

Investigating Impact Metrics for Performance for the US EPA National Center for Computational Toxicology

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The views expressed in this presentation are those of the author and do not necessarily reflect the views or policies of the U.S. EPA

*August 21-25, 2016
ACS Fall Meeting, Philadelphia, PA*

Who is NCCT?

- National Center for Computational Toxicology – part of EPA’s Office of Research and Development
- Research driven by the EPA’s *Chemical Safety for Sustainability Research Program*
 - Develop new approaches to **evaluate** the **safety** of chemicals
 - Integrate advances in biology, biotechnology, chemistry, exposure science and computer science
- Goal - To identify chemical exposures that may disrupt biological processes and cause adverse outcomes.
- Can we quickly and cheaply evaluate thousands of chemicals for potential risk?

What are our “products”?

- Our scientific publications and presentations
- Our research data
- Our software applications, code, algorithms and models
- Our collaborations
- Our trainings – postdoctoral researchers
- Our Scientific Leadership

What are our products?

- Our Scientific Publications and Presentations

https://cfpub.epa.gov/si/si_lab_search_results.cfm?fed_org_id=1267&SIType=PR&TIMSType=Journal&showCriteria=0&view=citation&sortBy=pubDateYear

Science Inventory Search Results

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2016

Judson, R., K. Houck, M. Martin, A. Richard, T. Knudsen, I. Shah, S. Little, J. Wambaugh, Woodrow Setzer, P. Kothiya, J. Phuong, D. Filer, D. Smith, D. Reif, D. Rotroff, N. Kleinstreuer, N. Sipes, M. Xia, R. Huang, K. Crofton, AND R. Thomas.

[Analysis of the Effects of Cell Stress and Cytotoxicity on In Vitro Assay Activity Across a Diverse Chemical and Assay Space.](#)
TOXICOLOGICAL SCIENCES. Society of Toxicology, 152(2):323-339, (2016).

Kuo, B., F. Webster, R. Thomas, AND C. Yauk. [BMDEExpress Data Viewer: A Visualization Tool to Analyze BMDEExpress Datasets.](#)
JOURNAL OF APPLIED TOXICOLOGY. John Wiley & Sons, Ltd., Indianapolis, IN, 36(8):1048-1059, (2016).

Ball, N., M. Cronin, J. Shen, M. Adenuga, K. Blackburn, E. Booth, M. Bouhifd, B. Donley, L. Egnash, J. Freeman, C. Hastings, D. Juberg, A. Kleinsang, N. Kleinstreuer, D. Kroese, T. Luechtefeld, A. Maertens, S. Marty, J. Naciff, J. Palmer, D. Pamies, M. Penman, A. Richarz, D. Russo, D. Steup, S. Stuard, G. Tier, B. van Ravenzwaay, S. Wu, H. Zhu, AND T. Hartung. CAAT Altex workshop paper entitled "Towards Good Read-Across Practice (GRAP) Guidance". ALTEX. Society ALTEX Edition, Kuesnacht, Switzerland, 33(2):149-166, (2016).

Widen Your Search

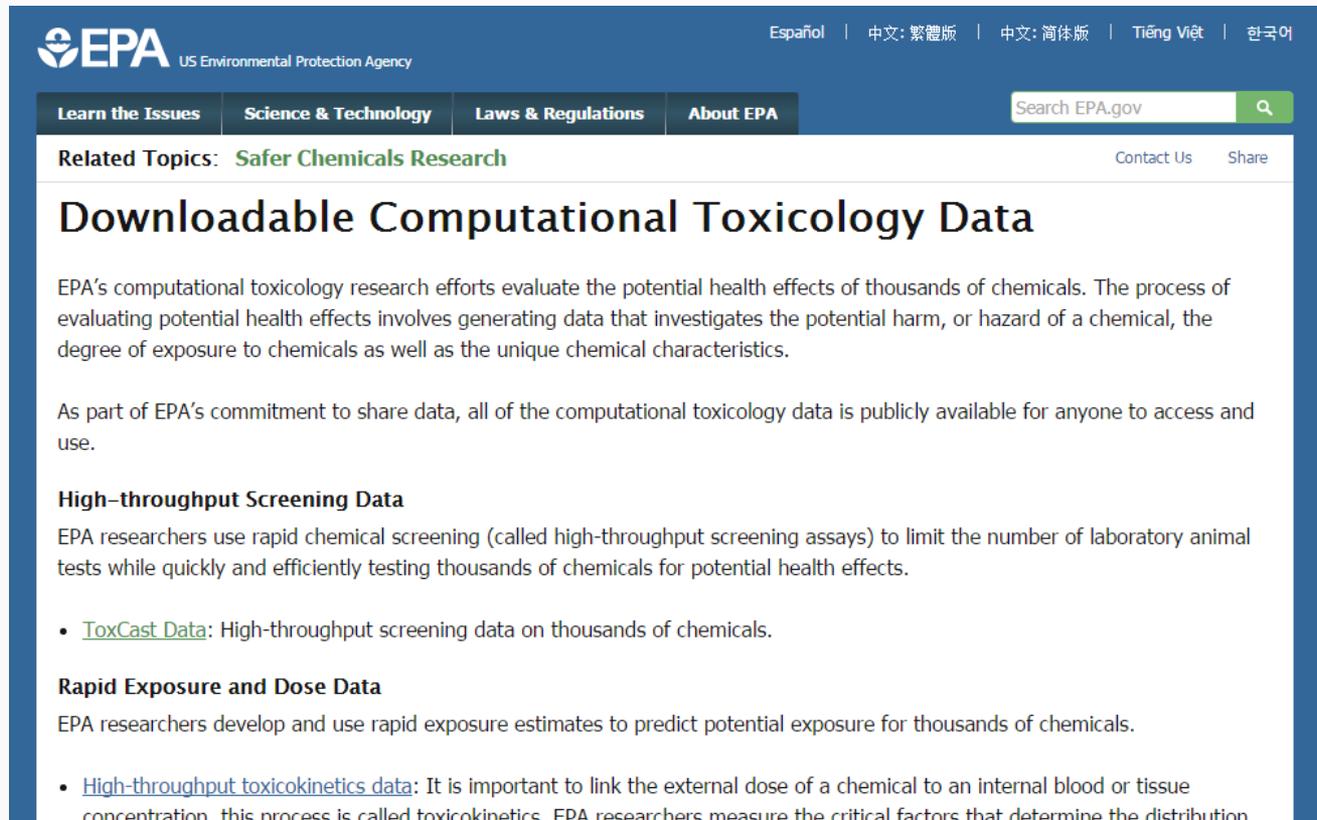
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What are our products?

- Our Data

<https://www.epa.gov/chemical-research/downloadable-computational-toxicology-data>



The screenshot shows the EPA website's 'Science & Technology' section. The page title is 'Downloadable Computational Toxicology Data'. The main text describes EPA's computational toxicology research, which evaluates the potential health effects of thousands of chemicals. It notes that the process involves generating data on potential harm, hazard, and exposure. A key point is that all this data is publicly available. The page is divided into three sub-sections: 'High-throughput Screening Data', 'Rapid Exposure and Dose Data', and 'High-throughput toxicokinetics data'. Each sub-section includes a brief description and a link to the relevant data.

EPA US Environmental Protection Agency

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Downloadable Computational Toxicology Data

EPA's computational toxicology research efforts evaluate the potential health effects of thousands of chemicals. The process of evaluating potential health effects involves generating data that investigates the potential harm, or hazard of a chemical, the degree of exposure to chemicals as well as the unique chemical characteristics.

As part of EPA's commitment to share data, all of the computational toxicology data is publicly available for anyone to access and use.

High-throughput Screening Data

EPA researchers use rapid chemical screening (called high-throughput screening assays) to limit the number of laboratory animal tests while quickly and efficiently testing thousands of chemicals for potential health effects.

- [ToxCast Data](#): High-throughput screening data on thousands of chemicals.

Rapid Exposure and Dose Data

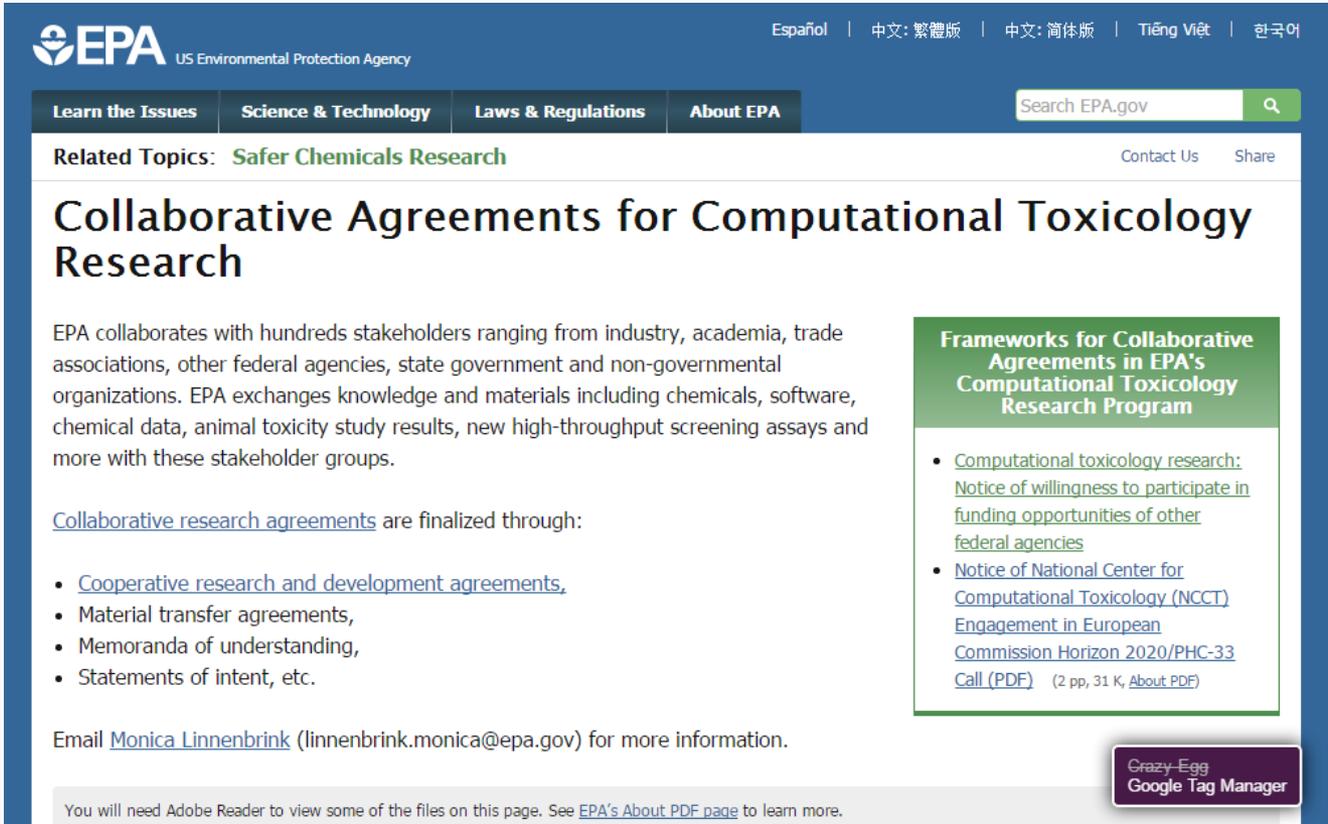
EPA researchers develop and use rapid exposure estimates to predict potential exposure for thousands of chemicals.

- [High-throughput toxicokinetics data](#): It is important to link the external dose of a chemical to an internal blood or tissue concentration this process is called toxicokinetics. EPA researchers measure the critical factors that determine the distribution

What are our products?

- Our collaborations

<https://www.epa.gov/chemical-research/collaborative-agreements-computational-toxicology-research>



The screenshot shows the EPA website page for 'Collaborative Agreements for Computational Toxicology Research'. The page features a blue header with the EPA logo and navigation links. The main content area includes a title, a paragraph describing EPA's collaborations, a list of agreement types, and a sidebar with a green box titled 'Frameworks for Collaborative Agreements in EPA's Computational Toxicology Research Program'. The sidebar lists two key documents: 'Computational toxicology research: Notice of willingness to participate in funding opportunities of other federal agencies' and 'Notice of National Center for Computational Toxicology (NCCT) Engagement in European Commission Horizon 2020/PHC-33 Call (PDF)'. A footer note mentions the need for Adobe Reader to view PDF files.

EPA US Environmental Protection Agency

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Collaborative Agreements for Computational Toxicology Research

EPA collaborates with hundreds stakeholders ranging from industry, academia, trade associations, other federal agencies, state government and non-governmental organizations. EPA exchanges knowledge and materials including chemicals, software, chemical data, animal toxicity study results, new high-throughput screening assays and more with these stakeholder groups.

[Collaborative research agreements](#) are finalized through:

- [Cooperative research and development agreements](#),
- Material transfer agreements,
- Memoranda of understanding,
- Statements of intent, etc.

Email [Monica Linnenbrink](mailto:linnenbrink.monica@epa.gov) (linnenbrink.monica@epa.gov) for more information.

You will need Adobe Reader to view some of the files on this page. See [EPA's About PDF page](#) to learn more.

Frameworks for Collaborative Agreements in EPA's Computational Toxicology Research Program

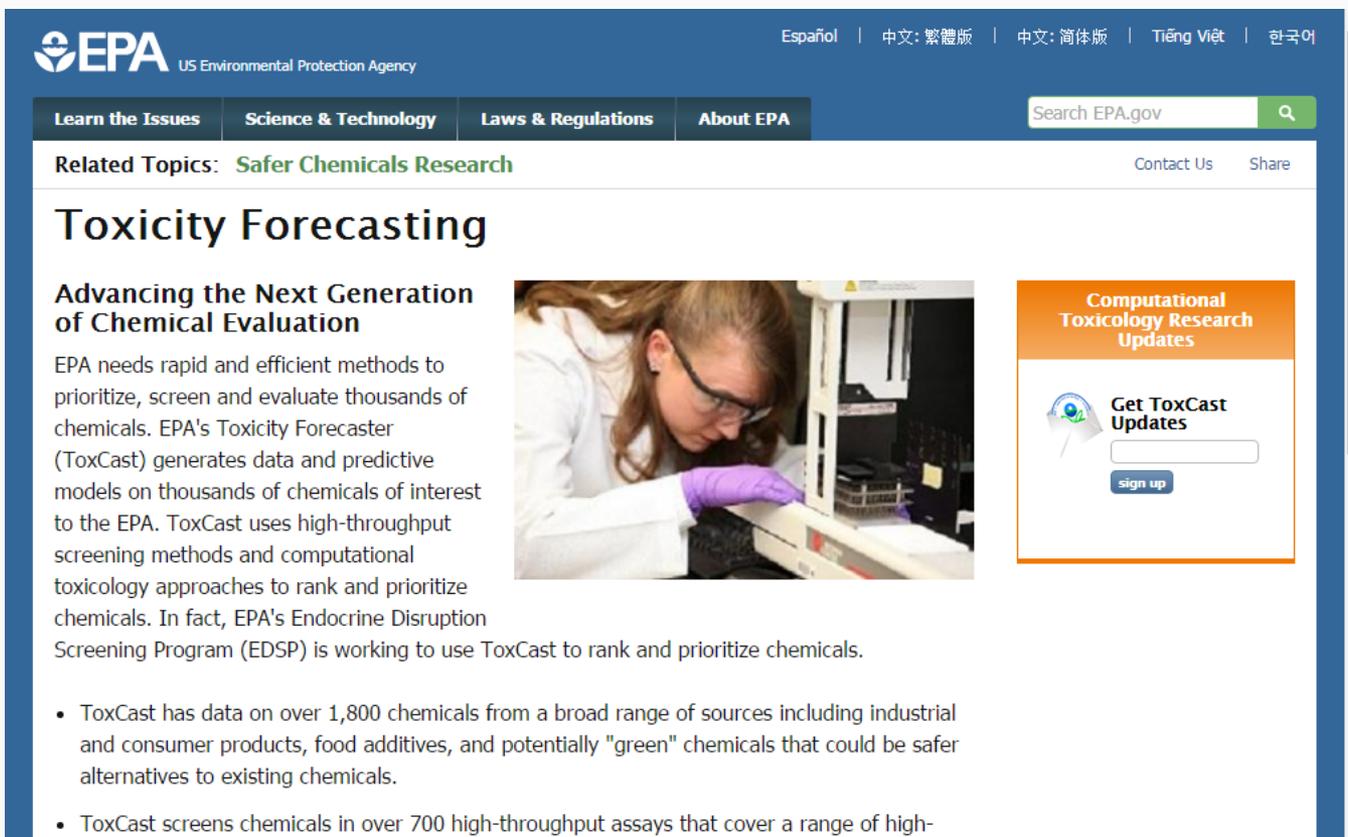
- [Computational toxicology research: Notice of willingness to participate in funding opportunities of other federal agencies](#)
- [Notice of National Center for Computational Toxicology \(NCCT\) Engagement in European Commission Horizon 2020/PHC-33 Call \(PDF\)](#) (2 pp, 31 K, [About PDF](#))

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What are our products?

- Our scientific leadership

<https://www.epa.gov/chemical-research/toxicity-forecasting>



The screenshot shows the EPA website page for Toxicity Forecasting. The header includes the EPA logo, navigation links for 'Learn the Issues', 'Science & Technology', 'Laws & Regulations', and 'About EPA', and a search bar. The main content area features the title 'Toxicity Forecasting' and a sub-header 'Advancing the Next Generation of Chemical Evaluation'. A paragraph describes the EPA's need for rapid and efficient methods to prioritize and evaluate thousands of chemicals, highlighting the use of the Toxicity Forecaster (ToxCast) and the Endocrine Disruption Screening Program (EDSP). A photograph of a scientist in a lab coat and purple gloves working in a laboratory is included. A sidebar on the right contains a 'Computational Toxicology Research Updates' section with a 'Get ToxCast Updates' button and a 'sign up' button.

EPA US Environmental Protection Agency

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Toxicity Forecasting

Advancing the Next Generation of Chemical Evaluation

EPA needs rapid and efficient methods to prioritize, screen and evaluate thousands of chemicals. EPA's Toxicity Forecaster (ToxCast) generates data and predictive models on thousands of chemicals of interest to the EPA. ToxCast uses high-throughput screening methods and computational toxicology approaches to rank and prioritize chemicals. In fact, EPA's Endocrine Disruption Screening Program (EDSP) is working to use ToxCast to rank and prioritize chemicals.



- ToxCast has data on over 1,800 chemicals from a broad range of sources including industrial and consumer products, food additives, and potentially "green" chemicals that could be safer alternatives to existing chemicals.
- ToxCast screens chemicals in over 700 high-throughput assays that cover a range of high-

Computational Toxicology Research Updates

Get ToxCast Updates

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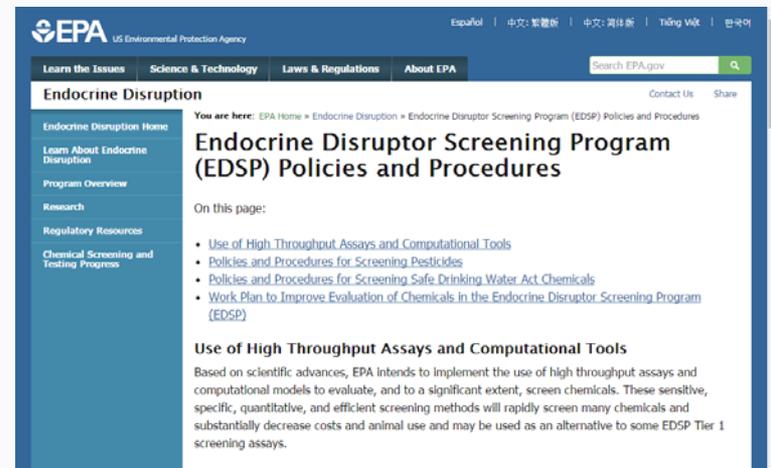
How should our impact be measured?

- **Classical measures** of impact – publications (How many, where published, how many times cited)
- The world of **AltMetrics** (<http://altmetrics.org/manifesto/>)



- **Scientific Publications and Presentations** – how many downloads, views, shares, tweets, embeds,
- **Research data** – downloads, uses, publications about and citations to data
- **Software applications, code, algorithms and models** – number of visitors, geography of visitors, number of searches, amount of data downloaded, integration to applications (web service access), reuse of code, algorithms and models

- **Collaborations** – funding of external work, provision of ToxCast plated materials,
- **Training – postdoctoral researchers** – what careers do they have when they leave NCCT?
- **Scientific Leadership** – contributions to EPA policy documents



Scientist AltMetrics

- Many Social and Altmetric platforms in recent

ImpactStory profile for Antony Williams, US Environmental Protection Agency Computational Chemist. The profile shows an overview, achievements, activity, and publications. Key metrics include 1333 saves and shares across 9 channels, with 495, 536, 57, 11, 14, 10, 3, 2, and 1 for various categories. A 'Global Reach' section notes that 31% of research is free to read online, and a 'Hot Streak' section mentions that people are talking about the research.

publons dashboard for Antony Williams. The dashboard shows a list of publications with columns for DATE, MANUSCRIPT, JOURNAL, ATTRIBUTES, and OPEN. The table lists several publications, including 'ADAMS - A Data Management System to Facilitate Process...', 'An Ensemble Model of QSAR Tests for Regulatory Risk Assess...', 'ChEMDataCrawler: A toolkit for automated extraction of ch...', 'URICON: A Powerful and Easy-to-Use Compound Library Con...', 'New open source tools for drug discovery', 'The ELF Forest Data Broker: informatics enabling public-pri...', 'The ELF Forest Data Broker: informatics enabling public-pri...', 'Identification of Novel Inhibitors of Organic Anion Transport...', and 'Chemical databases: creation or integration by user-defined...'. Each entry includes a journal name and various action icons.

ORCID profile for Antony Williams. The profile includes a biography, ORCID ID (0000-0002-3468-4821), and a list of keywords: NMR, Computer-assisted Structure Elucidation, Chemistry, ChemSpider. The biography states: 'Over the past decade I held many responsibilities including the direction of the development of scientific software applications for spectroscopy and general chemistry, directing marketing efforts, sales and business development collaborations for the company. Eight years experience of analytical laboratory leadership and management. Experienced in experimental techniques, implementation of new NMR technology, walk-up facility management, research and development, manufacturing support and teaching. Ability to provide innovative analysis, creative solutions and establish good working relationships. Prolific author with over a hundred and fifty peer-reviewed scientific publications, 3 patents and many public presentations.'

GPLOTIX profile for Antony J. Williams. The profile shows a list of connections in chemistry, including LinkedIn, ChemConnector Blog, Microsoft Academic Search, Impact Story, ResearchGate, Amazon.com, Votiv, Visualize.me, and Pinterest. A 'Researcher Profile' section includes a sample profile from the Royal Society of Chemistry and a bio: 'My passion is connecting people to chemistry. Over the past decade I held many jobs and responsibilities including the direction of the development of scientific software applications for spectroscopy and general chemistry, directing marketing efforts, sales and business development collaborations for the company. I have almost...'. A list of publications is shown at the bottom, including 'All 850', 'Lecture / Presentation (267)', 'Article (163)', 'Data (36)', 'Book Chapter (43)', 'Video (21)', 'Review (20)', 'Book (12)', 'Figure (10)', 'Research Article (4)', 'Patent (2)', 'Media (2)', 'Blog Post (1)', and 'Web resource (1)'.

KUDOS profile for Dr Antony John Williams. The profile shows a list of publications and co-authors. One publication is highlighted: 'Examining public datasets of antimicrobial "T102" and dr-gaps. Published in MelliChemCombin. Publication date: 2010-01-01'. Another publication is 'Precompetitive preclinical ADME/Tox data set 4 free on the web to facilitate computational model building and assist drug development. Published in eLab on a Chip. Publication date: 2010-01-01'. A 'What's it about?' section states: 'We have examined both intrinsic and predicted molecular properties across large sets of annotated screening for compounds and the associated bio...'. A 'Browser Update' notification for Google Analytics is visible.

Altmetric profile for the article 'Dispensing Processes Impact Apparent Biological Activity as Determined by Computational and Statistical Analyses'. The article has an attention score of 85. The profile shows a summary, news, blogs, twitter, peer reviews, and facebook. The title is 'Dispensing Processes Impact Apparent Biological Activity as Determined by Computational and Statistical Analyses'. The journal is 'PLoS ONE, May 2013'. The authors are 'Sean Evans, Joe Clements, Antony J. Williams'. The abstract states: 'Dispensing and dilution processes may profoundly influence estimates of biological activity of... [https://doi.org/10.1371/journal.pone.0062320]'. A 'Twitter Demographics' section is also visible.

- ...and publishers use these for tracking, assisting distribution and for amplification

Article Metrics: e.g. PLoS

<http://journals.plos.org/plosone/article?id=10.1371/journal.pone.0062325>

Dispensing Processes Impact Apparent Biological Activity as Determined by Computational and Statistical An...

Sean Ekins, Joe Olechno, Antony J. Williams



Article | Authors | **Metrics** | Comments | Related Content

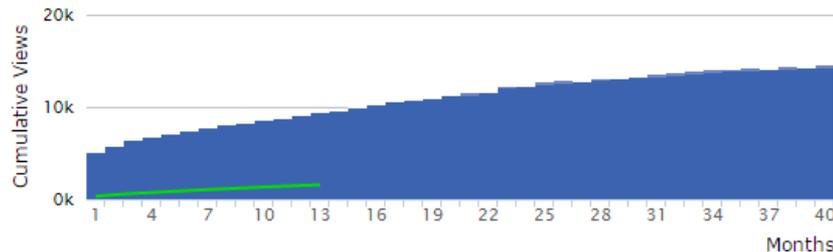
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	PMC	64	n.a.	291
	Totals	13,065	1,414	42

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Antony Williams

ORCID ID
 orcid.org/0000-0002-2668-4821
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Also known as
ChemSpiderman,
ChemConnector,
Tony Williams

Country
United States

Keywords

Biography    

Over the past decade I held many responsibilities including the direction of the development of scientific software applications for spectroscopy and general chemistry, directing marketing efforts, sales and business development collaborations for the company. Eight years experience of analytical laboratory leadership and management. Experienced in experimental techniques, implementation of new NMR technologies, walk-up facility management, research and development, manufacturing support and teaching. Ability to provide situation analysis, creative solutions and establish good working relationships. Prolific author with over a hundred and fifty peer-reviewed scientific publications, 3 patents and many public presentations.

 I am one of the Founders of ChemZoo Inc., the developers of the ChemSpider website (www.chemspider.com). ChemSpider is an open access online database of chemical structures and property transaction based services to enable chemists around the world to data mine chemistry databases. The Royal Society of Chemistry acquired ChemSpider in May 2009. I worked as a consortium member and work package leader for the Open PHACTS IMI project (<http://www.openphacts.org/>). This focuses on how drug discovery can utilize semantic technologies to link together public and private data for the drug discovery community. I have also worked as a member of the Pharmasea consortium (<http://www.pharmasea.eu/pharmasea.html>) focused on biodiscovery research and the development and commercialisation of new substances from marine organisms. 

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Chem. Res. Toxicol.

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Linking high resolution mass spectrometry data with exposure and toxicity forecasts to advance high-throughput environmental monitoring



Environment International

2016-03 | journal-article

DOI: [10.1016/j.envint.2015.12.008](https://doi.org/10.1016/j.envint.2015.12.008)

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Open drug discovery for the Zika virus [version 1; referees: awaiting peer review]



2016-02-09 | journal-article

DOI: [10.12688/f1000research.8013.1](https://doi.org/10.12688/f1000research.8013.1)

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Antony J. Williams

Connections in Chemistry

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Researcher from:
Sample Profiles / Royal Society of Chemistry

My passion is connecting people to chemistry. Over the past decade I held many jobs and responsibilities including the direction of the development of scientific software applications for spectroscopy and general chemistry, directing marketing efforts, sales and business development collaborations for the company. I have almost... + More

Artifact Summary

267	163	96	44	28
Lecture /	Article	Data	Chapters	Video

All (650) Lecture / Presentation (267) Article (163) Data (96) Book Chapter (44) Video (28) Review (20) Book (12) Figure (10) Research Artifact (4) Patent (2) Media (2) Blog Post (1) Web resource (1)

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Dispensing Processes Impact Apparent Biological Activity as Determined by Computational and Statistical Analyses

Citation data: PLoS ONE, ISSN: 1932-6203, Vol: 8, Issue: 5, Page: e62325
Publication Year: 2013
Researchers: Antony J. Williams

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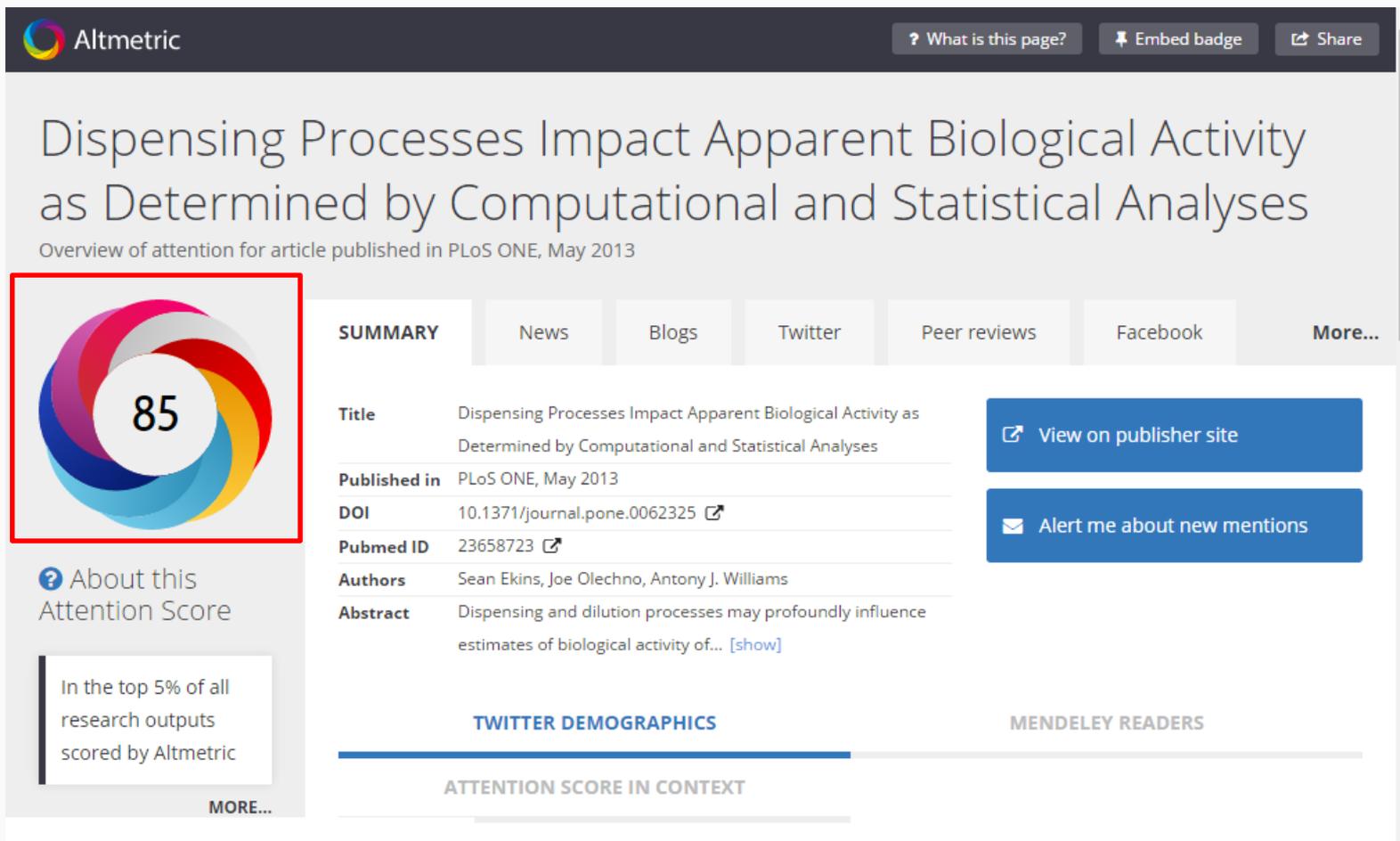
Sean Ekins
@collabchem

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Dispensing Processes Impact Apparent Biological Activity as Determined by Computational and Statistical Analyses

Overview of attention for article published in PLoS ONE, May 2013

85

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Title Dispensing Processes Impact Apparent Biological Activity as Determined by Computational and Statistical Analyses [View on publisher site](#)

Published in PLoS ONE, May 2013

DOI 10.1371/journal.pone.0062325 [↗](#)

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Authors Sean Ekins, Joe Olechno, Antony J. Williams

Abstract Dispensing and dilution processes may profoundly influence estimates of biological activity of... [\[show\]](#)

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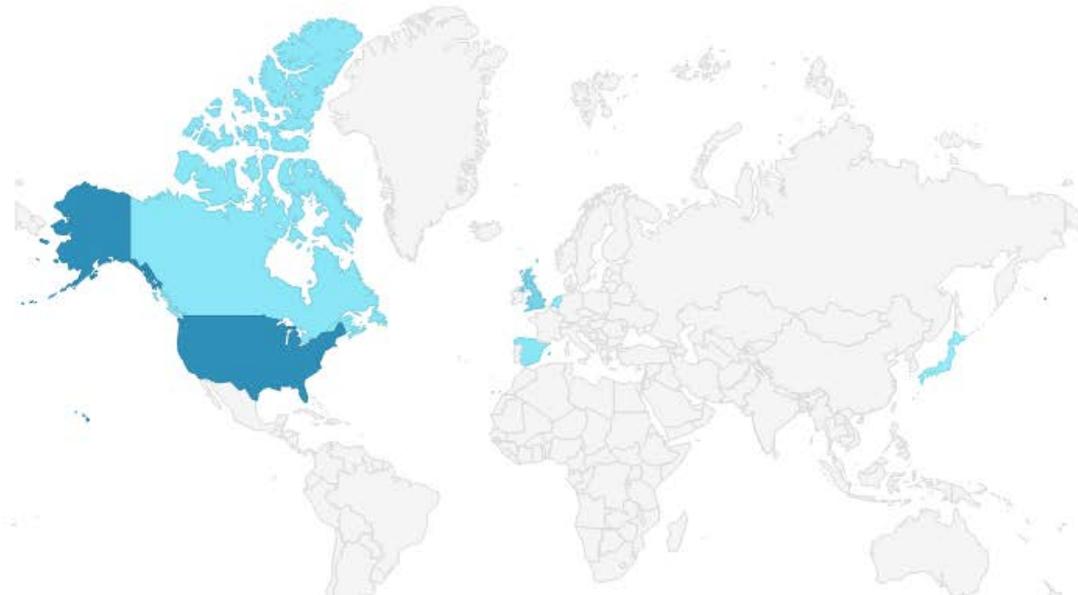
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What is this page?



Dr Antony John Williams | Menu ☰

Dispensing processes profoundly influence estimates of biological activity of compounds



Dispensing Processes Impact Apparent Biological Activity as Determined by Computational and Statistical Analyses

Sean Ekins, Joe Olechno, Antony J. Williams

Published in: PLoS ONE

Publication date: May 2013

Publisher: Public Library of Science (PLoS)

DOI: <http://dx.doi.org/10.1371/journal.pone.0062325>

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What's it about?



Dispensing processes profoundly influence estimates of biological activity of compounds. In this study using published inhibitor data for the tyrosine kinase EphB4, we show that IC50 values obtained via disposable tip-based serial dilution and dispensing versus acoustic dispensing differ by orders of magnitude with no correlation or ranking of datasets.

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Dispensing Processes Impact Apparent Biological Activity as Determined by Computational and Statistical Analyses

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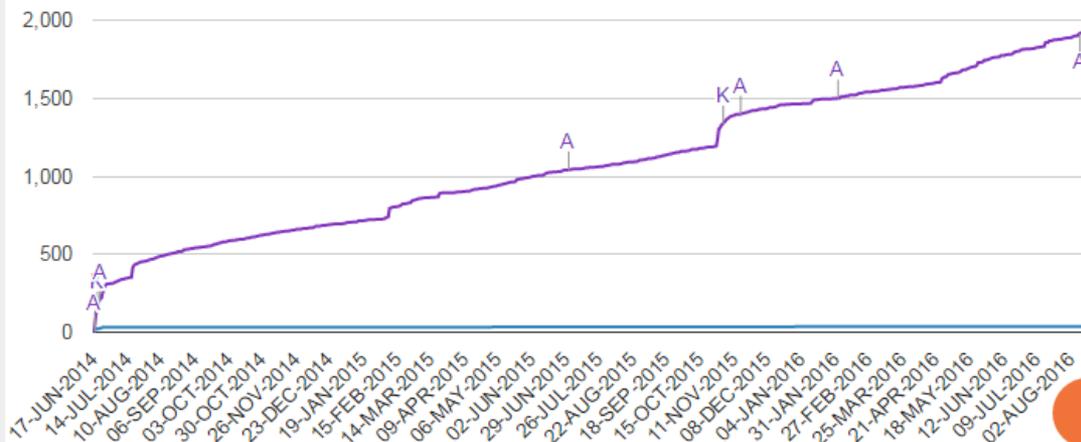
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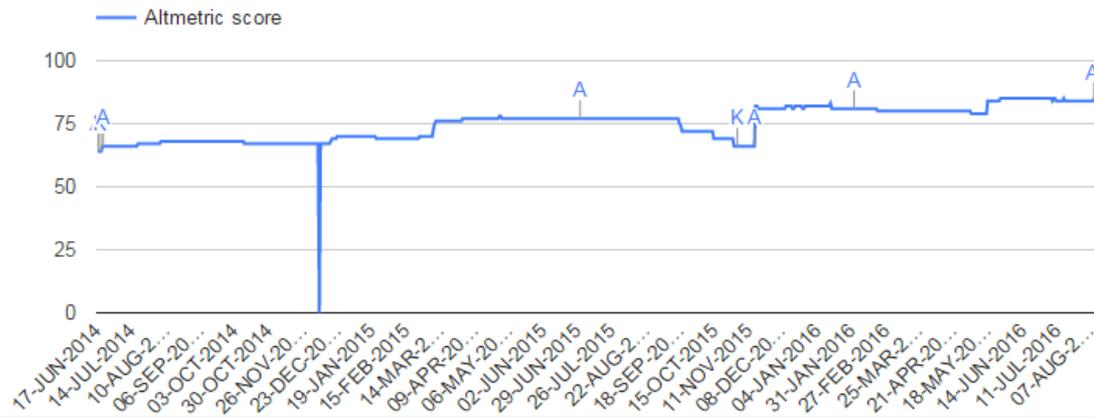


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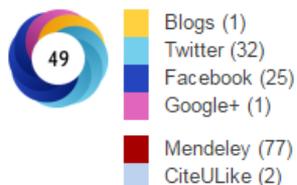
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In your HTML page, simply include a `<script src="//api.growkudos.com/widgets/article/DOI"></script>` tag, replacing the "DOI" with that of the publication you wish to link to. DOI is the Digital Object Identifier and can be found on the Kudos Publication page.

N.B. the "/" in the url ensures that the widget can function over both http and https protocols.

You can specify the following parameters for this widget: `omit_icons` will remove the icon next to the What's it about? and Why is it important? paragraphs - useful for narrow width integrations. `omit_read_more_btn` will remove the "Read more on Kudos..." button from the bottom.

You can pass these GET parameters by adding them to the address of the widget, e.g. `?omit_icons=true`, `?omit_read_more_btn=true` or `?omit_read_more_btn=true&omit_icons=true` for both at the same time. One complete example in this case would be `<script src="//api.growkudos.com/widgets/article/DOI?omit_icons=true"></script>`.

2. How to embed the Kudos Resources Widget

PLUMX
Groups ▾ Welcome ncct-epa ▾ 🔍

Artifact Pop-Up Widget

The popup widget is a small (~ 130x130px) widget that is well-suited for use in a sidebar.



Script

```
<script type="text/javascript" src="https://plumx.org/js/widget-popup.js"></script>
```

Placeholder and Link

```
<a href="https://plu.mx/plum/a/?doi=10.1371/journal.pone.0056506" class="plumx-plum-print-popup"></a>
```

PLUMX

Usage

Clicks: **76**
 Abstract Views: **171**
 PDF Views: **2530**
 HTML Views: **22535**
 Link-outs: **1**
 Downloads: **79**

Captures

Bookmarks: **1**
 Exports-Saves: **14**
 Readers: **88**

Mentions

Blog Mentions: **1**

Social Media

+1s: **7**
 Tweets: **33**

Citations

Citation Indexes: **44**

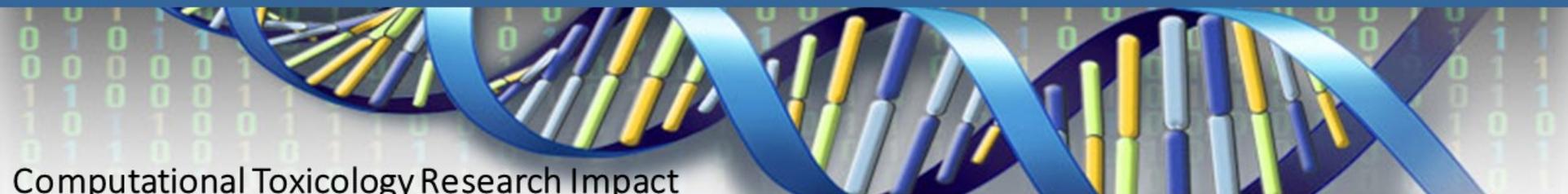
[see details](#)

attribute	default value	description
data-popup	top bottom left right hidden	The direction of the pop-up relative to the widget
data-hide-when-empty	true false	If true, hide the widget when no data is available
data-hide-when-empty	true false	If true, hide the widget when no data is available
data-size	tiny small medium large	Controls the size of the plumprint
data-badge	true false	If true, sets data-size to 'small', and appends a link to the artifact page.

https://plu.mx/plum/a/?doi=10.1371/journal.pone.0056506

- Tools can provide BOTH scientist level *and* article level metrics and activities
- NCCT wants to aggregate the **activities of the Center** – including through our scientists and our publications. But also all of our other “products”...
- Aggregation into one website is underway

What we are building... MOCKUP: Landing Page



Computational Toxicology Research Impact Ground-breaking science to advance chemical evaluation

Since 2005, EPA's computational toxicology research has developed ground-breaking approaches to evaluate chemicals for potential health effects. Using these new approaches, thousands of chemicals have been evaluated for potential risk at small cost in a very short amount of time. EPA collaborates with hundreds of partners from industry, regulators (Federal Agencies, State Agencies, etc), research institutions and others to use the data generated from these new approaches to better evaluate chemicals.



Our Scientists

- Entry point to papers and presentations associated with an individual scientist
- Connect to existing scientists page



Our Publications & Presentations

- Pubs and presentations segregated by year
- Search option
- Differentiate from STICS
- Link with Altmetric score and Kudos details



Our Data & Applications

- Link to stats for data downloads/usage
- Analytics for applications
- Publications about where our data has been used
- Link to FTP data download



Our Impact

- Summary view of our activities and impact
- Select most appropriate option, rather than use multiple with conflicts between widgets

What we would like... MOCKUP: Publications

Scientific Papers: All NCCT

National Center for Computational Toxicology

Researchers



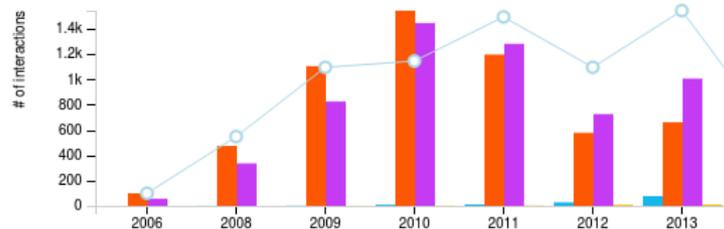
Artifact Summary

📄 Article: 171 📖 Book Chapter: 2
📄 Other: 7 📄 Letter: 1

Recent Artifacts

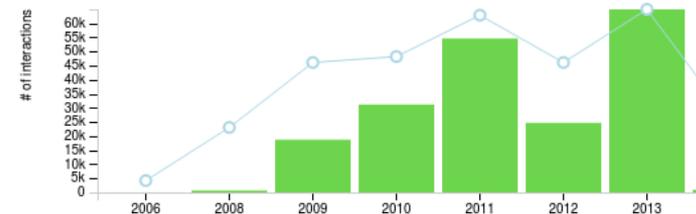
- 🌿 [A Workflow to Investigate Exposure and Pharmacokinetic Influences on High-Throughput in Vitro Chemical Screening Based on Adverse Outcome Pathways.](#)
- 🌿 [Identifiability of PBPK models with applications to dimethylarsinic acid exposure](#)
- 🌿 [Continuing harmonization of terminology and innovations for methodologies in developmental toxicology: Report of the 8th Berlin Workshop on Developmental Toxicity, 14-16 May 2014](#)
- 🌿 [Incorporating High-Throughput Exposure Predictions With Dosimetry-Adjusted In Vitro Bioactivity to Inform Chemical Toxicity Testing.](#)

Metrics by publication year



	Social Media	Citations	Captures	Mentions
2016	5	-	7	-
2015	25	78	230	2
2014	15	177	244	-
2013	77	661	1007	11
2012	28	578	725	9
2011	11	1197	1282	3
2010	9	1544	1446	2
2009	2	1105	825	1
2008	1	474	336	-
2006	-	99	57	-

Usage by publication year



	Usage	Artifacts
2016	2895	1
2015	2362	20
2014	909	12
2013	64941	31
2012	24687	22
2011	54604	30
2010	31165	23
2009	18719	22
2008	684	11
2006	30	2

What we would like... MOCKUP: Scientists

Scientific Papers: By Author

National Center for Computational Toxicology

Researchers



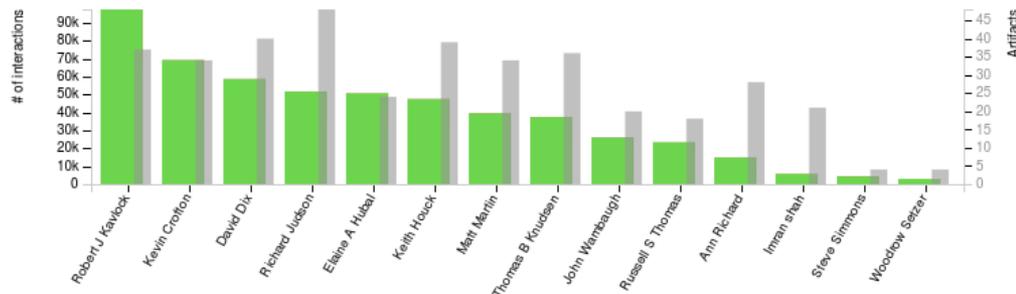
Artifact Summary

Article: 171 Book Chapter: 2
 Other: 7 Letter: 1

Recent Artifacts

- [A Workflow to Investigate Exposure and Pharmacokinetic Influences on High-Throughput in Vitro Chemical Screening Based on Adverse Outcome Pathways.](#)
- [Identifiability of PBPK models with applications to dimethylarsinic acid exposure](#)
- [Continuing harmonization of terminology and innovations for methodologies in developmental toxicology: Report of the 8th Berlin Workshop on Developmental Toxicity, 14-16 May 2014](#)
- [Incorporating High-Throughput Exposure Predictions With Dosimetry-Adjusted In Vitro Bioactivity to Inform Chemical Toxicity Testing.](#)

Usage



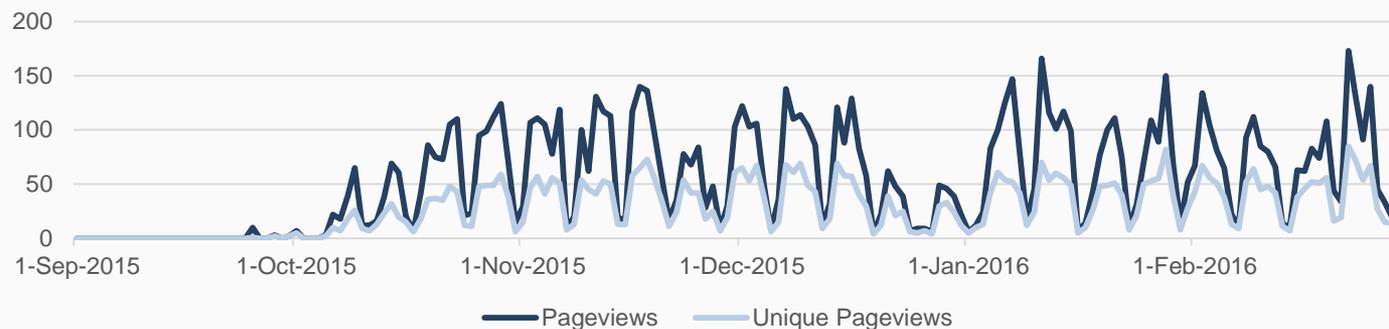
	Abstract Views	Link-outs	PDF Views	HTML Views	Clicks	Data Views	Artifacts
Robert J Kavlock	59504	91	4208	33416	214	-	37
Kevin Crofton	34610	45	3067	31293	168	-	34
David Dix	33175	60	4666	20660	41	-	40
Richard Judson	28823	79	3949	18765	41	-	48
Elaine A Hubal	29245	46	1428	19890	14	-	24
Keith Houck	26438	70	3239	17653	34	-	39
Matt Martin	24590	69	3215	11548	42	-	34
Thomas B Knudsen	19073	89	3712	14462	65	-	36
John Wambaugh	14131	22	1334	10498	9	-	20
Russell S Thomas	17657	39	629	5015	14	2	18
Ann Richard	10105	48	1669	2982	40	-	28
Imran shah	5091	17	504	73	9	-	21
Steve Simmons	1956	1	351	2031	1	-	4
Woodrow Setzer	2803	-	122	18	-	-	4

What we would like...

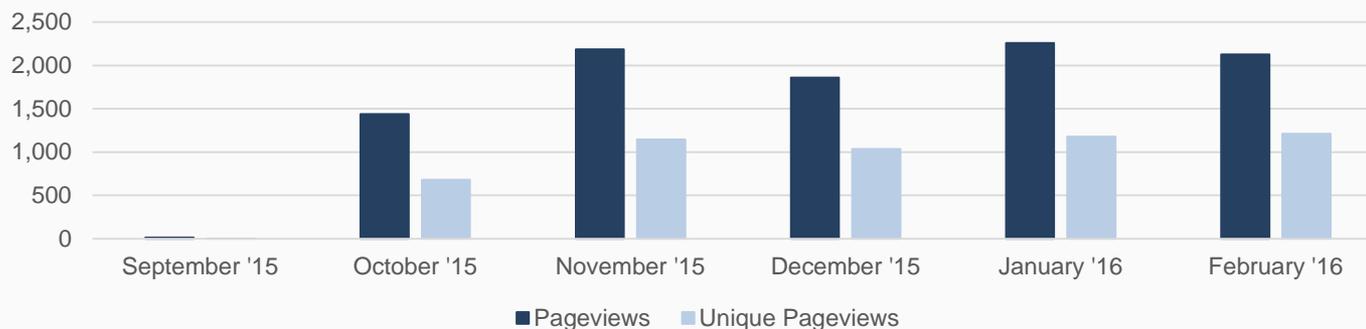
MOCKUP: Data Usage

Data & Tools: ToxCast Data Download Web

ToxCast Data Download Webpage Traffic (Daily)



ToxCast Data Download Webpage Traffic (Monthly)



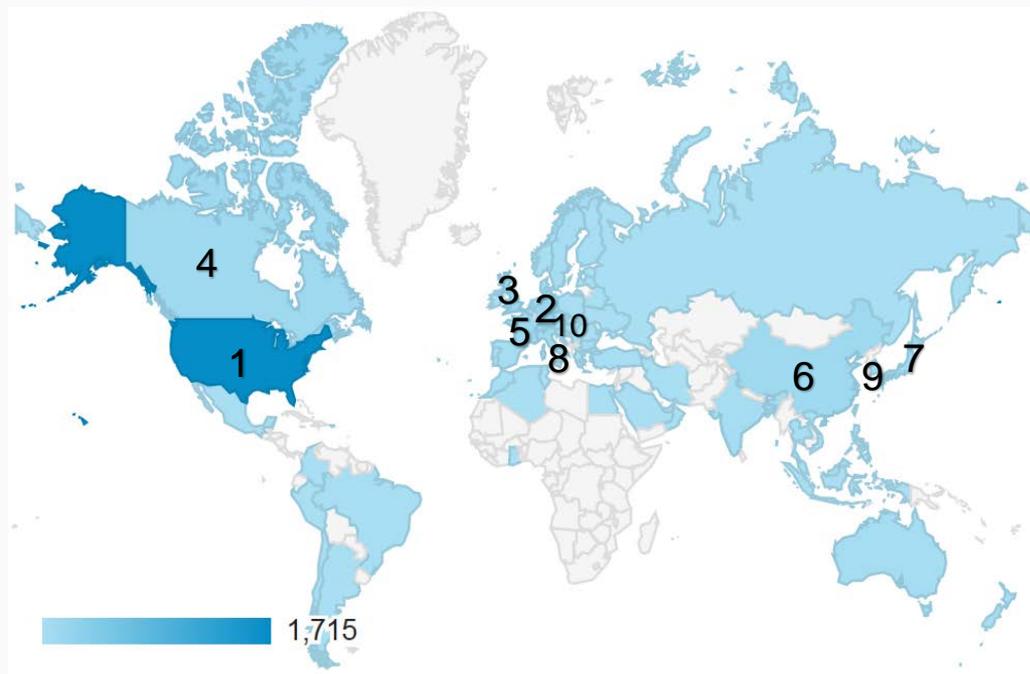
What we would like...

MOCKUP: Geographic Access

Data & Tools: ToxCast Data Download Web Demographics

Top Users by Country

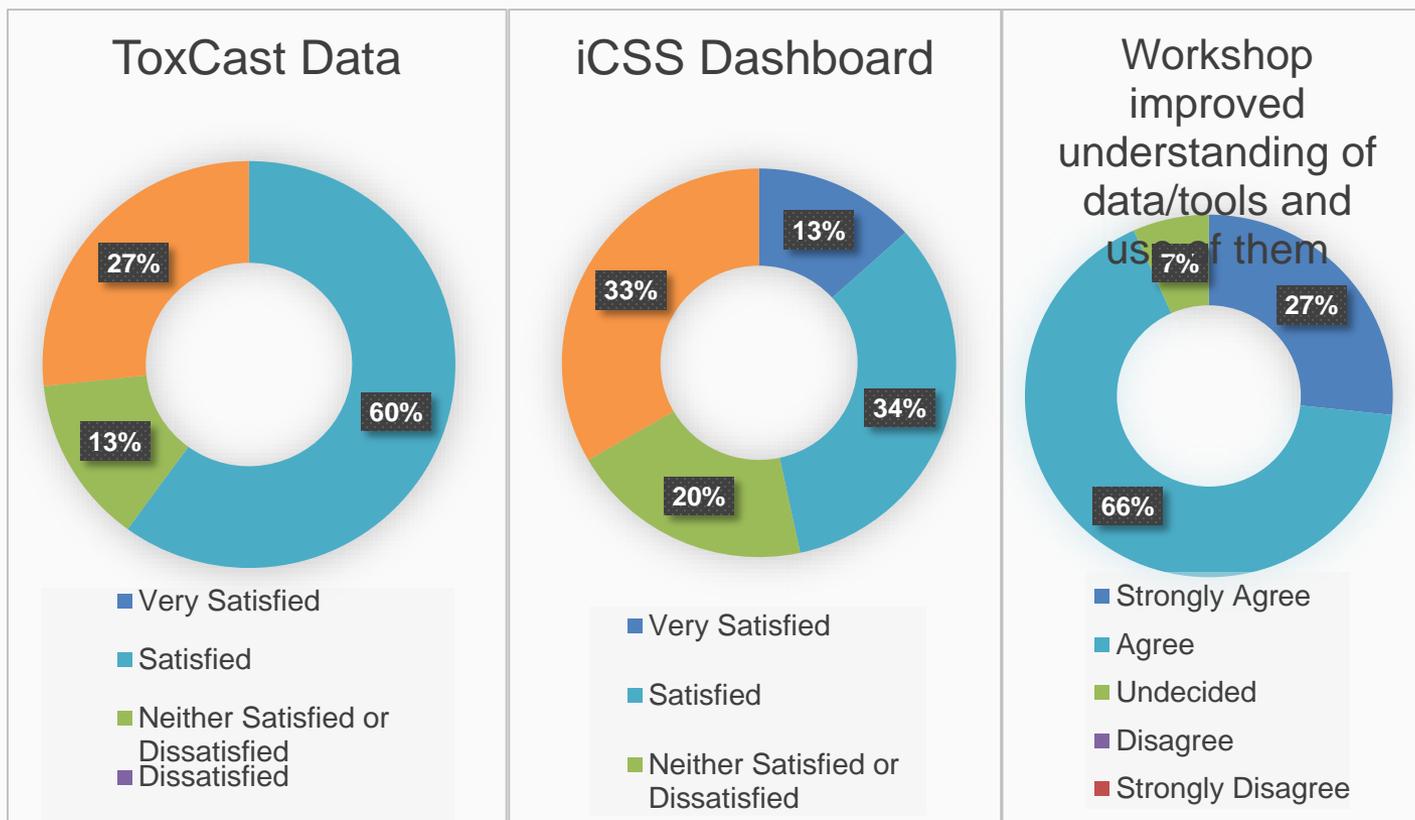
1. United States	1,715
2. Germany	170
3. United Kingdom	148
4. Canada	120
5. France	119
6. China	117
7. Japan	84
8. Italy	78
9. South Korea	60
10. Switzerland	56



What we would like...

MOCKUP: Aggregating Feedback

Interest and Use: 2014 Stakeholder Workshop Survey Results



Publications: Using Widgets

Leist, M., N. Hasiwa, C. Rovida, M. Daneshian, D. Basketter, I. Kimber, H. Clewell, T. Gocht, A. Goldberg, F. Busquet, A. Rossi, M. Schwarz, M. Stephens, R. Taalman, T. Knudsen, J. McKim, G. Harris, D. Pamies, AND T. Hartung. [Consensus report on the future of animal-free systemic toxicity testing](#). ALTEX. Society ALTEX Edition, Kuesnacht, Switzerland, 31(3):341-356, (2014).

Goldsmith, Rocky, Chris Grulke, R. Brooks, T. Transue, C. Tan, A. Frame, P. Egeghy, R. Edwards, D. Chang, R. Tornero-Velez, K. Isaacs, A. Wang, J. Johnson, K. Holm, M. Reich, J. Mitchell, D. Vallero, L. Phillips, M. Phillips, J. Wambaugh, R. Judson, T. Buckley, AND C. Dary. [Development of a Consumer Product Ingredient Database for Chemical Exposure Screening and Prioritization](#). FOOD AND CHEMICAL TOXICOLOGY. Elsevier Science Ltd, New York, NY, 65:269-279, (2014).

Paul, K., J. Hedge, D. Rotroff, M. Hornung, K. Crofton, AND Steve Simmons. [Development of a thyroperoxidase inhibition assay for high-throughput screening](#). CHEMICAL RESEARCH IN TOXICOLOGY. American Chemical Society, Washington, DC, 27(3):387-99, (2014).



- We are investigating AltMetric, PlumX and Kudos Widgets

Publications: AltMetric Widget

Leist, M., N. Hasiwa, C. Rovida, M. Daneshian, D. Basketter, I. Kimber, H. Clewell, T. Gocht, A. Goldberg, F. Busquet, A. Rossi, M. Schwarz, M. Stephens, R. Taalman, T. Knudsen, J. McKim, G. Harris, D. Pamies, AND T. Hartung. [Consensus report on the future of animal-free systemic toxicity testing](#). ALTEX. Society ALTEX Edition, Kuesnacht, Switzerland, 31(3):341-356, (2014).

Goldsmith, Rocky, Chris Grulke, R. Brooks, T. Transue, C. Tan, A. Frame, P. Egeghy, R. Edwards, D. Chang, R. Tornero-Velez, K. Isaacs, A. Wang, J. Johnson, K. Holm, M. Reich, J. Mitchell, D. Vallero, L. Phillips, M. Phillips, J. Wambaugh, R. Judson, T. Buckley, AND C. Dary. [Development of a Consumer Product Ingredient Database for Chemical Exposure Screening and Prioritization](#). FOOD AND CHEMICAL TOXICOLOGY. Elsevier Science Ltd, New York, NY, 65:269-279, (2014).

Paul, K., J. Hedge, D. Rotroff, M. Hornung, K. Crofton, AND Steve Simmons. [Development of a thyroperoxidase inhibition assay for high-throughput screening](#). CHEMICAL RESEARCH IN TOXICOLOGY. American Chemical Society, Washington, DC, 27(3):387-99, (2014).



- AltMetric will give us access to social sharing statistics and other stats

Publications: PlumX Widget

Leist, M., N. Hasiwa, C. Rovida, M. Daneshian, D. Basketter, I. Kimber, H. Clewell, T. Gocht, A. Goldberg, F. Busquet, A. Rossi, M. Schwarz, M. Stephens, R. Taalman, T. Knudsen, J. McKim, G. Harris, D. Pamies, AND T. Hartung. [Consensus report on the future of animal-free systemic toxicity testing](#). ALTEX. Society ALTEX Edition, Kuesnacht, Switzerland, 31(3):341-356, (2014).

Goldsmith, Rocky, Chris Grulke, R. Brooks, T. Transue, C. Tan, A. Frame, P. Egeghy, R. Edwards, D. Chang, R. Tornero-Velez, K. Isaacs, A. Wang, J. Johnson, K. Holm, M. Reich, J. Mitchell, D. Vallero, L. Phillips, M. Phillips, J. Wambaugh, R. Judson, T. Buckley, AND C. Dary. [Development of a Consumer Product Ingredient Database for Chemical Exposure Screening and Prioritization](#). FOOD AND CHEMICAL TOXICOLOGY. Elsevier Science Ltd, New York, NY, 65:269-279, (2014).

Paul, K., J. Hedge, D. Rotroff, M. Hornung, K. Crofton, AND Steve Simmons. [Development of a thyroperoxidase inhibition assay for high-throughput screening](#). CHEMICAL RESEARCH IN TOXICOLOGY. American Chemical Society, Washington, DC, 27(3):387-99, (2014).



PLUMX

Usage
 Clicks: 76
 Abstract Views: 171
 PDF Views: 2530
 HTML Views: 22535
 Link-outs: 1
 Downloads: 79

Captures
 Bookmarks: 1
 Exports-Saves: 14
 Readers: 88

Mentions
 Blog Mentions: 1

Social Media
 +1s: 7
 Tweets: 33

Citations
 Citation Indexes: 44
[see details](#)

- PlumX will give us access to social sharing statistics and other publication stats

Publications: Kudos Widget

Leist, M., N. Hasiwa, C. Rovida, M. Daneshian, D. Basketter, I. Kimber, H. Clewell, T. Gocht, A. Goldberg, F. Busquet, A. Rossi, M. Schwarz, M. Stephens, R. Taalman, T. Knudsen, J. McKim, G. Harris, D. Pamies, AND T. Hartung. [Consensus report on the future of animal-free systemic toxicity testing](#). ALTEX. Society ALTEX Edition, Kuesnacht, Switzerland, 31(3):341-356, (2014).

Goldsmith, Rocky, Chris Grulke, R. Brooks, T. Transue, C. Tan, A. Frame, P. Egeghy, R. Edwards, D. Chang, R. Tornero-Velez, K. Isaacs, A. Wang, J. Johnson, K. Holm, M. Reich, J. Mitchell, D. Vallerio, L. Phillips, M. Phillips, J. Wambaugh, R. Judson, T. Buckley, AND C. Dary. [Development of a Consumer Product Ingredient Database for Chemical Exposure Screening and Prioritization](#). FOOD AND CHEMICAL TOXICOLOGY. Elsevier Science Ltd, New York, NY, 65:269-279, (2014).

Paul, K., J. Hedge, D. Rotroff, M. Hornung, K. Crofton, AND Steve Simmons. [Development of a thyroperoxidase inhibition assay for high-throughput screening](#). CHEMICAL RESEARCH IN TOXICOLOGY. American Chemical Society, Washington, DC, 27(3):387-99, (2014).



- Kudos will provide details of social shares and article “enrichment”



Dispensing processes profoundly influence estimates of biological activity of compounds

Resources

- [Making People Aware of Biological Data Limitations](#)
A blog post on the Phoenix Next Inc. site by Sean Ekins, one of the authors of the paper
- [What data do we trust now in the world of high-throughput screening and public compound databases](#)
A blog post by myself on the ChemConnector blog regarding general issues of data quality and how this relates to high-throughput screening data and public compound databases
- [In the Pipeline Blog from Derek Lowe: Drug Assay Numbers, All Over the Place](#)
This blog post by Derek Lowe, who writes the In the Pipeline Blog, is best captured in terms of his opening sentence: "There's a truly disturbing paper out in PLoS ONE with potential implications for a lot of assay data out there in the literature."
- [Dispensing Processes Profoundly Impact Biological Assays and Computational and Statistical Analyses](#)
SlideShare Presentation: Dispensing processes profoundly influence estimates of biological activity of compounds. In this study using published inhibitor data for the tyrosine kinase EphB4, we show that IC50 values obtained via disposable tip-based serial dilution and dispensing versus acoustic dispensing differ by orders of magnitude with no correlation or ranking of datasets.

Read more on Kudos...

App Analytics: Google

CompTox
All Web Site Data ▾



HOME REPORTING CUSTOMIZATION ADMIN

Search reports & help

Audience Overview

Mar 13, 2016 - Aug 12, 2016 ▾

Email Export ▾ Add to Dashboard Shortcut

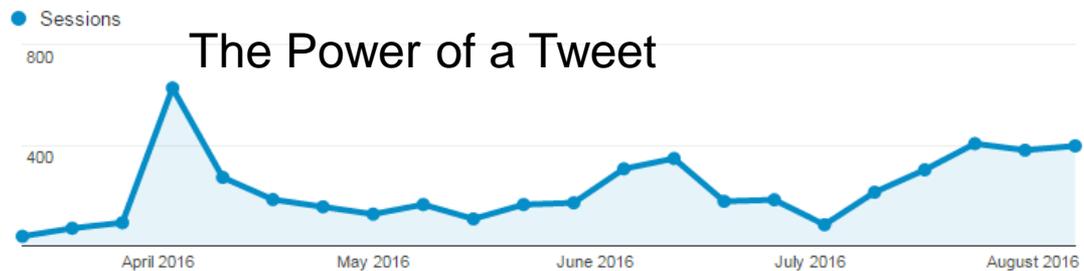
All Users
100.00% Sessions

+ Add Segment

Overview

Sessions ▾ vs. Select a metric

Hourly Day Week Month



- Dashboards
- Shortcuts
- Intelligence Events
- Real-Time
- Audience
 - Overview
 - Active Users
 - Cohort Analysis BETA
 - User Explorer
 - Demographics
 - Interests

- Investigating VIVO Open Source
- Data model in development
- **ORCiDs** for people, **DOIs** for papers
- Will integrate **AltMetric**, **PlumX** and **Kudos** embeddable widgets
- Integrate existing EPA tracking systems – e.g. EPA Science Inventory



Science Inventory Search Results

Search Criteria: the term 'Antony Williams' in any part of any record.
(Sorted by Relevance Rank)

Records 1 to 10 of 10

[The needs for chemistry standards, database tools and data curation at the chemical-biology interface \(SLAS meeting\)](#)

This presentation will highlight known challenges with the production of high quality chemical databases and outline recent efforts made to address these challenges. Specific examples will be provided illustrating these challenges within the U.S. Environmental Protection Agency ...

[The ToxCast Chemical Landscape - Paving the Road to 21st Century Toxicology](#)

The ToxCast high-throughput screening (HTS) program within the U.S. Environmental Protection Agency (EPA) was launched in 2007. Phase I of the program screened 310 chemicals, mostly pesticides, across hundreds of ToxCast assay endpoints. In Phase II, the ToxCast library was exp...

[An examination of data quality on QSAR Modeling in regards to the environmental sciences \(UNC-CH talk\)](#)

The development of QSAR models is critically dependent on the quality of available data. As part of our efforts to develop public platforms to provide access to predictive models, we have attempted to discriminate the influence of the quality versus quantity of data available to...

Search within these Results

Search

Our center – A BIG Impact! We are out to measure it...

