Poster Presentation

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Application of 3D-RISM to Water Placement

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Increasingly there is significant interest in understanding the behavior of water as it relates to ligand-receptor interactions. Ligand affinity and specificity appear to be influenced by the action of water molecules on the solvated ligand-receptor complex. As such, the ability to predict the location of water molecules is of significant importance. Here we apply 3D-RISM to elucidate the placement of water molecules given the solute 3D coordinates. A sum-of-Gaussians techniques is used to infer the water sites from the particle density calculated from 3D-RISM. The results of several computational experiments will be presented and discussed.

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