

## Supporting information

### Cationic Styryl Dyes for DNA Labelling and Selectivity Toward Cancer Cells and Gram-negative Bacteria

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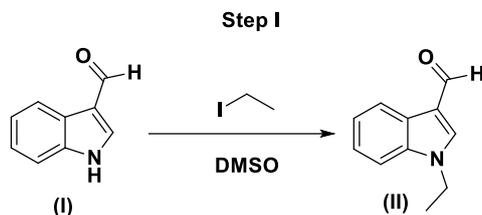
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#### Experimental Section

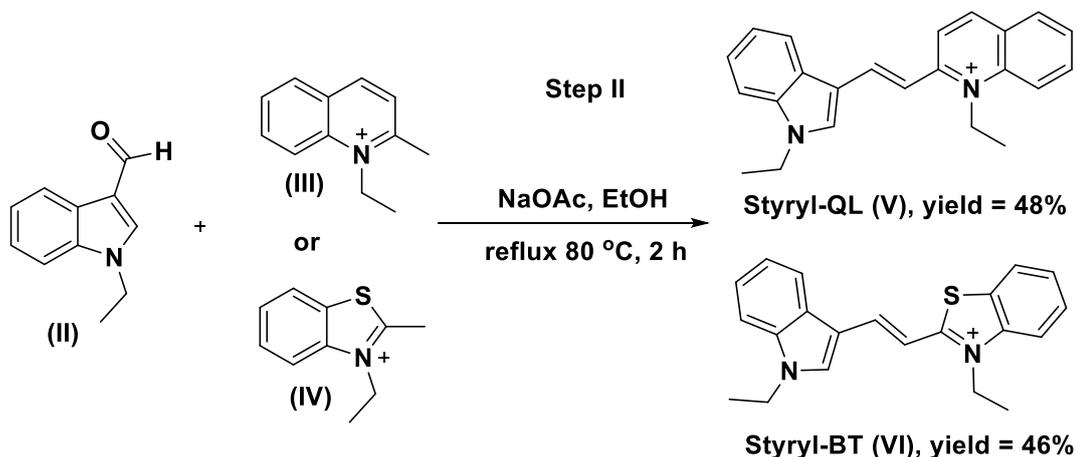
All glassware was oven-dried prior to use. All reagents were obtained from commercial suppliers (Sigma Aldrich, TCI, and Merck) and used without further purification. Column chromatography was performed with silica gel 60 F254 (Merck, mesh 300-400). <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra were recorded on a Bruker Avance 500 MHz spectrometer at room temperature in DMSO with Me<sub>4</sub>Si as an internal standard. Chemical shifts of <sup>1</sup>H NMR spectra were recorded and reported in ppm from the solvent resonance (DMSO at 2.54 ppm). Data were reported as follows: chemical shift in ppm ( $\delta$ ), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, quin = quintet, br = broad and m = multiplet), coupling constants, and number of protons. Proton decoupled <sup>13</sup>C NMR spectra were also recorded in ppm from tetramethylsilane (TMS) resonance (DMSO at 40.45 ppm). High-resolution mass spectra (HRMS) were recorded by an electrospray ionization mass (ESI-MS) spectrometer (MicrOTOF, Bruker, Rheinstetten, Germany).

## 1. $^1\text{H}$ NMR, $^{13}\text{C}$ NMR, and MS results of synthesized compounds

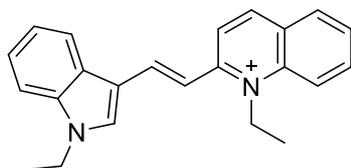
### Step I



1*H*-indole-3-carbaldehyde (2 g, 13.79 mmol) was dissolved in dimethyl sulfoxide (DMSO) (15 mL) with gentle warming. 20% NaOH (2 g NaOH, 2.76 mmol in 10 mL H<sub>2</sub>O) was slowly added to the solution at room temperature for 30 min. During this addition, the reaction temperature was maintained below 30 °C. After that, iodoethane (2.15 g, 13.79 mmol) was slowly added into the mixture at room temperature followed by stirring at 35 °C for 5 h. Finally, the mixture was poured into water (60 mL) followed by filtration to obtain a light-brown solid (1.5 g, 63%).<sup>1, 2</sup>



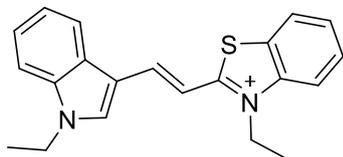
### Step II



### (*E*)-1-ethyl-2-(2-(1-ethyl-1*H*-indol-3-yl)vinyl)quinolin-1-ium

**Styryl-QL (V)**, was synthesized by the mixture of 1-ethyl-1*H*-indole-3-carbaldehyde (II) (100 mg, 0.58 mmol), 1-ethyl-2-methylquinolin-1-ium (III) (172 mg, 0.58 mmol) and anhydrous sodium acetate (95 mg, 1.16 mmol) in 4 mL EtOH at 80 °C for 3 h. After that, the solvent was removed followed by purification by silica gel column chromatography (5% v/v MeOH/CH<sub>2</sub>Cl<sub>2</sub>) to yield the pure product as an orange solid (90 mg, 48% yield); mp 244–246 °C. Characterization of **Styryl-QL**:  $^1\text{H}$  NMR (500 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  8.77 (d, *J* = 9.0 Hz, 1H), 8.65 (d, *J* = 15.5 Hz, 1H), 8.61 (d, *J* = 9.5 Hz, 1H), 8.48 (s, 1H), 8.41 (d, *J* = 9.0 Hz, 1H), 8.22 (d, *J* = 8.0 Hz, 1H), 8.15 (d, *J* = 6.5 Hz, 1H), 8.05 (t, *J* = 8.0 Hz, 1H), 7.81 (t, *J* =

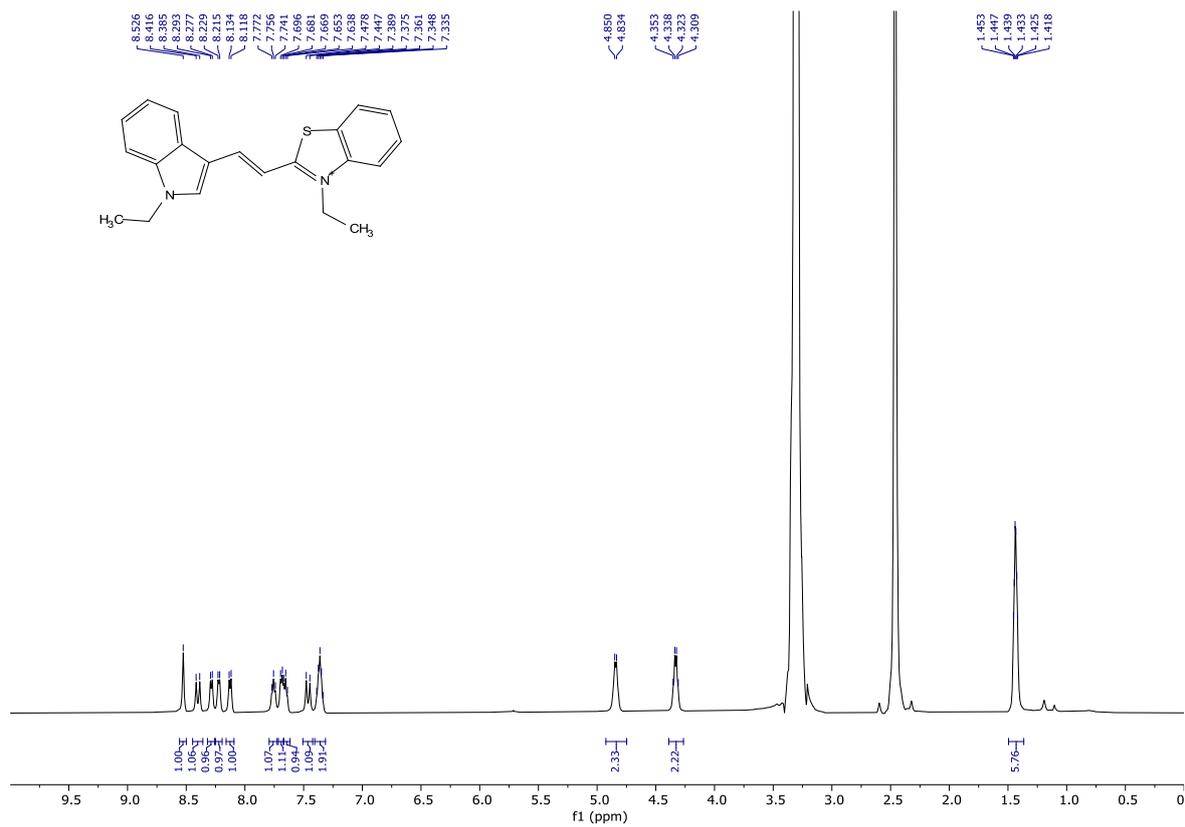
7.5 Hz, 1H), 7.66 (d,  $J = 6.5$  Hz, 1H), 7.46 (d,  $J = 15.5$  Hz, 1H), 7.33 (s, 2H), 5.01 (d,  $J = 7.5$  Hz, 2H), 4.34 (d,  $J = 7.0$  Hz, 2H), 1.57 (t,  $J = 7.0$  Hz, 3H), 1.44 (t,  $J = 7.0$  Hz, 3H),  $^{13}\text{C}$  NMR (125 MHz,  $\text{DMSO-}d_6$ )  $\delta$  156.0, 143.1, 142.3, 138.5, 137.6, 136.2, 134.8, 130.6, 128.4, 127.4, 126.6, 123.9, 122.7, 120.7, 120.4, 118.8, 114.1, 111.9, 110.9, 46.0, 41.9, 15.6, 14.0, HRMS (ESI) calcd for  $\text{C}_{23}\text{H}_{23}\text{N}_2^+$   $[\text{M}+\text{H}]^+$  327.1856, found 327.1853.



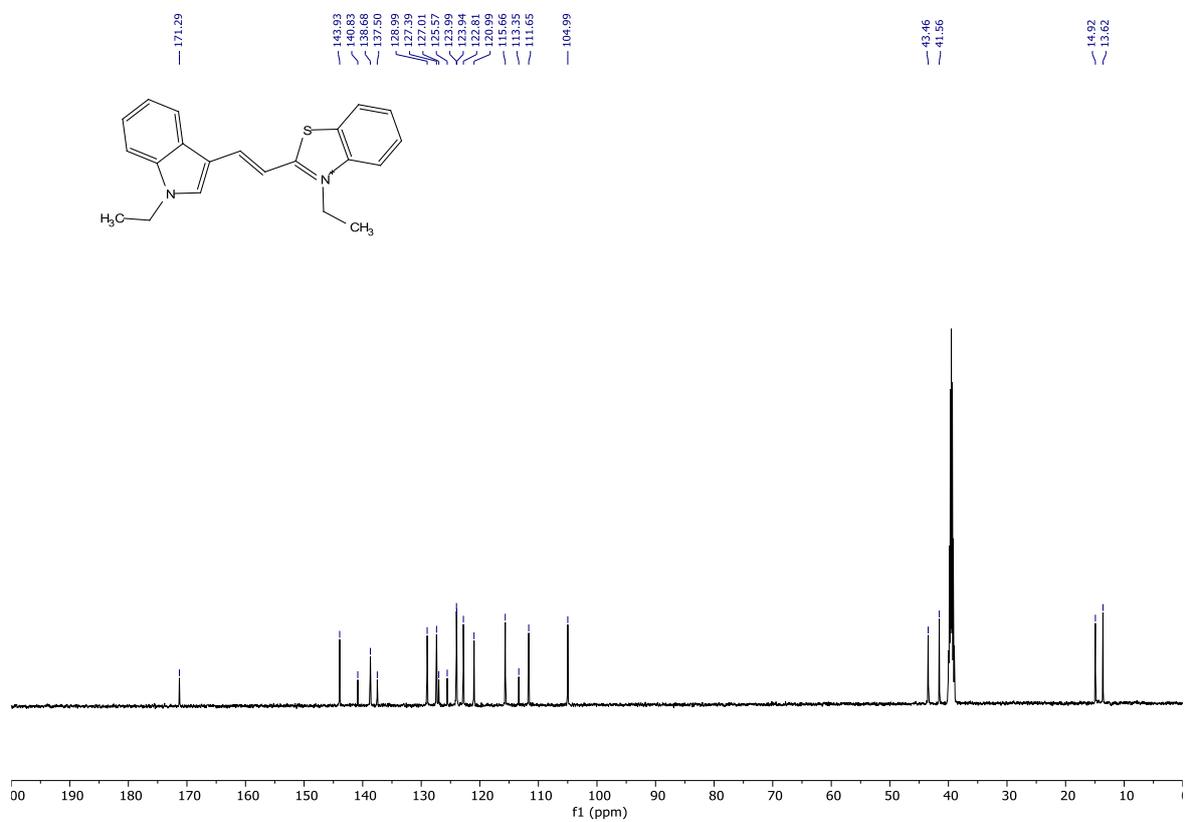
**(E)-3-ethyl-2-(2-(1-ethyl-1H-indol-3-yl)vinyl)benzo[d]thiazol-3-ium**

**Styryl-BT (VI)**, was synthesized by the mixture of 1-ethyl-1H-indole-3-carbaldehyde (II) (100 mg, 0.58 mmol), 3-ethyl-2-methylbenzo[d]thiazol-3-ium (IV) (102 mg, 0.58 mmol) and anhydrous sodium acetate (95 mg, 1.16 mmol) in 4 mL EtOH at 80 °C for 3 h. After that, the solvent was removed followed by purification by silica gel column chromatography (5% v/v MeOH/ $\text{CH}_2\text{Cl}_2$ ) to yield the pure product as an orange solid (88 mg, 46% yield); mp 236–238 °C. Characterization of **Styryl-BT**:  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO-}d_6$ )  $\delta$  8.53 (s, 1H), 8.40 (d,  $J = 15.5$  Hz, 1H), 8.29 (d,  $J = 8.0$  Hz, 1H), 8.22 (d,  $J = 7.0$  Hz, 1H), 8.13 (d,  $J = 8.0$  Hz, 1H), 7.76 (t,  $J = 8.0$  Hz, 1H), 7.68 (d,  $J = 7.5$  Hz, 1H), 7.65 (d,  $J = 7.5$  Hz, 1H), 7.46 (d,  $J = 15.5$  Hz, 1H), 7.36 (quin,  $J = 7.0$  Hz, 2H), 4.84 (d,  $J = 8.0$  Hz, 2H), 4.33 (q,  $J = 7.5$  Hz, 2H), 1.50 – 1.37 (m, 6H).  $^{13}\text{C}$  NMR (125 MHz,  $\text{DMSO-}d_6$ )  $\delta$  171.3, 143.9, 140.8, 138.7, 137.5, 129.0, 127.4, 127.0, 125.6, 124.0, 123.9, 122.8, 121.0, 115.7, 113.4, 111.7, 105.0, 43.5, 41.6, 14.9, 13.6, HRMS (ESI) calcd for  $\text{C}_{21}\text{H}_{21}\text{N}_2\text{S}_1^+$   $[\text{M}+\text{H}]^+$  333.1420, found 333.1429.

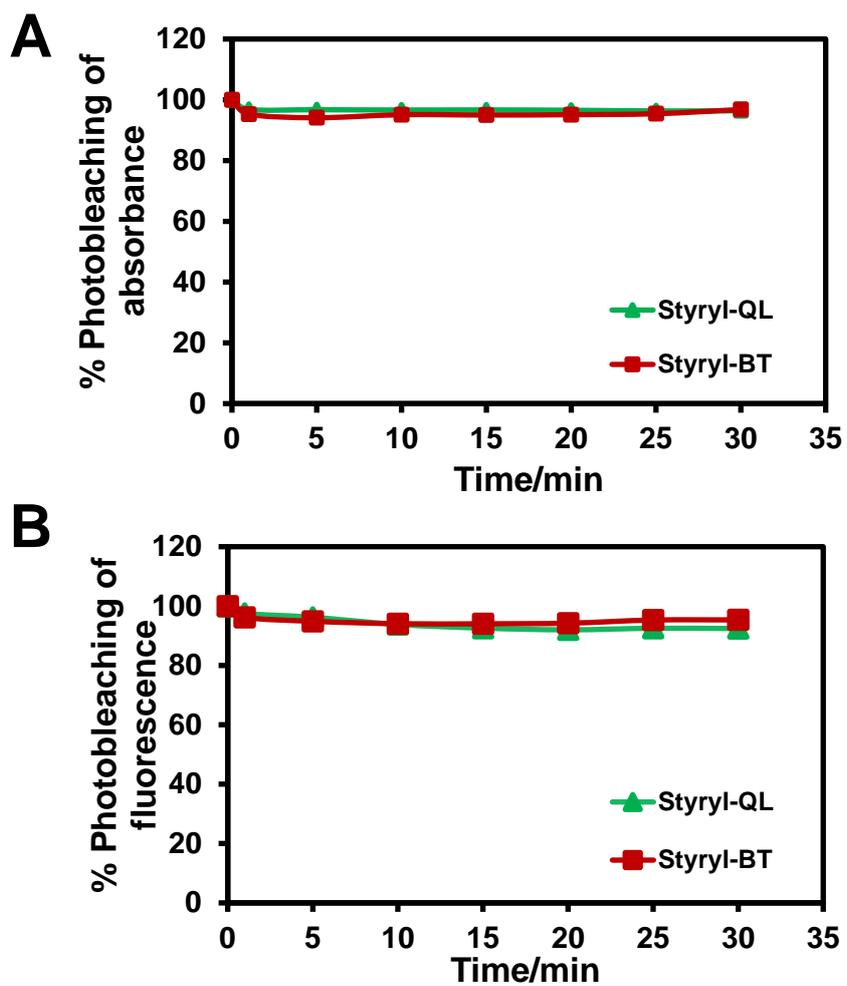




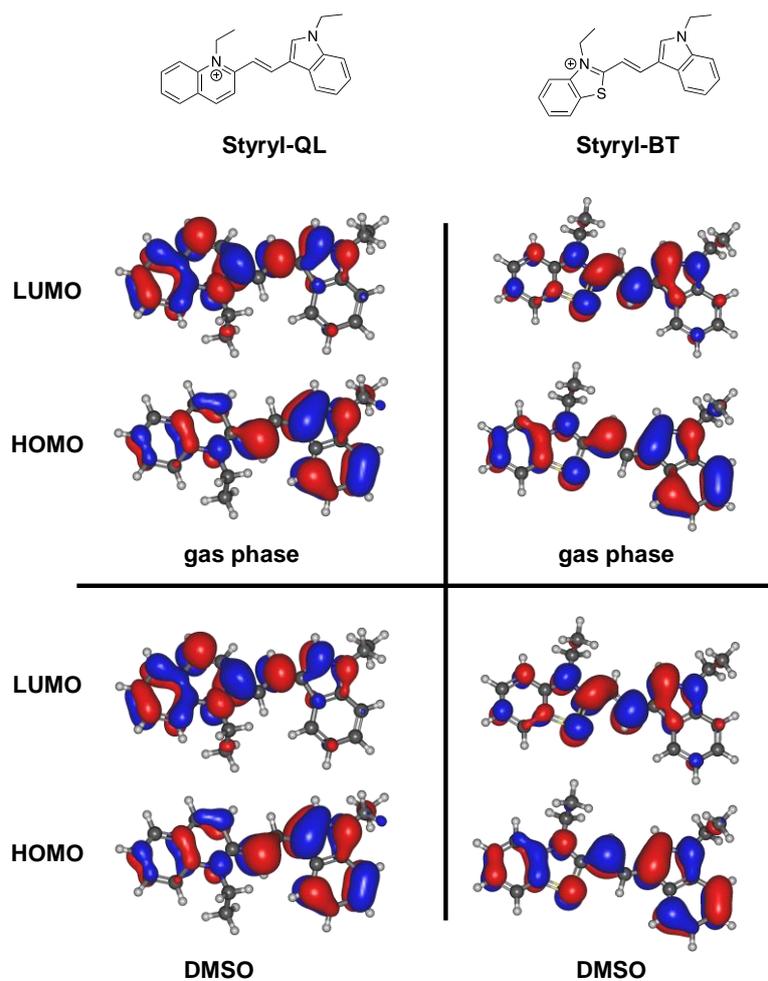
**<sup>1</sup>H NMR of compound Styryl-BT**



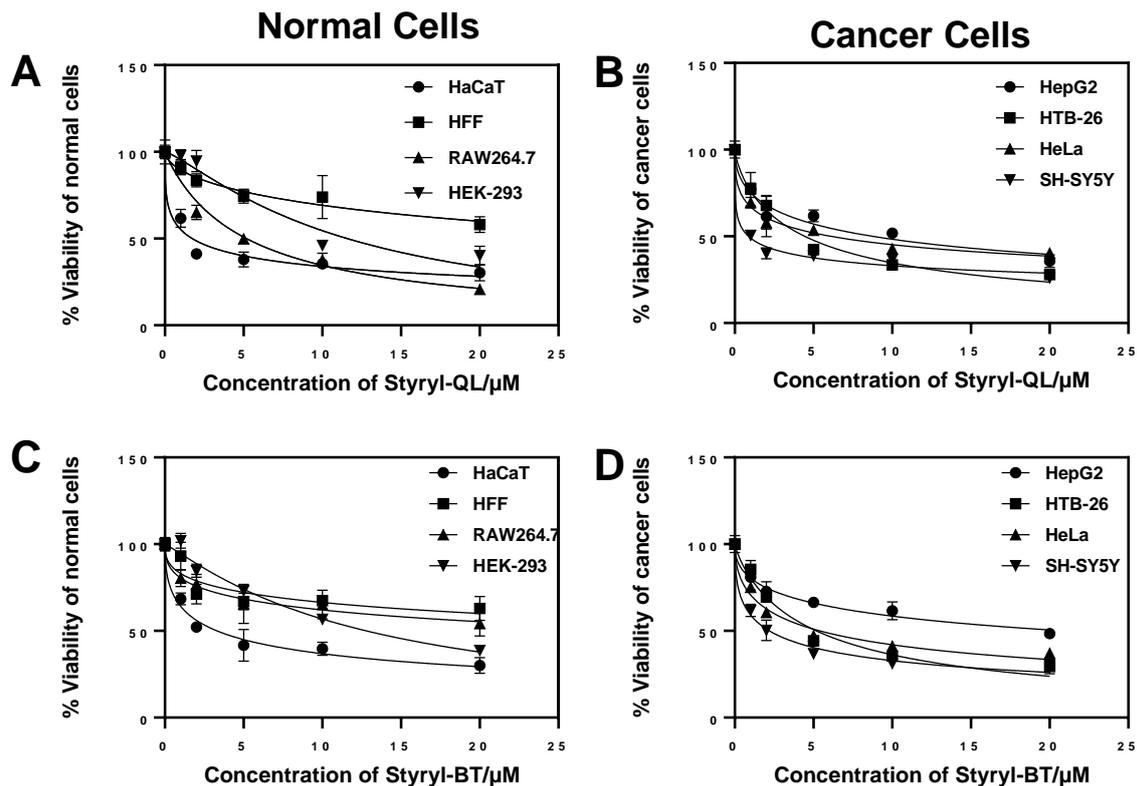
**<sup>13</sup>C NMR of compound Styryl-BT**



**Figure S1.** Photobleaching studies at 250 W blue light (450 nm) monitored at (A) the maximum absorbance and (B) emission intensity of styryl dyes in DMSO.



**Figure S2.** Frontier molecular orbital calculation obtained from DFT/B3-LYP/6-311G calculation in the gas phase and COSMO phase using the dielectric environment of DMSO (47.42).

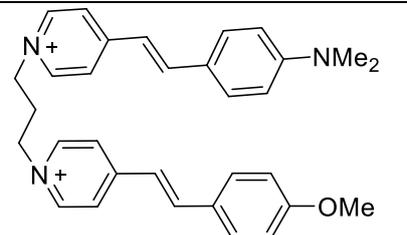
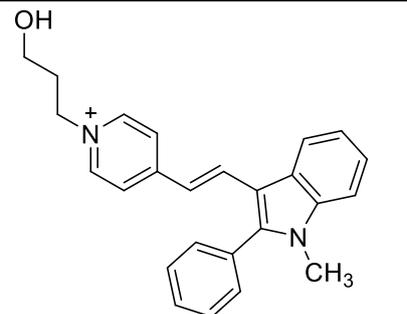
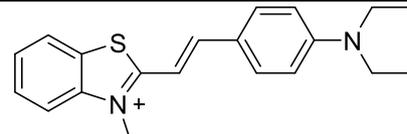
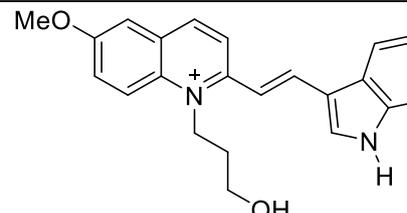
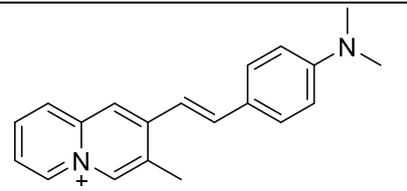
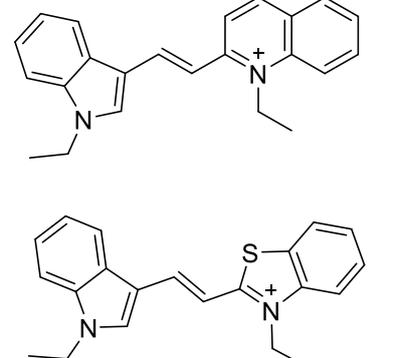


**Figure S3.** IC<sub>50</sub> of styryl dyes in (A, C) normal cells and (B, D) cancer cells, incubated for 24 h.

**Table S1.** MICs of 12 different drugs and our styryl dyes in two bacteria species.<sup>3</sup>

Name of antibiotic	MIC (μg/mL)	
	<i>E. Coli</i>	<i>S. Aureus</i>
Amoxicillin	32	1/8
Ceftiofur	1/8	2
Kamamycin	2	8
Colistin Sulfate	1/8	1
Doxycycline	32	32
A-tartrate	128	2
Florfenicol	2	64
Sulfadimidine	16	8
Enrofloxacin	16	0.5
Rifampicin	4	8
Berberine	512	128
Lincomycin	512	1
Styryl-QL	4	4
Styryl-BT	16	1

**Table S2.** Comparison of our cationic styryl dyes with the previous styryl systems.

structure	Wavelength of detection	Activity	Selectivity	Therapy property	Ref.
	Em= 620 nm	DNA templating	ct-DNA		Journal of Photochemistry and Photobiology A: Chemistry, 2021, 418, 113378.
	Em= 550 nm	DNA staining	dsDNA		Methods and applications in fluorescence, 2015, 3, 044003.
	Em= 599 nm	DNA staining	dsDNA	organelles in stem cells from apical papilla	Molbank 2022, 2022, M1392.
	Em= 558 nm	DNA staining	dsDNA		Organic & Biomolecular Chemistry, 2013, 11, 7458.
	Em= 629 nm	DNA detection	dsDNA	Chemosensor	Sensors and Actuators B: Chemical, 2014, 202, 483.
	Em= 565 and 547 nm	DNA detection	dsDNA, Cancer Cells and Gram-negative Bacteria ( <i>S. aureus</i> )	Yes (anti-cancer and anti-bacteria)	This work

## Reference

1. Q. K. Sun, W. Liu, S. A. Ying, L. L. Wang, S. F. Xue and W. J. Yang, *RSC advances*, 2015, **5**, 73046-73050.
2. K. Liu, Y. Ding and C. Kang, *Pharmaceutical Chemistry Journal*, 2020, **54**, 345-352.
3. B. Yang, Z. Lei, Y. Zhao, S. Ahmed, C. Wang, S. Zhang, S. Fu, J. Cao and Y. Qiu, *Frontiers in Microbiology*, 2017, **8**.