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The IUBMB enzyme nomenclature decision tree

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This project attempts to map the decisions involved in categorizing an enzyme using the International Union of Biochemistry and Molecular Biology (IUBMB) enzyme nomenclature. The recommendations of the Nomenclature Committee of IUBMB on the nomenclature and classification of enzyme-catalyzed reactions is complex and archaic, with rules that almost always have an exception. The IUBMB enzyme nomenclature was devised in 1961 by the first Enzyme Commission. It is a system of categorizing enzymes based on the biochemical reactions they catalyze. The system categorizes an enzyme into one of six main classes (oxidoreductases, transferases, hydrolases, lyases, isomerases, and ligases), a subclass, and a subclass based on the element of the biochemical reaction equation, such as the biochemical acceptor and donor. This research project looks at the IUBMB enzyme nomenclature with the purpose of defining a decision tree that would closely represent its taxonomy. The tree would be used in the programming of an automatic enzyme classifier, which when given the biochemical equation that an enzyme catalyzes, categorizes the enzyme in its final subclass. Techniques, such as the statistical analysis of chemical equation topologies and compound distribution, have been used to avoid the necessity of programming the underlying principals of chemistry, such as how to distinguish if a reaction is an oxidation-reduction reaction. This project is ongoing.