

Benzothiadiazole Based “Hot Exciton” Materials for Red Electroluminescence with Maximum External Quantum Efficiency Approaching 10%

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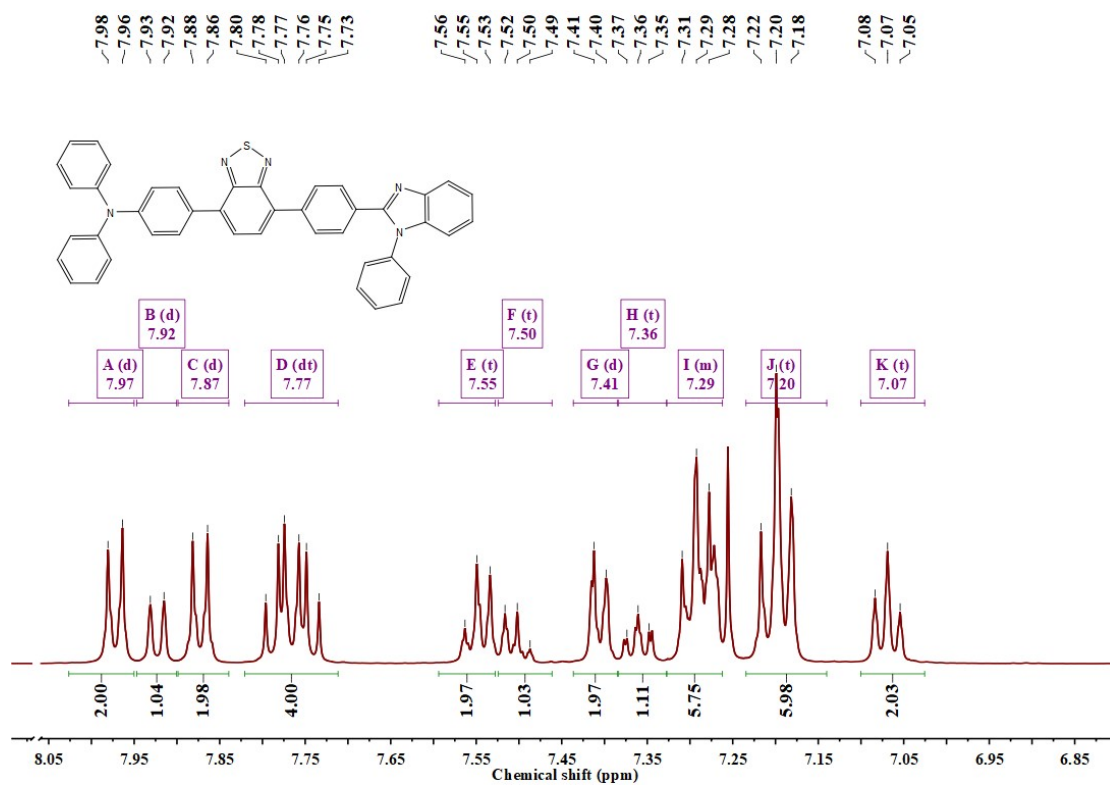


Fig. S1. ¹H-NMR spectra of TPA-BT-PBI in CD₂Cl₂.

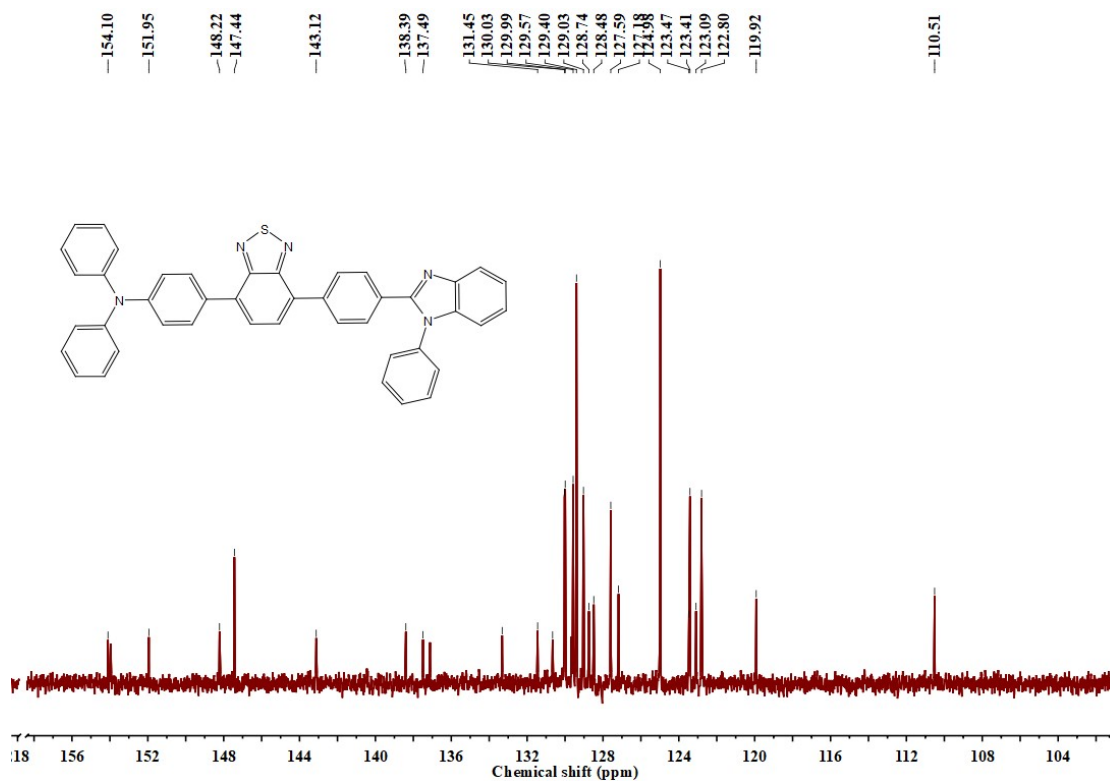


Fig. S2. ¹³C-NMR spectra of TPA-BT-PBI in CD₂Cl₂.

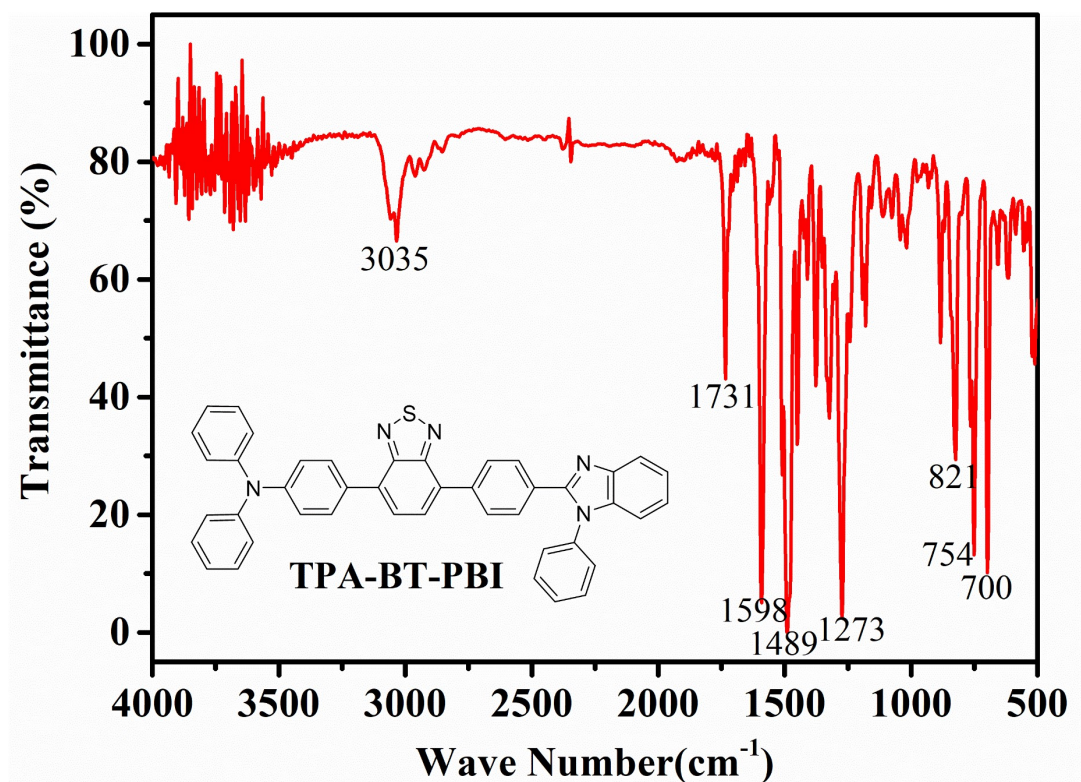


Fig. S3. FT-IR spectra of TPA-BT-PBI in the KBr matrix.

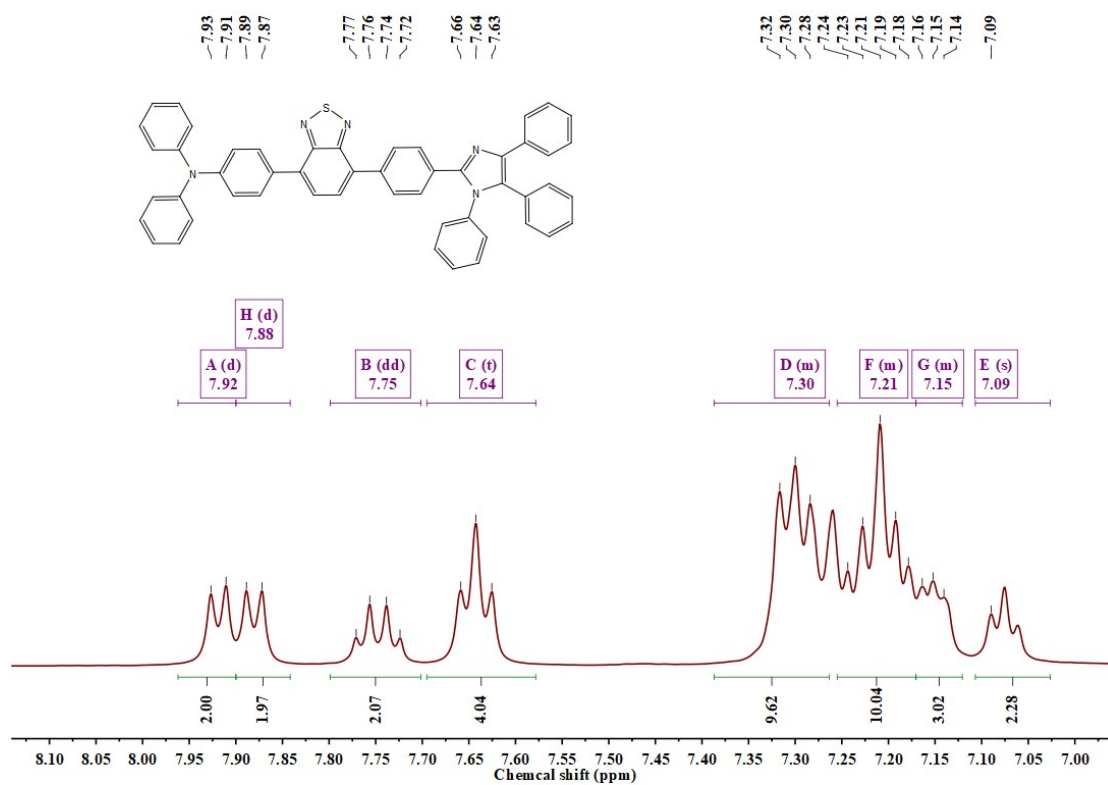
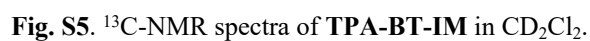


Fig. S4. ¹H-NMR spectra of TPA-BT-IM in CD₂Cl₂.



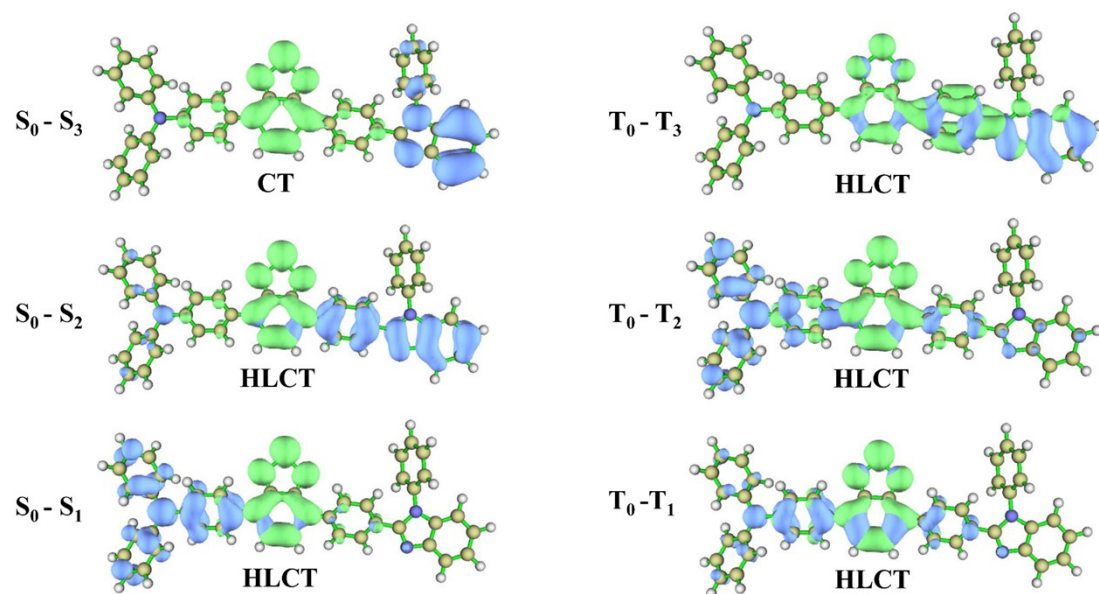


Fig. S7. Natural transition orbitals of $S_0 \rightarrow S_n$ and $T_0 \rightarrow T_n$ ($n = 1-3$) of TPA-BT-BPI. The blue and green isosurfaces present hole and electron distribution, respectively.

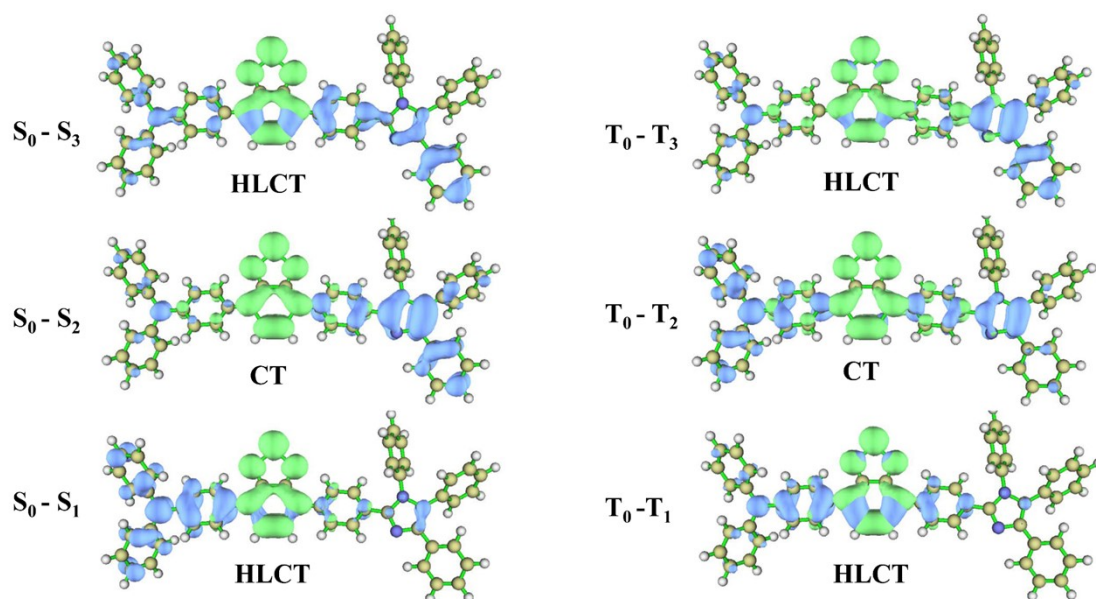


Fig. S8. Natural transition orbitals of $S_0 \rightarrow S_n$ and $T_0 \rightarrow T_n$ ($n = 1-3$) of TPA-BT-IM. The blue and green isosurfaces present hole and electron distribution, respectively.

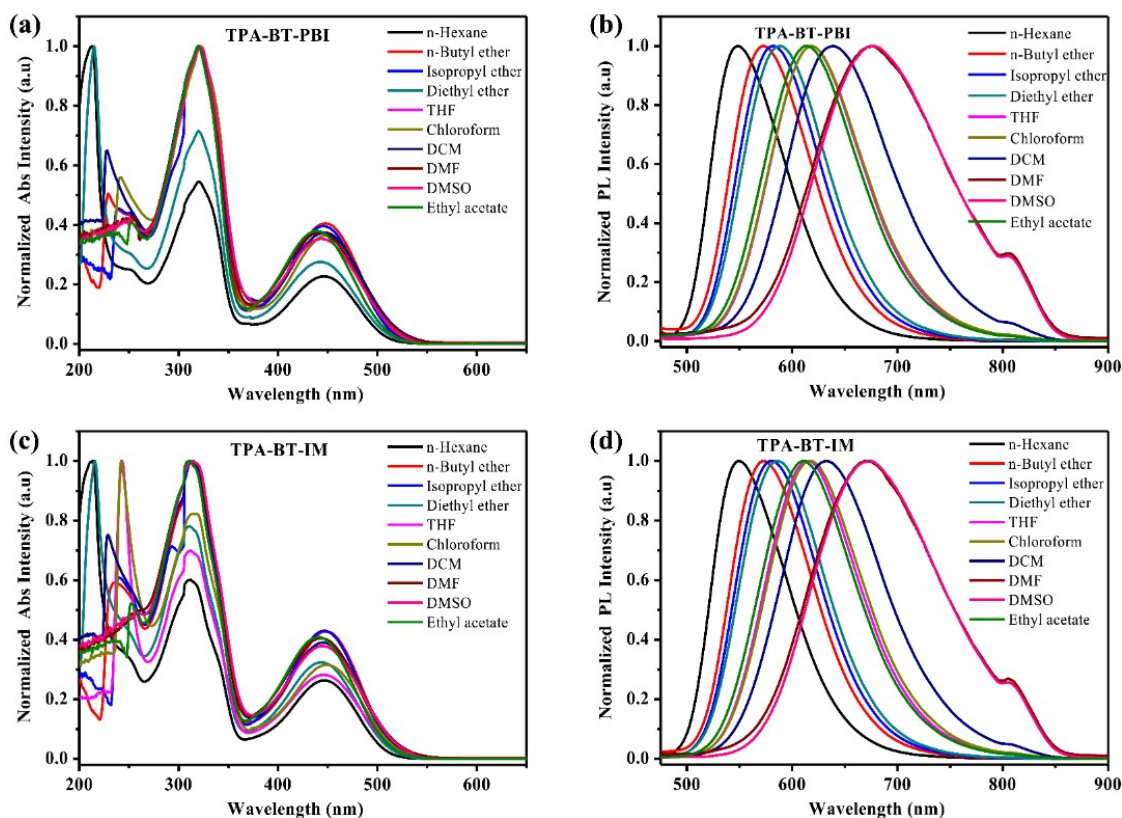


Fig. S9. Normalized UV-vis absorption and photoluminescence spectra of **TPA-BT-PBI** and **TPA-BT-IM** in different solvents.

Table S1. The absolute PLQY of **TPA-BT-PBI** and **TPA-BT-IM** in neat films or doped in various hosts (10 wt%).

Compounds	PLQY (%) ^a				
	Neat ^b	CBP ^c	CDBP ^d	mCP ^e	TPBi ^f
TPA-BT-PBI	55/56	80/87	51/56	71/83	77/85
TPA-BT-IM	51/54	74/86	77/88	76/87	75/95

^aPLQY of compounds tested with and without oxygen, respectively; ^bNeat means neat film; ^cCBP stands for 4,4'-Bis(N-carbazolyl)-1,1'-biphenyl; ^dCDBP stands for 4,4'-bis(9-carbazolyl)-2,2'-dimethylbiphenyl; ^emCP stands for 1,3-Di-(9-carbazolyl)benzene; ^fTPBi stands for 1,3,5-Tris(N-phenylbenzimidazol-2-yl)benzene.

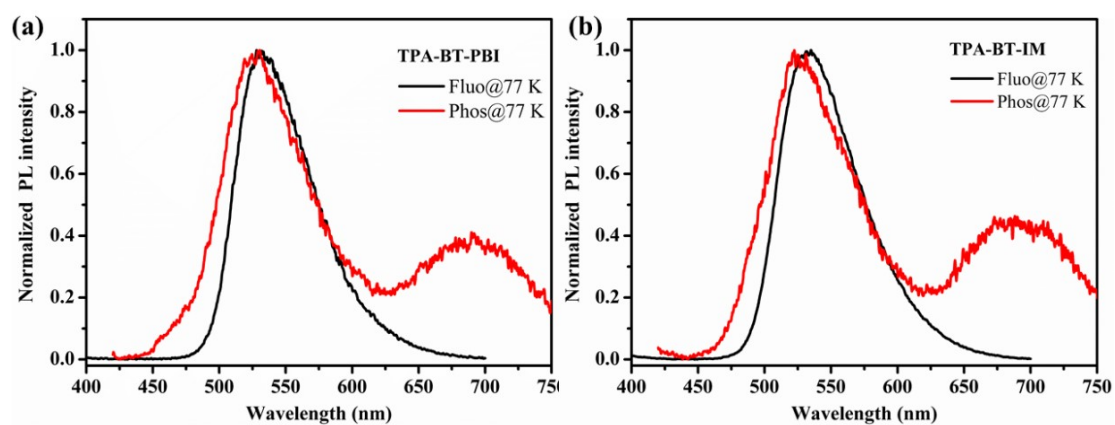


Fig. S10. Fluorescence and phosphorescence spectra of **TPA-BT-PBI** (a) and **TPA-BT-IM** (b) in toluene at 77 K.

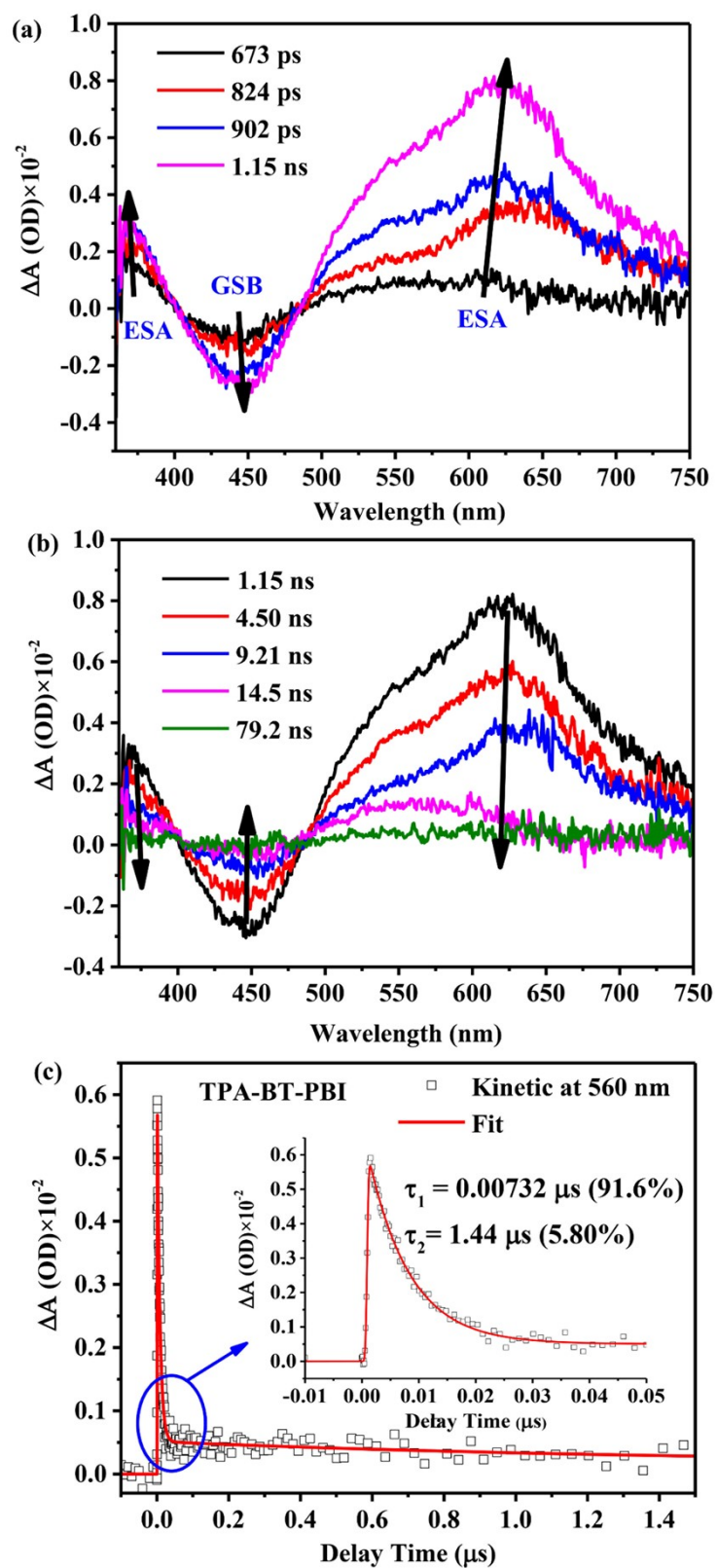


Fig. S11. TA spectra of TPA-BT-PBI in DCM solution were obtained after 320 nm excitation from 673 ps to 1.15 ns (a), 1.15 ns to 79.2 ns (b), and fitted kinetics at 560 nm of TA (the inset shows the enlarged time scale) (c).