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