NACRW 2025
July 27, 2025
4:00 – 5:30 pm

Workshop Outline

US-EPA Informatics Tools Supporting Chemical Residue Analysis

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The EPA utilizes mass spectrometry extensively in environmental monitoring and analysis, developing and implementing various methods to identify and quantify contaminants in air, water, and soil. Key EPA efforts include: 1) the development of standardized methods, drinking water analysis for various contaminants, including volatile and semi volatile organic compounds, pesticides, and pharmaceuticals; 2) PFAS Research to research and identify novel per- and polyfluorinated alkyl substances (PFAS) in various matrices; 3) air monitoring for analyzing toxic organic compounds in air; 4) to monitor the effectiveness of remediation efforts, such as the cleanup of contaminated sites.

The Center for Computational Toxicology and Exposure at the US-EPA supports many of these activities by the development of software and databases that are delivered as free access resources to the community. These provide access to data associated with 1.2 million chemical substances including chemical structures, identifiers/synonyms, physicochemical property data, toxicity, and bioactivity data. The primary application from the center is the CompTox Chemicals Dashboard (https://comptox.epa.gov/dashboard) but the chemical collection also provides the underpinning for the publicly accessible cheminformatics modules (https://hcd.rtpnc.epa.gov/), and the chemical transformation simulator (https://qed.epa.gov/cts/). Other tools in development and presently working towards public access, are the Analytical Methods and Open Spectra database (AMOS), the Chemical Transformations database (CheT), and the Non-Targeted Analysis WebApp.

This hands-on workshop will provide an overview of several of the publicly accessible software applications which can be of value to scientists working in the field of analysis of pesticides, veterinary drug residues, and other chemicals in food, animal feed, and environmental samples. This interactive workshop encourages attendees to bring their computers and work along with workshop examples as well as bring your own questions and challenges for consideration.

COMPTOX CHEMICALS DASHBOARD (https://comptox.epa.gov/dashboard/)

- Data sourcing and curation – assembling various types of data to support the applications: the challenges of chemical structures, names, and other identifiers
- Accessing chemical class related data via the CompTox Chemicals Dashboard
    - Searching – text, structures, substructures, and similarity searching
    - Mass and Formula searching
    - Sourcing property and hazard data
- The benefits of MS-Ready structures (https://jcheminf.biomedcentral.com/articles/10.1186/s13321-018-0299-2)
- Batch Searching (https://pmc.ncbi.nlm.nih.gov/articles/PMC8630643/)

CHEMINFORMATICS MODULES

- Hazard Comparison profiling - accessing toxicity hazard data for chemicals
- Safety Comparison profiling – accessing safety data (PPE, GHS, ignitability and reactivity)
- Coupling structure searching with hazard profiling
- Integration between the cheminformatics modules and the Dashboard

WORK-IN-PROGRESS

- The Analytical Methods and Open Spectra Database (hopefully released by the NACRW meeting)
    - Searching – chemicals, identifiers, sources
    - Searching – spectral searching against ~1 million spectra
    - Filtering methods by analytes, matrix, source, and technology
    - Finding methods based on structural similarity searching
    - Functional use classifications
- The Non-Targeted Analysis data processing and analysis web application (NTA WebApp)
    - aligning best practices for NTA, promoting standardization and reproducibility
    - data processing and reporting, ensuring consistency and reliability in the analysis of NTA data
    - integration with experimental and predicted mass spectral databases

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