

## SUPPORTING INFORMATION

### **A versatile, divergent route for the synthesis of ABAC tetraazaporphyrins, molecularly engineered, push-pull phthalocyanine-type dyes**

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## Copies of Spectra

Zn(II) [2,3-12,13-bis(benzo-4'(5')-iodo)-7,8,17,18-tetrapropyl-porphyrinato] (**3**)

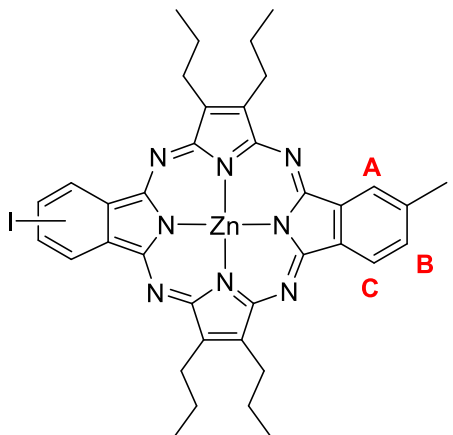
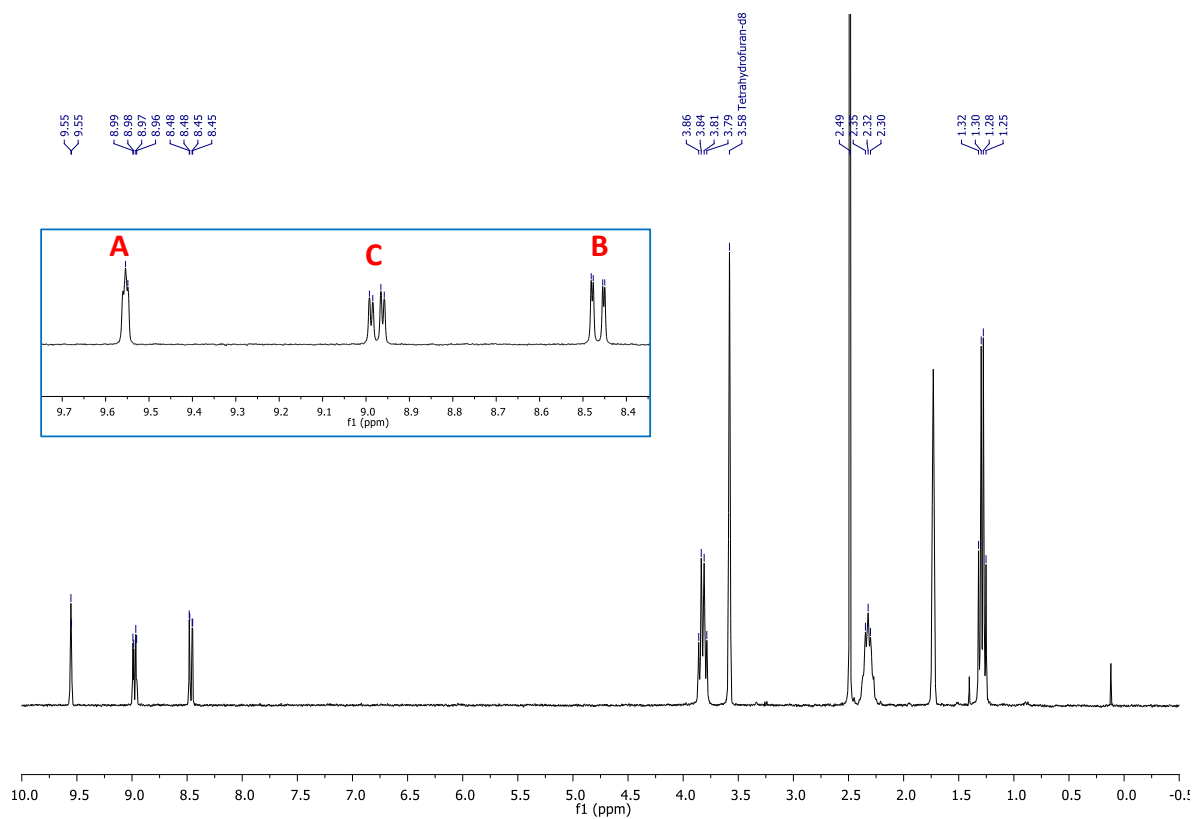


Figure S1.  $^1\text{H-NMR}$  spectrum of **3** in  $\text{THF-d}_4$ .



**Figure S2.**  $^{13}\text{C}$ -NMR spectrum of **3** in THF- $d_4$ .

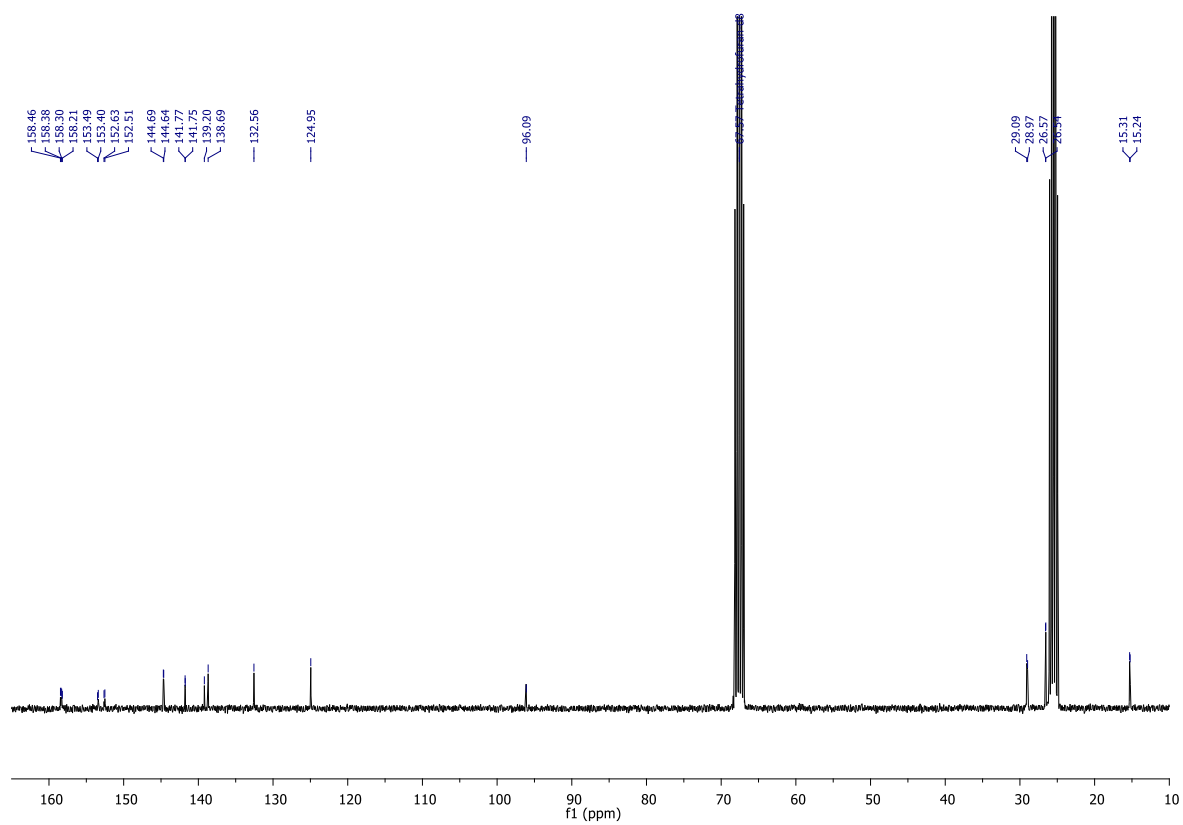


Figure S3. IR Spectrum (KBr) of **3**

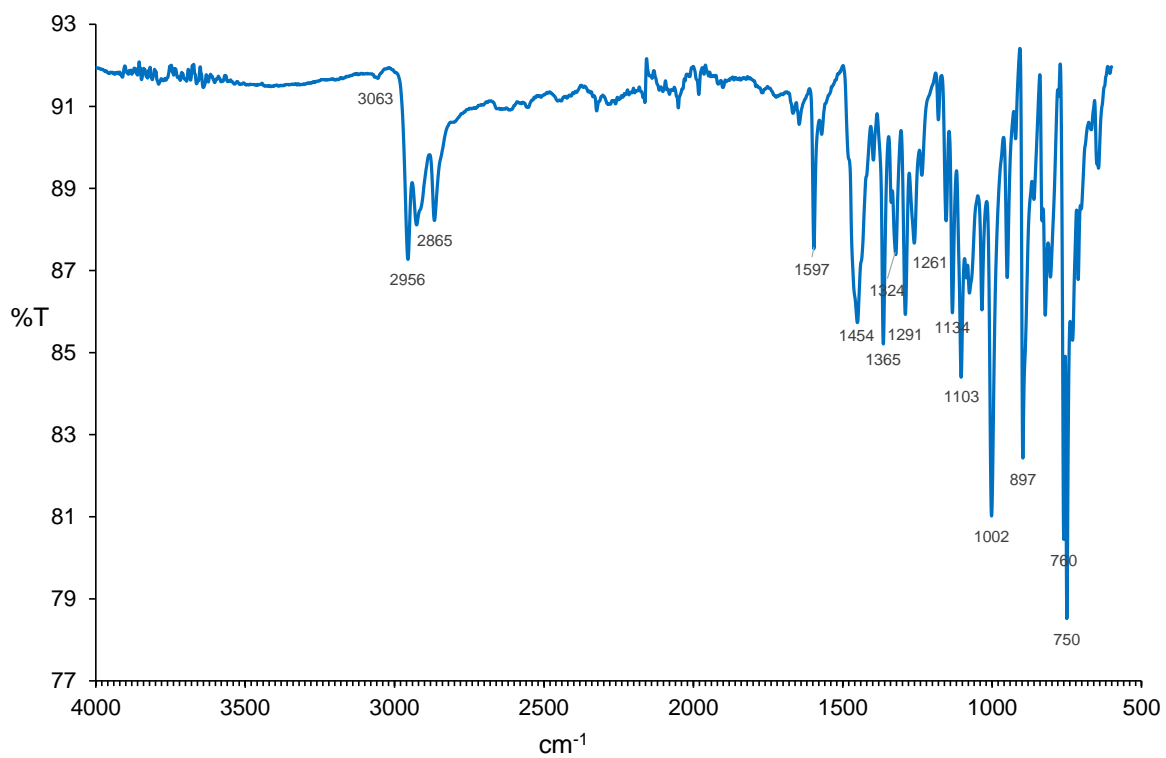
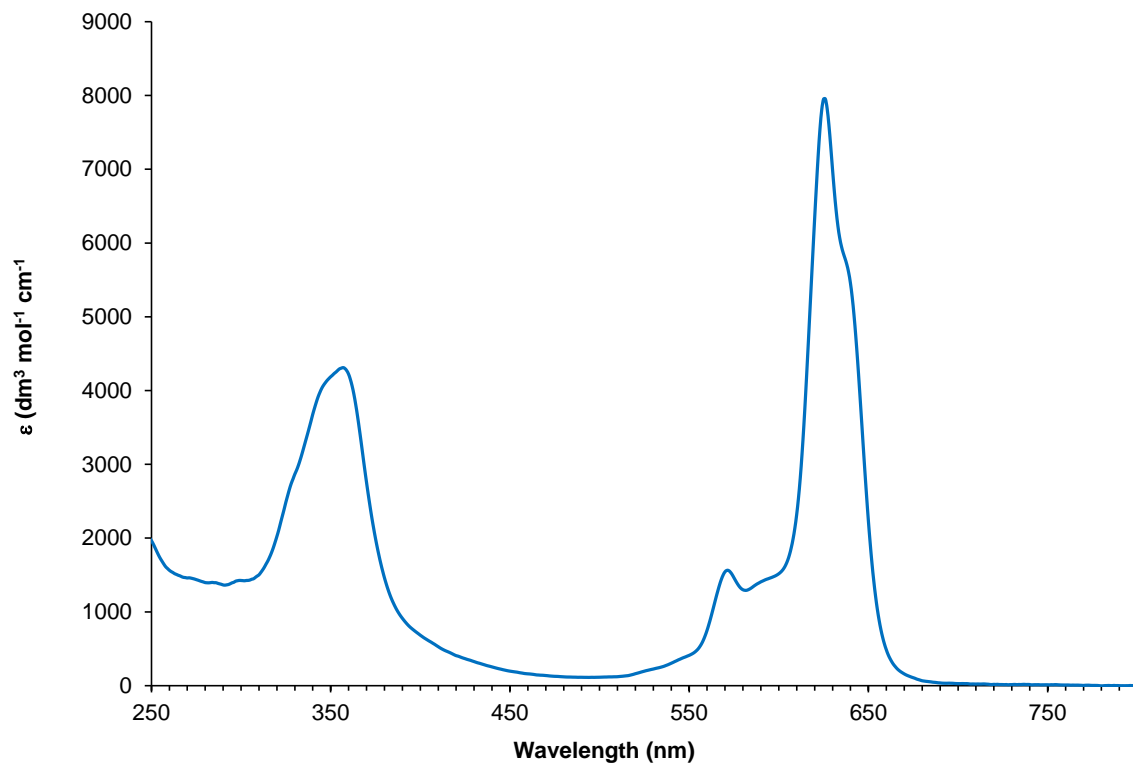
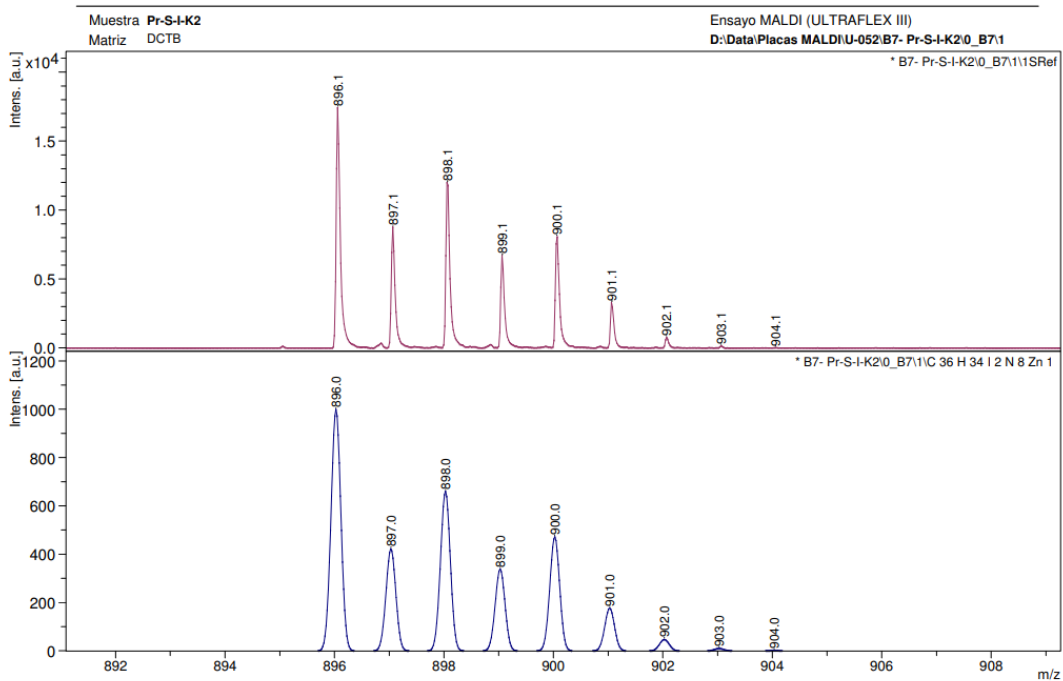
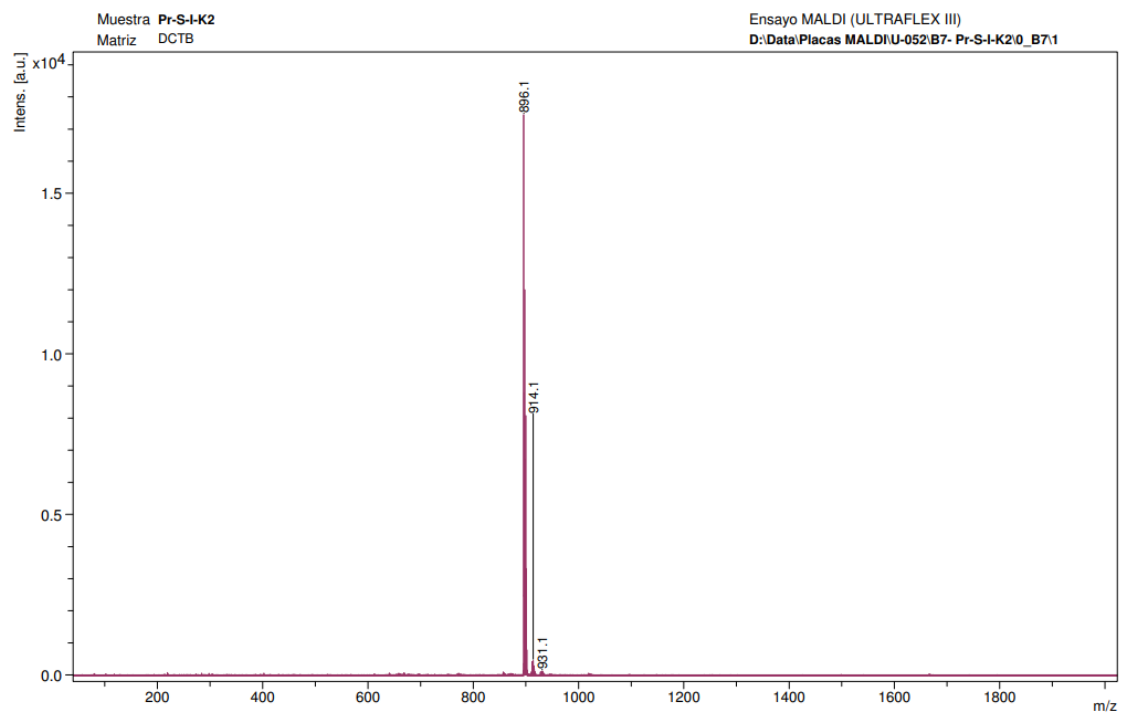


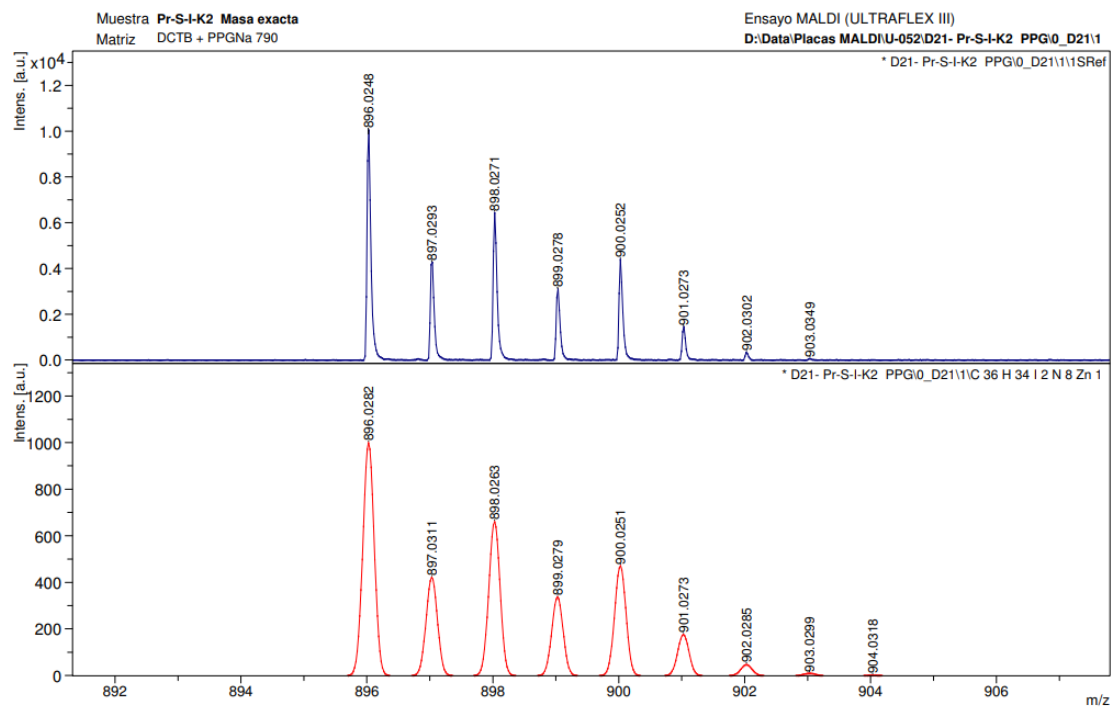
Figure S4. UV-Vis Spectrum of **3** in THF



**Figure S5.** MS (MALDI-TOF, DCTB) of **3**.



**Figure S6.** HRMS (MALDI-TOF, DCTB+ PPGNa 790) of **3**.





Zn(II) [2,3(benzo-4'-iodo)-12,13-benzo-7,8,17,18-tetrapropyl-porphyrinato] (4)

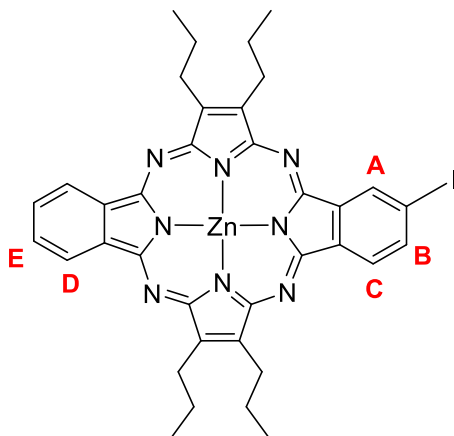
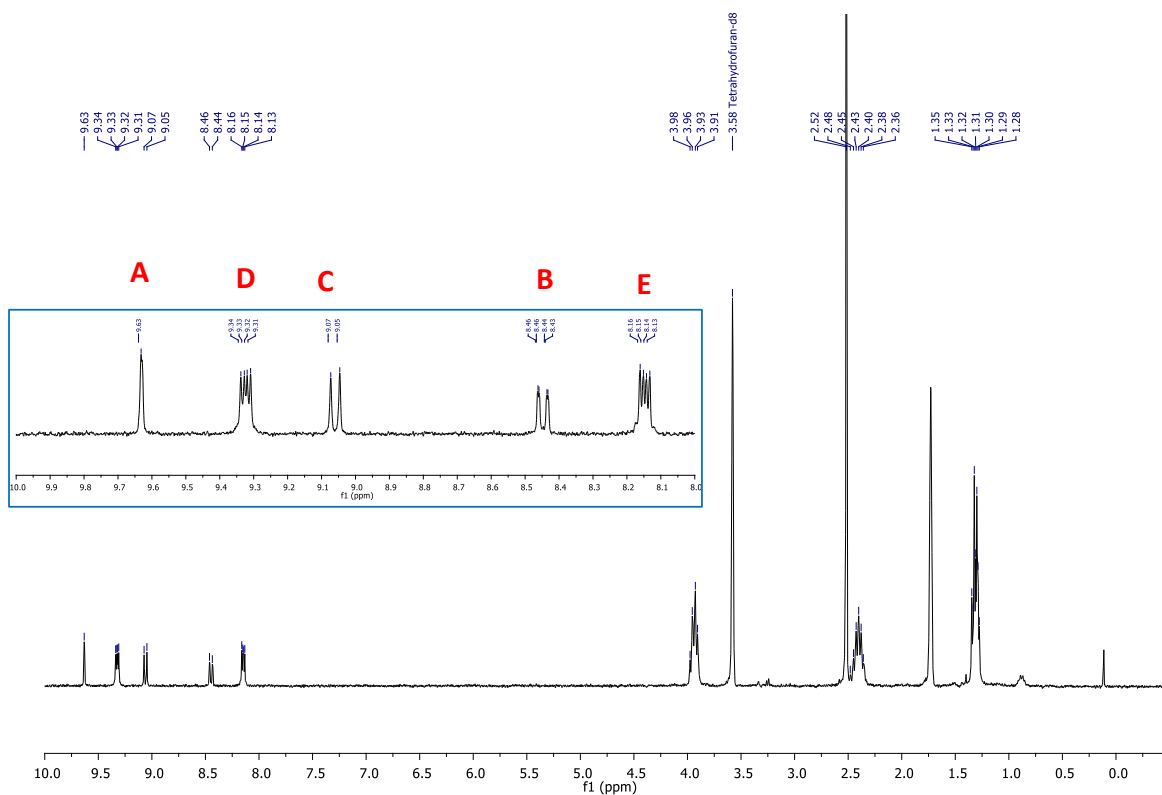
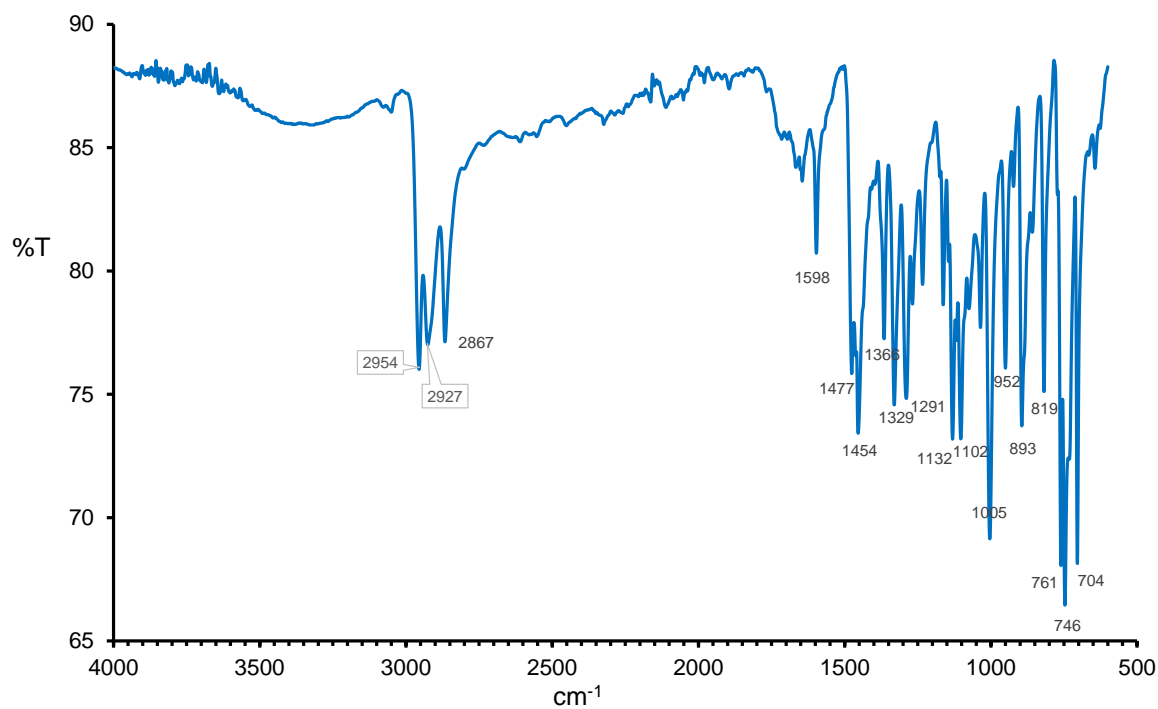


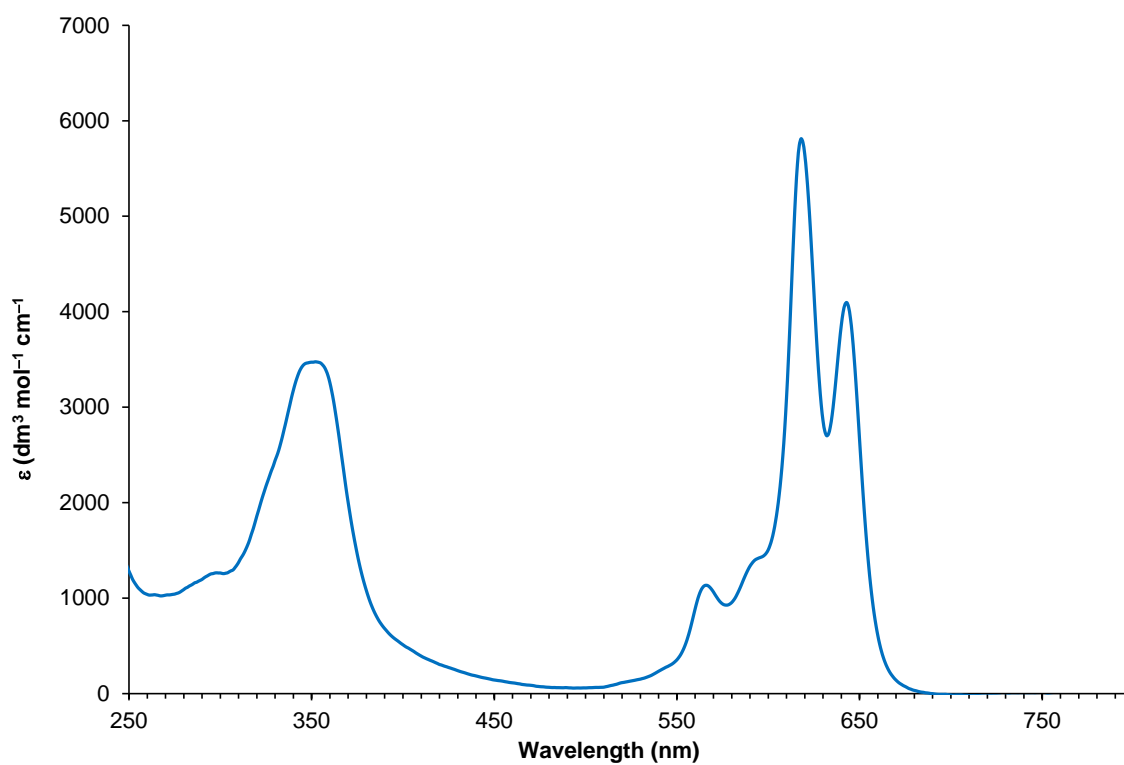
Figure S7.  $^1\text{H-NMR}$  spectrum of **4** in  $\text{THF-d}_4$ .



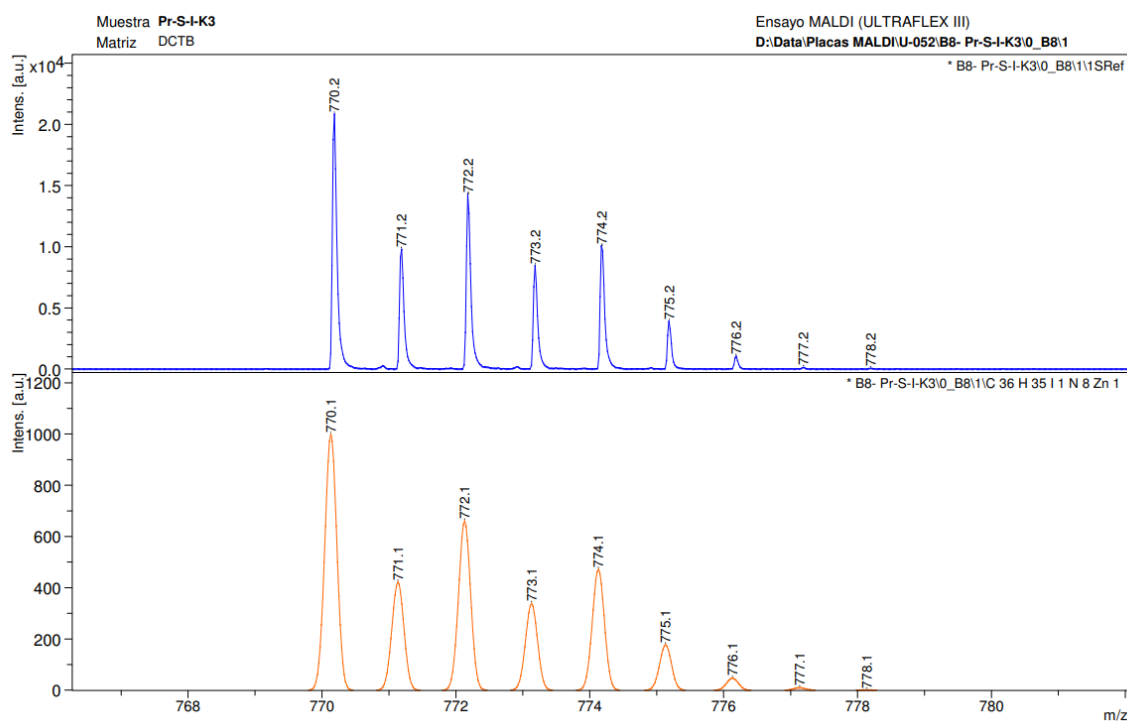
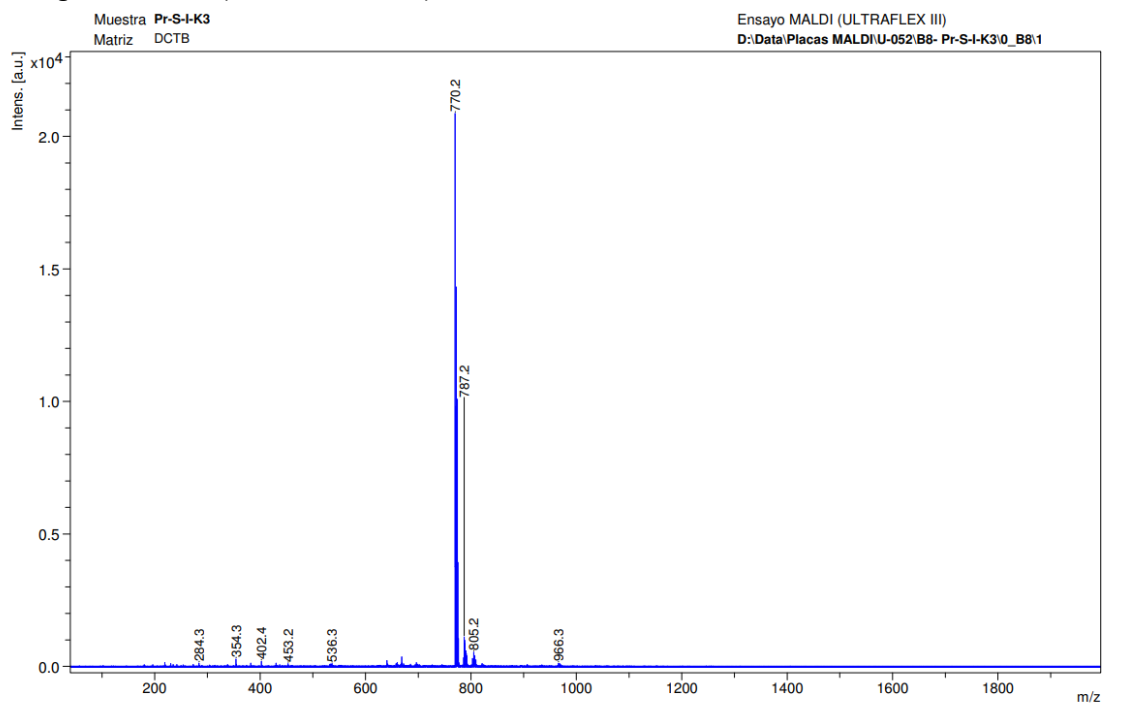
**Figure S8.** FTIR Spectrum (KBr) of **4**



**Figure S9.** UV-Vis Spectrum in THF of **4**



**Figure S10.** MS (MALDI-TOF, DCTB) of **4**.



Zn(II) [2,3-12,13-dibenzo-7,8,17,18-tetrapropyl-porphyrinato] (5)

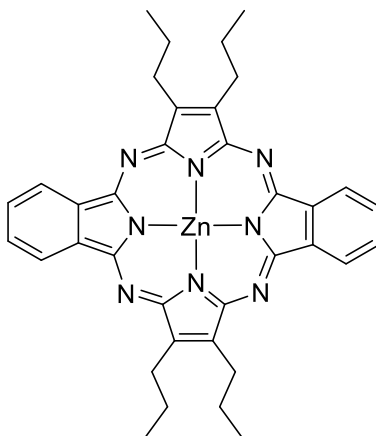
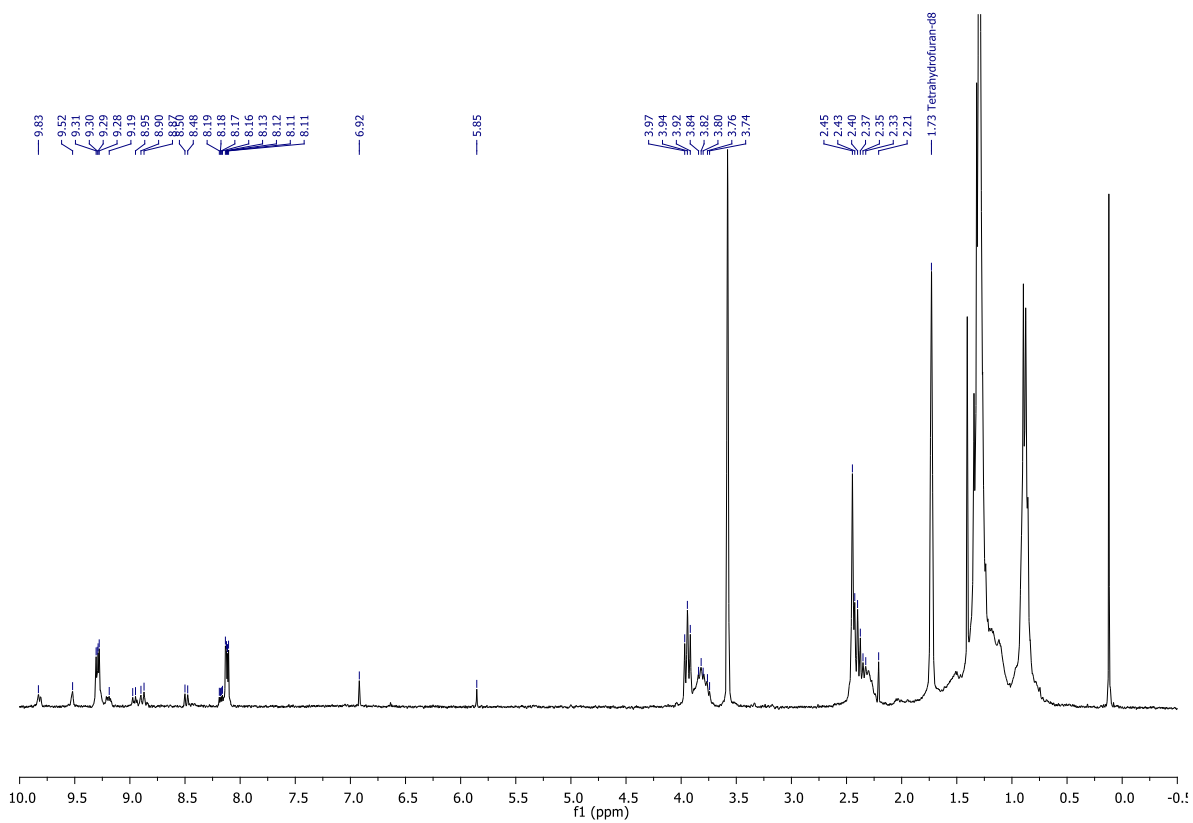
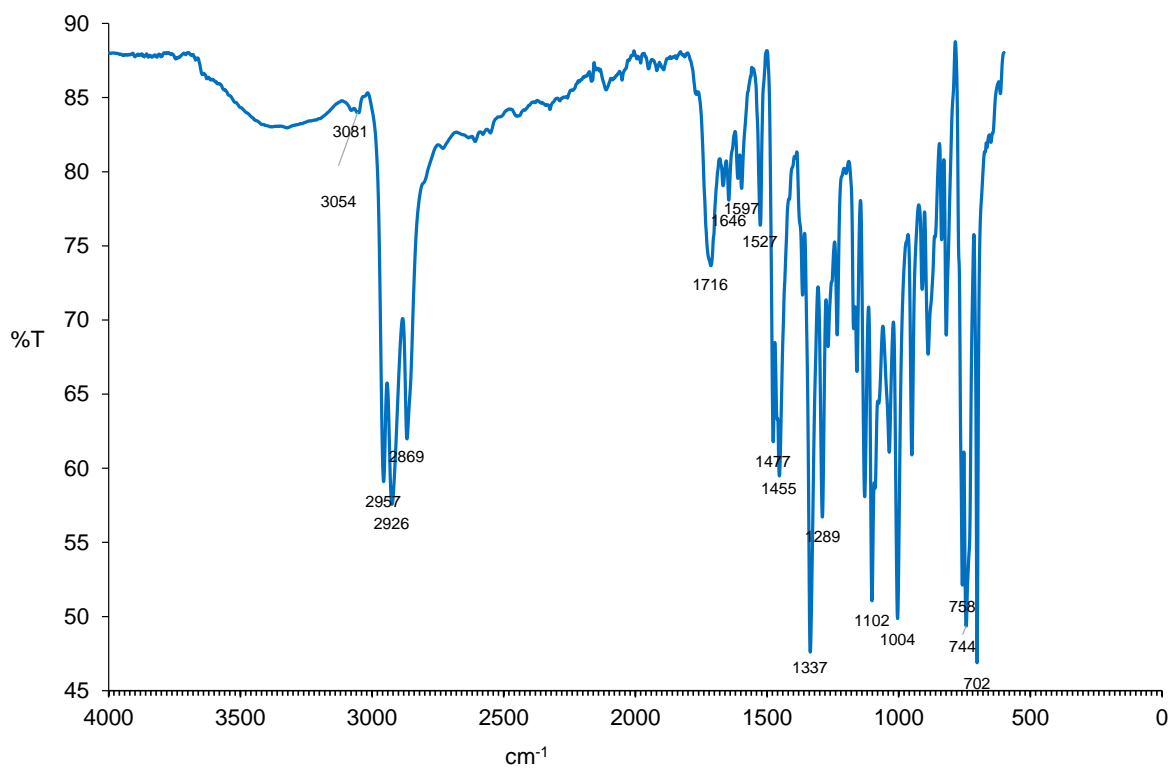


Figure S11. <sup>1</sup>H-NMR spectrum of 5 in THF-d<sub>4</sub>.



**Figure S12.** FTIR Spectrum (KBr) of **5**



**Figure S13.** UV/Vis Spectrum in THF of **5**

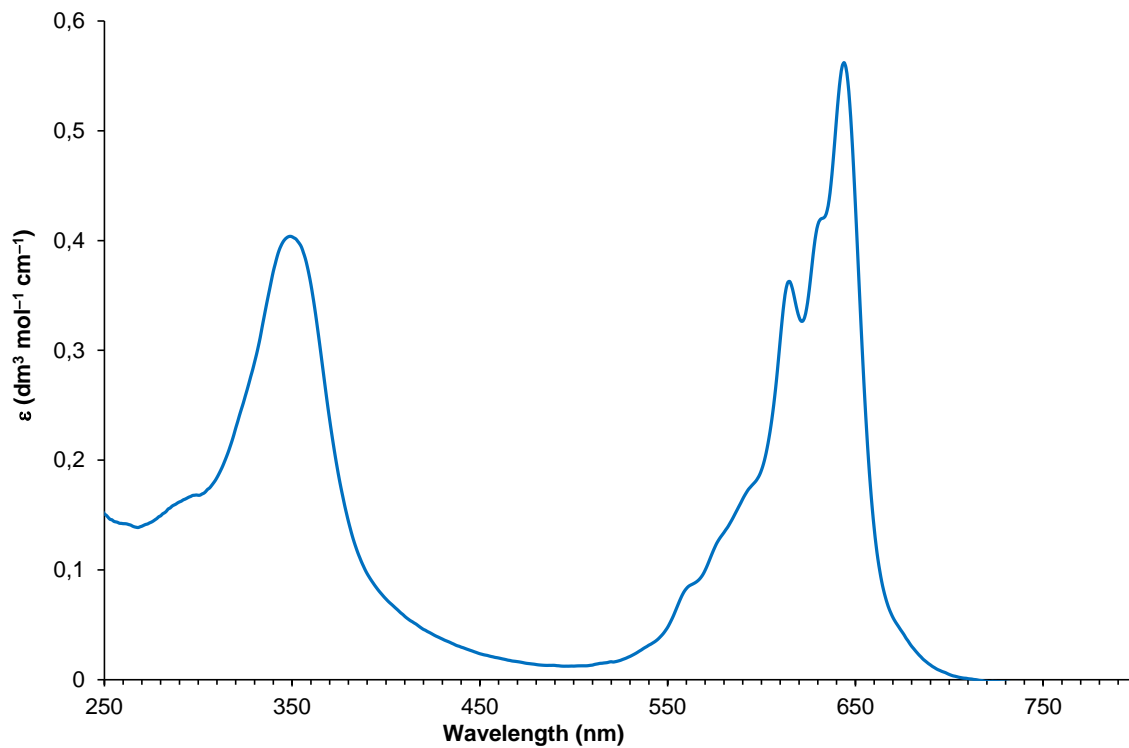
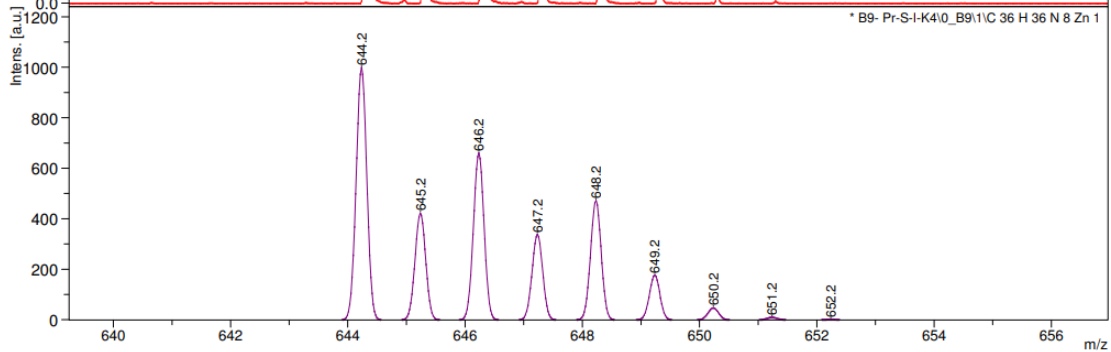
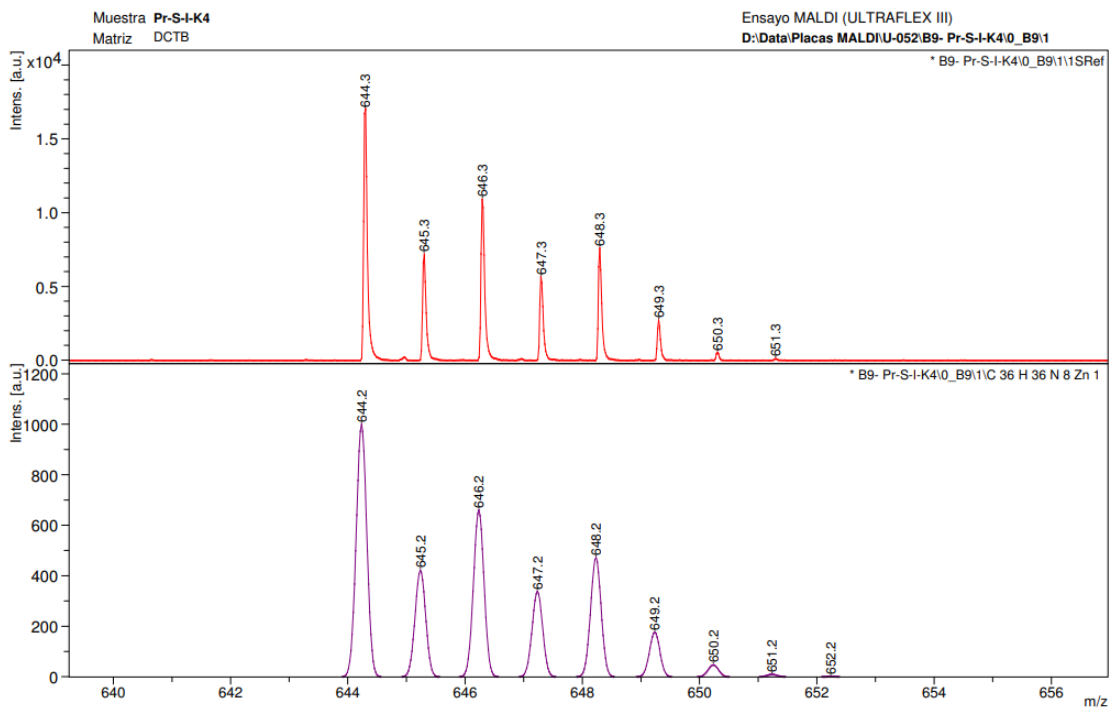
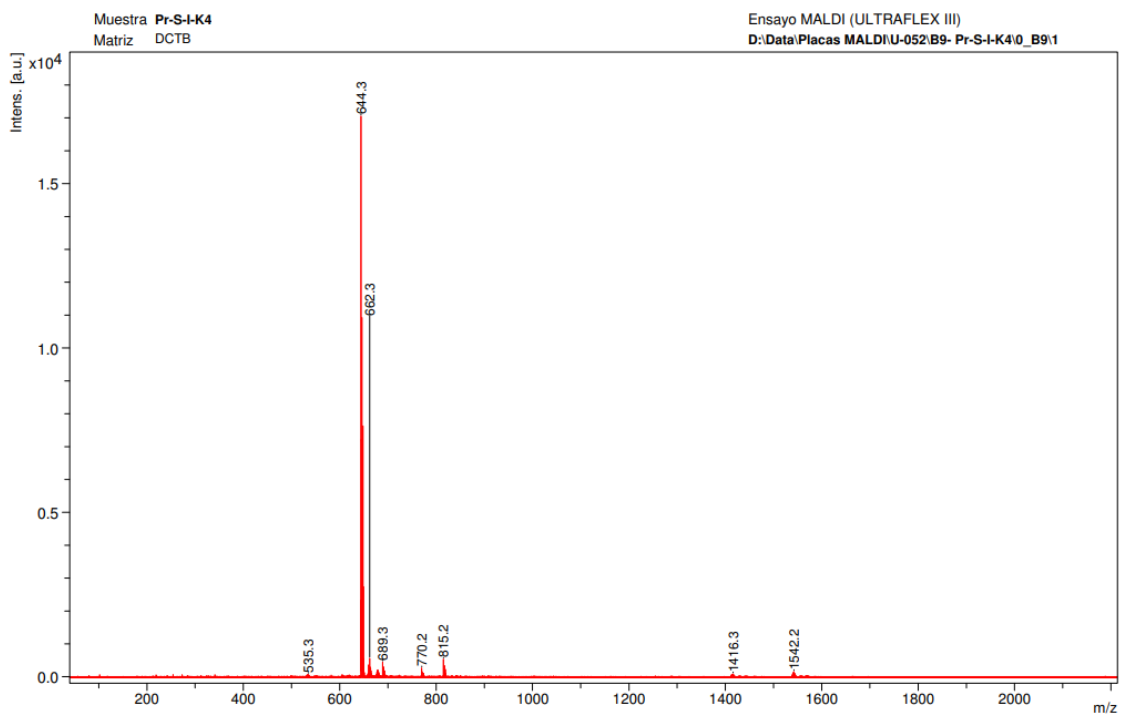


Figure S14. MS (MALDI-TOF, DCTB) of 5.



Zn(II) [2,3-(benzo-4'-ethynyltriisopropylsilane)-12,13-(benzo-4''(5'')-iodo)-7,8,17,18-tetrapropylporphyrinato] (6)

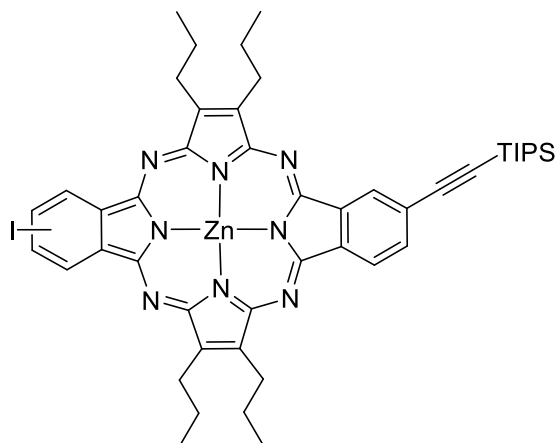
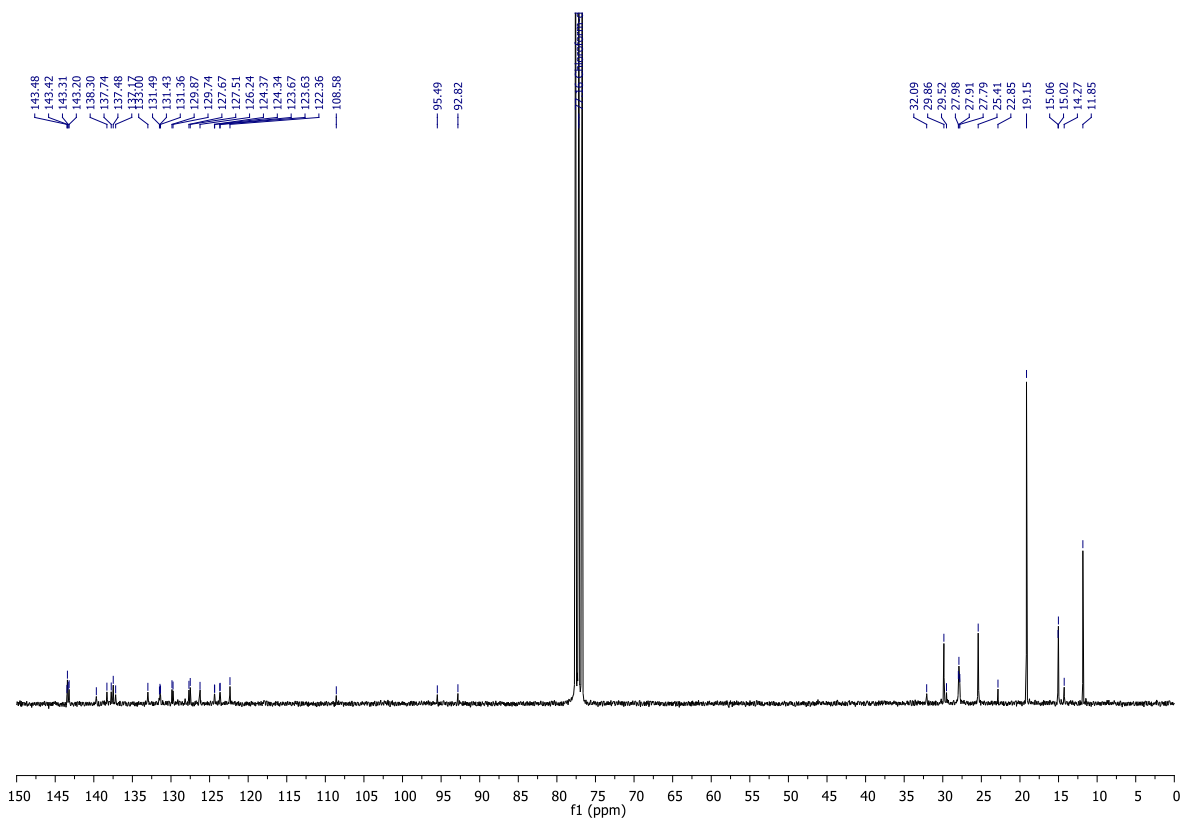
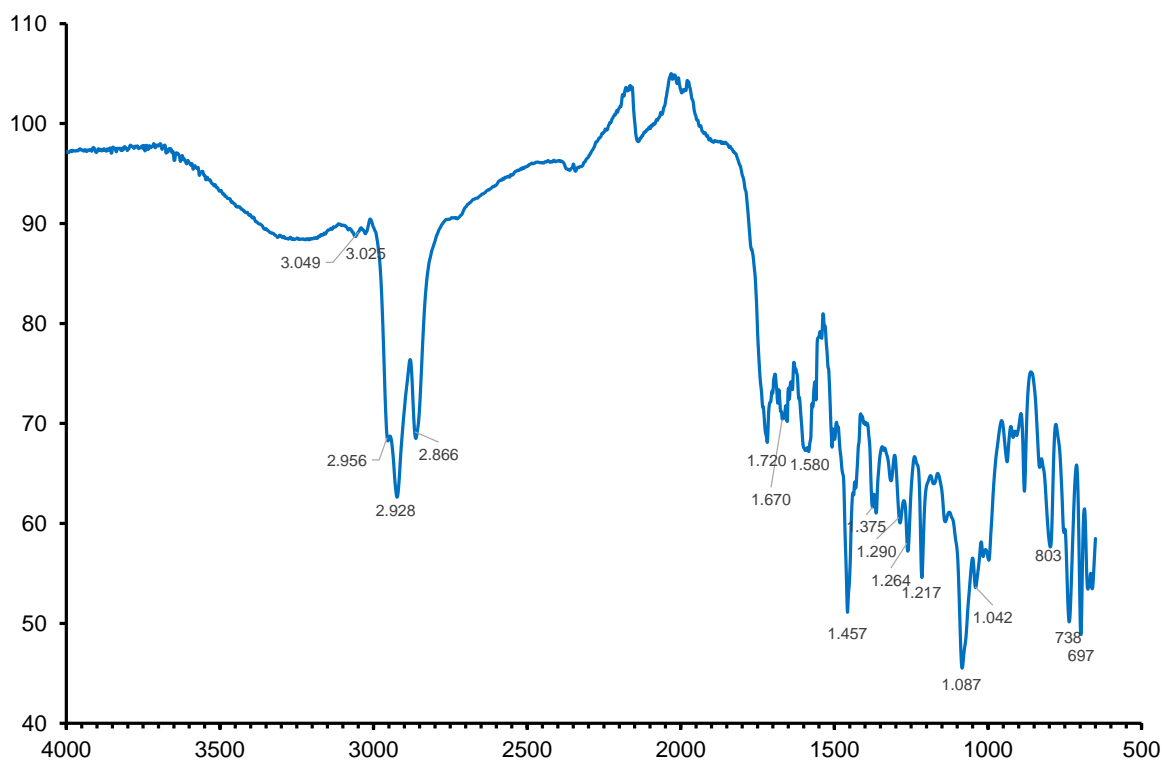


Figure S15.  $^{13}\text{C}$ -NMR spectrum of 6 in  $\text{CDCl}_3$ .



**Figure S16.** FT-IR (KBr) spectrum of **6**.



**Figure S17.** UV-Vis of **6** in  $\text{CHCl}_3$

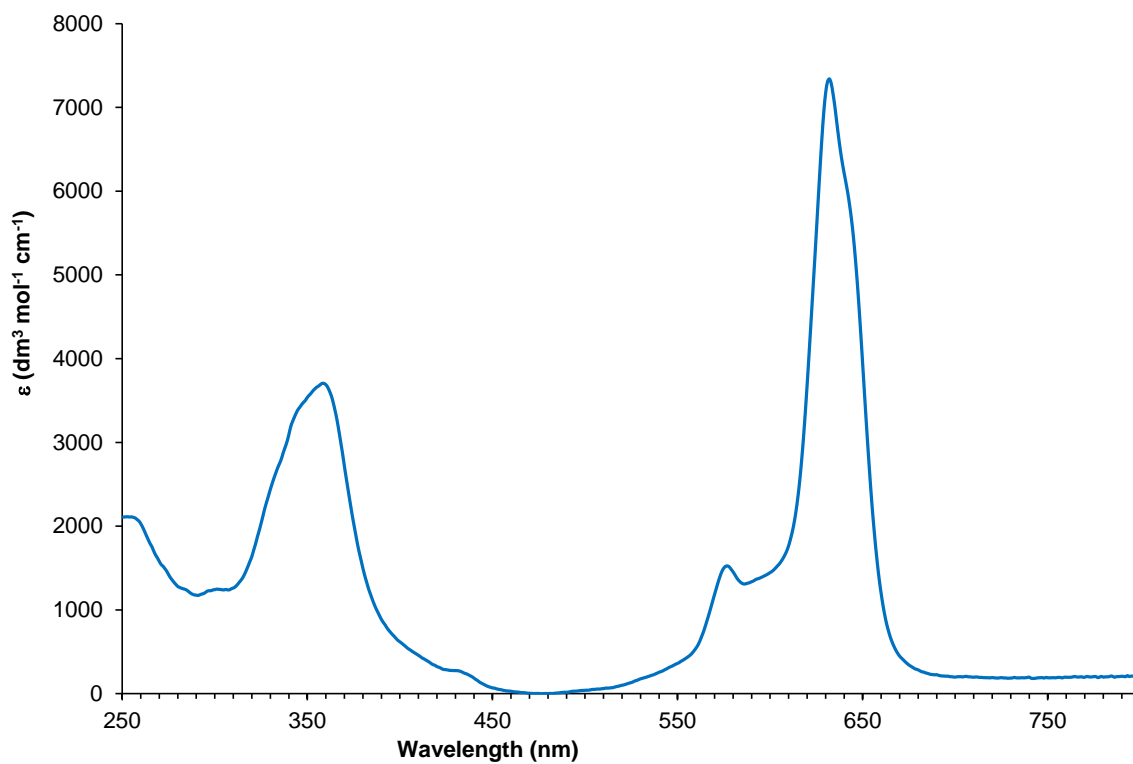
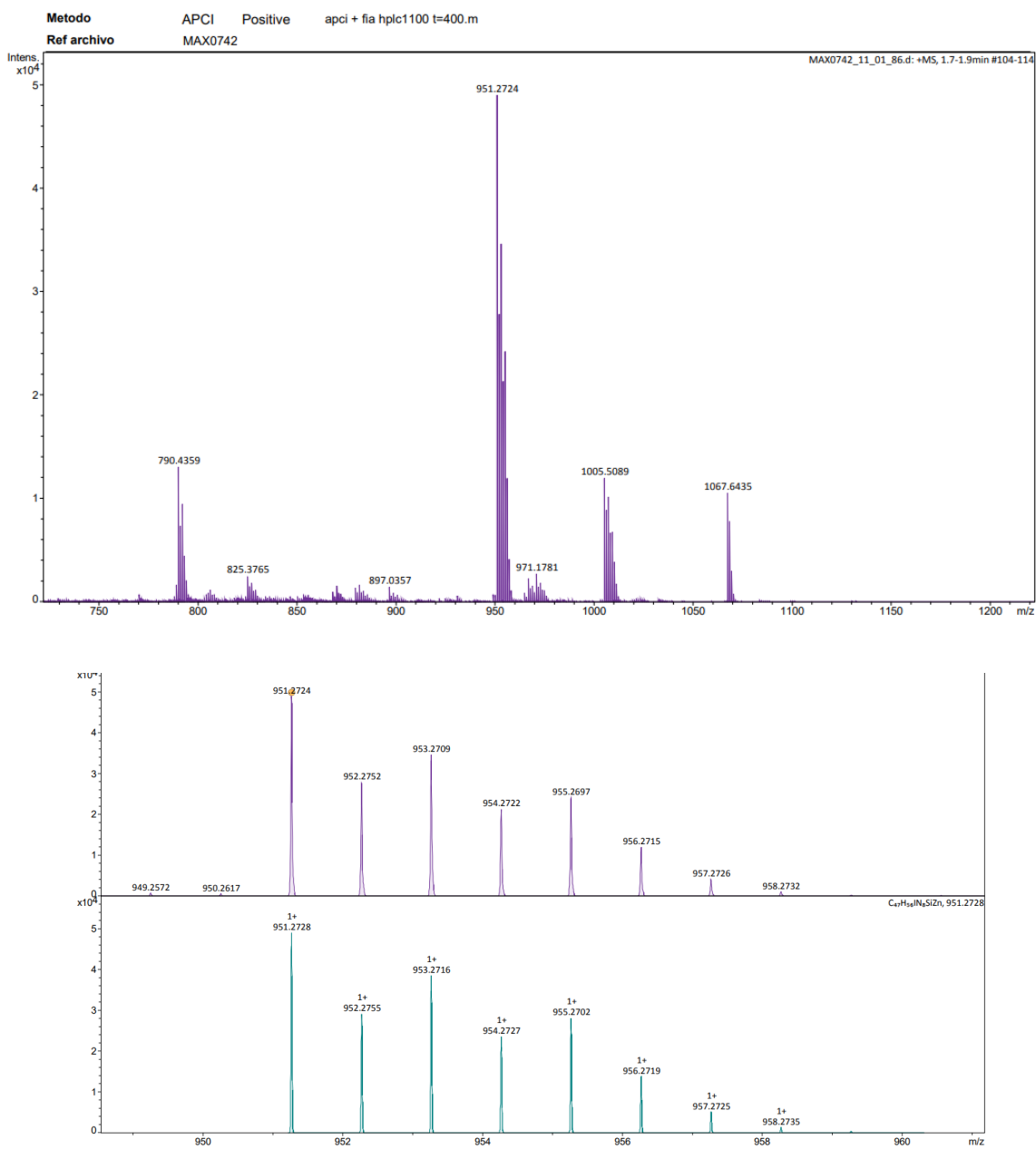




Figure S18. HRMS (APCI<sup>+</sup>) of 6.



Zn(II) [2,3-12,13-bis(benzo-4'(5')-ethynyltriisopropylsilane)-7,8,17,18-tetrapropylporfirazinato] (7)

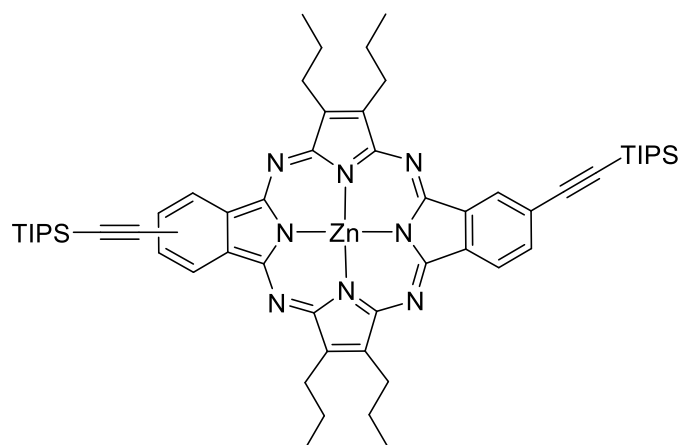
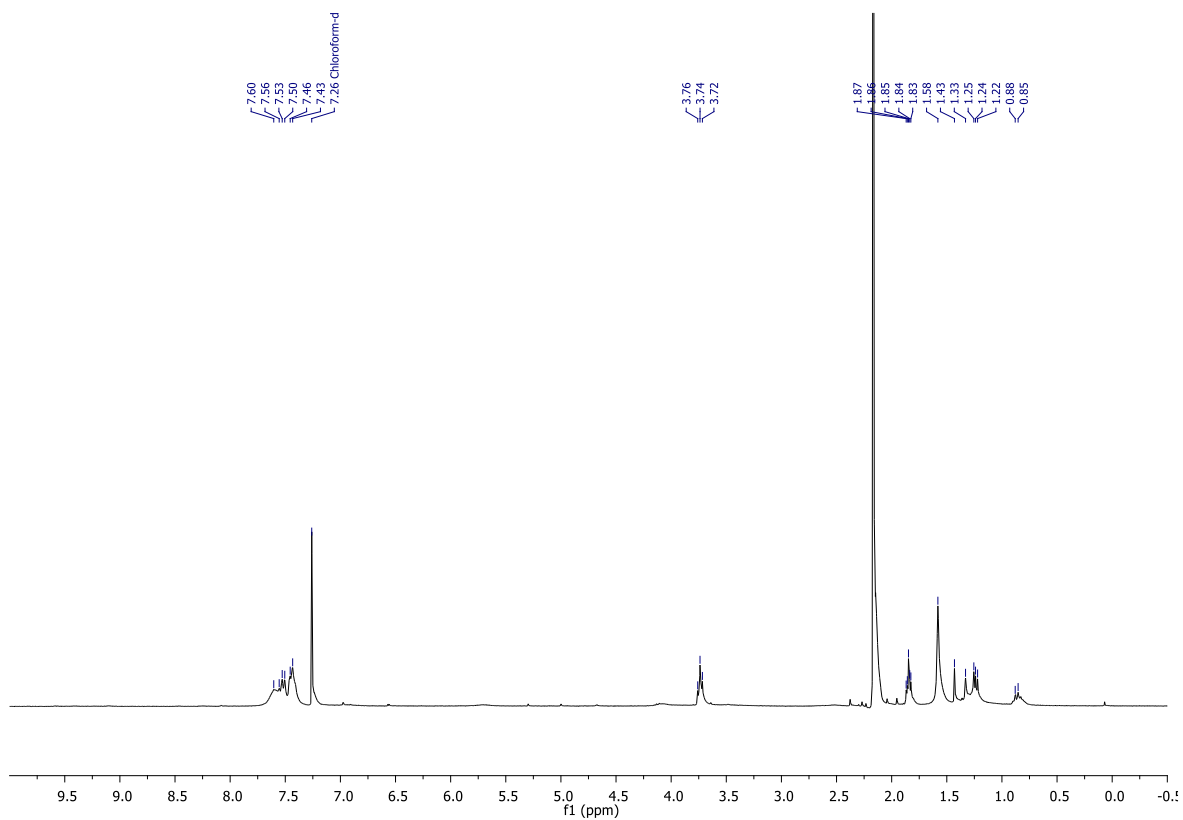
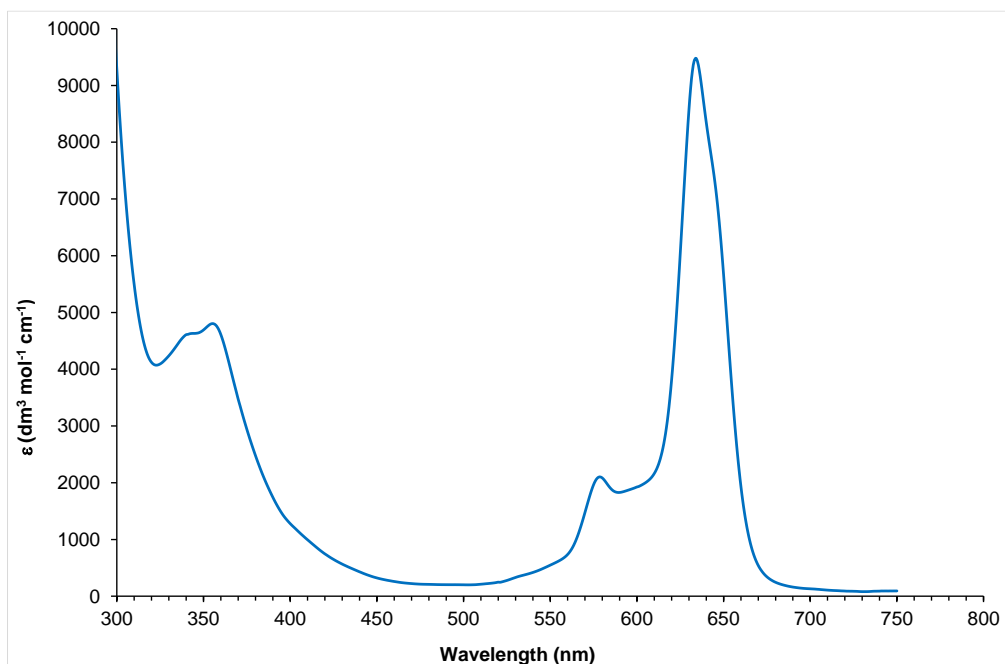


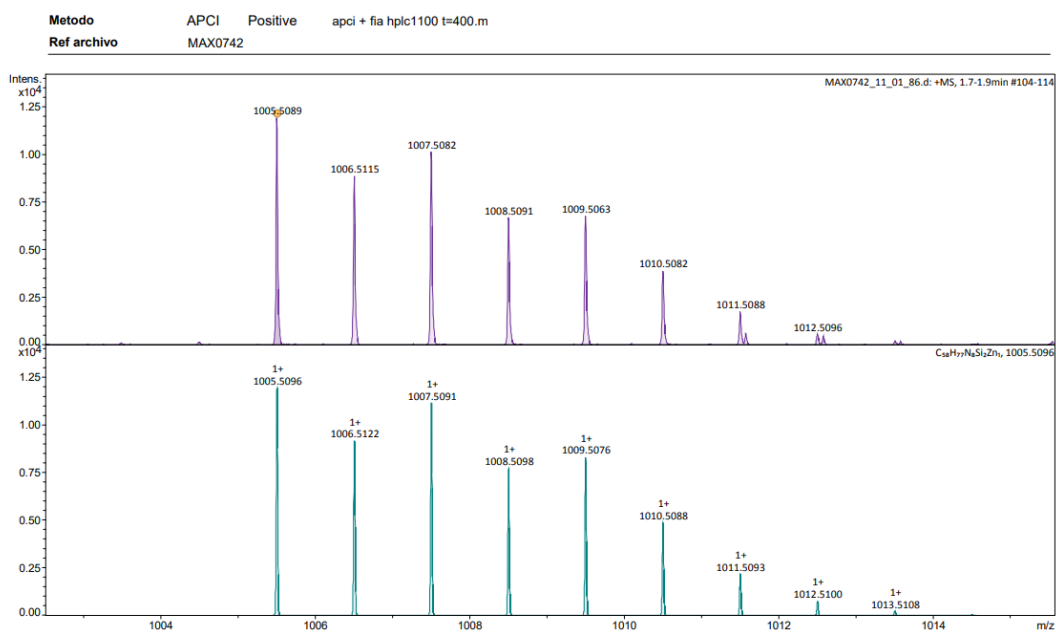
Figure S19.  $^1\text{H-NMR}$  spectrum of **7** in  $\text{CDCl}_3$ .



**Figure S20.** UV-Vis of **7** in CHCl<sub>3</sub>



**Figure S21.** HRMS (APCI<sup>+</sup>) of **7**.



Zn(II) [2,3-(benzo-4'(5')-ethynyltriisopropylsilane)-12,13-(benzo-4''-bis(2',4'''-dihexoxybiphenyl-4-yl)amine)-7,8,17,18-tetrapropylporphyrinato] (9)

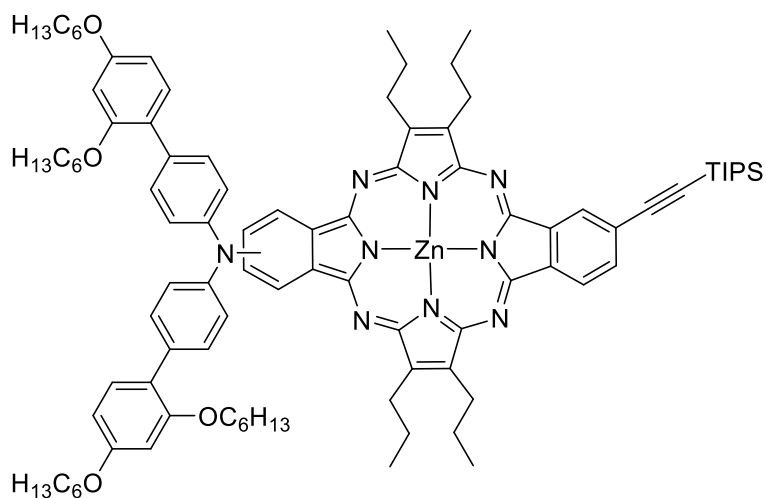
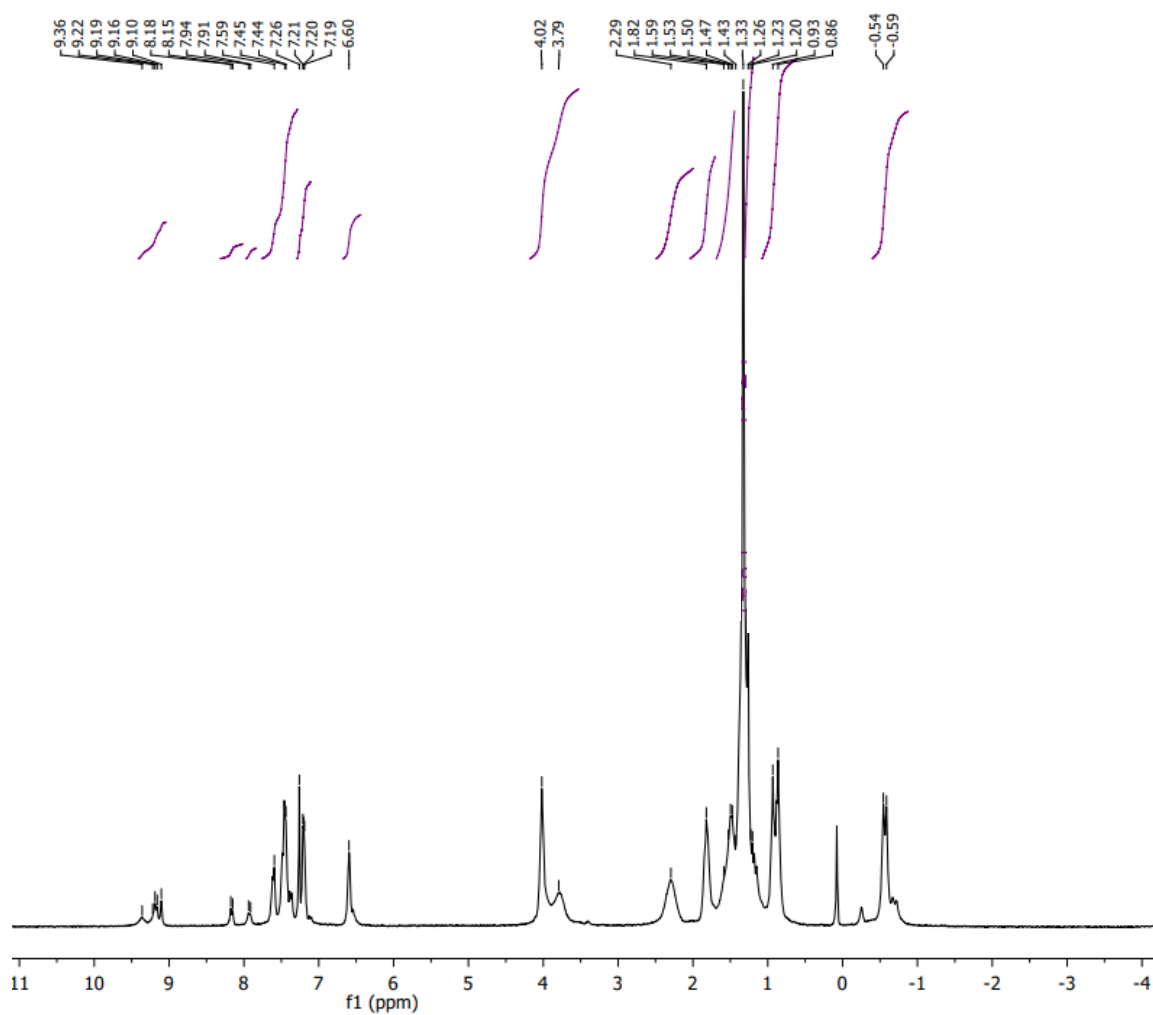
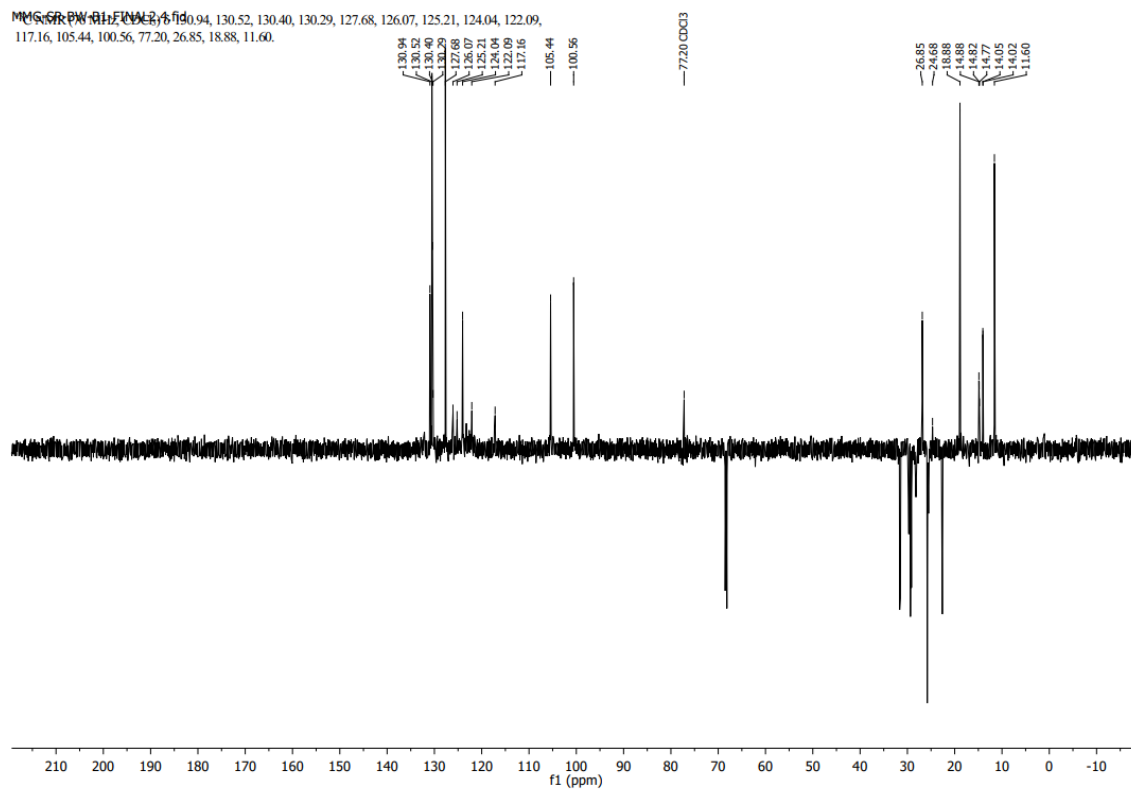


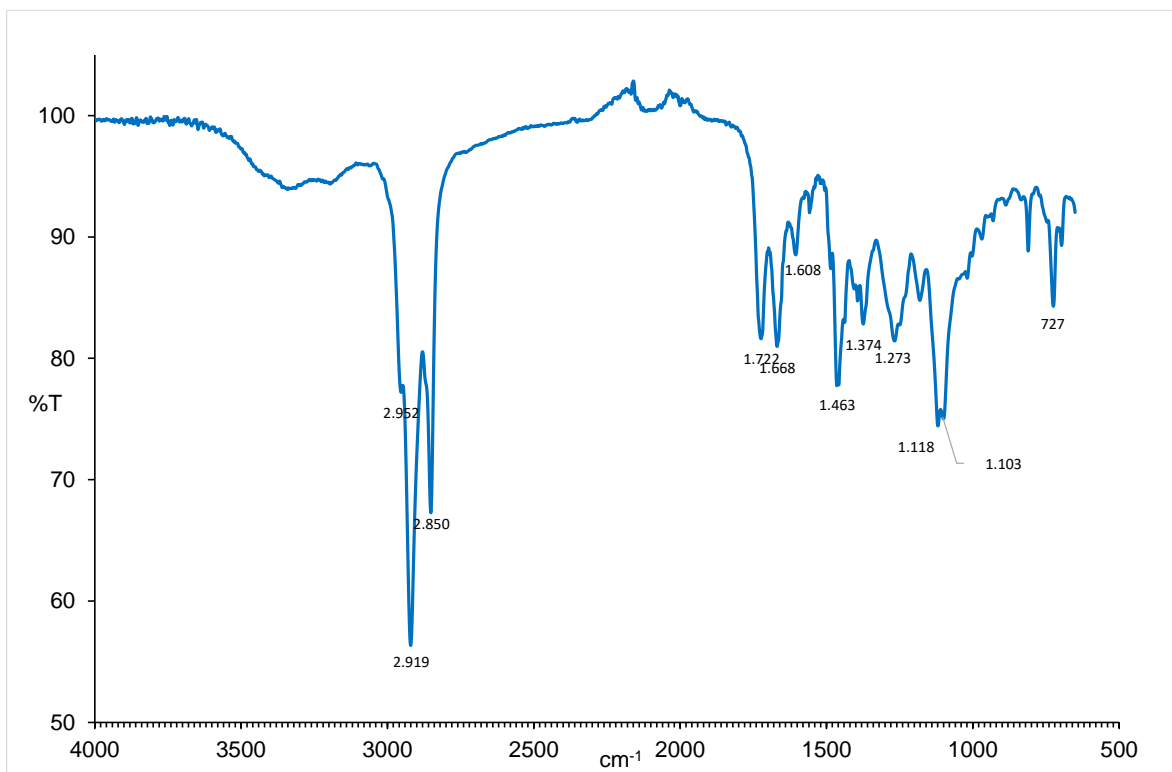
Figure S22.  $^1\text{H-NMR}$  spectrum of **9** in  $\text{CDCl}_3$ .



**Figure S23.** DEPT<sup>13</sup>C-NMR spectrum of **9** in CDCl<sub>3</sub>.



**Figure S24.** FT-IR (KBr) spectrum of **9**.



**Figure S25.** UV-Vis of **9** in CHCl<sub>3</sub>

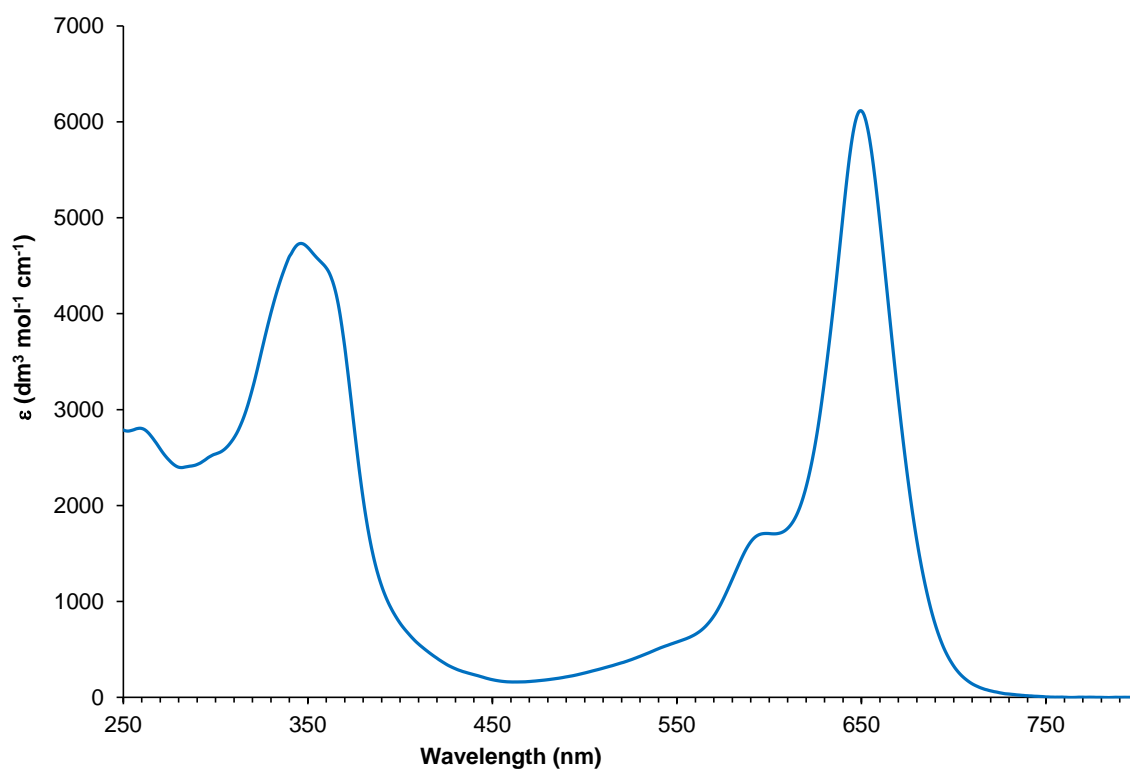
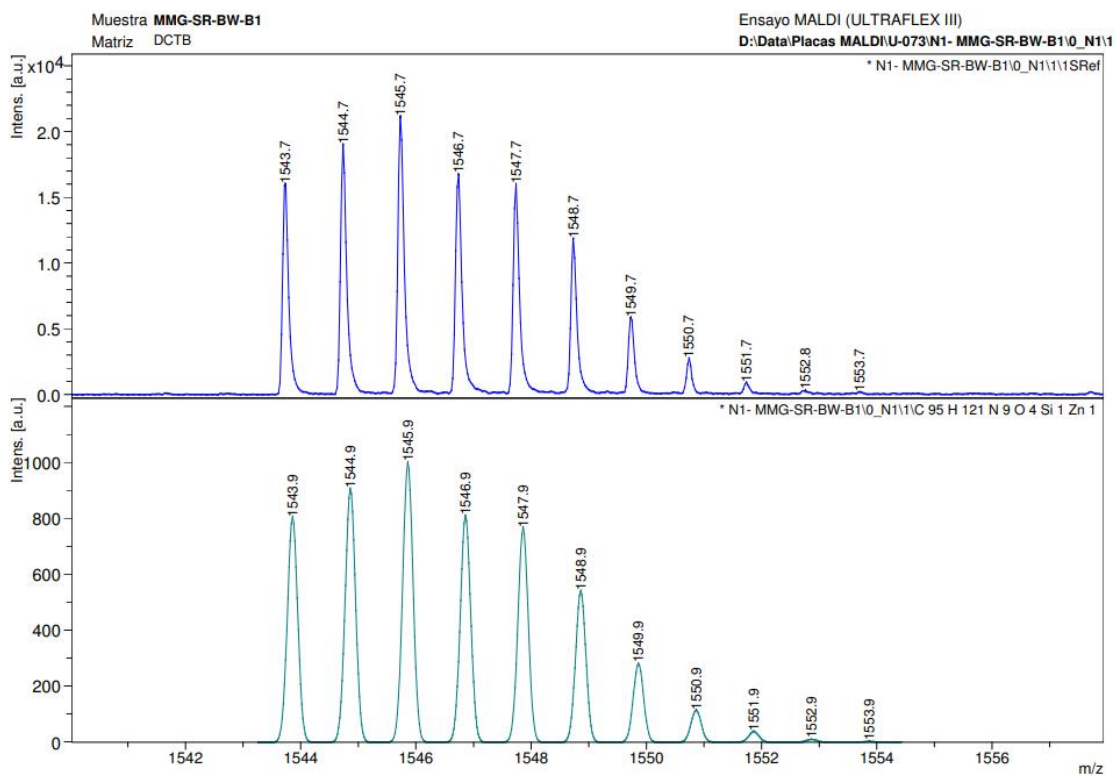
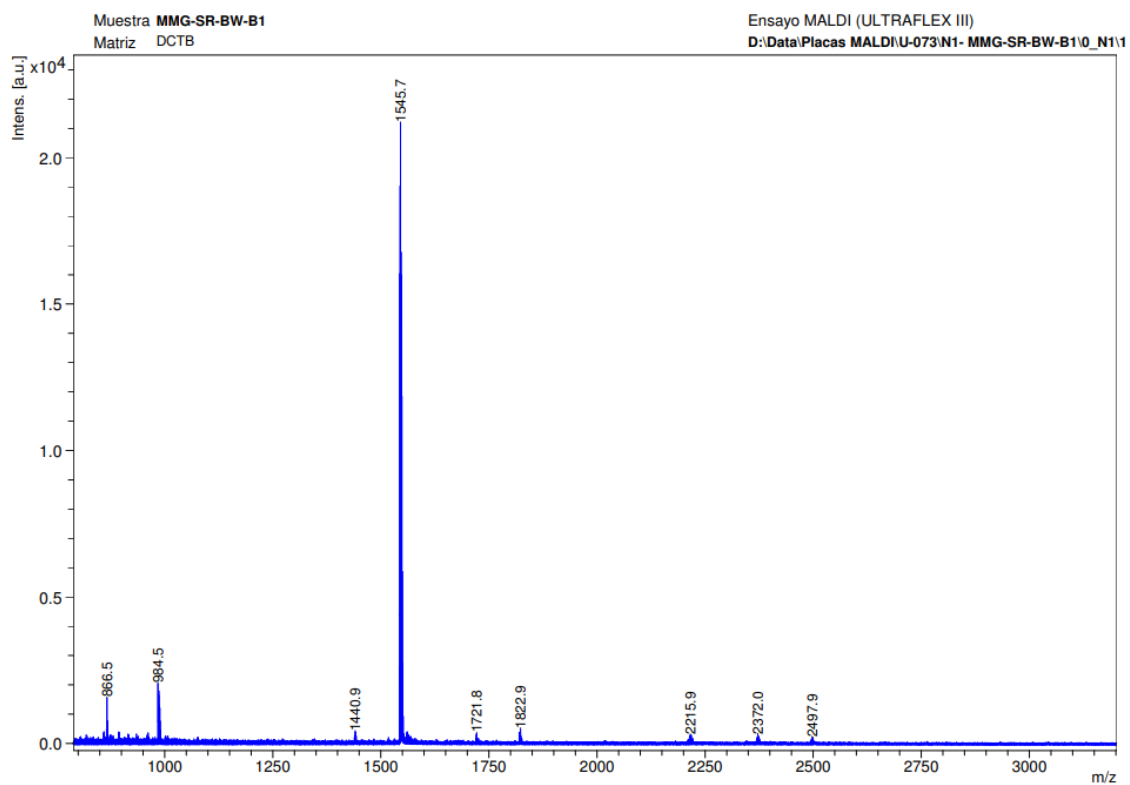
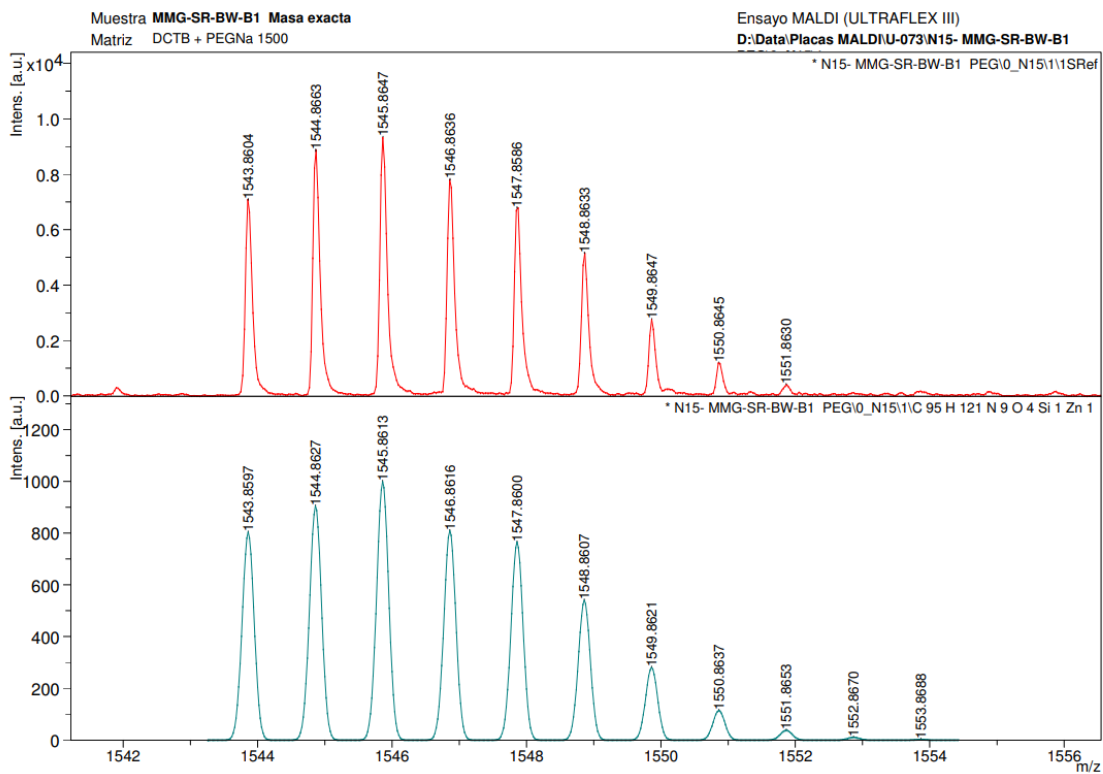


Figure S26. MS (MALDI-TOF, DCTB) of 9.

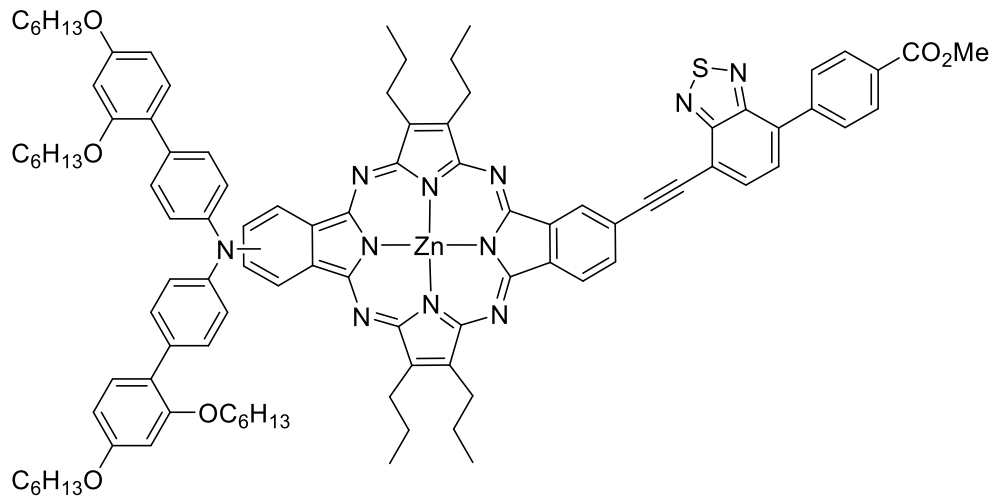


**Figure S27.** HRMS (DCTB + PEGNa 1500) of **9**.

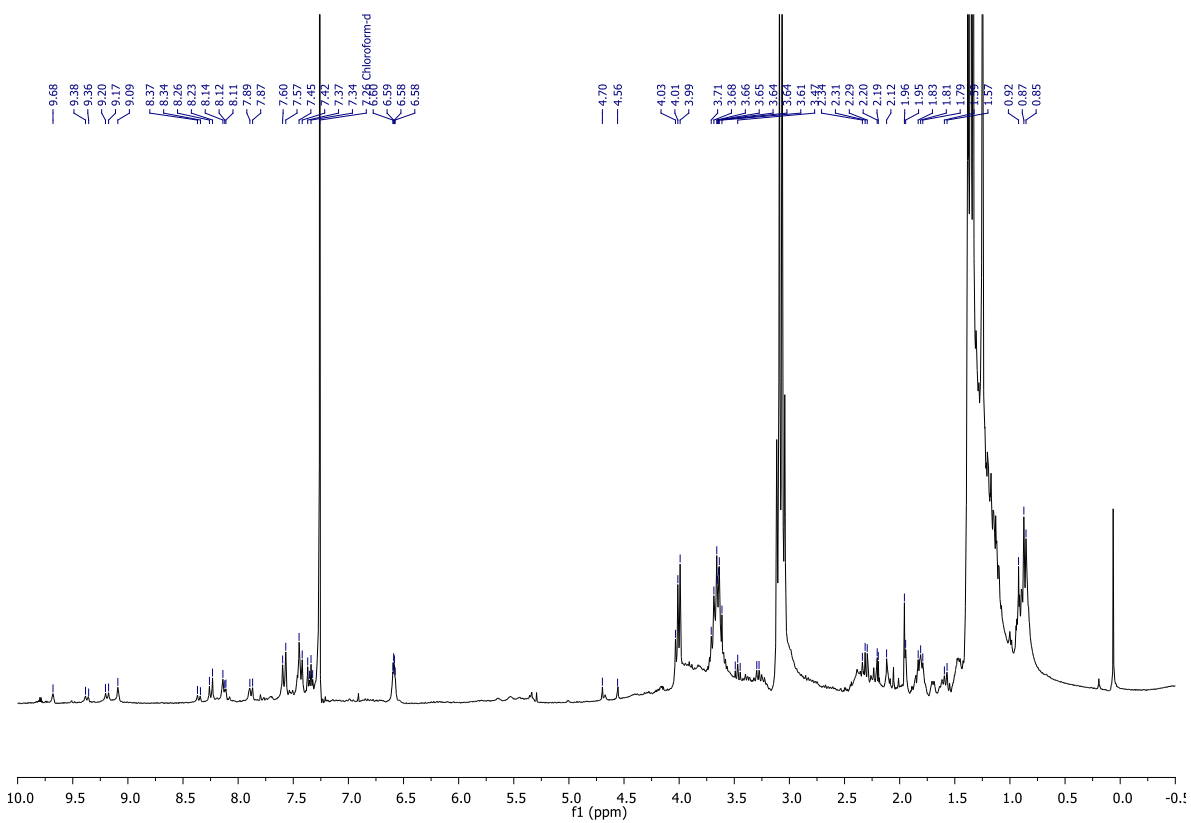




### Tetraazaporphyrin **11**



**Figure S28.**  $^1\text{H-NMR}$  spectrum of **11** in  $\text{CDCl}_3$ .



**Figure S29.** UV-Vis of **11** in  $\text{CHCl}_3$

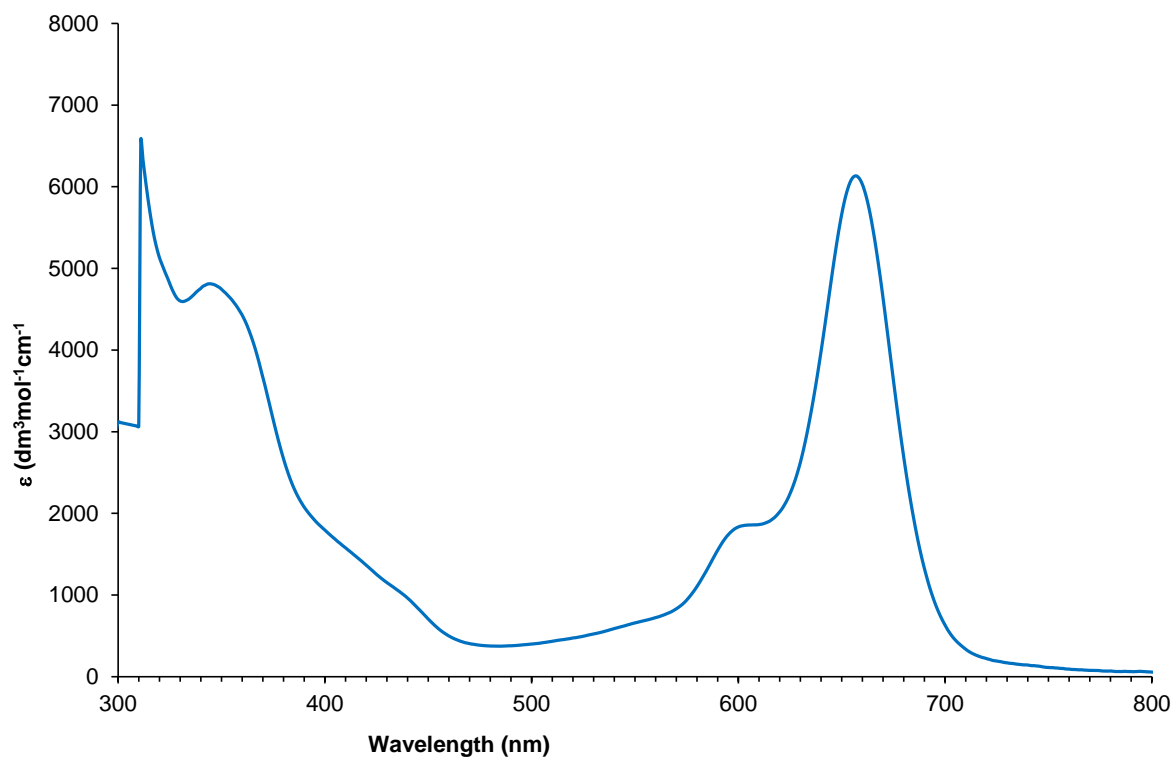
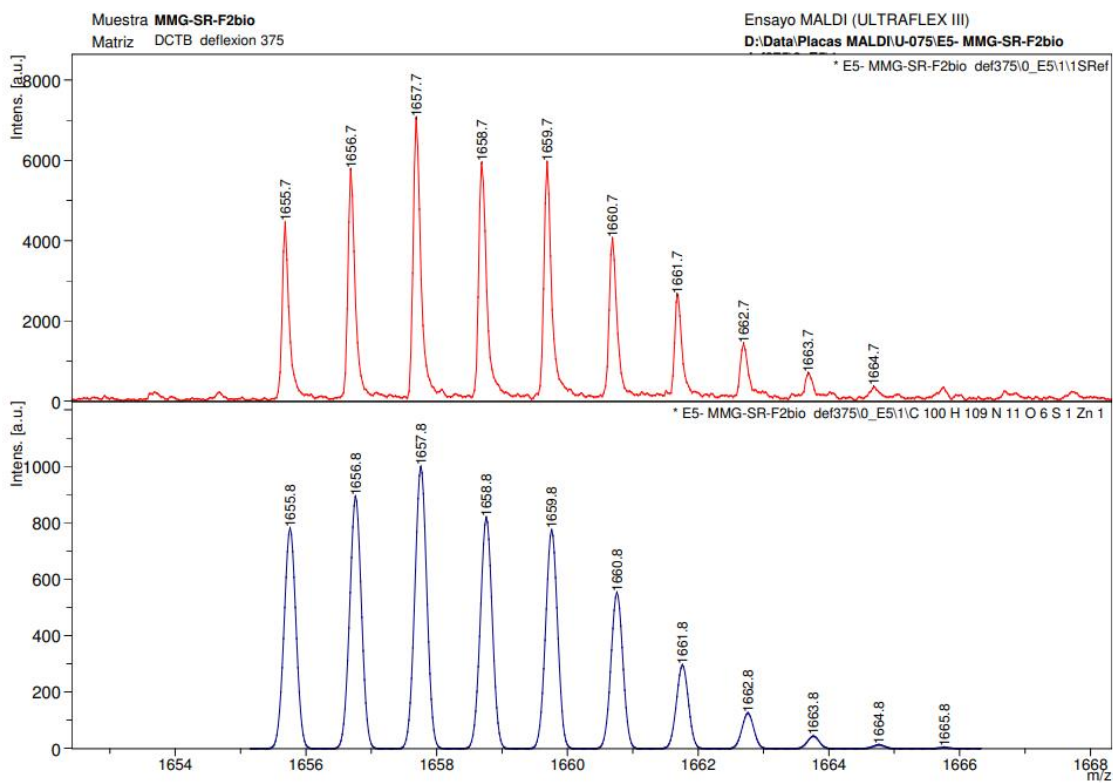
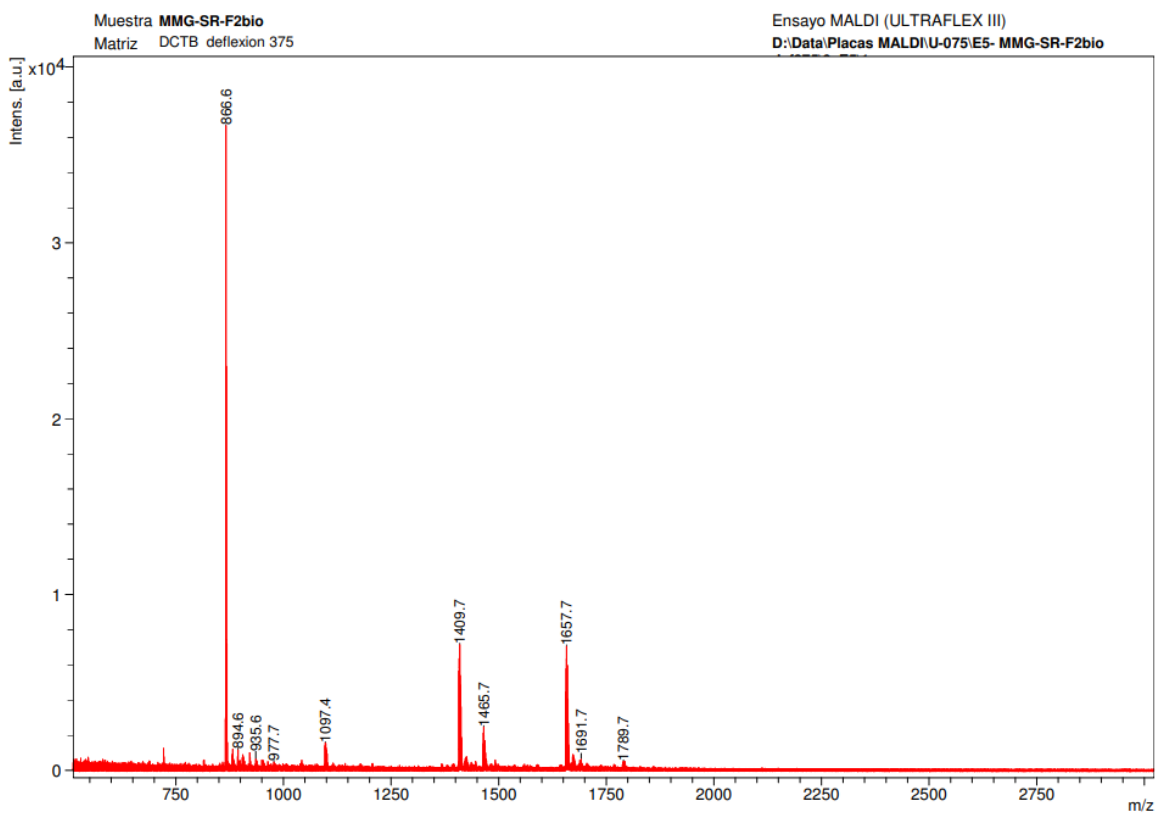
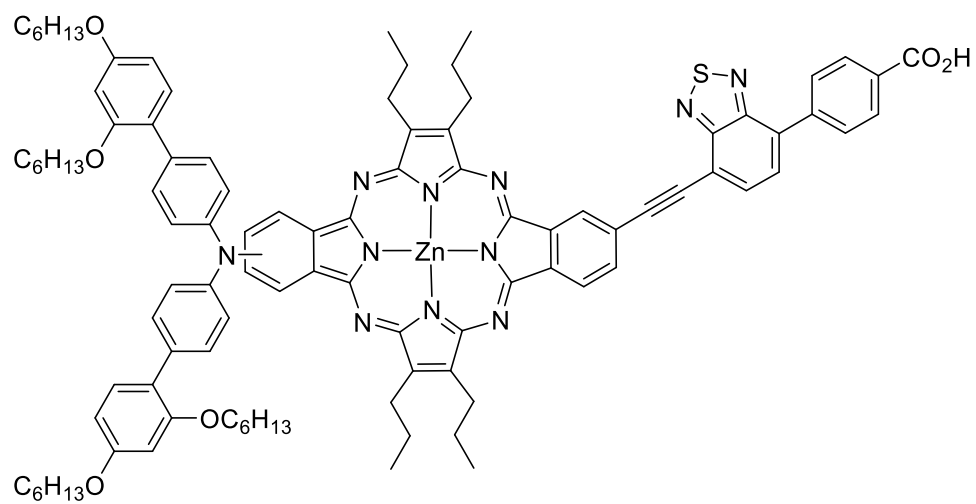


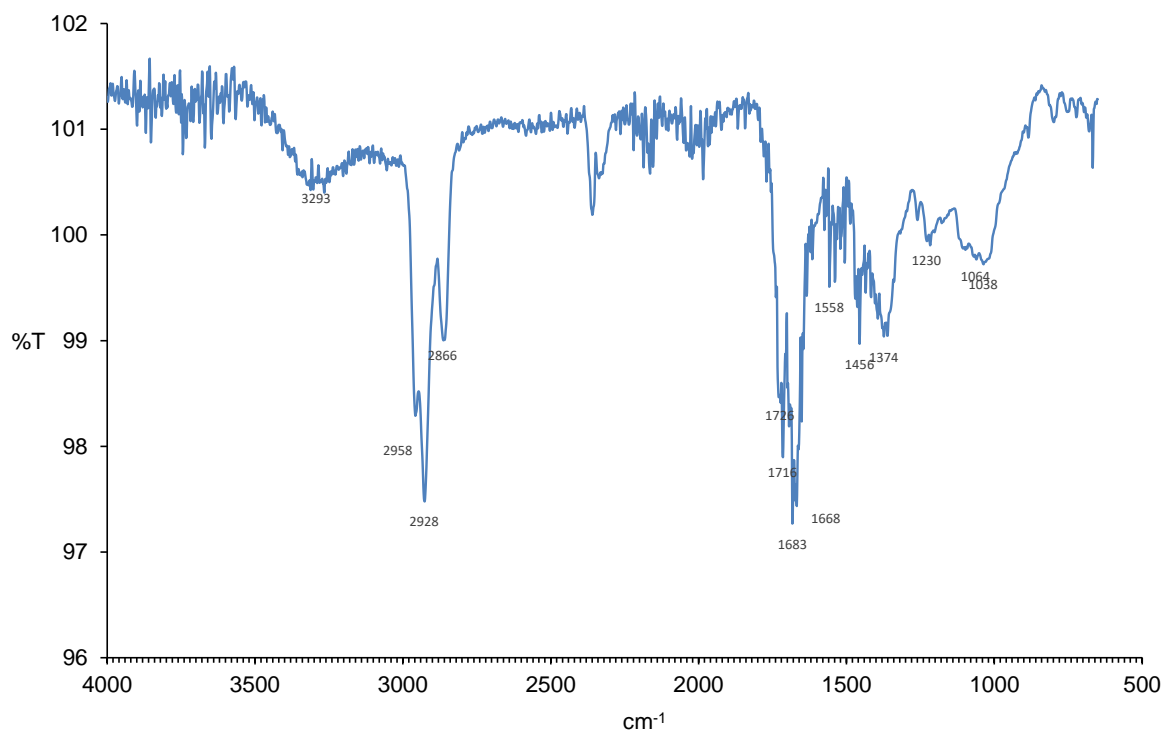
Figure S30. MS (MALDI-TOF, DCTB) of 11.



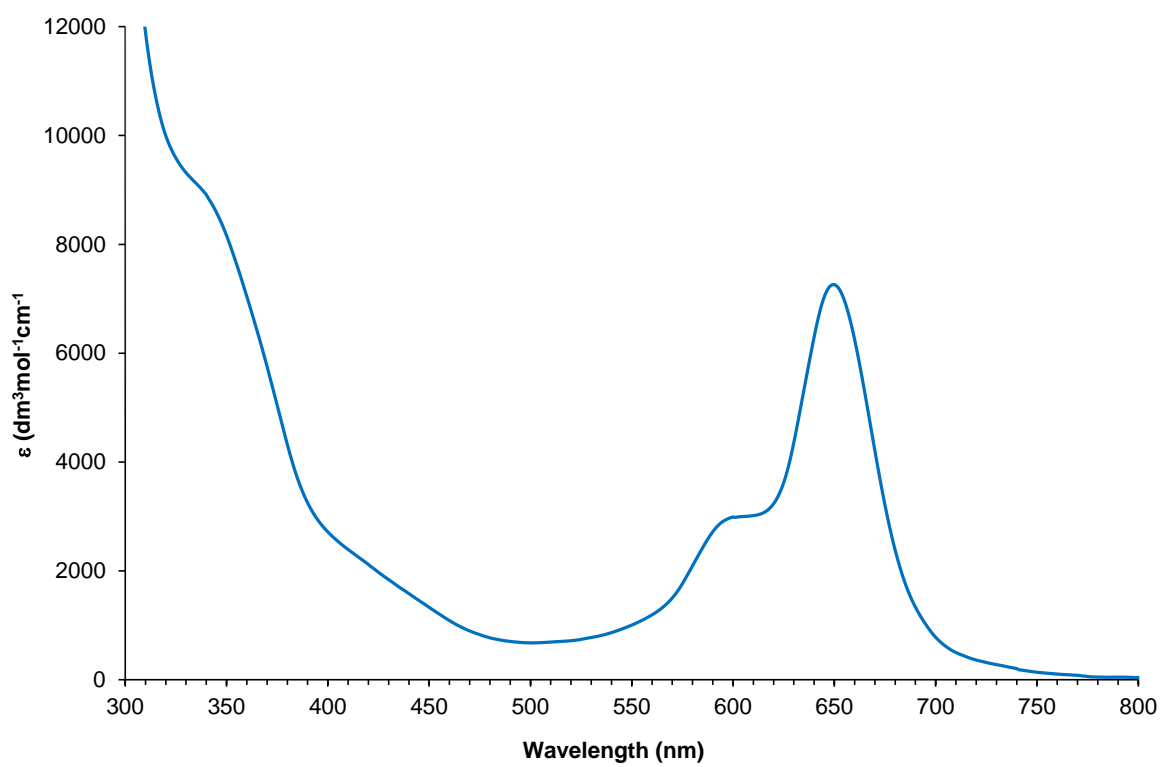
### Tetraazaporphyrin **12**



**Figure S31.** FT-IR spectrum of **12** in KBr.



**Figure S32.** UV-Vis Spectrum of **12** in CHCl<sub>3</sub>





**Figure S34.** HRMS (MALDI-TOF, DCTB + PPG2000) of **12**.

