Electronic Supplementary Information (ESI)

Probing Solvent-Solvent and Solute-Solvent Interactions in Surfactant Binary Mixtures: Solvatochromic Parameters, Preferential Solvation, and Quantum Theory of Atoms in Molecules Analysis

*Mona Kohantorabi, Mostafa Fakhraee, Hadi Salari, Mohammad Reza Gholami**

Department of Chemistry, Sharif University of Technology,
Tehran, 11365-11155, Iran

(*Corresponding author e-mail: gholami@sharif.edu)

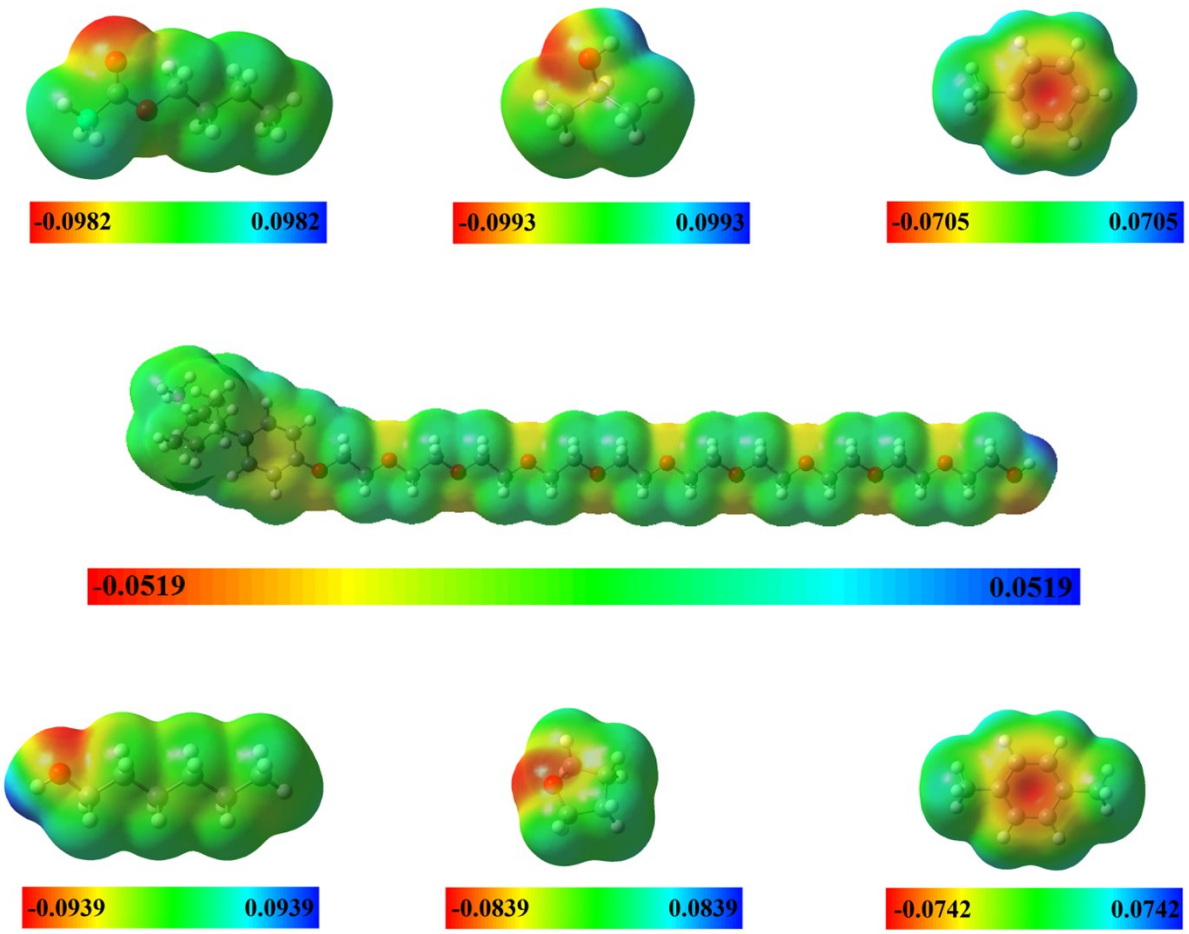

Figure S1. Electrostatic potential map (ESP) of Butyl acetate, 2-Propanol, Hexanol, THF, p-Xylene, Toluene, and TX-100 accompanied with their charge variation.

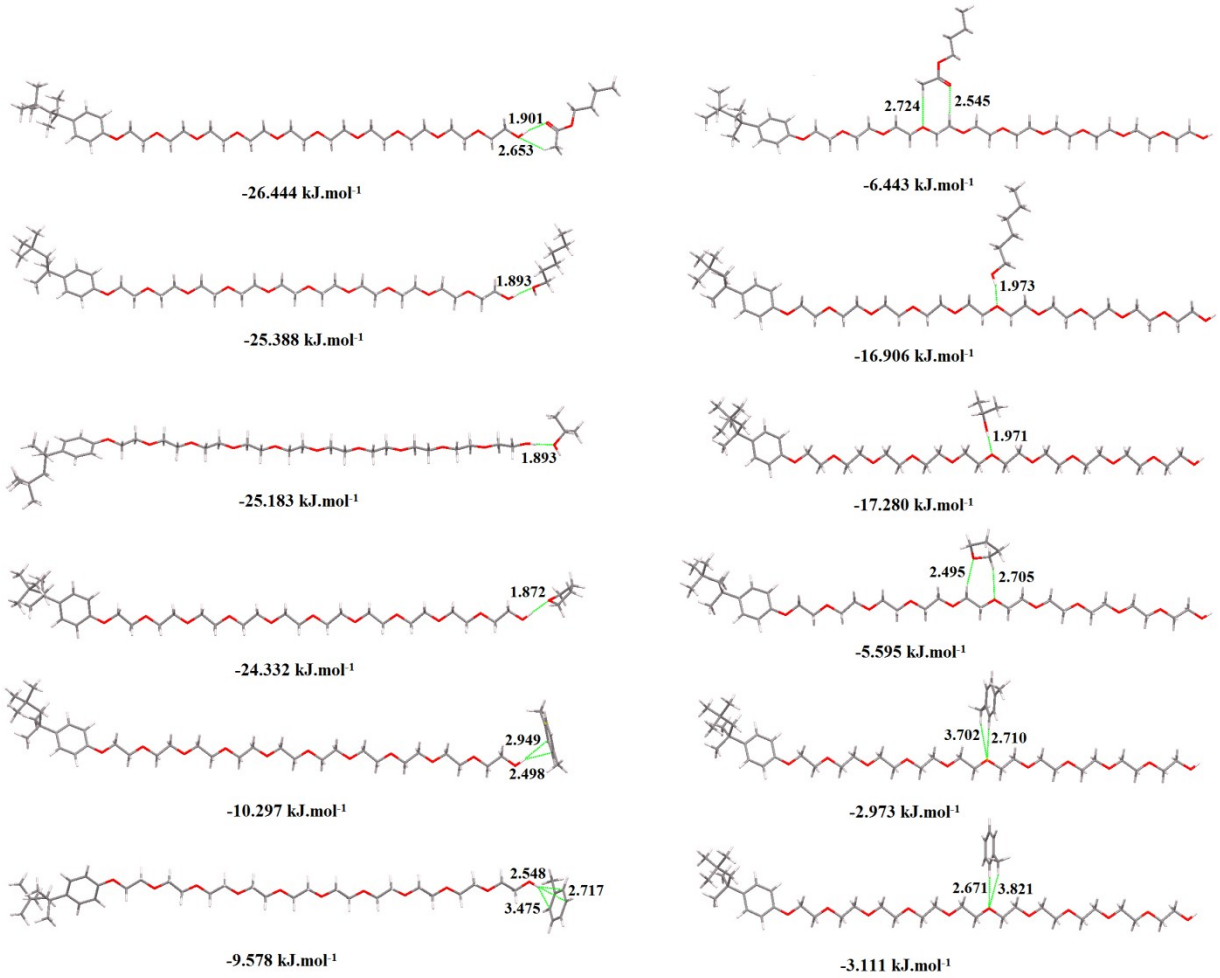

Figure S2. The optimized geometries of Butyl acetate/TX-100, Hexanol/TX-100, 2-Propanol/TX-100, THF/TX-100, p-Xylene/TX-100, and Toluene/TX-100 in binary mixtures accompanied with their interaction energies. The strong interactions are shown by dot line and distances are in Å.

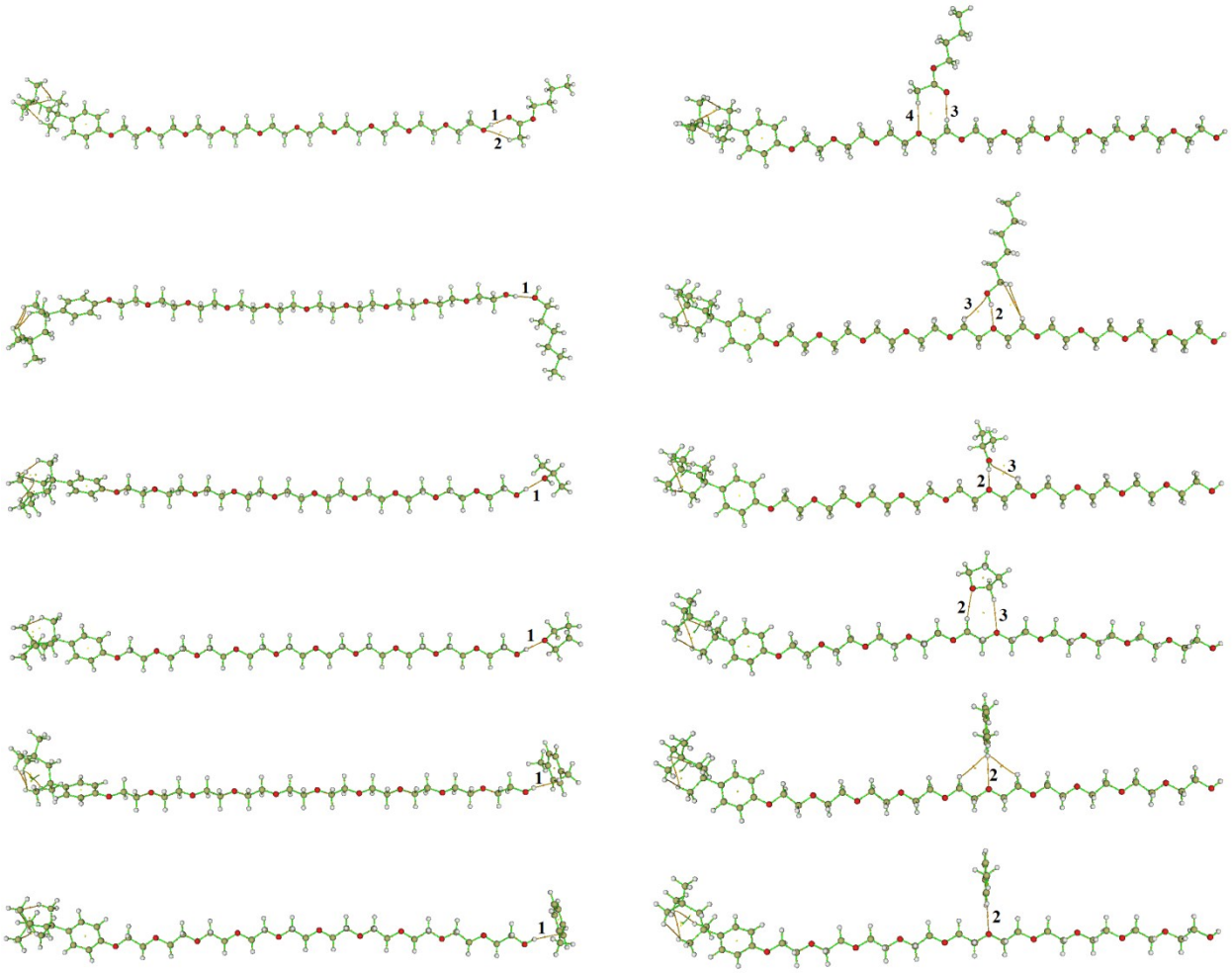

Figure S3. BCPs (in orange color), CCPs (in yellow color), and RCPs (in yellow color) of optimized structures for Butyl acetate/TX-100, Hexanol/TX-100, 2-Propanol/TX-100, THF/TX-100, p-Xylene/TX-100, and Toluene/TX-100 binary mixtures, performing at the B3LYP/6-311++G(d,p) level.

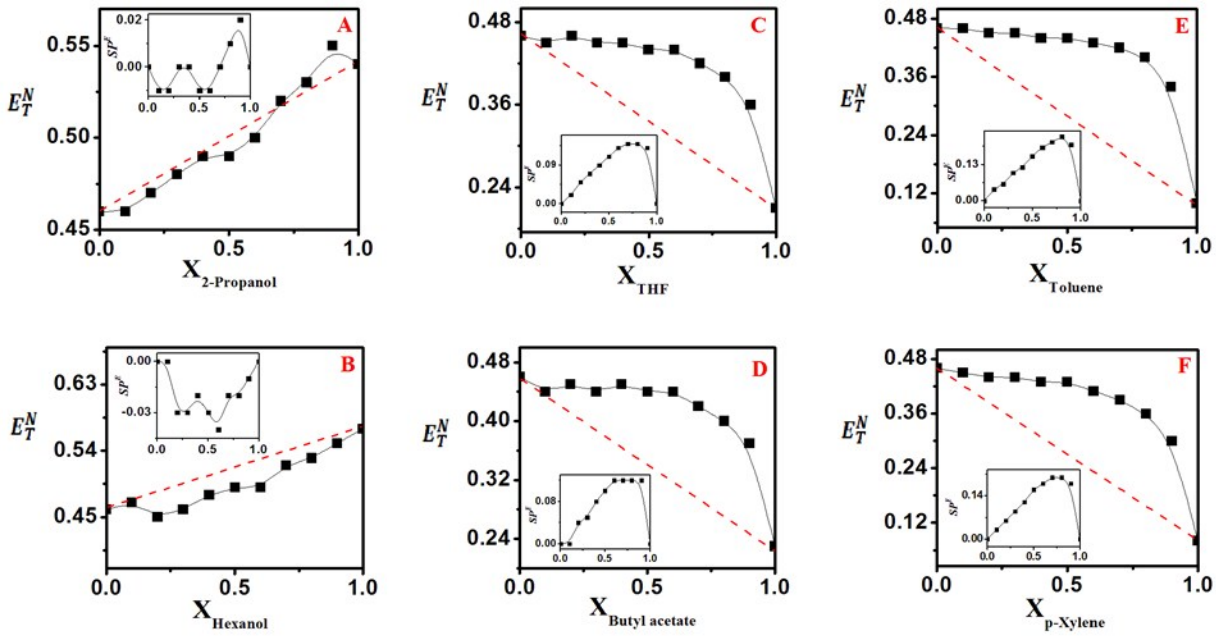

Figure S4. Variation in E_T^N and excess solvatochromic parameters (SP^E) with $X_{Solvent}$ in molecular solvents/TX-100 binary mixtures at ambient condition.

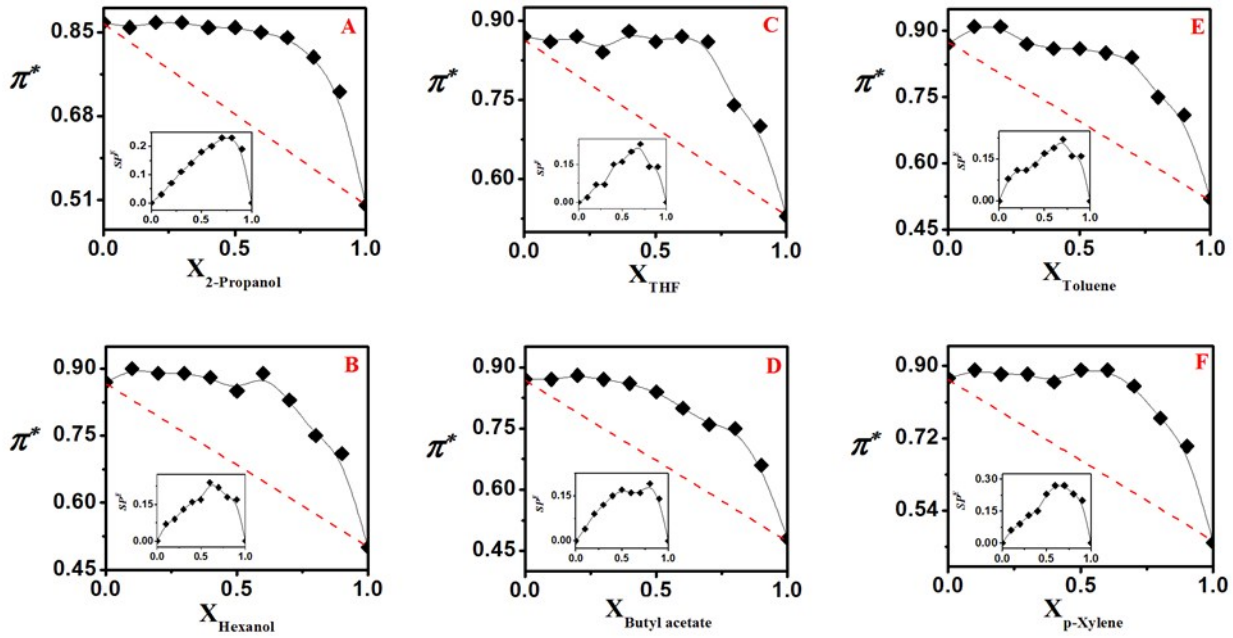

Figure S5. Variation in π^* and excess solvatochromic parameters (SP^E) with $X_{Solvent}$ in molecular solvents/TX-100 binary mixtures at ambient condition.

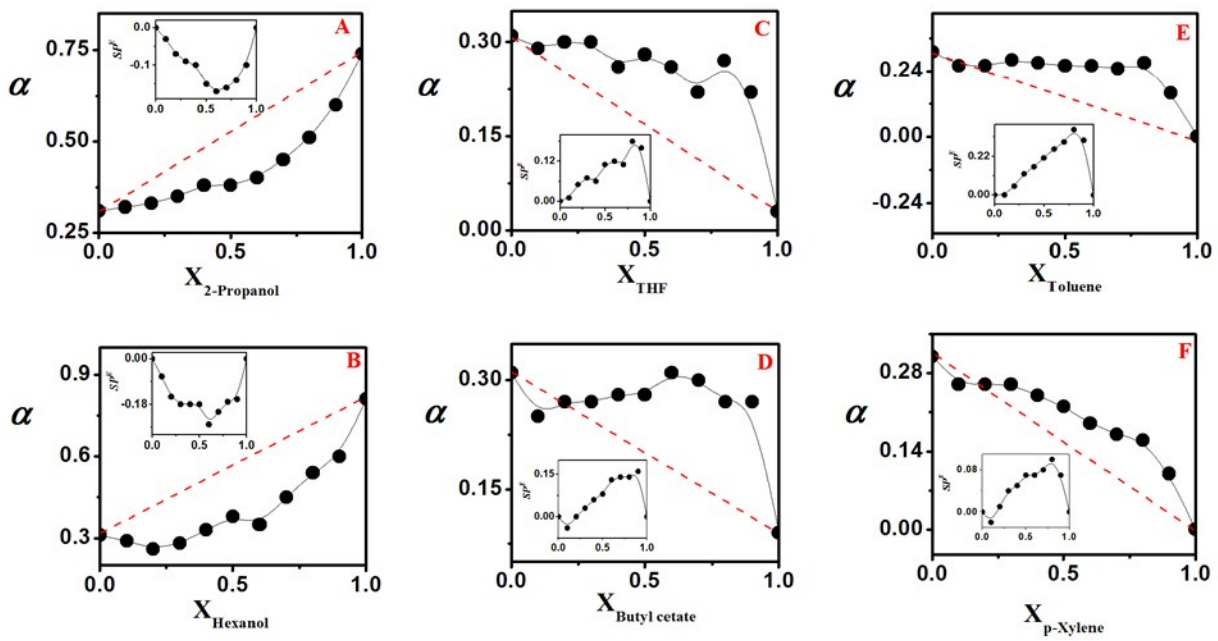

Figure S6. Variation in α and excess solvatochromic parameters (SP^E) with $X_{Solvent}$ in molecular solvents/TX-100 binary mixtures at ambient condition.

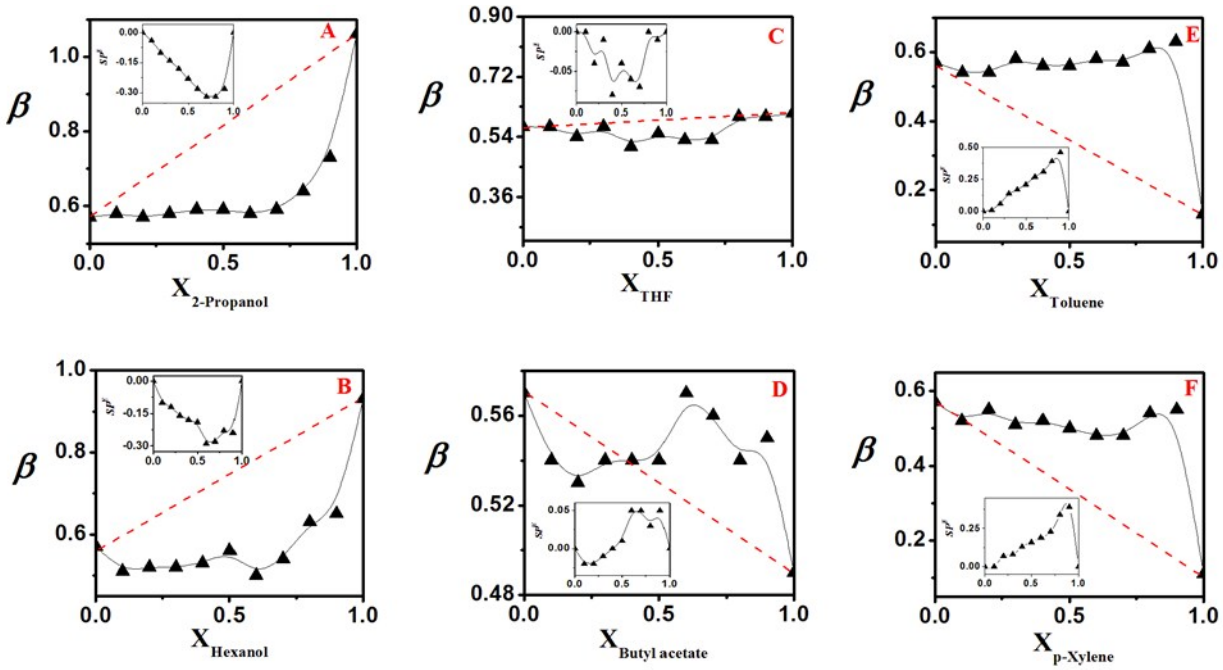

Figure S7. Variation in β and excess solvatochromic parameters (SP^E) with $X_{Solvent}$ in molecular solvents/TX-100 binary mixtures at ambient condition.