Solubilization of phenol and butanol by cationic surfactant micelles - molecular dynamic study

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Solubilization phenomenon has attracted attention and interest of many researchers over decades. This attention is due to a broad range of solubilization applications in biological, pharmaceutical and industrial processes. Despite the experimental and theoretical work, some aspects of the phenomenon remain poorly understood. One of the theoretical approaches to study surfactant micelles is using a realistic model of water and surfactant molecules (all atom simulations). The AA simulations provide detailed information of micelle structure i.e. radius of gyration, area per headgroup, etc. and are a promising way of micelle structure with solubilizate studies. In this work, all atom molecular dynamic simulations of hexadecyltrimethylammonium bromide (HTAB) in the presence of phenol and butanol molecule are presented. The simulations were performed for the systems with different solubilizate:surfactant and phenol:butanol:surfactant ratios.