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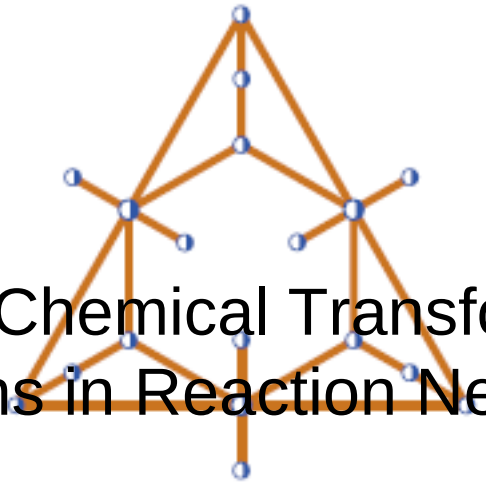

Finding Chemical Transformation Patterns in Reaction Networks

Content :

In this presentation we will discuss the analysis of chemical spaces that are spanned by grammar-based graph transformation of molecules. Given a set of input molecules (undirected graphs) and a set of rules (graph grammar rules) we derive a directed hypergraph that reflects all possible molecules that can be reached. To constraint the size of the hypergraph we consider only molecules that are smaller than a given maximal size. Based on this derivation graph we use integer linear programming approaches to automatically detect chemical patterns and pathways in the chemical space. The presented method will be applied i.) to automatically detect autocatalysis and ii.) to find chemical pathways that are optimal with respect to specific given criteria. As chemical example systems we will use i.) the formose reaction for the automatic detection of autocatalytic processes, and ii.) the non-oxidative phase of the pentose phosphate pathway for the inference of how six ribulose 5-phosphate molecules are modified by a series of chemical reactions to five fructose 6-phosphate molecules.

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