Synthesis, Photophysics, Ion Detection and DFT Investigation of

Novel Cyano-substituted Red-light Chromophores with

Triphenylamine Donor

Na Sun, Peng Zhang*, Yan-ling Hou

School of Chemistry and Chemical Engineering, Southwest University, Chongqing 400715, PR China

Supporting Information

Table S1. The electrochemical parameter of compounds 3-5

Fig.S1. TGA curves of compounds 3-5 at a heating rate of 10°C min⁻¹ under nitrogen

Fig.S2. DSC curves of compounds 3-5 at a heating rate of 10°C min⁻¹ under nitrogen

Fig.S3. X-ray powder diffraction patterns and d-space data for compounds 3-5

Fig.S4. The emission spectra in powder for compounds 3-5

Fig.S5. The images of the emissions in the powder for compounds 3-5

- **Fig.S6.** The dependence of the emission spectra of compounds **3** and **4** on their concentration in dichloromethane solution (mol/L)
- Fig.S7. The dependence of absorption spectra of the compounds 3-5 on the solvent polarity
- **Fig.S8.** The photographs of compounds **3-5** in different polar solvents (10⁻⁵M) (left to right, toluene, dichloromethane, THF, ethyl acetate and DMF).
- Fig.S9. The responses of absorption and fluorescence spectra of the compound 3 $(1 \times 10^{-5} \text{ M/L})$ in DMF with the addition of ion metal-DMF $(1 \times 10^{-4} \text{ M/L})$

Fig.S10. The responses of absorption and fluorescence spectra of the compound **4** $(1 \times 10^{-5} \text{ M})$ in DMF with the addition of ion metal-DMF $(1 \times 10^{-4} \text{ M/L})$

Fig.S11. The ion responses of absorption and fluorescence spectra of the compound **5** $(1 \times 10^{-5} \text{ M/L})$ in DMF with the addition of ion metal-DMF $(1 \times 10^{-4} \text{ M/L})$

Fig.S12. Fluorescence spectra of the compounds 3-5 $(1 \times 10^{-5} \text{ M/L})$ in DMF upon

^{*} Corresponding author. Tel: +86 023-68252360.

E-mail address: ybzhang@swu.edu.cn

addition of Hg^+-DMF solution ranging from $1{\times}10^{\text{-4}}$ to $9{\times}10^{\text{-4}}\,\text{M/L}$

Table S1

| Compd | $\mathbf{E}_{\text{ox, peak}}(\text{ev})$ | | $\mathbf{E}_{\text{red, peak}}(\text{ev})$ | |
|-------|-------------------------------------------|-------|--------------------------------------------|-------|
| 3 | 1.39 | -1.70 | _ | _ |
| 4 | 1.49 | -1.85 | -2.70 | _ |
| 5 | 1.48 | -1.94 | -2.27 | -2.57 |

Fig.S1



Fig.S2



Fig.S3



Fig.S4





Fig.S6





























Fig.S12



