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Synergetic effect of pyrene-based fluorescent probe for trace nitroaniline sensing

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1. NMR spectra

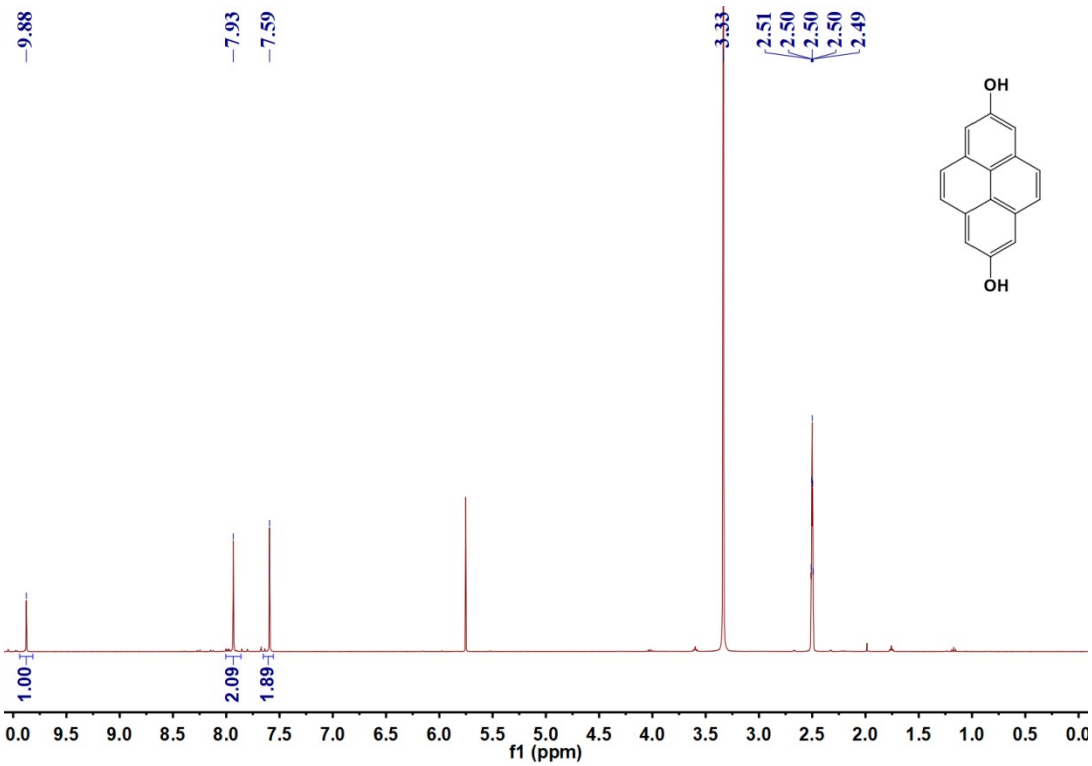

Figure S1 ^{1}H-NMR spectrum (400 MHz, 293 K, * $CDCl_3$) for **1**

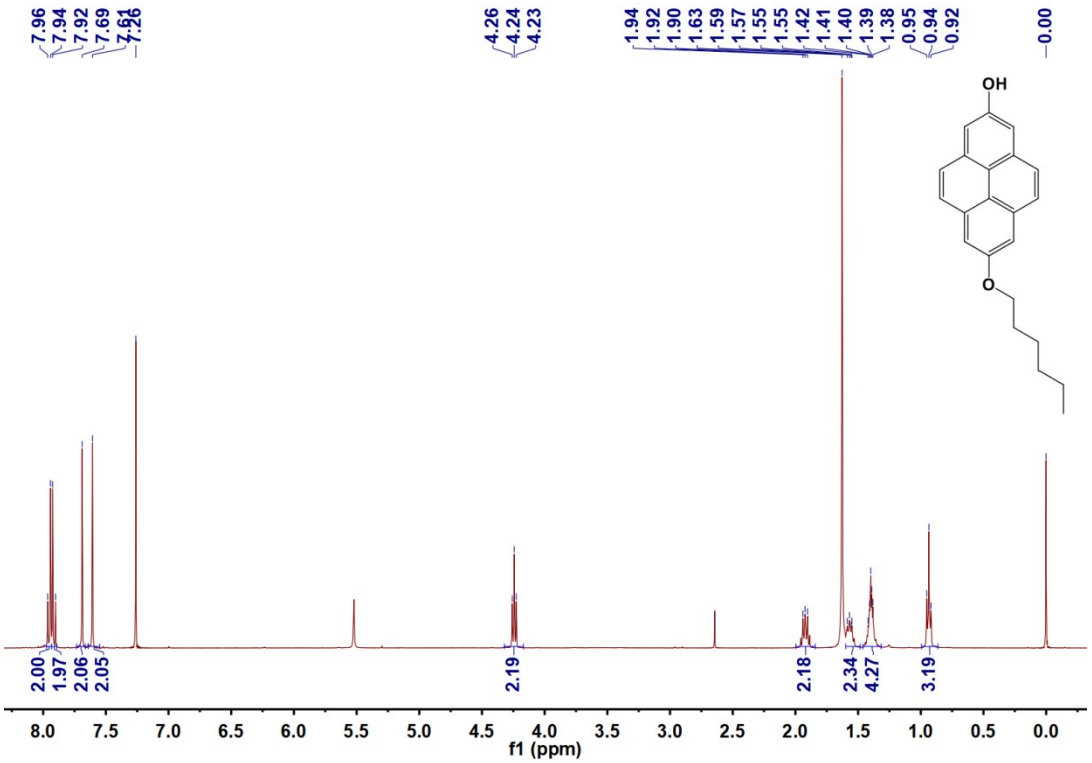

Figure S2 ^{1}H-NMR spectrum (400 MHz, 293 K, * $CDCl_3$) for **2**

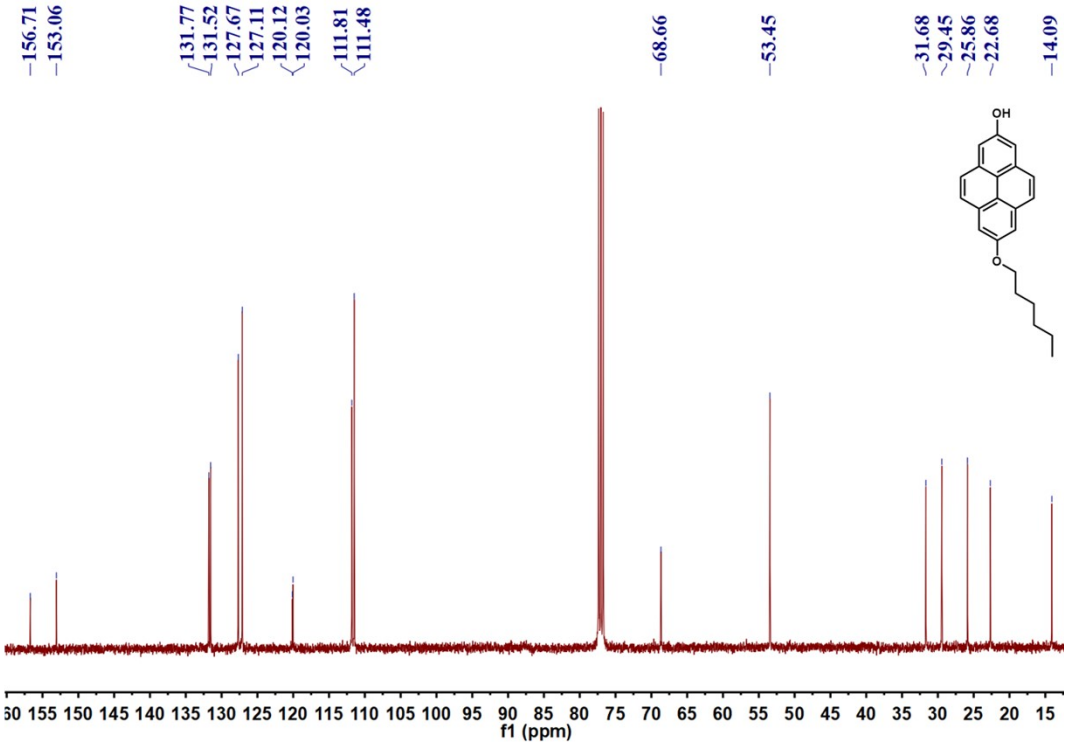

Figure S3 ^{13}C-NMR spectrum (100 MHz, 293 K, * $CDCl_3$) for **2**

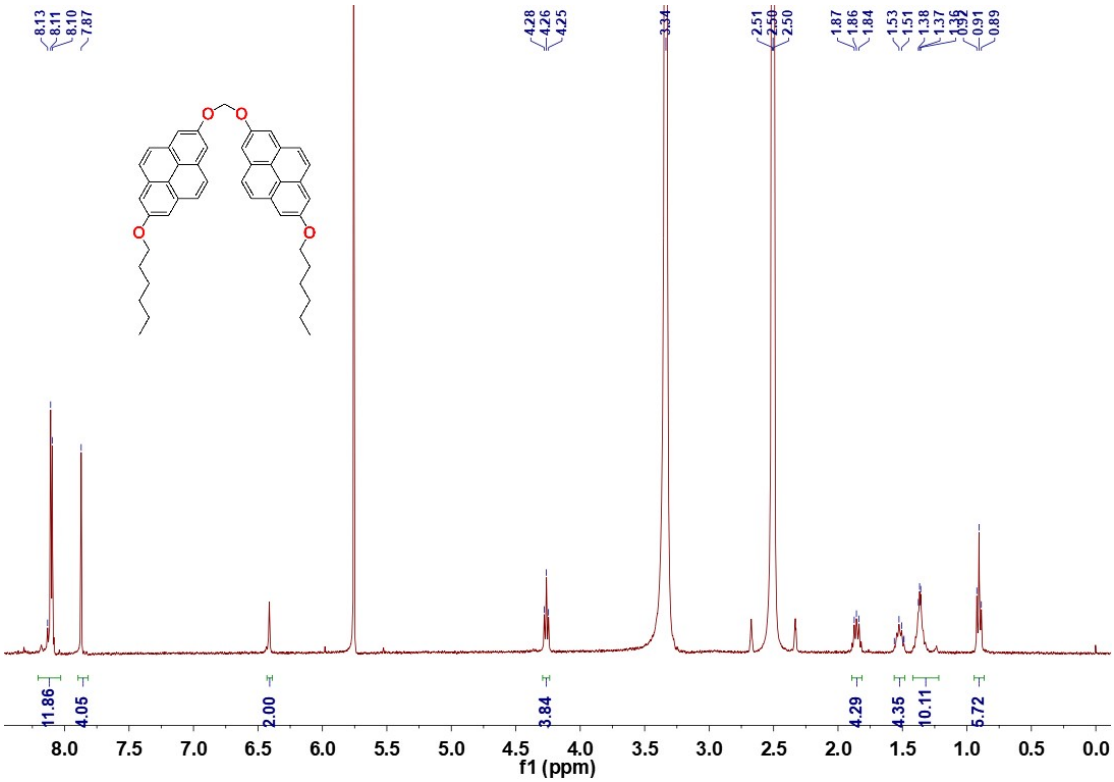

Figure S4 ^{1}H-NMR spectrum (400 MHz, 293 K, DMSO-d6) for **3a**

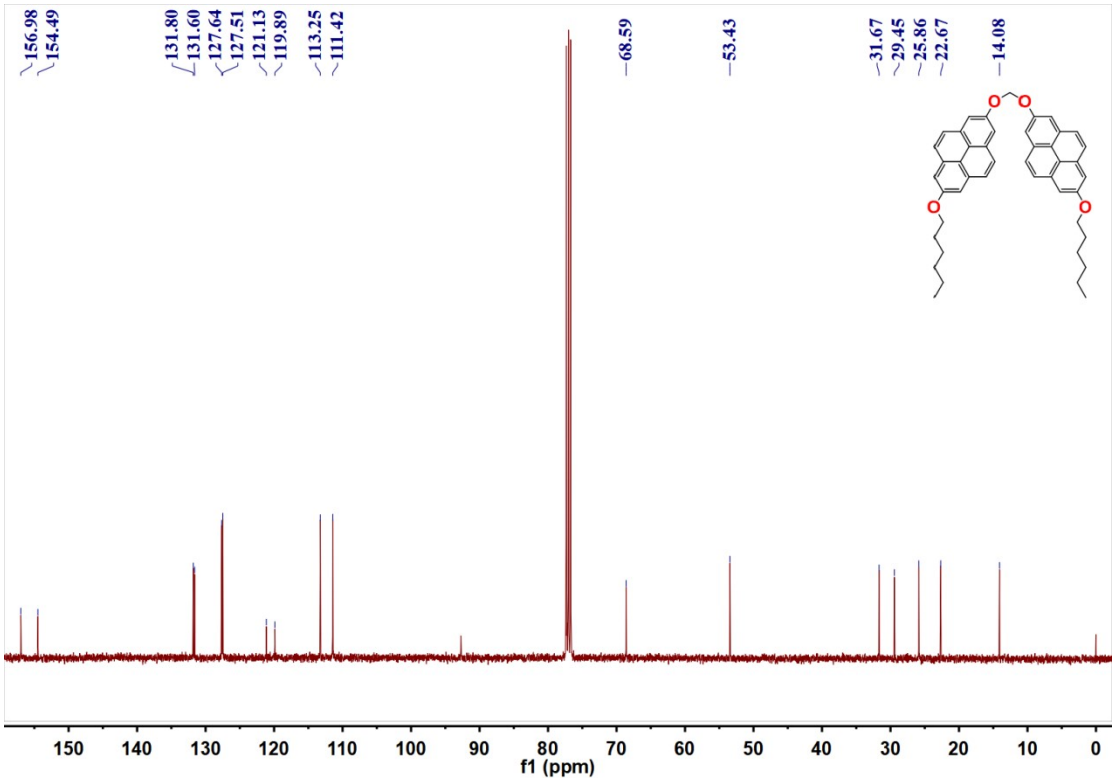

Figure S5 ^{13}C-NMR spectrum (100 MHz, 293 K, * $CDCl_3$) for **3a**

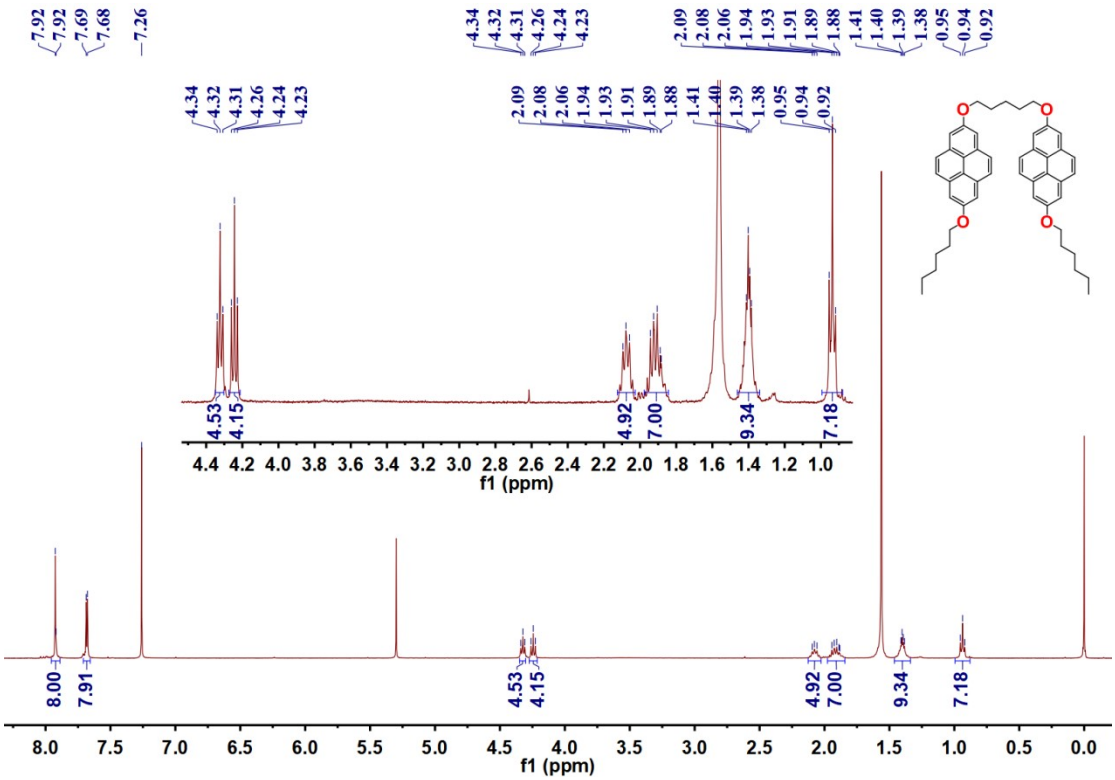

Figure S6 ^{1}H-NMR spectrum (400 MHz, 293 K, * $CDCl_3$) for **3b**

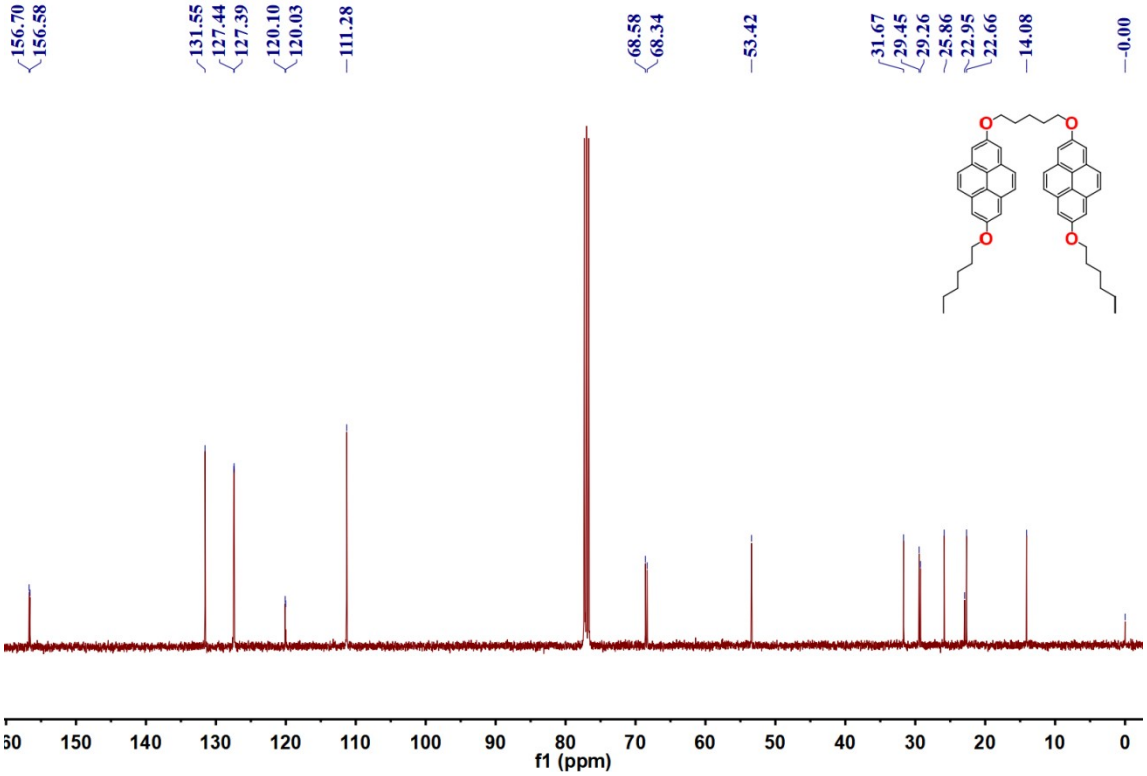

Figure S7 ^{13}C-NMR spectrum (100 MHz, 293 K, * $CDCl_3$) for **3b**

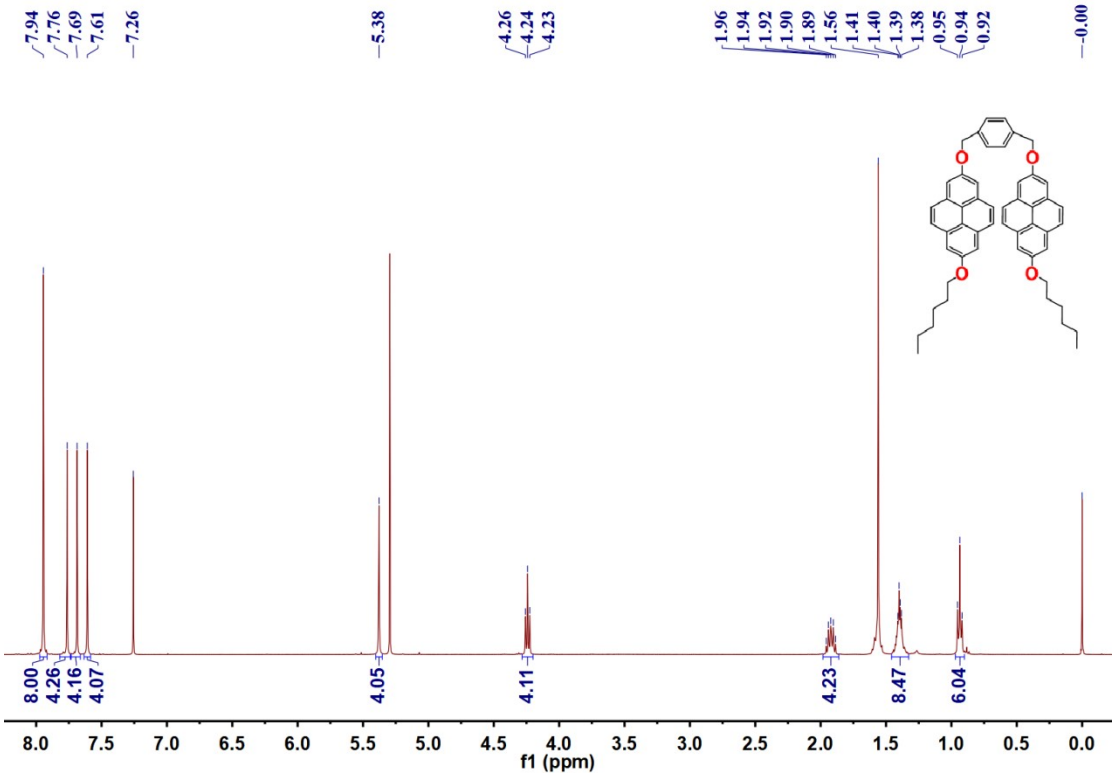

Figure S8 ^{1}H-NMR spectrum (400 MHz, 293 K, * $CDCl_3$) for **3c**

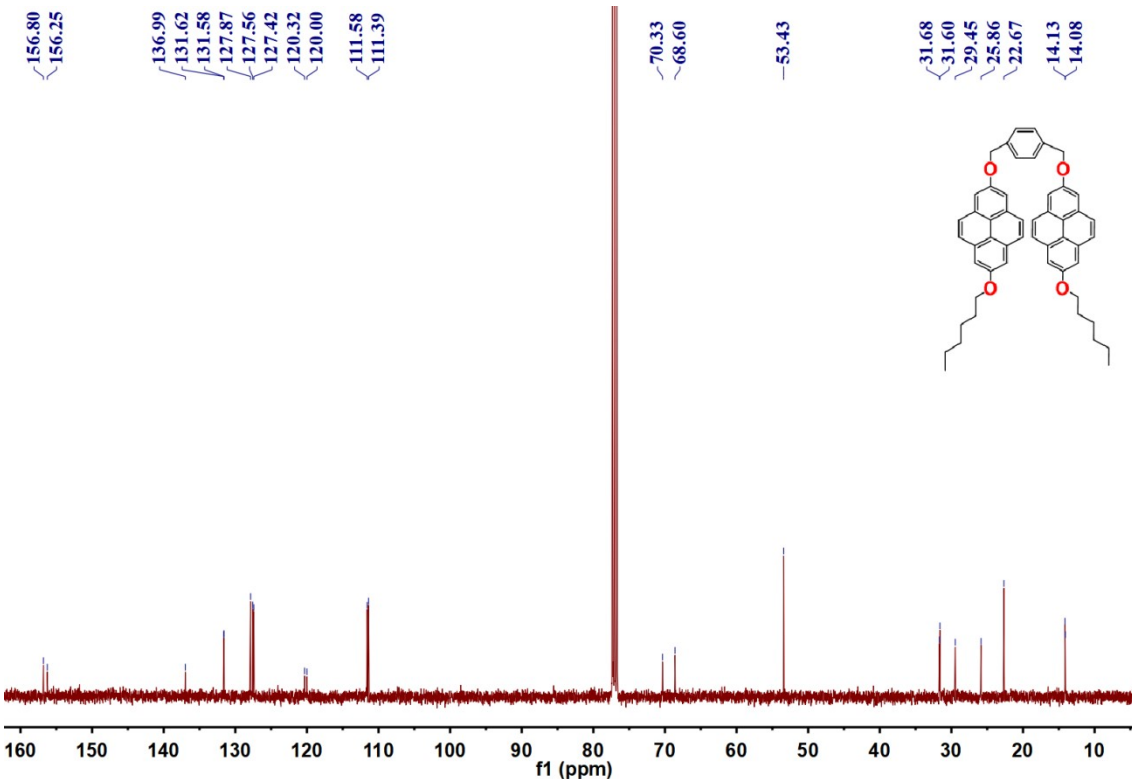

Figure S9 ^{13}C-NMR spectrum (100 MHz, 293 K, * $CDCl_3$) for **3c**

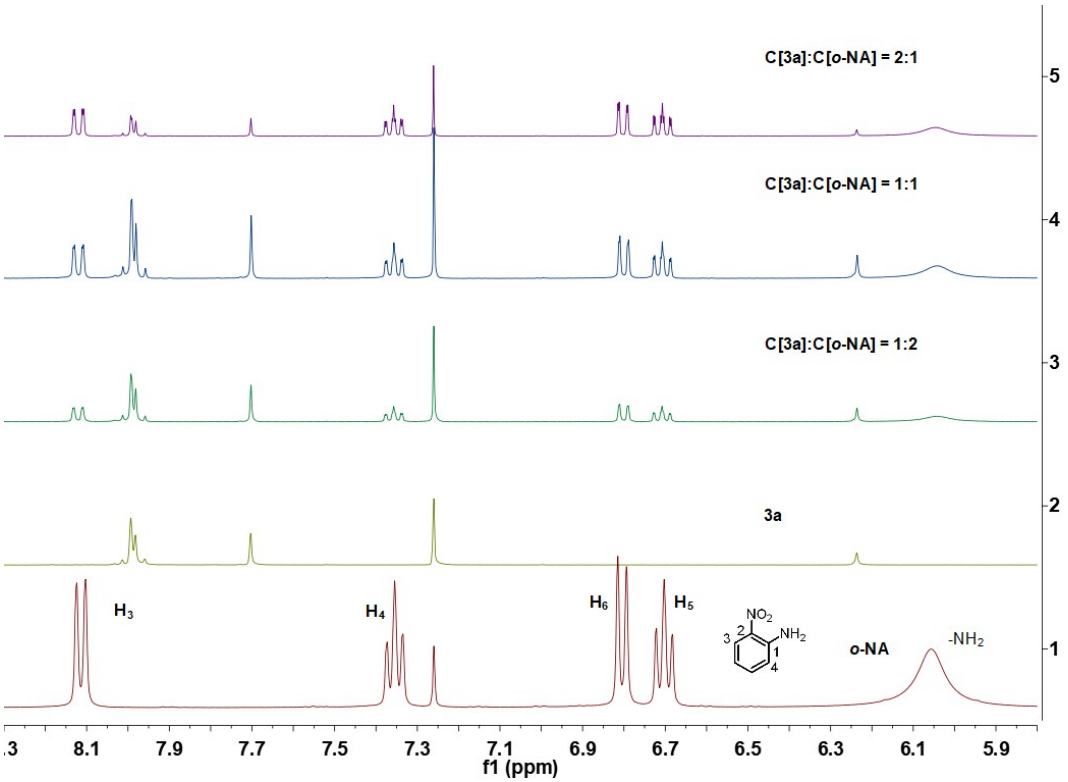

Figure S10 ^{1}H NMR spectrum (400 MHz, 293 K, * $CDCl_3$) of fluorescent probe **3a, and o-NA** with different concentration.

2. High Resolution Mass Spectroscopy

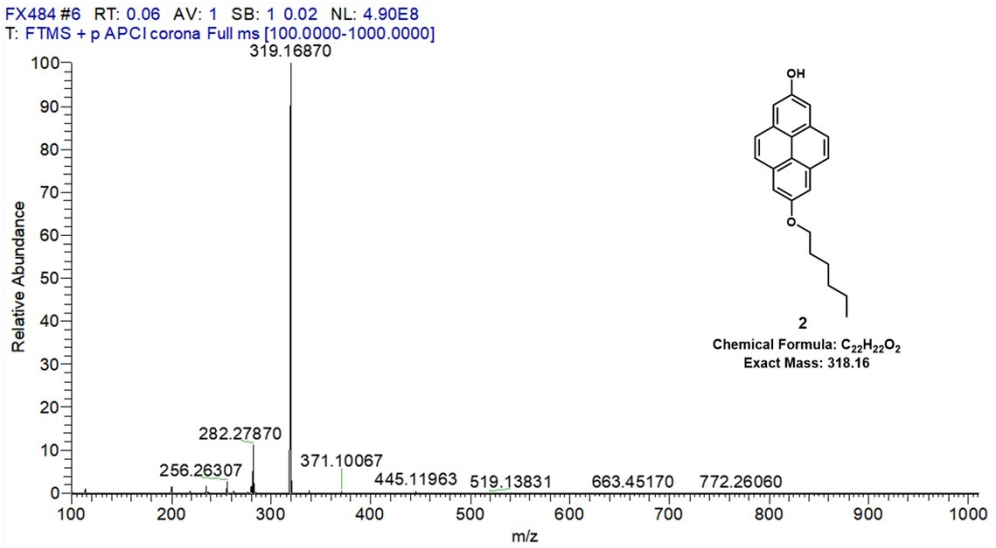

Figure S11 HRMS spectra of **2**

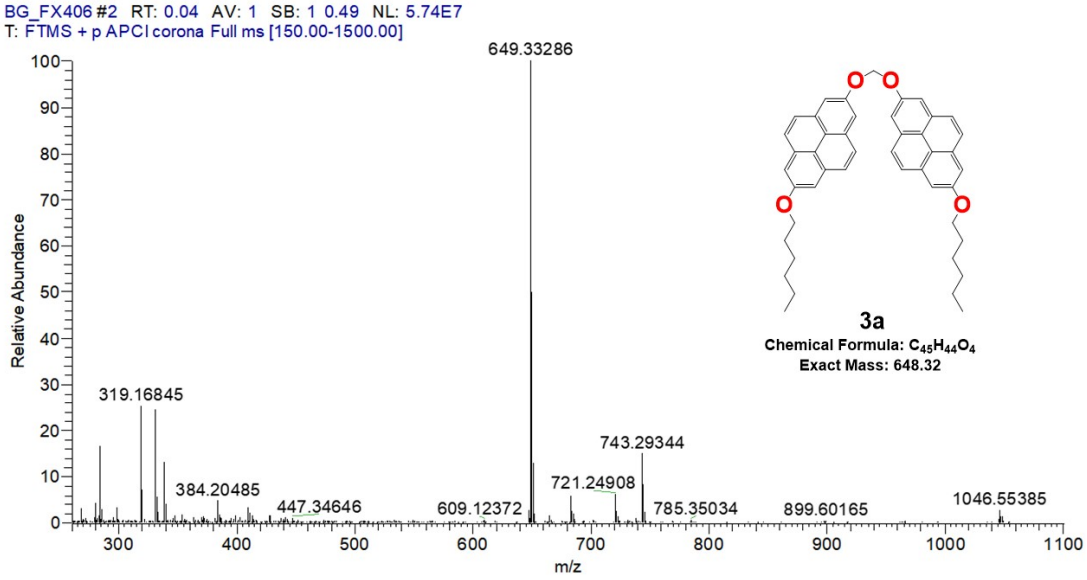

Figure S12 HRMS spectra of **3a**

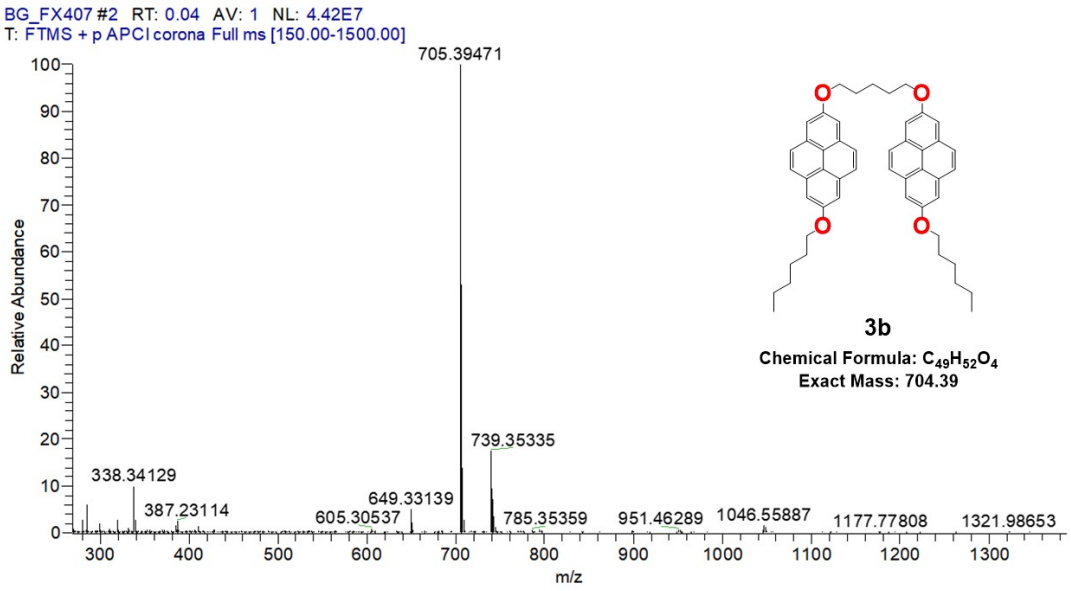

Figure S13 HRMS spectra of **3b**

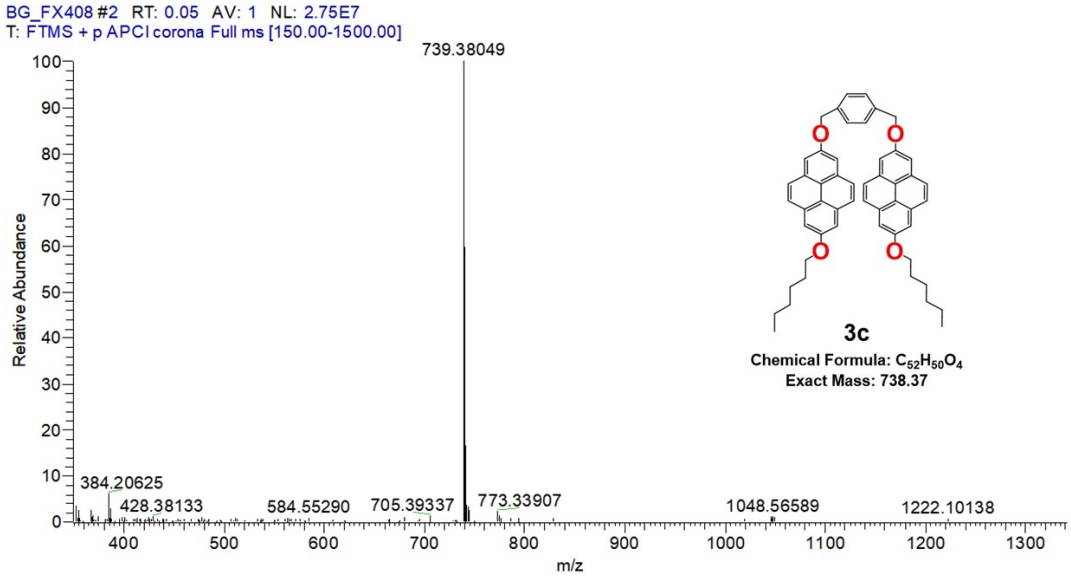

Figure S14 HRMS spectra of **3c**

3. TGA analysis

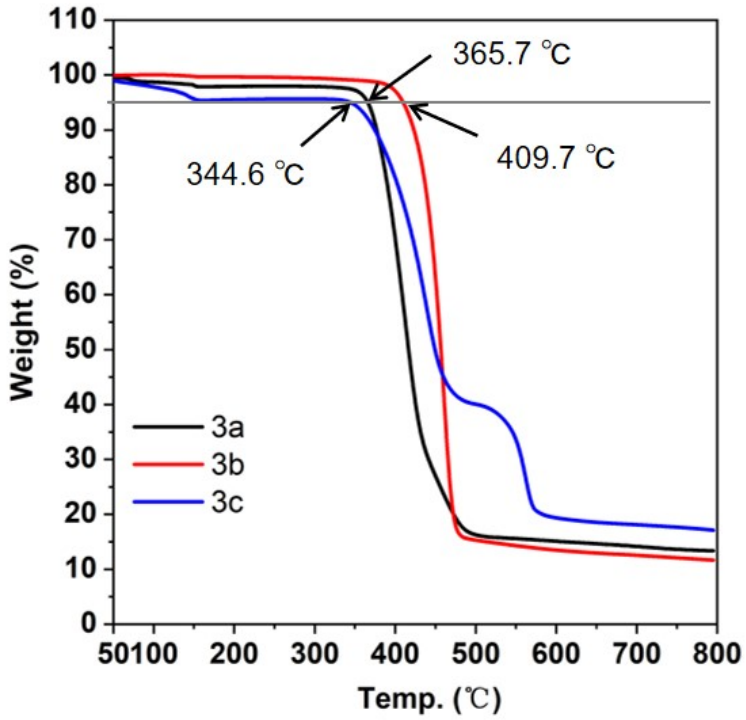

Figure S15 TGA thermogram of 3a-c recorded under nitrogen at a heating rate of 10 ℃/min.

4. Photophysical Properties

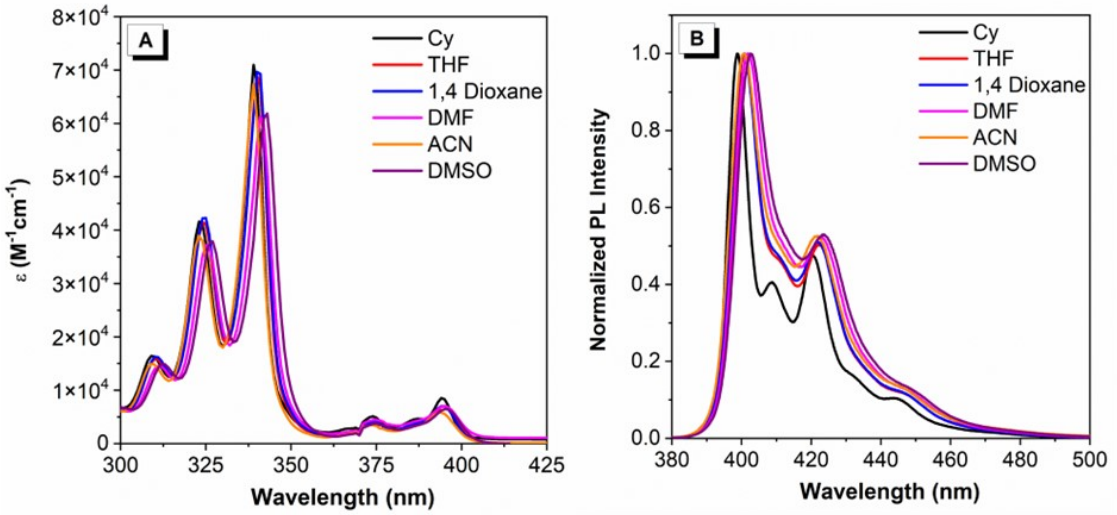

Figure S16 (A) UV-vis spectra and (B) Fluorescence spectra of **3a** recorded in six solvents at ~10^{-5} M and 25 °C.

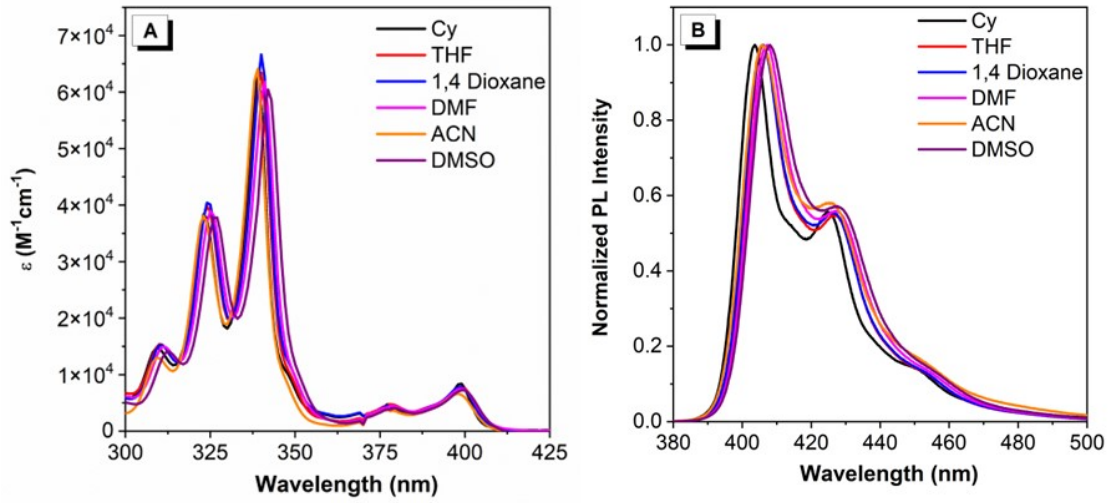

Figure S17 (A) UV-vis spectra and (B) Fluorescence spectra of **3b** recorded in six solvents at ~10^{-5} M and 25 °C.

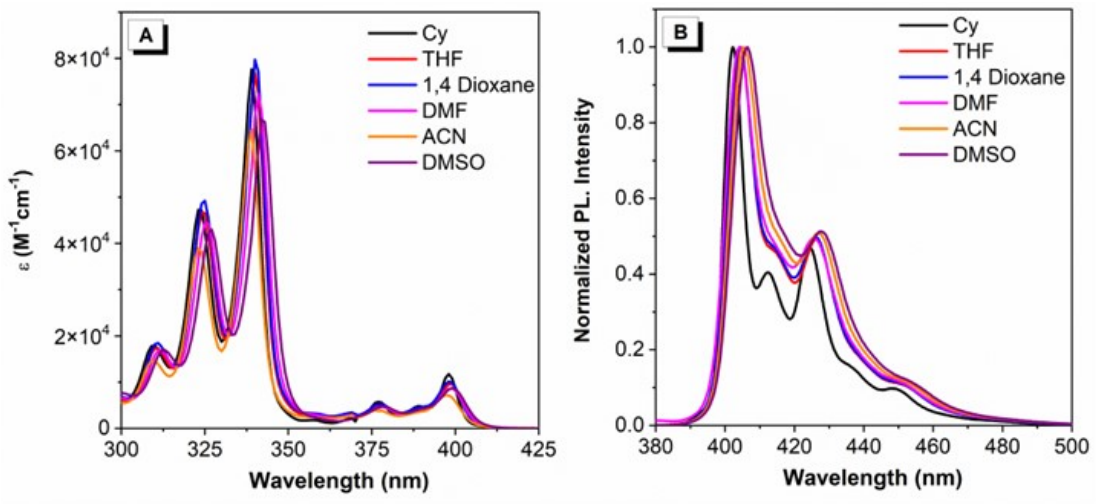

Figure S18 (A) UV-vis spectra and (B) Fluorescence spectra of **3c** recorded in six solvents at ~10^{-5} M and 25 °C.

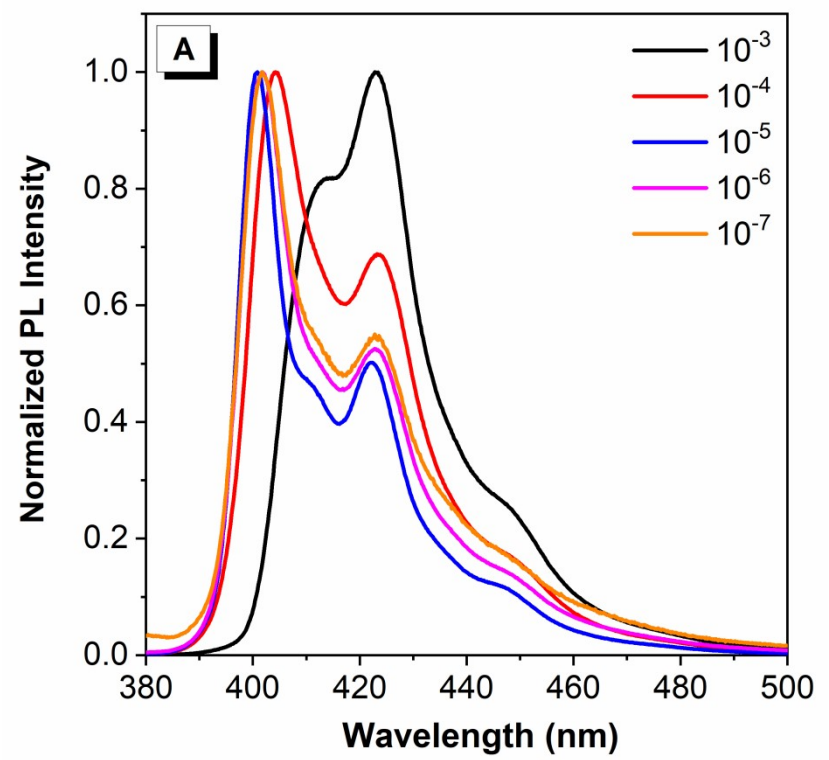

Figure S19 Concentration dependent fluorescence spectra of **3a** recorded in THF solvents at 25℃.

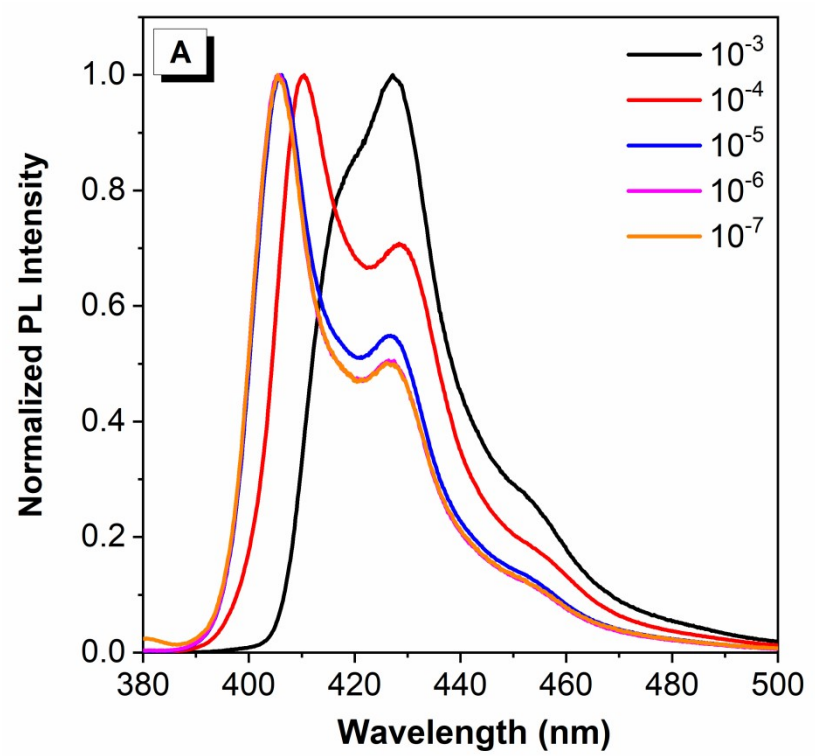

Figure S20 Concentration dependent fluorescence spectra of **3b** recorded in THF solvents at 25℃.

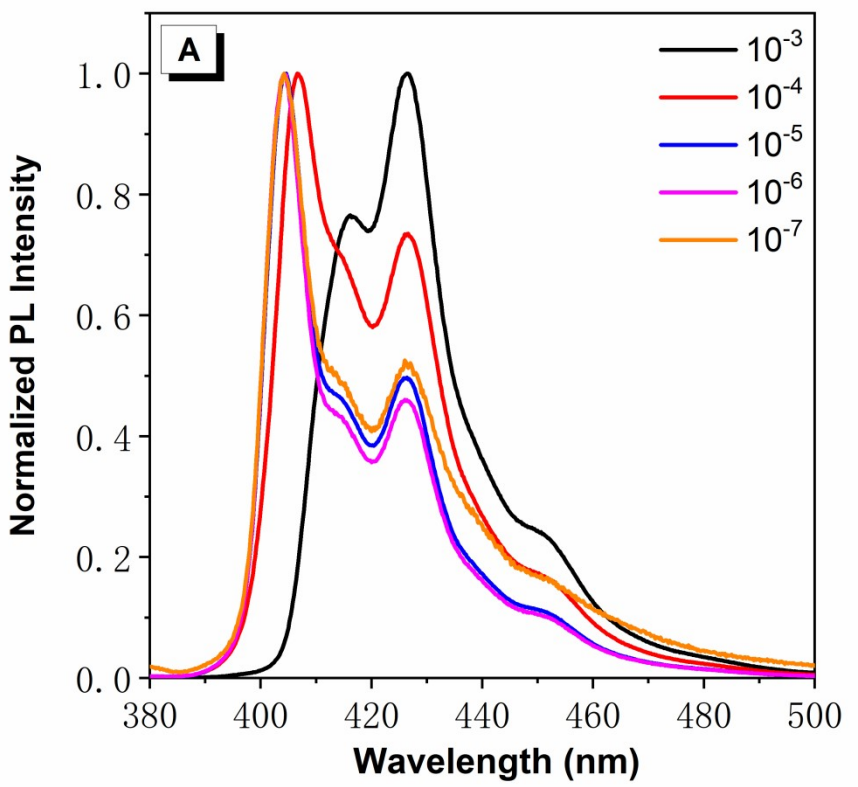

Figure S21 Concentration dependent fluorescence spectra of **3c** recorded in THF solvents at 25℃.

Table S1. UV-vis and emission spectroscopic data for **3a-c** in different solvents at 25 °C.

Comp.	Cy	THF	1,4-dioxane	DMF	ACN	DMSO
	λ_{abs} / λ_{em} (nm)	λ_{abs} / λ_{em} (nm)	λ_{abs} / λ_{em} (nm)	λ_{abs} / λ_{em} (nm)	λ_{abs} / λ_{em} (nm)	λ_{abs} / λ_{em} (nm)
3a	339; 394/ 399;420	340; 395/ 401; 422	340; 394/ 401; 422	341; 395/ 402; 423	339; 394/ 401; 421	343; 395/ 403; 423
3b	339; 399/ 404; 425	340; 399/ 406; 427	340; 399/ 406; 426	341; 399/ 407; 427	339; 398/ 406; 424	342; 399/ 408; 428
3c	339; 398/ 402; 424	340; 399/ 404; 426	340; 398/ 404; 426	341; 399/ 405; 427	339; 397/ 404; 426	342; 399/ 406; 428

5. Detection of nitroaniline

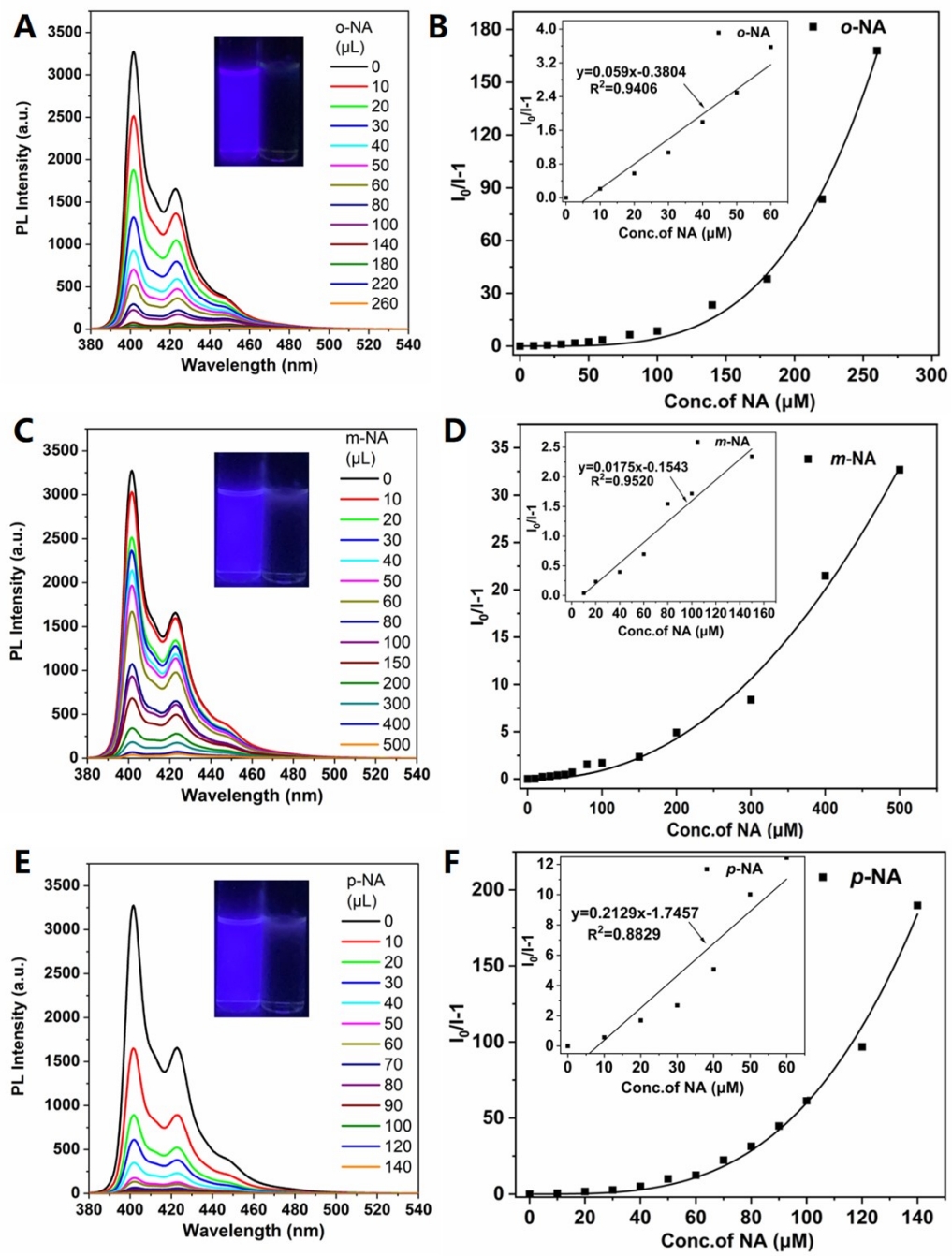

Figure S22 Fluorescence quenching of **3a** with incremental addition of A) o-NA, C) m-NA, E) p-NA, and inset photographs show the visible change in the fluorescence under UV light before and after addition of NA; Corresponding Sterne-Volmer plots for quenching of **3a** with (B) 0-NA, (D) m-NA, (F) p-NA as quencher in DCM. Inset shows the Sterne-Volmer plots at lower concentration of NA.

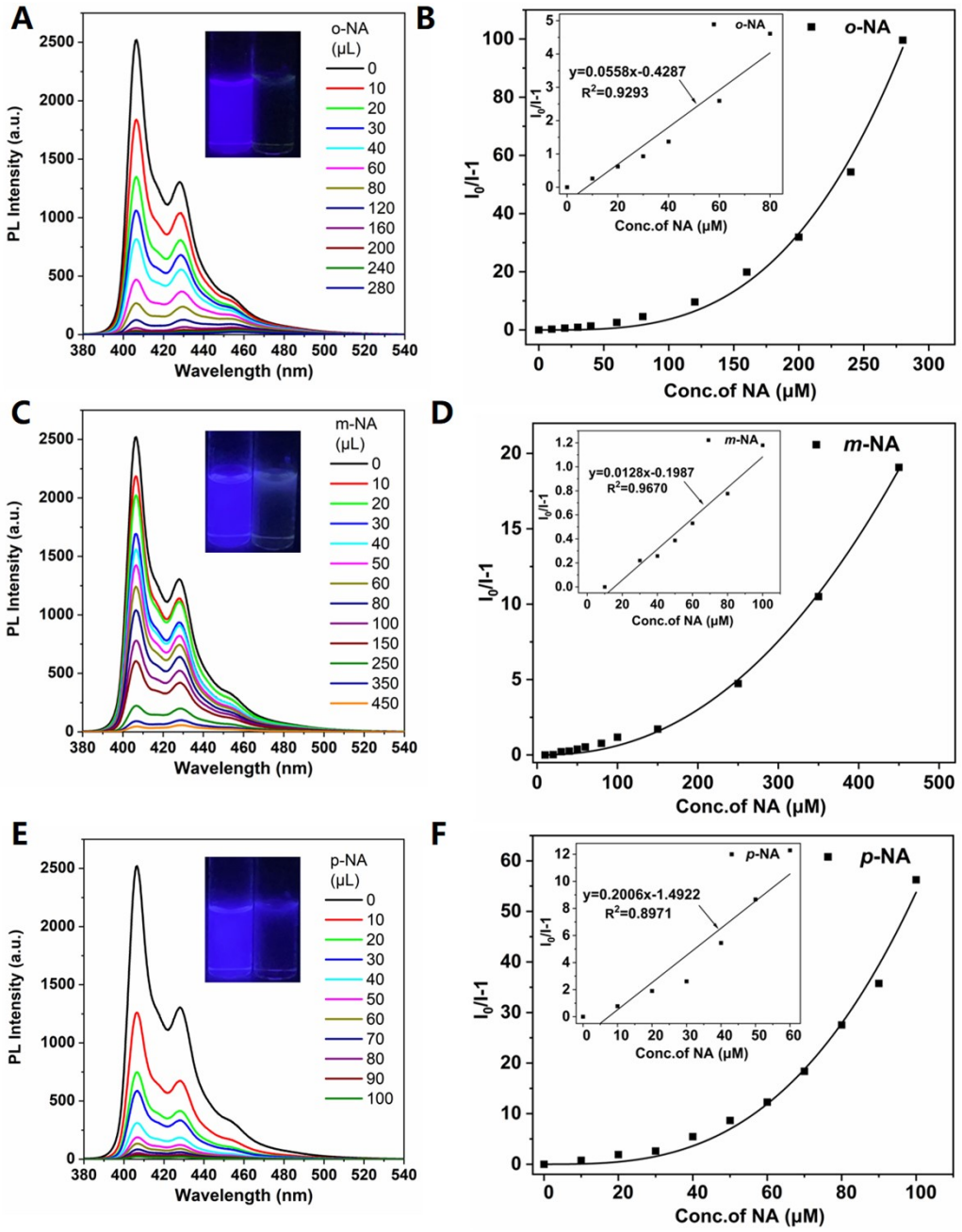

Figure S23 Fluorescence quenching of **3b** with incremental addition of A) o-NA, C) m-NA, E) p-NA, and inset photographs show the visible change in the fluorescence under UV light before and after addition of NA; Corresponding Sterne-Volmer plots for quenching of **3b** with (B) 0-NA, (D) m-NA, (F) p-NA as quencher in DCM. Inset shows the Sterne-Volmer plots at lower concentration of NA.

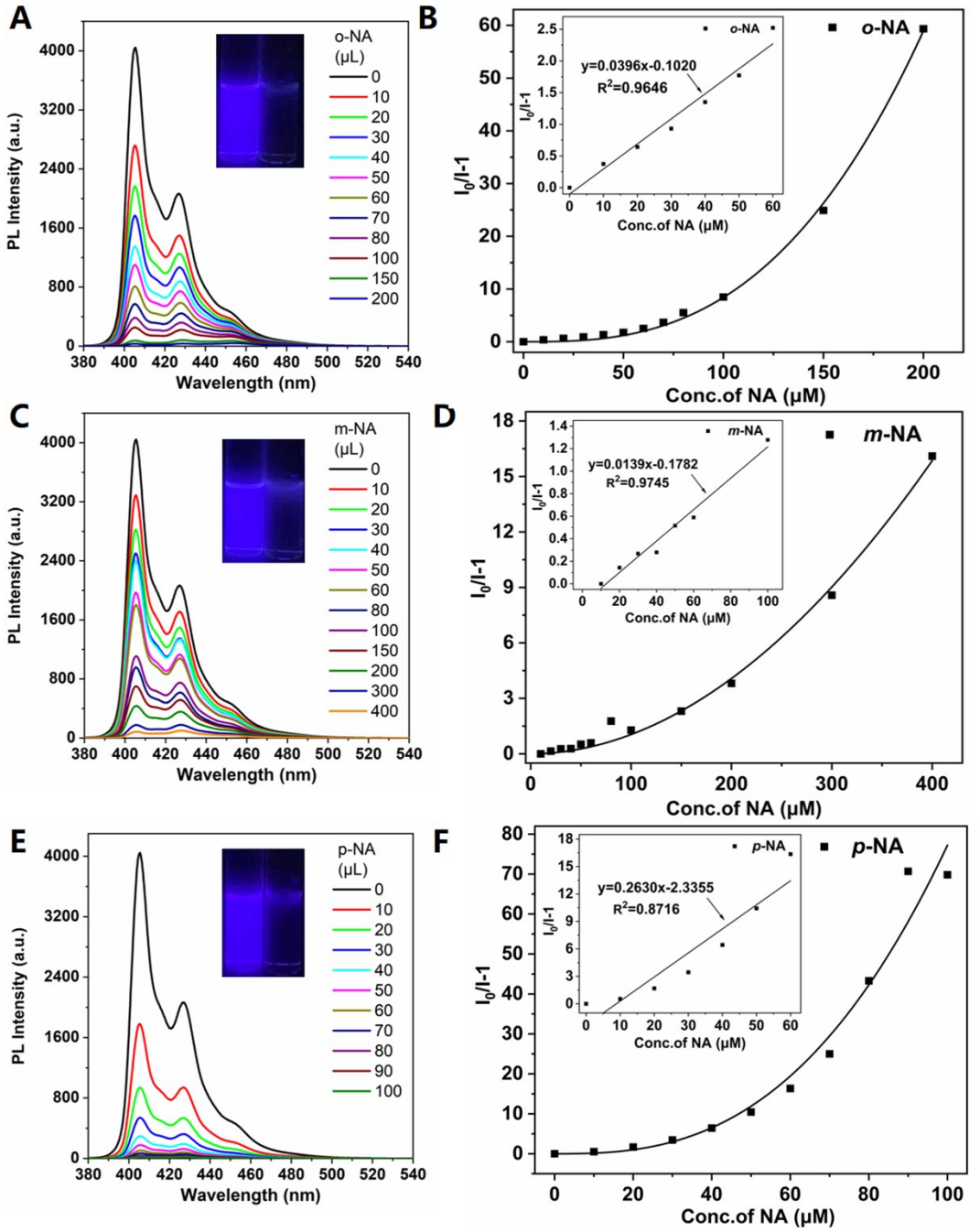

Figure S24 Fluorescence quenching of **3c** with incremental addition of A) o-NA, C) m-NA, E) p-NA, and inset photographs show the visible change in the fluorescence under UV light before and after addition of NA; Corresponding Sterne-Volmer plots for quenching of **3c** with (B) 0-NA, (D) m-NA, (F) p-NA as quencher in DCM. Inset shows the Sterne-Volmer plots at lower concentration of NA.

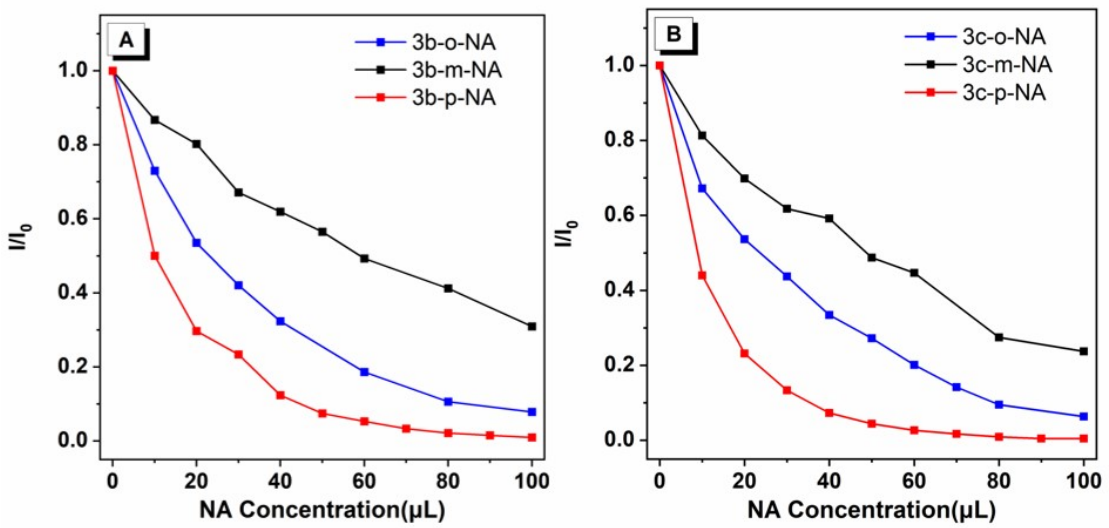

Figure S25 Compounds (A) **3b**, (B) **3c** with NA relative PL intensity I / I0 diagram.

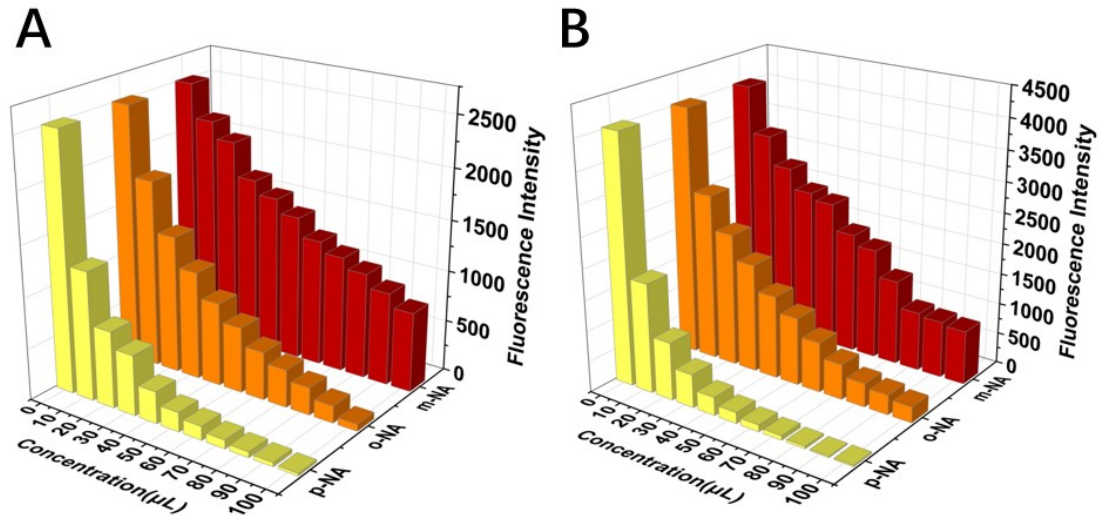

Figure S26 The histogram of fluorescence quenching of (A) **3b**, (B) **3c** with NA.

6. Interference experiment for detecting nitroaniline

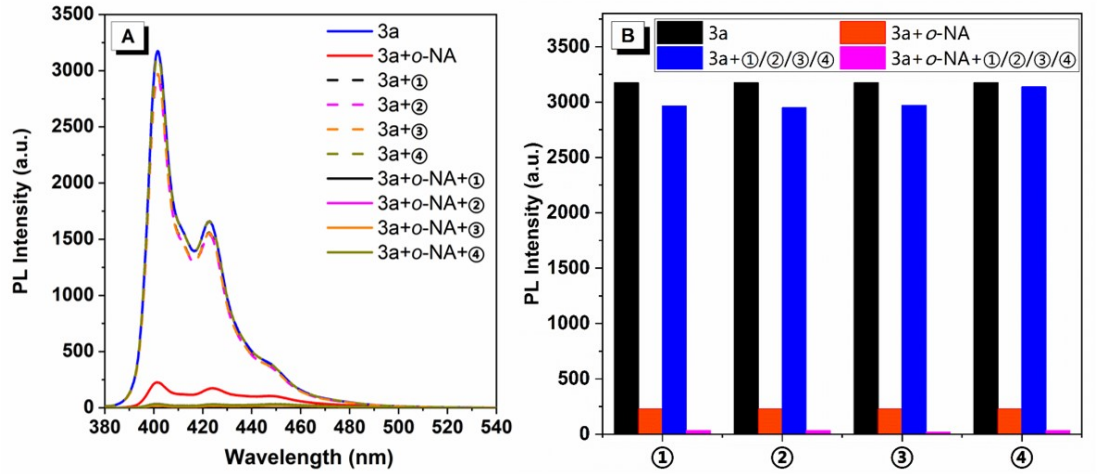

Figure S27 The Interference experiments of fluorescent probe **3a** toward *o*-NA. (A) The emission spectra of fluorescent probe **3a** (10^{-5} M) interacting with different interferent (10^{-5} M) (① hydroquinone, ② *p*-benzaldehyde, ③ *o*-phenylenediamine, and ④ 1,3,5-phenyltricarboxylic acid). (B) histogram of the fluorescence intensity of the fluorescent probe **3a** in presence of different species.

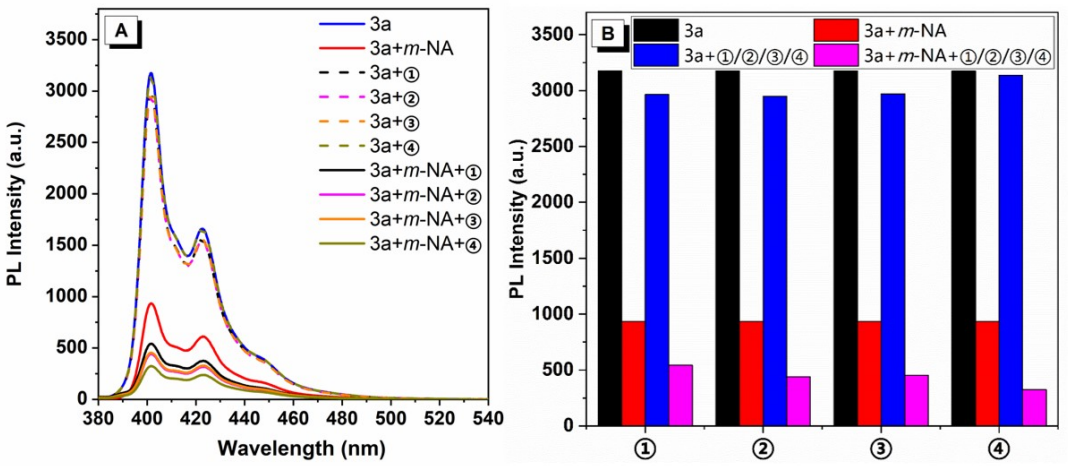

Figure S28 The Interference experiments of fluorescent probe **3a** toward *m*-NA. (A) The emission spectra of fluorescent probe **3a** (10^{-5} M) interacting with different interferent (10^{-5} M) (① hydroquinone, ② *p*-benzaldehyde, ③ *o*-phenylenediamine, and ④ 1,3,5-phenyltricarboxylic acid). (B) histogram of the fluorescence intensity of the fluorescent probe **3a** in presence of different species.

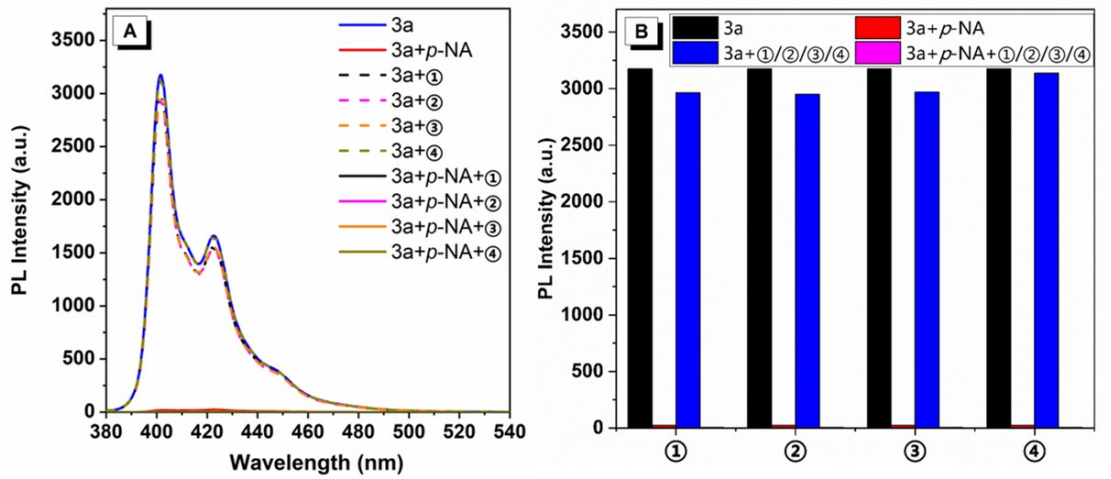

Figure S29 The Interference experiments of fluorescent probe **3a** toward *p*-NA. (A) The emission spectra of fluorescent probe **3a** (10^{-5} M) interacting with different interferent (10^{-5} M) (① hydroquinone, ② *p*-benzaldehyde, ③ *o*-phenylenediamine, and ④ 1,3,5-phenyltricarboxylic acid). (B) histogram of the fluorescence intensity of the fluorescent probe **3a** in presence of different species.

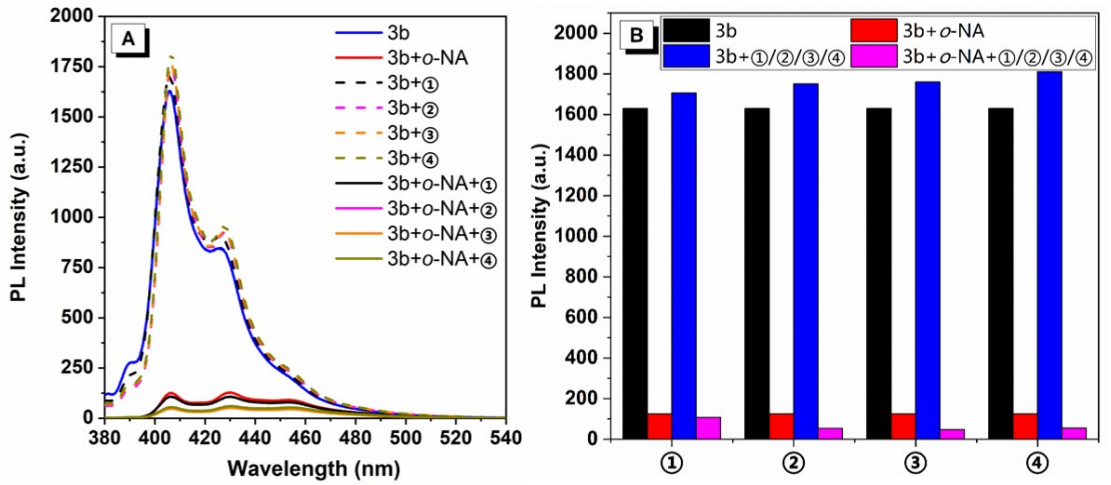

Figure S30 The Interference experiments of fluorescent probe **3b** toward *o*-NA. (A) The emission spectra of fluorescent probe **3b** (10^{-5} M) interacting with different interferent (10^{-5} M) (① hydroquinone, ② *p*-benzaldehyde, ③ *o*-phenylenediamine, and ④ 1,3,5-phenyltricarboxylic acid). (B) histogram of the fluorescence intensity of the fluorescent probe **3b** in presence of different species.

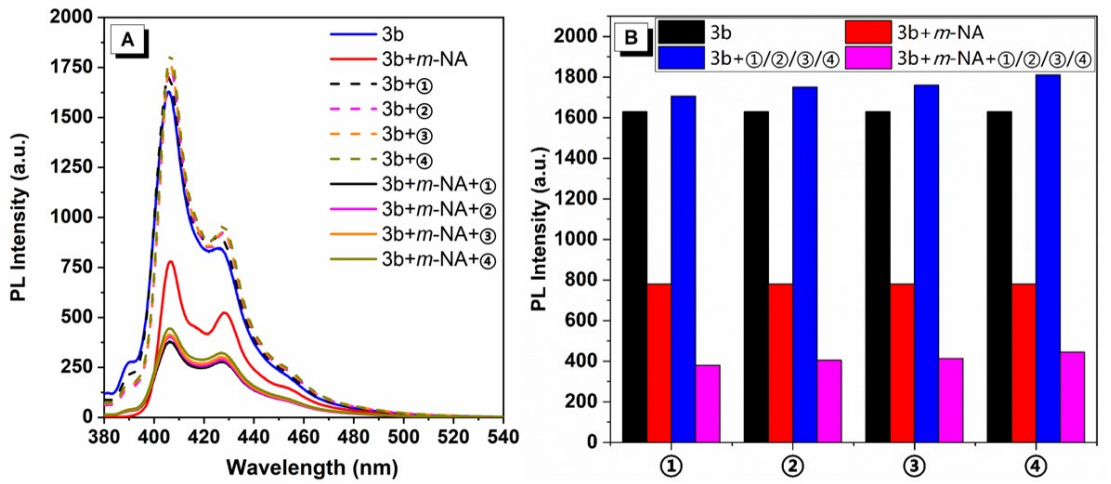

Figure S31 The Interference experiments of fluorescent probe **3b** toward *m*-NA. (A) The emission spectra of fluorescent probe **3b** (10^{-5} M) interacting with different interferent (10^{-5} M) (① hydroquinone, ② *p*-benzaldehyde, ③ *o*-phenylenediamine, and ④ 1,3,5-phenyltricarboxylic acid). (B) histogram of the fluorescence intensity of the fluorescent probe **3b** in presence of different species.

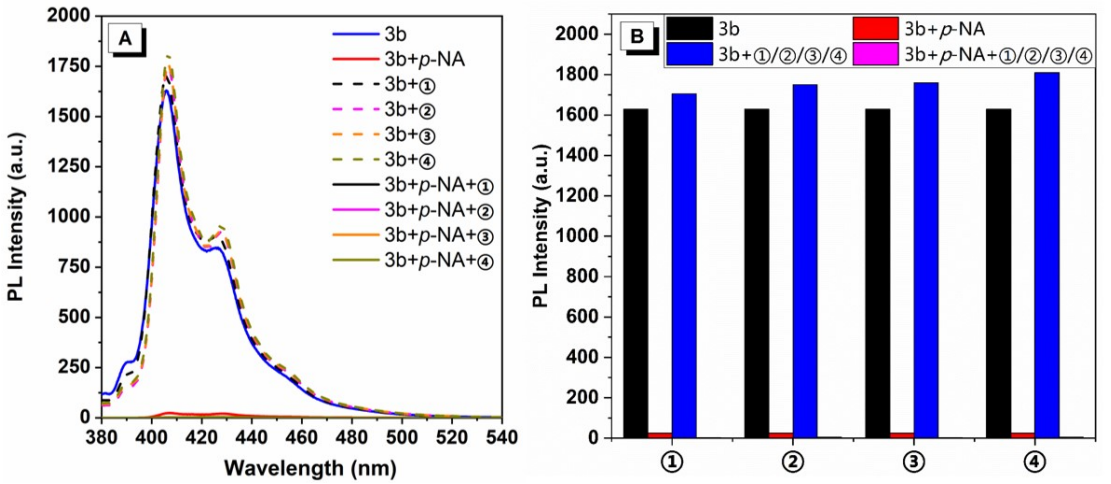

Figure S32 The Interference experiments of fluorescent probe **3b** toward *p*-NA. (A) The emission spectra of fluorescent probe **3b** (10^{-5} M) interacting with different interferent (10^{-5} M) (① hydroquinone, ② *p*-benzaldehyde, ③ *o*-phenylenediamine, and ④ 1,3,5-phenyltricarboxylic acid). (B) histogram of the fluorescence intensity of the fluorescent probe **3b** in presence of different species.

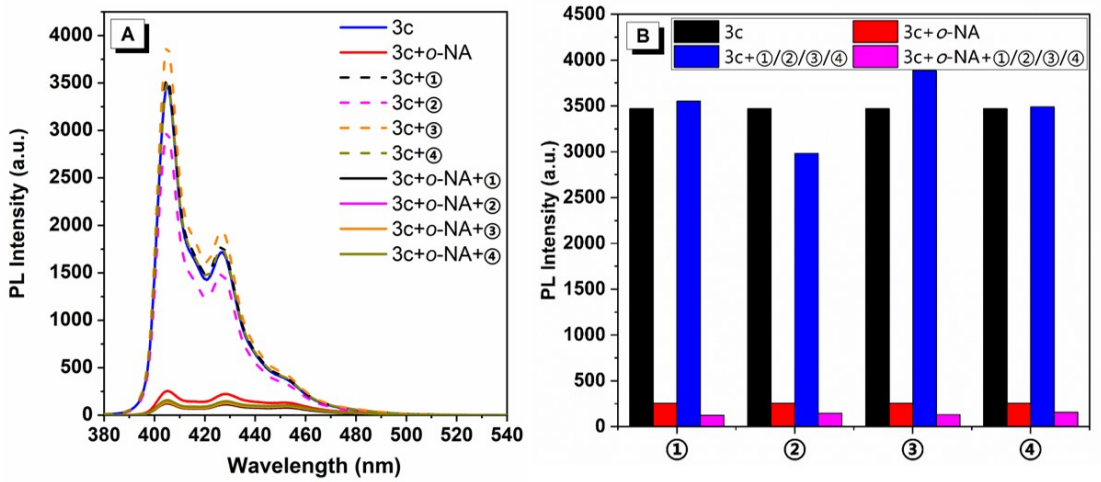

Figure S33 The Interference experiments of fluorescent probe **3c** toward *o*-NA. (A) The emission spectra of fluorescent probe **3c** (10^{-5} M) interacting with different interferent (10^{-5} M) (① hydroquinone, ② *p*-benzaldehyde, ③ *o*-phenylenediamine, and ④ 1,3,5-phenyltricarboxylic acid). (B) histogram of the fluorescence intensity of the fluorescent probe **3c** in presence of different species.

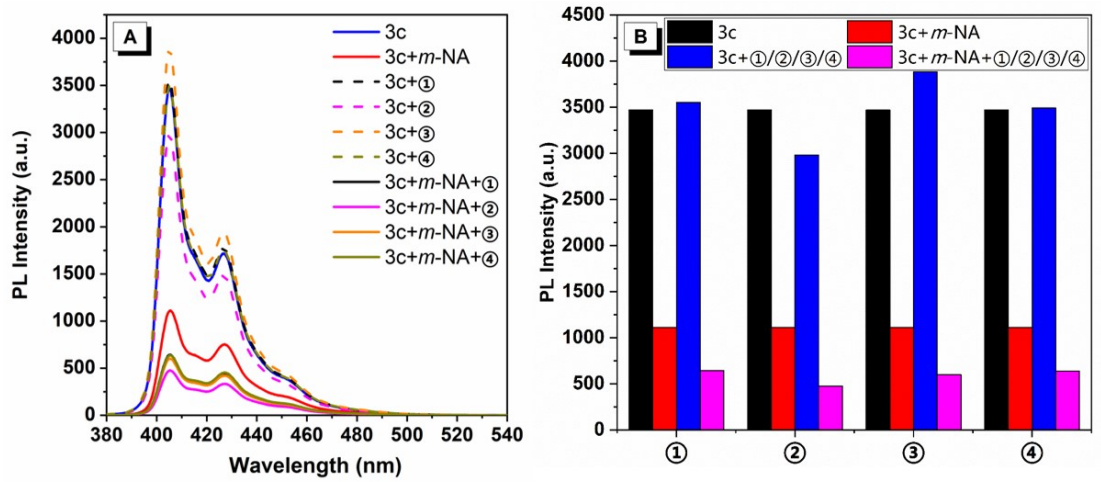

Figure S34 The Interference experiments of fluorescent probe **3c** toward *m*-NA. (A) The emission spectra of fluorescent probe **3c** (10^{-5} M) interacting with different interferent (10^{-5} M) (① hydroquinone, ② *p*-benzaldehyde, ③ *o*-phenylenediamine, and ④ 1,3,5-phenyltricarboxylic acid). (B) histogram of the fluorescence intensity of the fluorescent probe **3c** in presence of different species.

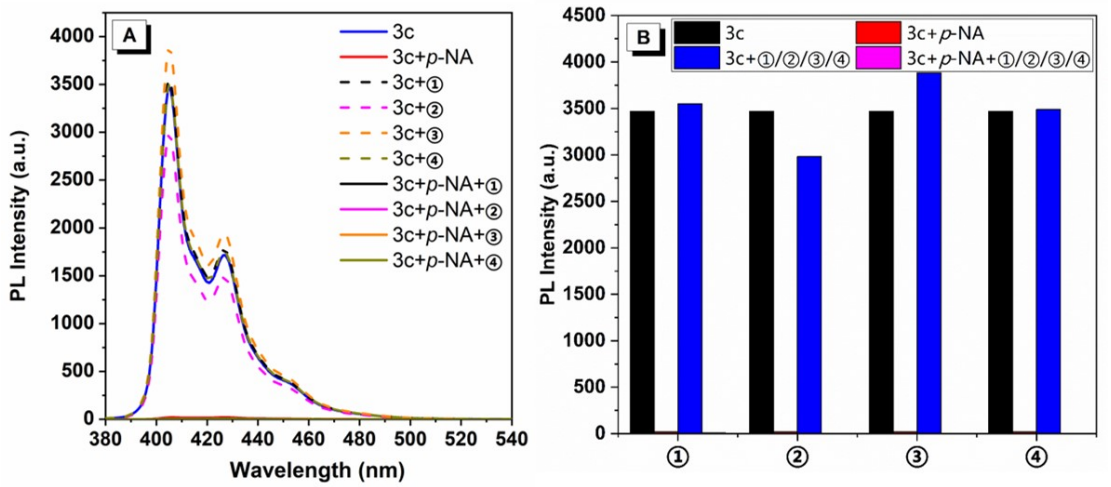

Figure S35 The Interference experiments of fluorescent probe **3c** toward *p*-NA. (A) The emission spectra of fluorescent probe **3c** (10^{-5} M) interacting with different interferent (10^{-5} M) (① hydroquinone, ② *p*-benzaldehyde, ③ *o*-phenylenediamine, and ④ 1,3,5-phenyltricarboxylic acid). (B) histogram of the fluorescence intensity of the fluorescent probe **3c** in presence of different species.