Electronic Supplementary Material (ESI) for RSC Advances.

Synthesis and photophysical properties of benzoxazolyl-imidazole and benzothiazolyl-imidazole conjugates

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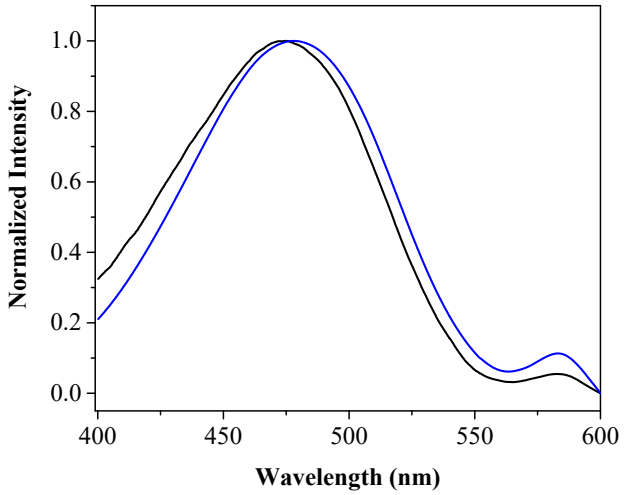


Fig. S1 Excitation spectra of **6b** with excitation wavelength at 620 nm. (black: 100 μM; blue: 500 μM)

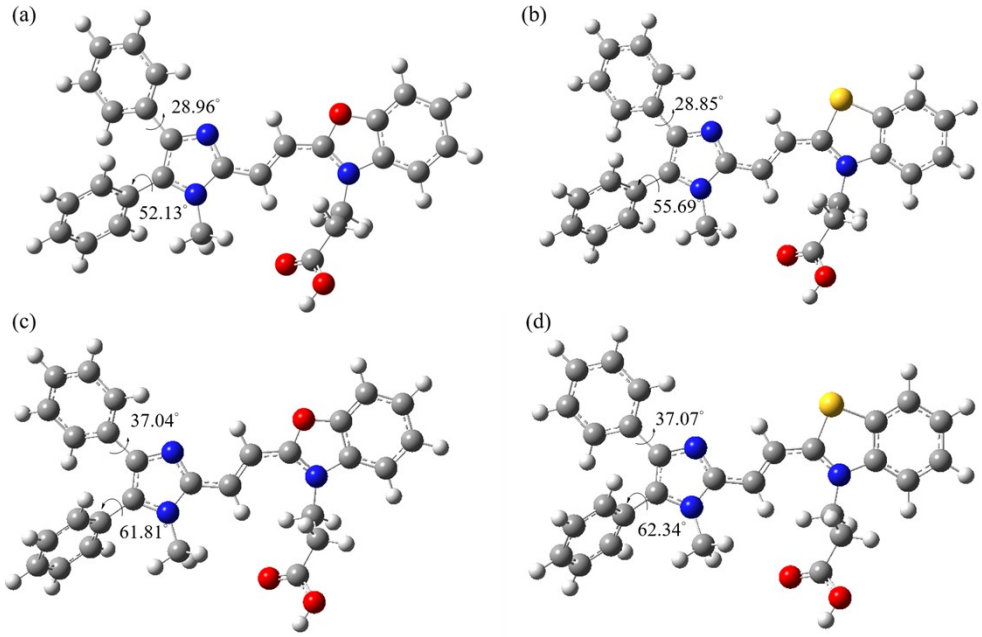


Fig. S2 The geometrical optimization structures of (a, c) **6a**$^{+}$ and (b, d) **6b**$^{+}$. (a, b) calculated by using DFT/B3LYP/6-31G (d,p); (c, d) calculated by using HF/6-31G (d,p). C: gray; H: white; N: blue; O: red; S: yellow.

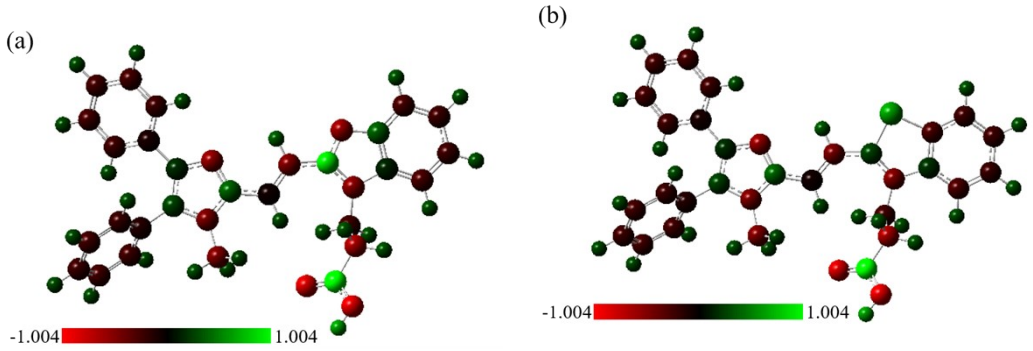


Fig. S3. NBO charge distribution on the optimized (a) **6a**$^+$ and (b) **6b**$^+$ designated by color change on the atoms with color scheme and scale (red for negative charge and green for positive charge), determined using HF/6-31G (d,p) level.

Table S1 Absorption spectra were obtained using TD-DFT methods for **6a**$^+$ and **6b**$^+$.[a]

	Optimized Geometries	Absorption (eV)	Electronic transitions	Oscillator strength
6a$^+$	DFT[b]	2.3319	H→L (0.69155)	0.7662
	HF[c]	2.3954	H→L (0.62171)	0.5869
6b$^+$	DFT[b]	2.2435	H→L (0.69333)	0.8094
	HF[c]	2.2707	H→L (0.61790)	0.6040

[a] For **6a**$^+$, X is oxygen atom; for **6b**$^+$, X is sulfur atom; [b] DFT/B3LYP/6-31G (d,p); [c] HF/6-31G (d,p).

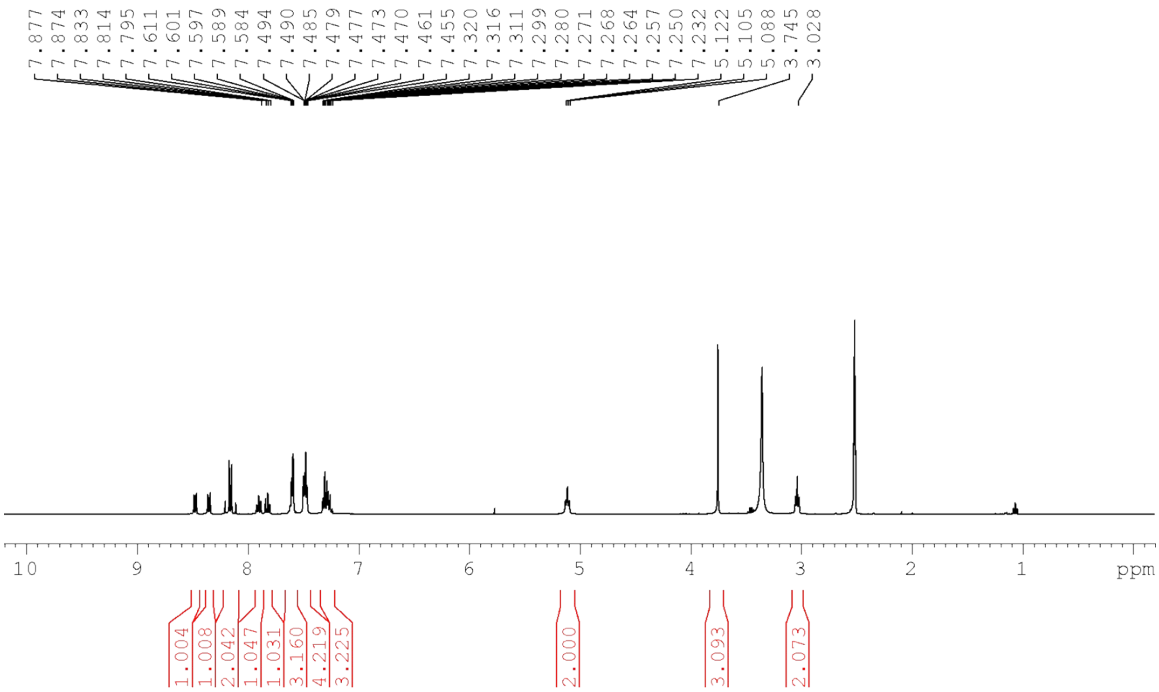


Fig. S4 ^{1}H NMR spectrum for **6a** in DMSO-d_6.

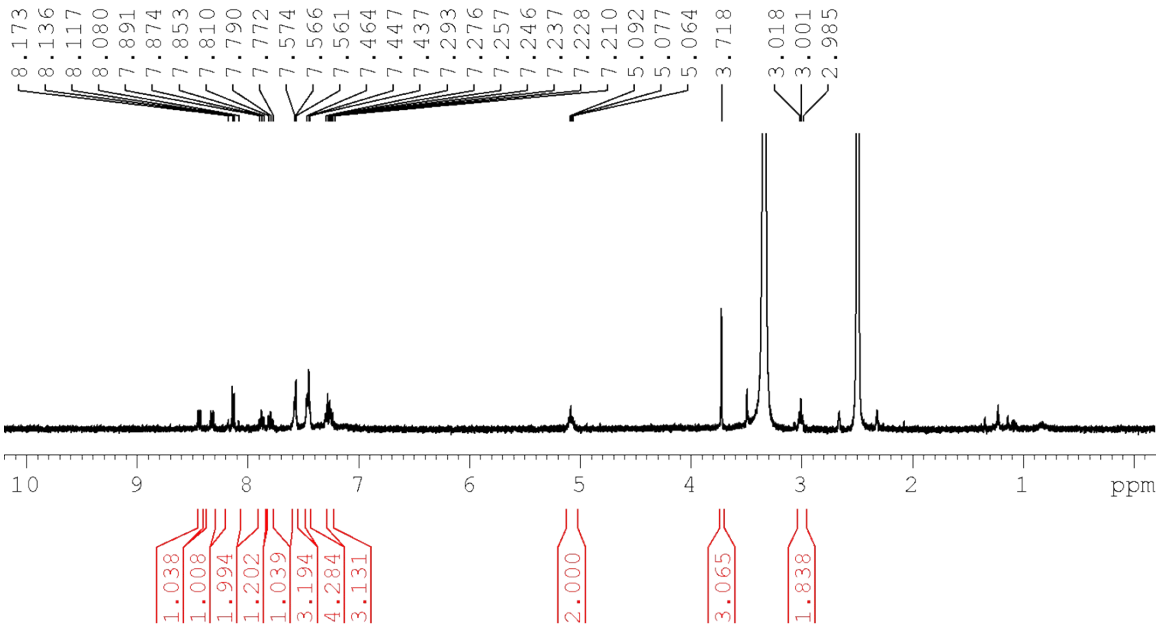
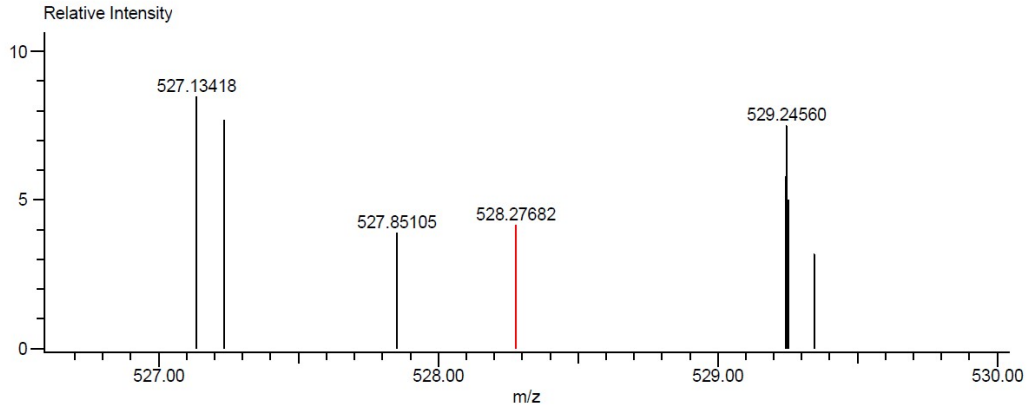
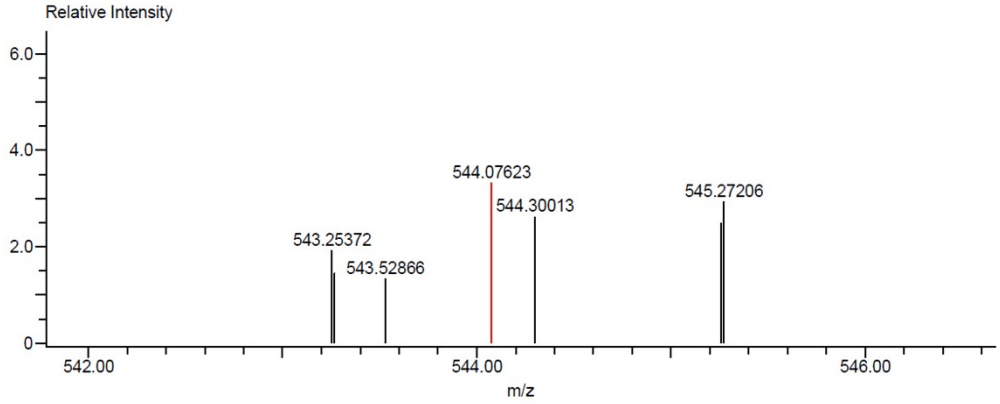


Fig. S5 ^{1}H NMR spectrum for **6b** in DMSO-d_6.



Mass	Intensity	Calc. Mass	Mass Difference [mDa]	Mass Difference [ppm]	Possible Formula
528.27682	82.57	528.09228	184.55	349.46	$^{12}C_{28}{}^{1}H_{23}{}^{79}Br_{1}{}^{14}N_{3}{}^{16}O_{3}$

Fig. S6. HRMS spectrum for **6a**.



Mass	Intensity	Calc. Mass	Mass Difference [mDa]	Mass Difference [ppm]	Possible Formula
544.07623	201.52	544.06943	6.79	12.49	$^{12}C_{28}{}^{1}H_{23}{}^{79}Br_{1}{}^{14}N_{3}{}^{16}O_{2}{}^{32}S_{1}$

Fig. S7. HRMS spectrum for **6b**.