

Published on BSC-CNS (https://www.bsc.es)

Inici > ParmBSC0: New force-field for molecular dynamics simulations of nucleic acids

ParmBSC0: New force-field for molecular dynamics simulations of nucleic acids

The Life Science Program (MMB-group) distributed the parmBSC0 force-field for simulation of nucleic acids. The force-field, an evolution of AMBER-parm99 was derived from high level QM data and was tested on near 1 usec of MD simulations. We found a high performance in this force-field, which was able to derive reliable trajectories in long simulation times.

Barcelona Supercomputing Center - Centro Nacional de Supercomputación

Source URL (retrieved on 22 des 2024 - 06:28): https://www.bsc.es/ca/news/bsc-news/parmbsc0-newforce-field-molecular-dynamics-simulations-nucleic-acids