Special Issue

Computational Modelling of Enzymatic Reaction Mechanisms

Message from the Guest Editor

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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The International Journal of Molecular Sciences (*IJMS*, ISSN 1422-0067) is an open access journal, which was established in 2000. The journal aims to provide a forum for scholarly research on a range of topics, including biochemistry, molecular and cell biology, molecular biophysics, molecular medicine, and all aspects of molecular research in chemistry. *IJMS* publishes both original research and review articles, and regularly publishes special issues to highlight advances at the cutting edge of research. We invite you to read recent articles published in *IJMS* and consider publishing your next paper with us.

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