# Hybrid Solvent Model for Ncd-Tubulin Ion Interactions

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## Abstract

Ncd proteins in Drosophila are motor proteins essential for spindle organization during cell division. Investigating the interactions between Ncd and tubulin dimers in the presence of ions is critical due to their highly charged nature. By using multi-scale computational approach, including Molecular Dynamics (MD) simulations, a machine learning-based Hybridizing Ions Treatment-2 (HIT-2) program, DelPhi, and DelPhiForce, we explored the interactions between the Ncd motor domain and tubulin dimers using a hybrid solvent model. This model accounts for bound ions explicitly while treating other ions implicitly within the solvent. The results indicate substantial differences in electrostatic properties when comparing the hybrid solvent model to purely implicit models. These findings highlight the importance of explicitly treating bound ions in highly charged regions for accurate electrostatic calculations. This machine learning-based approach is effective for kinesin-tubulin systems and can be extended to other biomolecules with similar electrostatic characteristics.