

# Investigating Reaction Mechanisms: from Quantum Chemistry to QM/MM and Force-Field Simulations

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To understand the chemical step in biological reactions, one has to use quantum mechanical methods to investigate the electronic structure. However, the environment (usually the protein) is too large to be handled by quantum mechanics, but too important to be neglected. Here it is shown how the reaction mechanisms of the enzyme PHBH and the ribosome are elucidated by means of QM/MM simulations.