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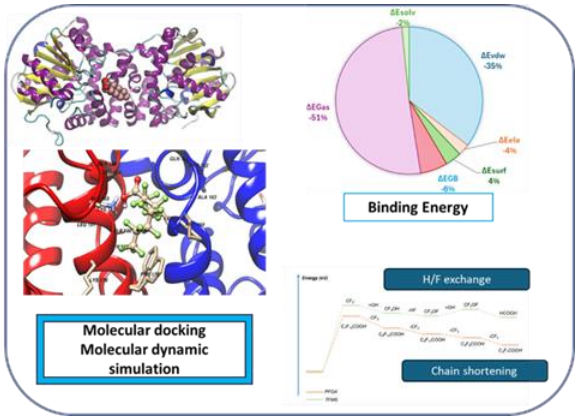
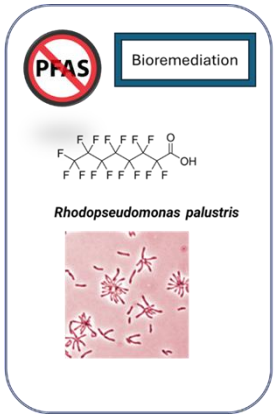
Molecular docking and molecular dynamics simulations for assessing biodegradation of PFAS

Aim: Per- and poly-fluoroalkyl substances (PFAS) have recently gained growing regulatory attention as emerging micropollutants, recognised for their exceptional resistance and environmental hazards to both human health and ecosystems. Often referred to as 'forever chemicals,' PFAS compounds exhibit extremely stable chemical structures. While numerous treatment technologies have been investigated to mitigate PFAS contamination, final remediation stages typically rely on thermal or incineration processes to achieve complete chemical breakdown. Recently, the *biodegradation* of PFAS has shown potential as a cost-effective alternative. This study employed molecular docking and molecular dynamics simulations as in silico tools to investigate interactions between enzymes (proteins) and PFAS compounds (ligands) and elucidate the biodegradation mechanisms of PFAS, bridging the gap between theoretical exploration and experimental validation.

This study focused on the microbial fluoroacetate dehalogenase enzyme (RPA1163) and its interaction with perfluorooctanoic acid (PFOA) as a long chain PFAS containing an acetate functional group, and a short chain PFAS (trifluoromethanesulfonic acid (TFMS)) which lacks an acetate functional group for comparison. Molecular docking was performed using AMBER 99SB force field to investigate the enzyme's binding affinity for PFAS, while molecular dynamic simulations provided insights into the stability and dynamics of the enzyme-ligand complex. The results revealed that van der Waals and gas-phase energy are the driving force of binding interaction between the enzyme and PFAS.

These findings provide critical insights into the molecular mechanisms underpinning PFAS biodegradation, which could contribute to the development of cost-effective biotechnologies for PFAS remediation. The deeper understanding of the catalytic mechanism can guide the rational engineering of enzymes to enhance the degradation of fluorochemicals, fostering more sustainable and effective approaches for environmental remediation of persistence pollutants.





Highlights

- Molecular docking simulations reveal the binding mechanisms of PFAS with the dehalogenase enzyme.
- PFOA exhibits stronger binding affinity with the enzyme but presents slower degradation.
- TFMS biodegradation relies on electron beam irradiation, which is limited in natural environments.
- Chain shortening of PFOA leads to the formation of less harmful and biodegradable carboxylic acids.
- Future engineering biotechnology approach should focus on optimising the binding pocket geometry.