

# Planning Organic Synthesis Using Reaction Types Derived from Reaction Databases

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A novel, reaction database-driven approach for a stepwise retrosynthetic analysis of a given target compound will be presented. The method uses a knowledge base of different reaction types that has been automatically derived from either a commercially available or in-house reaction database. New synthetic routes are suggested by applying appropriate reaction types to the target compound in a retrosynthetic and automated manner. At each step, the proposed precursors are automatically searched in integrated catalogs of available starting materials for their commercial availability. The rather general definition of chemical reactivity provides the user with new ideas for organic synthesis and deals with a broad range and diverse chemistry, including, *e.g.*, formation of heterocycles, pericyclic reactions, rearrangements and metathesis.

The method has been implemented in the web-based, easy-to-use program system THERESA (THE REtroSynthesis Analyser) and contains tools to browse the suggested syntheses and the corresponding published reaction data, such as literature data and experimental conditions, to build and display interactive synthesis trees and to generate reports.

The presentation will provide insights into the general algorithms of the approach and demonstrate the application of THERESA to some medicinally relevant synthetic targets.