North American Chemical Residue Workshop 2024
Workshop with Antony Williams US EPA

Sunday, July 14, 2024
Fort Lauderdale Marriott Harbor Beach
4:00-5:30 pm
Location: Grand Ballroom E, 3rd level

A Hands-On Experience of Accessing Data from EPA Dashboards to Support Analysis of Pesticides, Veterinary Drug Residues, and other Chemicals in Food, Animal Feed, and Environmental Samples

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The US-EPA Center for Computational Toxicology and Exposure has been developing software and databases that serve the chemistry community for many years. These provide access to an abundance of data for over 1.2 million chemical substances including structures, synonyms, physicochemical property data, toxicity and bioactivity data. This hands on workshop will provide an overview of several publicly accessible web-based software applications developed at the USEPA 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. While the primary software application from the Center is the CompTox Chemicals Dashboard almost a dozen proof-of-concept applications have been built serving various capabilities. The publicly accessible Cheminformatics Modules (https://www.epa.gov/chemicalresearch/cheminformatics) provides access to six individual modules to allow for hazard comparison for sets of chemicals, structure-substructure-similarity searching, structure alerts and batch QSAR prediction of both physicochemical and toxicity endpoints. A number of other applications in development include a chemical transformations database and a database of analytical methods and open mass spectral data. Each of these depends on the underlying DSSTox chemicals database, a rich source of chemistry data for over 1.2 million chemical substances. This workshop will provide an overview of existing publicly accessible Dashboards to access data to support pesticide research and pesticide residue analysis. An outline includes:

COMPTOX CHEMICALS DASHBOARD

- Data sourcing and curation – assembling pesticide data for distribution and tools: the challenges of chemical structures, names and other identifiers
- Introducing the DTXSID substance identifier
- Accessing pesticides related data via the CompTox Chemicals Dashboard
    - Searching – text, structures, substructures and similarity searching
    - Mass and Formula searching
    - Sourcing property and hazard data
- Linked Substances (using MS-Ready data mappings)
- Single versus Batch Searching
- Real time QSAR predictions

CHEMINFORMATICS MODULES

- What are proof-of-concept modules vs the Dashboard?
- Hazard Comparison profiling
- Coupling structure searching with hazard profiling
- Batch QSAR prediction

WORK-IN-PROGRESS

- The Analytical Methods and Open Spectra Database
    - Searching- chemicals, identifiers, “similar methods”
    - Filtering methods by analytes, matrix, source and technology
    - Integration to Dashboards

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