ABSTRACT

Metal-organic frameworks (MOFs) have emerged as promising materials for enzyme immobilization due to their high surface area, tunable pore sizes, and versatile chemical properties. In this study, we report the computational modeling and simulation of the interactions between the ZIF-8 MOF and the NAD-dependent formate dehydrogenase (FDH) enzyme. FDH is an important oxidoreductase that catalyzes the interconversion of formate and carbon dioxide, with applications in biofuel production and other biotechnological processes. Immobilizing FDH on a suitable support like ZIF-8 can enhance its stability, reusability, and catalytic efficiency. Using molecular docking and molecular dynamics simulations, we investigated the binding interactions between the FDH enzyme and the ZIF-8 framework. Our results show that the FDH enzyme can spontaneously adsorb onto the ZIF-8 surface, with the active site region forming stable contacts with the MOF. Key amino acid residues involved in the binding interface were identified, including hydrophobic, electrostatic, and hydrogen bonding interactions. These computational insights provide a rational basis for the design of ZIF-8-FDH biocatalytic systems and guide future experimental studies on the development of MOF-enzyme hybrids for sustainable chemical transformations. The methodology presented can be extended to other MOF-enzyme pairs of interest.

KEY WORDS

Metal-organic frameworks (MOFs) Enzyme immobilization. ZIF-8 MOF. Formate dehydrogenase (FDH) Computational modeling. Molecular docking. Molecular dynamics simulations. Catalytic efficiency. Biocatalytic systems. Sustainable chemical transformations. MOF-enzyme hybrids. Hydrophobic interactions. Electrostatic interactions