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ACCOUNTING FOR THE ANISOTROPY OF ELECTROSTATIC POTENTIAL OF HETEROATOMS IN DRUG DESIGN

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The systematic development of force fields and especially of their electrostatic components is one of the important tasks to improve the prediction quality of structural and energetic parameters for ligand biotarget interactions, which are key factors for successful modeling of the biological activity of molecules. The classical force fields presently used involve mainly the isotropic atomic potential approximation to model the electrostatic interactions. However further refinement of the interaction picture within the new generation force fields requires the anisotropic atom model to account for more subtle effects. The multipole expansion is one of the standard approaches to the description of anisotropy in properties. It permits the systematic improvement of a model until the required accuracy is reached.

The multipole anisotropy models were developed for halogen and sulfur atoms to reproduce the effects of halogen and chalcogen bonding. The suggested model was successfully applied, e.g. for the reproduction of solvation free energy differences in a series of halo substituted compounds. Currently we are developing similar approaches for the description of atoms of nitrogen and phosphorus as the most important organogenic elements. The systematic character of the model building approach allows its use within the commonly approved drug design protocols.

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