Supramolecular self-assemblies for bacterial cell agglutination driven by directional charge-transfer interactions[†]

Dan Wu,*a Jie Shen,^b Hongzhen Baia and Guocan Yu^c

^a Institute of Chemical Biology and Pharmaceutical Chemistry, Department of Chemistry, Zhejiang University, Hangzhou 310027, P. R. China; Email address: <u>21106180@zju.edu.cn</u>

^b School of Medicine, Zhejiang University City College, Hangzhou 310015, P. R. China;

^c Laboratory of Molecular Imaging and Nanomedicine, National Institute of Biomedical Imaging and Bioengineering, National Institutes of Health, Bethesda, Maryland 20892, United States.

Electronic Supplementary Information (7 pages)

1.	Materials and methods	S2
2.	Investigation of the charge-transfer interactions	S3
3.	Self-assembly of the bolaform amphiphiles	S6

1. Materials and methods

Compounds ND, NP1 and NP2 were synthesized according to literature procedures.^{S1} Solvents were either employed as purchased or dried according to procedures described in the literature. UV-vis spectra were taken on a Shimadzu UV-2550 UV-vis spectrophotometer. The fluorescence experiments were conducted on a RF-5301 spectrofluorophotometer (Shimadzu Corporation, Japan). Transmission electron microscopy (TEM) investigations were carried out on a HT-7700 instrument. The critical aggregation concentration (CAC) values of the building blocks and the self-assemblies were determined on a DDS-307 instrument (Shanghai Precision & Scientific Instrument Co., Ltd.). Scanning probe microscopy (SPM) investigations were carried out on a VECCO/PI-NAHOSCPEIVA instrument. Viscosity measurements were carried out on Cannon-Ubbelohde semi-micro dilution viscometers at room temperature.

2. Investigation of the charge-transfer interactions



Fig. S1 Photographs of NP2, ND and NP2-ND (molar ratio = 1:1) in water showing their colors. The concentrations of NP2 and ND were both 1.00×10^{-3} M.



Fig. S2 UV-vis spectra of NP2, ND and NP2-ND (molar ratio = 1:1) in water. The concentrations of NP2 and ND were both 1.00×10^{-3} M.



Fig. S3 UV-vis titration of ND (5.00×10^{-5} M) in water at room temperature with different

concentrations of **NP2** (0, 0.750, 1.50, 2.50, 3.75, 5.00, 7.50, 6.00, 10.0 and $15.0 \times 10^{-5} \text{ M}^{-1}$).



Fig. S4 A mole ratio plot of the absorbance at 425 nm versus $[NP2]/[ND]_0$ showing a 1:1 stoichiometry of the charge-transfer complex between NP2 and ND. $[ND]_0 = 5.00 \times 10^{-5}$ M.



Fig. S5 Fluorescence emission spectra of ND (1.00×10^{-5} M, $\lambda_{ex} = 387$ nm) in water at room temperature with different concentrations of NP1 (0, 2.00, 4.00, 8.00, 10.00, 15.0, 20.0, 25.0, 30.0 and 40.0×10^{-6} M).



Fig. S6 Fluorescence emission spectra of **ND** (1.00×10^{-5} M, $\lambda_{ex} = 387$ nm) in water at room temperature with different concentrations of **NP2** (0, 2.00, 4.00, 8.00, 10.00, 15.0, 20.0, 25.0, 30.0 and 40.0×10^{-6} M).



Fig. S7 ¹H NMR spectra (500 MHz, D₂O, room temperature): (a) **NP1** (1.00 mM); (b) **NP1** (1.00 mM) and **ND** (1.00 mM); (c) **NP2** (1.00 mM); (d) **NP2** (1.00 mM) and **ND** (1.00 mM).



Fig. S8 The concentration-dependent conductivity of (a) NP1 and (b) ND.^{S1}



Fig. S9 The concentration-dependent conductivity of (a) NP2 and (b) NP2-ND.^{S1}



Fig. S10 Scanning probe microscopy investigation of the nanoribbons formed by NP2-ND.



Fig. S11 (a) Concentration dependence of diffusion coefficient (*D*) of NP2-ND from DLS results. (b) Specific viscosity of the CT complex NP2-ND in water at room temperature versus the concentration of NP2-ND.



Fig. S12 (a) TEM image of the nanoribbons self-assembled from NP2-ND. (b) Enlarged image of a.

References:

S1. G. Yu, J. Li, W. Yu, C. Han, Z. Mao, C. Gao and F. Huang, *Adv. Mater.*, 2013, 25, 6373–6379.