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Poster presentation

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THERESA - a new reaction database-driven tool for stepwise retrosynthetic analysis

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The synthesis of new compounds is a quite time consuming and cost expensive task. The need to search and evaluate alternative synthetic paths is a mandatory step before going to the lab. Searching in reaction databases may provide some information about how a compound can be synthesized but often fails if the target is not present in the database.

The poster presents THERESA (THE REtro-Synthesis Analyser), a novel, web-based, easy-to-use tool for the stepwise retrosynthetic analysis of a given target compound. THERESA scans reaction databases to suggest new synthetic routes and simultaneously searches in catalogs of available starting materials for the proposed precursors. Furthermore, it provides the corresponding published reaction data for each suggested synthetic step. Due to the rather general definition of reactivity, it is able to provide the chemist with new ideas for organic synthesis as it deals with a broad range and diverse chemistry, including, e.g., formation of heterocycles, pericyclic reactions, rearrangements and metathesis.

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