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Accurate prediction of explicit solvent atom distribution in HIV-1 protease and F-ATP synthase by statistical theory of liquids DANIEL SINDHIKARA, NORIO YOSHIDA, FUMIO HIRATA, Institute for Molecular Science — We have created a simple algorithm for automatically predicting the explicit solvent atom distribution of biomolecules. The explicit distribution is coerced from the 3D continuous distribution resulting from a 3D-RISM calculation. This procedure predicts optimal location of solvent molecules and ions given a rigid biomolecular structure. We show examples of predicting water molecules near KNI-275 bound form of HIV-1 protease and predicting both sodium ions and water molecules near the rotor ring of F-ATP synthase. Our results give excellent agreement with experimental structure with an average prediction error of 0.45-0.65 angstroms. Further, unlike experimental methods, this method does not suffer from the partial occupancy limit. Our method can be performed directly on 3D-RISM output within minutes. It is useful not only as a location predictor but also as a convenient method for generating initial structures for MD calculations.

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