

ELECTRONIC SUPPLEMENTARY INFORMATION

Solution-phase molecular recognition of an azafullerene-quinoline dyad by a face-to-face porphyrin-dimer tweezer

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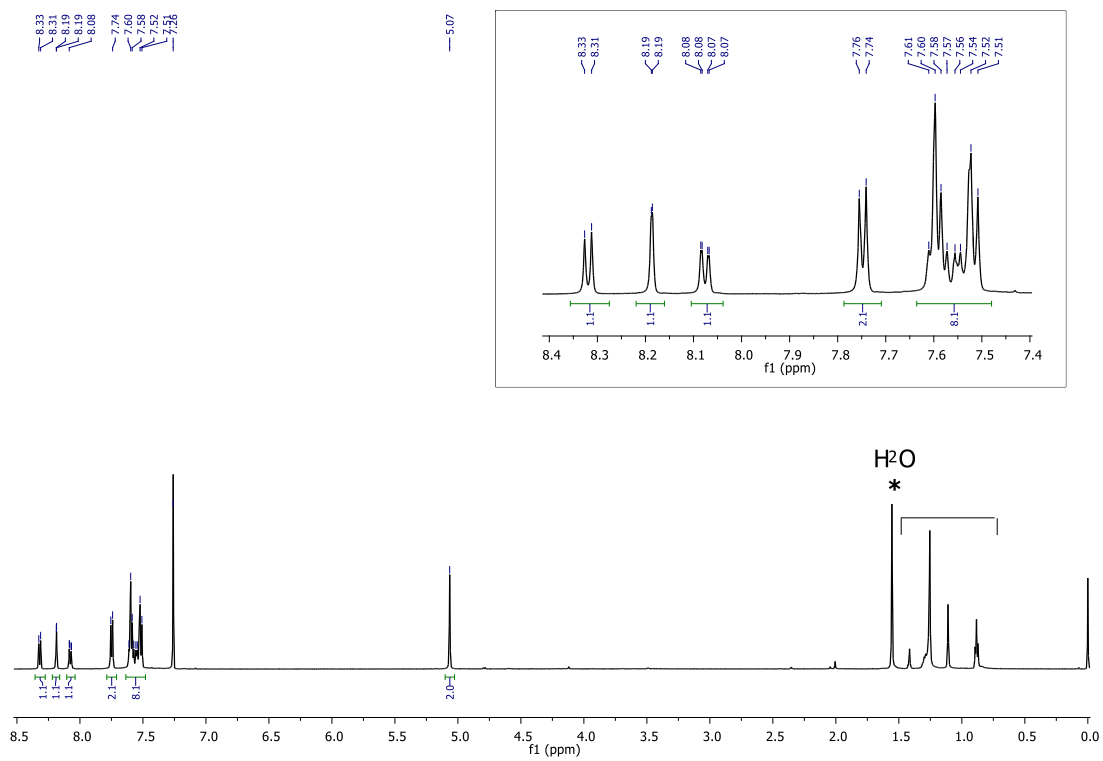


Figure S1. ^1H NMR spectrum of $\text{C}_{59}\text{N-FQ}$ recorded in CDCl_3 . The inset represents the region of the proton signals from the quinoline system.

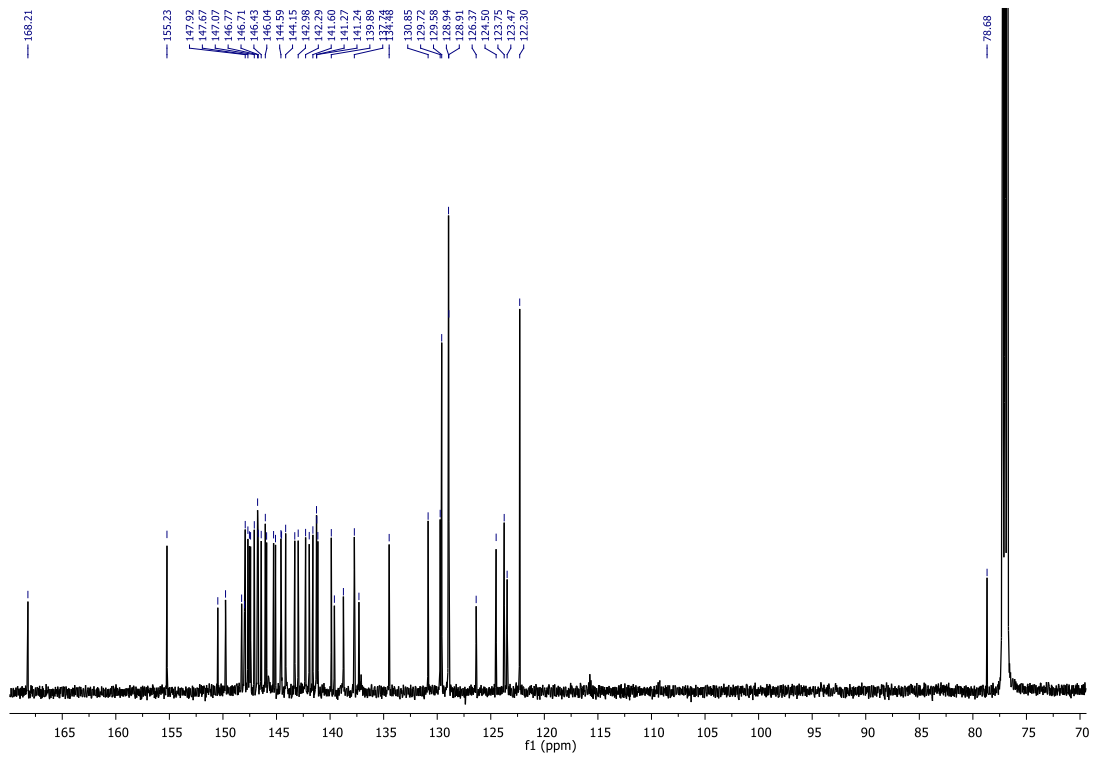


Figure S2. ^{13}C NMR spectrum of $\text{C}_{59}\text{N-FQ}$ recorded in CDCl_3 .

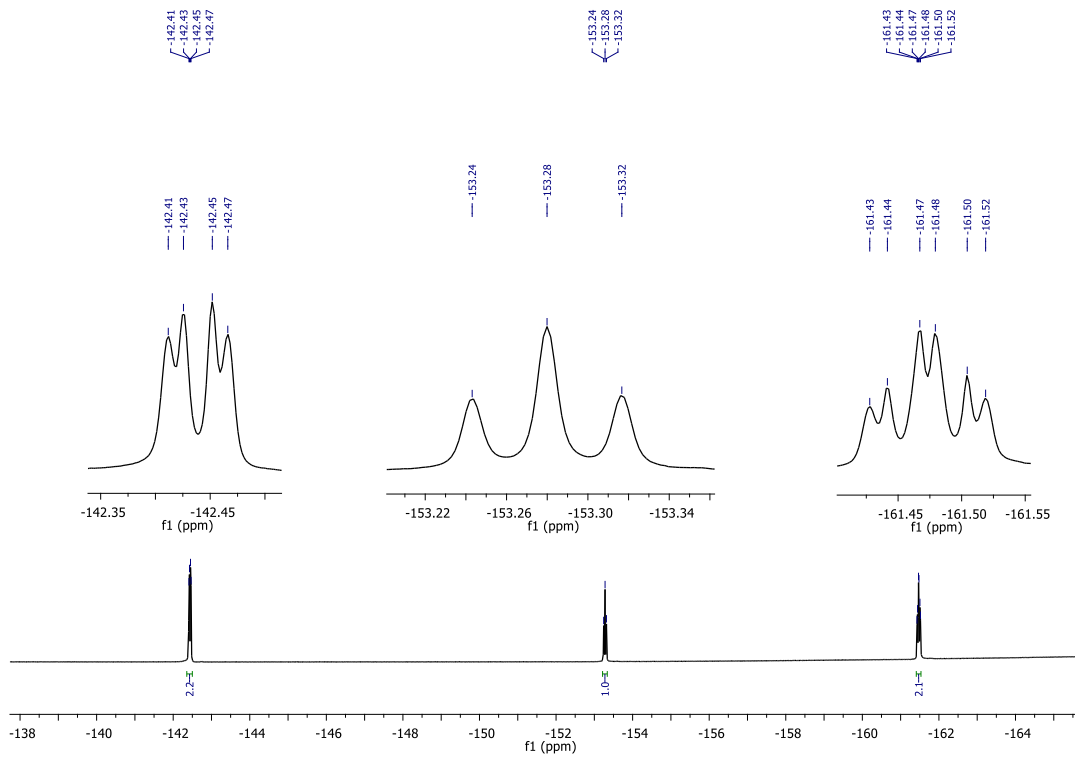


Figure S3. ^{19}F NMR spectrum of $\text{C}_{59}\text{N-FQ}$ recorded in CDCl_3 . The inset represents expanded areas of the recorded signals.

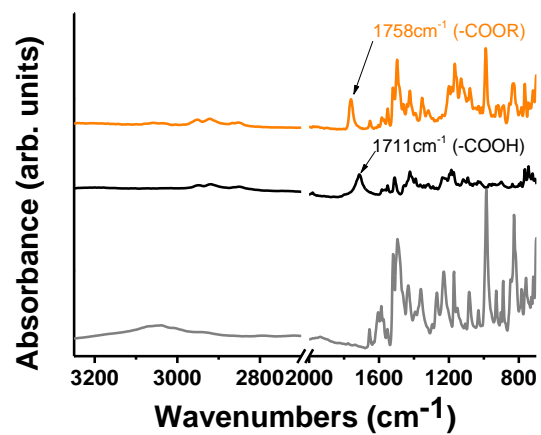


Figure S4. FT-IR spectra of FQ (grey), C₅₉N-COOH (black) and C₅₉N-FQ (orange).

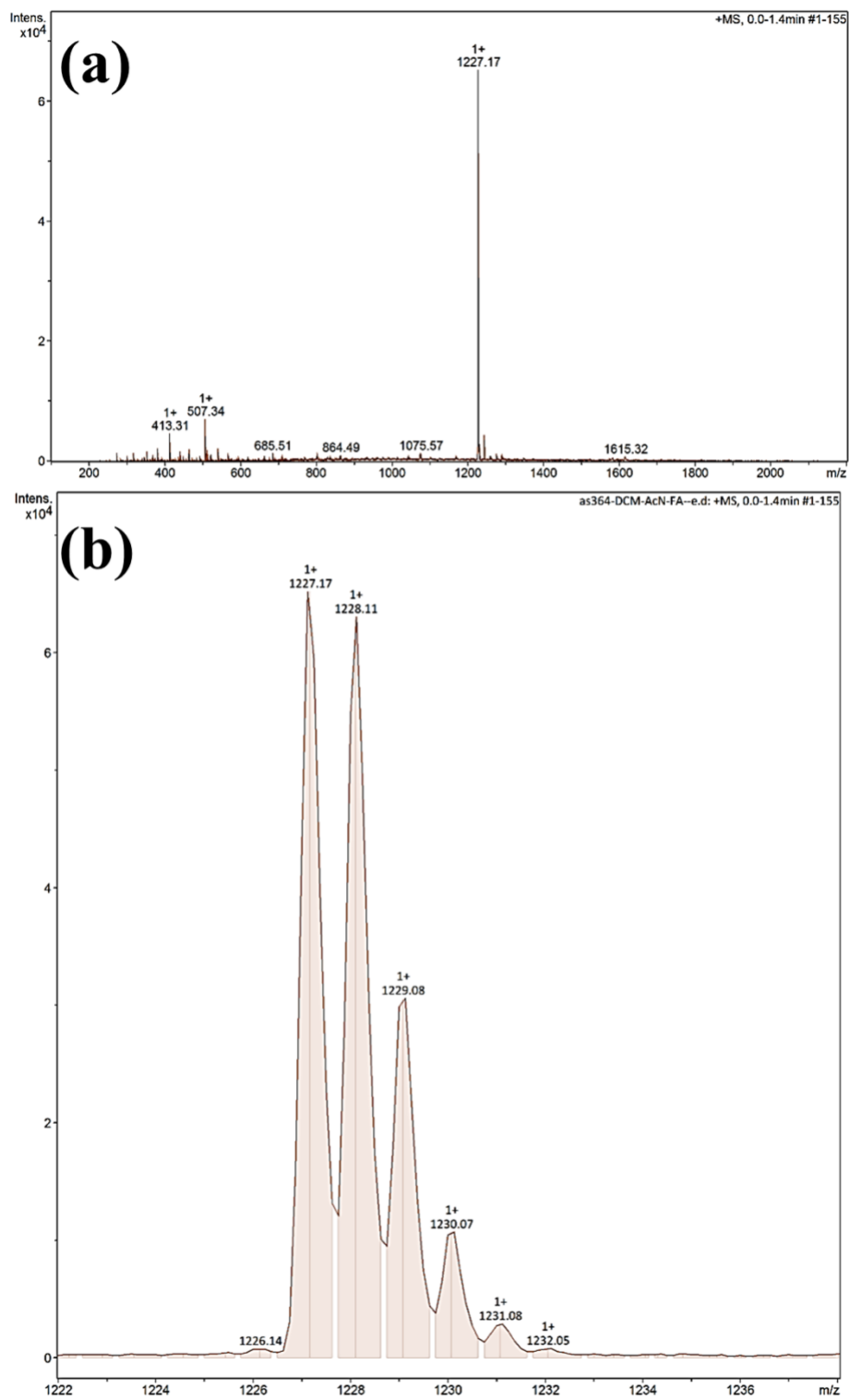


Figure S5. (a) ESI-MS mass spectrum, and (b) isotopic distribution pattern of $[C_{59}N-FQ+1]^+$.

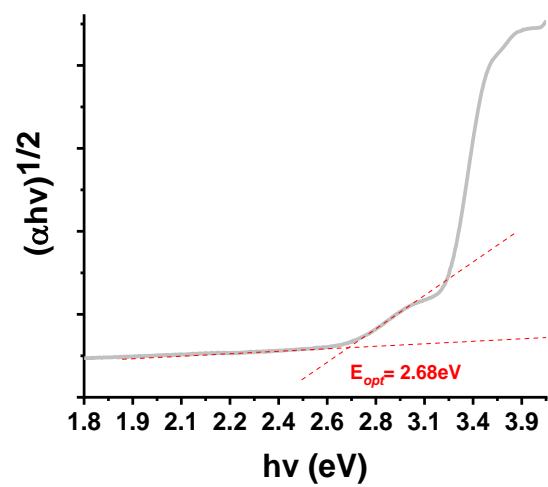


Figure S6. Tauc plot for the determination of the energy gap of FQ, based on the UV-Vis spectra presented in Figure 1a.

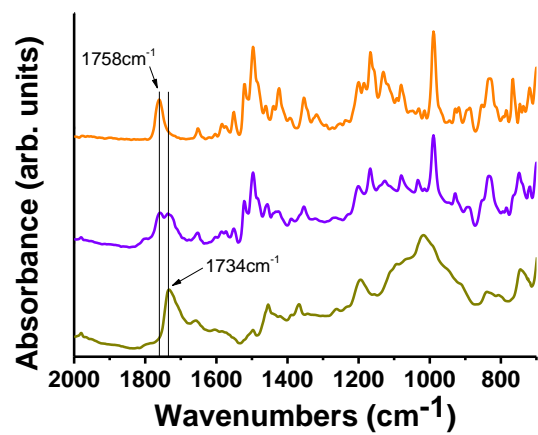


Figure S7. FT-IR spectra of C₅₉N-FQH⁺ (olive), C₅₉N-FQ (orange) and a mixture containing C₅₉N-FQH⁺ and C₅₉N-FQ (purple).

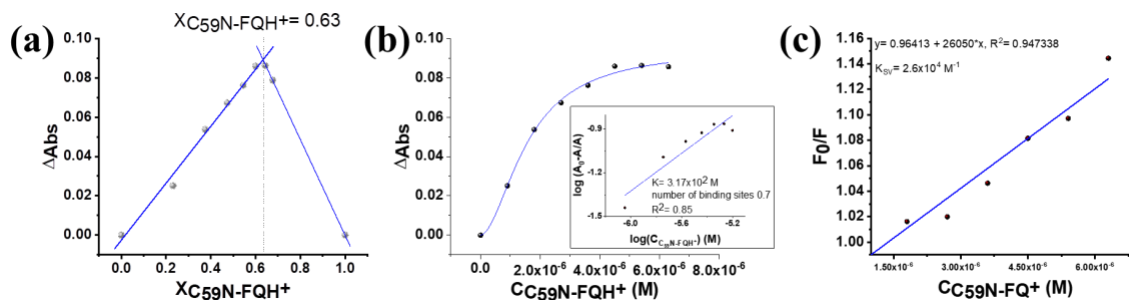


Figure S8. (a) Job's plot for the $(\text{H}_2\text{P})_2/\text{C}_{59}\text{N-FQH}^+$ system in benzonitrile, based on the absorbance changes of the Soret band of $(\text{H}_2\text{P})_2$ with respect to the $X_{\text{C}_{59}\text{N-FQH}^+}$. (b) Absorbance changes of the Soret band of $(\text{H}_2\text{P})_2$ with respect to the concentration of the guest $\text{C}_{59}\text{N-FQH}^+$, in benzonitrile. Inset: Hill plot for the $(\text{H}_2\text{P})_2/\text{C}_{59}\text{N-FQH}^+$ system.

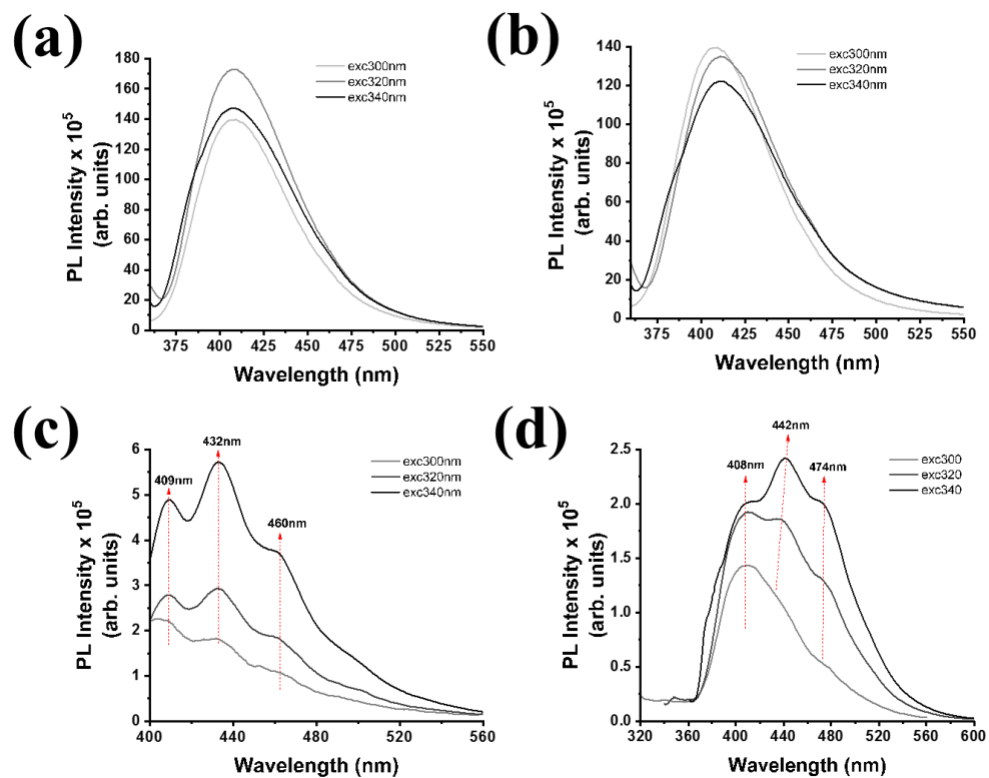


Figure S9. Fluorescence emission spectra of (a) FQ, (b) protonated FQH⁺, (c) C₅₉N-FQ and (d) C₅₉N-FQH⁺, recorded at three different excitation wavelengths (300, 320 and 340 nm) in toluene.

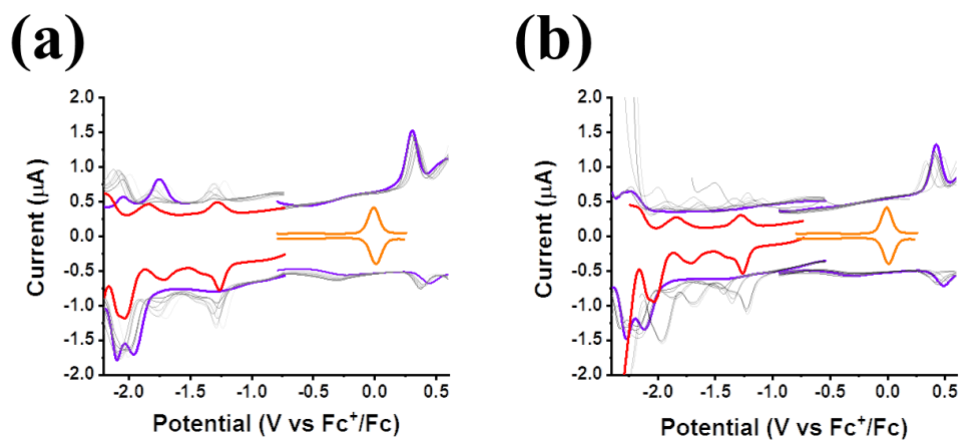


Figure S10. (a, b) DPV curves recorded upon incremental additions of up to 2.1 equivalents (gray lines) of C₅₉N-FQ and C₅₉N-FQH⁺, respectively. Purple line represents the DPV oxidation wave of free (H₂P)₂, red line refers to the reduction wave of the azafullerene cage within C₅₉N-FQ and C₅₉N-FQH⁺, while orange line displays the Fc⁺/Fc redox pair employed as internal reference. All graphs recorded in N₂-saturated solutions of 0.3 mM (H₂P)₂ in benzonitrile with 0.1 M TBAPF₆ as the supporting electrolyte at room temperature with scan rate 0.01 V/s.

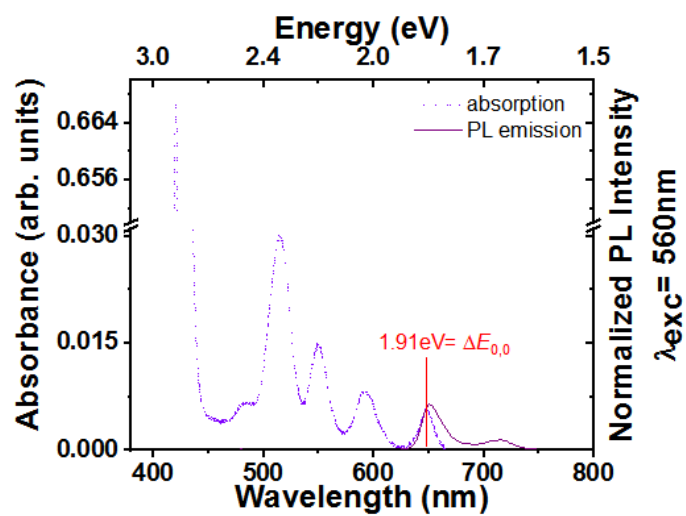


Figure S11. Absorption and emission spectra of $(\text{H}_2\text{P})_2$ in benzonitrile showing the spectral cross-section for the $0 \rightarrow 0$ transition.