Supporting Information

AIE-active multicolor tunable luminogens: Simultaneous mechanochromism and acidochromism with high contrast beyond 100 nm

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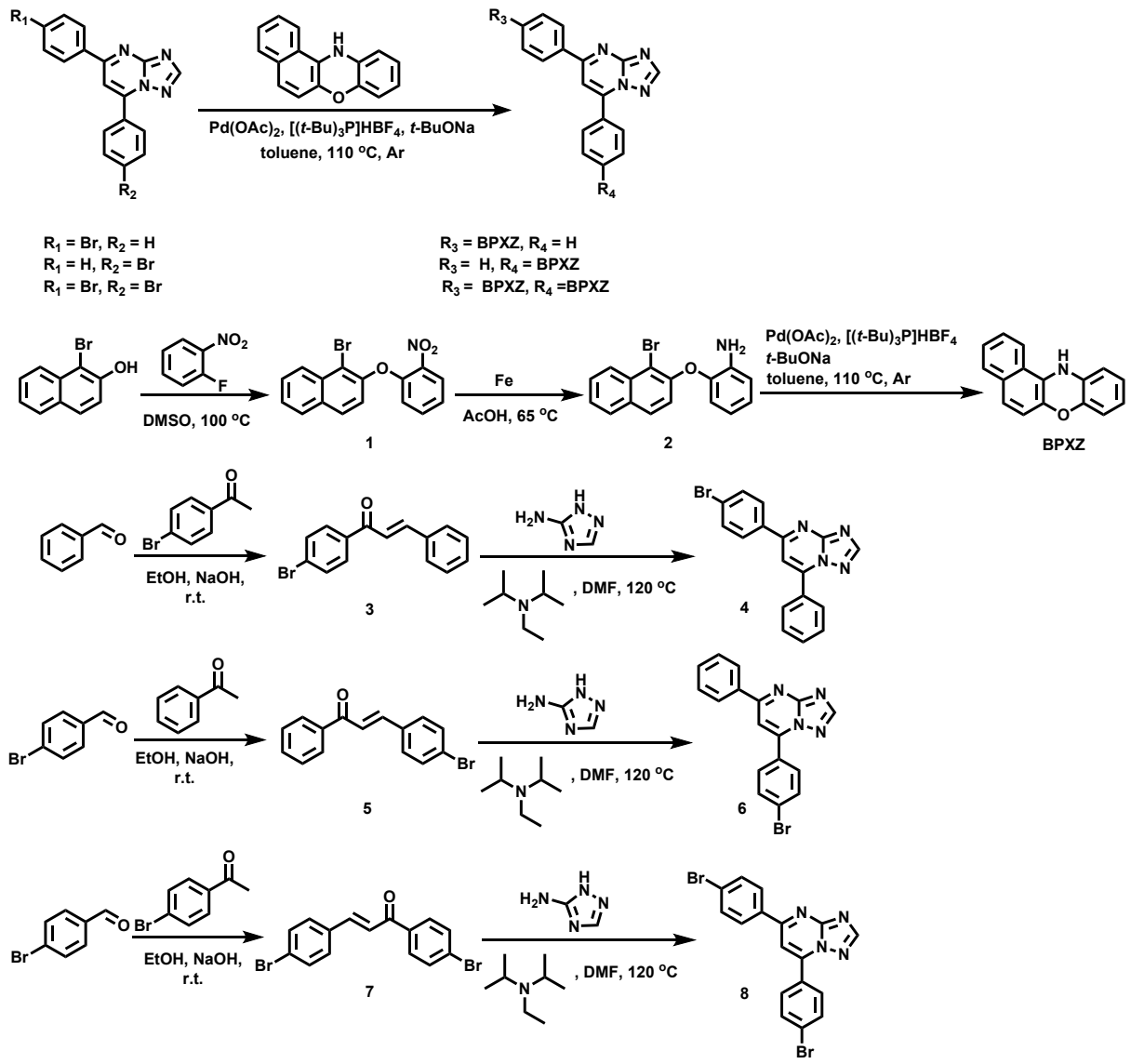
Synthesis



Scheme S1 Synthetic routes of the compounds.

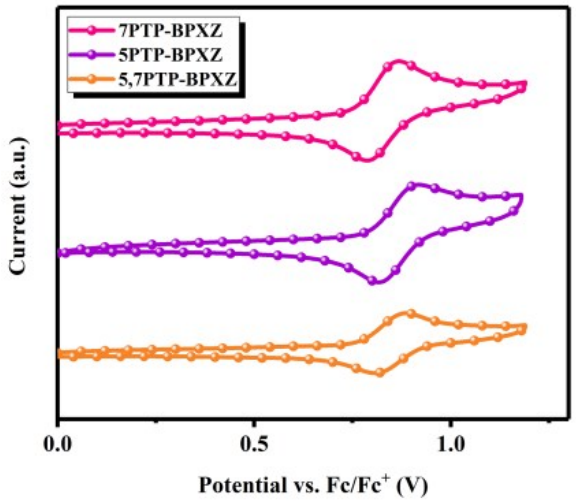


Fig. S1 Cyclic voltammograms: the oxidation experiments measured in THF solution.

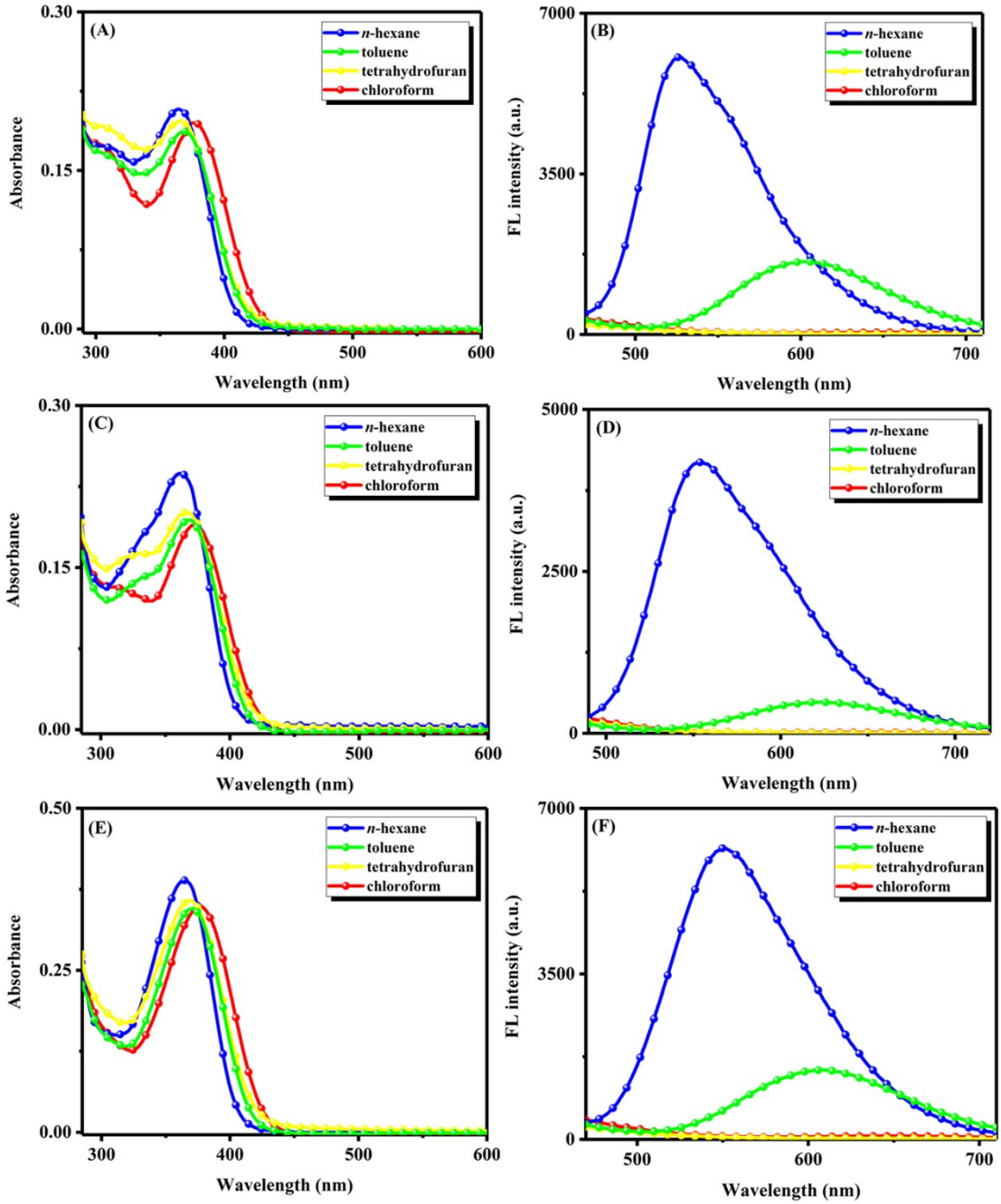


Fig. S2 The UV-vis and fluorescence spectra of the luminogens in different solvents (10.0 μM). A/B: **7PTP-BPXZ**; C/D: **5PTP-BPXZ**; E/F: **5,7PTP-BPXZ**.

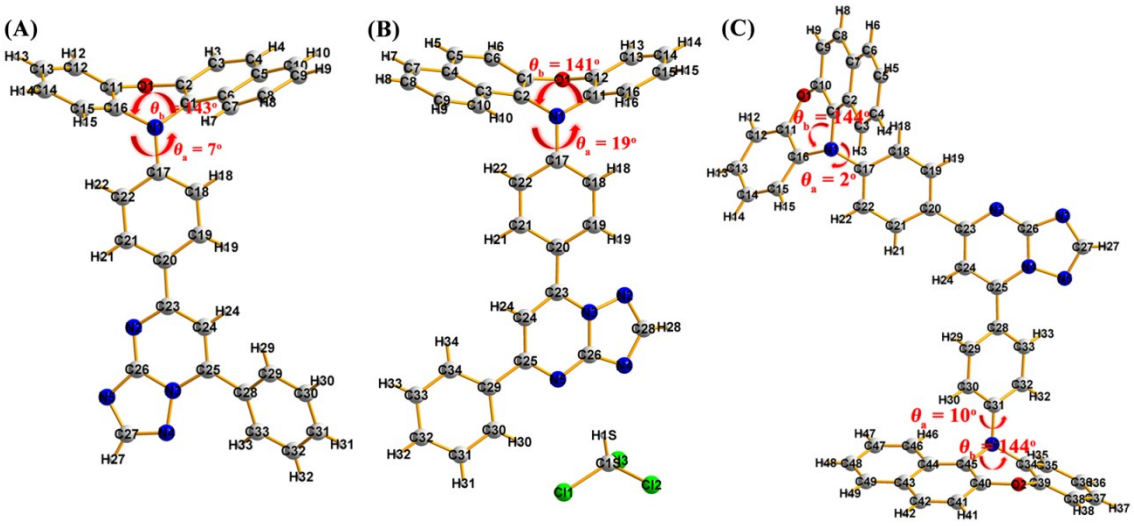


Fig. S3 Crystal structures of **7PTP-BPXZ** (A), **5PTP-BPXZ** (B) and **5,7TP-BPXZ** (C).

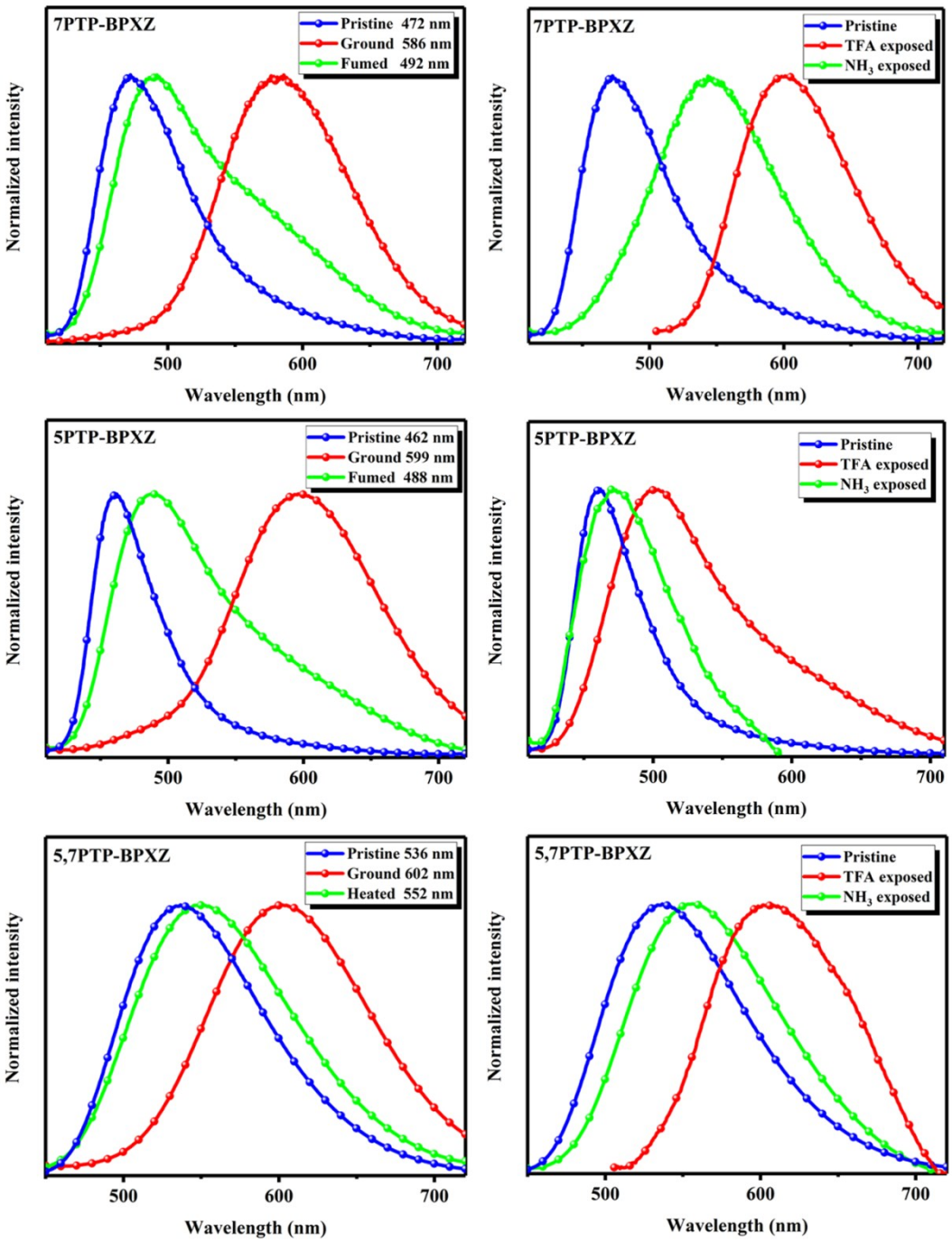


Fig. S4 Corresponding fluorescence spectra of the luminogens in different conditions.

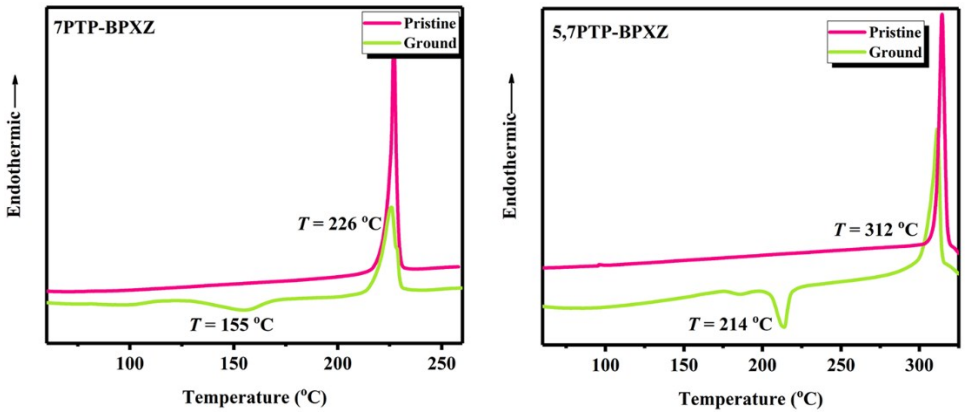


Fig. S5 DSC curves of the luminogens in the pristine and ground states.

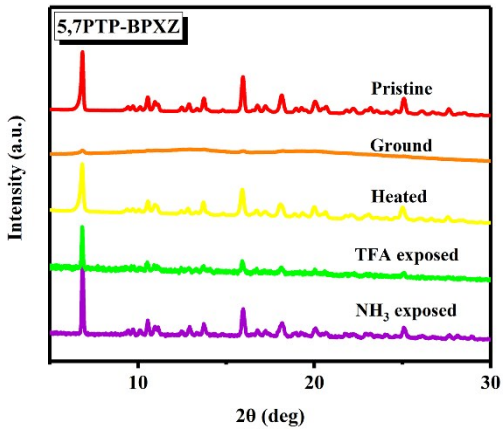


Fig. S6 PXRD curves of **5,7PTP-BPXZ** in different states.

Table S1 Photophysical data for the luminogens in different solvents.

Luminogen	Medium	λ_{abs} (nm)	λ_{em} (nm)	Stokes shift (cm^{-1})
7PTP-BPXZ	*n*-hexane	364	526	8016
	toluene	369	603	10443
	tetrahedrofuran	366	-	-
	chloroform	374	-	-
5PTP-BPXZ	*n*-hexane	361	555	9009
	toluene	368	624	11001
	tetrahedrofuran	367	-	-
	chloroform	371	-	-
5,7PTP-BPXZ	*n*-hexane	365	551	8878
	toluene	370	607	10552
	tetrahedrofuran	370	-	-
	chloroform	375	-	-

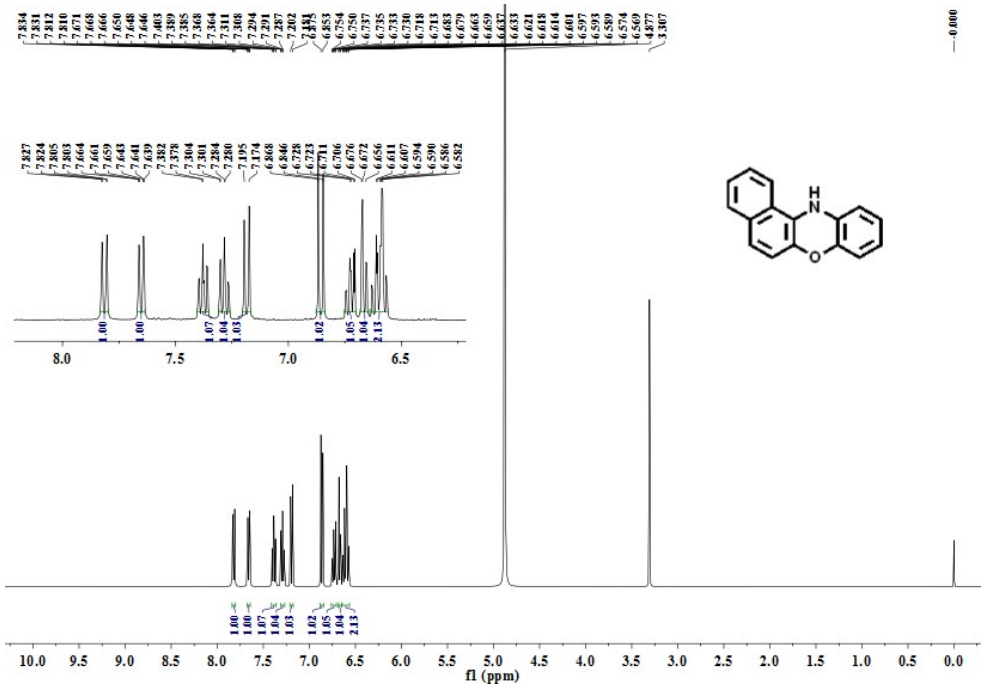
Table S2 Intermolecular interactions for **5PTP-BPXZ** crystal.

	Dimer	Adjacent dimers
Hydrogen bonds	C1S-H1S···N4 (*d* = 2.37 Å), C1S-H1S···N5 (*d* = 2.66 Å), C22-H22···Cl2 (*d* = 2.89 Å).	C13-H13···N4 (*d* = 2.88 Å), C14-H14···Cl3 (*d* = 2.96 Å), C32-H32···N2 (*d* = 2.65 Å).
C-H···π	C19-H19···π (ring1, C29-C30-C31-C32-C33-C34, *d* = 2.74 Å), C24-H24···π (ring2, C23-C24-C25-N5-C26-N3, *d* = 3.58 Å), C30-H30···π (ring3, C17-C18-C19-C20-C21-C22, *d* = 2.98 Å).	C5-H5···π (ring4, C1-C2-C3-C4-C5-C6, *d* = 3.24 Å), C6-H6···π (ring4, *d* = 3.30 Å), C6-H6···π (ring5, C3-C4-C7-C8-C9-C10, *d* = 3.01 Å), C7-H7···π (ring6, C11-C12-C13-C14-C15-C16, *d* = 2.99 Å), C33-H33···π (ring6, *d* = 3.14 Å), C34-H34···π (ring6, *d* = 3.59 Å).
π···π	ring2···ring2, *d* = 3.65 Å.	None.

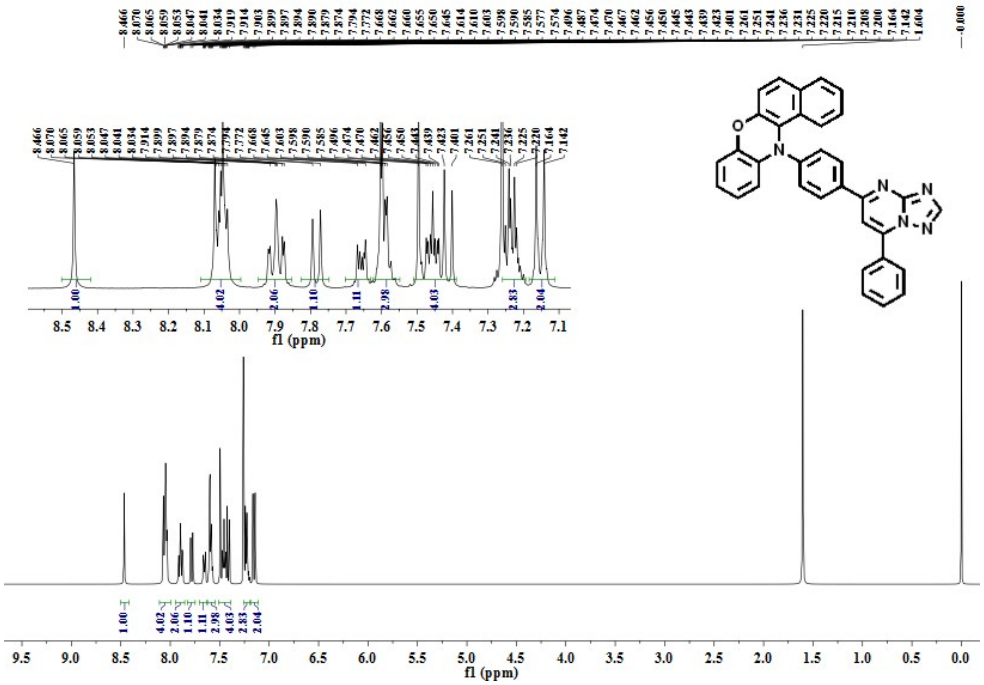
Table S3 Crystal data and structure refinements for **7PTP-BPXZ**, **5PTP-BPXZ** and **5,7PTP-BPXZ**.

Sample	**7PTP-BPXZ**	**5PTP-BPXZ**	**5,7PTP-BPXZ**.
Empirical formula	$C_{33}H_{21}N_5O$	$C_{34}H_{22}Cl_3N_5O$	$C_{49}H_{30}N_6O_2$
CCDC No.	1994907	1994908	1994909
Formula weight	503.55	622.91	734.79
Temperature	100 K	100 K	100 K
Crystal system	monoclinic	monoclinic	monoclinic
Space group	$P2_1/n$	$P2_1$	$P2_1/n$
	a=13.3125(11) Å	a=11.7716(3) Å	a=14.9283(2) Å
	b=6.9250(5) Å	b=6.9566(2) Å	b=14.0812(3) Å
Unit cell dimensions	c=32.282(2) Å	c=17.3812(5) Å	c=21.4884(4) Å
	α=90°	α=90°	α=90°
	β=94.065(7)°	β=95.546(3)°	β=94.7550(10)°
	γ=90°	γ=90°	γ=90°
Volume	2968.6(4) Å^3	1416.69(7) Å^3	4501.50(14) Å^3
Z, calculated density	4 Mg/m^3	2 Mg/m^3	4 Mg/m^3
Absorption coefficient	0.559 mm^{-1}	3.241 mm^{-1}	0.539 mm^{-1}
F(000)	1048.0	640.0	1528.0
2θ range for data	5.488-147.268°	5.108-147.318°	6.948-147.242°
	$-16 \le h \le 15$	$-10 \le h \le 14$	$-18 \le h \le 16$
Index ranges	$-5 \le k \le 8$	$-8 \le k \le 4$	$-17 \le k \le 15$
	$-39 \le l \le 35$	$-21 \le l \le 21$	$-26 \le l \le 23$
Data/parameters	5823/353	3971/388	8805/514
Final R indices	R_1=0.0859, W_{R2}=0.2442	R_1=0.0323, W_{R2}=0.0859	R_1=0.0541, W_{R2}=0.1529
Largest diff	0.52 e.Å^{-3}	0.19 e.Å^{-3}	0.25 e.Å^{-3}
peak and hole	-0.33 e.Å^{-3}	-0.39 e.Å^{-3}	-0.25 e.Å^{-3}
Goodness of fit on F^2	1.051	1.042	1.049
Refinement method	Full-matrix least-squares on F^2		

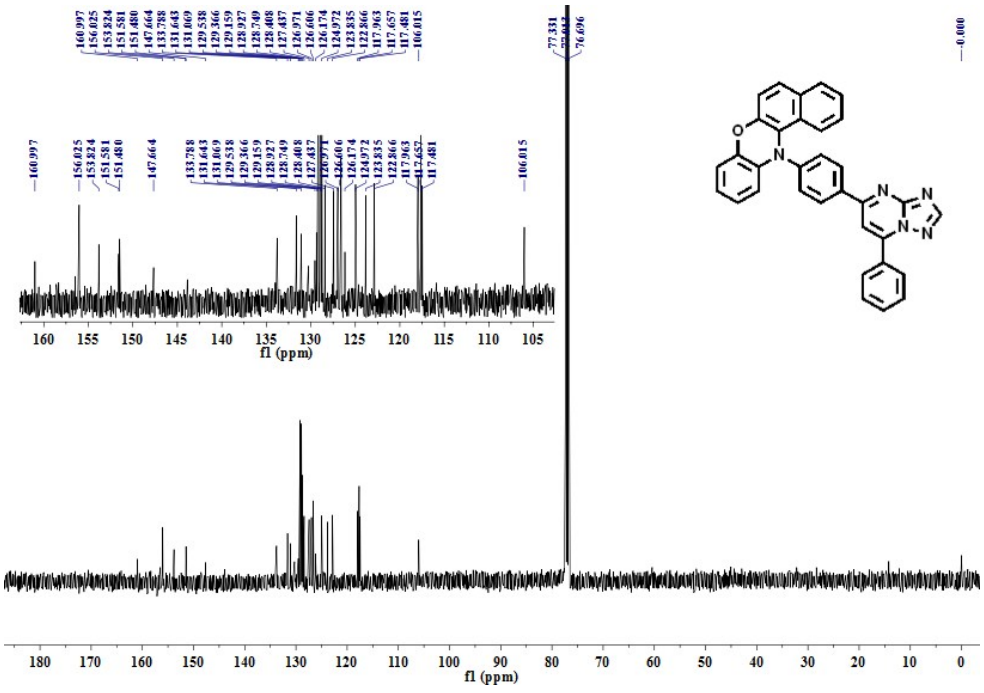
Spectral copies of ^{1}H NMR, ^{13}C NMR and HRMS



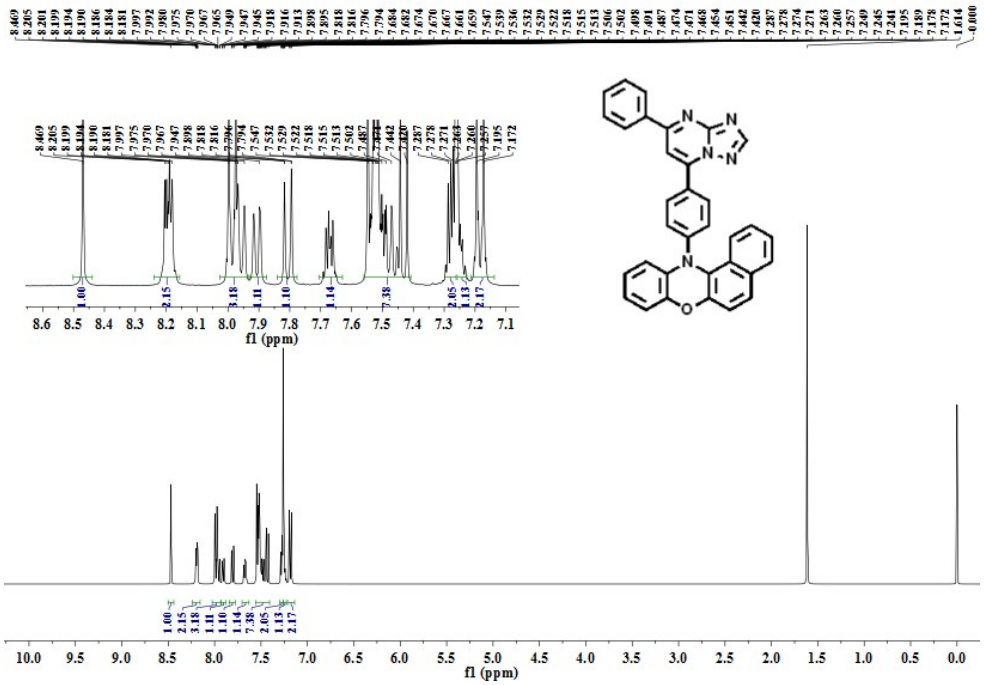
^{1}H NMR of **BPXZ** in CD_3OD.



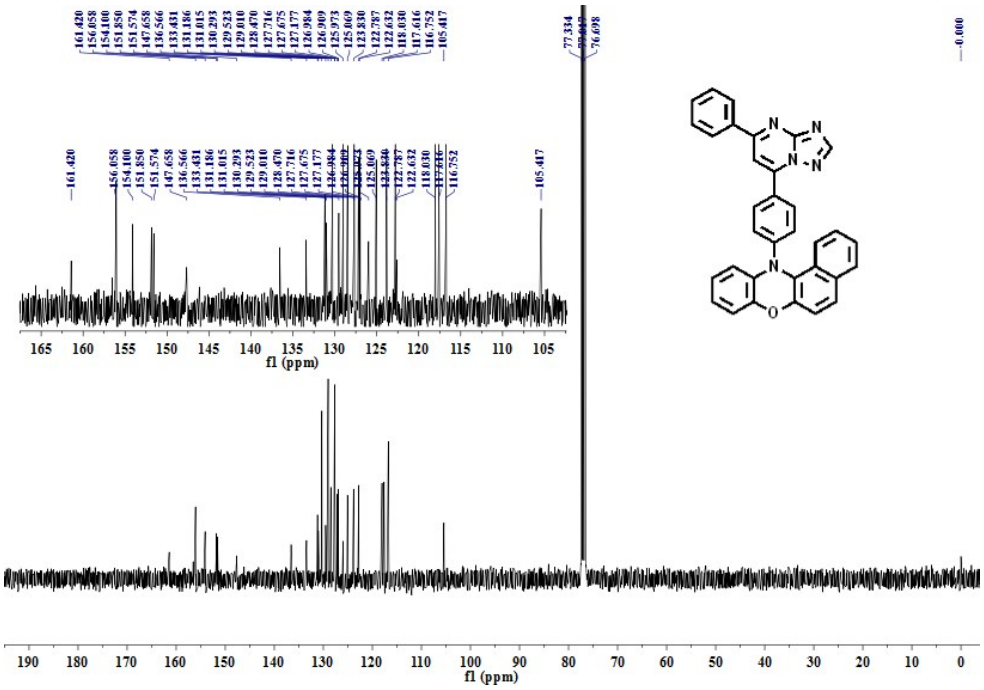
^{1}H NMR of **7PTP-BPXZ** in $CDCl_3$.



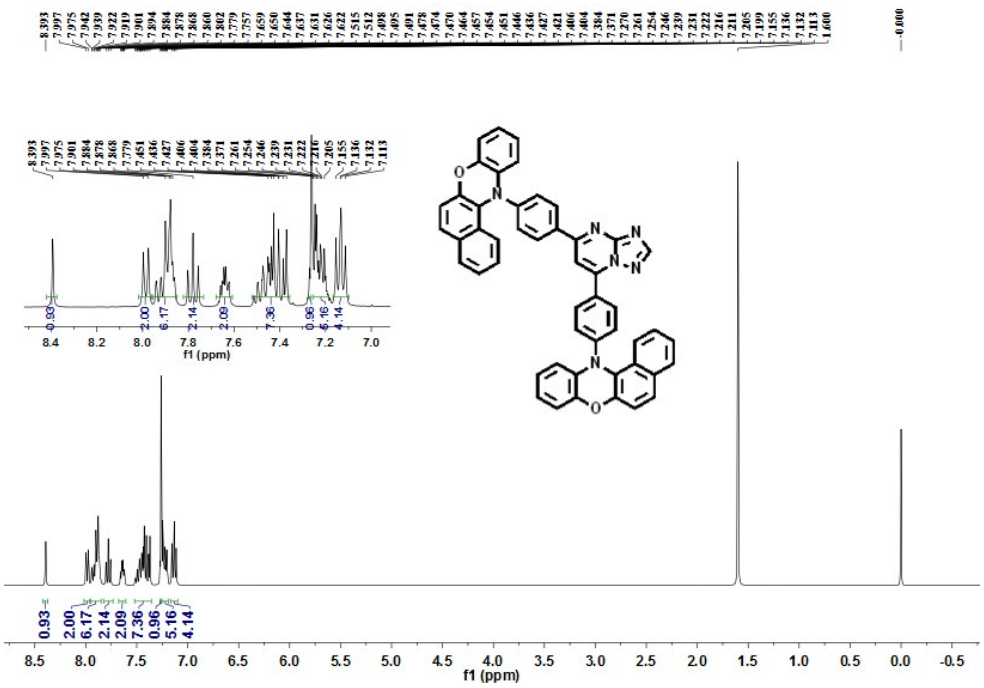
^{13}C NMR of **7PTP-BPXZ** in $CDCl_3$.



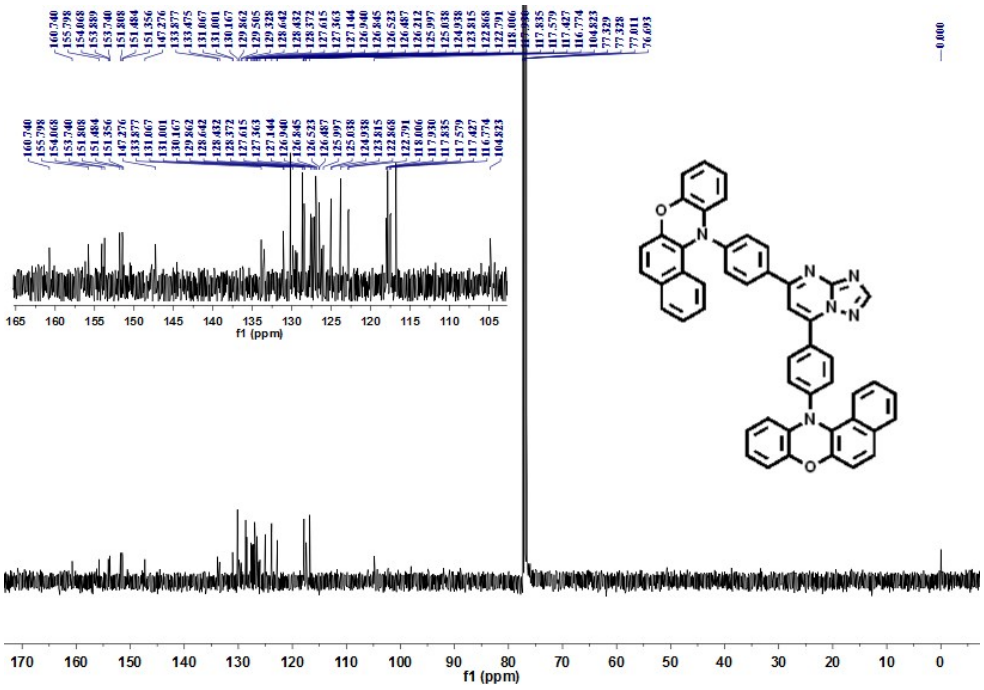
^{1}H NMR of **5PTP-BPXZ** in $CDCl_3$.



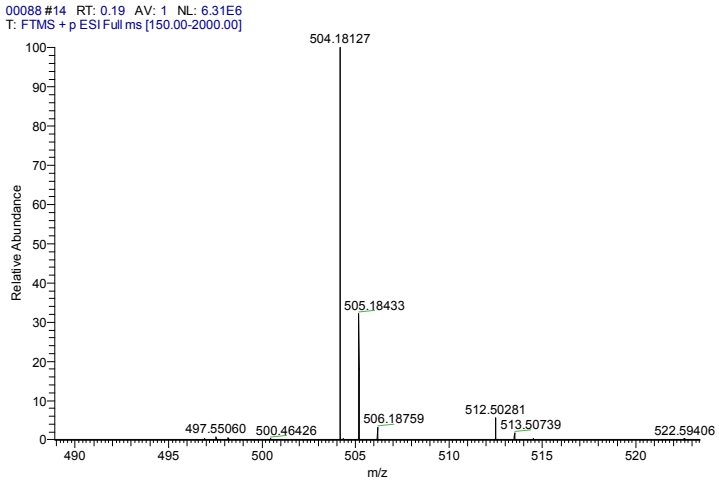
^{13}C NMR of **5PTP-BPXZ** in $CDCl_3$.



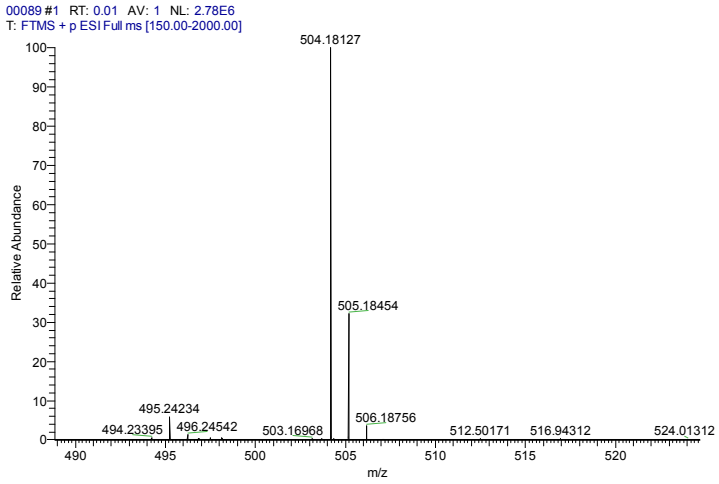
^{1}H NMR of **5,7PTP-BPXZ** in $CDCl_3$.



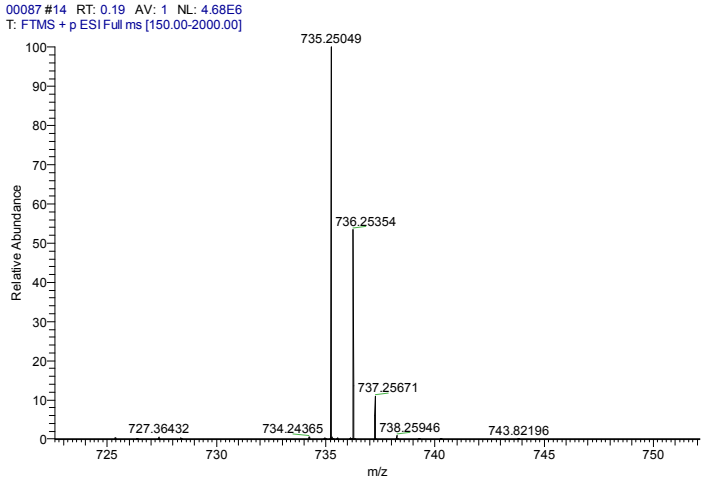
^{13}C NMR of **5,7PTP-BPXZ** in $CDCl_3$.



HRMS of **7PTP-BPXZ**.



HRMS of **5PTP-BPXZ**.



HRMS of **5,7PTP-BPXZ**.