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
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

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Science Inventory Search Results

Records 1 to 25 of 202

2016


What are our products?

- Our Applications
What are our products?

- Our Data

https://www.epa.gov/chemical-research/downloadable-computational-toxicology-data
What are our products?

• Our collaborations

https://www.epa.gov/chemical-research/collaborative-agreements-computational-toxicology-research
What are our products?

• Our scientific leadership
  https://www.epa.gov/chemical-research/toxicity-forecasting
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/](http://altmetrics.org/manifesto/))
Altmetrics impact

- **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), resuse of code, algorithms and models
Altmetrics impact

- **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
• Many Social and Altmetric platforms in recent years...

• ...and publishers use these for tracking, assisting distribution and for amplification
Antony Williams

ORCID ID

orcid.org/0000-0002-2668-4821

View public version

Get a QR Code for your ID

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.
### Works (3)

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PlumX: Scientists AltMetrics
https://plu.mx/u/awilliams/

Antony J. Williams
Connections in Chemistry

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

Lecture / Presentation (267)  Article (163)  Data (96)  Book Chapter (44)  Video (28)  Review (20)  Book (12)
Figuro (19)  Research Artifact (4)  Patent (2)  Media (2)  Blog Post (1)  Web resource (1)
PlumX: Scientists AltMetrics

https://plu.mx/u/awilliams/

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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

Altmetric: Article Level Metrics
https://www.altmetric.com/details/1425979?src=bookmarklet
AltMetric: Geographical Metrics

In the top 5% of all research outputs scored by Altmetric

Mentioned by
- 2 news outlets
- 5 blogs
- 53 tweeters
- 1 peer review site
- 1 Facebook page
- 2 Google+ users
- 1 research highlight platform

Readers on
- 74 Mendeley
- 4 CiteULike

What is this page?

The data shown below were collected from the profiles of 53 tweeters who shared this research output. Click here to find out more about how the information was compiled.
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.0062225

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.
GrowKudos: Article Level Metrics

Publications Metrics

KUDOS

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

IMPROVE MY RESULTS

Cumulative activity for publication: Dispensing Processes Impact Apparent Biological Activity as Determined by Computational and Statistical Analyses

- Full text downloads
- Abstract views
- Share referrals
- Kudos views

A = Author activity e.g. sharing. Hover over for more details.
P = Publisher activity. Hover over for more details.
K = Kudos admin activity. Hover over for more details.

Graph showing cumulative activity over time.
GrowKudos integrating AltMetric
Altmetric Widgets
http://api.altmetric.com/embeds.html
Kudos Widgets

There are three Kudos Widgets available for you to use on web pages, blog pages, publisher platforms and other online channels. The Kudos Publication Widget allows you to embed enhanced publication details including the title, lay summary and impact statement where present. The Kudos Resources Widget lists resources that have been added to the publication in Kudos. The Use Kudos widgets can be used to prompt authors to enhance their publication on Kudos by providing details such as title, lay summary and impact statement and will only appear for publications which do not have a lay summary or an impact statement on Kudos.

Note that widgets are responsive, just wrap the script tag in a container element (div is fine) and its width as you wish.

1. How to embed the Kudos Publication Widget

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
Artifact Pop-Up Widget

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

**Attr**

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<td>If true, hide the widget when no data is available</td>
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<td>Controls the size of the plumpprint</td>
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<td>data-badge</td>
<td>true</td>
<td>If true, sets data-size to 'small', and appends a link to the artifact page</td>
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[PlumX Widget](https://plum.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
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.

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

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

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

- 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

Metrics by publication year

Usage by publication year

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
Scientific Papers: By Author

National Center for Computational Toxicology

Researchers

Artifact Summary

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

Recent Artifacts

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- Incorporating High-Throughput Exposure Predictions With Dosimetry-Adjusted In Vitro Bioactivity to Inform Chemical Toxicity Testing.

Usage

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<th>PDF Views</th>
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Data & Tools: ToxCast Data Download Web

ToxCast Data Download Webpage Traffic (Daily)

ToxCast Data Download Webpage Traffic (Monthly)

What we would like…

MOCKUP: Data Usage
What we would like…

MOCKUP: Geographic Access

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
Interest and Use: 2014 Stakeholder Workshop Survey Results

ToxCast Data
- Very Satisfied: 27%
- Satisfied: 60%
- Neither Satisfied or Dissatisfied: 13%

iCSS Dashboard
- Very Satisfied: 33%
- Satisfied: 34%
- Neither Satisfied or Dissatisfied: 20%

Workshop improved understanding of data/tools and use of them
- Strongly Agree: 7%
- Agree: 66%
- Undecided: 27%
Publications: Using Widgets


• We are investigating AltMetric, PlumX and Kudos Widgets
Publications: AltMetric Widget


- AltMetric will give us access to social sharing statistics and other stats
PlumX will give us access to social sharing statistics and other publication stats.
Kudos will provide details of social shares and article “enrichment”
The Power of a Tweet
Work in Progress

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