http://www.orcid.org/0000-0002-2668-4821

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

Antony Williams, Monica Linnenbrink, Kevin Crofton, Russell Thomas and Jeffery Edwards*

National Center for Computational Toxicology
U.S. Environmental Protection Agency, RTP, NC

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

Records 1 to 25 of 202

Next >>

Widen Your Search

Stop filtering by organization

Expand results with the Science Inventory advanced search

2016

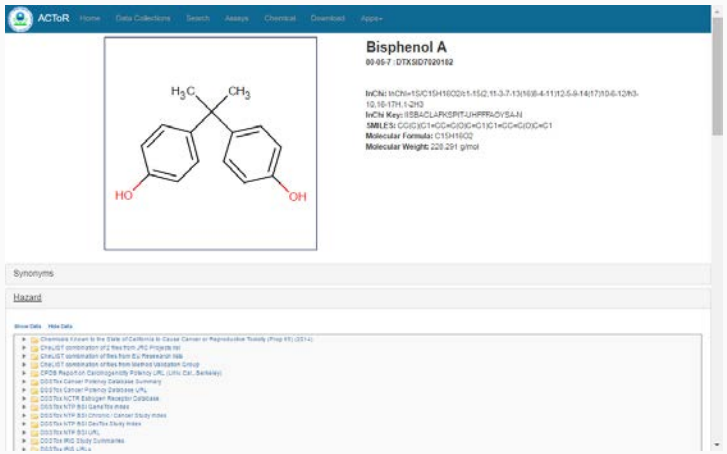
Judson, R., K. Houck, M. Martin, A. Richard, T. Knudsen, I. Shah, S. Little, J. Wambaugh, Woodrow Setzer, P. Kothiya, J. Phuong, D. Filer, D. Smith, D. Reif, D. Rotroff, N. Kleinstreuer, N. Sipes, M. Xia, R. Huang, K. Crofton, AND R. Thomas. Analysis of the Effects of Cell Stress and Cytotoxicity on In Vitro Assay Activity Across a Diverse Chemical and Assay Space. TOXICOLOGICAL SCIENCES. Society of Toxicology, 152(2):323-339, (2016).

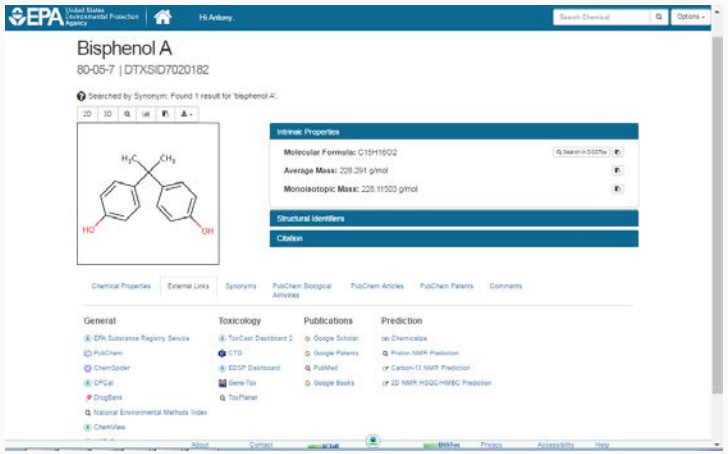
Kuo, B., F. Webster, R. Thomas, AND C. Yauk. BMDExpress Data Viewer: A Visualization Tool to Analyze BMDExpress Datasets. JOURNAL OF APPLIED TOXICOLOGY. John Wiley & Sons, Ltd., Indianapolis, IN, 36(8):1048-1059, (2016).

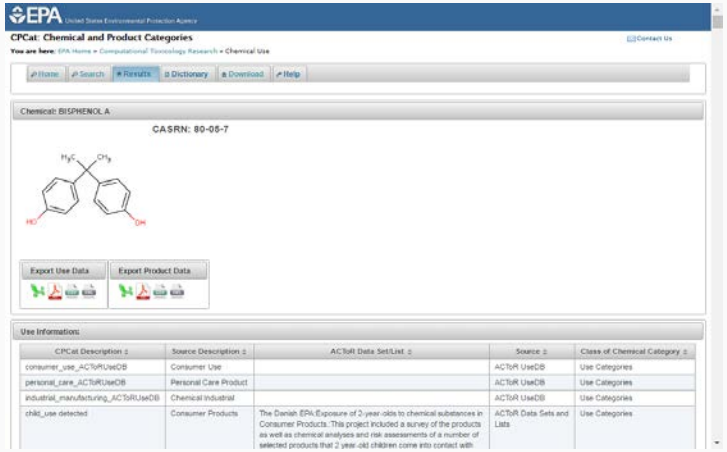
Ball, N., M. Cronin, J. Shen, M. Adenuga, K. Blackburn, E. Booth, M. Bouhifd, B. Donley, L. Egnash, J. Freeman, C. Hastings, D. Juberg, A. Kleensang, N. Kleinstreuer, D. Kroese, T. Luechtefeld, A. Maertens, S. Marty, J. Naciff, J. Palmer, D. Pamies, M. Penman, A. Richarz, D. Russo, D. Steup, S. Stuard, 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).

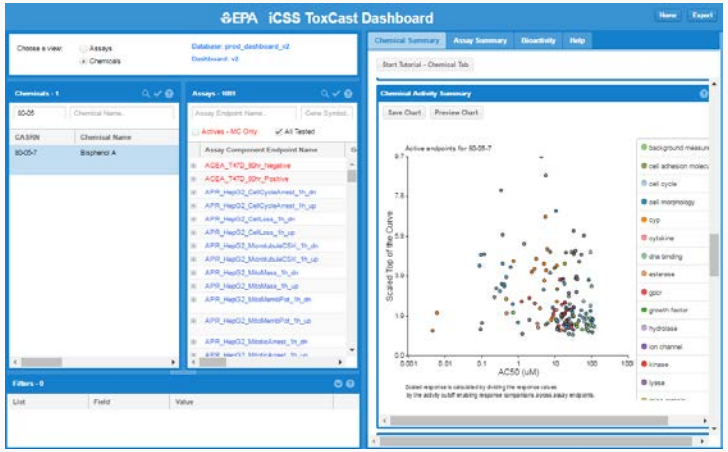
What are our products?

- Our Applications





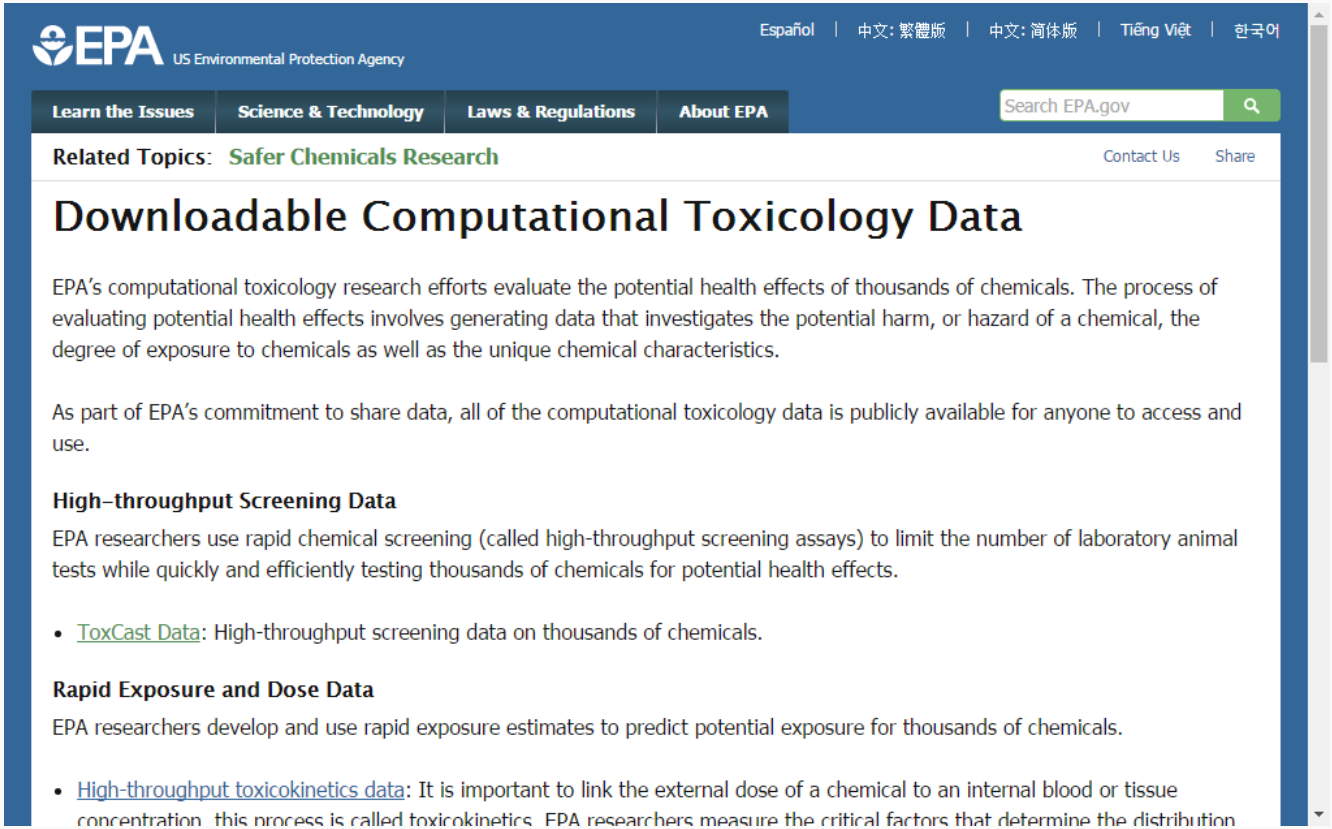




What are our products?

- Our Data

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

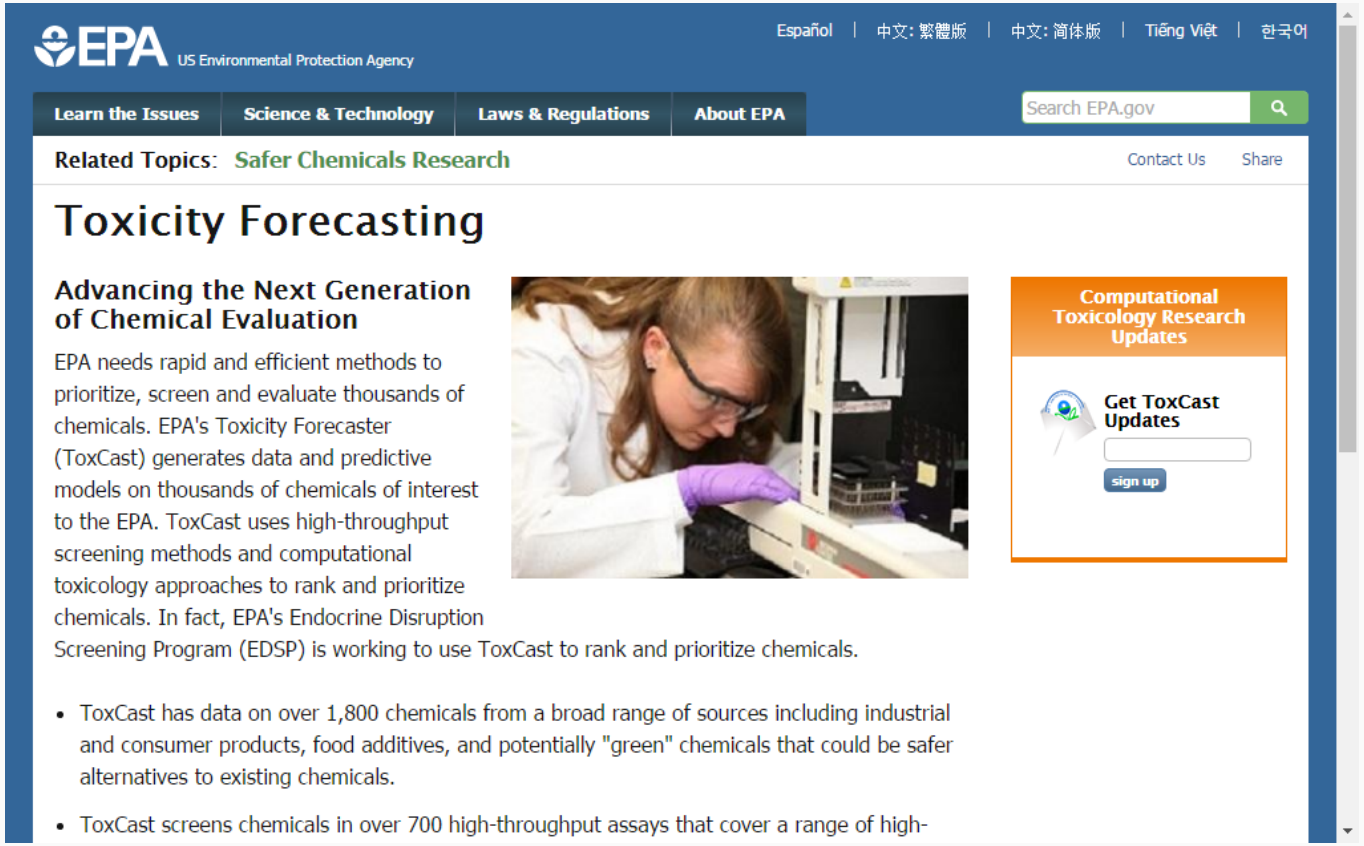
What are our products?

- Our collaborations

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

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/)

Altmetrics impact

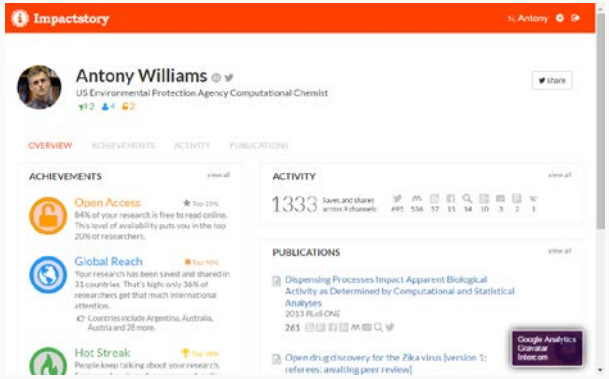
- **Scientific Publications and Presentations** – how many downloads, views, shares, tweets, embeds,
- **Research data** – downloads, uses, publications about and citations to data
- **Software applications, code, algorithms and models** – number of visitors, geography of visitors, number of searches,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

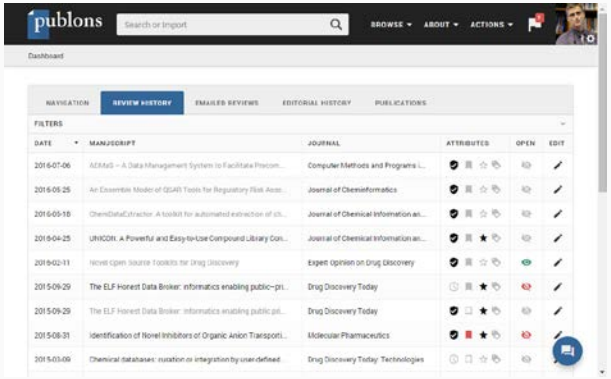
Altmetrics impact

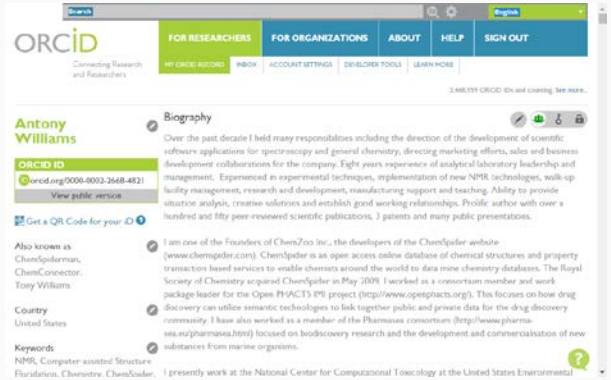
- **Collaborations** – funding of external work, provision of ToxCast plated materials,
- **Training – postdoctoral researchers** – what careers do they have when they leave NCCT?
- **Scientific Leadership** – contributions to EPA policy documents

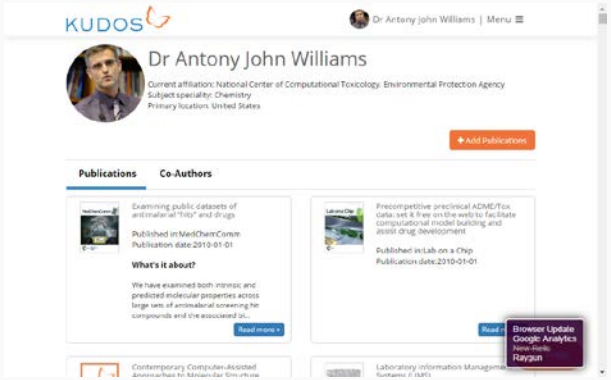
Scientist AltMetrics

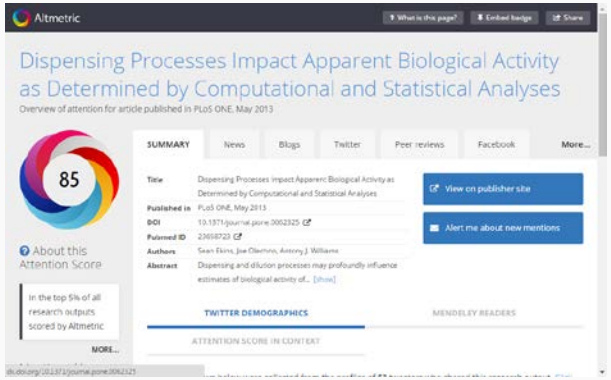
- Many Social and Altmetric platforms in recent











- …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

PLOS

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Total Article Views

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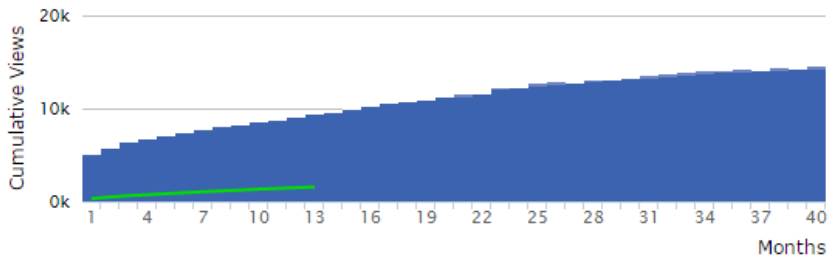
PMC	227	64	n.a.	291
Totals	13,065	1,414	42	14,521

10.82 % of article views led to PDF downloads



Compare average usage for articles published in **2013** in the subject area:

Computer and information sciences | Show reference set

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- Acoustics
- Hydrogen bonding
- Statistical data
- Bioacoustics
- Crystal structure
- Tyrosine kinases
- Molecular structure
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PLoS Article

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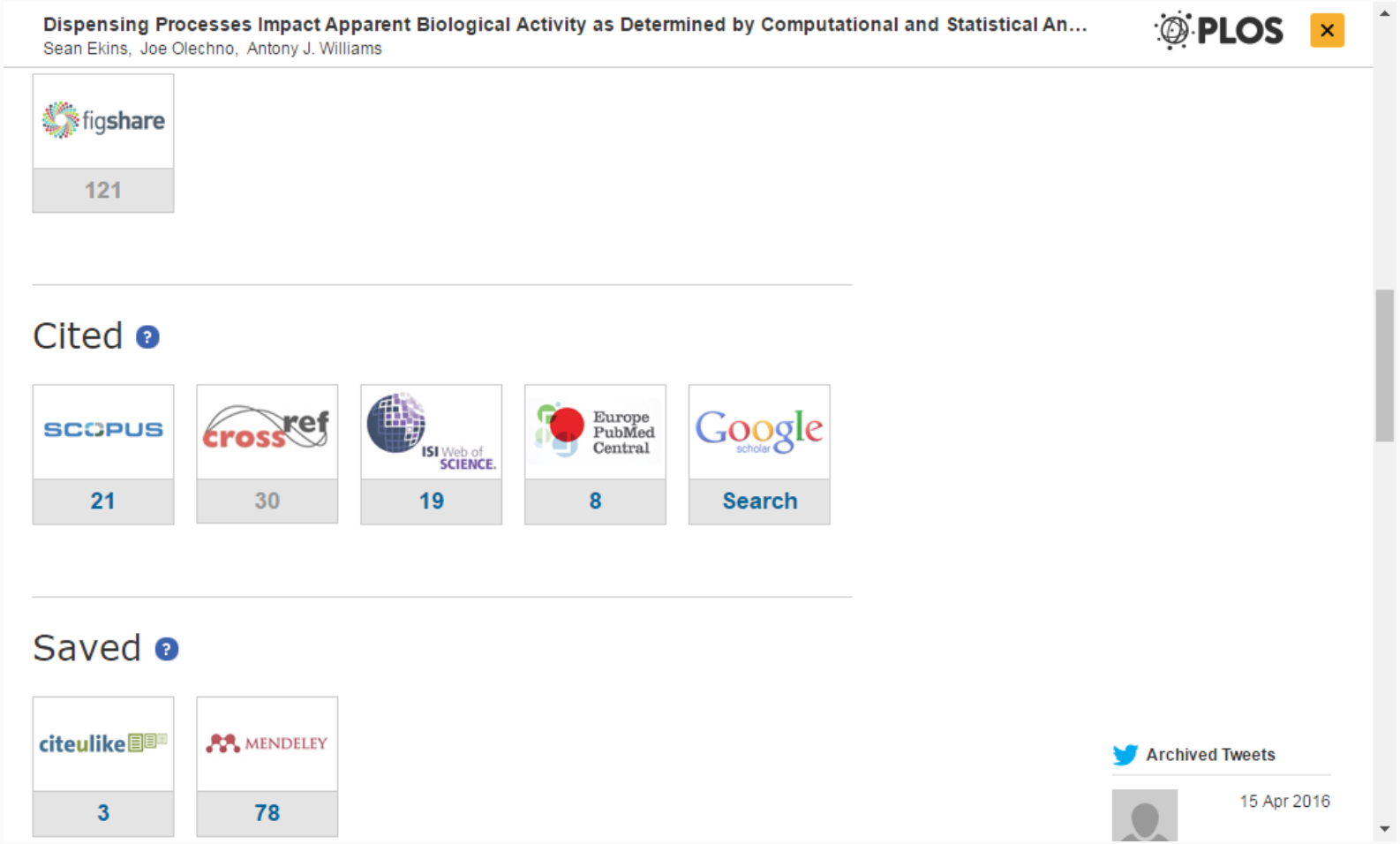
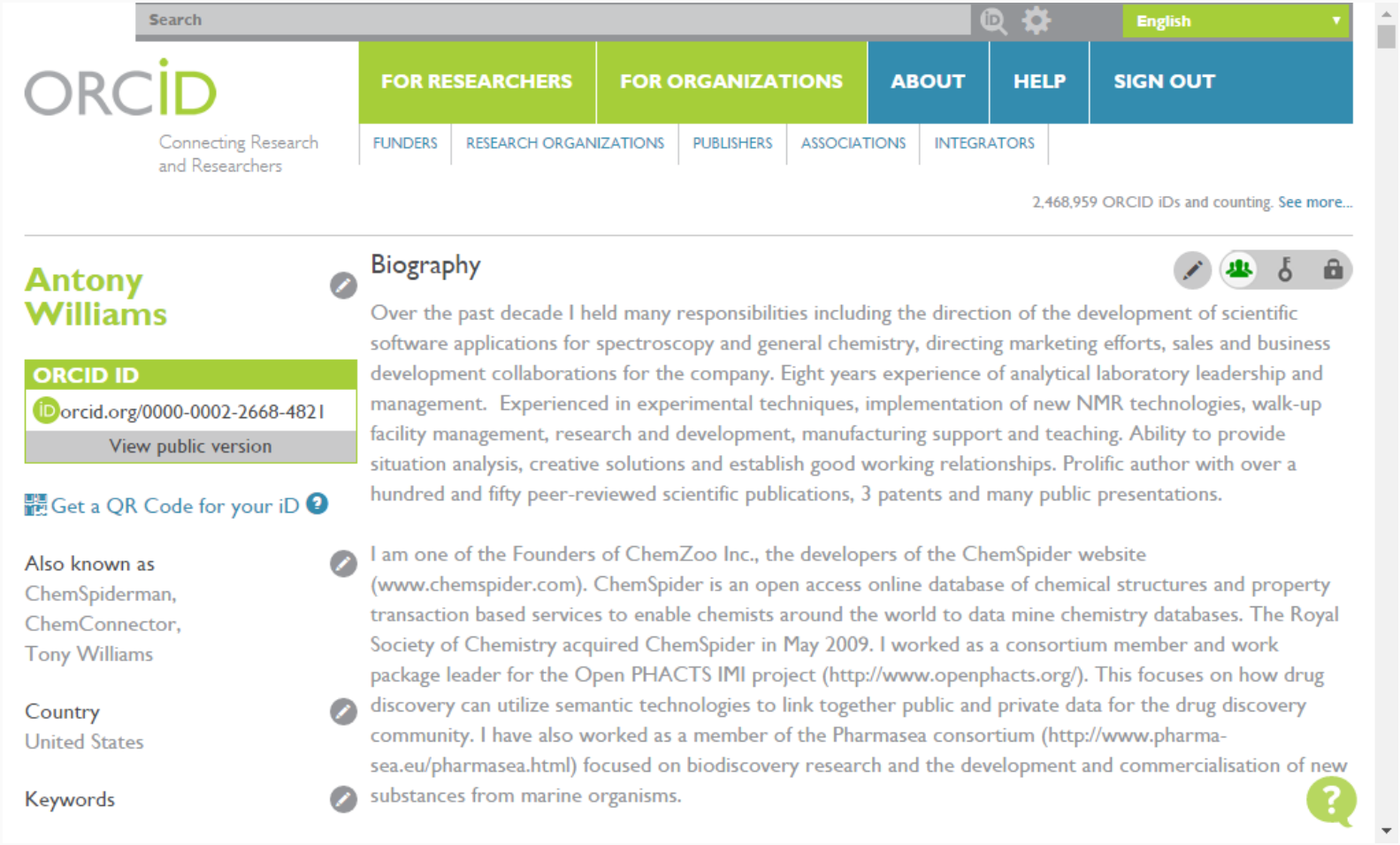
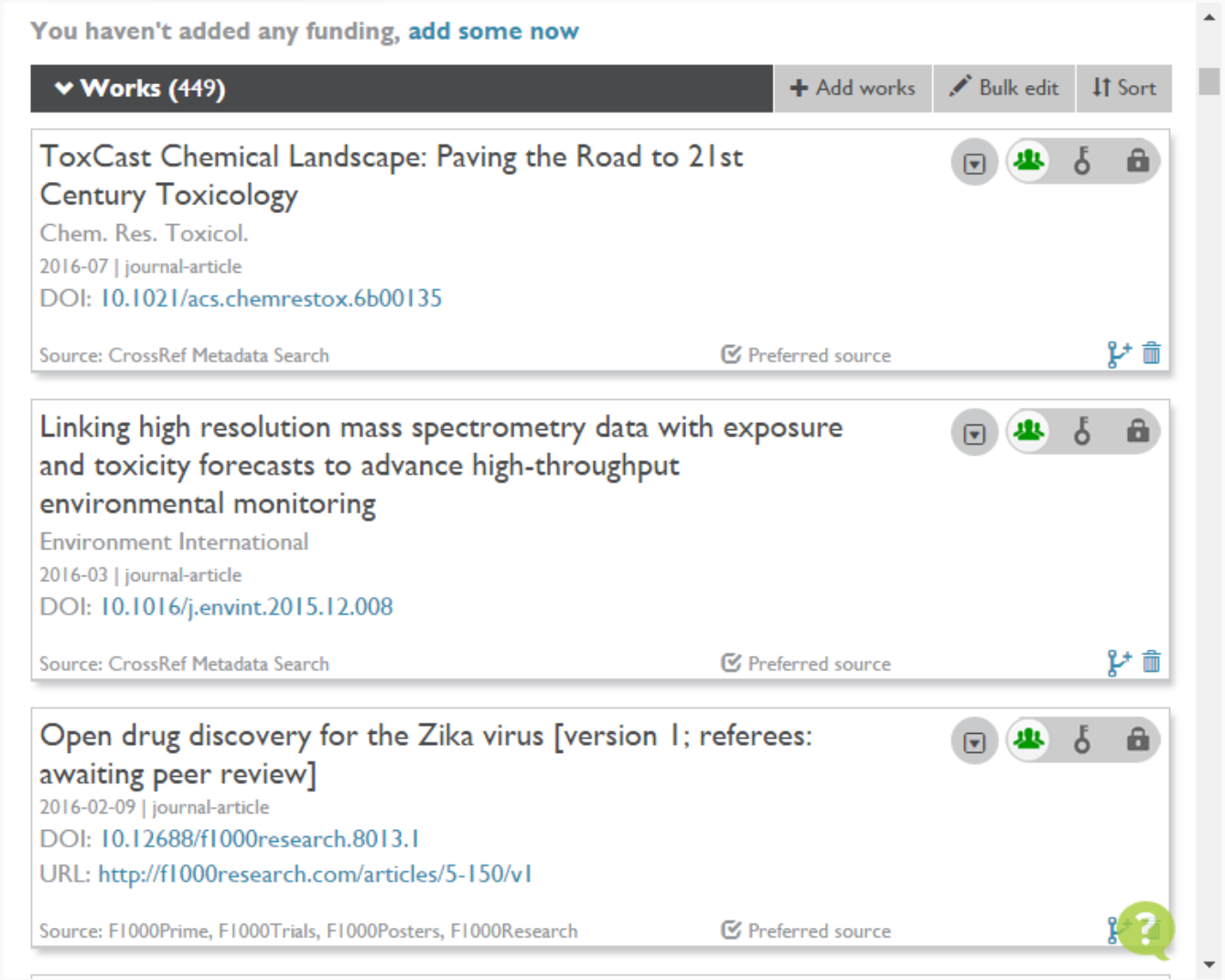


Scientists Identifier: ORCiD



ORCiD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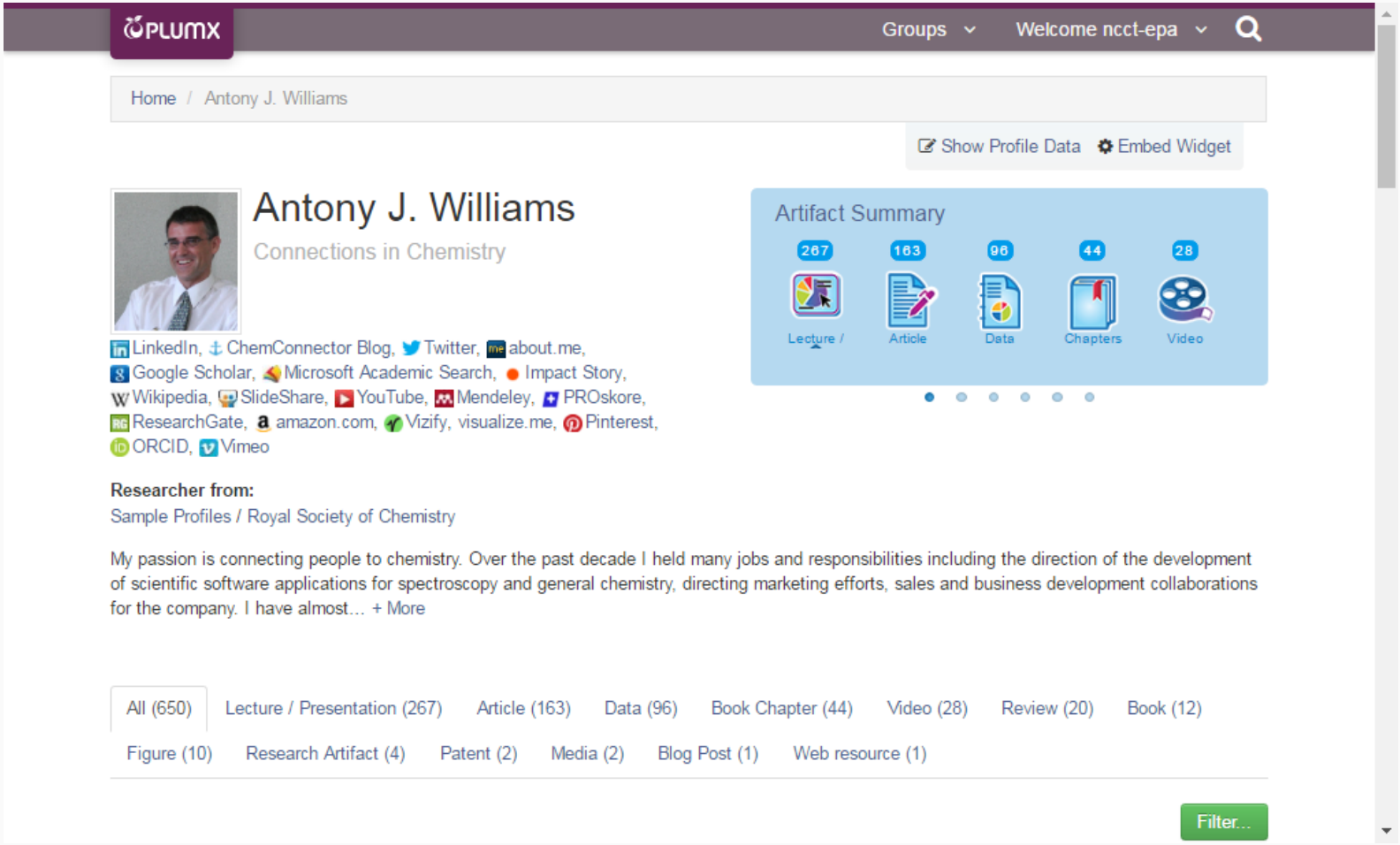
Works (449)
+ Add works
Bulk edit
Sort
ToxCast Chemical Landscape: Paving the Road to 21st Century Toxicology
Chem. Res. Toxicol.
2016-07 | journal-article
DOI: 10.1021/acs.chemrestox.6b00135
Source: CrossRef Metadata Search
Preferred source
Linking high resolution mass spectrometry data with exposure and toxicity forecasts to advance high-throughput environmental monitoring
Environment International
2016-03 | journal-article
DOI: 10.1016/j.envint.2015.12.008
Source: CrossRef Metadata Search
Preferred source
Open drug discovery for the Zika virus [version 1; referees: awaiting peer review]
2016-02-09 | journal-article
DOI: 10.12688/f1000research.8013.1
URL: http://f1000research.com/articles/5-150/v1
Source: F1000Prime, F1000Trials, F1000Posters, F1000Research
Preferred source

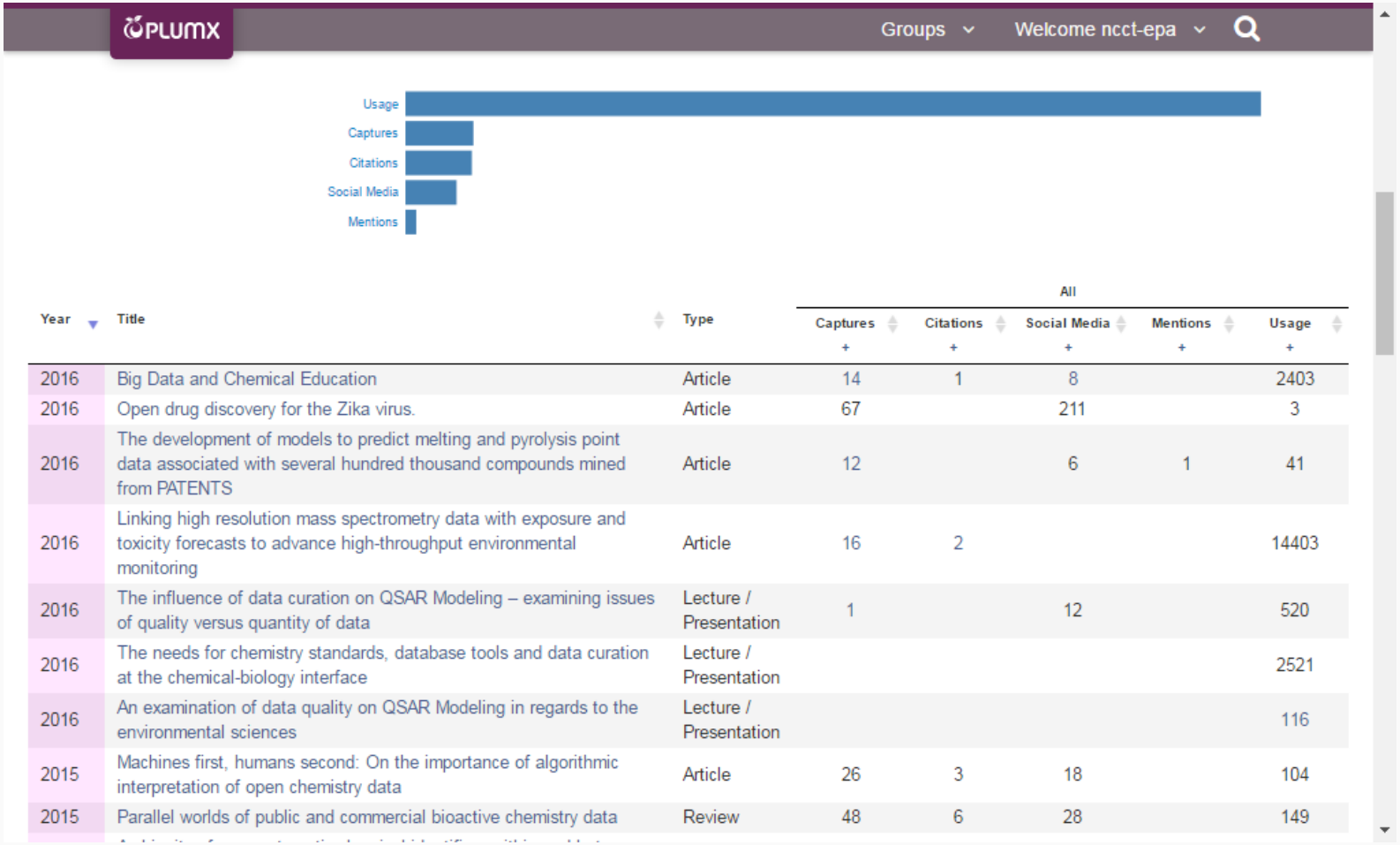
PlumX: Scientists AltMetrics

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



PlumX: Scientists AltMetrics

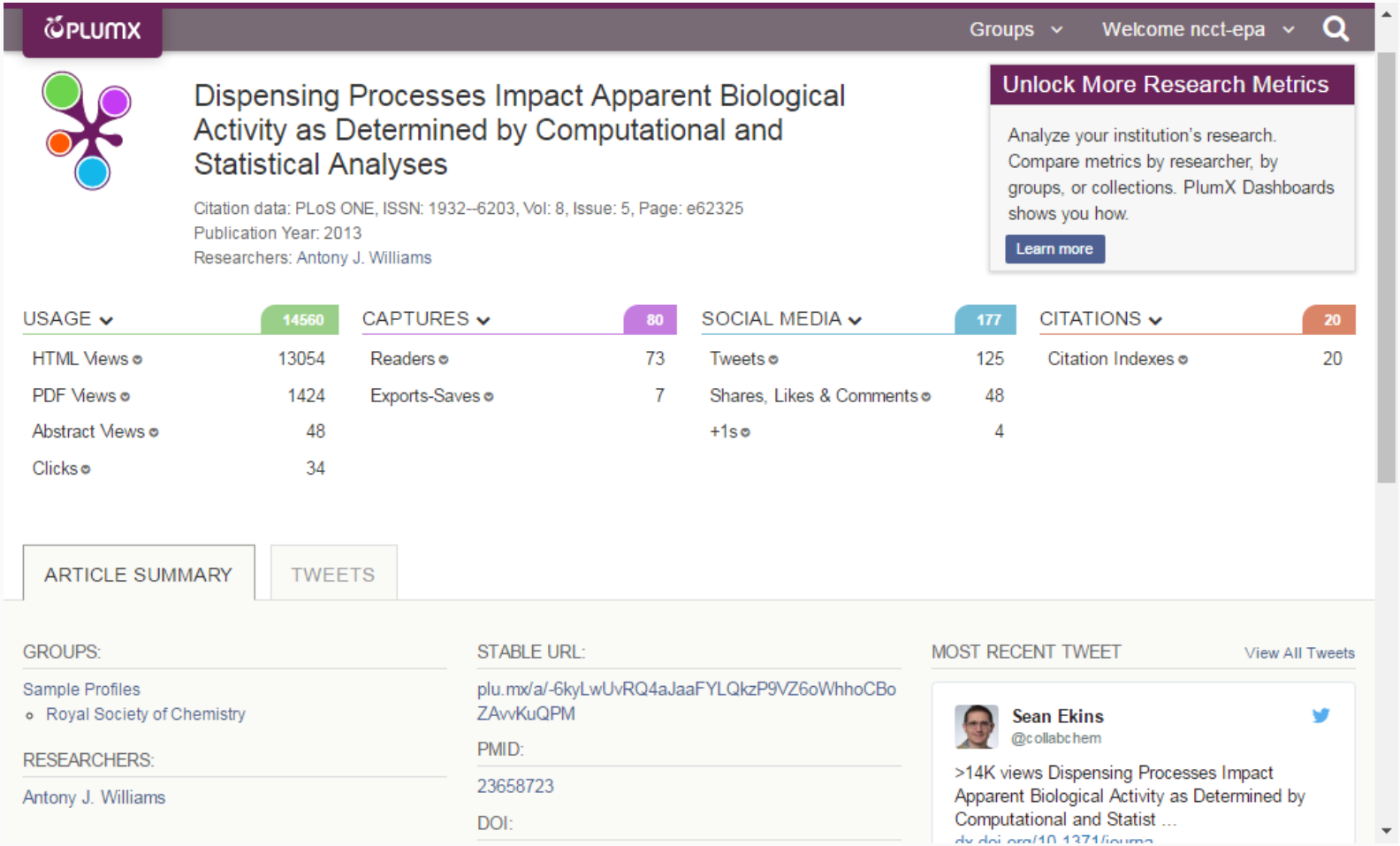
https://plu.mx/u/awilliams/



Year	Title	Type	All				
			Captures +	Citations +	Social Media +	Mentions +	Usage +
2016	Big Data and Chemical Education	Article	14	1	8		2403
2016	Open drug discovery for the Zika virus.	Article	67		211		3
2016	The development of models to predict melting and pyrolysis point data associated with several hundred thousand compounds mined from PATENTS	Article	12		6	1	41
2016	Linking high resolution mass spectrometry data with exposure and toxicity forecasts to advance high-throughput environmental monitoring	Article	16	2			14403
2016	The influence of data curation on QSAR Modeling – examining issues of quality versus quantity of data	Lecture / Presentation	1		12		520
2016	The needs for chemistry standards, database tools and data curation at the chemical-biology interface	Lecture / Presentation					2521
2016	An examination of data quality on QSAR Modeling in regards to the environmental sciences	Lecture / Presentation					116
2015	Machines first, humans second: On the importance of algorithmic interpretation of open chemistry data	Article	26	3	18		104
2015	Parallel worlds of public and commercial bioactive chemistry data	Review	48	6	28		149

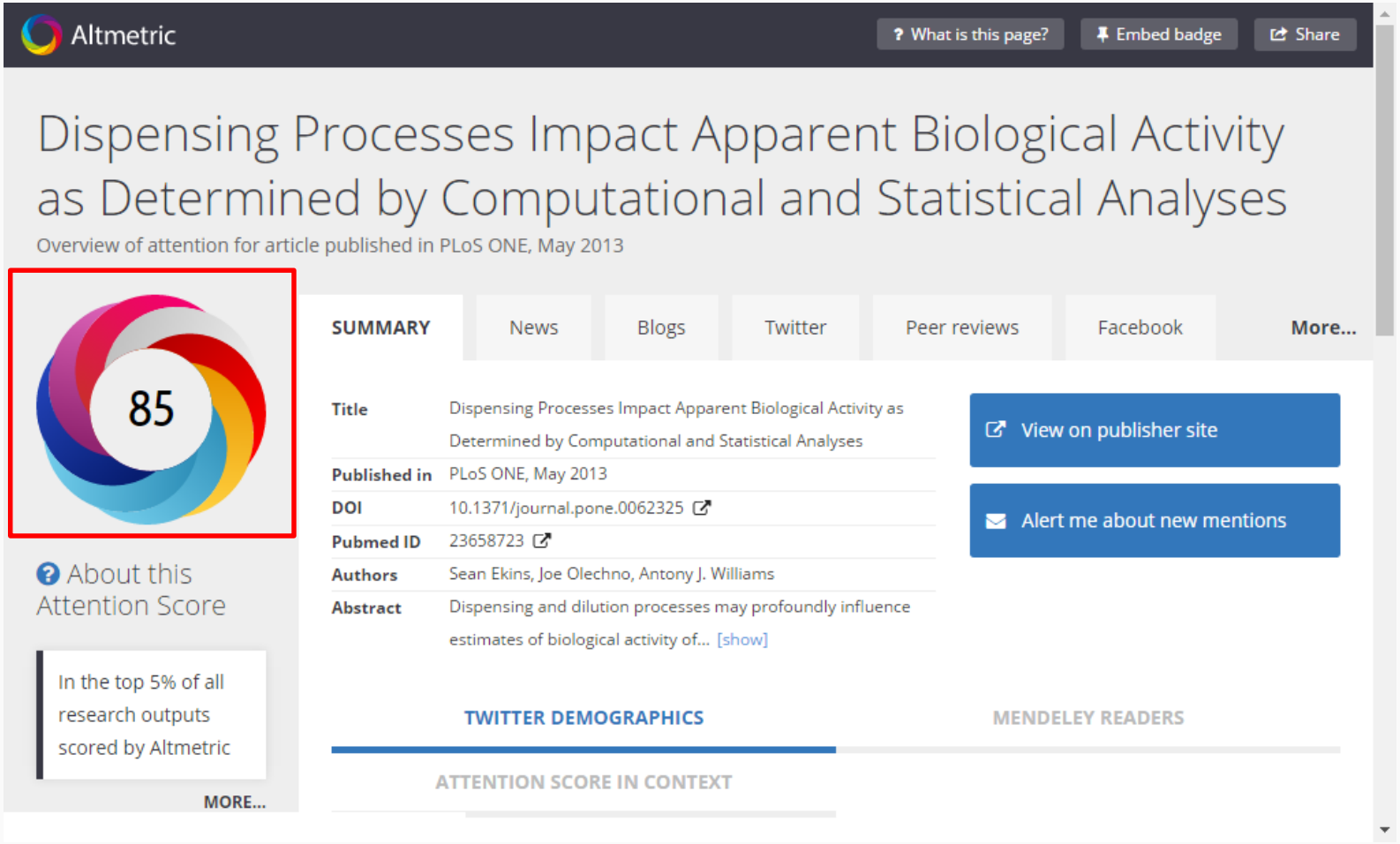
PlumX: Article Level Metrics

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

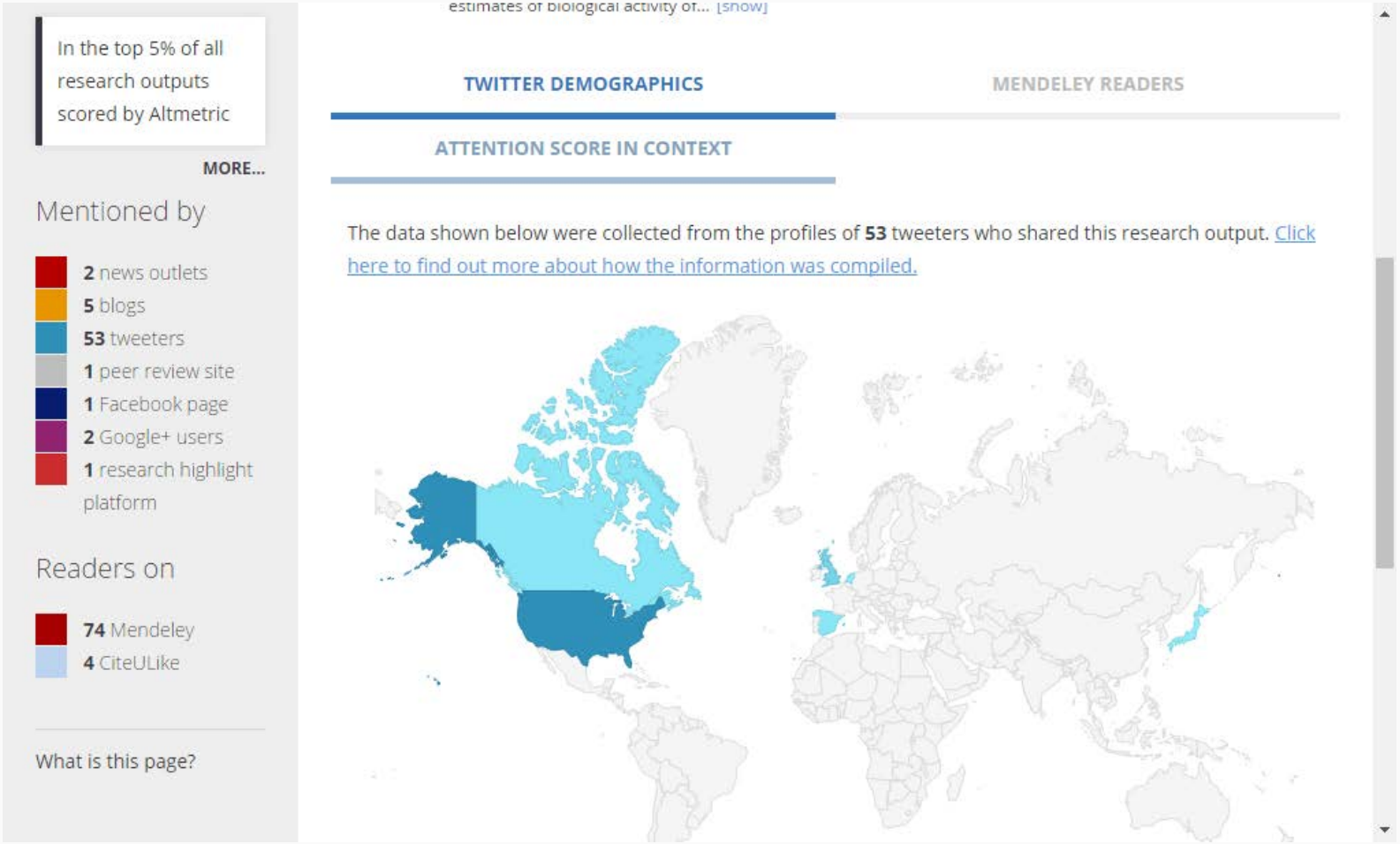


AltMetric: Article Level Metrics

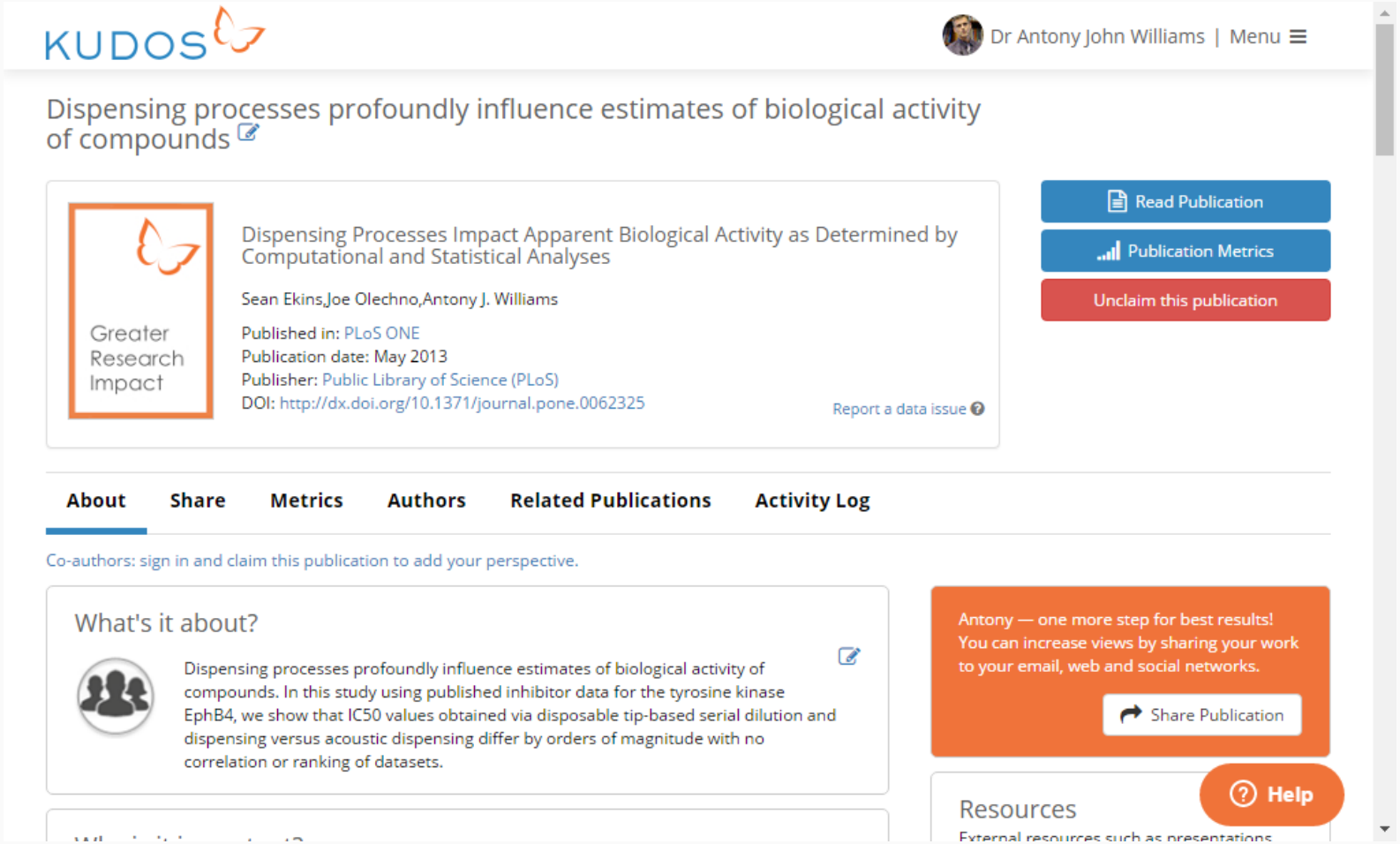
https://www.altmetric.com/details/1425979?src=bookmarklet



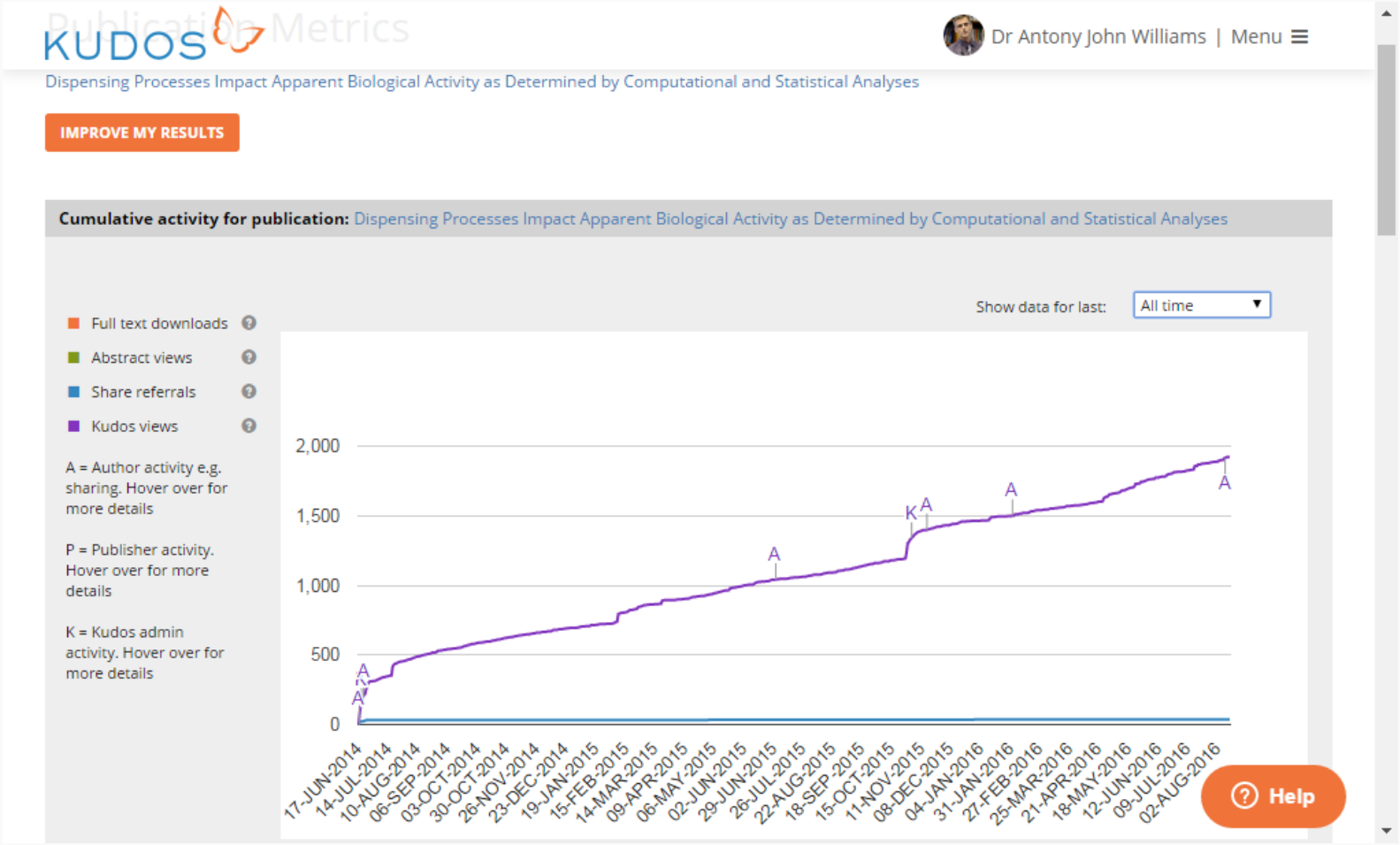
AltMetric: Geographical Metrics



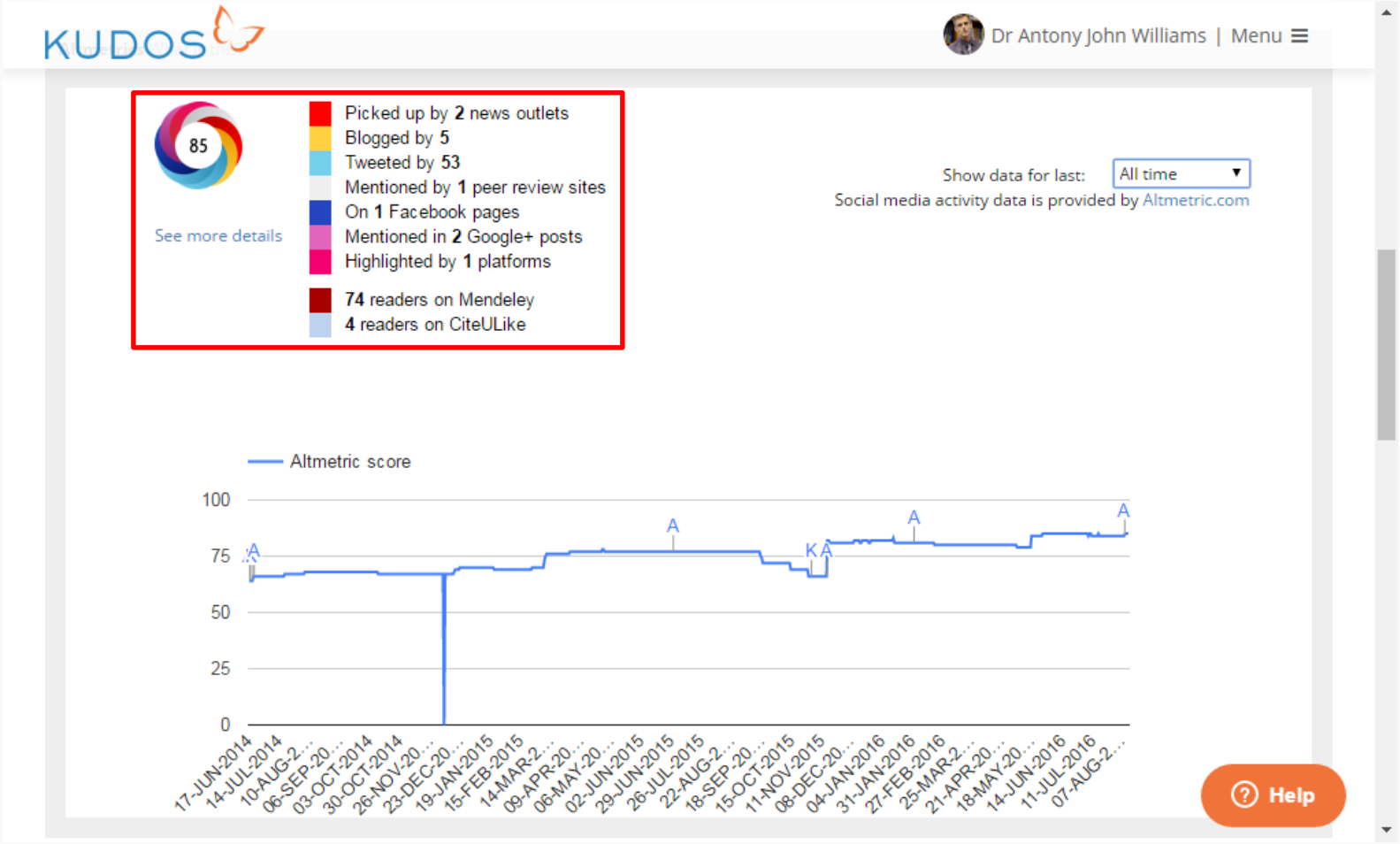
GrowKudos: Article Level Data



GrowKudos: Article Level Metrics

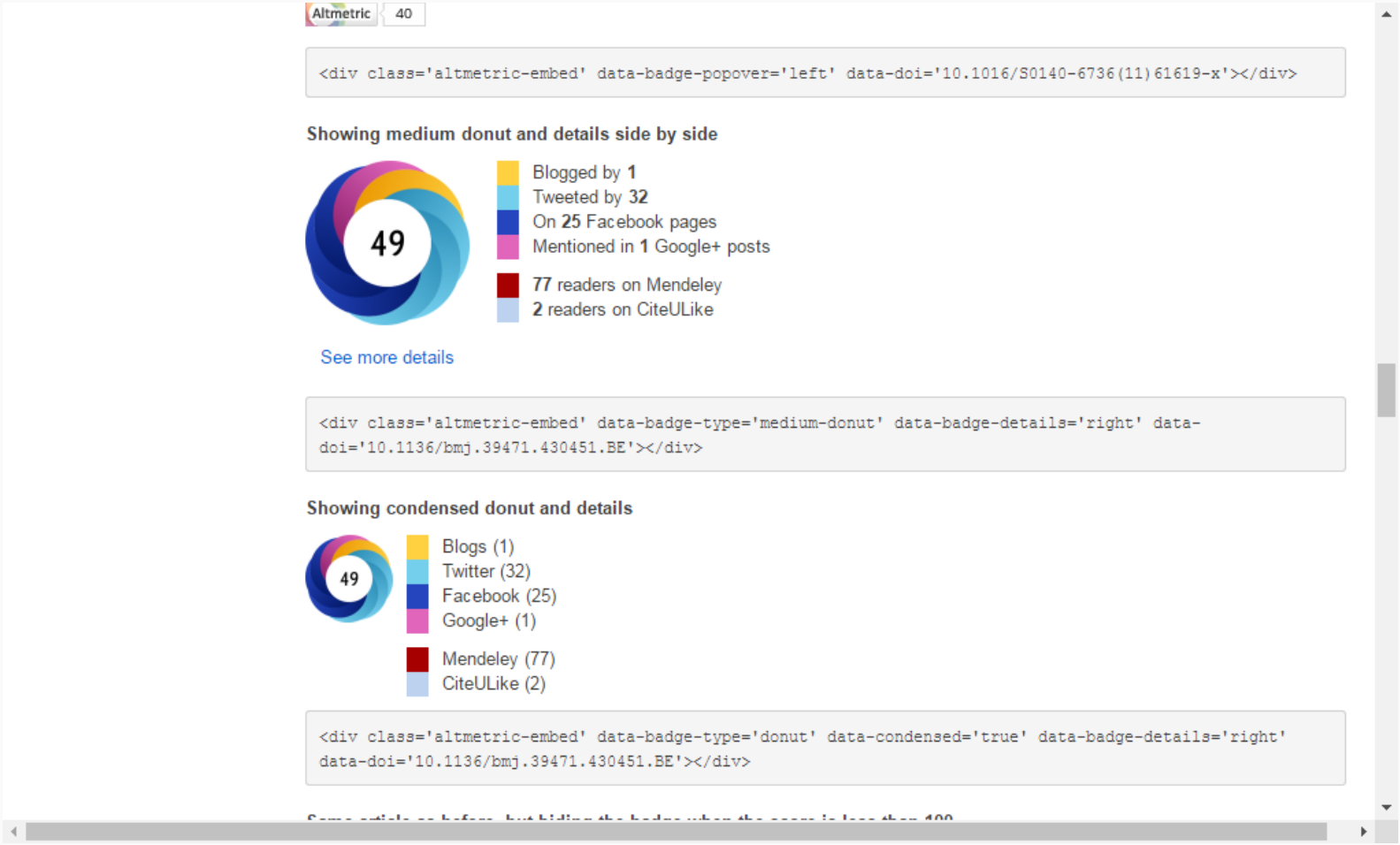


GrowKudos integrating AltMetric



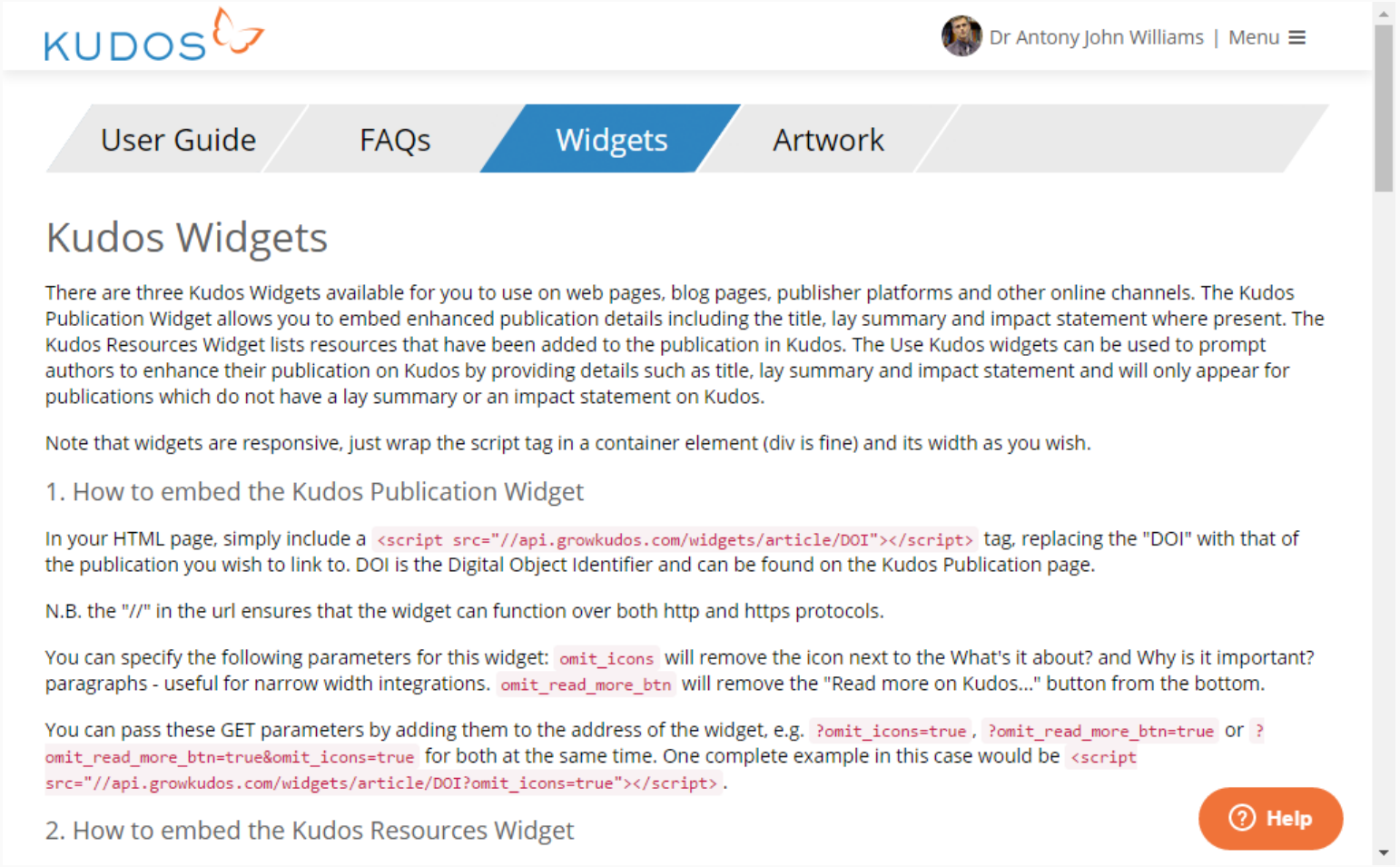
Altmetric Widgets

http://api.altmetric.com/embeds.html



Kudos Widgets

https://www.growkudos.com/about/user_guide



KUDOS

Dr Antony John Williams | Menu

User Guide | FAQs | Widgets | Artwork

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.

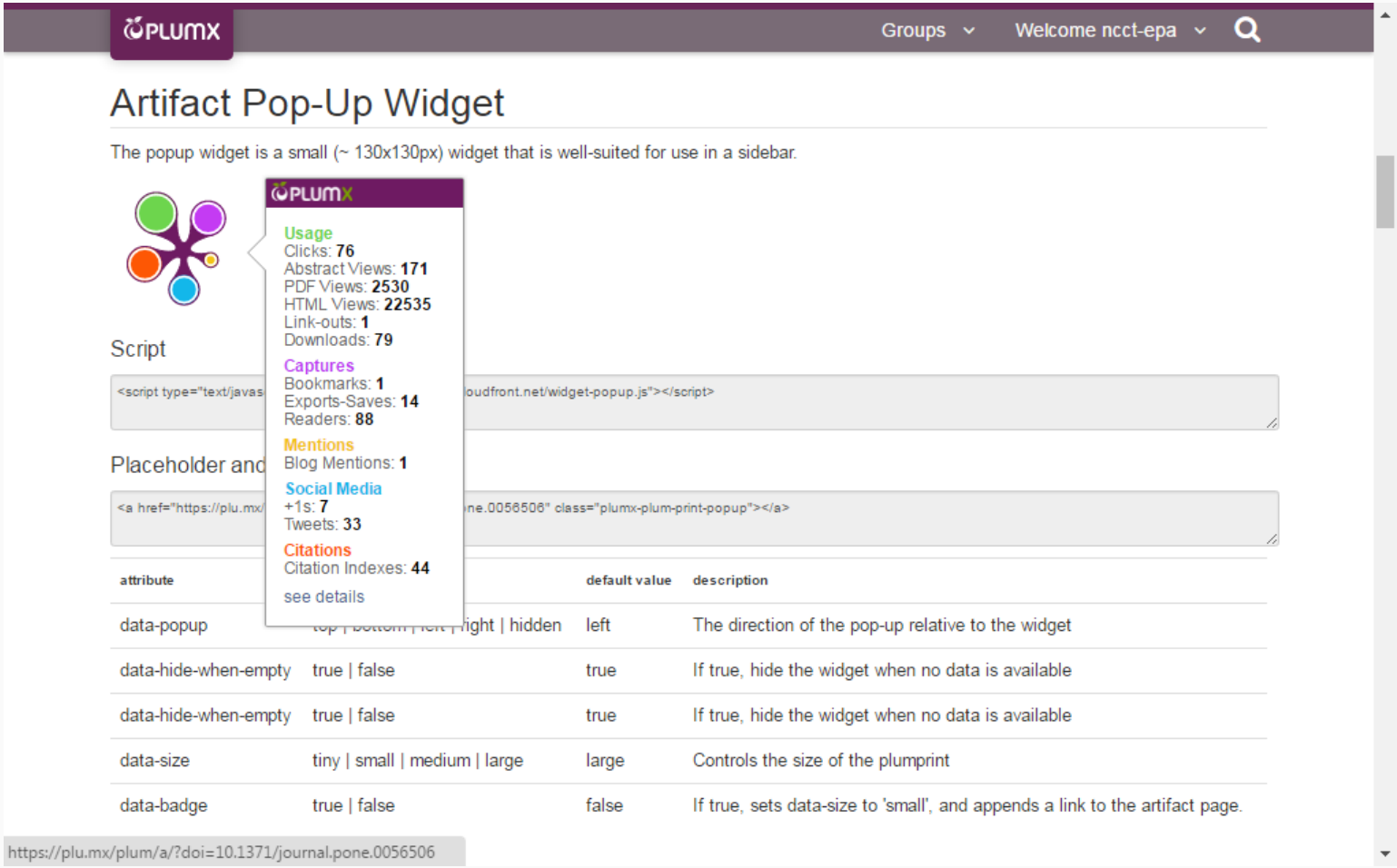
You can specify the following parameters for this widget: `omit_icons` will remove the icon next to the What's it about? and Why is it important? paragraphs - useful for narrow width integrations. `omit_read_more_btn` will remove the "Read more on Kudos..." button from the bottom.

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

Help

PlumX Widget



Integrating Data

- 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

EPA United States Environmental Protection Agency

EPA United States Environmental Protection Agency | Español | 中文: 繁體版 | 中文: 简体版 | Tiếng Việt | 한국어

Computational Toxicology Research Impact

Ground-breaking science to advance chemical evaluation

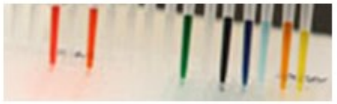
Since 2005, EPA's computational toxicology research has developed ground-breaking approaches to evaluate chemicals for potential health effects. Using these new approaches, thousands of chemicals have been evaluated for potential risk at small cost in a very short amount of time. EPA collaborates with 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

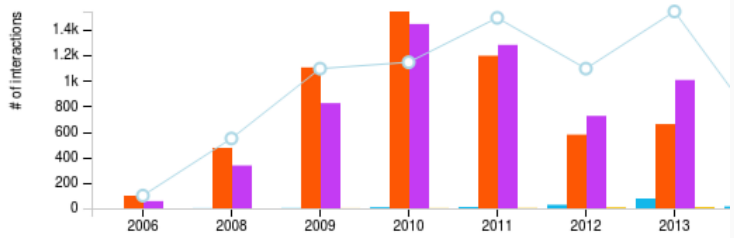
Artifact Summary

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

Recent Artifacts

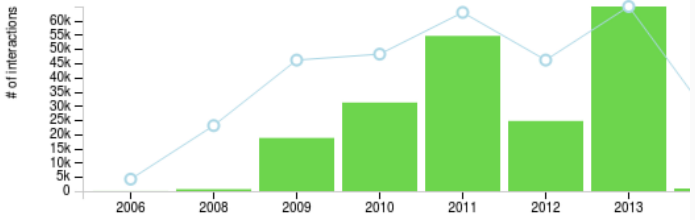
- A Workflow to Investigate Exposure and Pharmacokinetic Influences on High-Throughput in Vitro Chemical Screening Based on Adverse Outcome Pathways.
- Identifiability of PBPK models with applications to dimethylarsinic acid exposure
- Continuing harmonization of terminology and innovations for methodologies 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.
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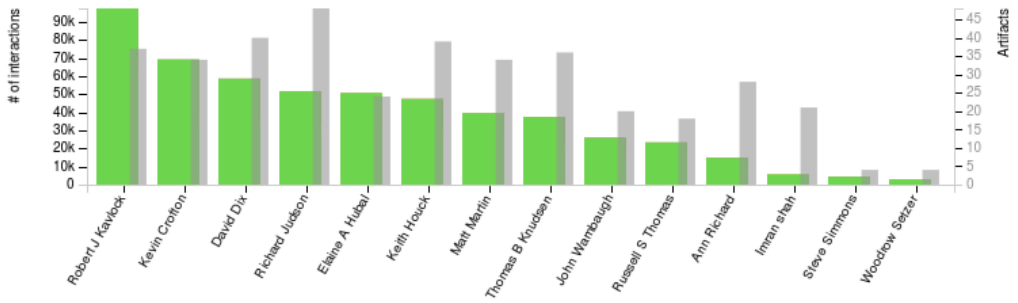
- Incorporating High-Throughput Exposure Predictions With Dosimetry-Adjusted In Vitro Bioactivity to Inform Chemical Toxicity Testing.

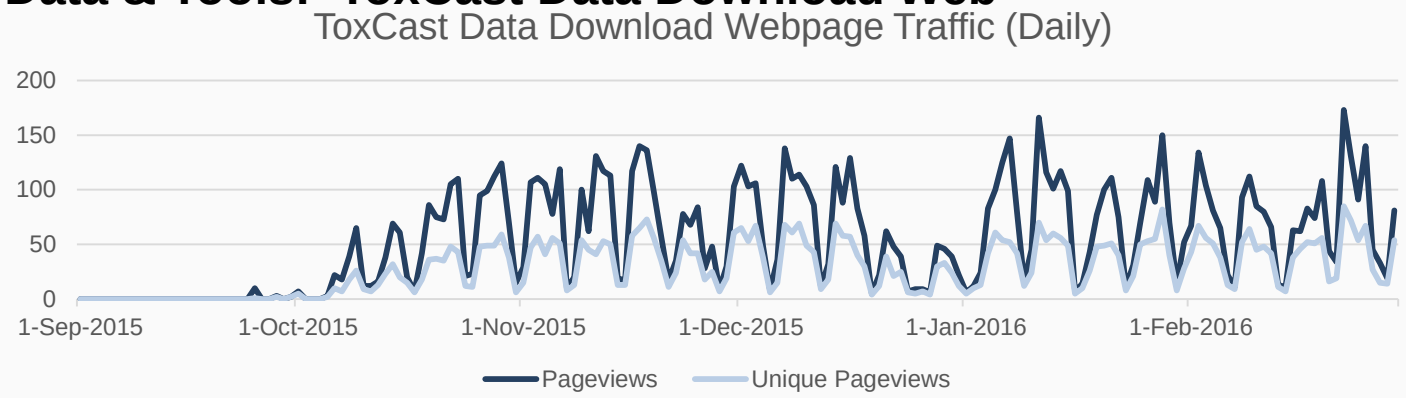
Usage

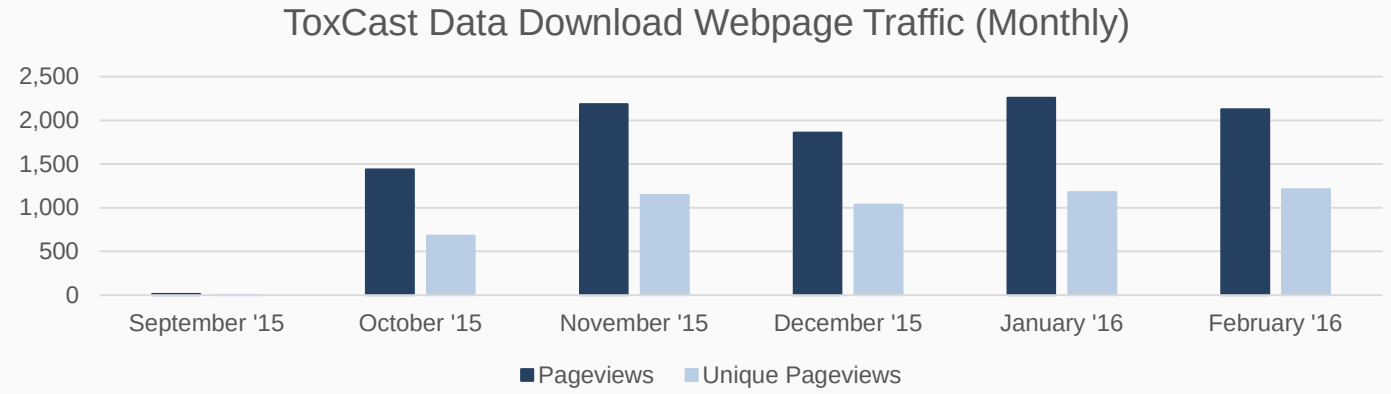


	Abstract Views	Link-outs	PDF Views	HTML Views	Clicks	Data Views	Artifacts
Robert J Kavlock	59504	91	4208	33416	214	-	37
Kevin Crofton	34610	45	3067	31293	168	-	34
David Dix	33175	60	4666	20660	41	-	40
Richard Judson	28823	79	3949	18765	41	-	48
Elaine A Hubal	29245	46	1428	19890	14	-	24
Keith Houck	26438	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

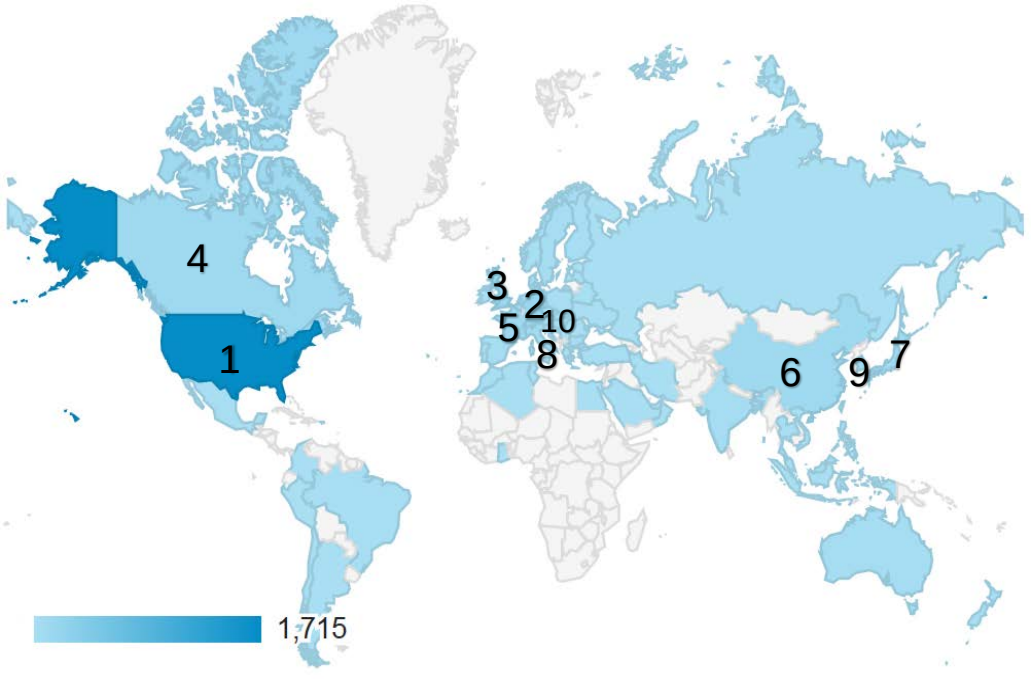




What we would like…
MOCKUP: Geographic Access

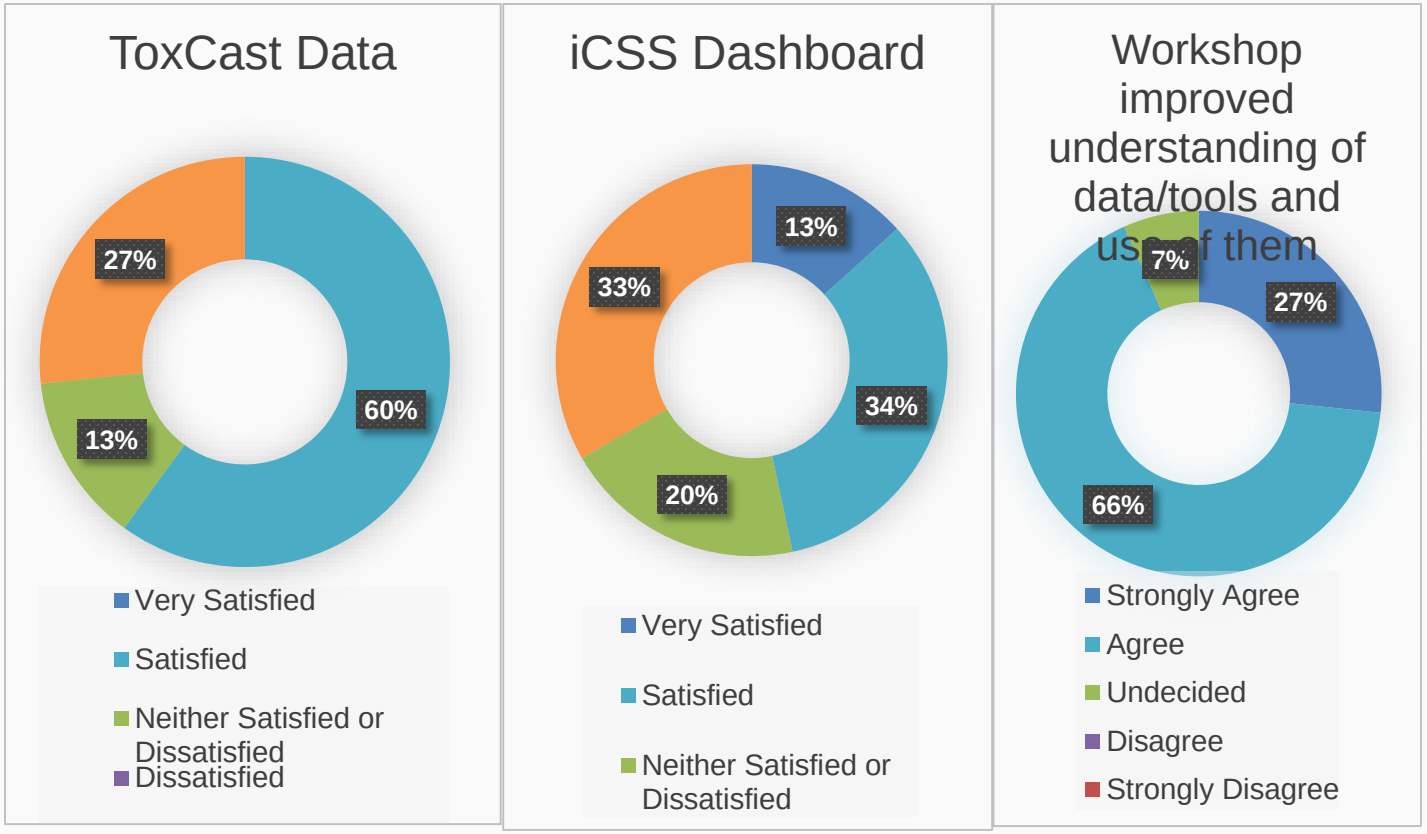
Data & Tools: ToxCast Data Download Web Demographics

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 ExposureScreening 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).

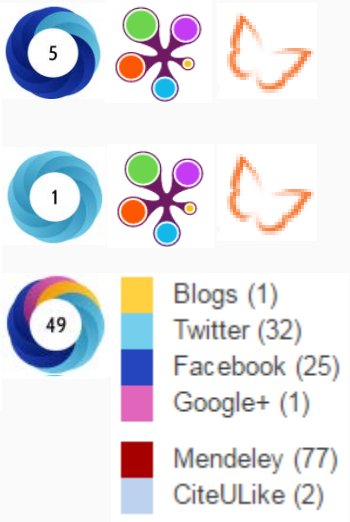
- We are investigating AltMetric, PlumX and Kudos Widgets

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 ExposureScreening 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).



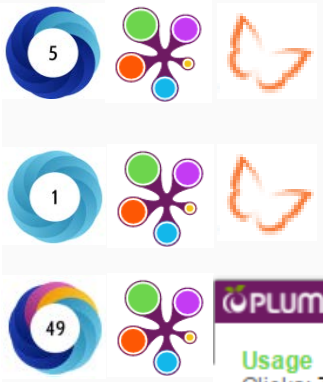
- AltMetric will give us access to social sharing statistics and other stats

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 ExposureScreening 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).



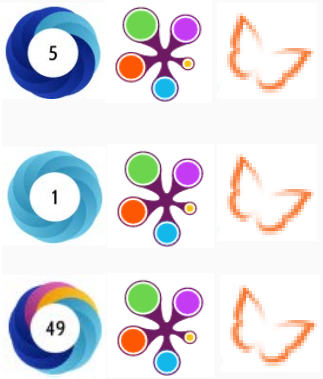
- PlumX will give us access to social sharing statistics and other publication stats

Publications: Kudos Widget

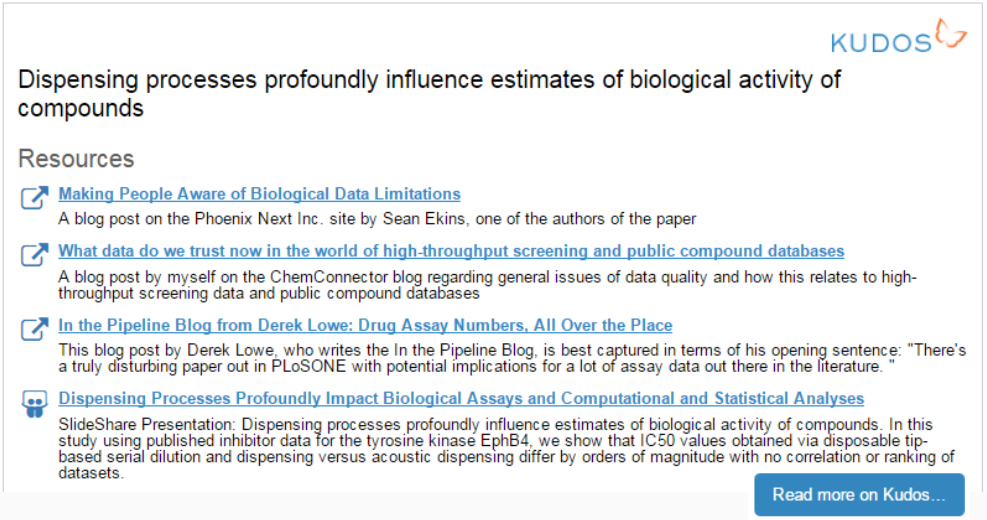
Leist, M., N. Hasiwa, C. Rovida, M. Daneshian, D. Basketter, I. Kimber, H. Clewell, T. Gocht, A. Goldberg, F. Busquet, A. Rossi, M. Schwarz, M. Stephens, R. Taalman, T. Knudsen, J. McKim, G. Harris, D. Pamies, AND T. Hartung. Consensus report on the future of animal-free systemic toxicity testing. ALTEX. 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. Vallero, L. Phillips, M. Phillips, J. Wambaugh, R. Judson, T. Buckley, AND C. Dary. Development of a Consumer Product Ingredient Database for Chemical ExposureScreening 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”

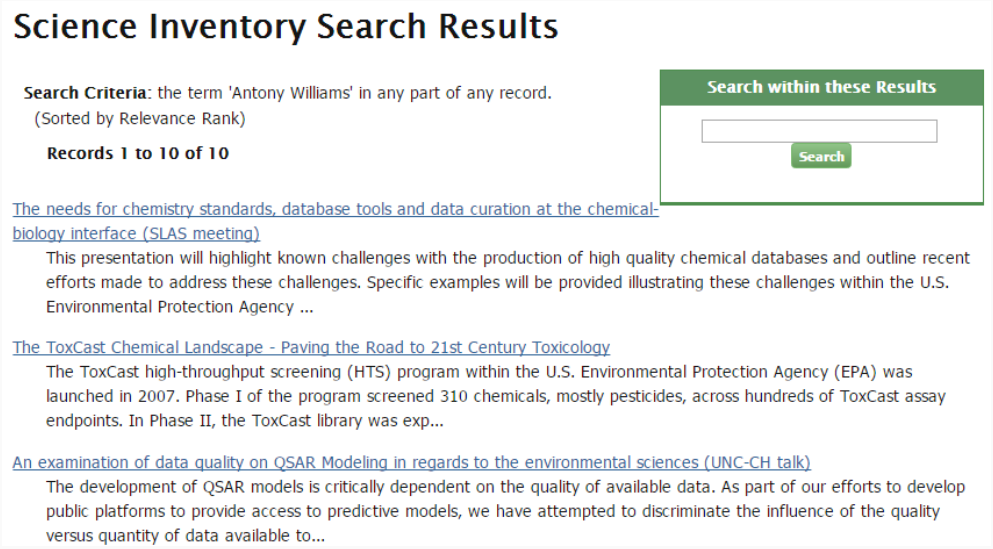


App Analytics: Google

The Power of a Tweet

Work in Progress

- Investigating VIVO Open Source
- Data model in development
- **ORCiD**s for people, **DOI**s 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…