Electronic Supplementary Information

Porphyrin Sensitizers with Modified Indoline Donors for Dye-Sensitized Solar Cells

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1. Emission spectra

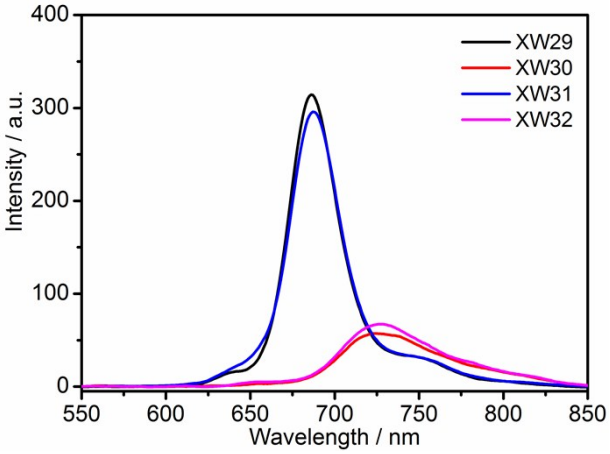


Fig. S1 Emission spectra of **XW29-XW32** in THF. The spectra were used to estimate the $E_{0\text{-}0}$ values.

2. Normalized absorption spectra of the dyes in THF and on TiO_2 films

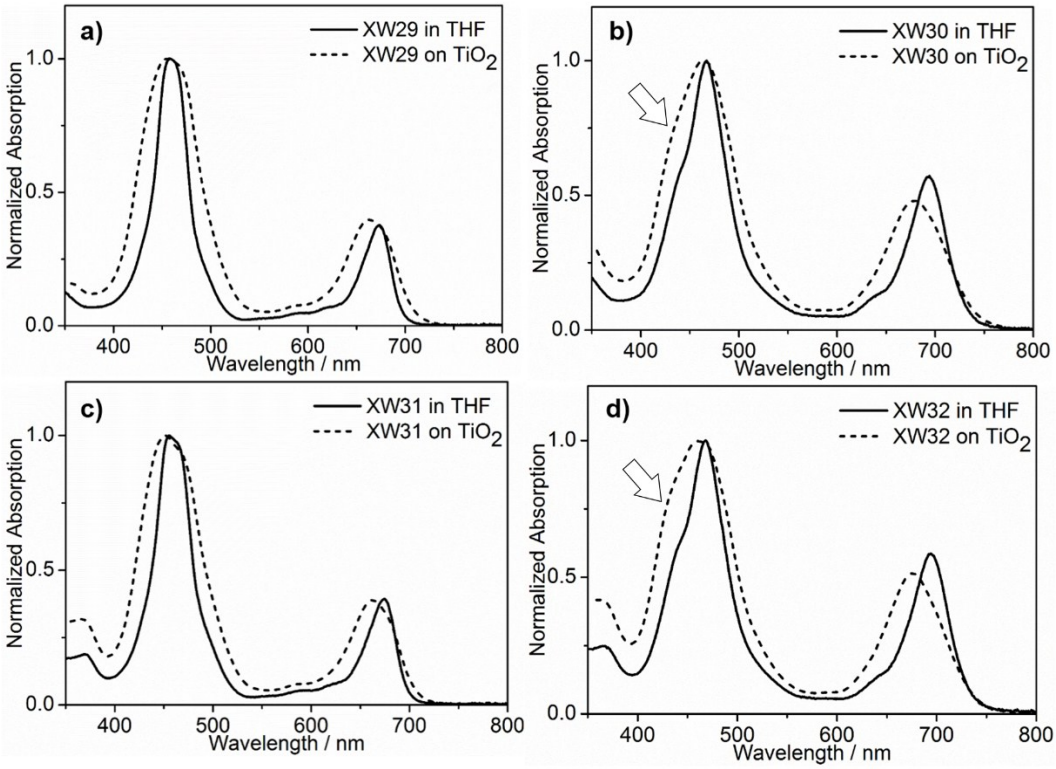


Fig. S2 Normalized absorption spectra of **XW29-XW32** in THF and on TiO_2 films.

3. Cyclic voltammetry curves

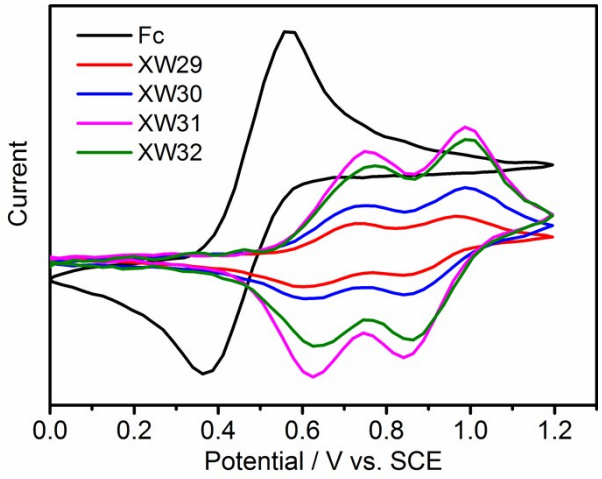


Fig. S3 Cyclic voltammetry curves of **XW29-XW32**.

4. Raw data of photovoltaic parameters

Table S1. Original *J-V* data of DSSC devices based on the individual porphyrin dyes.

Sensitizer	V_{oc} [mV]	J_{sc} [mA·cm^{-2}]	*FF* [%]	PCE [%]
XW29	723	20.71	67.0	10.03
	717	21.73	66.1	10.30
	713	21.56	66.7	10.25
	712	21.05	66.7	10.00
XW30	678	19.90	64.3	8.67
	678	19.18	66.3	8.61
	678	19.85	65.7	8.84
	679	19.76	64.2	8.61
XW31	715	21.85	65.8	10.28
	717	21.71	66.3	10.33
	724	22.46	64.3	10.45
	724	22.22	67.0	10.78
XW32	676	20.45	65.3	9.03
	680	20.11	64.7	8.85
	675	19.94	64.2	8.64
	676	20.01	64.8	8.76

Table S2. Original *J-V* data of DSSC devices based on the porphyrin dyes coadsorbed with 1 mM CDCA.

Dyes	V_{oc} [mV]	J_{sc} [mA·cm^{-2}]	*FF* [%]	PCE [%]
XW29+CDCA	700	21.94	64.4	9.90
	702	22.16	65.9	10.25

	701	21.91	64.6	9.93
	702	22.01	65.2	10.07
XW30+CDCA	689	21.51	66.6	9.86
	687	21.21	66.4	9.68
	689	21.60	67.5	10.05
	688	21.61	66.6	9.90
XW31+CDCA	695	21.91	65.3	9.95
	695	21.93	64.9	9.89
	696	22.48	65.2	10.19
	696	21.61	64.6	9.71
XW32+CDCA	688	21.81	66.0	9.90
	688	21.66	66.7	9.94
	688	22.01	65.9	9.98
	690	22.07	65.2	9.92

5. PL decay traces of the dye-grafted zirconia and titania films

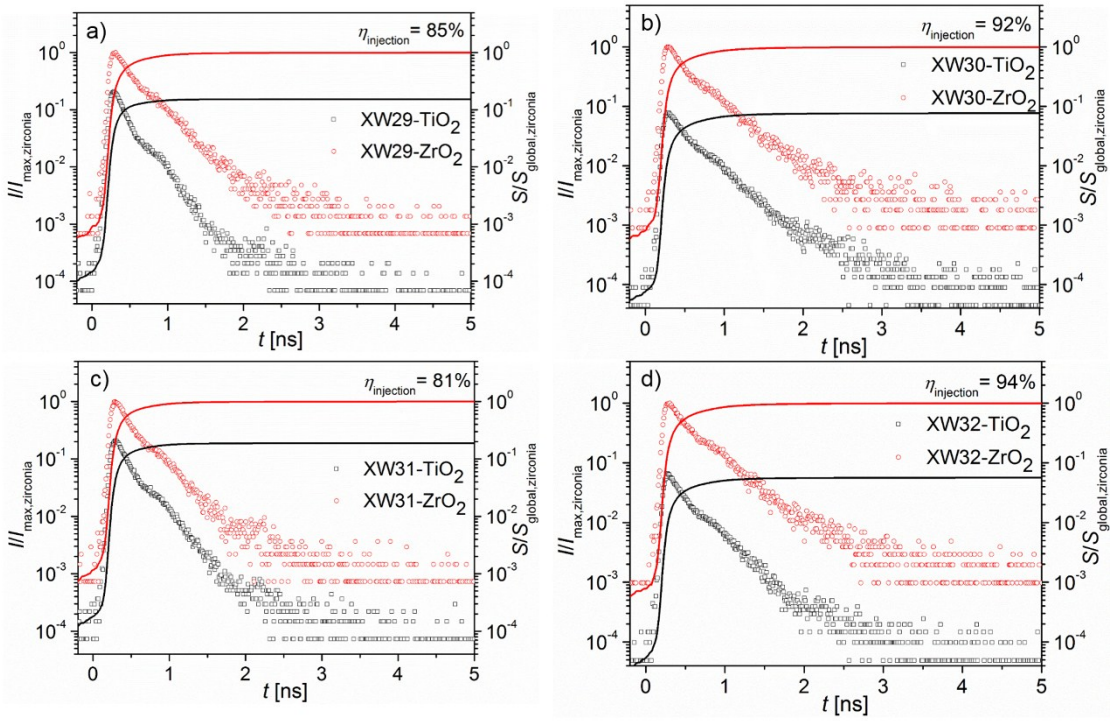


Fig. S4 PL decay traces of dye-grafted zirconia and titania films immersed in an iodine electrolyte. The PL intensity (I) was corrected in term of the absorbance at 670 nm and further normalized with respect to the PL maximum of a corresponding dye-grafted zirconia film ($I_{max,\ zirconia}$). The PL integral areas (S) of the zirconia and titania films were normalized with respect to the global PL integral area of a corresponding dye-grafted zirconia film ($S_{global,\ zirconia}$). Excitation wavelength: 670 nm; probe wavelength: 740 nm.

6. Nyquist plots and estimated charge collection efficiencies of the devices based on XW29-32

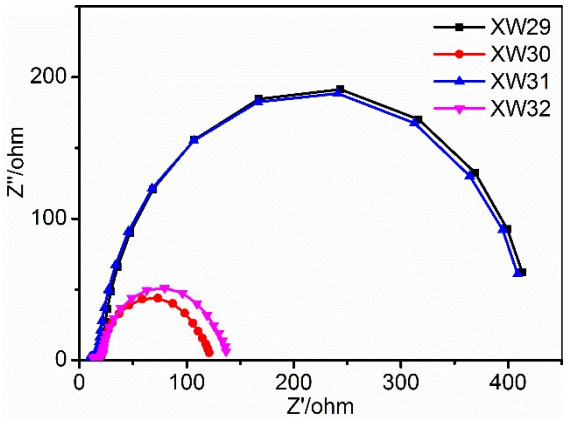


Fig. S5 Nyquist plots of the devices based on **XW29-XW32** measured at -0.70 V in the dark.

Table S3. Charge collection efficiencies estimated from the EIS measurements at a bias potential of -0.7 V.

Device	R_{tr} / Ω	R_{rec} / Ω	Estimated η_{coll}
XW29	4.1	408	99%
XW30	3.2	98.4	97%
XW31	4.2	409	99%
XW32	3.2	114	97%

R_{tr}: transport resistance; R_{rec}: charge recombination resistance. η_{coll} was estimated by $\eta_{coll} = (1 + R_{tr} / R_{rec})^{-1}$.

7. ^{1}H NMR, ^{13}C NMR and MS spectra for the compounds

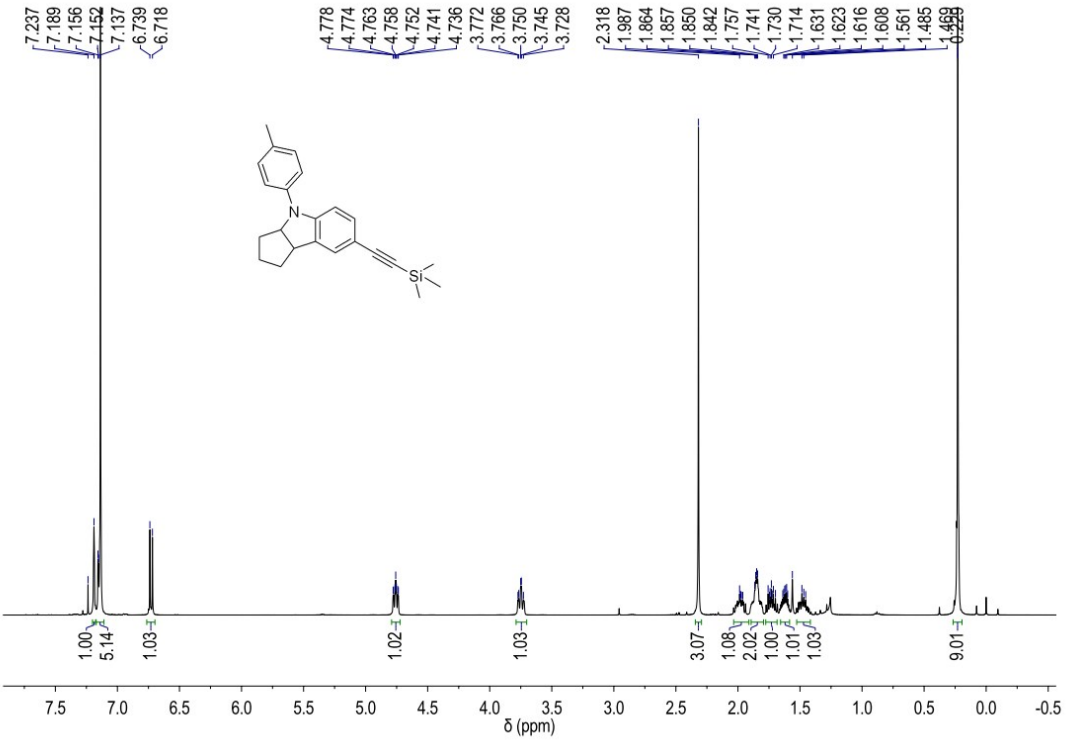


Fig. S6 ^{1}H NMR spectrum of compound **3a** in $CDCl_3$.

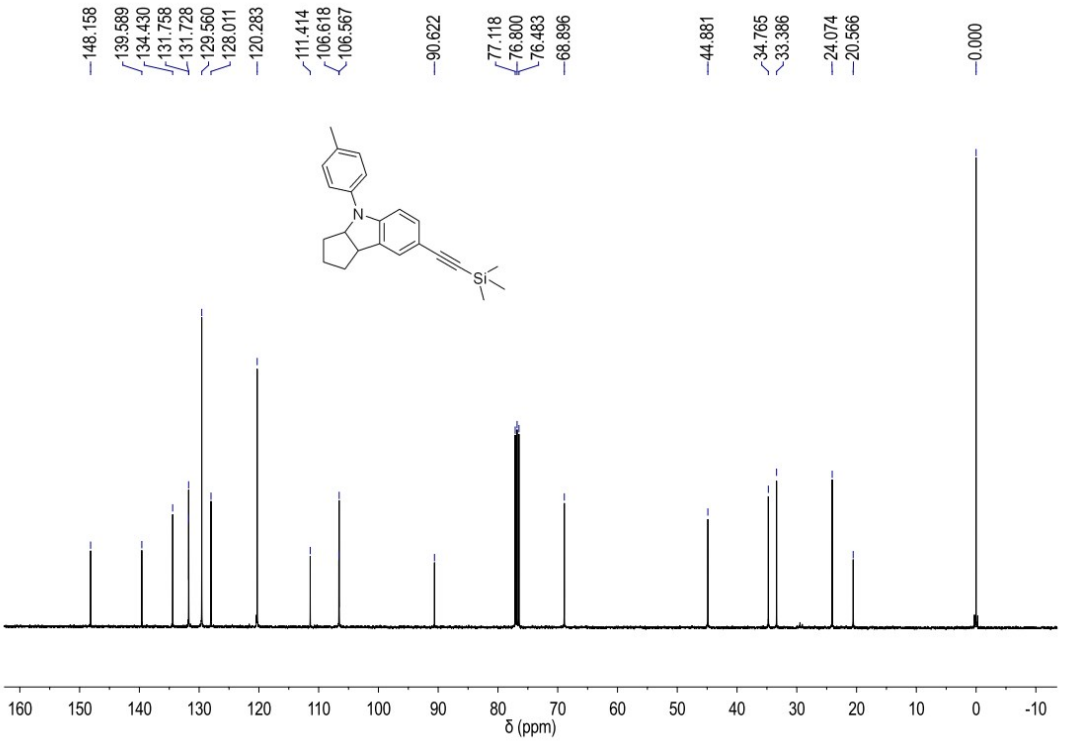


Fig. S7 ^{13}C NMR spectrum of compound **3a** in $CDCl_3$.

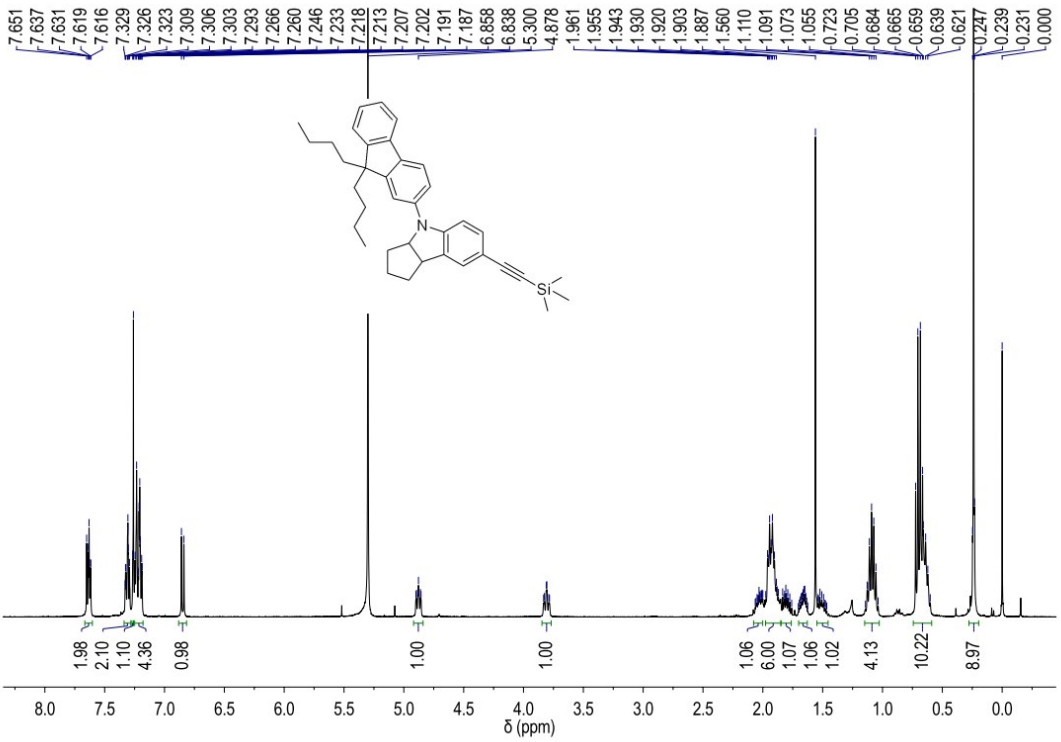


Fig. S8 ^{1}H NMR spectrum of compound **3b** in $CDCl_3$.

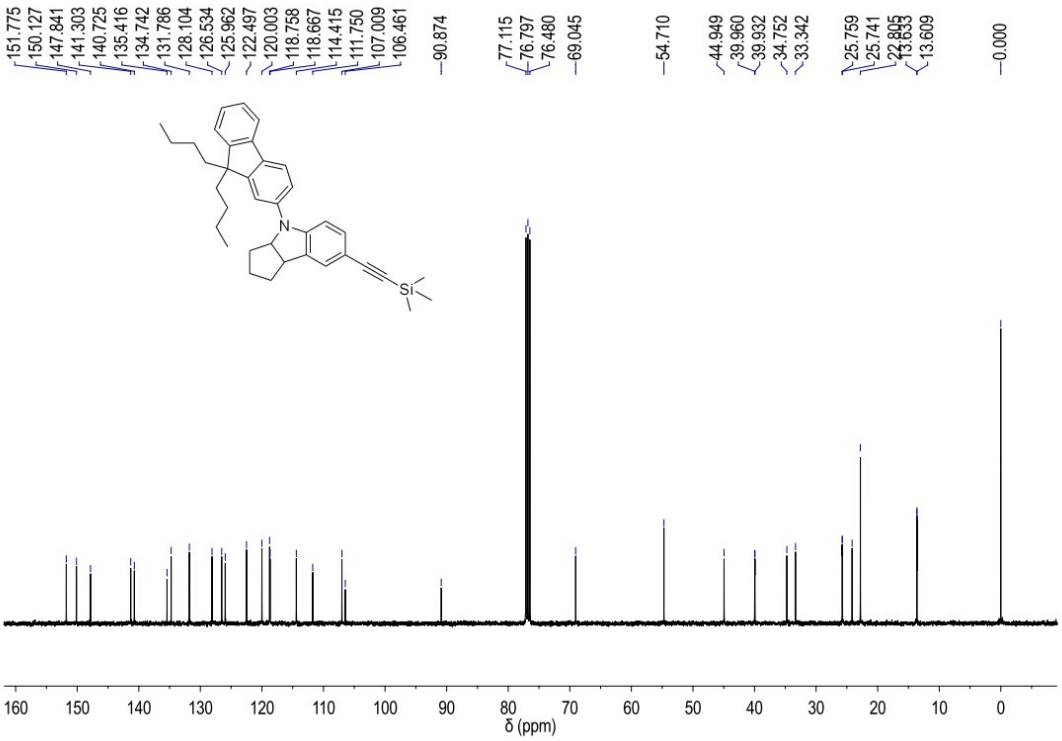


Fig. S9 ^{13}C NMR spectrum of compound **3b** in $CDCl_3$.

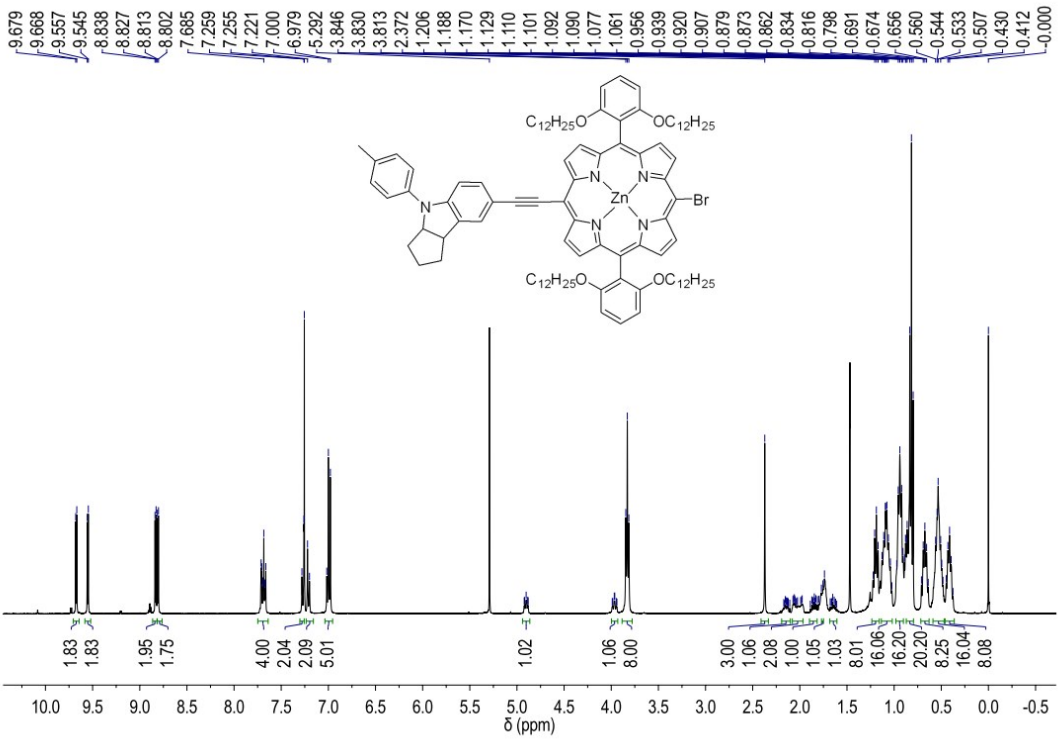


Fig. S10 ^{1}H NMR spectrum of compound **5a** in $CDCl_3$.

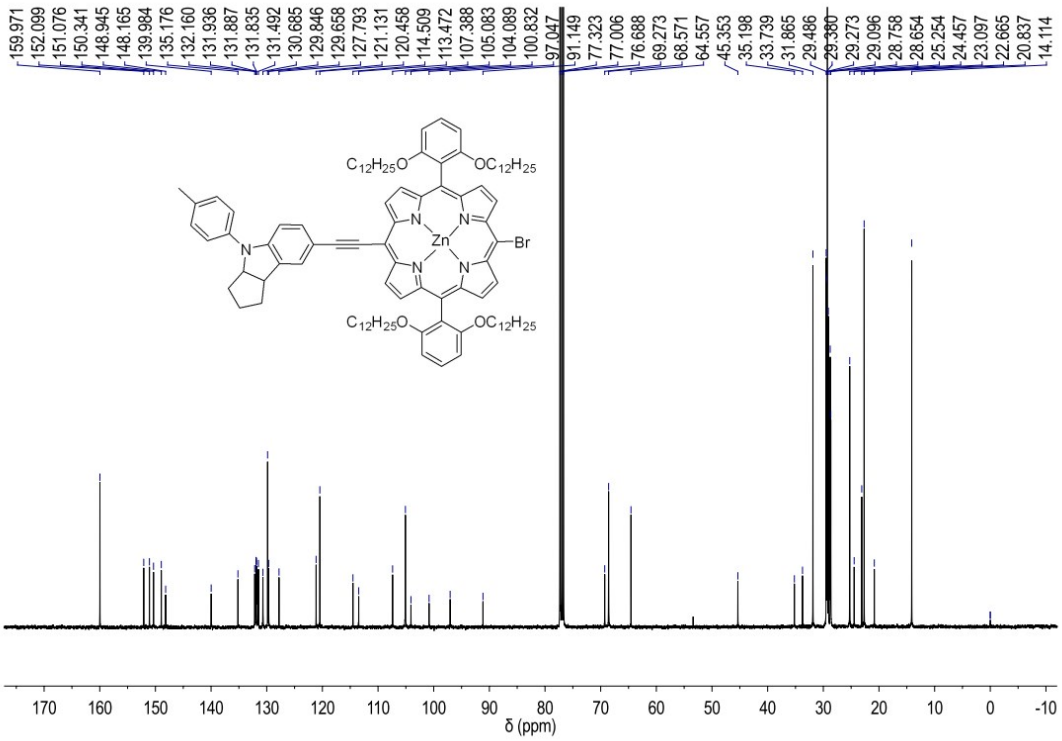


Fig. S11 ^{13}C NMR spectrum of compound **5a** in $CDCl_3$.

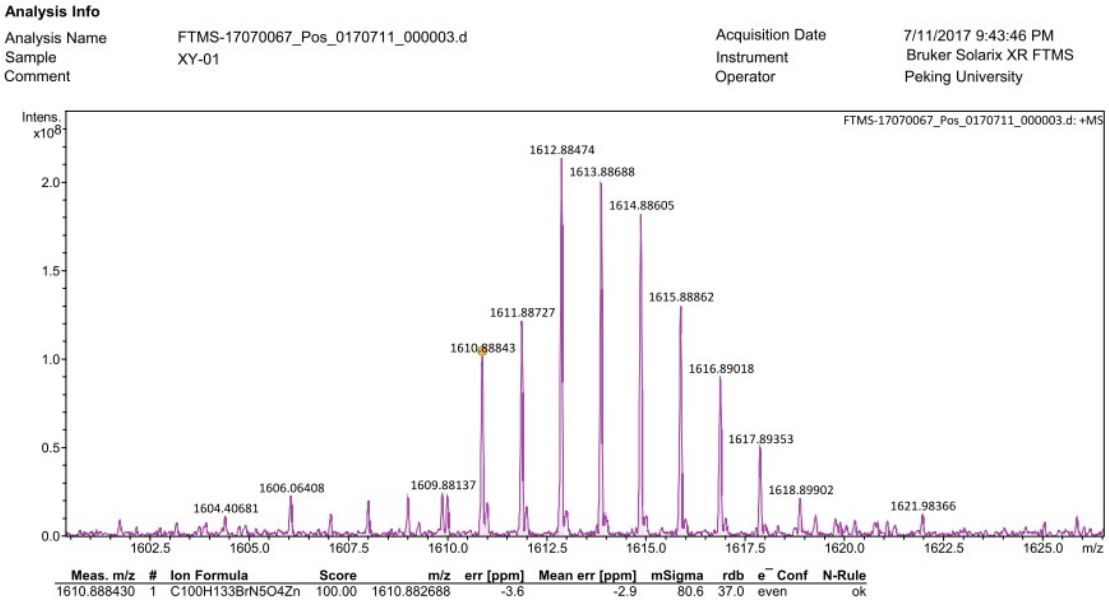


Fig. S12 FTICR-MS of **5a**.

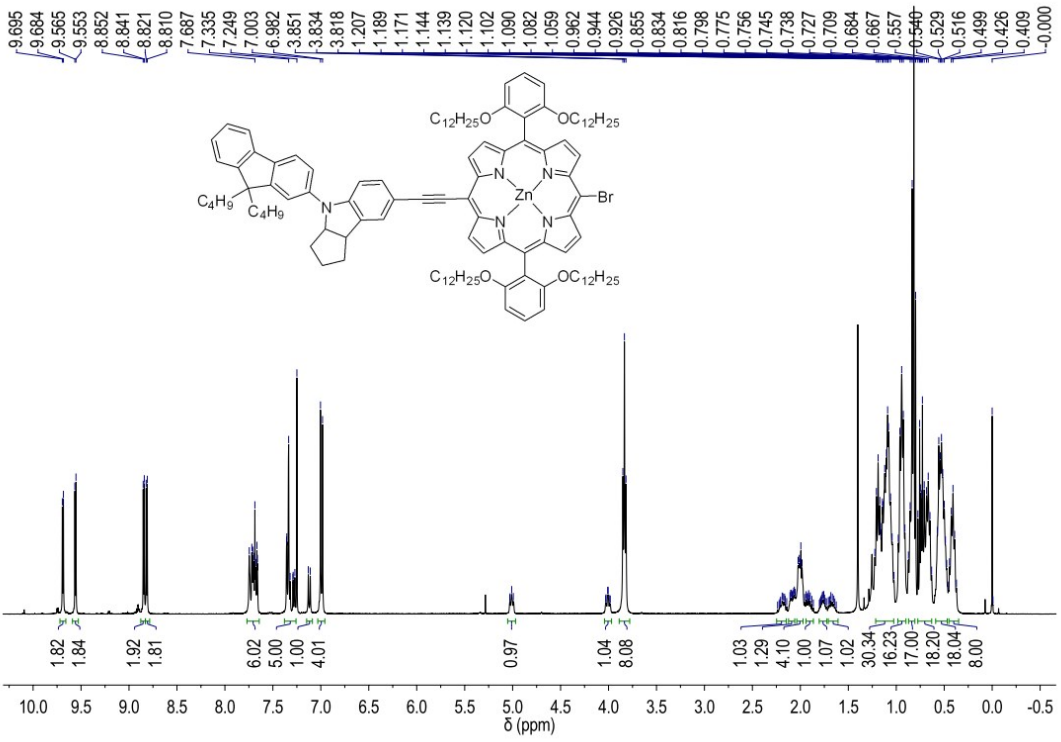


Fig. S13 ^{1}H NMR spectrum of compound **5b** in $CDCl_3$.

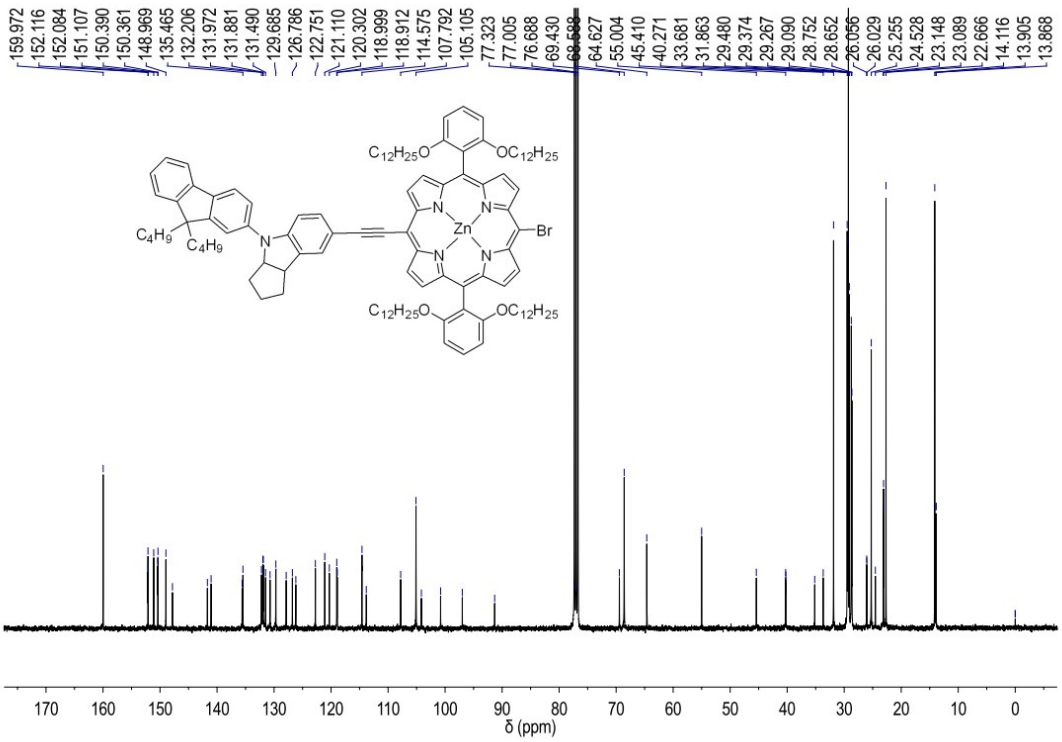


Fig. S14 ^{13}C NMR spectrum of compound **5b** in $CDCl_3$.

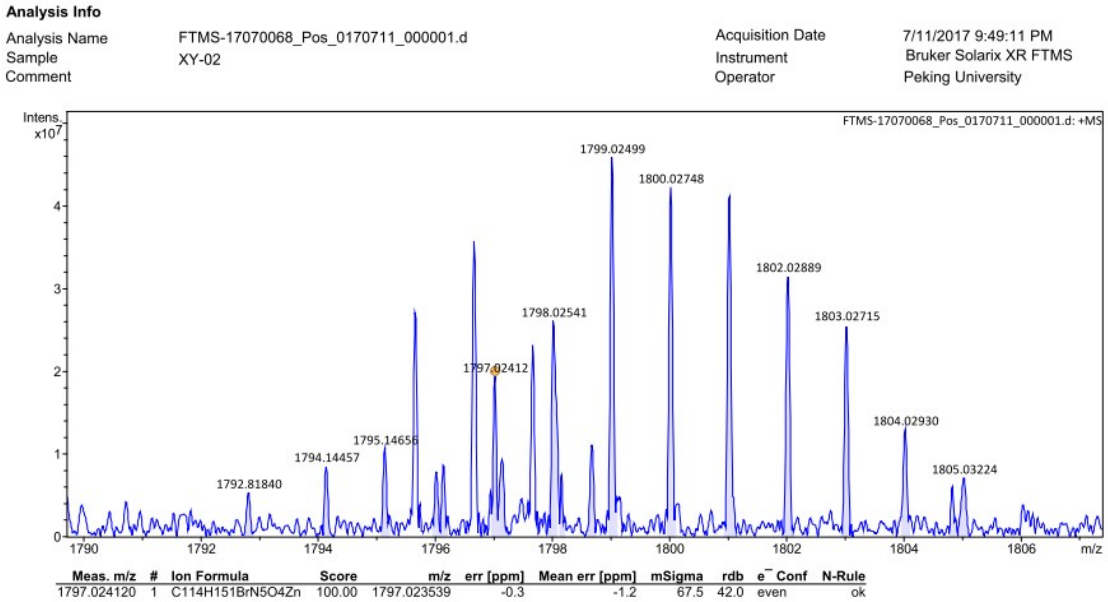


Fig. S15 FTICR-MS of **5b**.

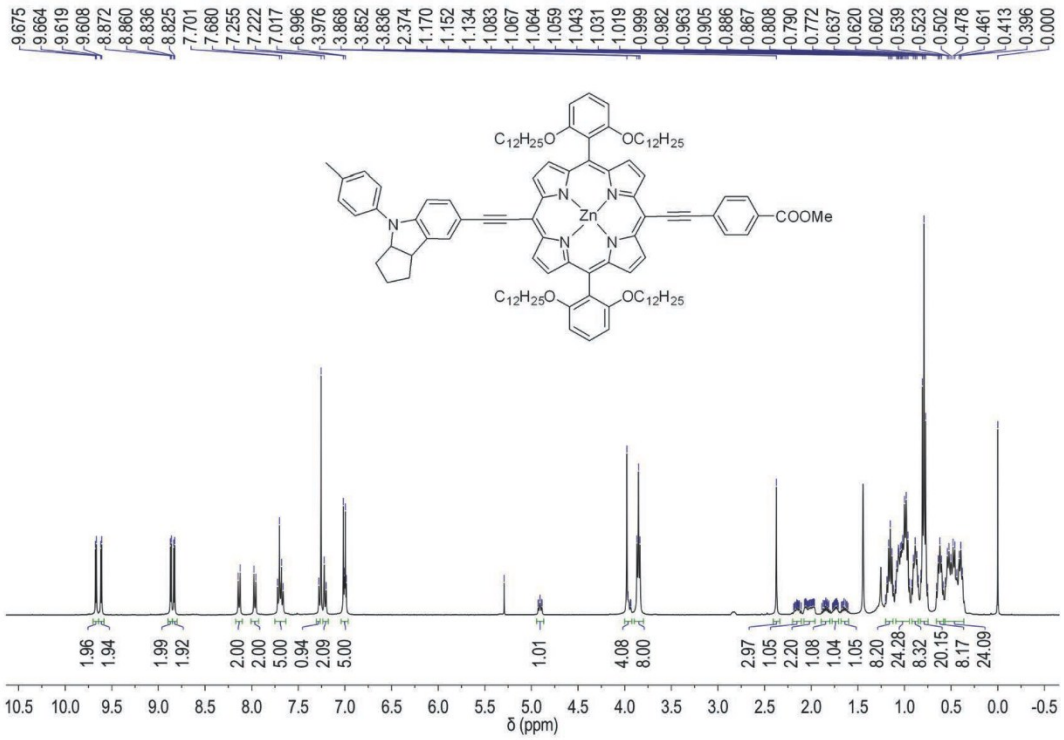


Fig. S16 ^{1}H NMR spectrum of compound **6a** in $CDCl_3$.

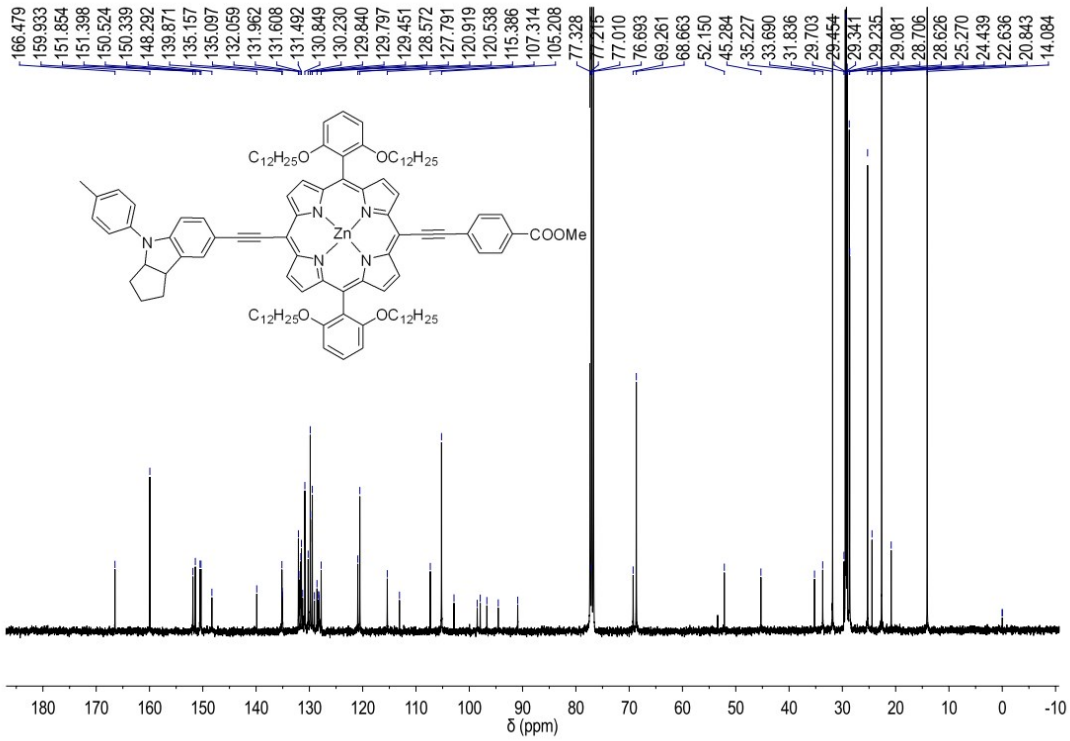


Fig. S17 ^{13}C NMR spectrum of compound **6a** in $CDCl_3$.

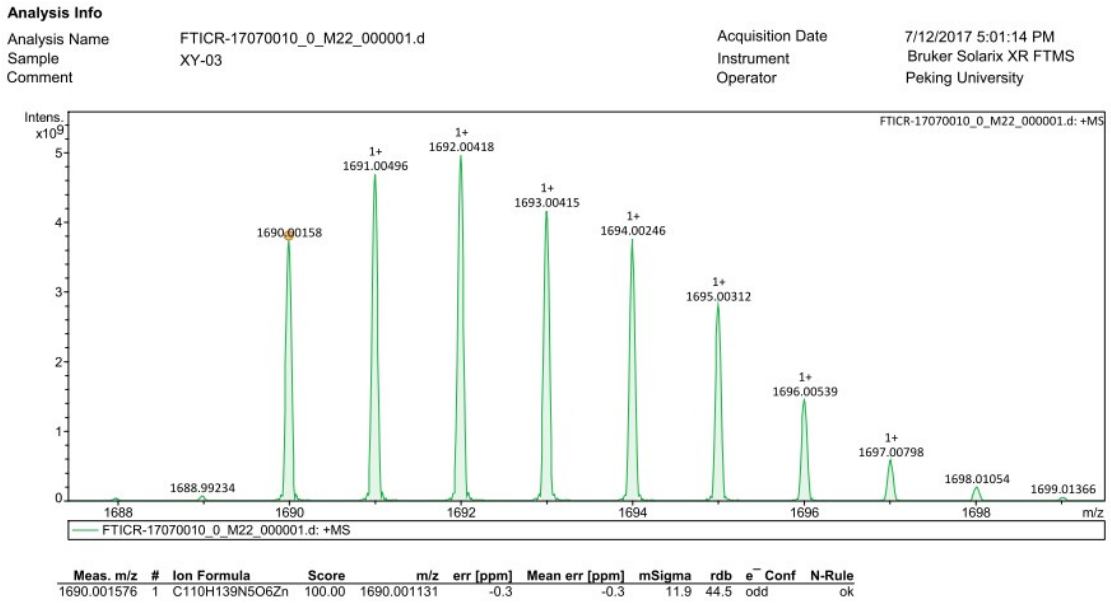


Fig. S18 FTICR-MS of **6a**.

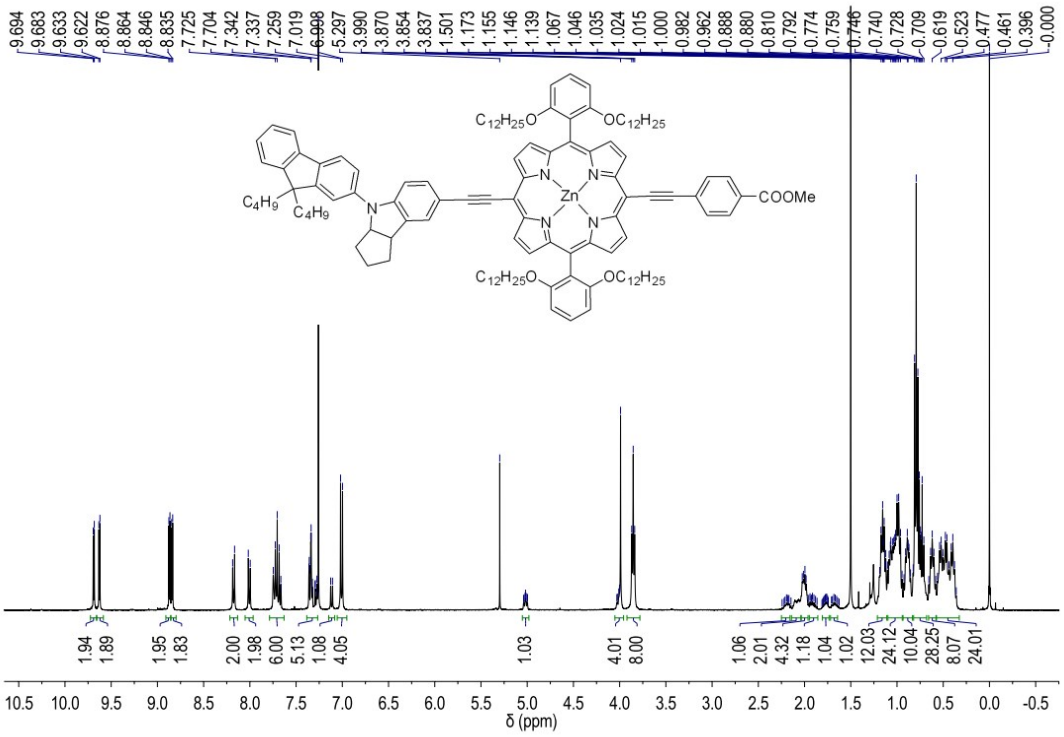


Fig. S19 ^{1}H NMR spectrum of compound **6b** in $CDCl_3$.

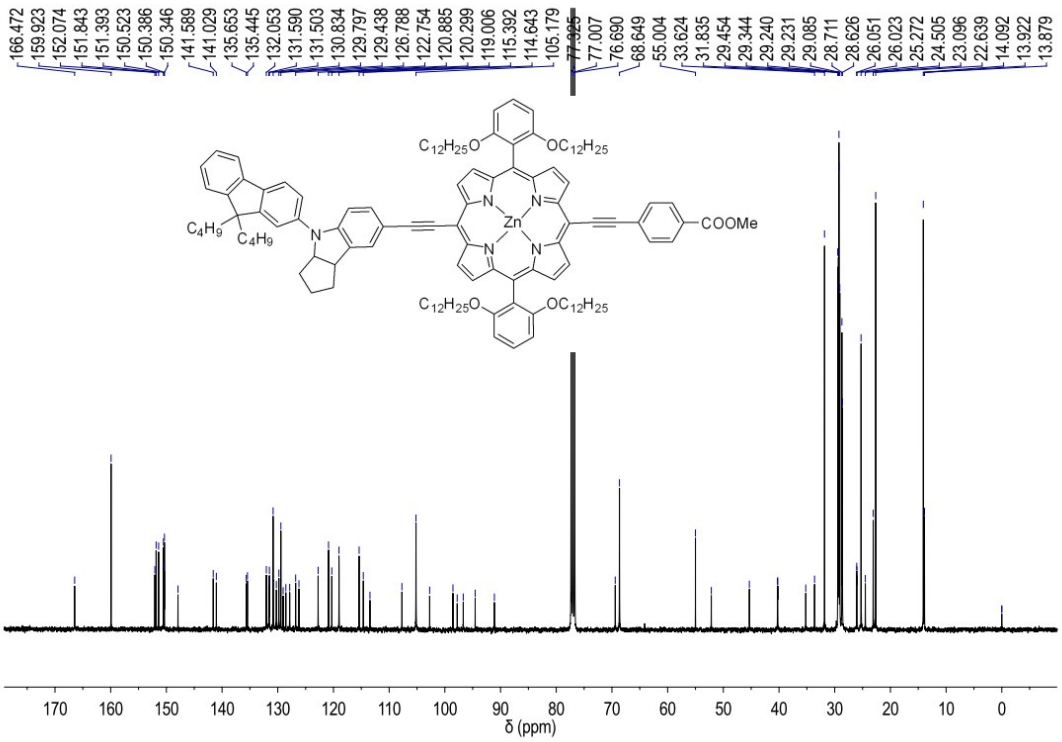


Fig. S20 ^{13}C NMR spectrum of compound **6b** in $CDCl_3$.

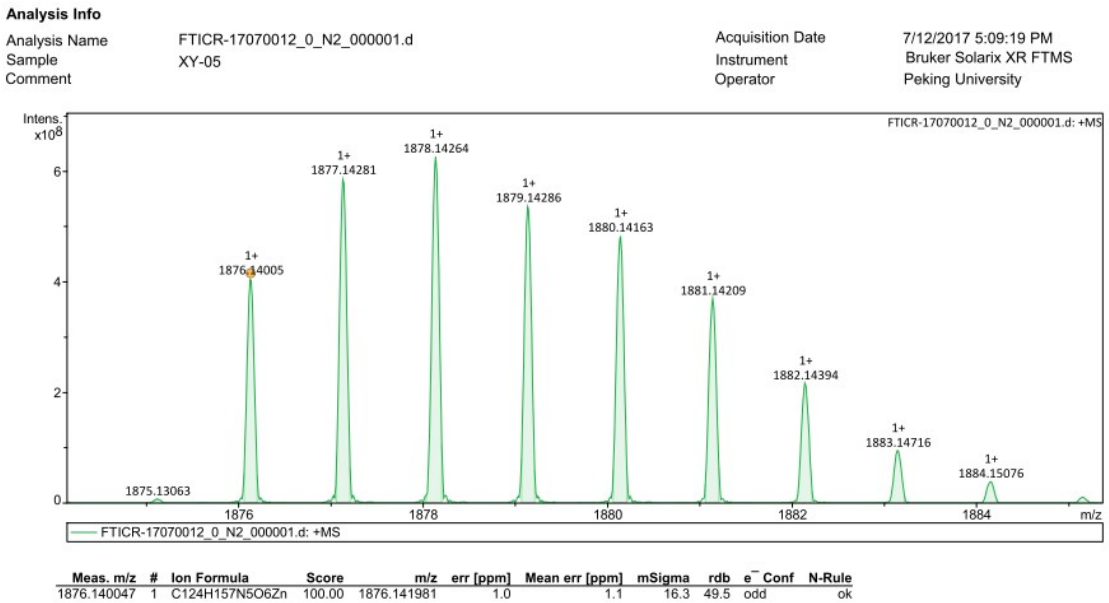


Fig. S21 FTICR-MS of **6b**.

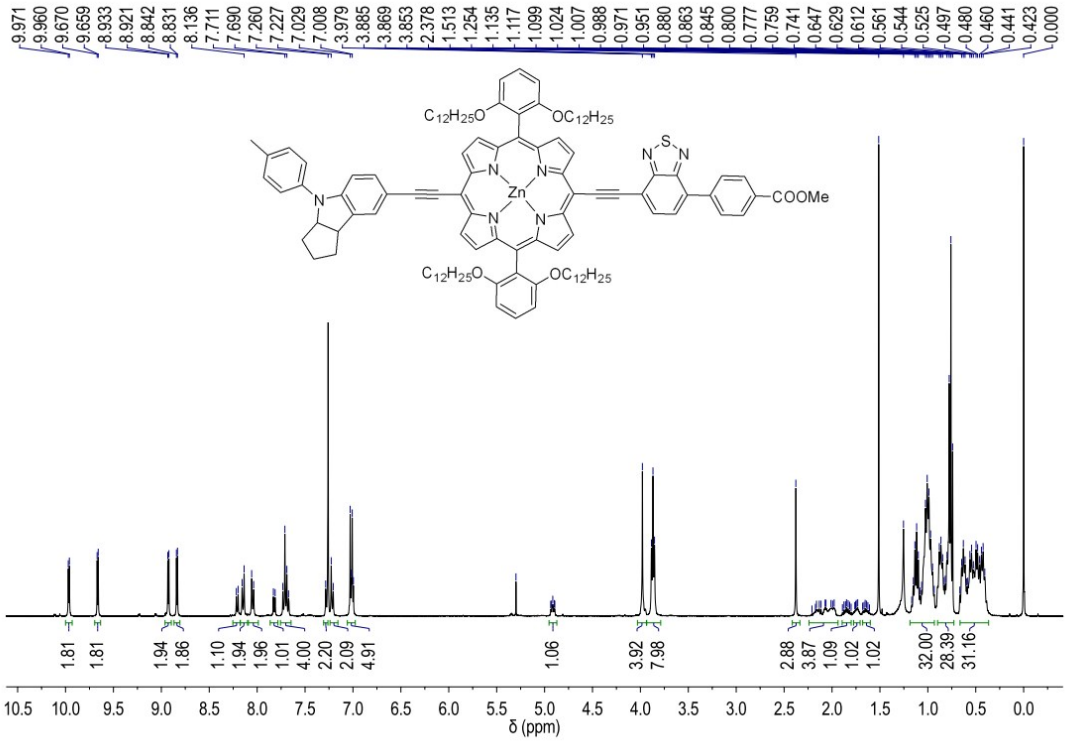


Fig. S22 ^{1}H NMR spectrum of compound **6c** in $CDCl_3$.

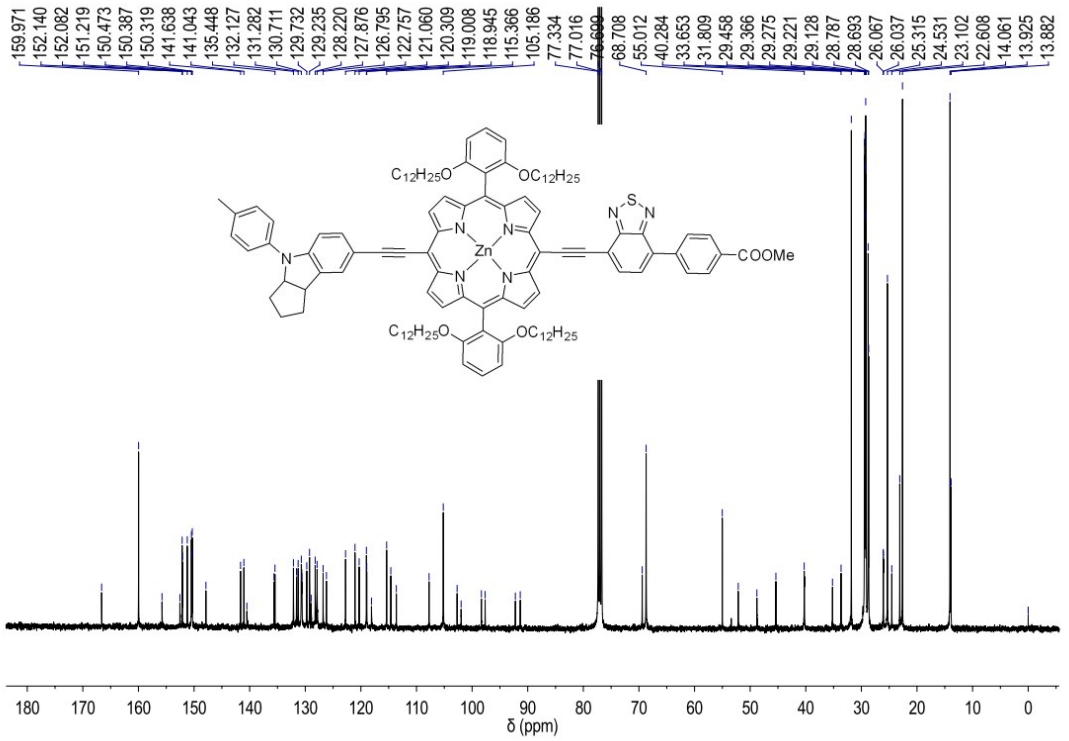


Fig. S23 ^{13}C NMR spectrum of compound **6c** in $CDCl_3$.

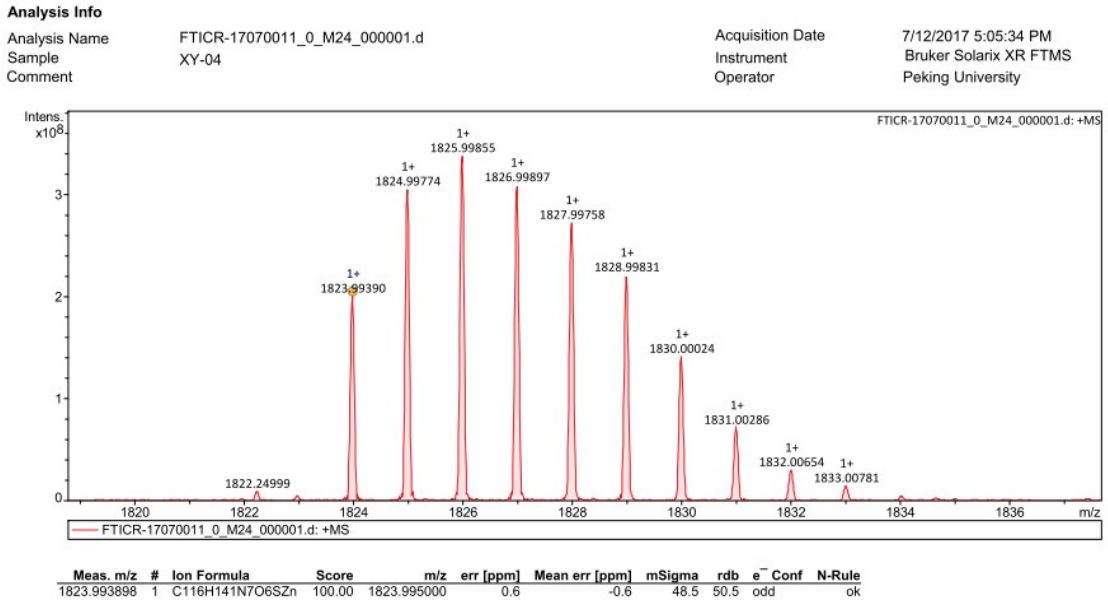


Fig. S24 FTICR-MS of **6c**.

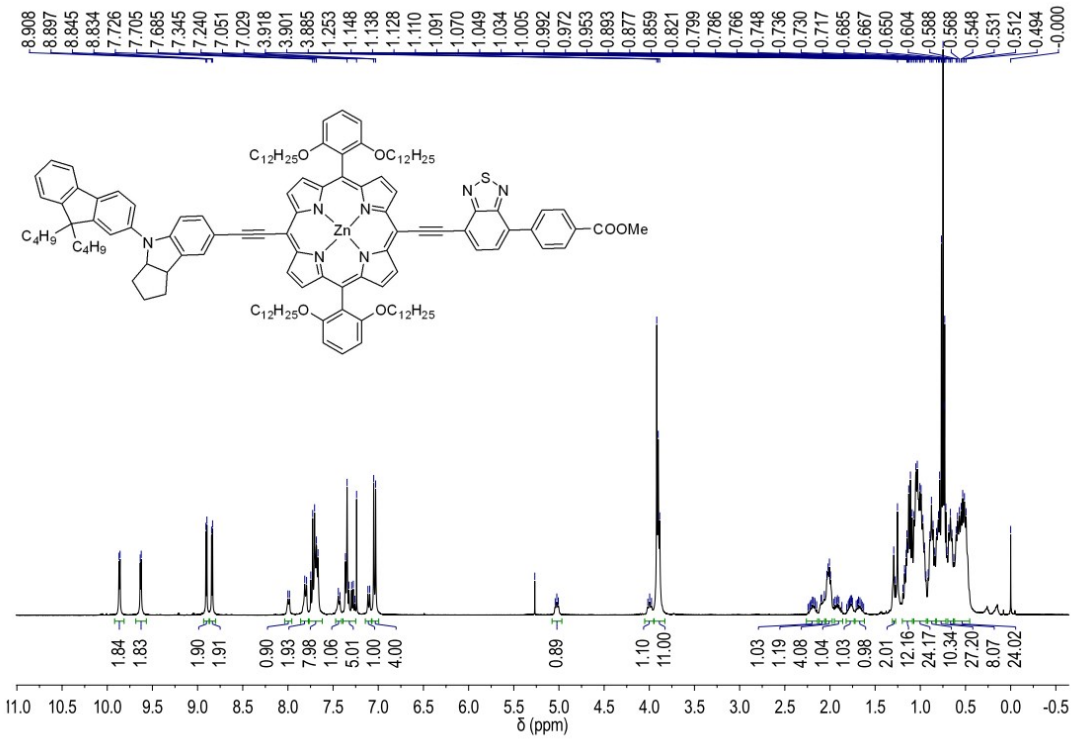


Fig. S25 ^{1}H NMR spectrum of compound **6d** in $CDCl_3$.

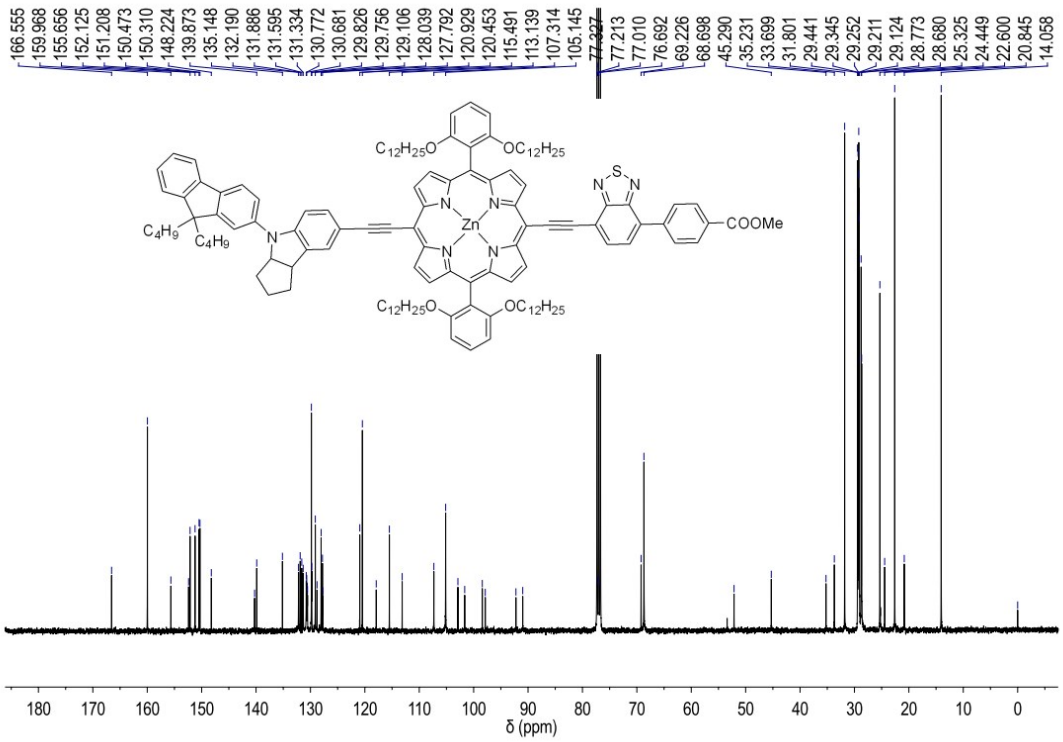


Fig. S26 ^{13}C NMR spectrum of compound **6d** in $CDCl_3$.

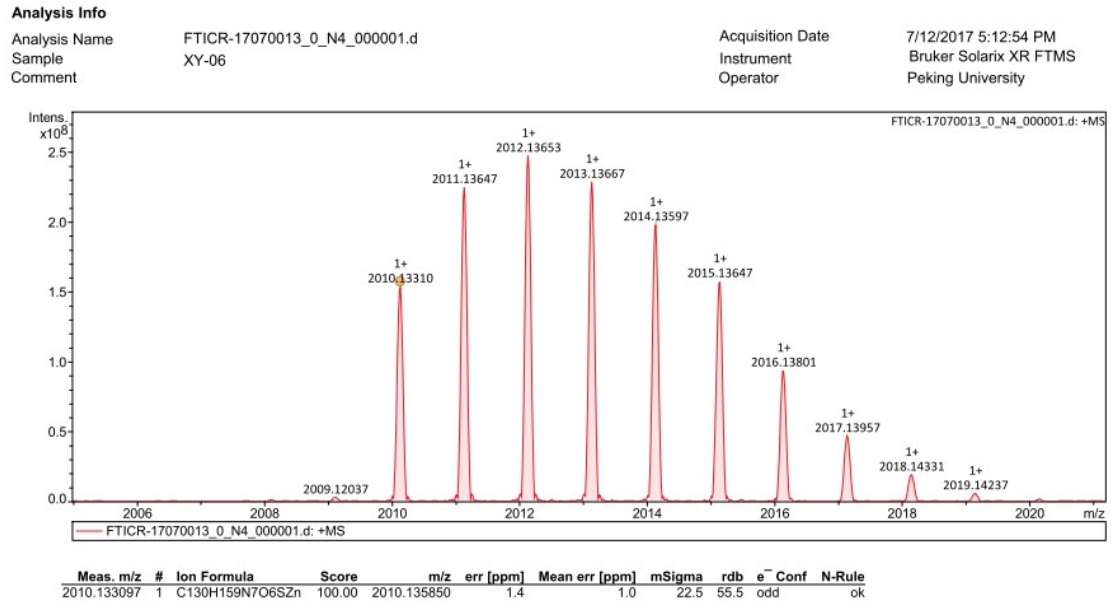


Fig. S27 FTICR-MS of **6d**.

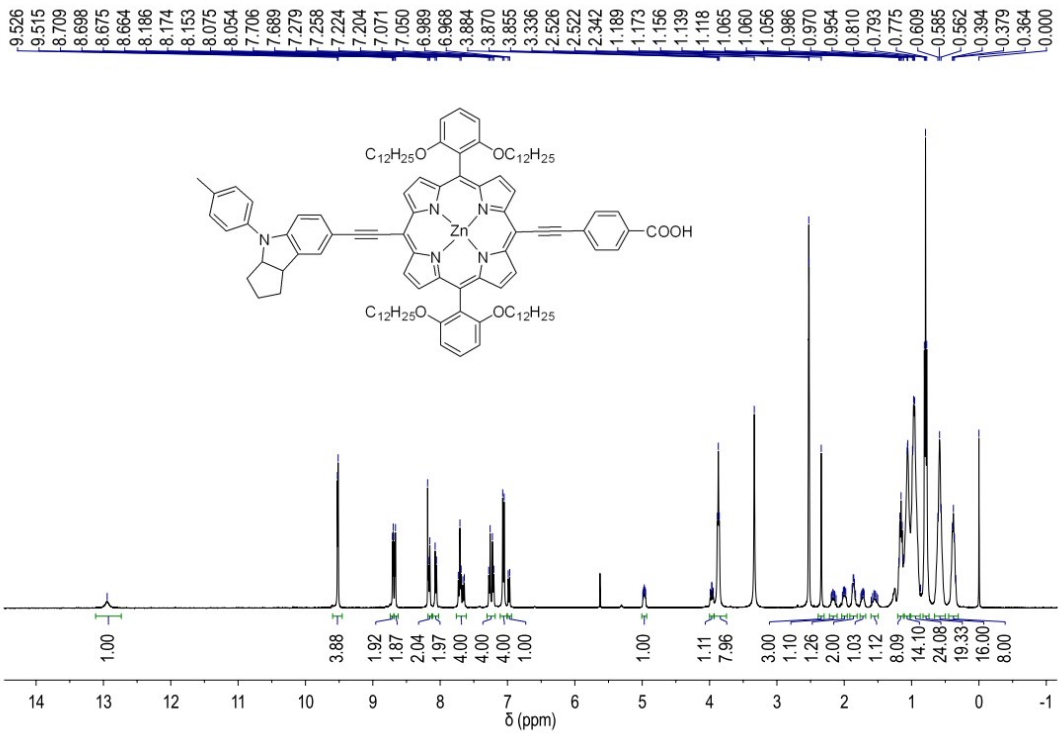


Fig. S28 ^{1}H NMR spectrum of **XW29** in $CDCl_3$: DMSO-d_6 (1:2, v/v).

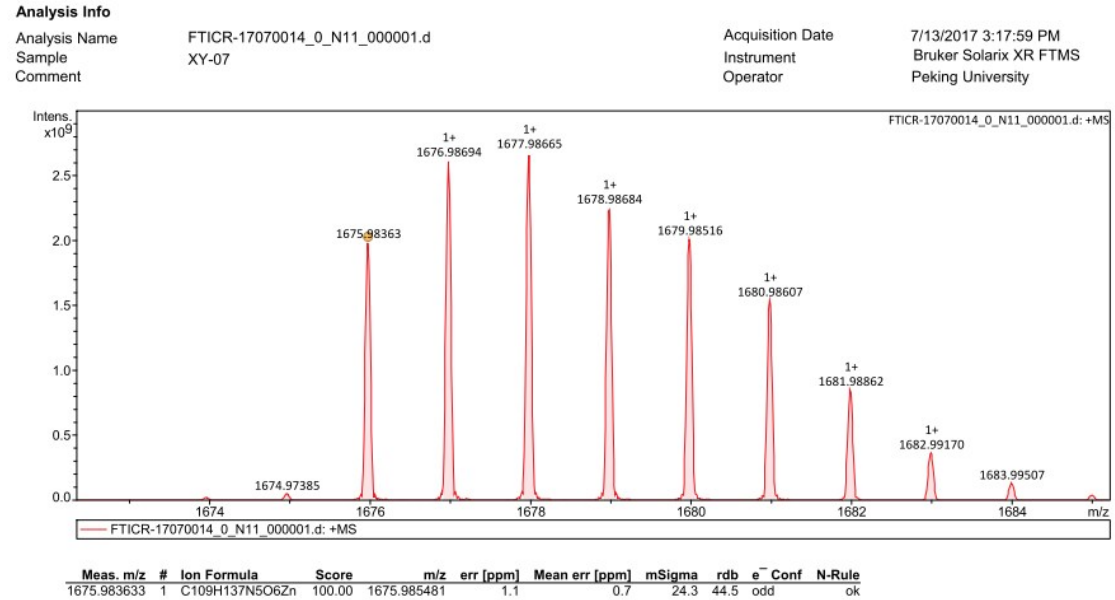


Fig. S29 FTICR-MS of **XW29**.

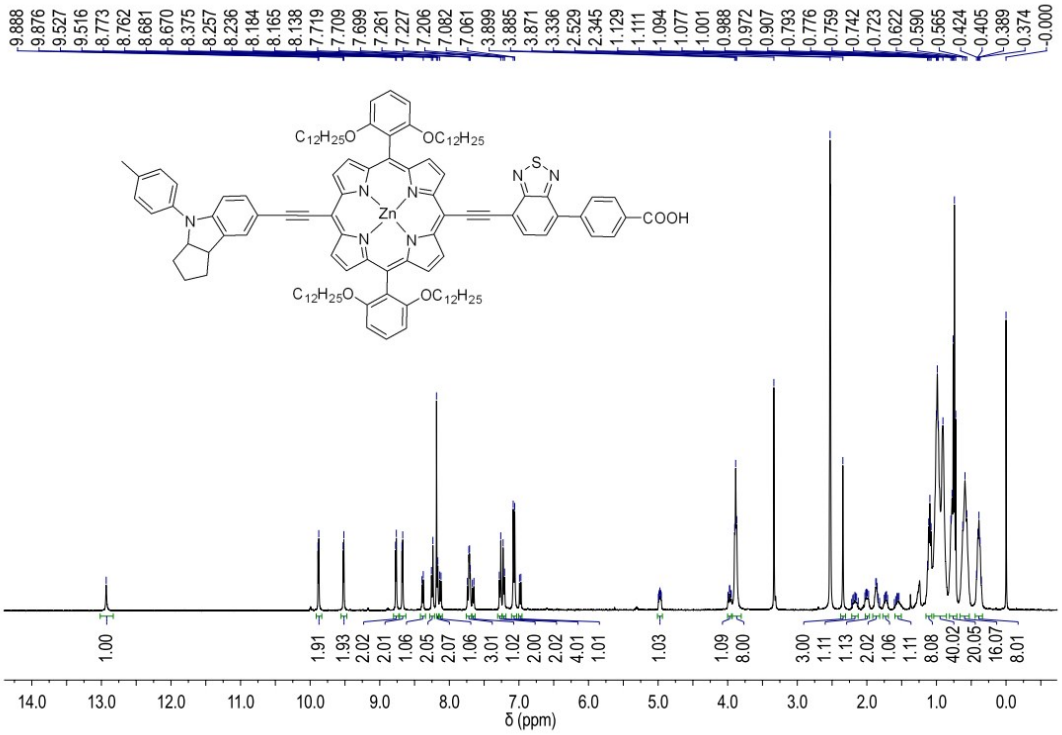


Fig. S30 ^{1}H NMR spectrum of **XW30** in $CDCl_3$: DMSO-d_6 (1:2, v/v).

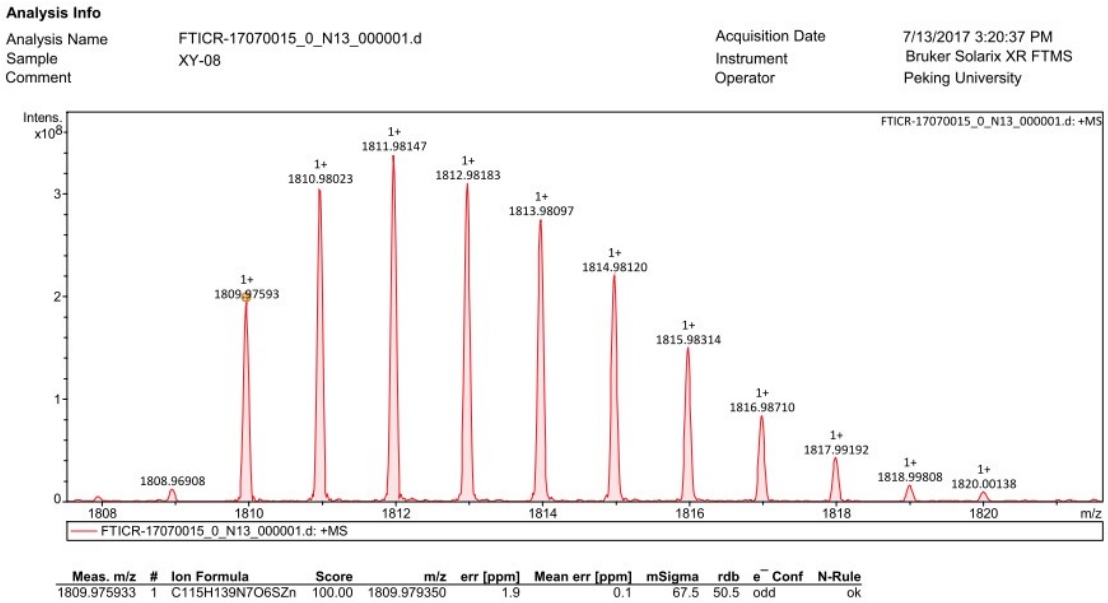


Fig. S31 FTICR-MS of **XW30**.

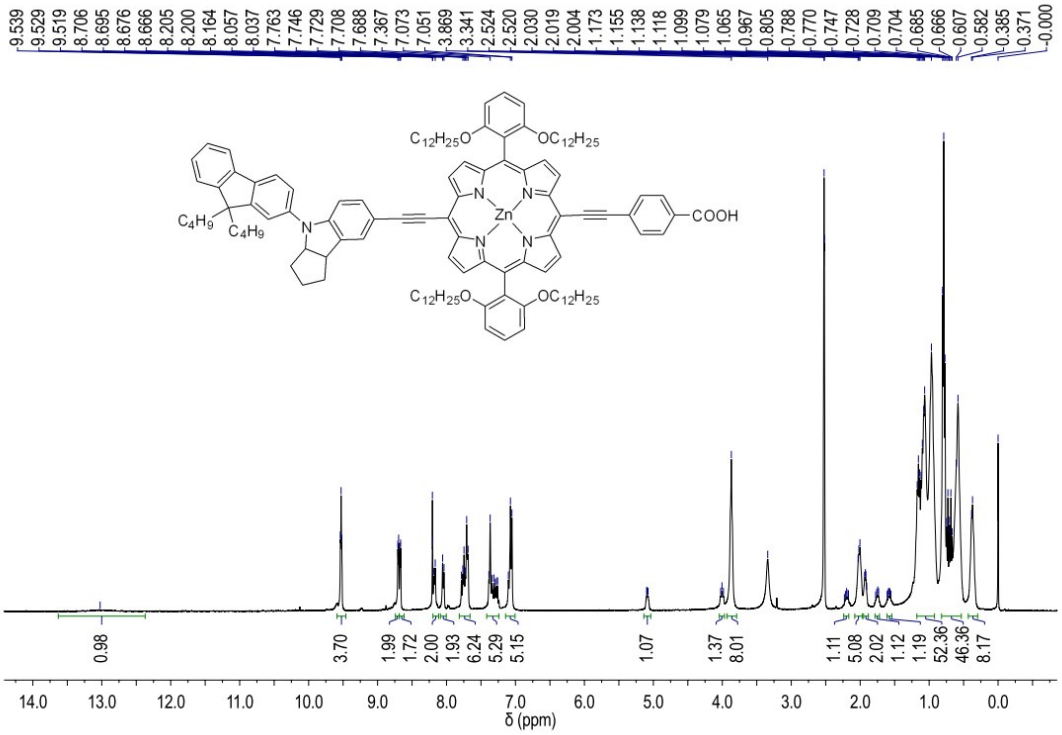
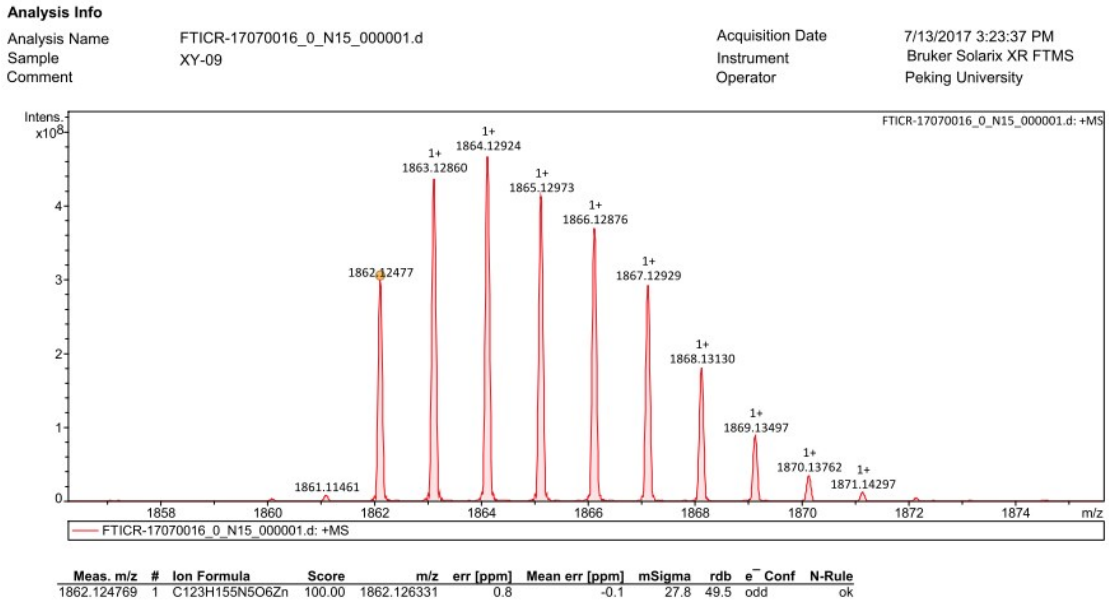


Fig. S32 ^{1}H NMR spectrum of **XW31** in $CDCl_3$: DMSO-d_6 (1:2, v/v).



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
1862.124769	1	C123H155N5O6Zn	100.00	1862.126331	0.8	-0.1	27.8	49.5	odd	ok

Fig. S33 FTICR-MS of **XW31**.

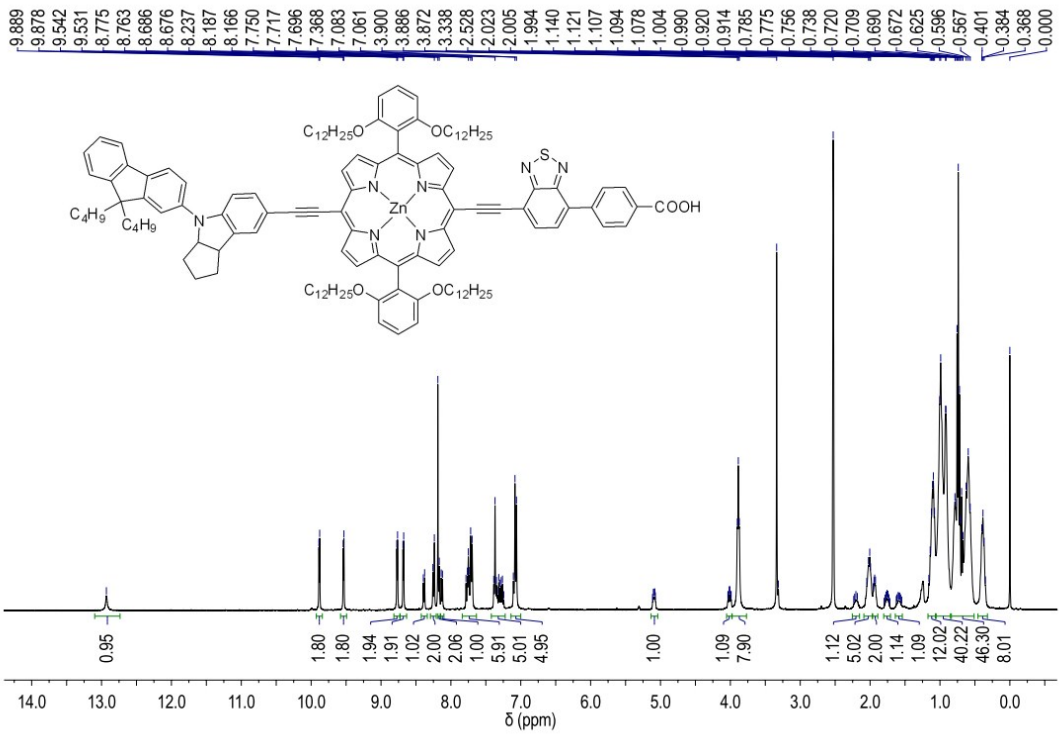


Fig. S34 ^{1}H NMR spectrum of **XW32** in $CDCl_3$: DMSO-d_6 (1:2, v/v).