

## Supporting Information

# Studies of the Functionalized $\alpha$ -Hydroxy-*p*-Quinone Imine Derivatives Stabilized by Intramolecular Hydrogen Bond

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## 1. NMR spectroscopy data

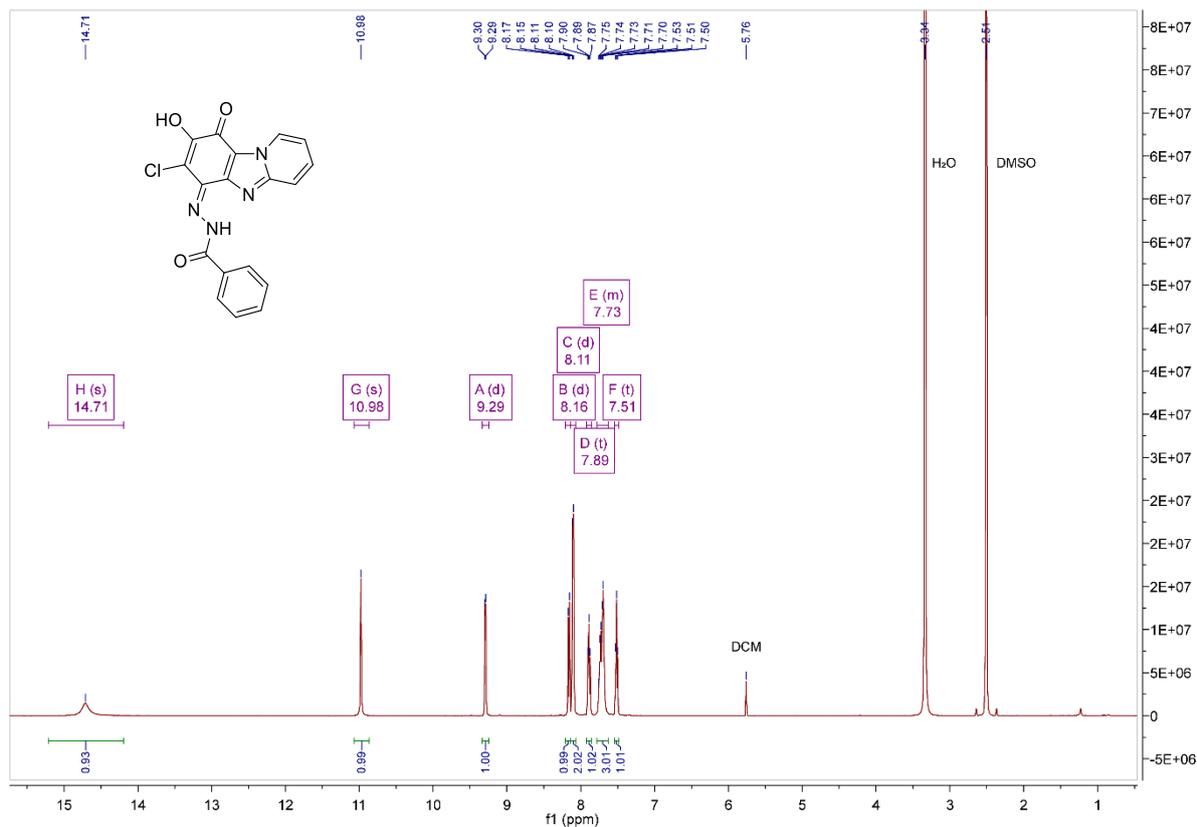


Figure S1. <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>) spectrum of compound 3a.

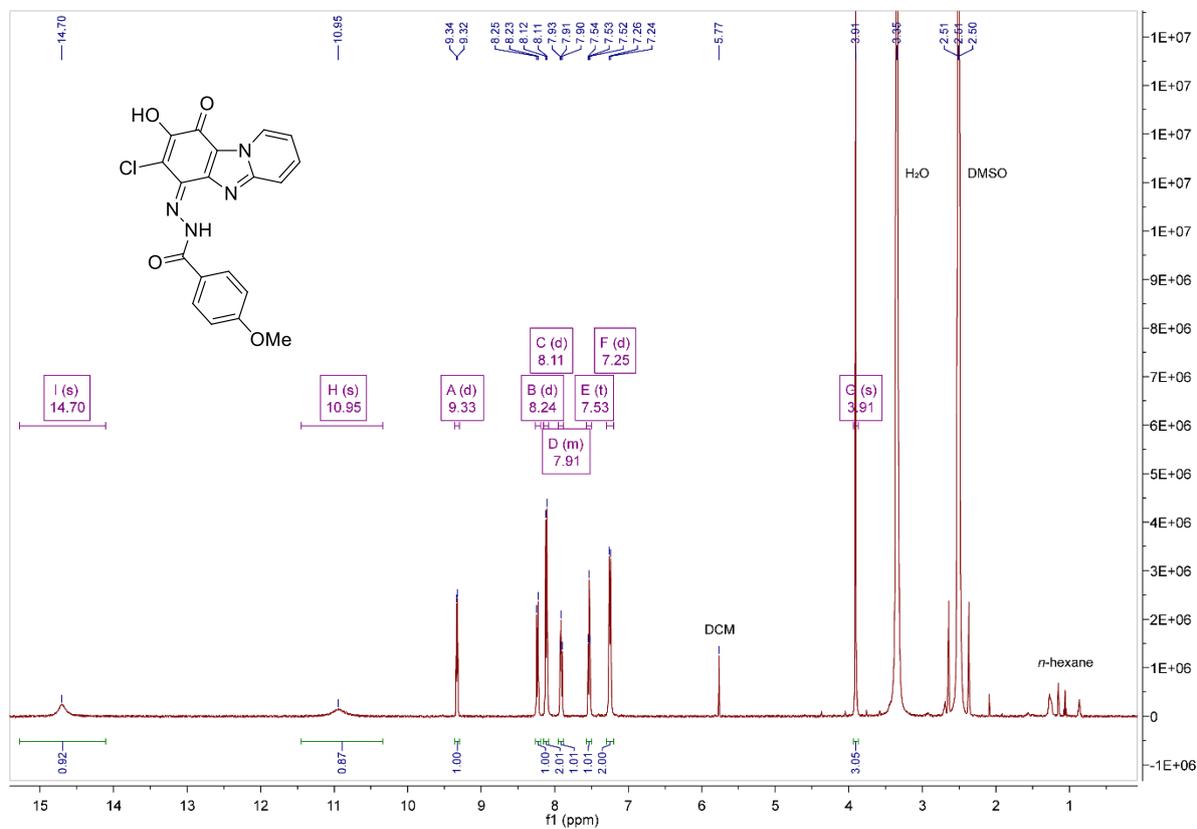


Figure S2. <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>) spectrum of compound 3b.

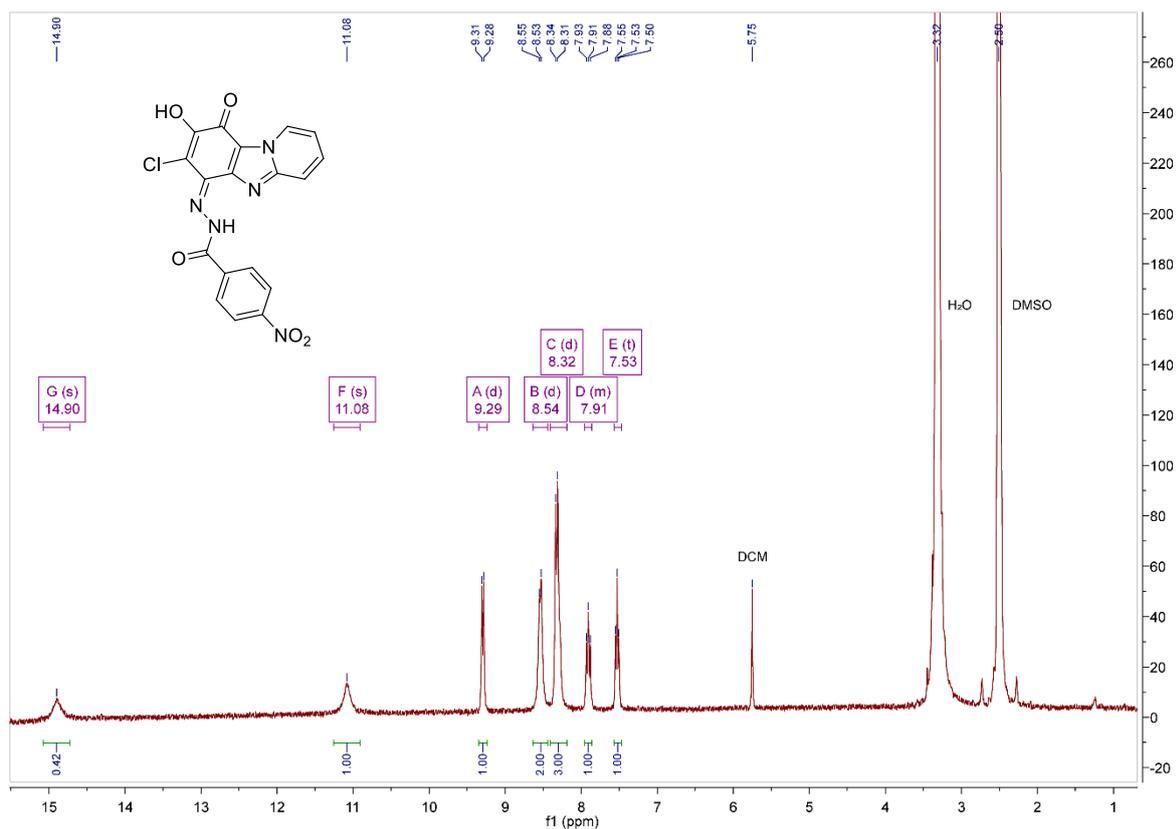


Figure S3.  $^1\text{H}$  NMR (300 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound 3c.

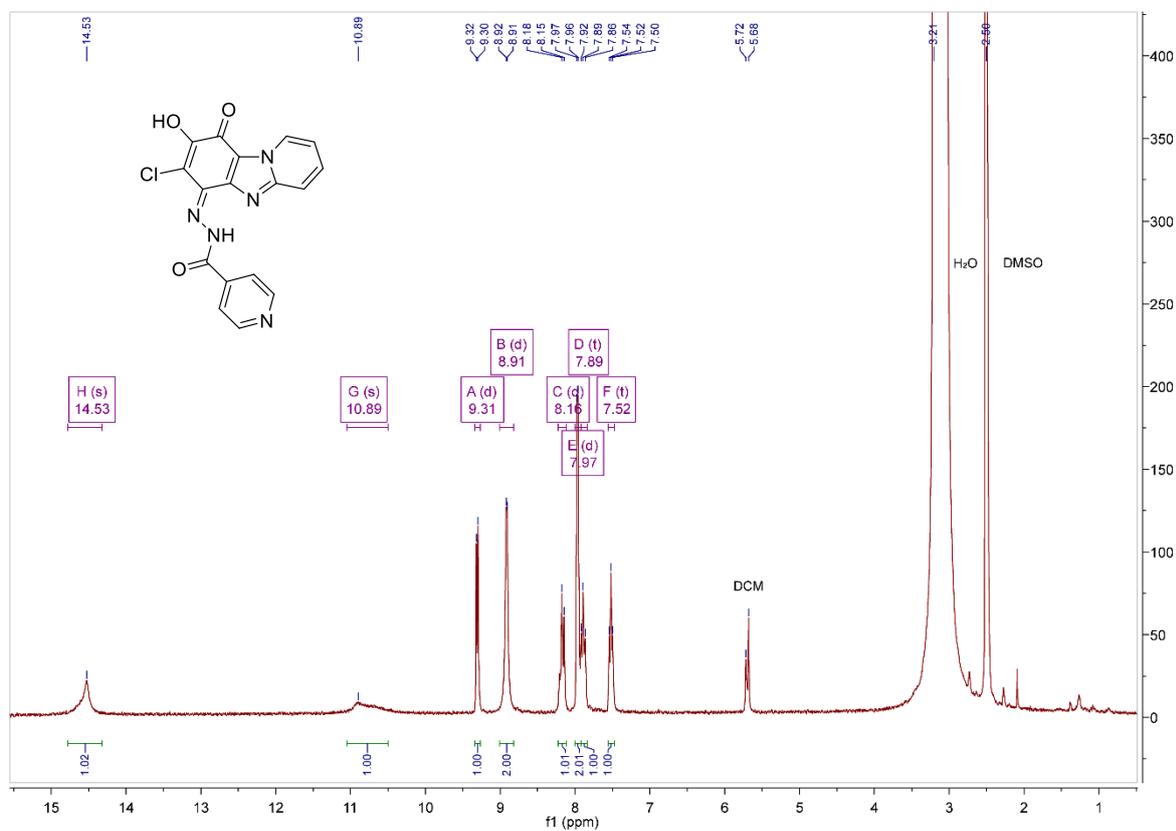


Figure S4.  $^1\text{H}$  NMR (300 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound 3d.

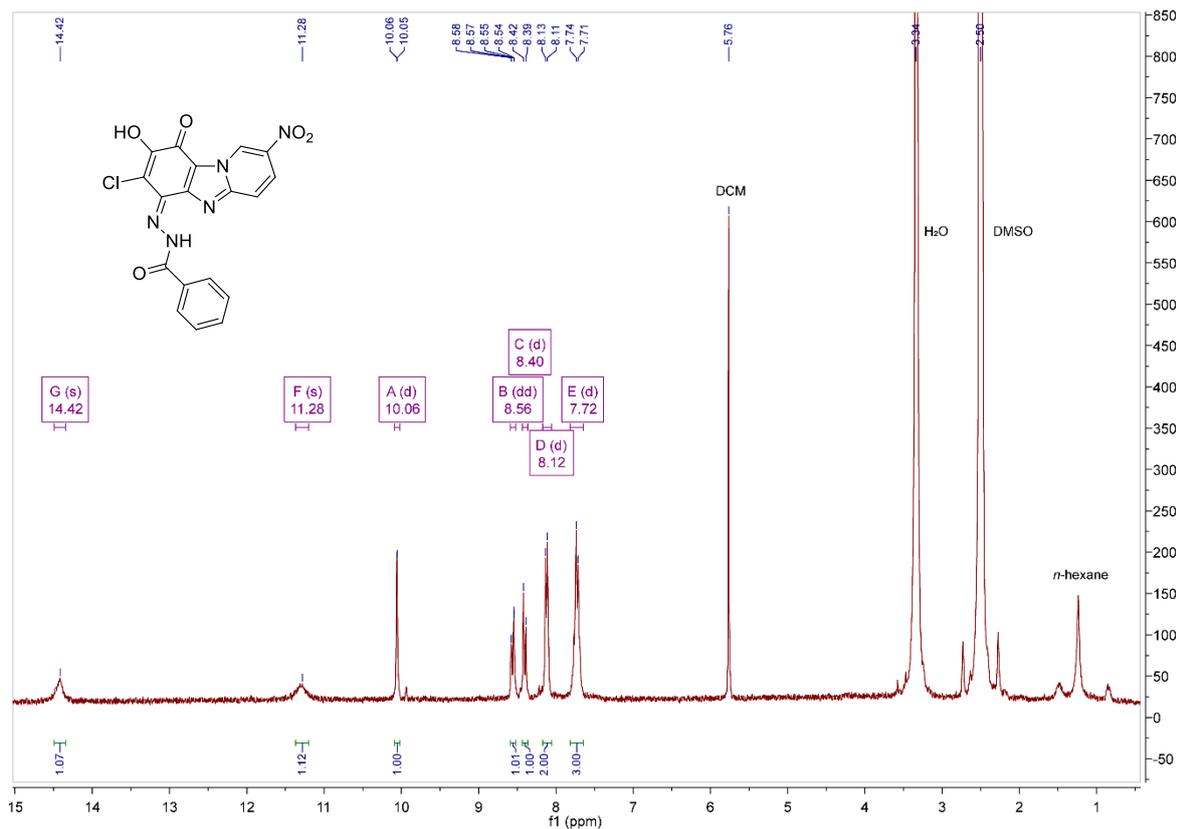


Figure S5.  $^1\text{H}$  NMR (300 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound 3e.

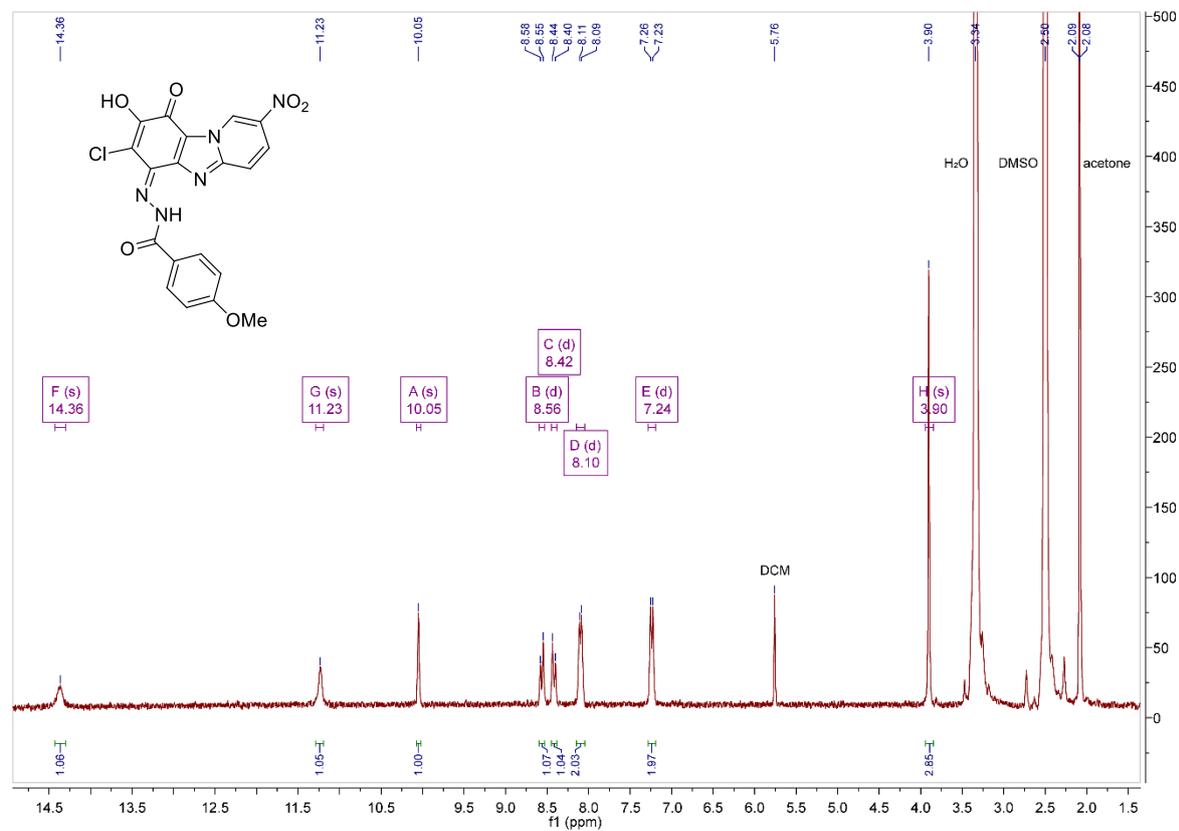
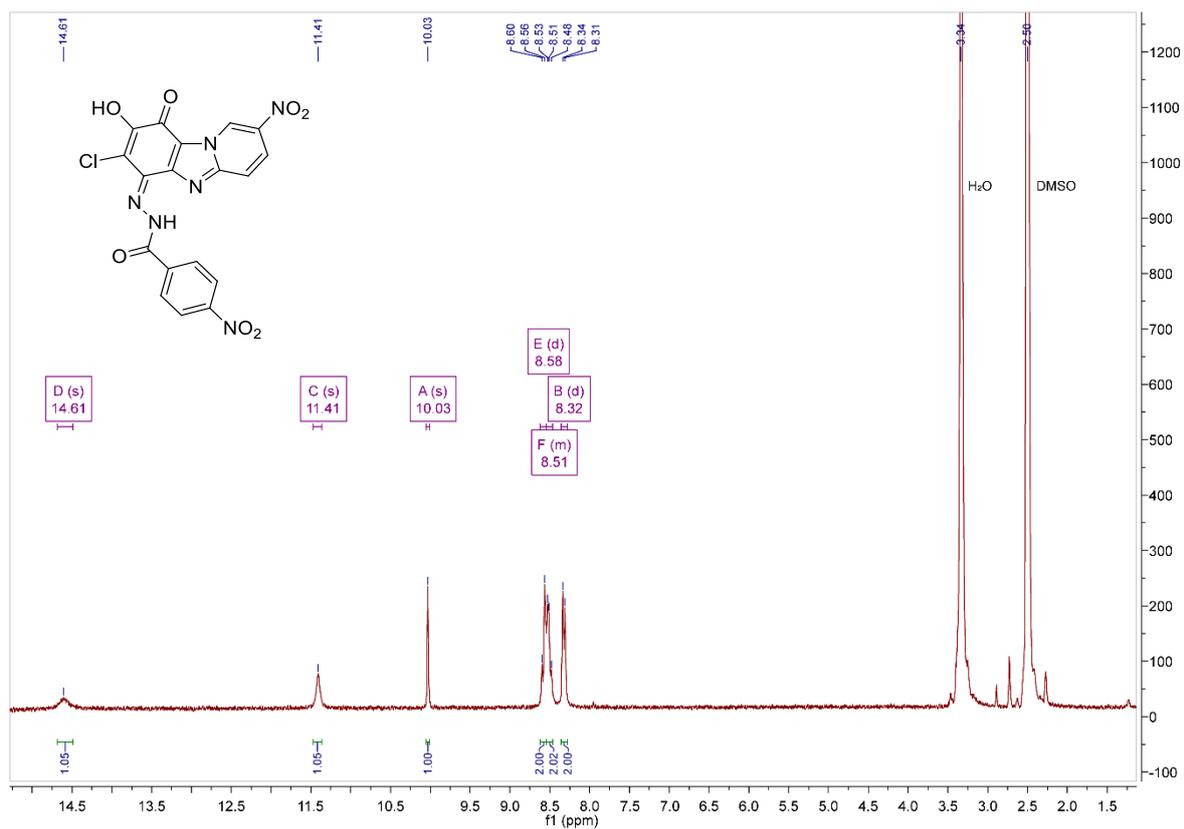
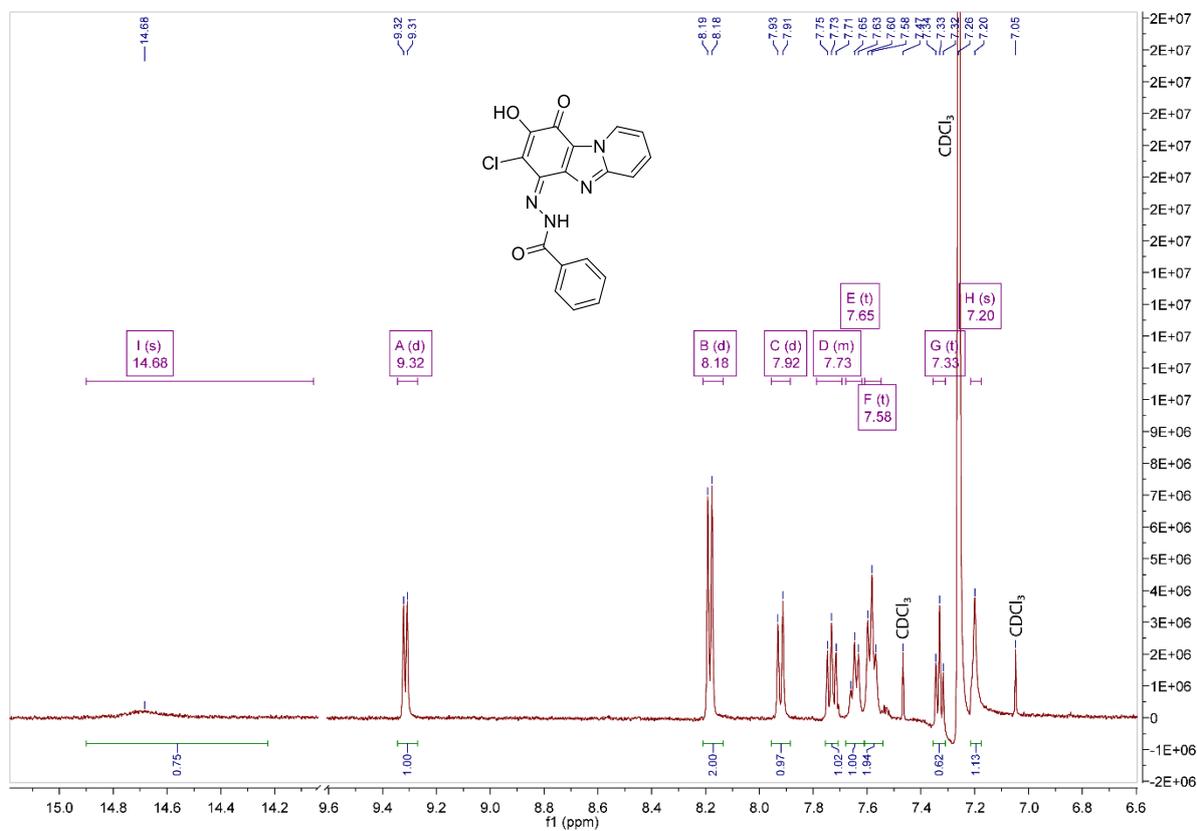


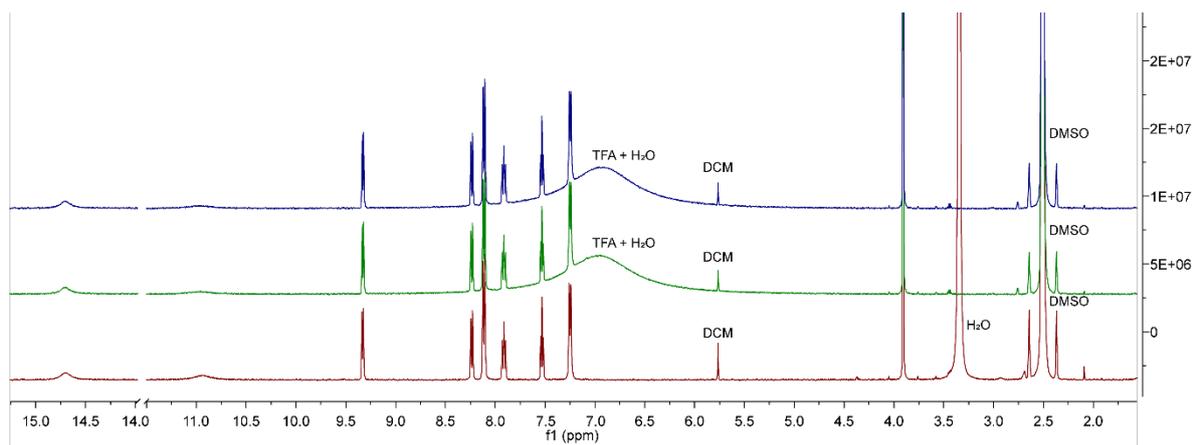
Figure S6.  $^1\text{H}$  NMR (300 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound 3f.



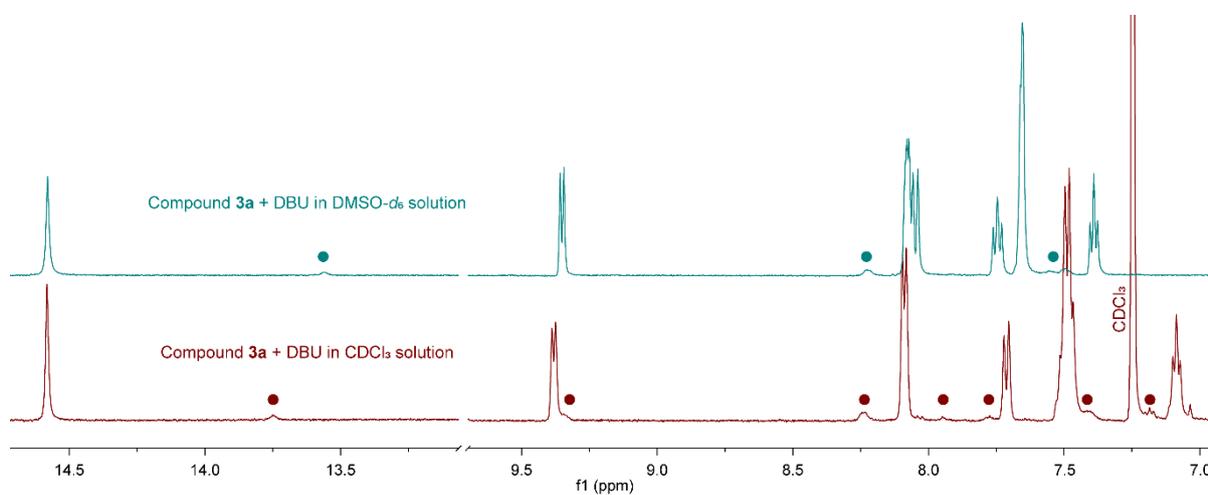
**Figure S7.** <sup>1</sup>H NMR (300 MHz, DMSO-*d*<sub>6</sub>) spectrum of compound **3g**.



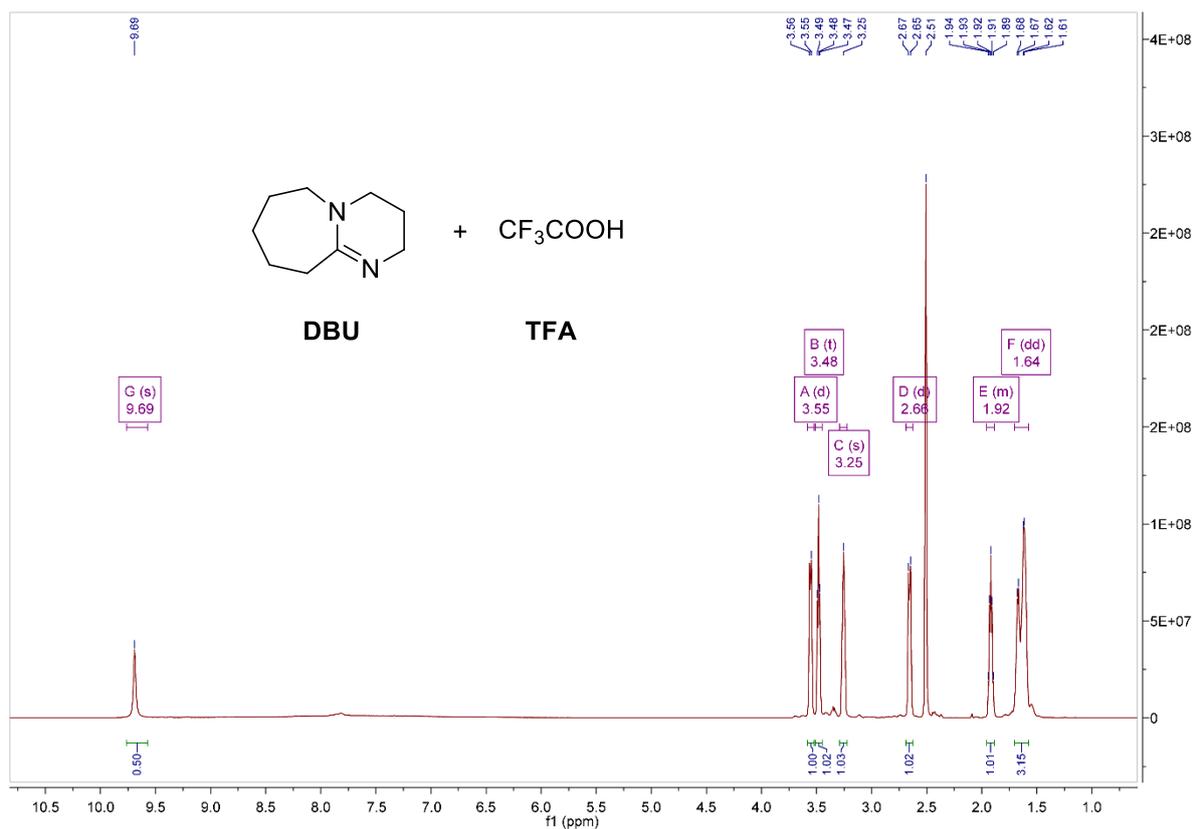
**Figure S8.** <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of compound **3a**.



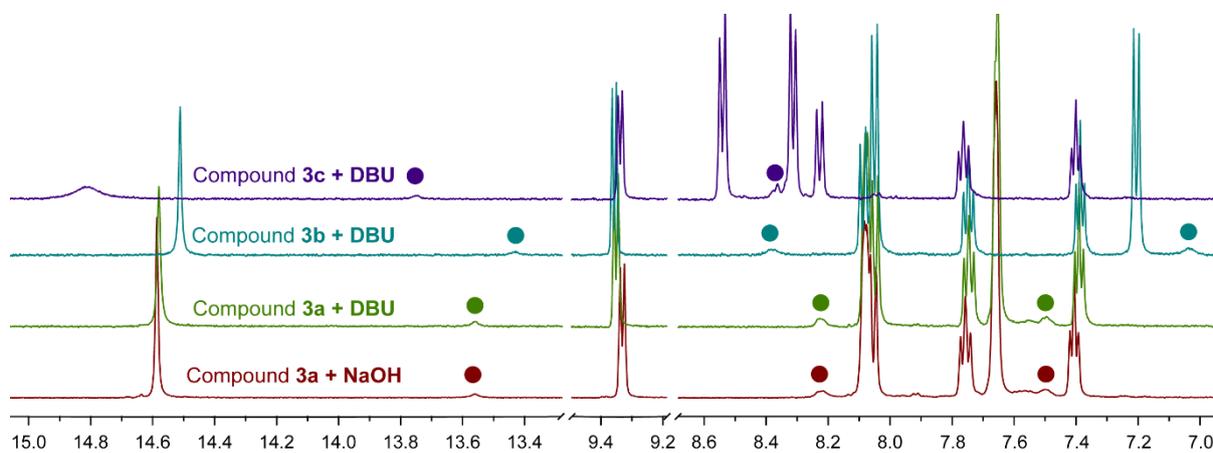
**Figure S9.**  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO-}d_6$ ) spectra of compound **3b** (red line) after addition of TFA (green line) and UV irradiation (blue line).



**Figure S10.** An expansion of  $^1\text{H}$  NMR spectra (500 MHz) upon the addition of excess DBU to the solution of compound **3a** in  $\text{DMSO-}d_6$  solution (blue line) or in  $\text{CDCl}_3$  solution (red line). The signals of minor form of deprotonated compound **3a** are marked with circles.

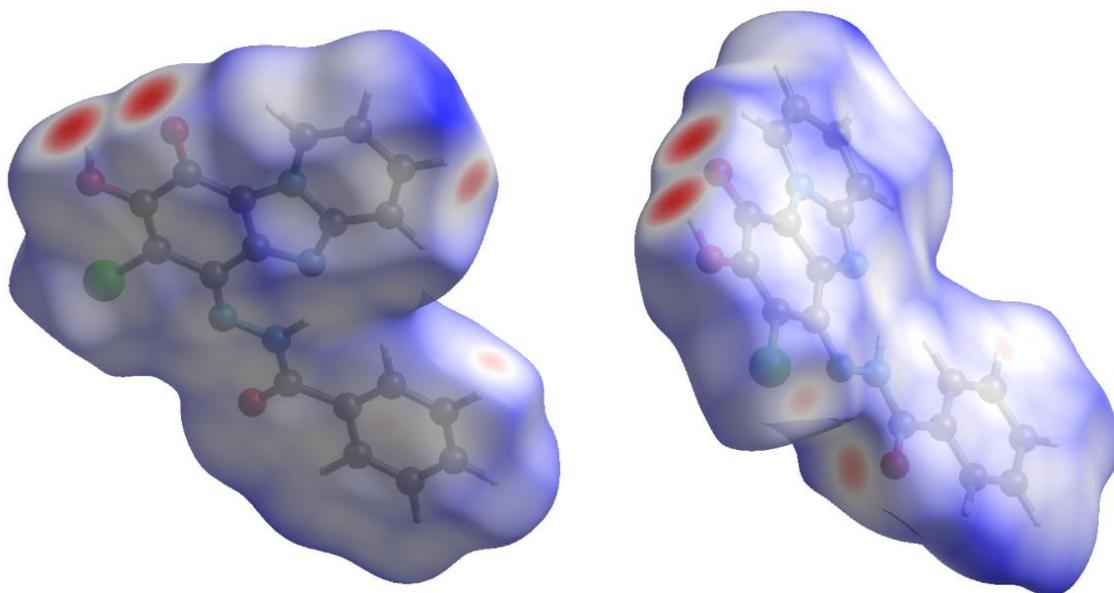


**Figure S11.**  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO-}d_6$ ) spectrum of 1,8-diazabicyclo(5.4.0)undec-7-ene (**DBU**) mixture with trifluoroacetic acid (**TFA**).

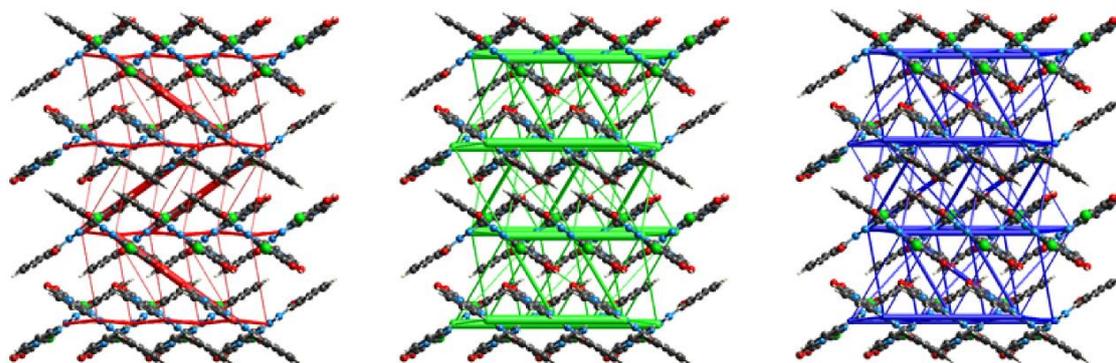


**Figure S12.** An expansion of  $^1\text{H}$  NMR spectra (500 MHz,  $\text{DMSO-}d_6$ ) upon the addition of excess NaOH (to the solution of compound **3a** (red line)) or excess of DBU (to the solutions of compound **3a** (green line), **3b** (blue line) or **3c** (purple line)). The signals of minor form of deprotonated compounds **3a-c** are marked with circles.

## 2. Crystal Explorer: Hirshfeld Surfaces and Energy frameworks

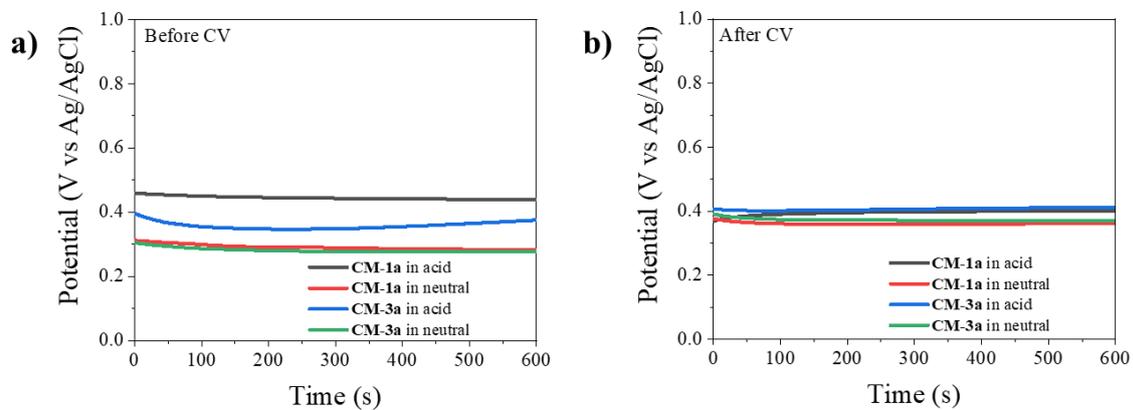


**Figure S13.** Hirshfeld surface for compound **3a**.

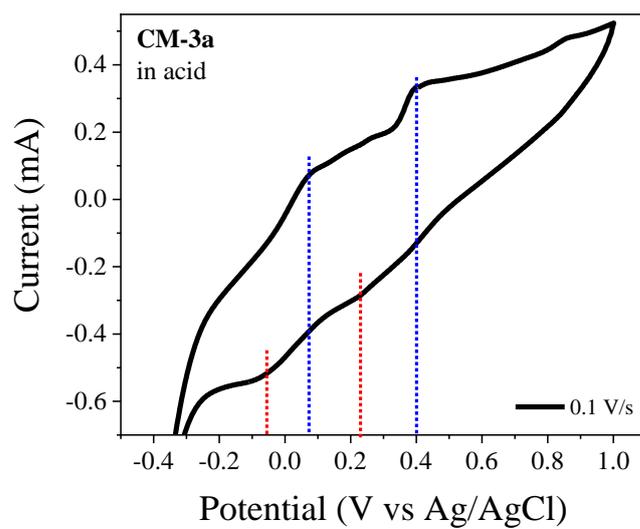


**Figure S14.** Energy frameworks of compound **3a**. Energy frameworks for separate electrostatic (red) and dispersion (green) contributions to the total nearest neighbor pairwise interaction energies (blue). All energies with a magnitude less than 5 kJ mol<sup>-1</sup> have been omitted from the frameworks.

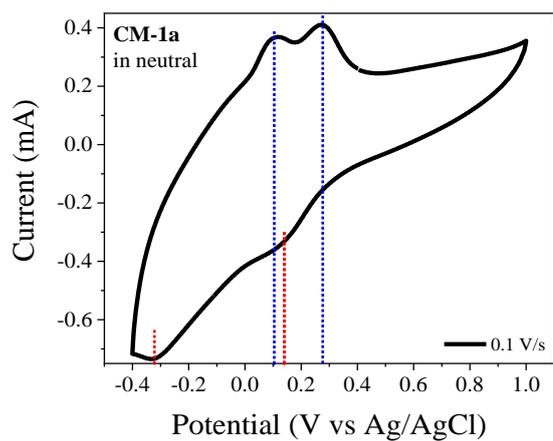
### 3. Redox properties



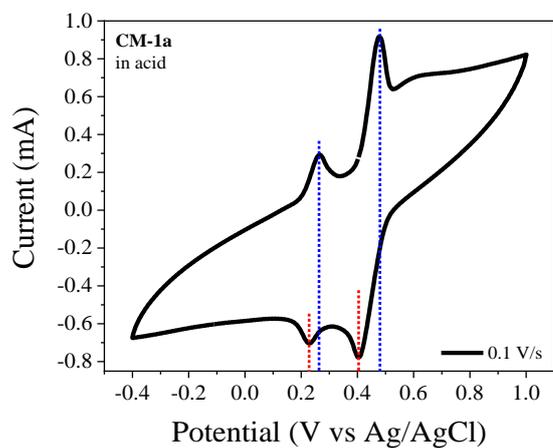
**Figure S15.** OCP measurements of samples **CM-1a** and **CM-3a** before and after CV measurements.



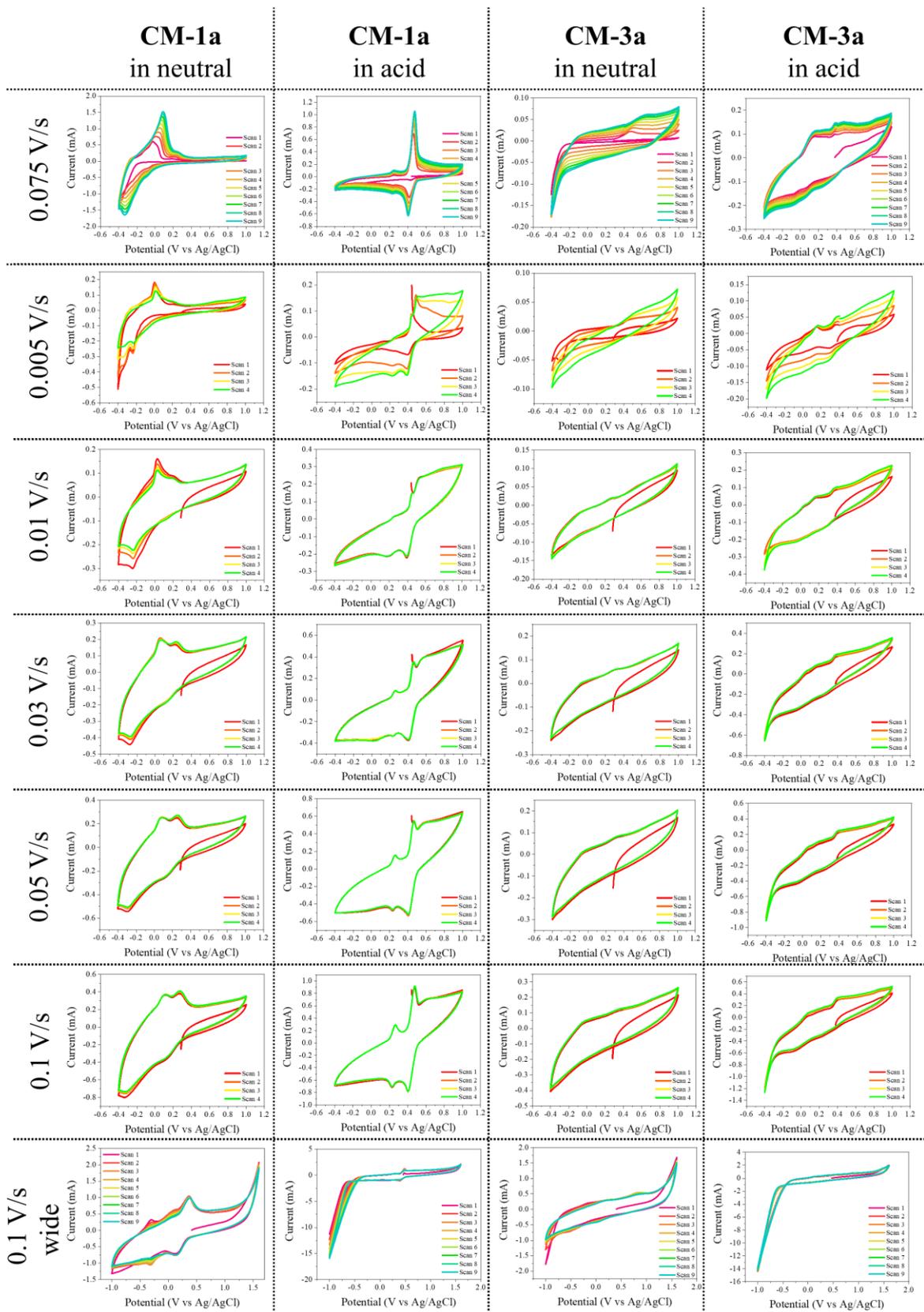
**Figure S16.** CV curve of sample **CM-3a** in acidic electrolyte at 0.1V/s scan speed.



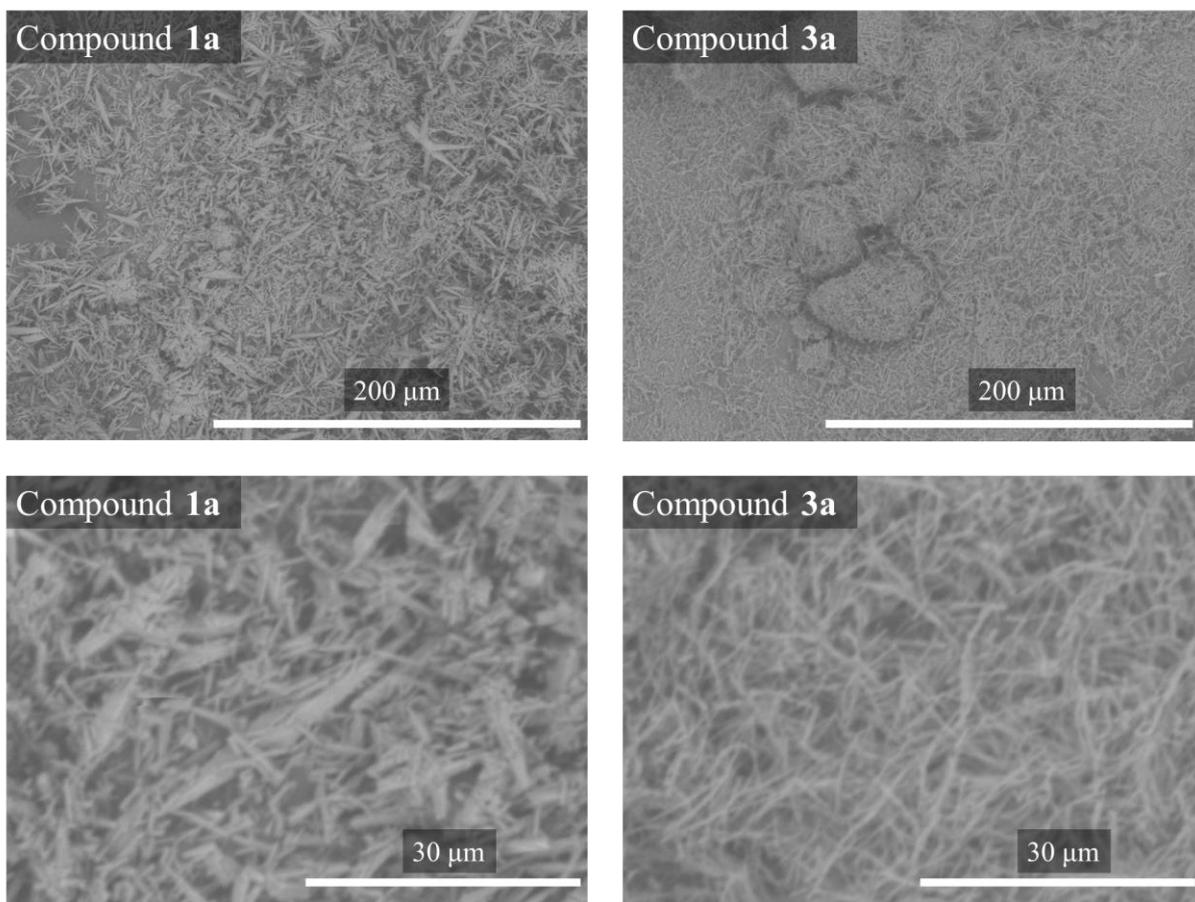
**Figure S17.** CV curve of sample **CM-1a** in neutral electrolyte at 0.1V/s scan speed.



**Figure S18.** CV curve of sample **CM-1a** in acidic electrolyte at 0.1V/s scan speed.



**Figure S19.** CV curves of samples **CM-1a** and **CM-3a** in neutral and acidic electrolyte at various scan speeds.



**Figure S20.** Scanning electron microscopy images of compounds **1a** and **3a** at different magnifications (x500 and x2500).