

Computational Study of Enzymatic Lignin β-O-4 cleavage

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Abstract: The first challenge in production of lignocellulosic biofuel is to disrupt the complex polymeric matrix of lignin that surrounds cellulose and hemicellulose chains in plant cell walls. Typically, thermo-mechano-chemical pretreatments of biomass are used to break lignin barrier, but developing alternative strategies is of major interest today to avoid the release of toxic compounds and valorize lignin as feedstock. Enzymatic degradation of lignin represents a promising approach to selectively valorize lignin derivatives to the production of fuel, chemicals and materials. In this work, we studied two enzymes that act on the early and last stages in the lignin β-aryl ether cleavage pathway from *Sphingobium sp* SYK-6 [1,2]. Using docking, molecular dynamics, QM/MM simulations and QM calculations, we shed light on the key interactions for substrate binding and came up with strong suggestions for the mechanism of action of these enzymes, named LigF and LigG. Further studies can make use of these results to identify other lignin degrading enzymes in other organisms, as well as to optimize these biocatalysts for future application in biorefineries.

Key-words: quantum mechanics / molecular mechanics, quantum mechanics, ligninase, bioethanol

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