



Showcasing Impact of Science and Technology

US EPA's Computational Toxicology pilot effort using traditional and alternative metrics

Presented by:

Monica Linnenbrink, Acting Deputy Director
US EPA National Center for Computational Toxicology



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Data and Tools



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The views expressed in this presentation are those of the presenter and do not necessarily reflect the views or policies of the U.S. Environmental Protection Agency

- **Classical metrics**
- **Alternative metrics**
- **Usage of research**
 - **Usage of research for decision-making**
 - **Presence of research or reference to it in influential documents such as budget or statutory language.**



Home Page

EPA Computational Toxicology Impact

EPA Computational Toxicology Research Impact Chemical safety has been a major priority for EPA since it was established in 1970. As the number of chemicals entering the marketplace has increased, evaluating chemicals for potential health effects has become a formidable challenge. Today, some 80,000 chemicals are listed or registered under the Toxic Substance Control Act (TSCA), and hundreds of new chemicals are introduced every year. EPA's computational toxicology research has had successes addressing this challenge by developing scientific approaches that can be used to evaluate thousands of chemicals for potential health effects. Approaches are faster, more efficient, and far less costly than traditional methods. Learn more about how EPA's Computational Toxicology research has made tremendous impacts by exploring the successes achieved and metrics demonstrating those successes.



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ORAU Student Services
Contractor-Laboratory Support
Technician



Antony Williams

Chemist

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Bio

Area of Expertise:

Dr. Williams' present focus at NCCT is as part of the Chemical Safety for Sustainability (CSS) Research Program to develop a cheminformatics architecture for the center. This work has already produced the publicly accessible website, the ICSS Chemistry Dashboard, providing access to chemistry related data for over 700,000 chemicals (<https://comptox.epa.gov/dashboard>).

Education:

- B.S., Liverpool University, Liverpool, UK; Chemistry, 1985
- Ph.D., University of London, London, UK; Chemistry, 1988

Professional Experience:

- North Carolina ACS Distinguished Lecturer, 2016
- Microsoft eScience Jim Gray Award, 2012
- Fellow of the Royal Society of Chemistry, 2009
- University of London Bourne Medal for best Chemistry Thesis, 1988
- Morris Ranger Undergraduate scholarship, 1983

Publications

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Publications

Baker, N; Williams, A; Grulke, C; Edwards, J; McEachran, A; Mansouri, K; Patlewicz, G; Shah, I; Wambaugh, J; Judson, R; Richard, A; The CompTox Chemistry Dashboard - A Community Data Resource for Environmental Chemistry. *Journal of Cheminformatics*. Springer, New York, NY, USA, 9(61) doi:10.1186/s13321-017-0247-6

 Abstract Views **3** Citations **34** Downloads **N/A**

Newton, S; McMahan, R; Sobus, J; Strynar, M; Mansouri, K; Williams, A; McEachran, A; Suspect Screening and Non-Targeted Analysis of Drinking Water Using Point-Of-Use Filters. *ENVIRONMENTAL POLLUTION*. Elsevier Science Ltd, New York, NY, USA, 234: 297-306, [2018]. doi:10.1016/j.envpol.2017.11.033

 Abstract Views **N/A** Citations **18** Downloads **N/A**

Sauer, S J; Tarpley, M; Save, A V; Lyerly, H K; Patierno, S R; Devi, G R; Shah, I; Williams, K P; Bisphenol A activates EGFR and ERK promoting proliferation, tumor spheroid formation and resistance to EGFR pathway inhibition in estrogen receptor negative inflammatory breast cancer cells. *CARCINOGENESIS*. Oxford University Press, Cary, NC, USA, 38(3) doi:10.1093/carcin/bgx003

 Abstract Views **13** Citations **14** Downloads **N/A**

Mansouri, K; Grulke, C; Richard, A; Judson, R; Williams, A; An automated curation procedure for addressing chemical errors and inconsistencies in public datasets used in QSAR modeling. *SAR AND QSAR IN ENVIRONMENTAL RESEARCH*. Taylor & Francis, Inc., Philadelphia, PA, USA, 27(11) doi:10.1016/j.tiv.2016.12.006

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Kudos





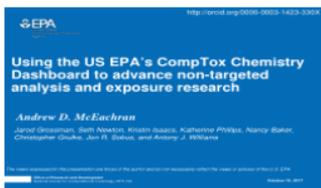
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Using the US EPA's CompTox Chemistry Dashboard to advance non-targeted analysis and exposure research

10.23645/epacomptox.6807404
2018-07-11

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The CompTox Dashboard & Emerging Contaminants in the Superfund Program

10.23645/epacomptox.6807212
2018-07-11

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Identification of Androgen Receptor Antagonists Using Tox21 qHTS Data and the MARCoNI Assay

10.23645/epacomptox.6791795.v2
2018-07-09

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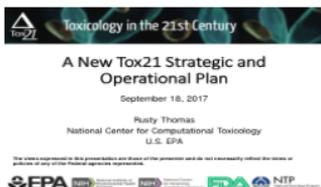
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Quantifying uncertainty in read-across assessment - an algorithmic approach

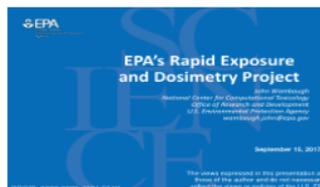
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2018-07-05

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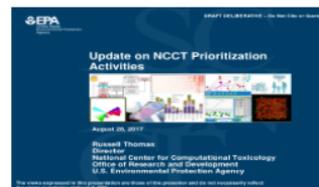
A New Tox21 Strategic and Operational Plan

10.23645/epacomptox.6744008
2018-07-05



EPA's Rapid Exposure and Dosimetry Project

10.23645/epacomptox.6743933
2018-07-05



Update on NCCT Prioritization Activities

10.23645/epacomptox.6743855
2018-07-05



Navigating through the minefield of read-across: from research to practical tools

10.23645/epacomptox.6743792
2018-07-05

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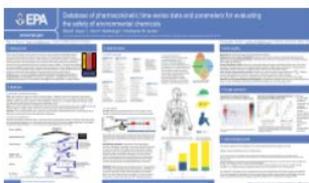
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Database of Pharmacokinetic Time-Series Data and Parameters for Evaluating the Safety of Environmental Chemicals

10.23645/epacomptox.8023229
2019-04-22

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Generation of hydrolyzed complement component C3 is substantially elevated in SLE

10.6084/m9.figshare.7963052
2019-04-06

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Characterization of cell-bound complement activation products on SLE PBMCs using mass cytometry

10.6084/m9.figshare.7939055
2019-04-02

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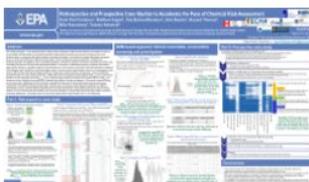


Assessing data-related practices in the field of psychology: Survey design and preliminary results

10.1184/r117928705
2019-04-01

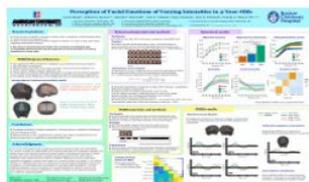
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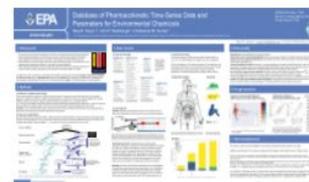
Retrospective and Prospective Case Studies to Accelerate the Pace of Chemical Risk Assessment

10.23645/epacomptox.7873742
2019-03-21



Perception of Facial Emotions of Varying Intensities in 3-Year-Olds

10.6084/m9.figshare.7871774
2019-03-21



Database of Pharmacokinetic Time-Series Data and Parameters for Environmental Chemicals

10.23645/epacomptox.7844492
2019-03-14



QSAR Modeling of Caco-2 Permeability for the Estimation of Oral Bioavailability

10.23645/epacomptox.7841102
2019-03-13



CompTox Online Tools Usage

CompTox Research Data and Tools Usage

CompTox Chemistry Dashboard

ACToR

CPCat

EDSP21

ToxCast

DSSTox

CompTox Data Download

The CompTox Dashboard contains information on over 700,000 chemicals currently in use. Users can access chemical structures, experimental, and predicted physiochemical and toxicity data, and additional links to relevant websites and applications.

CompTox Chemistry Dashboard Usage

Page Views

Unique Page Views

Users

Geographics

CompTox Chemistry Dashboard FTP Data Downloads

Region:

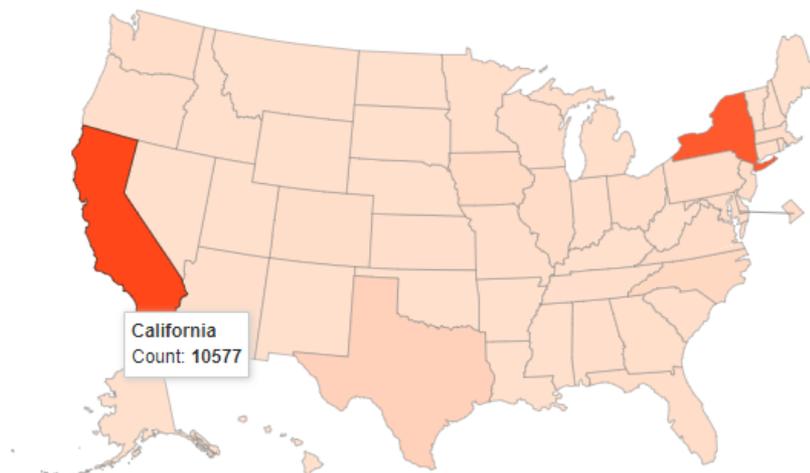
USA

World

Time Period:

Apr 2019

2018

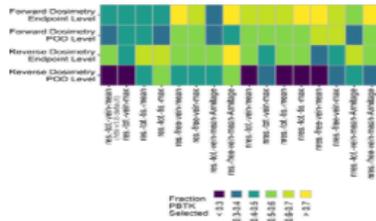


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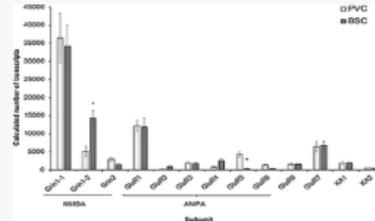
Altered expression of ionotropic L-Glutamate receptors in aged sensory neurons of *Aplysia californica*

Plos.org
2019-05-23



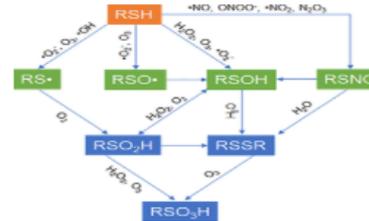
Using the concordance of in vitro and in vivo data to evaluate extrapolation

Plos.org
2019-05-28



Altered expression of ionotropic L-Glutamate receptors in aged sensory

Plos.org
2019-05-23



Nitrosylation vs. oxidation – How to modulate cold physical plasmas for

Plos.org
2019-05-08



What Are the Alternatives to Animal Testing?

Livescience.com
2019-05-04



Take Home Messages

- **Identify the research products to track**
- **Determine the appropriate and available metrics**
- **Investigate metric sources such as Web of Science, PlumX, AltMetric, Dimensions, VIVO, Google Analytics**
- **Gather metrics through APIs and other existing sources**
- **Products may need a Digital Object Identifier (DOI) for tracking purposes**
- **Use lessons learned to continually refine approach**