

Supporting Information

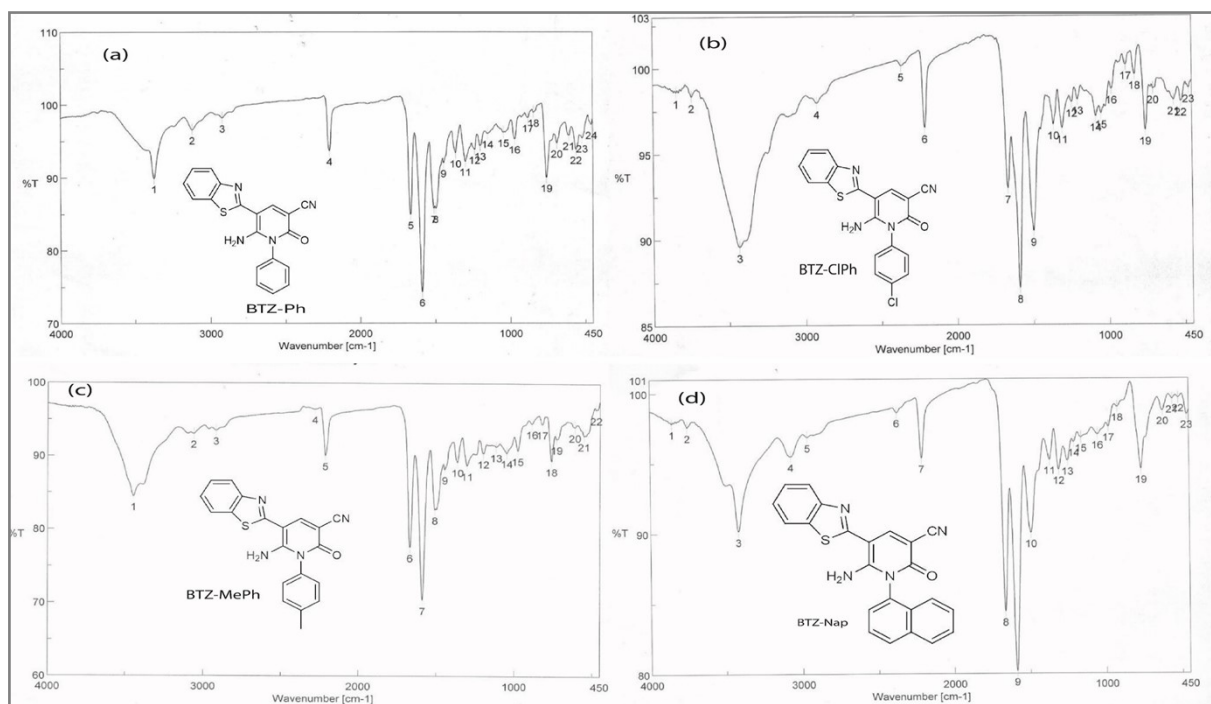


Fig S1. FT-IR Spectra of a) BTZ-Ph, b) BTZ-ClPh, c) BTZ-MePh, and d) BTZ-Nap.

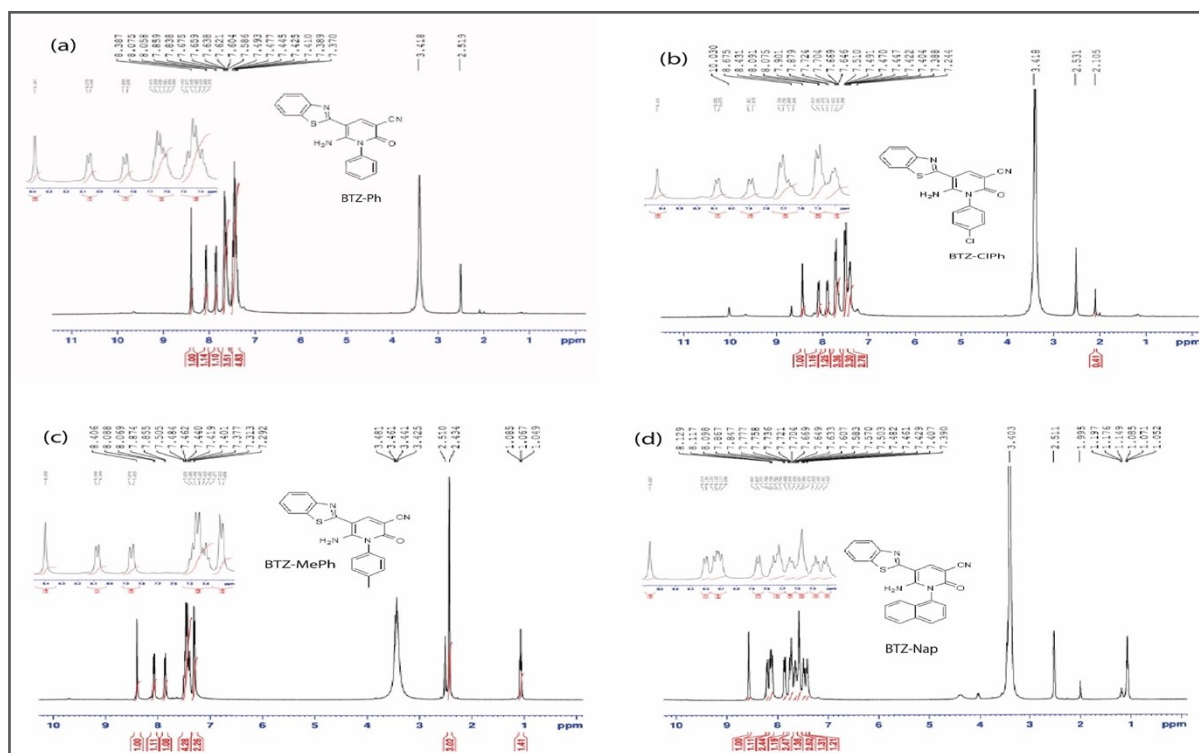


Fig S2. ¹H NMR spectra of a) BTZ-Ph, b) BTZ-ClPh, c) BTZ-MePh, and d) BTZ-Nap.

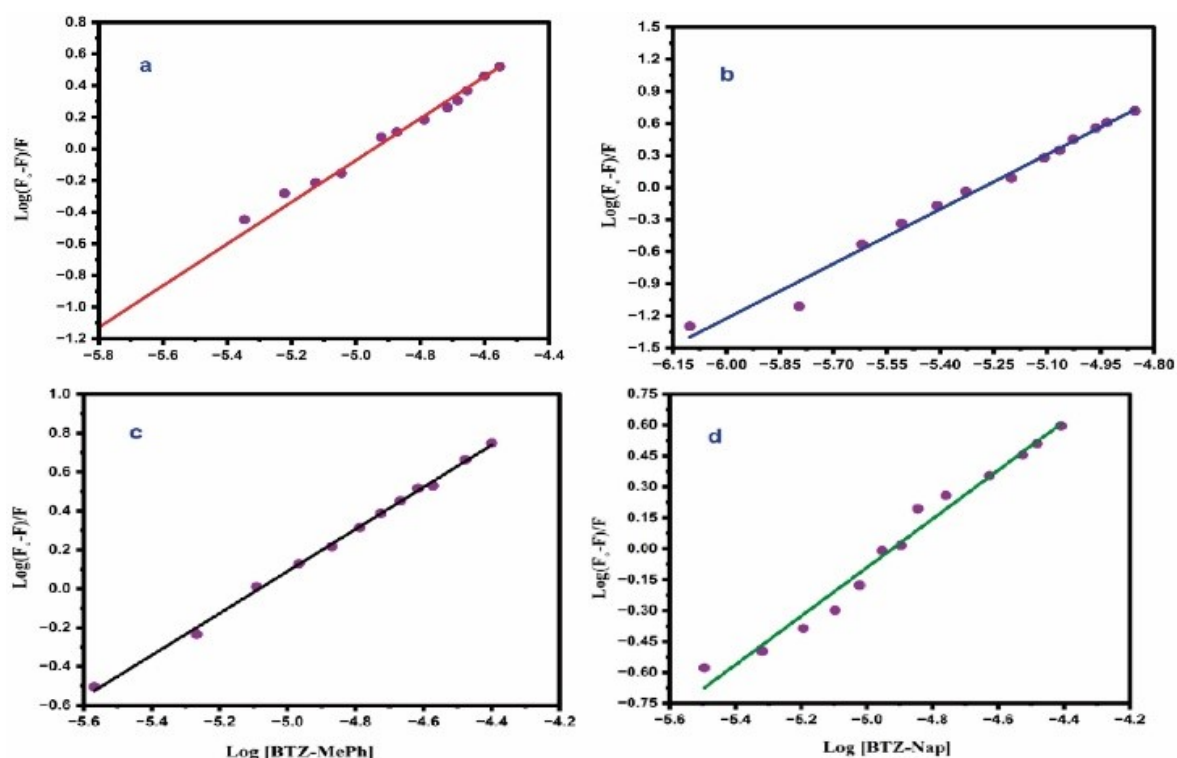


Figure S3. Plots of $\log(F_0 - F)/F$ versus $\log[Q]$ for a) BTZ-Ph, b) BTZ-ClPh, c) BTZ-MePh, and d) BTZ-Nap.

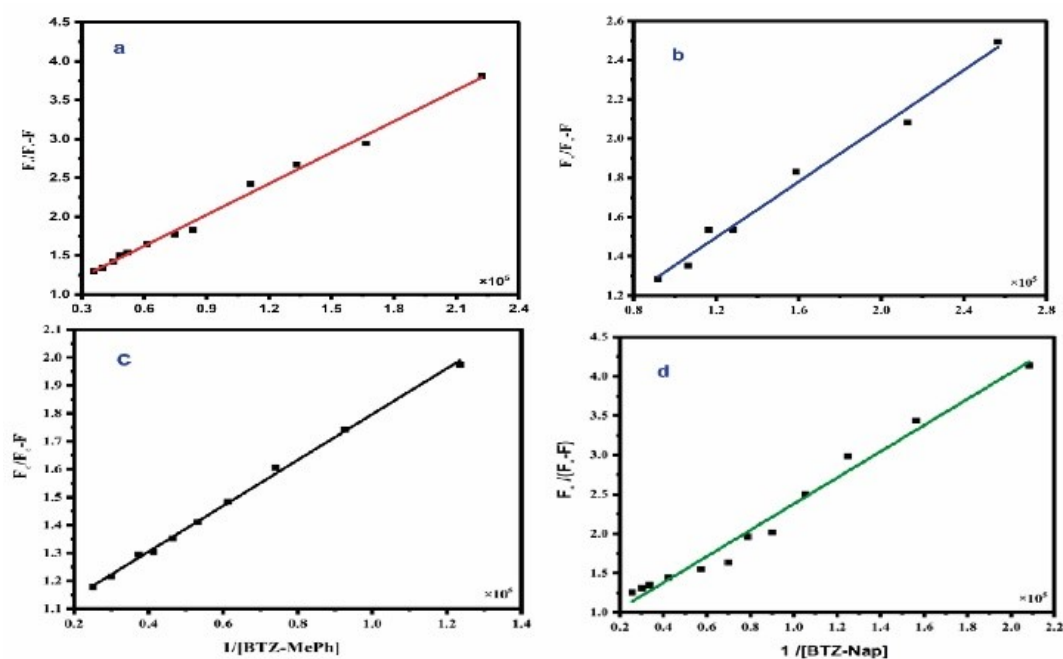


Figure S4. Modified Stern-Volmer plots for quenching of BSA by a) BTZ-Ph, b) BTZ-ClPh, c) BTZ-MePh, and d) BTZ-Nap.

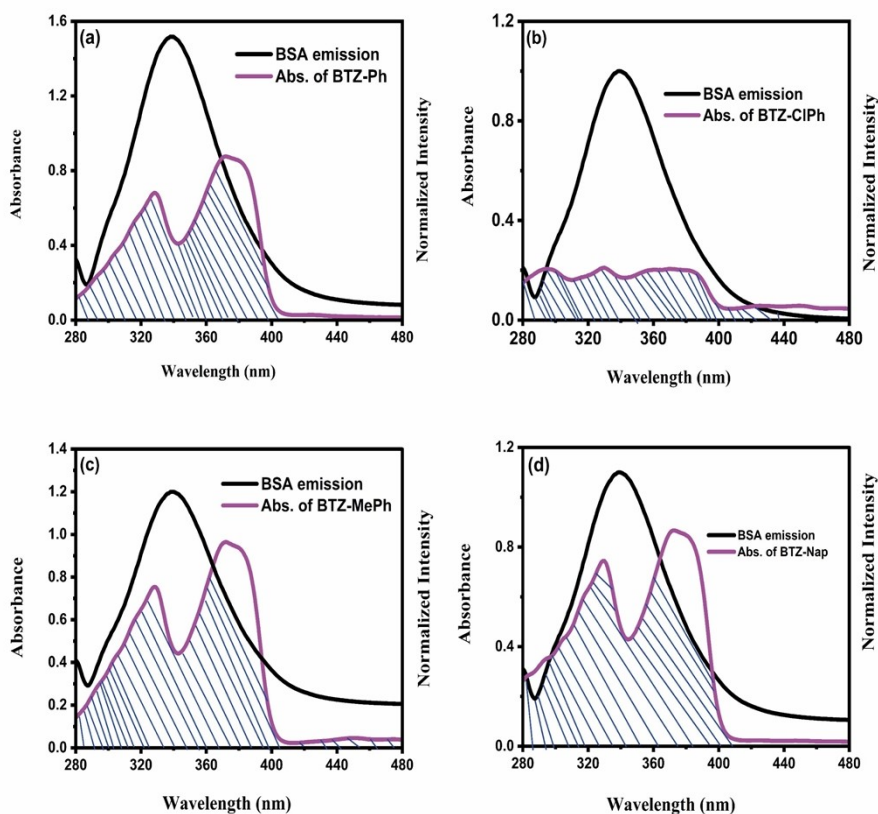


Fig. S5. The overlap of the fluorescence spectrum of BSA, and the absorbance spectrum of a) BTZ-Ph, b) BTZ-ClPh, c) BTZ-MePh, and d) BTZ-Nap; $\lambda_{\text{ex}} = 279$ nm and $\lambda_{\text{em}} = 339$ nm.

Table S1. The efficacy of energy transfer, the overlap integral, and the distance parameters of BTZ-Ph, BTZ-ClPh, BTZ-MePh, and BTZ-Nap.

Compound	J (10^{-16} L mol $^{-1}$ cm 3)	R_0 (nm)	r (nm)	E (%)
BTZ-Ph	1.17	1.22	1.26	0.45
BTZ-ClPh	1.71	1.30	1.45	0.34
BTZ-MePh	1.23	1.23	1.28	0.44
BTZ-Nap	1.56	1.28	1.40	0.36

Table S2. In silico docking results of benzothiazolyl-pyridinecarbonitrile derivatives in potential docking sites.

Docking site (method)	BTZ-MePh	BTZ-Ph	BTZ-CIPh	BTZ-Nap	Docking Score Order
Site 1 (Template)	-13.62	-15.27	-16.75	-11.49	BTZ-CIPh > BTZ-Ph > BTZ-MePh > BTZ-Nap
Site 1 (No-Template)	-13.79	-19.76	-19.98	-11.03	BTZ-CIPh > BTZ-Ph > BTZ-MePh > BTZ-Nap
Site 2 (Template)	-14.76	-18.40	-22.66	-12.24	BTZ-CIPh > BTZ-Ph > BTZ-MePh > BTZ-Nap
Site 2 (No-Template)	-14.76	-18.4	-22.66	-12.24	BTZ-CIPh > BTZ-Ph > BTZ-MePh > BTZ-Nap
Site 3 (Template)	-18.22	-14.56	-10.05	-12.99	BTZ-MePh > BTZ-Ph > BTZ-Nap > BTZ-CIPh
Site 3 (No-Template)	-20.45	-26.34	-26.77	-16.76	BTZ-CIPh > BTZ-Ph > BTZ-MePh > BTZ-Nap
DLID_5	-21.03	-23.68	-22.13	-20.07	BTZ-Ph > BTZ-CIPh > BTZ-MePh > BTZ-Nap
DLID_3	-16.59	-18.47	-15.17	-15.7	BTZ-Ph > BTZ-MePh > BTZ-Nap > BTZ-CIPh
DLID_6	-22.55	-18.71	-12.95	-18.4	BTZ-MePh > BTZ-Ph > BTZ-Nap > BTZ-CIPh
DLID_1	-27.47	-28.51	-27.04	-5.99	BTZ-Ph > BTZ-MePh > BTZ-CIPh > BTZ-Nap
DLID_12	-16.78	-18.48	-17.13	-17.12	BTZ-Ph > BTZ-CIPh > BTZ-MePh > BTZ-Nap

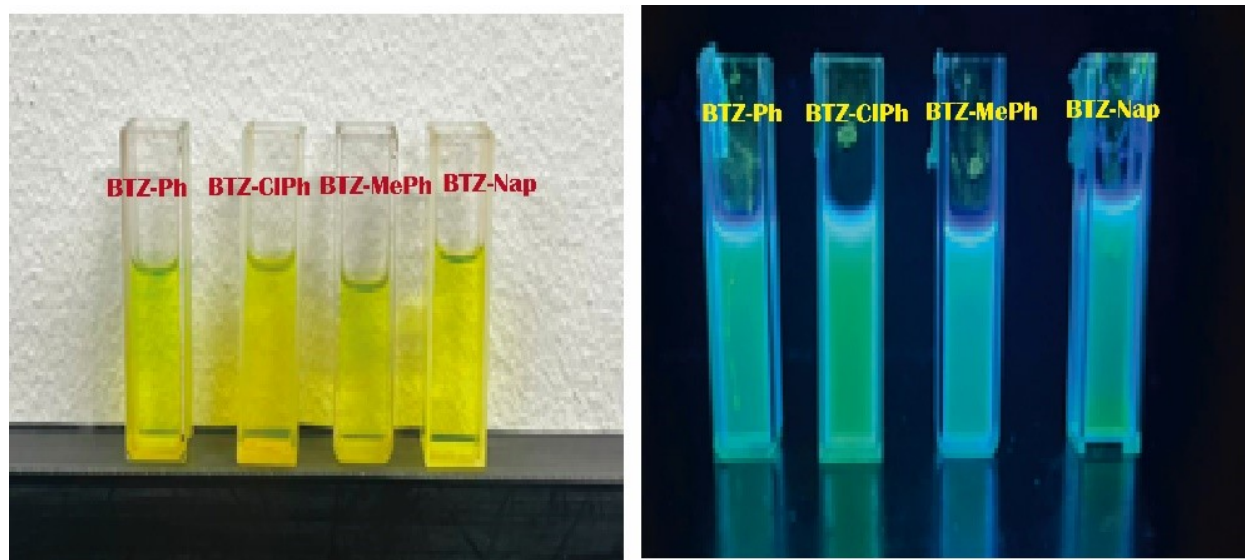


Fig S6. Solutions of BTZ derivatives in acetonitrile under visible light (left), and UV irradiation (right).

Equations

Equation S1: $F_o/F = 1 + K_q \tau_o [Q] = 1 + K_{sv}$

Equation S2: $\log \frac{F_o - F}{F} = \log K_b + n \log [Q]$

Equation S3: $K_q = K_{sv} / \tau_o$

Equation S4: $\frac{F_o}{F_o - F} = \frac{1}{faKa[Q]} + \frac{1}{fa}$