

Supporting Information

Table S1 The S_1 - T_1 gap value of M-Porphyrin and M-Porphyrin-PDI.

	$\Delta E_{ST} / \text{eV}$
Porphyrin	0.85
Fe¹-Porphyrin	3.34
Fe²-Porphyrin	1.13
Zn-Porphyrin	0.74
Mg-Porphyrin	0.71
PDI	1.14
Porphyrin-PDI	0.71
Fe¹-Porphyrin-PDI	3.54
Fe²-Porphyrin-PDI	0.67
Zn-Porphyrin-PDI	0.73
Mg-Porphyrin-PDI	0.70

Table S2 The S_1 - T_1 gap value of Compound 1-5

	$\Delta E_{ST} / \text{eV}$
Compound 1	0.25
Compound 2	0.34
Compound 3	0.73
Compound 4	0.31
Compound 5	0.31