

SI 1: The quantitative experiment spectra for the fluorescent spectra at different concentrations of the investigated drug.



**SI 2:** MFX-induced CPB quenching depicted in the Stern–Volmer graph at three temperature levels.



SI 3: The Modified Stern–Volmer charting for the MFX and CPB stain binding.



SI 4: The charting of log  $\Delta F/F$  to log [M] at operating temperature to determine the binding site(s).



SI 5: Van't Hoff charting for the thermodynamic criteria



SI 6: FTIR spectra of the drug, dye, and newly formed product.

SI 7: A list of equations.

| The equation   | Equ. No. |
|--|----------|
| $f_0/f = 1 + k_{sv}[M] = 1 + k_{q\tau_o}[M]$   | (1)      |
| $k_q = k_{sv} / \tau_o$  | (2)      |
| $f_0 / \Delta f = \left[ \frac{1}{f_a K_a} \right] \left[ \frac{1}{[M]} \right] + 1 / f_a$ | (3)      |
| $\log \frac{(f_0 - f)}{f} = \log k_d + n \log[M]$  | (4)      |
| $\ln K_T = -\Delta H/RT + \Delta S/R$  | (5)      |
| $\Delta G^{\circ} = \Delta H^{\circ} - T \Delta S^{\circ}$                                 | (6)      |

 $F_0$  / F: The relative fluorescence amplitudes of the dye and analyte-dye.

K<sub>SV</sub>: Volmer dynamic suppressing constant.

k<sub>q</sub>: The bimolecular suppressing rate constant.

[M]: the analyte molar concentration.

K<sub>a</sub>: The suppression constant.

F<sub>a</sub>: The initial fluorescence that can be quenched by the quencher.

 $\Delta F :$  The fluorescence difference.

n: The number of linking sites.

R: The gas constant, K<sub>T</sub> is the coupling constant, and T is the temperature (in kelvin scale).

 $\Delta G:$  free energy,  $\Delta S,$  entropy changes, and  $\Delta H$  is enthalpy change.