Optimal Yield Pathways in Complex Reaction Networks

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Advanced methods for constructing complex chemical reaction networks include graph transformation models, which are based on rigorous mathematical foundation. In such models, molecules are represented by graphs, and reactions by graph transformations. As such, chemical reaction networks are hypergraphs where reaction arcs connect educt molecules to product molecules. By using graph transformations to model reactions, one is able to extrapolate reaction mechanisms to novel compounds, thus introducing a predictive aspect when expanding networks. We use the graph transformation model to rapidly expand complex spaces for the purpose of yield analysis.

Finding potential synthesis pathways, especially ones with optimal yield from a given set of input compounds in such complex systems is of high interest in many areas of chemistry and biotechnology. We exploit the fact that reachability is polynomial in continuous Petri nets to introduce an algorithm for computing the maximal yield of a molecule in a chemical reaction network. Our algorithm does not return only the maximum theoretical yield, but rather the maximum yield pathway, allowing for easy identification of the reactions which contribute to synthesis.