



## Computational Modelling of Enzymatic Reaction Mechanisms

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### Message from the Guest Editor

Dear Colleagues,

Computational tools have advanced dramatically in recent years and now large (bio)chemical systems can be studied accurately with density functional theory as well as quantum mechanics/molecular mechanics methods. A popular use of the techniques is of a predictive nature in biotechnology and biocatalysis, where catalytic cycles and reaction schemes of enzymes are established that predict the formation of products and by-products and determine the rate determining steps in a reaction mechanism. This Special Issue in the *International Journal of Molecular Science* will be dedicated to the modelling of reaction mechanisms and reaction profiles relevant to biochemistry and aimed to elucidate biochemical reaction processes in enzymes and biocatalysts using computational tools.

Prof. Dr. Sam de Visser  
*Guest Editor*





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