

Electronic Supporting Information for
Two-photon absorption behavior of conjugated oligomers suitable
for low colour temperature LEDs

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S1 ¹H-NMR and elemental analysis data

#1: ¹H-NMR (500 MHz, CDCl₃) δ 7.82 (s, 2H), 7.51 (d, *J* = 9.3 Hz, 2H), 7.44 (d, *J* = 7.7 Hz, 2H), 7.38 (d, *J* = 8.7 Hz, 4H), 7.30–7.26 (m, 6H), 7.26 (s, 2H), 7.14–7.10 (m, 10H), 7.07–7.02 (m, 8H), 6.97 (d, *J* = 16.2 Hz, 2H). Elemental analysis calculated for C₅₃H₃₈N₂O: C, 88.55; H, 5.33; N, 3.90; O, 2.23. Found: C, 88.62; H, 5.26; N, 3.86. MS, *m/z*: cal: 718.9, found: 718.9.

#2: ¹H-NMR (500 MHz, CDCl₃) δ 7.80–7.70 (m, 2H), 7.48–7.34 (m, 4H), 7.26–7.18 (m, 4H), 7.17–7.10 (m, 4H), 7.03–6.75 (m, 10H), 3.81 (s, 4H), 1.79 (s, 4H), 1.42 (s, 4H), 1.34–1.23 (m, 16H), 0.87 (t, *J* = 6.9 Hz, 6H). Elemental analysis calculated for C₅₇H₅₈N₂OS₂: C, 80.43; H, 6.87; N, 3.29; O, 1.88; S, 7.53. Found: C, 80.36; H, 6.92; N, 6.89. MS, *m/z*: cal: 851.2, found: 851.3.

#3: ¹H-NMR (500 MHz, CDCl₃) δ 7.93 (s, 2H), 7.69–7.65 (m, 4H), 7.62 (d, *J* = 7.6 Hz, 2H), 7.50 (dd, *J* = 10.3, 7.6 Hz, 8H), 7.47–7.42 (m, 6H), 7.32–7.26 (m, 10H), 7.20–7.03 (m, 22H), 2.09–1.98 (m, 8H), 1.22–1.06 (m, 40H), 0.81 (t, *J* = 7.1 Hz, 12H), 0.70 (s, 8H). Elemental analysis calculated for C₁₁₅H₁₂₂N₂O: C, 89.21; H, 7.94; N, 1.81; O, 1.03. Found: C, 89.33; H, 7.86; N, 1.76. MS, *m/z*: cal: 1548.2, found: 1548.8.

#4: ¹H-NMR (500 MHz, CDCl₃) δ 7.92 (s, 2H), 7.68–1.64 (m, 1H), 7.61 (d, *J* = 7.7 Hz, 2H), 7.54–7.39 (m, 11H), 7.35 (s, 2H), 7.31–7.26 (m, 4H), 7.20–6.99 (m, 10H), 6.84 (s, 5H), 3.89 (s, 4H), 2.02 (s, 8H), 1.82 (s, 4H), 1.47–1.41 (m, 4H), 1.32–1.05 (m, 56H), 0.87 (t, *J* = 5.8 Hz, 6H), 0.80 (t, *J* = 7.1 Hz, 12H), 0.69 (s, 6H). Elemental analysis calculated for C₁₁₉H₁₄₂N₂OS₂: C, 85.05; H, 8.827; N, 1.67; O, 0.95; S, 3.82. Found: C, 85.12; H, 8.43; N, 1.59. MS, *m/z*: cal: 1680.5, found: 1681.0.

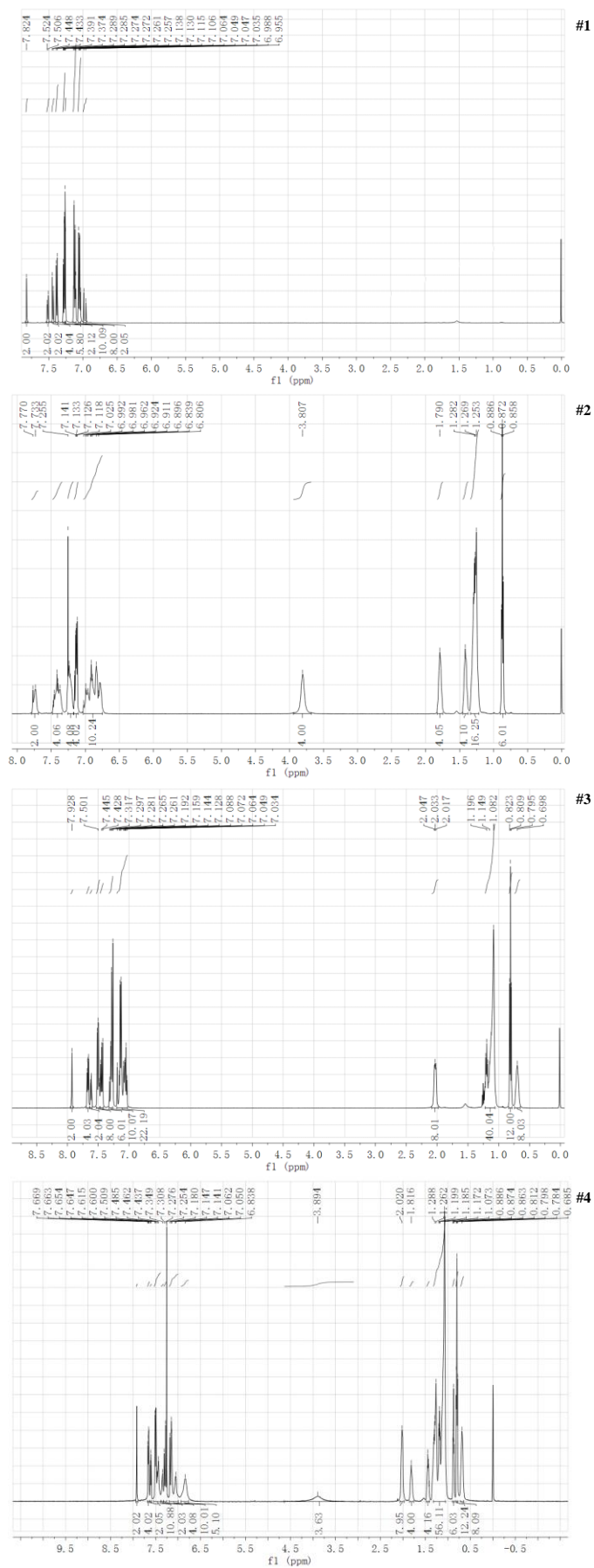


Fig. S1 500MHz $^1\text{H-NMR}$ spectra of compound #1–#4.

Table S1 Spectral parameters obtained from the absorption spectra, employing multi-peaks Gaussian fit.

Samples	Parameters	Peak assignments		
		$n-\pi^*$	$\pi-\pi^*$	ICT
#1	Center / nm	307, 317	385, 415	487
	Width / nm	13.1, 36.0	50.4, 34.1	80.9
	Height / a.u.	0.08, 0.29	0.40, 0.53	0.14
	Area / %	18.8	62.5	18.7
#2	Center / nm	311, 318	366, 410	484
	Width / nm	15.8, 38.5	36.1, 42.8	83.5
	Height / a.u.	0.16, 0.26	0.27, 0.51	0.13
	Area / %	22.6	57.2	20.2
#3	Center / nm	319	402, 429	489
	Width / nm	41.3	63.9, 35.0	57.3
	Height / a.u.	0.31	0.87, 0.52	0.19
	Area / %	13.2	75.9	10.9
#4	Center / nm	325	407, 431	489
	Width / nm	43.1	65.8, 29.2	60.3
	Height / a.u.	0.30	0.95, 0.29	0.18
	Area / %	13.9	75.0	11.1

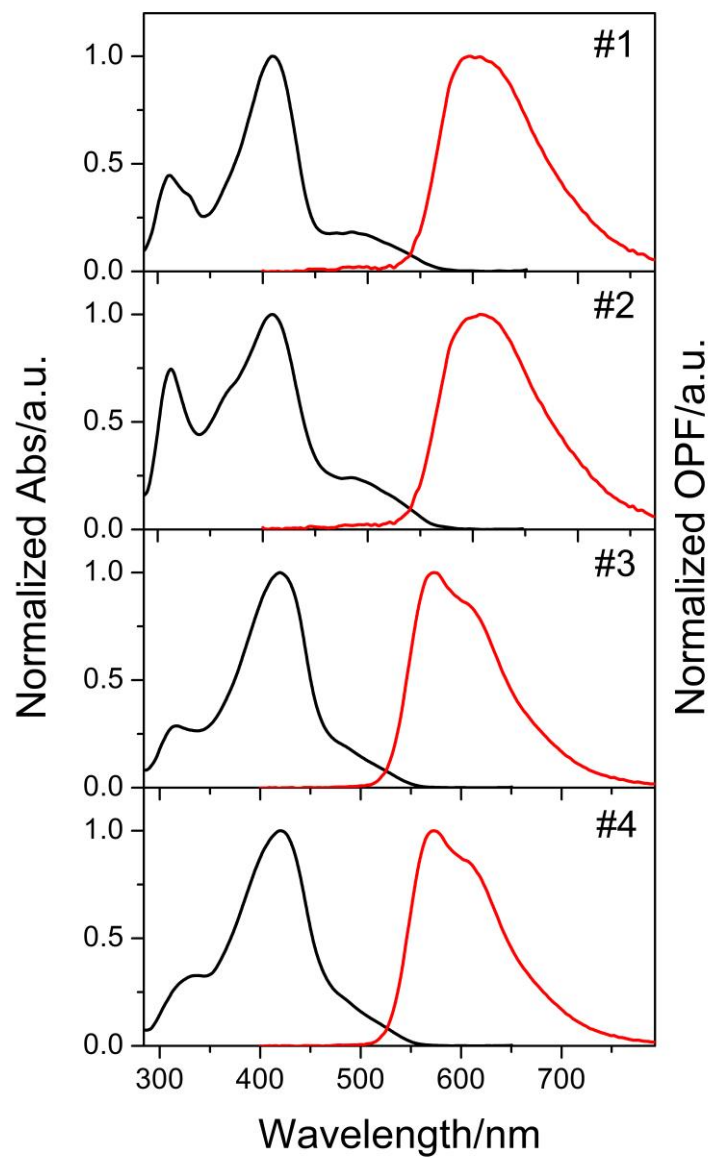


Fig. S2 Normalized absorption and OPF spectra of #1–#4.

Table S2 Linear optical parameters derived from the normalized absorption and OPF spectra.

Linear optical parameters	Samples			
	#1	#2	#3	#4
$\lambda_{\max}(\text{Abs})/\text{nm}$	409	409	424	423
$\lambda_{\max}(\text{OPF})/\text{nm}$	597	607	573	571
OPF intensity/ 10^5	3.4	3.3	8.6	8.6
$E_g^{\text{opt}}/\text{eV}$	2.30	2.29	2.36	2.36
Stokes shift/ cm^{-1}	7705	7981	6137	6132
