Benzothiazole derivatives with varied π-conjugation: Synthesis, tunable solid-state emission, and application in single-component LEDs

Yuwei Song, Lai Hu, Qian Cheng, Zhiyuan Chen, Huan Su, Hao Liu, Rui Liu*, Senqiang Zhu* and Hongjun Zhu

School of Chemistry and Molecular Engineering, Nanjing Tech University, Nanjing 211816, China

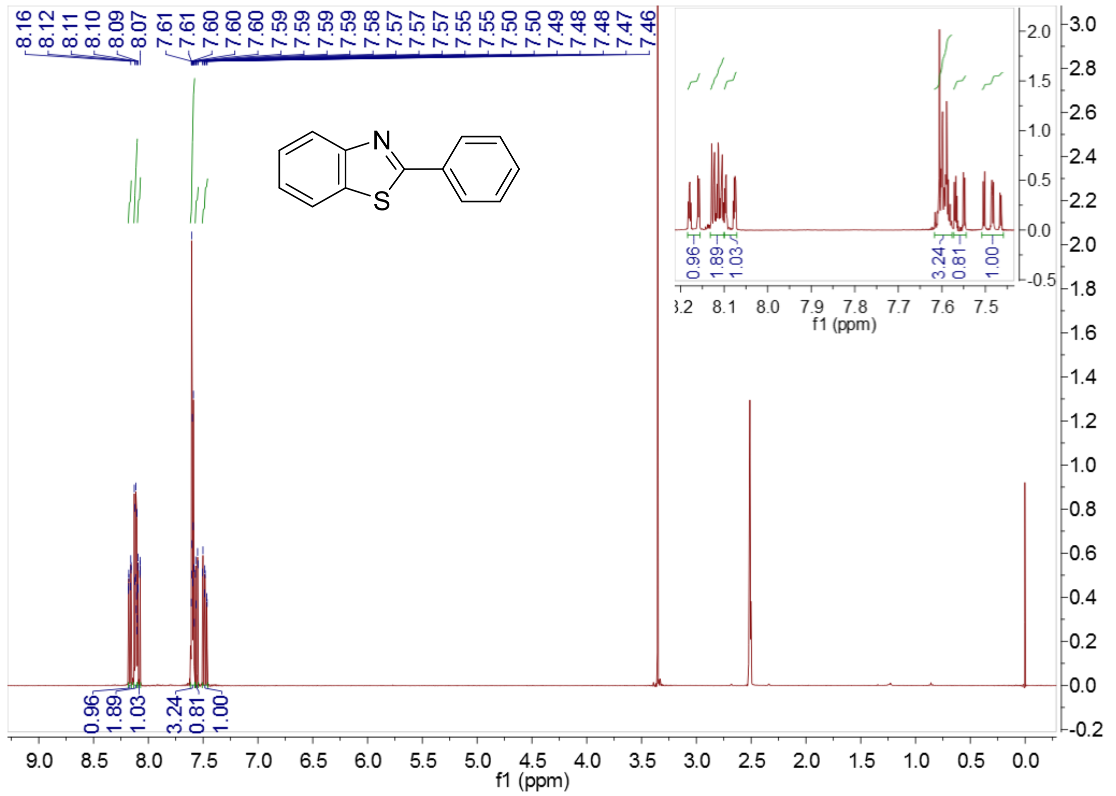

Figure S1. ^{1}H NMR spectrum of **ATZ1** (400 MHz, DMSO-d_6)

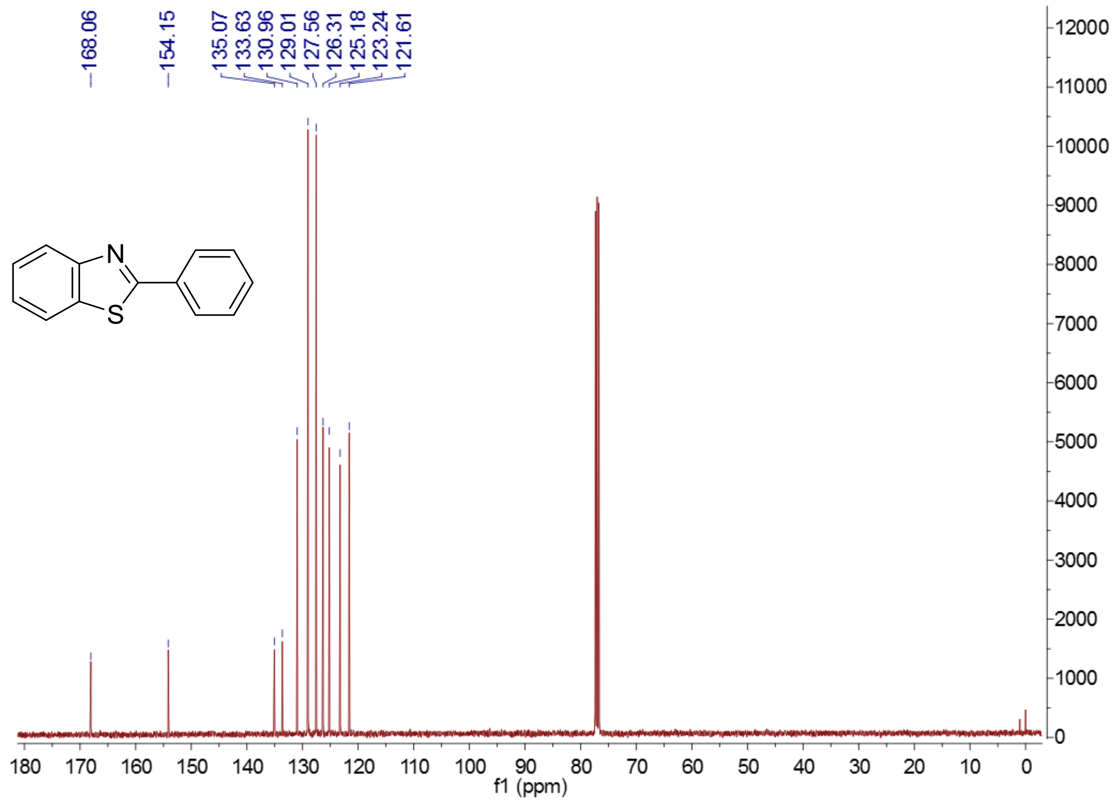

Figure S2. ^{13}C NMR spectrum of **ATZ1** (400 MHz, $CDCl_3$)

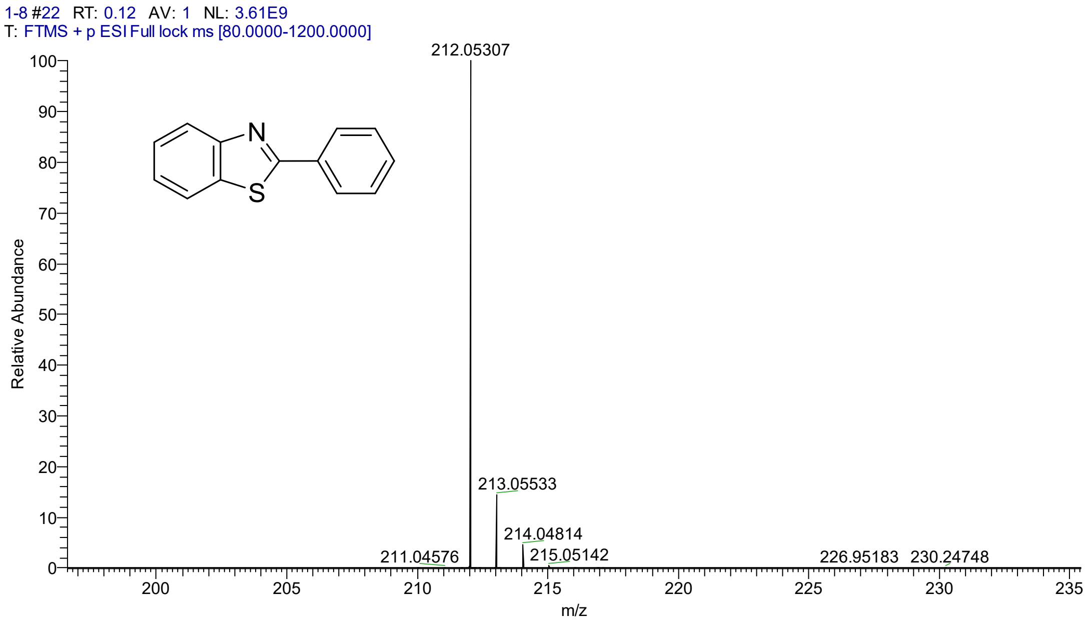

Figure S3. Mass spectrum of **ATZ1**

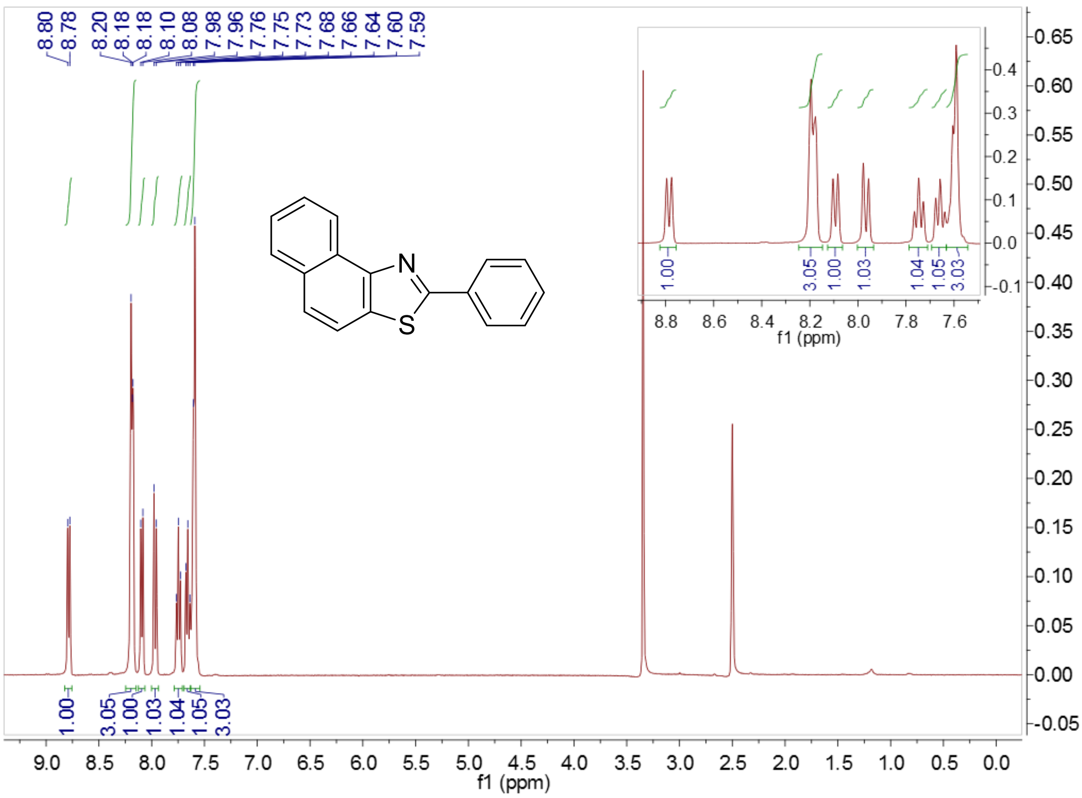

Figure S4. ^{1}H NMR spectrum of **ATZ2** (400 MHz, DMSO-d_6)

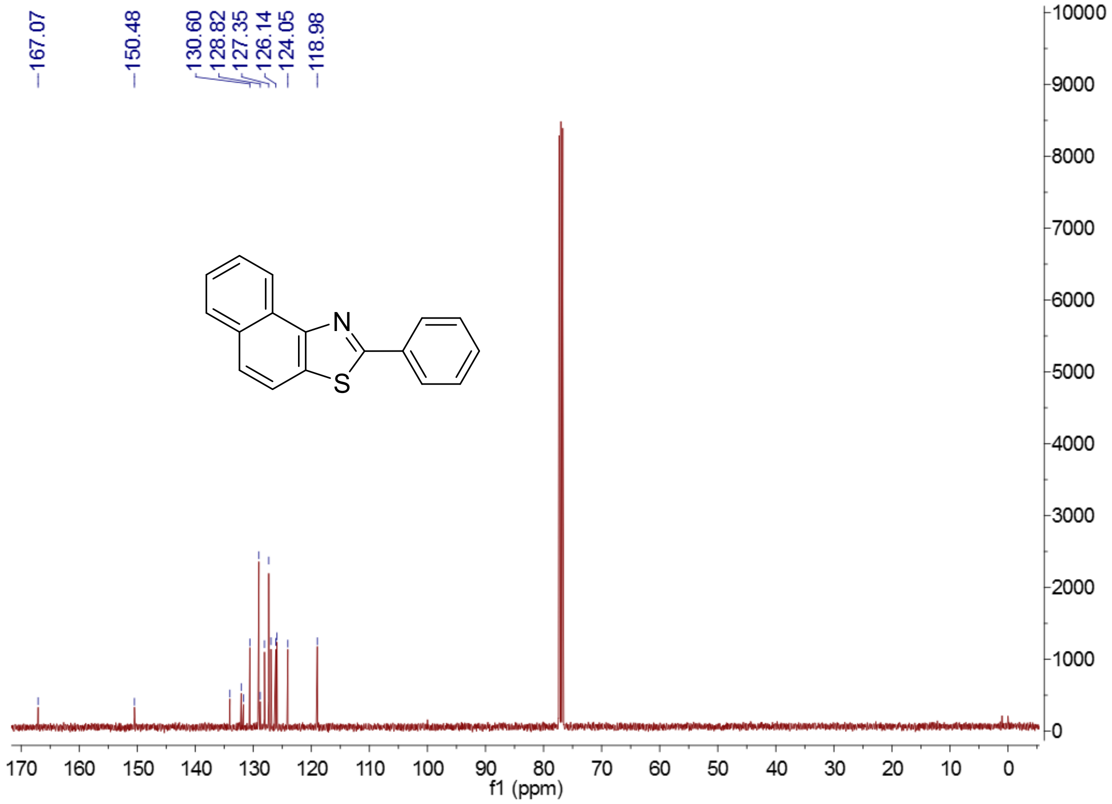

Figure S5. ^{13}C NMR spectrum of **ATZ2** (400 MHz, $CDCl_3$)

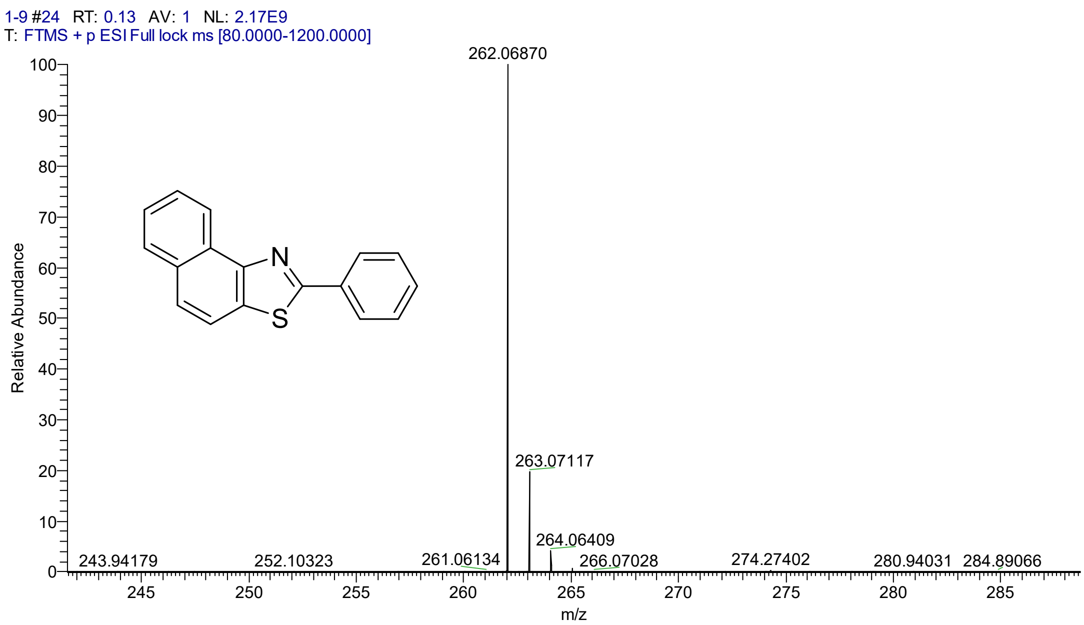

Figure S6. Mass spectrum of **ATZ2**

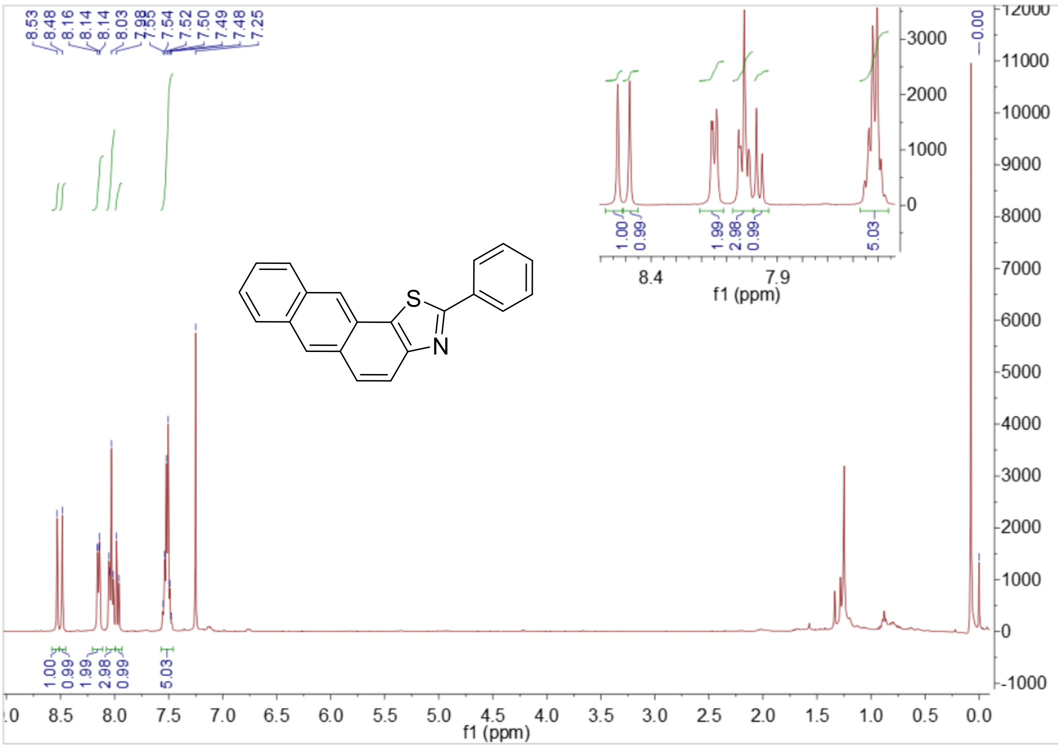

Figure S7. ^{1}H NMR spectrum of **ATZ3** (400 MHz, $CDCl_3$)

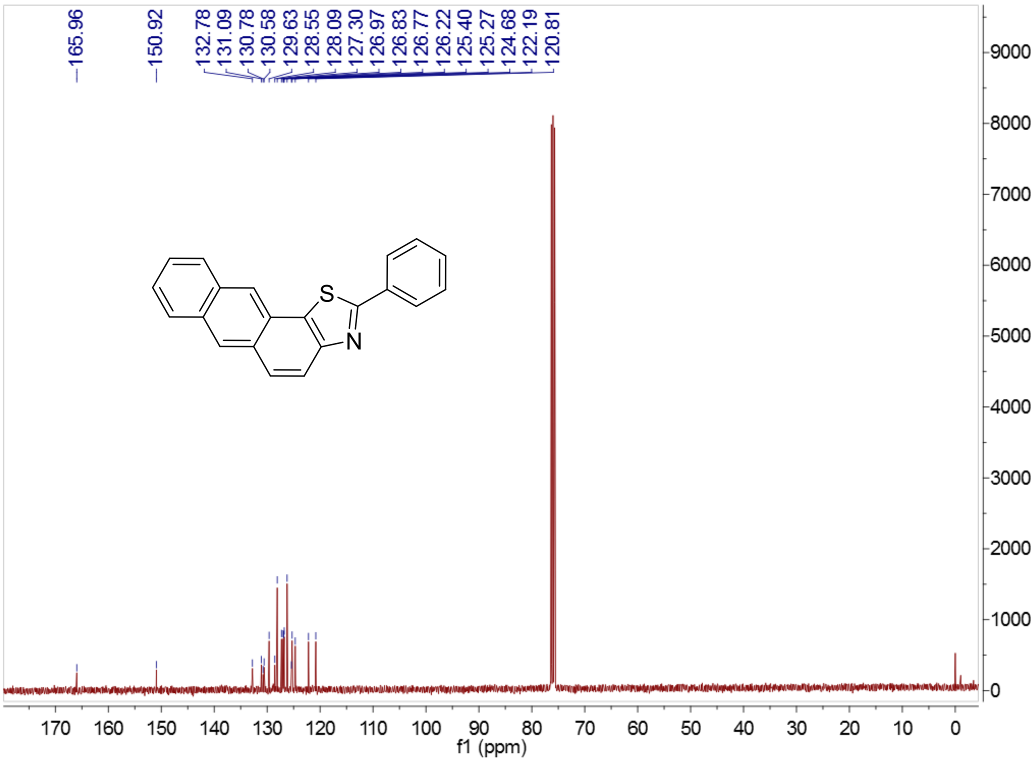

Figure S8. ^{13}C NMR spectrum of **ATZ3** (400 MHz, $CDCl_3$)

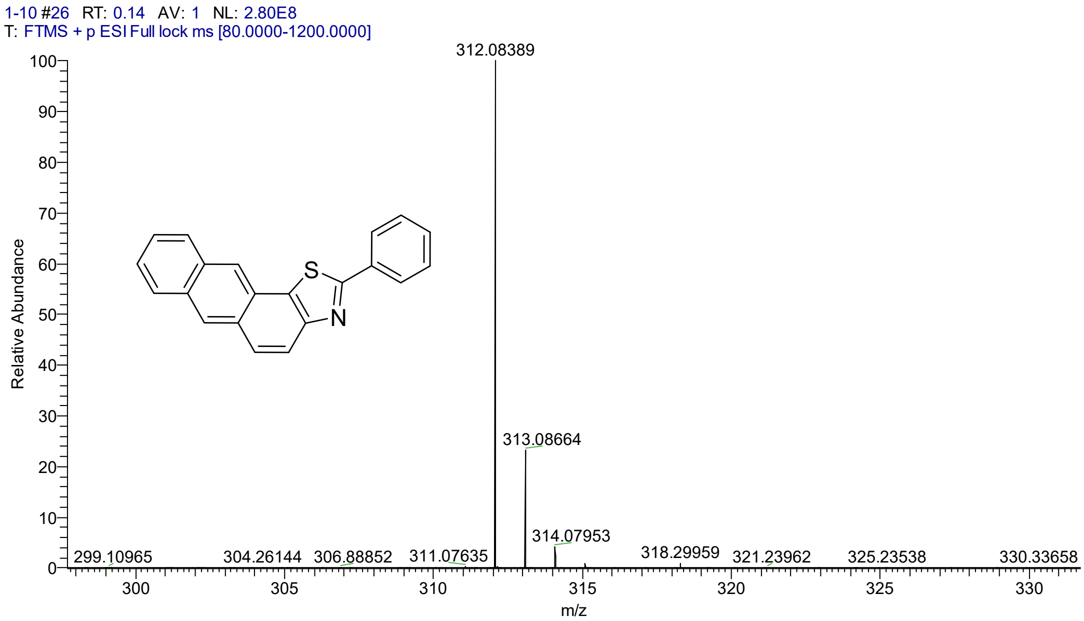

Figure S9. Mass spectrum of **ATZ3**

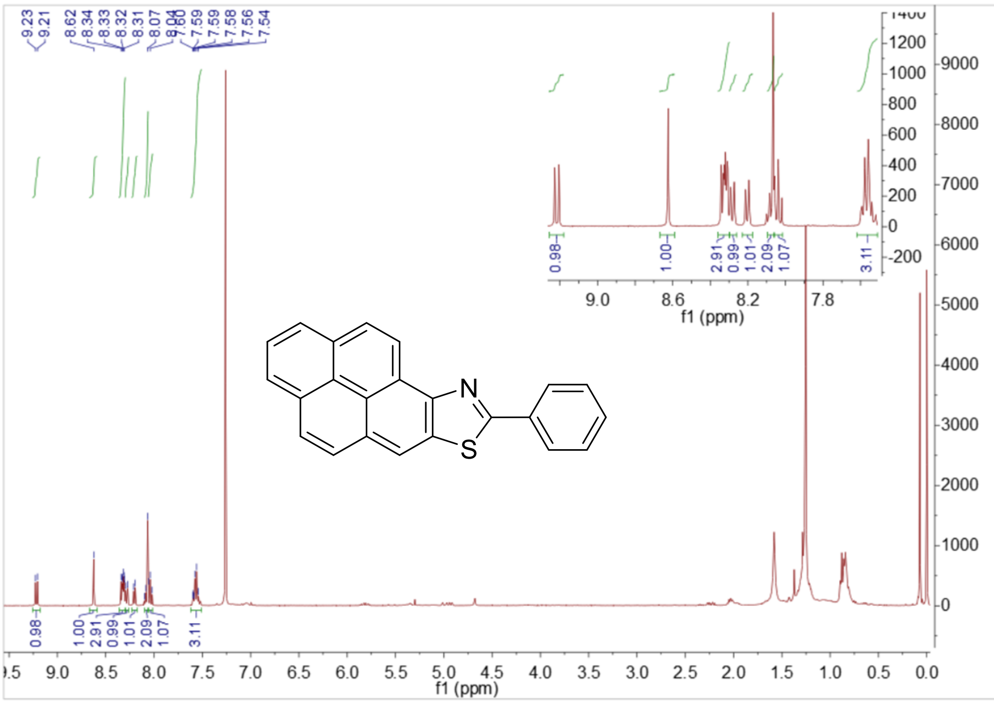

Figure S10. [1]H NMR spectrum of **ATZ4** (400 MHz, $CDCl_3$)

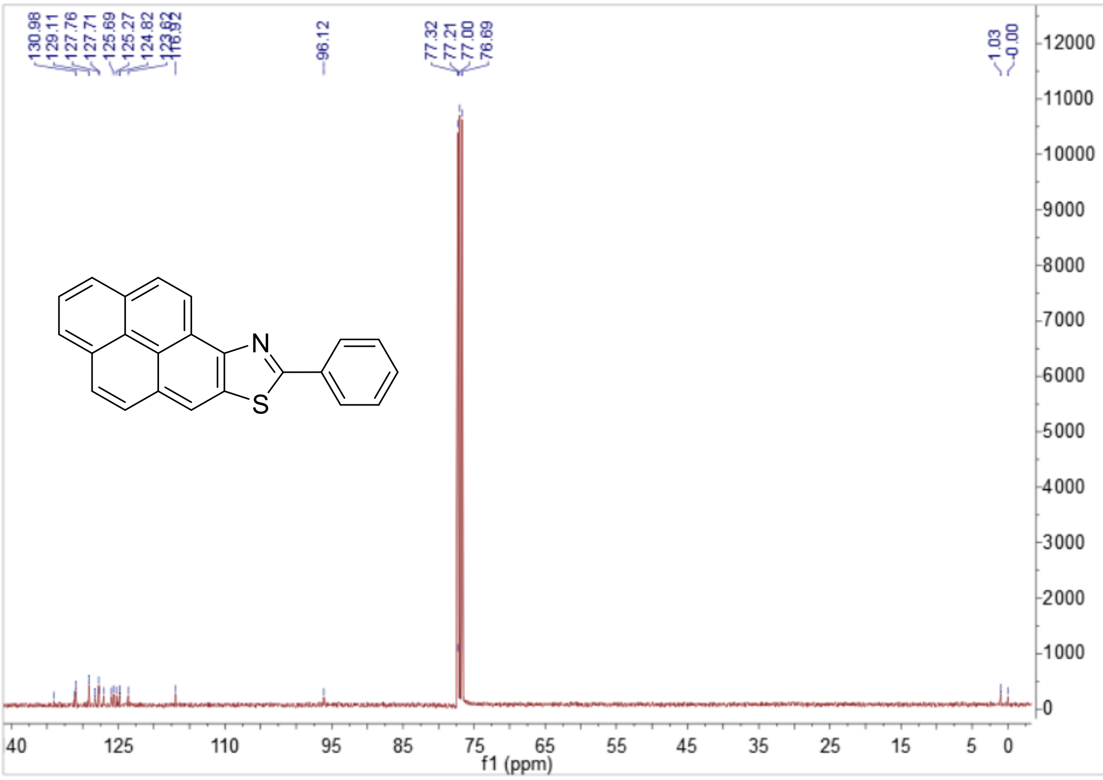

Figure S11. ^{13}C NMR spectrum of **ATZ4** (400 MHz, $CDCl_3$)

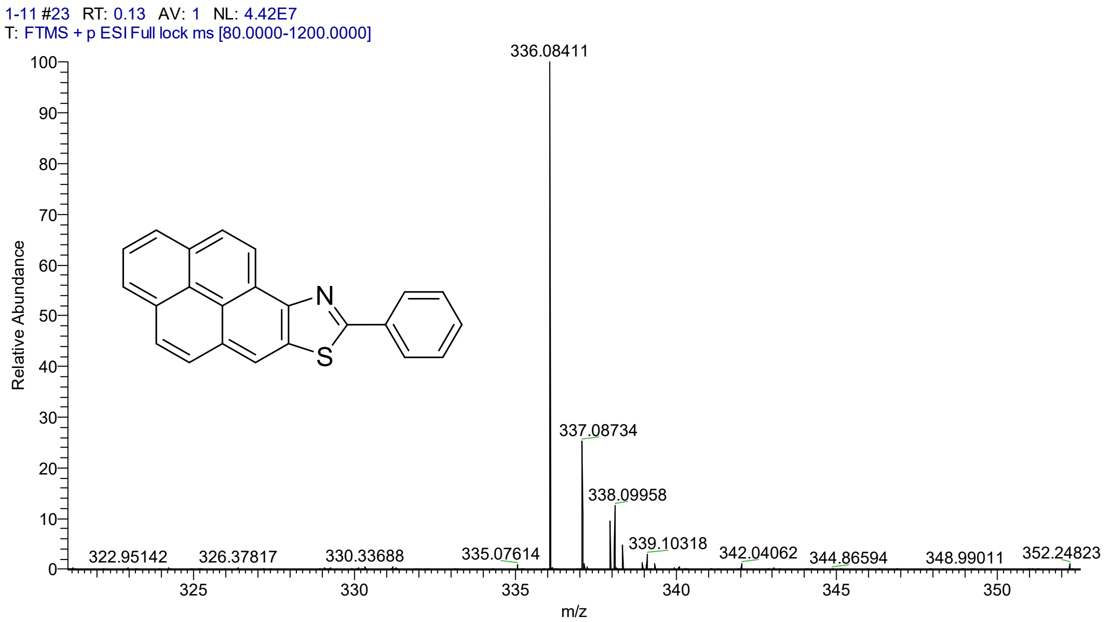

Figure S12. Mass spectrum of **ATZ4**

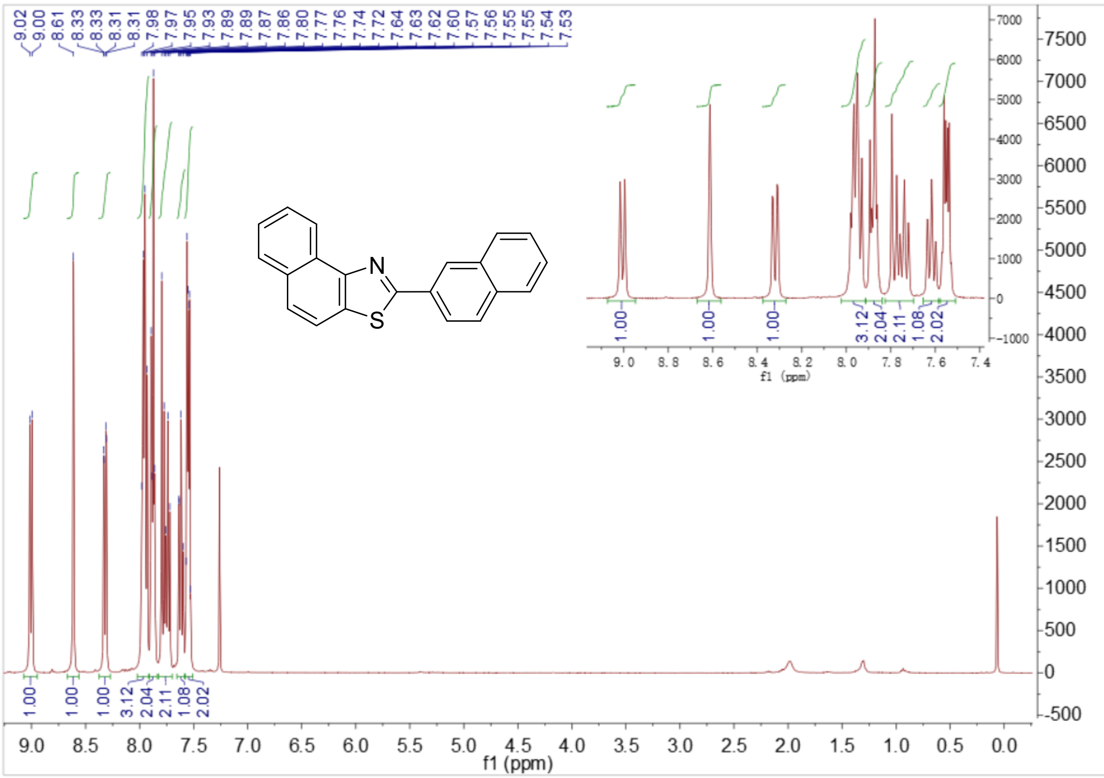

Figure S13. ^{1}H NMR spectrum of **ATZ5** (400 MHz, $CDCl_3$)

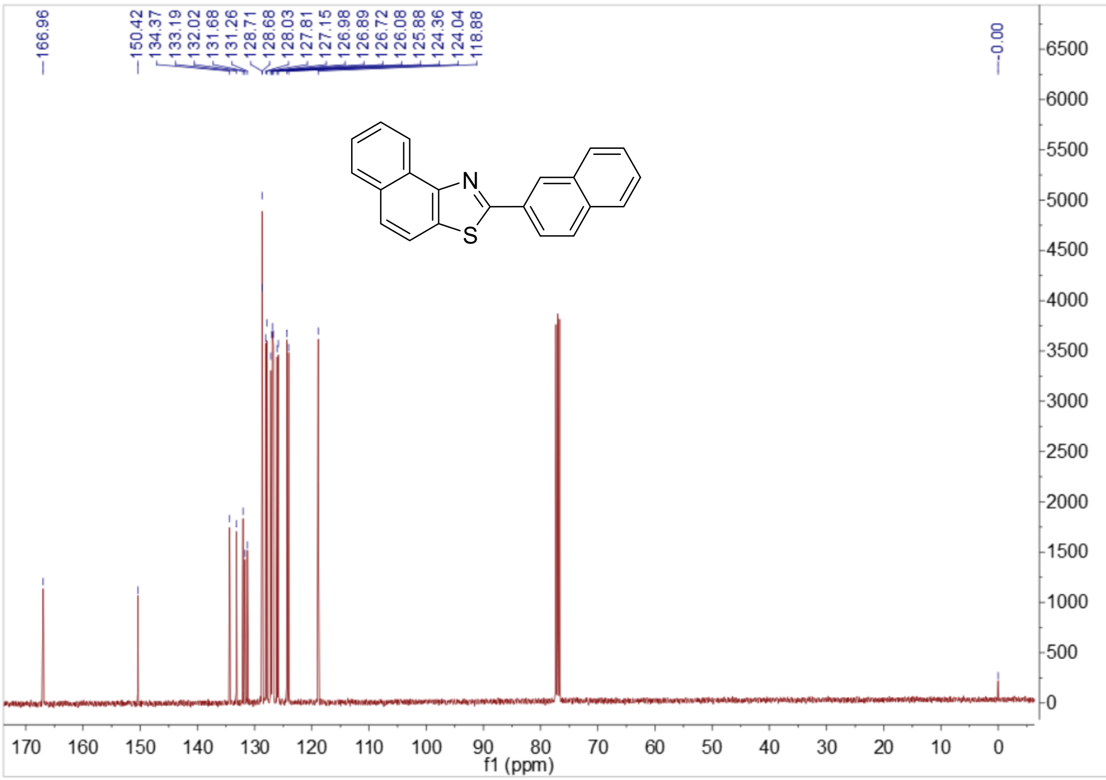

Figure S14. ^{13}C NMR spectrum of **ATZ5** (400 MHz, $CDCl_3$)

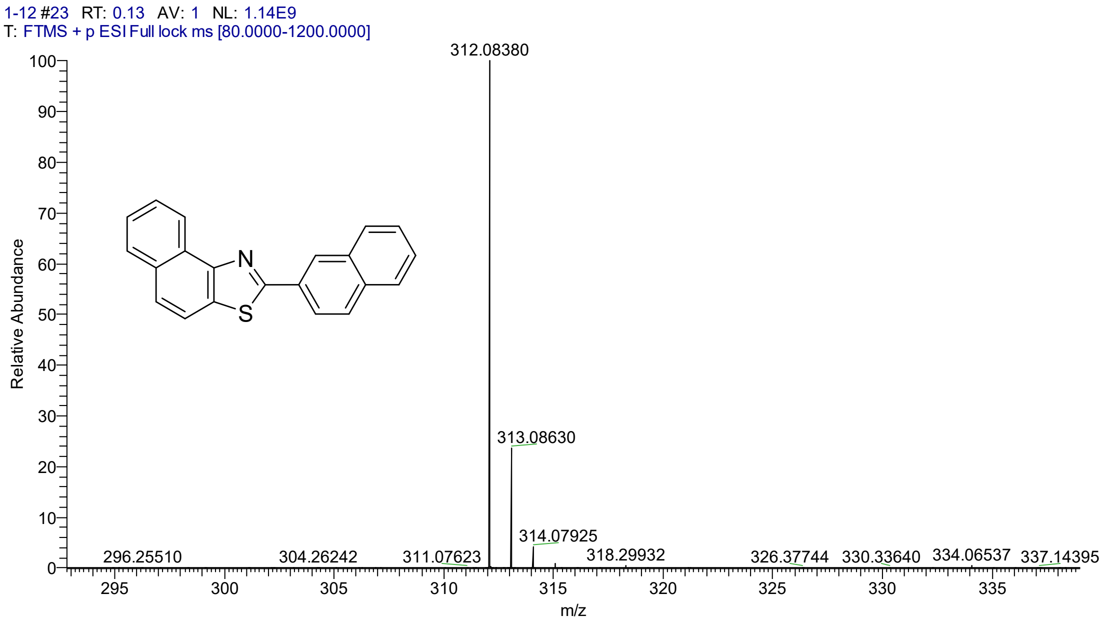

Figure S15. Mass spectrum of **ATZ5**

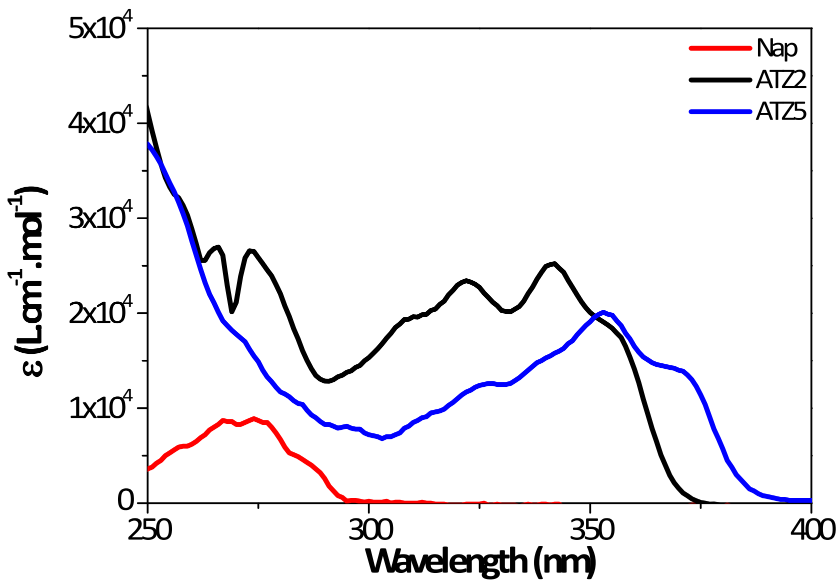

Figure S16. The UV-vis absorption spectra of **ATZ2, ATZ5,** and naphthalene in dichloromethane solution (1×10^{-5} mol L^{-1}) measured at room temperature.

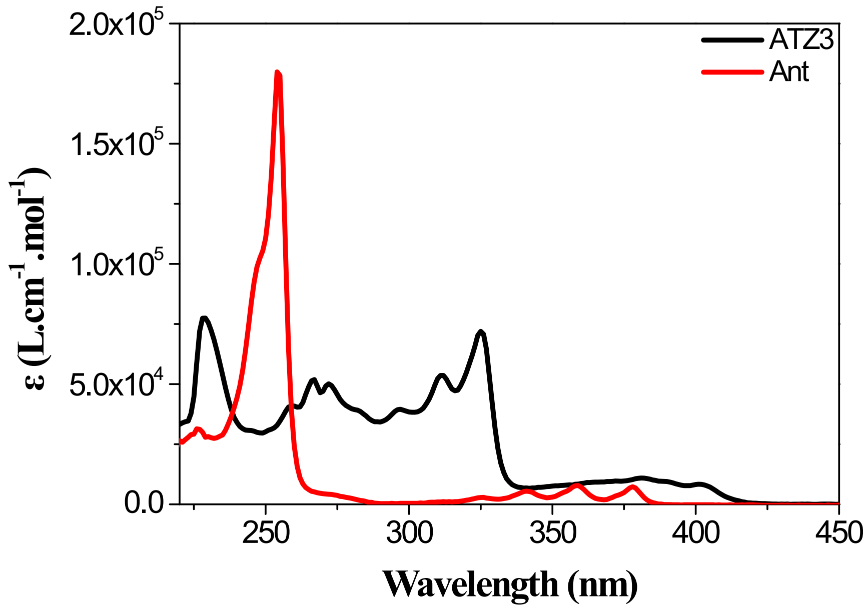

Figure S17. The UV-vis absorption spectra of **ATZ3** and anthracene in dichloromethane solution (1×10^{-5} mol L^{-1}) measured at room temperature.

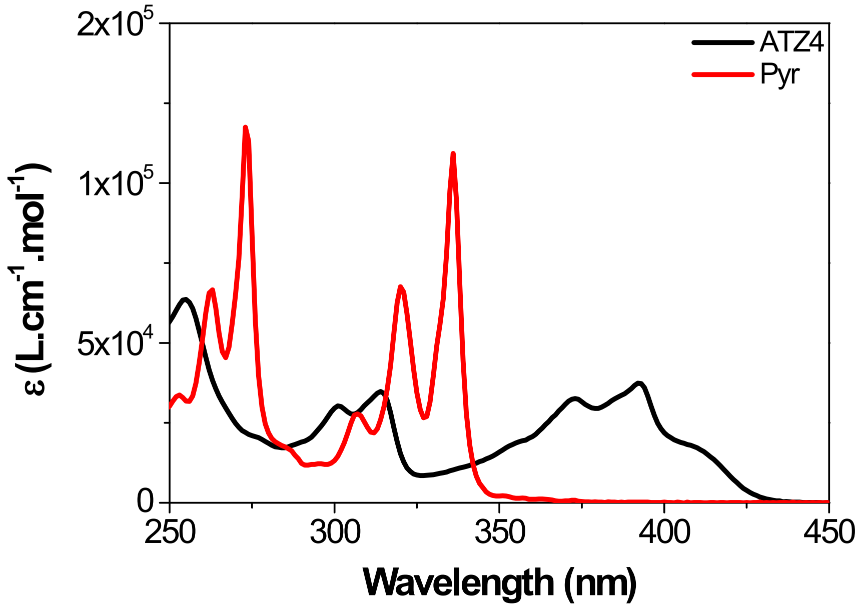

Figure S18. The UV-vis absorption spectra of **ATZ4** and pyrene in dichloromethane solution (1×10^{-5} mol L^{-1}) measured at room temperature.

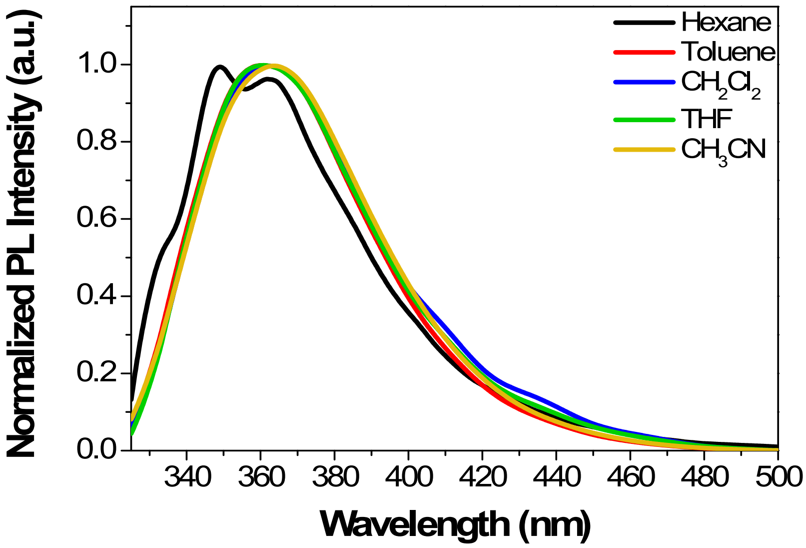

Figure S19. Photoluminescence spectra of **ATZ1** in different polar solvents

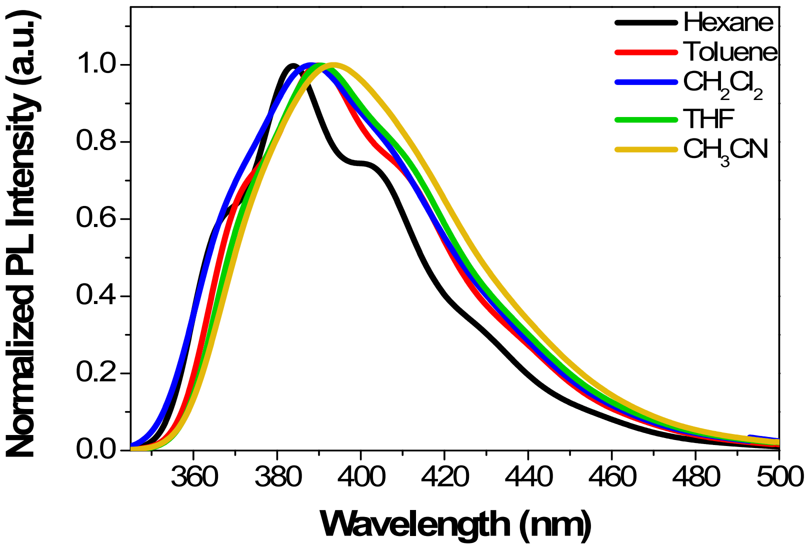

Figure S20. Photoluminescence spectra of **ATZ2** in different polar solvents

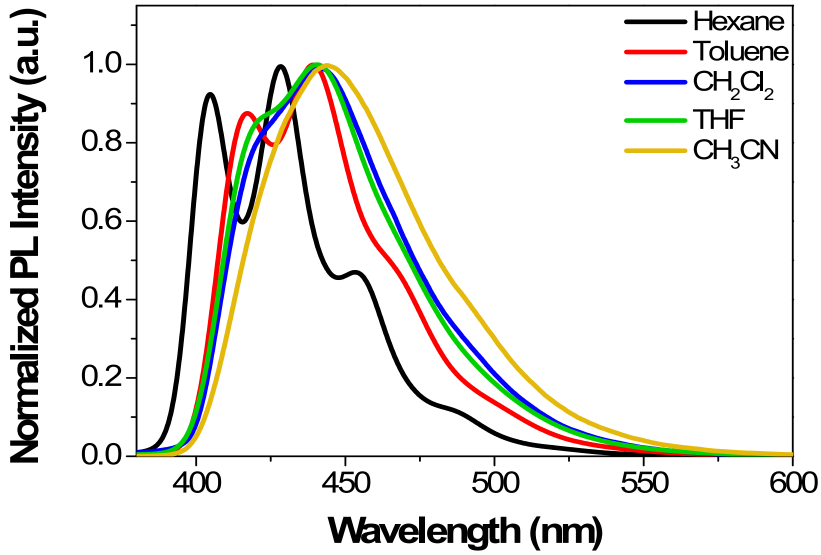

Figure S21. Photoluminescence spectra of **ATZ3** in different polar solvents

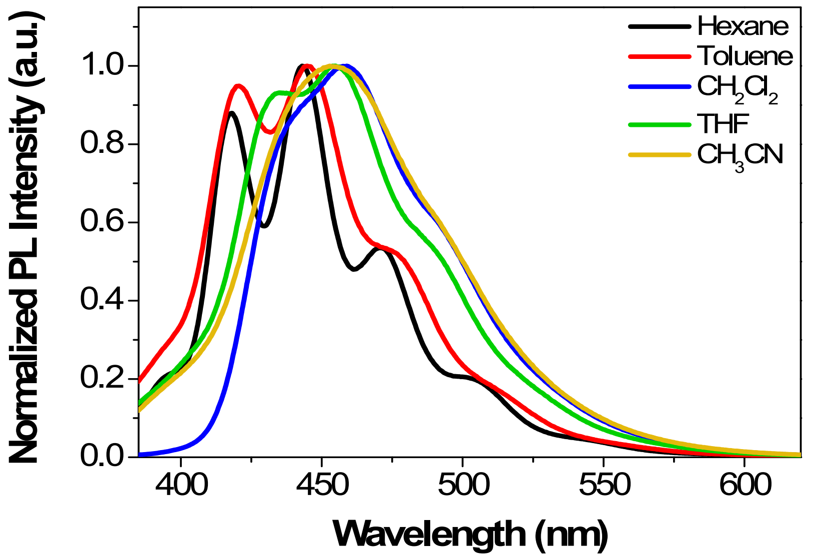

Figure S22. Photoluminescence spectra of **ATZ4** in different polar solvents

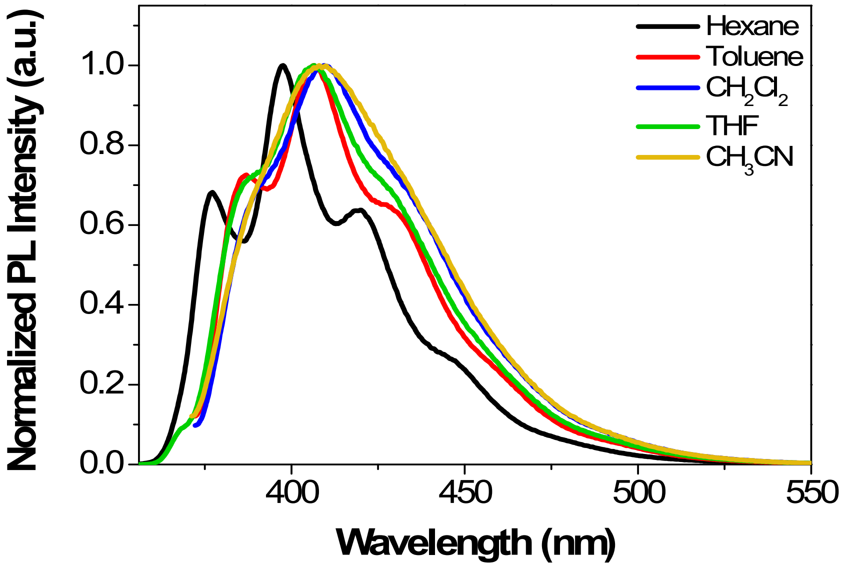

Figure S23. Photoluminescence spectra of **ATZ5** in different polar solvents

Table S1. Relative fluorescence quantum yield of **ATZ1~ATZ5** in different polar solvents

	Hexane	Toluene	CH_2Cl_2	THF	ACN
ATZ1	0.035	0.019	0.027	0.019	0.017
ATZ2	0.204	0.213	0.194	0.122	0.188
ATZ3	0.247	0.261	0.210	0.110	0.175
ATZ4	0.284	0.311	0.247	0.321	0.169
ATZ5	0.264	0.249	0.192	0.230	0.138

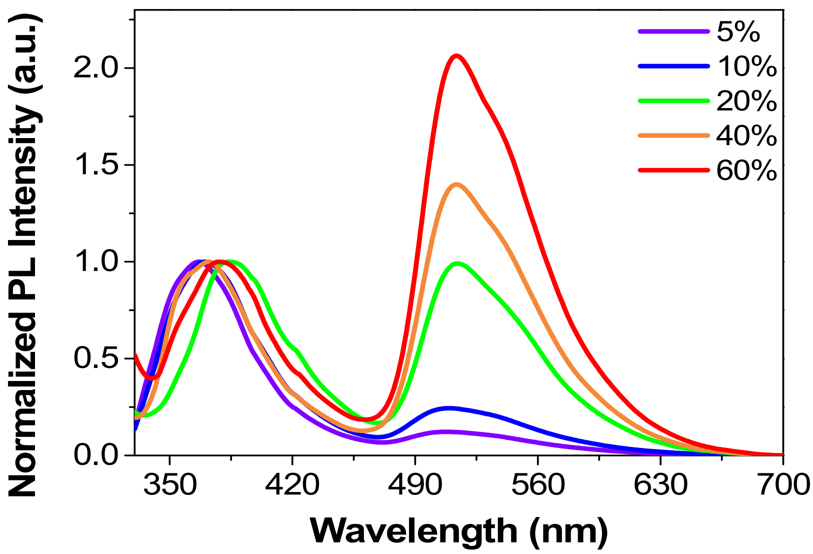

Figure S24. Photoluminescence spectra of the thin films prepared by doping different proportions of **ATZ1** in PMMA.

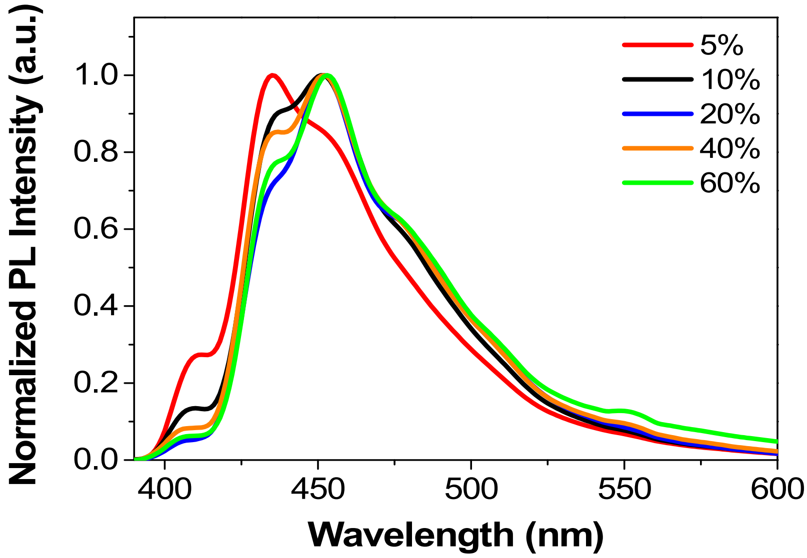

Figure S25. Photoluminescence spectra of the thin films prepared by doping different proportions of **ATZ3** in PMMA.

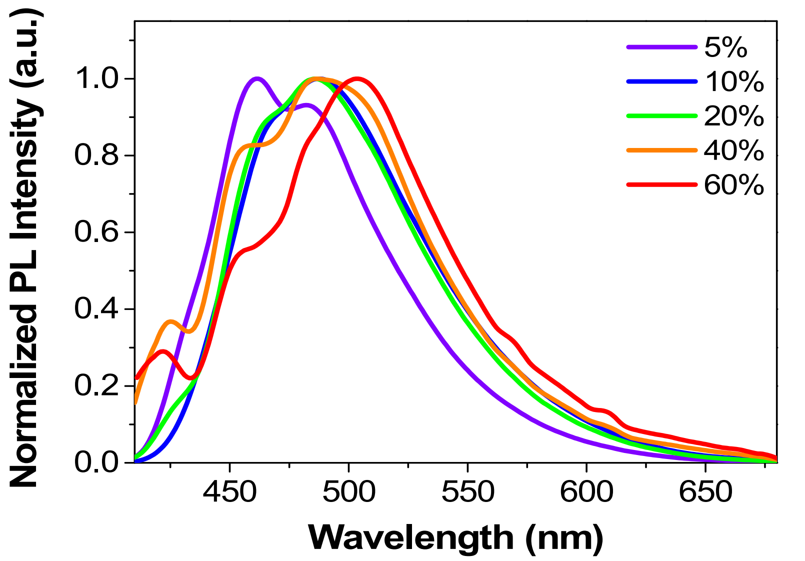

Figure S26. Photoluminescence spectra of the thin films prepared by doping different proportions of **ATZ4** in PMMA.

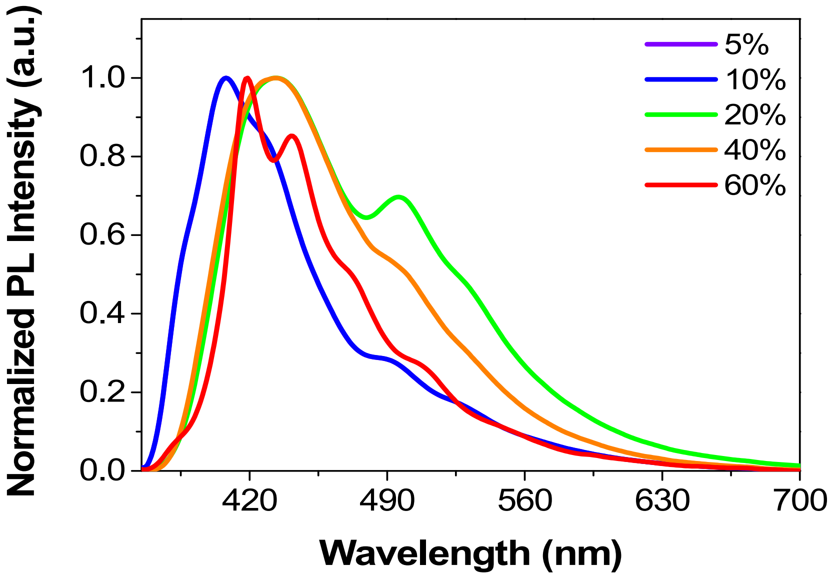

Figure S27. Photoluminescence spectra of the thin films prepared by doping different proportions of **ATZ5** in PMMA.

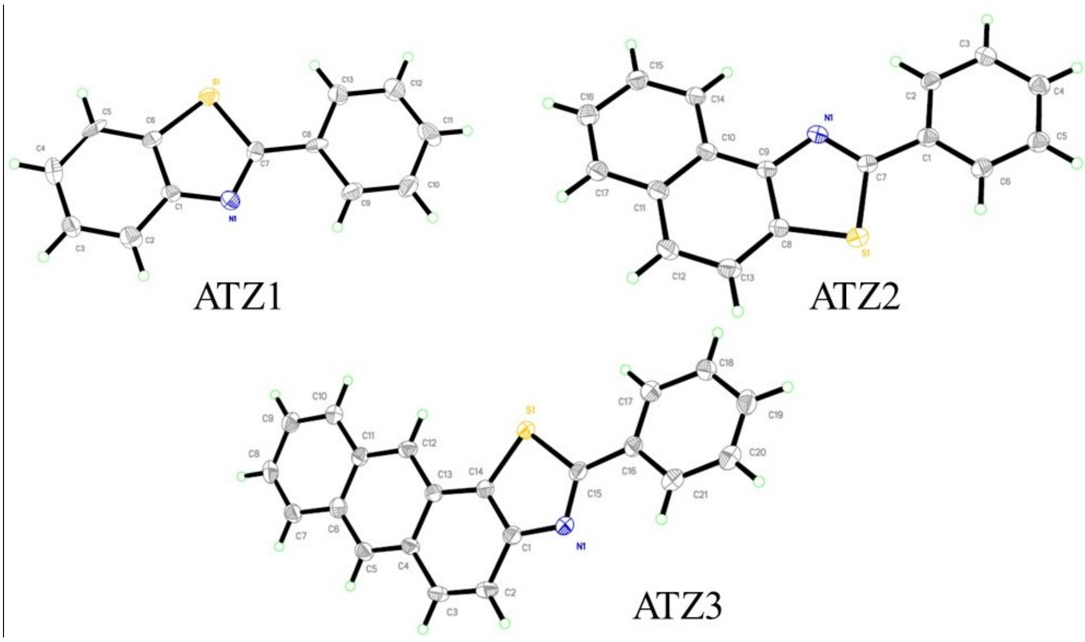

Figure S28. Crystal structure of **ATZ1**, **ATZ2**, and **ATZ3**.

Table S2. Crystallographic data of **ATZ1**, **ATZ2**, and **ATZ3**.

	ATZ1	**ATZ2**	**ATZ3**
formula	$C_{13}H_9NS$	$C_{17}H_{11}NS$	$C_{21}H_{13}NS$
Formula weight	211.27	261.33	311.38
Crystal system	orthorhombic	monoclinic	monoclinic
Space group	P n a 2_1	P 2_1/m	P 2_1/n
a, Å	16.1420(19)	11.7214(6)	4.0231(3)

b, Å	11.0866(14)	3.8718(2)	28.291(2)
c, Å	5.7979(8)	13.6211(8)	12.8877(10)
α, deg	90	90	90
β, deg	90	94.355(3)	91.515(4)
γ, deg	90	90	90
V, Å^3	1037.6(2)	616.38(6)	1466.35(19)
Z	4	2	4
ρ_{calcd}, g cm^{-3}	1.352	1.408	1.410
T / K	296(2)	193(2)	193(2)
μ, mm^{-1}	0.272	1.422	1.258
θ	2.229-28.457	2.83-48.85	2.718 - 52.991
F (000)	440	272	648
Index ranges	$-21 \leq h \leq 15$ $-14 \leq k \leq 14$ $-7 \leq l \leq 7$	$-13 \leq h \leq 13$ $0 \leq k \leq 4$ $0 \leq l \leq 16$	$-4 \leq h \leq 4$ $-33 \leq k \leq 33$ $-12 \leq l \leq 15$
Data / restraints / parameters	2552//22/248	1261/1317/285	2560/0/208
GOF (F^2)	1.079	1.056	1.095
R, wR	0.0650, 0.1433	0.0553, 0.1388	0.0850, 0.2343

Table S3. Properties of single-component white light emitting materials based on small organic molecules.

Compound	Molecular weight	Φ (%)	CIE (x, y)	CRI	CCT (K)	Ref.
3	820	0.9	0.30, 0.43	56		1
TIM	153	11.8	0.33, 0.35	85	5669	2
1	189	2	0.31, 0.35	83	6218	3
TPO-Br	454		0.31, 0.33			4
PTZ-Ph-TTR	477	11	0.33, 0.33	92		5
2PQ-PTZ	479		0.32, 0.34	89	5850	6
rac-BINAP	622	7.6	0.37, 0.44	73		7
CTM	453		0.35, 0.35	88.8		8
D1c	356	32	0.34, 0.36			9
Cz9PhAn	600	47	0.30, 0.33	75.6		10
2	293	16	0.31, 0.34			11
OPC	544	23	0.35, 0.35			12
PTZ-BP	379	8	0.28, 0.30			13
DPPZ	280	1	0.28, 0.33			14
ClBDBT	322	7.2	0.33, 0.35			15
ImBr	369	4.1	0.29, 0.35			16
3-DPH-XO	363	40	0.27, 0.35			17
SDB2t	582	13	0.27, 0.27			18
P3	310	36	0.28, 0.31			19
ATZ2	**262**	**4.8**	**0.28, 0.34**	**73**	**8401**	**This work**

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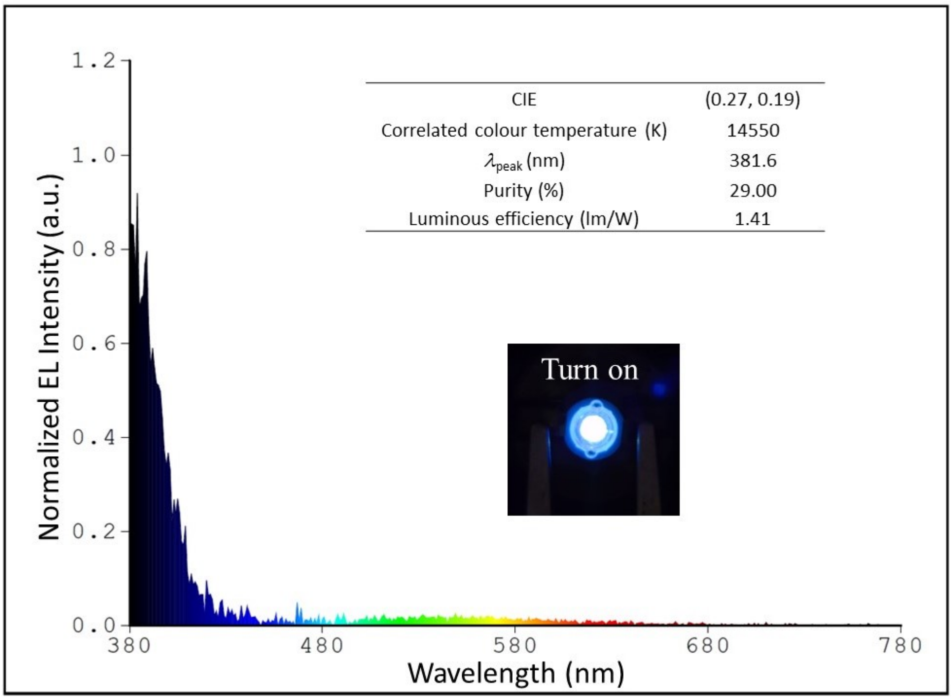

Figure S29. Electroluminescent spectra, energized photo (inset) and the electroluminescent data (inset) of commercial UV LED.

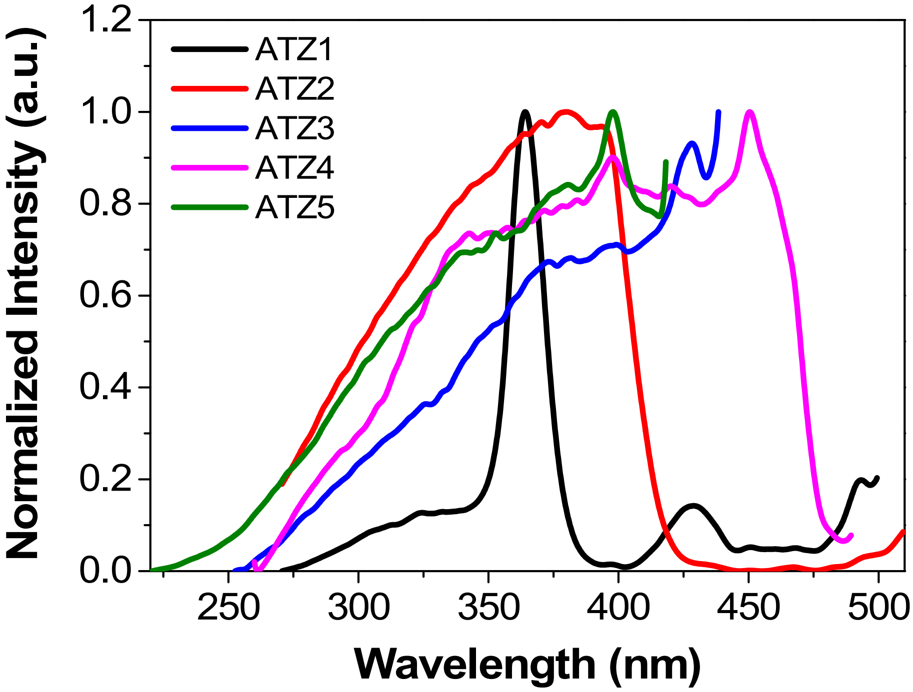

Figure S30. Normalized excitation spectra of **ATZ1~ATZ5**. **ATZ1**: λ_{em} = 520 nm, **ATZ2**: λ_{em} = 526 nm, **ATZ3**: λ_{em} = 455 nm, **ATZ4**: λ_{em} = 505 nm, **ATZ5**: λ_{em} = 428 nm.