On computational (and other) studies aiding our understanding of reaction mechanisms by non-heme iron enzymes

T. Borowski*,
A. Miłaczewska, A. Kluza, Z. Wojdyła
Jerzy Haber Institute of Catalysis and Surface Chemistry, Polish Academy of Sciences, Kraków, Poland
tomasz.borowski@ikifp.edu.pl

Non-heme iron enzymes constitute a large group of biocatalysts, which are present in all forms of life and catalyze a wide array of chemical transformations, usually involving oxidation of the substrate. Their reaction mechanisms, which still hold many secrets, are the subject of study by many research groups, including our team. In this talk we will present selected results from our works showcasing how computational investigations can aid, guide and supplement experimental studies focusing on enzymatic reaction mechanisms. More specifically, we will discuss reactions between dioxygen, or its surrogate (HNO), and reactive (co-)substrate: 2-oxoglutarate, acireductone, quercetin facilitated by, respectively: 2-oxoglutarate dependent enzymes, acireductone and quercitin dioxygenases. Examples of T6ODM and FtmF enzymes we will show how docking and molecular dynamics simulations can help to model enzyme-substrate complex when such is difficult to get by experimental methods, whereas results of QM/MM studies on AsqJ, CAS and H6H enzymes will exemplify how a question about reaction specificity can be tackled. Computational results will be presented in the context of experimental findings, obtained by us or other research groups.

References

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