

[Inici](#) > Importance of accurate charges in molecular docking: quantum mechanical/molecular mechanical (QM/MM) approach.

Importance of accurate charges in molecular docking: quantum mechanical/molecular mechanical (QM/MM) approach.

Authors: [Cho, Art](#) / [Guallar, Victor](#) / [Berne, Bruce](#) / [Friesner, Richard](#)

Publication: Journal of computational chemistry

Volume / Pagination: 26 / 915-31

Paraules clau: [Algorithms](#), [Binding Sites](#), [Electrochemistry](#), [Ligands](#), [Models](#), [Molecular](#), [Molecular Conformation](#), [Protein Binding](#), [Proteins](#), [Thermodynamics](#)

Barcelona Supercomputing Center - Centro Nacional de Supercomputación

Source URL (retrieved on 12 nov 2024 - 16:56): <https://www.bsc.es/ca/research-and-development/publications/importance-accurate-charges-molecular-docking-quantum>