
Title: Improved Modeling of Halogenated Ligand-Protein Interactions using the Drude Polarizable and CHARMM Additive Empirical Force Fields.

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Abstract: Halogenated ligands can participate in nonbonding interactions with proteins via halogen bonding. Here, we evaluate the use of two empirical force fields, the Drude polarizable force field and the CHARMM additive force field, for this type of interaction. The Drude force field is based on the Drude model and is designed to properly capture nonbonding interactions in liquid water. The CHARMM force field is widely used for protein simulations, but it has not been explicitly designed to handle halogen-bonding interactions. The Drude force field provides clear improvement over the CHARMM force field, particularly for interactions of iodinated compounds.

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