

**AIE-active molecule based self-assembled nano-fibrous films  
for sensitive detection of volatile organic amines**

Jinyang Hu, Rui Liu\*, Shengliang Zhai, Yanan Wu, Haozhe Zhang, Hanting Cheng  
Hongjun Zhu\*

*Department of Applied Chemistry, College of Chemistry and Molecular Engineering,  
Nanjing Tech University, Nanjing, 211816, China*

\*Corresponding author.

Phone: +86-25-83172358. Fax: +86-25-83587428. E-mail: rui.liu@njtech.edu.cn (R.  
Liu), zhuhj@njtech.edu.cn (H. Zhu).

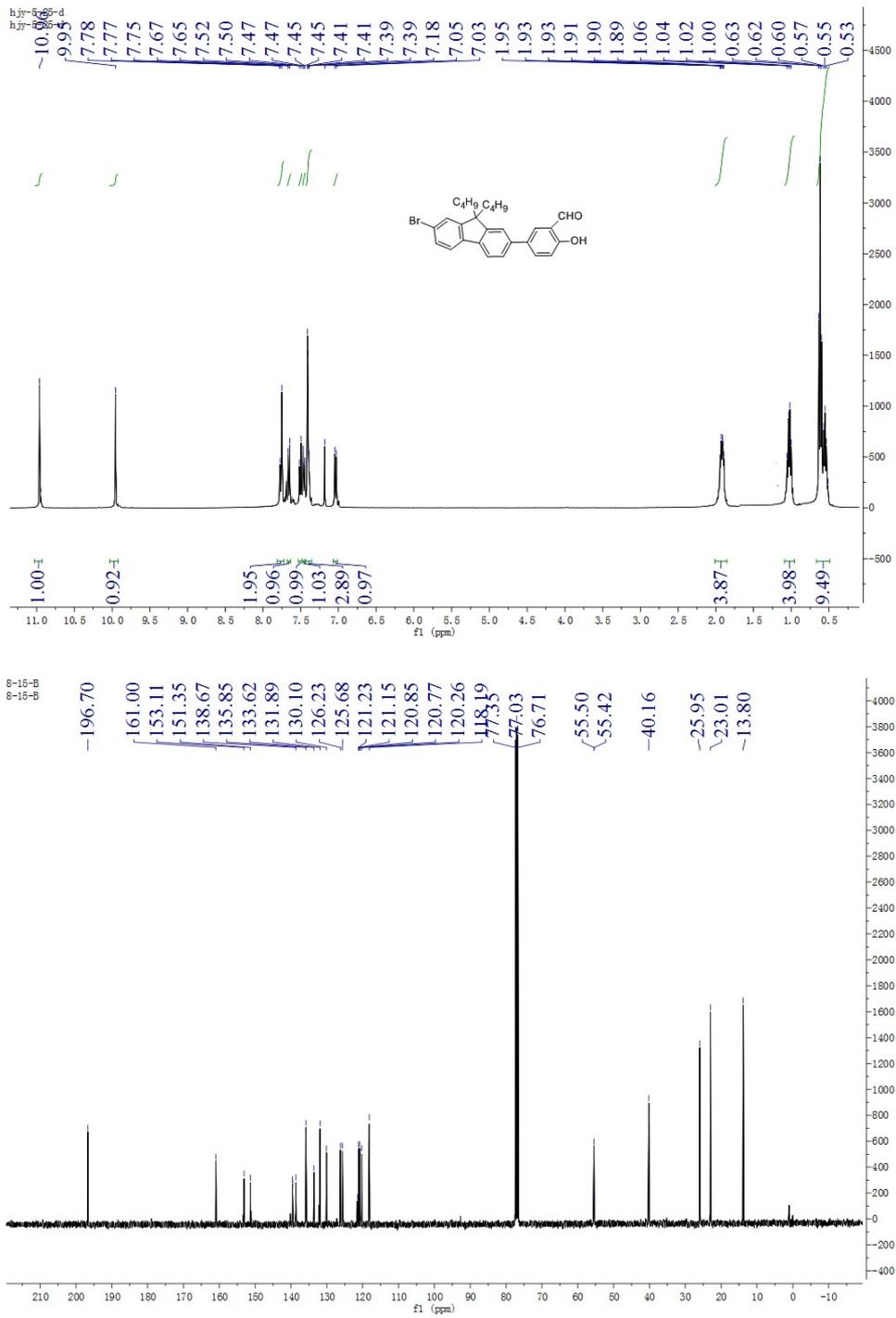
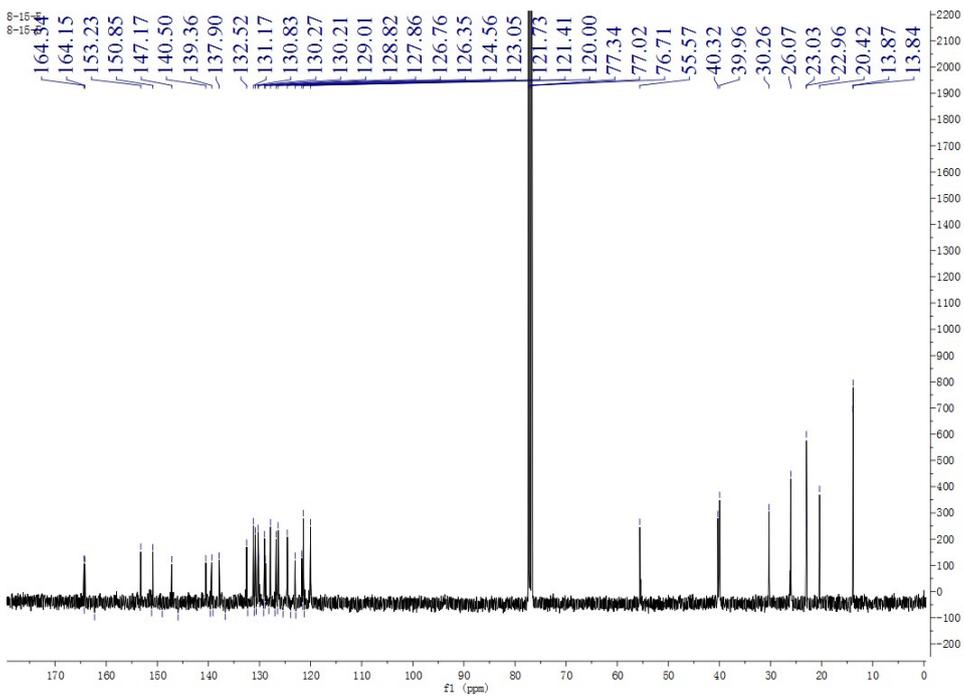
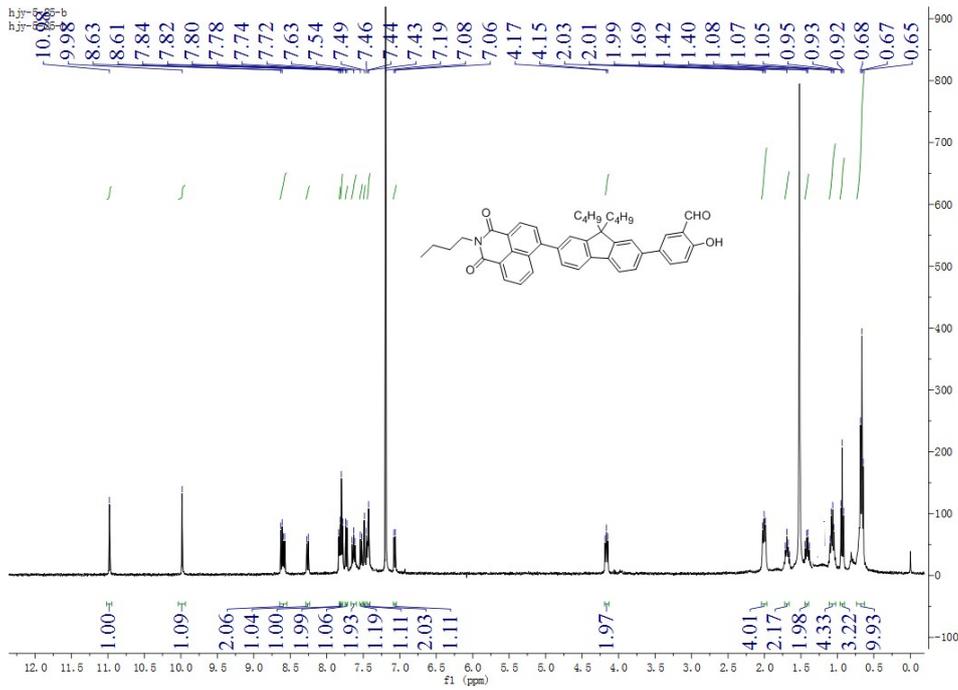
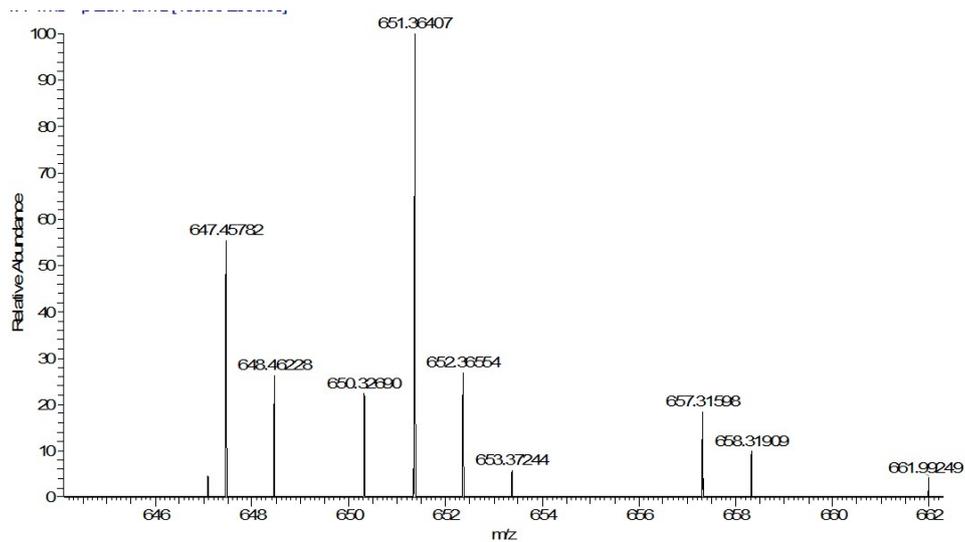
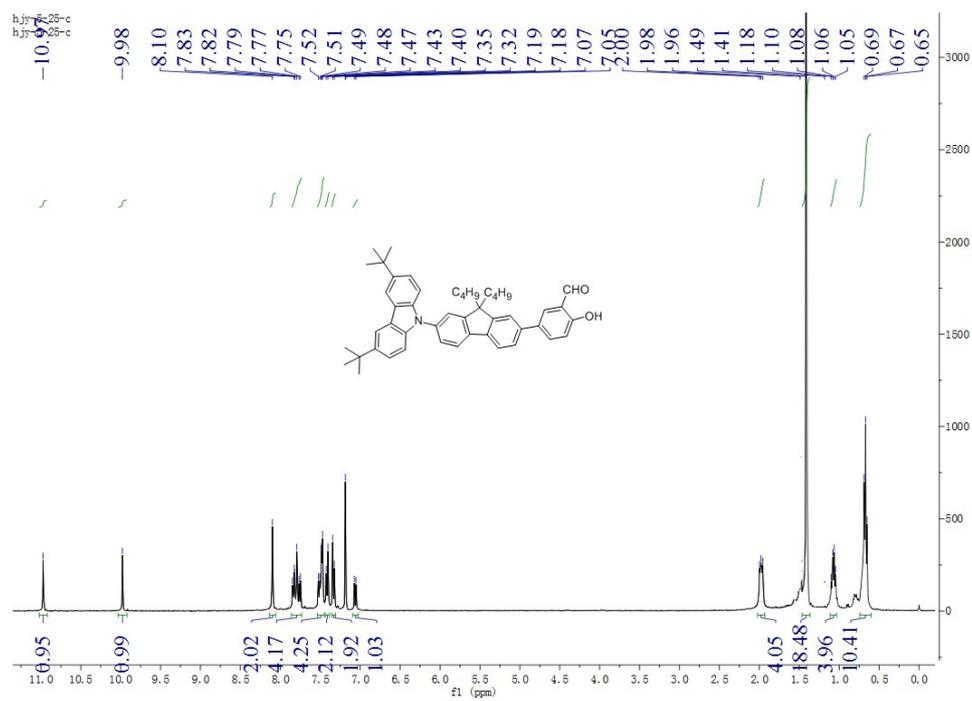


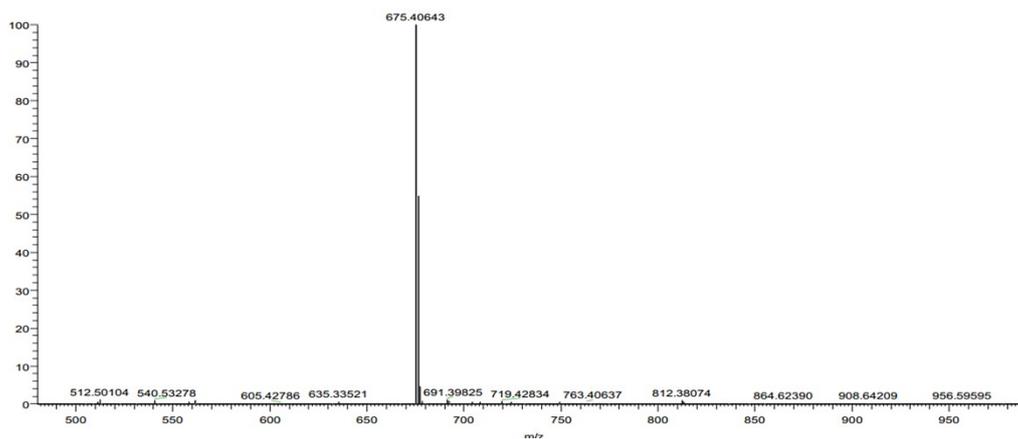
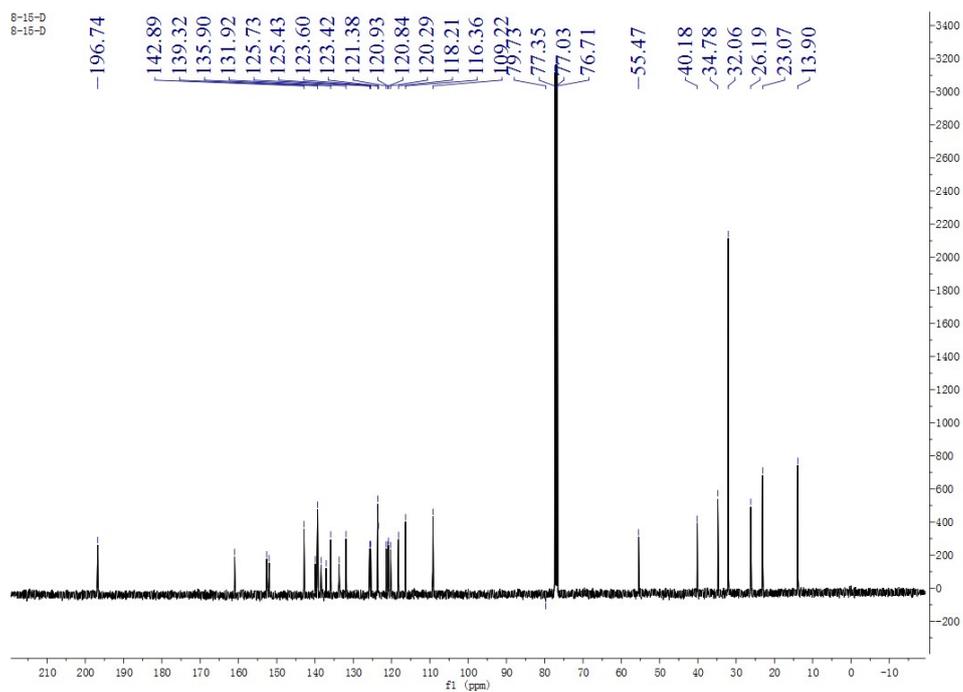
Fig.S1 <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compounds SFB





**Fig.S2**  $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR and high resolution mass spectrometry of compounds SFN



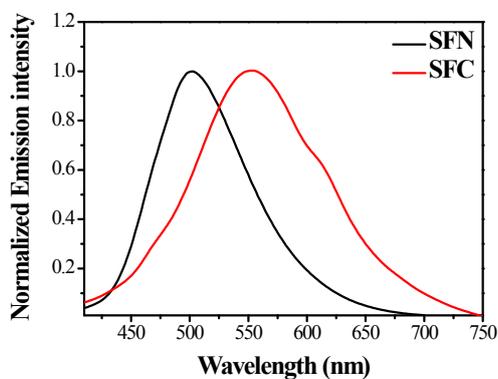


**Fig.S3**  $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR and high resolution mass spectrometry of compounds **SFC**

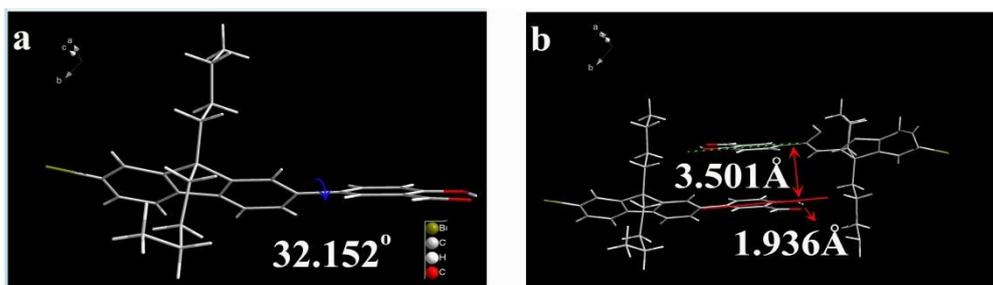
**Table S1** Emission wavelength and quantum yield of SFN and SFC in different solvents at R.T. and their solid quantum yield.

	$\lambda_{\text{em}}/\text{nm} (\Phi_{\text{em}})^{\text{a}}$					
	Hexane	Toluene	THF	$\text{CH}_2\text{Cl}_2$	$\text{CH}_3\text{CN}$	Solid
SFN	431(0.77)	460(0.56)	496(0.41)	507(0.39)	536(0.37)	502(0.61)
SFC	389/527(0.05)	396/538(0.04)	407/542(0.02)	413/557(0.012)	436(0.008)	553(0.08)

a Determined in different solvents using 0.1 M sulfuric acid solution of quinine sulfate ( $\Phi_{em}=0.54$ , excited at 365 nm) was used as the reference.



**Fig. S4** Normalized emission spectra of SFN and SFC in solid state.

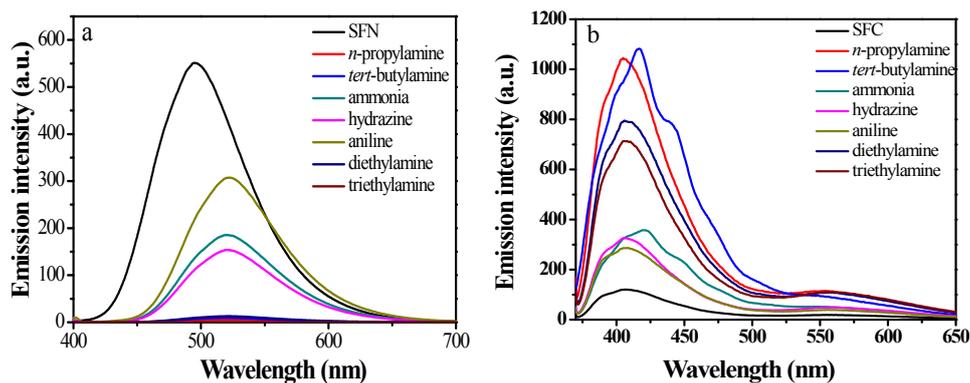


**Fig. S5** (a) Molecular structure and (b) crystal packing mode of SFB. The inter/intramolecular weak interactions (O-H...O and  $\pi$ - $\pi$ ) were shown as dashed lines.

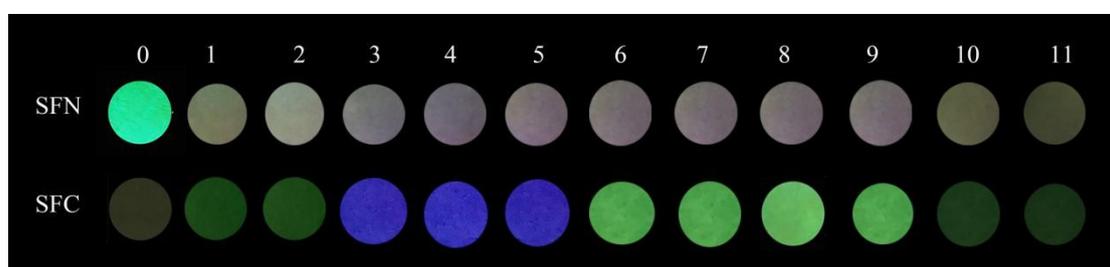
**Table S2** Crystallographic data of SFB, SFN and SFC (1558696-1558698)

	SFB	SFN	SFC
formula	C <sub>28</sub> H <sub>29</sub> Br O <sub>2</sub>	C <sub>44</sub> H <sub>43</sub> NO <sub>4</sub>	C <sub>48</sub> H <sub>53</sub> NO <sub>2</sub>
fw	477.42	649.32	675.41
crystal system	Triclinic	Triclinic	Triclinic
space group	P-1 (2)	P-1 (2)	P-1 (2)
<i>a</i> , Å	8.7300(7)	11.742(5)	11.417(3)

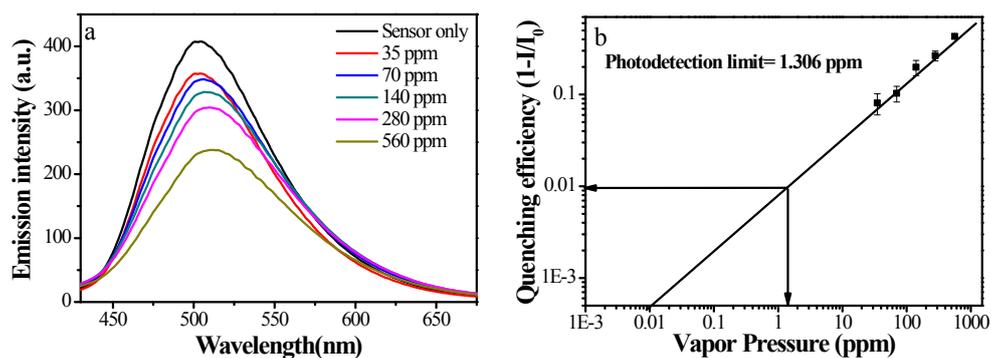
$b$ , Å	10.4348(8)	12.270(5)	14.259(4)
$c$ , Å	13.1284(13)	13.311(5)	14.489(4)
$a$ , deg	99.414(3)	67.566(10)	100.327(4)
$\beta$ , deg	97.111(3)	84.865(11)	110.851(4)
$\gamma$ , deg	97.020(2)	77.303(12)	112.865(4)
$V$ , Å <sup>3</sup>	1158.30(17)	1729.25(122)	1887.88(90)
$Z$	2	1	2
$\rho_{\text{calcd}}$ , g cm <sup>-3</sup>	1.369	1.16471	1.09507
$T$ / K	296(2)	296(2)	296(2)
$\mu$ , mm <sup>-1</sup>	1.248	1.248	1.189
$\theta$ , deg	2.32 to 25	2.42 to 26.98	2.3 to 27.39
$F(000)$	496	692	728
index ranges	$-10 \leq h \leq 10,$ $-11 \leq k \leq 12, -15$ $\leq l \leq 13$	$-13 \leq h \leq 9,$ $-14 \leq k \leq 14, -15$ $\leq l \leq 15$	$-13 \leq h \leq 13,$ $-10 \leq k \leq 16, -17$ $\leq l \leq 14$
data/restraints/parameters	4068 / 0 / 283	6022 / 278 / 445	6447 / 0 / 469
GOF ( $F^2$ )	1.064	1.024	1.047
$R_1^a, wR_2^b$ ( $I > 2\sigma(I)$ )	0.0461, 0.1143	0.0221, 0.2258	0.0541, 0.1435
$R_1^a, wR_2^b$ (all data)	0.0574, 0.1198	0.0315, 0.2114	0.0712, 0.1611



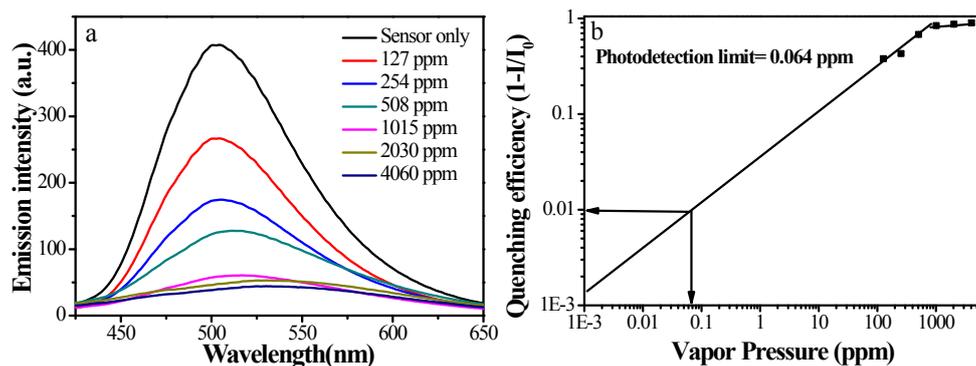
**Fig. S6** Changes in fluorescence intensity of SFN (a) and SFC (b) in THF solution with addition of 100 eq. different amines.



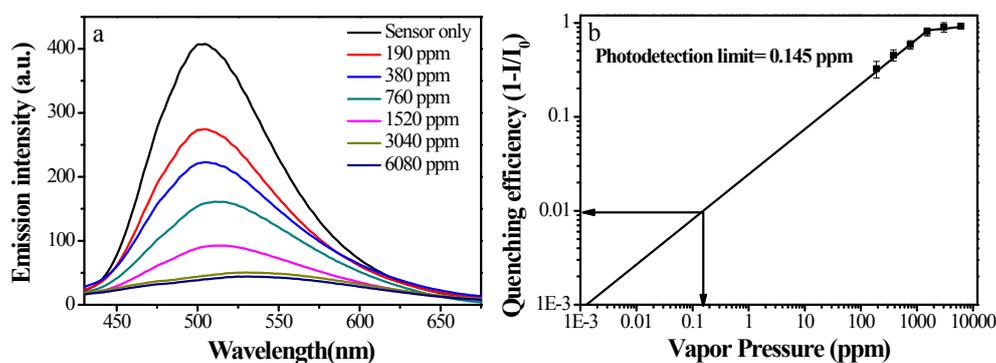
**Fig.S7** Photographs of SFN and SFC on test papers upon exposure to different saturated amine vapors for 30 s under 365 nm lamp: (0) blank; (1) ammonia; (2) hydrazine; (3) *n*-propylamine; (4) *tert*-butylamine; (5) *n*-butylamine; (6) diethylamine; (7) diisopropylamine; (8) *N,N*-diisopropylethylamine; (9) triethylamine; (10) aniline; (11) pyridine.



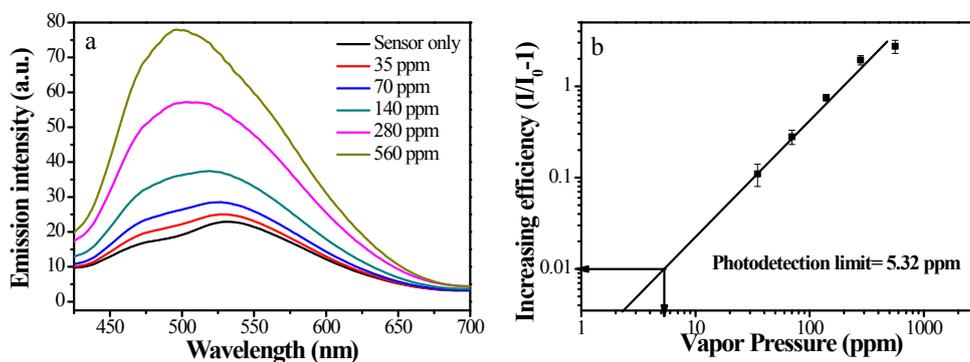
**Fig. S8** (a) Changes in fluorescence intensity of SFN films exposed to aniline vapor with different concentrations; (b) The concentration-dependent fluorescence quenching efficiency ( $1-I/I_0$ ) for SFN as a function of the vapor pressure of aniline, fitted with the Langmuir equation.



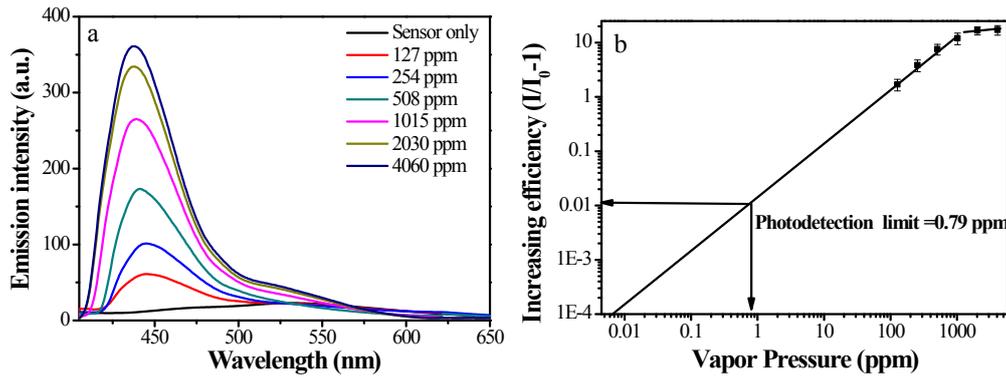
**Fig. S9** (a) Changes in fluorescence intensity of SFN films exposed to *n*-propylamine vapor with different concentrations; (b) The concentration-dependent fluorescence quenching efficiency ( $1-I/I_0$ ) for SFN as a function of the vapor pressure of *n*-propylamine, fitted with the Langmuir equation.



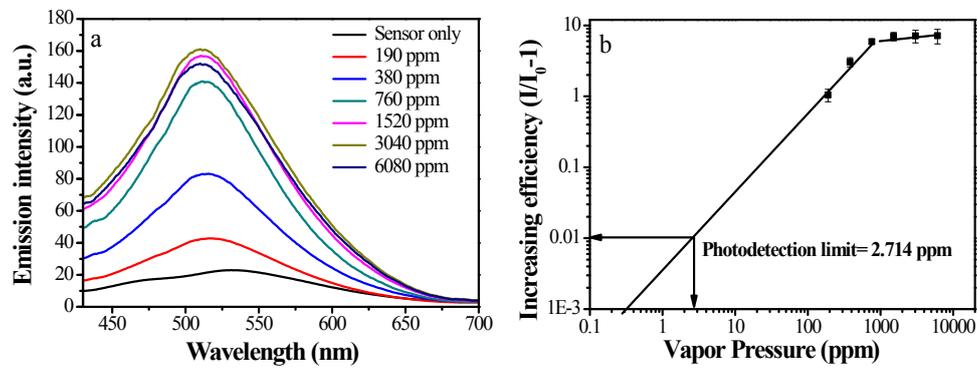
**Fig. S10** (a) Changes in fluorescence intensity of SFN films exposed to triethylamine vapor with different concentrations; (b) The concentration-dependent fluorescence quenching efficiency ( $1-I/I_0$ ) for SFN as a function of the vapor pressure of triethylamine, fitted with the Langmuir equation.



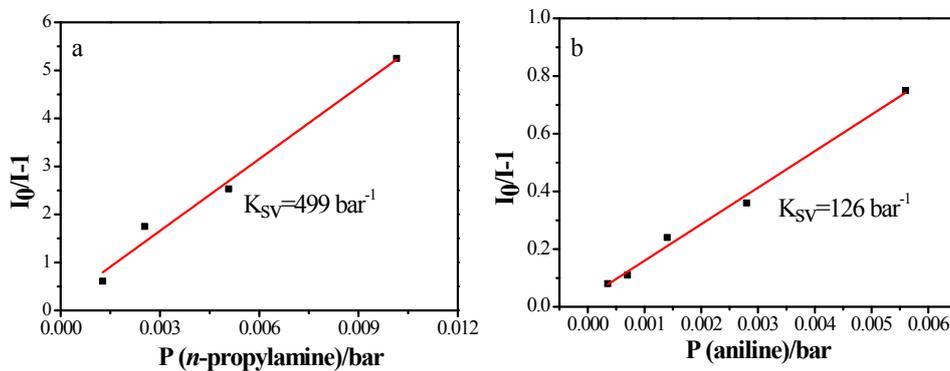
**Fig. S11** (a) Changes in fluorescence intensity of SFC films exposed to aniline vapor with different concentrations; (b) The concentration-dependent fluorescence increasing efficiency ( $I/I_0 - 1$ ) for SFC as a function of the vapor pressure of aniline, fitted with the Langmuir equation.

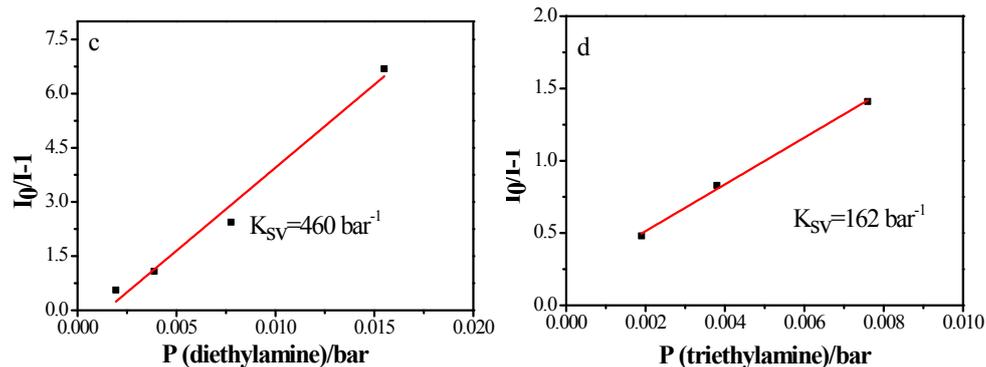


**Fig. S12** (a) Changes in fluorescence intensity of SFC films exposed to *n*-propylamine vapor with different concentrations; (b) The concentration-dependent fluorescence increasing efficiency ( $I/I_0 - 1$ ) for SFC as a function of the vapor pressure of *n*-propylamine vapor.

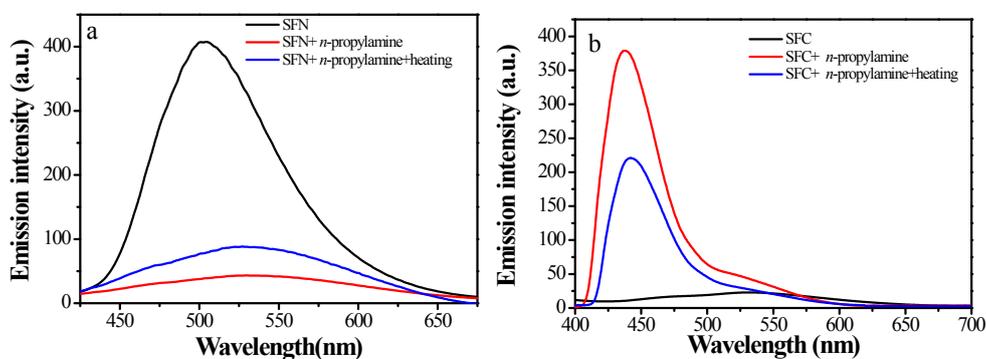


**Fig. S13** (a) Changes in fluorescence intensity of SFN films exposed to triethylamine vapor with different concentrations; (b) The concentration-dependent fluorescence increasing efficiency ( $I/I_0 - 1$ ) for SFC as a function of the vapor pressure of triethylamine, fitted with the Langmuir equation.

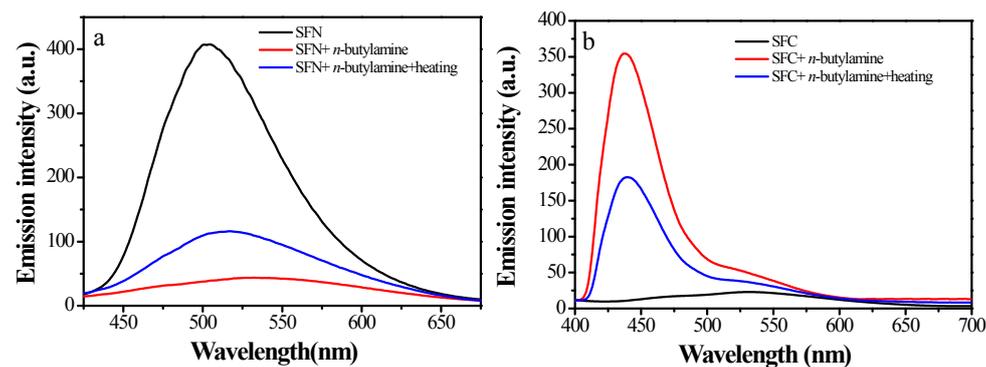




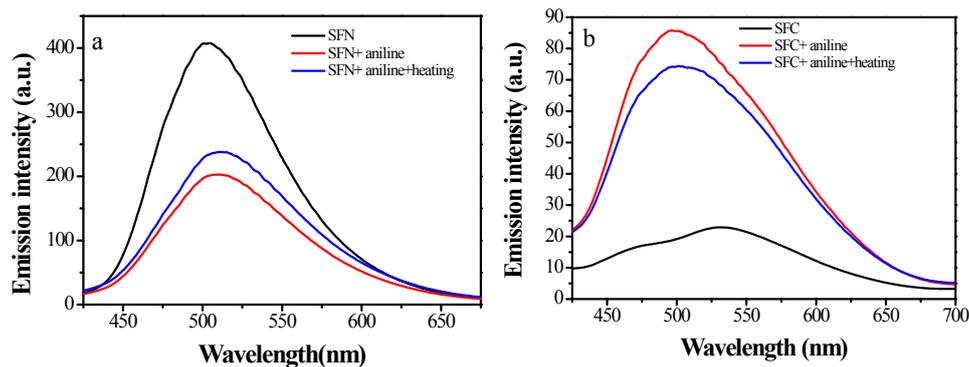
**Fig. S14** Stern-Volmer plot of SFN in *n*-propylamine (a), aniline (b), diethylamine (c) and triethylamine (d) vapor.



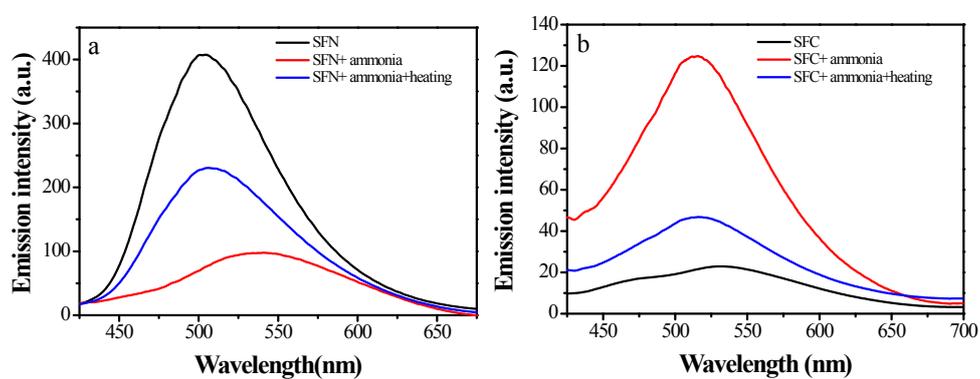
**Fig. S15** Emission spectra of SFN(a) and SFC(b) films exposed to *n*-propylamine vapor and then heating.



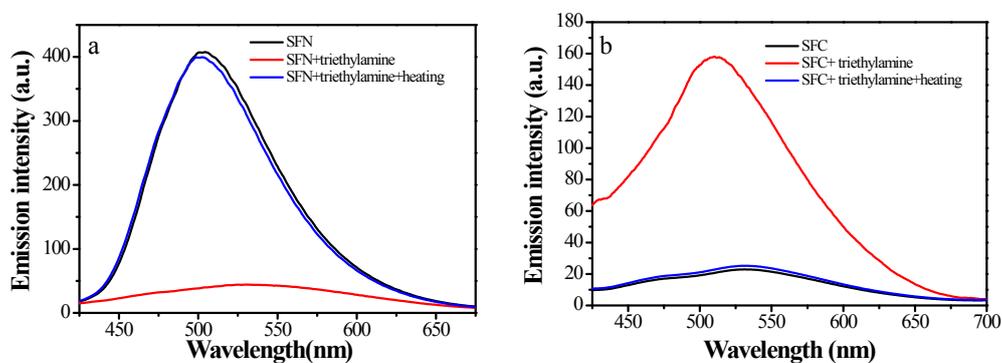
**Fig. S16** Emission spectra of SFN(a) and SFC(b) films exposed to *n*-butylamine vapor and then heating.



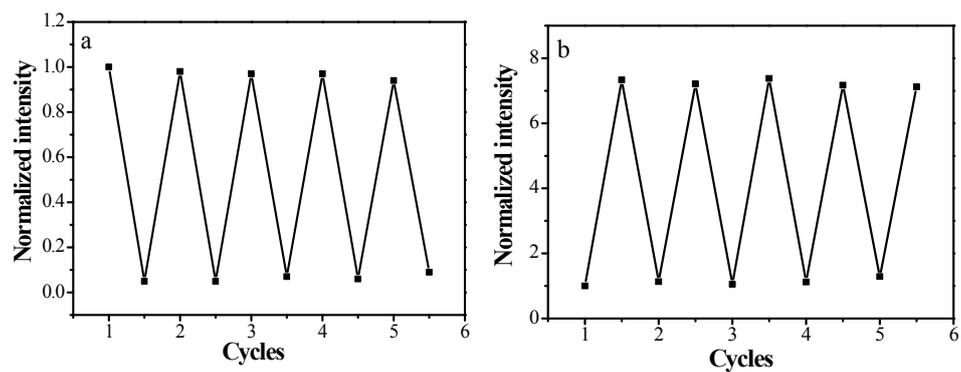
**Fig. S17** Emission spectra of SFN(a) and SFC(b) films exposed to aniline vapor and then heating.



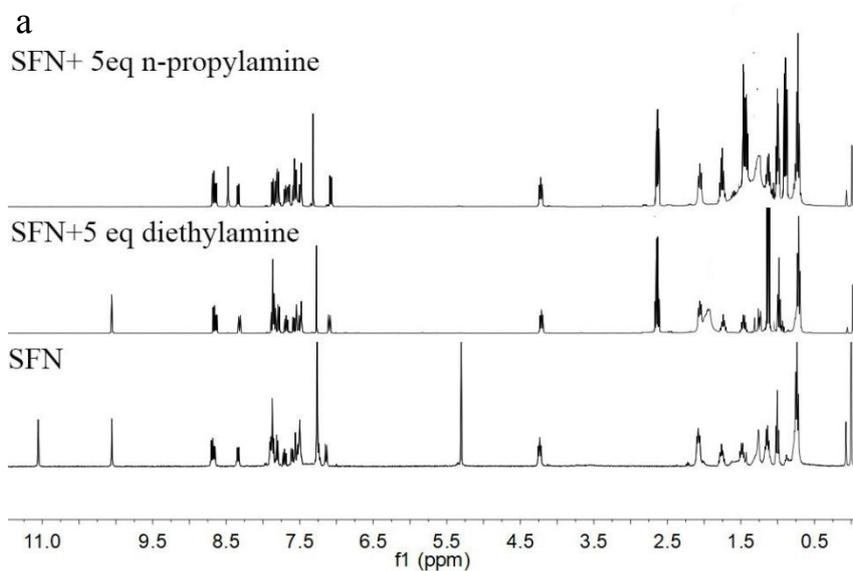
**Fig. S18** Emission spectra of SFN(a) and SFC(b) films exposed to ammonia vapor and then heating.

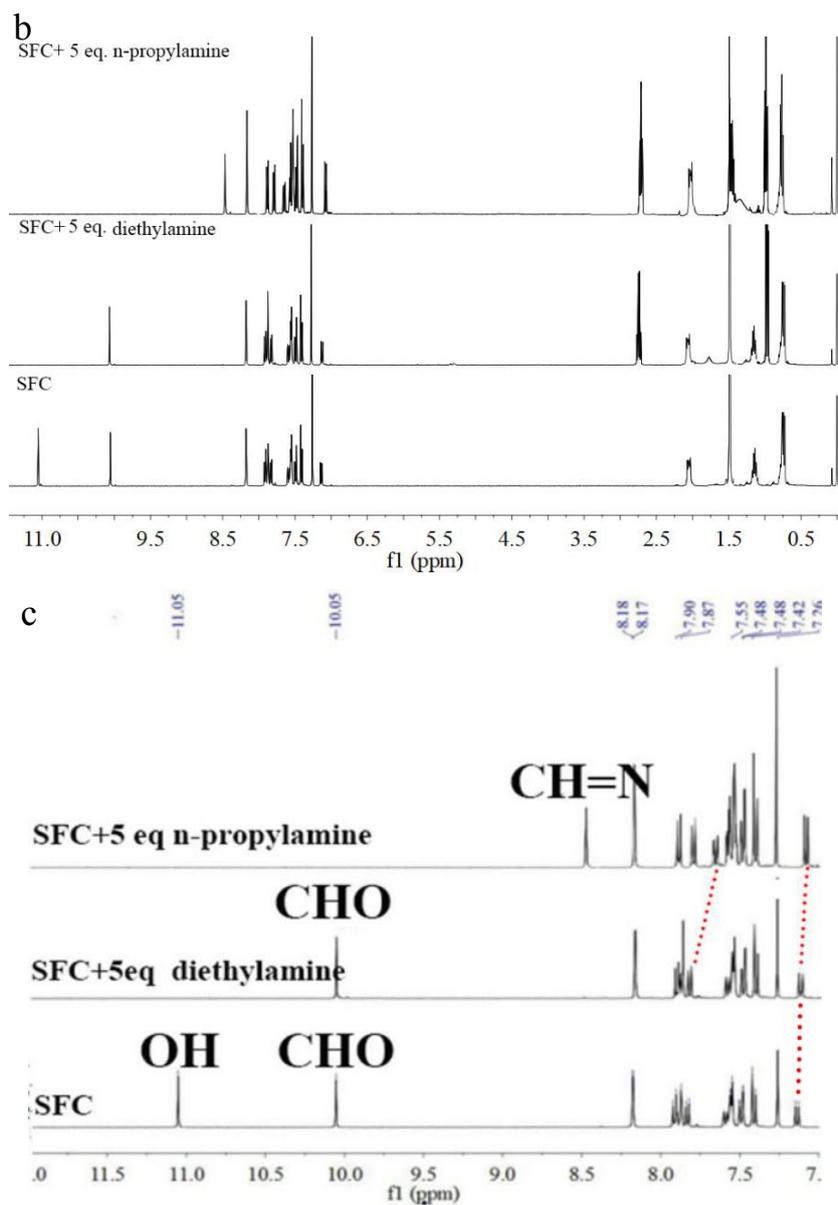


**Fig. S19** Emission spectra of SFN(a) and SFC(b) films exposed to triethylamine vapor and then heating.



**Fig. S20** Cycles of the emission (a) quenching/ (b) increasing by exposure to the saturated of triethylamine vapors and recovery by the heating, respectively.





**Fig. S21** Changes in  $^1\text{H}$  NMR spectra of SFN(a), SFC(b) and enlarged  $^1\text{H}$  NMR spectra of SFC(c) upon addition of *n*-propylamine and diethylamine in  $\text{CDCl}_3$  solvent.