

[Inicio](#) > Ab initio quantum chemical and mixed quantum mechanics/molecular mechanics (QM/MM) methods for studying enzymatic catalysis.

---

## [Ab initio quantum chemical and mixed quantum mechanics/molecular mechanics \(QM/MM\) methods for studying enzymatic catalysis.](#)

**Authors:** [Friesner, Richard](#) / [Guallar, Victor](#)

**Publication:** Annual review of physical chemistry

**Volume / Pagination:** 56 / 389-427

**Palabras clave:** [Antibodies](#), [Binding Sites](#), [Catalysis](#), [Cytochrome P-450 Enzyme System](#), [Enzyme Activation](#), [Oxygenases](#), [Quantum Theory](#), [Solvents](#), [Triose-Phosphate Isomerase](#)

Barcelona Supercomputing Center - Centro Nacional de Supercomputación

---

**Source URL (retrieved on 14 Dic 2024 - 19:43):** <https://www.bsc.es/es/research-and-development/publications/ab-initio-quantum-chemical-and-mixed-quantum>