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Molecular dynamics analysis of the binding mechanism of veratryl alcohol at the protein surface of lignin peroxidase (*P. chrysosporium*) and its mutants E168Q and D264N.

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Abstract: Lignin peroxidase (LiP), a fungal heme-containing peroxidase, first discovered in the basidiomycete *Phanerochaete chrysosporium*, plays an important role in the degradation of lignin and lignin model compounds[1-3] due to its high redox potential. Veratryl alcohol (VA), is a secondary metabolite of the fungus *P. chrysosporium* and is the main substrate of LiP. Also, VA acts as a redox mediator in the oxidation of lignin and other phenolic and non-phenolic compounds, after being oxidized to a radical species ($VA^{\bullet+}$) by Trp171, a catalytic residue located at the protein surface.[4, 5] In a previous report, we explored through molecular docking, MD and MM-GBSA simulations the way VA (in its neutral state) interacted with Trp171 and how it was stabilized by other residues at the protein surface.[6] Furthermore, VA in a neutral and cationic state, was used to run long molecular dynamics of 1μs for LiP-$VA^{\bullet+}$ and LiP-VA complexes with the Desmond software. Interaction profiles for each state of VA were obtained showing that there exists a clear difference in the interaction dynamics of both species. For a further understanding of the stabilization mechanism of $VA^{\bullet+}$ at the protein surface, in this work are reported new MD simulations of 1 μs that take into account a higher substrate concentration and explore its affinity by WT LiP and the E168Q and D264N mutants.

Conflicts of Interest

The authors declare no conflict of interest.

References and Notes

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