

Discovery and Analysis of Novel Biochemical Transformations

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We have developed a computational discovery platform for identifying and analyzing novel biochemical pathways to target chemicals. Automated network generation that defines and implements the chemistry of what we have coined “generalized enzyme functions” based on knowledge compiled in existing biochemical databases is employed. The output is a set of compounds and the pathways connecting them, both known and novel. To identify the most promising of the thousands of different pathways generated, we link the automated network generation algorithms with pathway evaluation tools. The simplest screening metrics to rank pathways are pathway length and number of known reactions. More sophisticated screening tools include thermodynamic feasibility and potential of known enzymes for carrying out novel reactions. Our method for automated generation of pathways creates *novel compounds and pathways* that have not been reported in biochemical or chemical databases. Thus, our method goes beyond a survey of existing compounds and reactions and provides an alternative to the conventional approaches practiced to develop novel biochemical processes. This presentation will focus on the components of this computational discovery platform and its application.