

FA4-MS10-O1

Towards Knowledge - Based Design of Pharmaceutical Crystal Forms. Peter A. Wood. *Cambridge Crystallographic Data Centre, Cambridge, UK.*

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The technique of co-crystallisation as a means to produce a solid dosage form of an active pharmaceutical ingredient (API) has been gaining popularity within the pharmaceutical industry. Co-crystals have the potential for greater flexibility and diversity in the created forms than salts or hydrates due to their compatibility with non-ionisable APIs and the large range of pharmaceutically acceptable coformers that are potentially available. The effective use of co-crystallisation for this purpose is clearly affected by the capacity with which the solid forms produced can be controlled and predicted.

The structural knowledge stored within the Cambridge Structural Database (CSD, [1]) is highly relevant to all aspects of crystal engineering and the understanding of intermolecular interactions at a fundamental level. The study of appropriate structural data is of prime importance when investigating these areas.

Recent software advances [2] have broadened the opportunities for using the CSD for design and control of crystal forms. This study focuses on the analysis of a large family of pharmaceutical co-crystals containing a consistent API component [3] to provide insight into intermolecular interactions in general as well as co-crystal design in particular.

[1] Allen, F. H. A.; *Acta Cryst. B*, **2002**, 58, 380-388. [2] Macrae, C. F.; Bruno, I. J.; Chisholm, J. A.; Edgington, P. R.; McCabe, P.; Pidcock, E.; Rodriguez-Monge, L.; Taylor, R.; van de Streek, J.; Wood, P. A.; *J. Appl. Cryst.*, **2008**, 41, 466-470. [3] Childs, S. L.; Wood, P. A.; Rodriguez-Hornedo, N.; Reddy, L. S.; Hardesty, K. I.; *Cryst. Growth Des.*, **2009**, 9, 1869-1888.

Keywords: knowledge-based design; packing analysis; crystal form

FA4-MS10-O2

Chemical Semantic Web Concepts, Ontology, Software, Database for 2D and 3D Structures from Resources such as the Protein Data Bank, PubChem and HIVSDB. Talapady N. Bhat^a, Anh-Dao Nguyen^a, Glen Noble^b, L. Cooney^b, Mohamed Nasr^c, Alex Wlodawer^d, Kalyan Das^d, Edy Arnold^d. ^aBiochemical Science Division, NIST, Gaithersburg, MD 20899, USA. ^bCygnus Corporation, Inc, Rockville, MD 20852, USA. ^cNIAID, Bethesda, MD 20892, USA. ^dNCI/FCRDC, Frederick, MD 21702, USA. ^eCABM/Rutgers University, 679 Hoes Lane, Piscataway, NJ 08854, USA.

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The HIV structural databases (HIVSDB, http://bioinfo.nist.gov/SemanticWeb_pr2d/chemblast.do, [\[niaid.nih.gov\]\(http://niaid.nih.gov\)\) 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\[1\]\) 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. Recently we have extended \(<http://xpdn.nist.gov/pdb/chemblast.html>\) the Chem-BLAST technology to cover all the ligands held in the PDB. This new effort provides a versatile ligand gateway for data available in the PDB. Another structural database that includes thermodynamics data for Biofuels \(<http://bioinfo.nist.gov/biofuels>\) will also be presented.](http://chemdb2.</p>
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[1] Prasanna, M.D., et al., *Chemical compound navigator: a web-based chem-BLAST, chemical taxonomy-based search engine for browsing compounds*. *Proteins*, 2006. **63**(4): p. 907-17.

Keywords: bioinformatics; AIDS inhibitors; structural database and drug design

FA4-MS10-O3

Identification of Crystalline Phases of Cements Using X-ray Microdiffraction Techniques. Dmitry Popov^a, Rainer Daehn^a, Daniel Grolimund^a, Philip Pattison^b, Erich Wieland^a. ^aPaul Scherrer Institut, 5232 Villigen PSI, Switzerland. ^bEuropean Synchrotron Radiation Facility, Swiss-Norwegian beamline, Grenoble France.

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Micro X-ray diffraction (microXRD) is a powerful tool to investigate spatially resolved micro-scale heterogeneous systems. The aim of the present study was to develop microXRD data collection and reduction techniques to study heterogeneous materials with typical features on the micro-meter scale. MicroXRD was exemplarily applied to cementitious materials to gain structural information from selected micron-sized crystals within the whole matrix. Case studies and test measurements performed at the SLS microXAS and ESRF Swiss-Norwegian beamlines showed the feasibility of this task: major crystalline components of selected area of the samples and selected microcrystals