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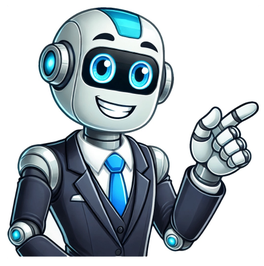

To better understand how different solvents influence the behavior of cholesterol, researchers conducted molecular dynamics simulations on the molecule in four various solvents: water, methanol, dimethyl sulfoxide, and benzene. Their main focus was on analyzing how the hydrophilic and hydrophobic parts of cholesterol interact with these solvents. The study found that both types of groups were interacting with some solvents, such as methanol and dimethyl sulfoxide, which exhibit polar and non-polar interactions. In contrast, water showed extreme behavior due to hydrogen bonding with the hydroxyl group, while benzene formed strong van der Waals interactions only. The researchers also looked at how the hydrophobic effect of cholesterol affected its solubility in different solvents. They discovered that the hydrophobic character was more pronounced in polar environments, which limited solvent mobility in the solvation layer. Furthermore, they analyzed the dynamical properties of cholesterol, such as lateral diffusion and hydrogen bond dynamics, as well as free energies of solvation. Their results suggested that the polarity of the solvents significantly influenced cholesterol's aggregation properties. Notably, they found that highly polar solvents like water facilitated the aggregation of cholesterol. This is particularly important from a clinical perspective due to its role in cardiovascular diseases. The mass fraction of ethanol in the solvent mixture was found to be approximately 10%. In terms of solubility, cholesterol exhibits greater affinity for methyl isobutyl ketone (MIBK), ethyl acetate, and anisole compared to methanol, heptane, and acetic acid. The experimental solubilities were correlated with various models, including the van't Hoff, modified Apelblat, Yaws, van’t Hoff–Jouyban–Acree, and modified UNIQUAC models. Among these, the modified UNIQUAC model provided a better fit to the data, exhibiting an average relative error (ARD) of less than 9%. In contrast, the other models showed ARD values below 12%. Note: The text has been paraphrased while maintaining its original content and language.

Cholesterol solubility in ethanol.  Cholesterol solubility in water.