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Title (English)

Relating surface potentials to cation and anion exchange retention of proteins

Title (Swedish)

Abstract

This work reports the development of a new program (SCARP) for the calculation of electrostatic potentials in proteins. The program is based on the linearized Poisson-Bolzmann equation and takes protein structure (PDB) files as input. Several electrostatic potentials are calculated by the program. Among these, the average surface potential has been used as a descriptor for the modelling of ion exchange chromatography. For cation exchange, previously published results describing a clear relation between average surface potentials and retention times have been reproduced and extended to a wider set of proteins. For some proteins, the same principles seem to apply also for anion exchange chromatography, whereas for other proteins this is not the case.

Keywords

Electrostatic potential, Poisson-Bolzmann equation, ion-exchange chromatography, proteins

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