Pulverizing PFOA: Analyzing Molecular Dynamics Simulations Between Perfluorooctanoic Acid and a Fluoroacetate Dehalogenase Enzyme

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Perfluorooctanoic acid (PFOA) has been connected to changes in liver function, immunity issues, thyroid disease, and kidney and testicular cancer. Due to these effects, PFOA is banned for use in the United States. However, in over 30 American states, PFOA remains in the environment and drinking water due to its hard-to-break carbon-fluorine bonds. Developing a method to destroy this substance is critical. The fluoroacetate dehalogenase enzyme is one of few enzymes that can break apart carbon-fluorine bonds. It was hypothesized that if PFOA is introduced to fluoroacetate dehalogenase as a substrate, then the enzyme chemistry will change in such a way as to favor the degradation of PFOA. Enzyme chemistry is evaluated through molecular modeling software PyMOL and UCSF Chimera. After optimizing the parameters for the molecular dynamics simulations, the simulation was performed five times, and the average of atom distances was taken for evaluation. In spite of some close interactions between the carboxylic acid group of PFOA and the enzyme's active site, large distances between the nucleophile and PFOA as well as the fluorine atom and the fluoride pocket of the active site suggest that the enzyme may not biodegrade PFOA as those interactions are essential for weakening the C-F bond. Research focused on verifying simulation data through wet-lab experiments is currently being performed. Successful transformation of fluoroacetate dehalogenase plasmids into E. coli BL21 Star (DE3) has been achieved. In tandem with these experiments, possible mutations to the enzyme's active site for more favorable enzyme chemistry are being examined.

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