Supporting Information

for

Effects of Temperature and Host Concentration on the Supramolecular Enantiodifferentiating [4+4] Photodimerization of 2-Anthracenecarboxylate through Triplet-Triplet Annihilation Catalyzed by Pt-Modified Cyclodextrins

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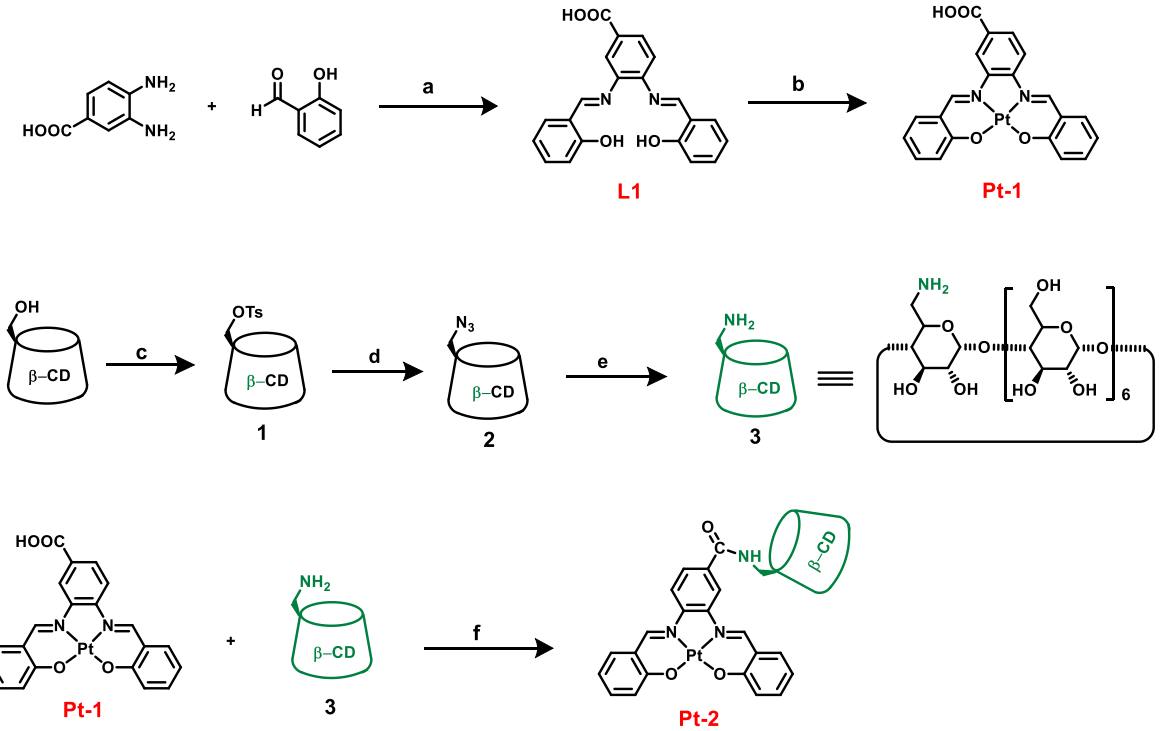
Contents

1. Synthetic route



Scheme S1. Synthesis of **Pt-1**, **Pt-2**: a) EtOH, RT, 2 h; b) K_2PtCl_4, K_2CO_3, DMSO, 80 ^oC; c) Pyridine, Paratoluensulfonyl Chloride, RT, 6 h; d) NaN_3, DMF/H_2O (10/1, v/v), 80 ^oC; e) 1) PPh_3, DMF, RT, 6 h; 2) NH_3•H_2O, RT, 1 h; f) 1) EDC, HOBT, -20 ^oC, 2 h; 2) **3**, RT, 6 h;

2. NMR and HRMS spectra of Pt-2 and AC

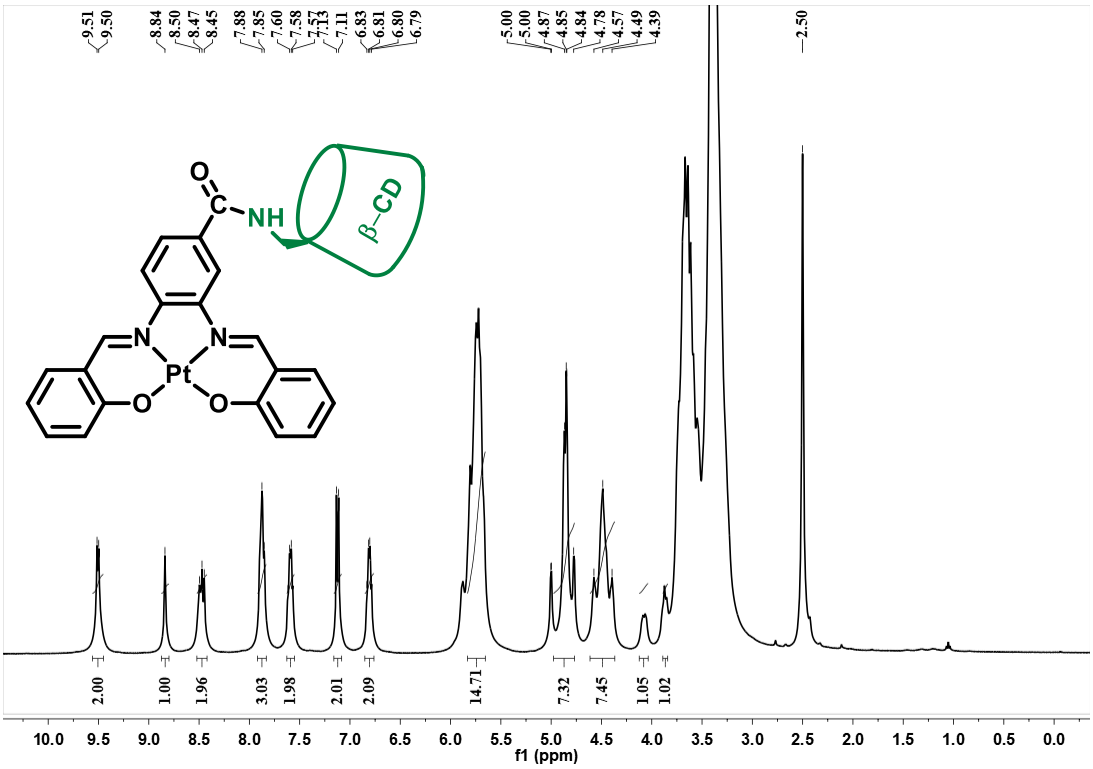


Figure S1. ^{1}H NMR spectrum (400 MHz, DMSO-d_6, room temperature) of **Pt-2.**

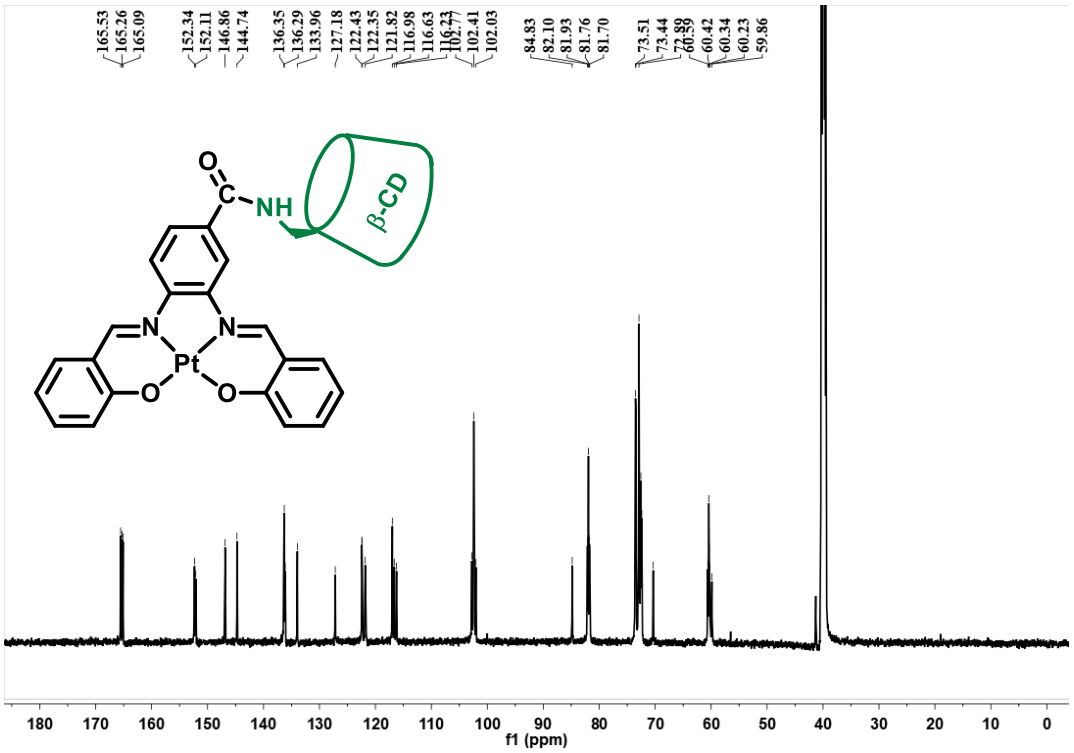


Figure S2. ^{13}C NMR spectrum (151 MHz, DMSO-d_6, room temperature) of **Pt-2.**

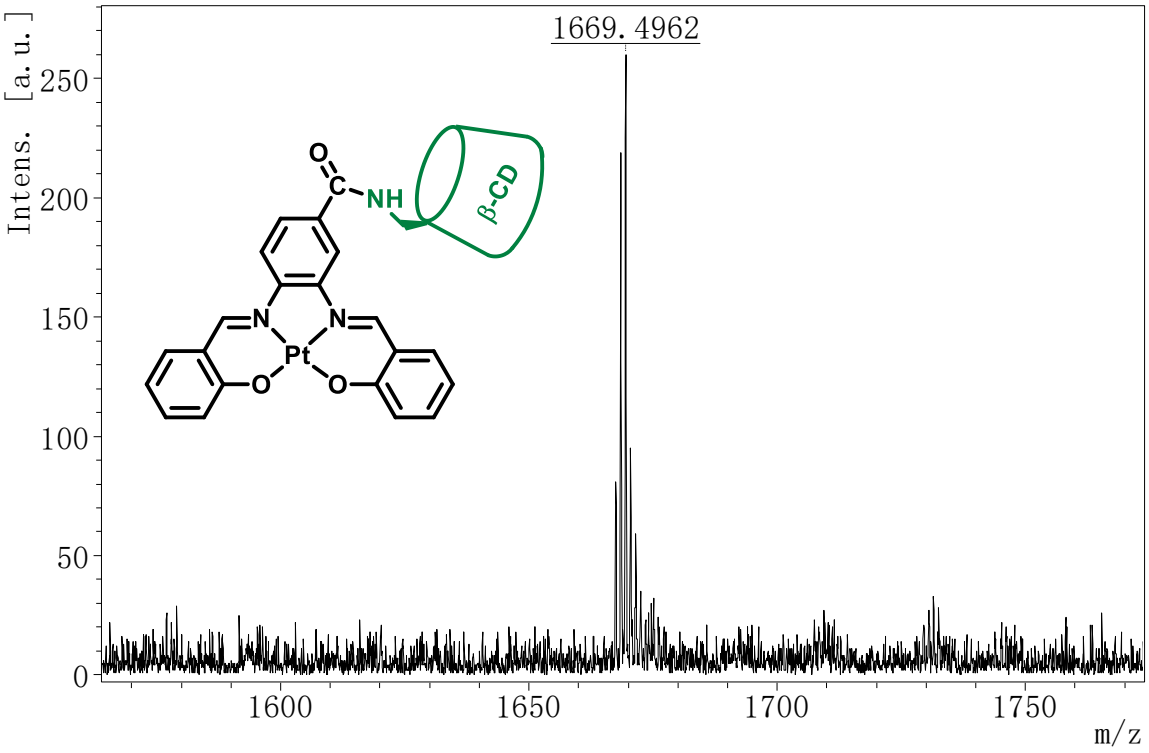


Figure S3. MALDI-TOF-MS of **Pt-2.**

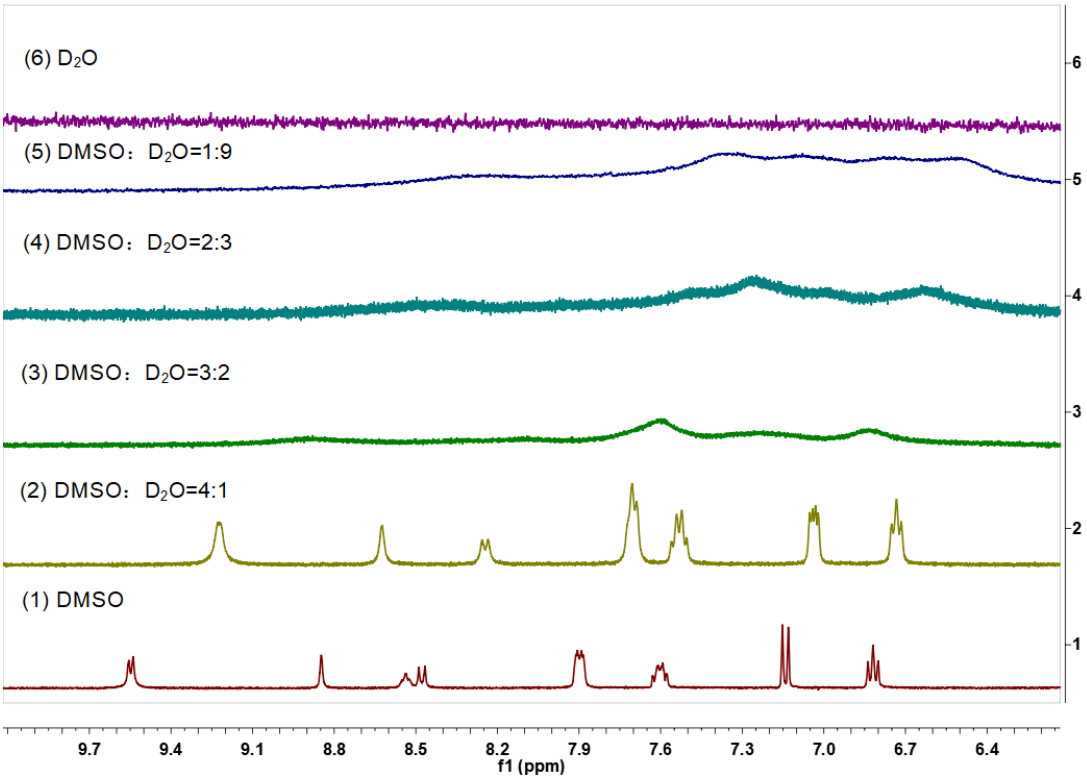


Figure S4. ^{1}H NMR spectra (400 MHz, room temperature) of **Pt-2**. (1) DMSO-d_6, (2) DMSO-d_6 : D_2O=1:4 (v:v), (3) DMSO-d_6 : D_2O=2:3 (v:v) , (4) DMSO-d_6 : D_2O=3:2 (v:v), (5) DMSO-d_6 : D_2O=1:9 (v:v), (6) D_2O.

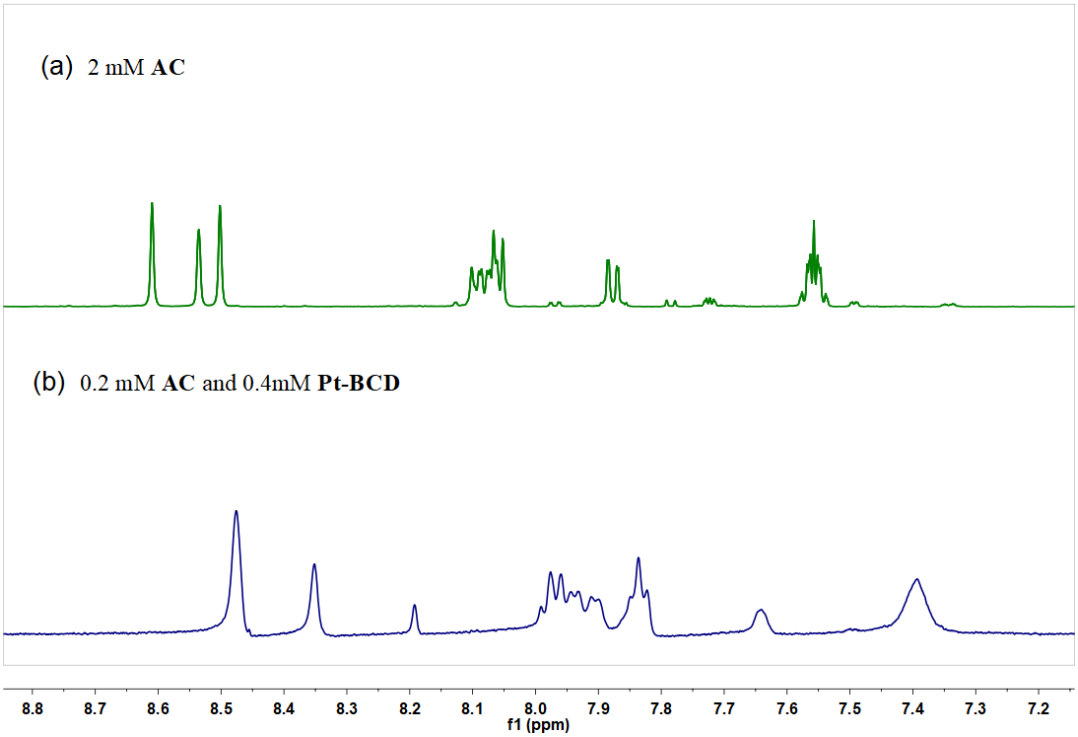


Figure S5. ^{1}H NMR spectra (600 MHz, room temperature) of (a) 2 mM **AC,** (b) 0.2 mM **AC** and 0.4mM **Pt-BCD**, measured in D_2O.

3. Absorption and emission spectra of Pt-1, Pt-2 and Pt-3

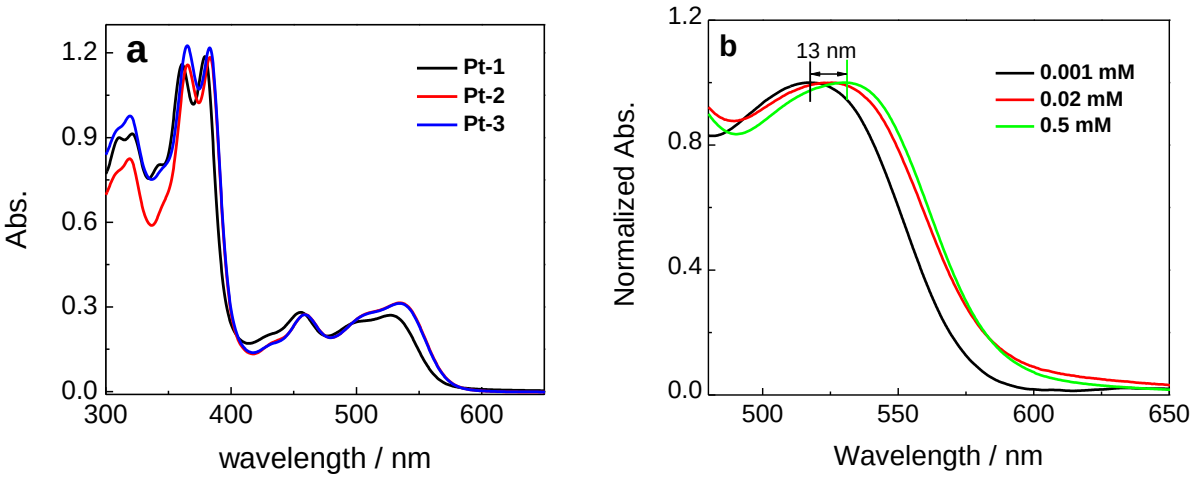


Figure S6. (a) UV-vis absorption spectra of **Pt-1, Pt-2,** and **Pt-3** in DMF solution, $c = 5 \times 10^{-5}$ M, 20 °C. (b) Normalized UV-vis absorption spectra of **Pt-2** at different concentrations in aqueous solution, 20 °C.

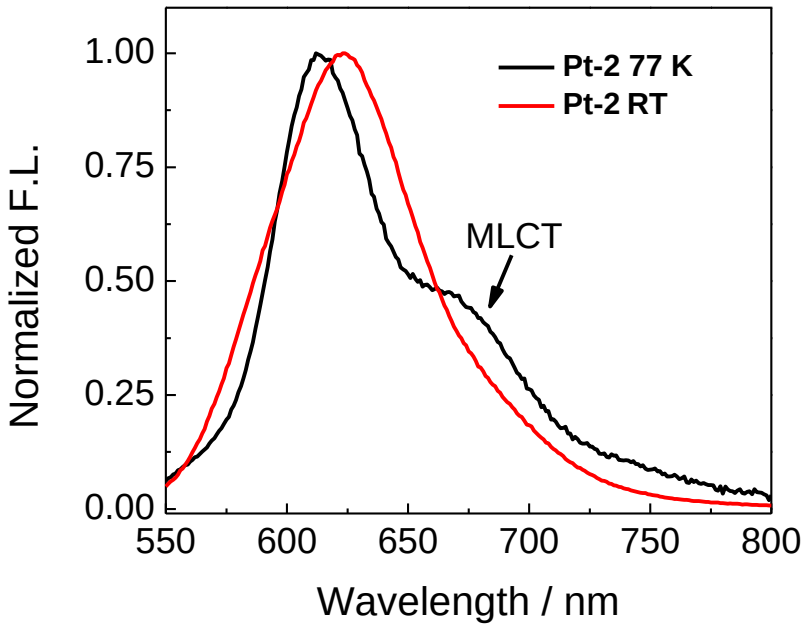


Figure S7. Emission spectra of **Pt-2** measured in ethanol-methanol (4:1, v/v) glass at 77 K (black) and in aqueous solution at room temperature (red) (298 K), λ_{ex} = 532 nm.

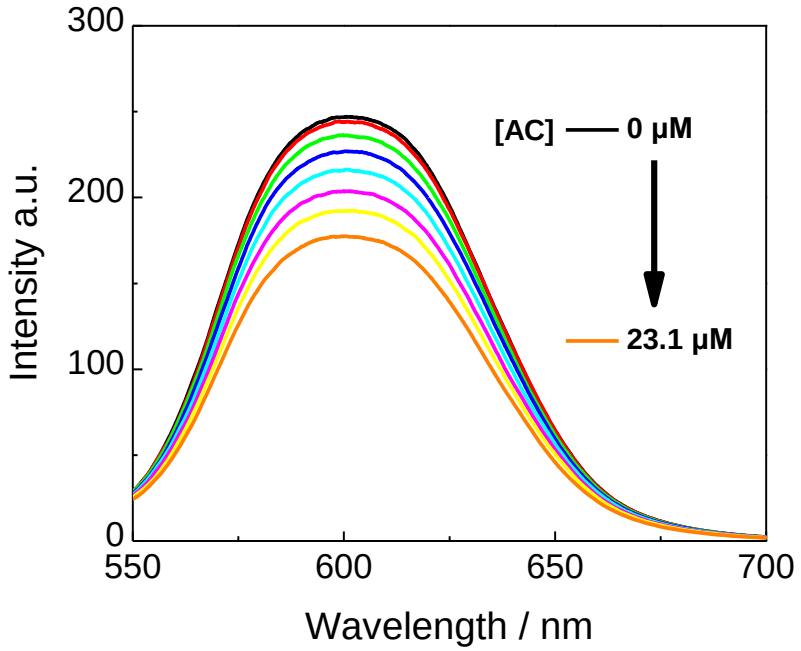


Figure S8. Phosphorescence spectral change of 5×10^{-5} M **Pt-2** upon increasing the concentration of AC (0 – 23.1 x 10^{-6} M), λ_{ex} = 532 nm, T = 20 °C.

4. Photophysical properties of the sensetizers/hosts Pt-1, Pt-2, and Pt-3

Table S1. Photophysical properties of the sensetizers/hosts **Pt-1, Pt-2,** and **Pt-3**, and Stern-Volmer quenching constant (K_{SV}) between sensitizers/host and **AC** at 20 °C.

	Abs[a]/nm	ε^b	**Em[c]/nm**	$\Phi_F{}^d$	$\tau_p{}^e$/μs	$K_{sv}/10^4$ M	$K_q/10^9$ $M^{-1}s^{-1}$
Pt-1	529	5396	599	0.13	2.0	1.28	6.46
Pt-2	533	6286	621	0.19	3.1	1.57	5.06
Pt-3	533	6267	611	0.20	4.1	2.29	5.65

[a] In DMF at 5×10^{-5} M. [b] Molar absorption coefficient at the absorption maxima. [c] Emission in water at RT. [d] Fluorescence quantum yield, rose bengal as standard (Φ_F = 0.11 in EtOH). [e] Phosphorescence lifetimes in deaerated water, 20°C.

5. Binding constants of Pt-3 and AC at different temperature

Table S2. Association Constants for the 1:1 and 1:2 Inclusion Complexes of **Pt-3** with AC Obtained by ITC at Various Temperature.

T/°C	Association constants [a] / M^{-1}		K_2 / K_1	K_1K_2 (10^6 M^{-2})
	K_1 [b]	K_2 [c]		
0	3810 (68)	5350 (88)	1.4	20.38 (0.006)
25	10400 (160)	719 (25)	0.07	7.48 (0.004)

[a] The values in parentheses the errors. [b] Association constant for **Pt-3** and **AC** making 1:1 complex. [C] Association constant for 1:1 complex and **AC** making 1:2 complex

6. CD spectra of Pt-2 and Pt-3

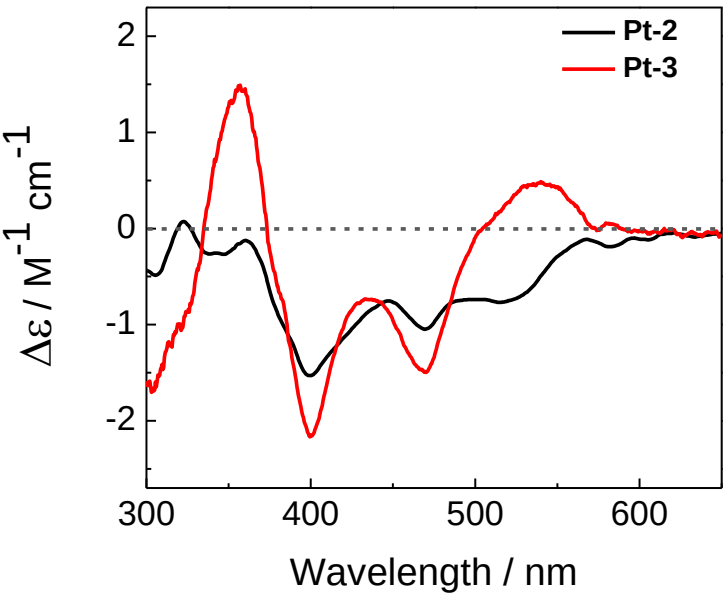


Figure S9. CD Spectra of **Pt-2, Pt-3** in aqueous solution, T=20 °C.

7. Job Plots of Pt-2 and Pt-3

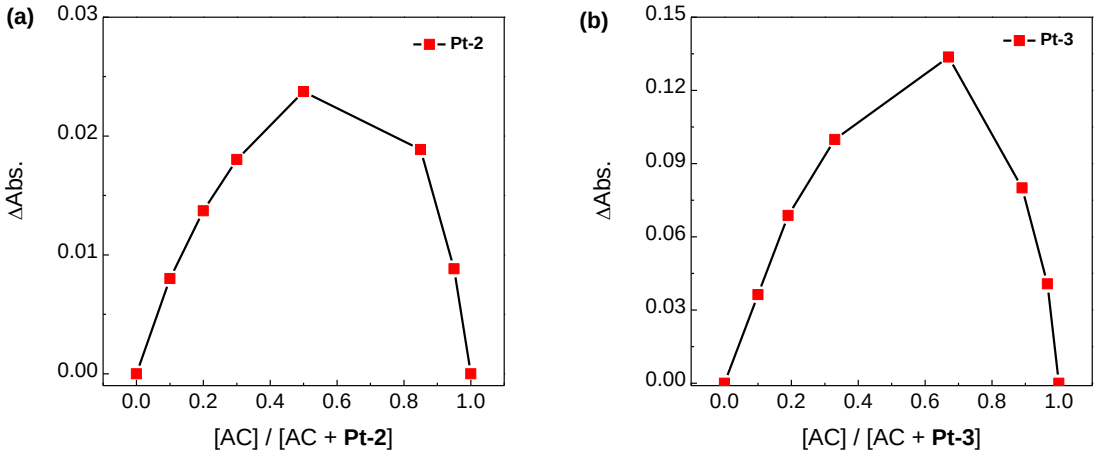


Figure S10. Job plots of the absorption changes at 532 nm of (a) **Pt-2**, (b) **Pt-3** measured by holding the total concentration of [AC]+[sensitizer]=0.2 mM

8. Stern-Volmer plots of Pt-3

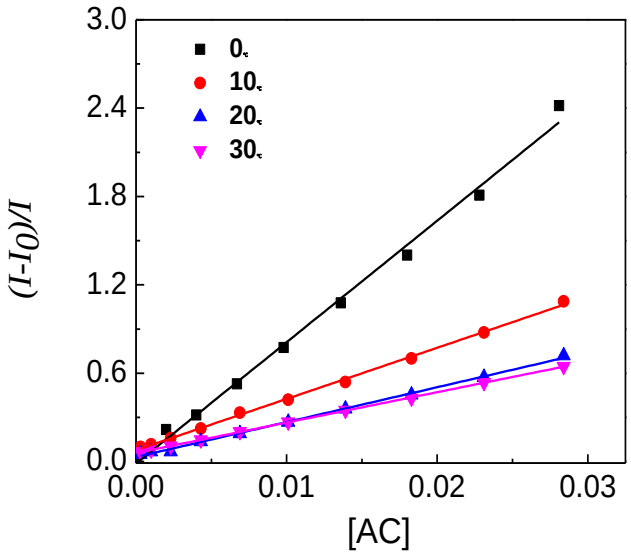


Figure S11. Stern-Volmer plots of **Pt-3** of $(I-I_0)/I$ versus [AC] in dearated water, $C_{[Pt\text{-}3]}=5 \times 10^{-5}$ M,$C_{[AC]}$ = 0 - 2.8 × 10^{-5} M, T=0, 10, 20, 30 °C.