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Modelling of catalytic activity and enzyme-MOF interactions using combined in silico approach

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Enzymes as industrial biocatalysts offer numerous advantages over traditional chemical processes concerning sustainability and process efficiency. Immobilization of enzymes on solid supporters is one of the key strategies for improving the practical performances of enzymes.
Metal-organic frameworks (MOFs) are promising candidates for enzyme immobilization. MOFs are porous coordination polymers consisting of metal-containing nodes and organic ligands linked through coordination bonds. It has been demonstrated that proteins can be successfully immobilized even in MOF pores whose apertures are smaller than the molecular dimension of the protein due to its conformational flexibility.
For our study, we selected horseradish peroxidase (HRP) encapsulated in MOF PCN-888(Al). We report the modelling of PCN-888(Al) MOF and the design of novel HRP mutants, which determine their enzymatic activity and magnitude of intermolecular interactions with MOF. Using a combined in silico approach, consisting of Informational Spectrum Method (ISM) bioinformatics method, molecular docking and molecular dynamics simulations, we propose new HRP mutants, which show higher/lower specific catalytic activity and higher/lower MOF-HRP dissociation constant, compared to the wild type of enzyme.

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