

Abstract

Functional Group Ontology is an important source of prior knowledge that may be automatically integrated to support predictive data analysis tasks. The assessment of similarity of functional groups provides the basis for the implementation of classification tools and the automated validation of functional associations. This study discusses alternative techniques for measuring ontology-driven similarity of functional groups. Thus a novel approach for functional group ontology based on chemical functional group creation has been automated, which can be identified by a computer program, useful to categorize small molecules.

Small molecules play crucial role in the modulation of biological functions. Besides serving as metabolites these also serve as building blocks of larger biopolymers such as DNA and proteins. Small molecule interactions are studied by a variety of experimental methods. An organic molecule along with information of their biological activities is a widely studied topic. The tremendous increase in publicly available small molecules is driving new efforts to better understand their interaction particularly in area of drug docking and pharmacogenomics.

Functional group ontology is a structured classification of chemical compounds of biological relevance. Hence, functional group ontology provides the framework to define chemical components of each chemical compound. Every compound will have parents and children's (if available) displayed. If not available the compound will be listed as unclassified. It gives framework for studying the functional groups of chemical compound.

We have assessed a functional group of any small molecule on the basis of their atom types, bond information and properties of molecule that can be useful for designing Pharmacophore.