Cosolubilization of phenanthrene and pyrene in surfactant micelles: experimental and atomistic simulations studies

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Methods to compute $K_m$ for single and mixed PAH solubilization systems

Detailed methods to compute $K_m$ for single and mixed PAH solubilization systems are described as below.

The micelle-water partition coefficient, $K_m$, a thermodynamic parameter that represents the affinity of a given solubilize within the micellar phase, can be expressed by the following equations[1, 2]:

\[ K_m = \frac{55.4 \times \text{MSR}}{S_{\text{CMC}} \times (1 + \text{MSR})} \]  \hspace{1cm} (S1)

For cosolubilization, partition coefficient of the PAH$_i$ in the presence of the PAH$_j$, $K_{mi}$, is given by with the following relation [1]:

\[ K_{mi} = \frac{55.4 \times \text{MSR}_i}{S_{\text{CMC}} \times (1 + \text{MSR}_i + \text{MSR}_j)} \]  \hspace{1cm} (S2)
Fig. S1 Radius of gyration of the micelle-PAH complexes in System I as a function of the simulation time. PYR and PHE are abbreviations for pyrene, and phenanthrene, respectively.

Fig. S2 Radius of gyration of the micelle and micelle-PAH complexes in Systems II and III as a function of the simulation time. PYR and PHE are abbreviations for pyrene, and phenanthrene, respectively.
Fig. S3 Instantaneous distance between the center of mass (COM) of (a) phenanthrene (PHE)/(b) pyrene (PYR) and micelle as function of time in System III.
Fig. S4 Enhanced solubility of phenanthrene (PHE) and pyrene (PYR) as individual compounds and their respective binary mixtures in TX. Symbols represent experimental values, and lines represent linear regression. The error bars stand for the standard deviation of the triplicate samples at each concentration and are, in most cases, smaller than the symbols.
Fig. S5 Enhanced solubility of phenanthrene (PHE) and pyrene (PYR) as individual compounds and their respective dual mixtures in TX/SDS (1/1) mixed surfactant systems. Symbols represent experimental values, and lines represent linear regression. The error bars stand for the standard deviation of the triplicate samples at each concentration and are, in most cases, smaller than the symbols.
Fig. S6 Enhanced solubility of phenanthrene (PHE) and pyrene (PYR) as individual compounds and their respective dual mixtures in TX/SDS (2/3) mixed surfactant systems. Symbols represent experimental values, and lines represent linear regression. The error bars stand for the standard deviation of the triplicate samples at each concentration and are, in most cases, smaller than the symbols.
Fig. S7 Enhanced solubility of phenanthrene (PHE) and pyrene (PYR) as individual compounds and their respective dual mixtures in SDS surfactant systems. Symbols represent experimental values, and lines represent linear regression. The error bars stand for the standard deviation of the triplicate samples at each concentration and are, in most cases, smaller than the symbols.
Fig. S8 Normalized probability distribution of the distance between the center of mass (COM) of phenanthrenes (PHEs)/pyrenes (PYRs) in Systems I and III. The legends from top and down mean the distance distribution of two PHEs, two PYRs and mixed PHE-PYR in each panel.
Fig. S9 Distribution of dimer angle ($\theta$) as a function of dimer distance for (a) phenanthrene (PHE), (b) pyrene (PYR) and (c) PHE-PYR in System I.
Fig. S10 Distribution of dimer angle (θ) as a function of dimer distance for (a) phenanthrene (PHE), (b) pyrene (PYR) and (c) PHE-PYR in System III.

References