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Title (English)

Proton binding in proteins: pK_a calculations with explicit and implicit solvent

Title (Swedish)

Abstract

Accurate and reliable pK_a prediction is of significant interest, because it provides direct information of the protonation state of a protein and can be compared to experimental data. In this work pK_a shifts of three aminoacids in proteins have been calculated using molecular dynamics free energy simulations with an explicit solvent and implicit Generalized Born solvent model. The direction of the shifts were correctly predicted in both the explicit and implicit solvent calculations, but the results were not in perfect agreement with experimental data.

Keywords

Proton binding, pK_a, free energy calculations, molecular dynamics

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