POSTER 36

A LIGAND FACEBOOK FOR AIDS AND BEYOND

T.N. Bhat

Biochemical Science Division, NIST, Gaithersburg, MD 20899, USA

Efficient and user friendly data management systems that support state-of-the-art annotation and query capabilities are crucial for the effective use of structural data. Semantic Web and rule-based data management techniques are the vision of the W3C for enabling seamless integration of electronic data. Here we describe an approach towards this goal for structural data on chemical compounds. In this approach, chemical compounds are recursively dissected into scaffolds. From these scaffolds, first RDF and then ontological tree to describe their relationships are generated. Ontology is used to display data in a predictable fashion. Elements at the lowest level of the ontological tree are used to group distantly related compounds and the elements at higher levels of the ontology tree are used to hold closely related compounds. This technique is called Chem-BLAST – Chemical Block Layered Alignment of Substructure Technique and it generates ontology in layers of low to high level of precision to define queries. This method has been used to develop the following databases.

- HIV structural database (HIVSDB) distributes one of the largest comprehensive collections of structural data obtained from many resources.
    - http://bioinfo.nist.gov/SemanticWeb_pr2d/chemblast.do
- A ligand gateway for PDB that cover many diseases ranging from Cancer to TB, malaria to neural diseases.
    - http://xpdb.nist.gov/chemblast/pdb.html
    - This database is now also available from the PDB Website http://www.rcsb.org/pdb/explore/externalReferences.do?structure=3BC3