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Supporting Information

Highly Emissive Water-Soluble Polysulfurated Pyrene-Based Chromophores as Dual Mode Sensors of Metal Ions

Marco Villa,* Myriam Roy,* Giacomo Bergamini, Paola Ceroni, and Marc Gingras

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1. Characterization of compounds

The characterization data and synthetic procedures for **3O**, **3M** and **3P** were previously published[1]

1a. Characterization and spectroscopic data for 2O, 2M and 2P

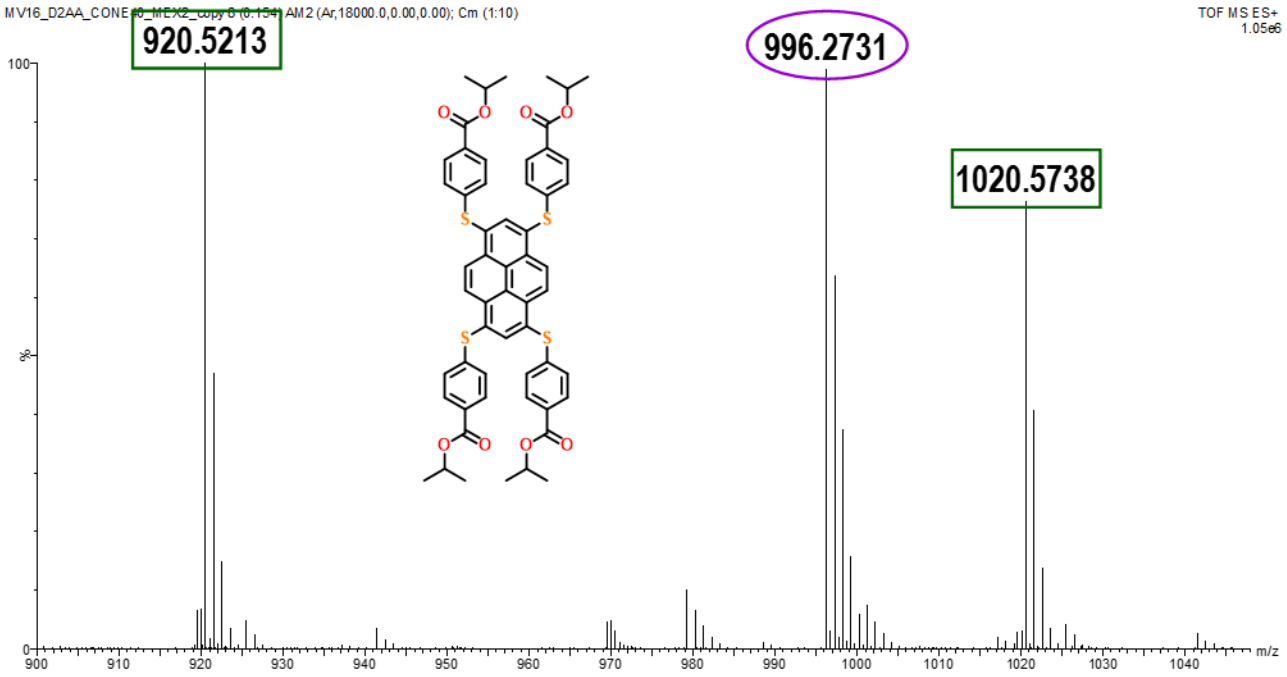

Figure S 1 HR-MS ESI of **2P**. Ion detected atm/z 996.2731 and internal standard at m/z 920.5213 et m/z 1020.5738.

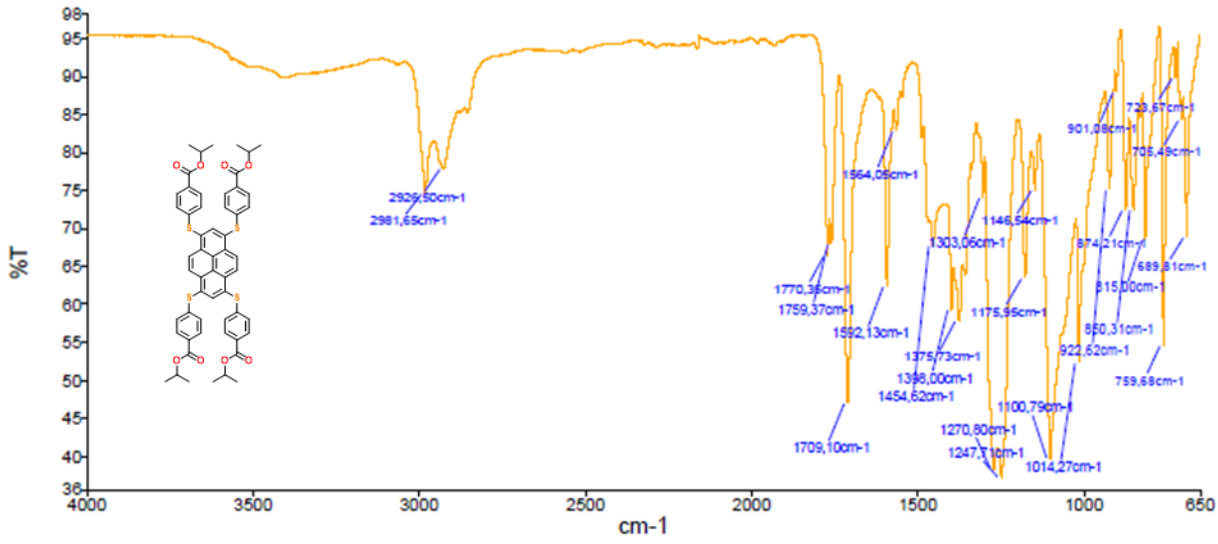

Figure S 2 FT-IR ATR (diamond) spectra of **2P** (solid)

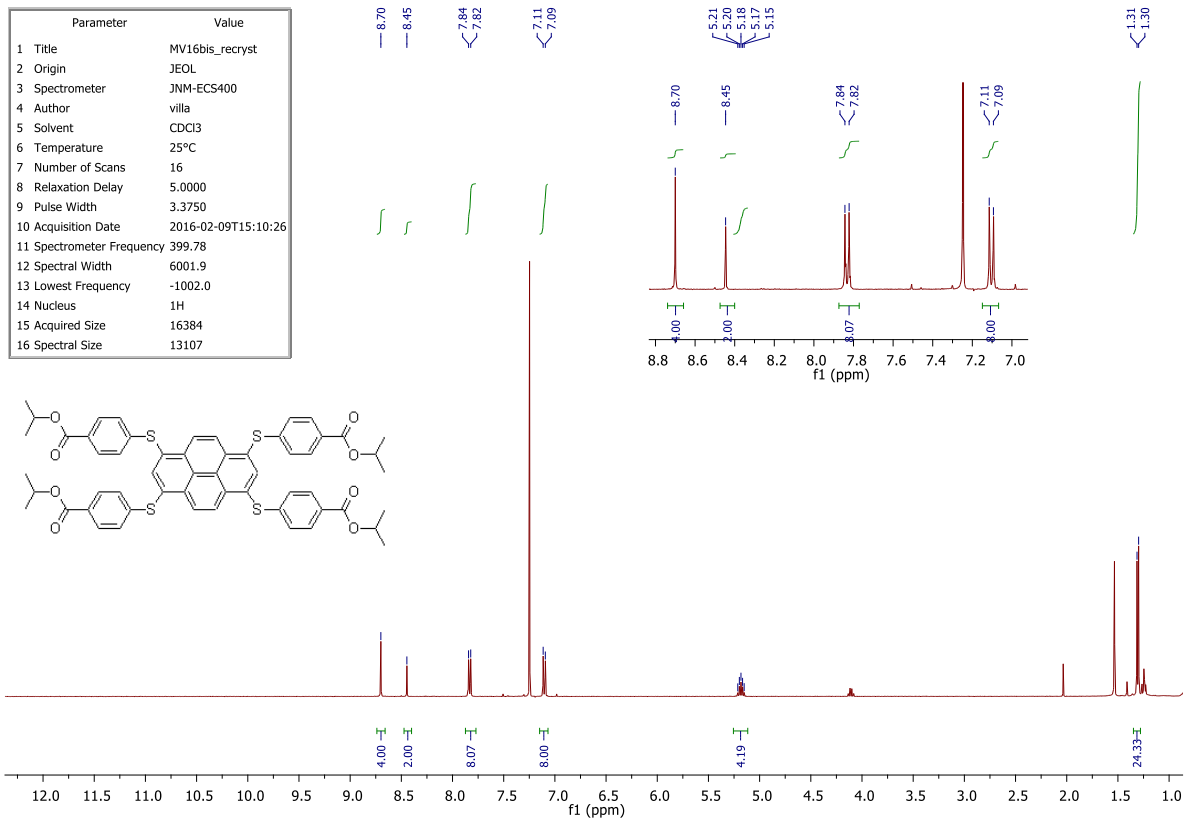

Figure S 3 ^{1}H-NMR spectra of **2P** ($CDCl_3$, 399.78 MHz)

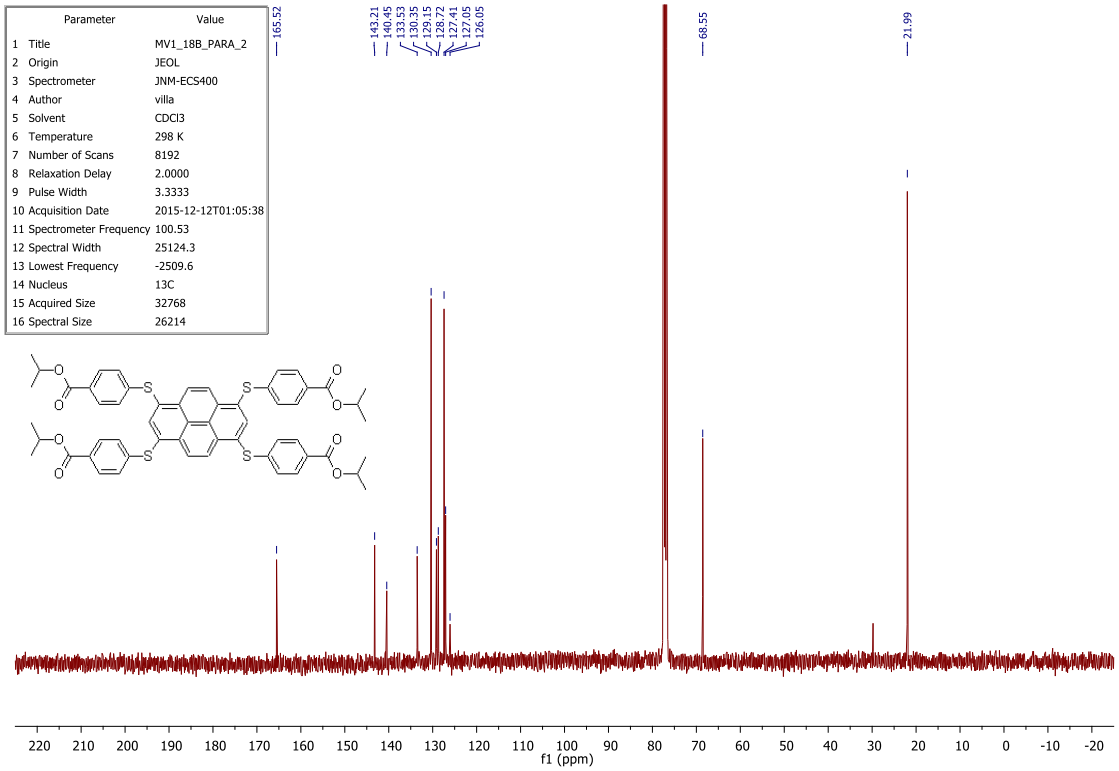

Figure S 4 ^{13}C-NMR spectra of **2P** ($CDCl_3$, 100.53 MHz)

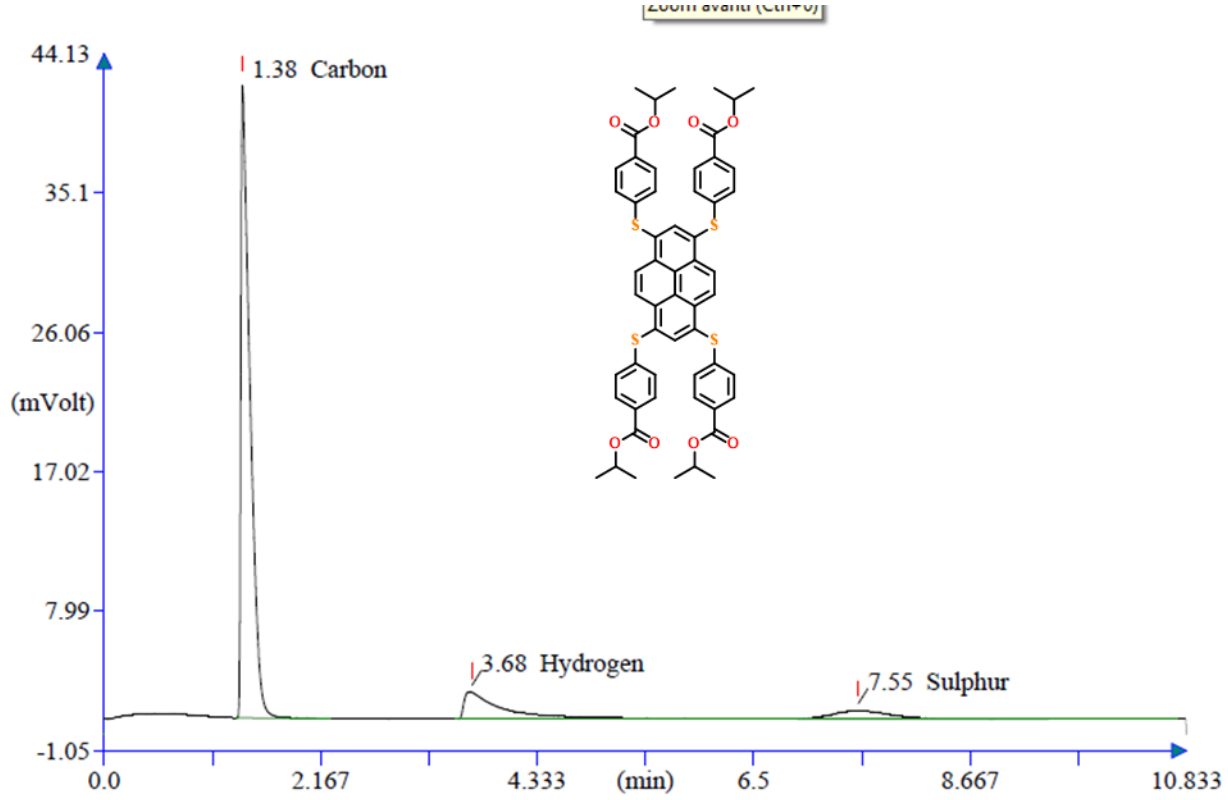

Figure S 5 Elemental analysis for **2P**. Calculated : 68.69%C 5.15%H 13.10%S Found: 68.42%C 5.05%H 13.02%S

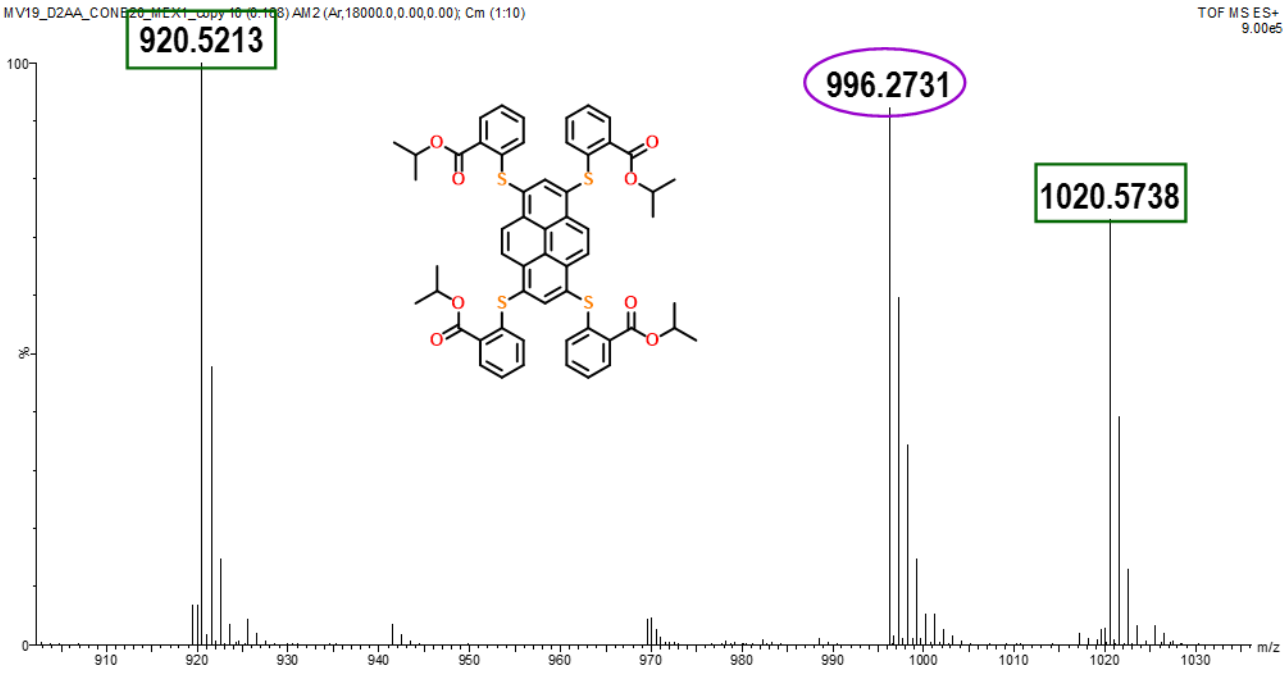

Figure S 6 HR-MS ESI of **2O**. Ion detected atm/z 996.2731 and internal standard at m/z 920.5213 et m/z 1020.5738.

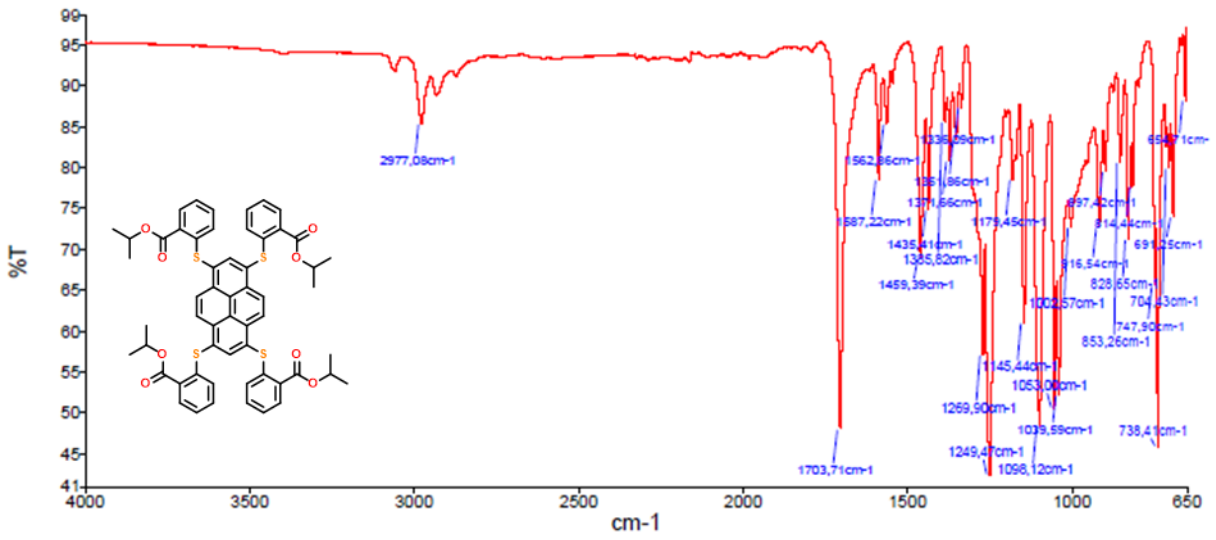

Figure S 7 FT-IR ATR (diamond) spectra of **2O** (solid)

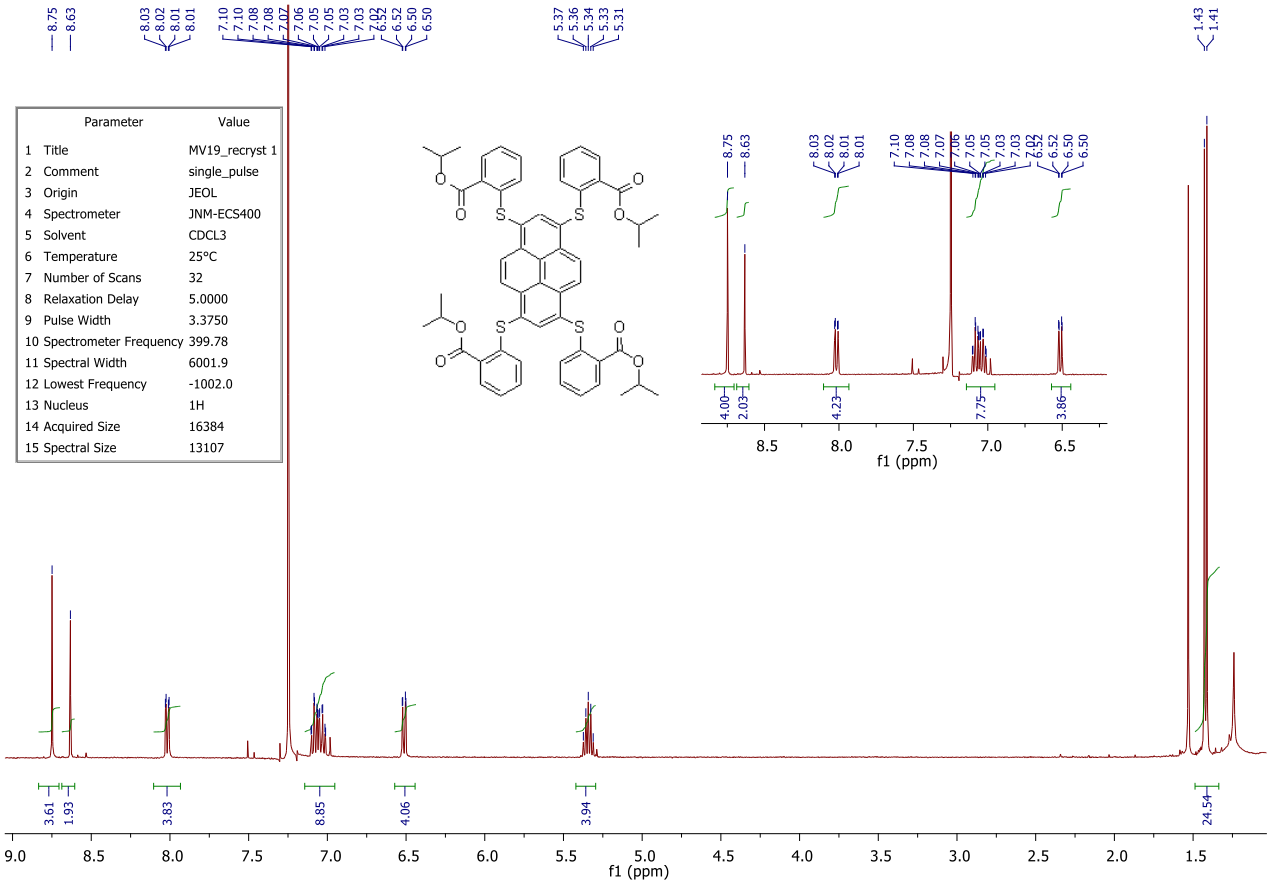

Figure S 8 ^{1}H-NMR spectra of **2O** ($CDCl_3$, 399.78 MHz)

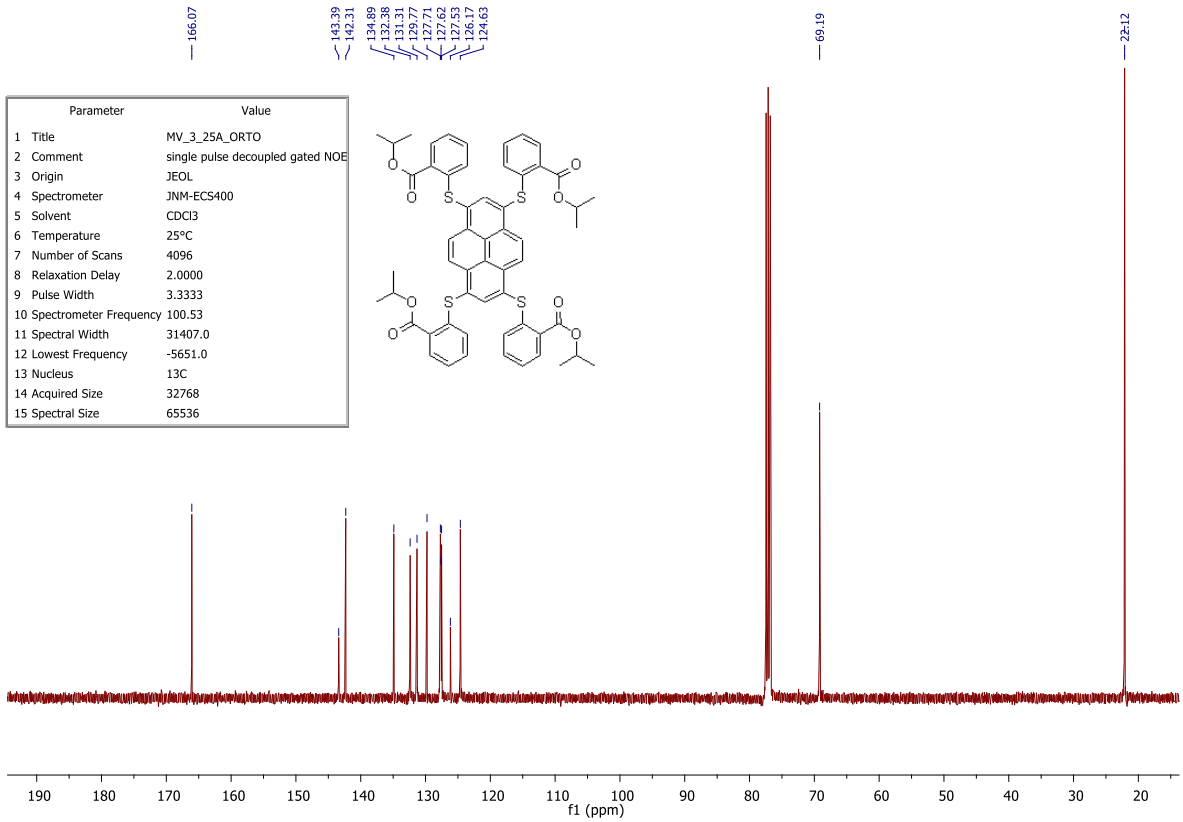

Figure S 9 ^{13}C-NMR spectra of **2O** ($CDCl_3$, 100.53 MHz)

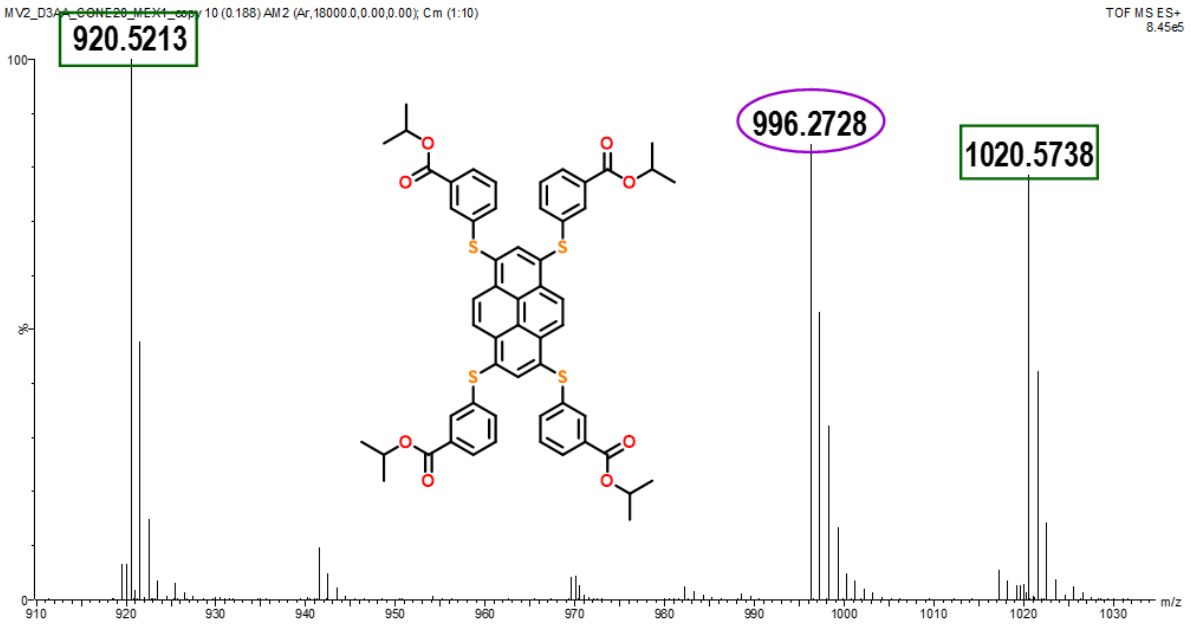

Figure S 10 HR-MS ESI of **2M**. Ion detected atm/z 996.2728 and internal standard at m/z 920.5213 et m/z 1020.5738.

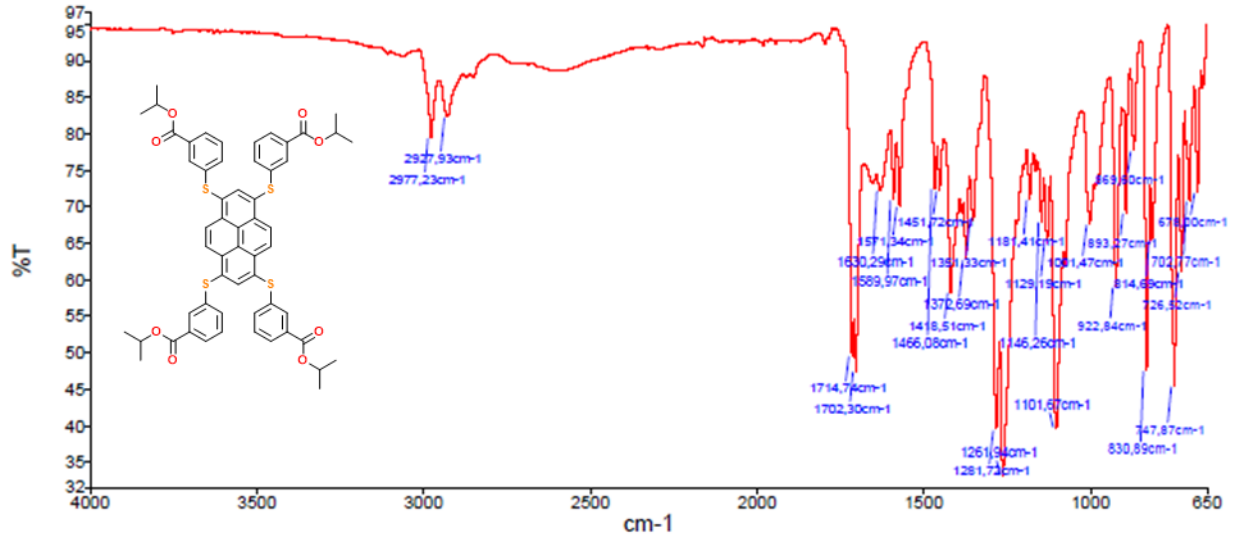

Figure S 11 FT-IR ATR (diamond) spectra of **2M** (solid)

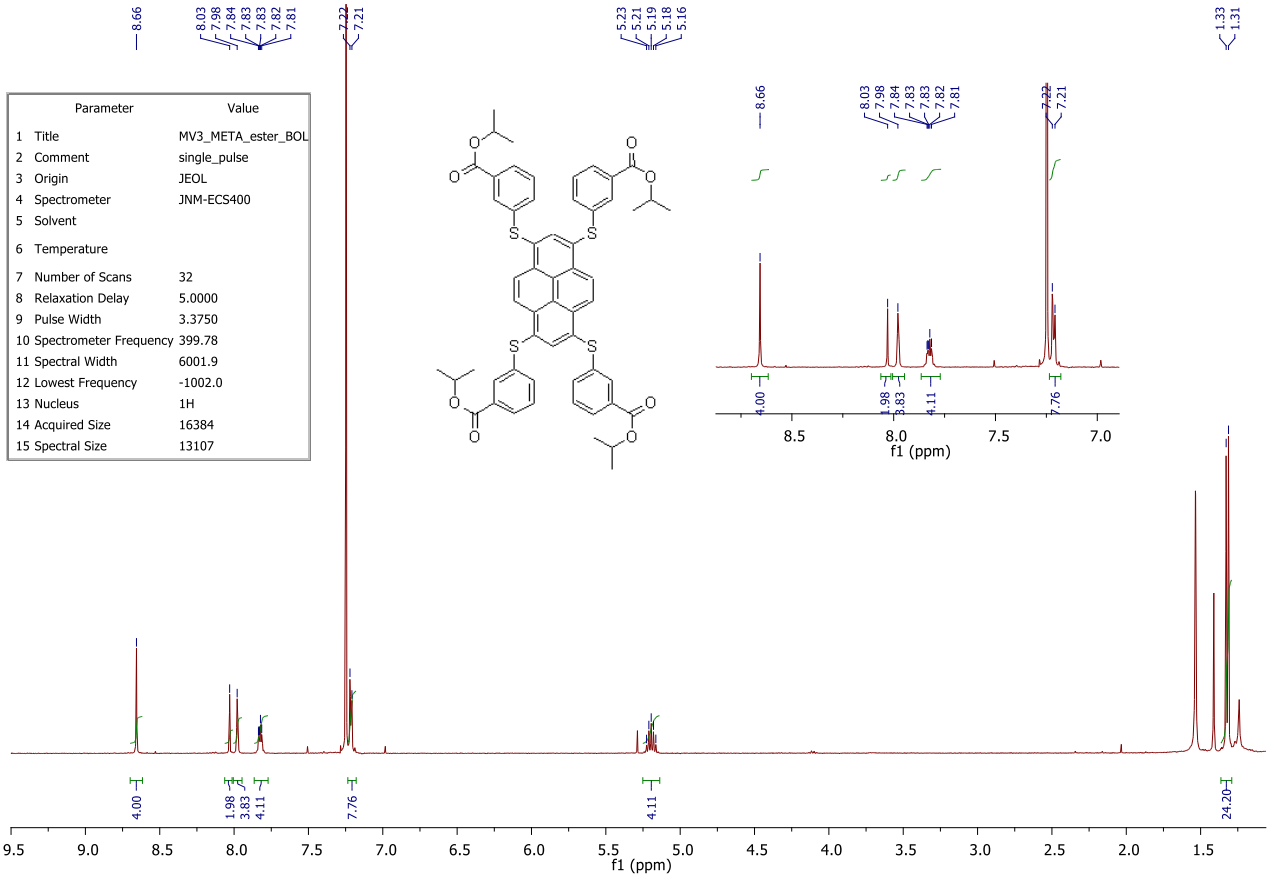

Figure S 12 ^{1}H-NMR spectra of **2M** ($CDCl_3$, 399.78 MHz)

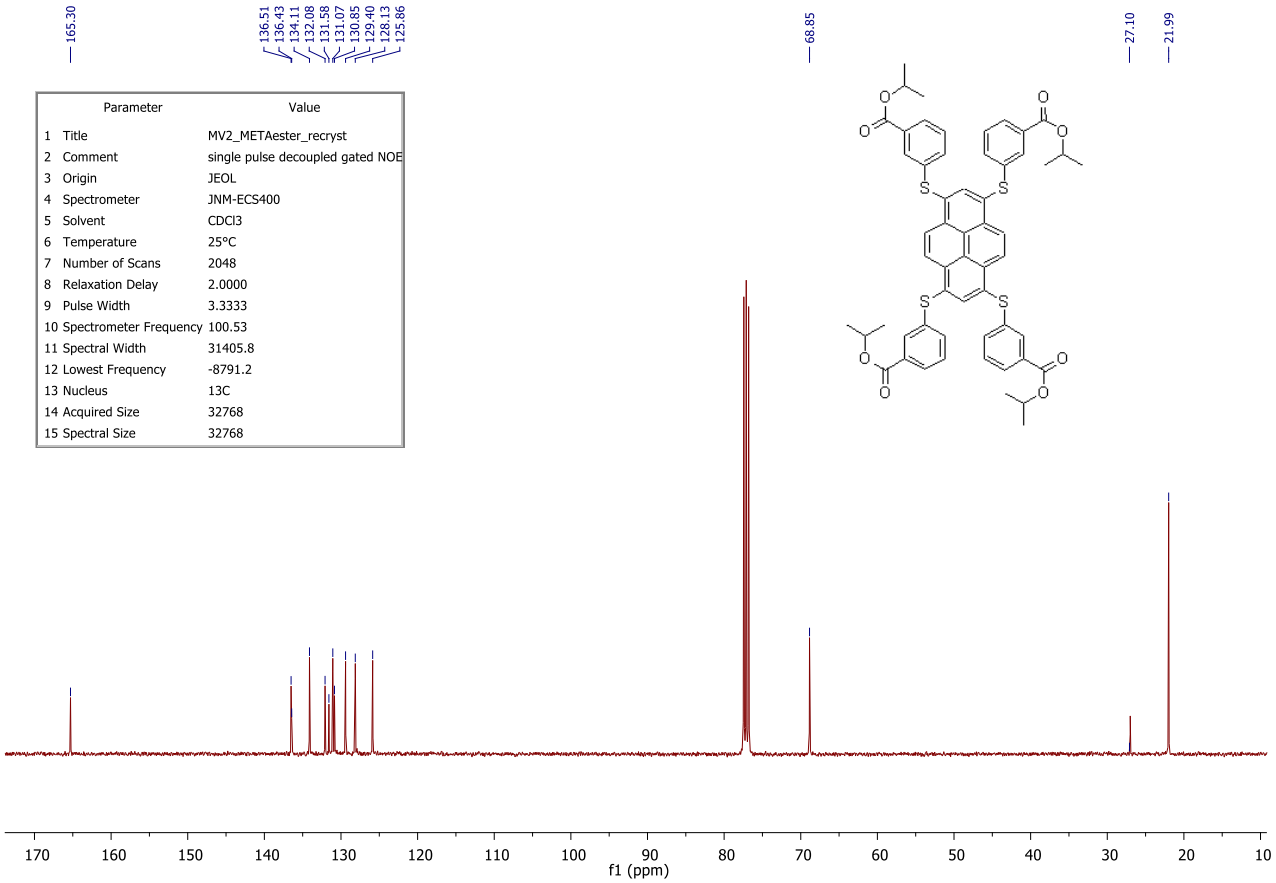

Figure S 13 ^{13}C-NMR spectra of **2M** ($CDCl_3$, 100.53 MHz)

1b. Characterization and spectroscopic data for 1O, 1M and 1P

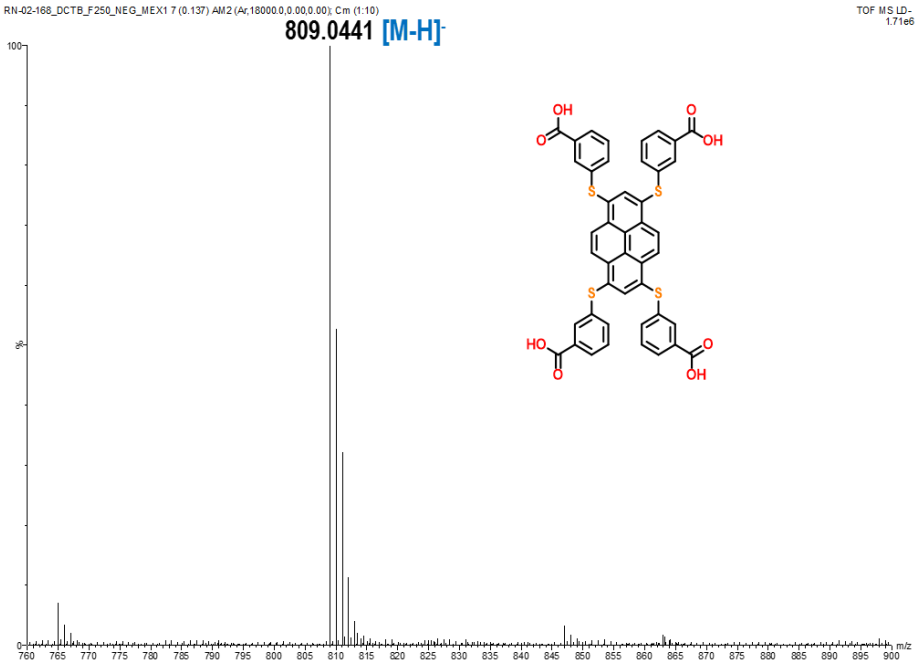

Figure S 14 HR-MS MALDI- ToF (DTCB matrix, negative mode, laser 355 nm) of **1M**

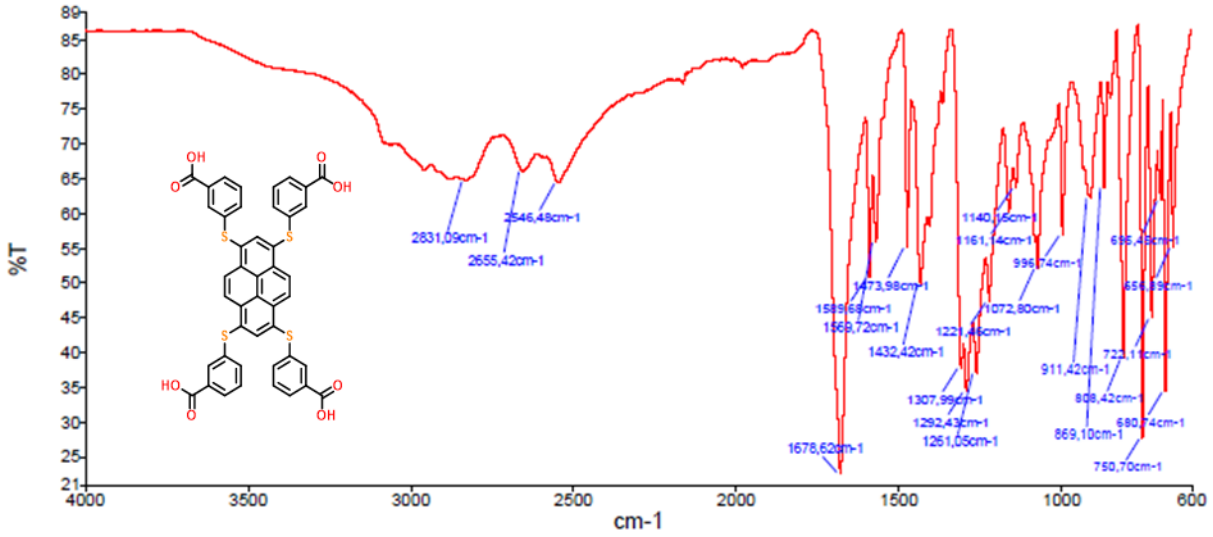

Figure S 15 FT-IR ATR (diamond) spectra of **1M** (solid)

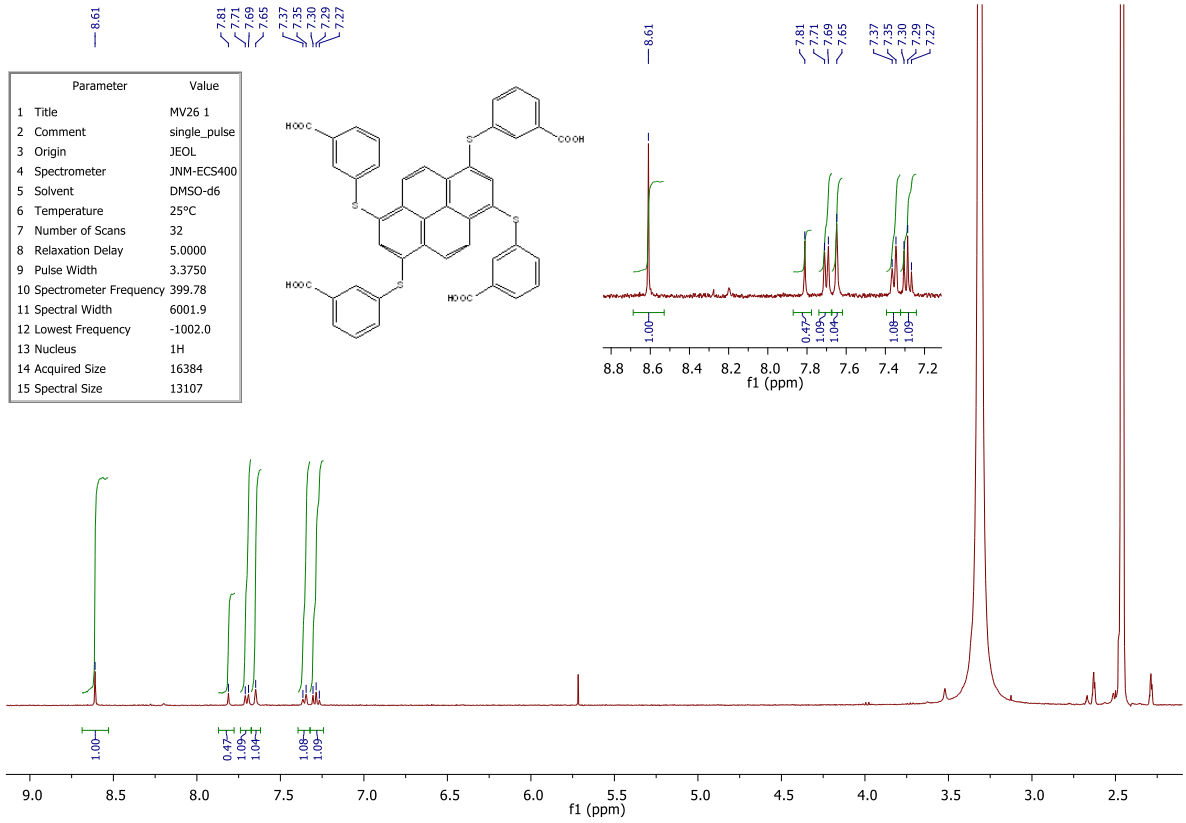

Figure S 16 ^{1}H-NMR spectra of **1M** (DMSO-d_6, 399.78 MHz)

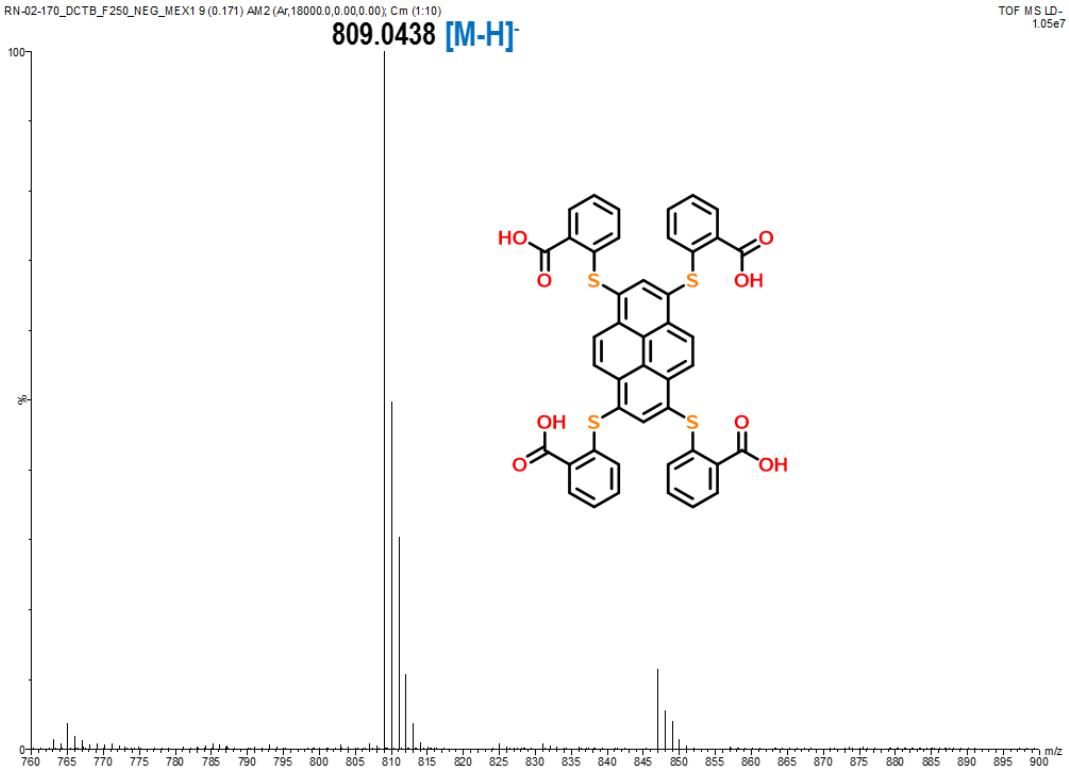

Figure S 17 HR-MS MALDI- ToF (DCTB matrix, negative mode, laser 355 nm) of **1O**

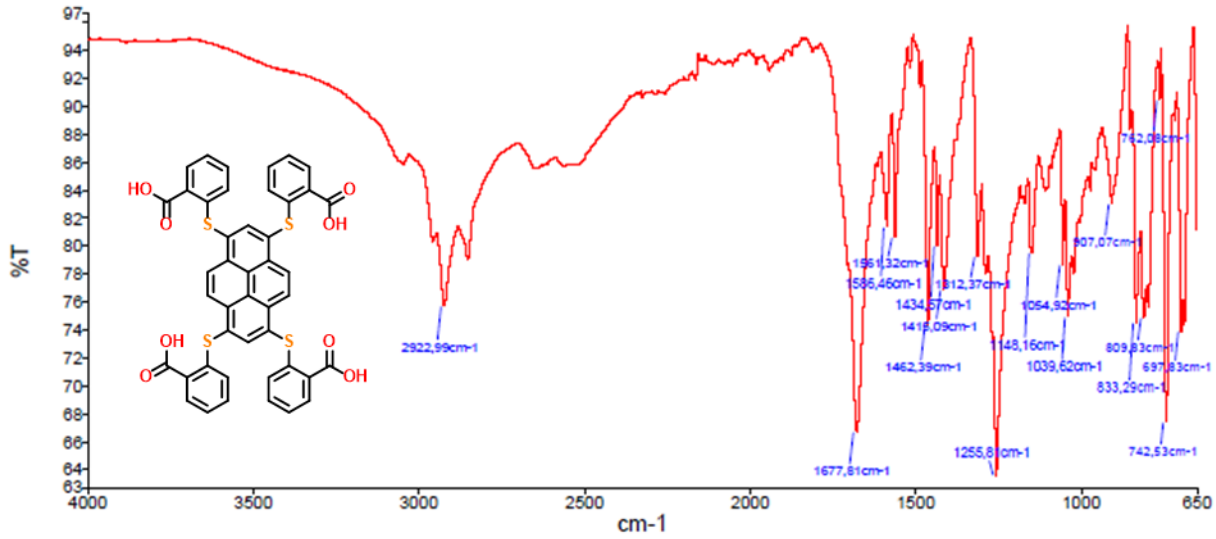

Figure S 18 FT-IR ATR (diamond) spectra of **1O** (solid)

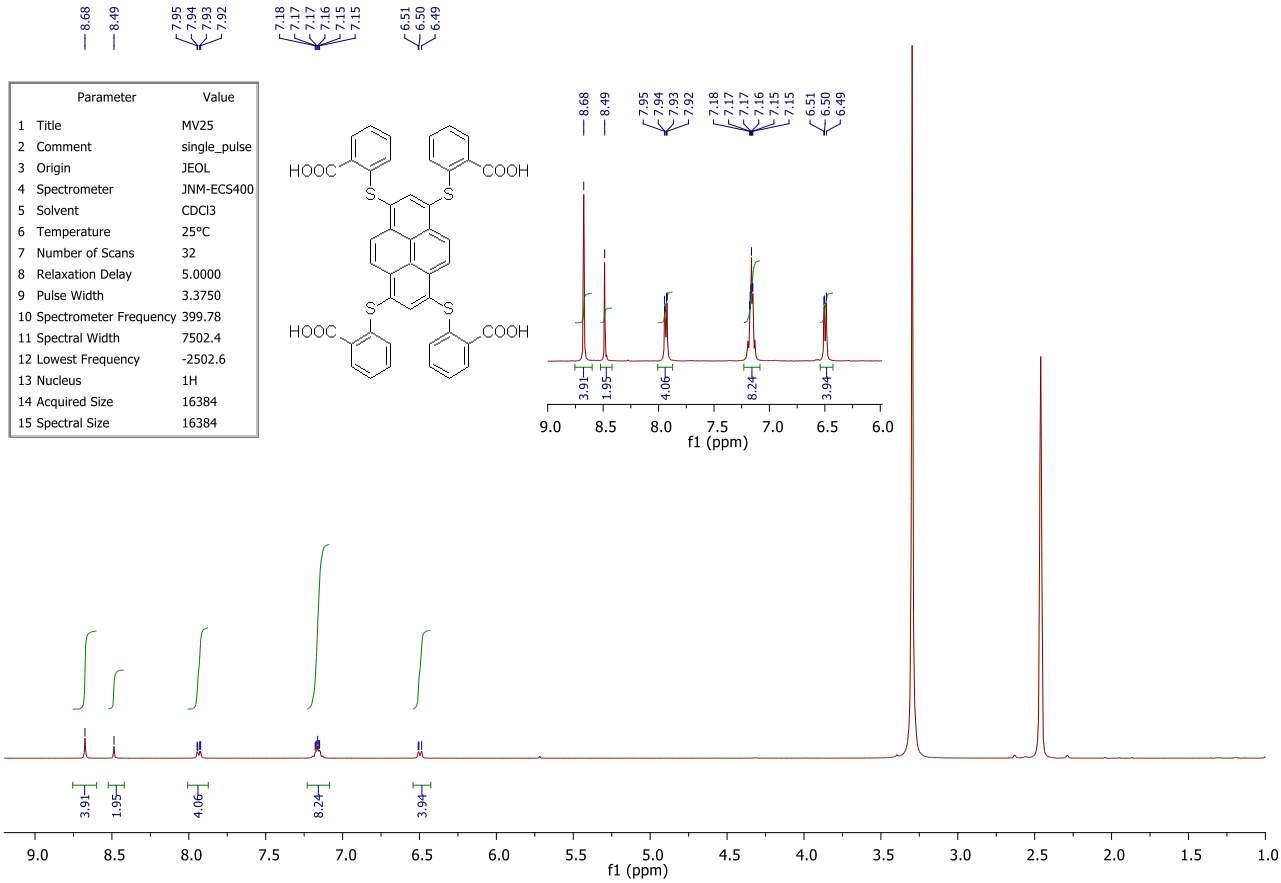

Figure S 19 ^{1}H-NMR spectra of **1O** (DMSO-d_6, 399.78 MHz)

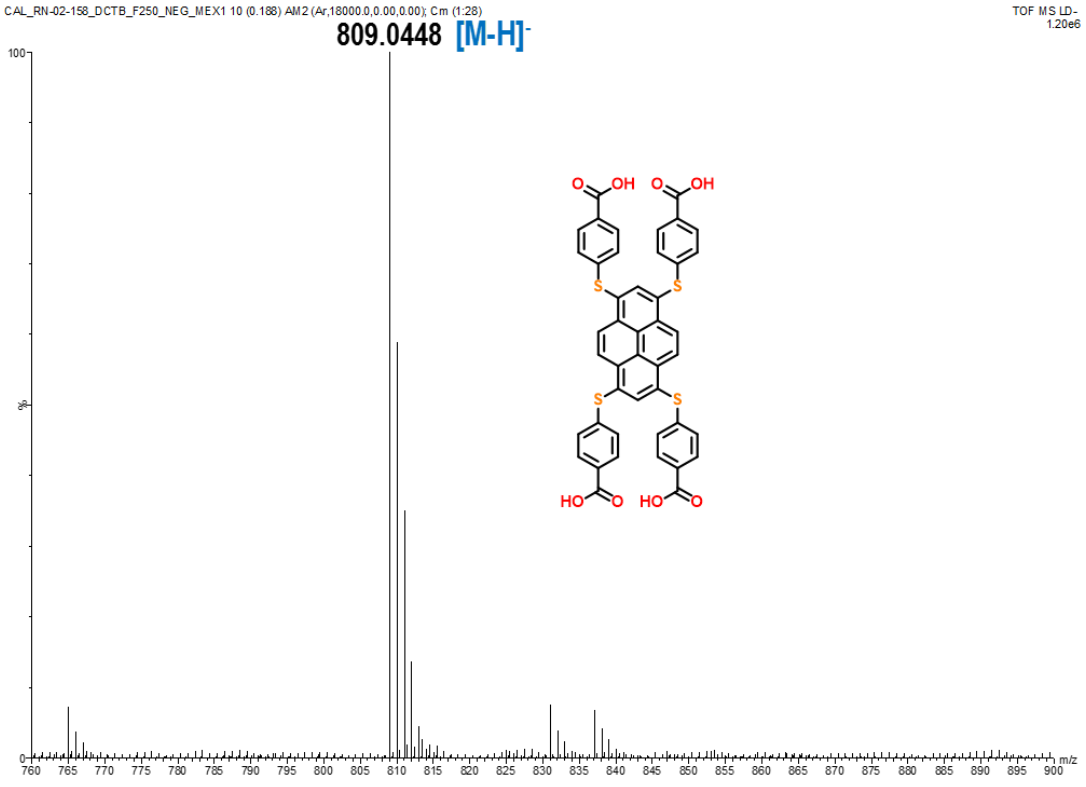

Figure S 20 HR-MS MALDI-ToF (DHB matrix, negative mode, laser 355 nm) of **1P**

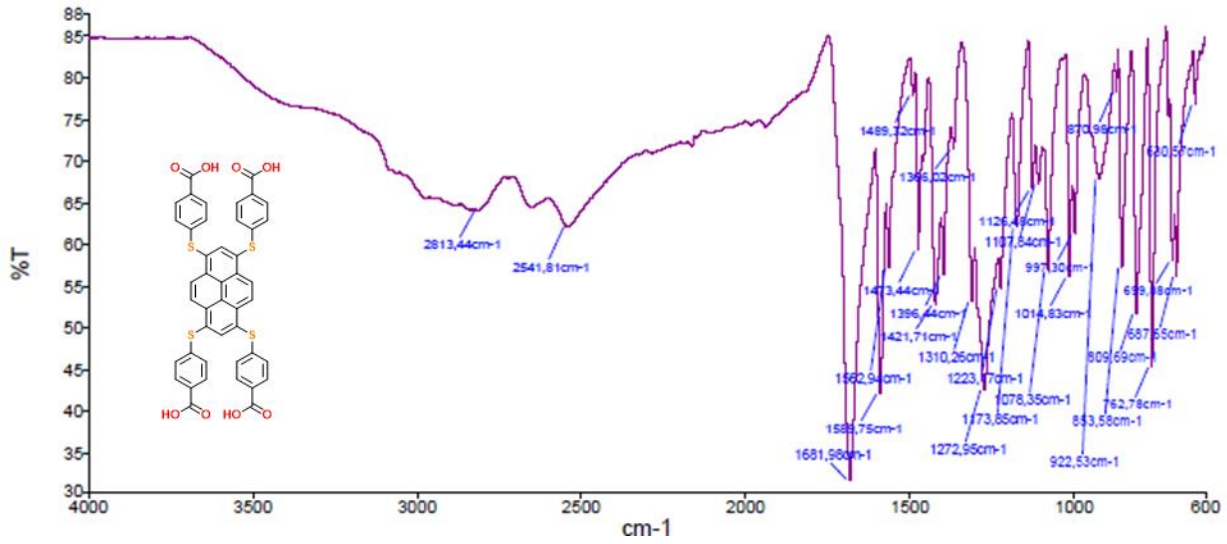

Figure S 21 FT-IR ATR (diamond) spectra of **1P** (solid)

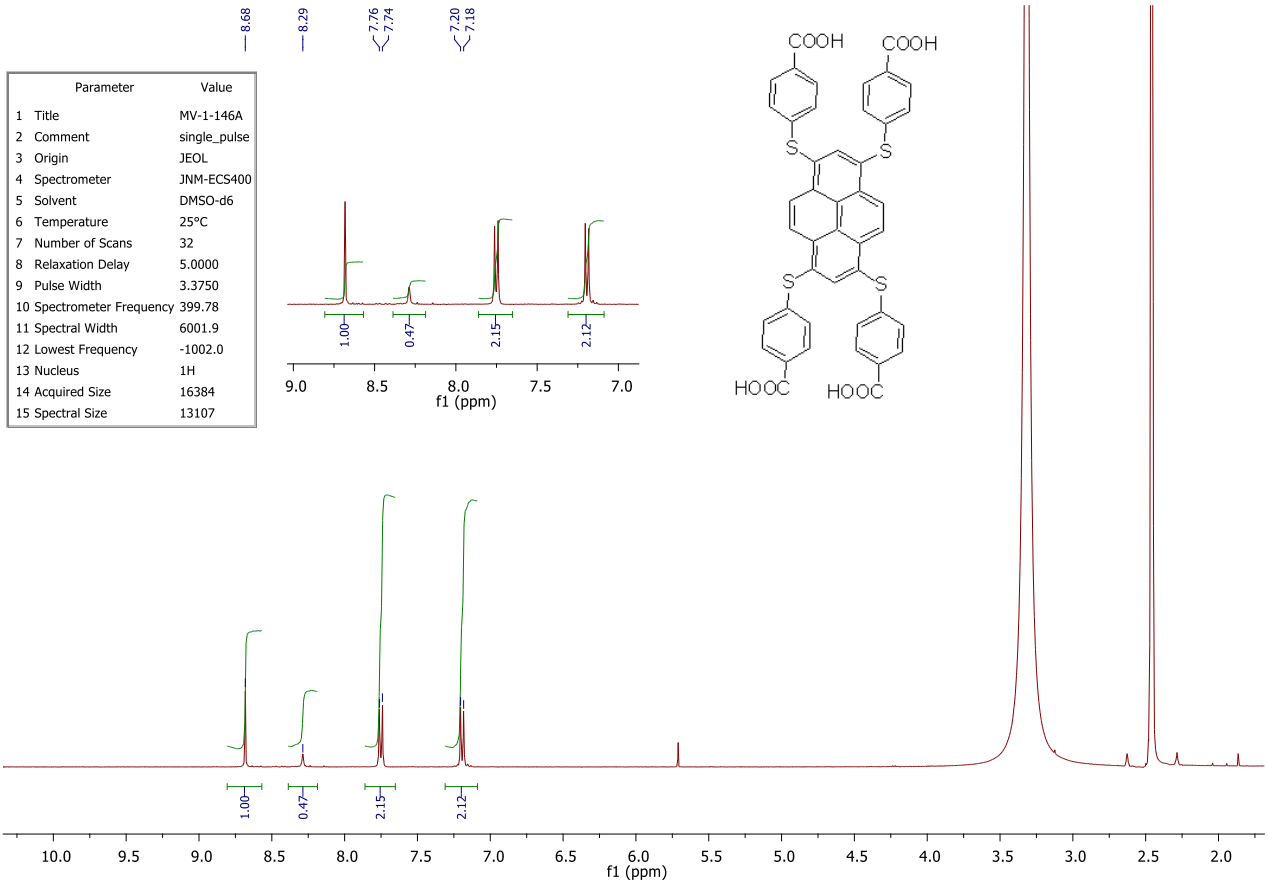

Figure S 22 ^{1}H-NMR spectra of **1P** (DMSO-d_6, 399.78 MHz)

2. Photophysical measurements

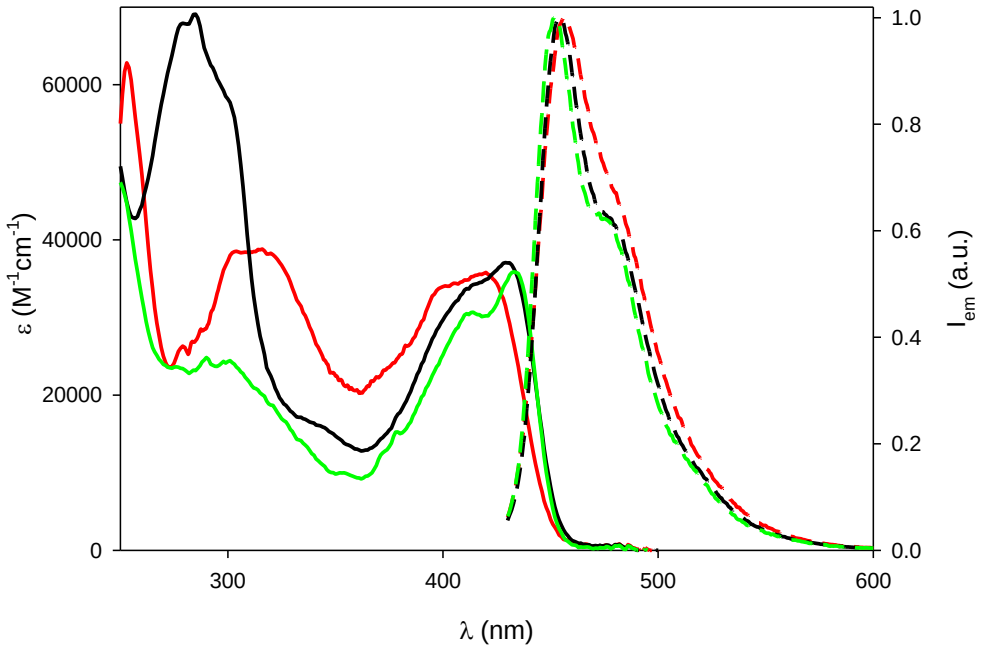

Figure S23 Absorption spectra (solid lines) and normalized emission spectra (dashed lines) in air-equilibrated THF solution (λ_{exc}= 400 nm) of **2P** (black), **2O** (red), and **2M** (green).

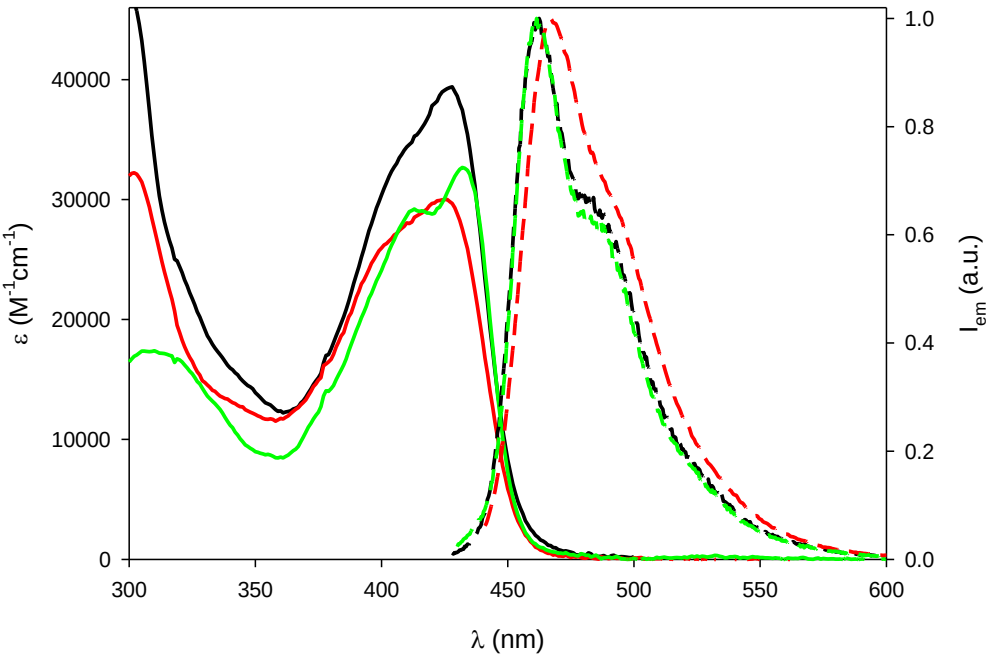

Figure S24 Absorption spectra (solid lines) and normalized emission spectra (dashed lines) in air-equilibrated THF solution (λ_{exc}= 410 nm) of **1P** (black), **1O** (red) and **1M** (green).

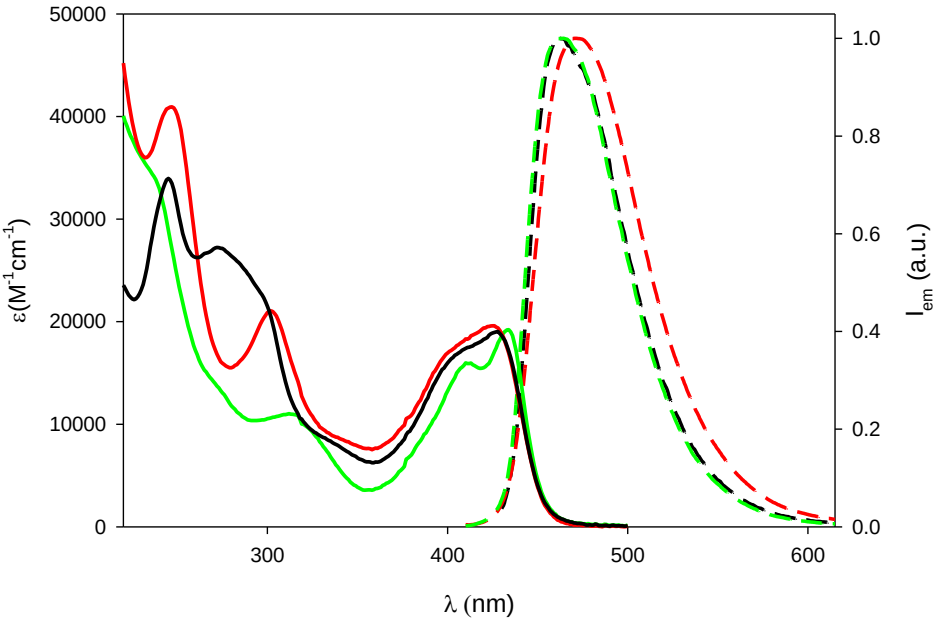

Figure S25 Absorption spectra (solid lines) and normalized emission spectra (dashed lines) in air-equilibrated aqueous solution at pH=8 (λ_{exc}= 390 nm) of **1P** (black), **1O** (red) and **1M** (green).

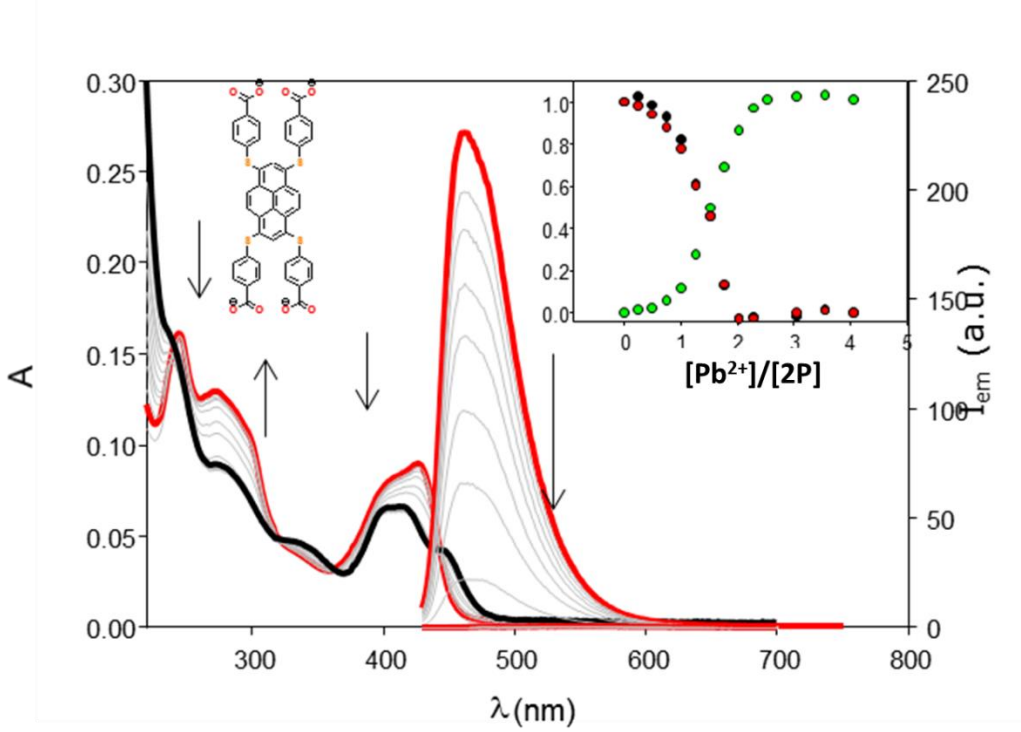

Figure S26 Absorption (left) and fluorescence (right) of a 4.8x10^{-6} M solution of **1P** in air equilibrated NaOH 0.1mM water solution upon titration with a 3.73 mM water solution of $Pb(NO_3)_2$: red line (0 eq), black line (2 eq). Inset show the normalized absorption changes at 400 nm (black) and 470 nm (green) and emission intensity changes at 470 nm (green).

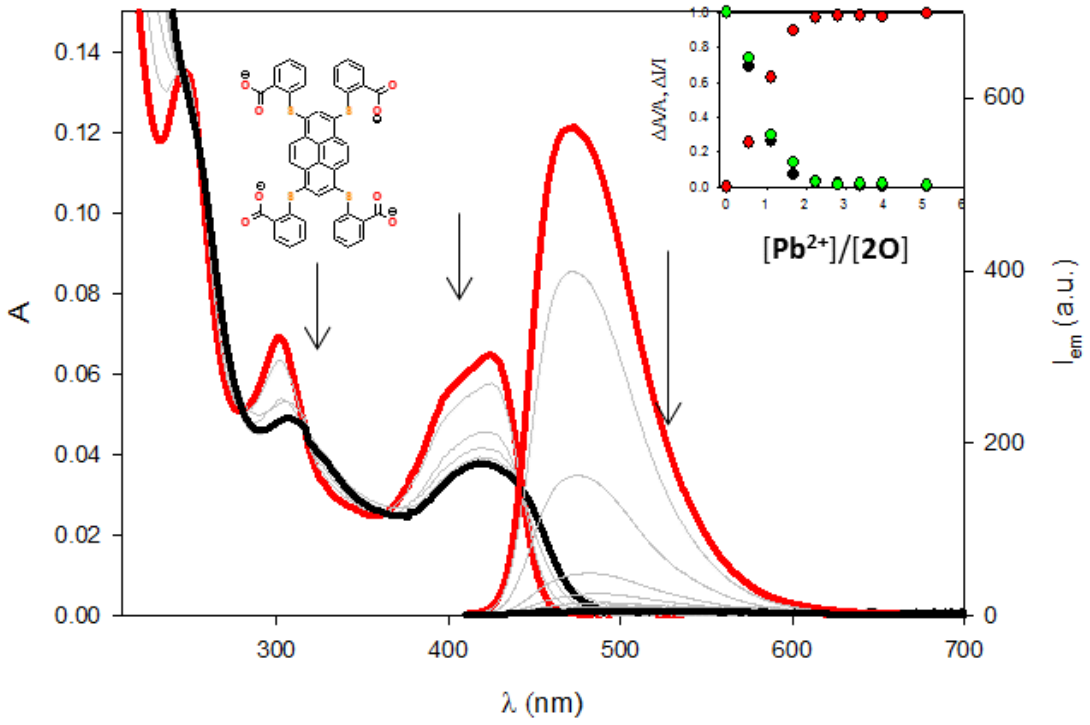

Figure S27 Absorption (left) and fluorescence (right) of a 3.3×10^{-6} M solution of **1O** in air equilibrated NaOH 0.1mM water solution upon titration with a 3.73 mM water solution of $Pb(NO_3)_2$: red line (0 eq), black line (2 eq). Inset show the normalized absorption changes at 400 nm (black) and 470 nm (red) and emission intensity changes at 470 nm (green).

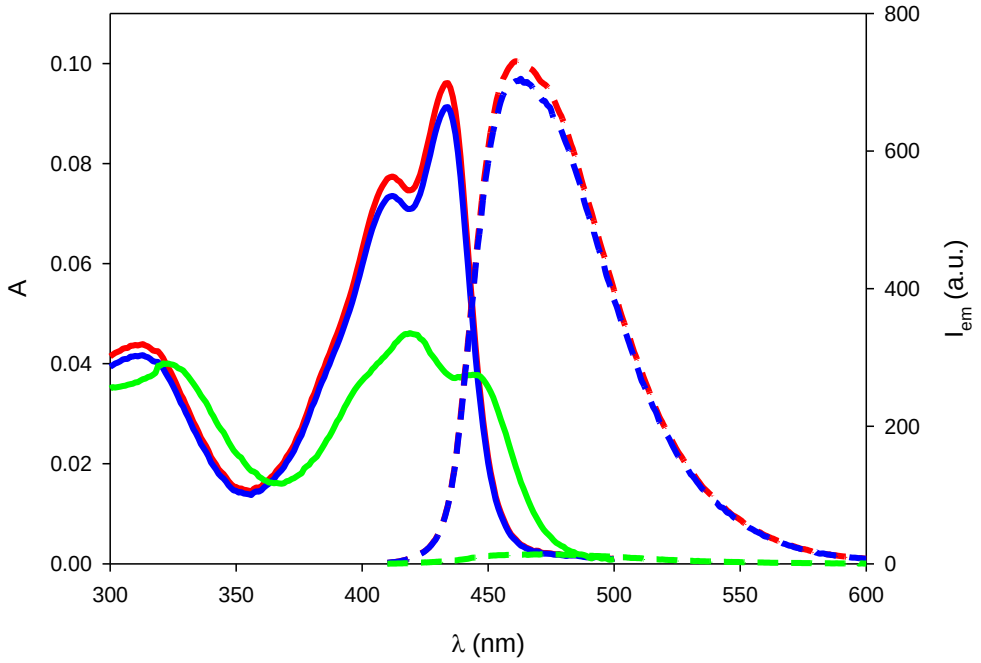

Figure 28 Absorption (left) and emission (right) spectra of a solution of **1M** in air-equilibrated aqueous solution (pH=8) (red line) upon addition of 2.5 eq of $Pb(NO_3)_2$ (green line) and 5 eq of EDTA (blue line). λ_{em} = 390 nm.

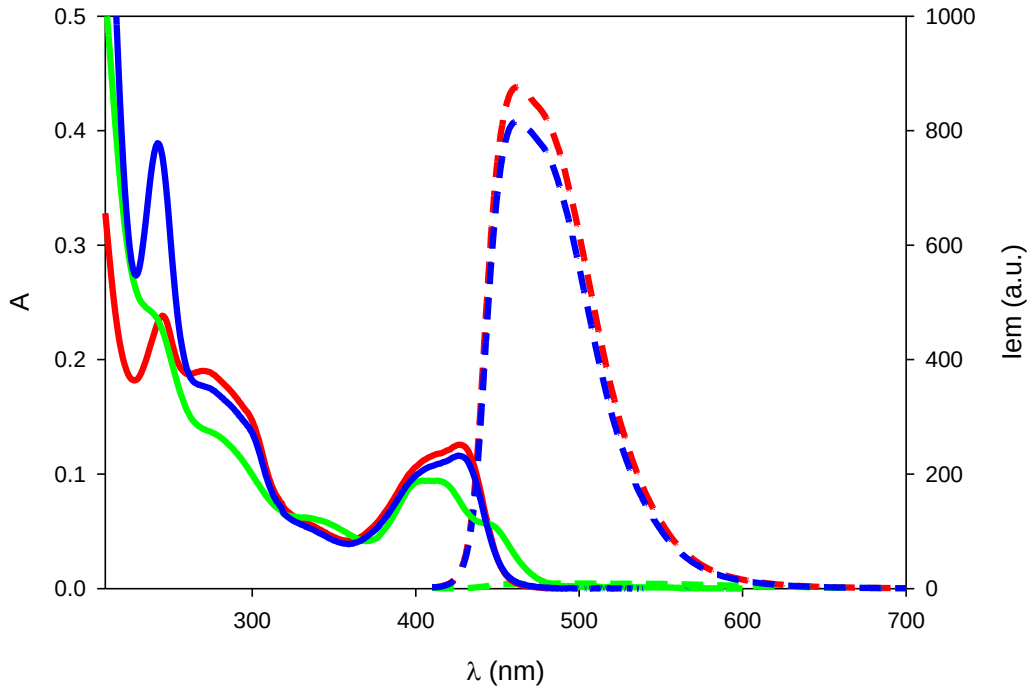

Figure S29 Absorption (left) and emission (right) spectra of a solution of **1P** in air-equilibrated aqueous solution (pH=8) (red line) upon addition of 2.5 eq of $Pb(NO_3)_2$ (green line) and 5 eq of EDTA (blue line). λ_{em} = 390 nm.

		Size (d.nm):	% Intensity:	St Dev (d.nm):
Z-Average (d.nm): 101.3	Peak 1:	181.6	100.0	129.1
PdI: 0.473	Peak 2:	0.000	0.0	0.000
Intercept: 0.743	Peak 3:	0.000	0.0	0.000
Result quality : Good				

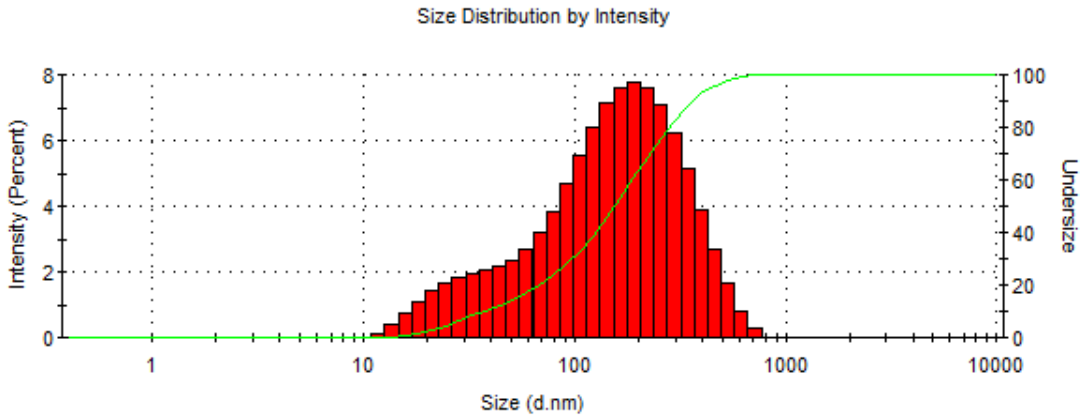

Figure S30 Size distribution by DLS analysis on a 3.0 x 10^{-6} M solution of **1M** in aqueous solution (pH=8) upon addition of 2.5 equiv. of $Pb(NO_3)_2$.

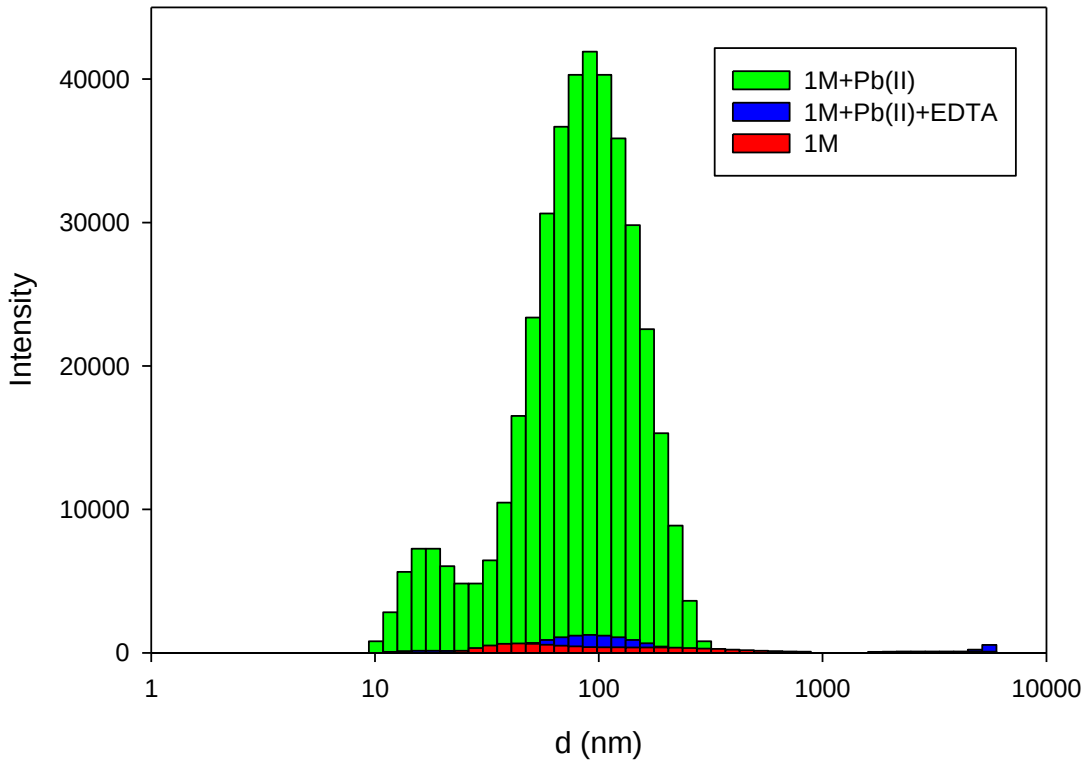

Figure S31. Size distribution by DLS analysis of scattered intensity of a 3.0 x 10^{-6} M solution of **1M** in air-equilibrated aqueous solution (pH=8) (red) upon addition of 2.5 equiv. of $Pb(NO_3)_2$ (green) and 5 equiv. of EDTA (blue).

3. References:

[1] M. Villa, M. Roy, G. Bergamini, M. Gingras, P. Ceroni, *Dalton Trans.* **2019**, *48*, 3815-3818.