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Incorporation of a hydration layer in the ab initio modeling of Biological Macromolecules using Small Angle Scattering data.

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Abstract:
Ab initio algorithms for the restoration of bio-macromolecular structure from small angle scattering data, have gained increasing popularity in the last 15 years. Especially ”dummy atom” models that require minimal information about the system under study have been proven capable of recovering the low- resolution shape of proteins and nucleic acids in many published works. However consideration of solvated biological molecules as particles of uniform electron or scattering length density contrast relative to the solvent, neglects the presence of an inherent hydration layer around their surface, leading to an overall apparent swelling of the obtained models and to a large overestimation of the particle’s volume. By the development of a new algorithm [*Koutsioubas & Perez, J. Appl. Cryst. 46, 1884*] we address this problem by the introduction of an additional type of ”dummy atoms” representing the hydration layer. Successful applications of this new approach are illustrated for several proteins while the complementarity of treating x-ray and neutron scattering data is discussed.

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