Supporting Information

Highly Selective Fluorescent Sensing for CN⁻ in Water:
Utilization of the Supramolecular Self-assembly

BingBing Shi, Peng Zhang, TaiBao Wei, Hong Yao, Qi Lin, YouMing Zhang*

E-mail: zhangnwnu@126.com

Key Laboratory of Eco-Environment-Related Polymer Materials, Ministry of Education of China; Key Laboratory of Polymer Materials of Gansu Province; College of Chemistry and Chemical Engineering, Northwest Normal University, Lanzhou, Gansu, 730070, P. R. China
General experimental section

Fresh double distilled water was used throughout the experiment. All other reagents and solvents were commercially available at analytical grade and were used without further purification. $^1$H NMR spectra were recorded on a Mercury-400BB spectrometer at 400 MHz. Chemical shifts are reported in ppm downfield from tetramethylsilane (TMS, $\delta$ scale with solvent resonances as internal standards) UV–vis spectra were recorded on a Shimadzu UV-2550 spectrometer. Photoluminescence spectra were performed on a Shimadzu RF-5301 fluorescence spectrophotometer.

All Fluorescence spectroscopy was carried out after the addition of tetrabutylammonium salts in DMSO, while keeping the ligand concentration constant ($4.0 \times 10^{-6}$ M) on a Shimadzu RF-5301 fluorescence spectrometer. The excitation wavelength was 346 nm. The solution of anions were prepared from the tetrabutylammonium salts of F$^-$, Cl$^-$, Br$^-$, I$^-$, AcO$^-$, H$_2$PO$_4^-$, HSO$_4^-$, ClO$_4^-$, CN$^-$.

The $^1$H NMR titration experiment was investigated by addition increasing concentrations of CN$^-$ in H$_2$O to the solution of S$_4$ (DMSO-$d_6$) in NMR tube. The spectra were recorded after mixing and the temperature of the NMR probe was kept constant at 298K.

XRD patterns were recorded at a scanning rate of 5o/min in the 2θ range of 2° to 50° with Cu-Kα radiation.

The association constants (Ka) were determined based on the fluorescent titration curve using the equation as follows: where $A$ and $A_0$ represent the fluorescent
intensity of host in the presence and absence of ions, respectively, \( A_{\text{max}} \) is the saturated intensity of host in the presence of excess amount of ions; \([G]\) is the concentration of ions added.[1]

\[
\frac{1}{A_{\text{max}} - A_0} = \frac{1}{A_1 - A_0} \left[ \frac{1}{K[G]^2} + 1 \right]
\]
**Figure S1** Absorbance spectra of $S_4$ (20μM) in H$_2$O in the presence of CN$^-$. Inset: photograph from left to right shows the change in the absorbance of only $S_4$, $S_4$-CN$^-$ in H$_2$O.
Figure S2 Benesi-Hilderbrand plot of $S_4$ with $CN^-$. 
Figure S3 ESI-MS spectrum of S₄.
Figure S4 $^1$H NMR spectra (400 MHz, DMSO-$d_6$) of free $S_4$ and in the presence of $OH^-$ or $CN^-$. 

References