# MultiScale Modelling of Biochemical Reactions

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In this course we will explore the possibilities offered by hybrid quantum mechanics / molecular mechanics (or QM/MM) methodologies for the study of chemical reactions in biological environments. We will introduce the need of these methods, the theoretical basis of the different QM/MM variants and their use for the calculation of energy and free energy reaction profiles of biochemical reactions. [1] The outline of the class will be:

1- Introduction
2- QM/MM schemes
3- Geometry optimization in Biochemical reactions
4- Free energy calculations in Biochemical reactions

The practical part of the course will be devoted to the computation of the energy profile for the enzymatic conversion of chorismite into prephenate [2] using Amber.

[1] Combined Quantum Mechanics/Molecular Mechanics (QM/MM) Methods in Computational Enzymology
M.W. van der Kamp and A. J. Mulholland
*Biochemistry* **2013** *52*, 2708-2728

QM/MM Methods for Biomolecular Systems
H. M. Senn and W. Thiel (2009), QM/MM Methods for Biomolecular Systems.
*Angewandte Chemie Int. Ed.* **2009** 48,1198-1229

[2] A Hybrid Potential Reaction Path and Free Energy Study of the Chorismate Mutase Reaction
S. Martí, J. A., V. Moliner, E. Silla, I. Tuñón, J. Bertrán, and M. J. Field
*Journal of the American Chemical Society* **2001** *123*, 1709-1712