

Supporting Information (SI)

A simple and effective strategy *via* aggregation-induced to improve two-photon absorption

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Fig. S1: The characterization data of compounds **T1**, **T2** and **T3**

Fig. S2: Linear absorption (a) and fluorescence (b) spectra of **T2** in five organic solvents with different polarities at a concentration of $5 \times 10^{-5} \text{ mol L}^{-1}$.

Fig. S3: Linear absorption (a) and fluorescence (b) spectra of **T3** in five organic solvents with different polarities at a concentration of $5 \times 10^{-5} \text{ mol L}^{-1}$.

Fig. S4: Lippert-Mataga plots for **T1**, **T2** and **T3**.

Fig. S5: Particle size distribution of **T2** in mixtures with different water fractions: (a) Water/DMF (40/60, v/v); (b) Water/ DMF (50/50, v/v); (c) Water/ DMF (90/10, v/v).

Fig. S6: The 2D layer structures of **T1** and **T2**

Fig. S7: The open aperture Z-scan data of **T1** (a) in pure solution and **T3** in aggregates (b) and in pure solution (c)

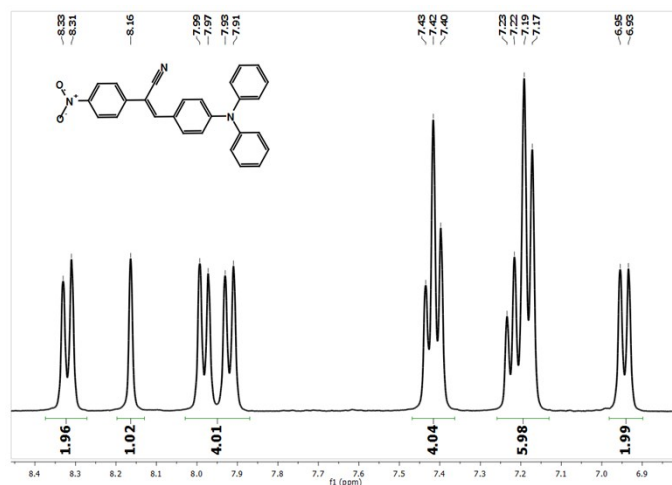
Fig. S8: Photon-bleach experiment of **T1**, **T2** and **T3** over continued laser scanning.

Table S1: The linear optical properties of **T1**, **T2** and **T3**.

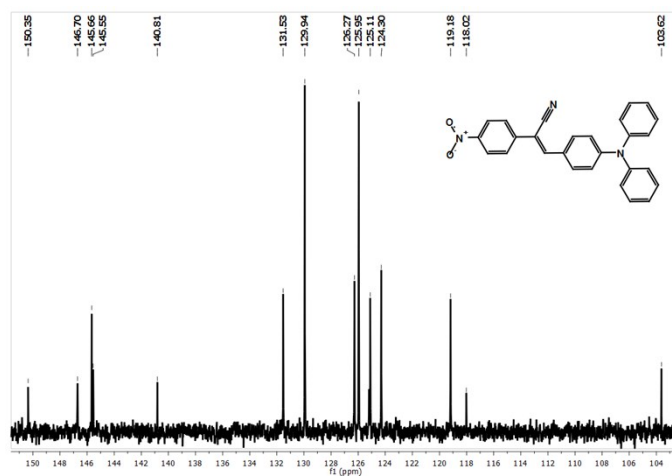
Table S2: The transition dipole moment calculation results of **T1**, **T2** and **T3**

Table S3: Crystal data of **T1** and **T2**.

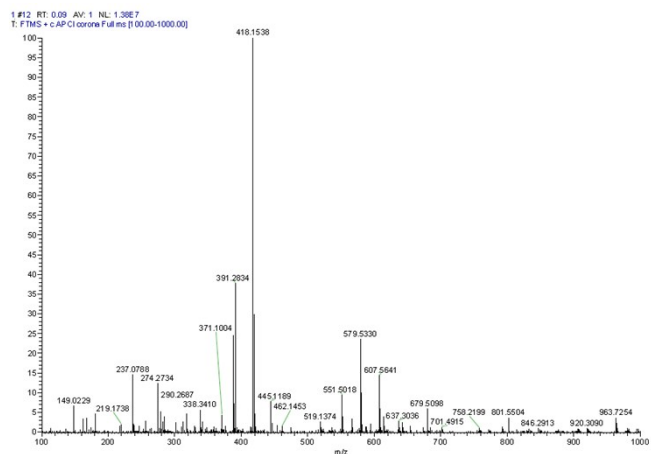
Fig. S1a: ^1H NMR, ^{13}C NMR and MS spectra of **T1**.



The ^1H NMR (400MHz) spectra of **T1** in $\text{DMSO-}d_6$

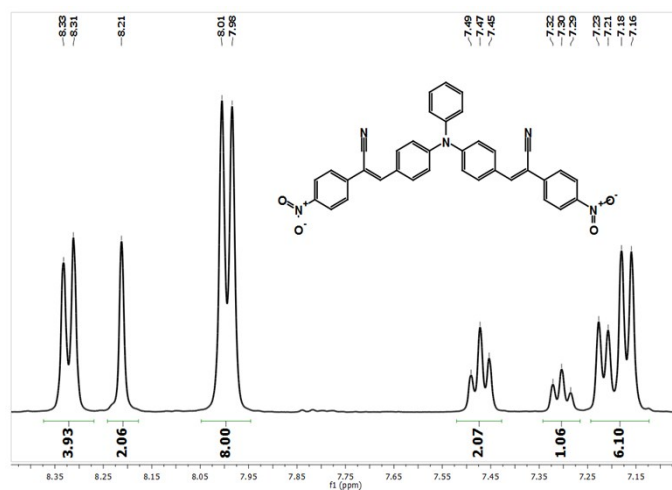


The ^{13}C NMR (100 MHz) spectra of **T1** in $\text{DMSO-}d_6$

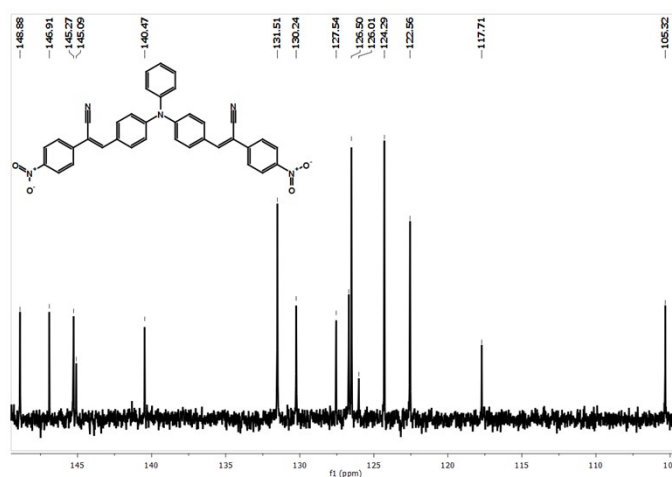


MS of **T1**

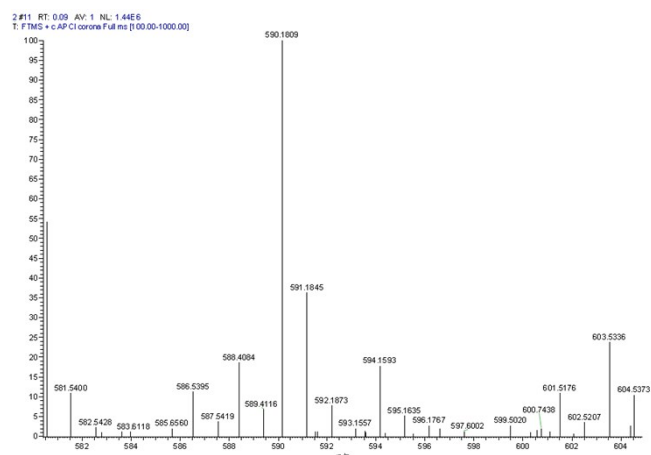
Fig. S1b: ^1H NMR, ^{13}C NMR and MS spectra of **T2**.



The ^1H NMR (400MHz) spectra of **T2** in $\text{DMSO-}d_6$

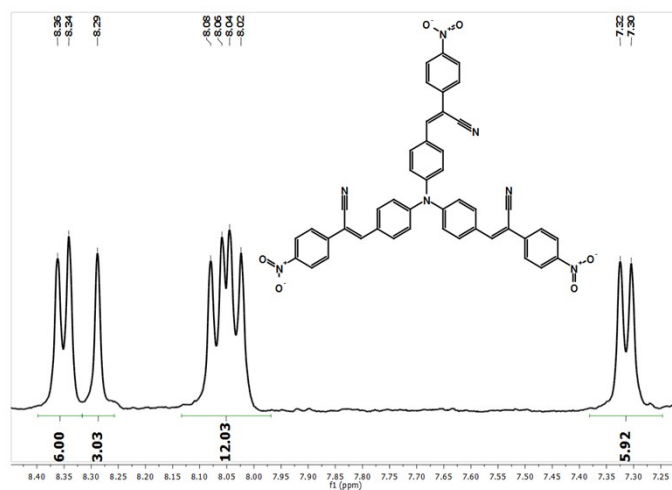


The ^{13}C NMR (100 MHz) spectra of **T2** in $\text{DMSO-}d_6$

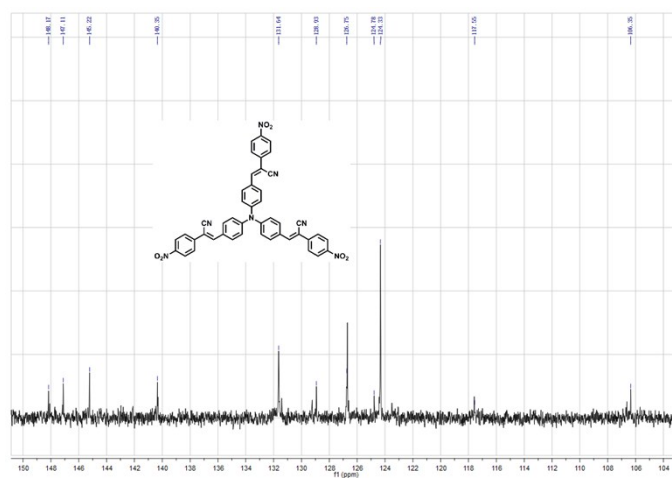


MS of **T2**

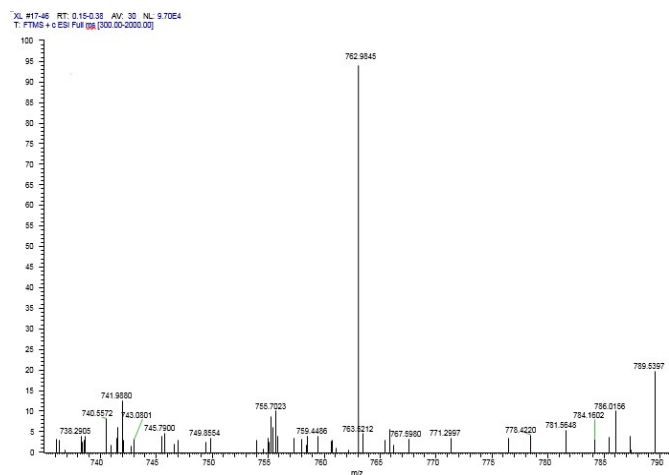
Fig. S1c: ^1H NMR, ^{13}C NMR and MS spectra of **T3**.



The ^1H -NMR of **T3** ($\text{DMSO}-d_6$, 400 MHz)



The ^{13}C NMR (100 MHz) spectra of **T3** in $\text{DMSO}-d_6$



MS of T3

Fig. S2: Linear absorption (a) and fluorescence (b) of **T2** in five organic solvents with different polarities at a concentration of $5 \times 10^{-5} \text{ mol L}^{-1}$.

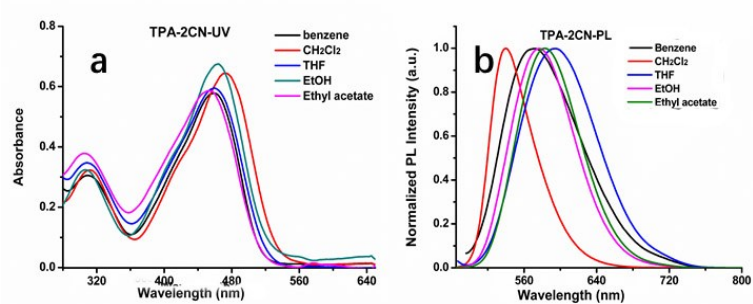


Fig. S3: Linear absorption (a) and fluorescence (b) of **T3** in five organic solvents with different polarities at a concentration of $5 \times 10^{-5} \text{ mol L}^{-1}$.

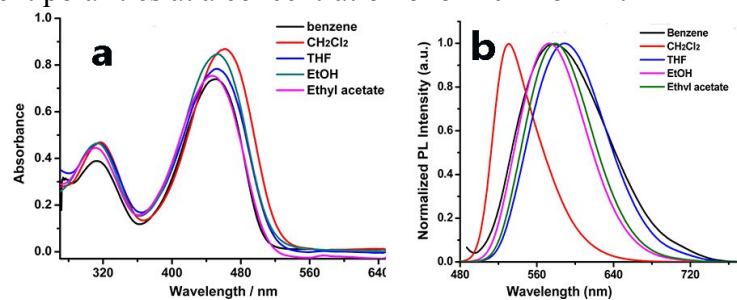


Fig. S4: Lippert-Mataga plots for T1, T2 and T3

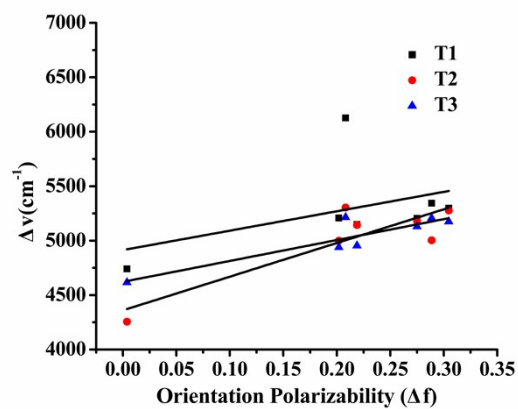


Fig. S5: Particle size distribution of T2 in mixtures with different water fractions: (a) Water/DMF (40/60, v/v); (b) Water/DMF (50/50, v/v); (c) Water/DMF (90/10, v/v).

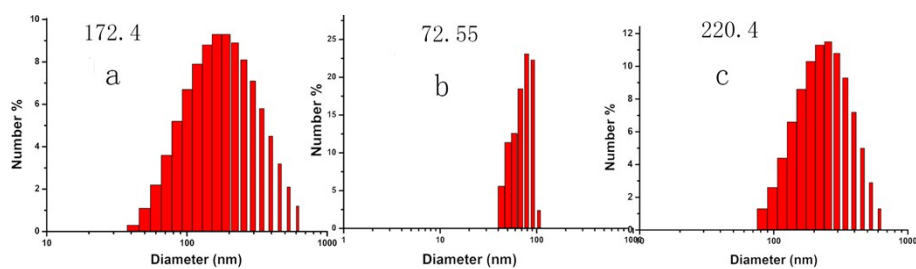


Fig. S6: The 2D structures of T1 (a) and T2 (b)

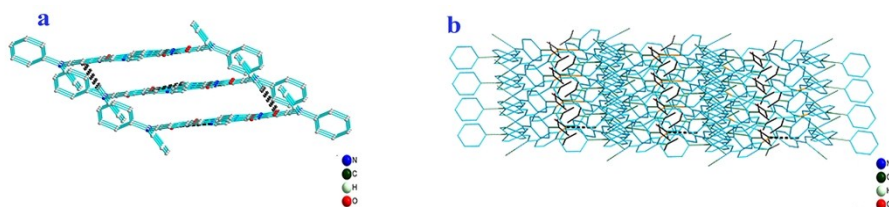


Fig. S7: The open aperture Z-scan data of **T1** (a) and **T3** (b, c) in aggregates and in pure solution

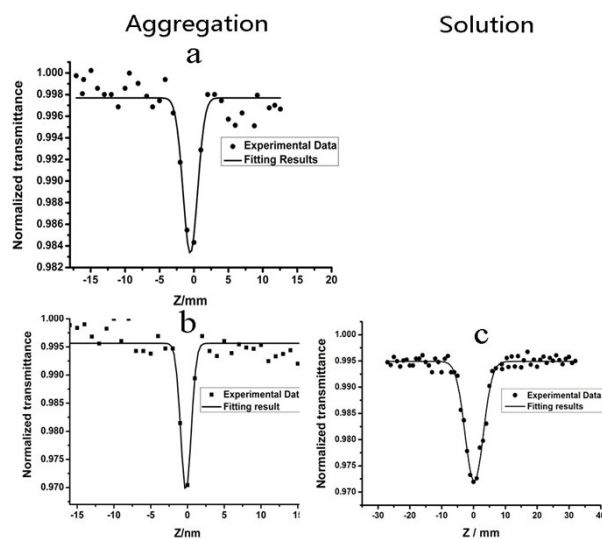


Fig. S8: Photon-bleach experiment of **T1**, **T2** and **T3**.

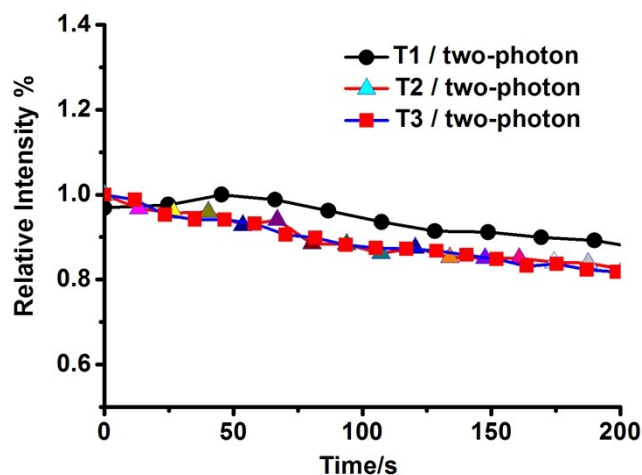


Table S1: The Linear absorption properties of **T1**, **T2** and **T3**.

Compounds	Solvents	$\lambda_{\max}^{[a]}$	$\lambda_{\max}^{[b]}$	$\Delta\nu^{[c]}$
T1	Benzene	296, 435	548	4740.33
	Dichloromethane	297, 451	549	3958.01
	Tetrahydrofuran	294, 434	572	5558.96
	Ethanol	293, 441	586	5585.21
	Ethyl acetate	293, 426	593	6610.77
T2	Benzene	310, 460	572	4256.61
	Dichloromethane	312, 472	540	2667.92
	Tetrahydrofuran	309, 460	594	4904.11
	Ethanol	307, 463	577	4267.25
	Ethyl acetate	306, 453	583	4922.40

T3	Benzene	312, 450	568	4616.59
	Dichloromethane	317, 461	531	2859.58
	Tetrahydrofuran	315, 451	588	5166.15
	Ethanol	313, 453	573	4623.05
	Ethyl acetate	307, 454	580	4785.05

^a Absorption peak position in nm (5×10^{-5} mol L⁻¹). ^b Emission Peak position of **T1-T3** in nm (5×10^{-5} mol L⁻¹), excited at the absorption maximum. ^c Stokes shift in cm⁻¹.

Table S2: The transition dipole moment calculation results of **T1**, **T2** and **T3**

Compounds	Angstrom radius with optimized structure(Å)	$\mu_e - \mu_g$ (D)
T1	5.66	4.79
T2	6.27	8.35
T3	6.99	6.42

Table S3: Crystal data of compounds **T1** and **T2**

Compounds	T1	T2
Empirical formula	C ₂₇ H ₁₉ N ₃ O ₂	C ₃₆ H ₂₃ N ₅ O ₄
Formula weight	417.45	589.59
Crystal system	Monoclinic	Monoclinic
Space group	P2(1)/c	C2/c
a[Å]	11.165(5)	34.868(3)
b[Å]	7.545(5)	9.7729(9)
c[Å]	25.708(5)	29.980(3)
α [°]	90.000(5)	90
β [°]	96.505(5)	119.721(3)
γ [°]	90.000(5)	90
<i>V</i> [Å ³]	2151.7 (18)	8871.9(15)
<i>Z</i>	4	12
<i>T</i> [K]	296(2)	296(2)
<i>D</i> _{calcd} [g·cm ⁻³]	1.289	1.055
F(000)	872	884
μ [mm ⁻¹]	0.08	0.089
θ range[°]	2.6–22.3	1.34–25.00
Total no. data	14789	30908
No. unique data	3774	7833
<i>R</i> _{int}	0.030	0.0489
<i>R</i> ₁	0.0454	0.0515
<i>wR</i> ₂	0.1559	0.1475
GOF	1.136	0.919

