Cheminformatics Analysis Modules

NAMs Training Workshop

RTP, NC

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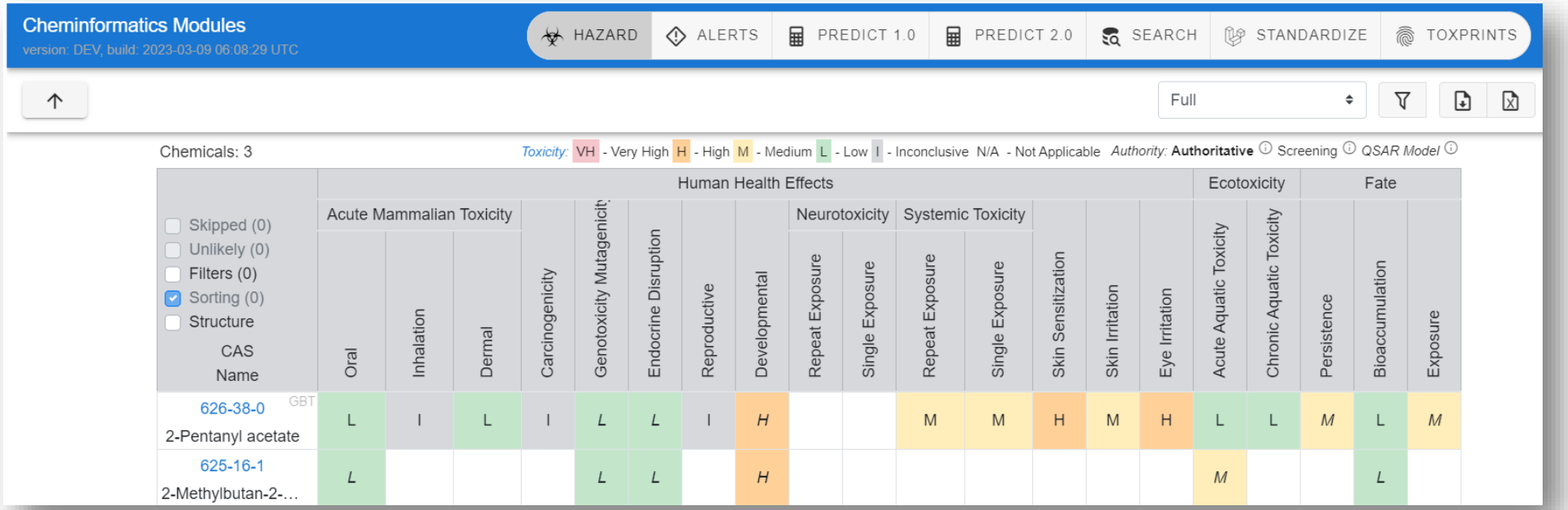
Purpose of the Cheminformatics Modules

- PoCs are research software builds to **prove approaches** before moving into production software environments
- Assemble data, develop data model(s), **test** user interface **approaches**, work with test user base to **garner feedback**
- PoCs are internal access data refreshes and application updates can be more frequent

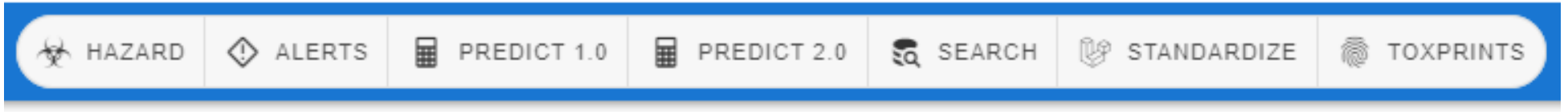
Accessing the Cheminformatics Analysis Modules

- https://www.epa.gov/comptox-tools/cheminformatics



Purpose of the Cheminformatics Modules

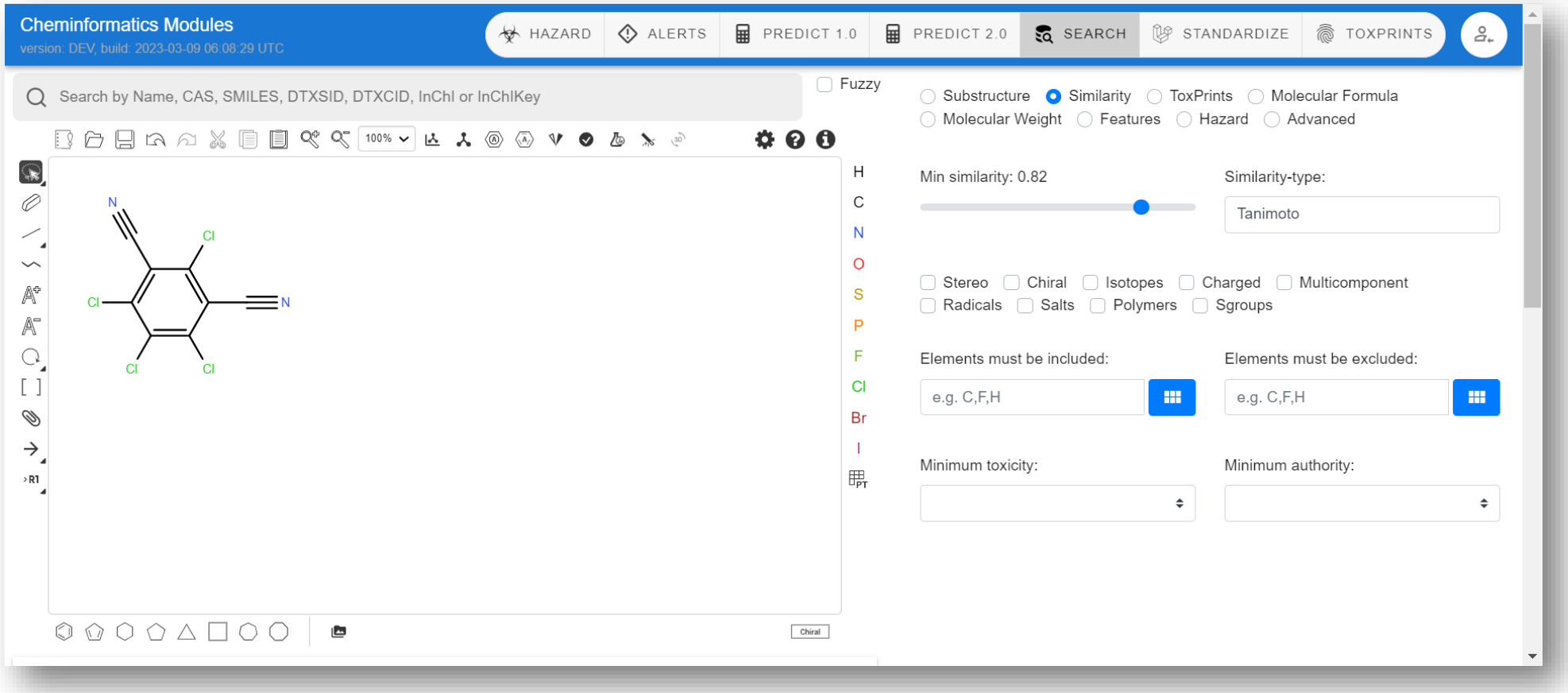
- The Cheminformatics Modules includes:
  - Hazard Comparison
  - Batch QSAR Predictions
  - Structure/Substructure/Similarity Search
  - ToxPrints



- These modules allow for user testing and feedback and provide inspiration for implementation into production systems

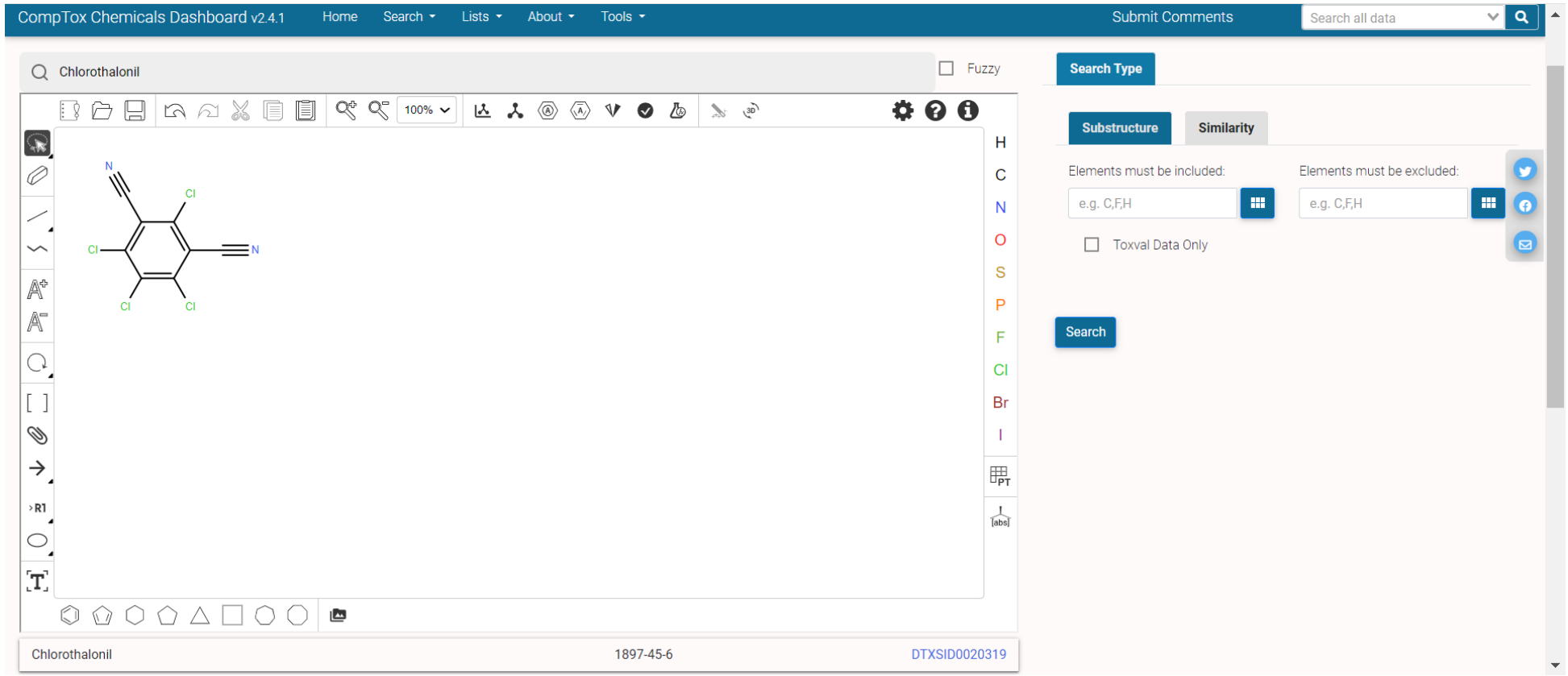
Initiated in Cheminformatics Modules

- Structure/substructure/similarity search module



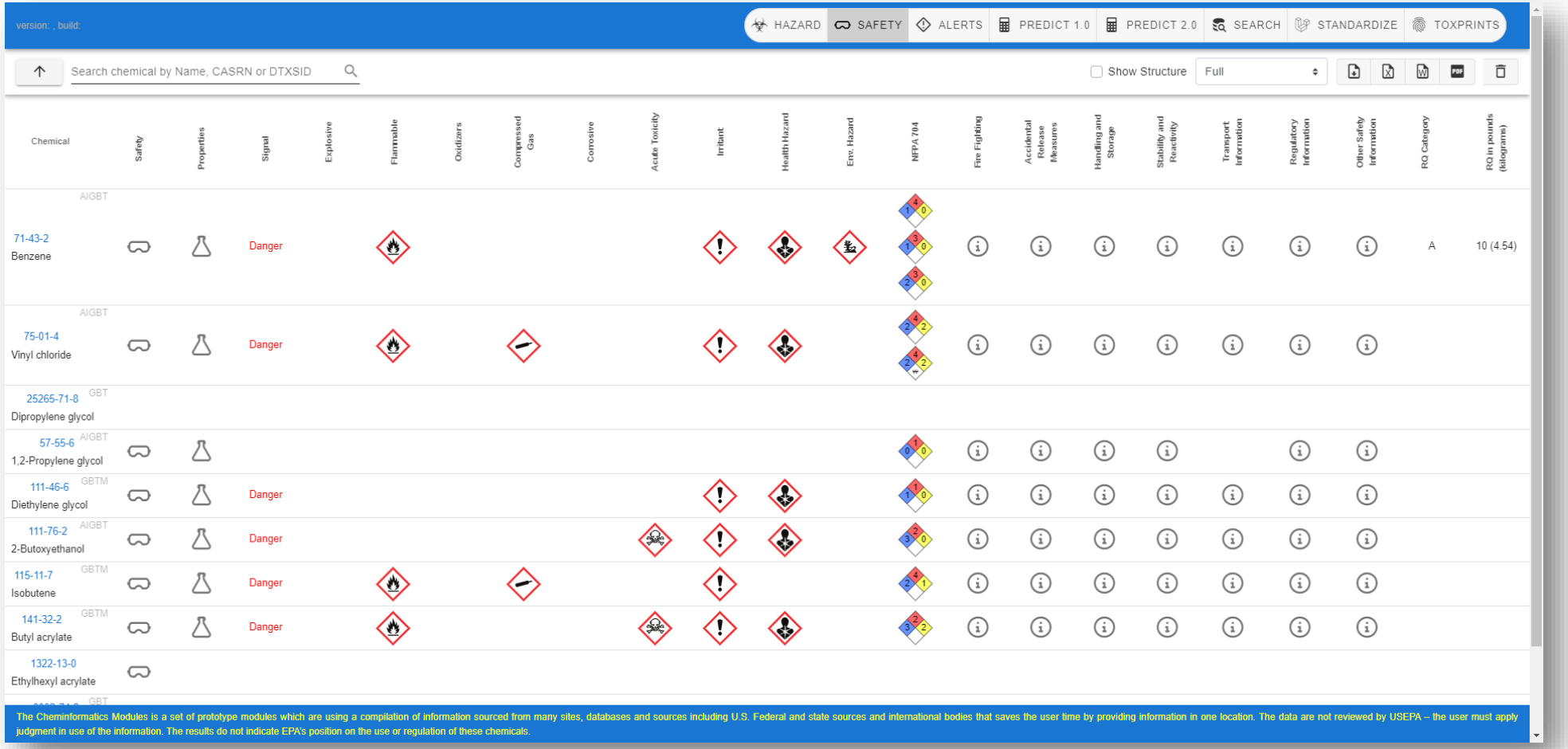
Reimplemented in the Dashboard

- A subset of functionality was moved to the Dashboard



Not all PoCs are Public: Work-In-Progress

- Safety Module



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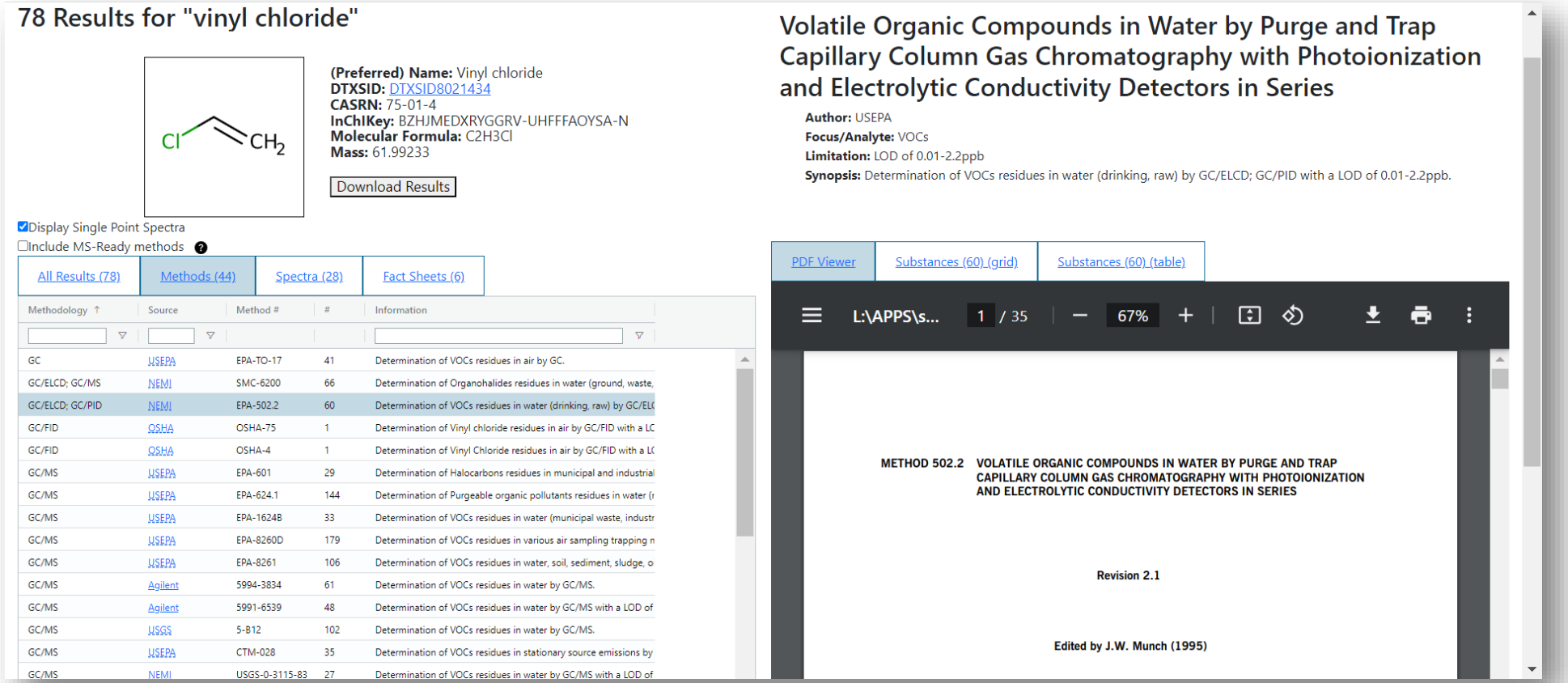
- Analytical Methods and Open Spectral Database



Interested in a demo?

- Cheminformatics Modules: https://www.epa.gov/comptox-tools/cheminformatics

- Contact for follow up demo: Antony Williams williams.antony@epa.gov