First symposium on chemistry of the Mittelbau at the Faculty of Chemistry, University of Vienna

Exploring the biosynthetic pathway design space.

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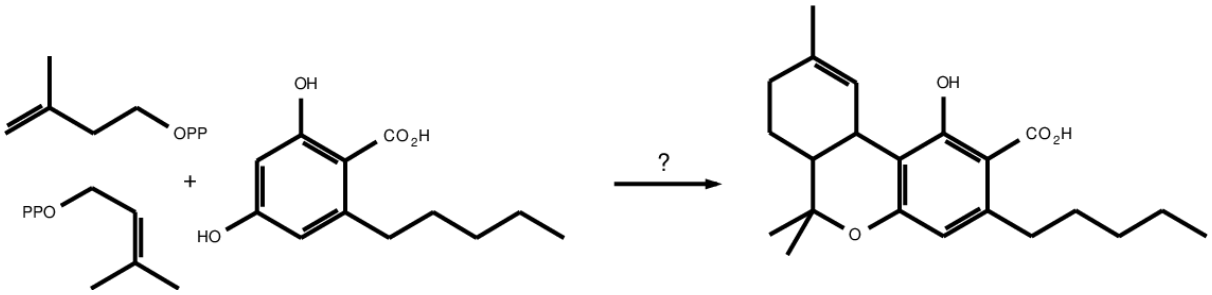
The design and implementation of *de-novo* biosynthetic pathways is a costly and rather slow endeavor due to the expanse and combinatorial complexity of the biosynthetic chemical space. Therefore efficient computational approaches are required to explore the diversity of biosynthetic routes towards target compounds. Designing biosynthetic pathways is a variant of the classical synthesis planning problem from organic chemistry, where construction



operations are restricted to enzyme reactions. I will introduce our graph rewriting framework, that provides a powerful set of techniques to specify, construct, and search through chemical spaces. A chemical space is defined by a collection of start compounds and a "reaction chemistry" defined as a set of graph transformation rules. This algebraic model of chemical transformation in combination with mathematical optimization techniques makes it possible to explore the biosynthetic design space in a systematic manner. The question of interest e.g. "Does the specified chemical space harbor multiple, possibly competing, routes to the target molecule?" is rephrased in the mathematical language of integer flows on hypergraphs offering an efficient way to identify networks in the chemical space that optimize a predefined objective function. I will illustrate this approach with the help of examples from carbohydrate and polyketide chemistry.

References: Jakob L Andersen *et al* (2017), Chemical Transformation Motifs – Modelling Pathways as Integer Hyperflows doi:10.1109/TCBB.2017.2781724.