Supplementary Materials

Molecular Dynamics Simulation of Drug Solubilization Behavior in Surfactant and Cosolvent Injections

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Table S1. The significance test between the number of hydrogen bonds between water–water (per water) in formulations without cosolvents and the formulations containing cosolvents.

Systems	$\bar{x} \pm S$	95% CI	P (Student's t-Test)	P (Mann–Whitney U Test)
Cyc [1]	2.4292+_0.0066	0.0058~0.0139	<0.001	<0.001
Cyc [2]	2.4194+_0.0089			
Doc [1]	2.4505+_0.0046	0.0113~0.0163	<0.001	<0.001
Doc [2]	2.4367+_0.0050			
Eto [1]	2.4597+_0.0039	−0.0003~0.0041	0.093	0.050
Eto [2]	2.4578+_0.0046			
Pac [1]	2.4284+_0.0064	0.0602~0.0668	<0.001	<0.001
Pac [2]	2.3649+_0.0062			
Val [1]	2.2791+_0.0166	0.0591~0.0851	<0.001	<0.001
Val [2]	2.2070+_0.0311			
Cab [1]	2.4790+_0.0029	0.0023~0.0053	<0.001	<0.001
Cab [2]	2.4752+_0.0029			

[1] The system without cosolvents. [2] The system with cosolvents.

Table S2. The significance test between the average R_g values of different systems without cosolvents and containing cosolvents during the last 30 ns simulation time.

Systems	$\bar{x} \pm S$	95% CI	P (Student's t-Test)	P (Mann–Whitney U Test)
Cyc [1]	15.68 ± 0.43	−0.53~−0.50	<0.001	<0.001
Cyc [2]	16.20 ± 0.80			
Doc [1]	17.90 ± 0.65	−0.22~−0.19	<0.001	<0.001
Doc [2]	18.10 ± 0.50			
Eto [1]	9.52 ± 0.78	−0.90~−0.84	<0.001	<0.001
Eto [2]	10.38 ± 1.20			
Pac [1]	28.53 ± 2.26	−7.13~−7.05	<0.001	<0.001
Pac [2]	35.62 ± 1.10			
Val [1]	14.19 ± 0.54	−0.50~−0.48	<0.001	<0.001
Val [2]	14.68 ± 0.49			
Cab [1]	17.80 ± 0.63	−0.17~−0.15	<0.001	<0.001
Cab [2]	17.96 ± 0.42			

[1] The system without cosolvents. [2] The system with cosolvents.