# Chemical Compounds with Path Frequency Using Multi-Core Technology

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## Abstract

Drug design is the approach of finding drugs by design using computational tools. When designing a new drug, the structure of the drug molecule can be modeled by classification of potential chemical compounds. Kernel Methods have been successfully used in classifying chemical compounds, within which the most popular one is Support Vector Machine (SVM). In order to classify the characteristics of chemical compounds, methods such as frequency of labeled paths have been proposed to map compounds into feature vectors. In this study, we analyze the path frequencies computed from chemical compounds, and reconstruct all possible compounds that share the same path frequency with the original ones, but differ in their molecular structures. Since the computation time for reconstructing such compounds increase greatly along with the size increase of the compounds, we propose an efficient algorithm based on multi-core processing technology. We report here that our algorithm can infer chemical compounds from path frequency while effectively reduce computation time and obtained high speed up.

Keyword：Chemical compound, feature space, Multi-Core Processing, Branch-and-Bound, OpenMP