

Electronic Supplementary Information

Pyrrolopyrrole aza boron dipyrromethene based two-photon fluorescent probes for subcellular imaging

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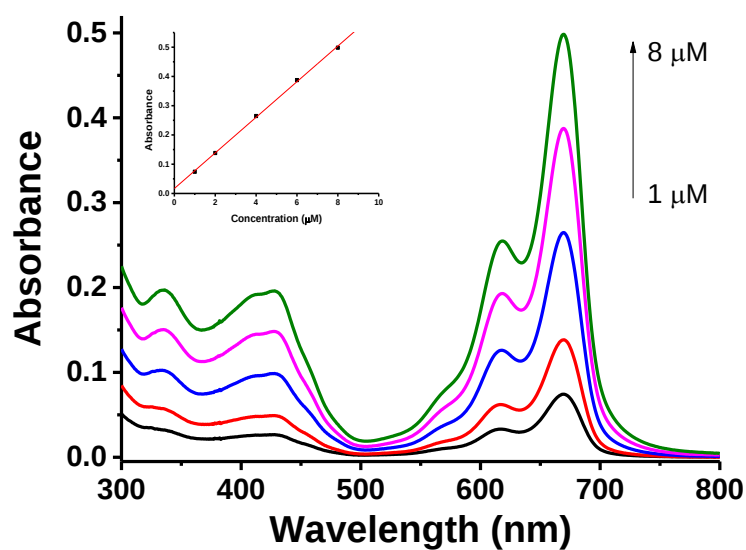


Fig. S1 Electronic absorption spectra of **17** at various concentrations in deionised water (with 0.3% v/v Tween 80 and 1% v/v DMF). The inset plots the Q-band absorbance versus the concentration of **17**.

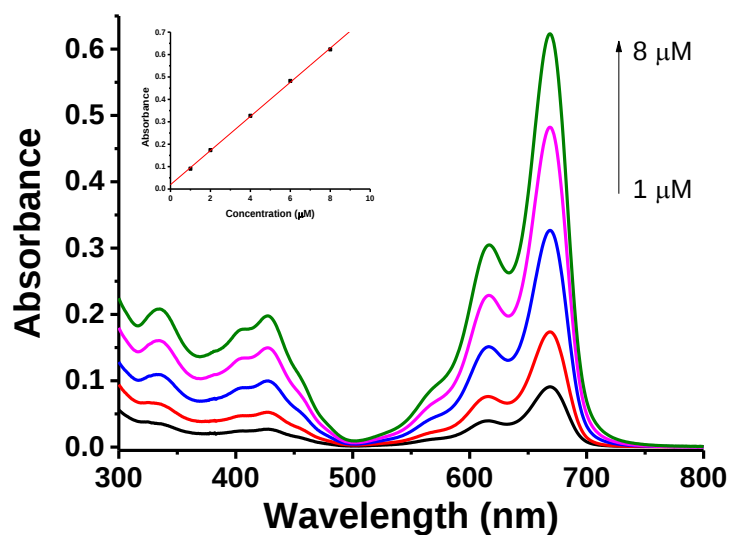


Fig. S2 Electronic absorption spectra of **18** at various concentrations in deionised water (with 0.3% v/v Tween 80 and 1% v/v DMF). The inset plots the Q-band absorbance versus the concentration of **18**.

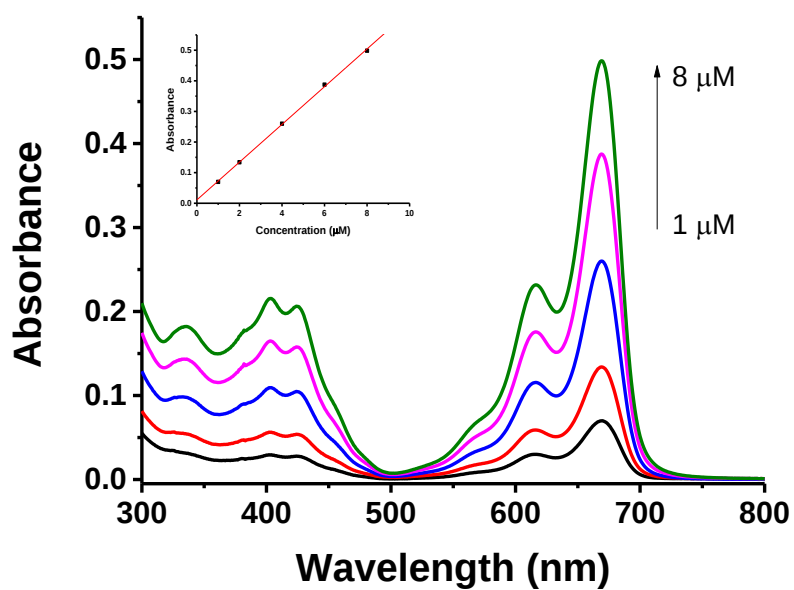


Fig. S3 Electronic absorption spectra of **19** at various concentrations in deionised water (with 0.3% v/v Tween 80 and 1% v/v DMF). The inset plots the Q-band absorbance versus the concentration of **19**.

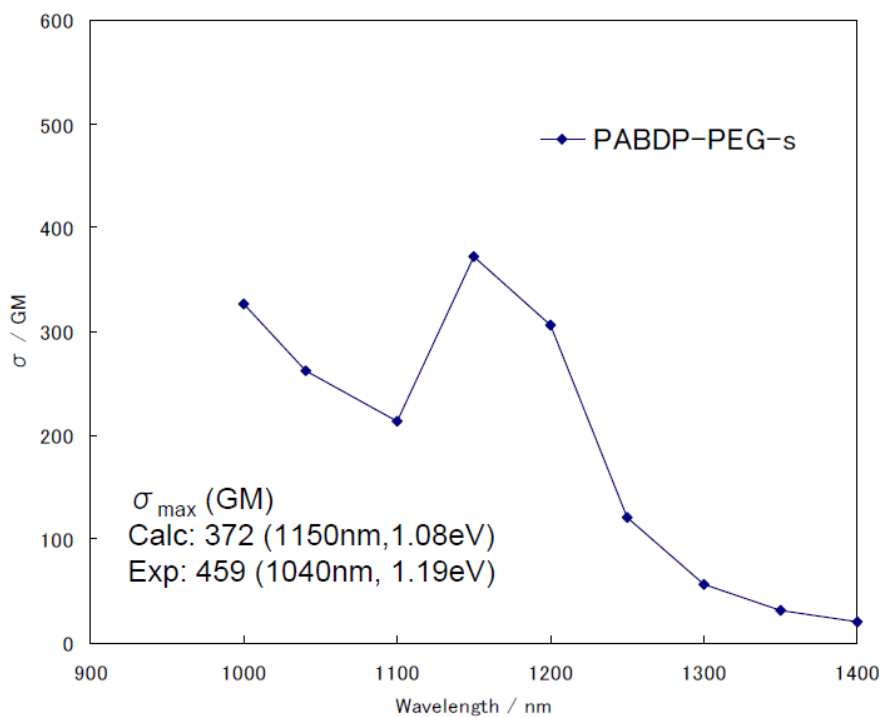


Fig. S4 Simulation of the TPA cross-sections of the model compound for **19** with reduced chain length using the ADF programme on the PBE/DZ basis condition.

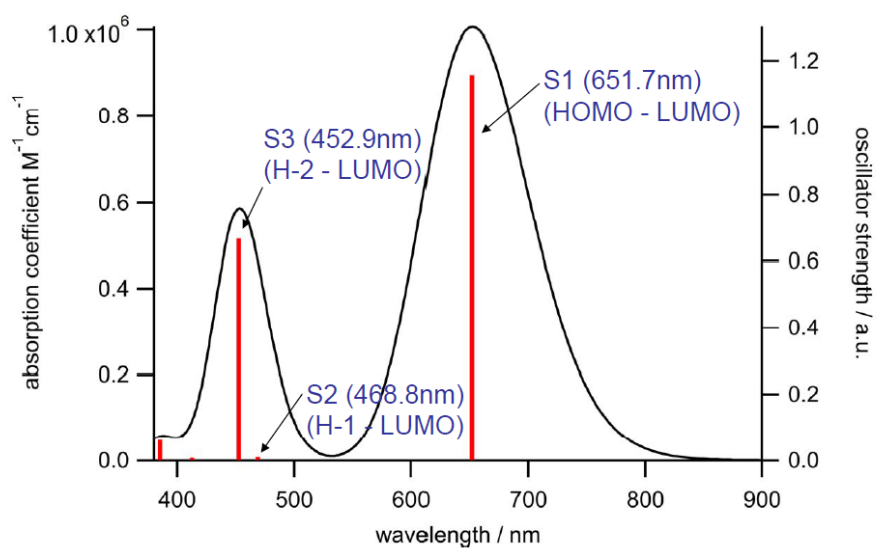


Fig. S5 Simulation of the one-photon absorption spectrum of the model compound for **19** with reduced chain length using a time-dependent DFT method.

In all the following ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra, residual solvent (or solvent) signals are marked with asterisks.

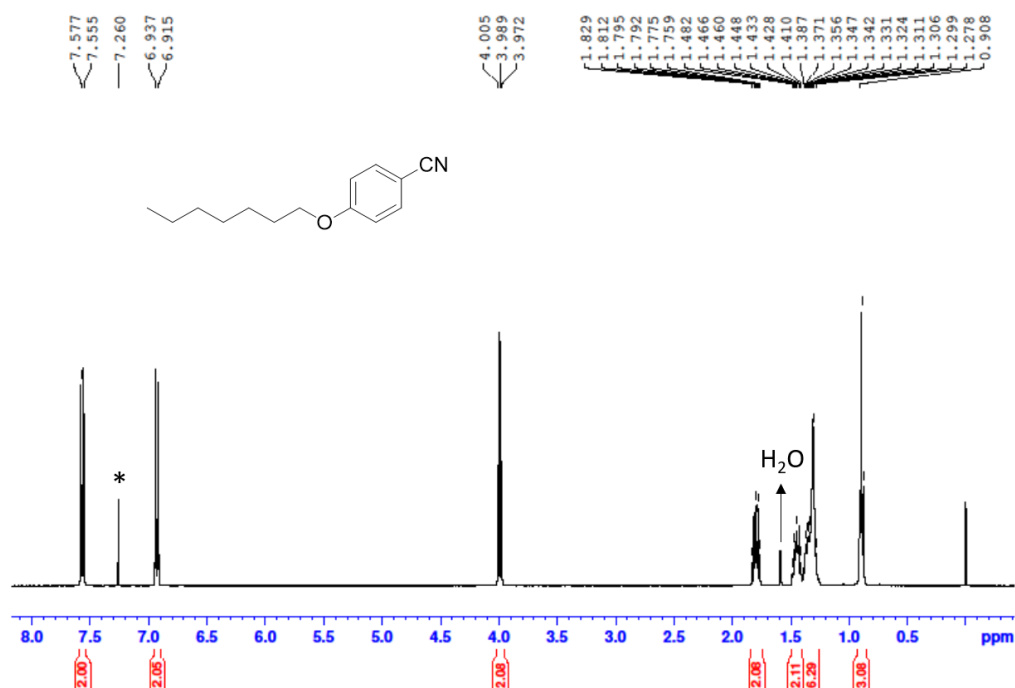


Fig. S6 ^1H NMR spectrum of **1** in CDCl_3 .

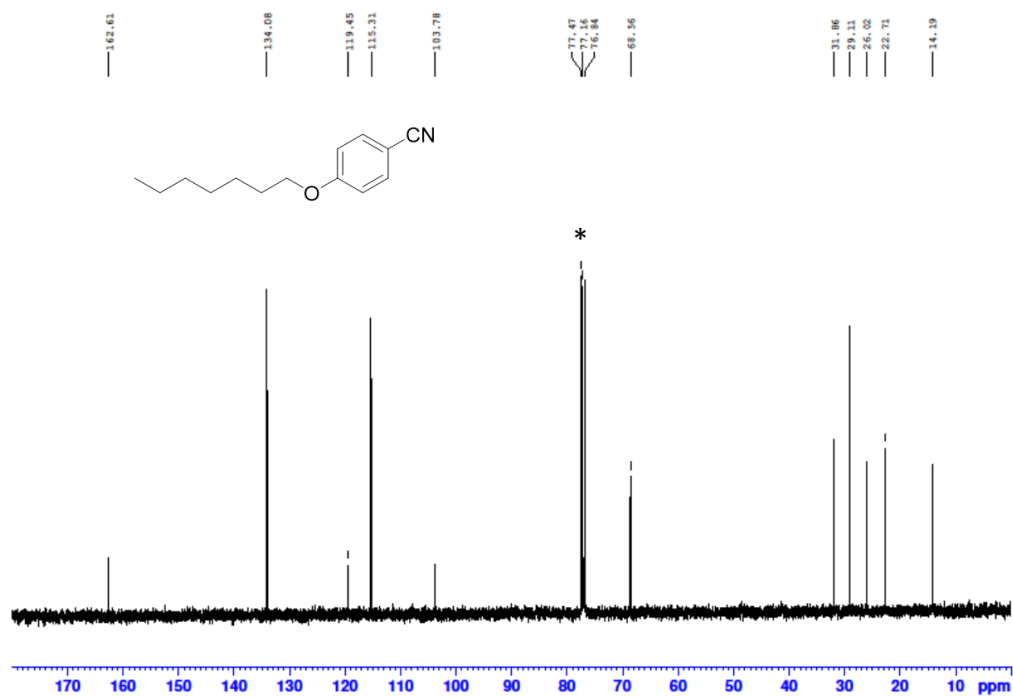


Fig. S7 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **1** in CDCl_3 .

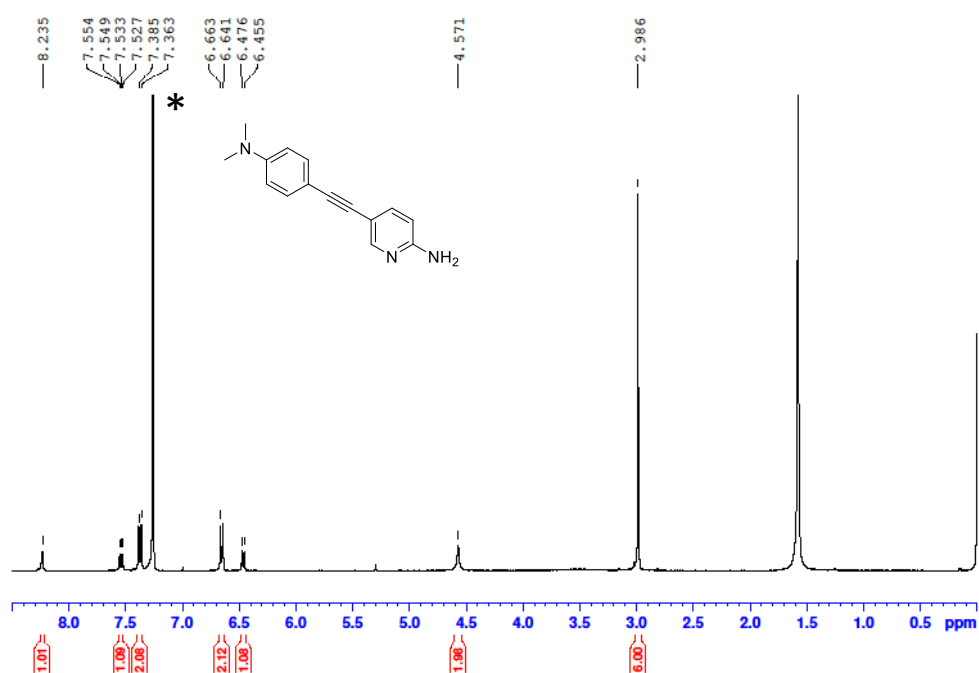


Fig. S8 ¹H NMR spectrum of 7 in CDCl₃.

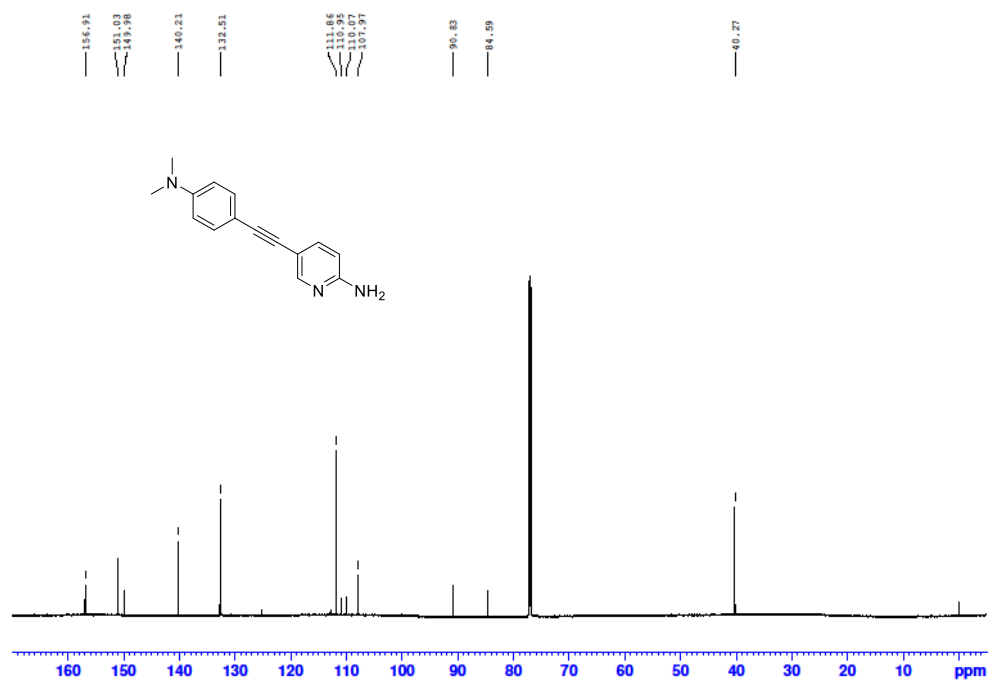


Fig. S9 ¹³C{¹H} NMR spectrum of 7 in CDCl₃.

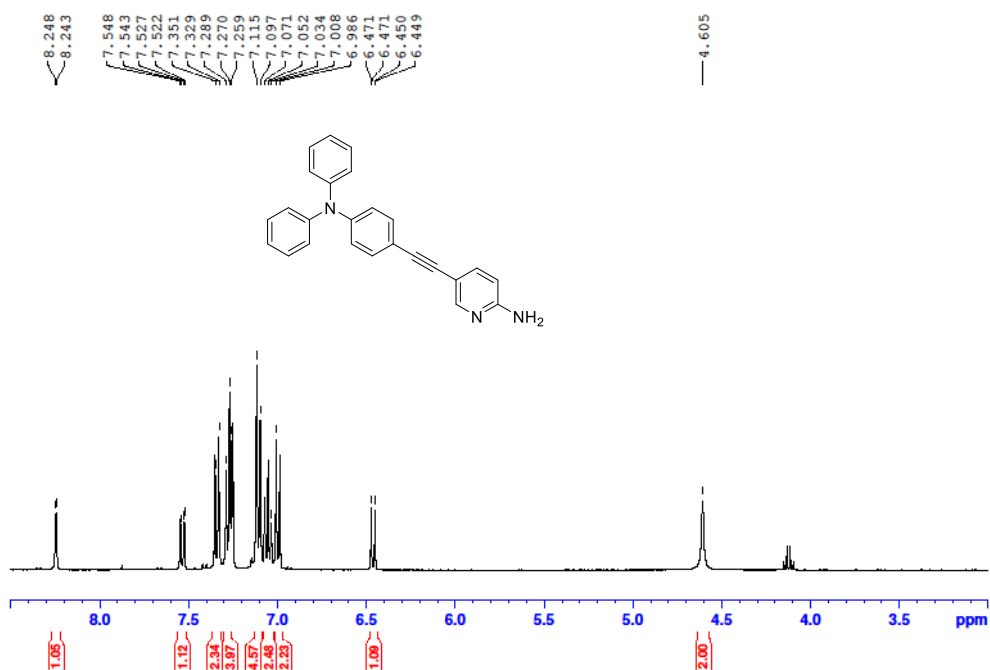


Fig. S10 ¹H NMR spectrum of **8** in CDCl₃.

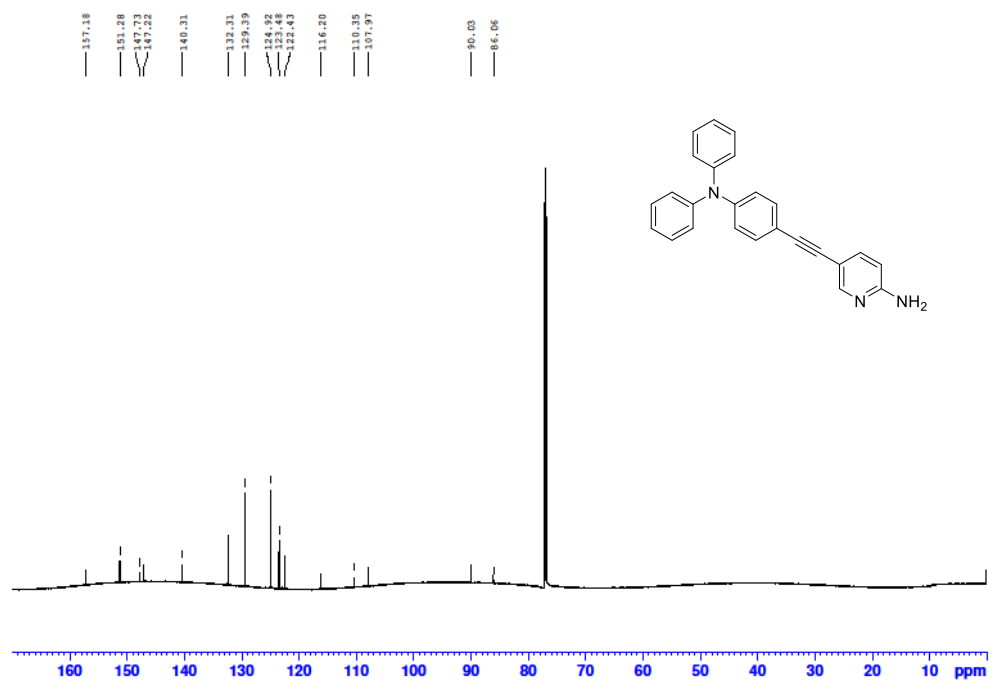


Fig. S11 ¹³C{¹H} NMR spectrum of **8** in CDCl₃.

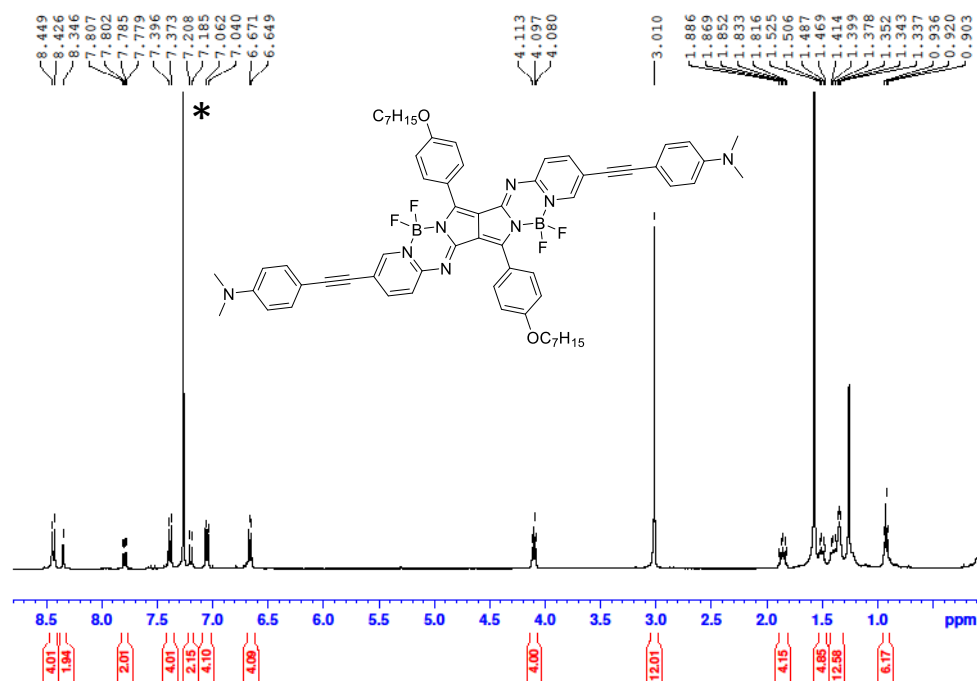


Fig. S12 ¹H NMR spectrum of **9** in CDCl₃.

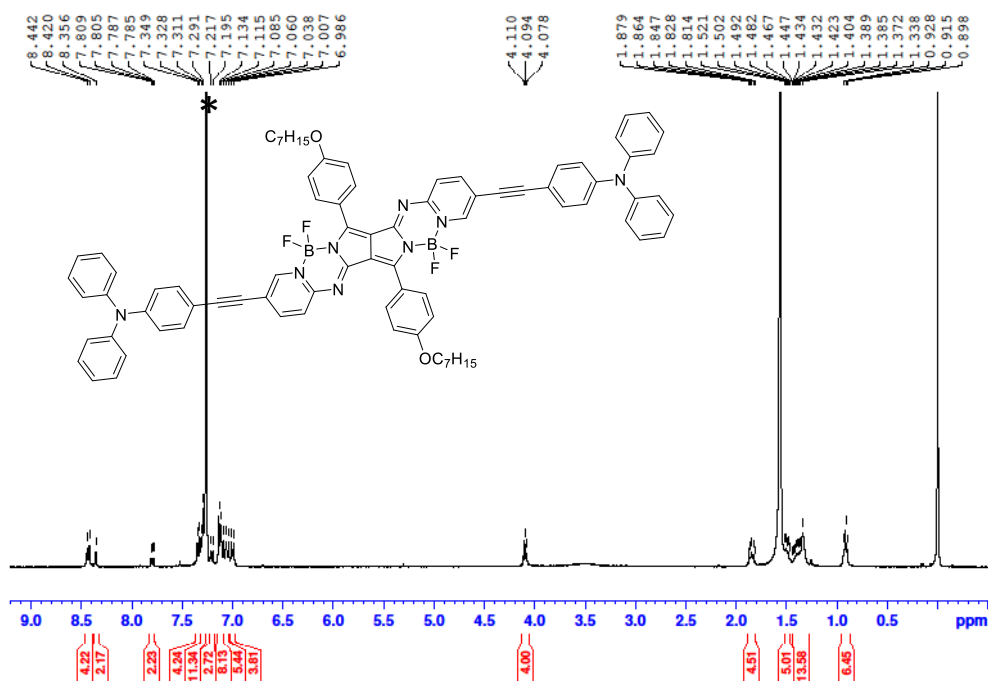


Fig. S13 ¹H NMR spectrum of **10** in CDCl₃.

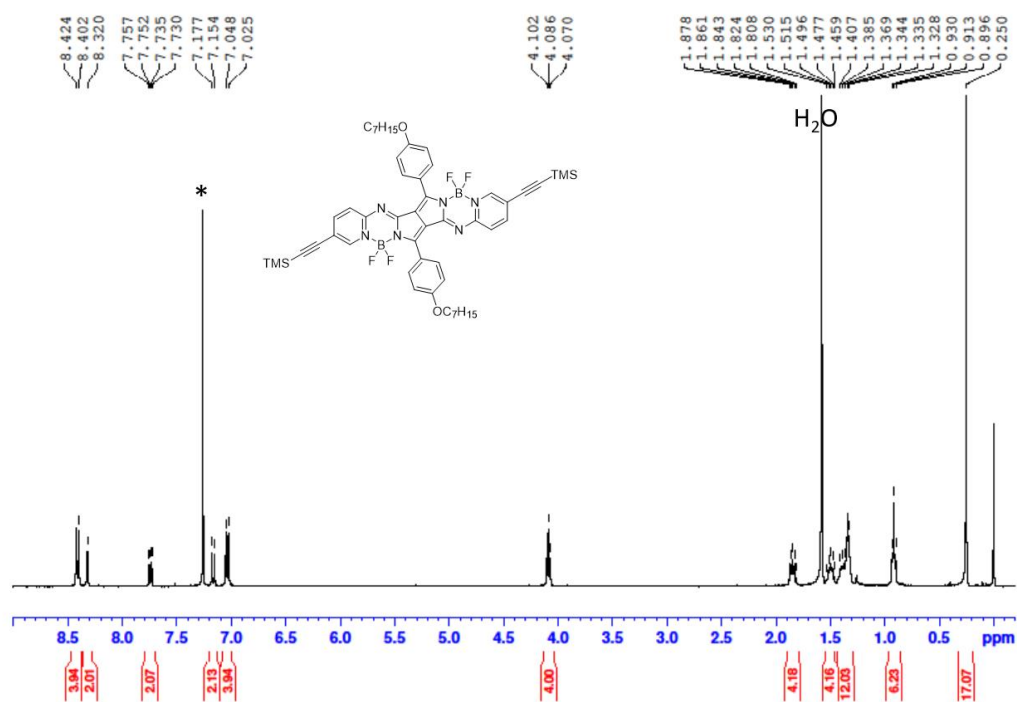


Fig. S14 1H NMR spectrum of 12 in $CDCl_3$.

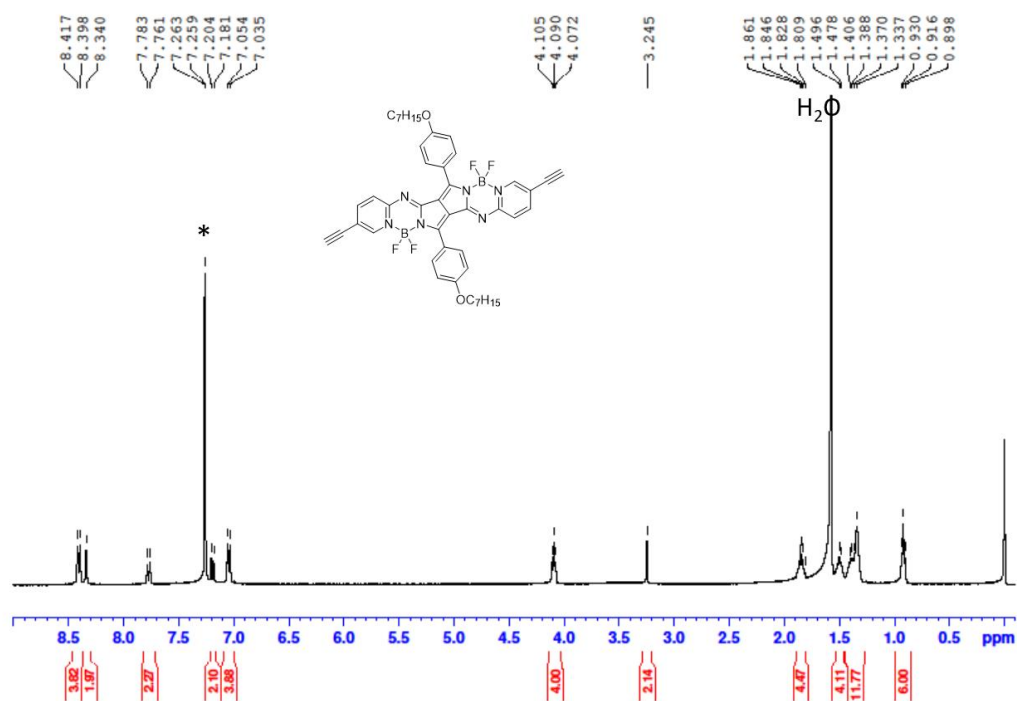


Fig. S15 1H NMR spectrum of 13 in $CDCl_3$.

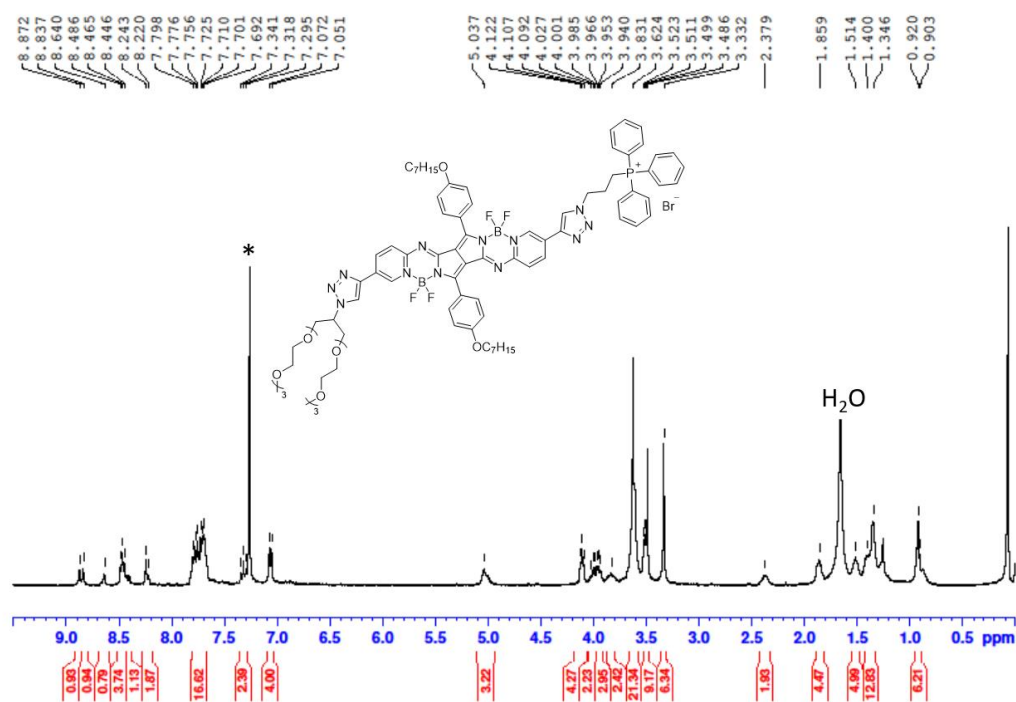


Fig. S16 ¹H NMR spectrum of **17** in CDCl₃.

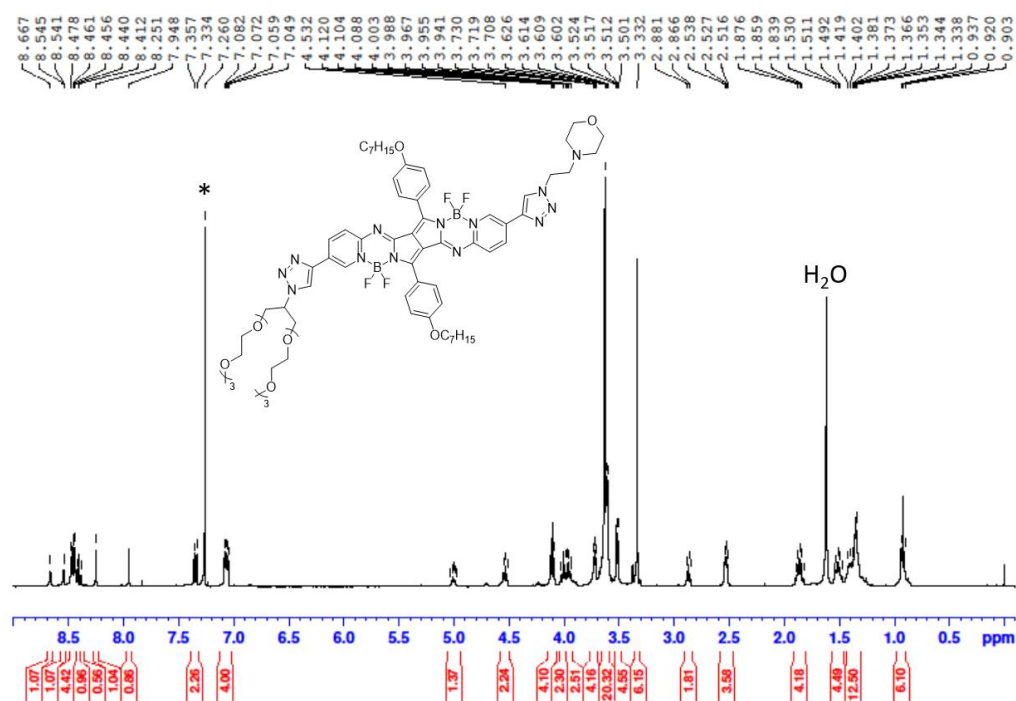


Fig. S17 ¹H NMR spectrum of **18** in CDCl₃.

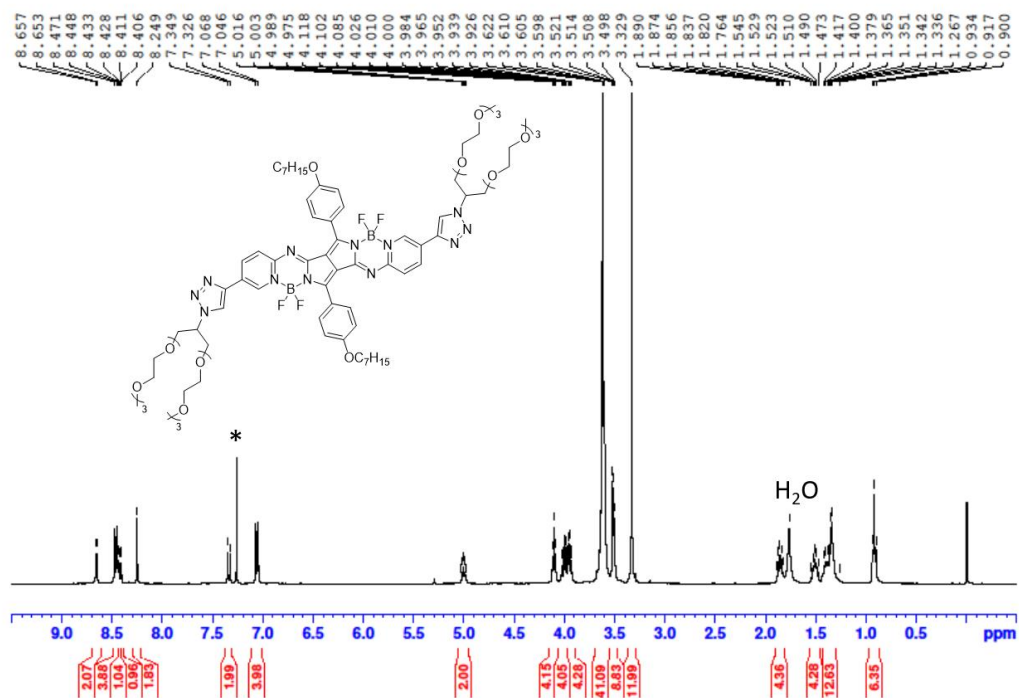


Fig. S18 ¹H NMR spectrum of **19** in CDCl₃.

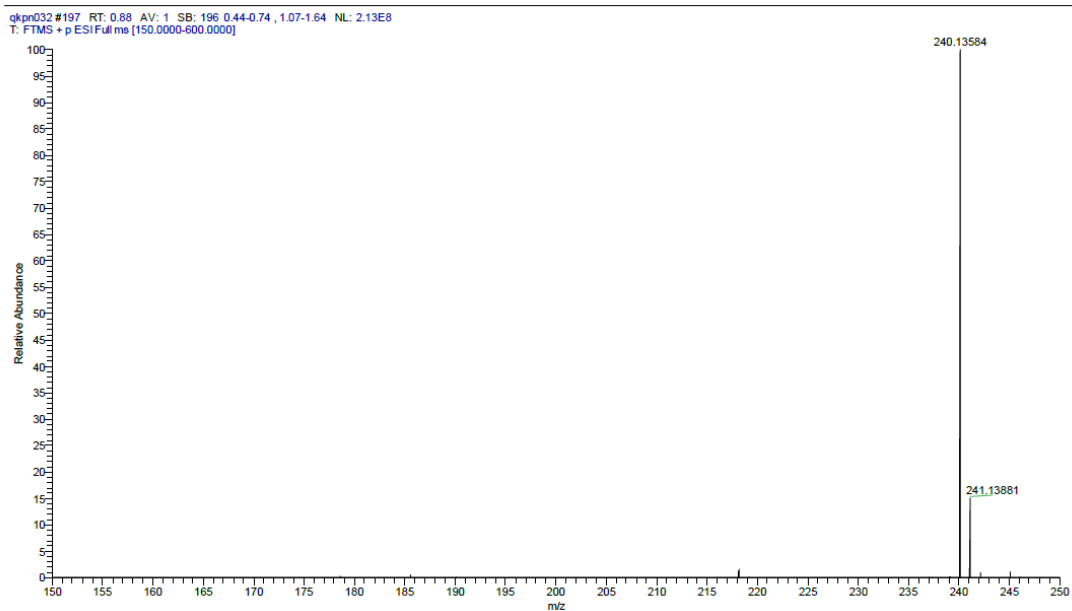


Fig. S19 ESI mass spectrum of **1**.

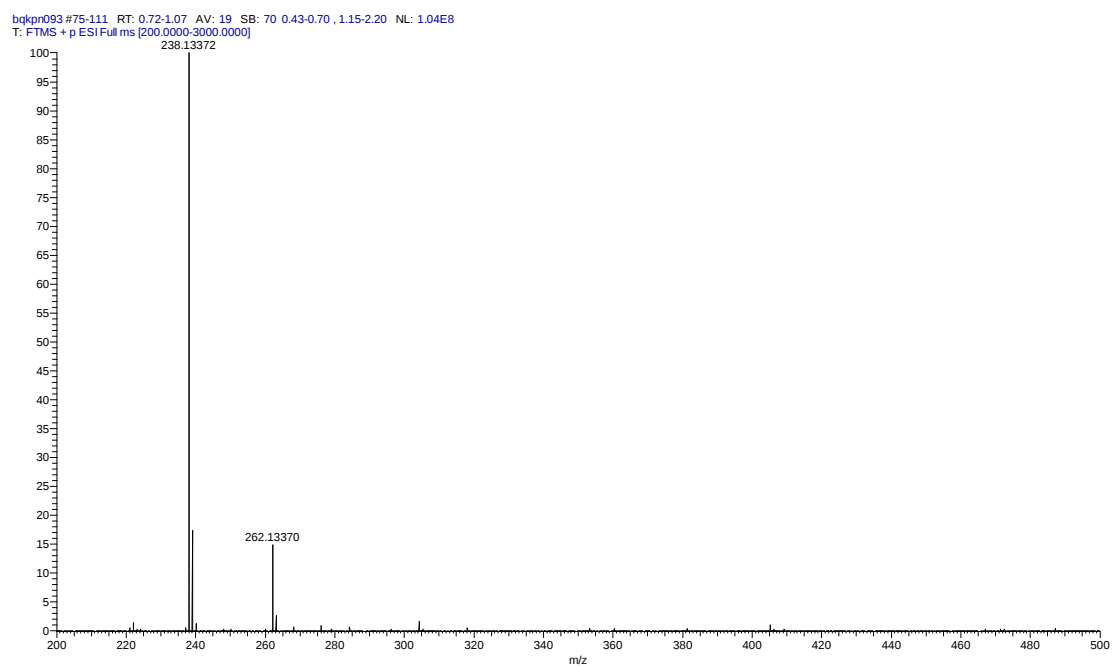


Fig. S20 ESI mass spectrum of **7**.

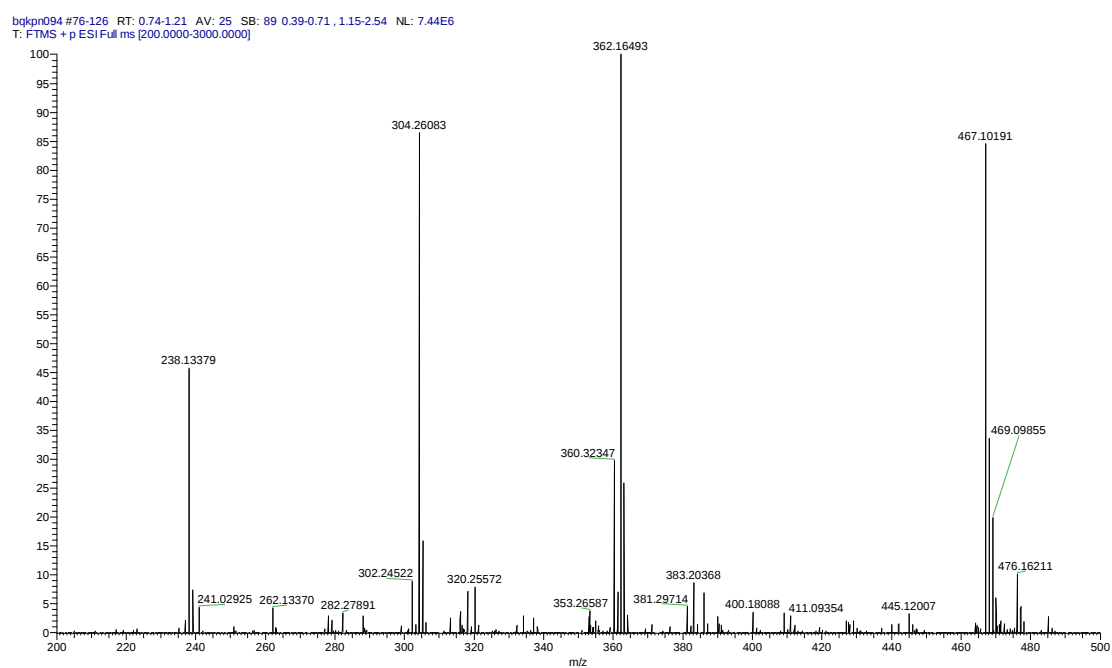


Fig. S21 ESI mass spectrum of **8**.

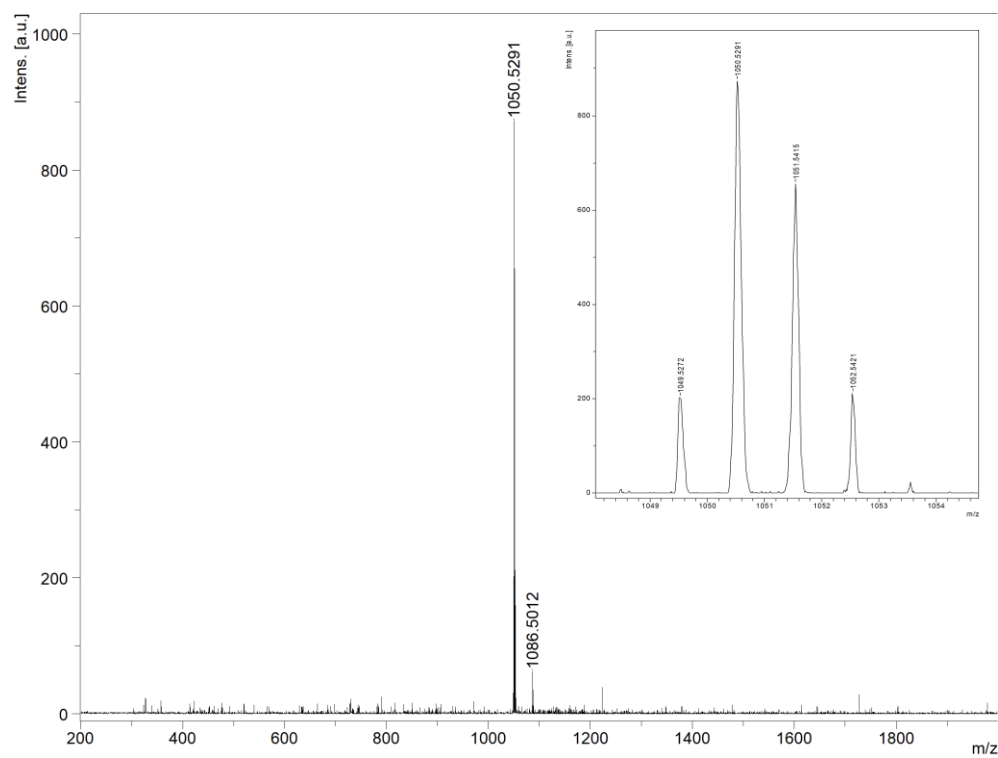


Fig. S22 MALDI-TOF mass spectrum of **9**. The inset shows the enlarged isotopic envelop of the molecular ion peak.

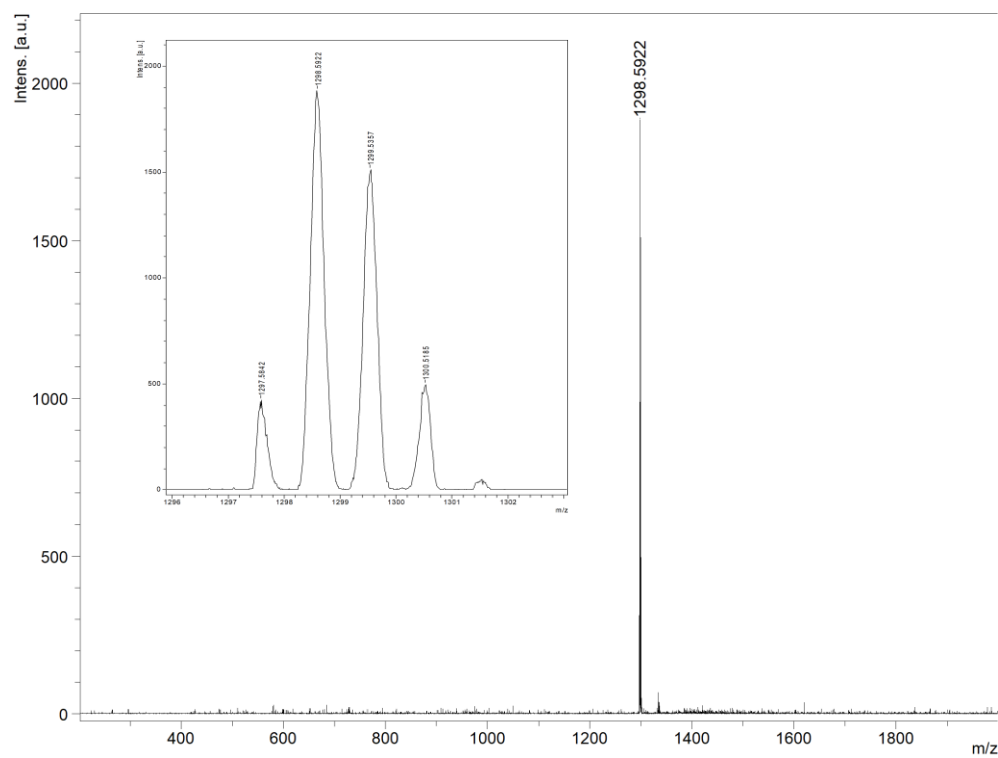


Fig. S23 MALDI-TOF mass spectrum of **10**. The inset shows the enlarged isotopic envelop of the molecular ion peak.

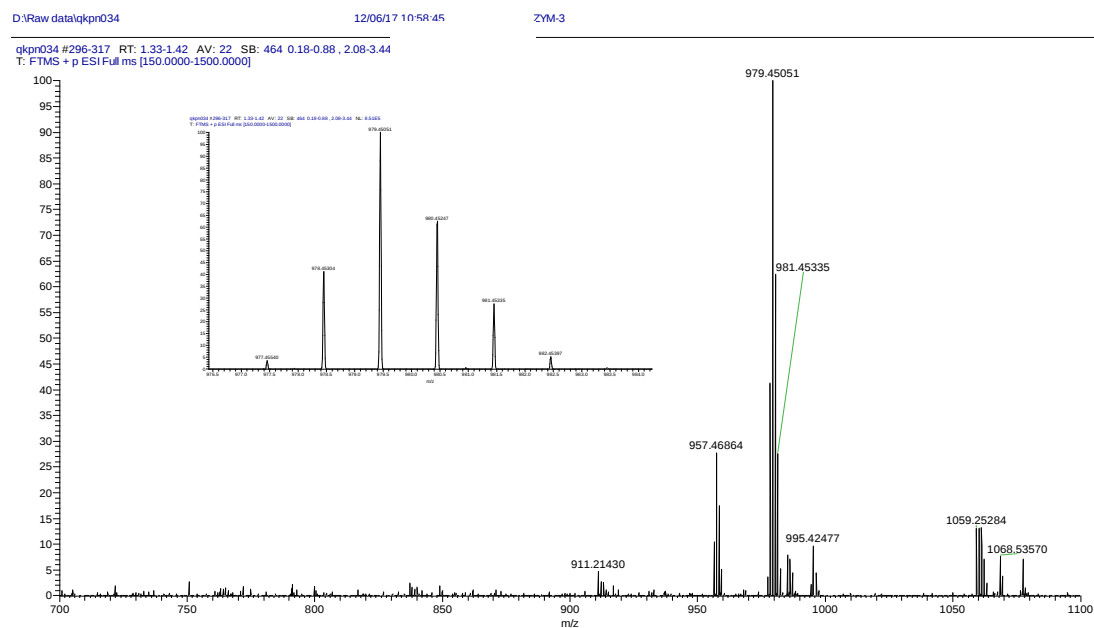


Fig. S24 ESI mass spectrum of **12**. The inset shows the enlarged isotopic envelope of the molecular ion peak.

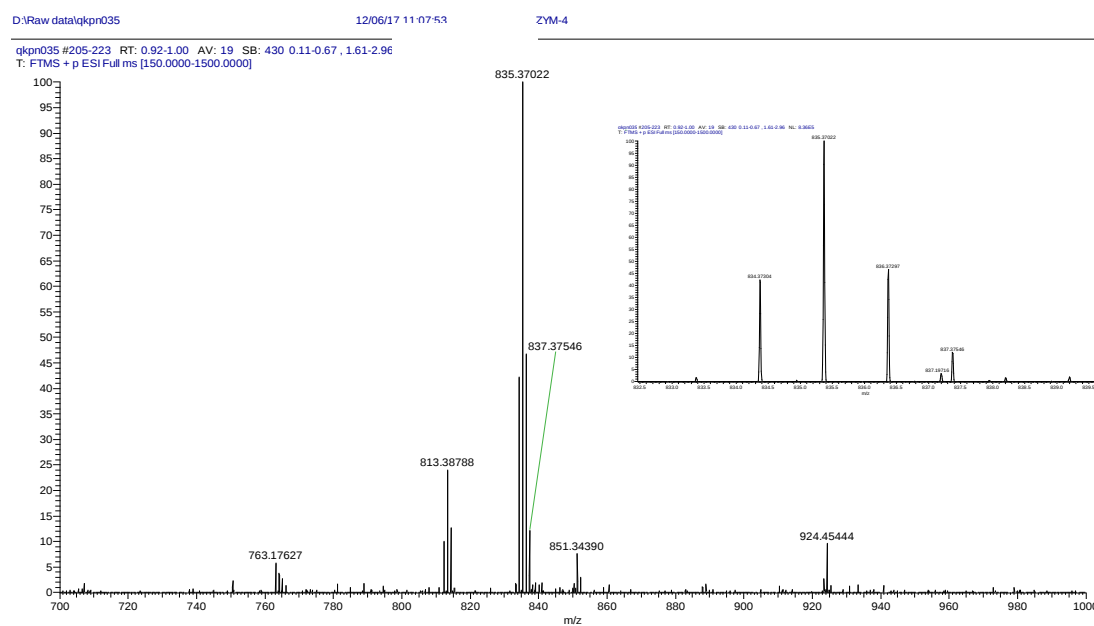


Fig. S25 ESI mass spectrum of **13**. The inset shows the enlarged isotopic envelope of the molecular ion peak.

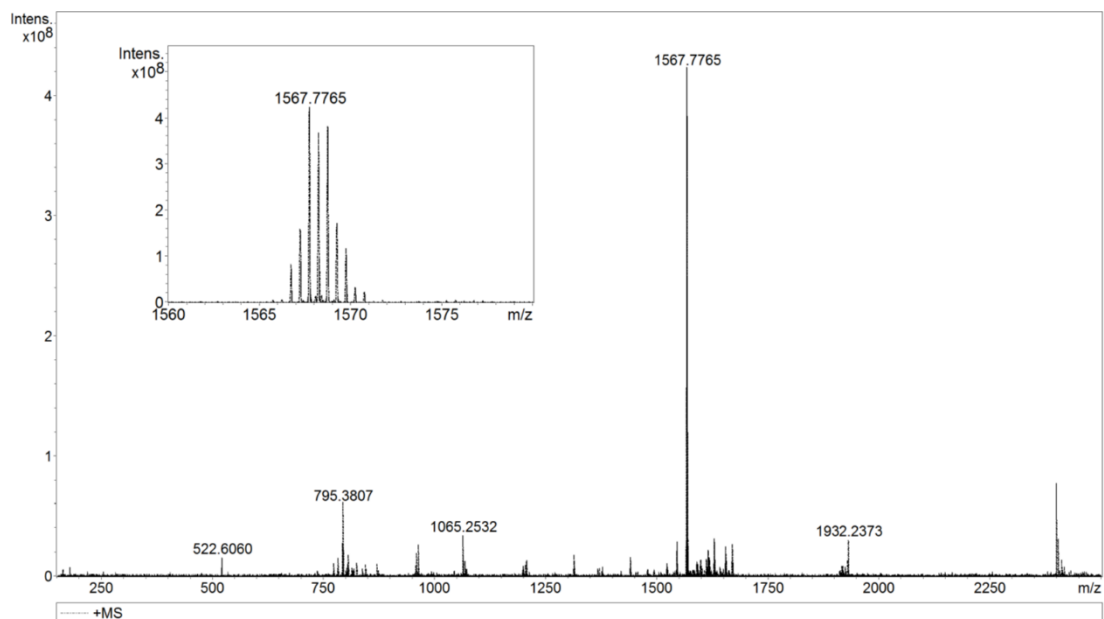


Fig. S26 ESI mass spectrum of **17**. The inset shows the enlarged isotopic envelop of the molecular ion peak.

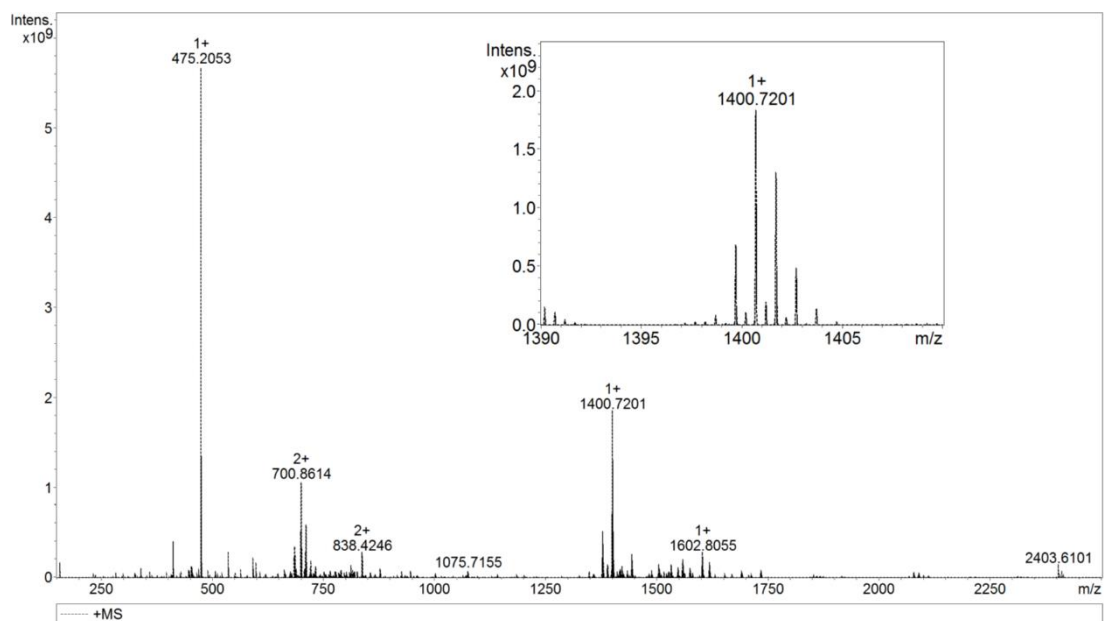


Fig. S27 ESI mass spectrum of **18**. The inset shows the enlarged isotopic envelop of the molecular ion peak.

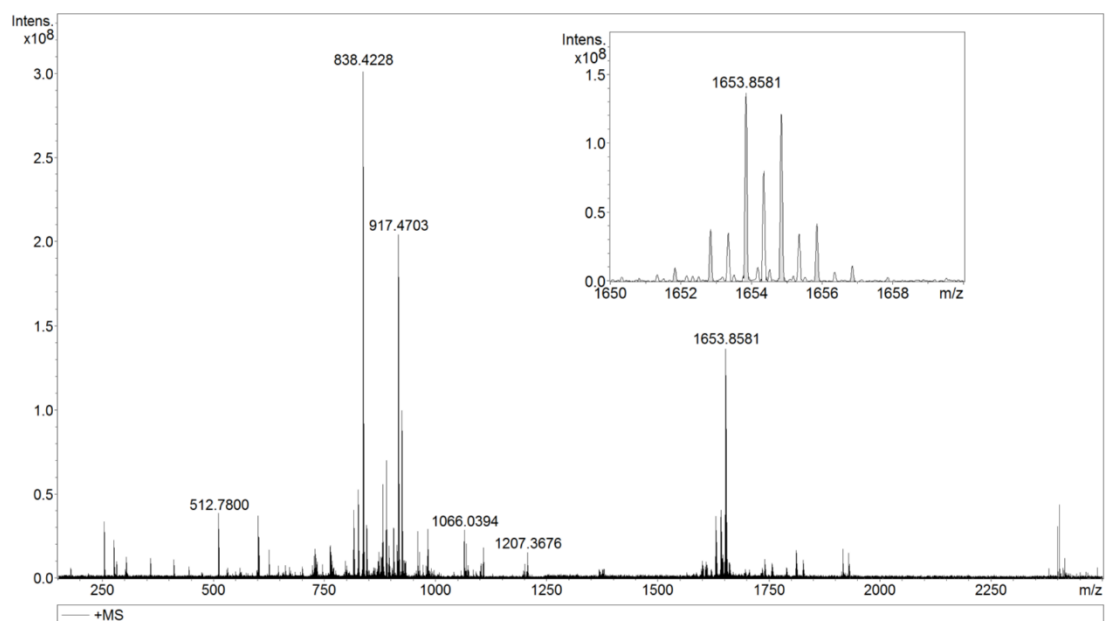


Fig. S28 ESI mass spectrum of **19**. The inset shows the enlarged isotopic envelop of the molecular ion peak.