

Electronic Supporting Information for:
New Tetralactam Hosts for Squaraine Dyes

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A. ^1H and ^{13}C NMR Spectra

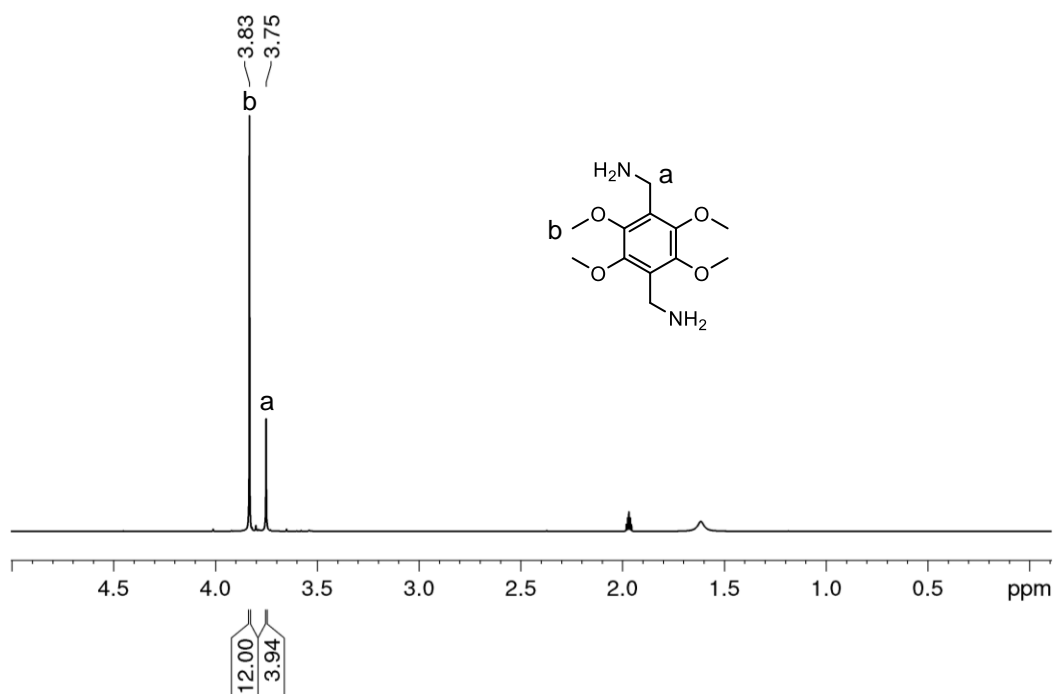


Figure S1: ^1H NMR (400 MHz, CD_3CN , 25 °C) of **4**.

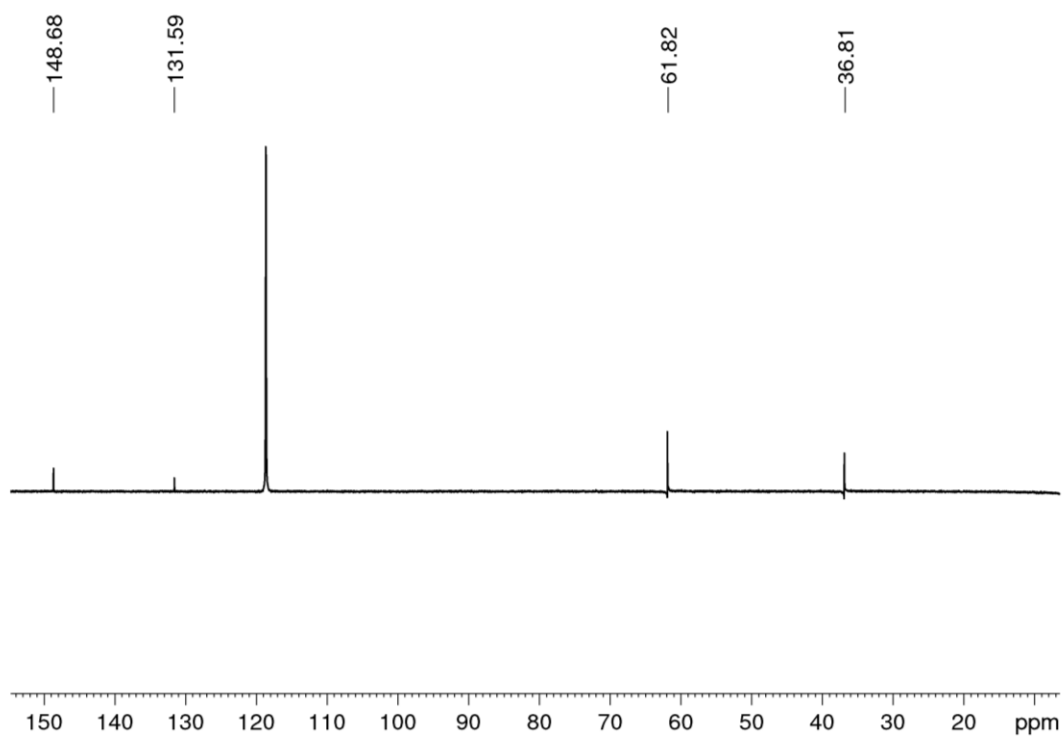


Figure S2: ^{13}C NMR (100 MHz, CD_3CN , 25 °C) of **4**.

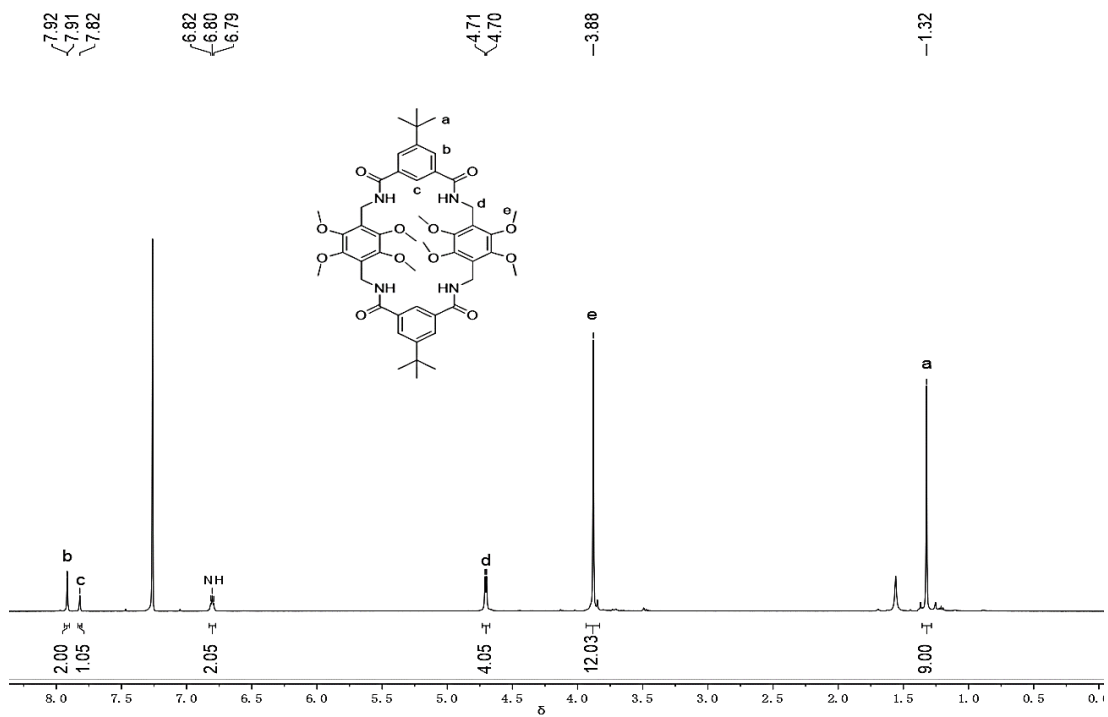


Figure S3: ^1H NMR (500 MHz, CDCl_3 , 25 $^\circ\text{C}$) of **M4a**.

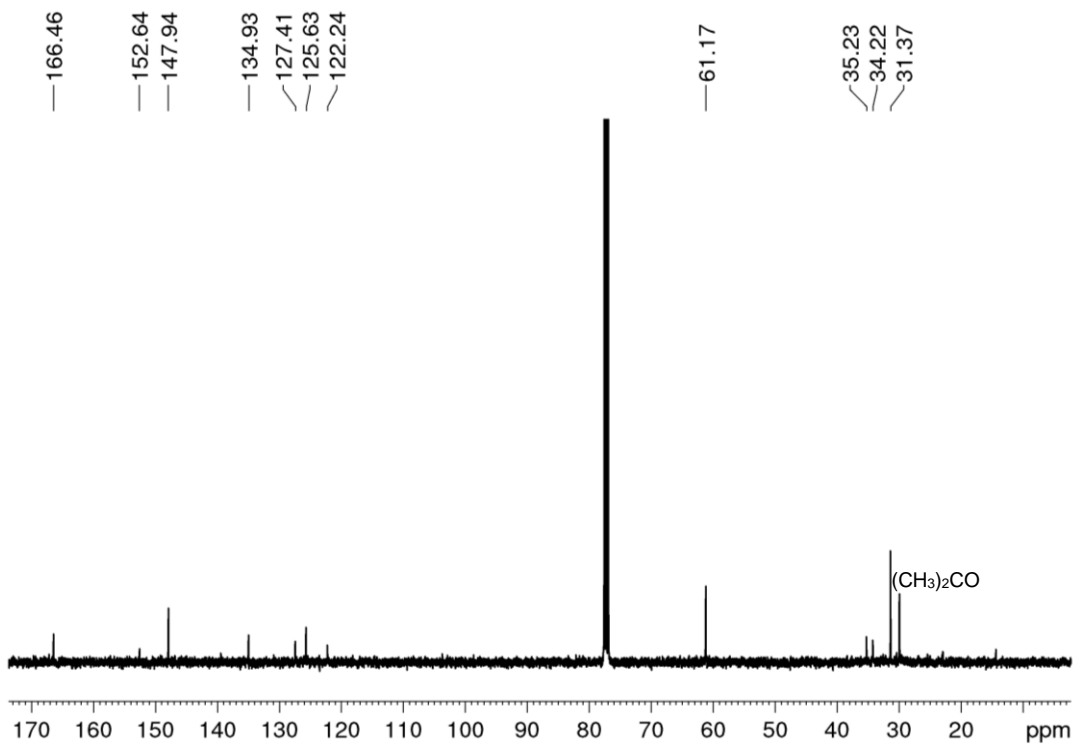


Figure S4: ^{13}C NMR (100 MHz, CDCl_3 , 25 $^\circ\text{C}$) of **M4a**.

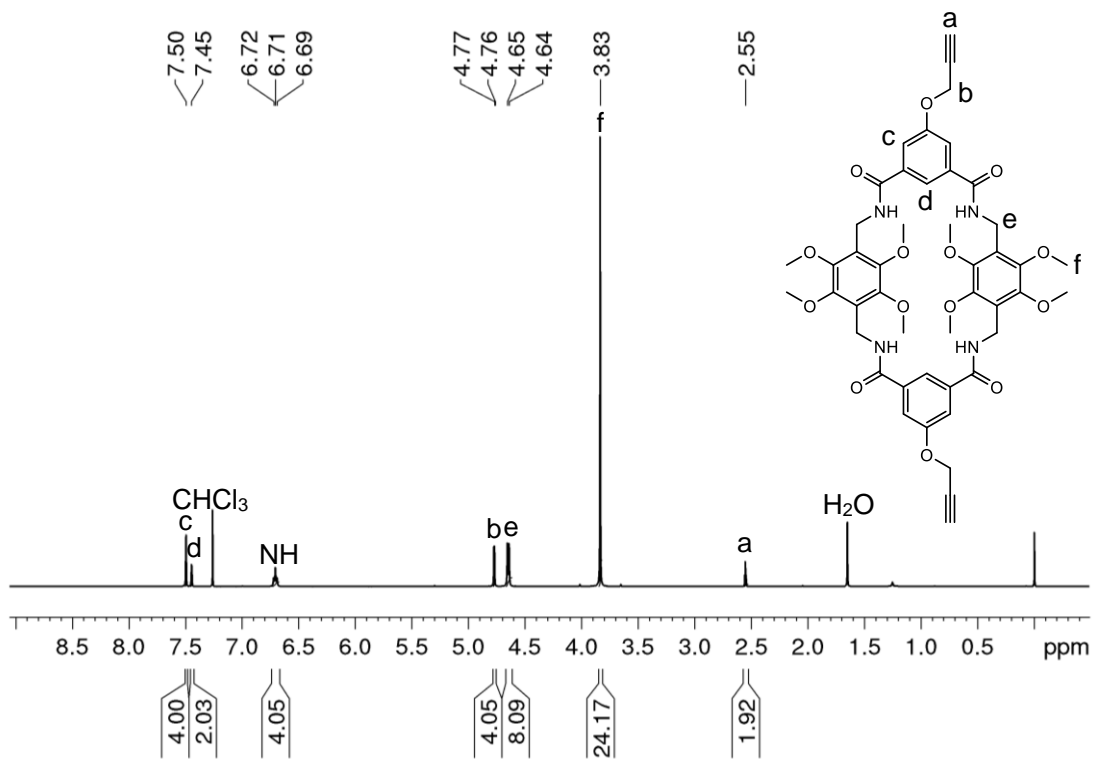


Figure S5: ^1H NMR (400 MHz, CDCl_3 , 25 °C) of **M4b**.

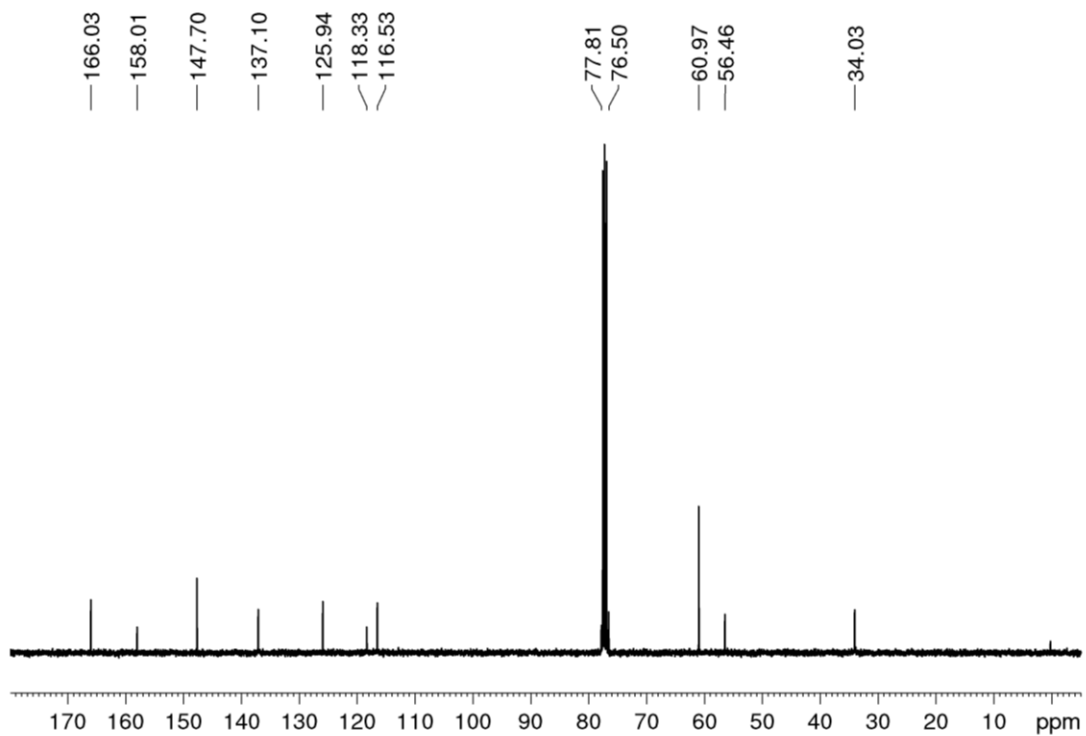
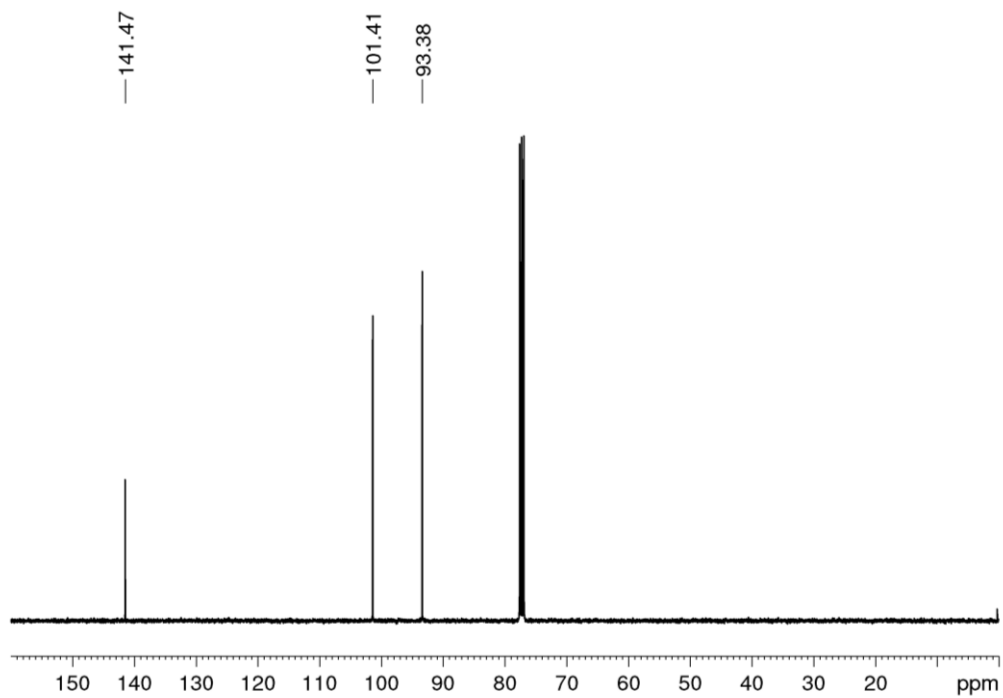
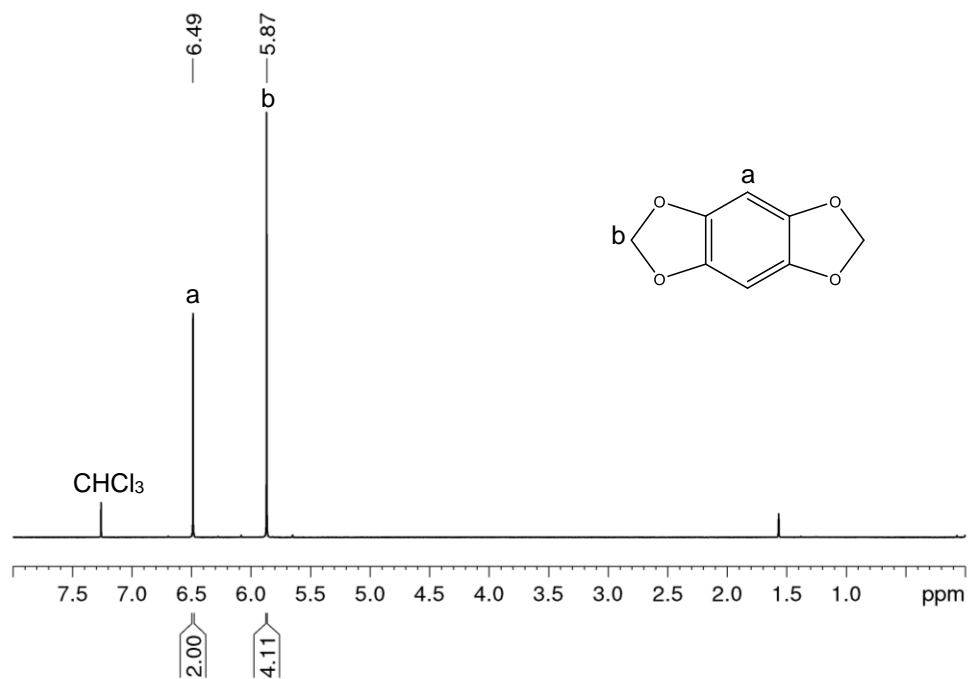


Figure S6: ^{13}C NMR (100 MHz, CDCl_3 , 25 °C) of **M4b**.



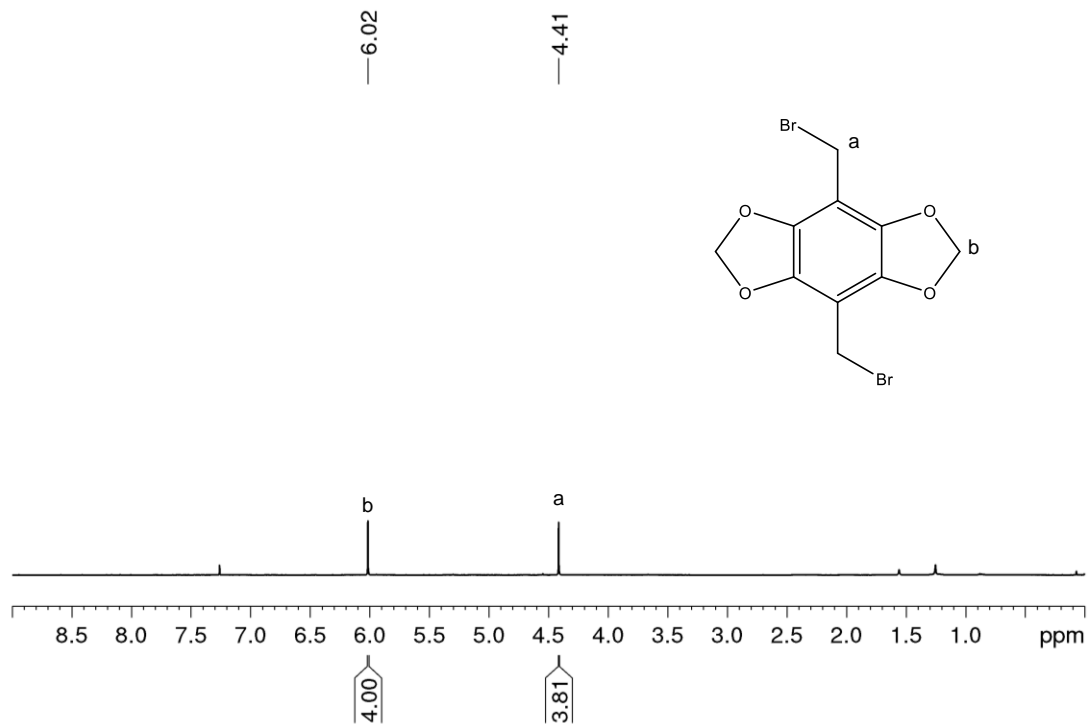


Figure S9: ^1H NMR (500 MHz, CDCl_3 , 25 $^\circ\text{C}$) of **8**.

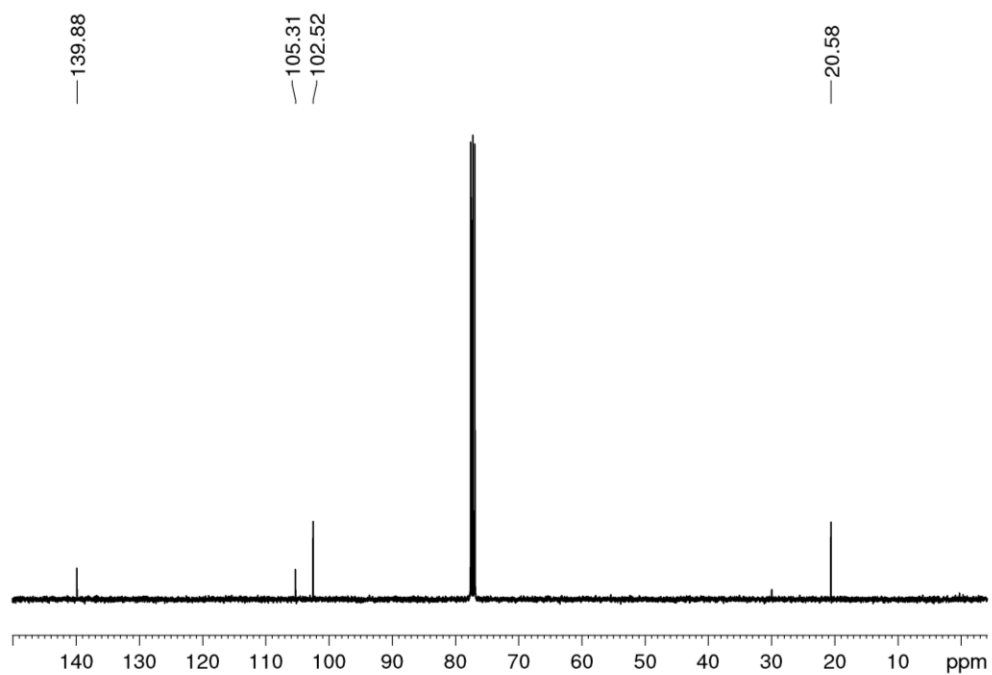


Figure S10: ^{13}C NMR (100 MHz, CDCl_3 , 25 $^\circ\text{C}$) of **8**.

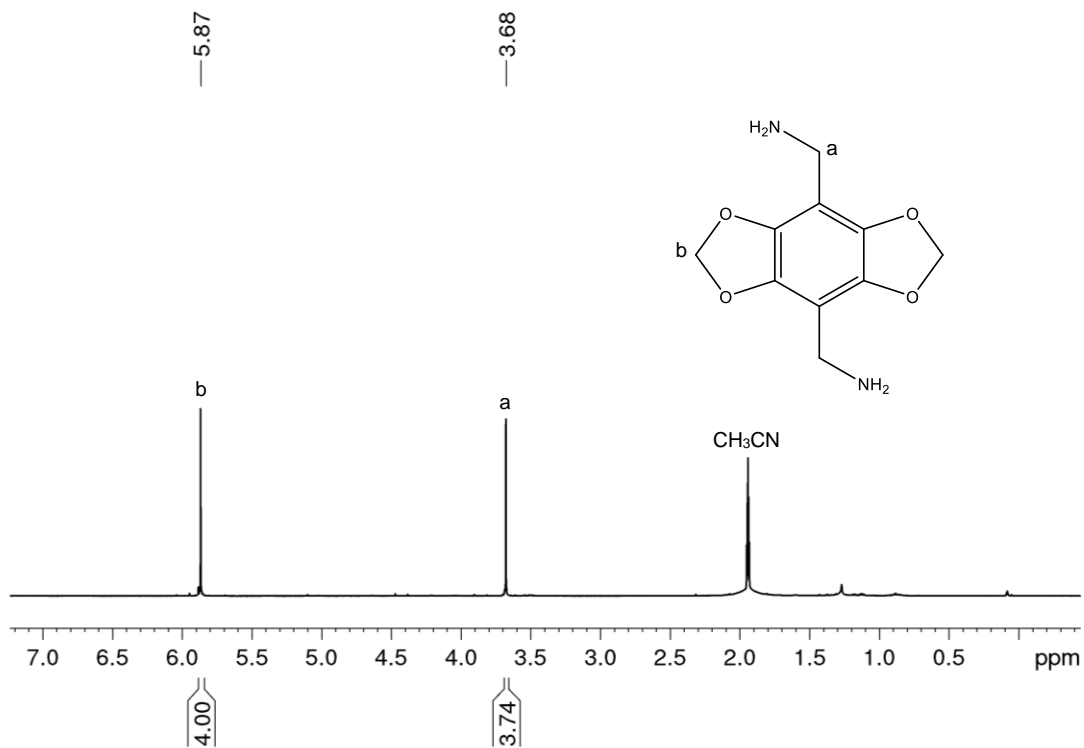


Figure S11: ^1H NMR (500 MHz, CD_3CN , 25 °C) of **9**.

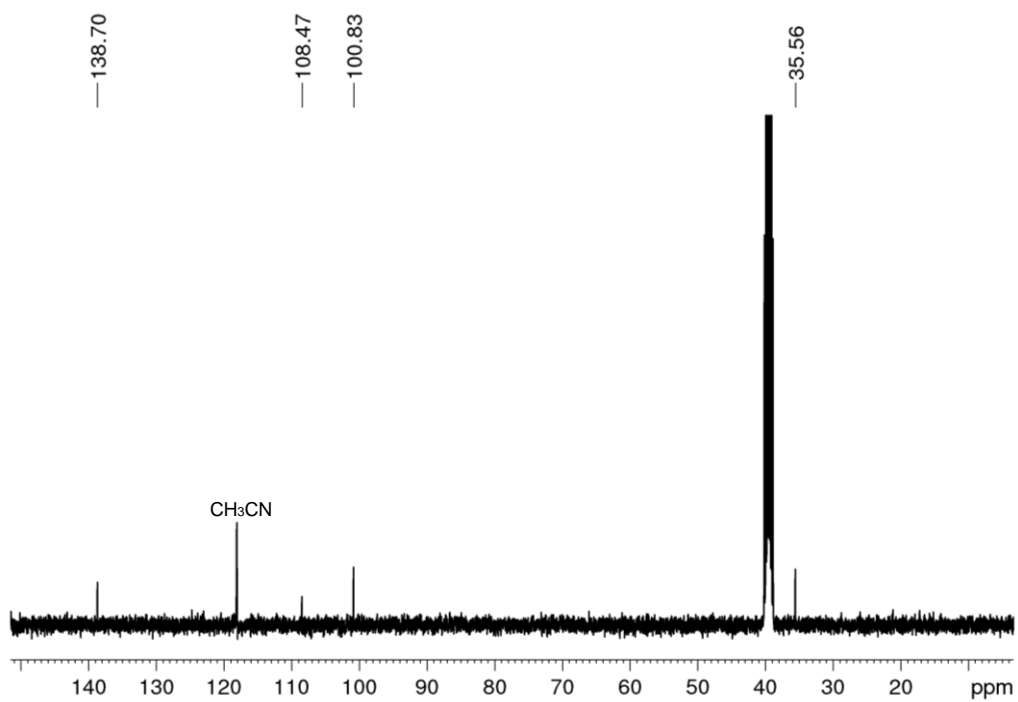


Figure S12: ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$, 25 °C) of **9**.

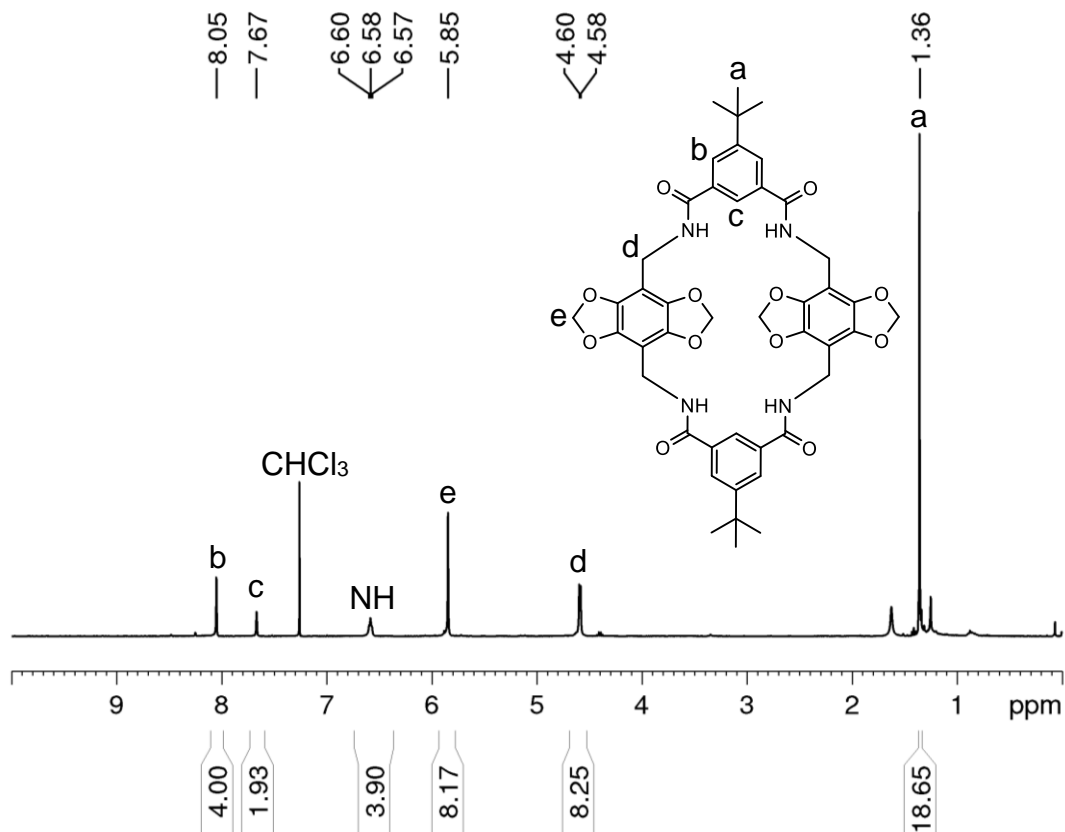


Figure S13: ^1H NMR (400 MHz, CDCl_3 , 25 °C) of **M5**.

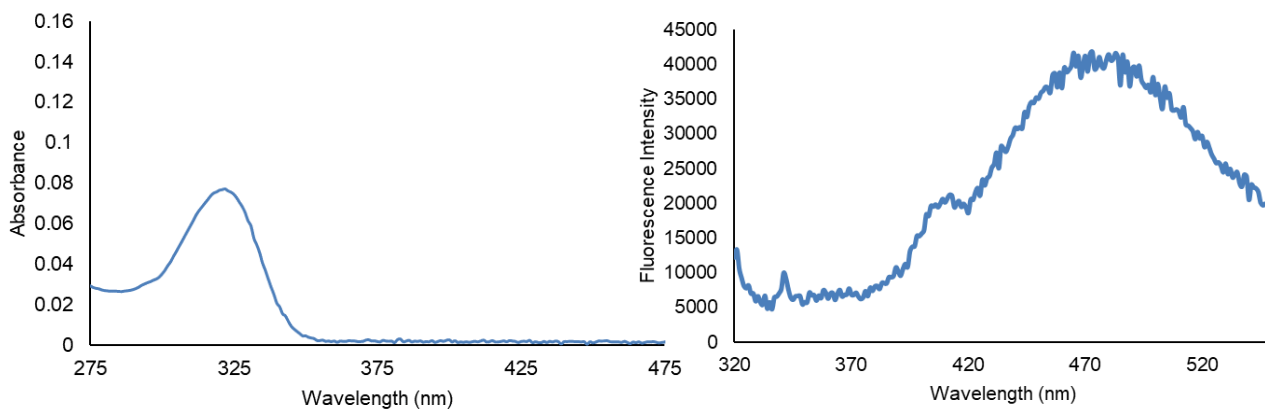


Figure S14: Absorbance and fluorescence spectra (ex. 310 nm, slit width: 2 nm) of 5.0 μM **M5** in CHCl_3 .

B. Threading of M3

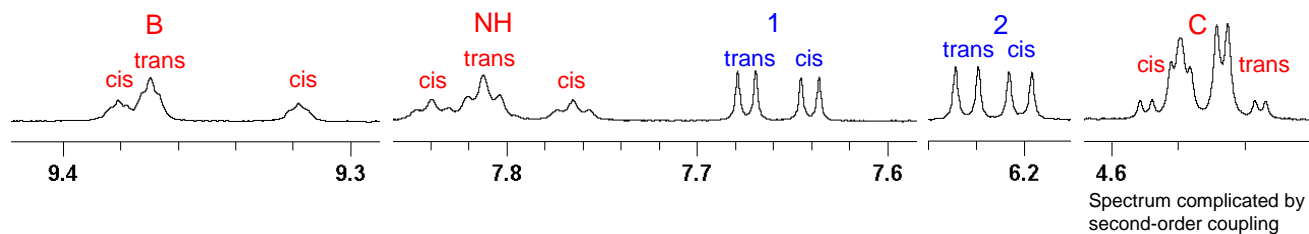


Figure S15: Expansion of manuscript Figure 1 showing labels of peaks corresponding to cis and trans conformations of encapsulated **S1**.

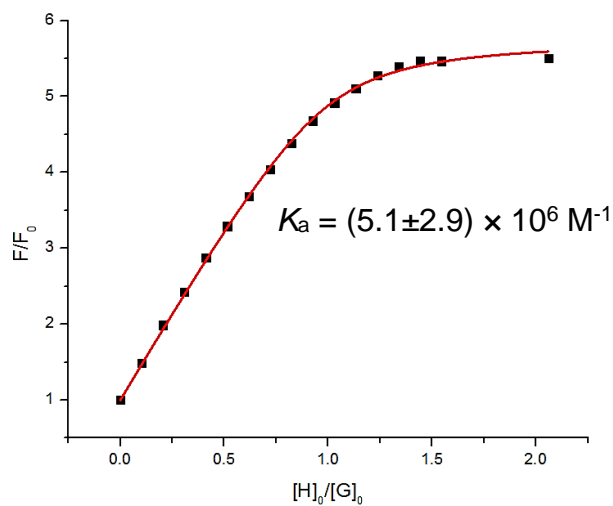


Figure S16: Representative titration of 3.0 μM **S1** with increasing equivalents of **M3** in CHCl_3 fitted to a 1:1 binding model (ex. 600 nm, em. 690 nm, slit width: 2 nm at 22 $^\circ\text{C}$). K_a is the average and standard deviation of three independent measurements.

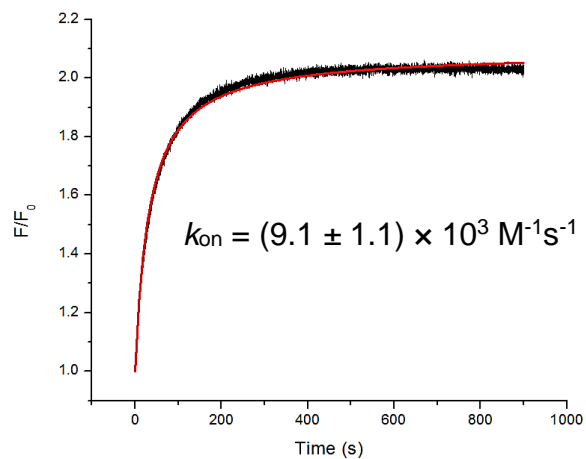


Figure S17: Representative curve for association of 3.0 μM **S1** with 1.5 equivalents **M3** in CHCl_3 fitted to second-order kinetics (ex. 600 nm, em. 690 nm, slit width: 2 nm at 22 $^\circ\text{C}$). k_{on} is the average and standard deviation of three independent measurements.

C. Evidence Showing No Threading of M4a

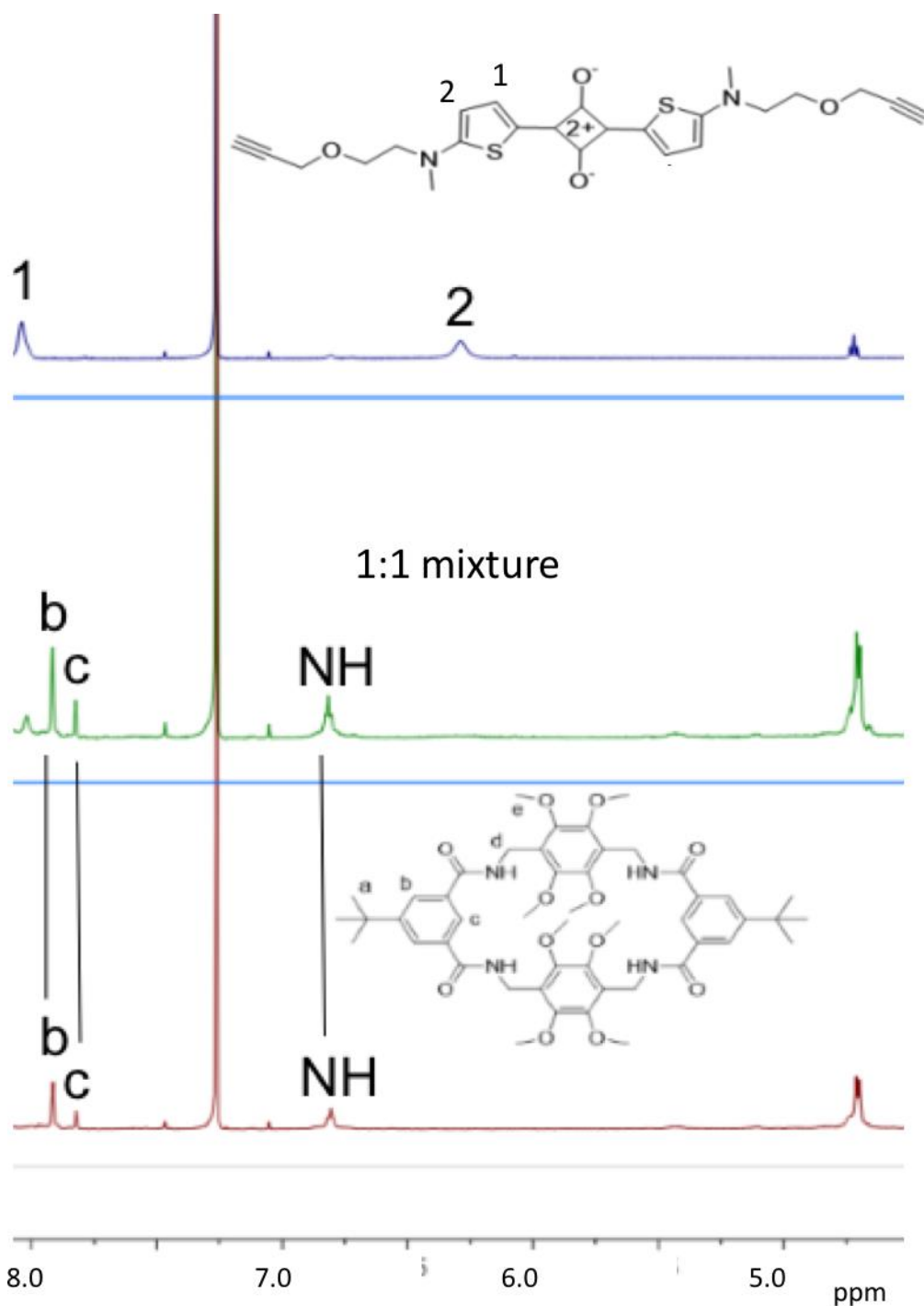


Figure S18: Partial ¹H NMR (500 MHz, CDCl₃, 25 °C) indicating lack of change in chemical shift upon mixing **S1** and **M4a** at 1.0 mM concentration. Furthermore, dye protons 2 remain broad due to slow bond rotation in CDCl₃ and conformational exchange; this is in contrast to manuscript Figure 1 where protons 2 become sharper upon encapsulation inside **M3** which inhibits dye bond rotation.

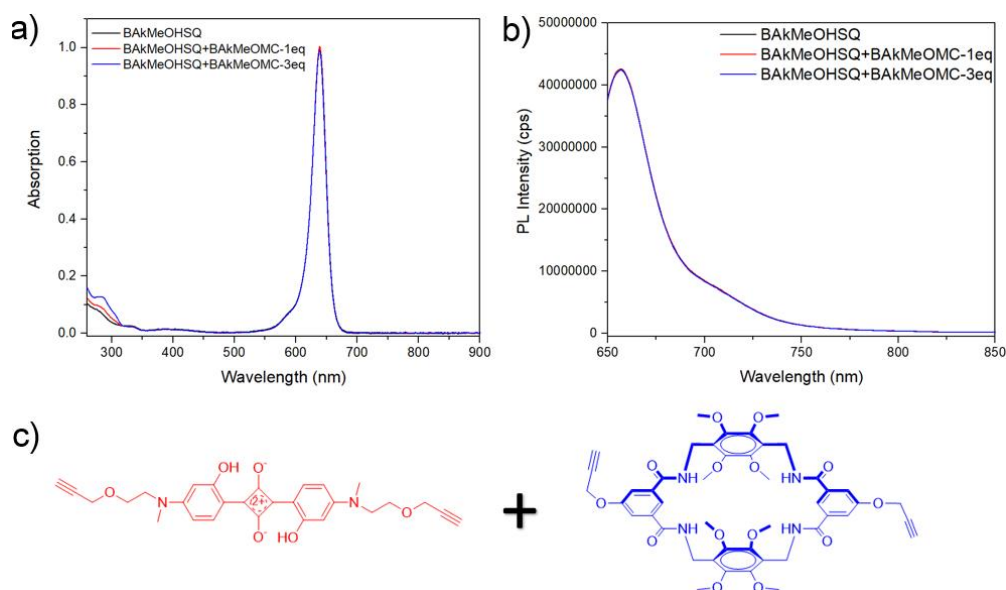


Figure S19: a) Absorbance and b) fluorescence spectra of 3.0 μM squaraine **S2**^{S1} indicating no spectral change upon addition of **M4b** (ex. 640 nm, slit width: 2 nm).

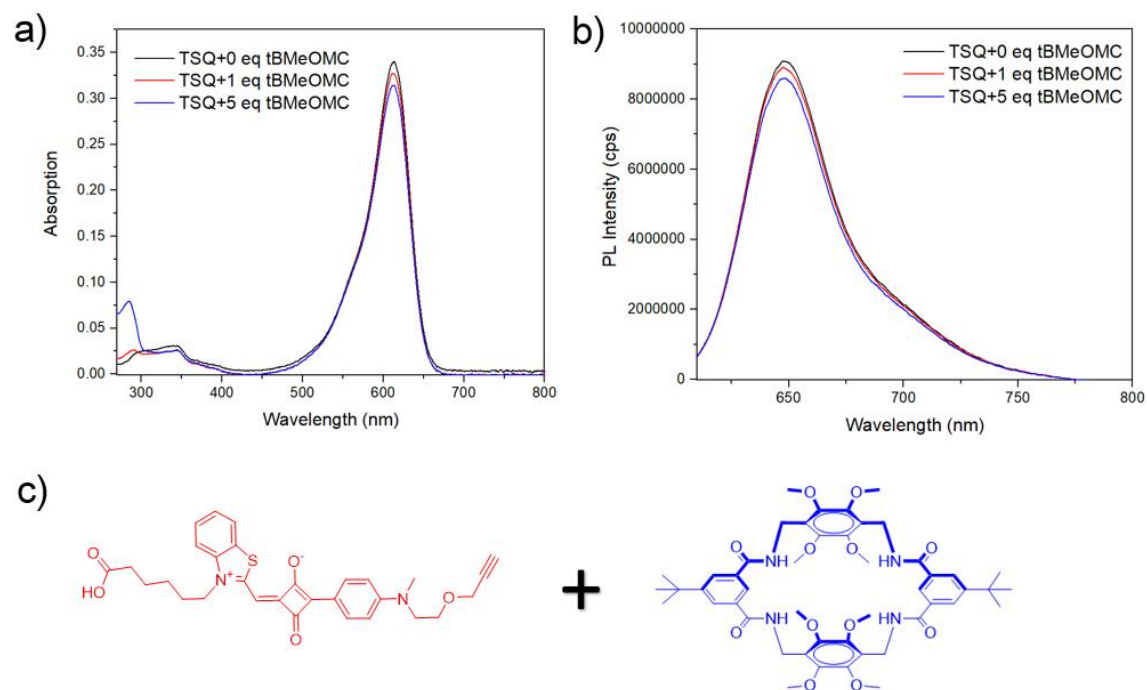


Figure S20: a) Absorbance and b) fluorescence spectra of 3.0 μM squaraine **S3**^{S2} indicating no spectral change upon addition of **M4a** (ex. 600 nm, slit width: 2 nm).

D. Threading of M5

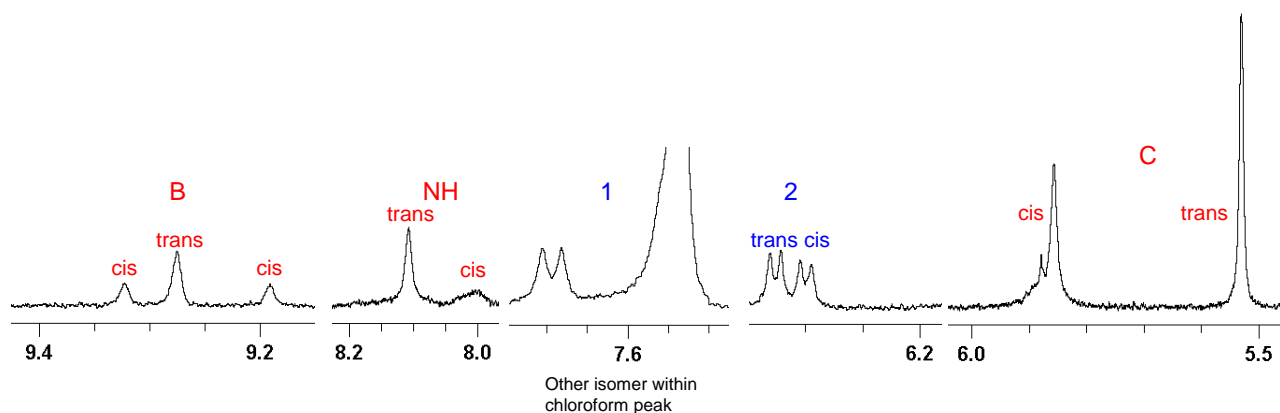


Figure S21: Expansion of manuscript Figure 5 now showing labels of peaks corresponding to cis and trans conformations of encapsulated **S1**.

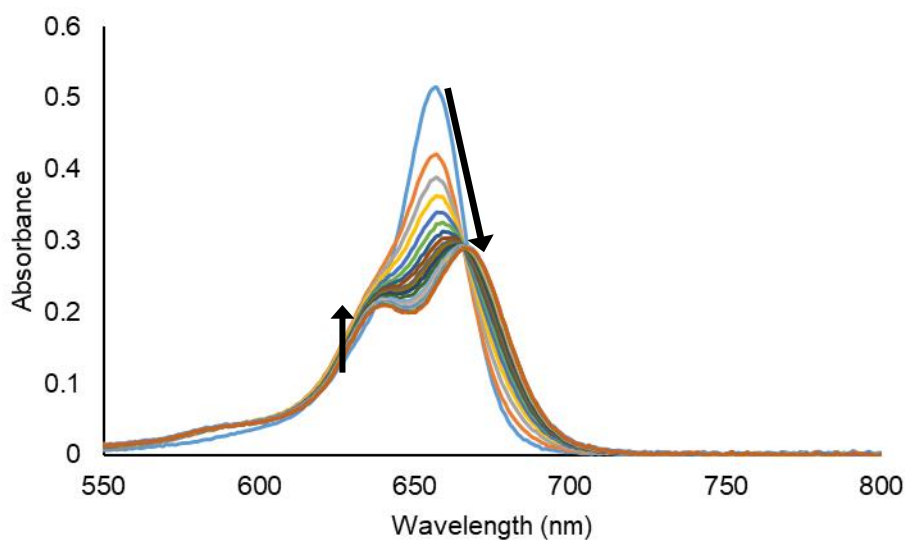


Figure S22: Absorbance spectrum of 3.0 μM **S1** upon sequential addition of 0-4.0 equiv. **M5**, indicating appearance of a red-shifted absorption maxima band and also a blue-shifted band due to self-aggregation of the complex.

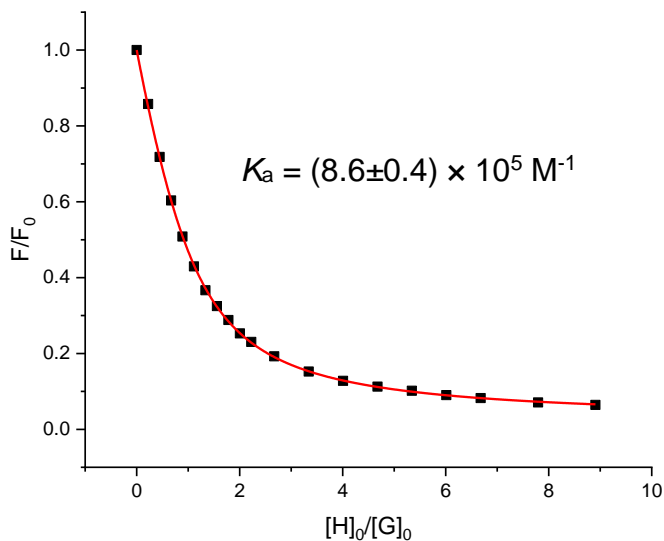


Figure S23: Representative titration of 3.0 μM **S1** with increasing equivalents of **M5** in CHCl_3 fitted to a 1:1 binding model (ex. 650 nm, em. 668 nm, slit width: 2 nm at 25 $^\circ\text{C}$). K_a is the average and standard deviation of three independent measurements.

E. References

- S1. Liu, W.; Gómez-Durán, C. F. A.; Smith, B. D. Fluorescent Neuraminidase Assay Based on Supramolecular Dye Capture after Enzymatic Cleavage. *J. Am. Chem. Soc.* **2017**, *139* (18), 6390–6395.
- S2. Jarvis, T.; Roland, F.; Dubiak, K.; Huber, P.; Smith, B. Time-Lapse Imaging of Cell Death in Cell Culture and Whole Living Organisms Using Turn-on Deep-Red Fluorescent Probes. *J. Mater. Chem. B* **2018**, 4963–4971.