

Cheminformatics Resources of U.S. Governmental Organizations

MAY 9 - 11, 2022
Workshop Agenda

Day 1

Session 1			
Time	Name	Agency	Title
9:05	Yulia Borodina	FDA/OC	Opening remarks, introduction of session chairs: Huixiao Hong (FDA/NCTR) and Patra Volarath (FDA/CDER)
9:15	Steve Heller	NIH	The IUPAC InChI Chemical Identifier Standard Project
9:40	Jian Zhang	NIH/NCBI	Open access chemical information integration in PubChem
10:05	Tyler Peryea	FDA/OC	FDA's Global Substance Registration System
10:30-10:45	Coffee break		
10:45	Huixiao Hong or Patra Volarath		Welcome back
10:50	Akshay Narang	EPA	Where to find Regulated Substances at EPA: The Substance Registry Service
11:15	Christopher Ellis	DOD	The Threat Agent Science Chemical Space
11:40	Tammy Page	FDA/CFSAN	Food and Food Packaging Substances at FDA
12:05-13:05	Lunch		

Session 2

Time	Name	Agency	Title
13:05	Evan Bolton	NIH/NCBI	Welcome back. Introduction of session chairs: Gergely Zahoranszky-Kohalmi (NIH/NCATS) and Jung Lee (FDA/CDER)
13:10	Anubhav Jain	DOE/LBNL	The Materials Project: A Community Data Resource for Accelerating New Materials Design
13:35	Jessie Carder	USDA	USDA's AWIC: How to Conduct a Literature Search for Chemoinformatics Information to Find Animal Use Alternatives
14:00	Louise Sumner or Margaret Rush	NIH/NIAID	ChemDB: NIH NIAID's Therapeutics Database for Compounds Tested against HIV, Tuberculosis, HBV, and Other Opportunistic Infections
14:25-14:40	Coffee break		
14:40	Zahoranszky-Kohalmi or Jung Lee		Welcome back
14:45	Eugene Demchuk	CDC/ATSDR	Per- and polyfluoroalkyls – a new class of persistent organic pollutants
15:10	Ann Richard	EPA	The strategic role and requirements of chemical curation in support of EPA's DSSTox database
15:35	Marc Nicklaus	NIH/NCI	NCI CADD Group cheminformatics resources: From web tools to billion-molecule databases

16:00

Evan Bolton

NIH/NCBI

Adjourn

Day 2

Session 3

Time	Name	Agency	Title
9:05	Patra Volarath	FDA/CDER	Opening remarks, introduction of session chairs Ann Richard (EPA) and Huixiao Hong (FDA/NCTR)
9:15	Jie Liu	FDA/NCTR	Development of cheminformatics systems for facilitating application of computational chemistry in regulatory sciences
9:40	Michael Appell	USDA	Quantum chemical and quantitative structure-activity relationship studies to reduce exposure to mycotoxins in food and feed
10:05	Yitong Liu	FDA/CFSAN	In silico evaluation of biokinetics and toxicity of phytochemicals
10:30-10:45	Coffee break		
10:45	Ann Richard (EPA) and Huixiao Hong (FDA)		Welcome back
10:50	Nathan Mahynski	NIST	Chemometric Trends for Persistent Anthropogenic Toxins found in Seabirds of the Northern Pacific
11:15	Minjun Chen	FDA/NCTR	QSAR modeling for drug-induced liver injury
11:40	Jahan Cooper	FDA/CDER	The FDA/CDER Computational Toxicology Consultation Service Chemical Dictionary and Consult Database
12:05-13:05	Lunch		

Session 4

Time	Name	Agency	Title
13:05	Gergely Zahoranszky-Kohalmi	NIH/NCATS	Welcome back. Introduction of session chairs: Jie Liu (FDA/NCTR) and Tony Williams (EPA)
13:10	Eric Stahlberg	FNLCR	ATOM: Integrated AI Modeling to Accelerate Cancer Drug Discovery
13:35	Sankalp Jain	NIH/NCATS	A hybrid in silico approach reveals novel inhibitors of multiple SARS-CoV-2 variants
14:00	Naomi Kruhlak	FDA/CDER	Application of (Quantitative) Structure-Activity Relationships to pharmaceuticals at FDA/CDER
14:25-14:40	Coffee break		
Time	Name	Agency	Title
14:40	Jie Liu or Tony Williams		Welcome back
14:45	Jacob Monroe	NIST	Bayesian Methods for Enhanced Model Fitting and Uncertainty Analysis of Simulation Data
15:10	Mike Mikailov	FDA/CDRH	Scaling Cheminformatics Applications on CDRH HPC clusters
15:35	Raul Cachau	NIH/NIAID	Encoding chemical information in the age of AI
16:00	Gergely Zahoranszky-Kohalmi	NIH/NCATS	Adjourn

Day 3

Session 5

Time	Name	Agency	Title
9:05	Huixiao Hong	FDA/NCTR	Opening remarks, introduction of session chairs: Iwona Weidlich (FDA/CDER) and Evan Bolton (NIH/NCBI)
9:15	Antony Williams	EPA	Delivering chemical-associated data via EPA web applications
9:40	Andrei Kazakov	NIST	Overcoming Scarcity in the Scientific Literature
10:05	Mitch Miller	NIH/NLM	Structures in ChemIDplus: continuous improvement in small steps
10:30-10:45	Coffee Break		
10:45	Evan Bolton	NIH/NCBI	Welcome back
10:50	Gergely Zahoranszky-Kohalmi	NIH/NCATS	Reaction Informatics Innovations in ASPIRE
11:15	Lewis Geer	NIST	NIST mass spectral libraries
11:40	Yulia Borodina	FDA/OC	PrecisionFDA – a platform where Government cheminformaticians can collaborate with Academia and Industry
12:05-13:05	Lunch		
13:05	Iwona Weidlich	FDA/CDER	Welcome back. Introduction of panelists.
13:10-14:40	Panel discussion		Andrei Kazakov Marc Nicklaus Evan Bolton Ann Richard Tony Williams Raul Cachau Tammy Page
14:40	Iwona Weidlich	FDA/CDER	Adjourn