

POSTER 47**STRUCTURAL DATABASE USING SEMANTIC WEB CONCEPTS TO SUPPORT STRUCTURE-BASED DRUG DESIGN FOR AIDS**

T.N. Bhat¹, Anh-Dao Nguyen¹, G. Noble², L. Cooney², M. Nasr³, A. Wlodawer⁴, K. Das⁴, E. Arnold⁴

¹Biochemical Science Division, NIST, Gaithersburg, MD 20899, USA; ²Cygnus Corporation, Inc, Rockville, MD 20852, USA; ³NIAID, Bethesda, MD 20892, USA; ⁴NCI-Frederick, Frederick, MD 21702, USA; ⁵CABM/Rutgers University, Piscataway, NJ 08854, USA

The HIV structural databases (HIVSDB, http://bioinfo.nist.gov/SemanticWeb_pr2d/chemblast.do, <http://chemdb2.niaid.nih.gov>) distribute one of the largest comprehensive collections of structural, biological and pre-clinical data on inhibitors, drug leads and clinical drugs for AIDS. These databases contain info on several thousand biologically active compounds from all classes (HIV PR, RT, CCR5, Integrase) of FDA approved drugs. Efficient and yet user friendly data management systems that support state-of-the-art annotation, visualization and query capabilities are crucial for the effective use of data for fragment based structural pharmacology and rational drug design. Semantic Web is the vision of the World Wide Web Consortium for enabling seamless integration of electronic data for data mining and knowledge generation across the Web. Robust and functionally relevant ontology plays a critical role in developing the data elements for a Semantic Web. Presentation will illustrate how Semantic Web concepts are used for novel annotation, data integration, storage, and query to manage and display structural (fragments, 2-D images and text-based) biological, and pre-clinical data. One of these techniques (Chem-BLAST¹) developed allows rapid comparison of structural fragments using the Semantics commonly used in drug discovery process. At present majority of the data in HIVSDB are obtained by us by weaning through publications. Our intension is to seek greater participation by the community by depositing data to HIVSDB at the time of publication.

¹Prasanna, M.D., J. Vondrasek, et al. (2006). "Chemical compound navigator: a web-based chem-BLAST, chemical taxonomy-based search engine for browsing compounds." *Proteins* 63(4): 907-17.