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# AUTOMATIC CIRCUIT TERMINAL OF ORGANIC COMPOUND SYNTHESIS BASED ON ITS STRUCTURAL FORMULA

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## Abstract

The study suggests software implementation for analytical work in solving the problem of planning substance synthesis based on the structural formula. This software makes it possible to get ways to synthesize a given organic compound using a small knowledge base. We consider this software implementation by means of two programming languages (Prolog and Python). The input data is the target substance structure, written in SMILES notation. The output data is the set of reactions necessary to obtain the given structure. The result of this work is a module in Python language, which can be used to automatically output ways of synthesizing organic compounds.

## Keywords

Synthesis planning, chemoinformatics, RDKit, Prolog, OpenBabel, molecular graph, reaction graph, SMILES, Python

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