

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

[Inici](#) > Performance of the IEF-MST solvation continuum model in the SAMPL2 blind test prediction of hydration and tautomerization free energies

Performance of the IEF-MST solvation continuum model in the SAMPL2 blind test prediction of hydration and tautomerization free energies

URL: <http://www.springerlink.com/content/t04014112597w443/>

Authors: [Soteras,](#) / [Orozco, Modesto](#) / [Luque, Francisco Javier](#)

Barcelona Supercomputing Center - Centro Nacional de Supercomputación

Source URL (retrieved on 23 abr 2024 - 20:04): <https://www.bsc.es/ca/research-and-development/publications/performance-the-ief-mst-solvation-continuum-model-the-sampl2>