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A Molecular Dynamics Study to Predict Protonation Sites on the Xylanase Surface.

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Xylanase enzyme families play an important role in many industries due to its ability to digest the hemicellulose within plant cell walls. Developing the enzyme that can withstand extreme conditions under an industrial process and in a stomach requires an extended information in molecular scale for further protein engineering. In this study, atomistic molecular dynamics simulation and analysis was performed to assess the positive ion distribution patterns on the surface of a Xylanase enzyme molecule. The simulations were carried out at three different temperatures, representing room temperature (303K), optimum temperature (333K) and high temperature within an extruding machine (378K). Three sites with highest ion occupancy and temperature effects were identified. The results enable us to predict the most probable regions for amino acid protonation under acidic conditions at different temperatures.

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