

## Supplementary Material (SM)

# Scaffold Hopping and Structural Modification of NSC 663284: Discovery of Potent (Non)Halogenated Aminobenzoquinones

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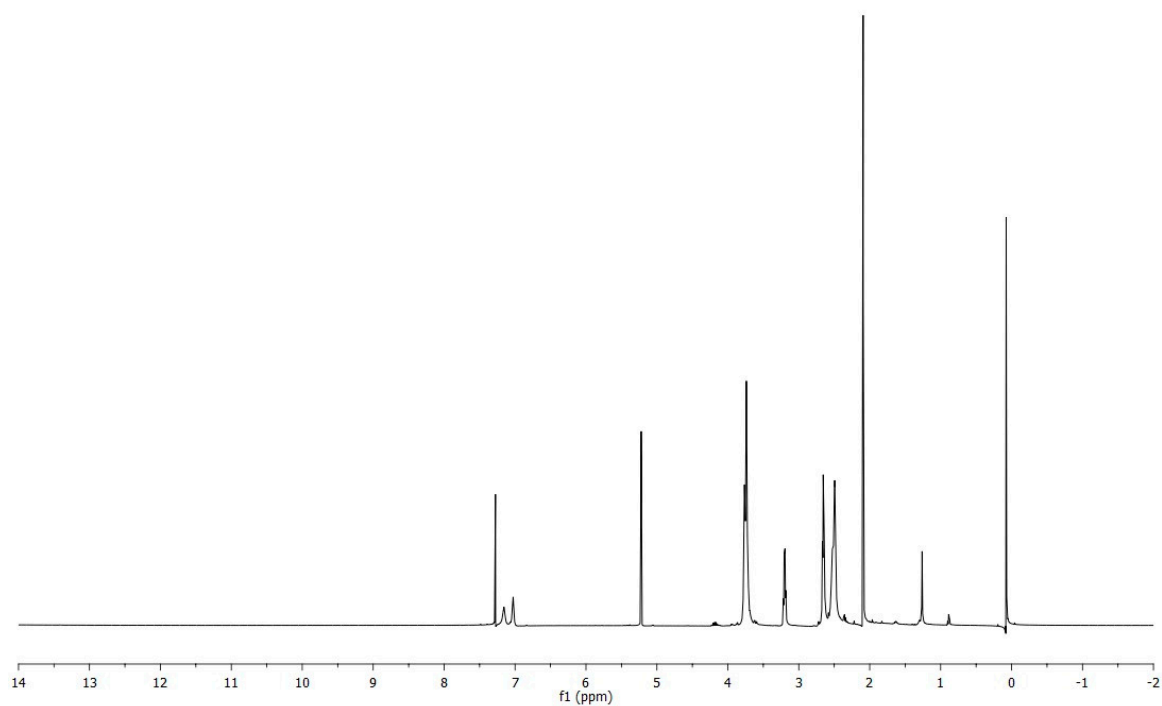
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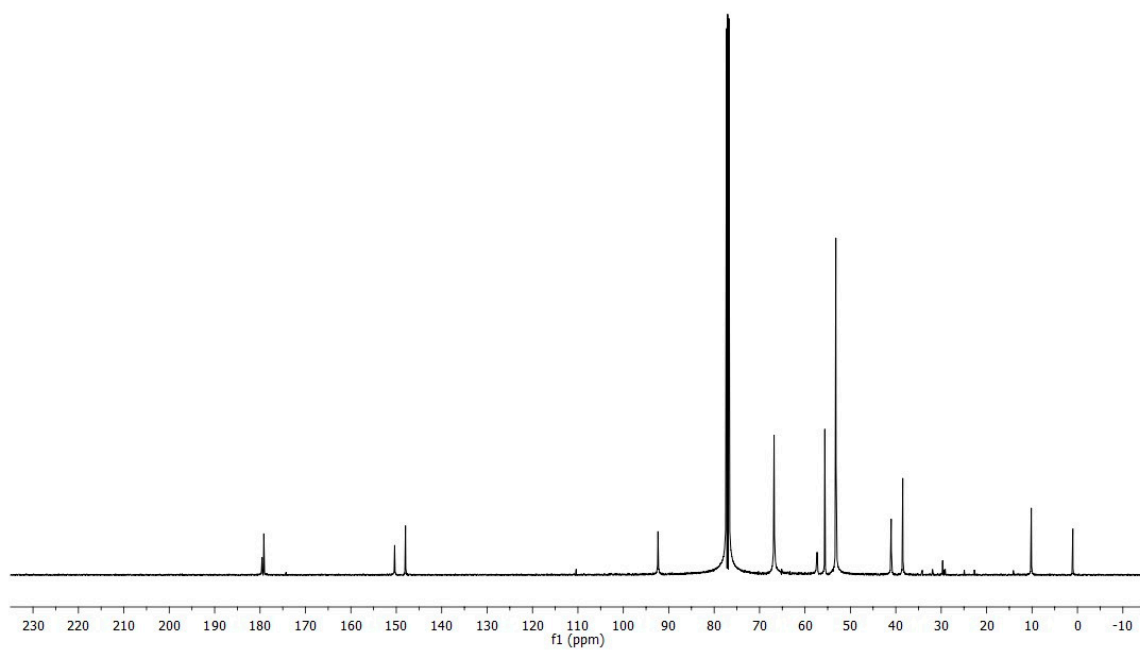
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## Contents

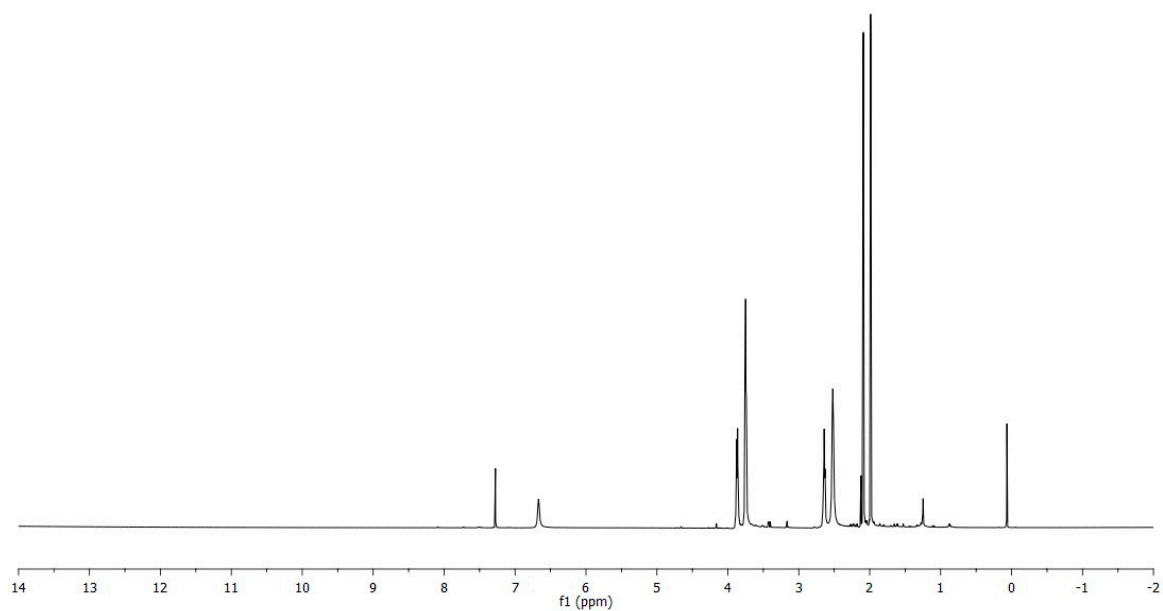
$^1\text{H}$ and $^{13}\text{C}$ spectra of the PQ analogs ( <b>PQ1-4</b> )	S3-6
HRMS spectra of the PQ analogs ( <b>PQ1-4</b> )	S7



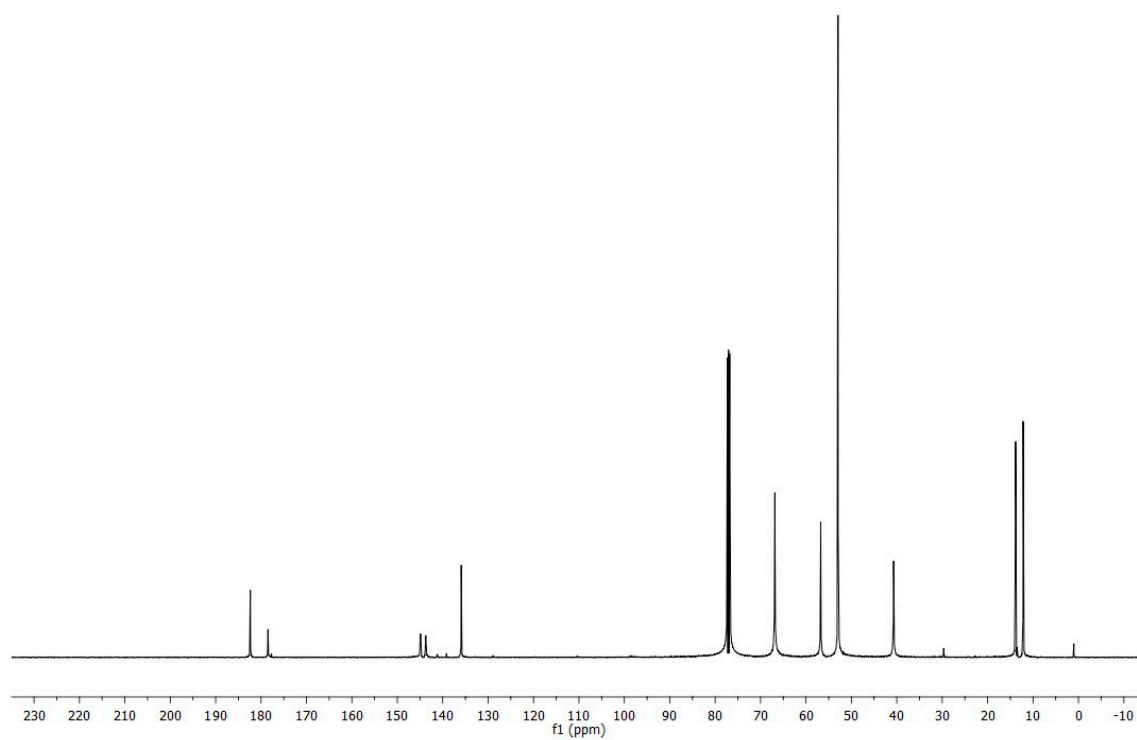
**Figure S1:**  $^1\text{H}$  NMR (500 MHz) spectrum of the **PQ1** in  $\text{CDCl}_3-d_1$



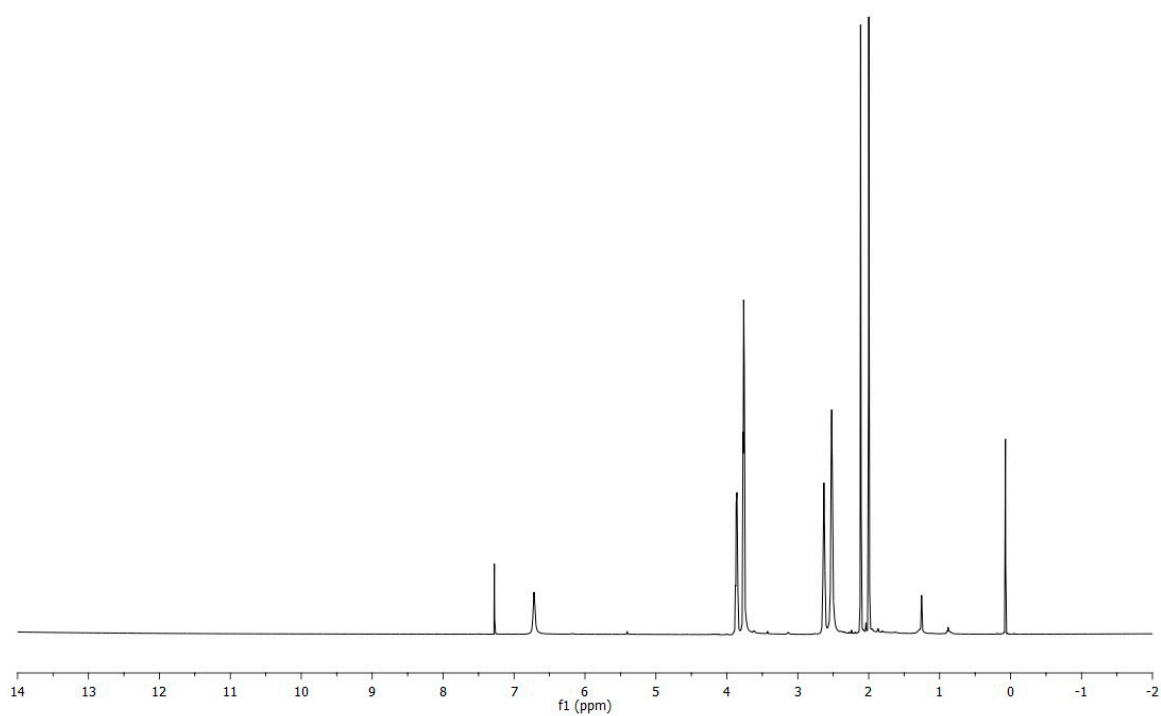
**Figure S2:**  $^{13}\text{C}$  NMR (125 MHz) spectrum of the **PQ1** in  $\text{CDCl}_3-d_1$



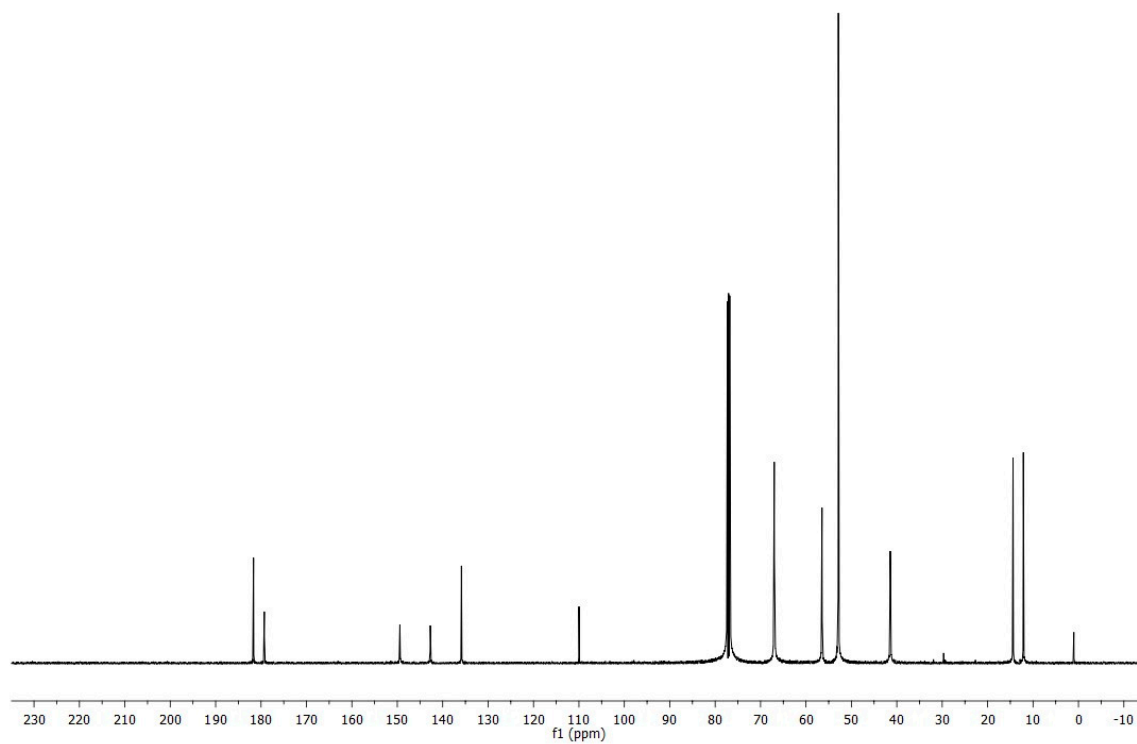
**Figure S3:**  $^1\text{H}$  NMR (500 MHz) spectrum of the **PQ2** in  $\text{CDCl}_3\text{-}d_1$



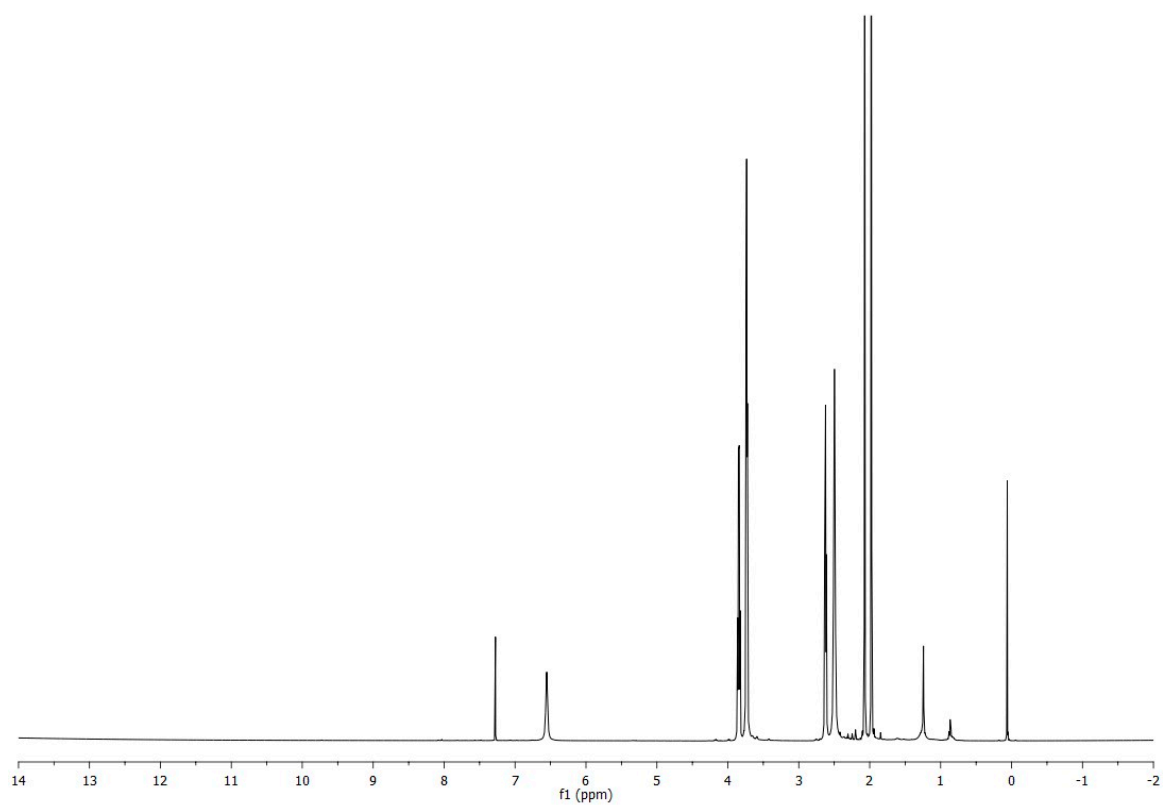
**Figure S4:**  $^{13}\text{C}$  NMR (125 MHz) spectrum of the **PQ2** in  $\text{CDCl}_3\text{-}d_1$



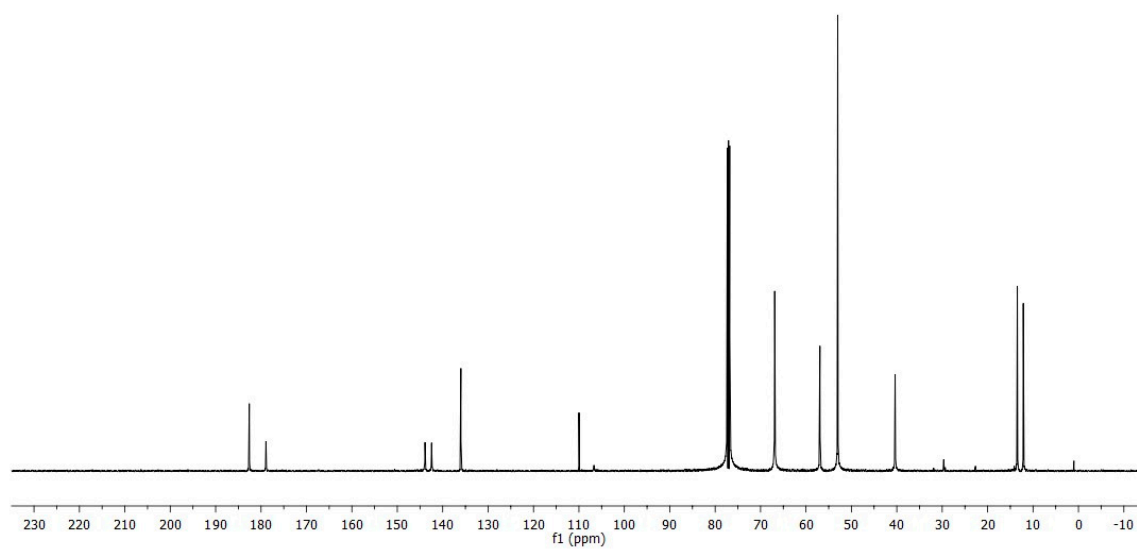
**Figure S5:**  $^1\text{H}$  NMR (500 MHz) spectrum of the **PQ3** in  $\text{CDCl}_3-d_1$



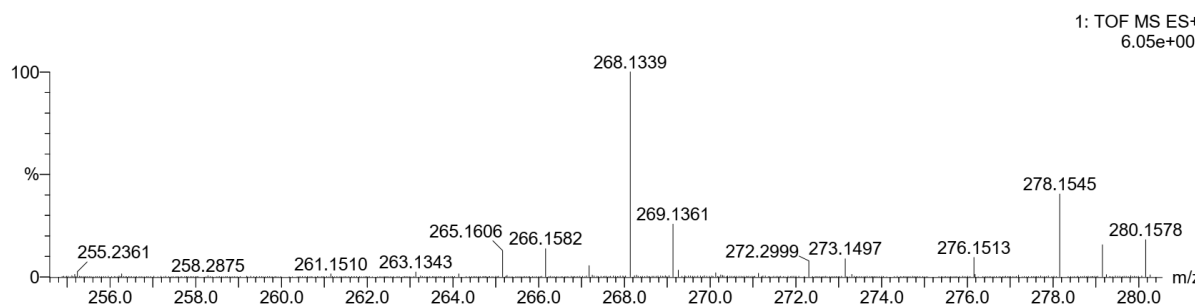
**Figure S6:**  $^{13}\text{C}$  NMR (125 MHz) spectrum of the **PQ3** in  $\text{CDCl}_3-d_1$



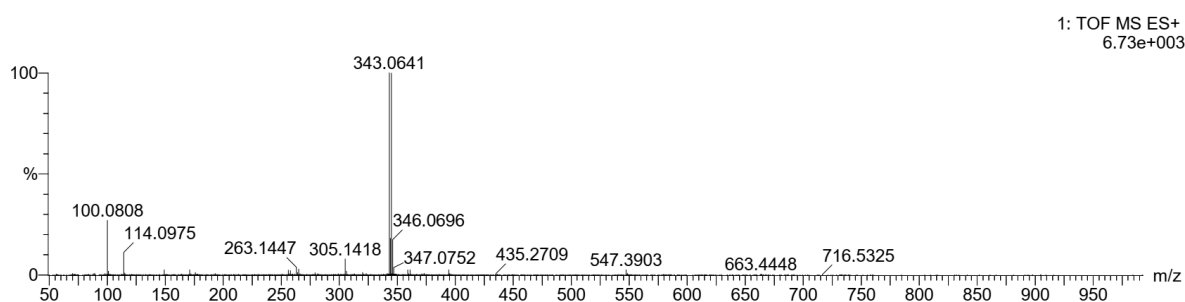
**Figure S7:**  $^1\text{H}$  NMR (500 MHz) spectrum of the **PQ4** in  $\text{CDCl}_3-d_1$



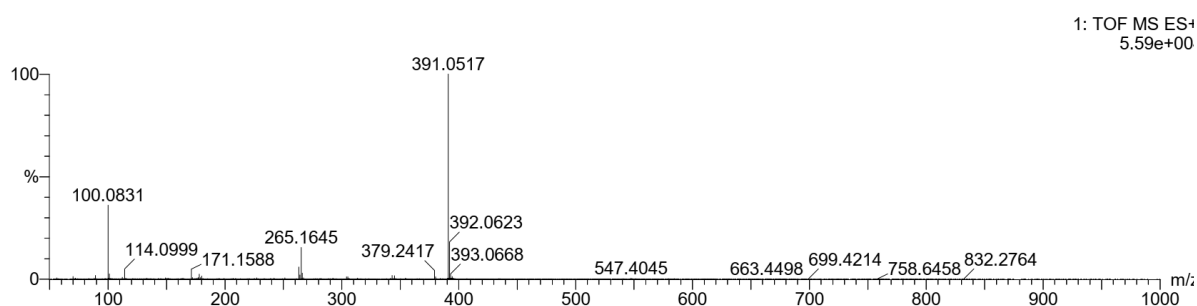
**Figure S8:**  $^{13}\text{C}$  NMR (125 MHz) spectrum of the **PQ4** in  $\text{CDCl}_3-d_1$



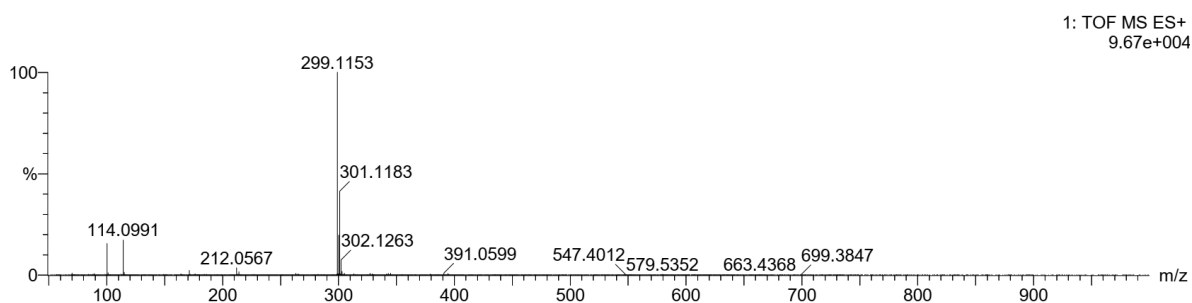
**Figure S9: HRMS spectrum of the PQ1**



**Figure S10: HRMS spectrum of the PQ2**



**Figure S11: HRMS spectrum of the PQ3**



**Figure S12: HRMS spectrum of the PQ4**