

Implicit solvation



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Reviews

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(Mitchell Kuhn III)

IMPLICIT SOLVATION



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Alphascript Publishing Dez 2009, 2009. Taschenbuch. Condition: Neu. Neuware - Implicit solvation is a method of representing solvent as a continuous medium instead of individual explicit solvent molecules most often used in molecular dynamics simulations and in other applications of molecular mechanics. The method is often applied to estimate free energy of solute-solvent interactions in structural and chemical processes, such as folding or conformational transitions of proteins, DNA, RNA, and polysaccharides, association of biological macromolecules with ligands, or transport of drugs across biological membranes. The implicit solvation model is justified in liquids, where the potential of mean force can be applied to approximate the averaged behavior of many highly dynamic solvent molecules. However, the interiors of biological membranes or proteins can also be considered as media with specific solvation or dielectric properties. These media are continuous but not necessarily uniform, since their properties can be described by different analytical functions, such as polarity profiles of lipid bilayers 68 pp. Englisch.



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