ISTITUTO ITALIANO
DI TECNOLOGIA

TITLE

Studying Molecular Interaction Via Enhanced Molecular Dynamics Simulations: A Novel Collective Variable And The Md-Dock Algorithm

INVENTORS

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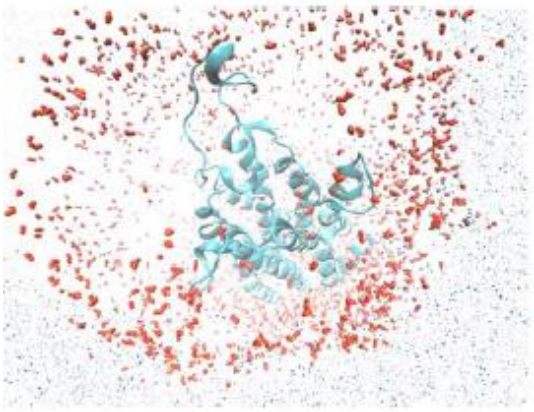
DESCRIPTION

The invention relates to a method to facilitate the acceleration of the configurationally sampling of molecular interaction in molecular dynamics (MD) simulation. This method makes use of an auxiliary (Yukawa-like)
screened electrostatic interaction potential acting between the subsets of a molecular system the interaction of which one wants to sample. This potential can be easily implemented in MD plugins and smears the interaction over all the atoms of the two subsets, leading to a concerted global movement.



APPLICATIONS

Biotech, pharma, drug discovery

KEYWORDS

Electrostatic Collective variable, adaptive binding protocol

BIBLIOGRAPHIC DATA

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Applicants	Fondazione Istituto Italiano di Tecnologia

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