9, 38042, France, [2]Department of Chemistry, The University of Manchester, Brunswick Street, Manchester, M13 9PL, UK, E-mail：fisher@ill.fr

Per-deuteration of proteins is becoming more common place and the assumption is in general that deuteration does not affect protein structure. It should be noted that functional changes upon deuteration are known, e.g. D_2O is toxic to living systems, reaction kinetics change [1], proteins stiffen in D_2O [2] and ferroelectrics alter their properties [3]. There are two exceptions known to us for protein structures. Firstly in Kuhn et al [4] they observe a difference in position of a critical H versus D atom for subtilisin versus trypsin respectively. Secondly in haloalkane dehydrogenase Liu et al 2007 [5] observe a rotation of an Asp towards a His for the deuterated enzyme. In the absence of a statistical database of protein neutron AND ultra-high resolution X-ray crystal structures we have instead examined the effect of deuteration on structure by data-mining of the Cambridge Structural Database [6] for deuterated and hydrogenated pairs of small molecule structures which have been analysed by neutron or X-ray crystallography. There are, mainly, examples of isomorphous crystal pairs but also some non-isomorphous pairs. Differences between these structures for both types have been calculated and their statistical significance assessed. There are precisely enough measured structural differences but we find that they are in each case small enough that they do not upset the general assumption that deuteration does not affect protein structure.

1. P. Atkins & J. de Paula (2002). Atkins' Physical Chemistry, 7th ed.
2. P. Cioni and G. B. Strambini (2002) Biophysical Journal 82, 3246-3253.
3. A. Katrusiak (1995). Physical Review B 51, 589.
4. P. Kuhn et al Biochemistry 1998, 37, 13446-13452
5. X. Liu et al Acta Cryst. (2007). D63, 1000-1008
6. CCDC (2007). http://www.ccdc.cam.ac.uk

Keywords: structure mining, deuterated structures, neutron protein crystallography

MS.98.5

Acta Cryst. (2008). A**64**, C164

Structural database using semantic Web concepts to support structure-Based drug design for AIDS

Talapady N Bhat[1], Talapady N Bhat[1], A Nguyen[1], G Noble[2], L Cooney[2], M Nasr[3], A Wlodawer[4], K Das[5], E Arnold[5]
[1]NIST, Biochemical Science Division, Bldg 227, 100 Bureau Drive, Gaithersburg, MD, 20899, USA, [2]Cygnus Corporation, Inc, Rockville, MD 20852, USA, [3]NIAID, Bethesda, MD 20892, USA, [4]NCI/FCRDC, Frederick, MD 21702, USA, [5]CABM/Rutgers University, 679 Hoes Lan Picatway, NJ 08854, USA, E-mail：bhat@nist.gov

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-BLAST(Prasanna, Vondrasek et al. 2006)) 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.

Prasanna, 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.

Keywords: bioinformatics: the future, knowledge-based applications in structural chemist, structure-based drug design, structural informatics