Electronic supplementary information (ESI)
(11 pages)

^{13}C and ^{1}H NMR spectroscopic investigation on the structure of the iminium ion with a dipolar form in metal complexes of 2-N substituted N-confused porphyrins

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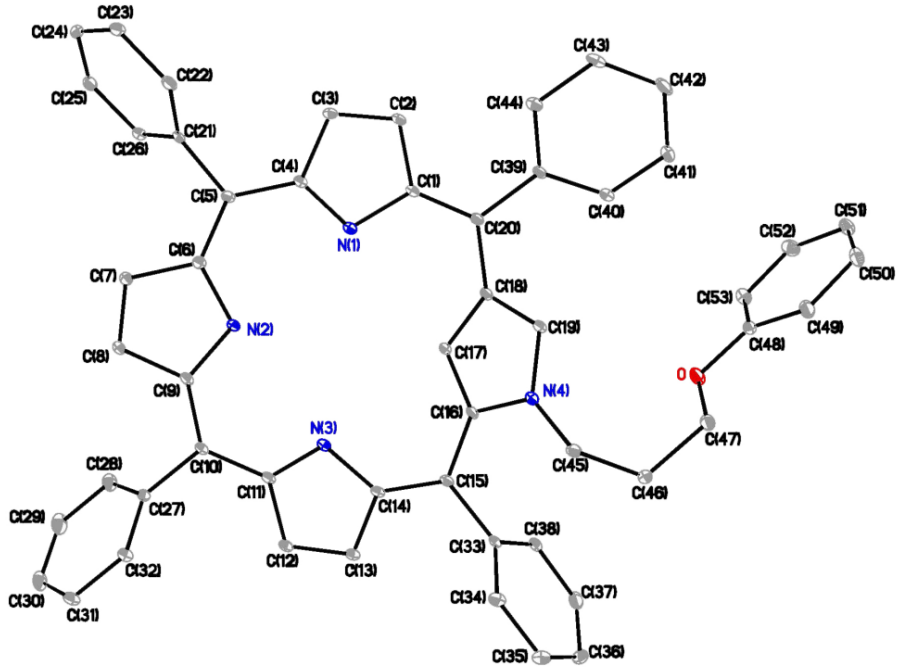
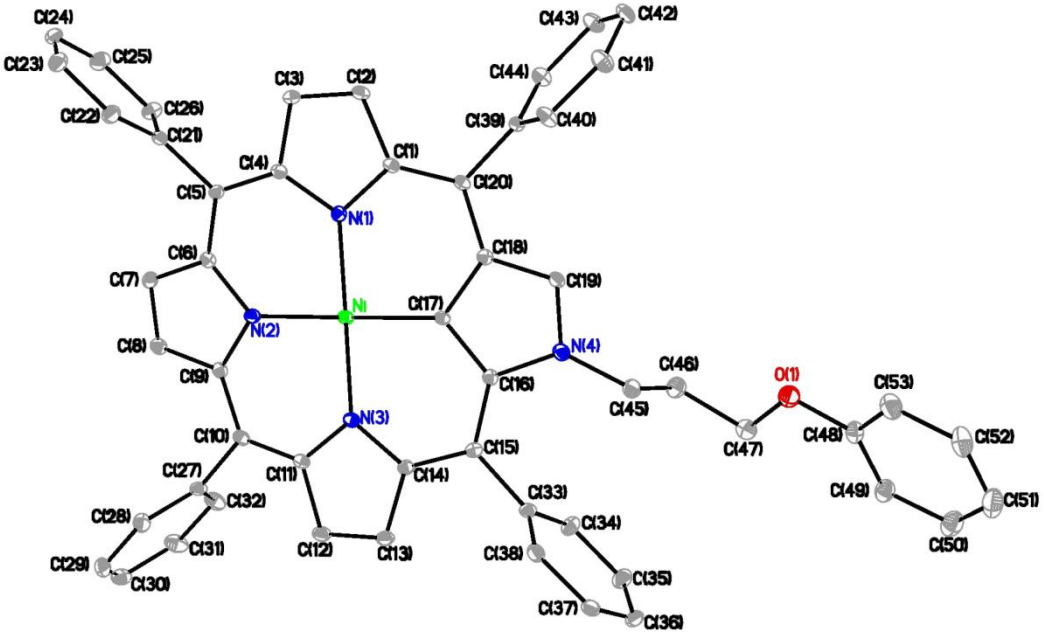
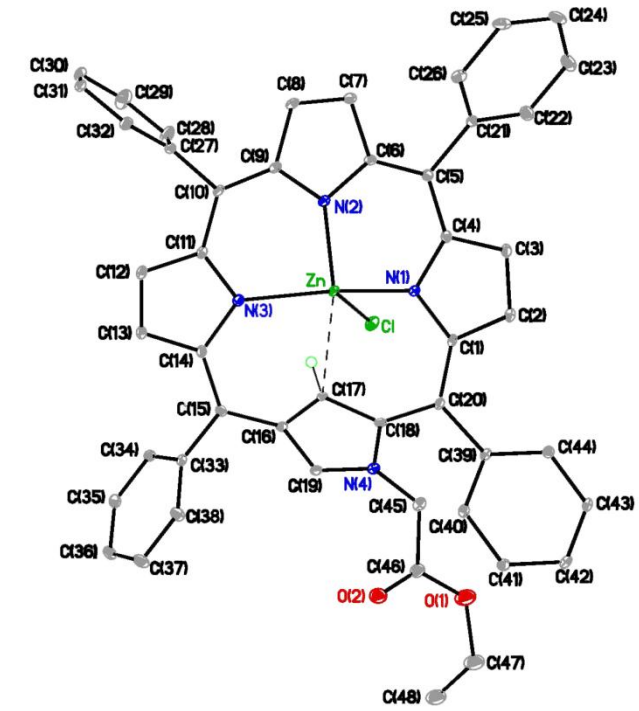


(a) (**2**)

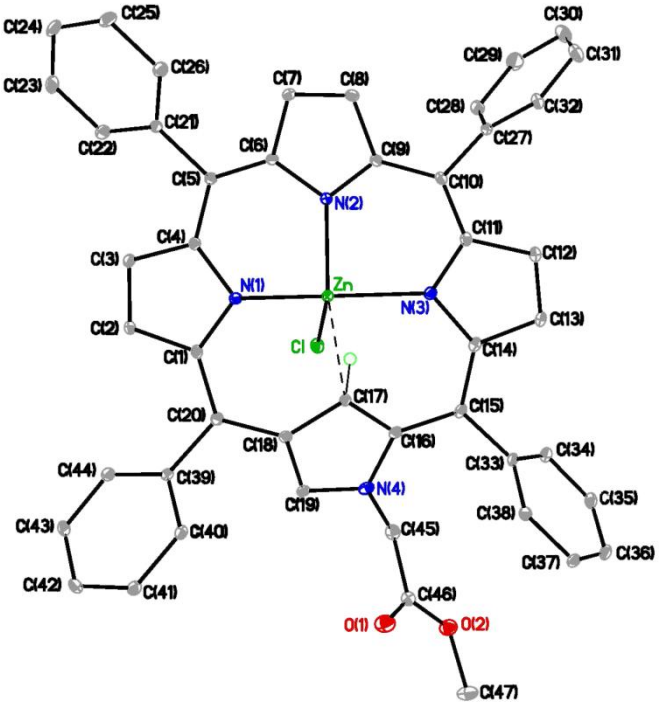


(b) (**7**)

Figure S1. Molecular configuration and atom-labeling scheme for (a) 2-$NCH_2CH_2CH_2OC_6H_5NCTPPH$ **(2)** and (b) Ni(2-$NCH_2CH_2CH_2OC_6H_5NCTPP$) **(7)**, with 30% thermal ellipsoids. Hydrogen atoms are omitted for clarity.

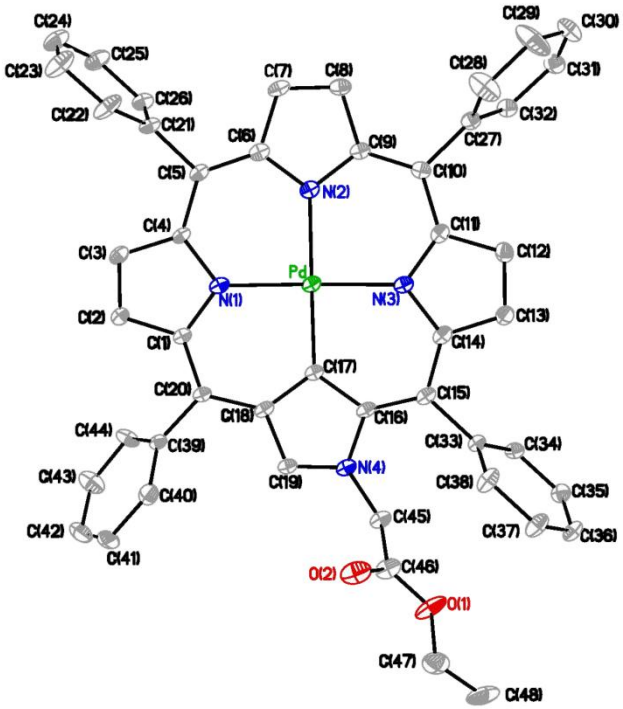


(a) (**4**)

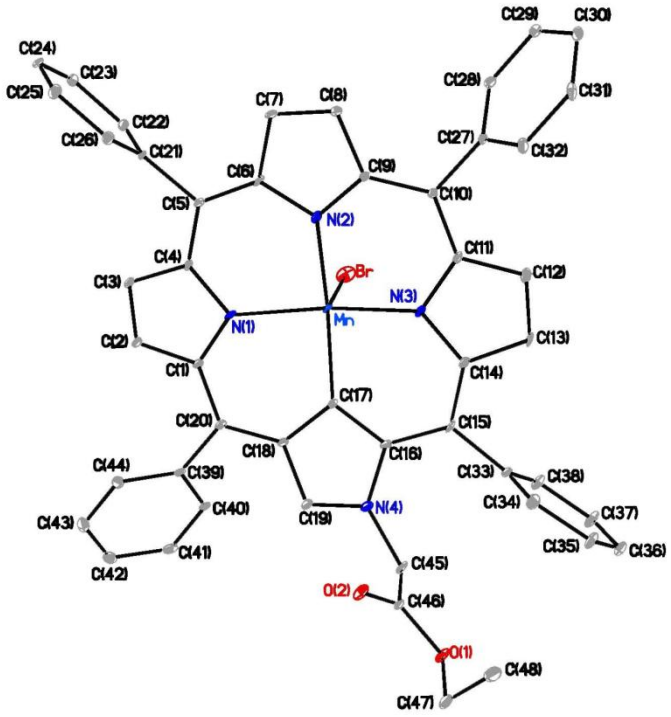


(b) (**8**)

Figure S2. Molecular configuration and atom-labeling scheme for (a) Zn(2-$NCH_2COOC_2H_5$NCTPP)Cl (**4**) and (b) Zn(2-NCH_2COOCH_3NCTPP)Cl (**8**), with 30% thermal ellipsoids. Hydrogen atoms except H(17A) for **4** and **8** are omitted for clarity.

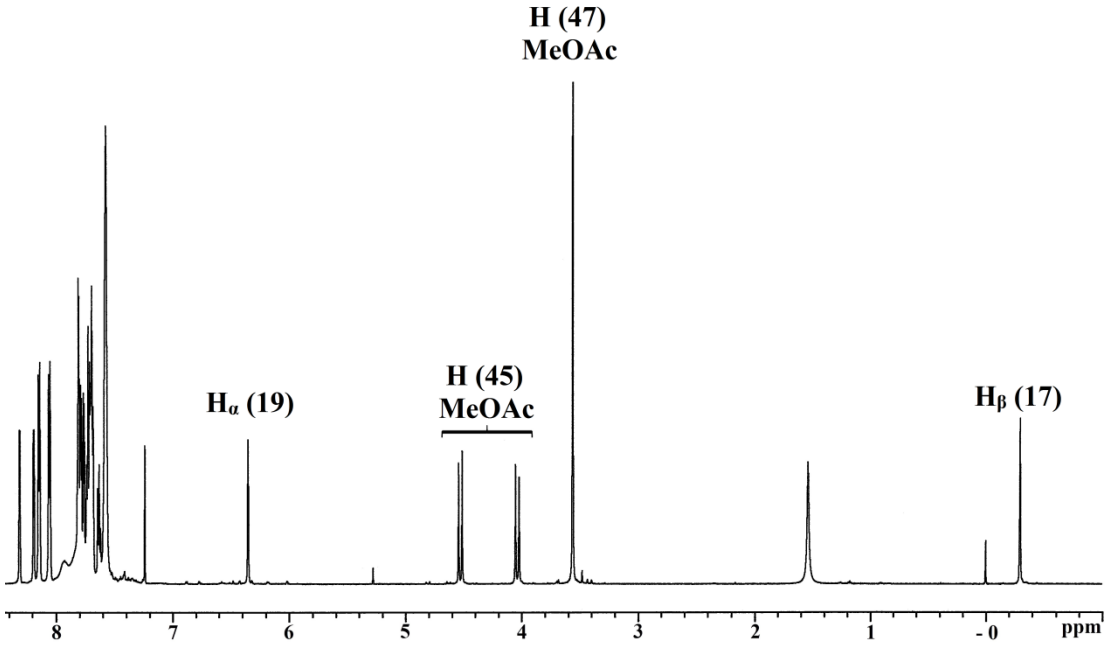


(a) (**5**)

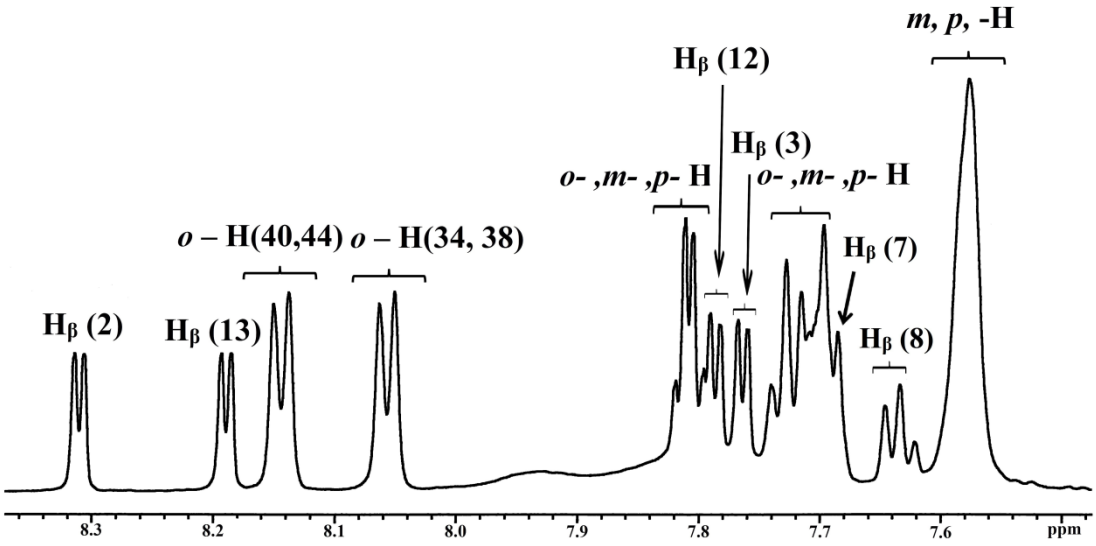


(b) (**6**)

Figure S3. Molecular configuration and atom-labeling scheme for (a) Pd(2-$NCH_2COOC_2H_5$NCTPP) (**5**) and (b) Mn(2-$NCH_2COOC_2H_5$NCTPP)Br (**6**), with 30% thermal ellipsoids. Hydrogen atoms are omitted for clarity.



(a)

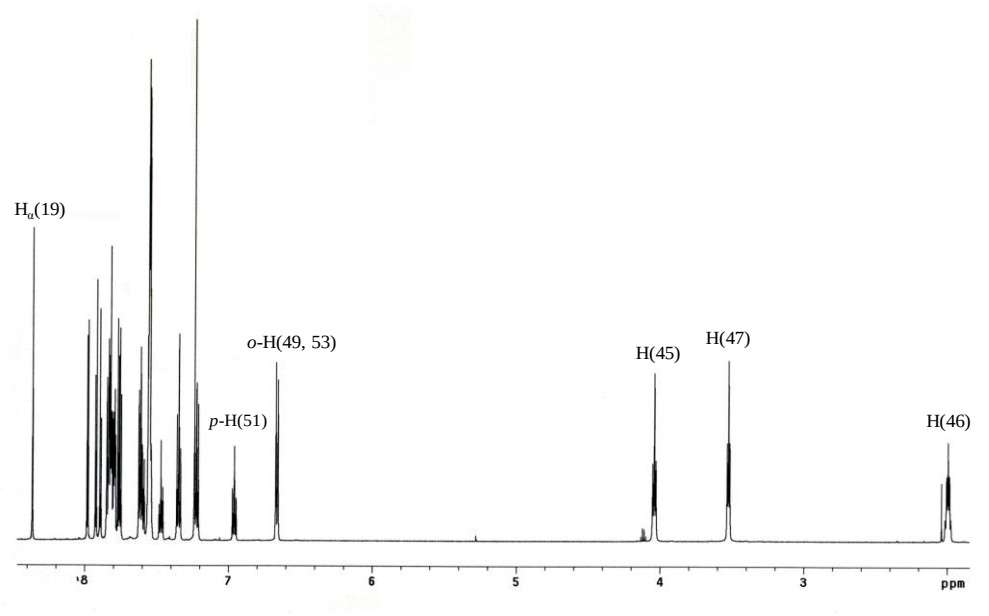


(b)

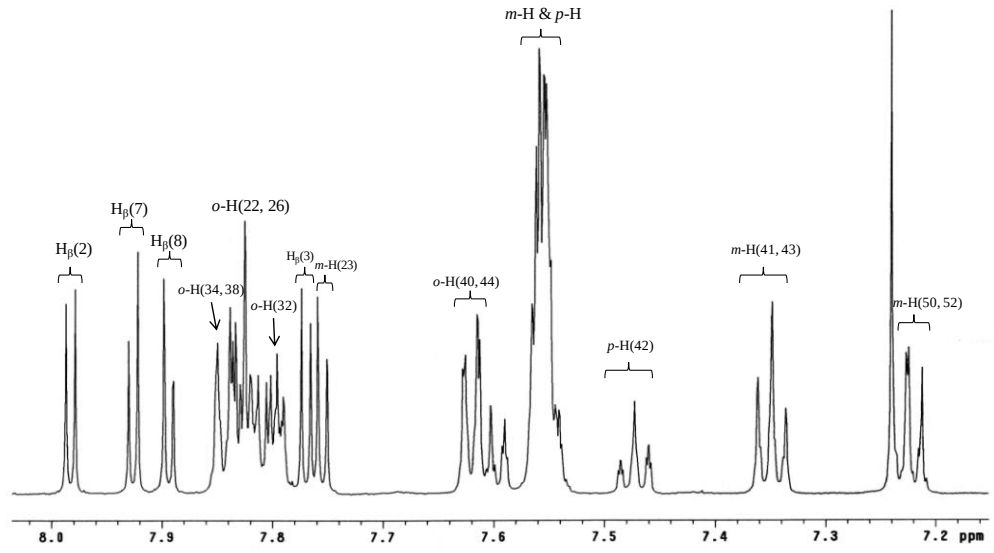
Figure S4. ^{1}H NMR spectra for **8** at 599.95 MHz in $CDCl_3$ at 20 ℃ :
(a) entire spectrum; (b) expansion of the region 7.50-8.30 ppm in (a) showing seven different β-pyrrole protons H_β and phenyl protons (*o*-H, *m*, *p*-H). Chemical shifts are in ppm from $CDCl_3$ at 7.24 ppm.

The description for the ^{1}H NMR of H_{β} in 8.

The doublet at 8.30 ppm is assigned to $H_{\beta}(2)$ with ^{3}J(H-H) = 4.5 Hz and the other doublet at 7.76 ppm is due to $H_{\beta}(3)$ with ^{3}J(H-H) = 4.5 Hz. The doublet at 8.19 ppm is assigned to $H_{\beta}(13)$ with ^{3}J(H-H) = 4.8 Hz and the other doublet at 7.78 ppm is due to $H_{\beta}(12)$ with ^{3}J(H-H) = 4.8 Hz. The doublet at 7.69 ppm is assigned to $H_{\beta}(7)$ with ^{3}J(H-H) = 5.7 Hz and the other doublet at 7.62 ppm is due to $H_{\beta}(8)$ with ^{3}J(H-H) = 5.7 Hz.



(a)

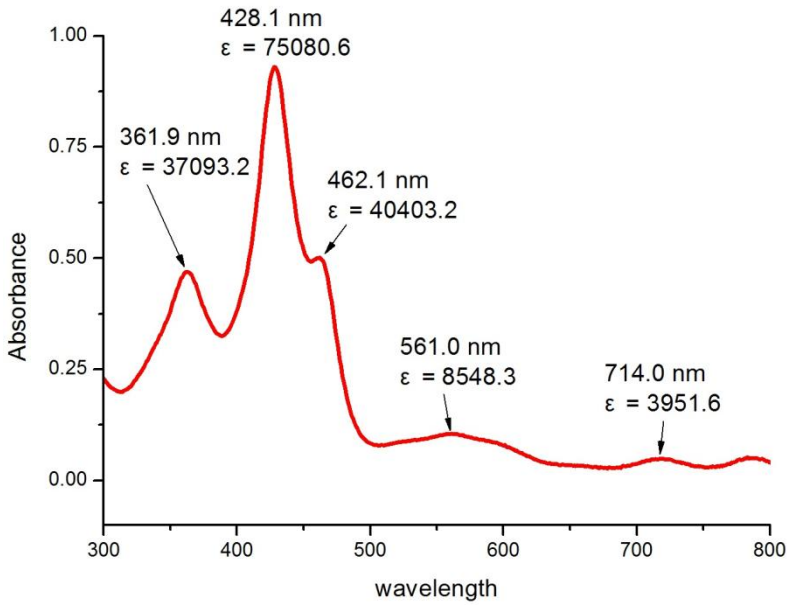


(b)

Figure S5. ^{1}H NMR spectra of **7** at 599.94 MHz in $CDCl_3$ at 20 ℃
(a) entire spectrum; (b) expansion of the region 7.20-8.00 ppm in (a) showing β-pyrrole protons H_β and phenyl protons (*o*-H, *m*, *p*-H)

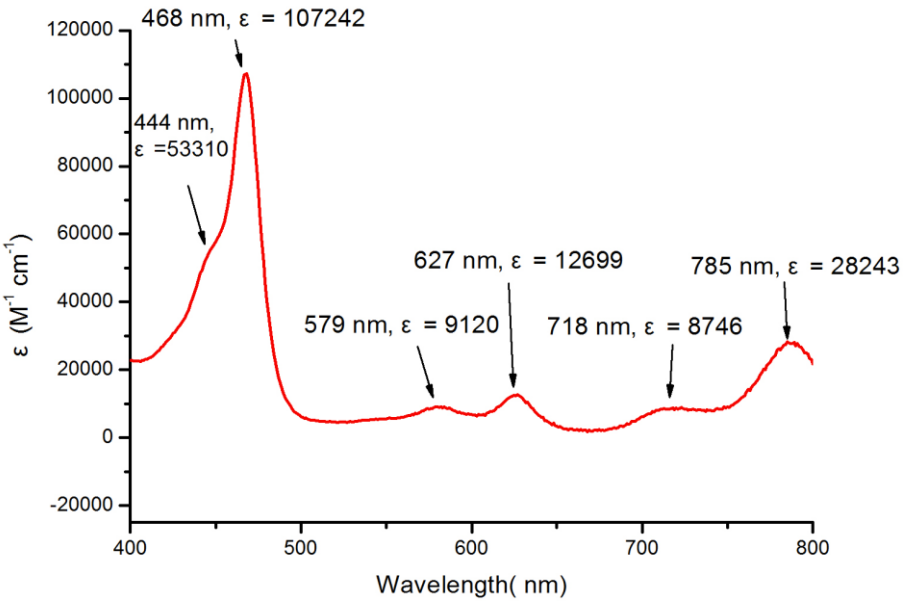
The description for the ^{1}H NMR of H_{β} in 7.

The doublet at 7.99 ppm is assigned to $H_{\beta}(2)$ with ^{3}J(H-H) = 4.8 Hz and the other doublet at 7.77 ppm is due to $H_{\beta}(3)$ with ^{3}J(H-H) = 4.8 Hz. The doublet at 7.93 ppm is assigned to $H_{\beta}(7)$ with ^{3}J(H-H) = 5.1 Hz and the other doublet at 7.89 ppm is due to $H_{\beta}(8)$ with ^{3}J(H-H) = 5.1 Hz.

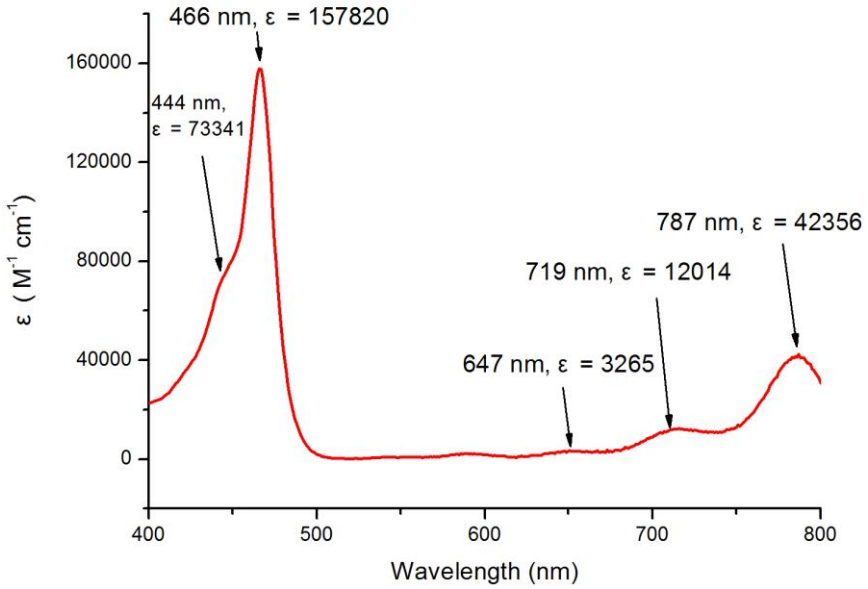


(7)

Figure S6. The UV/vis spectrum of Ni(2-$NCH_2CH_2CH_2OC_6H_5$NCTPP) **(7)** in CH_2Cl_2 at 20 ℃.

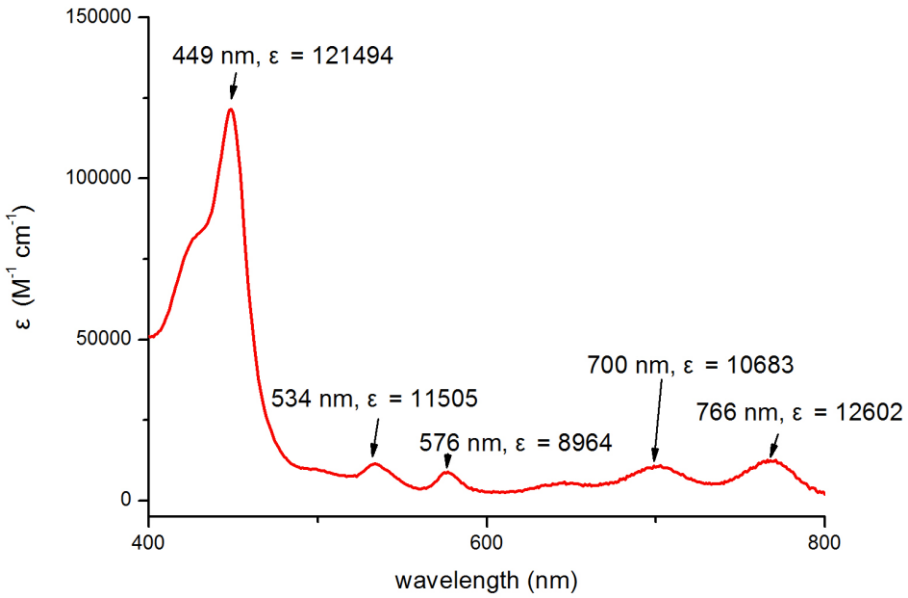


(a) (**4**)

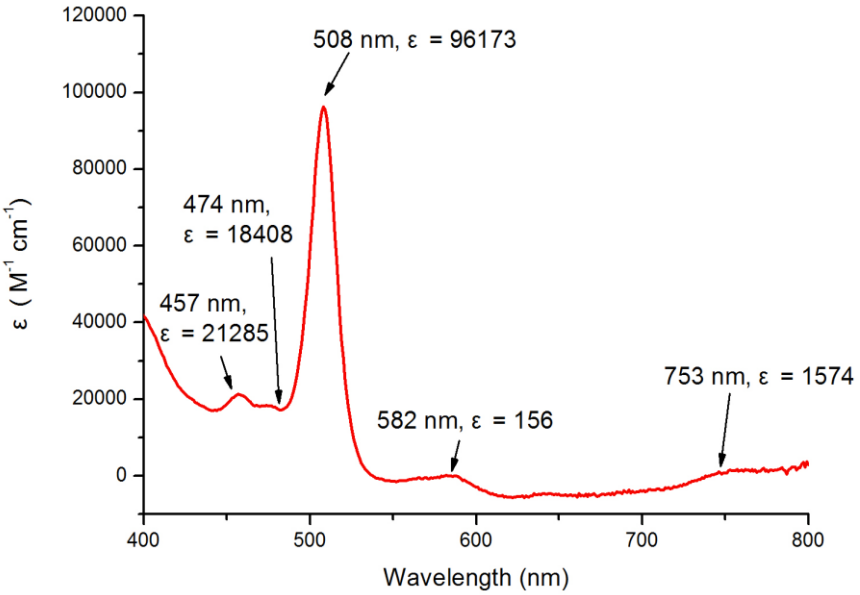


(b) (**8**)

Figure S7. The UV/vis spectra of (a) Zn(2-$NCH_2COOC_2H_5$NCTPP)Cl (**4**) and (b) Zn(2-NCH_2COOCH_3NCTPP)Cl (**8**) in CH_2Cl_2 at 20 ℃.



(a) (**5**)



(b) (**6**)

Figure S8. The UV/vis spectra of (a) Pd(2-$NCH_2COOC_2H_5$NCTPP) (**5**) and (b) Mn(2-$NCH_2COOC_2H_5$NCTPP)Br (**6**) in CH_2Cl_2 at 20 ℃.