

## Supplementary Information

### Synthesis, photophysical and electrochemical properties of new star-shaped molecule with 1,3,5-triethynylbenzene core and diketopyrrolopyrrole arms

Chunpeng Li, Qingfen Niu\*, Shanshan Zhang, Tianduo Li, Qingxin Yang,

*Shandong Provincial Key Laboratory of Molecular Engineering, School of Chemistry and Pharmaceutical Engineering, Qilu University of Technology (Shandong Academy of Sciences), Jinan 250353, People's Republic of China*

#### Supplementary captions

**Fig. S1**  $^1\text{H}$  NMR spectra of **BDPP-1**.

**Fig. S2**  $^{13}\text{C}$  NMR spectra of **BDPP-1**.

**Fig. S3** IR spectra of **BDPP-1**.

**Fig. S4** The MALDI-TOF mass spectra of **BDPP-1**.

**Table S1** Elemental analysis of **BDPP-1**.

**Fig. S5.** Differential Pulse Voltammetry experiments of **BDPP-1** in 0.1 M  $\text{Bu}_4\text{NClO}_4$  solution under  $\text{N}_2$ , pulse height 50 mV; step time 0.1 s; scan increment 5 mV; scan rate 50  $\text{mV s}^{-1}$ .

**Fig. S6(a)** DFT calculated optimized geometry (left) and conformations (right) of the star-shaped molecule; **(b)** The frontier molecular orbital distributions of the star-shaped molecule optimized by DFT calculations at the B3LYP/6-31G level.

**Fig. S7** Fluorescent emission spectra of **BDPP-1** in  $\text{CHCl}_3$  solution with different concentrations ranged from  $2.0 \times 10^{-4}$  to  $5.0 \times 10^{-6}$  M.

**Fig. S8** Fluorescent spectra of **BDPP-1** in different water fractions (fw) at a concentration of  $1.0 \times 10^{-5}$  M.

Fig. S1

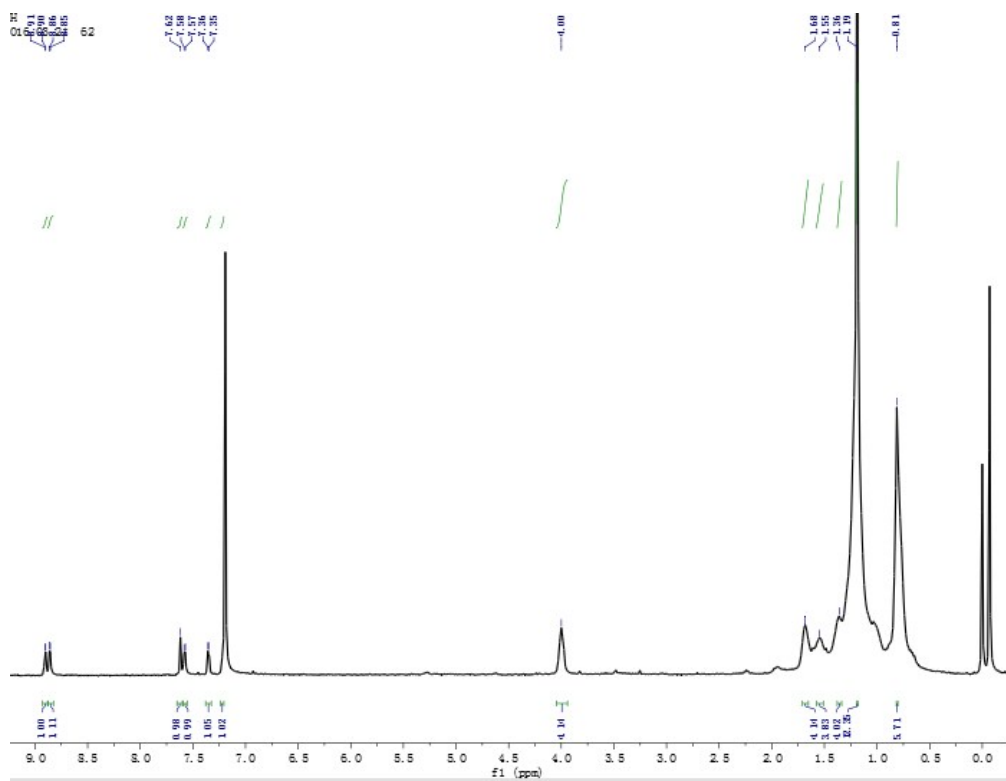


Fig. S2

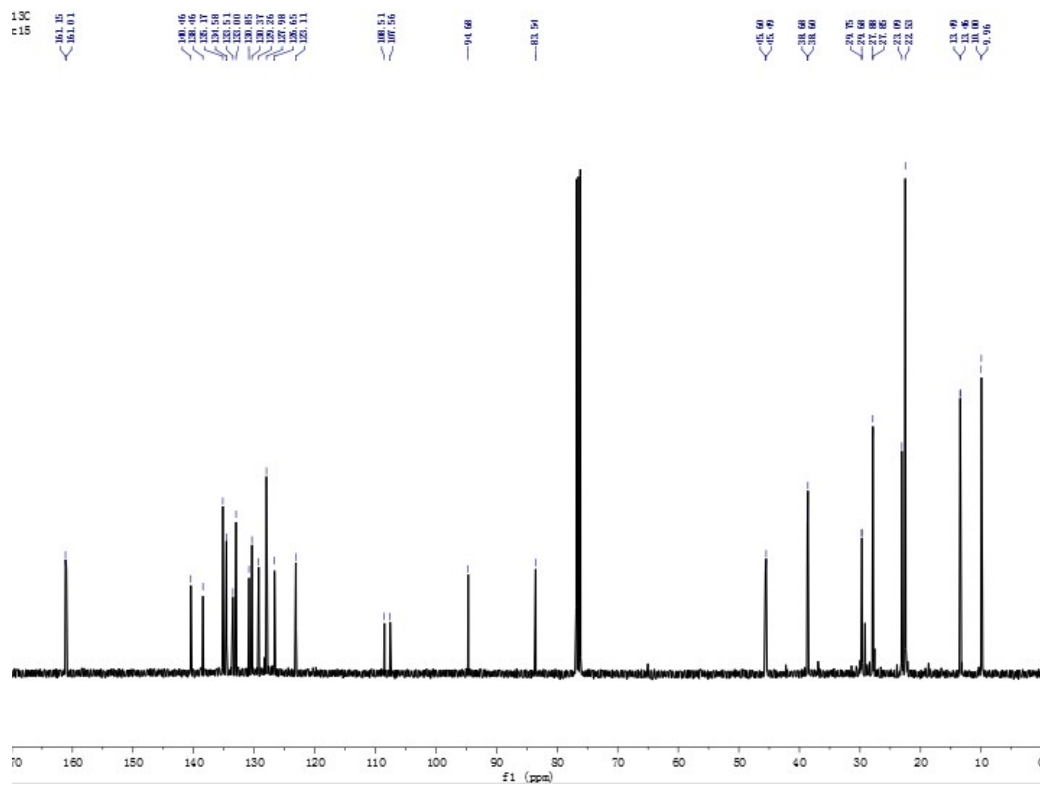


Fig. S3

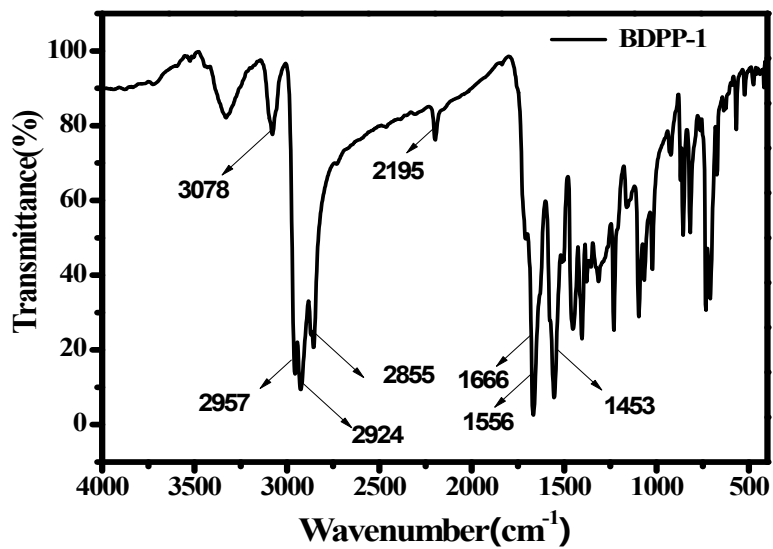


Fig. S4

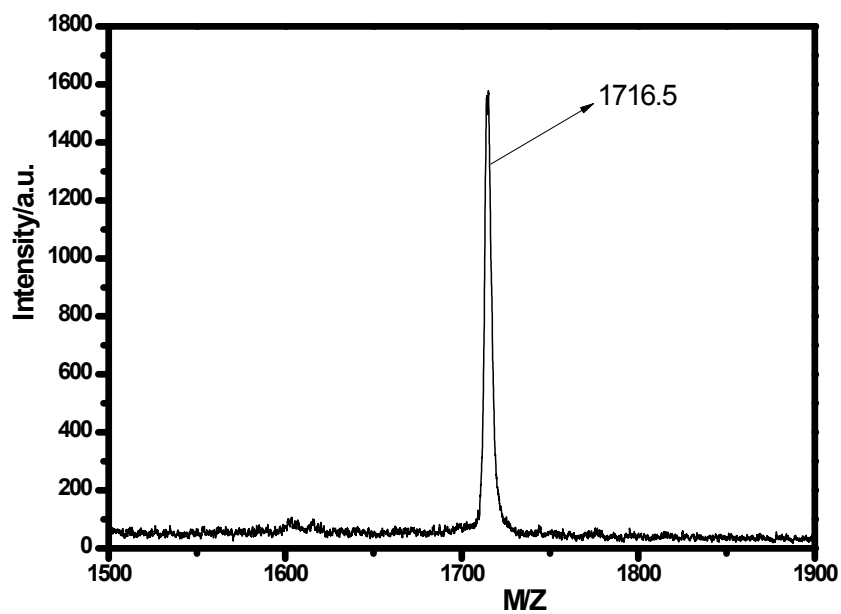
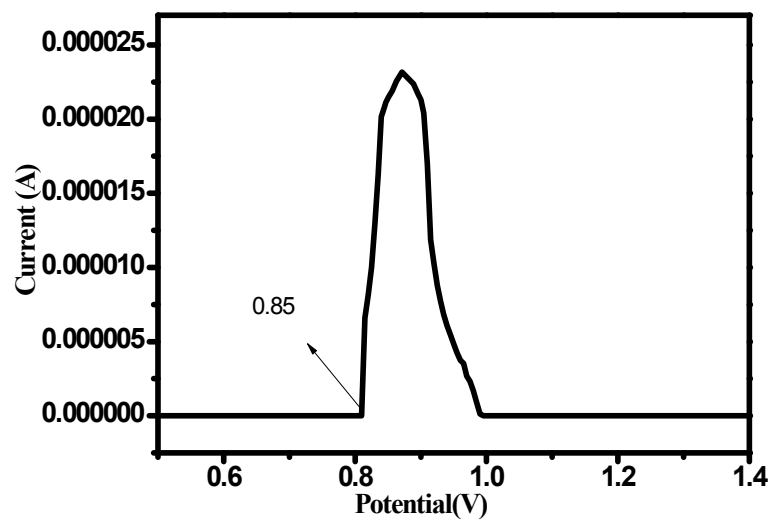


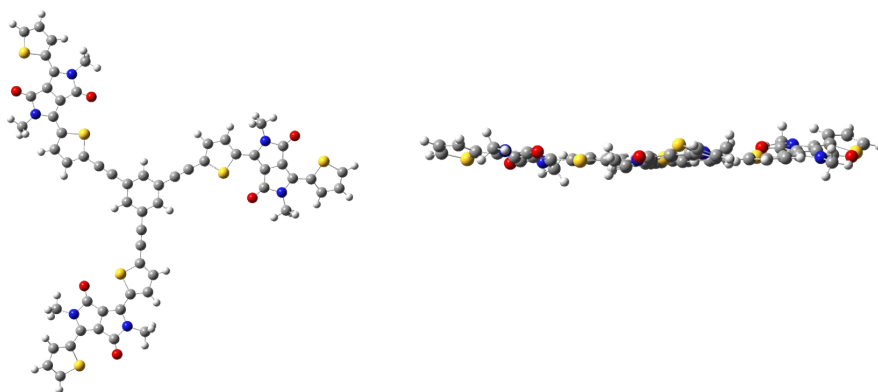
Table S1

Anal. (%)		Calc. (%)	
C	71.21	C	71.29
H	7.11	H	7.04
N	4.86	N	4.89
S	11.18	S	11.20

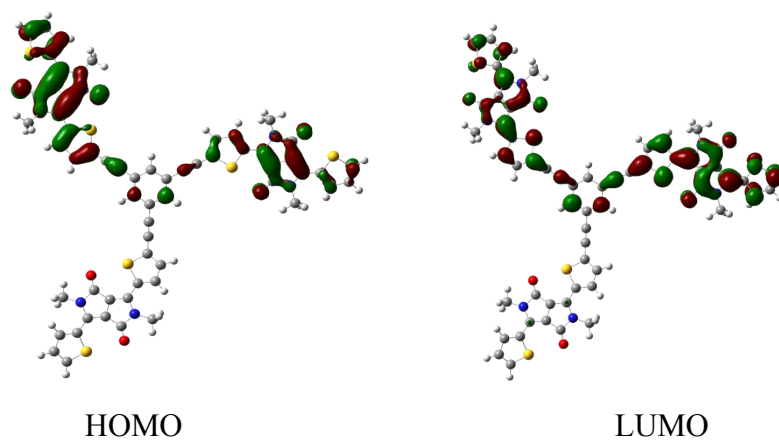
**Fig. S5**



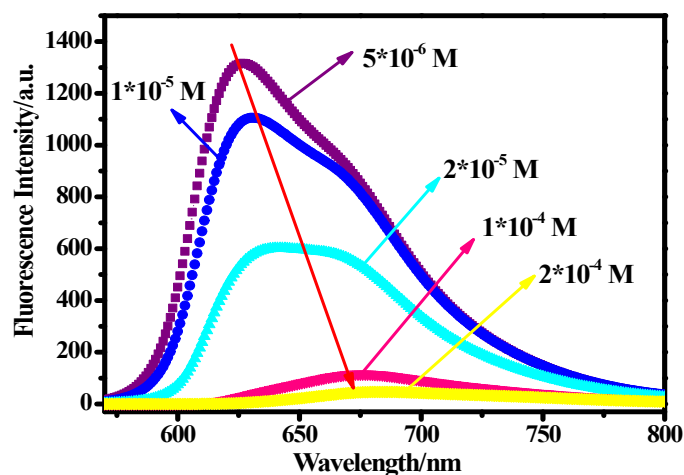
**Fig. S6 (a)**



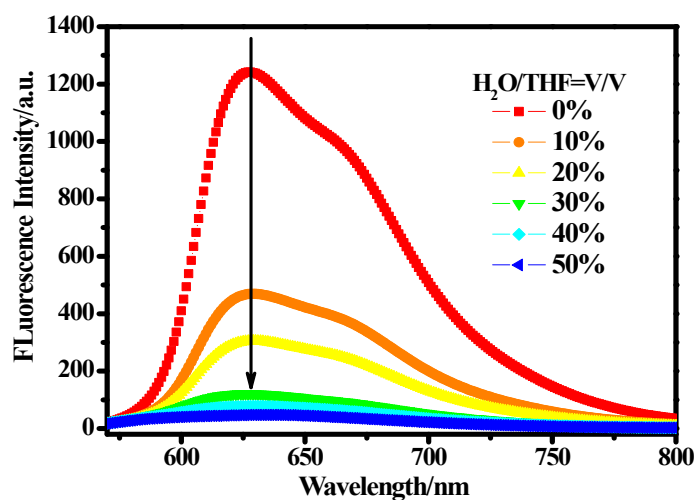
**Fig. S6 (b)**



**Fig. S7**



**Fig. S8**



The corresponding fluorescence spectra of **BDPP-1** with different concentrations in CHCl<sub>3</sub> solution ranged from  $2.0 \times 10^{-4}$  to  $5.0 \times 10^{-6}$  M was performed to further study its fluorescence properties. As shown in **Fig. S7**, the **BDPP-1** exhibited strong fluorescence intensity (620 nm) at the low concentration of  $5.0 \times 10^{-6}$  M, indicating strong red fluorescence. However, the fluorescence intensity of **BDPP-1** decreased significantly as the concentration increases and the emission peak also red-shifted from 620 to 675 nm. Surprisingly, when the concentration arrived at  $2.0 \times 10^{-4}$  M, the fluorescence was almost completely quenched, suggesting the so-called concentration aggregation-induced quenching (ACQ) effect [1].

To further investigate the aggregation-induced quenching properties, the fluorescence behavior of **BDPP-1** in THF-water mixtures were carried out and the great changes were

shown in **Fig. S8**. The **BDPP-1** displayed bright red fluorescence at 628 nm in pure THF solution. The emission intensity of **BDPP-1** decreased significantly when the fraction of water (fw) reached 10%. Whereas, as the fw arrived at 30%, the fluorescence quenched completely. These great changes in emission intensity of **BDPP-1** suggested a typical ACQ behavior. The distinct decrease of emission intensity against the increase of fw, which could be induced by the formation of aggregates and quenched the fluorescence through the intermolecular  $\pi$ - $\pi$  interaction.

**Reference:**

[1] Z. Wang, H. Shao, J. Ye, L. Tang and P. Lu, *J. Phys. Chem. B*, 2005, 109, 19627–19633.