Supporting Materials

Microwave-Assisted Synthesis, Optical and Theoretical Characterization of Novel 2-(imidazo[1,5-*a*]pyridine-1-yl)pyridnium Salts

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NMR characterization

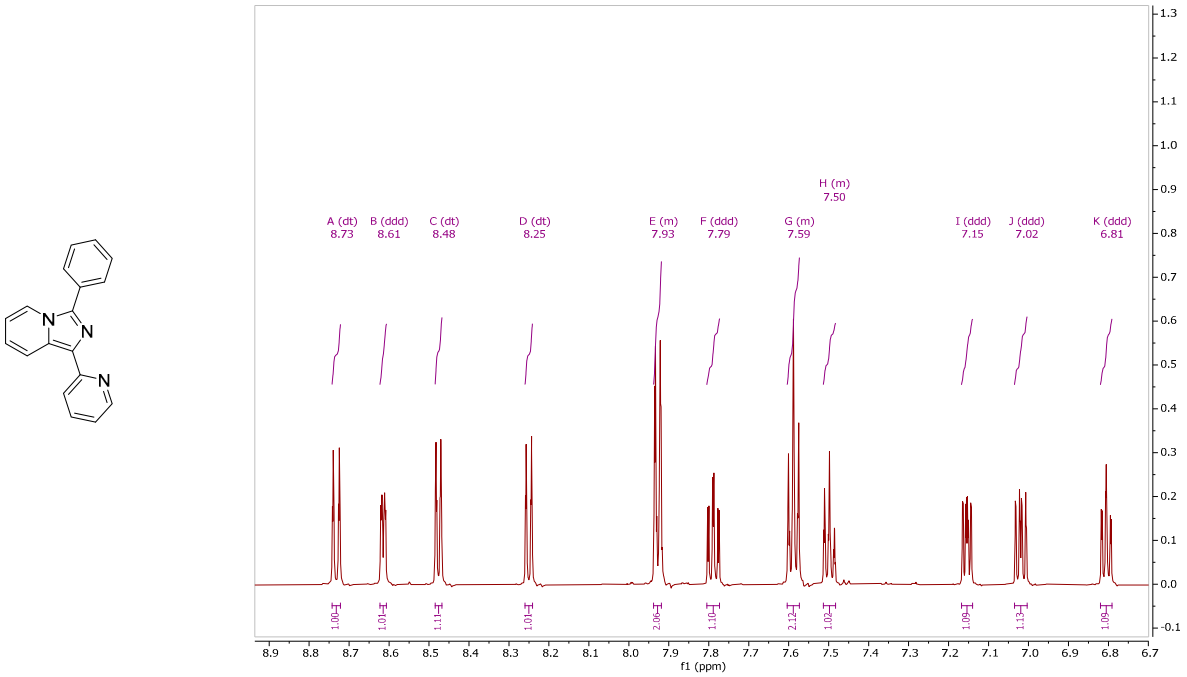

Figure S1. ^{1}H NMR spectrum of Acetone-d_6 solution of **1**

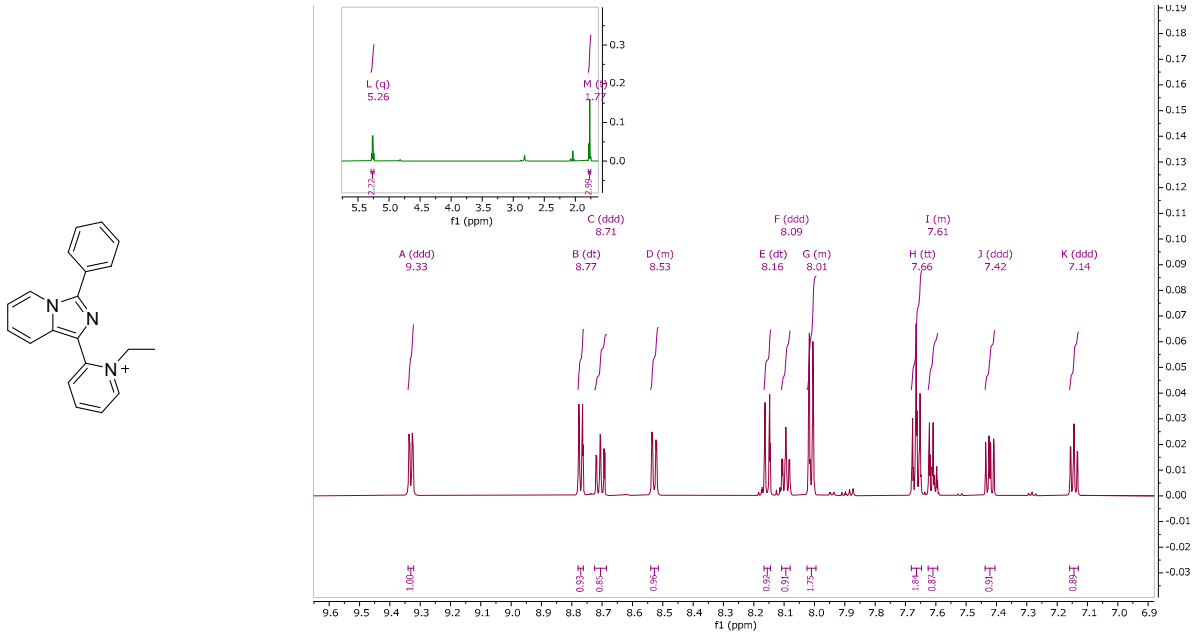

Figure S2. ^{1}H NMR spectrum of Acetone-d$_6$ solution of **1q**. The aliphatic region is shown in the inset.

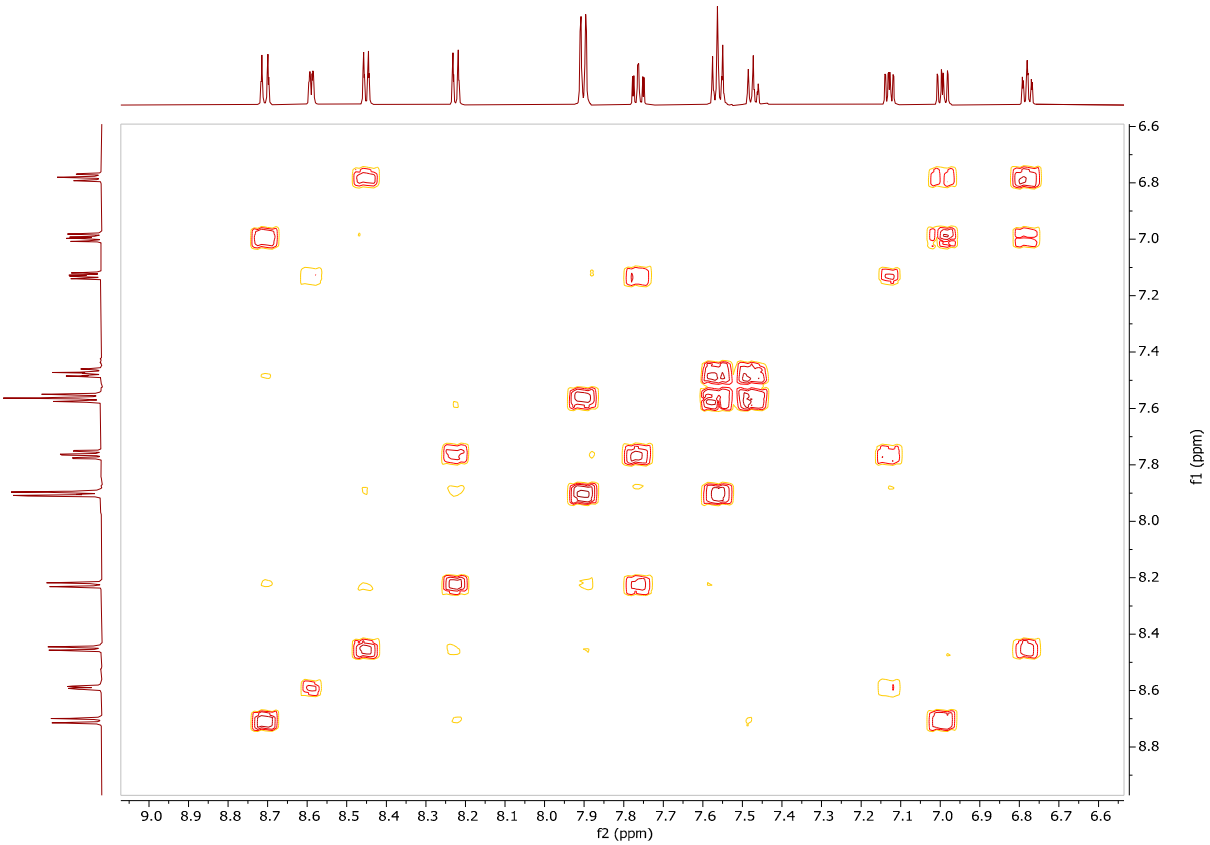

Figure S3. 2D ^{1}H-COSY NMR spectrum of Acetone-d$_6$ solution of **1**

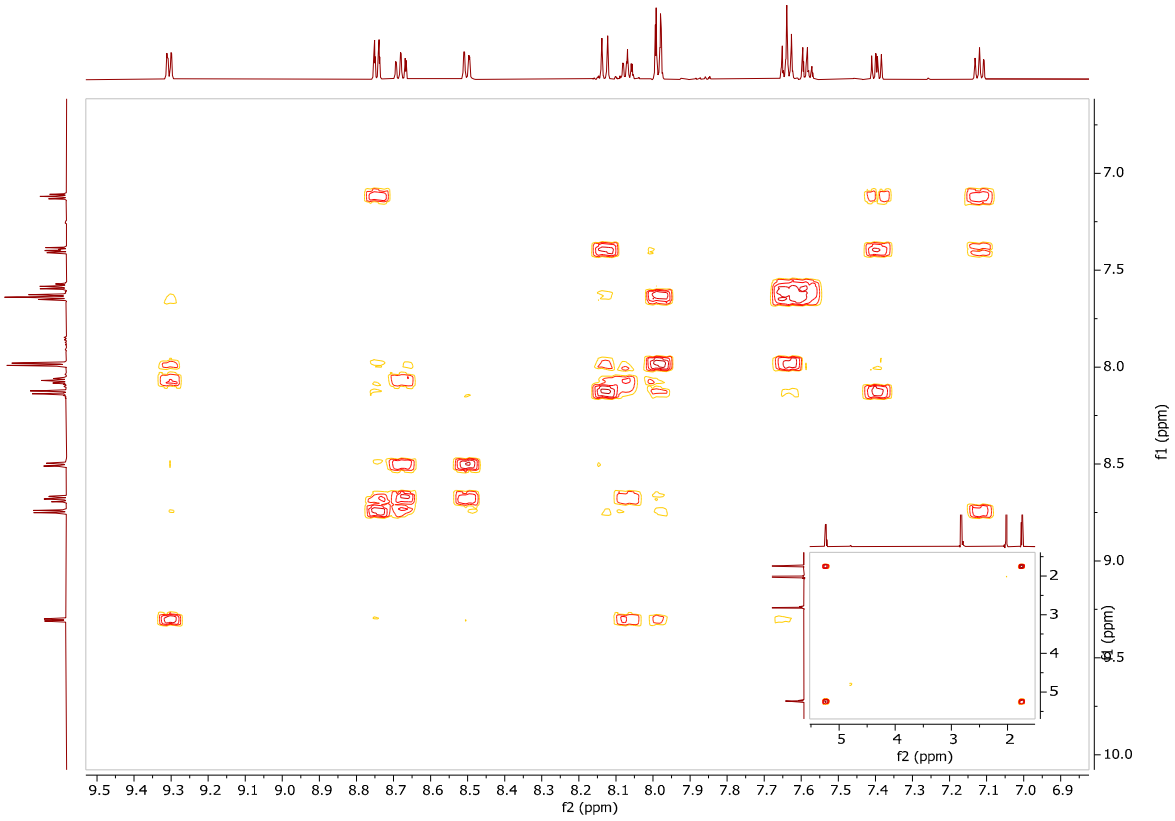

Figure S4. 2D ^{1}H-COSY NMR spectrum of Acetone-d$_6$ solution of **1q.** The aliphatic region is shown in the inset.

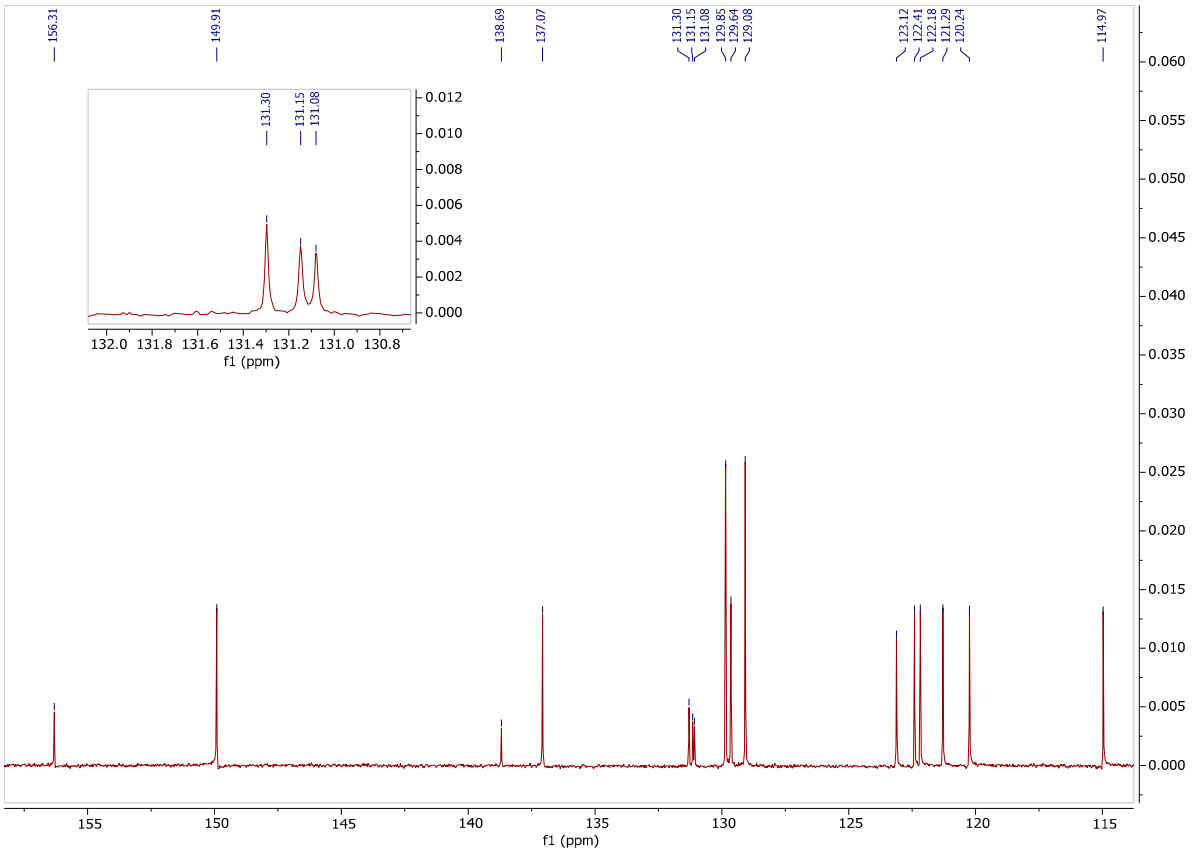

Figure S5. ^{13}C NMR spectrum of Acetone-d$_6$ solution of **1**

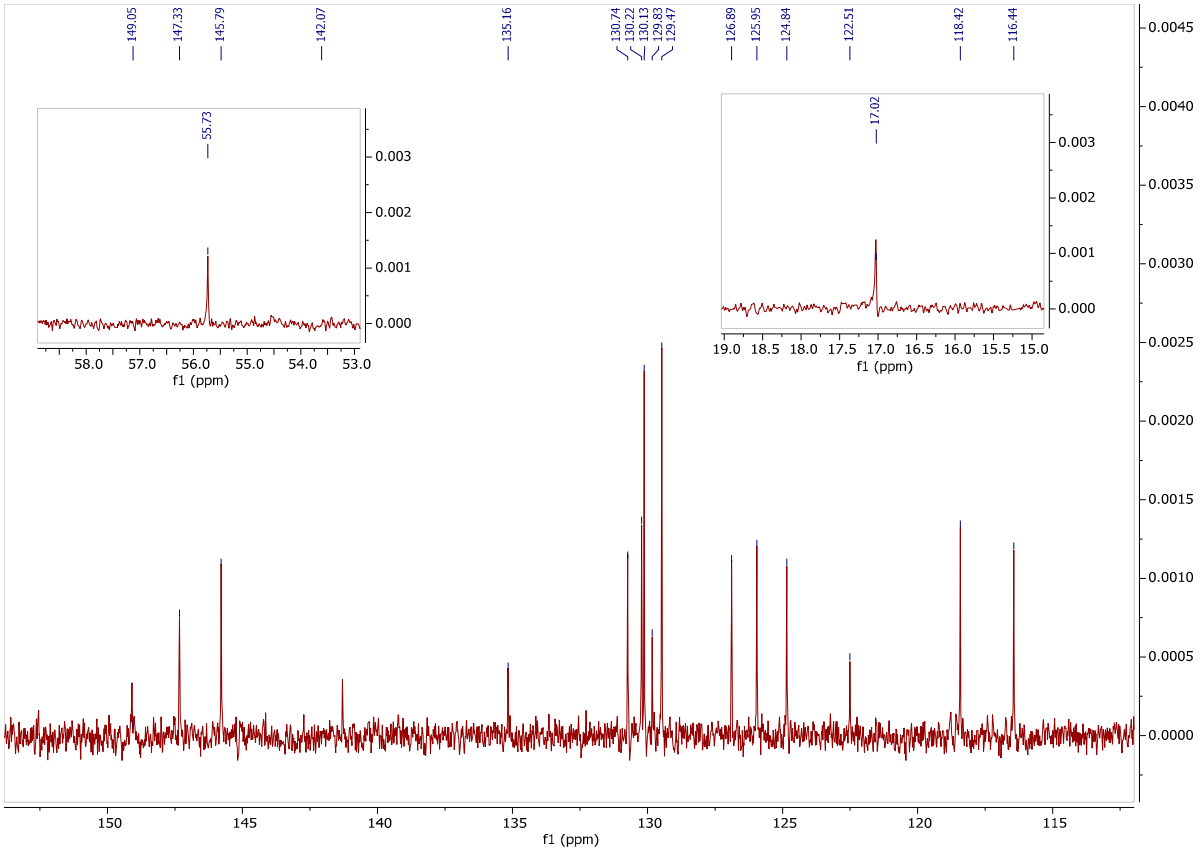

Figure S6. ^{13}C NMR spectrum of Acetone-d_6 solution of **1q.** The aliphatic region is shown in the inset.

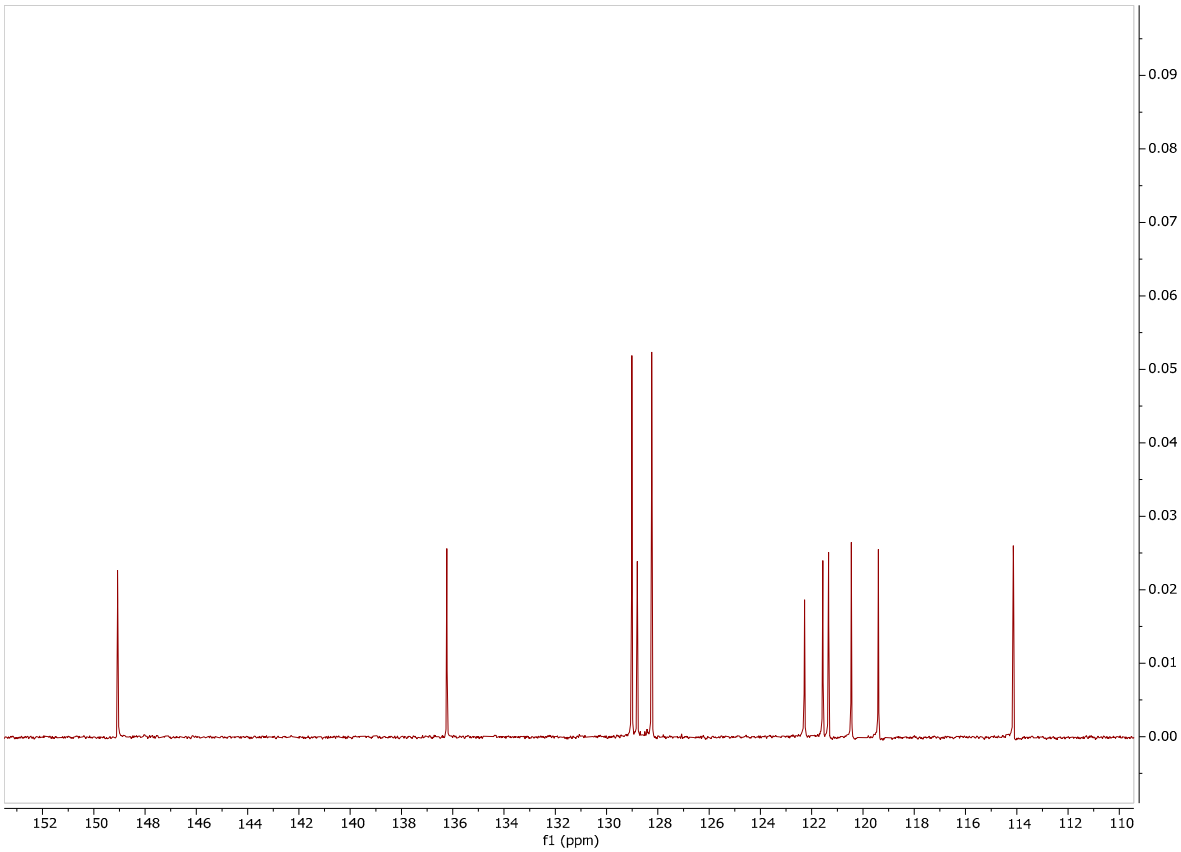

Figure S7. ^{13}C DEPT-135 NMR spectrum of Acetone-d_6 solution of **1.**

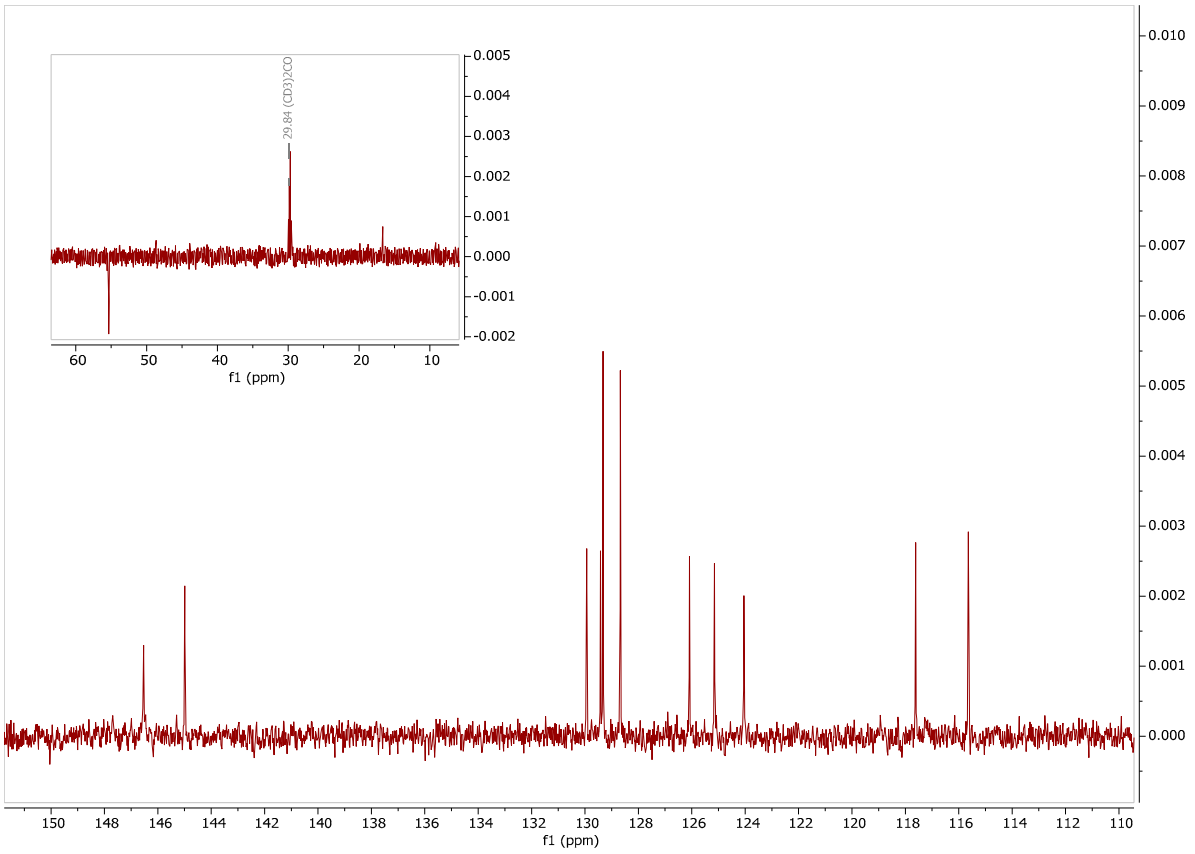

Figure S8. ^{13}C DEPT-135 NMR spectrum of Acetone-d$_6$ solution of **1q.** The aliphatic region is shown in the inset.

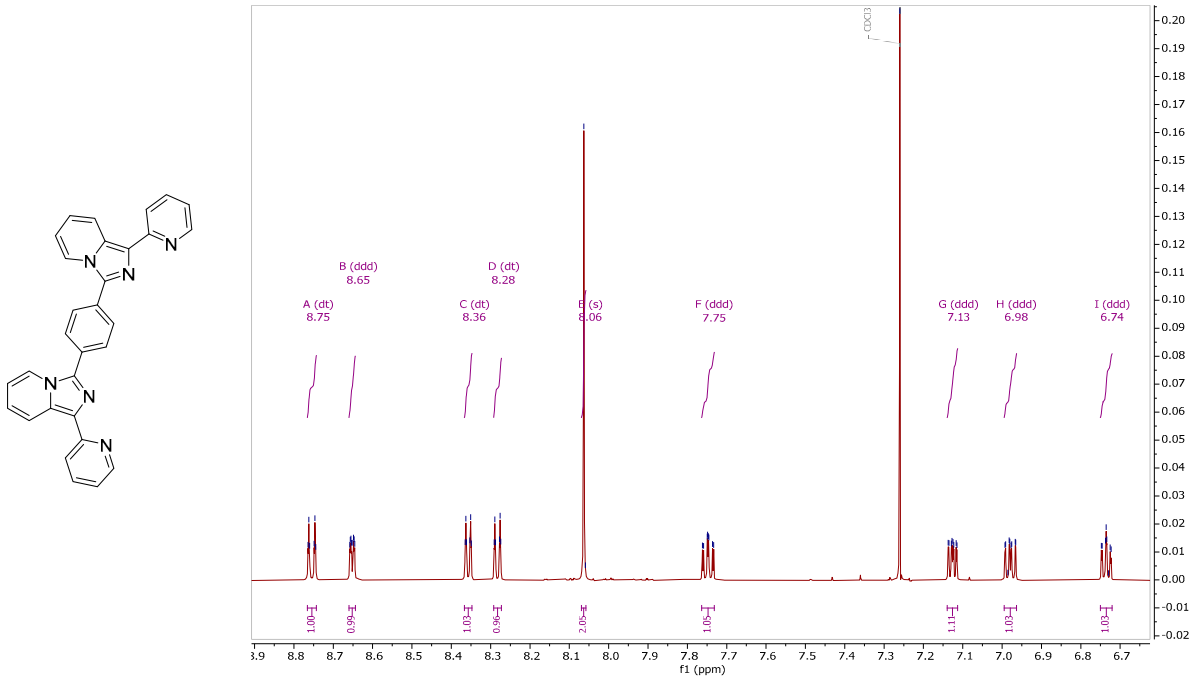

Figure S9. ^{1}H NMR spectrum of Chloroform-d$_3$ solution of **2.**
Due to the symmetry of the system only half of the ^{1}H nuclei are shown.

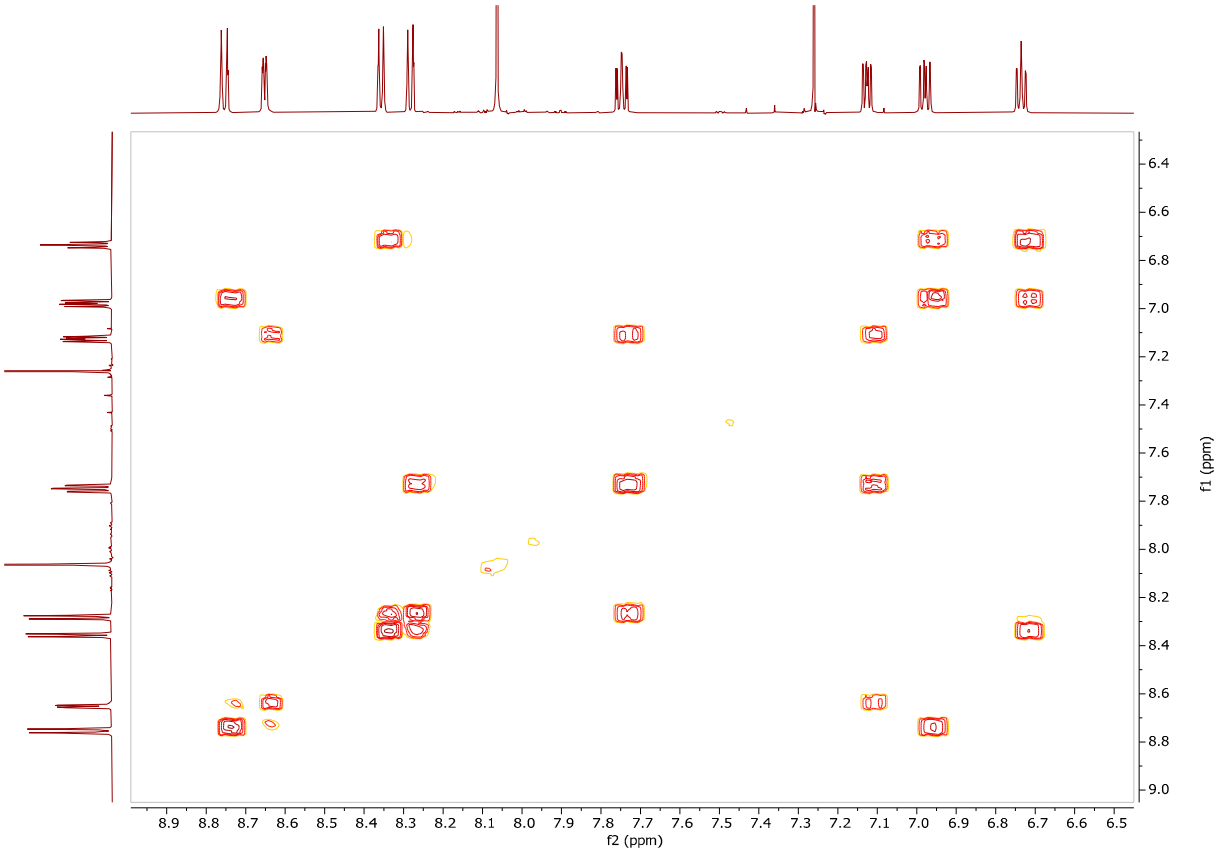

Figure S10. 2D ^{1}H COSY-NMR spectrum of Chloroform-d$_3$ solution of **2.**

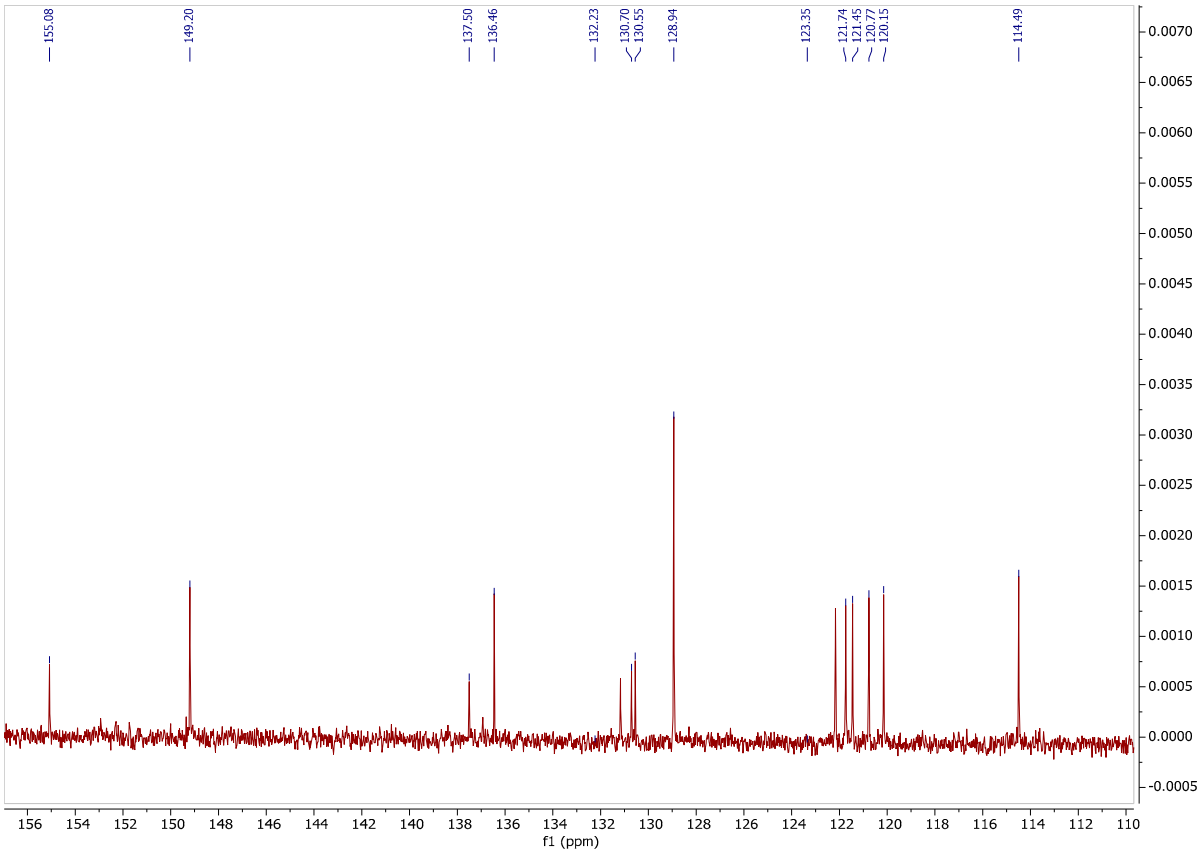

Figure S11. ^{13}C NMR spectrum of Chloroform-d$_3$ solution of **2.**

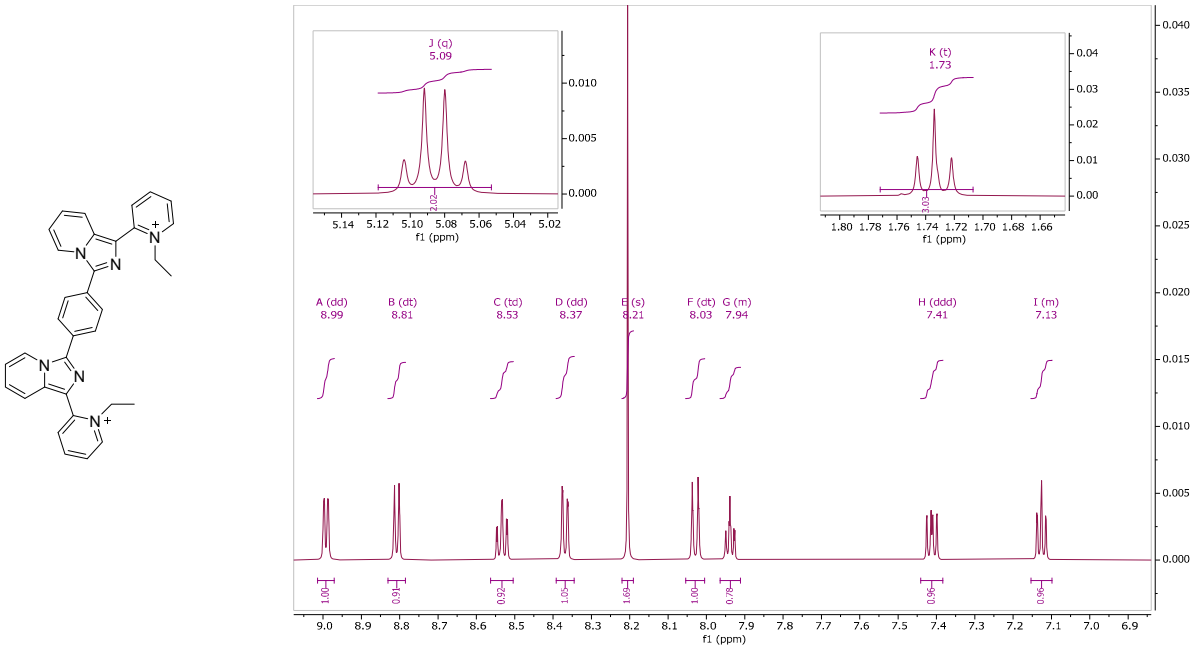

Figure S12. ^{1}H NMR spectrum of Methanol-d$_4$ solution of **2q.** The aliphatic region is shown in the inset. Due to the symmetry of the system only half of the ^{1}H nuclei are shown.

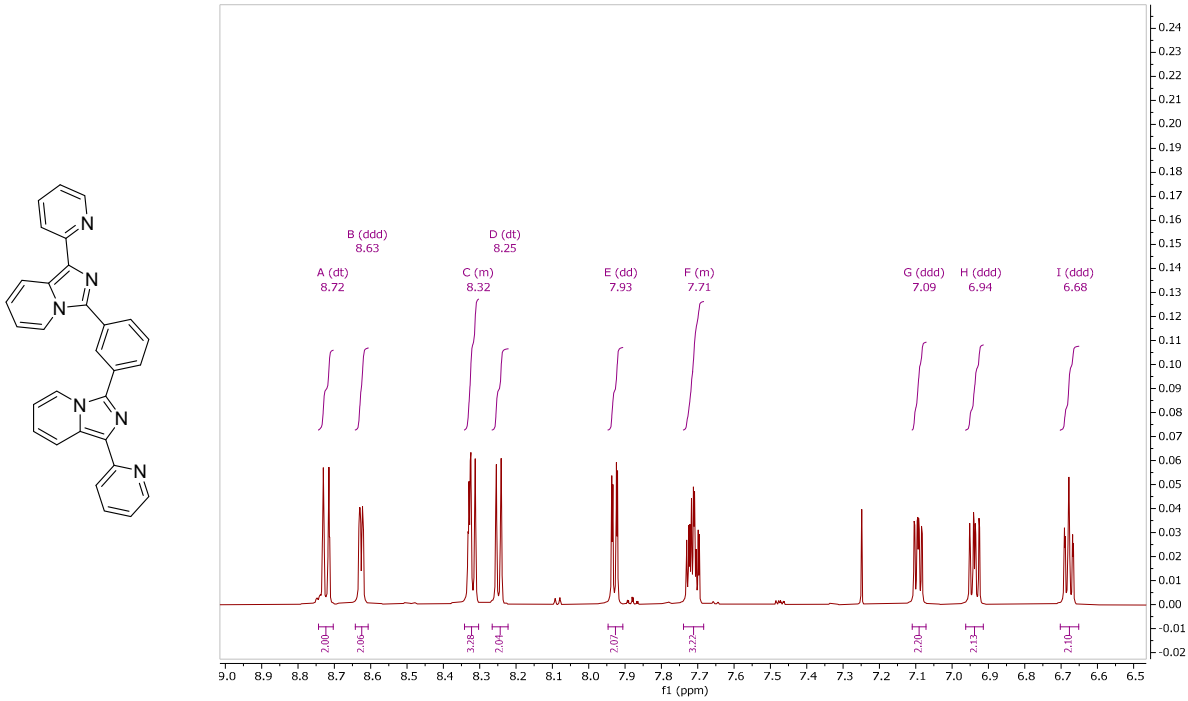

Figure S13. ^{1}H NMR spectrum of Chloroform-d$_3$ solution of **3.**

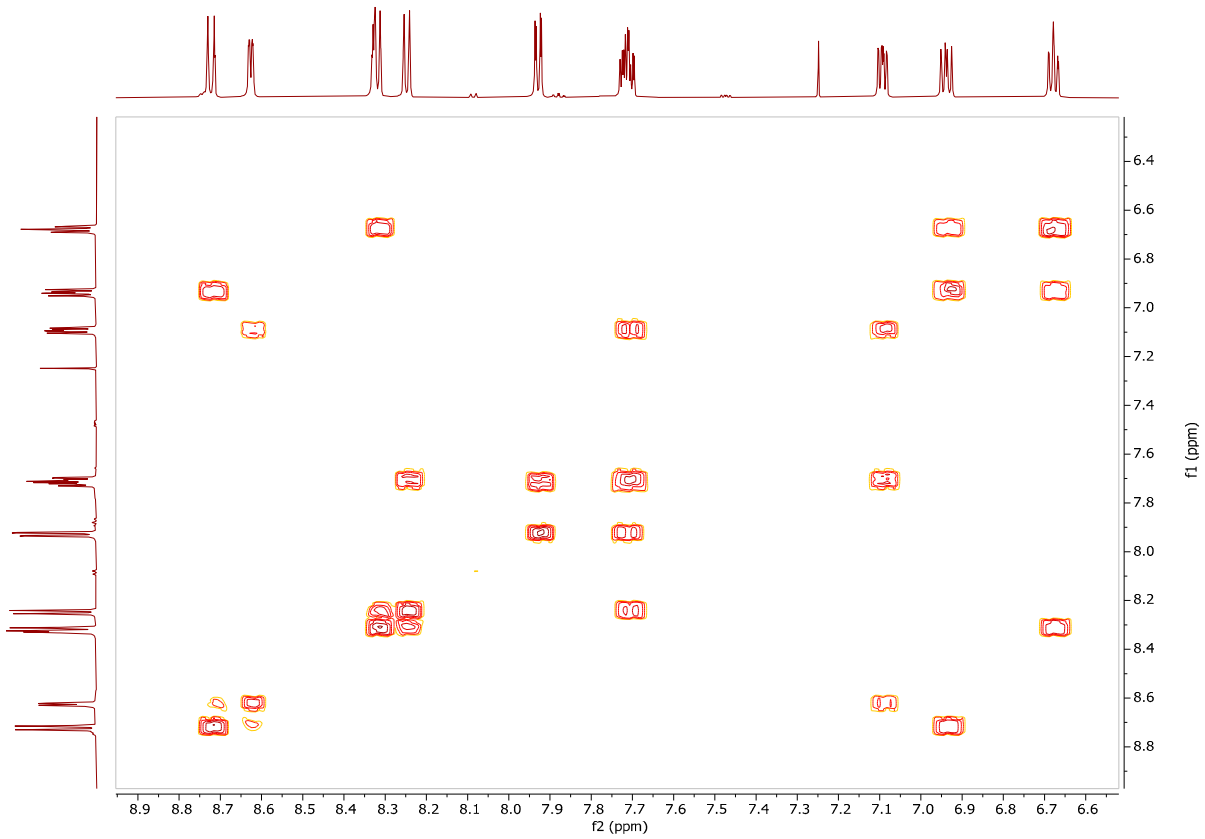

Figure S14. 2D ^{1}H COSY-NMR spectrum of Chloroform-d$_3$ solution of **3.**

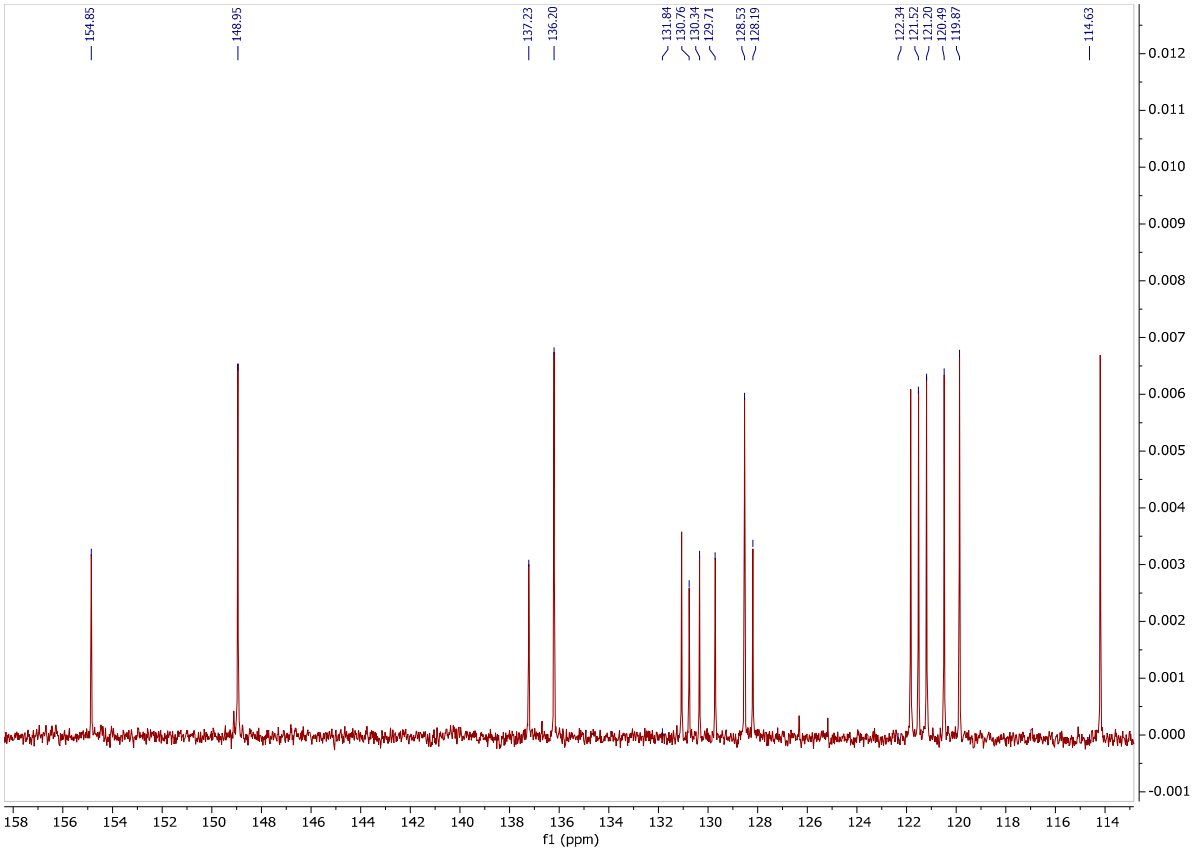

Figure S15. ^{13}C NMR spectrum of Chloroform-d$_3$ solution of **3.**

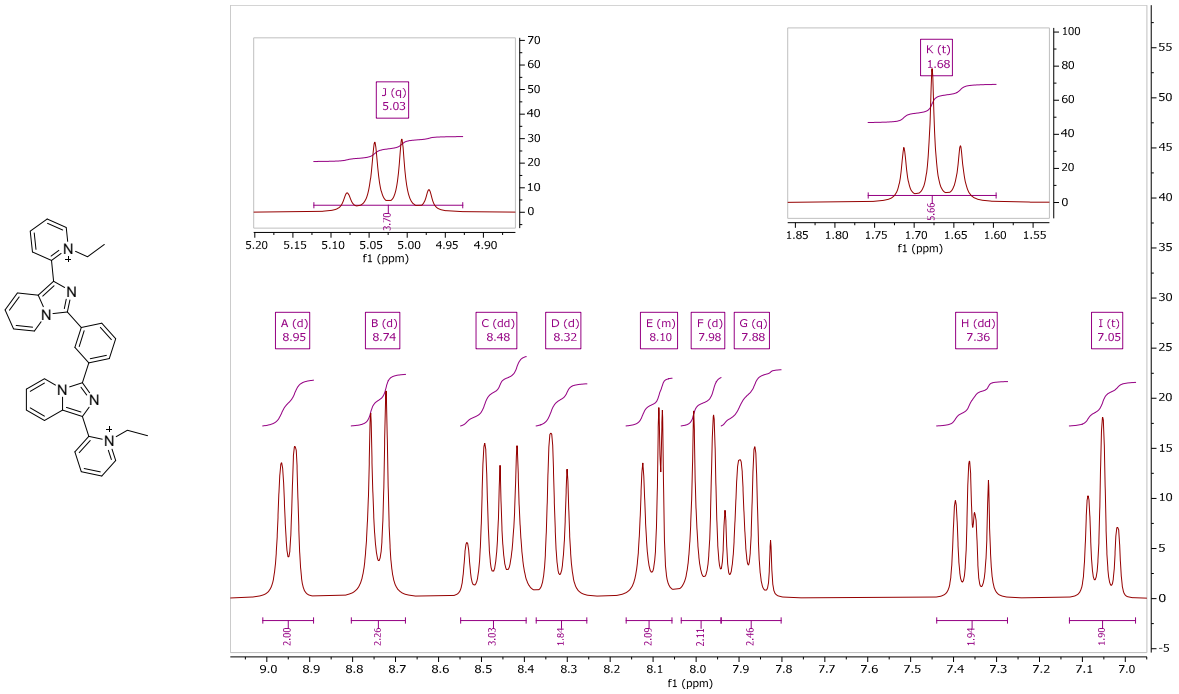

Figure S16. ^{1}H NMR spectrum of Methanol-d$_4$ solution of **3q.** The aliphatic region is shown in the inset.

Computational details

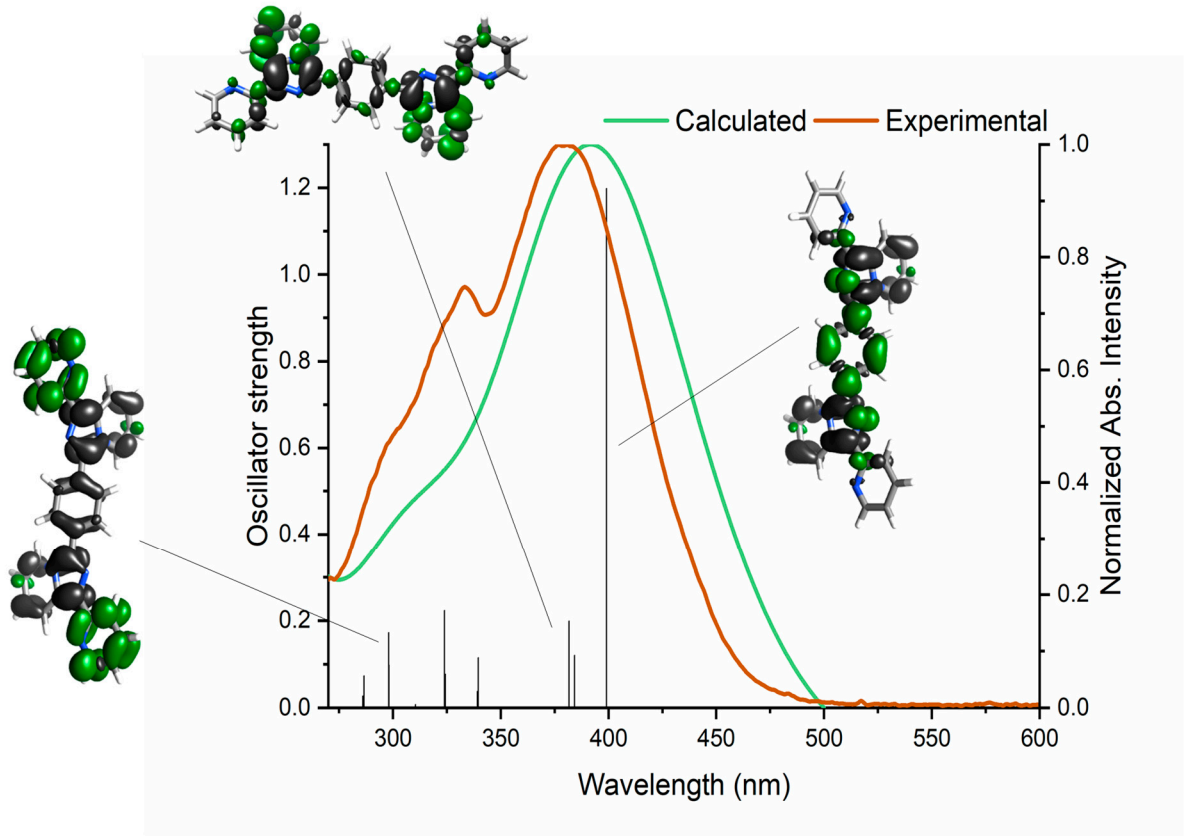

Figure S17. Experimental (orange) and calculated (green) absorption spectra of **2**. The EDDMs of the most relevant transitions are shown.

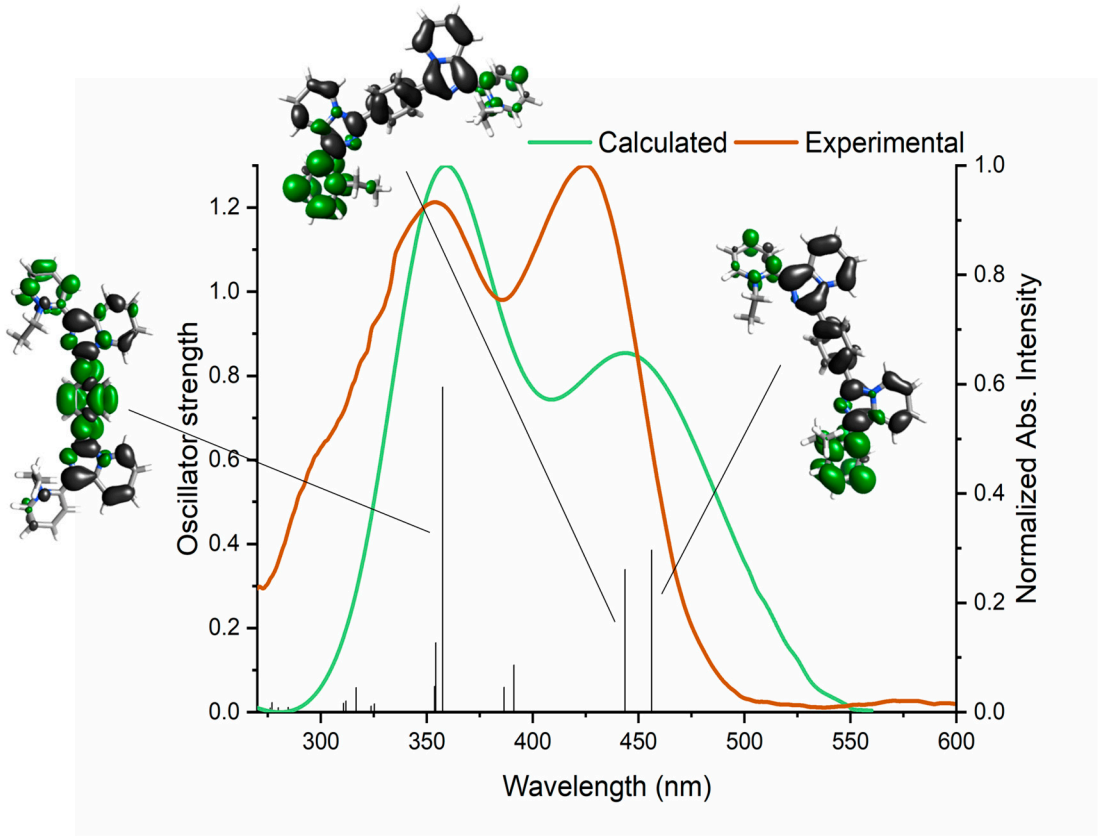

Figure S18. Experimental (orange) and calculated (green) absorption spectra of **2q**. The EDDMs of the most relevant transitions are shown.

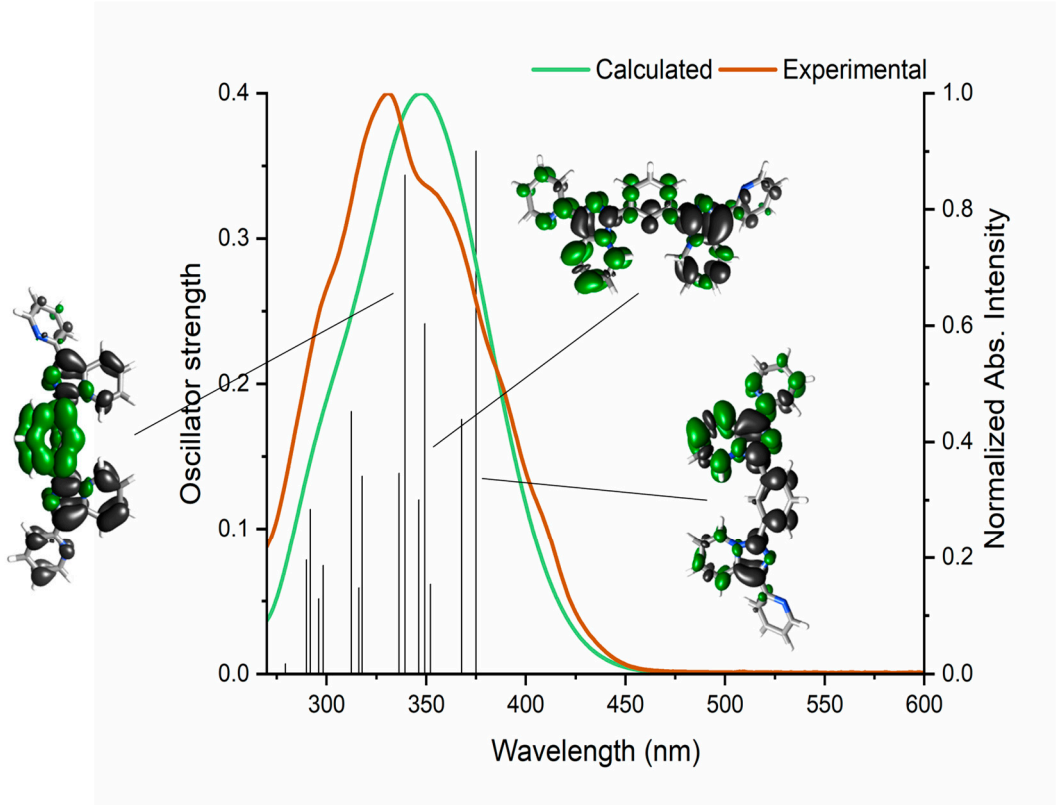

Figure S19. Experimental (orange) and calculated (green) absorption spectra of **3**. The Electron Density Difference Map (EDDM) of the most relevant transitions are shown.

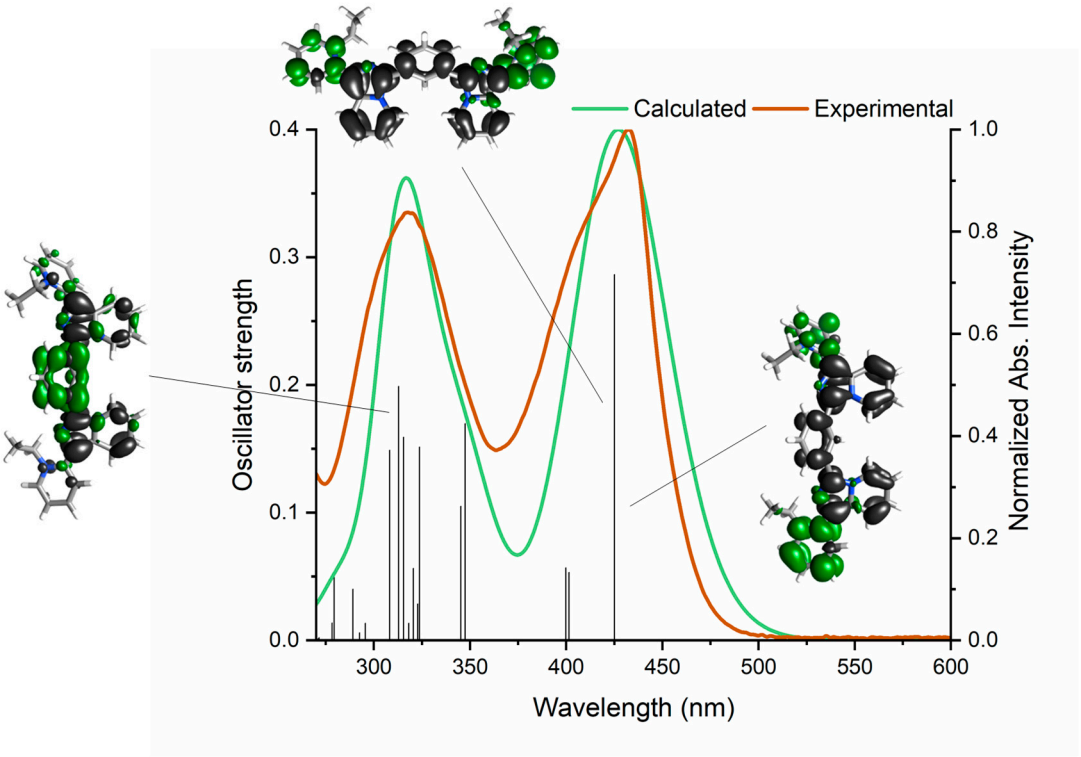

Figure S20. Experimental (orange) and calculated (green) absorption spectra of **3q**. The Electron Density Difference Map (EDDM) of the most relevant transitions are shown.

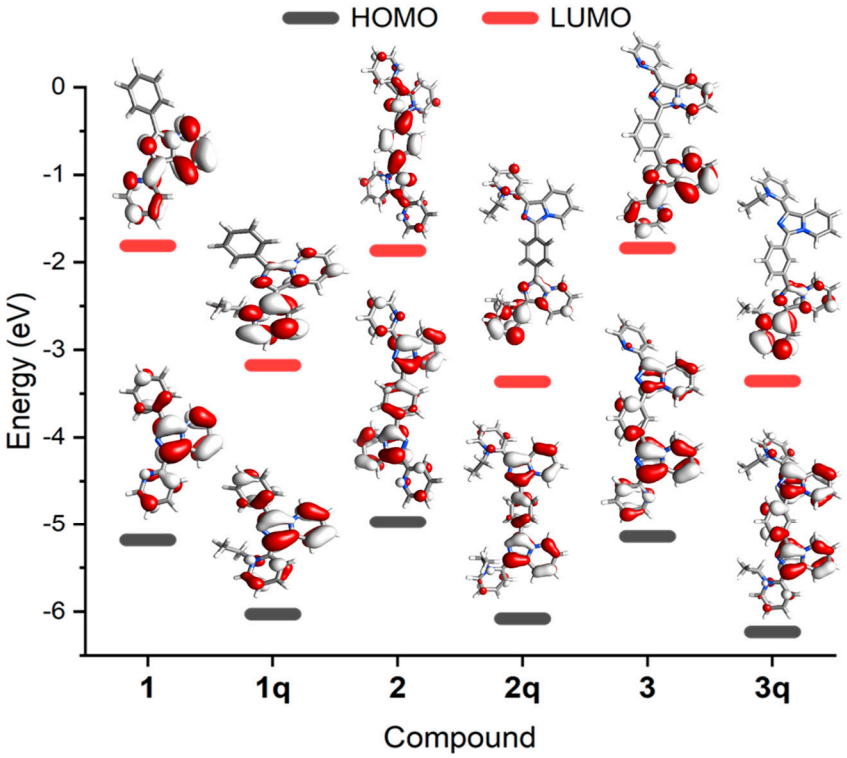

Figure S21. Molecular orbital plots (LUMO and HOMO) of the reported compounds.

Photophysical characterization in thin film

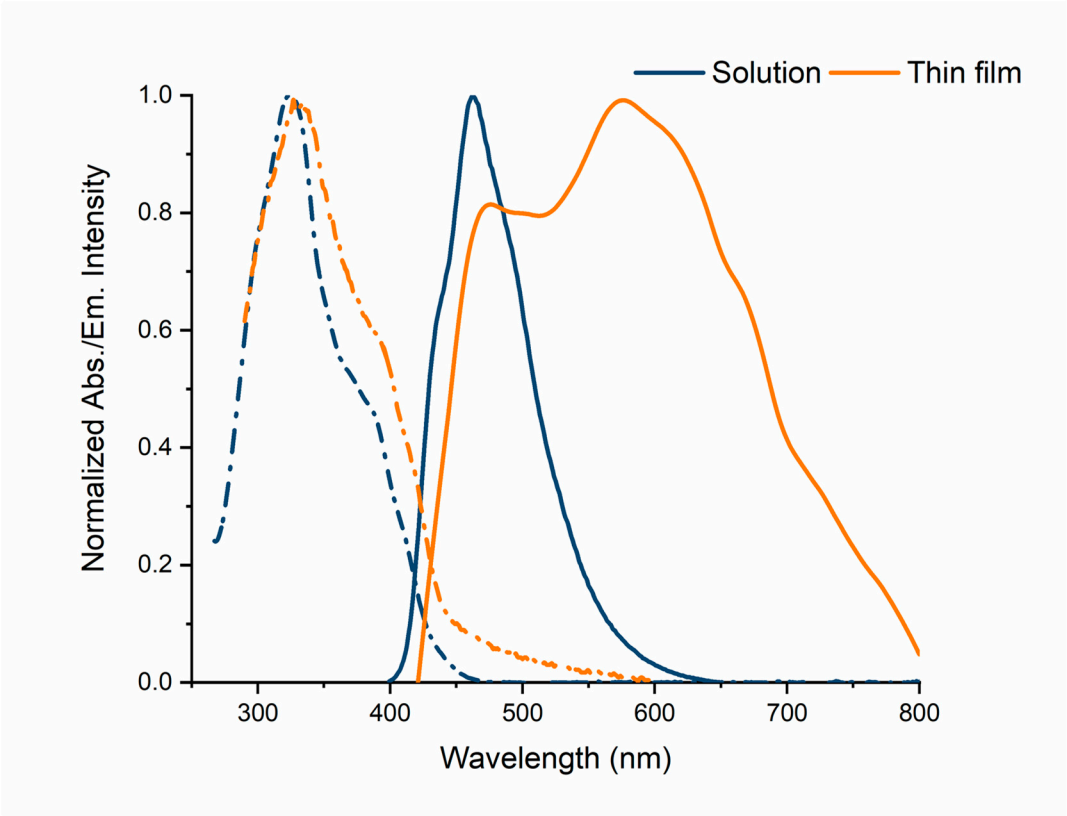

Figure S22. Absorption (dashed lines) and emission (solid lines) spectra of **1** recorded in DCM solution (concentration 10^{-5} M) (blue) and in thin film (orange)

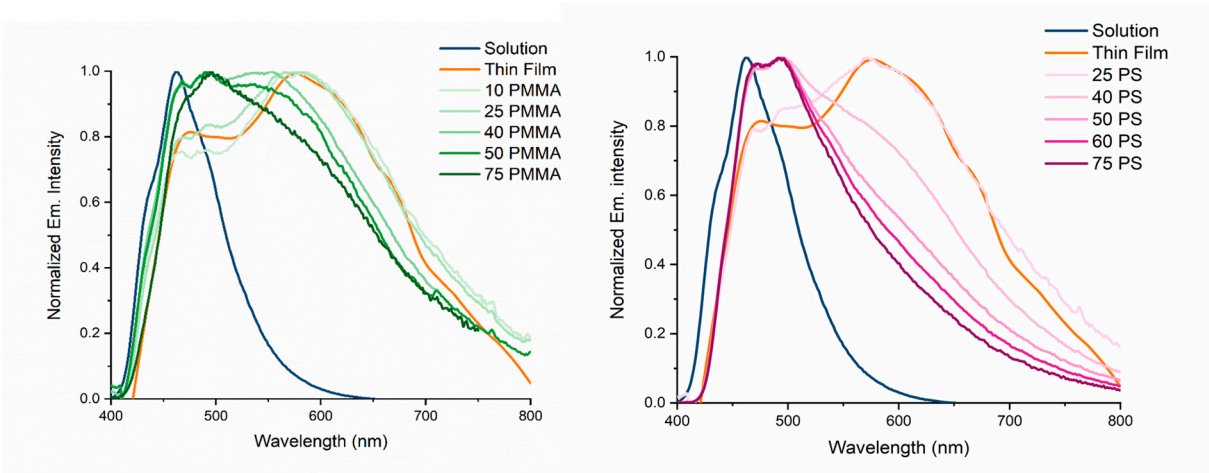

Figure S23. Emission spectra of **1** recorded in different conditions: DCM solution, thin film, blended in PMMA and in PS – See Legend.

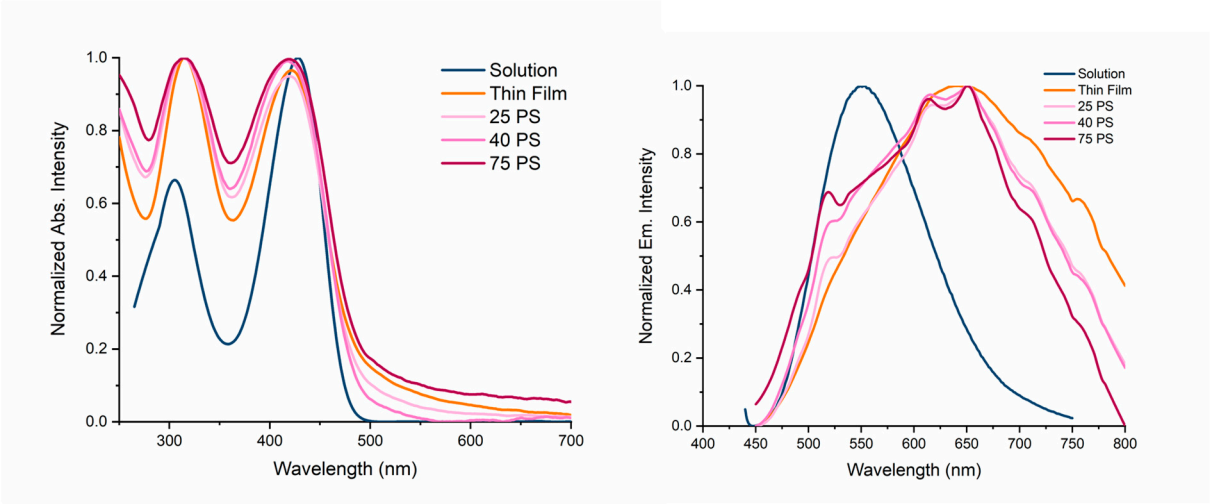

Figure S24. Absorption (left) and emission (right) spectra of **1q** recorded in DCM solution (concentration 10^{-5} M), in thin film and blended in PS matrix

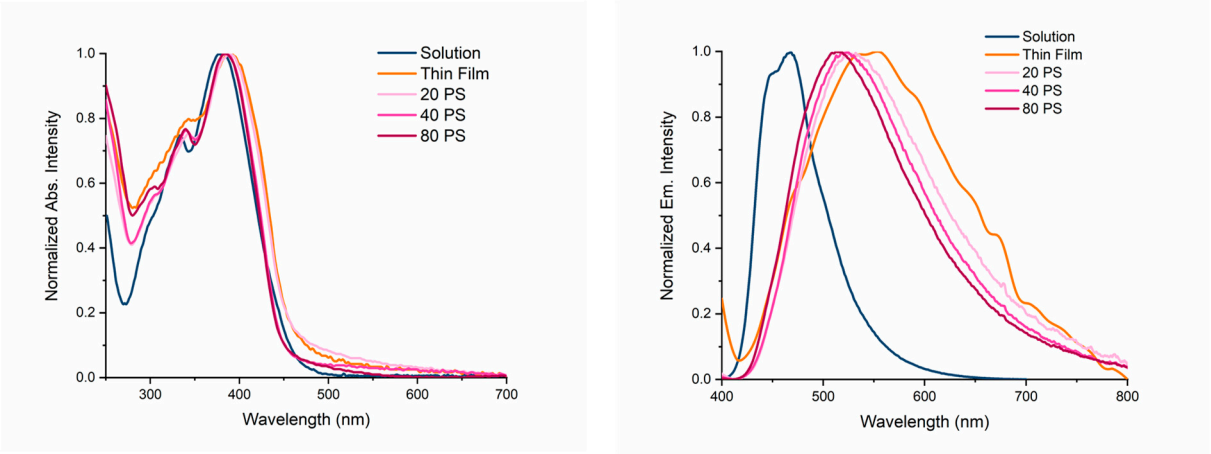

Figure S25. Absorption (left) and emission (right) spectra of **2** recorded in DCM solution (concentration 10^{-5} M), in thin film and blended in PS matrix

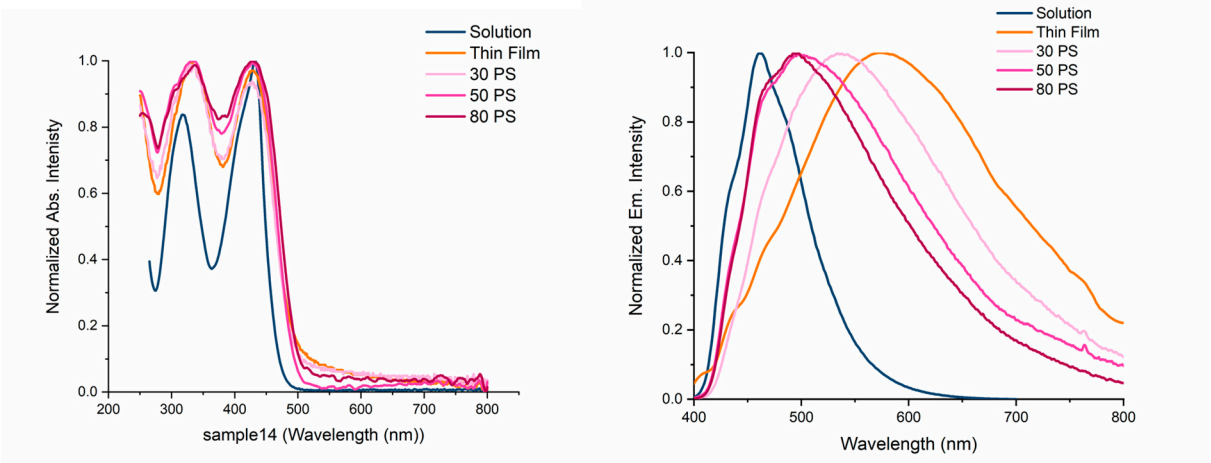

Figure S26. Absorption (left) and emission (right) spectra of **3** recorded in DCM solution (concentration 10^{-5} M), in thin film and blended in PS matrix

Table S1. Photophysical characterization of **2** and **3** in pristine thin film or with different %wt of polymeric matrices.

Compound	Conditions	λ_{em} /nm	ϕ/% (λ_{ex}/nm)	<τ> /ns	k_{rad} /s^{-1}	k_{nrad} /s^{-1}
2	**Solution**	466	22 (380)	6.27	3.51E+07	1.24E+08
	Thin film	550	<5 (385)	2.56	5.31E+06	3.85E+08
	25% PS	530	<5 (385)	2.34	9.75E+06	4.18E+08
	40% PS	525	<5 (385)	2.96	1.27E+07	3.26E+08
	80% PS	515	<5 (385)	2.4	2.45E+07	3.92E+08
3	**Solution**	461	19 (330)	5.76	3.30E+07	1.41E+08
	Thin film	572	<5 (340)	4.21	1.74E+06	2.36E+08
	25% PS	538	<5 (340)	3.99	6.09E+06	2.45E+08
	40% PS	492	<5 (340)	2.83	1.30E+07	3.41E+08
	80% PS	492	<5 (340)	3.32	1.34E+07	2.88E+08