

Supporting Information

Studies of the Functionalized α -Hydroxy-*p*-Quinone Imine Derivatives Stabilized by Intramolecular Hydrogen Bond

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1. NMR spectroscopy data

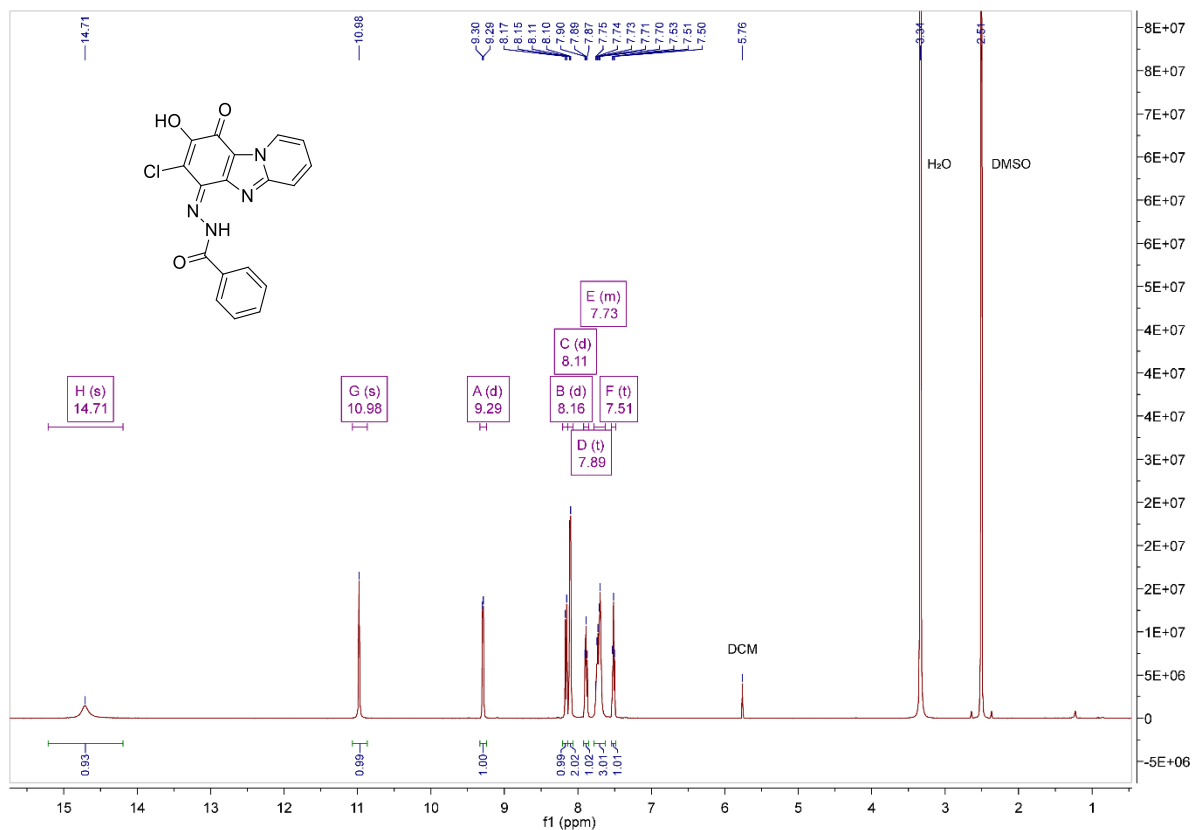


Figure S1. ¹H NMR (500 MHz, DMSO-*d*₆) spectrum of compound **3a**.

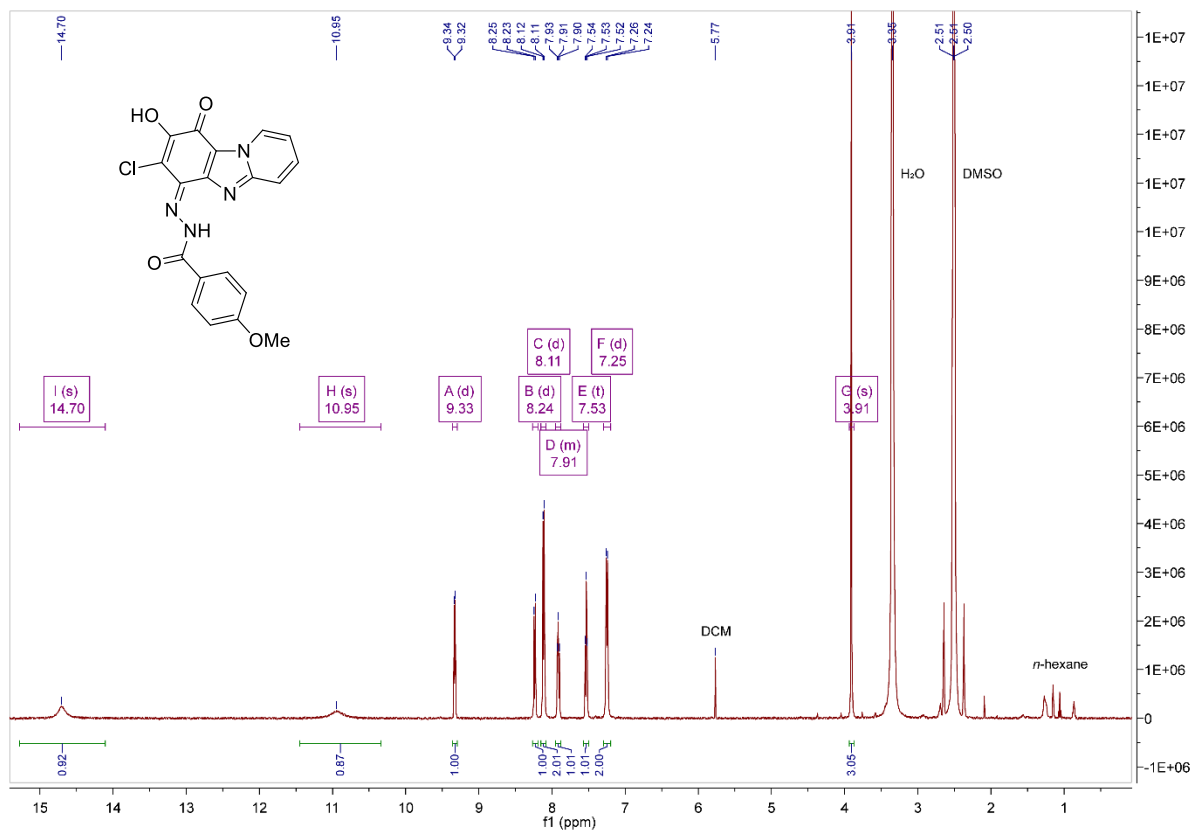


Figure S2. ¹H NMR (500 MHz, DMSO-*d*₆) spectrum of compound **3b**.

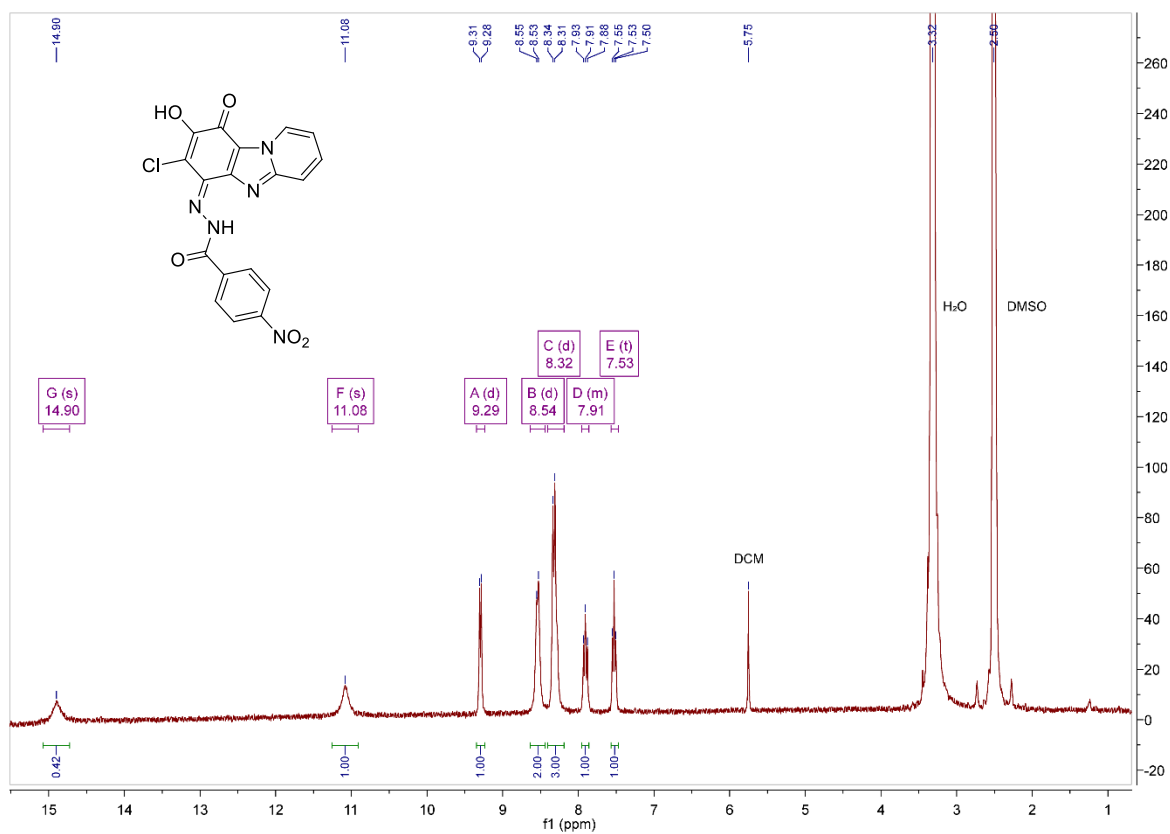


Figure S3. ¹H NMR (300 MHz, DMSO-*d*₆) spectrum of compound **3c**.

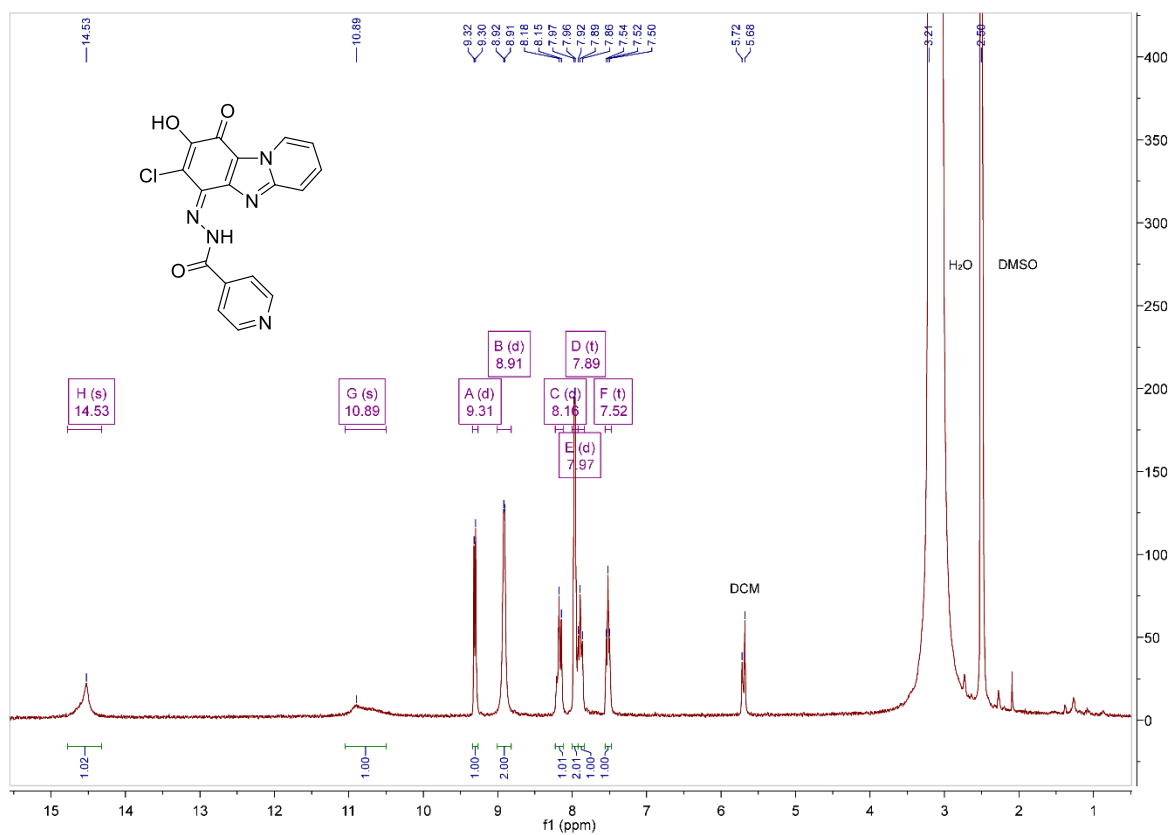


Figure S4. ¹H NMR (300 MHz, DMSO-*d*₆) spectrum of compound **3d**.

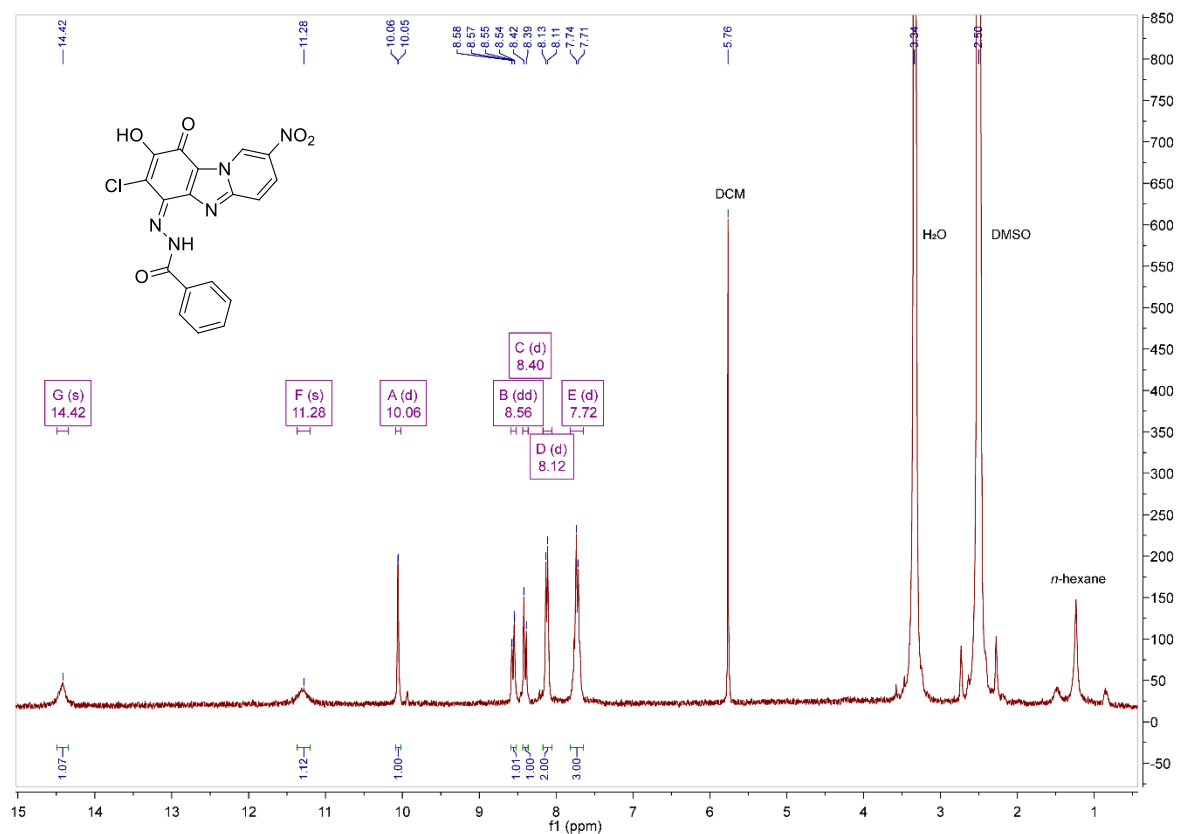


Figure S5. ¹H NMR (300 MHz, DMSO-*d*₆) spectrum of compound **3e**.

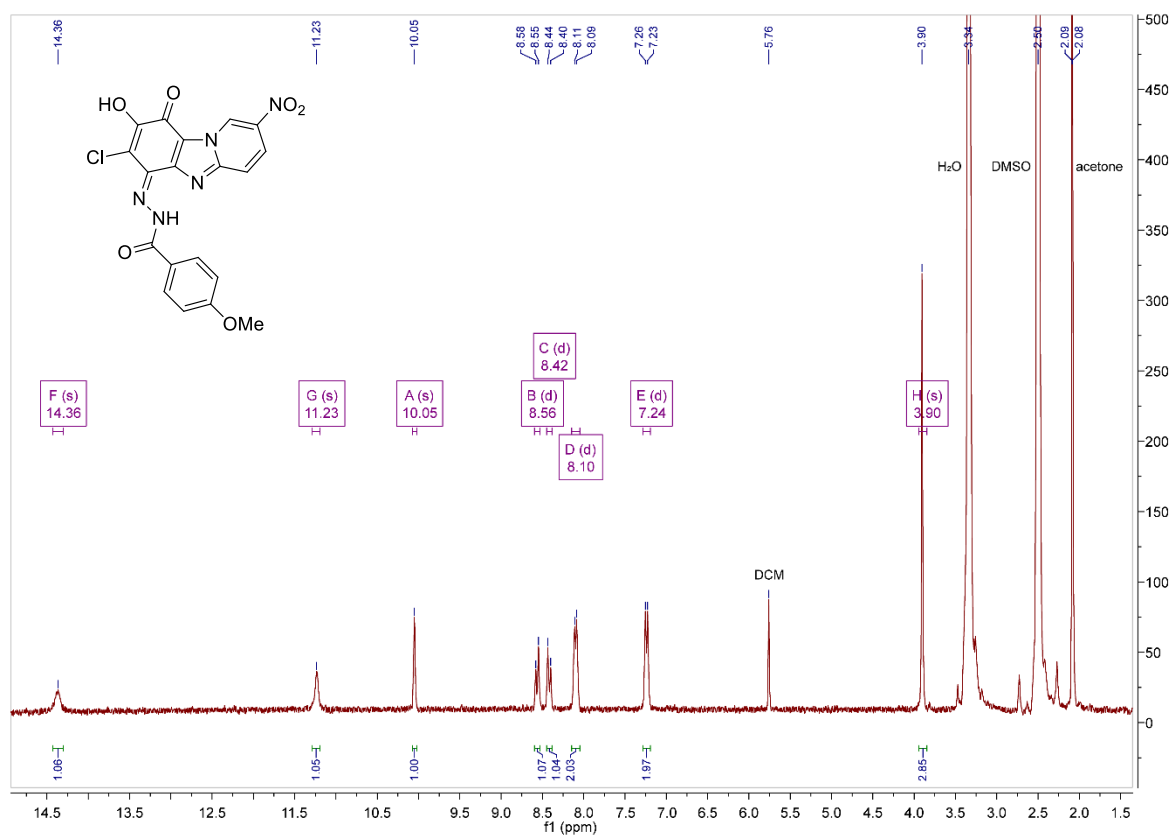


Figure S6. ¹H NMR (300 MHz, DMSO-*d*₆) spectrum of compound **3f**.

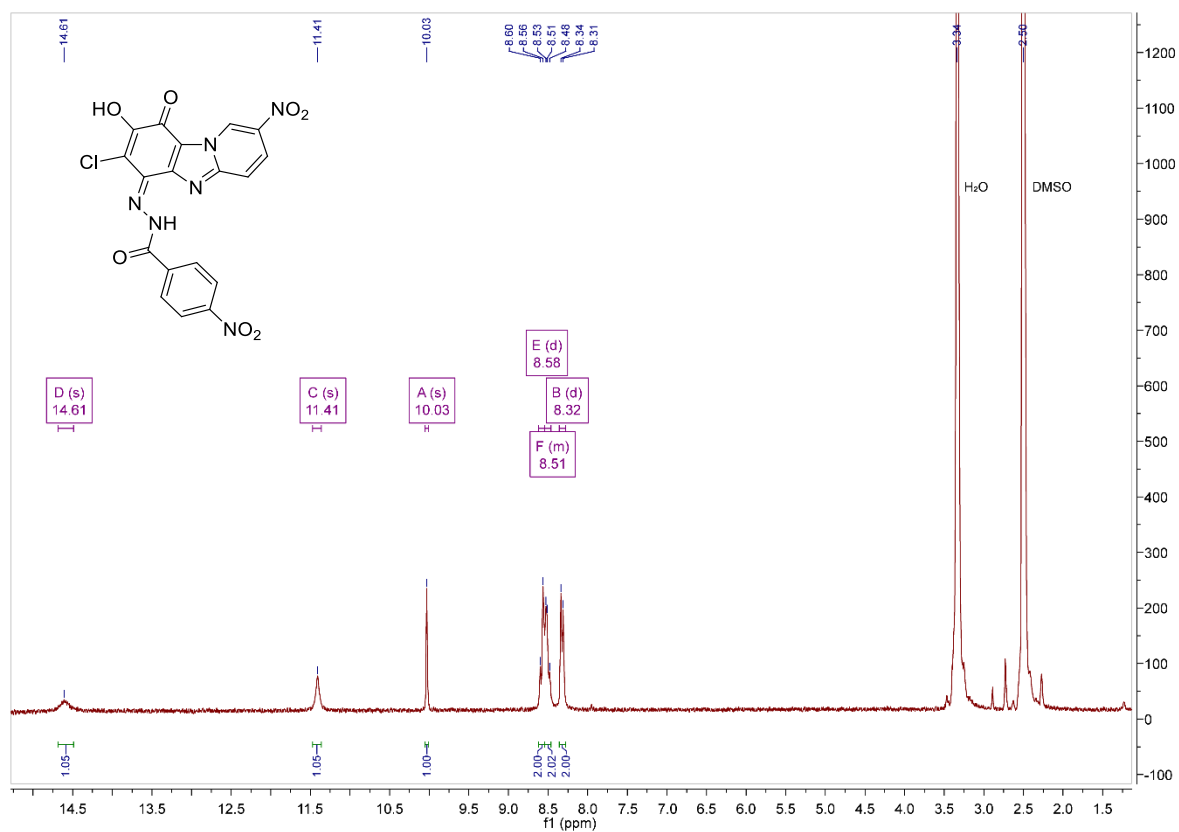


Figure S7. ¹H NMR (300 MHz, DMSO-*d*₆) spectrum of compound **3g**.

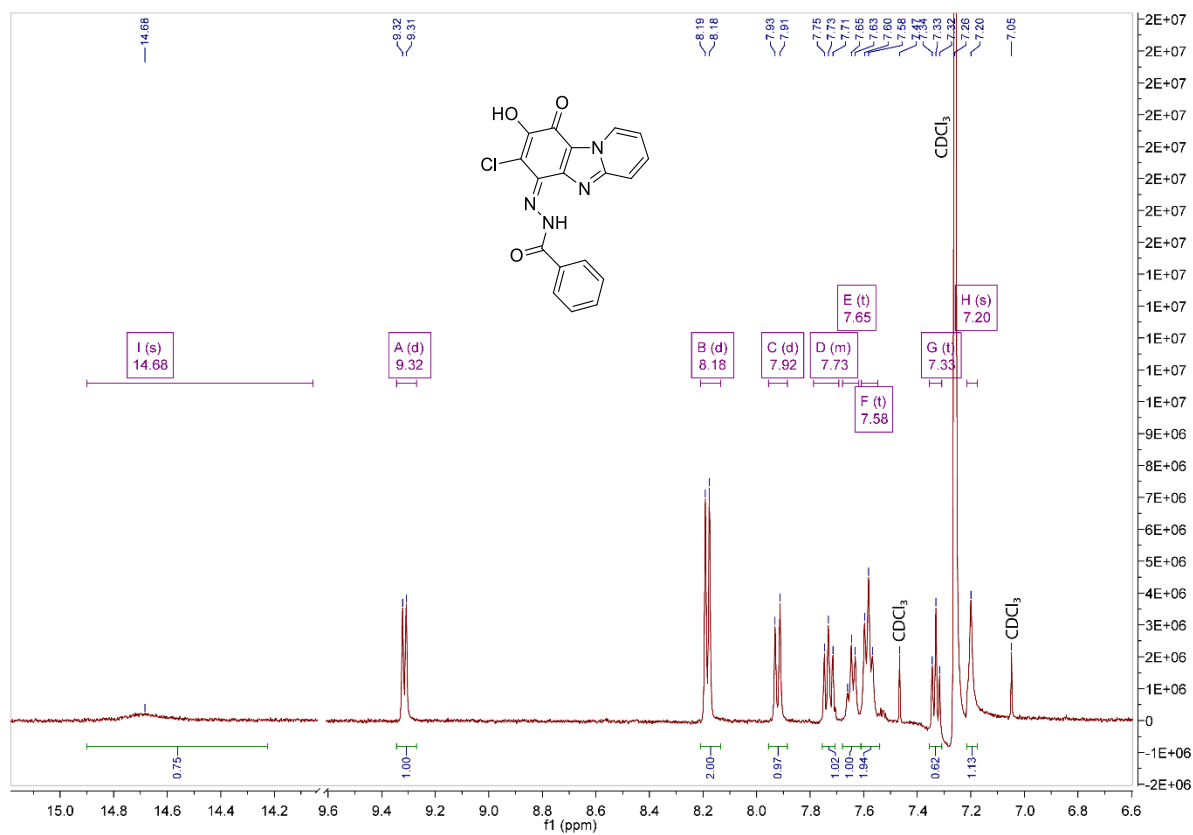


Figure S8. A fragment of ¹H NMR (500 MHz, CDCl₃) spectrum of compound **3a**.

Table S1. Substituents R_1 and R_2 , the Hammett constant (for R_2) and chemical shifts of NH and OH protons in ^1H NMR spectra ($\text{DMSO-}d_6$) of the compounds **3a-c** and **3e-g**.

Compound	R_1	R_2	The Hammett constant of R_2 substituent (σ_p)	Chemical shift of NH proton (δ_{NH}), ppm	Chemical shift of OH proton (δ_{OH}), ppm
3a	H	H	0	14.71	10.98
3b	H	OMe	-0.27	14.70	10.95
3c	H	NO_2	0.78	14.90	11.08
3e	NO_2	H	0	14.42	11.28
3f	NO_2	OMe	-0.27	14.36	11.23
3g	NO_2	NO_2	0.78	14.61	11.41

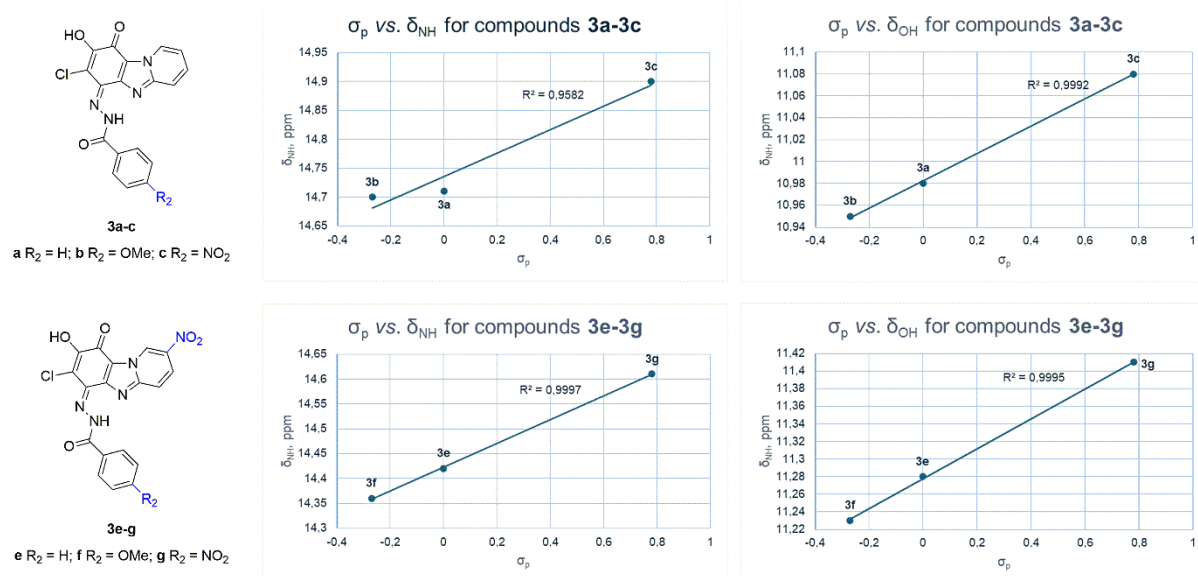


Figure S9. Structures of compounds **3a-c** and **3e-g** and correlations between the Hammett constants (σ_p) of substituent R_2 and the chemical shifts of NH proton (δ_{NH}) or OH proton (δ_{OH}) in ^1H NMR spectra ($\text{DMSO-}d_6$) of compounds **3a-c** and **3e-g**.

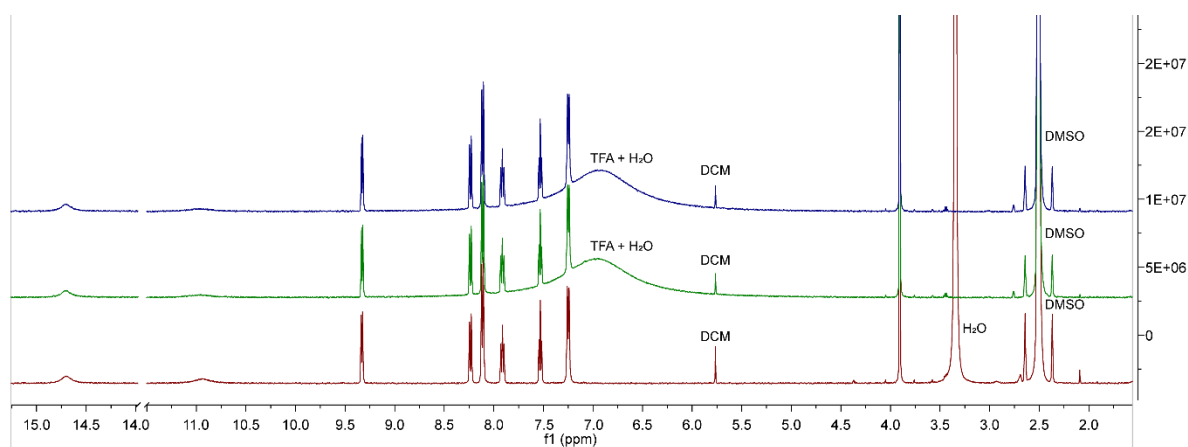


Figure S10. ^1H NMR (500 MHz, $\text{DMSO-}d_6$) spectra of compound **3b** (red line) after addition of TFA (green line) and UV irradiation (blue line).

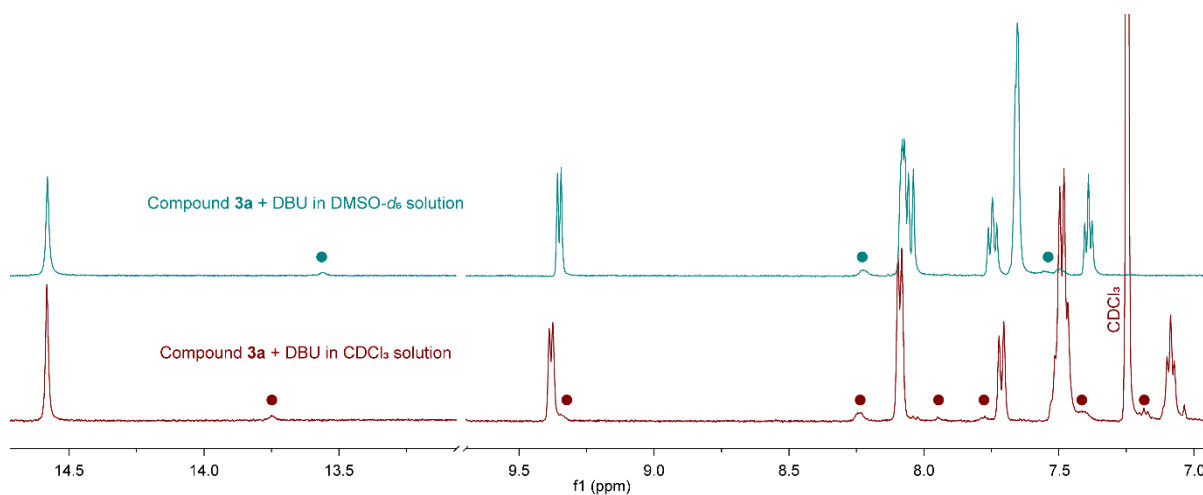


Figure S11. An expansion of ¹H NMR spectra (500 MHz) upon the addition of excess DBU to the solution of compound **3a** in DMSO-*d*₆ solution (blue line) or in CDCl₃ solution (red line). The signals of minor form of deprotonated compound **3a** are marked with circles.

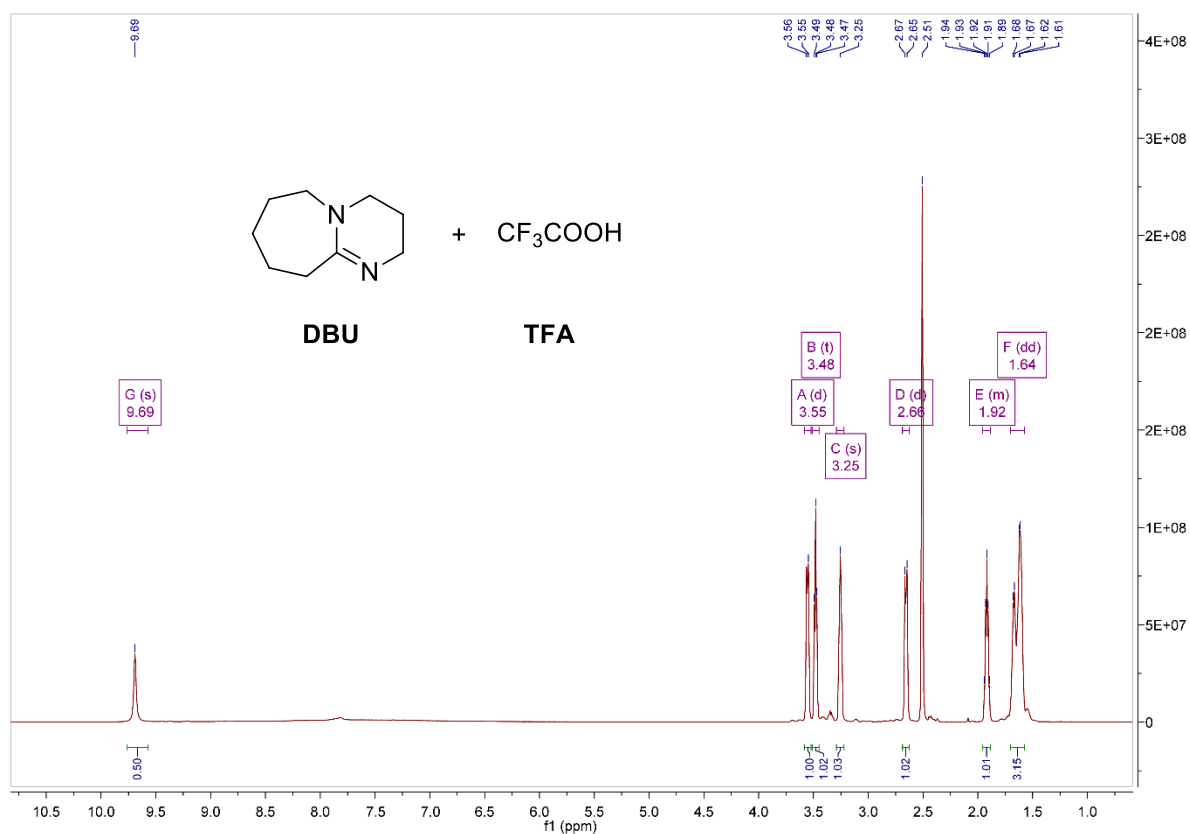


Figure S12. ¹H NMR (500 MHz, DMSO-*d*₆) spectrum of 1,8-diazabicyclo(5.4.0)undec-7-ene (**DBU**) and trifluoroacetic acid (**TFA**) mixture.

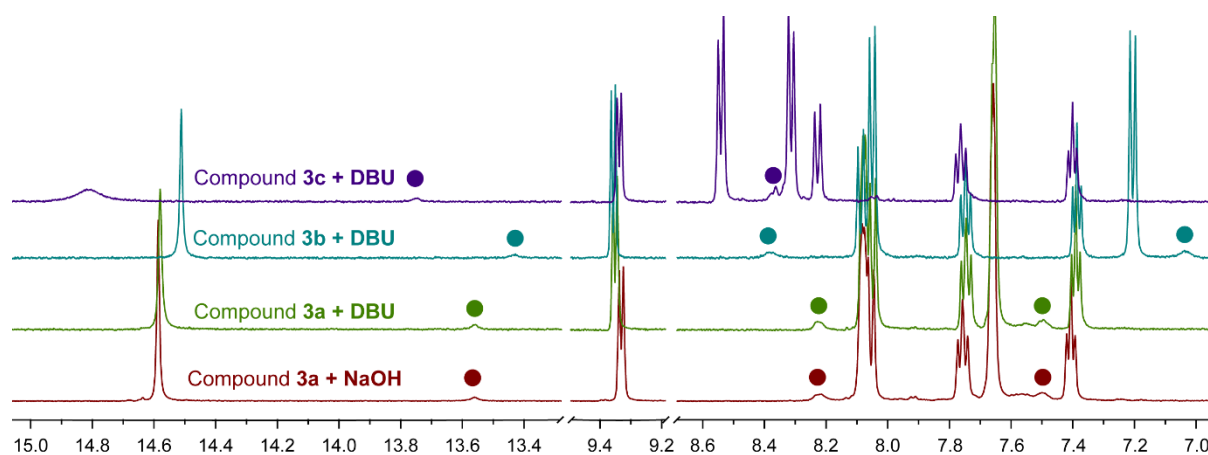


Figure S13. An expansion of ^1H NMR spectra (500 MHz, $\text{DMSO-}d_6$) upon the addition of excess NaOH (to the solution of compound **3a** (red line)) or excess of DBU (to the solutions of compound **3a** (green line), **3b** (blue line) or **3c** (purple line)). The signals of a minor form of deprotonated compounds **3a-c** are marked with circles.

2. Crystal Explorer: Hirshfeld Surfaces and Energy frameworks

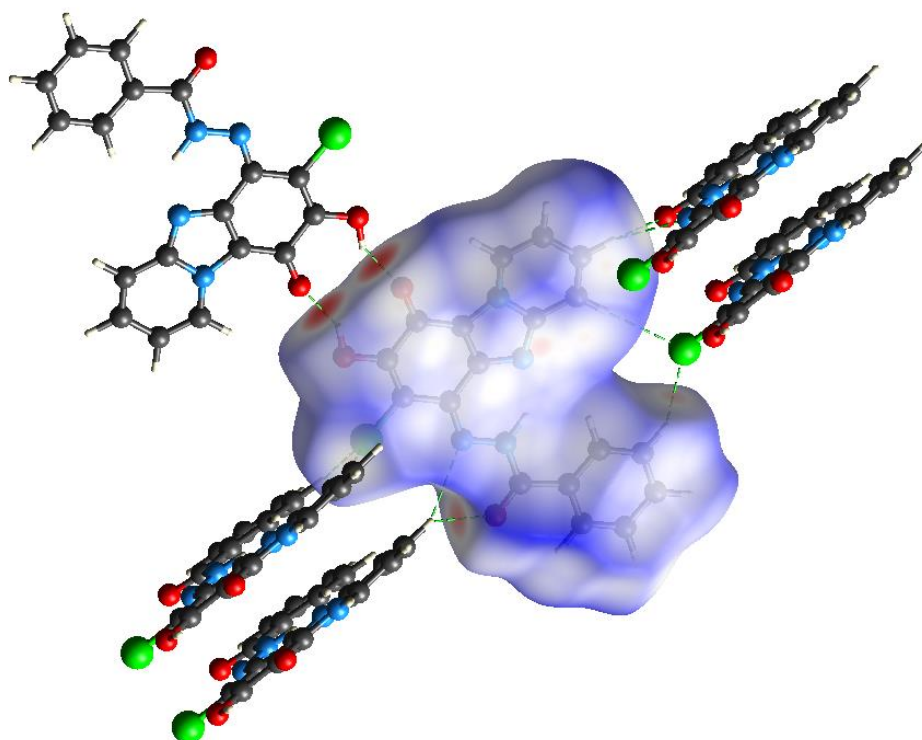


Figure S14. Hirshfeld surface for compound **3a**.

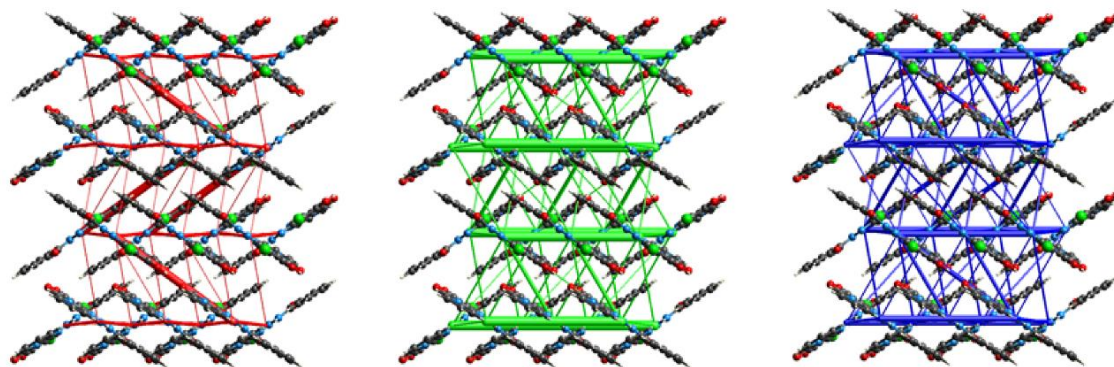


Figure S15. Energy frameworks of compound **3a**. Energy frameworks for separate electrostatic (red) and dispersion (green) contributions to the total nearest neighbor pairwise interaction energies (blue). All energies with a magnitude less than 5 kJ mol⁻¹ have been omitted from the frameworks.

3. UV-Vis spectroscopy data

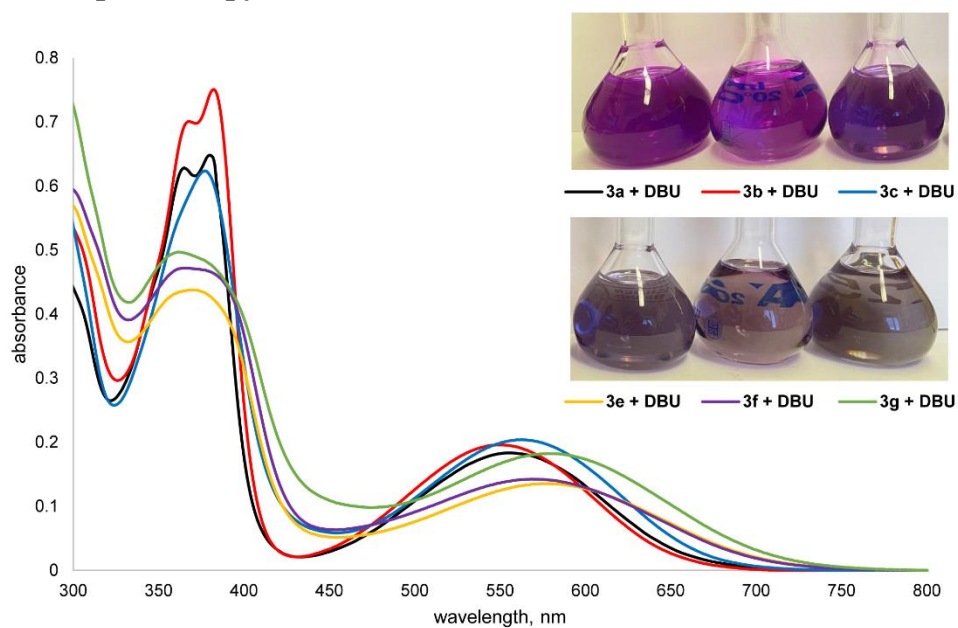


Figure S16. UV-Vis spectra of compounds **3a-c** and **3e-g** in CHCl_3 solution upon addition of DBU (excess).

Table S2. UV-Vis spectroscopy data of compounds **3a-c** and **3e-g** in the presence of DBU (CHCl_3).

Compound	λ_{max} (lg ϵ)
3a	365 (4.40), 380 (4.41), 556 (3.87)
3b	368 (4.45), 382 (4.48), 551 (3.89)
3c	377 (4.40), 563 (3.91)
3e	371 (4.24), 575 (3.73)
3f	365 (4.28), 569 (3.76)
3g	361 (4.30), 578 (3.86)

4. Redox properties

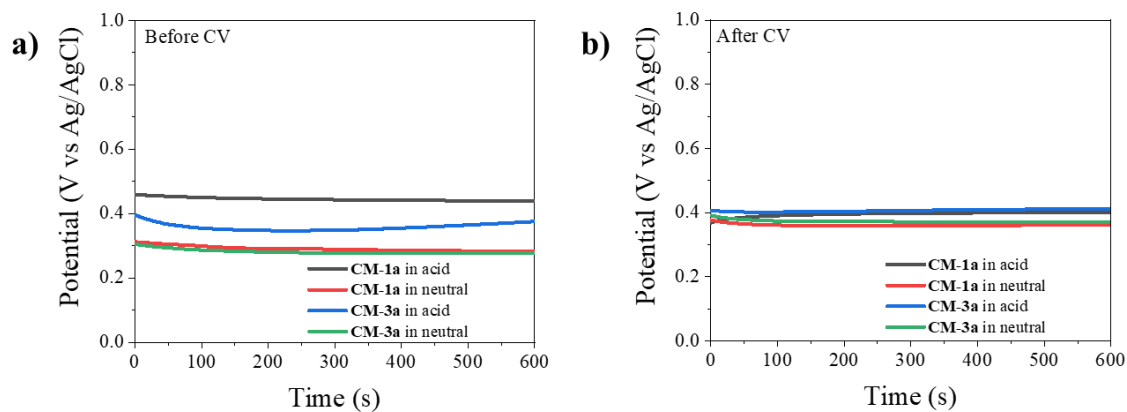


Figure S17. OCP measurements of samples **CM-1a** and **CM-3a** before and after CV measurements.

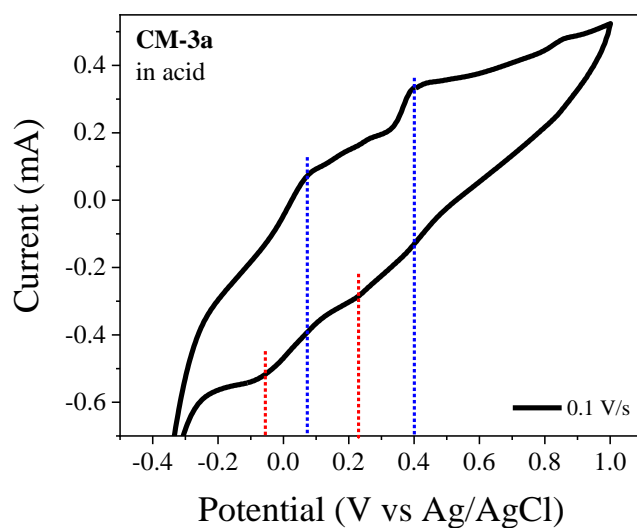


Figure S18. CV curve of sample **CM-3a** in acidic electrolyte at 0.1 V/s scan speed.

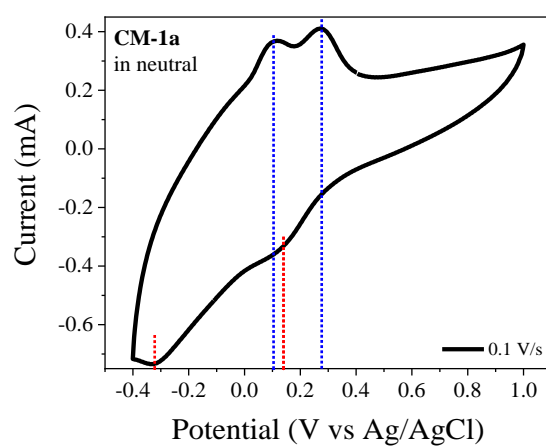


Figure S19. CV curve of sample **CM-1a** in neutral electrolyte at 0.1V/s scan speed.

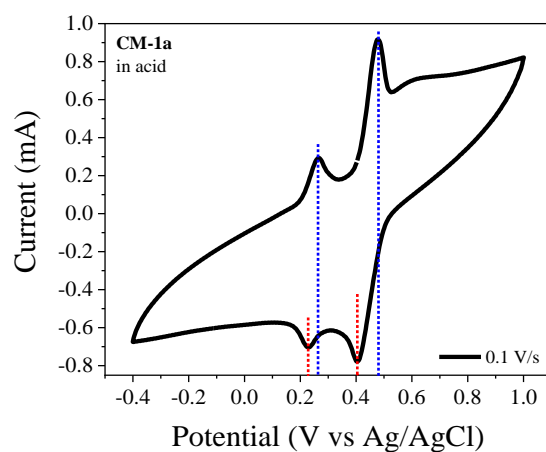


Figure S20. CV curve of sample **CM-1a** in acidic electrolyte at 0.1V/s scan speed.

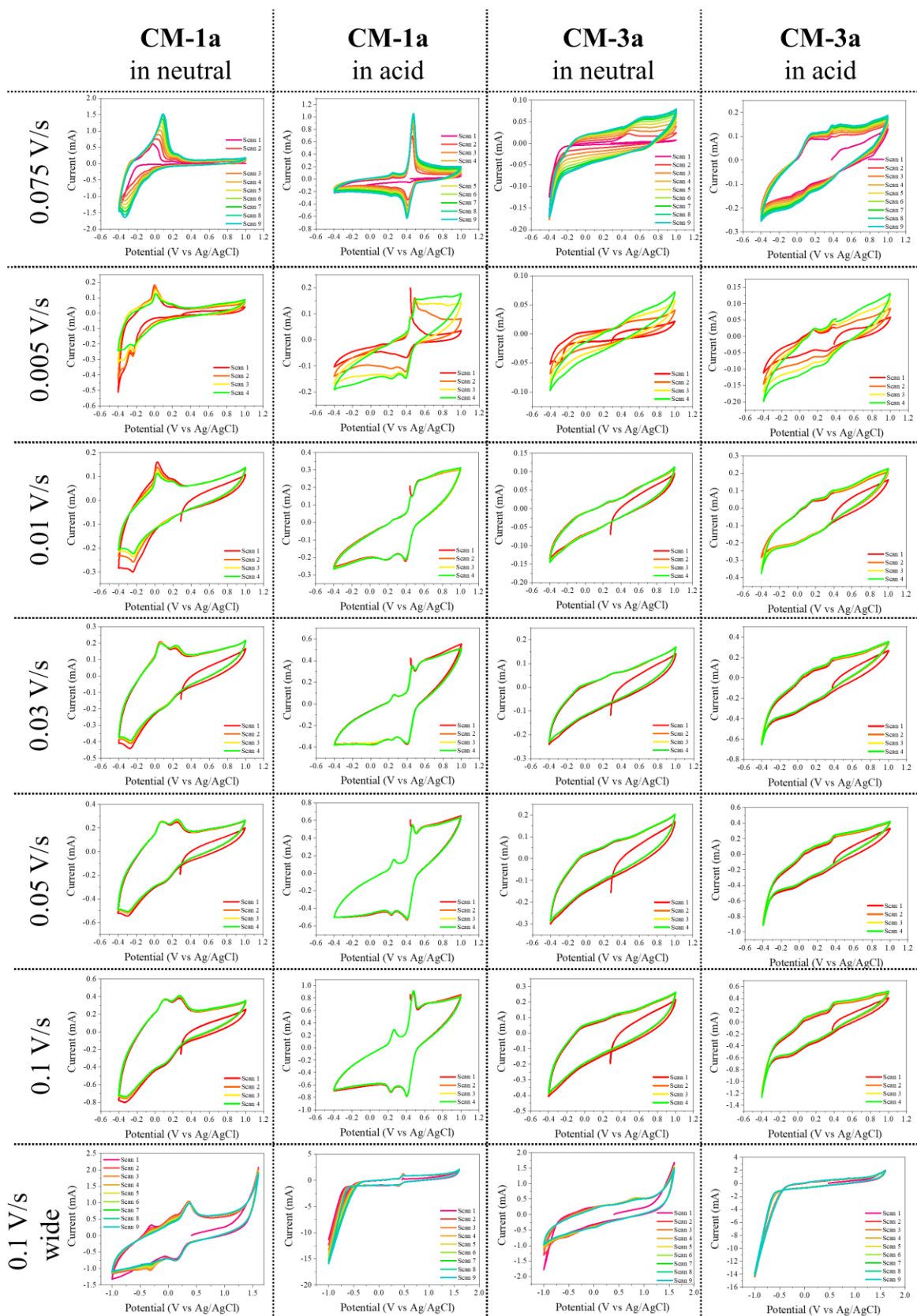


Figure S21. CV curves of samples **CM-1a** and **CM-3a** in neutral and acidic electrolyte at various scan speeds.

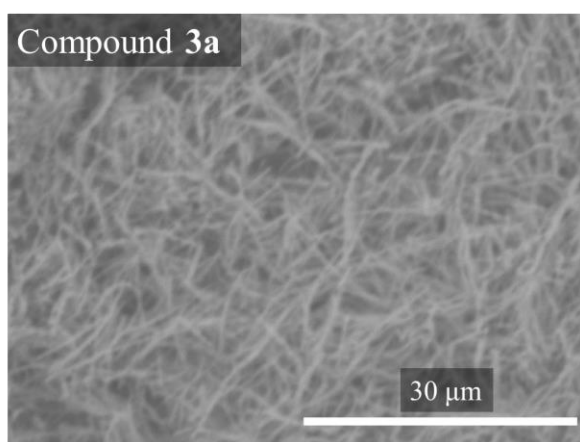
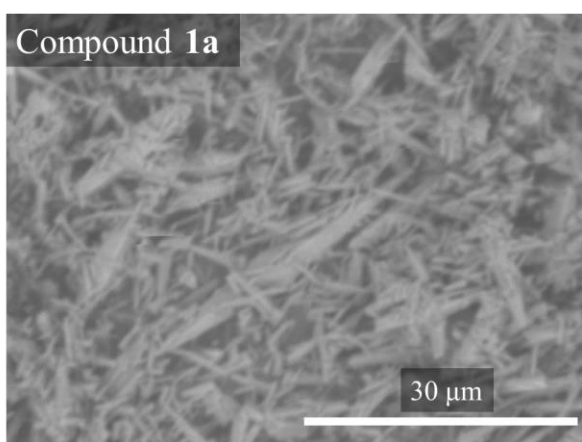
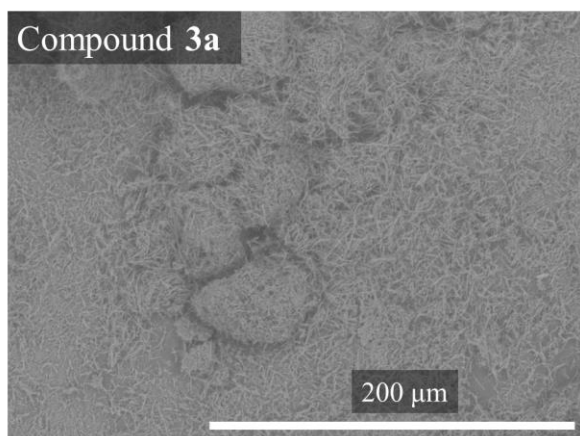
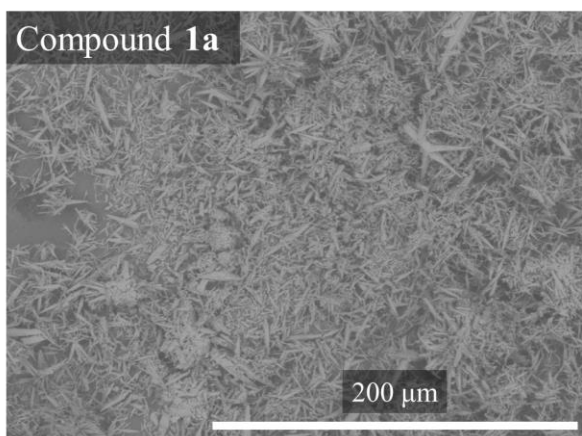


Figure S22. Scanning electron microscopy images of compounds **1a** and **3a** at different magnifications (x500 and x2500).