Cheminformatics Resources of U.S. Governmental Organizations

OCTOBER 18 - 20, 2023

Workshop Agenda

Day 1. Session: FAIR-ifying and Sharing Chemical-Related Data

Session chairs: Dr. Evan Bolton, Dr. Huixiao Hong

Time	Name	Agency	Title
9:05	Yulia Borodina	FDA/OC	Opening remarks, introduction of session chairs
9:15	Jian Zhang	NIH/NCBI	Chemical literature in PubChem
9:40	Akshay Narang	EPA	EPA's Substance Registry Services: https://cdxapps.epa.gov/oms-substance-registry-services/search
10:05	Steve Heller	NIH	Status of the IUPAC InChI project
10:30-10:45	**Coffee break**		
10:45	Huixiao Hong	FDA/NCTR	Welcome back
10:50	Margaret Rush	Gryphon Scientific	The National Institute for Allergy and Infectious Diseases' Anti HIV/OI/TB Therapeutics Database: ChemDB
11:15	Todd Martin	EPA	Dissemination of model metadata via the WebTEST2.0
11:40	Ewy Mathe	NIH/NCATS	Knowledge sources and approaches to guide analysis and interpretation of metabolomics (and other omics) data
12:05-13:35	**Lunch**		
13:35	Evan Bolton	NIH/NCBI	Welcome back
13:40	Kevin Snyder	FDA/CDER	SEND Sanitizer: Generation of Synthetic SEND Data from Existing Studies
14:05	Antony Williams	EPA	Chemistry data delivery from the US-EPA Center for Computational Toxicology and Exposure to support environmental chemistry
14:30	Tyler Peryea	FDA/OC	FDA GSRS: Systematically Describing Substances and Chemical Synthetic Schemes
14:55-15:10	**Coffee break**		
15:10	Huixiao Hong	FDA/NCTR	Welcome back
15:15	Panel discussion		
16:30	Yulia Borodina	FDA/OC	Adjourn

Day 2. Session: Application of Cheminformatics to Support Analytical Chemistry

Session chairs: Dr. Antony Williams, Dr. Tytus Mak

Time	Name	Agency	Title
9:05	Huixiao Hong	FDA/NCTR	Opening remarks, introduction of session chairs
9:15	Antony Williams	EPA	Diving into the depths of decade old analytical QC data associated with the Tox21 Project
9:40	Nathaniel Charest	EPA	ChemSTER: Visualizing Chemical Space for Non-Targeted Analysis
10:05	Charles Lowe	EPA	The Complexities of Chemical Information regarding Predicting Compound Amenability with Liquid Chromatography Mass Spectrometry
10:30-10:45	**Coffee break**		
10:45	Tytus Mak	NIST	Welcome back
10:50	Gregory Janesch	EPA	Developing an EPA database of open spectra to support non-targeted analysis
11:15	Ann Knolhoff	FDA/CFSAN	Non-Targeted Analysis using LC/HR-MS for Food Safety Applications: Capabilities, Challenges, and Potential Opportunities
11:40	Alex Chao	EPA	EPA's Non-Targeted Analysis WebApp: Linking cheminformatics resources with NTA workflows
12:05-13:05	**Lunch**		
13:05	Antony Williams	EPA	Welcome back
13:10	Tytus Mak	NIST	MetaboPique: A High-Throughput Workflow for Validating, Annotating, and Organizing Tandem LC-MS Spectra Derived from Biological Samples
13:35	Frank Delaglio	NIST	Chemometrics and Machine Learning to Enable Applications of NMR in Biomanufacturing
14:00	Brian Cooper	NIST	Beyond the top hit: interactive visual interpretation of hybrid similarity search hit lists
14:25-14:40	**Coffee break**		
14:40	Tytus Mak	NIST	Welcome back
14:45	Goncalo Gouveia	NIST	NMR metabolomics from design to metabolite ID
15:10	Hani Habra	NIST	Disparately Acquired LC-MS Alignment with Applications in Metabolomics

15:35	Eric Miller	CDRH	Confident Identification of Extractables in Medical Devices: The need for a standardized approach for chemical characterization to facilitate toxicological risk assessment.
15:45	Panel discussion		
16:30	Huixiao Hong	FDA/NCTR	Adjourn

Day 3. Session: The Path Forward for Machine Learning with Chemical Data and Molecular Representations

Session chairs: Dr. Eric A Stahlberg, Dr. Samir Lababidi

Time	Name	Agency	Title
9:05	Evan Bolton	NIH/NCBI	Opening remarks, introduction of session chairs: Eric A Stahlberg (FNLCR), Dr. Samir Lababidi (FDA/ODAR)
9:15	Eric Stahlberg	FNLCR	Using AI to Improve Predictive Models for Chemistry
9:40	Rick Stevens	Argonne National Laboratory	The DOE/NCI IMPROVE Framework for AI Model Improvement and its Potential Application to AI Toxicology Models
10:05	Marc Nicklaus	NIH/NCI	SAVI - Going Back to Beyond AI
10:30-10:45	**Coffee Break**		
10:45	Eric Stahlberg	FNLCR	Welcome back
10:50	Jie Liu	FDA/NCTR	Machine Learning Models for Rat Multigeneration Reproductive Toxicity Prediction
11:15	Katherine Phillips	EPA	Development, Evaluation, and Application of Quantitative Structure-Use Relationship Models
11:40	Samir Lababidi	FDA/OC	AI Methods for Chemical Datasets
12:05-13:35	**Lunch**		
13:35	Samir Lababidi	FDA/OC	Welcome back
13:40	Neeraj Kumar	Pacific Northwest National Laboratory	Machine Learning with Chemical Data and Molecular Representations
14:05	Felice Lightstone	Lawrence Livermore National Laboratory	Data and Computing Resources for Building Predictive Safety Models
14:30	Mike Mikailov and Yulia Borodina	FDA/CDRH; FDA/OC	Scalable Workflow for On-Demand Lead Optimization - A Pilot

15:00-15:15	**Coffee Break**		
15:15	Eric Stahlberg	FNLCR	Welcome back
15:20	Panel discussion		
16:30	Samir Lababidi	FDA/OC	Adjourn