Block Copolymer and Organic Salts in Forming Aqueous Biphases: A Platform to Identify Molecular Interactions in Aqueous Medium

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Determination of Tie line (TL): Each TL was determined by the lever-arm rule through the relationship between the top phase composition and the overall system composition. For this the following system of four equations (eqns S1 - S4) and four unknown factors were solved.

$$Y_T = Aexp\left[\left(B \times X_T^{0.5}\right) - \left(C \times X_T^3\right)\right]$$
(S1)

$$Y_B = Aexp\left[\left(B \times X_B^{0.5}\right) - \left(C \times X_B^3\right)\right]$$
(S2)

$$Y_T = \left(\frac{Y_M}{\alpha}\right) - \frac{1 - \alpha}{\alpha} \times Y_B \tag{S3}$$

$$X_T = \left(\frac{X_M}{\alpha}\right) - \frac{1 - \alpha}{\alpha} \times X_B \tag{S4}$$

Where T, B, and M, are assigned to the top phase, the bottom phase and the mixture, respectively; X and Y represent the equilibrium weight fraction percentages of the salt and tri block copolymer; α is the ratio between the mass of the top phase and the total mass of the mixture. Each tie-line length (TLL) and slope of the tie-lines (STL) could be obtained using the following equations:

$$TLL = \sqrt{(X_T - X_B)^2 + (Y_T - Y_B)^2}$$
(S5)

$$STL = (Y_T - Y_B) / (X_T - X_B)$$
(S6)



Figure S1: Othmer-Tobias plot of PPG-PEG-PPG – sodium acetate system.



Figure S2: Bancroft plot of PPG-PEG-PPG – sodium acetate system.



Figure S3: Othmer-Tobias plot of PPG-PEG-PPG – sodium citrate system.



Figure S4: Bancroft plot of PPG-PEG-PPG – sodium citrate system.



Figure S5: Fluorescence quenching plot of PPG-PEG-PPG



Figure S6: Plot for obtaining aggregation number of PPG-PEG-PPG



Figure S7: Fluorescence quenching plot of PPG-PEG-PPG obtained from PPG-PEG-PPG/ Na-acetate ABS.



Figure S8: Fluorescence plot for aggregation number of PPG-PEG-PPG from PPG-PEG-PPG acetate ABS.



Figure S9: Fluorescence quenching plot of PPG-PEG-PPG obtained from PPG-PEG-PPG/ Na-citrate ABS.



Figure S10: Fluorescence plot for aggregation number of PPG-PEG-PPG from PPG-PEG-PPG citrate ABS.



Figure S11: Absorbance spectrum of thiamine in polymer medium.



Figure S12: Absorbance spectrum of riboflavin in polymer medium.



Figure S13: Absorbance spectrum of cholecalciferol in polymer medium.



Figure S14: Absorbance spectrum of caffeine in polymer medium.



Figure S15: Multi-wavelength linear regression plot of caffeine and vitamin D mixture at pH 5.



Figure S16: Multi-wavelength linear regression plot of caffeine and vitamin D mixture at pH 5.5.



Figure S17: Multi-wavelength linear regression plot of caffeine and vitamin D mixture at pH 6.5.



Figure S18: Multi-wavelength linear regression plot of caffeine and vitamin D mixture at pH 7.5.



Figure S19: Multi-wavelength linear regression plot of caffeine and vitamin D mixture at pH 8.5.



Figure S20: ¹H NMR spectral study of inter molecular interactions (a) caffeine (b) cholecalciferol (c) caffeine+ cholecalciferol



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Figure S21: ESI MS study of inter molecular interactions (a) caffeine (b) cholecalciferol (c) caffeine+ cholecalciferol