

Study of Interfacial Properties of Anionic–Nonionic Surfactants Based on Succinic Acid Derivatives via Molecular Dynamics Simulations and the IGMH Method

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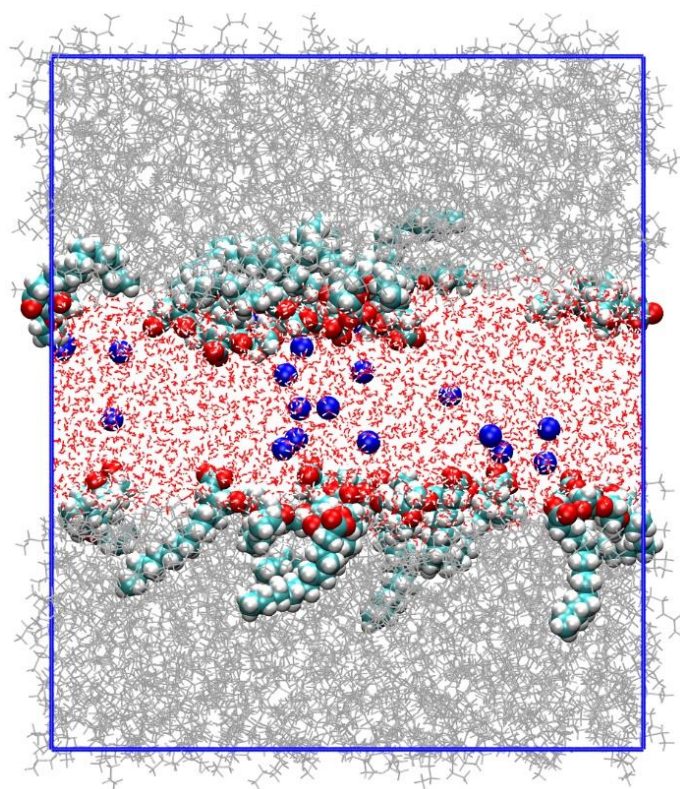
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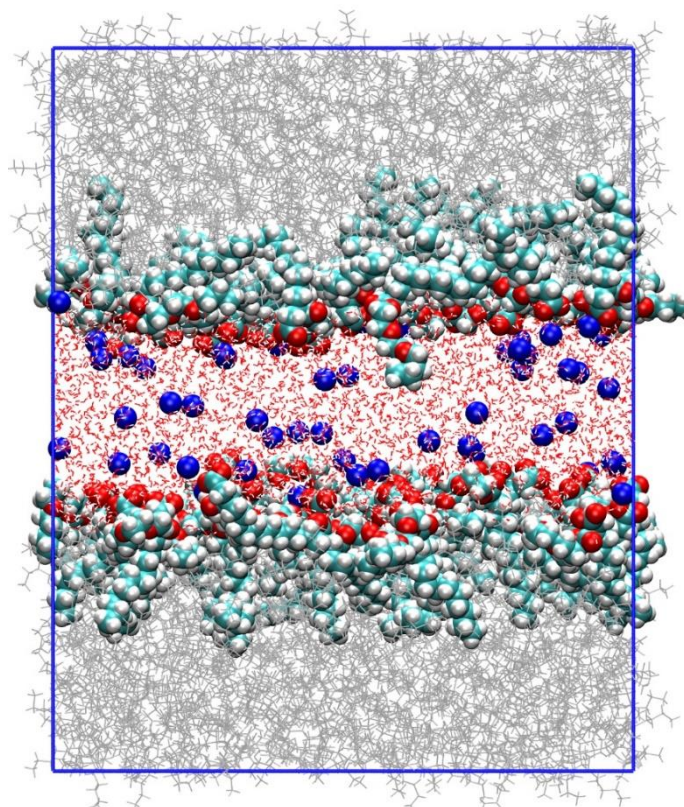
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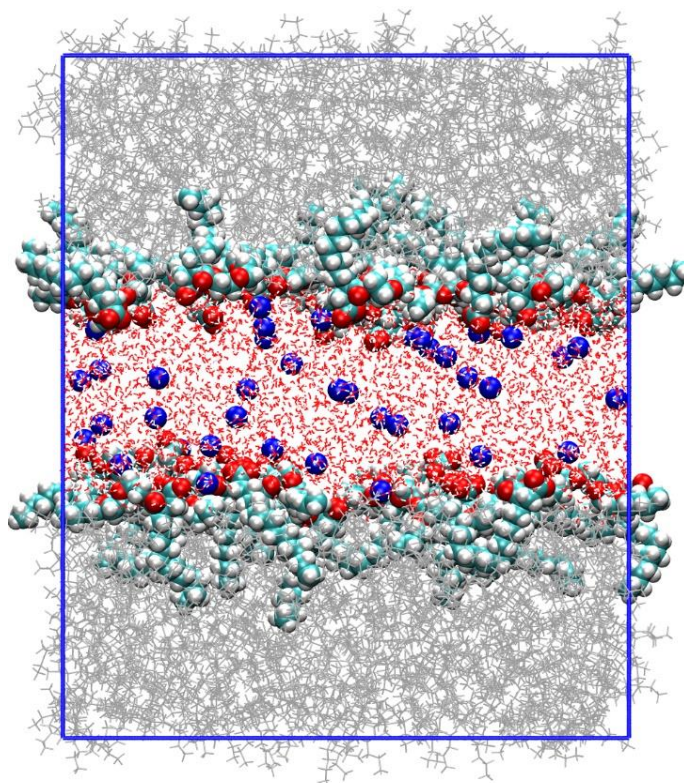
Table s1 Number of molecules for each component in the MD model

	BEMA	DTOA
	oil/surfactant/water	oil/surfactant/water
20	800/20/4000	800/20/4000
40	800/40/4000	800/40/4000
60	800/60/4000	800/60/4000
80	800/80/4000	800/80/4000
100	800/100/4000	800/100/4000
120	800/120/4000	800/120/4000
140	800/140/4000	800/140/4000
160	800/160/4000	800/160/4000
180	800/180/4000	-
200	800/200/4000	-

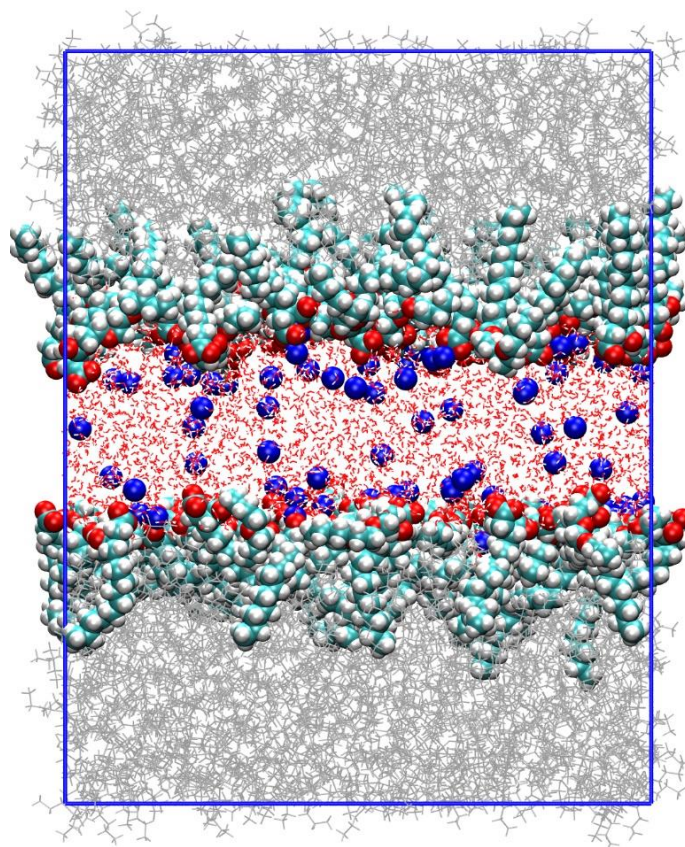
**20 BEMA**



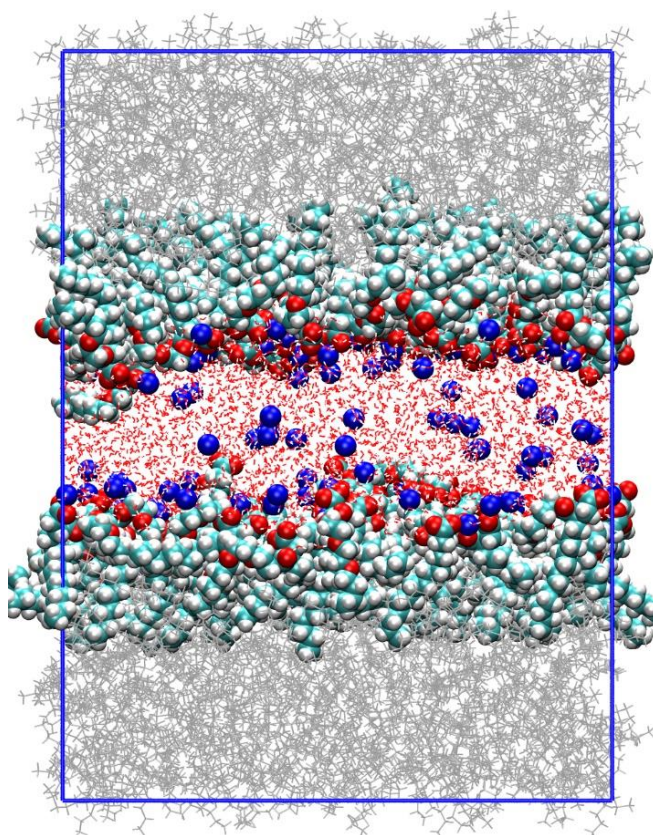
40 BEMA



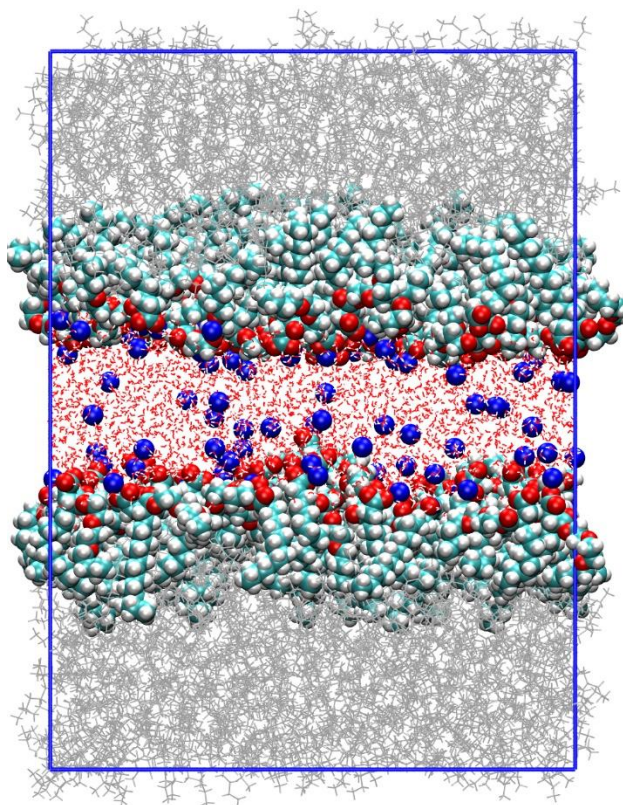
60 BEMA



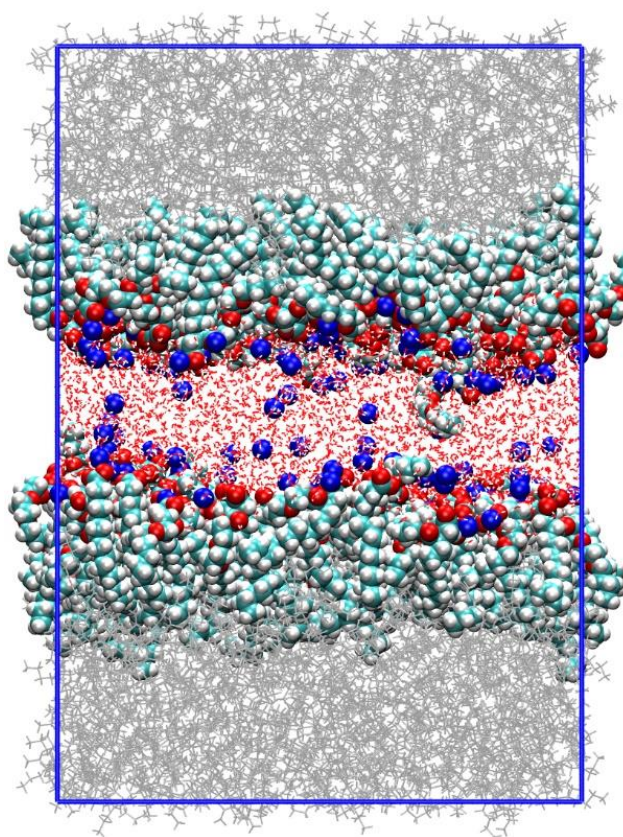
80 BEMA



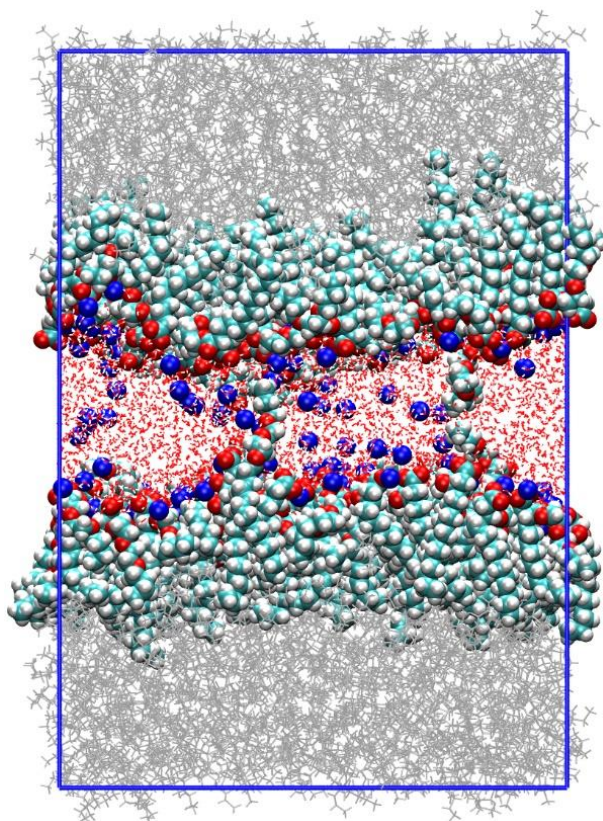
100 BEMA



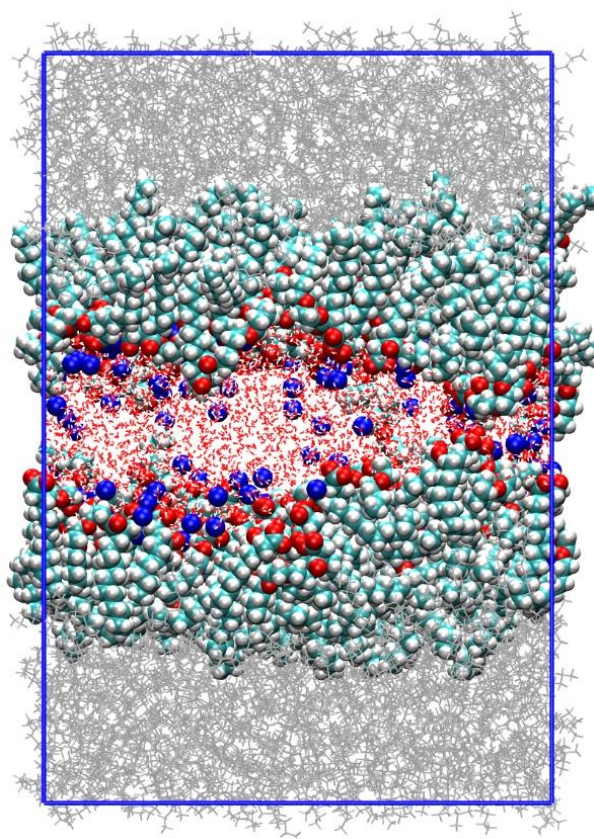
120 BEMA



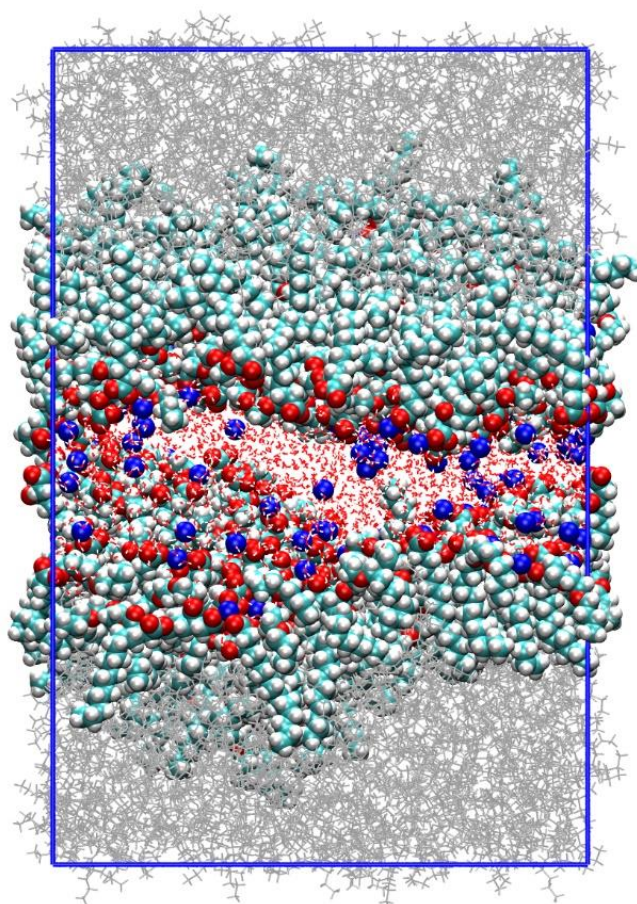
140 BEMA



160 BEMA

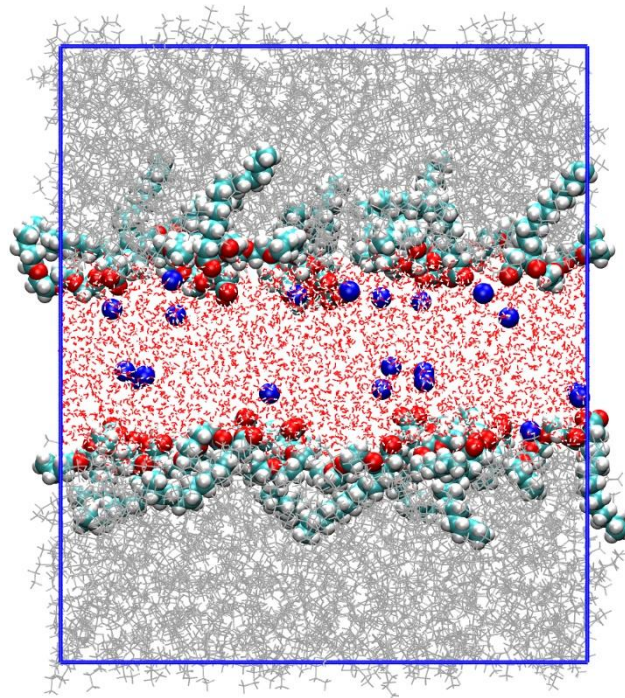


180 BEMA

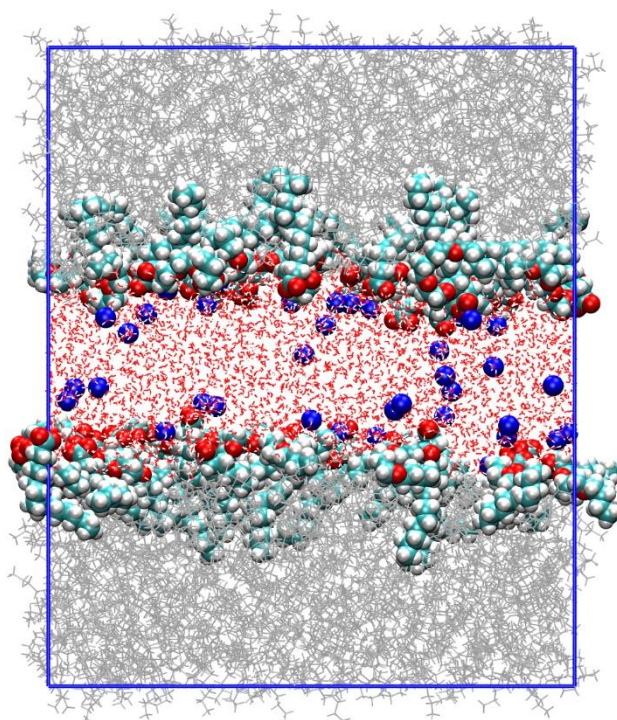


200 BEMA

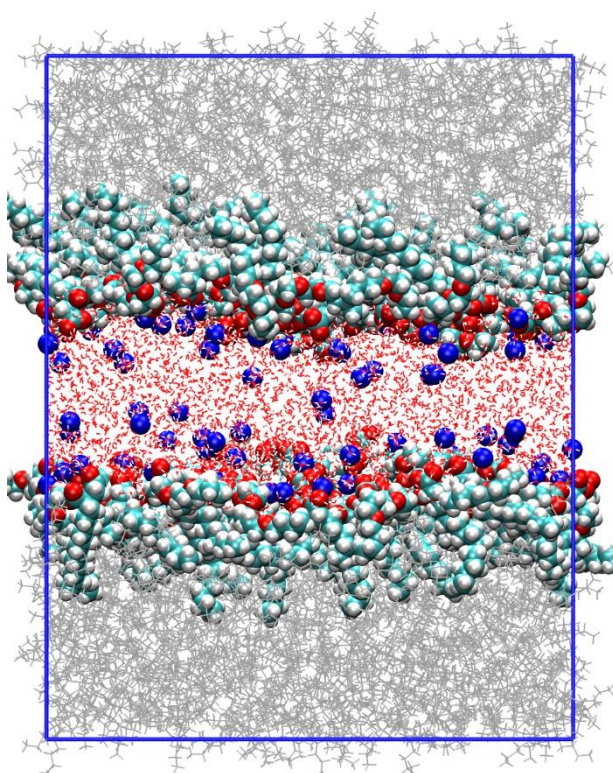
Figure s1 Snapshots of the equilibrium state of MD simulations with different concentrations of BEMA, grey lines were used to represent oil, blue balls to describe sodium ions, red dots to mean water molecules and surfactant molecules were represented using three colors (red balls for oxygen atoms, white balls for hydrogen atoms, and cyan balls for carbon atoms).



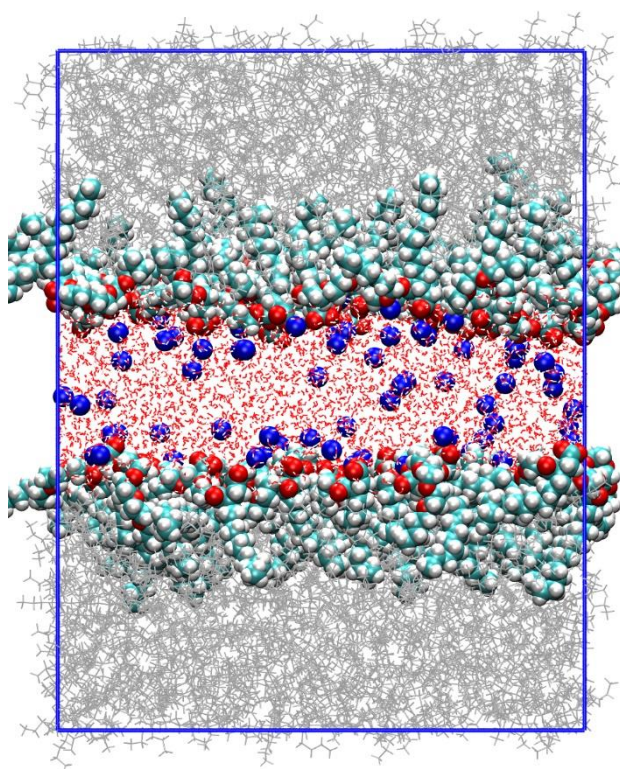
20 DTOA



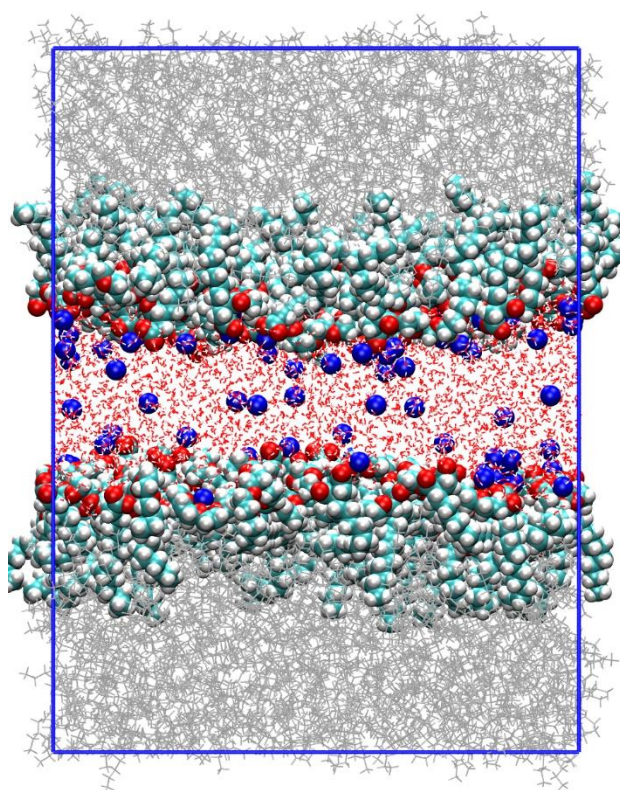
40 DTOA



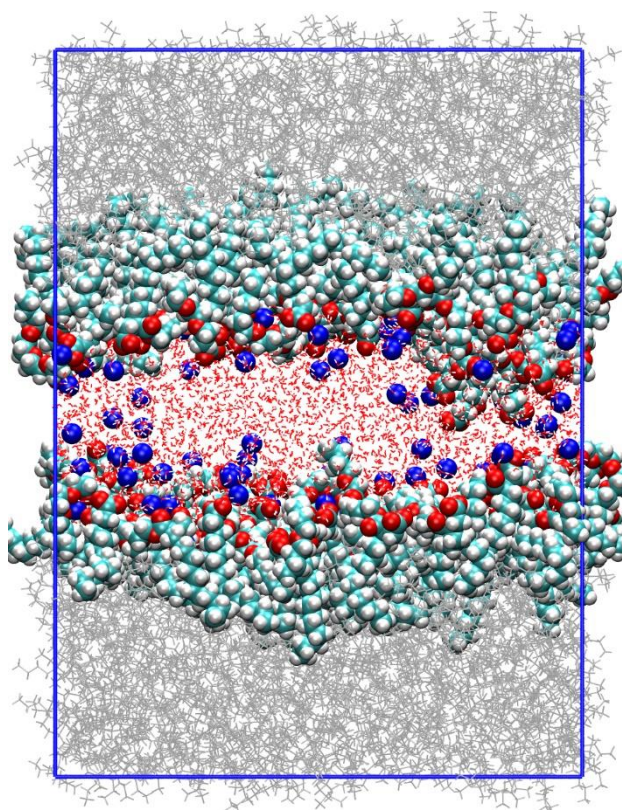
60 DTOA



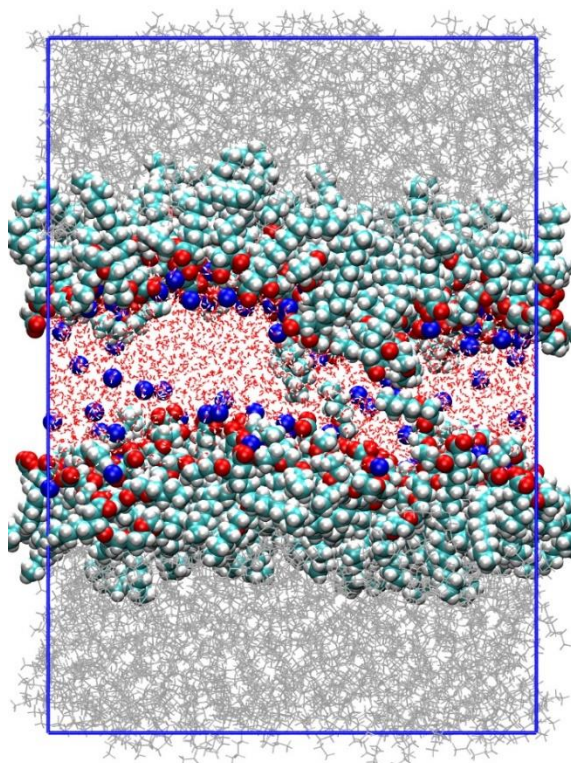
80 DTOA



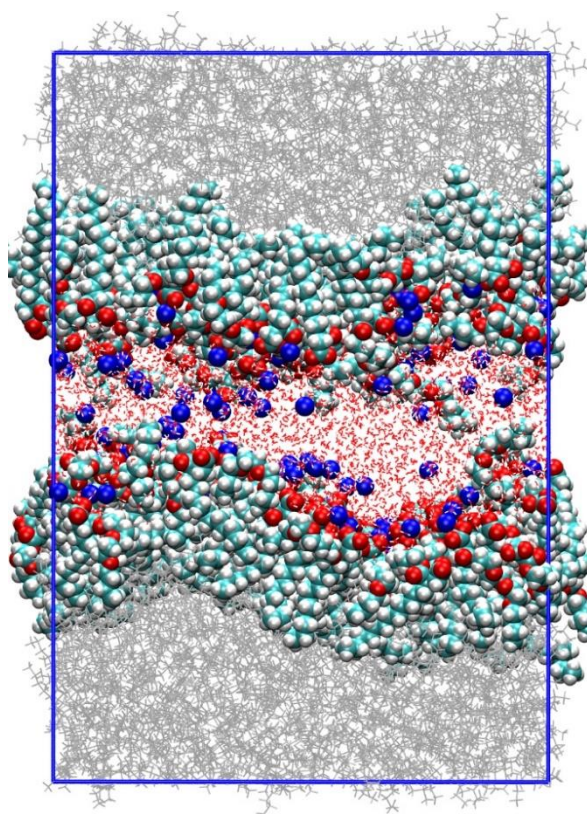
100 DTOA



120 DTOA



140 DTOA



160 DTOA

Figure s2 Snapshots of the equilibrium state of MD simulations with different concentrations of **DTOA**, grey lines were used to represent oil, blue balls to describe sodium ions, red dots to mean water molecules and surfactant molecules were represented using three colors (red balls for oxygen atoms, white balls for hydrogen atoms, and cyan balls for carbon atoms).