Graph Algorithms for Decision Support in Molecular Construction

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Abstract

The objective of this research project is to propose and evaluate on real chemical data new algorithms of prediction of a reaction chain for the synthesis of a new molecule. These algorithms consist first in the selection of a set of molecules sufficiently similar to the target one in a database of reactions. This measure of similarity is based on a specific metric of comparison of graphs modeling the structure of molecules at a high level of granularity. The second algorithmic phase consists in solving an edition problem for the prediction of the target reaction chain from existing reaction chains in the data base, selected by using the similarity of the molecules.