Peripheral substitution as a tool for tuning electron-accepting properties of phthalocyanine analogs in intramolecular charge transfer

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Fig. S1 TLC (chloroform/THF (20 : 1)) of the mixture of congeners arising from reaction of precursor 6 and 10 with zinc acetate in pyridine.

Fig. S2 Influence of extinction coefficient of $1\text{Zn}$ at 652 nm on concentration (a) and the absorption spectra of the $1\text{Zn}$ ($\lambda_{\text{max}} = 652$ nm) (b) at different concentrations (0.8 µM to 100 µM). The comparison of normalized absorption spectra of $1\text{Zn}$ at 100 µM (green line) and 0.8 µM (orange line) (c).
Fig. S3 Absorption spectra of 2H (a), 3H (b), 4H (c), 5H (d) in THF at 1 μM concentration.
Fig. S4 Normalized absorption (blue), excitation (black) and emission (red) spectra of 1Zn (a), 2Zn (b), 3Zn (c), 4Zn (d), and 5Zn (e) in THF. The emission of 1Zn was too weak to obtain excitation spectra of sufficient quality.
Fig. S5 The changes of absorption spectra of s1Zn (a), s2Zn (b), s4Zn (c) and s5Zn (d) in DMSO (1 μM) upon addition of sulfuric acid. Insets: Dependence of absorption in Q-band maximum (black line) and quantum yields of fluorescence (ΦF, red line) on amount of sulfuric acid.

Fig. S6 Changes of ΦF values of studied TPyzPzs (1 μM) in DMSO after addition of sulfuric acid. s1Zn (square, red dashed line), s2Zn (triangle, orange dashed line), s4Zn (asterisk, green dashed line), s5Zn (dot, magenta dashed line).
Fig. S7 $^1$H NMR spectrum of 12 in CDCl$_3$.

Fig. S8 $^1$H NMR spectrum of 1Zn in the mixture of CDCl$_3$ and pyridine-d$_5$. Asterisk indicates signal of residual water.
Fig. S9 $^1$H NMR spectrum of $2H$ in the mixture of CDCl$_3$ and pyridine-d$_5$.

Fig. S10 $^1$H NMR spectrum of $2Zn$ in the mixture of CDCl$_3$ and pyridine-d$_5$. 
Fig. S11 $^1$H NMR spectrum of 3H in the mixture of CDCl$_3$ and pyridine-d$_5$. Asterisk indicates signal of residual water.

Fig. S12 $^1$H NMR spectrum of 3Zn in the mixture of CDCl$_3$ and pyridine-d$_5$. Asterisk indicates signal of residual water.
Fig. S13 $^1$H NMR spectrum of 4H in the mixture of CDCl$_3$ and pyridine-d$_5$. Asterisk indicates signal of residual water.

Fig. S14 $^1$H NMR spectrum of 4Zn in the mixture of CDCl$_3$ and pyridine-d$_5$. Asterisk indicates signal of residual water.
Fig. S15 $^1$H NMR spectrum of 5H in the mixture of CDCl$_3$ and pyridine-d$_5$. Asterisk indicates signal of residual water.

Fig. S16 $^1$H NMR spectrum of 5Zn in the mixture of CDCl$_3$ and pyridine-d$_5$. Asterisk indicates signal of residual water.