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Title (English)

Implementation of a generalized Born/surface area algorithm for solvation energy calculations in the molecular dynamics program *Q*

Title (Swedish)

Abstract

The generalized Born/surface area (GB/SA) method for calculating free energies of solvation was implemented in the molecular dynamics program package Q. The implementation is based on an analytical method for calculating Born radii and the Linear Combination of Pairwise Overlaps (LCPO) algorithm for calculating solvent accessible surface areas. A set of nine molecules, ranging in size from 6 to 1029 atoms, was used to test the implementation against the results from similar studies and experimentally determined energies. Using this test set of molecules, the GB/SA implementation in Q produces solvation energies with an average unsigned error of 0.99 kcal mol^{-1}, to be compared with a reported implementation with an average unsigned error of 1.06 kcal mol^{-1}.

Keywords

Computer simulations, molecular dynamics, solvation energy, generalized Born equation, solvent accessible surface area

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