Supporting Information

For

The environment-sensitivity of fluorescent ZTRS-Cd(II) complex was applied to discriminate different types of surfactants

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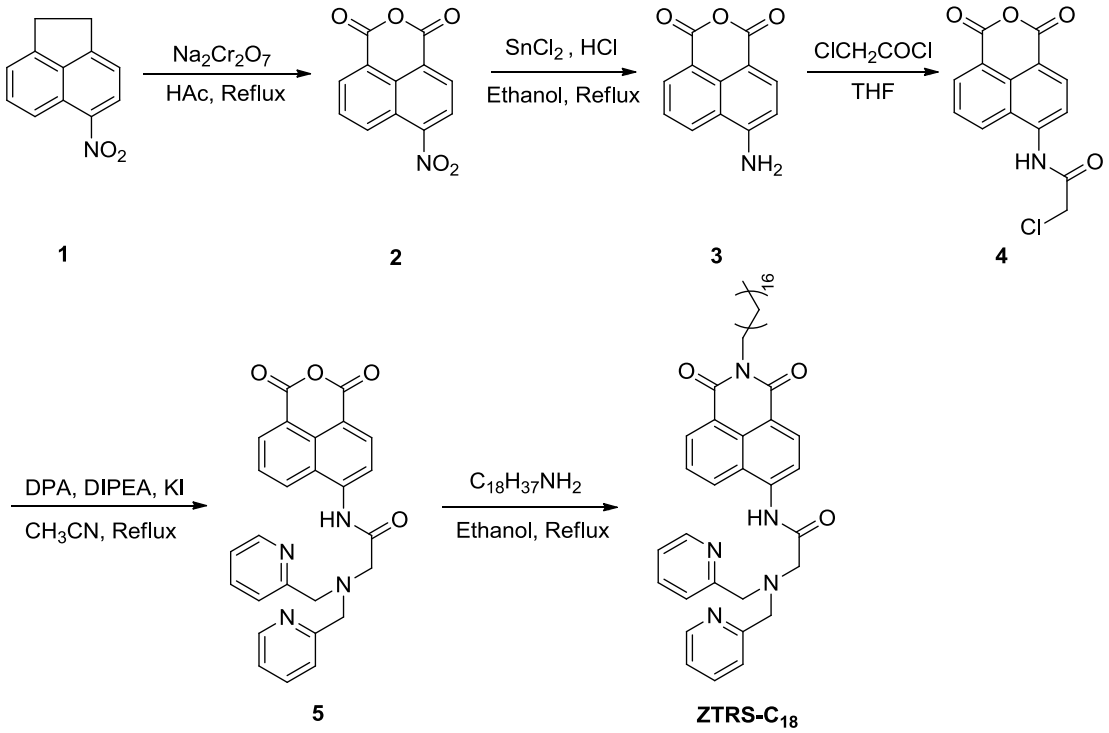
CONTENTS:

1. Materials and Instruments

Unless otherwise stated, all reagents were purchased from commercial suppliers and used without further purification. ^{1}H-NMR and ^{13}C-NMR spectra were recorded on Bruker 400 spectrometer with Chemical shifts reported in ppm and coupling constants (*J*) reported in Hz. Mass spectrometry data were performed on a HP1100LC/MSD mass spectrometer and a LC/Q-TOF MS spectrometer. UV-vis absorption spectra were obtained on an Agilent Cary 60 UV-Vis Spectrophotometer. Fluorescence measurements were performed on VAEIAN CARY Eclipse fluorescence spectrophotometer and Horiba FluoroMax 4 spectrometer. The dynamic light scatterings were measured by Malvern Zetasizer Nano. Transmission electron microscopes were performed on JEOL JEM-2100.

2. Synthesis



Scheme S1. Synthesis of compound **ZTRS-C$_{18}$**.

Synthesis of compound 2 and 3.

Compounds **2** and **3** were synthesized from 5-nitroacenaphthene according to the published procedure.[1, 2]

Synthesis of compound 4.

A solution of 170 mg (1.5 mmol) of 2-chloroacetyl in 5mL of dry THF was added dropwise to a solution of 63 mg (0.3 mmol) **3** in 30 mL of dry THF stirred at room temperature. After stirred 3h at room temperature, the solvents were removed under reduced pressure. The crude product was dissolved in 150 mL CH_2Cl_2, and washed with water and brine subsequently. Then the organic layer was separated, dried with Na_2SO_4, and finally removed under reduced pressure to give product **4** as pale solid in 97% yield (122 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.25 (s, 1H), 8.71 (d, *J* = 7.2 Hz, 1H), 8.69 – 8.60 (m, 2H), 8.31 (d, *J* = 8.8 Hz, 1H), 7.94 – 7.90 (m, 1H), 4.42 (s, 2H).

Synthesis of 5.

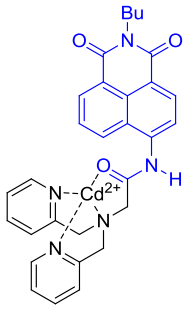
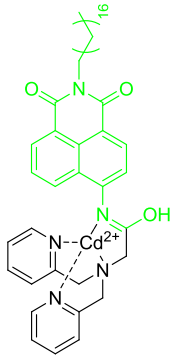
Compound **4** (185 mg, 0.64 mmol) was dissolved in 70 mL acetonitrile. Then Di-(2-picolyl) amine (DPA) (116 mg, 0.58 mmol, 0.9 eq), DIPEA (250 mg, 1.92 mmol, 3 eq) and potassium iodide were added. After stirred and refluxed for 3h under nitrogen atmosphere, the mixture was cooled to room temperature and filtered. The solvent was removed under reduced pressure to obtain yellow solid, which was purified by silica column chromatography with CH_2Cl_2/CH_3OH (50:1). (130 mg, yield 90%). ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.62 (s, 1H), 9.08 (d, J = 8.5 Hz, 1H), 8.62 (d, J = 7.1 Hz, 1H), 8.55 (dd, J = 17.9, 8.4 Hz, 2H), 8.40 (d, J = 4.5 Hz, 2H), 8.09 – 8.03 (m, 1H), 7.75 (t, J = 7.5 Hz, 2H), 7.46 (d, J = 7.7 Hz, 2H), 7.29 – 7.20 (m, 2H), 4.06 (s, 4H), 3.66 (s, 2H).

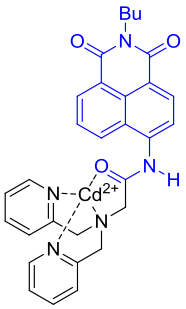
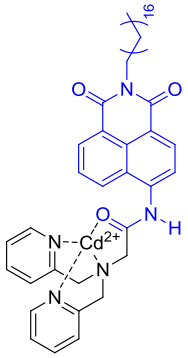
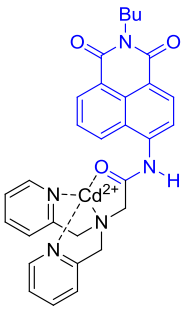
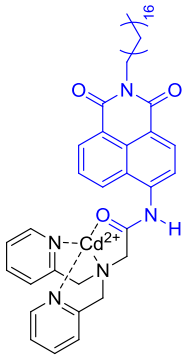
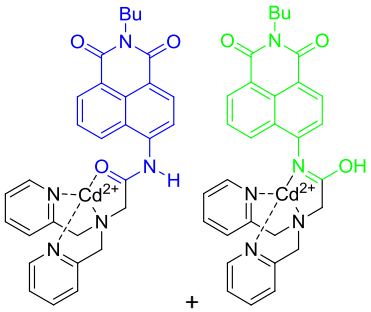
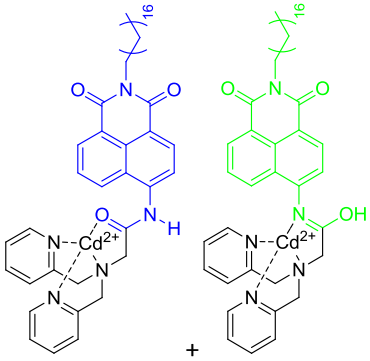
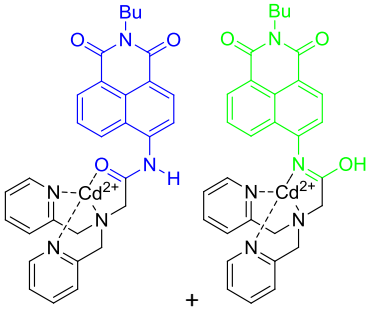
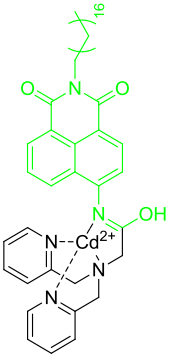
Synthesis of ZTRS-C_{18}.

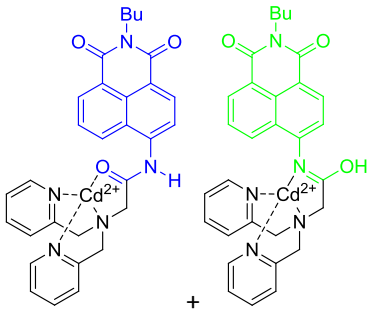
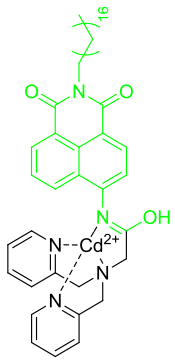
Compound **5** (45 mg, 0.1 mmol) and Octadecylamine (53 mg, 0.2 mmol, 2 eq.) were dissolved in 20 mL ethanol. After stirred and refluxed for 8h, the solvent was removed under reduced pressure. The crude product was purified by column chromatography with CH_2Cl_2/CH_3OH (50:1) and afforded the target product **ZTRS-C_{18}** as pale yellow solid (55 mg, yield 79%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.74 (s, 1H), 9.09 (d, J = 8.5 Hz, 1H), 8.69 (d, J = 7.0 Hz, 1H), 8.62 (dd, J = 25.9, 8.3 Hz, 2H), 8.45 (d, J = 4.4 Hz, 2H), 7.86 – 7.81 (m, 1H), 7.62 (t, J = 6.9 Hz, 2H), 7.31 (d, J = 7.7 Hz, 2H), 7.18 – 7.12 (m, 2H), 4.20 – 4.14 (m, 2H), 4.08 (s, 4H), 3.62 (s, 2H), 1.73 (d, J = 6.7 Hz, 2H), 1.25 (s, 30H), 0.88 (t, J = 6.7 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.79, 164.40, 163.78, 157.67, 149.60, 139.80, 136.73, 132.72, 131.05, 128.19, 126.13, 123.55, 123.39, 123.12, 122.72, 117.76, 117.14, 60.69, 59.15, 40.44, 31.92, 29.70, 29.36, 28.17, 27.20, 22.69, 14.13 ppm. MS (ESI) m/z: calcd for $C_{44}H_{58}N_5O_3$ $[M+H]^+$ 704.4540; observed 704.4553.

3. Supplementary Tables and Figures

Table S1. Binding modes of **ZTRS-Cd(II)** and **ZTRS-C_{18}-Cd(II)** in different surfactants.

	ZTRS-Cd(II)	**ZTRS-C_{18}-Cd(II)**
HEPES		

SDS		
SDBS		
BS-12		
DTAB		

Triton X-100		

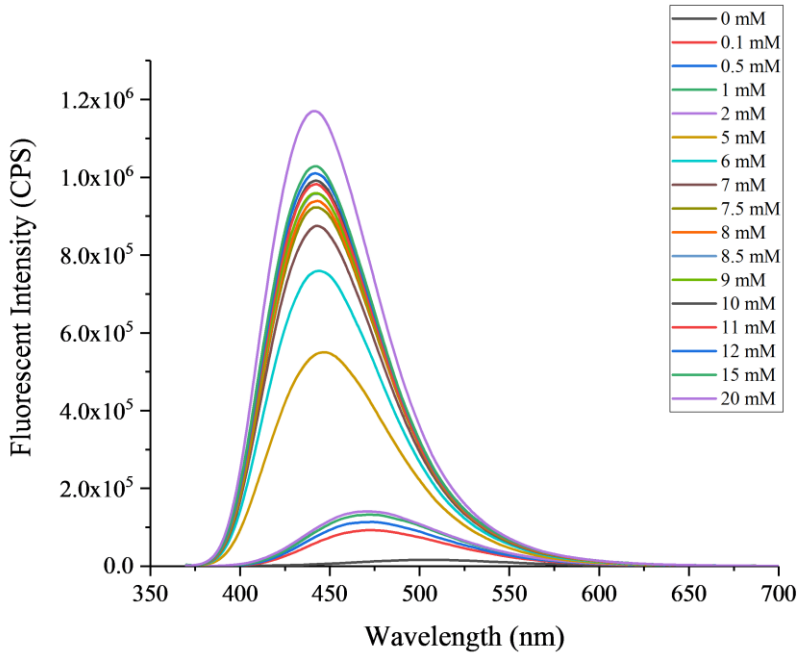


Figure S1. Fluorescence spectra of 10 μM **ZTRS-C_{18}-Cd(II)** in different concentrations of SDS.

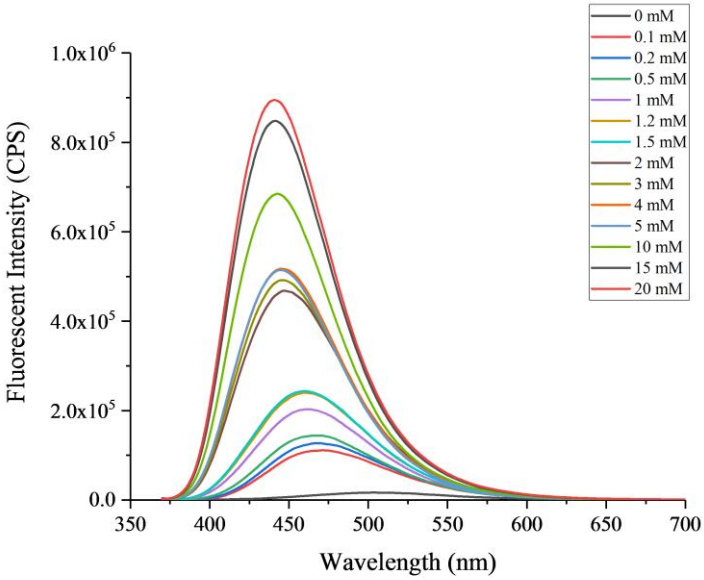


Figure S2. Fluorescence spectra of 10 μM **ZTRS-C_{18}-Cd(II)** in different concentrations of SDBS.

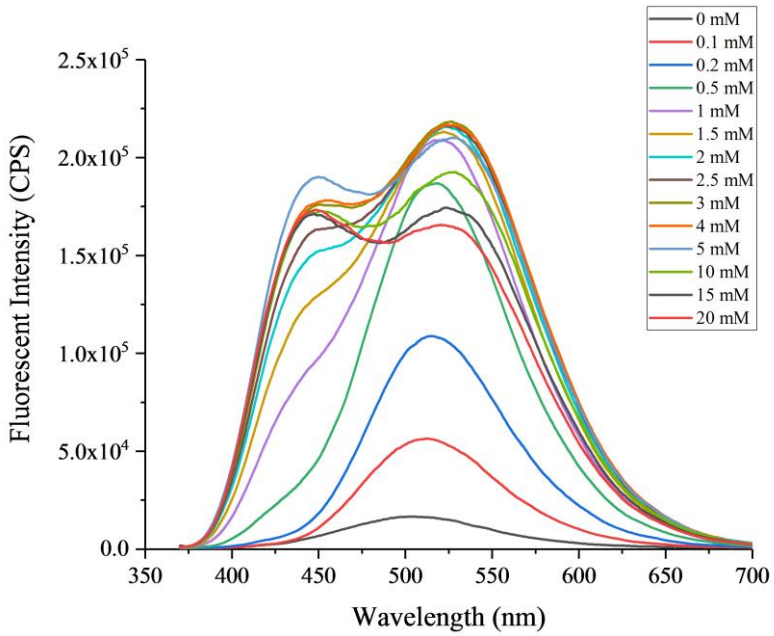


Figure S3. Fluorescence spectra of 10 μM **ZTRS-C_{18}-Cd(II)** in different concentrations of BS-12.

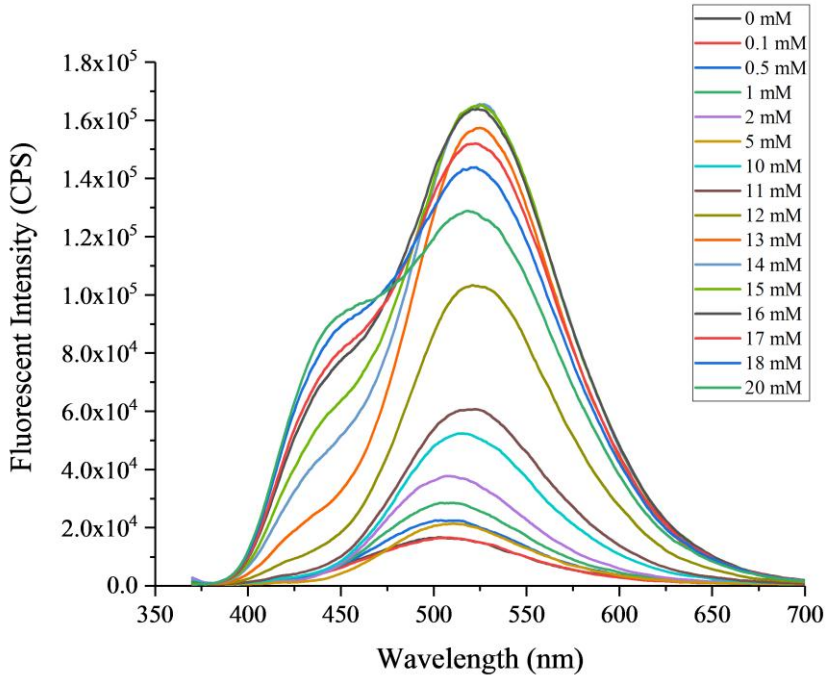


Figure S4. Fluorescence spectra of 10 μM **ZTRS-C_{18}-Cd(II)** in different concentrations of DTAB.

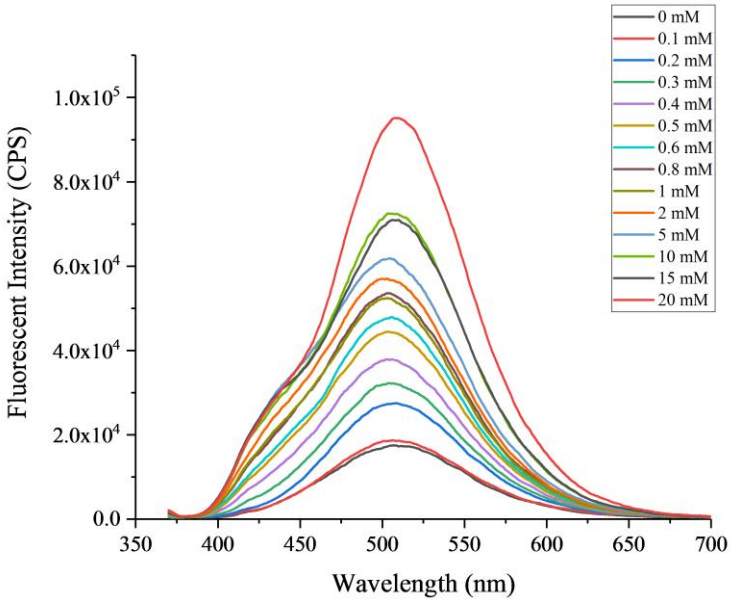


Figure S5. Fluorescence spectra of 10 μM **ZTRS-C_{18}-Cd(II)** in different concentrations of Triton X-100.

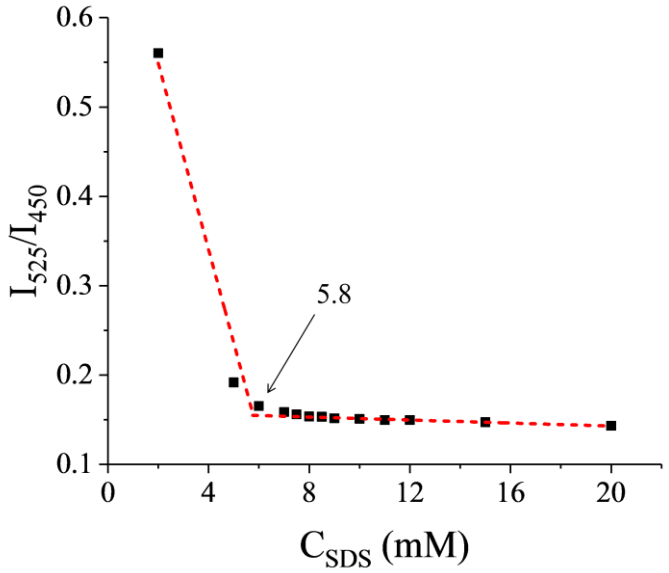


Figure S6. The ratio of I_{525}/I_{450} as a function to determine the CMC value of SDS.

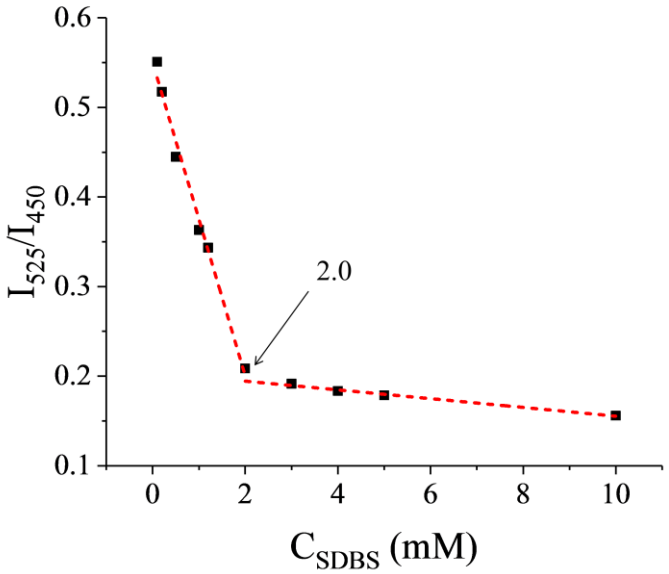


Figure S7. The ratio of I_{525}/I_{450} as a function to determine the CMC value of SDBS.

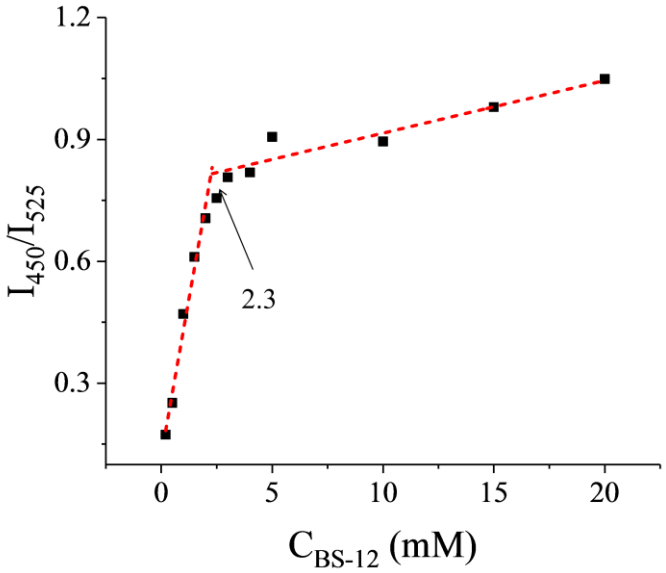


Figure S8. The ratio of I_{450}/I_{525} as a function to determine the CMC value of BS-12.

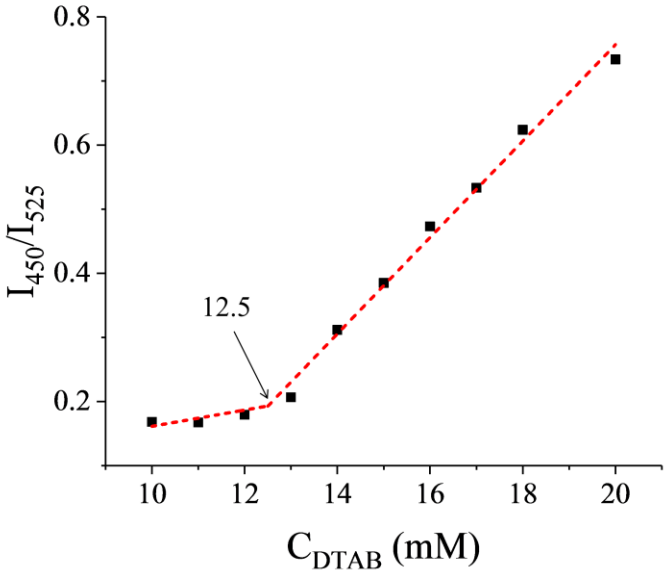


Figure S9. The ratio of I_{450}/I_{525} as a function to determine the CMC value of DTAB.

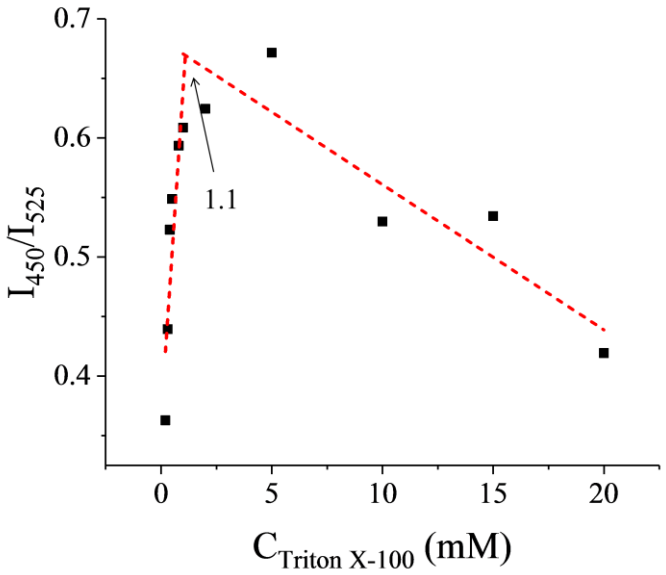


Figure S10. The ratio of I_{450}/I_{525} as a function to determine the CMC value of Triton X-100.

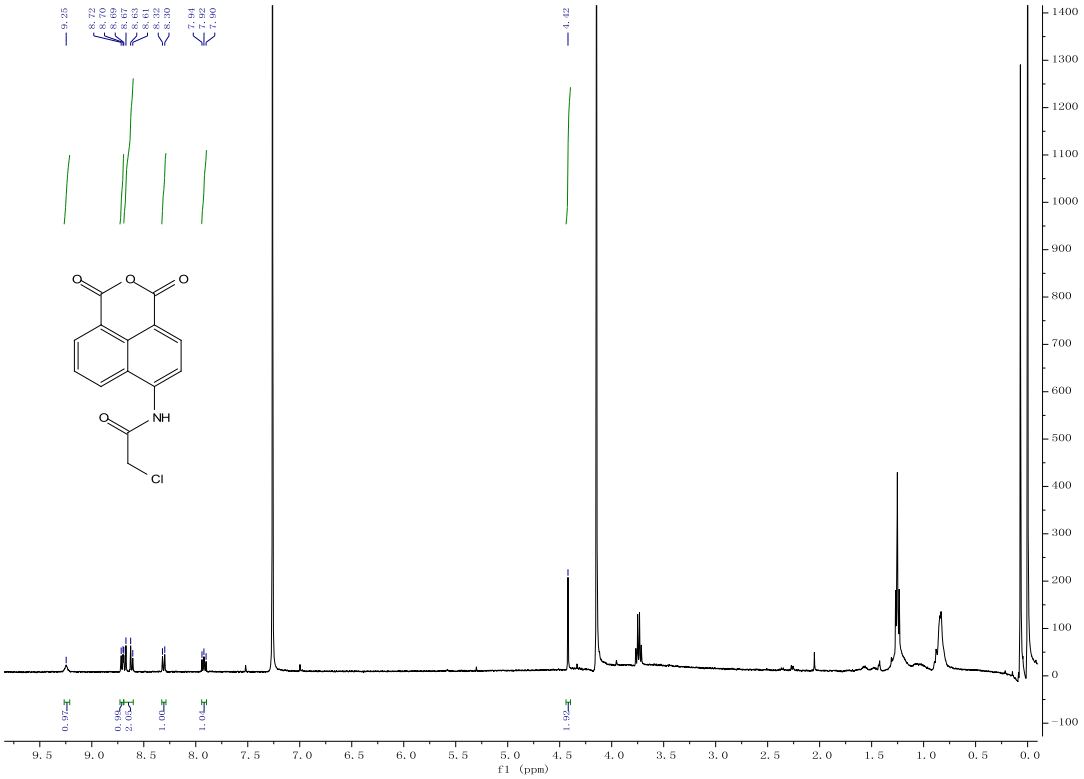


Figure S11. ^{1}H NMR spectra of compound **4** in $CDCl_3$.

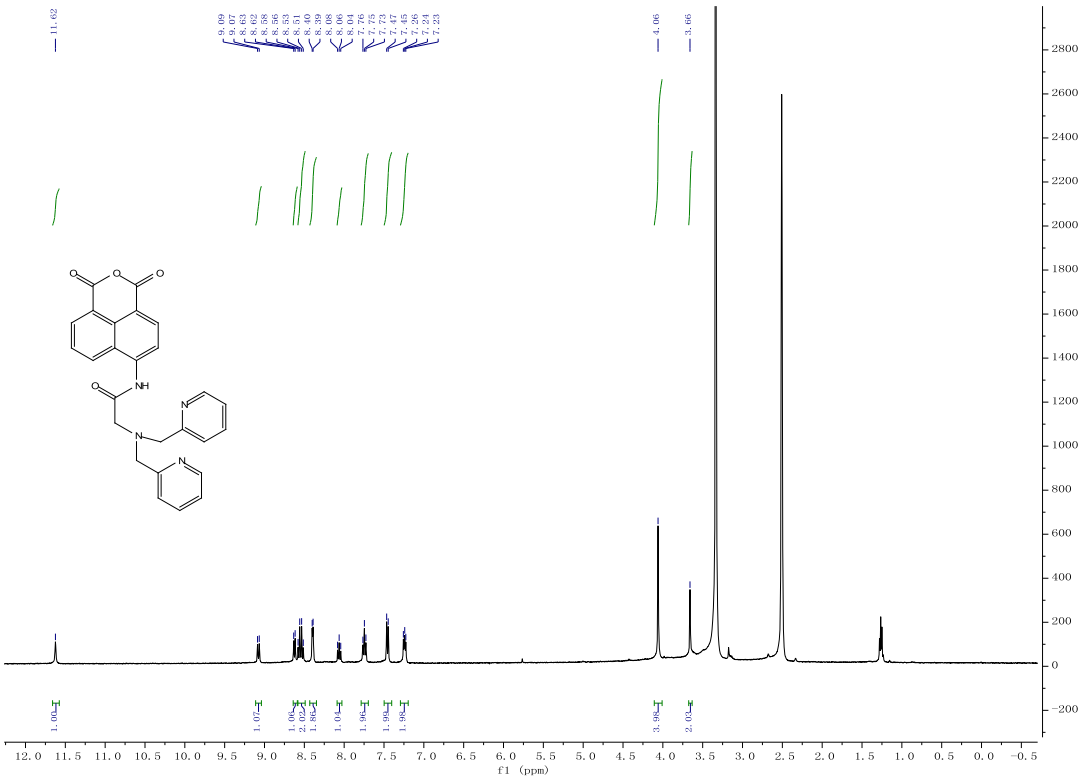


Figure S12. ^{1}H NMR spectra of compound **5** in DMSO-d_6.

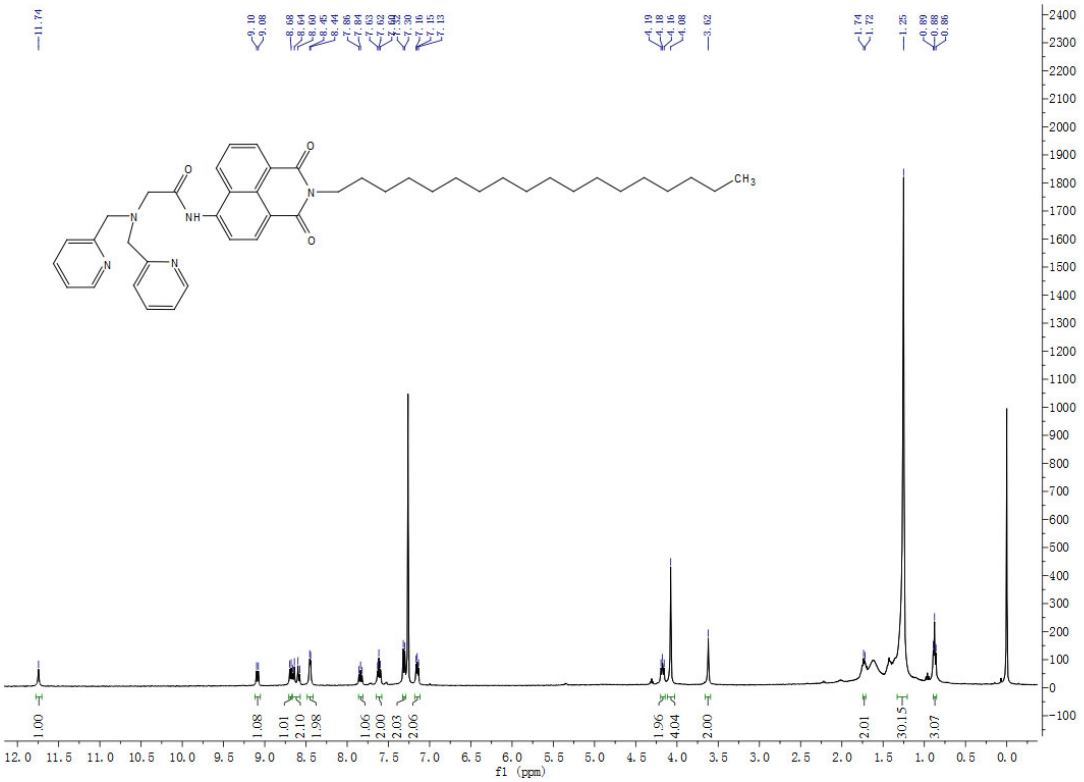


Figure S13. ^{1}H NMR spectra of **ZTRS-C$_{18}$** in $CDCl_3$.

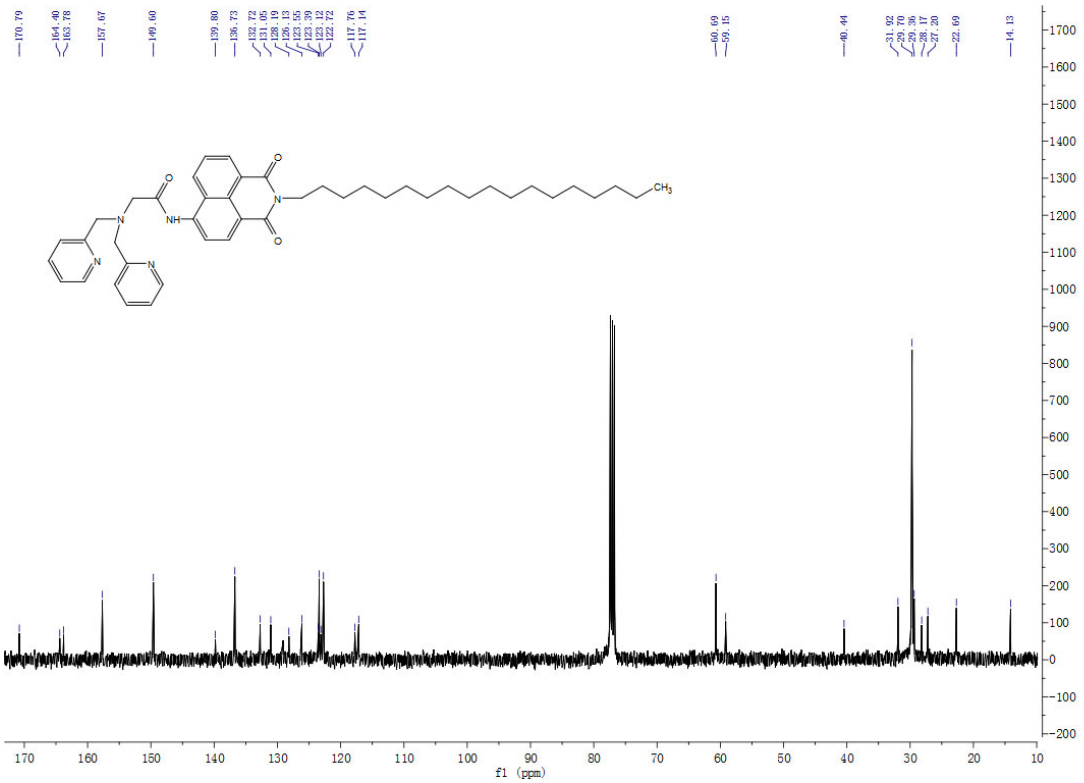


Figure S14. ^{13}C NMR spectra of **ZTRS-C$_{18}$** in $CDCl_3$.

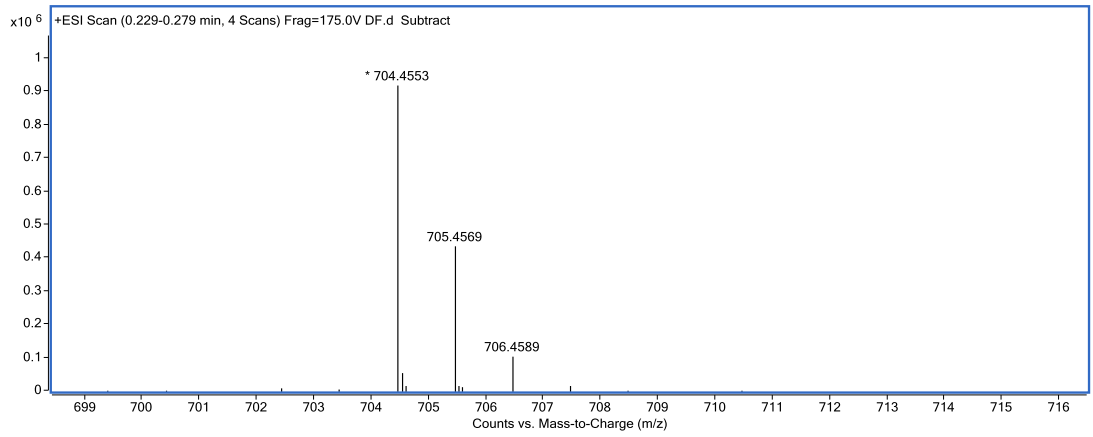


Figure S15. MS spectrum of **ZTRS-C$_{18}$**.

4. References

1. M. Dong, Y. W. Wang and Y. Peng, *Org Lett*, 2010, **12**, 5310-5313.
2. K. A. MacGregor, M. J. Robertson, K. A. Young, L. von Kleist, W. Stahlschmidt, A. Whiting, N. Chau, P. J. Robinson, V. Haucke and A. McCluskey, *J Med Chem*, 2014, **57**, 131-143.