ISTITUTO ITALIANO
DI TECNOLOGIA

TITLE

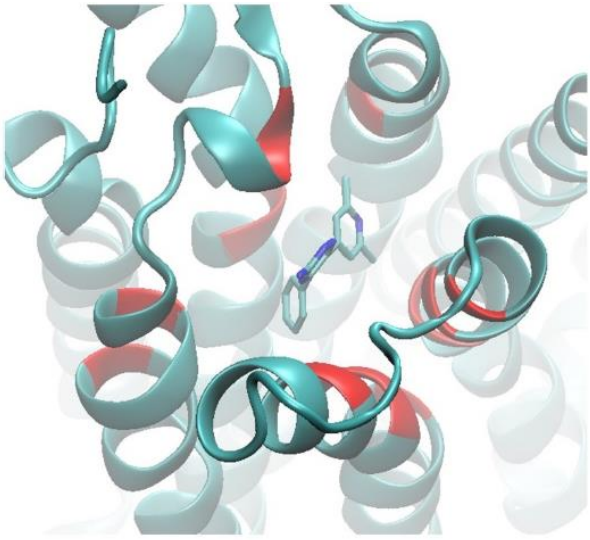
Kinetics of protein-ligand unbinding via smoothed potential molecular dynamics simulations

INVENTORS

Walter Rocchia

DESCRIPTION

A computational methodology to estimate the unbinding kinetics inherent in biomolecular interaction, also tested in the case of protein-ligand binding, is provided. This method couples smoothed potential molecular dynamics simulations with a statistical treatment. A method is further provided for use on systems of pharmacological interest, including those for which kinetic experimental data are available, including heat shock proteins (HSP70 and HSP90) that bind two distinct classes of ligands and the Adenosine A2A G-Protein Coupled Receptor in complex with congeneric inhibitors. The method provides the ability to rank ligands in consistent agreement with experimental kinetic data and to provide residence time estimates that correlate well with corresponding experimental measurements obtained from surface plasmon resonance experiments.



APPLICATIONS

Pharmacology, kinetics

KEYWORDS

Biomolecule, kinetics, dynamic simulation, statistical, proteins, ligands

BIBLIOGRAPHIC DATA

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