Cheminformatics Resources of U.S. Governmental Organizations
OCTOBER 16 - 18, 2024
Workshop Agenda

Day 1 (Oct. 16, 2024). Session: Application of Cheminformatics to Support Analytical Chemistry

Session Chairs: Dr. Tytus Mak (NIST/MSDC), Dr. Karen E. Butler (FDA/CFSAN)
Session Moderators: Dr. Margaret Rush (NIAID), Dr. Yulia Borodina (FDA/ODT)

Time	Name	Agency	Title
9:00	Yulia Borodina	FDA	Opening remarks, introduction of session chairs
9:10	Tytus Mak	NIST	Welcome session 1
9:15	Karen Butler	FDA	Investigating the Impact of Replicates for Different Food Matrices on Non-Targeted Analysis Results
9:40	Anh Tran	NIST	Evaluation of Peptide Isotopologue Envelope for Enhancement of Trapped Ion Mobility Data
10:05	E. Tyler Carr	EPA	Curating and Visualizing the Analytical Methods and Open Spectra Database's Functional Use Chemical Taxonomy
10:30-10:45	**Coffee Break**		
10:45	Karen Butler	FDA	Welcome back
10:50	Tytus Mak	NIST	Moleculyzer: A High-Performance Algorithm for Untargeted LC-MS Metabolomics Chromatogram Deconvolution and Metabolite Identification
11:15	Alix Rodowa	NIST	Per- and Polyfluoroalkyl Substances (PFAS): Development of Reference Materials and Ongoing Efforts
11:40	Marc Nicklaus	NCI	We Don't Forget Tautomers
12:05-13:05	**Lunch**		
13:05	Tytus Mak	NIST	Welcome back
13:10	Tony Williams	EPA	3 years, 30,000 spectra, 9,000 chemicals – What did we learn?
13:40	Nathaniel Charest	EPA	Landscapes of Chemistry: Visualizing Chemical Space with ChemSTER
14:10-14:25	**Coffee Break**		
14:25	Karen Butler	FDA	Welcome back
14:30	Gregory Janesch	EPA	Applying Cheminformatics to Develop a Structure Searchable Database of Analytical Methods
15:00	Alex Chao	EPA	EPA's Non-Targeted Analysis WebApp: A web-based software tool for production-level NTA
15:30	Meg Rush (moderator)	NIAID	Panel Discussion
16:30	Meg Rush	NIAID	Adjourn

Day 2 (Oct. 17, 2024). Session: Predictive Models and Protected Data

Session Chairs: Dr. Eric A Stahlberg (FNLCR/CDSI), Dr. Samir Lababidi (FDA/ODT)
Session Moderators: Dr. Margaret Rush (NIAID), Dr. Tytus Mak (NIST)

Time	Name	Agency	Title
9:00	Tytus Mak	NIST	Opening remarks, introduction of session chairs
9:05	Eric Stahlberg	FNLCR	Welcome session 2
9:10	Mohamed AbdulHamee	DoD	Development of open toxicity prediction tools for countermeasure discovery
9:40	Michael Appell	USDA	Predictive quantitative structure–activity relationship modeling the antifungal and antimicrobial properties of GRAS food compounds
10:10-10:25	**Coffee break**		
10:25	Eric Stahlberg	FDA	Welcome back
10:30	Charlie Lowe	EPA	Structural peculiarities of quaternary ammonium compounds and how their representation effects QSAR modeling
11:00	Samir Lababidi	FDA	Predicting Active and Inactive Substances
11:30	Dan Vallero	EPA	Evaluation of quantitative structure activity relationship for predicting plasma protein binding of per- and polyfluoroalkyl substances in humans
12:00-13:15	**Lunch**		
13:15	Samir Lababidi	FDA	Welcome back
13:20	Yulia Borodina	FDA	Deidentification of Chemistry Data for Training Predictive Models: A Pilot on precisionFDA
13:50	Debsindhu Bhowmik	ORNL	SLGE-MoDe: Synergizing Language Models, GANs, and Evolutionary Algorithms for Molecular Design
14:20	Eric Stahlberg	FNLCR	Sharing, Improving and Evaluating Predictive Cheminformatics Models
14:50-15:05	**Coffee break**		
15:05	Xiang Yu	FDA	Fragment Nitrosamine Risks Based on Quantity, Extent of Conversion Rate and CPCA Calculations
15:30	Tytus Mak (Moderator)	NIST	Panel discussion
16:30	Tytus Mak	NIST	Adjourn

Day 3 (Oct. 18, 2024). Session: Data Science Interfaces to Chemistry-oriented Resources

Session Chairs: Dr. Evan Bolton (NIH/NLM/NCBI), Dr. Jie Liu (FDA/NCTR)
Session Moderators: Dr. Huixiao Hong (FDA/NCTR), Dr. Eric A Stahlberg (FNLCR/CDSI)

Time	Name	Agency	Title
9:00	Eric Stahlberg	FNLCR	Opening remarks, introduction of session chairs
9:05	Jie Liu	FDA	Welcome session 3
9:10	Jian Zhang	NIH	PubChem classification browser
9:35	Souvik Dey	DoD	Enhancing Classification of Imbalanced Muscarinic Receptor M1 Datasets Using Transfer Learning and Generative AI Techniques
10:00	Antony Williams	EPA	Consuming and Delivering Government APIs for EPA Application
10:30-10:45	**Coffee break**		
10:45	Evan Bolton	NIH	Welcome back.
10:50	Ewy Mathe	NIH	Improving interoperability of knowledge sources to advance translational research efforts
11:15	Keith Kelleher Jessica Maine	NIH	Comprehensive Annotations on Drug Targets with Pharos
11:45	Kamel Mansouri	NIH	Democratizing Cheminformatics Using Guided Automated Workflows
12:05-13:05	**Lunch**		
13:05	Evan Bolton	NIH	Welcome back.
13:10	Paul Kruse	EPA	A Cheminformatics Workflow for Higher-Throughput Modeling of Chemical Exposures From Biosolids
13:35	Debsindhu Bhowmik	ORNL	AI-MoDe (AI-Driven Molecular Design): Integrating CompBio with FAIR Cheminformatics and Data Science Interfaces
14:00	Margaret Rush	NIAID	The ChemDB HIV, Opportunistic Infection and Tuberculosis Therapeutics Database
14:25	Debananda Das	NIH	Schrodinger molecular modeling software at NCI and NIH
14:35-14:50	**Coffee break**		
14:50	Jie Liu	FDA	Welcome back.
14:55	Tyler Peryea	FDA	FDA's Global Substance Registration System: Overview and Recent Developments
15:25	Nancy Baker	EPA	PubMed Abstract Sifter version 8 integrates chemistry data APIs from EPA's DSSTox database and PubChem
15:55	Eric Stahlberg	FNLCR	Adjourn