

Degradation of High Energy Materials Using Biological Reduction: A Rational Way to Reach Bioremediation

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Explosives molecules have been widely used since World War II, leading to considerable contamination of soil and groundwater. Recently, bioremediation has emerged as an environmentally friendly approach to solve such contamination issues. However, the 1,3,5,7-tetranitro-1,3,5,7-tetrazocane (HMX) explosive, which has very low solubility in water, does not provide satisfying results with this approach. In this study, we used a rational design strategy for improving the specificity of the nitroreductase from *E. Cloacae* (PDB ID 5J8G) toward HMX. We used the Coupled Moves algorithm from Rosetta to redesign the active site around HMX. Molecular Dynamics (MD) simulations and affinity calculations allowed us to study the newly designed protein. Five mutations were performed. The designed nitroreductase has a better fit with HMX. We observed more H-bonds, which productively stabilized the HMX molecule for the mutant than for the wild type enzyme. Thus, HMX's nitro groups are close enough to the reductive cofactor to enable a hydride transfer. Also, the HMX affinity for the designed enzyme is better than for the wild type. These results are encouraging. However, the total reduction reaction implies numerous HMX derivatives, and each of them has to be tested to check how far the reaction can go.

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