Organic fluorescent compounds that display efficient aggregation-induced emission enhancement and intramolecular charge transfer

Ruibin Hou^{1,2}, Baohua Zhao¹, Yan Xia^{1,2,*} and Dongfeng Li^{1,*}

¹School of Chemistry and Life Science, Changchun University of Technology, Changchun, 130012, China ²Advanced Institute of Materials Science, Changchun University of Technology, Changchun 130012, China

Figure S1-S4: Characterization of compounds 1a-c.

Figure S5: Absorption spectra of 1a-c.

Figure S6: PL emission spectra of 1b.

Figure S7: PL emission spectra of **1a-b** in DMF/H₂O mixtures.

Figure S8: Cyclic voltammograms of 1a.

Figure S9: Electron density contours and orbital energies calculated for the HOMOs and LUMOs of

1b-c

Characterization

¹H NMR





Figure S1 (3) ¹H NMR spectra of 1c.

¹³C NMR



Figure S2 (1) 13 C NMR spectra of 1a.



Figure S2 (3) 13 C NMR spectra of 1c.

FT-IR



Figure S3 (2) IR spectra of 1b.



Figure S3 (3) IR spectra of 1c.

TOF Ms



Figure S4 (1) TOF MS spectra of 1a.











Figure S5 (1) Absorption spectra of 1a in different solutions at the same concentration(10⁻⁵molL⁻¹).



Figure S5 (2) Absorption spectra of **1b** in different solutions at the same concentration(10⁻⁵molL⁻¹). DMSO=dimethylsulfoxide.



Figure S5 (4) Absorption spectra of **1c** in different solutions at the same concentration(10⁻⁵molL⁻¹). DMSO=dimethylsulfoxide.



Figure S6 (1) PL emission spectra of **1b** in different solutions at the same concentration (10⁻⁶molL⁻¹, excitation wavelength:327nm). DMSO=dimethylsulfoxide.



Figure S6 (1) PL emission spectra of **1b** in different solutions at the same concentration (10⁻⁵molL⁻¹, excitation wavelength:325nm). DMSO=dimethylsulfoxide.



Figure S7 (1) PL emission spectra of **1b** THF/H₂O mixtures at the same concentration (5×10^{-6} molL⁻¹, excitation wavelength:325nm).



Figure S7 (2) PL emission spectra of **1b** THF/H₂O mixtures at the same concentration (10⁻⁶molL⁻¹, excitation wavelength:327nm).



Figure S7 (3) PL emission spectra of **1a** DMF/H₂O mixtures at the same concentration (10^{-5} molL⁻¹, excitation wavelength:325nm).



Figure S7 (4) PL emission spectra of **1b** DMF/H₂O mixtures at the same concentration (10^{-6} molL⁻¹, excitation wavelength:327nm).



Figure S8 Cyclic voltammograms of 1a inCHCl₃(1×10⁻³ M).



Figure S9 (1) Electron density contours and orbital energies calculated for the HOMOs and LUMOs of **1b** at the B3LYP/DZP level. H and L denote HOMO and LUMO, respectively.



Figure S9 (2) Electron density contours and orbital energies calculated for the HOMOs and LUMOs of **1c** at the B3LYP/DZP level. H and L denote HOMO and LUMO, respectively.