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Fluorescent Nanofiber Film Based on Simple Organogelator for Highly Efficient Detection of TFA Vapour

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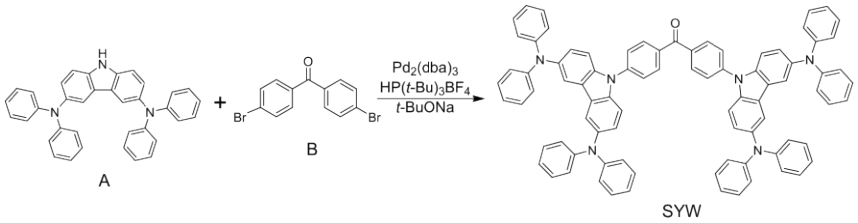
1. Synthesis of SYW



Scheme S1. The synthesis procedure of **SYW**.

Synthesis of bis(4-(3,6-bis(diphenylamino)-9*H*-carbazol-9-yl)phenyl)methanone (SYW):

The synthesis of compound **SYW** is obtained by Buchwald-Hartwig reaction. A solution of N^3,N^3,N^6,N^6-tetraphenyl-9*H*-carbazole-3,6-diamine (371 g, 0.74 mmol), bis(4-bromophenyl)methanone (95 mg, 0.28 mmol), $Pd_2(dba)_3$ (13 mg, 0.014 mmol), $[HP(t\text{-}Bu)_3]BF_4$ (8 mg, 0.028 mmol) and sodium *t*-butoxide (161 mg, 1.68 mmol) in anhydrous toluene (15 mL) was refluxed for 12 h under argon atmosphere. After cooling, the suspension was poured into water. Then, the mixture was extracted with dichloromethane and washed with brine several times. The combined organic phase was dried over $MgSO_4$. After removal of the solvent under reduced pressure, the crude product was purified by chromatography (dichloromethane : petroleum ether = 2 : 1) to give **SYW** (265 mg, 80 %) as a yellow solid. ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm): 8.15 (d, J = 8.4 Hz, 4H), 7.80-7.77 (m, 8H), 7.46 (d, J = 8.4 Hz, 4H), 7.26-7.20 (m, 22H), 7.08 (d, J = 7.8 Hz, 16H), 6.95 (t, J = 7.2 Hz, 8H). ^{13}C NMR (150 MHz, $CDCl_3$): δ(ppm): 194.22, 148.47, 141.87, 141.41, 137.73, 135.79, 131.89, 129.14, 126.14, 125.98, 124.73, 122.95, 121.90, 118.55, 110.88. MS (MALDI): *m/z*: 1180.4820

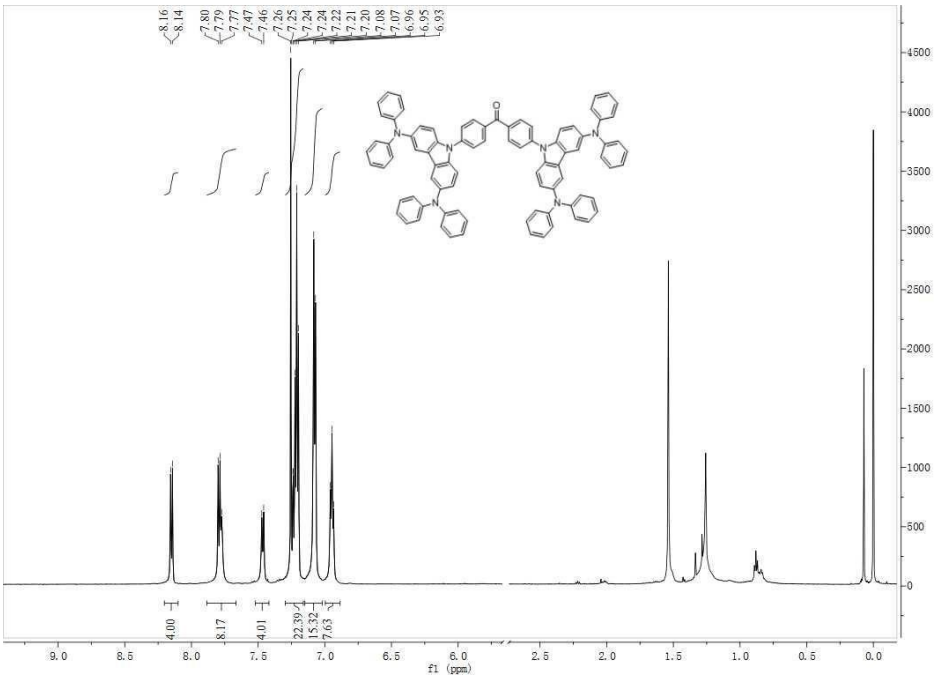


Figure S1. ^{1}H NMR of **SYW**.

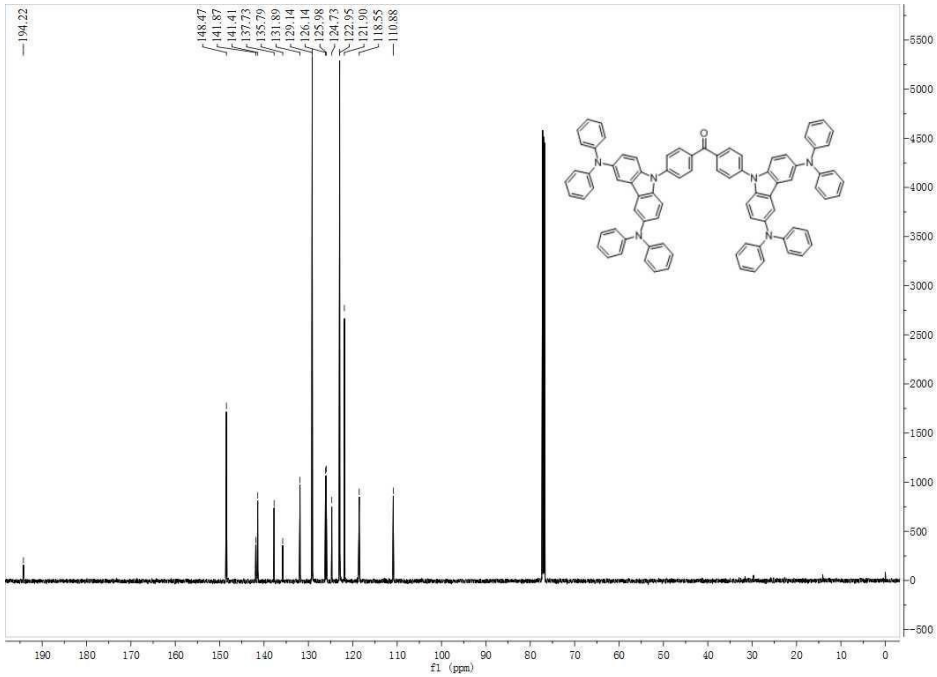


Figure S2. ^{13}C NMR of **SYW**.

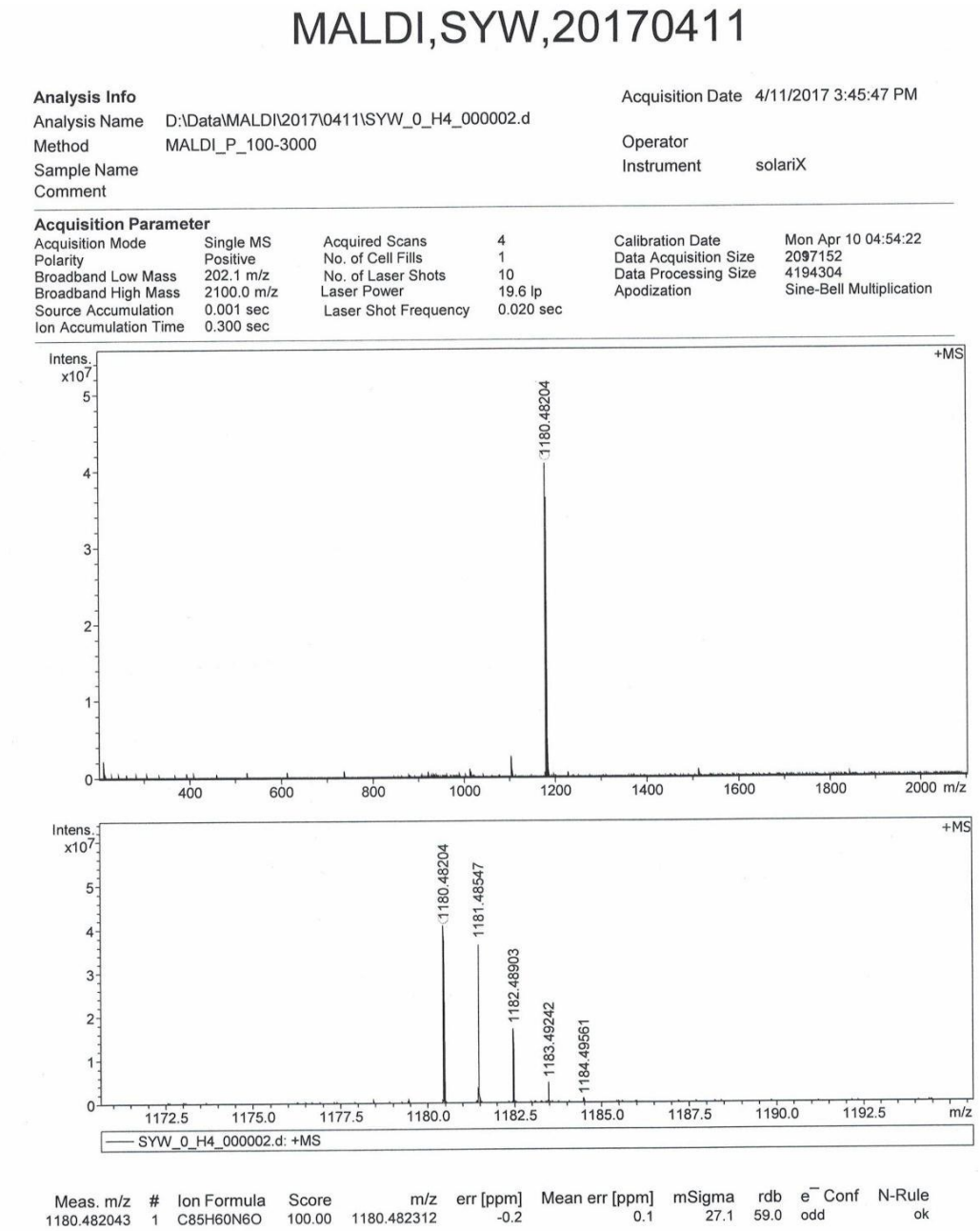


Figure S3. MALDI-TOF spectrum of **SYW**.

Table S1. Gelation properties of **SYW** in selected organic solvents[a].

Solvent	CGC(m/v)	T_{gel}(℃)
n-hexane	I	-
acetonitrile	I	-
chloroform	P	-
THF	UG	-
DMF	P	-
1,4-dioxane	P	-

toluene	G(6)	57
DMSO	P	-
acetone	I	-
dichlormethane	P	-
methanol	I	-
ethanol	I	-
EA	UG	-
chlorobenzene(CB)	G(8)	45
1,2-dichloroethane(DCE)	P	-
bromobenzene(BB)	G(8)	46
1,2-dichlorobenzene(DCB)	G(10)	43

[a] G = stable gel; S = soluble; I = insoluble; P = precipitation. UG = unstable gel; The values in parentheses are the critical gelation concentrations (CGCs) in mg/mL.

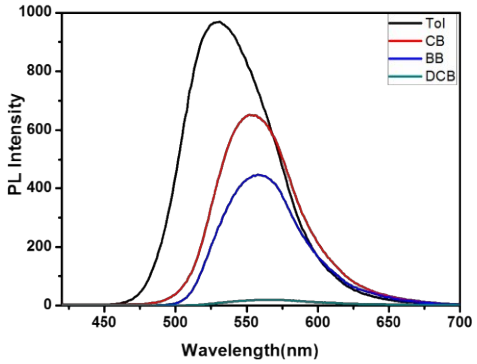


Figure S4. Fluorescence spectra of **SYW** gels formed in toluene, chlorobenzene, bromobenzene and 1,2-dichlorobenzene.

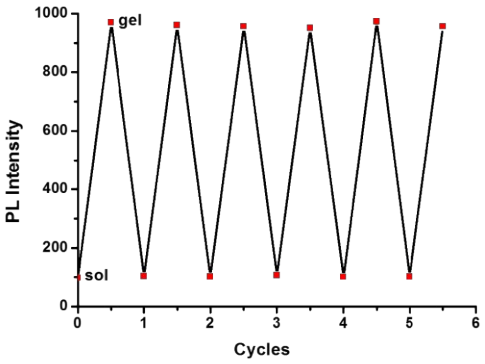


Figure S5. Reproducible reversibility of emission intensity in solution to gel conversion.

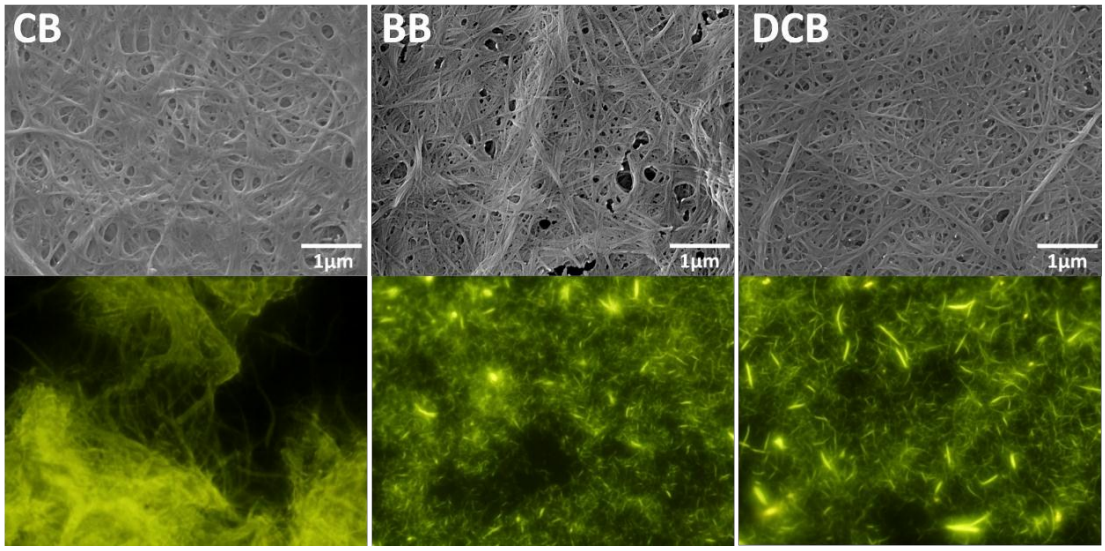


Figure S6. FE-SEM photographs and fluorescence microscopy of xerogels formed from **SYW** in different solvents.

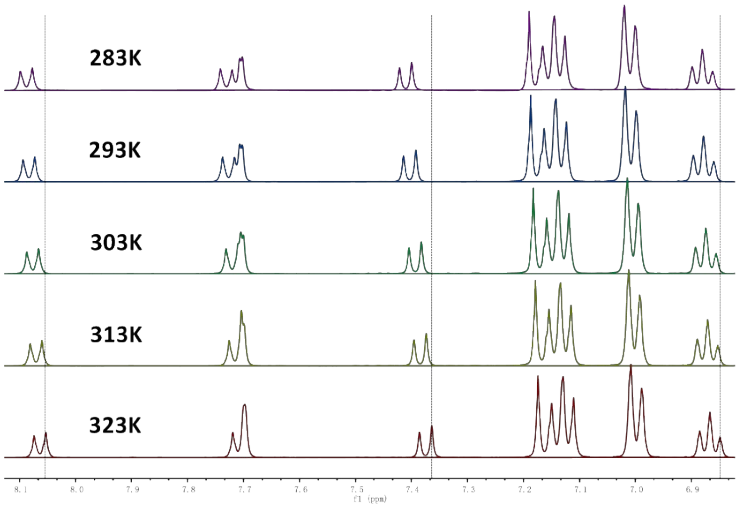


Figure S7. ^{1}H NMR spectra of **SYW** from 283-323 K in $CDCl_3$.

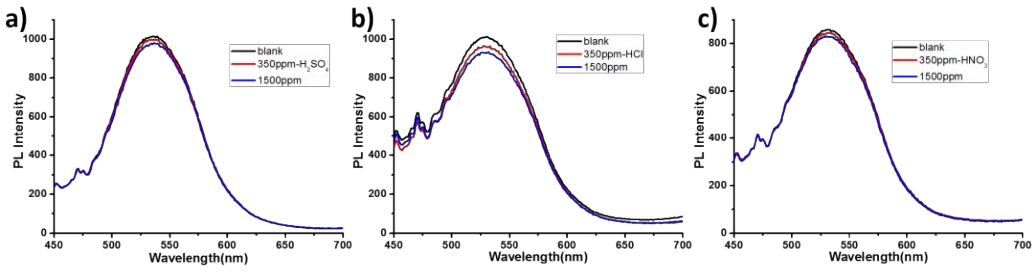


Figure S8. Emission spectral change of **SYW** xerogel film obtained from toluene (λ_{ex} = 360 nm) with the increasing vapor concentration of a) H_2SO_4, b) HCl, c) HNO_3.

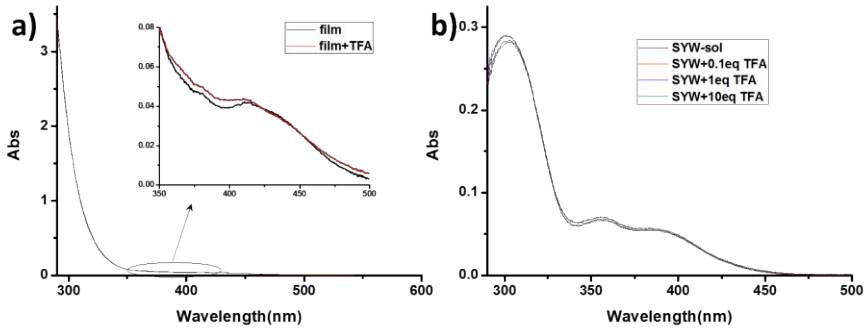


Figure S9. UV-Vis spectra of **SYW** a) in xerogel film obtained from toluene before and after expose TFA vapor; b) in toluene solution (3×10^{-6} M) upon increasing the amount of TFA.

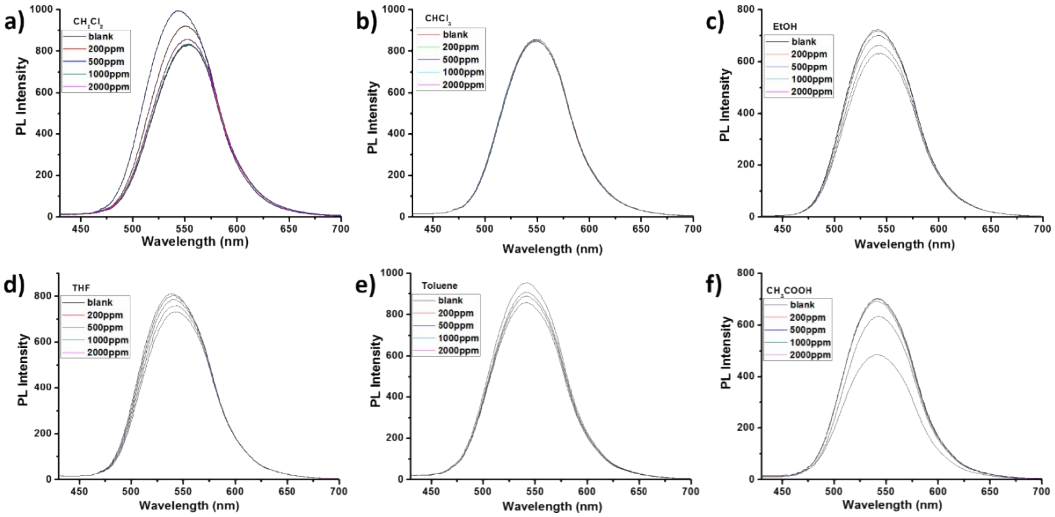


Figure S10. Fluorescence emission spectra of xerogel-based film (λ_{ex} = 360 nm) upon exposure towards different vapor of a) CH_2Cl_2, b) $CHCl_3$, c) C_2H_5OH, d) THF, e) toluene and f) CH_3COOH.