Cheminformatics Resources of U.S. Governmental Organizations
JANUARY 5 - 7, 2026
Workshop Agenda

Day 1 (Jan. 5, 2026). Session: Applications of AI/ML in Cheminformatics Research

Session Chairs: Dr. Samir Lababidi (FDA/ODT), Dr. Huixiao Hong (FDA/NCTR)
Session Moderators: Dr. Evan Bolton (NIH/NBCI), Dr. Yulia Borodina (FDA/ODT)

Time	Name	Agency	Title
9:00	Yulia Borodina	FDA	Opening remarks
9:10	Huixiao Hong	FDA	Welcome session 1
9:15	Samir Lababidi	FDA	Introduction to AI/ML
9:25	Michael Santillo	FDA	Combining in silico and in vitro toxicological data for profiling chemicals in foods and dietary supplements: A case study
9:50	Yitong Liu	FDA	Integration of computational models to predict botanical phytochemical constituent clearance routes by the Extended Clearance Classification System (ECCS)
10:15-10:30			**Coffee Break**
10:30	Samir Lababidi	FDA	Welcome back
10:35	Kamel Mansouri	NIH	Democratizing Computational Toxicology tools with Automated Workflows
11:00	Alexey Zakharov	NIH	AI-Driven Drug Discovery: Bridging Medicinal Chemistry and Machine Learning
11:25	Debsindhu Bhowmik	ORNL	GEMMINI: A Generative AI Platform for Custom Molecular Design, Validation, and Discovery
11:55-13:30			**Lunch**
13:30	Samir Lababidi	FDA	Welcome back
13:35	Huixiao Hong	FDA	Empower Tobacco Constituent Screening for nAChR α7 Binding with Machine Learning and 3D Interaction Descriptors
14:00	Ruili Huang	NIH	Application of Tox21 data in machine learning models for chemical safety assessment
14:25	Raul E. Cachau	NIH	AI as a Molecular Translator: Bridging Chemical Space, Biological Function, and Drug Discovery
14:50-15:05			**Coffee break**
15:05			Panel discussion
16:30	Samir Lababidi		Adjourn

Day 2 (Jan. 6, 2026). Session: Cloudization of Cheminformatics and Data Sharing

Session Chairs: Dr. Ewy Mathé (NIH/NCATS), Dr. Evan Bolton (NIH/NCBI)
Session Moderators: Dr. Tytus Mak (NIST/MSDC), Dr. Jie Liu (FDA/NCTR)

Time	Name	Agency	Title
9:00	Tytus Mak	NIST	Opening remarks
9:05	Ewy Mathé	NIH	Welcome session 2
9:15	Evan Bolton	NIH	PubChem, Cloud, and more!
9:40	Marlene Kim	FDA	Global Substance Registration System (GSRS), Home of the Unique Ingredient Identifier (UNII) and More
10:05	Tyler Peryea	FDA	Lightweight Client-Side Cheminformatics with JSChemify and GSRS (this talk should precede Mitch's)
10:30	Mitch Miller	NIH	JavaScript tools for chemistry inside Excel: one add-in's experience
10:55-11:10			**Coffee Break**
11:10	Evan Bolton	NIH	Welcome back
11:15	Mark Williams	NIH	Data Accessibility and Findability with Government Cloud Resources
11:40	Mike Mikailov, Yulia Borodina	FDA	Cheminformatics Scientific Computing: On-Prem HPC versus Cloud
12:05	Ewy Mathé	NIH	Harmonization, analysis, and interpretation of metabolomic and other research data
12:30-14:00			**Lunch**
14:00	Ewy Mathé	NIH	Welcome back
14:05	Katherine Heal	PNNL	National Microbiome Data Collaborative: Metadata harmonization to enhance data reuse of mass spectrometry data
14:30	Jessica Maine, Keith Kelleher	NIH	Standards-Aligned, Interoperable Data Integration Across Translational Sciences: Modular ETL Pipelines and Harmonization Approaches in IFX/ODIN
14:55	Chris Mungall	LBNL	CHEMROF: An AI-ready ontological framework for managing information about chemical entities
15:20-15:35			**Coffee Break**
15:35			Panel Discussion
16:30	Evan Bolton		Adjourn

Day 3 (Jan. 7, 2026). Session: Application of Cheminformatics to Support Analytical Chemistry

Session chairs: Dr. Tytus Mak (NIST/MSDC), Dr. Karen E. Butler (FDA/HFP)
Session Moderators: Dr. Evan Bolton (NIH/NCBI), Dr. Samir Lababidi (FDA/ODT)

Time	Name	Agency	Title
9:00	Evan Bolton	NIH	Opening remarks
9:05	Tytus Mak	NIST	Welcome session 3
9:15	Ann Knolhoff	FDA	Non-Targeted Analysis: Capabilities, Quality, and Opportunities for Compound Identification
9:45	Zachary Kralles	FDA/JHU	Quantitative Non-Targeted Analysis of Pesticide Residues in Food Crops
10:15	Ben Place	NIST	The DIMSpec Project: developing a FAIR open-source database for analytical chemistry data
10:45-11:00			**Coffee Break**
11:00	Karen Butler	FDA	Welcome back
11:05	Anh Tran	NIST	Towards Accurate TIMS-Derived Peptide Ion Mobility Measurements: Calibration Strategy and MS1/MS2 Discrepancies
11:35	Aivett Bilbao	PNNL	AI-powered molecular profiling for Ion Mobility-Mass Spectrometry
12:05-13:35			**Lunch**
13:35	Tytus Mak	NIST	Welcome back
13:40	Szabina Stice	FDA	Building the Expanded Decision Tree: Enhancing Predictive Toxicology through Cheminformatics and Expert Rules
14:10	David Sheen	NIST	PyChemAuth: Python-based Chemometric Authentication
14:40	Yufang Zheng	NIST	Enhancing the Coverage and Quality of Spectra of Per- and Polyfluoroalkyl Substances (PFAS) in a Comprehensive Electron Ionization (EI) Mass Spectral Library
15:10-15:25			**Coffee Break**
15:25			Panel Discussion
16:30	Karen Butler	FDA	Adjourn