Public Abstract

First Name:Nandini

Middle Name:

Last Name:Basu

Adviser's First Name:Toni

Adviser's Last Name:Kazic

Co-Adviser's First Name:

Co-Adviser's Last Name:

Graduation Term:WS 2007

Department:Computer Science

Degree:MS

Title:Heuristics for searching chemical structures

Structure search tools are the most important part of chemical and biochemical structure databases allowing the user to search for specific structures or make varied structural comparisons. Even though a number of such available databases provide varied structure search methods, a detailed isomer search tool has not been developed to our knowledge. Our database, Klotho, consists of biochemical compounds defined with rules depicting the relations between atoms in the molecules. We have developed methods to recognize multiple types of isomerism among molecules. In addition to isomer recognition, we have also implemented standard isomorphism and substructure searches. The methods exploit grammatical rules defining molecular structure and searches for specific structures in the database using graph similarity algorithms. Heuristics and pre-processed relevant structure information has been employed to improve the performance level of the search methods by increasing the speed. The search methods are isomer search, substructure search, isoconnected structure search and general structure search. Isomer search matches those compounds which are structural and configurational isomers of the query compounds. Substructure search retrieves those compounds which has the query compound as a part of its structure. Isoconnected structure search retrieves compounds which are isoconnected to the structure and are exact structures of the query structure. General structure search retrieves structural property information for compounds.