A Comprehensive Primer for the CompTox Chemicals Dashboard

- **Antony Williams –** General chemistry capabilities and advanced search, predicted model and experimental data, real time modeling, advanced searches based on mass, formula, formula generation (15 minutes)
- **Katie Paul Friedman –** Hazard and Bioactivity Functionality (15 minutes)
- **John Wambaugh –** Absorption, Distribution, Metabolism and Excretion Data (10 minutes)
- **Kathie Dionisio –** Exposure Functionality including Product Use Categories, Chemical Weight Fraction and Chemical Functional Use (10 minutes)
- **Kristin Isaacs –** Exposure Functionality including Toxics Release Inventory, Monitoring Data, Production Volume and Exposure Predictions (10 minutes)
- **Grace Patlewicz –** GenRA, Similar Compounds and Related Substances (10 minutes)
- **Nancy Baker –** Literature Search Functionality (15 minutes)
- **Antony Williams –** Batch search and lists (10 mins)

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General chemistry capabilities and advanced search, predicted model and experimental data, real time modeling, advanced searches based on mass, formula, formula generation

Antony Williams

Center for Computational Toxicology and Exposure

MS-Ready

Journal of Cheminformatics

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Methodology | Open Access | Published: 30 August 2018

"MS-Ready" structures for non-targeted high-resolution mass spectrometry screening studies

Andrew D. McEachran, Kamel Mansouri, Chris Grulke, Emma L. Schymanski, Christoph Ruttkies & Antony J. Williams

Journal of Cheminformatics **10**, Article number: 45 (2018) | Cite this article

2910 Accesses | **10** Citations | **13** Altmetric | Metrics

Our Curation Process

Computational Toxicology 12 (2019) 100096

Contents lists available at ScienceDirect

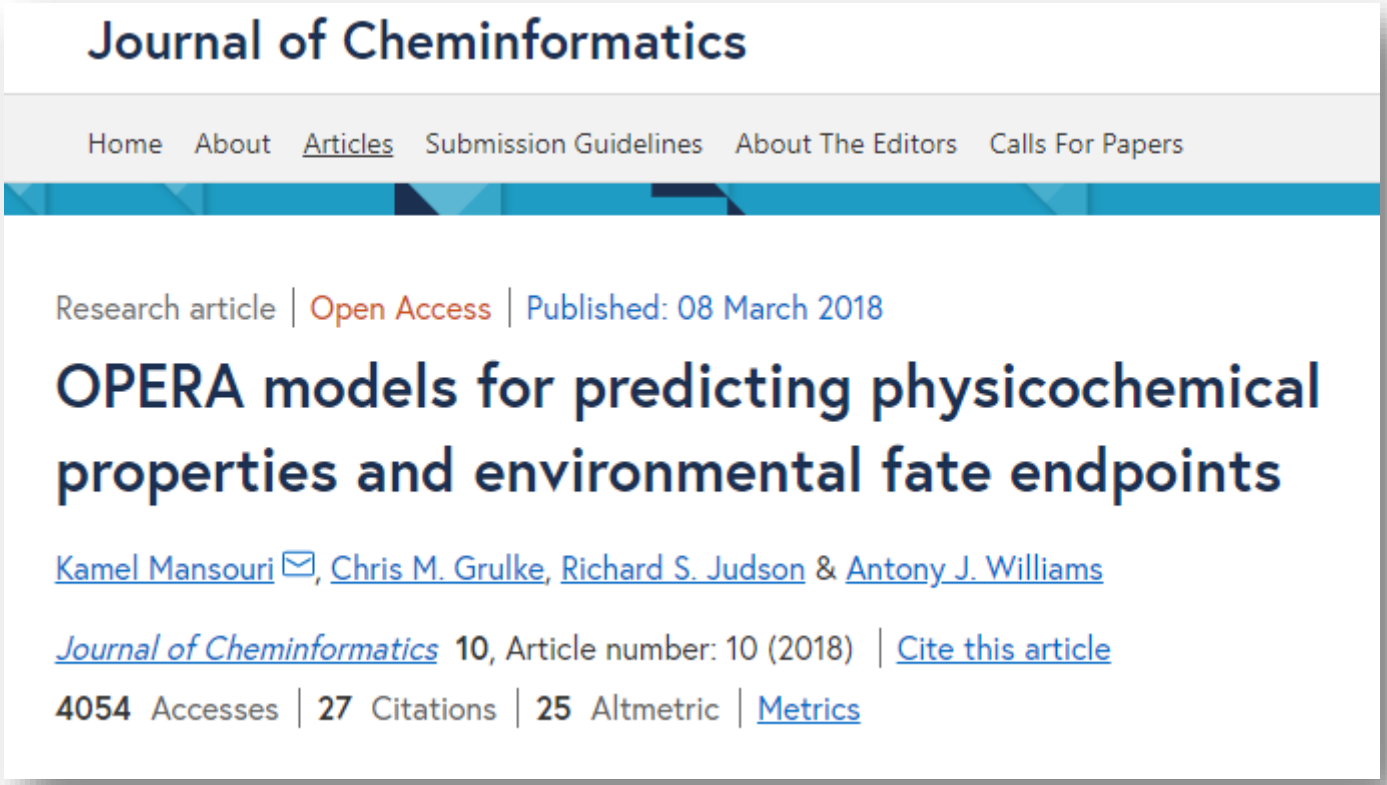
Computational Toxicology

journal homepage: www.elsevier.com/locate/comtox

EPA's DSSTox database: History of development of a curated chemistry resource supporting computational toxicology research

Christopher M. Grulke[a], Antony J. Williams[a], Inthirany Thillanadarajah[b], Ann M. Richard[a,*]

OPERA Models



Journal of Cheminformatics

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Research article | Open Access | Published: 08 March 2018

OPERA models for predicting physicochemical properties and environmental fate endpoints

Kamel Mansouri, Chris M. Grulke, Richard S. Judson & Antony J. Williams

Journal of Cheminformatics **10**, Article number: 10 (2018) | Cite this article

4054 Accesses | **27** Citations | **25** Altmetric | Metrics

TEST – Toxicity Estimation Software Tool
https://www.epa.gov/chemical-research/toxicity-estimation-software-tool-test

Toxicity Estimation Software Tool (TEST)

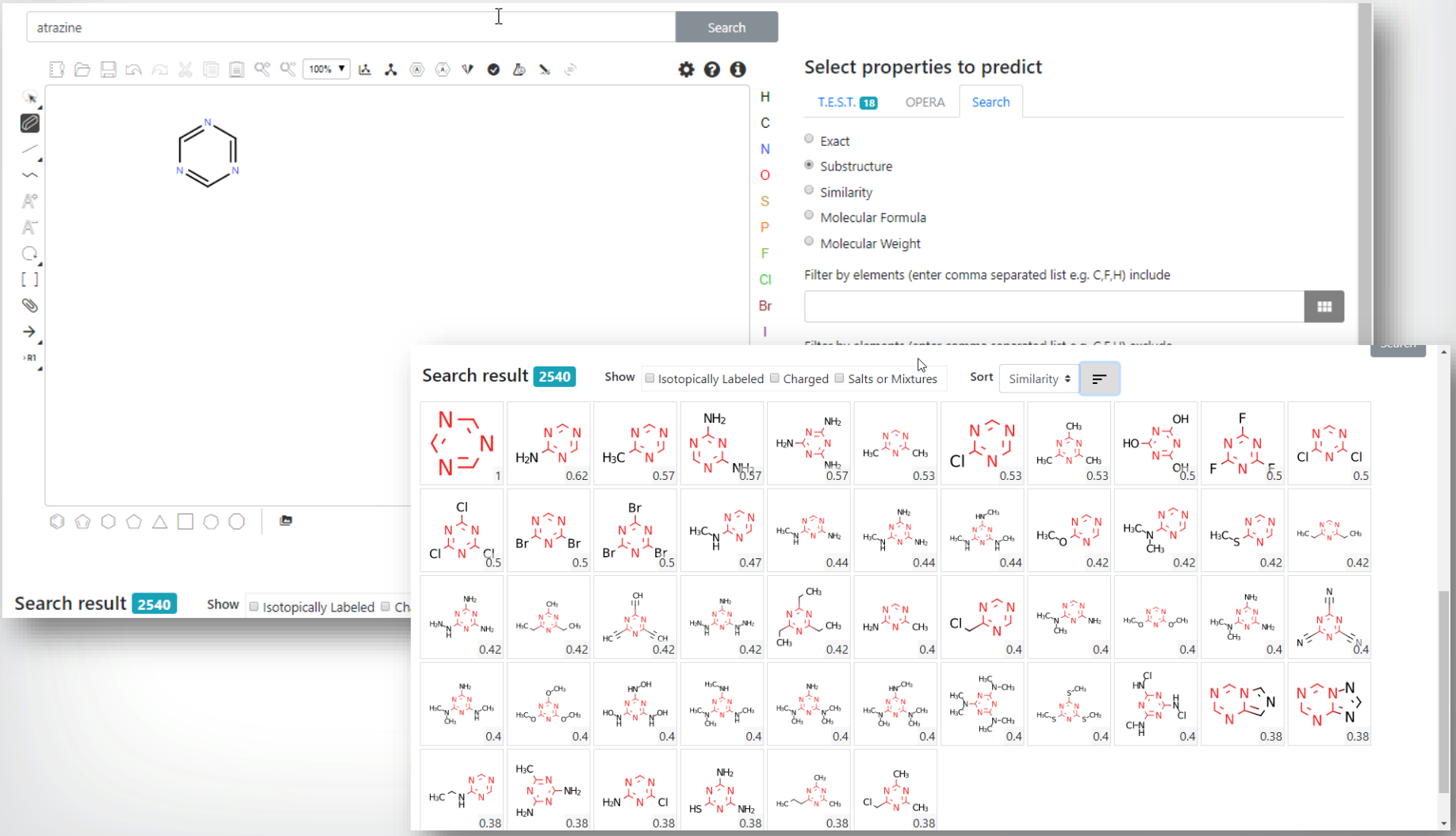
On this page:

The Toxicity Estimation Software Tool (TEST) was developed to allow users to easily estimate the toxicity of chemicals using Quantitative Structure Activity Relationships (QSARs) methodologies. QSARs are mathematical models used to predict measures of toxicity from the physical characteristics of the structure of chemicals (known as molecular descriptors). Simple QSAR models calculate the toxicity of chemicals using a simple linear function of molecular descriptors:

Ask a Technical Expert

Got a question about our research model? Want to give us feedback? Contact a technical expert about TEST.

Structure/Substructure Search



Spectral Searching against Predicted Fragmentation

Non Target Analysis Prototype

Mass Search

± | Min/Max

321.136493476 Da ± 0.0000002 Da | ppm

Molecular Formula Search

Molecular Formula

Mass or Formula must be entered before searching spectrum

Ionization Type

ESI+ ▼

ESI+
ESI-
EI

Spectra Input

Single Energy | Multiple

304.1332052 11.6199475
198.0913404 7.306439699
123.0440559 6.538348292
196.0756904 5.269463115
216.1019051 4.700461978

Peak Match Window: 0.02 Da | ppm

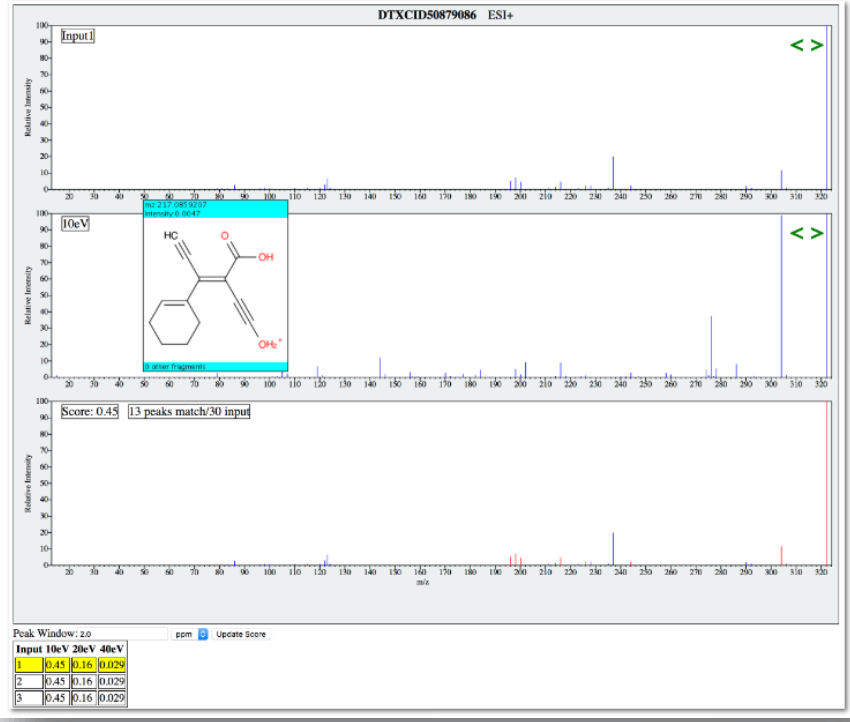
Search

Data Descriptor | OPEN | Published: 02 August 2019

Linking *in silico* MS/MS spectra with chemistry data to improve identification of unknowns

Andrew D. McEachran, Ilya Balabin, Tommy Cathey, Thomas R. Transue, Hussein Al-Ghoul, Chris Grulke, Jon R. Sobus & Antony J. Williams

Scientific Data **6**, Article number: 141 (2019) | Download Citation



Hazard and Bioactivity Functionality

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