

Understanding the Conformational Preference of Tenside Surfactants

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Surfactants are agents that are used to lower the surface tension of a liquid or the interfacial tension between two liquids. Often, surfactants are amphiphilic molecules, containing both greasy non-polar regions as well as polar regions. Here, the conformational preferences for a few novel surfactants will be presented.

Conformational searching was used to evaluate the surfaces of the molecules. Clustering was performed to evaluate the resulting ensembles, and quantum mechanics was used to verify the low energy structures that resulted.

