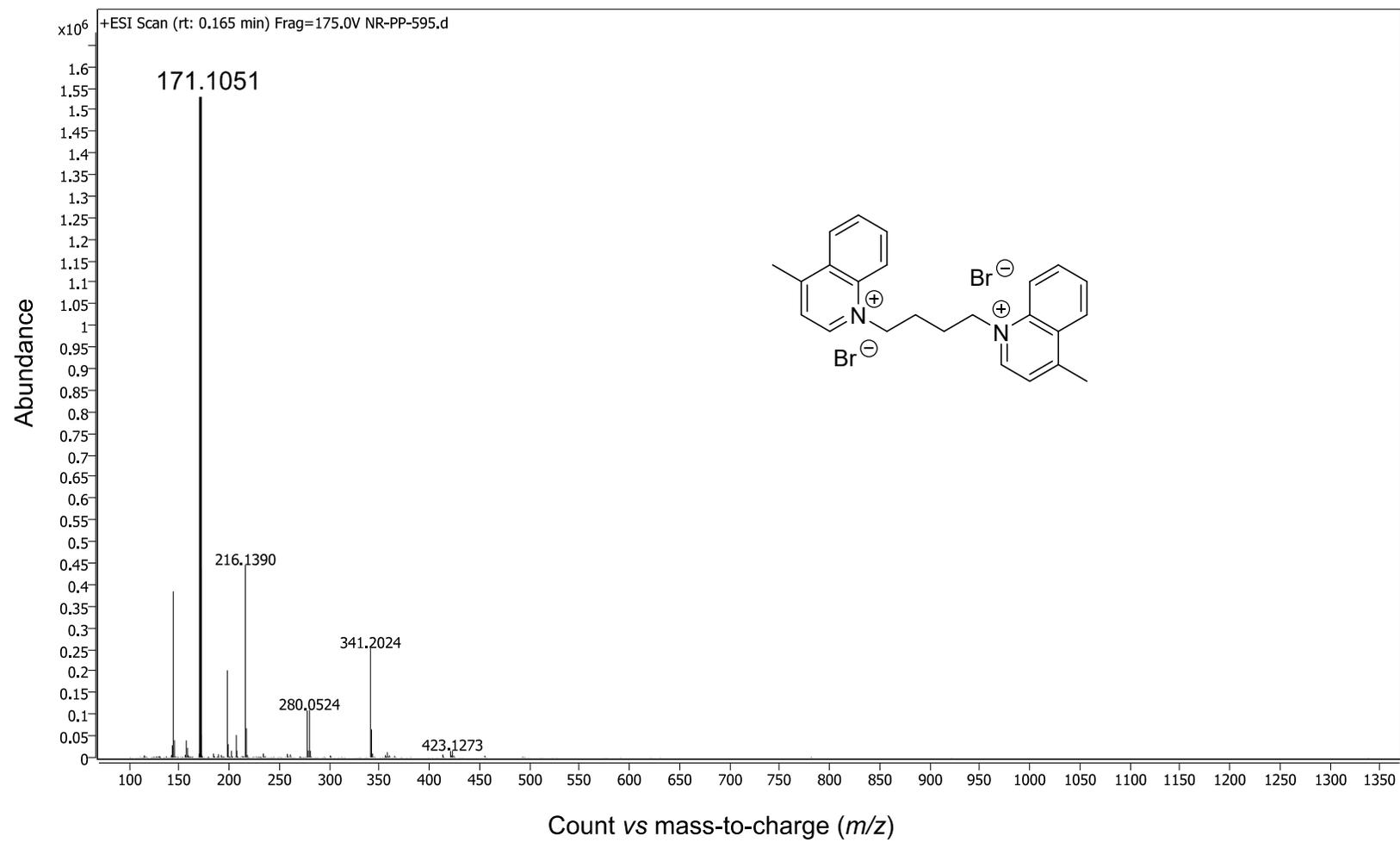


Figure S2. <sup>13</sup>C NMR spectrum of compound 4a



**Figure S3.** HRMS spectrum of compound **4a**

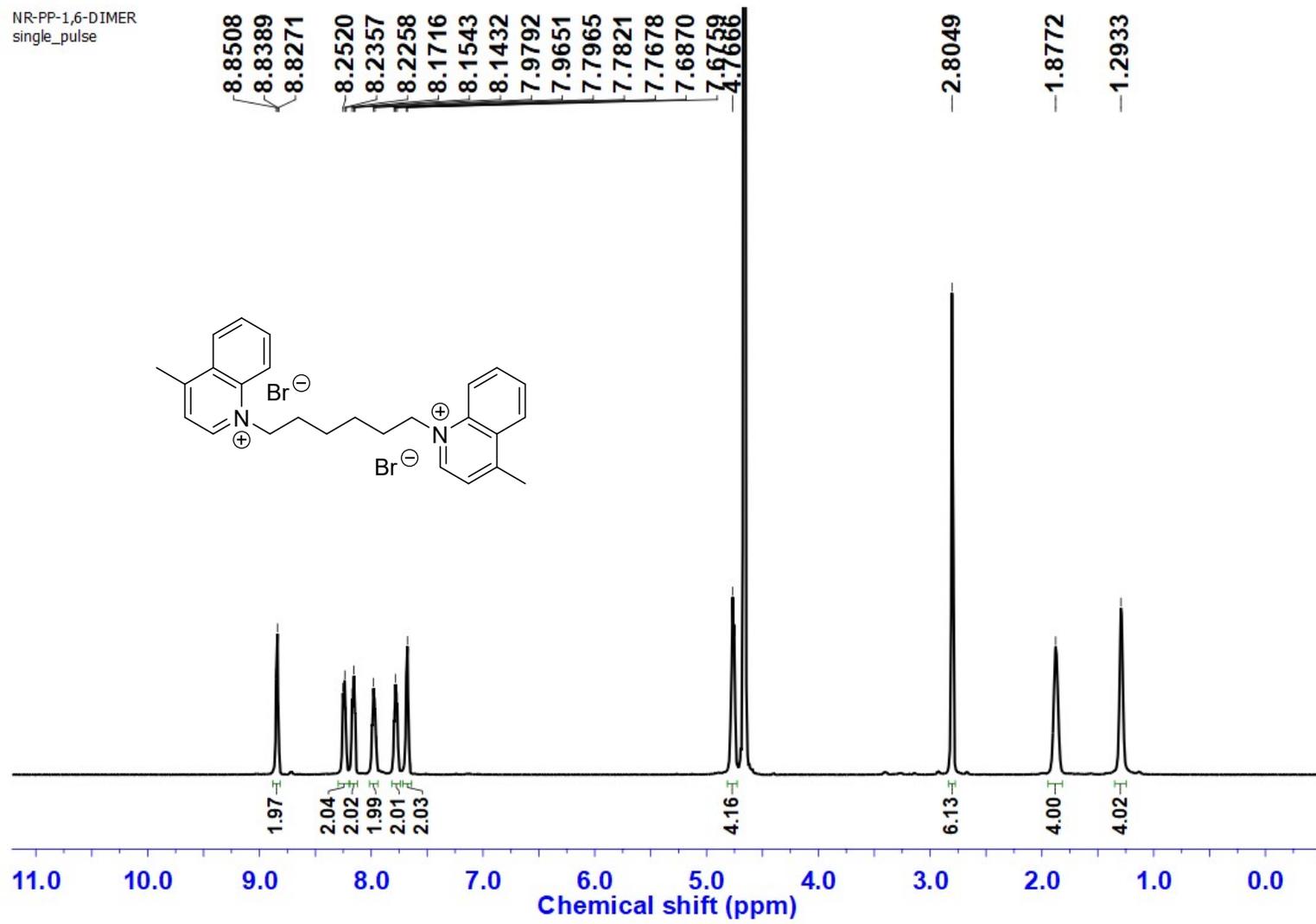


Figure S4. <sup>1</sup>H NMR spectrum of compound **4b**

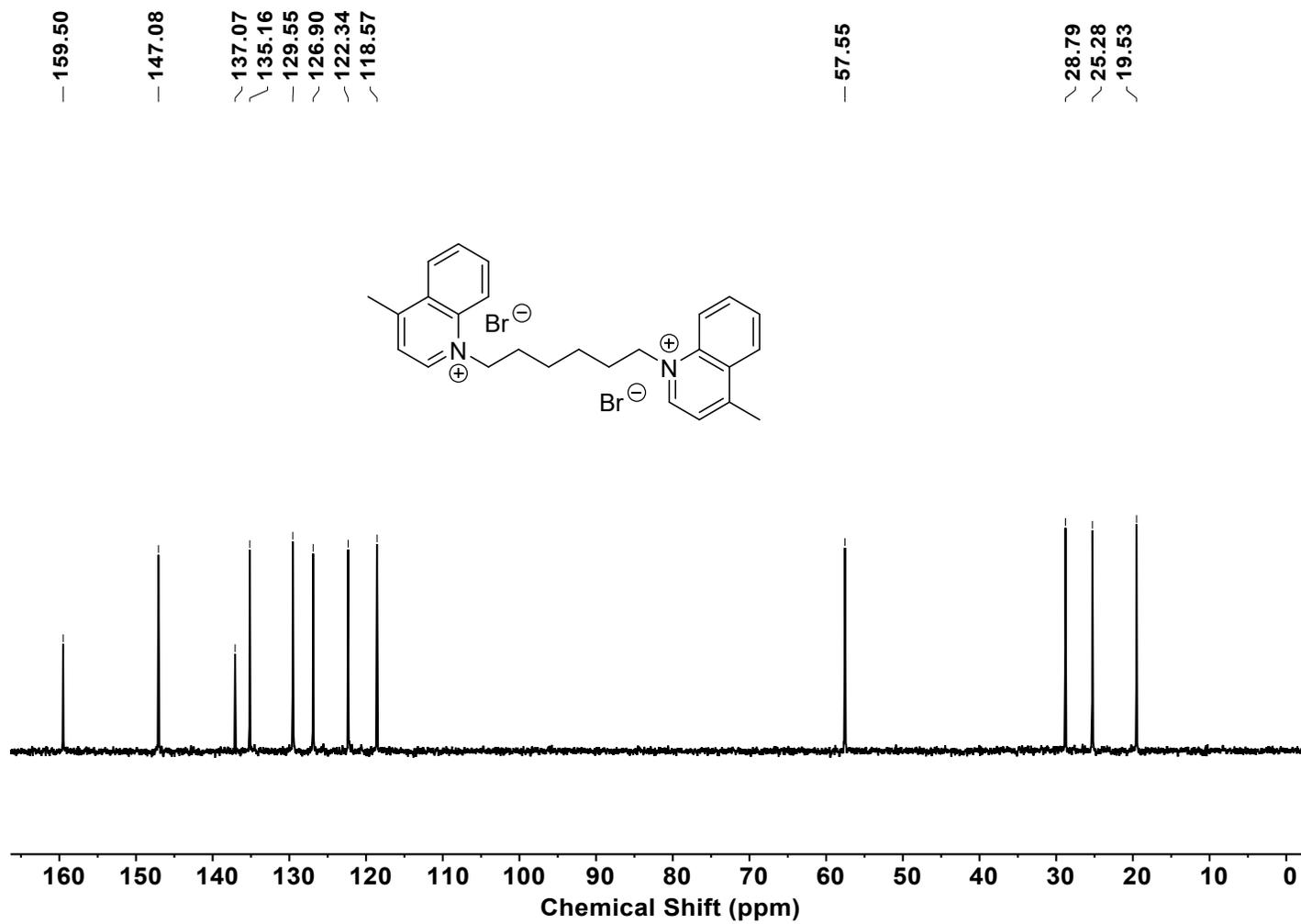
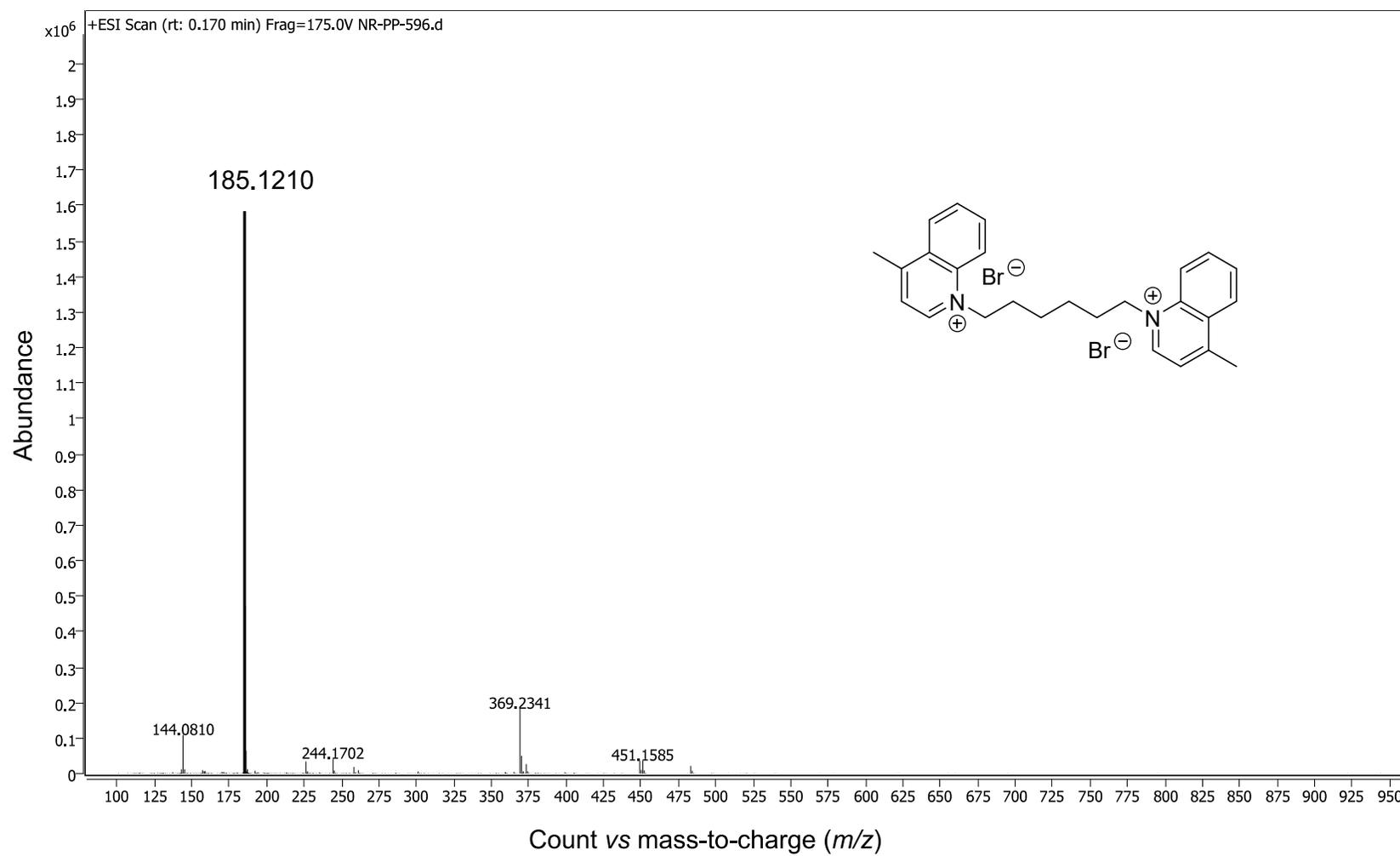


Figure S5. <sup>13</sup>C NMR spectrum of compound 4b



**Figure S6.** HRMS spectrum of compound **4b**

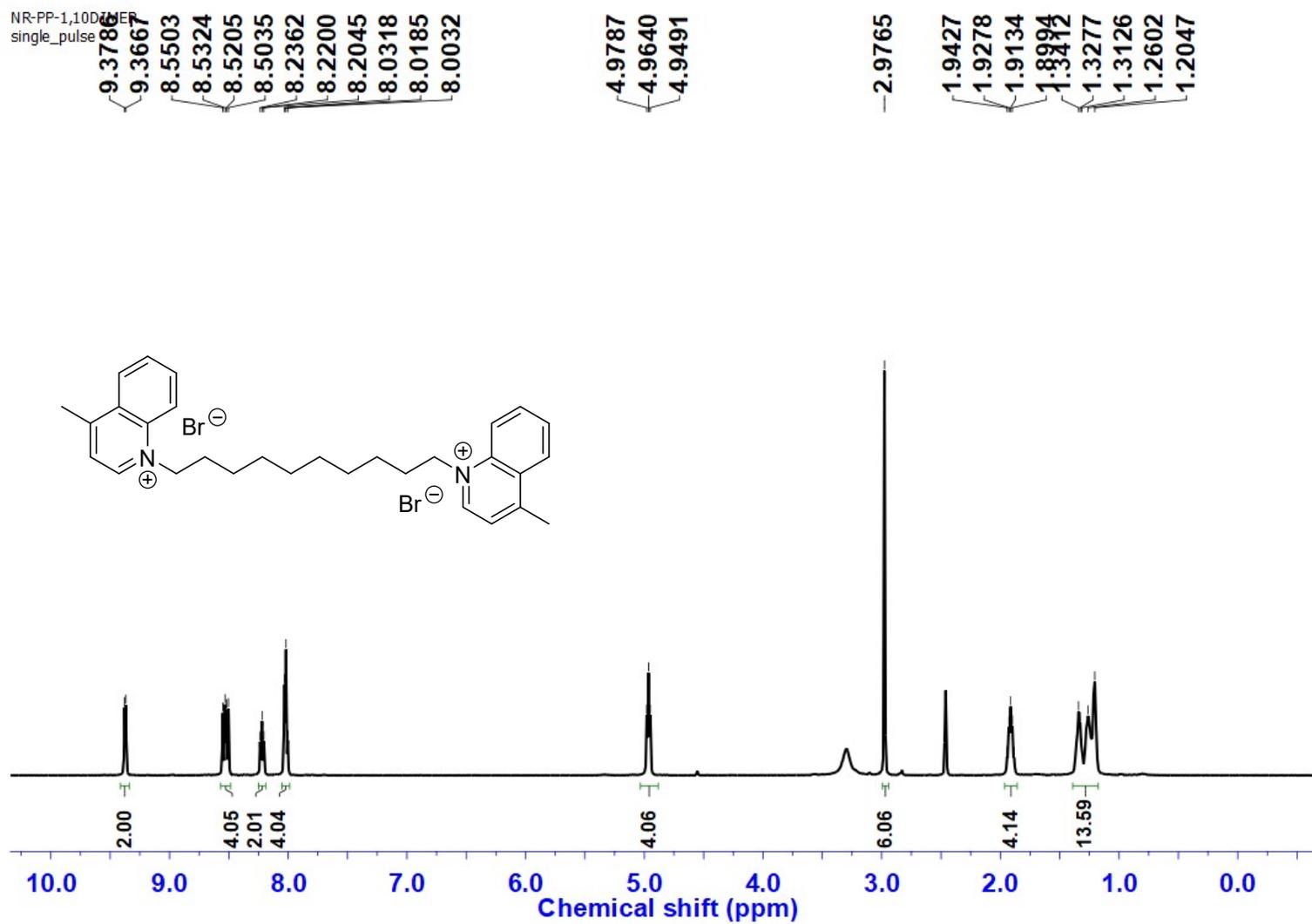


Figure S7. <sup>1</sup>H NMR spectrum of compound 4c

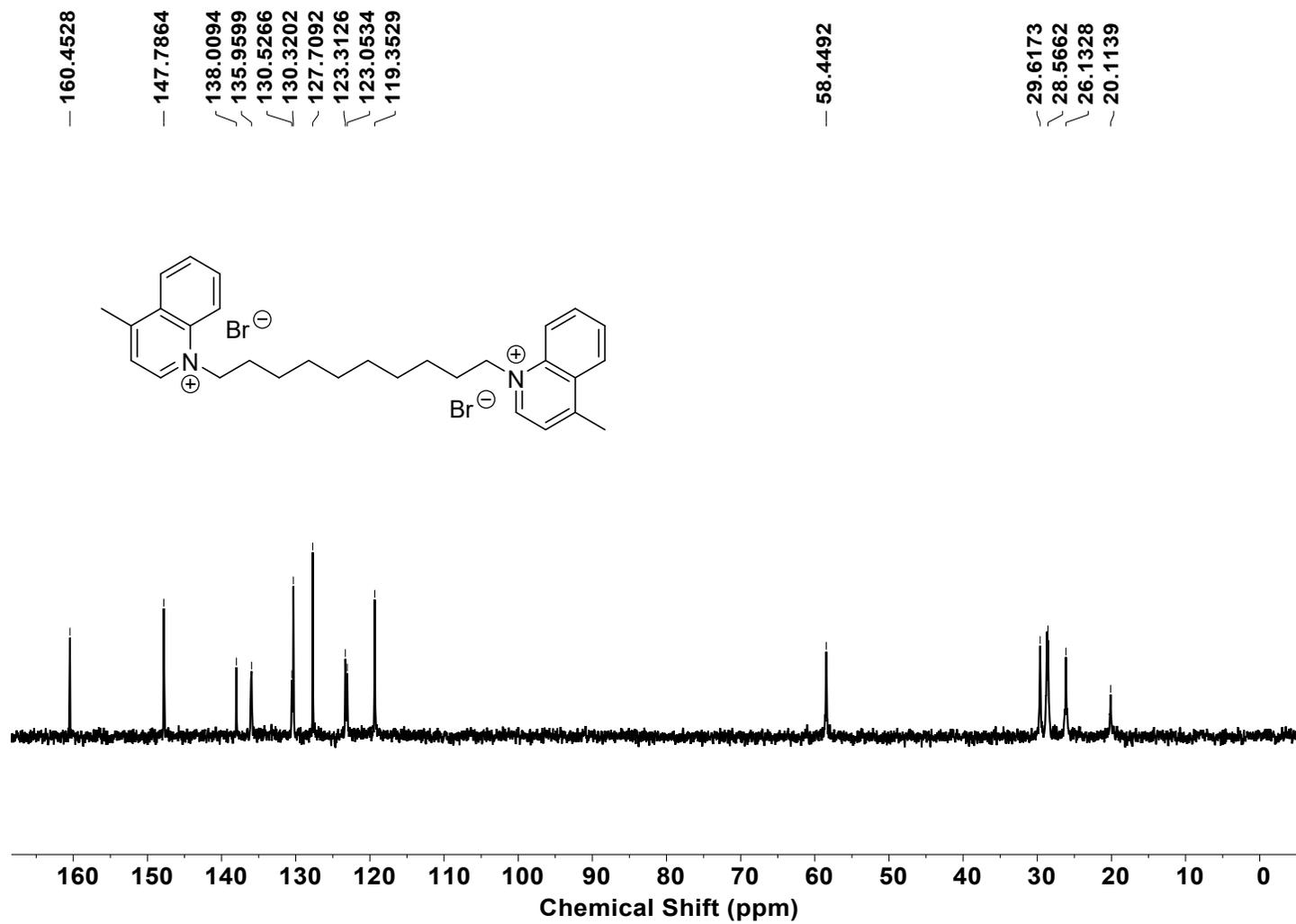
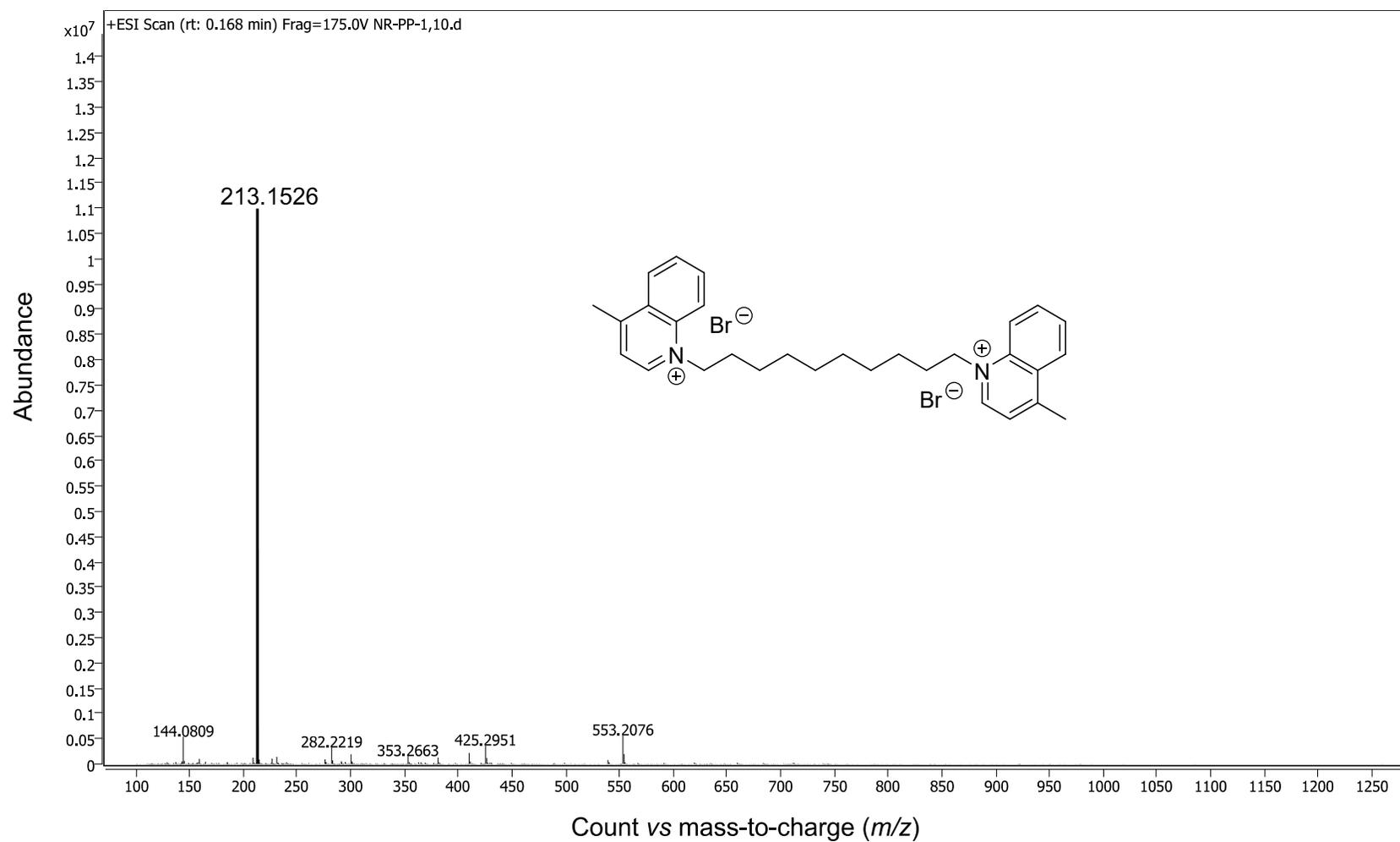


Figure S8.  $^{13}\text{C}$  NMR spectrum of compound 4c



**Figure S9.** HRMS spectrum of compound **4c**

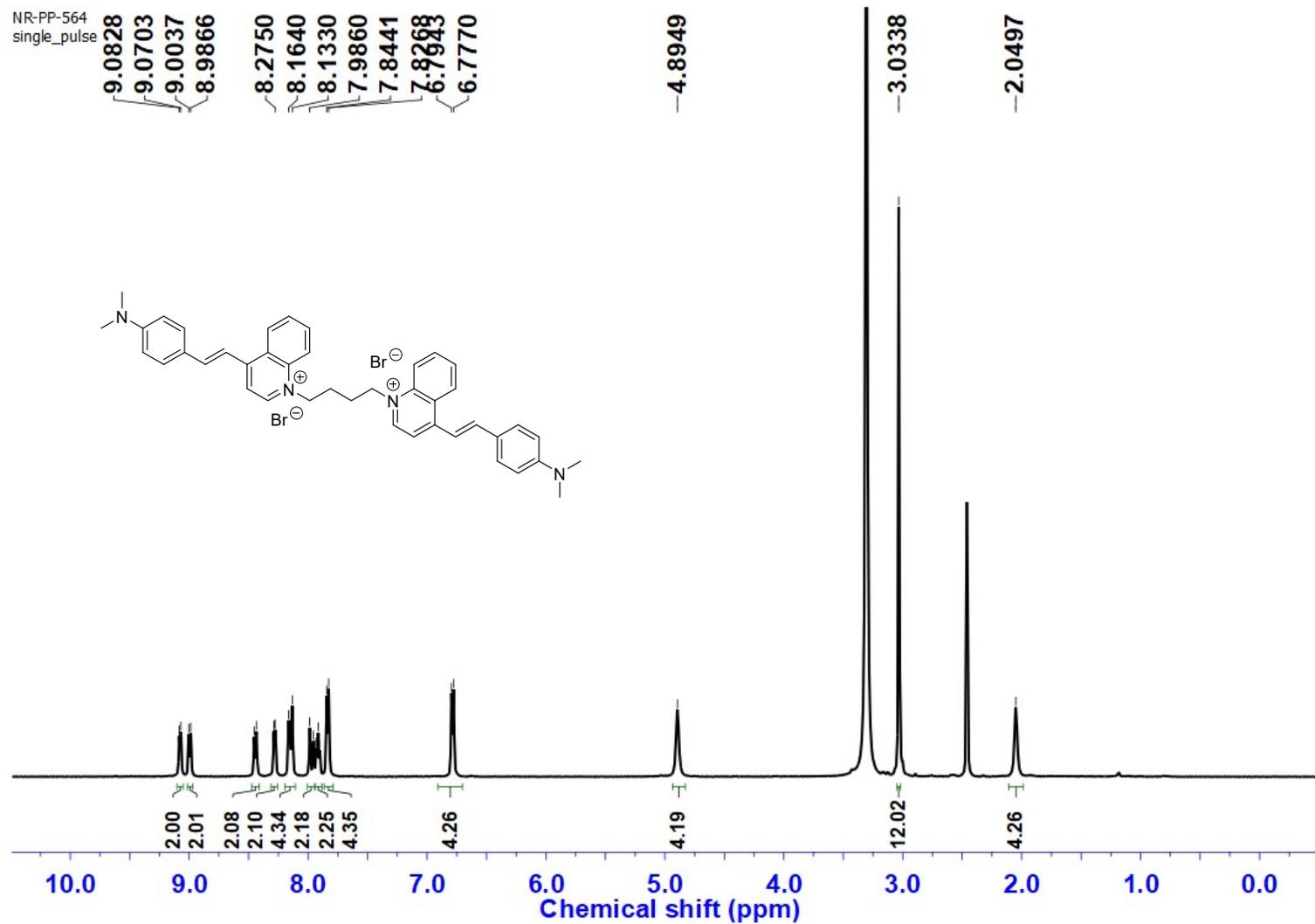


Figure S10. <sup>1</sup>H NMR spectrum of compound 6a.

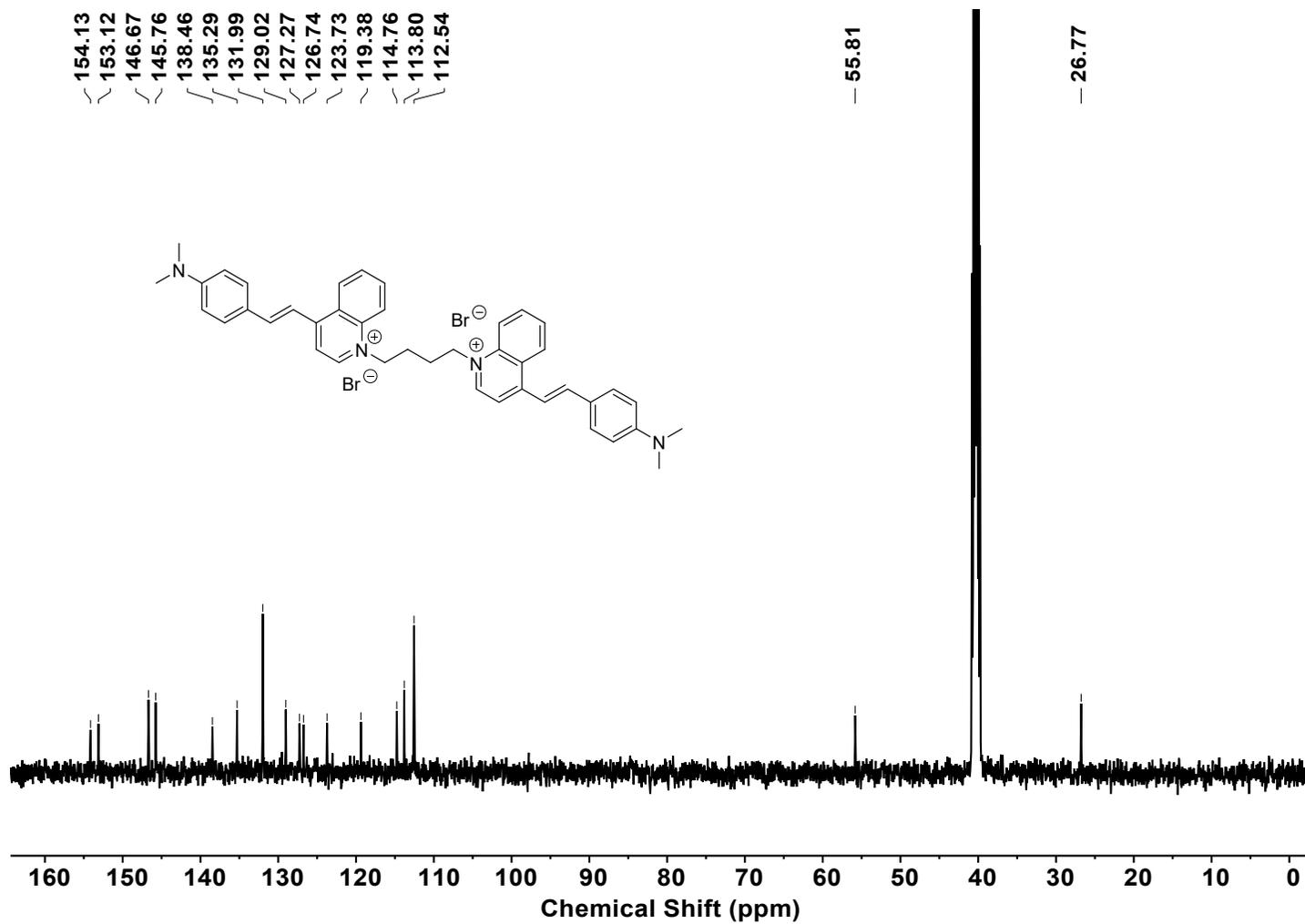
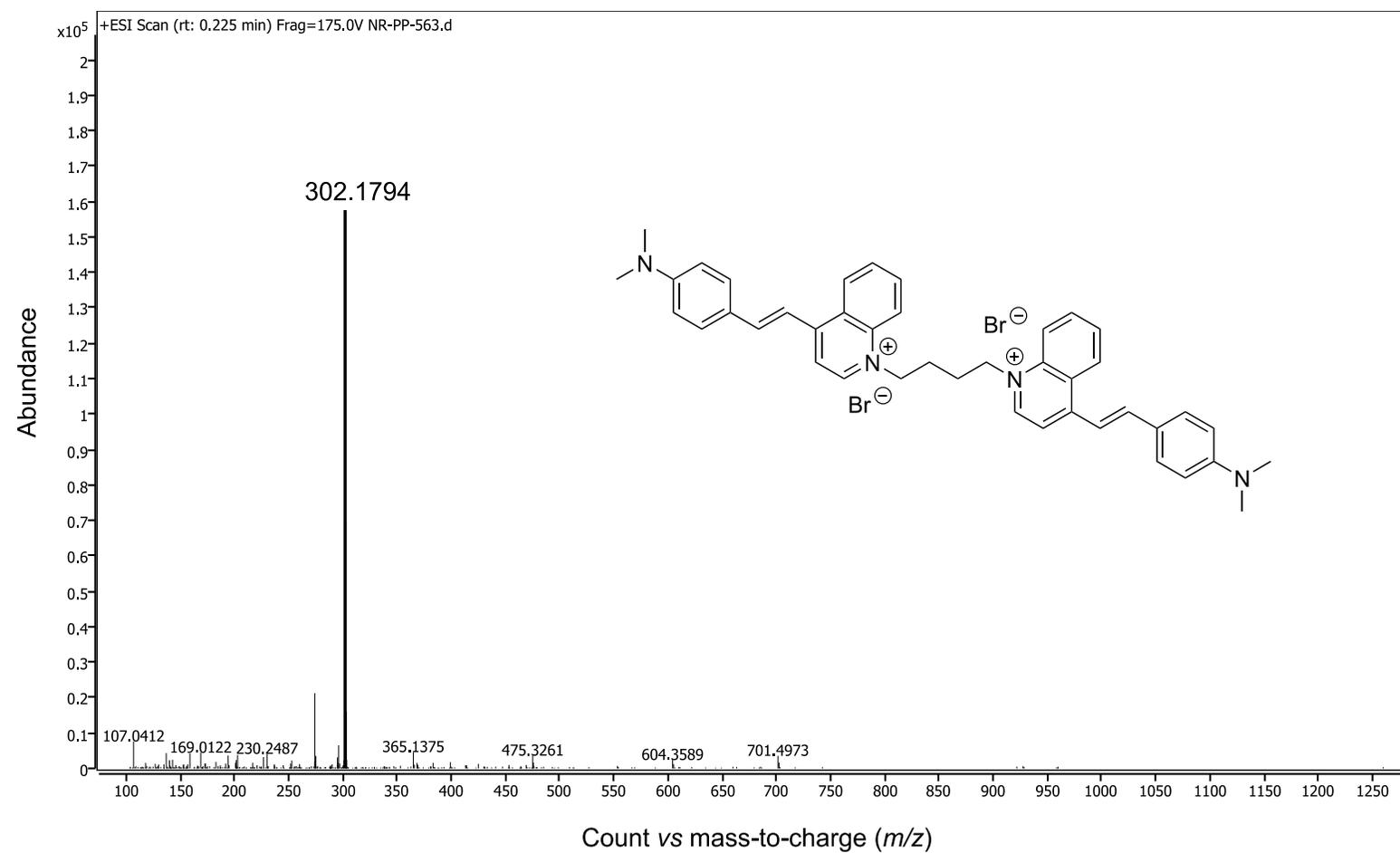
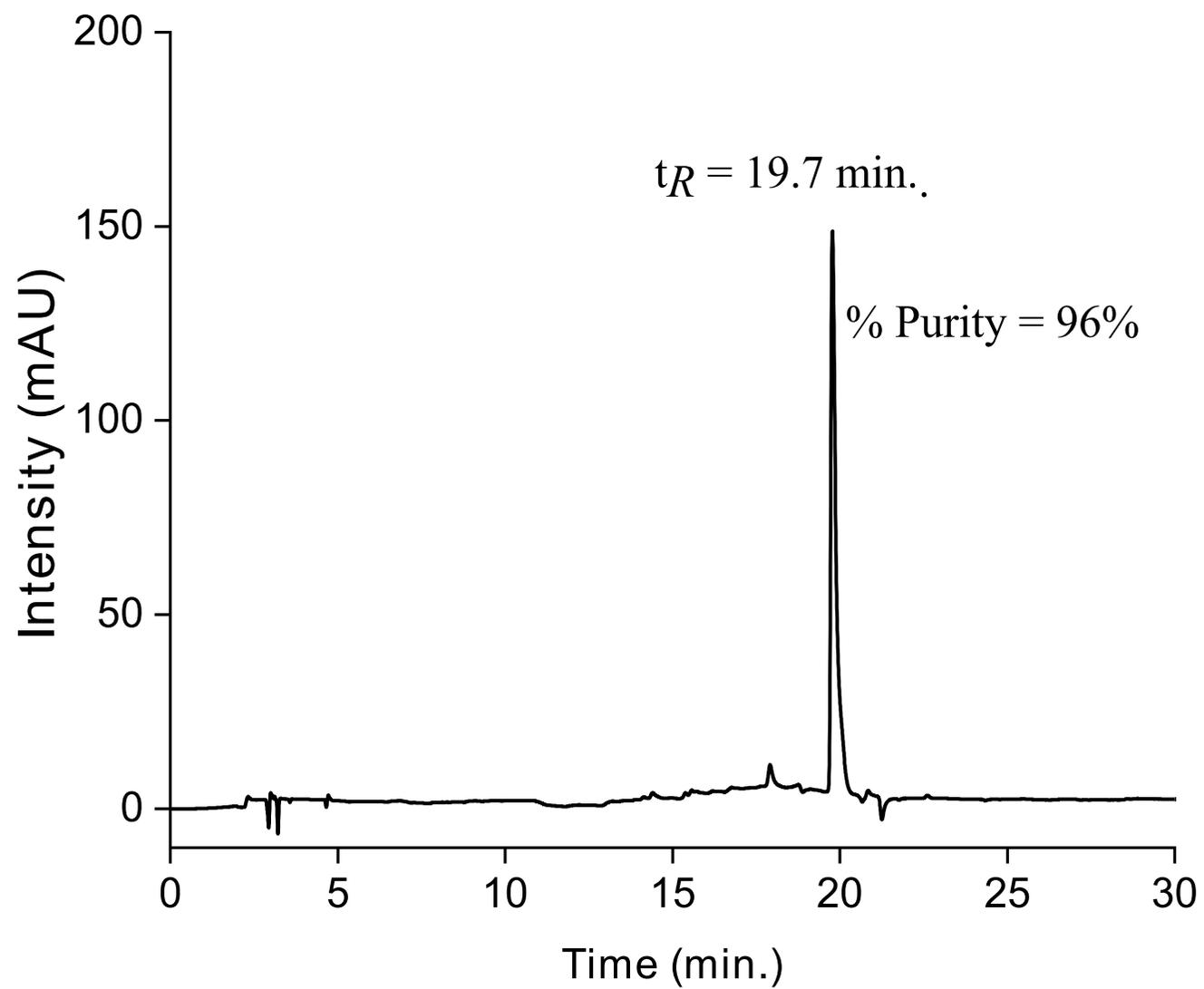


Figure S11. <sup>13</sup>C NMR spectrum of compound 6a



**Figure S12.** HRMS spectrum of compound **6a**



**Figure S13.** HPLC plot of compound **6a**

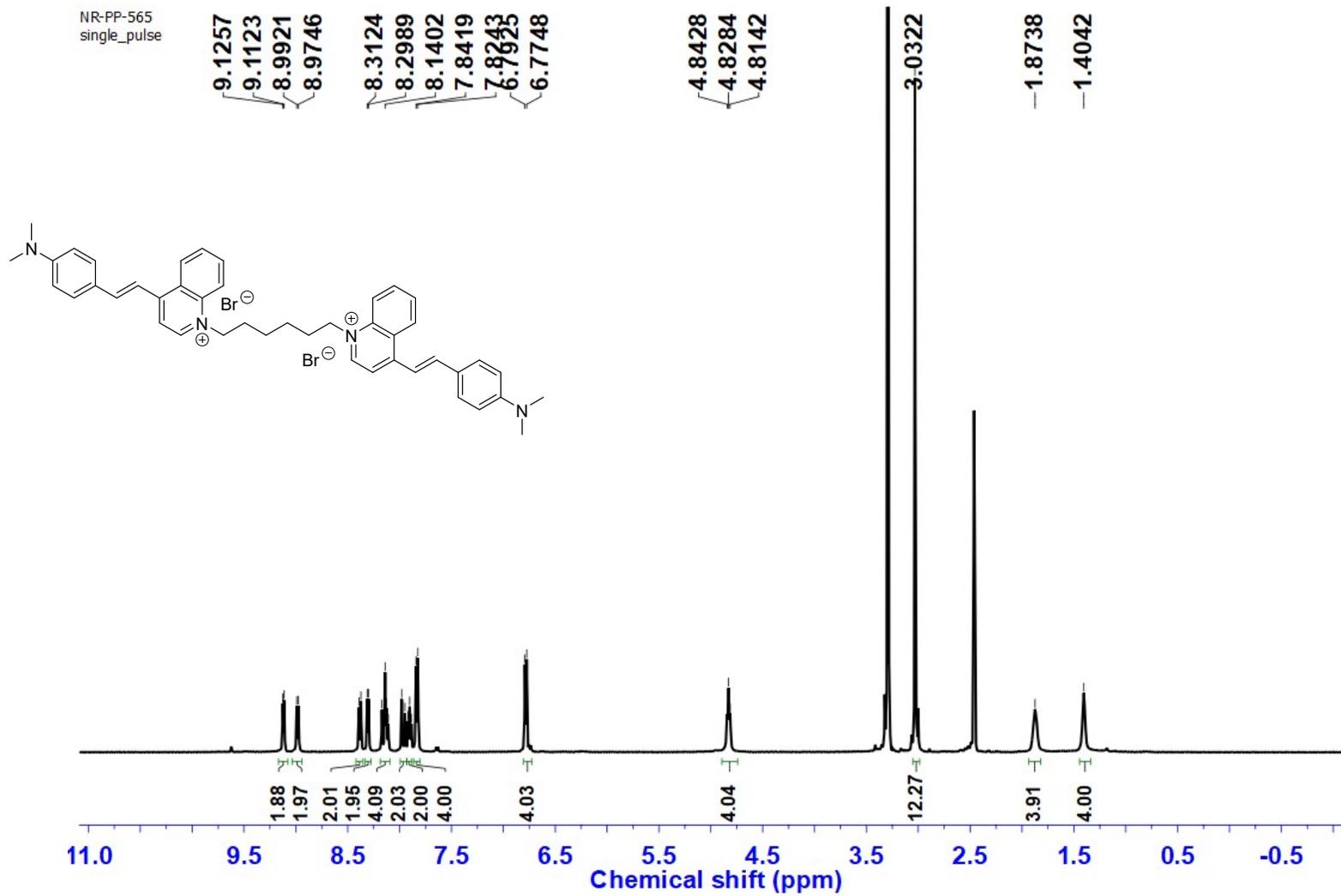


Figure S14.  $^1\text{H}$  NMR spectrum of compound **6b**

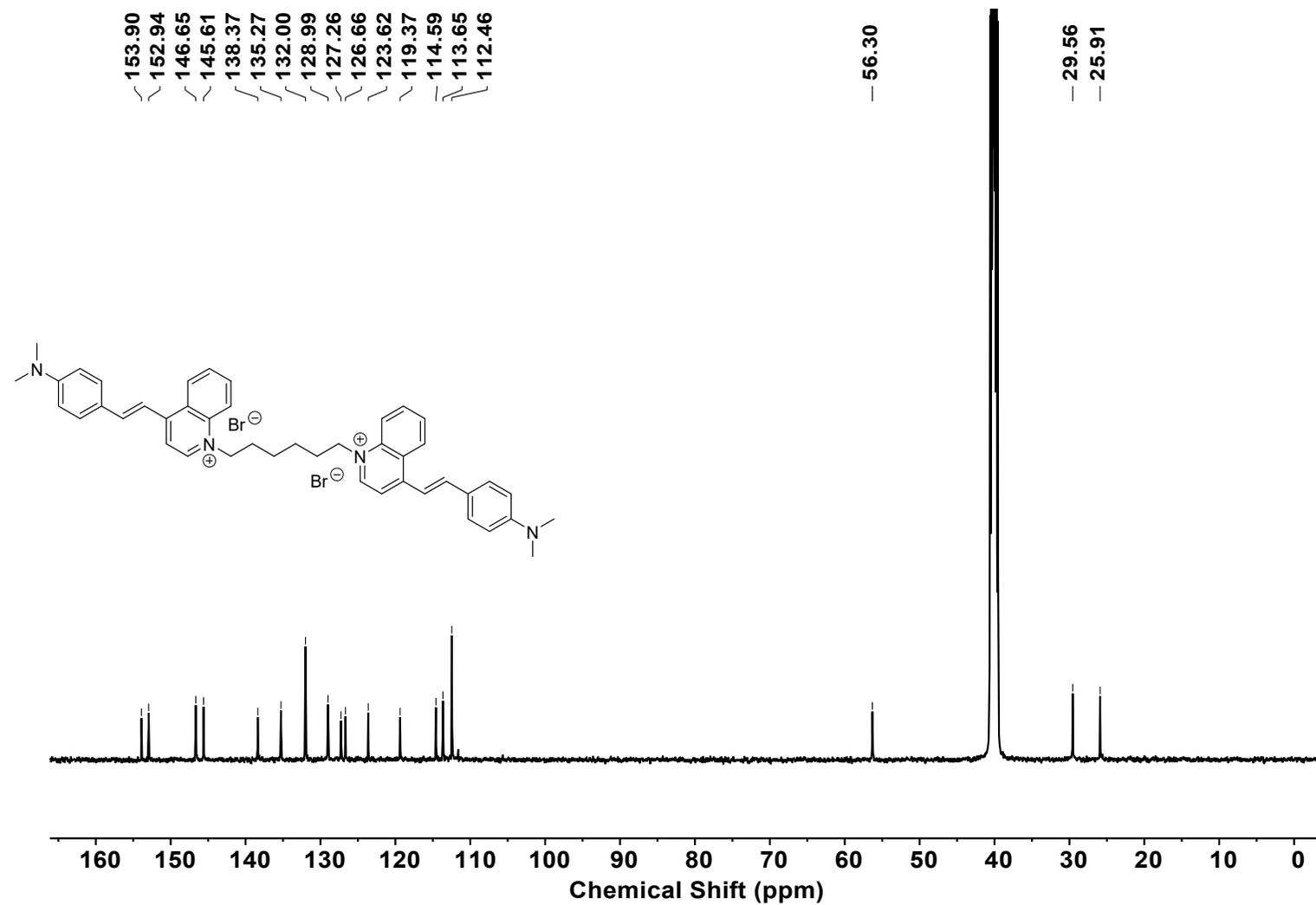


Figure S15.  $^{13}\text{C}$  NMR spectrum of compound **6b**

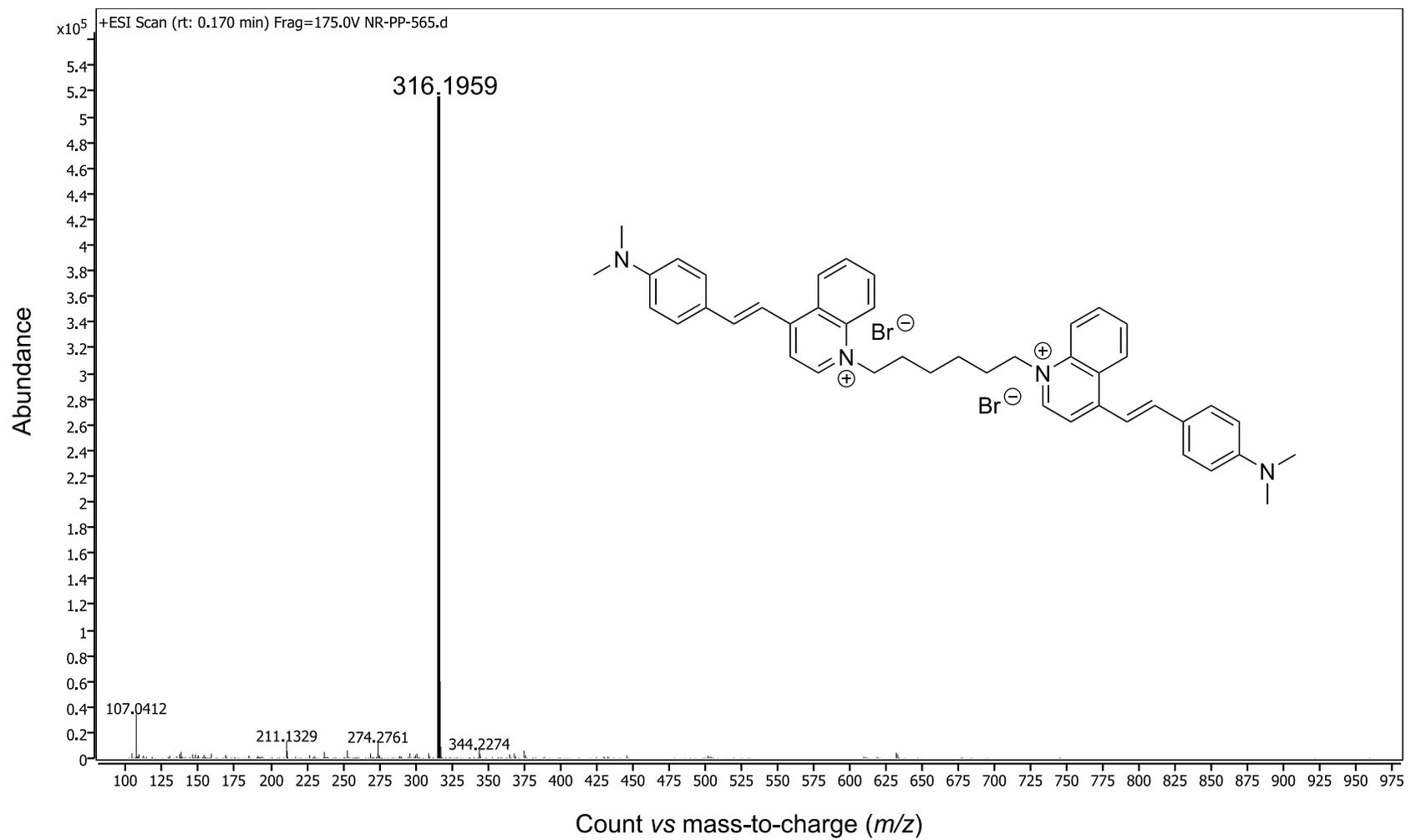


Figure S16. HRMS spectrum of compound 6b

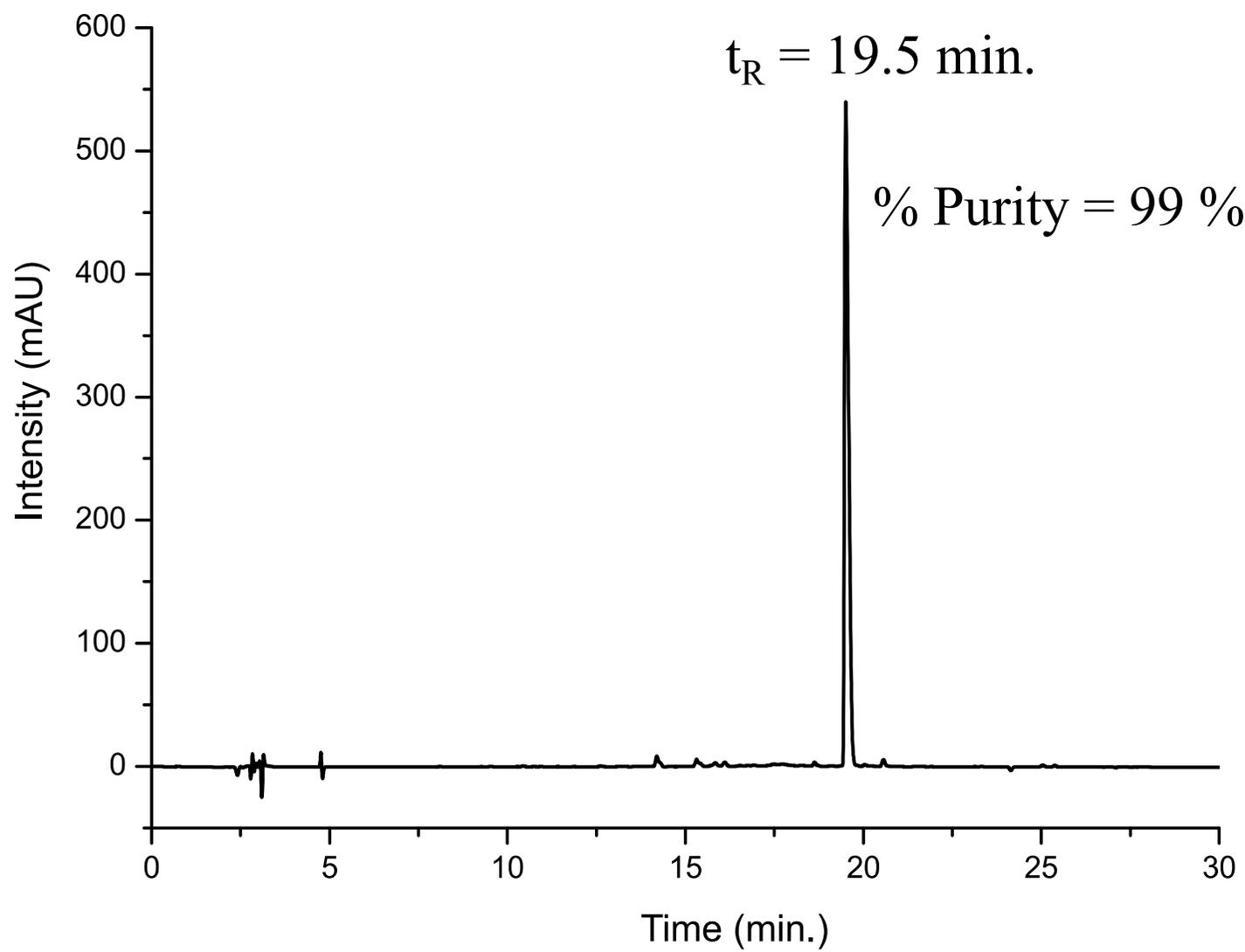


Figure S17. HPLC plot of compound **6b**

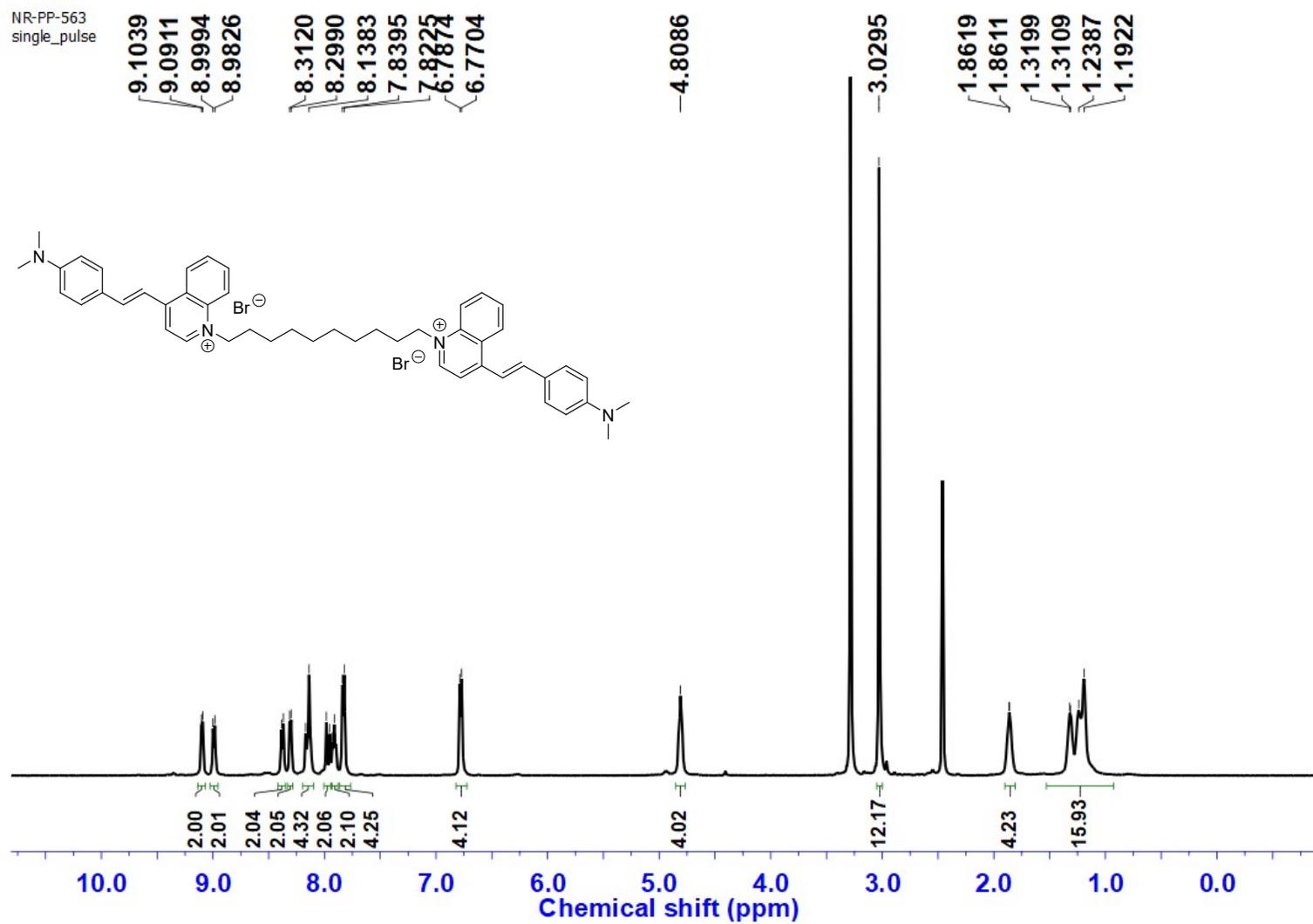


Figure S18.  $^1\text{H}$  NMR spectrum of compound 6c

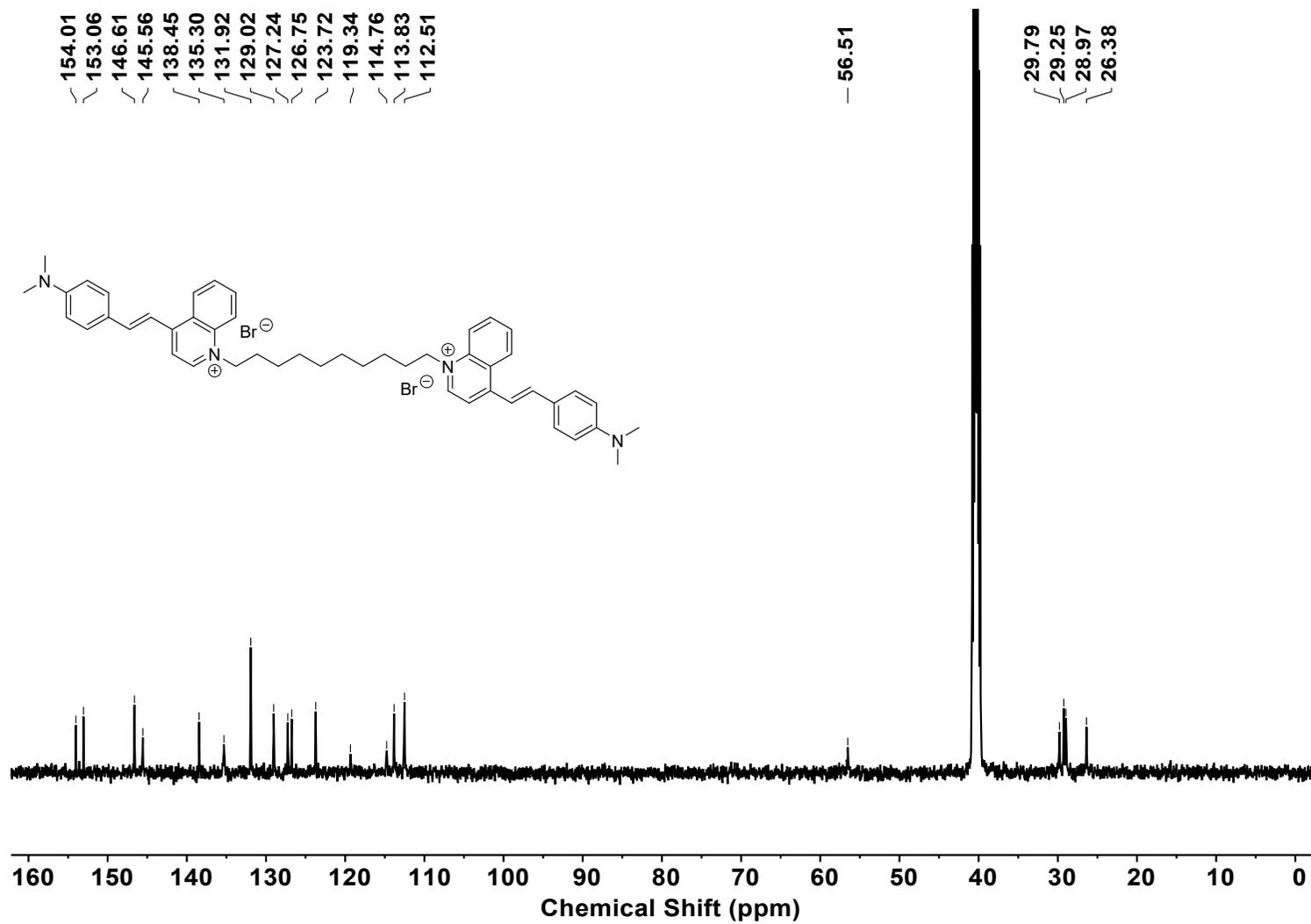
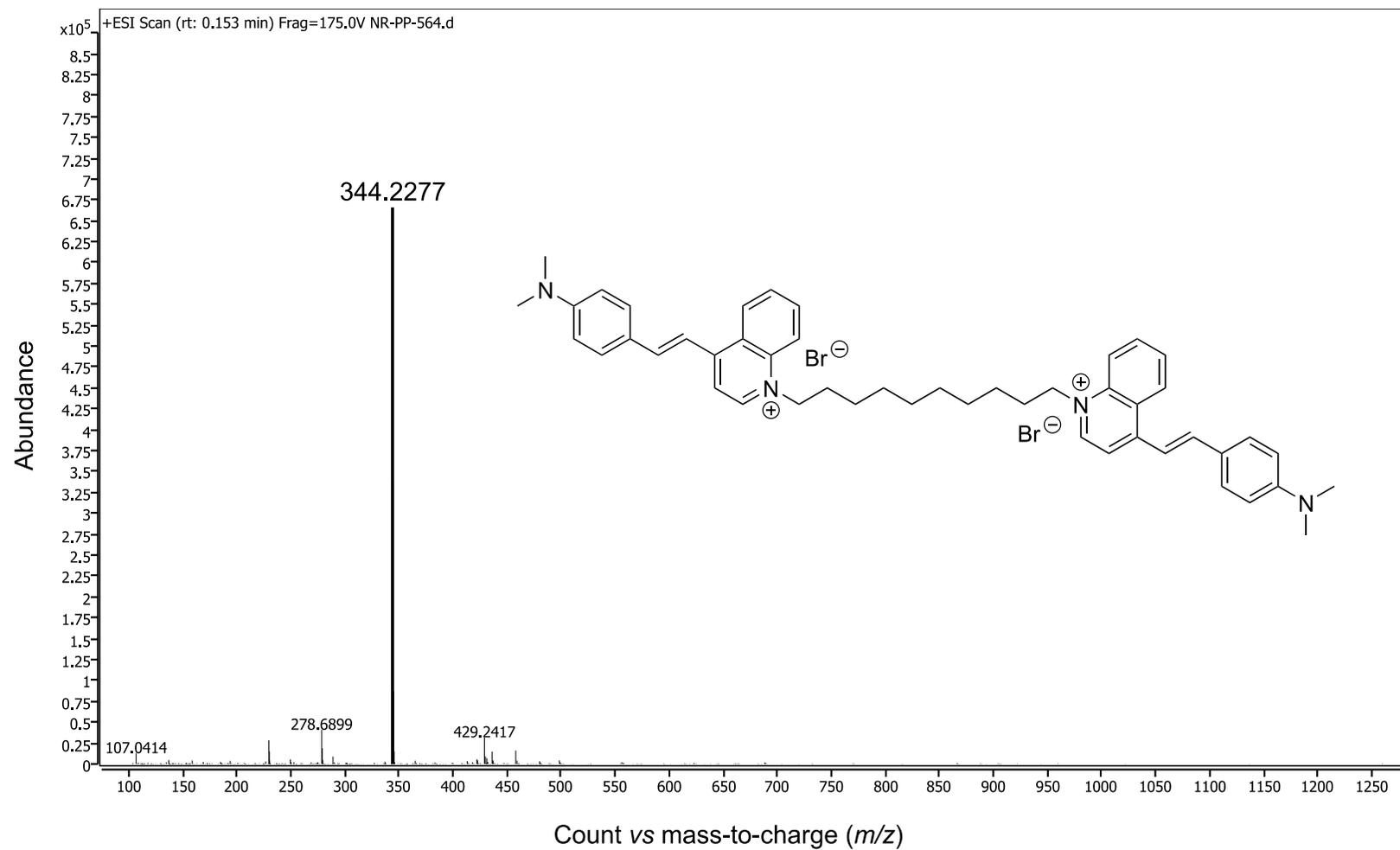
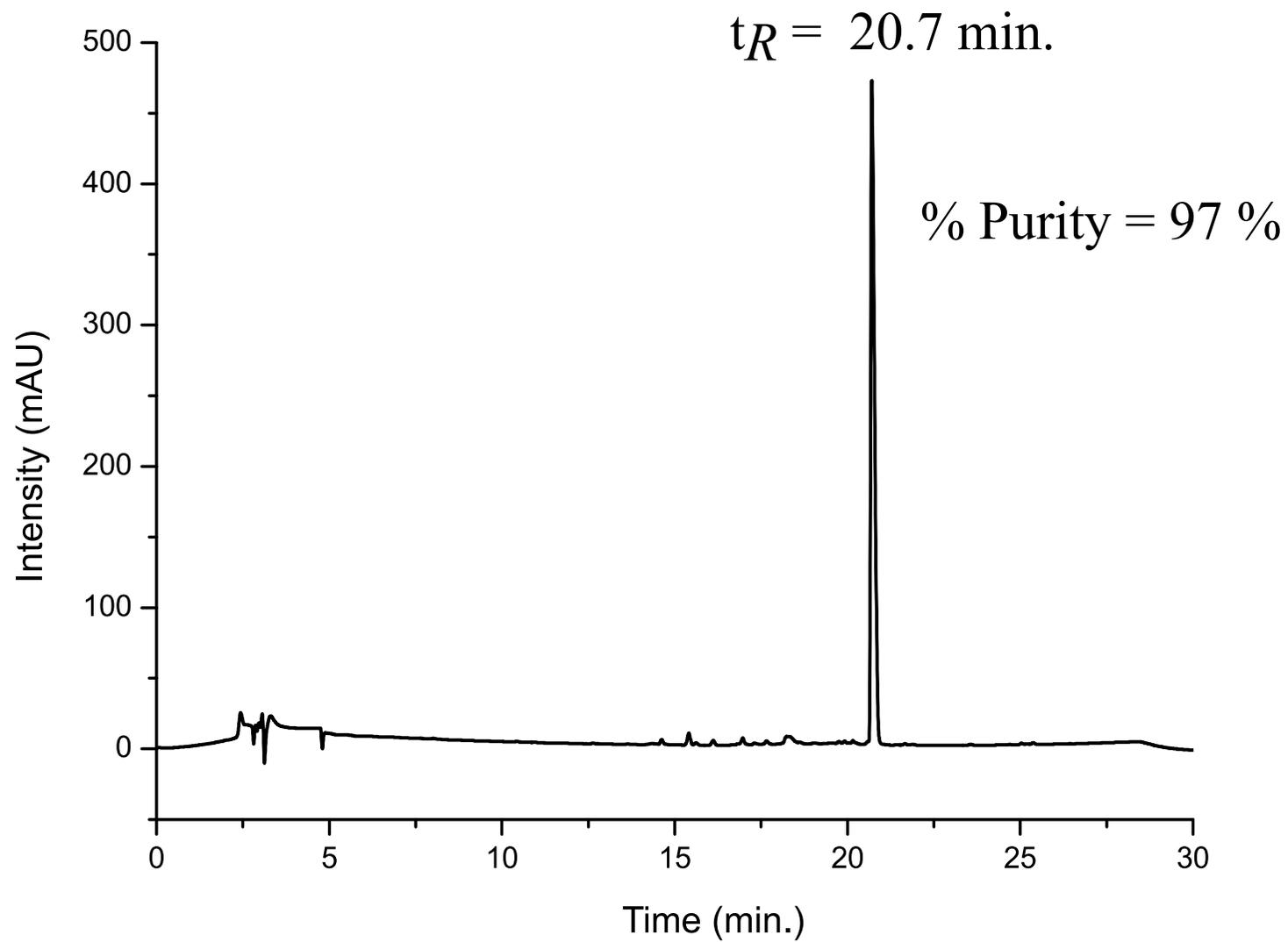


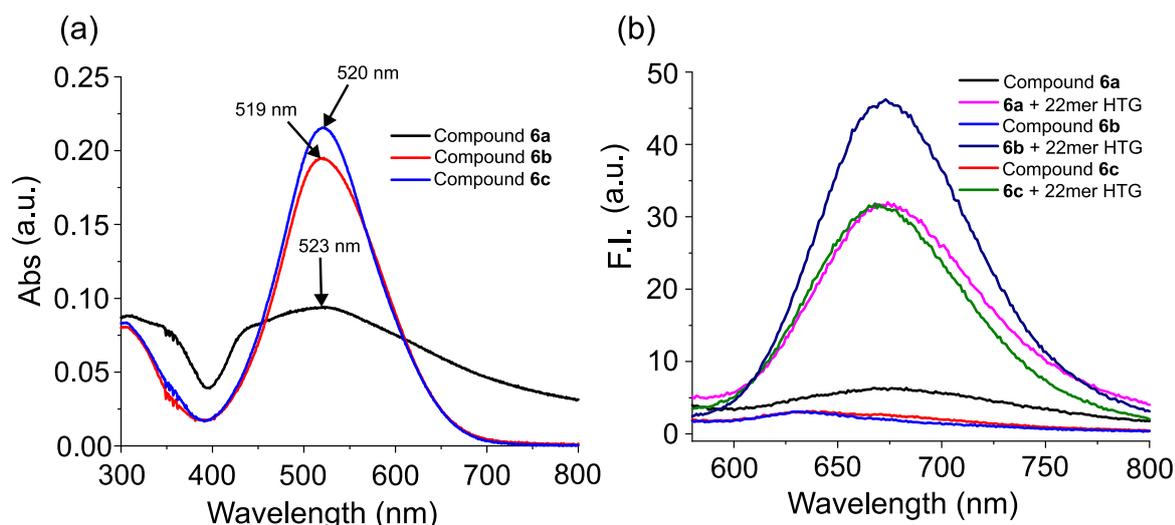
Figure S19. <sup>13</sup>C NMR spectrum of compound 6c



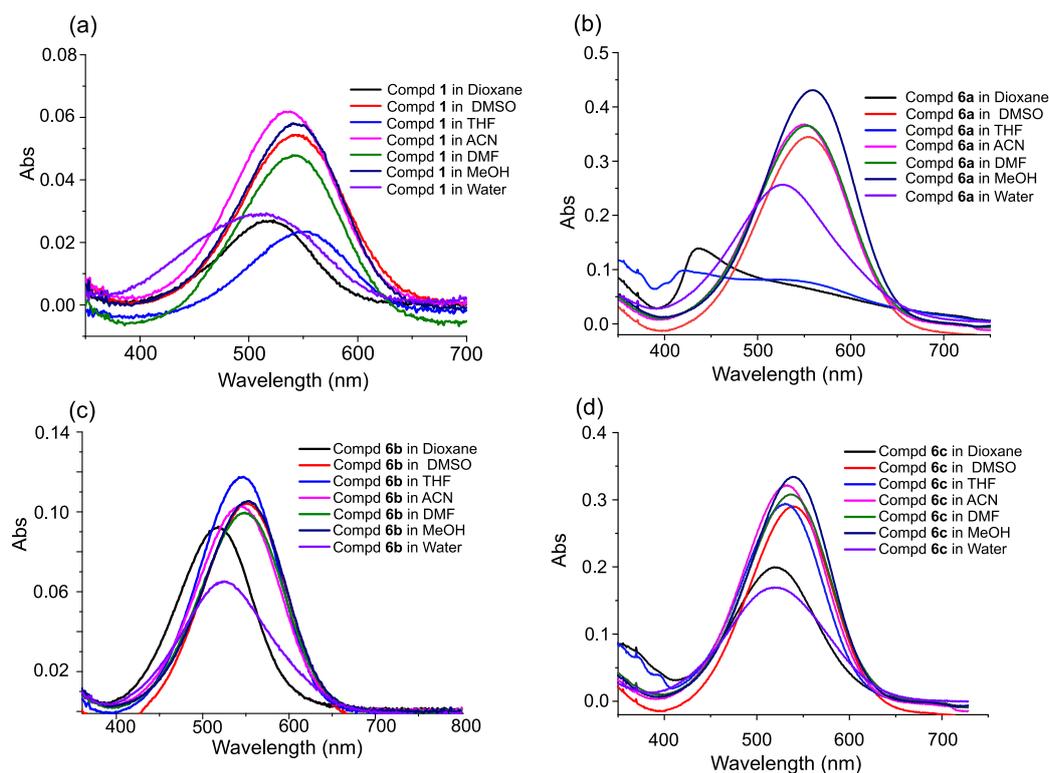
**Figure S20.** HRMS spectrum of compound **6c**



**Figure S21.** HPLC plot of compound **6c**

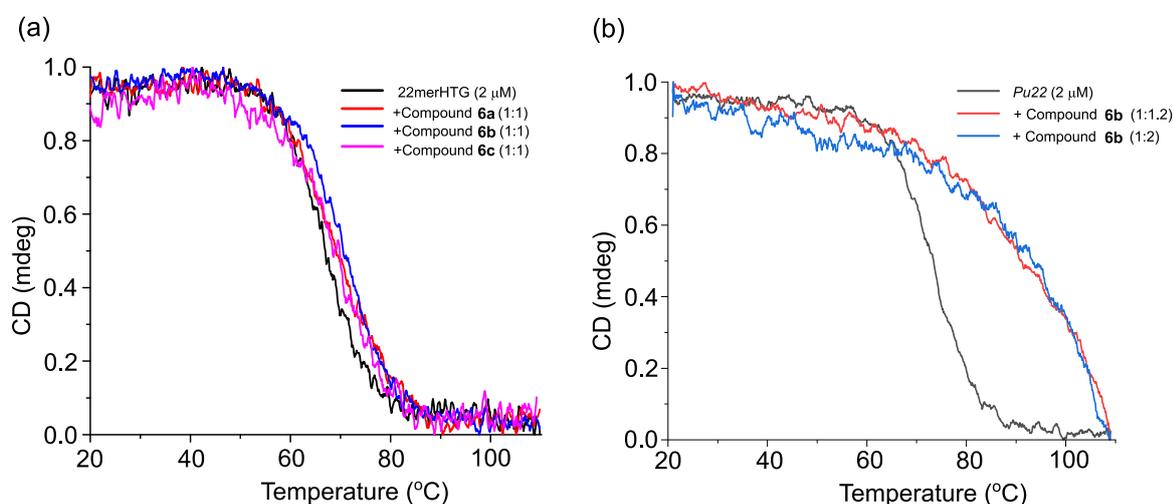


**Figure S22.** (a) UV-vis absorption spectra of compounds **6a-c** (b) emission spectra of compound **6a-c** alone and with 22mer HTG G-quadruplex. Experiments were conducted in buffer 10 mM potassium phosphate, 0.5 mM EDTA, and 100 mM KCl at pH 7.0 ( $T = 25$  °C).



**Figure S23.** UV-vis absorption spectra of compounds (a) compound **1** (b) **6a** (c) **6b** (d) **6c** in various solvents.

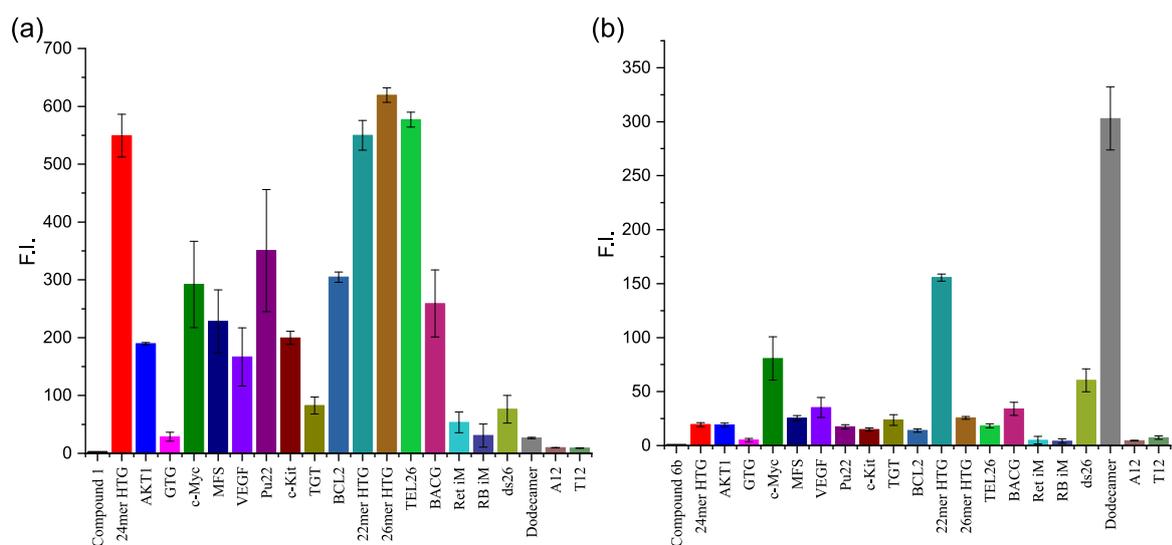
S.No.	Solvent	Compound <b>1</b> (nm)	Compound <b>6a</b> (nm)	Compound <b>6b</b> (nm)	Compound <b>6c</b> (nm)
1.	1,4-dioxane	518	436	517	529
2.	DMSO	543	554	551	551
3.	THF	536	420	545	541
4.	ACN	550	550	543	544
5.	MeOH	542	559	553	550
6.	DMF	541	553	549	547
7.	Water	513	528	524	529



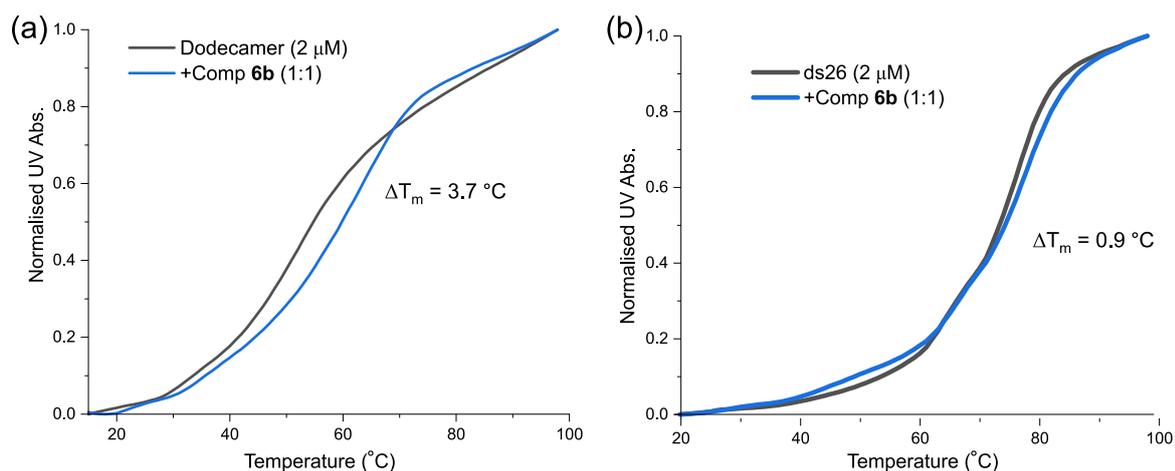
**Figure S24.** CD thermal denaturation curves for (a) 22merHTG G-quadruplex (5  $\mu$ M) in the absence (black line) and presence of compound **6a** at 1:1 (red line) and **6b** at 1:1 (blue line) and compound **6c** (pink line) (b) *Pu22* G-quadruplex (5  $\mu$ M) in the absence (black line) and presence of compound **6a-b** at 1:1 (red, blue) DNA to ligand ratios. The experiments for 22merHTG were performed in 10 mM potassium phosphate, 0.5 mM EDTA, and 100 mM KCl buffer and for *Pu22* were performed in a buffer of 2 mM potassium phosphate, 0.1 mM EDTA, and 12 mM KCl at pH 7.0. The DNA was thermally denatured between 20  $^{\circ}$ C to 110  $^{\circ}$ C at the rate of 1.0  $^{\circ}$ C/min.

<b>Table S2.</b> CD thermal melting studies of compound <b>6b</b> with <i>Pu22</i> at
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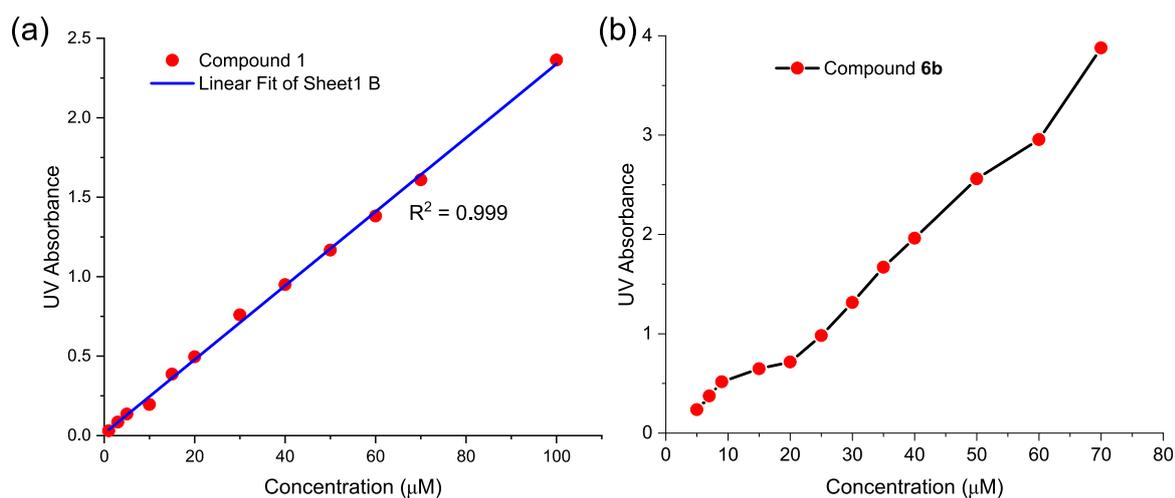
different ratios.				
DNA	Compound	DNA: Ligand ratio	<i>Pu22</i>	
<i>Pu22</i>	Compound <b>6b</b>		$T_m$ (°C)	$\Delta T_m$ (°C)
		-	73.8	-
		1:1	87.6	13.8
		1:1.2	93.07	19.2
		1.2	96.0	22.2



**Figure S25.** (a) Fluorescence emission bar plot showing the emission intensities of compound **1** ( $\lambda_{\text{ex}} = 580 \text{ nm}$ ,  $\lambda_{\text{em}} = 660 \text{ nm}$ ) and (b) compound **6b** ( $\lambda_{\text{ex}} = 521 \text{ nm}$ ,  $\lambda_{\text{em}} = 670 \text{ nm}$ ) upon binding to different nucleic acid sequences at a 1:1 DNA: ligand ratio. All experiments were performed in triplicate, and the corresponding standard deviations were calculated. Measurements were carried out in 10 mM potassium phosphate buffer containing 0.5 mM EDTA and 100 mM KCl (pH 7.0) at 20 °C. The concentration of compound **1** and **6b** was 1.0  $\mu\text{M}$ .



**Figure S26.** UV-vis-based thermal denaturation studies of (a) dodecamer and (b) ds26 DNA duplex in the absence and presence of compound **6b** in 10 mM potassium phosphate buffer containing 0.5 mM EDTA and 100 mM KCl (pH 7.0) at a 1:1 DNA: ligand ratio. The duplex DNA was used at a concentration of 2 μM per duplex.



**Figure S27.** The absorbance versus concentration plots of (a) compound **1** and (b) compound **6b** showing the effect of concentration on linearity of their absorbance values.