Biomimetic modifications on the bridging cys residue ligand of an FeNi Hydrogenase

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This study attempts to computationally determine biomimetic modifications that can be made to the native enzyme active site of FeNi Hydrogenase, which is used to catalyze the conversion of hydrogen to protons and electrons. Previous research has been conducted on propanedithiol, a common biomimetic ligand, and I am altering these bridging cys residues computationally, then optimizing them using a Density Functional Theory method. Based on a similar ligand found in the native FeFe Hydrogenase active site, I replaced the center carbon in the propane with an amine group and later, a methyl-amine group. To make alterations to the hydrogenase, we use a computational chemistry software called Gaussian 16 that simulates chemistry that one does not necessarily have the time or resources to complete in a laboratory setting. The results determined computationally are able to direct chemists working in the lab towards potentially favorable biomimetic catalysts. Practically, a catalyst with FeNi Hydrogenase properties could be used to sustainably oxidize hydrogen, which would be a great renewable alternative energy source.