

Supplementary Materials

# Post Synthetic Modification of Planar Antiaromatic Hexaphyrin(1.0.1.0.1.0) By Regio-selective, Squential S<sub>N</sub>Ar

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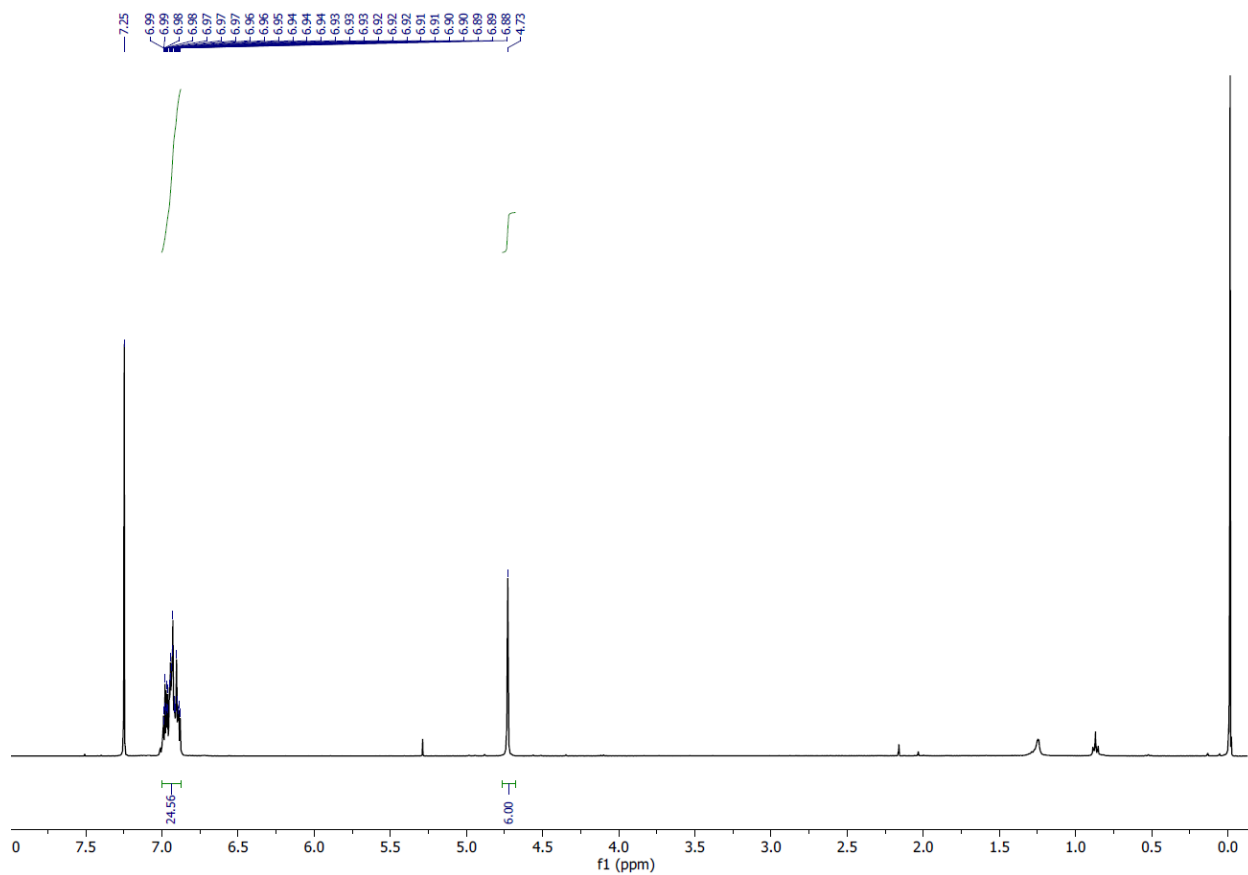


Figure S1. <sup>1</sup>H NMR of **3** in CDCl<sub>3</sub>.

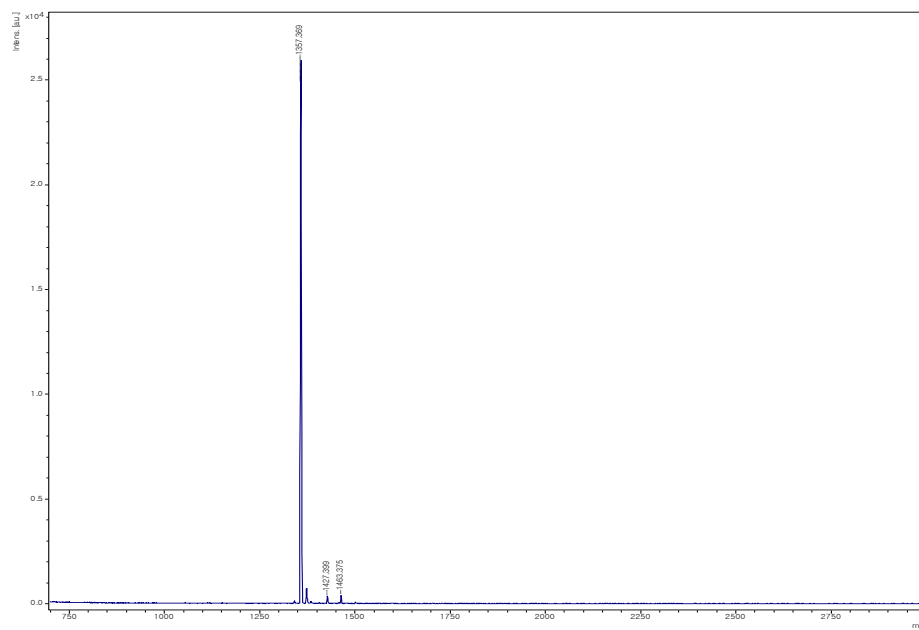


Figure S2. MALDI-TOF spectrum of 3.

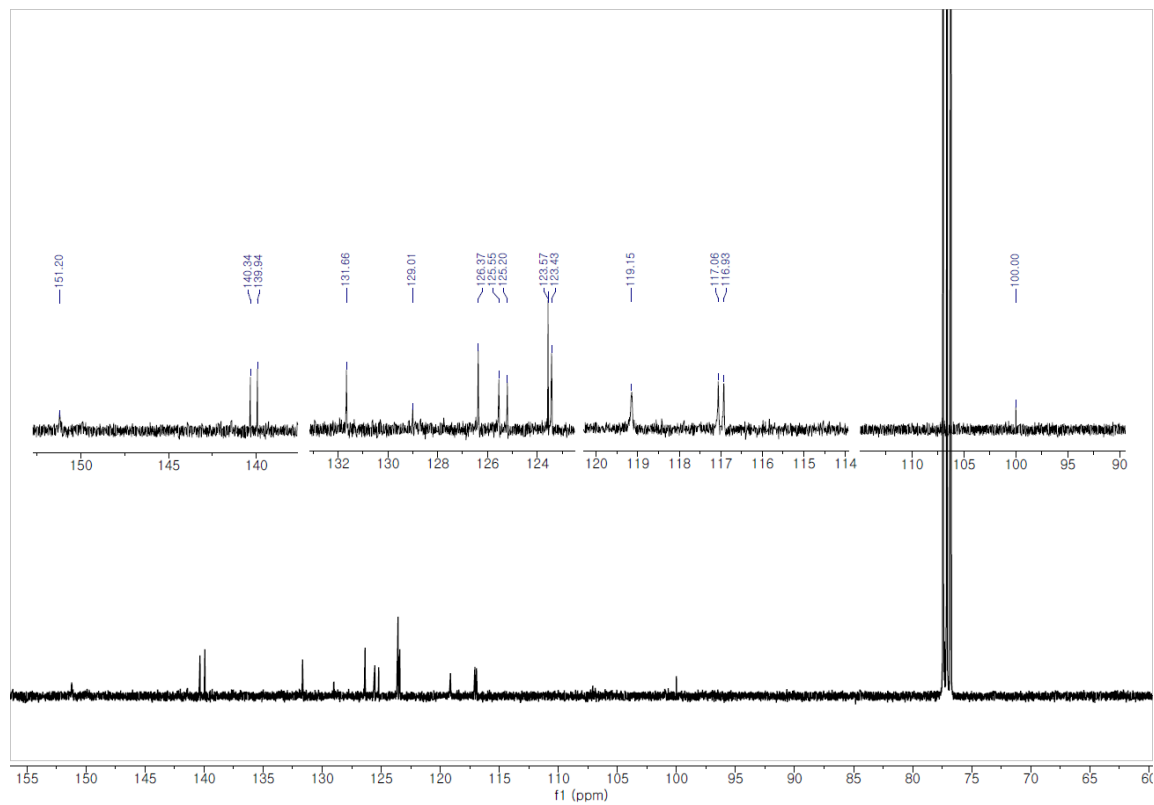
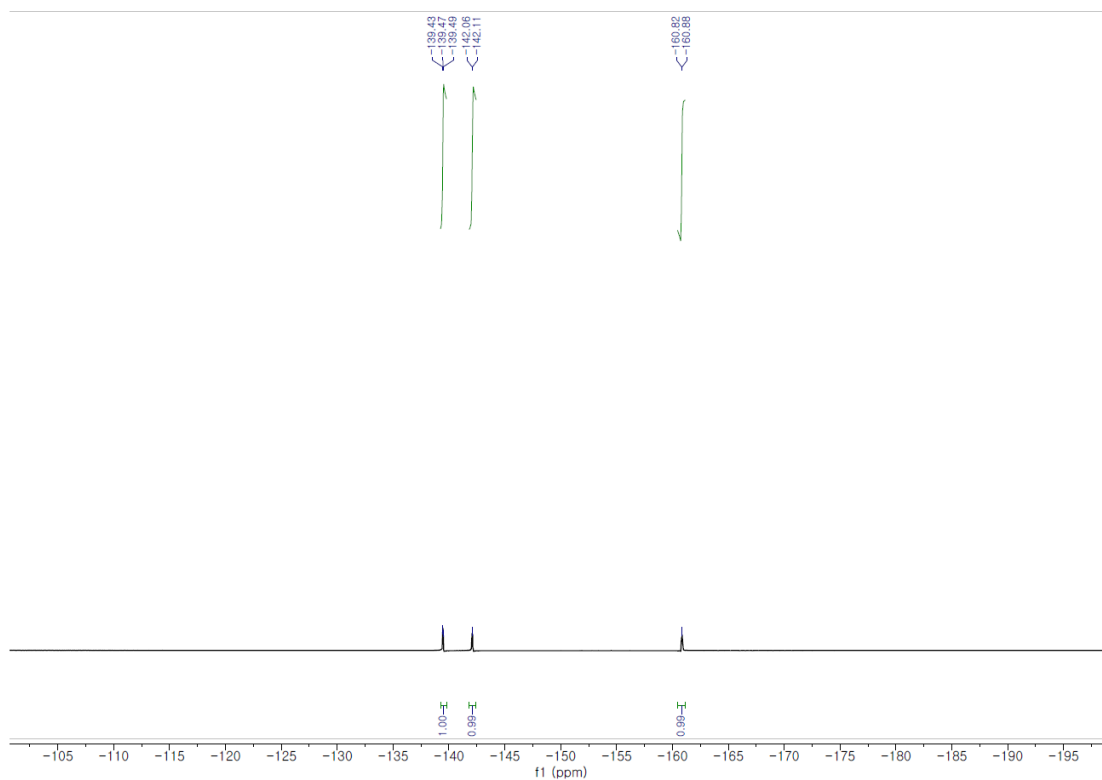
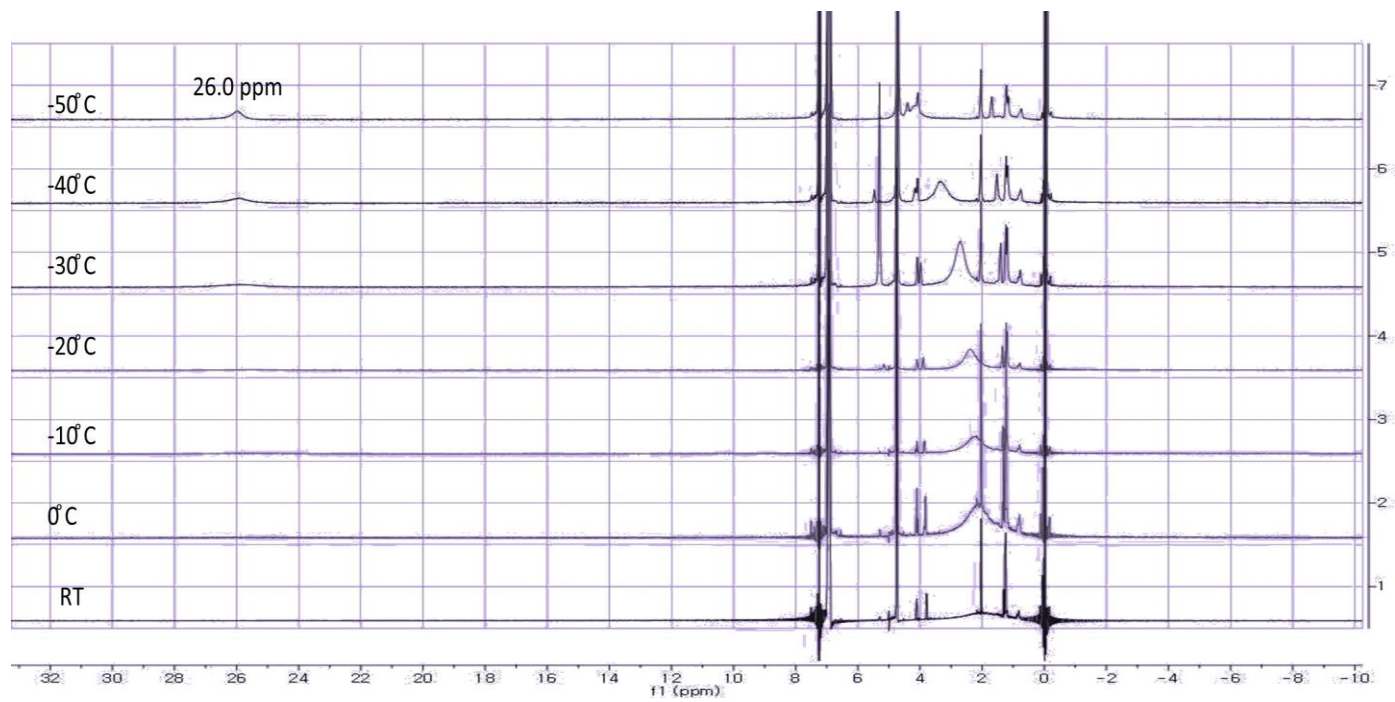


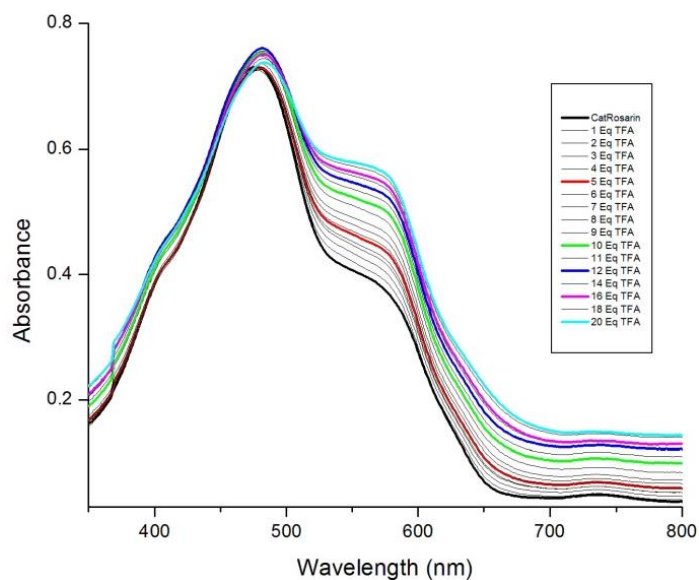
Figure S3. <sup>13</sup>C NMR of 3 in CDCl<sub>3</sub> (expanded region is included).



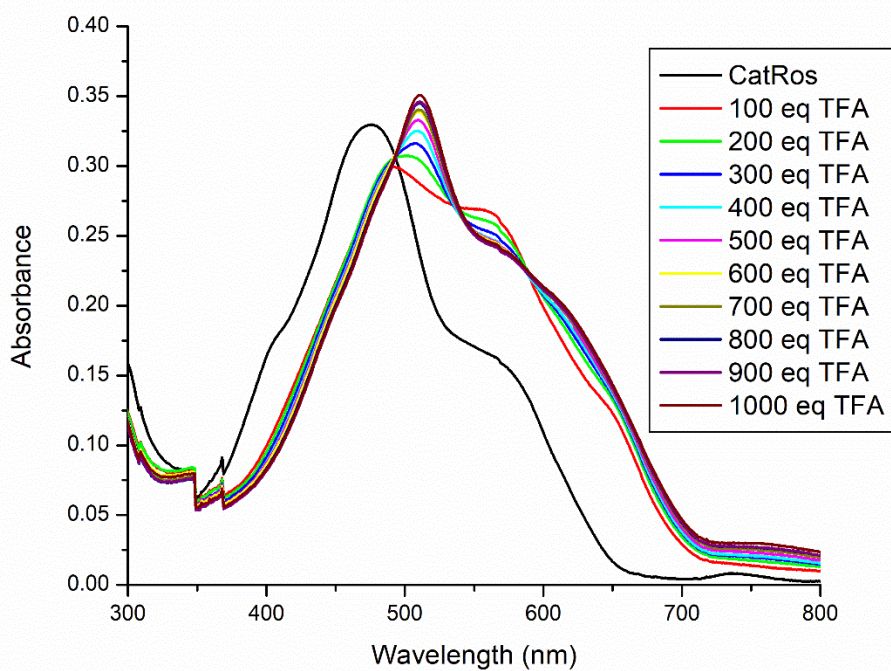
**Figure S4.**  $^{19}\text{F}$  NMR of **3** in  $\text{CDCl}_3$ .



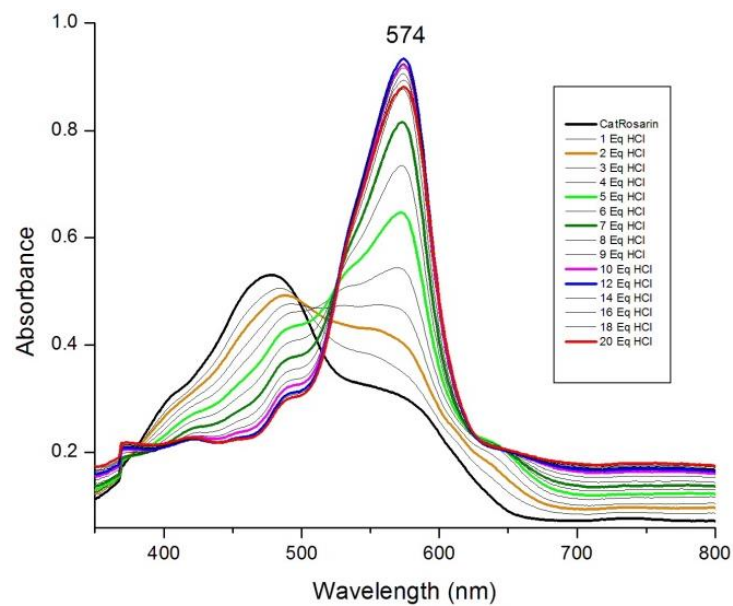
**Figure S5.** Low temperature  $^1\text{H}$  NMR of **3** in  $\text{CDCl}_3$ .



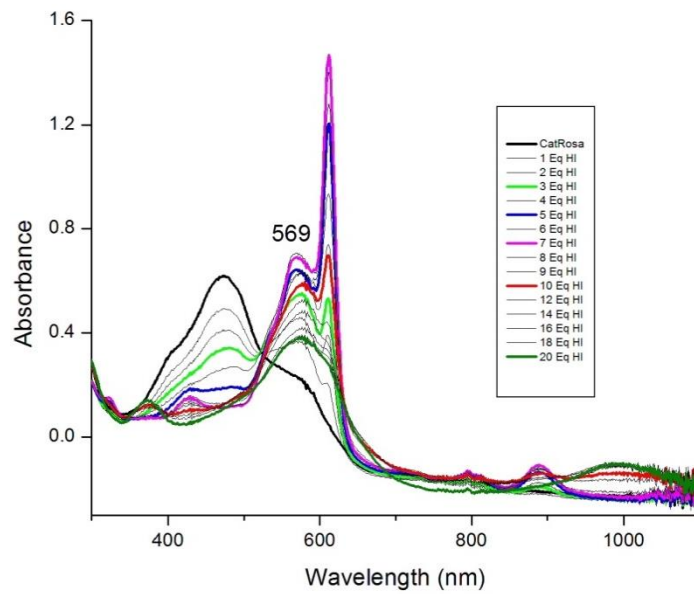
**Figure S6.** UV-vis absorption spectra of **3** [ $7.36 \times 10^{-6}$  M] upon addition of TFA (20 eqv.) in  $\text{CH}_2\text{Cl}_2$ .



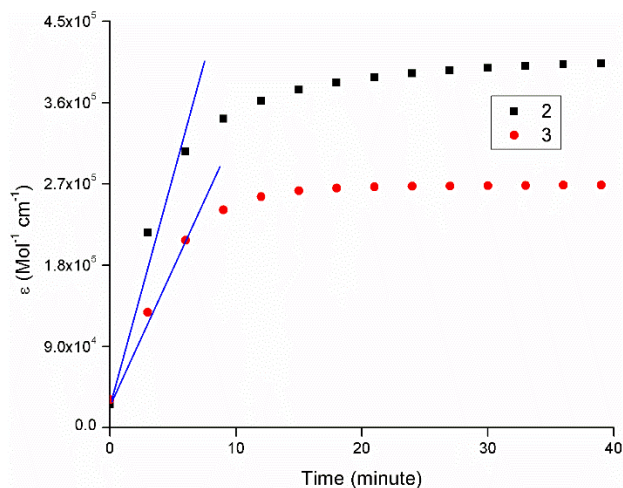
**Figure S7.** UV-vis absorption spectra of **3** [ $7.36 \times 10^{-6}$  M] upon addition of TFA (1000 eqv.) in  $\text{CH}_2\text{Cl}_2$ .



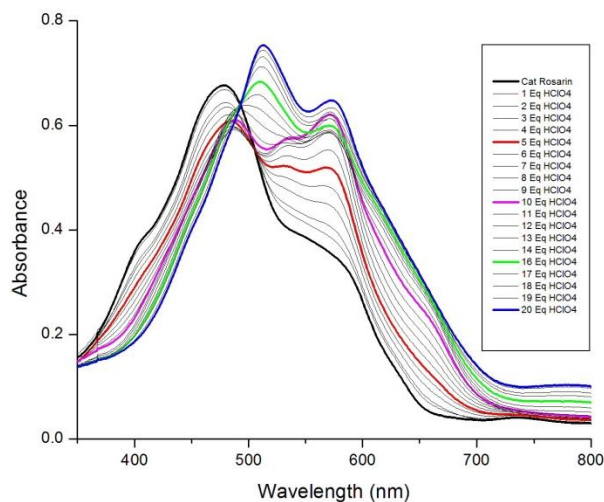
**Figure S8.** UV-vis absorption spectra of **3** [7.36 × 10<sup>-6</sup> M] upon addition of HCl in CH<sub>2</sub>Cl<sub>2</sub>.



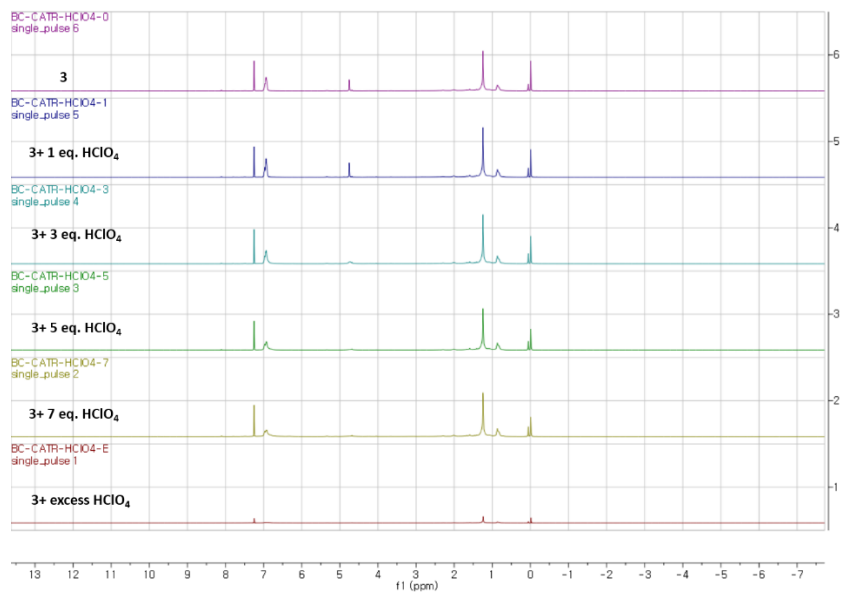
**Figure S9.** Change in UV-vis absorption spectra of **3** [7.36 × 10<sup>-6</sup> M] upon addition of HI in CH<sub>2</sub>Cl<sub>2</sub>.



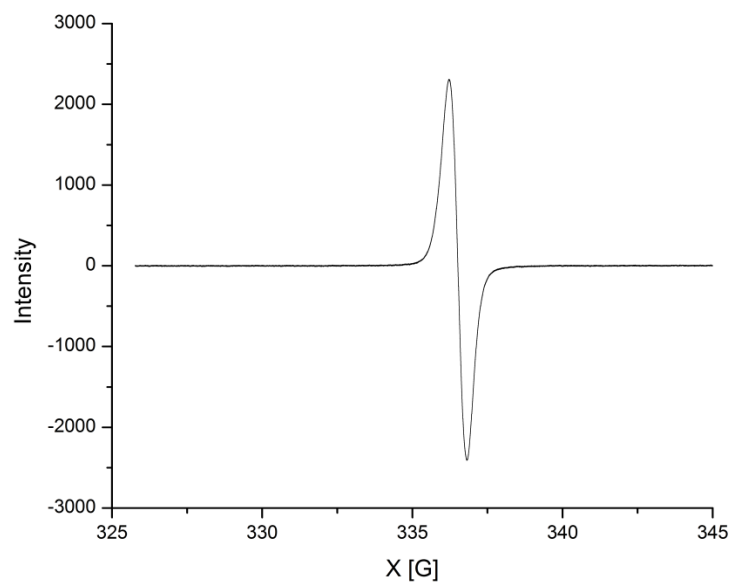
**Figure S10.** Conversion rate of **2** and **3** to their respective 26-pi analogues with 3eqv. HI in  $\text{CH}_2\text{Cl}_2$  followed at 613 nm.



**Figure S11.** UV-vis absorption spectrum of **3** [ $7.36 \times 10^{-6}$  M] upon addition of  $\text{HClO}_4$  in  $\text{CH}_2\text{Cl}_2$ .



**Figure S12.**  $^1\text{H}$  NMR spectra of **3** upon addition of  $\text{HClO}_4$  in  $\text{CDCl}_3$ .



**Figure S13.** EPR spectrum of **3** upon addition of excess  $\text{HClO}_4$  in  $\text{CH}_2\text{Cl}_2$ .

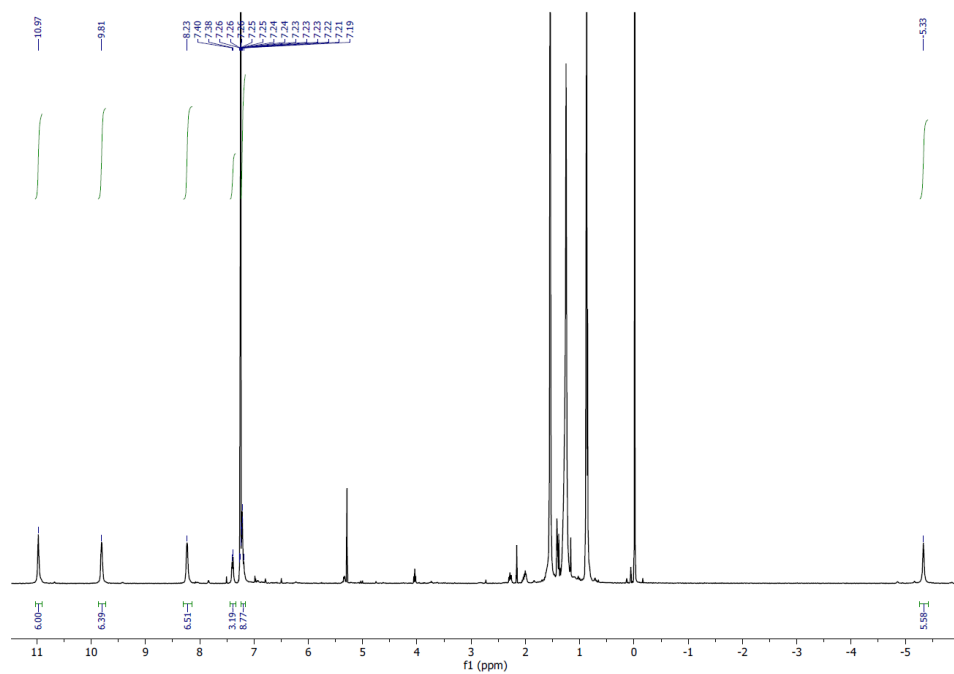


Figure S14.  $^1\text{H}$  NMR spectra of  $4\text{H}^+\cdot\text{Cl}^-$  in  $\text{CDCl}_3$ .

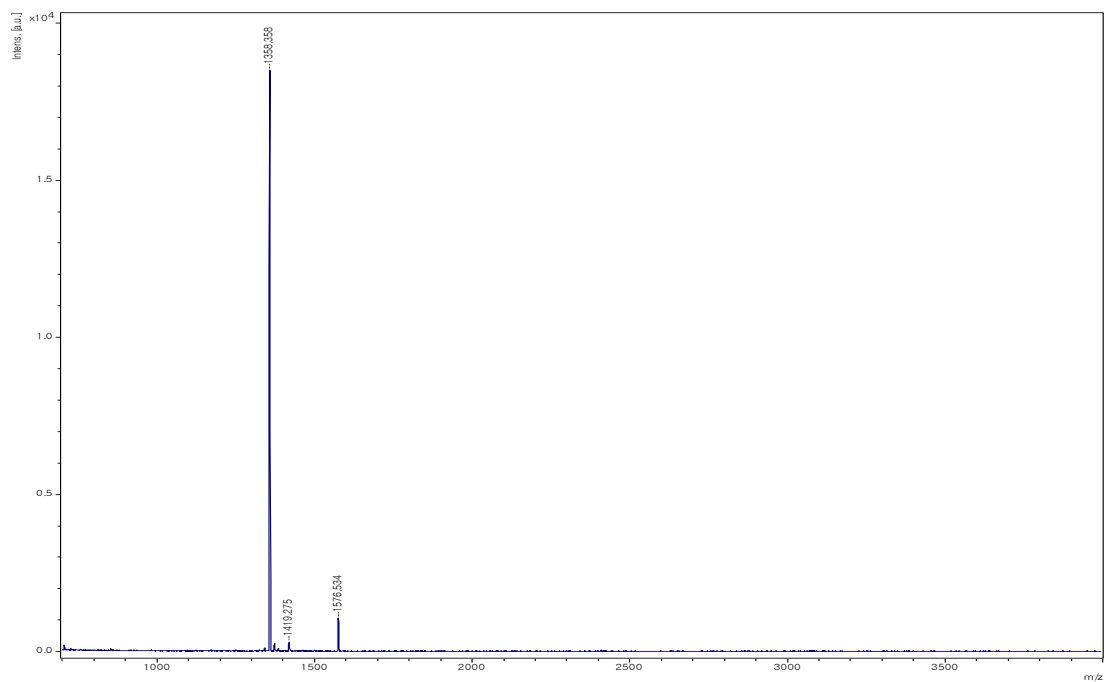
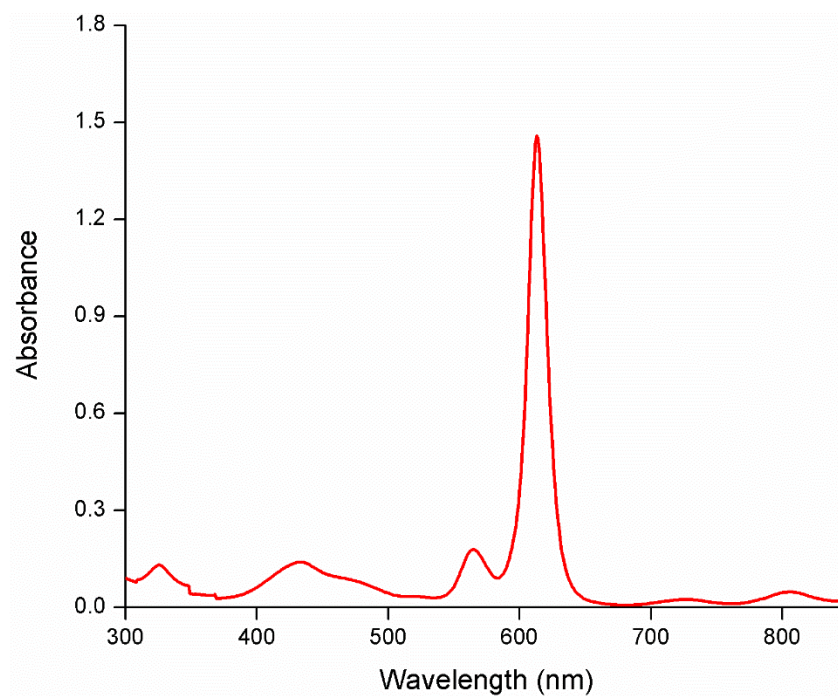


Figure S15. MALDI-TOF spectrum of  $4\text{H}^+\cdot\text{Cl}^-$ .





**Figure S16.** UV-vis absorption spectra of  $4\text{H}^+\cdot\text{Cl}^-$  [ $1.8 \times 10^{-6}$  M] in  $\text{CH}_2\text{Cl}_2$ .