Agenda
5th Meeting on U.S. Government Chemical Databases and Open Chemistry

Thursday, August 25, 2011

MORNING
Chairperson: Ann Richard

9:00-9:15 AM  Registration, Check-In

9:15-9:30 AM  Introduction: Marc Nicklaus

9:30-11:15 AM  Morning Session I – FDA Databases & Projects

9:30-9:50  Kirk Arvidson, FDA/CFSAN, "Development of an Institutional Knowledge-base at FDA’s Center for Food Safety and Applied Nutrition”

9:50-9:55  Discussion


10:15-10:20  Discussion

10:20-10:40  Huixiao Hong, FDA/NCTR, “EDKB: Endocrine Disruptors Knowledge Base at the FDA”

10:40-10:45  Discussion

10:45-11:05  Frank Switzer, FDA/OC, “The FDA/USP Substance Registration System as an Informational Bridge Between Chemistry and Biology”

11:05-11:15  Discussion

11:15-11:30 AM  Morning Break

11:30-12:45 PM  Morning Session II – Toxicology

11:30-11:50  Eugene Demchuk, CDC, “Chemical Toxicity Databases at NCEH/ATSDR”

11:50-11:55  Discussion


12:15-12:20  Discussion

12:20-12:40  Nina Jeliazkova, Ideaconsult Ltd., “Seamless and uniform access to chemical data and tools: Experience gained in developing the OpenTox framework”

12:40-12:45  Discussion

12:45-1:45 PM  Lunch Break & Poster Session
THURSDAY, AUGUST 25, 2011

AFTERNOON
Chairperson: Michael Gilson

1:45-2:45 PM  Afternoon Session I – Identifiers

1:45-2:05
Steve Heller, NIST, “The Status of the InChI Project”
2:05-2:15
Discussion
2:15-2:35
Jonathan Goodman, IUPAC & RSC, “InChI and Reactions”
2:35-2:45
Discussion

2:45-3:00 PM  Afternoon Break

3:00-4:45 PM  Afternoon Session II – NIH Resources and How to Access Them

3:00-3:20
Evan Bolton, NCBI/NLM, “PubChem: A significant resource for scientists”
3:20-3:25
Discussion
3:25-3:45
Wolf-D. Ihlenfeldt, Xemistry GmbH, “Accessing U.S. Government Databases with the CACTVS Toolkit”
3:45-3:50
Discussion
3:50-4:10
Markus Sitzmann, NCI, “NCI/CADD Chemical Identifier Resolver: Indexing and Analysis of Available Chemistry Space”
4:10-4:15
Discussion
4:15-4:35
Marcus Hanwell, Kitware, Inc., “Chemical Databases and Open Chemistry on the Desktop”
4:35-4:45
Discussion

4:45-6:00 PM  Panel Discussion

Topic: “How do we get (authors to put, and publishers to accept if not require) chemistry information in a computer-readable format into primary chemical literature?”

Jasmine Young, Rutgers; RCSB PDB
Michael Gilson, UCSF; Binding DB database
Steve Heller, NIST; InChI
Dušanka Janežič, NIC, Ljubljana; JCIM, Associate Editor
Jay Schneekloth, CBL, NCI; Synthetic Chemistry & Screening
Markus Sitzmann, CADD Group, NCI; Chem. Identifier Resolver
Antony Williams, RSC; ChemSpider
MORNING  

Chairperson: Heather Carlson

9:00-9:15 AM  
Registration, Check-In

9:15-11:00 AM  
Morning Session I – Ligands and Binding Data

9:15-9:35  
Jasmine Young, RCSB, “Management and Distribution of Chemical Data in the PDB”

9:35-9:40  
Discussion

9:40-10:00  
James Dunbar, UMich, “CSAR and Binding MOAD: Two different databases, two different aims, one common goal provide the best protein-ligand data”

10:00-10:05  
Discussion

10:05-10:25  

10:25-10:30  
Discussion

10:30-10:50  
Michael Gilson, UCSD, “BindingDB: A Protein-Ligand Database for Drug Discovery”

10:50-11:00  
Discussion

11:00-11:15 AM  
Morning Break

11:15-12:30 AM  
Morning Session II – Drug Design; Validation of Chemistry Data

11:15-11:35  
John Overington, EMBL-EBI, “ChEMBL - An Open Data resource for drug discovery”

11:35-11:40  
Discussion

11:40-12:00  
Antony Williams, RSC, “ChemSpider: A Crowdsourcing Environment for Hosting and Validating Chemistry Resources”

12:00-12:05  
Discussion

12:05-12:25  
Talapady N Bhat, NIST, “Managing 2D and 3D Ligand Fragments from Disparate Large Resources”

12:25-12:30  
Discussion

12:30-1:30 PM  
Lunch Break & Poster Session
Friday, August 26, 2011

AFTERNOON

Chairperson: Markus Sitzmann

1:30-4:00 PM

Afternoon Session I – Drug Design; Validation of Chemistry Data

1:30-1:50  John Irwin, UCSF, “ZINC – A database of commercially available compounds for virtual screening”

1:50-1:55 Discussion

1:55-2:15 Scott Hutton, ChemNavigator/Sigma-Aldrich, “Aldrich Market Select Chemistry Portal, a new publicly accessible resource under development at Sigma-Aldrich”

2:15-2:20 Discussion

2:20-2:50 Noel O’Boyle, Open Babel Development Team, “Improving the quality of chemical databases with community-developed tools (and vice versa)”

2:50-2:55 Discussion

2:55-3:15 Andrew Lang, Oral Roberts Univ., and Jean-Claude Bradley, Drexel Univ., “The collection, curation and modeling of open melting point measurements”

3:15-3:20 Discussion

3:20-3:50 Martin Walker, SUNY, “Validation of Wikipedia Chemical Data”

3:50-4:00 Discussion

4:00-4:15 PM

Afternoon Break

4:15-5:55 PM

Afternoon Session II – Open Tools; OSR and Patents


4:35-4:40 Discussion

4:40-5:00 Koji Nakagawa, Kyushu Univ., “Digitizing Chemical Structure Images of Japanese Published Patent Applications into a Searchable Format”

5:00-5:05 Discussion

5:05-5:25 Marc Zimmermann, Univ. Bonn, “Evaluation of different benchmark sets and evaluation methods for automatic extraction of chemical entities from text and image”

5:25-5:30 Discussion

5:30-5:50 Stephen Boyer, IBM, “Computer Curation of WW Intellectual Property (patents) and the Scientific Literature”

5:50-5:55 Discussion

5:55-6:00 PM

Concluding Remarks
POSTER SESSION

1. XML-based description and uniqueness check for complex substances in the FDA Substance Registration System - Or: How to assure a UNII is actually UNIIque
Yulia Borodina, Frank Switzer, Tyler Peryea, and Lawrence Callahan
OCPP, OCS, OC, FDA

2. ToxML: A Format for Toxicology Data and Analysis Results -
R. Daniel Benz¹, Kevin P. Cross² and David A. Bower²
¹FDA/CDER/OTR/DDS and ²Leadscope, Inc

3. Chemical Evaluation and Risk Estimation System (CERES) Data Model Overview
Dimitar Hristozov, Annette McCarthy, Kirk Arvidson, and Chihae Yang
Office of Food Additive Safety, Center for Food Safety and Applied Nutrition, U.S. Food and Drug Administration, College Park, MD

4. FDI: Flexible Database Integrator for integrating multiple databases
Uma Mudunuri, Anney Che and Robert Stephens
Advanced Biomedical Computing Center, SAIC-Frederick, NCI-Frederick, MD

5. A Suite of Web Resources for Computational RNA Analysis, Prediction and Design
Eckart Bindewald¹, Wojciech Kasprzak¹, Bruce A. Shapiro²
¹Basic Science Program, SAIC-Frederick, Inc., NCI-Frederick, Frederick, Maryland, ²Center for Cancer Research Nanobiology Program, NCI-Frederick, MD

6. NIST Computational Chemistry Comparison and Benchmark Database
Russell Johnson
NIST, Gaithersburg, MD

7. Automating the process of 3D structure generation for 2D registration into a chemical cartridge database
Mitchell Miller¹, George (Mike) Hazard², Chuchu Lan¹
¹Scientific Thinking, LLC, Fairfax, VT. ²National Library of Medicine, Specialized Information Services, Bethesda, MD

8. The NIAID ChemDB HIV/AIDS Database
Margaret Rush¹, Danna Huffman², Glen Noble¹, Matthew Whiting¹, Mohamed Nasr³
¹Gryphon Scientific LLC, Takoma Park, MD; ²SRA International, Inc., Fairfax, VA; ³NIH, NIAID, Bethesda, MD

9. Development of Virtual Screening Models Based on NIH Roadmap Assay Data - Experimental Validation
Iwona E Weidlich¹, Igor Filippov³, and Marc C Nicklaus¹
¹Chemical Biology Laboratory, Center for Cancer Research, NCI, NIH, DHHS, Frederick, MD; ²University of Maryland, Baltimore County, Chemistry and Biochemistry Department, 1000 Hilltop Circle, Baltimore, MD; ³Chemical Biology Laboratory, SAIC-Frederick, Inc., NCI-Frederick, MD
10. Chemoinformatics infrastructure for drug discovery
   Kamal Kumar, Li Cheng, Jason Smith, Sid Chaudhury, Narender Singh, Mohamed
   Diwan AbdulHameed, Gregory Tawa, and Anders Wallqvist
   Biotechnology HPC Software Applications Institute, Telemedicine and Advanced
   Technology Research Center, U.S. Army Medical Research and Materiel Command,
   Fort Detrick, MD

11. A Physicochemical Descriptor-based Scoring Scheme for Effective and Rapid
    Filtering of Kinase-like Chemical Space Extracted from the ChEMBL Database
    Narender Singh, Sidhartha Chaudhury, Mohamed Diwan M. AbdulHameed, Anders
    Wallqvist, and Gregory Tawa
    DoD Biotechnology High Performance Computing Software Applications Institute,
    Telemedicine and Advanced Technology Research Center, U.S. Army Medical
    Research and Materiel Command, Fort Detrick, MD

12. BindingDB: A Protein-Ligand Database for Drug Discovery
    George Nicola, Tiqing Liu, Linda Hwang and Michael K. Gilson
    University of California San Diego

13. Databases and Tools Developed by LIPID MAPS Consortium
    Manish Sud, Eoin Fahy, Dawn Cotter, Robert Byrnes, Shakti Gupta, Mano
    Maurya, H. Alex Brown, Christopher K. Glass, Alfred H. Merrill, Jr., Robert C.
    Murphy, Christian R.H. Raetz, David W. Russell, Edward A. Dennis, Shankar
    Subramaniam
    LIPID MAPS Bioinformatics Core, SDSC/UCSD, 9500 Gilman Dr, La Jolla, CA
    92093; Department of Bioengineering, UCSD, 9500 Gilman Dr, La Jolla, CA,
    92093; Department of Pharmacology, Vanderbilt University Medical Center,
    Nashville, TN 37232; Department of Cellular and Molecular Medicine,
    UCSD, 9500 Gilman Dr, La Jolla, CA 92093; School of Biology, Georgia Institute of Technology,
    Atlanta, GA 30332; University of Colorado Health Sciences Center, Aurora, CO
    80045; Department of Biochemistry, Duke University Medical Center, Durham, NC
    27710; Department of Molecular Genetics, University of Texas Southwestern
    Medical Center, Dallas, Texas 75390; Department of Chemistry and Biochemistry,
    and Department of Pharmacology, UCSD, La Jolla, CA 92093.

14. Chemical eCommerce
    Klaus Gubernator
    eMolecules, Inc.

15. Optical Structure Recognition Application: development timeline and the status quo
    Igor Filippov, and Marc C Nicklaus
    1Chemical Biology Laboratory, SAIC-Frederick, Inc., NCI-Frederick, MD; 2Chemical
    Biology Laboratory, Center for Cancer Research, NCI, NIH, DHHS, Frederick, MD

16. Image-Based Automated Annotation of Chemical Database: Development and
    Application
    Jungkap Park, Gus Rosania, and Kazuhiro Saitou
    1Department of Mechanical Engineering, University of Michigan, Ann Arbor, MI;
    2Department of Pharmaceutical Sciences, University of Michigan, Ann Arbor, MI
Akio Fujiyoshi\textsuperscript{1}, Koji Nakagawa\textsuperscript{2}, and Masakazu Suzuki\textsuperscript{2}.
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\textsuperscript{2}Faculty of Mathematics, Kyushu University, Nishi-ku, Fukuoka, 819-0395 Japan