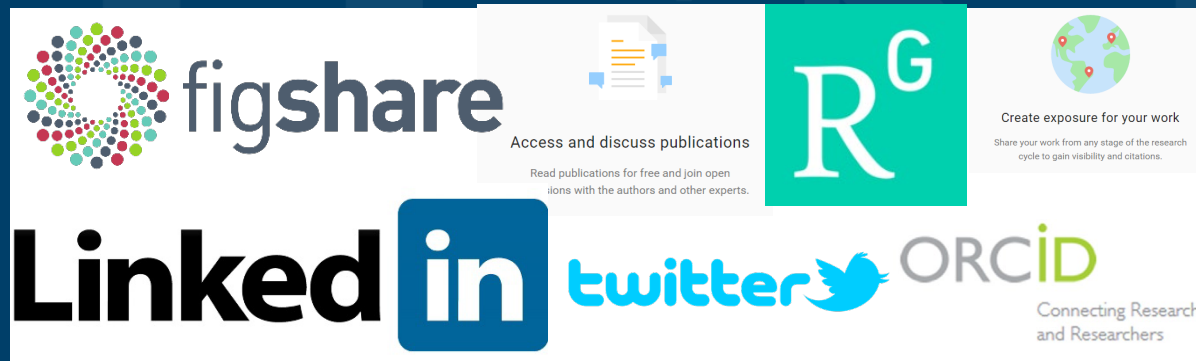


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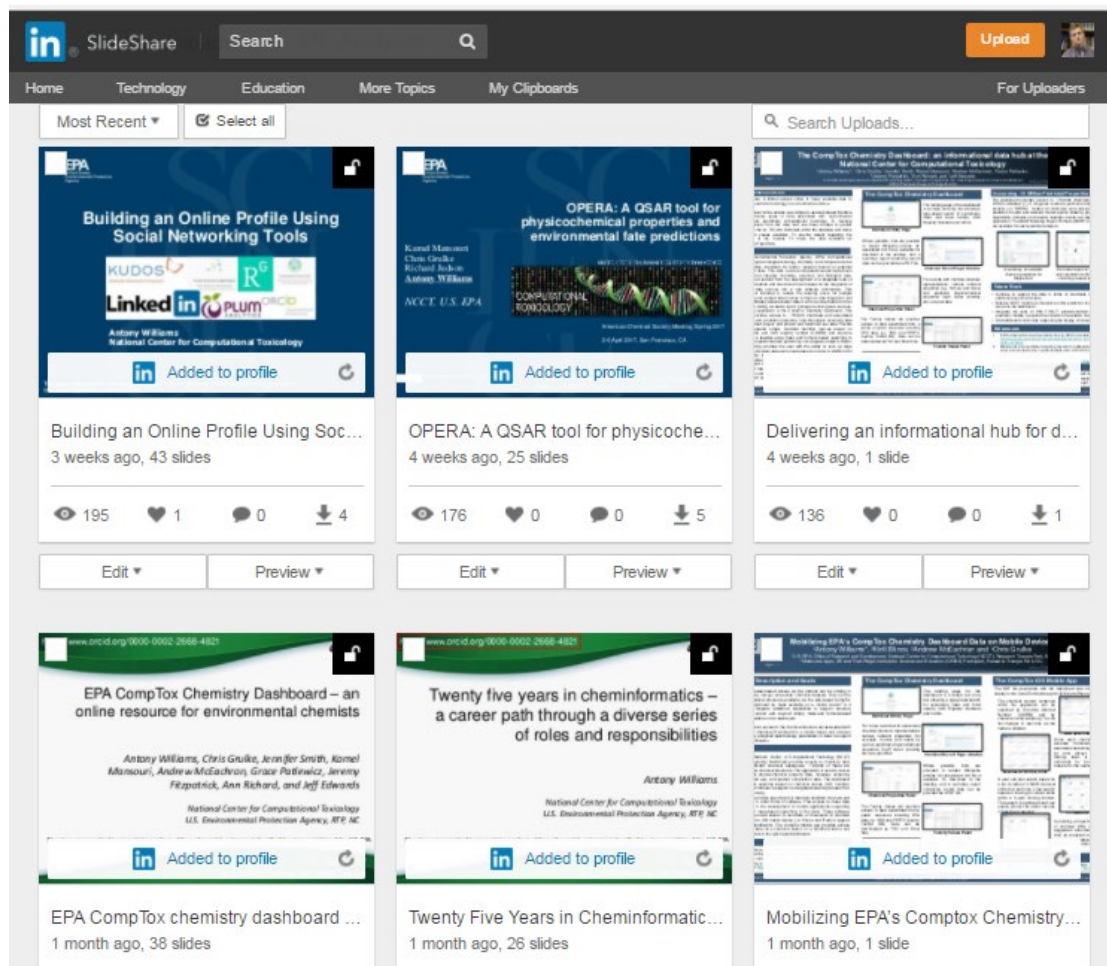


**Antony Williams, US-EPA
Center for Computational Toxicology and Exposure**

**Johns Hopkins University
November 13th 2022**

Various Versions of This Talk

www.slideshare.net/AntonyWilliams



The screenshot displays a SlideShare profile for Antony Williams, a National Center for Computational Toxicology (NCCT) scientist at the U.S. Environmental Protection Agency (EPA). The profile features six presentations:

- Building an Online Profile Using Social Networking Tools** (3 weeks ago, 43 slides): A presentation about leveraging social media for professional networking, featuring logos for KUDOS, LinkedIn, and R6.
- OPERA: A QSAR tool for physicochemical properties and environmental fate predictions** (4 weeks ago, 25 slides): A presentation about the OPERA tool, developed by NCCT, U.S. EPA, and the National Center for Computational Toxicology.
- Delivering an informational hub for d...** (4 weeks ago, 1 slide): A presentation about the EPA's CompTox Chemistry Dashboard.
- EPA CompTox chemistry dashboard – an online resource for environmental chemists** (1 month ago, 38 slides): A presentation about the EPA's CompTox Chemistry Dashboard, an online resource for environmental chemists.
- Twenty Five Years in Cheminformatics – a career path through a diverse series of roles and responsibilities** (1 month ago, 26 slides): A presentation about the author's career path in cheminformatics.
- Mobilizing EPA's CompTox Chemistry...** (1 month ago, 1 slide): A presentation about mobilizing EPA's CompTox Chemistry resources.

Each presentation card includes a thumbnail image, a title, a brief description, the number of slides, and engagement metrics (views, likes, comments, downloads). The presentations are all marked as "Added to profile".

A related publication...




 F1000Research

F1000Research 2017, 6:1315 Last updated: 19 DEC 2018



OPINION ARTICLE

The new alchemy: Online networking, data sharing and research activity distribution tools for scientists [version 1; referees: 2 approved, 1 approved with reservations]

Antony J. Williams ¹, Lou Peck ², Sean Ekins ³

¹National Center for Computational Toxicology, Environmental Protection Agency, Durham, NC, 27711, USA

²Lou Peck Consulting, Swansea, SA4 3JQ, UK

³Collaborations Pharmaceuticals, Inc., Raleigh, NC, 27606, USA

Some Questions for you...

- Consider...
 - How many of you have an ORCID?
 - How many of you have LinkedIn?
 - How many of you have SlideShare?
 - How many of you have published >3 papers?
 - How many of you share your work online?
- Maybe after this it will change...

Who markets your work???

If not you, then who?

- **“It's not the job of researchers to become experts in public relations — that's why universities have press offices, says Matt Shipman, research communications lead at North Carolina State University in Raleigh. But he recommends scientists toot their own horns as well.”**

- <http://www.nature.com/news/kudos-promises-to-help-scientists-promote-their-papers-to-new-audiences-1.20346>

My Hopes for Today

- Encourage you in the “era of participation”
 - Provide an overview of some tools available
 - Share some stories, statistics and strategies
 - Encourage you to “share for the sake of community/science as well as for yourself”
-
- **OUTCOMES**
 - You will claim an **ORCiD**
 - You will invest ~2 hours per month on your profile
 - You have a bigger “Impact” online....

ORCID – The Scientists SSN

ORCID

Connecting Research
and Researchers

Antony Williams

ORCID ID



orcid.org/0000-0002-2668-4821

What's the value of ORCID?

- ORCIDs are now expected for many publications

 Antony J. Williams ¹, Lou Peck ², Sean Ekins ³

- Single click through to your ORCID page – how rich is your ORCID biography??? See

<https://orcid.org/0000-0002-2668-4821>

Publishers Requiring ORCIDs...

<https://orcid.org/content/mandating-orcid-publication-workflows-open-letter>

Requiring ORCID in Publication Workflows: Open Letter

Major publishers have committed to requiring ORCID iDs in the publishing process for their journals and invite other publishers to do the same.

In November, 2015, a group of publishers asked ORCID to help facilitate communications about their plans to require authors to use an ORCID iD, including hosting this open letter explaining their rationale, developing best practices for using iDs in publishing, and maintaining the signatory list. The publishers' goal is to encourage others to join them in supporting the adoption of ORCID. Publishers signing this open letter are committing to requiring ORCID iDs during 2016 following specific implementation standards.

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Antony Williams (0000-0002-2668-4821) - ORCID | Connecting ...

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Antony (Tony) J. Williams received his BSc in 1985 from the University of Liverpool (UK) and PhD in 1988 from the University of London (UK). His PhD research ...

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Antony Williams - Academic Karma

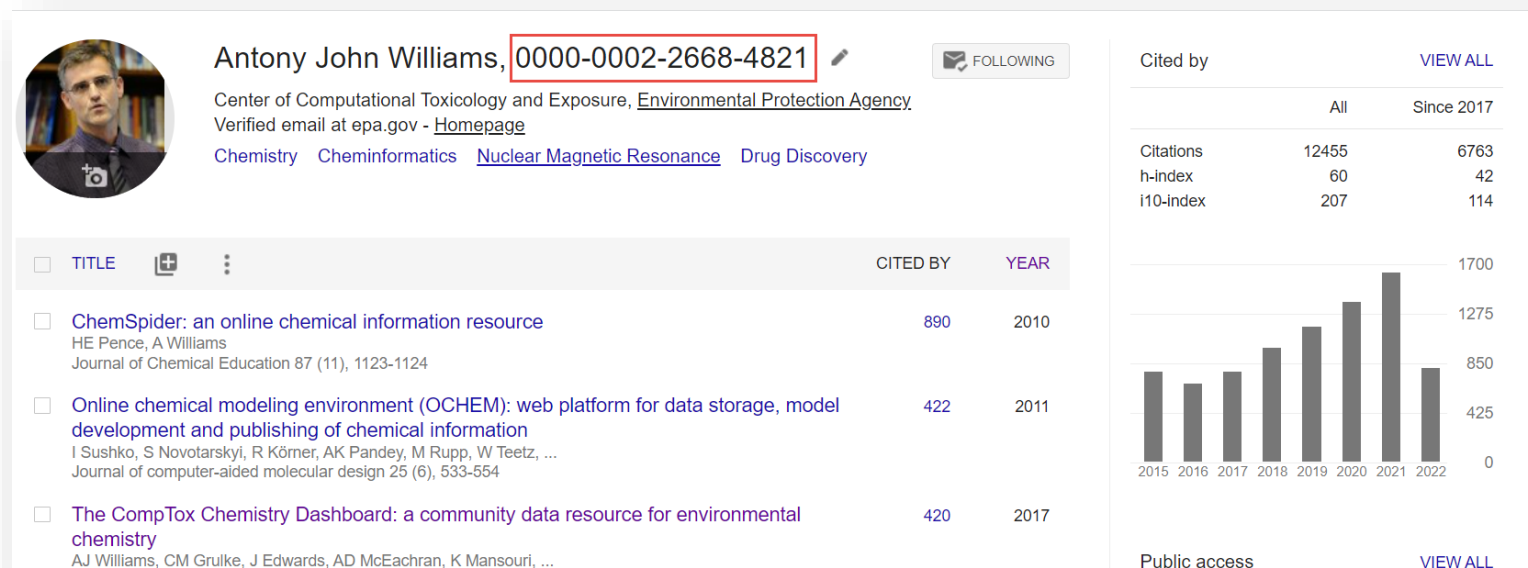
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


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


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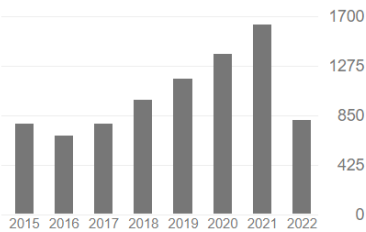
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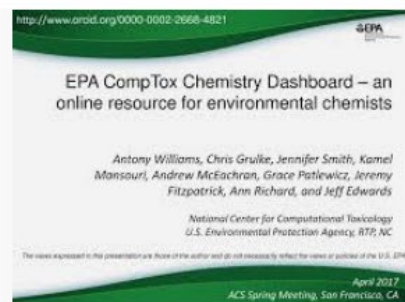


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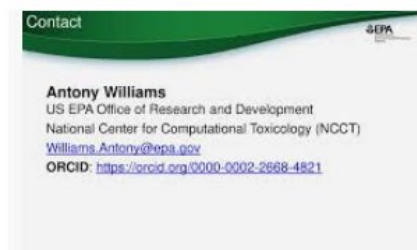
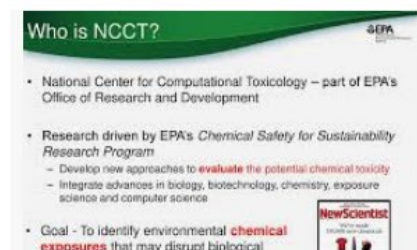
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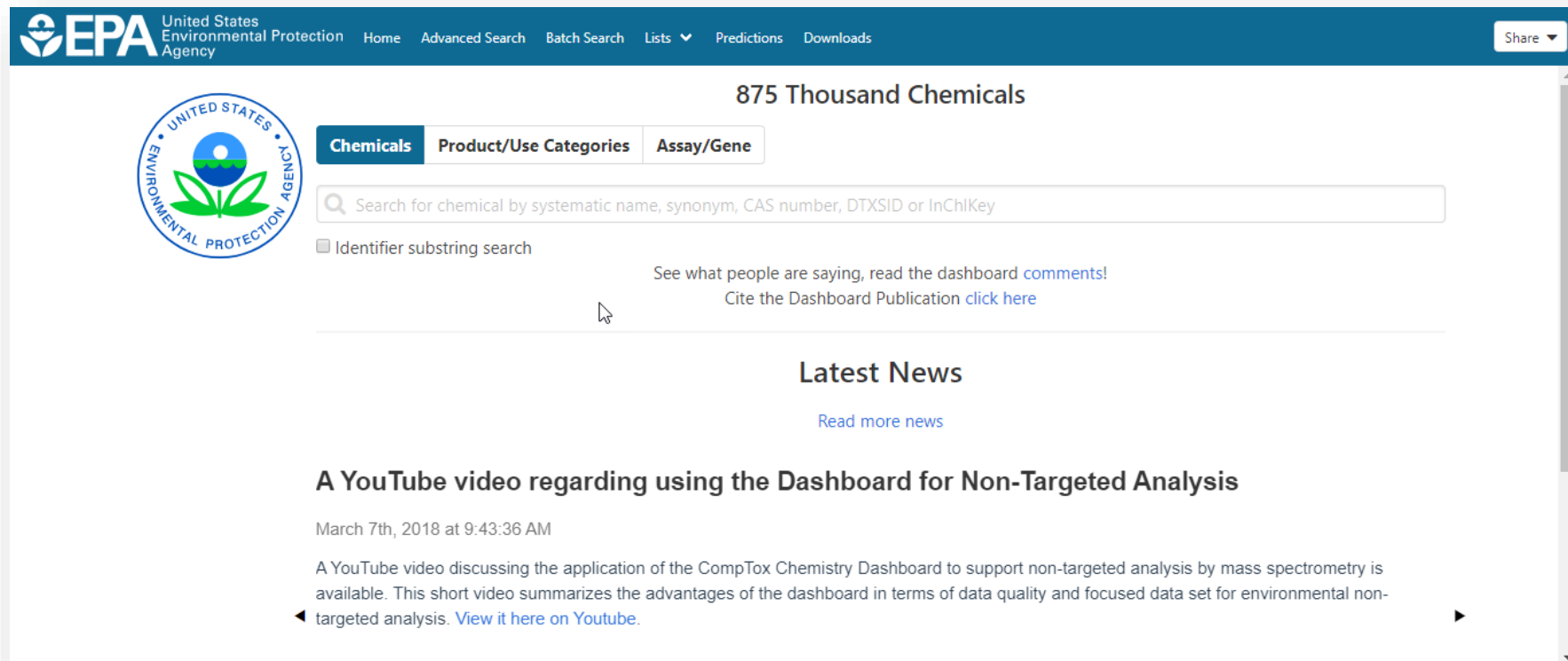


Scientists are Evaluated: “Statistics”

- Research datasets
- Scientific software
- Publications – peer-reviewed and many others
- Posters and presentations at conferences
- Electronic theses and dissertations
- Performances in film and audio
- Other forms of research
- **CAVEAT: Make sure you are *allowed* to share**

<http://www.linkedin.com/in/AntonyWilliams>

Something I worked on...



The screenshot shows the EPA CompTox Chemistry Dashboard. The header includes the EPA logo and navigation links: Home, Advanced Search, Batch Search, Lists, Predictions, and Downloads. A 'Share' button is in the top right. The main content area is titled '875 Thousand Chemicals' and features three tabs: 'Chemicals' (selected), 'Product/Use Categories', and 'Assay/Gene'. Below the tabs is a search bar with the placeholder text 'Search for chemical by systematic name, synonym, CAS number, DTXSID or InChIKey'. A checkbox for 'Identifier substring search' is present. To the right of the search bar, there are links to 'See what people are saying, read the dashboard comments!' and 'Cite the Dashboard Publication click here'. Below this is a 'Latest News' section with a link to 'Read more news'. The news item is titled 'A YouTube video regarding using the Dashboard for Non-Targeted Analysis' and is dated 'March 7th, 2018 at 9:43:36 AM'. The text of the news item describes a YouTube video discussing the application of the CompTox Chemistry Dashboard to support non-targeted analysis by mass spectrometry. It mentions that the video summarizes the advantages of the dashboard in terms of data quality and focused data set for environmental non-targeted analysis. A link 'View it here on Youtube.' is provided. The dashboard is displayed within a browser window with a scrollbar on the right.

EPA United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

Share

875 Thousand Chemicals

Chemicals Product/Use Categories Assay/Gene

Search for chemical by systematic name, synonym, CAS number, DTXSID or InChIKey

☐ Identifier substring search

See what people are saying, read the dashboard [comments!](#)
Cite the Dashboard Publication [click here](#)

Latest News

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A YouTube video regarding using the Dashboard for Non-Targeted Analysis

March 7th, 2018 at 9:43:36 AM

A YouTube video discussing the application of the CompTox Chemistry Dashboard to support non-targeted analysis by mass spectrometry is available. This short video summarizes the advantages of the dashboard in terms of data quality and focused data set for environmental non-targeted analysis. [View it here on Youtube.](#)

Ability to Highlight Projects

7 Projects

The CompTox Chemicals Dashboard

Dec 2015 – Present

The CompTox Chemicals Dashboard is an integration hub for chemistry and biology data of interest to environmental scientists and toxicologists. The dashboard was released as a beta on April 1st 2016 and formally as version 1 to the community in August 2016. The dashboard is free to use and presently provides access to data for ~875,000 chemicals.

The definitive article regarding the development of the dashboard is published in the Journal of Cheminformatics as <https://jcheminf.biomedcentral.com/articles/10.1186/s13321-017-0247-6>.

There are a number of derivative and related articles that have come from the related research and application development. These include:

- 1) OPERA models for predicting physicochemical properties and environmental fate endpoints - <https://jcheminf.biomedcentral.com/articles/10.1186/s13321-018-0263-1>
- 2) An automated curation procedure for addressing chemical errors and inconsistencies in public datasets used in QSAR modelling <https://doi.org/10.1080/1062936X.2016.1253611>
- 3) Generalized Read-Across (GenRA): A workflow implemented into the EPA CompTox Chemicals Dashboard <https://www.altex.org/index.php/altex/article/view/1202>
- 4) A Chemical Category-Based Prioritization Approach for Selecting 75 Per- and Polyfluoroalkyl Substances (PFAS) for Tiered Toxicity and Toxicokinetic Testing <https://ehp.niehs.nih.gov/doi/10.1289/EHP4555>

Other creators



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64

Publications

Generalized Read-Across (GenRA): A workflow implemented into the EPA CompTox Chemicals Dashboard


Feb 4, 2019 • ALTEX-Alternatives to animal experimentation

Generalized Read-Across (GenRA) is a data driven approach which makes read-across predictions on the basis of a similarity weighted activity of source analogues (nearest neighbors). GenRA has been described in more detail in the literature (Shah et al., 2016; Helman et al., 2018). Here we present its implementation within the EPA's CompTox Chemicals Dashboard to provide public access to a GenRA module structured as a read-across workflow. GenRA assists researchers in identifying source analogues, evaluating their validity and making predictions of in vivo toxicity effects for a target substance. Predictions are presented as binary outcomes reflecting presence or absence of toxicity together with quantitative measures of uncertainty. The approach allows users to identify analogues in different ways, quickly assess the availability of relevant in vivo data for those analogues and visualize these in a data matrix to evaluate the consistency and concordance of the available experimental data for those analogues before making a GenRA prediction. Predictions can be exported into a tab-separated value (TSV) or Excel file for additional review and analysis (e.g., doses of analogues associated with production of toxic effects). GenRA offers a new capability of making reproducible read-across predictions in an easy-to use-interface.

Other authors





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 **CompTox Chemicals Dashboard Release March 2019** ×


397 views


3 reshares

 **David Grawoig, Ph.D.** • 1st
Entrepreneur ♦ Scientist ♦ RNA-drug discovery expert
2d


 **Antony Williams**
Scientist at National Center of Computational Toxicology at EPA
3d

A new version of the [#CompTox](#) Chemicals dashboard was released today in time for [#sot2019](#). A summary overview of what's new is on [#SlideShare](#) at

**CompTox Chemicals Dashboard Release March 2019**
Antony Williams
National Center for Computational Toxicology
slideshare.net



1 Like

 **Kamel Mansouri** • 1st
Lead Computational Chemist at Integrated Laboratory Systems, Inc. (ILS)
2d • Edited

New OPERA (<https://lnkd.in/eX5BtBj>) predictions as well as CERAPP (<https://lnkd.in/edt87EG>) and CoMPARA (<https://lnkd.in/eWpQzjK>) data are available on the [#CompTox](#) Chemicals dashboard and ICE (<https://lnkd.in/epW6jYy>). Visit us at [#sot2019](#) [#ToxExpo](#) for more info.

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Elin Ulrich · 1st

Supervisory chemist at US EPA

September 19, 2021, Elin worked with Antony but on different teams

Tony ROCKS! We have worked together on non-targeted analysis projects since about 2015. His knowledge of chemistry, cheminformatics, and ability to design useful tools is phenomenal. He is patient as a trainer/teacher, unselfish with his time, and makes a substantial and tangible difference in the projects he's part of. Tony's vision and ability to pull together chemistry information in a useful way for a broad ...see more



Seth Newton · 1st

Physical Scientist at US Environmental Protection Agency (EPA)

August 31, 2021, Seth worked with Antony but on different teams

I have had the pleasure of working with Tony for the past five years on several different projects and I am constantly impressed with his ability to add value to everything he touches. Tony is an effective leader when managing large projects, but also a helpful contributor to any collaboration. As the product owner of the Comptox Chemicals Dashboard, he would consult with me regularly to make sure new features me ...see more



Andrew McEachran · 1st

Product Owner at Agilent Technologies

August 26, 2021, Andrew reported directly to Antony

I had the absolute pleasure of working with Tony for 3 years at the EPA while I was a postdoctoral researcher. Tony was my mentor, colleague, advocate, and cheerleader. Navigating life as an early career postdoc can be challenging, but Tony steered me in the right direction and provided me opportunities I would not have had otherwise. Tony put me in the position to lead collaborative projects and papers, work directly with ...see more

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Endorsed by james little and 44 others who are highly skilled at this



Endorsed by 11 colleagues at US Environmental Protection Agency (EPA)



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Analytical Chemistry



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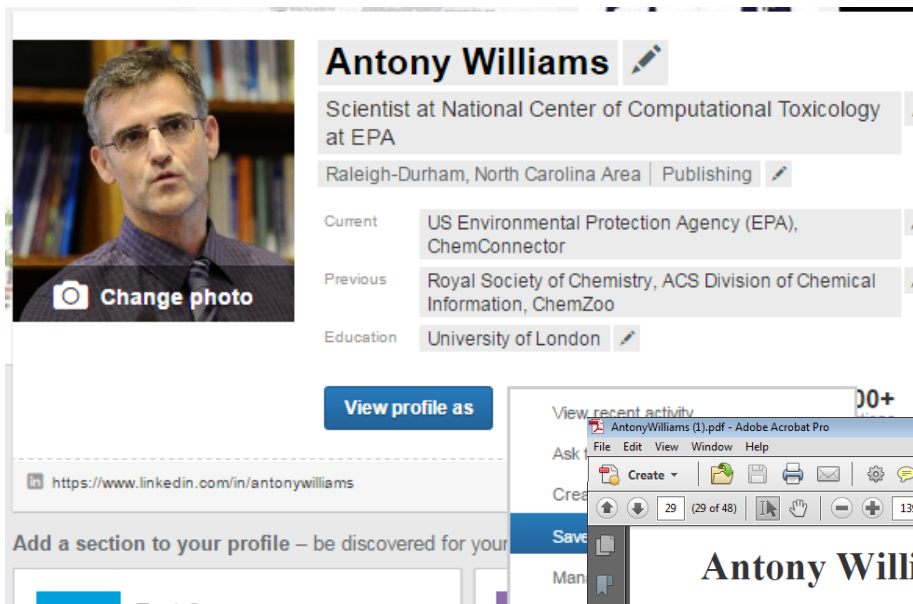



Endorsed by 6 colleagues at US Environmental Protection Agency (EPA)




99+ endorsements

Instant Summary as a PDF




Antony Williams 

Scientist at National Center of Computational Toxicology at EPA

Raleigh-Durham, North Carolina Area | Publishing 

Current US Environmental Protection Agency (EPA), ChemConnector

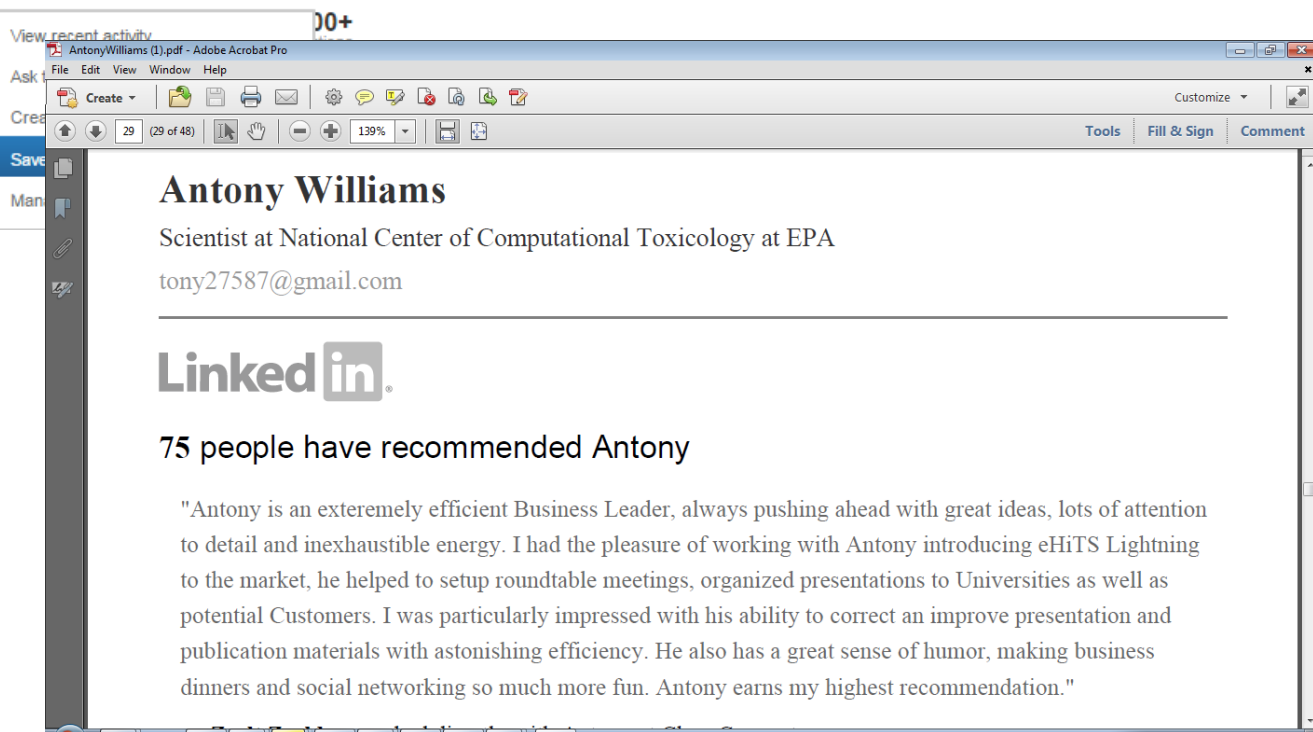
Previous Royal Society of Chemistry, ACS Division of Chemical Information, ChemZoo

Education University of London 

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<https://www.linkedin.com/in/antonywilliams>



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Antony Williams

Scientist at National Center of Computational Toxicology at EPA

tony27587@gmail.com

LinkedIn

75 people have recommended Antony

"Antony is an extremely efficient Business Leader, always pushing ahead with great ideas, lots of attention to detail and inexhaustible energy. I had the pleasure of working with Antony introducing eHiTS Lightning to the market, he helped to setup roundtable meetings, organized presentations to Universities as well as potential Customers. I was particularly impressed with his ability to correct an improve presentation and publication materials with astonishing efficiency. He also has a great sense of humor, making business dinners and social networking so much more fun. Antony earns my highest recommendation."

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US Environmental Protection Agency (EPA), National Center for Computational Toxicology

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- Raleigh-Durham, North Carolina Area, North Carolina, United States
- www.chemconnector.com
- 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,

US Environmental Protection Agency (EPA), National Center for Computational Toxicology

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

Translating research into practical tools: A case study of GenRA, a new read-across tool

Antony Williams¹, George Helman², Jeff Edwards¹, Jeremy Dunne¹,
Imran Shah¹ and Grace Patlewicz¹

1) National Center for Computational Toxicology, U.S. Environmental Protection Agency, RTP, NC
2) Oak Ridge Institute of Science and Education (ORISE) Research Participant, RTP, NC

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

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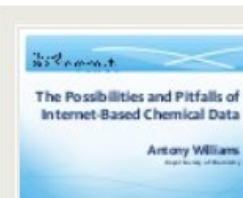
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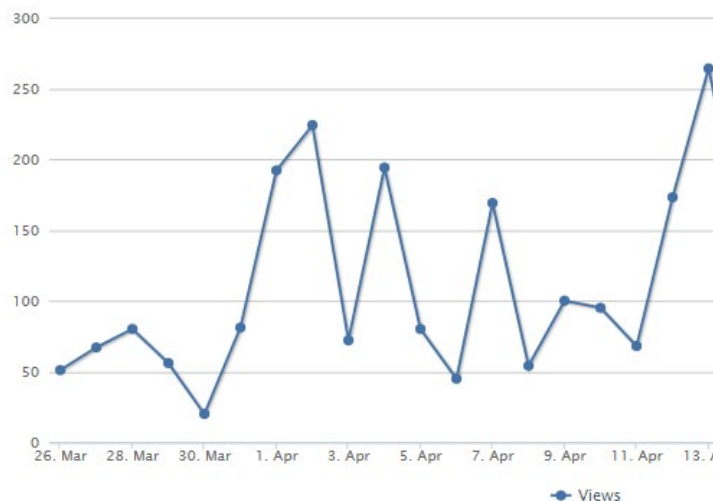
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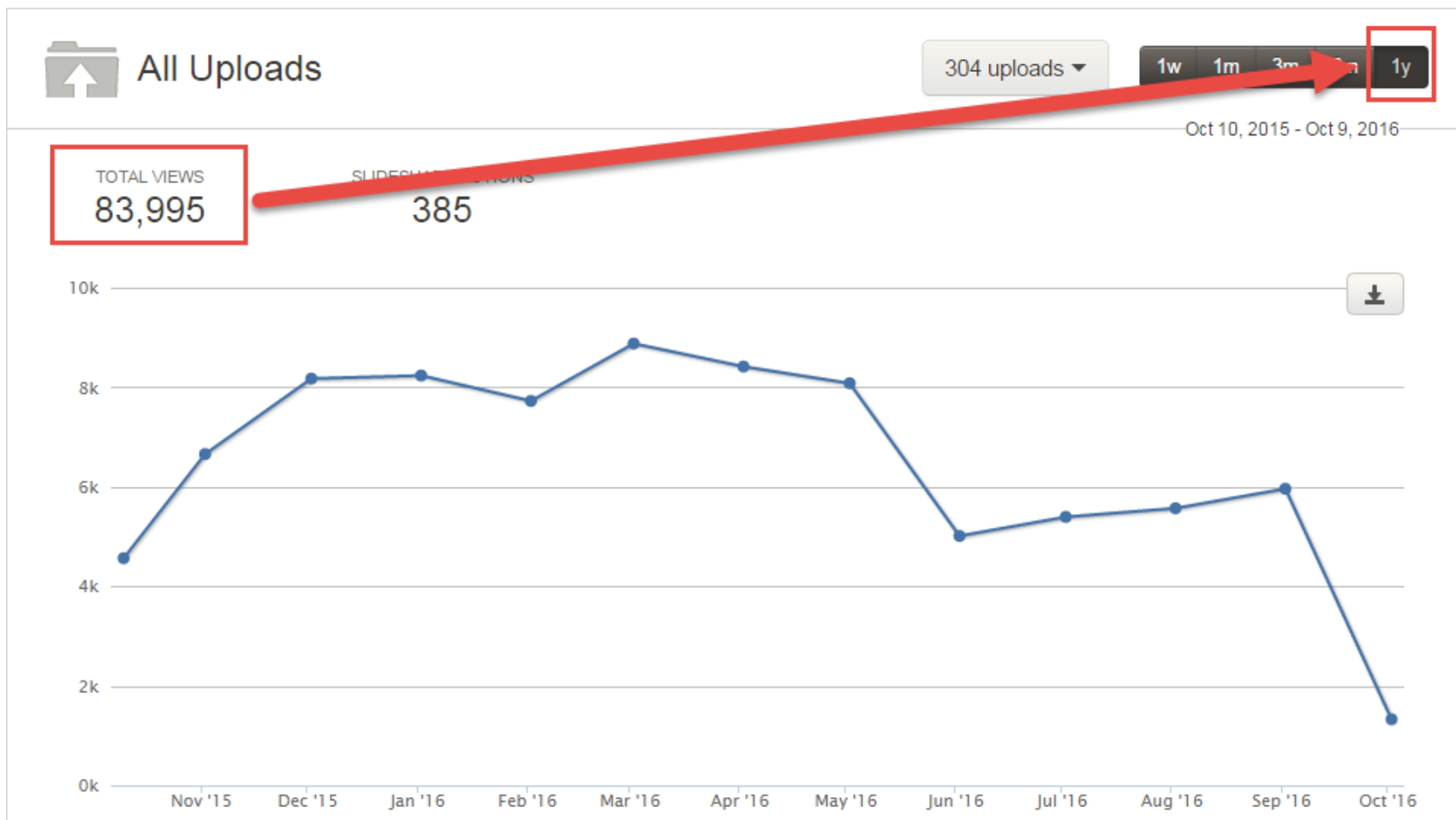
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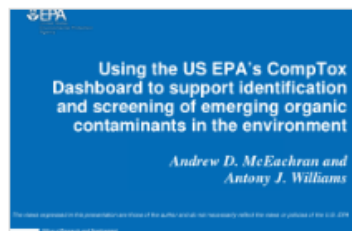
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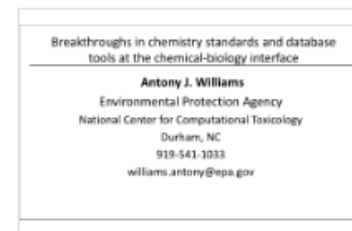
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Building an Online Profile Using Social Networking Tools

Antony Williams

30/05/2018



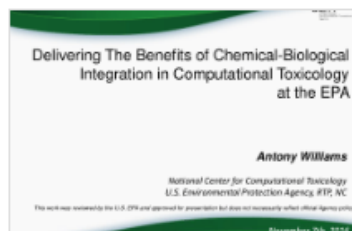
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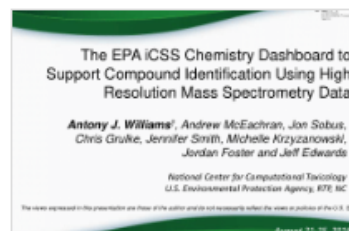
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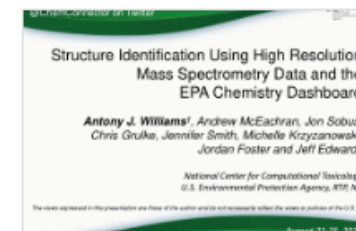
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Antony Williams*, Kamel Mansouri, Ann M. Richard and Chris Grulke

U.S. Environmental Protection Agency, Office of Research and Development, National Center for Computational Toxicology (NCCT), Research Triangle Park, NC
Oak Ridge Institute for Science and Education (ORISE) Participant, Research Triangle Park, NC

2627/P125

Society of Toxicology Annual Meeting
New Orleans, LA

March 13-17, 2016

ORCID: 0000-0002-2668-4821

Antony Williams | williams.antony@epa.gov | 919-541-1033

Automated Analysis Using KNIME

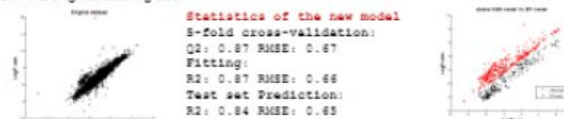
The manual investigation of the data allowed us to develop a KNIME³ workflow for automated processing. This workflow was derived from earlier work by Mansouri et. al.⁴ and is represented in the figure below as a series of blocks representing, for example:

- Compare Mol-Block and SMILES (2268 different)
- Check for duplicates (657 structures, 531 names)
- Check CASRN Numbers (3646 invalid CASRN)
- Check names against dictionary (555 invalid)
- Assign Quality flags based on consistency among data fields



Model Performance

The LogKow prediction model delivered by EPI Suite used a smaller dataset (of 2700 chemicals). The curation of the available data, utilization of a larger dataset (>14,000 chemicals) and application of novel machine-learning approaches produced a better and simpler model with only 10 descriptors. The figures below illustrate the difference between the original EPI Suite model and the newly derived predictive model. The red data points indicate the outliers from the original modeling approach, the majority not included in the original training set.



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5	2018	Journal of cheminformatics 10 (1), 10	Article	https://doi.org/10.1186/s13321-018-0263-1
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12	2018	Drug discovery today 23 (3), 661-672	Article	https://doi.org/10.1016/j.drudis.2018.01.018
13	2018	Computational Toxicology: Risk Assessment for Chemicals, 211-244	Chapter	https://doi.org/10.1002/9781119282594.ch8
14	2018	Environmental science & technology 52 (5), 3125-3135	Article	https://doi.org/10.1021/acs.est.7b04781
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I am presently a Computational Chemist at the National Center for Computational Toxicology with the US Environmental Protection Agency in Research Triangle Park, North Carolina. I am one of the founders of the ChemSpider database (<http://www.chemspider.com>), one of the top chemistry databases in the world that was acquired by the Royal Society of Chemistry in 2009. Prolific author with almost 200 peer-reviewed scientific publication and book chapters, 3 patents and 100s of public presentations.

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The CompTox Chemicals Dashboard

Antony John Williams · Christopher M Grulke · Mansouri Ka

Goal: The CompTox Chemicals Dashboard is a web-based application that integrates chemistry and biology data of different types including experimental and computational data, in vivo and in vitro toxicity data, real time predictions across approaches. The dashboard, available at <https://comptox.epa.gov>, contains data for 875,000 chemicals as of March 2019

Date: 30 March 2016

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An update to the dashboard has been released in March 2019 to coincide with the meeting of Toxicology and American Chemical Society Spring meetings. Six months of effort resulted in the addition of 110,000 new chemical substances being added (bringing total of chemical substances to 876k), improved support for Toxcast bioassay data (integrating data from the invitroDB_v3 release), the addition of multiple chemical new user interface enhancements across the application. A list of release notes available for review at https://comptox.epa.gov/dashboard/comptox_release_notes

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EPA Comptox Chemistry Dashboard "MS-Ready" File of Structures

17.02.2017, 11:27 by Antony Williams

The EPA CompTox Chemistry Dashboard (at <https://comptox.epa.gov>) can be used by mass spectrometrists for the purpose of structure identification. A normal formula search would search the exact formula associated with any chemical, whether it include solvents of hydration, salts or multiple components. However, mass spectrometry detects ionized chemical structures and molecular formulae searches should be based on desalted, and desolvated structures with stereochemistry removed. We refer to these as "MS ready structures" and the MS-ready mappings are delivered as Excel Spreadsheets containing the Preferred Name, CAS-RN, DTXSID, Formula, Formula of the MS-ready structure and associated masses, SMILES and InChI Strings/Keys.

REFERENCES

- <http://link.springer.com/article/10.1007/s00216-016-0139-z>

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


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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

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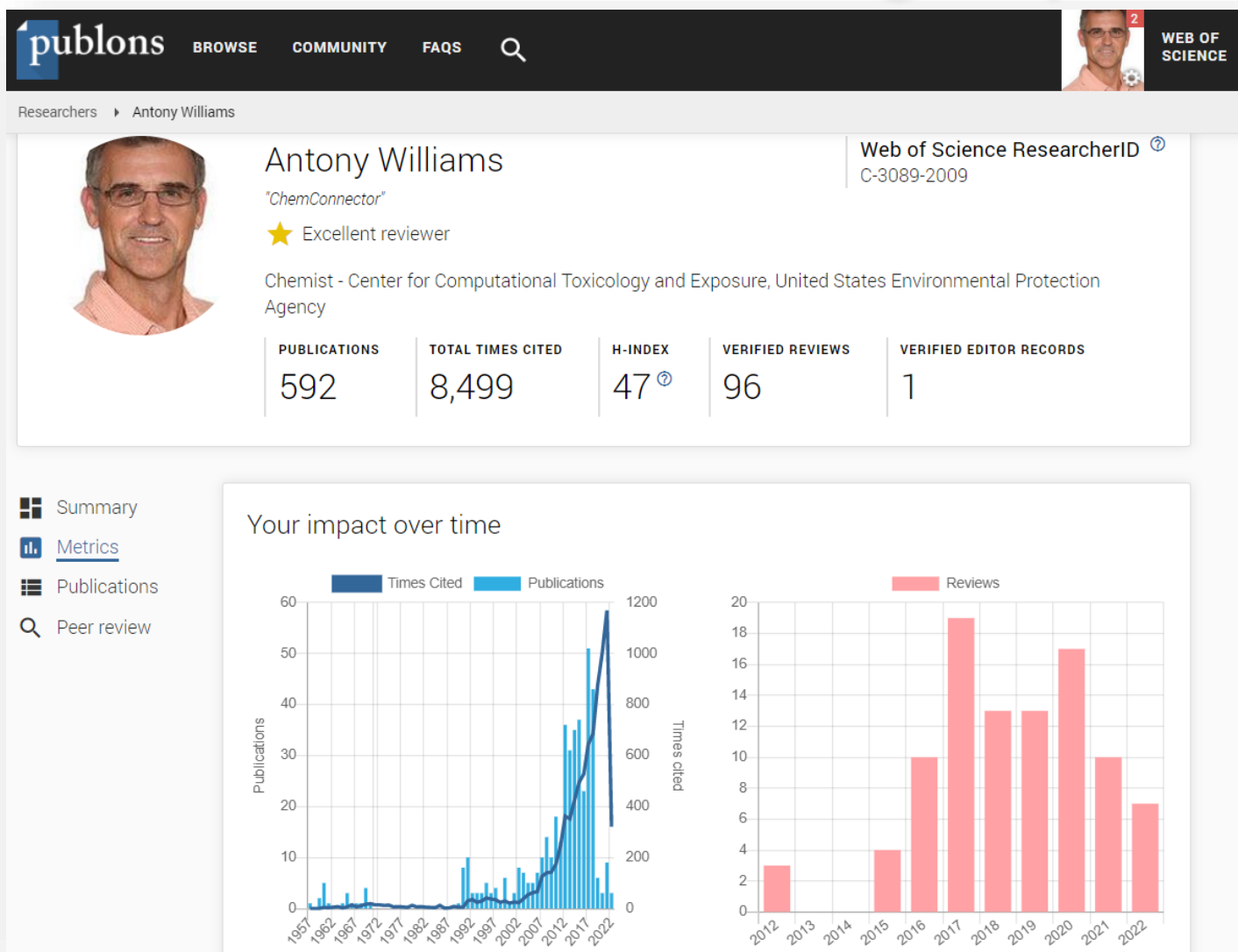


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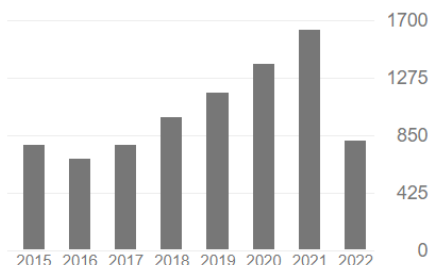
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I Sushko, S Novotarskyi, R Körner, AK Pandey, M Rupp, W Teetz, ...
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Author Updates

I am a Computational Chemist at the National Center for Computational Toxicology, part of the Environmental Protection Agency.

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 peer-reviewed scientific publications, 3 patents and many public presentations.

Founder of ChemZoo Inc., the host of ChemSpider (www.chemspider.com). ChemSpider is an open access online database of chemical structures and



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PRESENTATION ACS SPRING 2018: Structure identification by Mass Spectrometry Non-Targeted Analysis using the US EPA's CompTox Chemistry Dashboard


Structure identification by Mass Spectrometry Non-Targeted Analysis using the US EPA's CompTox Chemistry Dashboard

Identification of unknowns in mass spectrometry based non-targeted analyses (NTA) requires the integration of complementary pieces of data to arrive at a confident, consensus structure. Researchers use chemical reference databases, spectral matching, fragment prediction tools, retention time prediction tools, and a variety of other data to arrive at tentative, probable, and confirmed, if possible, identifications. With the diverse, robust data contained within the US EPA's CompTox Chemistry Dashboard (<https://comptox.epa.gov>), the goal of this research is to identify and implement a harmonized identification tool and workflow using previously generated chemistry data. Data has been compiled from product use, functional use prediction models, environmental media occurrence prediction models, and PubMed references, among other sources. We will report on our development of a visualization tool whereby users can visualize the relative contribution of identification-based metrics on a list of candidate structures and observe the greatest likelihood of occurrence. These data and visualization tools support NTA identification via the Dashboard and demonstrate an open, accessible tool for all users of HRMS data. This abstract does not necessarily represent the views or policies of the U.S. Environmental Protection Agency.

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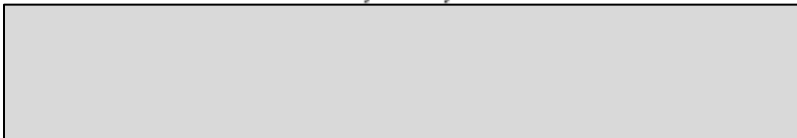
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Structure identification by Mass Spectrometry Non-Targeted Analysis using the US EPA's CompTox



But the top of my CV...

ANTONY JOHN WILLIAMS, PhD, FRSC



Blog: <http://www.chemconnector.com>

Complete CV: http://www.chemconnector.com/antonywilliams_cv/

Google Citations: <http://scholar.google.com/citations?user=O2L8nh4AAAAJ>

LinkedIn profile: <http://www.linkedin.com/in/antonywilliams>

ImpactStory AltMetrics: <http://impactstory.org/ChemConnector>

SlideShare profile: <http://www.slideshare.net/AntonyWilliams>

Wikipedia profile: http://en.wikipedia.org/wiki/Antony_John_Williams

Amazon Author Page: <http://www.amazon.com/Antony-J.-Williams/e/B004YRPRV2>

Publons Profile Page: <https://publons.com/author/306575/antony-williams#profile>

SUMMARY SCIENTIST, ONLINE CHEMISTRY EVANGELIST AND SENIOR EXECUTIVE

- ♦ Experienced in senior leadership and management
- ♦ Expert at bridging science and community
- ♦ Thought leader and evangelist for "Open Access Chemistry"

What Next?

My Recommendations

- Register for an ORCID ID
- **Enhance** your LinkedIn profile
- Use Google Scholar Citations and **curate**
- **Choose:** ResearchGate **or** Academia.edu
- **Use:** Publons
- **Participate** building your profile – share data, papers, presentations, etc..

Various Versions of This Talk

www.slideshare.net/AntonyWilliams



The screenshot shows a SlideShare profile for the US Environmental Protection Agency (EPA). The profile includes a header with the EPA logo and name, a search bar, and navigation links. The main content area displays the profile picture, name, location (Raleigh-Durham, North Carolina Area, North Caroli United States), and statistics (310 SlideShares, 237 Followers, 0 Clipboards). A bio section describes the user's responsibilities and experience. Below the bio are social media links for Twitter, LinkedIn, and Google+. A list of followers is also visible. To the right, a presentation slide is displayed with the title "Environmental Chemistry Compound Identification Using High Resolution Mass Spectrometry Data Integrated to the EPA Chemistry Dashboard". The slide lists authors: Antony J. Williams, Andrew McEachran, Jon Sobus, Seth Newton, Elin Ulrich, Chris Grukke, Kamel Mansouri, Jennifer Smith, and Jeff Edwards. The slide also mentions the Eastern Analytical Symposium 2016 and includes a date of November 14th, 2016. A sidebar on the right shows counts for Presentations (241), Documents (66), Infographics (0), and Videos (0). At the bottom, there is a section for "Likes (24)" with a "View all" link and a grid of related presentations.

Email: williams.antony@epa.gov