Supporting Information

A New Type of Light-Emitting Naphtho[2,3-*c*][1,2,5]thiadiazole Derivatives: Synthesis, Photophysical Characterization, and Transporting Property

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Single-crystal structure: Single-crystal X-ray experiment of **1** was performed on a Bruker P4 diffractometer equipped with graphite monochromatized Mo K_α radiation at the room temperature (295±2 K). Single-crystal X-ray experiment of **3** was performed on a Bruker SMART APEX-CCD based diffractometer equipped with graphite monochromatized Mo Kα radiation at the room temperature (295±2 K). The structures were solved by direct method using SHELXS NT ver. 5.10 (Bruker, 1997).

Table S1. Crystal Data of **1**

Sample code	**1**-single crystal		
Molecular formula	$C_{50}H_{34}N_2S$		
Molecular weight	694.85		
Color and habit	red prism		
Crystal size	$0.2 \times 0.3 \times 0.4$ mm^3		
Crystal system	triclinic		
Space group	$P\bar{1}$ (No. 2)		
Unit cell parameters	a = 6.0191(11) Å		α = 100.69(2)°
	b = 9.059(2) Å		β = 95.305(19)°
	c = 17.191(6) Å		γ = 91.741(15)°
	V = 916.1(4) Å^3	Z = 1	F(000) = 364
Density (calcd)	1.259 g/cm^3		
Temperature	295±2 K		
Scan type	ω-scan		
Data collection range	$-1 < h < 7$, $-10 < k < 10$, $-20 < l < 20$;		θ_{max} = 25.00º
Reflections measured	Total: 4199	Unique (n): 3211	Observed [$I \geq 2\sigma(I)$]: 1256
Absorption coefficient	0.127 mm^{-1}		
No. of variables, p	309		
Weighting scheme	$w = \frac{1}{\sigma^2(F_o^2) + (0.001P)^2 + 2.0P}$		$P = (F_o^2 + 2F_c^2)/3$
$R_1 = \frac{\Sigma \lvert\lvert F_o \rvert - \lvert F_c \rvert\rvert}{\Sigma \lvert F_o \rvert}$	(for all reflections)	0.2145	0.1114 (for observed data)
$wR_2 = \sqrt{\frac{\Sigma[w(F_o^2 - F_c^2)^2}{\Sigma w(F_o^2)^2}}$	(for all reflections)	0.2355	0.2111 (for observed data)
$\text{Goof} = \text{S} = \sqrt{\frac{\Sigma[w(F_o^2 - F_c^2)^2]}{n - p}}$	1.069		
Largest and mean Δ/σ	0.000, 0.000		

Table S2. Crystal Data of **3**

Sample code	**3**-single crystal		
Molecular formula	$C_{34}H_{22}N_2S$		
Molecular weight	490.60		
Color and habit	red prism		
Crystal size	0.1 × 0.3 × 0.4 mm^3		
Crystal system	monoclinic		
Space group	*C*2/*c*		
Unit cell parameters	*a* = 9.3698(10) Å		*α* = 90.00º
	b = 28.450(3) Å		*β* = 107.178(3)º
	c = 9.4857(11) Å		*γ* = 90.00º
	V = 2415.8(5) $Å^3$	Z = 4	F(000) = 1024
Density (calcd)	1.349 g/cm^3		
Temperature	295±2 K		
Scan type	ω-scan		
Data collection range	$-7 < h < 11$, $-35 < k < 33$, $-11 < l < 11$;		θ_{max} = 26.37º
Reflections measured	Total: 6151	Unique (*n*): 2463	Observed [$I \geq 2\sigma(I)$]: 1585
Absorption coefficient	0.162 mm^{-1}		
No. of variables, *p*	192		
Weighting scheme	$w = \frac{1}{\sigma^2(F_0^2) + (0.001P)^2 + 2.0P}$		$P = (F_o^2 + 2F_c^2)/3$
$R_1 = \frac{\Sigma \lvert\lvert F_o \rvert - \lvert F_c \rvert\rvert}{\Sigma \lvert F_o \rvert}$	(for all reflections)	0.1079	0.0727 (for observed data)
$wR_2 = \sqrt{\frac{\Sigma[w(F_o^2 - F_c^2)^2}{\Sigma w(F_o^2)^2}}$	(for all reflections)	0.1501	0.1376 (for observed data)
$\text{Goof} = \text{S} = \sqrt{\frac{\Sigma[w(F_o^2 - F_c^2)^2]}{n - p}}$	1.032		
Largest and mean Δ/σ	0.048, 0.002		

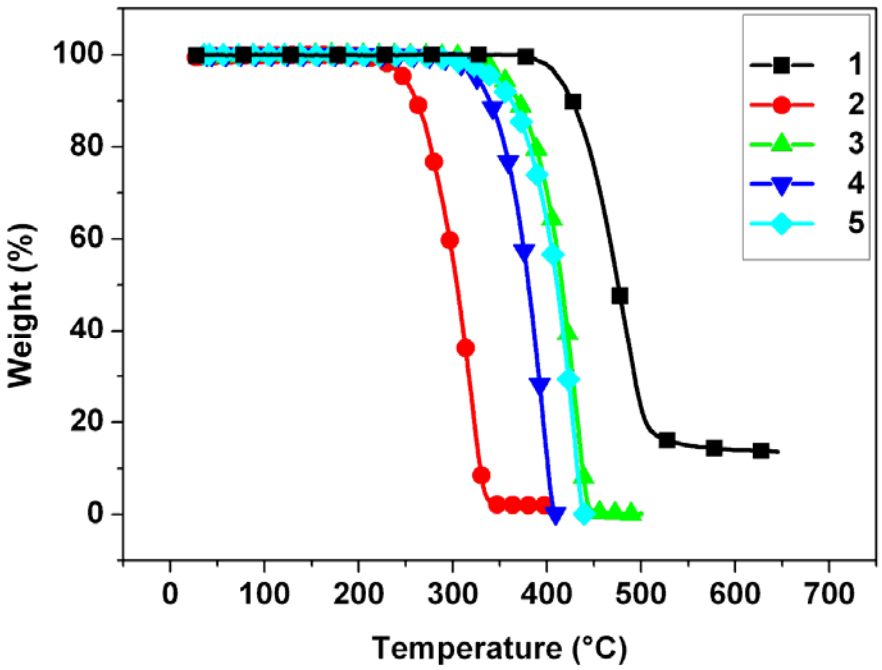

Figure S1. TGA curve for **1**~**5**.

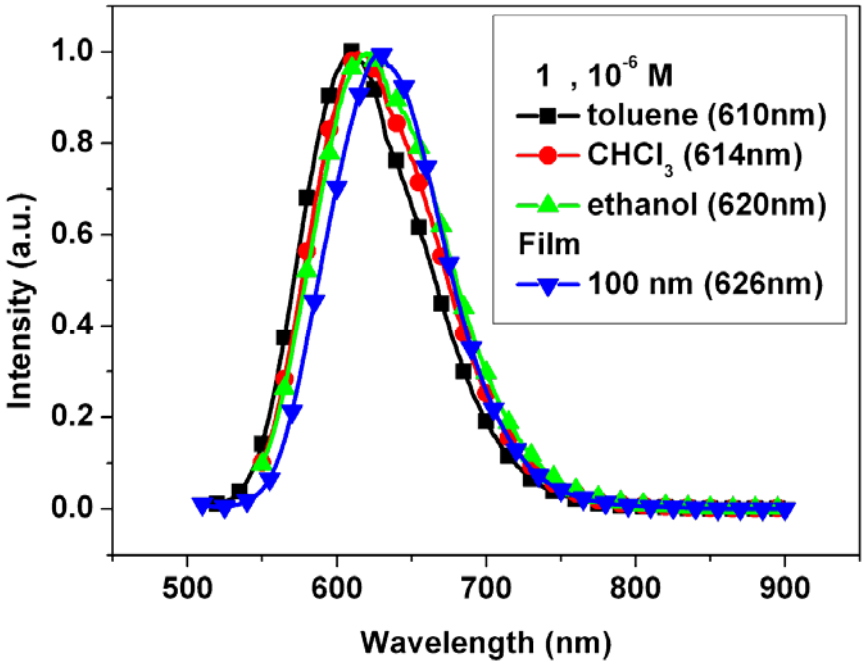

Figure S2. PL spectra of **1** in different solvents (1×10^{-6} M).

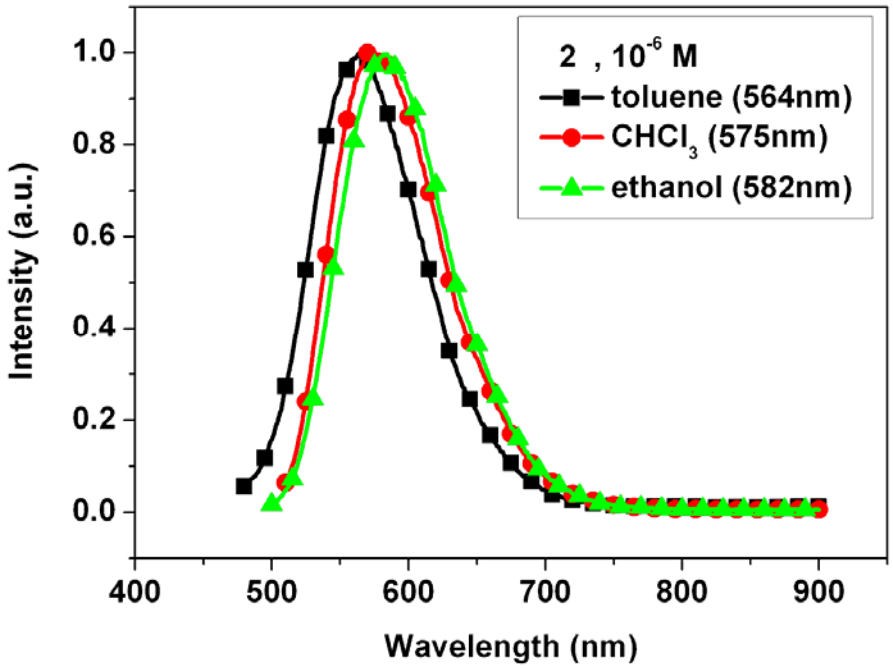

Figure S3. PL spectra of **2** in different solvents (1×10^{-6} M).

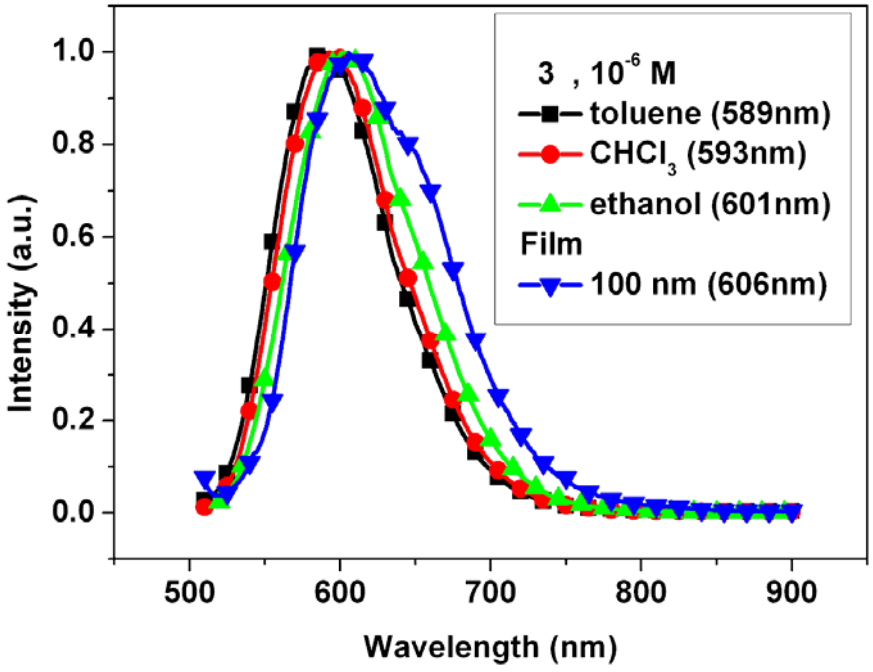

Figure S4. PL spectra of **3** in different solvents (1×10^{-6} M).

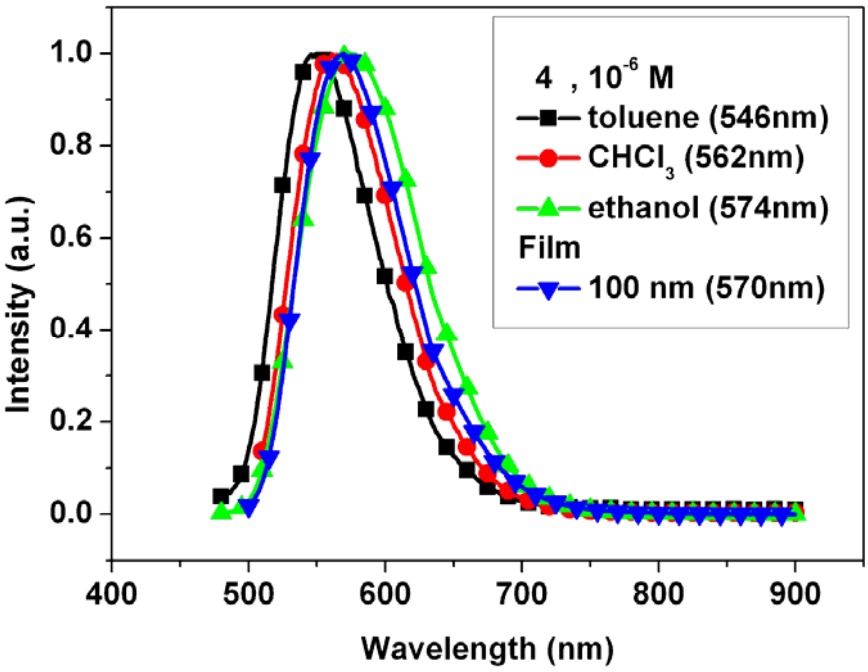

Figure S5. PL spectra of **4** in different solvents (1×10^{-6} M).

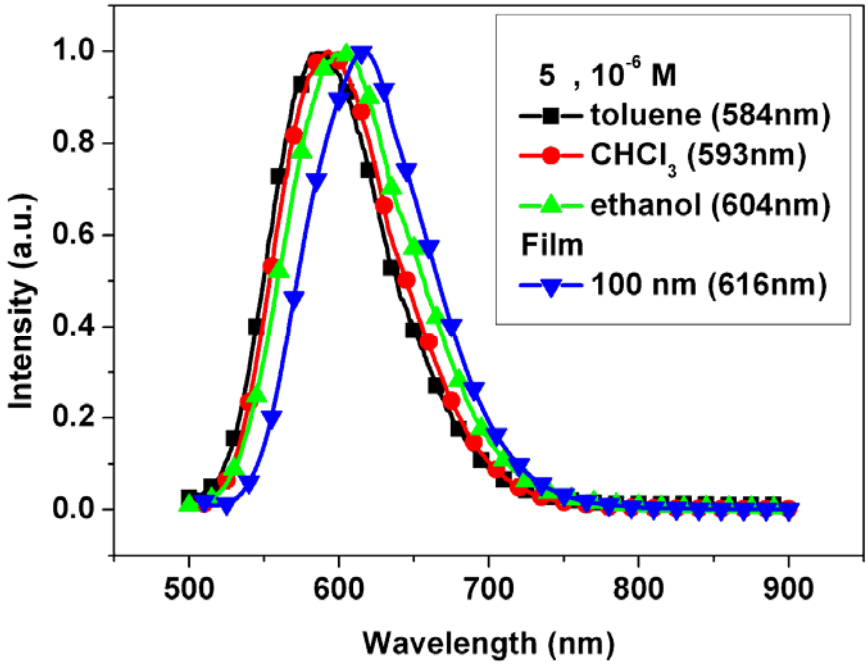

Figure S6. PL spectra of **5** in different solvents (1×10^{-6} M).

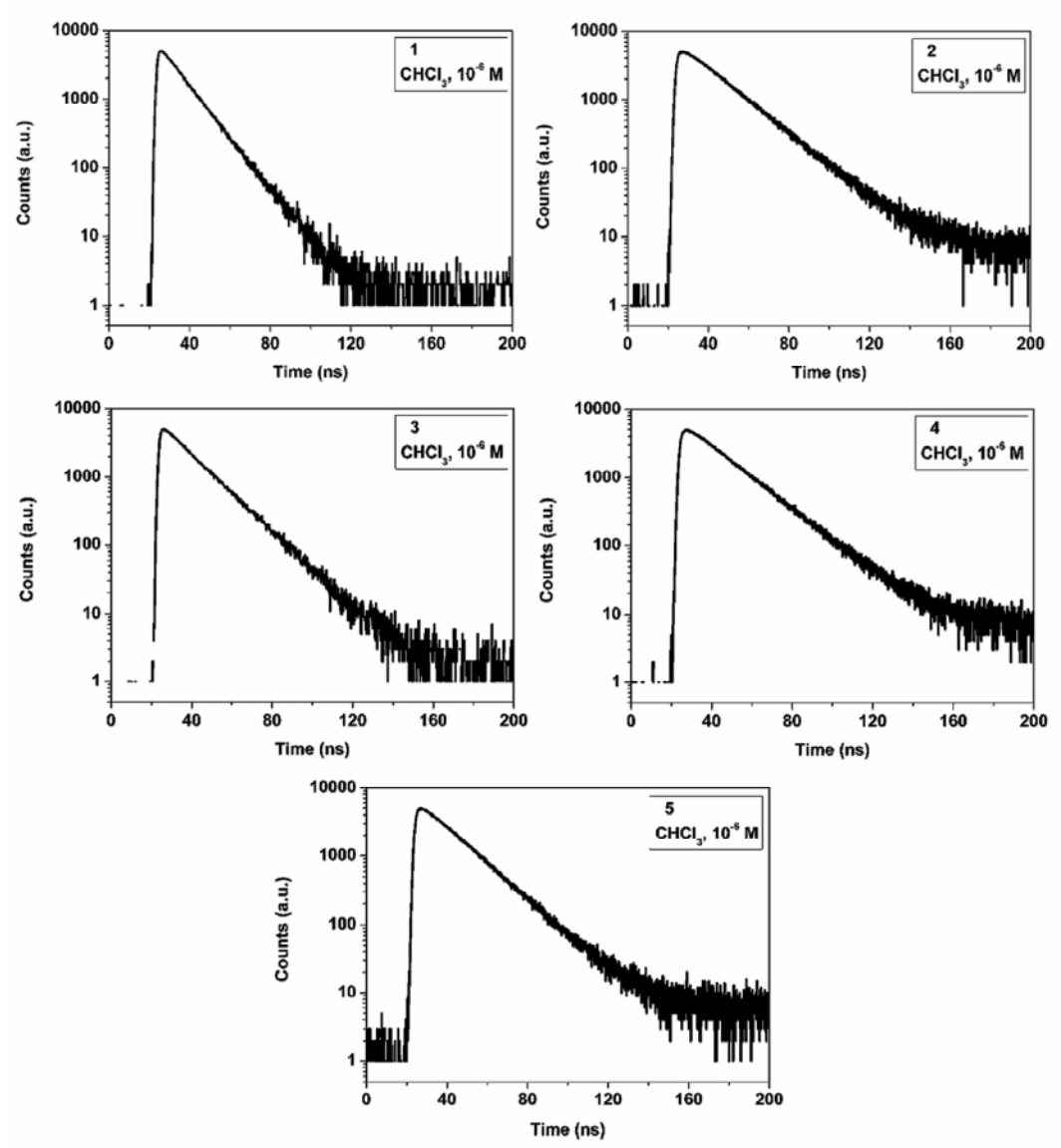

Figure S7. Fluorescence transients of **1**~**5** in $CHCl_3$ solutions