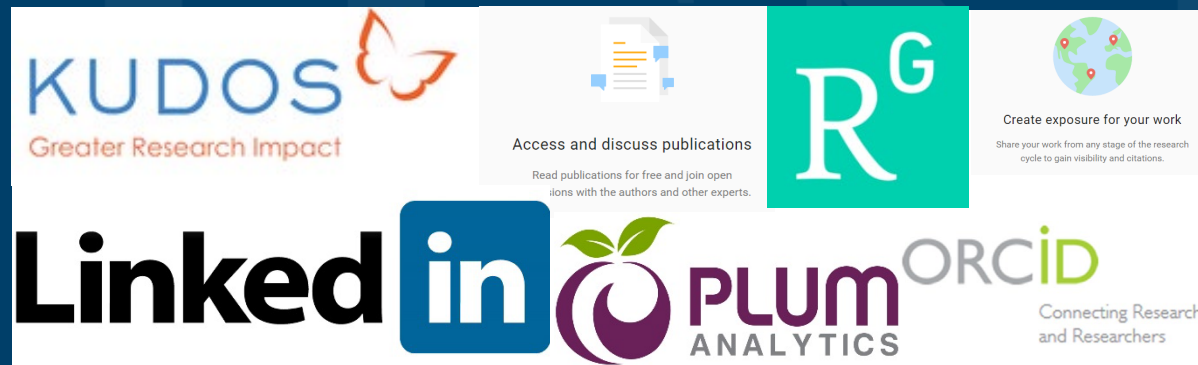


Sharing Yourself and Your Science using Social Media Tools for Scientists



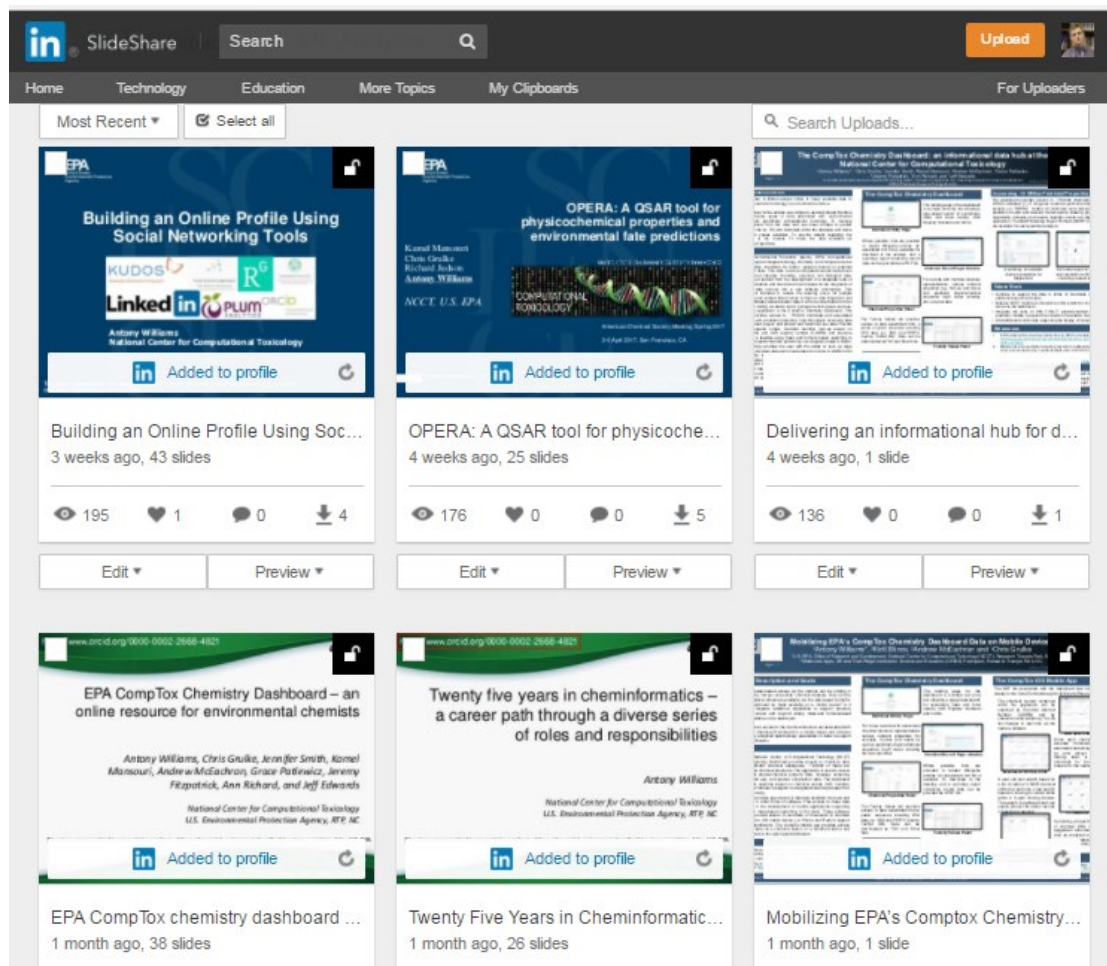
Antony Williams
Center for Computational Toxicology and Exposure

Feel free to take notes but..

- All slides will be made available later
- Contact me directly if I can help –
williams.antony@epa.gov

Various Versions of This Talk

www.slideshare.net/AntonyWilliams



The screenshot displays the SlideShare profile of Antony Williams, a member of the National Center for Computational Toxicology at the U.S. Environmental Protection Agency. The profile shows six presentations, each with a thumbnail, title, description, and engagement metrics (views, likes, comments, and downloads). The presentations are:

- Building an Online Profile Using Social Networking Tools**: 3 weeks ago, 43 slides, 195 views, 1 like, 0 comments, 4 downloads.
- OPERA: A QSAR tool for physicochemical properties and environmental fate predictions**: 4 weeks ago, 25 slides, 176 views, 0 likes, 0 comments, 5 downloads.
- Delivering an informational hub for d...**: 4 weeks ago, 1 slide, 136 views, 0 likes, 0 comments, 1 download.
- EPA CompTox Chemistry Dashboard – an online resource for environmental chemists**: 1 month ago, 38 slides, 136 views, 0 likes, 0 comments, 1 download.
- Twenty five years in cheminformatics – a career path through a diverse series of roles and responsibilities**: 1 month ago, 26 slides, 136 views, 0 likes, 0 comments, 1 download.
- Mobilizing EPA's CompTox Chemistry...**: 1 month ago, 1 slide, 136 views, 0 likes, 0 comments, 1 download.

Each presentation thumbnail includes the EPA logo and the title. The descriptions provide more details about the content, including the authors and the organization. The engagement metrics are shown at the bottom of each presentation card.

A related publication...






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.

It's a Scientists SSN – use it in various places



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

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

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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B Lam, A Baer, M Alae, B Lefebvre, A Moser, A Williams, AJ Simpson. Environmental science & technology 41 (24), 8240-8247, 2007. 155, 2007. Smart phones ...

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Antony Williams - Academic Karma


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0000-0002-2668-4821. Keywords: nmr. chemistry. chemspider.

computer_assisted_structure_elucidation. cheminformatics. systematic_naming. open_data.

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HE Pence, A Williams
Journal of Chemical Education 87 (11), 1123-1124
470 2010
- ☐ [Open PHACTS: semantic interoperability for drug discovery](#)
AJ Williams, L Harland, P Groth, S Pattifer, C Chichester, EL Willighagen, ...
Drug discovery today 17 (21-22), 1188-1198
252 2012
- ☐ [Online chemical modeling environment \(OCHEM\): web platform for data storage, model development and publishing of chemical information](#)
I Sushko, S Novotarskyi, R Körner, AK Pandey, M Rupp, W Teetz, ...
214 2011

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Google will index all of your works...even if ORCID doesn't



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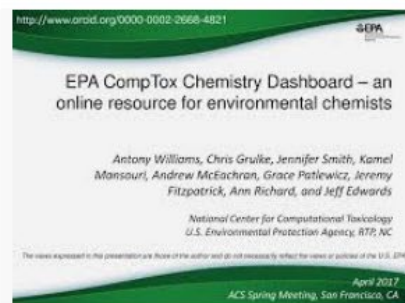


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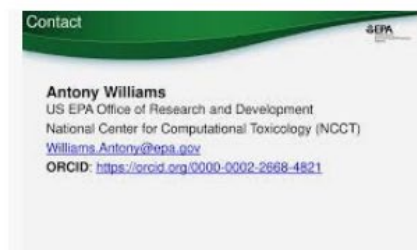
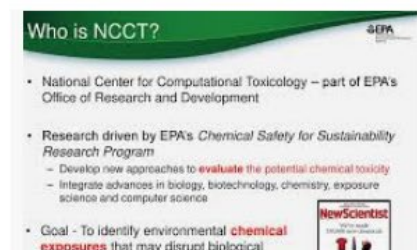
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promise of a chemistry data repository ...
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ChemConnector on Twitter: "First talk ...
twitter.com



Think about it...

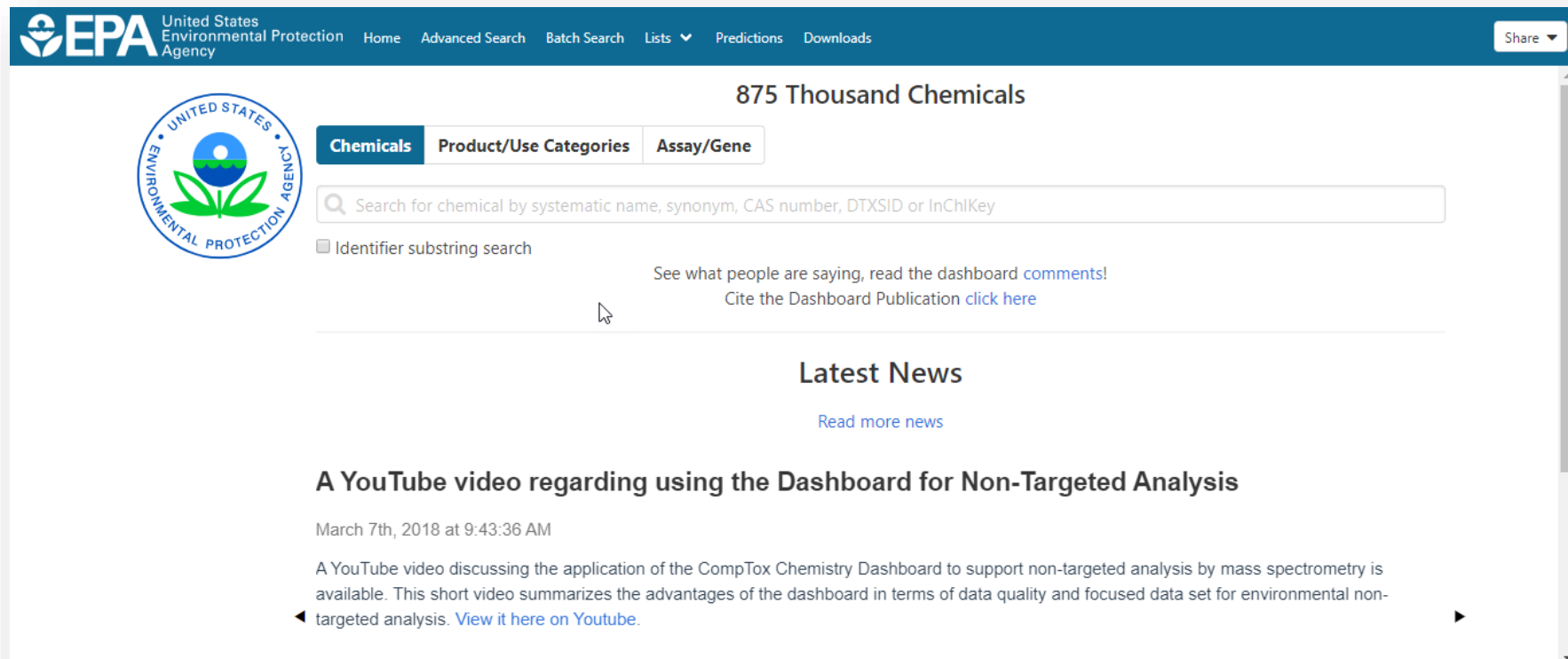
- 100s if not 1000s of hours of research behind a paper. How much work is the PUBLISHER going to do to make sure people find out about your article?? How do you find out about an article???
- Shouldn't **YOU** and your **CO-AUTHORS** invest some time in getting it out to the network???
- A presentation given to a small room of people has a lifetime of “20-30 mins”. A presentation shared online for all to see lives a lot longer. An article shared in the network has a much wider audience.

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 section titled 'Latest News' with a link to 'Read more news'. The news section features a video titled 'A YouTube video regarding using the Dashboard for Non-Targeted Analysis' dated March 7th, 2018. The video description states: '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.'

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



Manage Articles Here Too...

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





Your Postings Get Networked

 **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
Version 3/2019
[https://comp.tox.us/chemicals/](#)
Antony Williams
National Center for Computational Toxicology

CompTox Chemicals Dashboard Release March 2019
slideshare.net



1 Like

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

What do you want to be recommended for?

Scientist in the National Center of Computational T

2

Who do you want to ask?

Your connections: (You can add up to 3 people)

Jeff Edwards

3



Jeff Edwards

What's your relationship?

You worked with Jeff in the same group

What was Jeff's position at the time?

Software Architect & Engineer at US EPA

4

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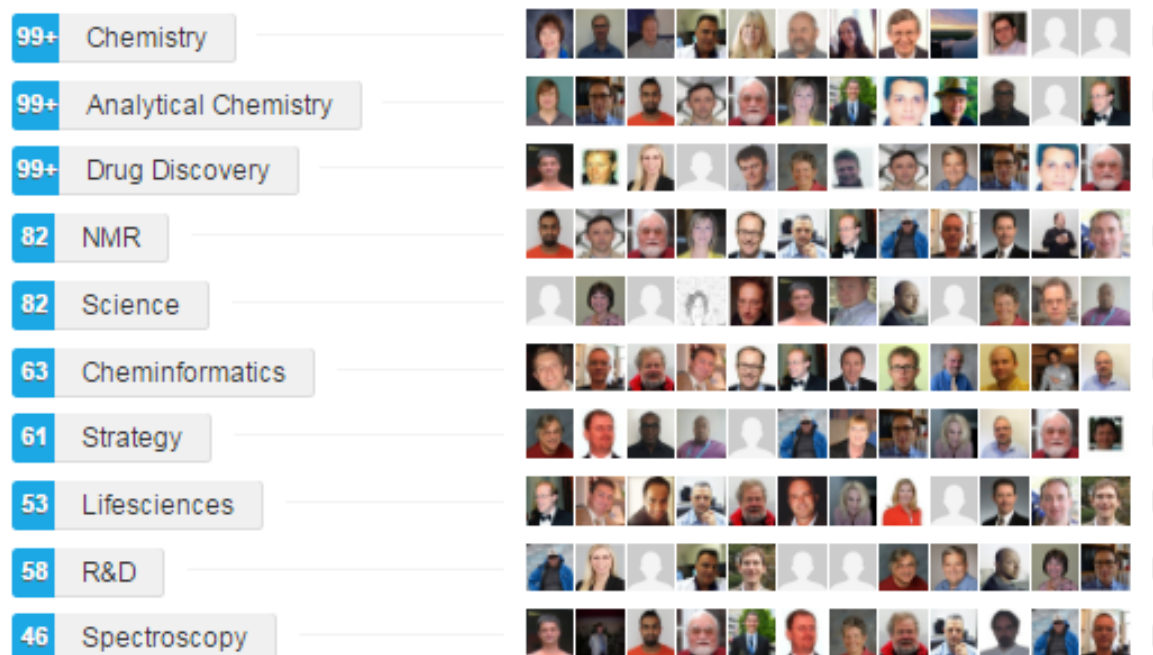
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Skills & Endorsements

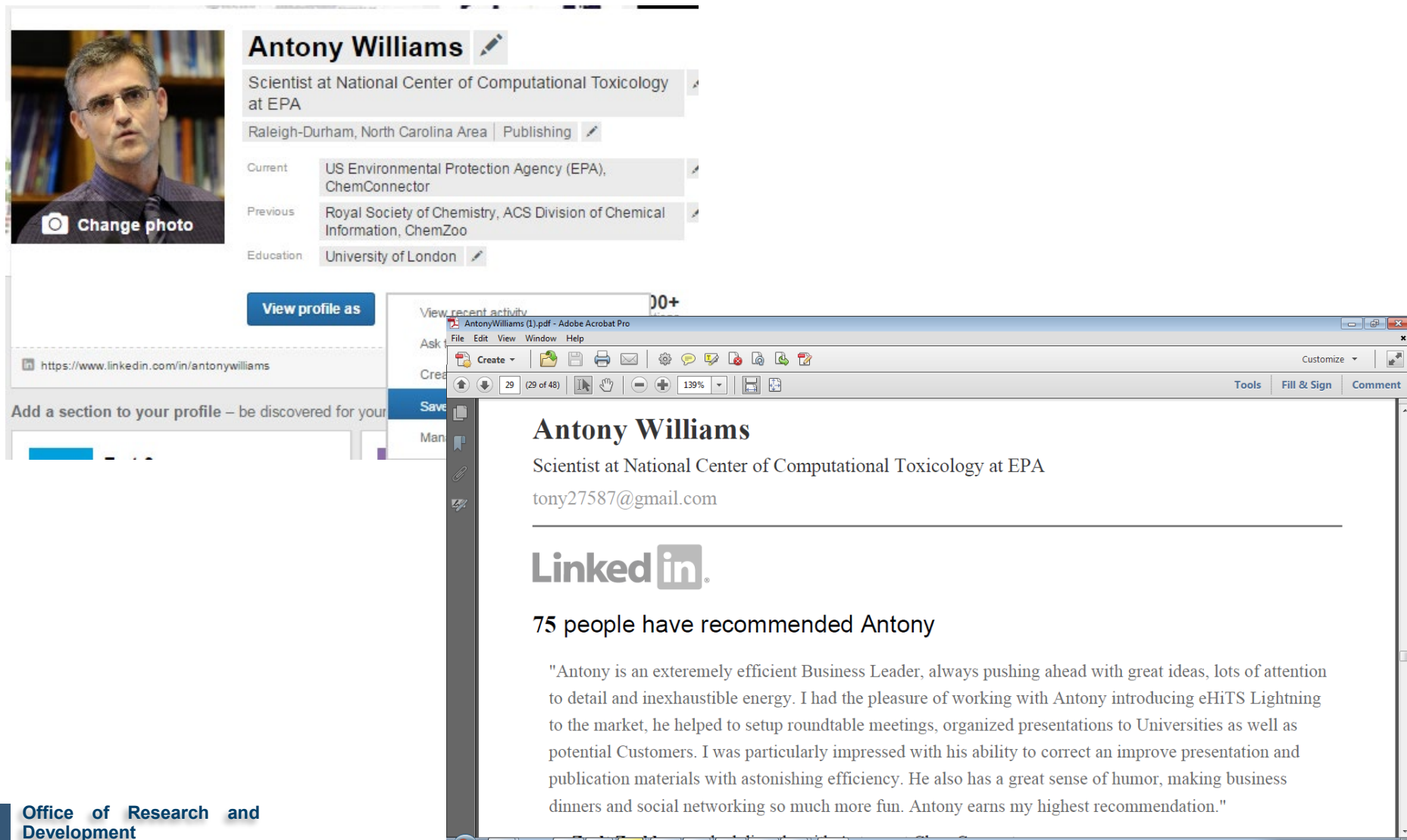
Top Skills




Antony also knows about...




Instant Summary as a PDF



The image shows a LinkedIn profile for Antony Williams, a Scientist at the National Center of Computational Toxicology at EPA. The profile includes a photo, a "Change photo" button, and a "View profile as" button. The URL <https://www.linkedin.com/in/antonywilliams> is visible. Below the profile, a PDF summary of the profile is shown, generated by Adobe Acrobat Pro. The PDF summary includes the name "Antony Williams", title "Scientist at National Center of Computational Toxicology at EPA", email "tony27587@gmail.com", and a recommendation from 75 people. The recommendation text reads: "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."


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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tony27587@gmail.com

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75 people have recommended Antony

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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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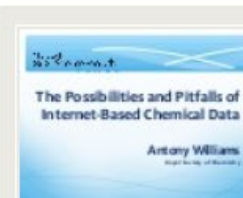
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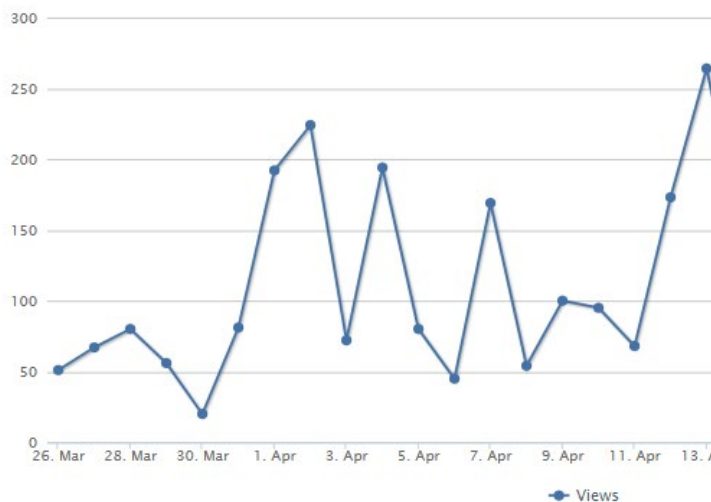
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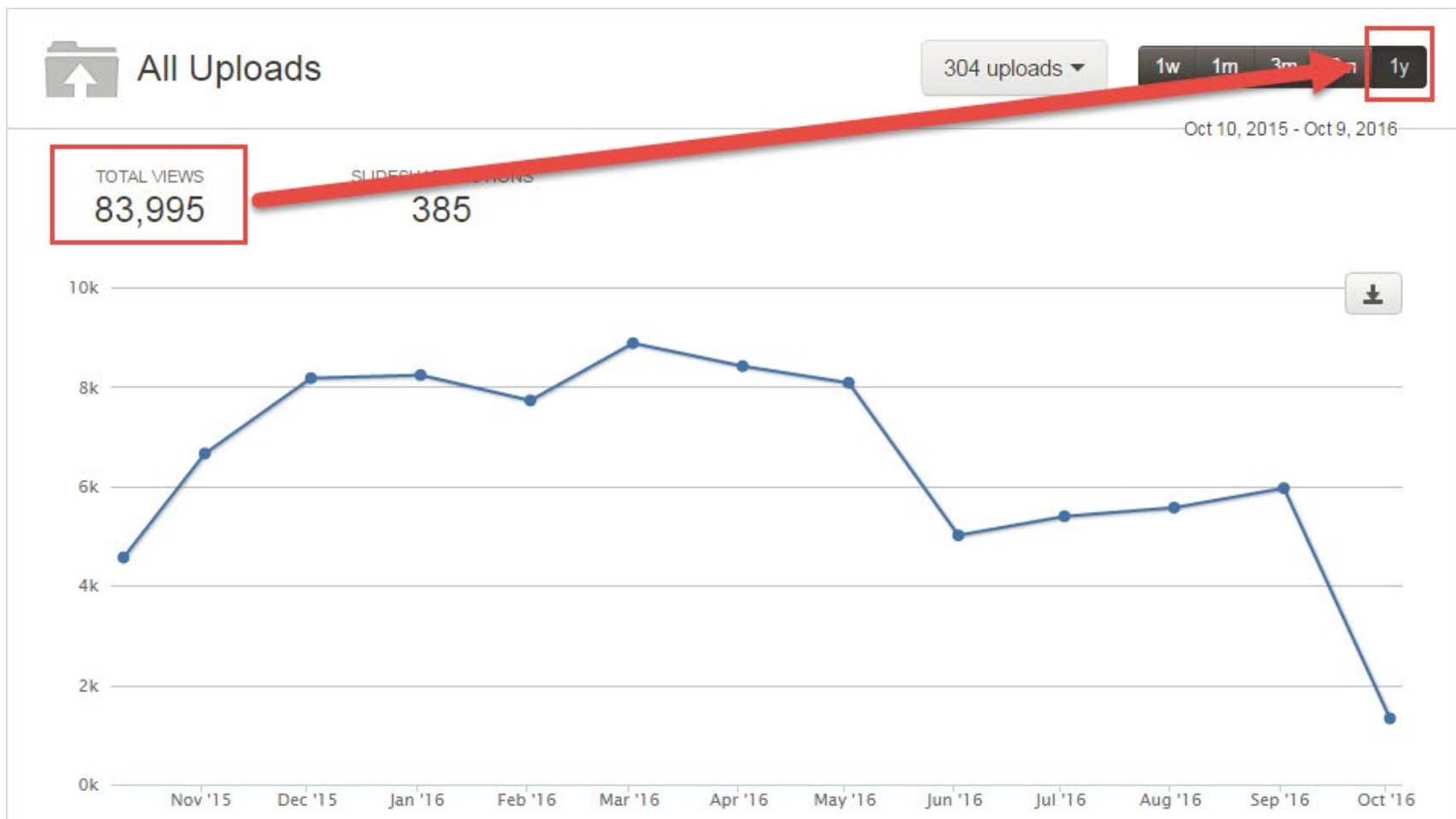
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Chemical identification of unknowns in high resolution mass spectrometry using the CompTox Chemicals Dashboard	240
Structure identification by Mass Spectrometry Non-Targeted Analysis using the US EPA's CompTox Chemistry Dashboard	189
New developments in delivering public access to data from the National Center for Computational Toxicology at the EPA	189
US EPA CompTox Chemistry Dashboard as a source of data to fill data gaps for chemical sources of risk	185
Development of a Tool for Systematic Integration of Traditional and New Approach Methods for Prioritizing Chemical Lists	183

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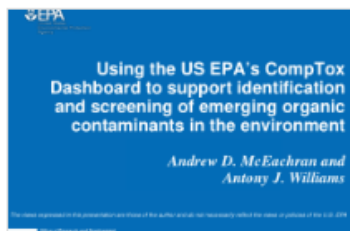
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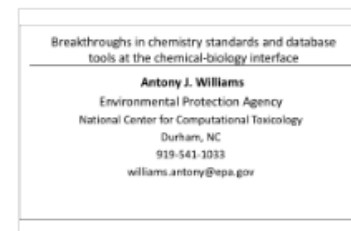
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Building an Online Profile Using Social Networking Tools

Antony Williams

30/05/2018



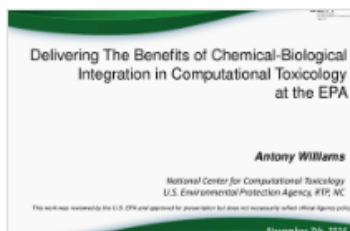
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Antony Williams

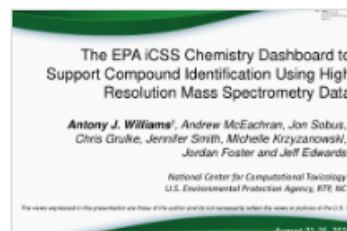
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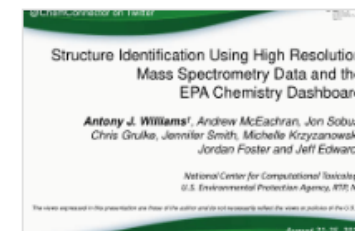
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Structure Identification Using High Resolution Mass Spectrometry Dat...

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Influence of data curation on QSAR Modeling – examining issues of quality versus quantity of data

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

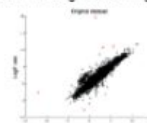
The manual investigation of the data allowed us to develop a KNIME³ workflow for automated processing. This workflow was derived from earlier work by Mansouri et. al.⁴ and is represented in the figure below as a series of blocks representing, for example:

- 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

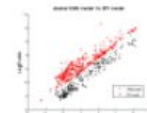


Model Performance

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.



Statistics of the new Model
5-fold cross-validation:
Q2: 0.87 RMSE: 0.67
Fitting:
R2: 0.87 RMSE: 0.66
Test set Prediction:
R2: 0.84 RMSE: 0.65



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4	2018	Analytical and bioanalytical chemistry, 1-14	Article	https://doi.org/10.1007/s00216-018-1435-6
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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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Project

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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Dec 26, 2018 ▾

EPA's non-targeted analysis collaborative trial (ENTACT): genesis, design, and initial findings

Article Dec 2018

 Elin M Ulrich ·  Jon R. Sobus ·  Christopher M Grulke · [...] ·  Antony John Williams

In August 2015, the US Environmental Protection Agency (EPA) convened a workshop entitled "Advancing non-targeted analyses of xenobiotic chemicals in environmental and biological media." The purpose of the workshop was to bring...

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New update to CompTox Chemicals Dashboard released March 2019





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 is available for review at https://comptox.epa.gov/dashboard/comptox_release_notes

 [comptox_release_notes.pdf](#) · 48.41 KB

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"MS-Ready" structures for non-targeted high-resolution mass spectrometry screening studies

Article Dec 2018

 Andrew McEachran ·  Mansouri Kamel ·  Christopher M Grulke · [...] ·  Antony John Williams

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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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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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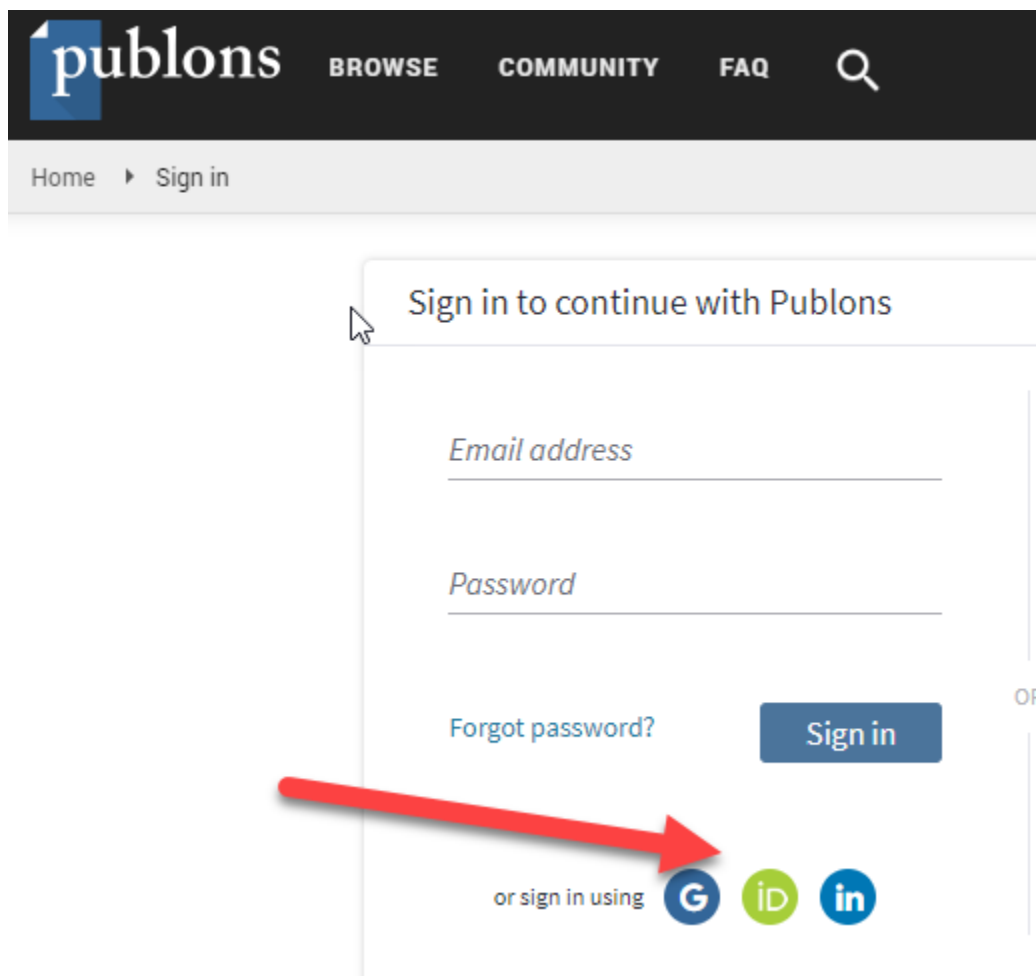
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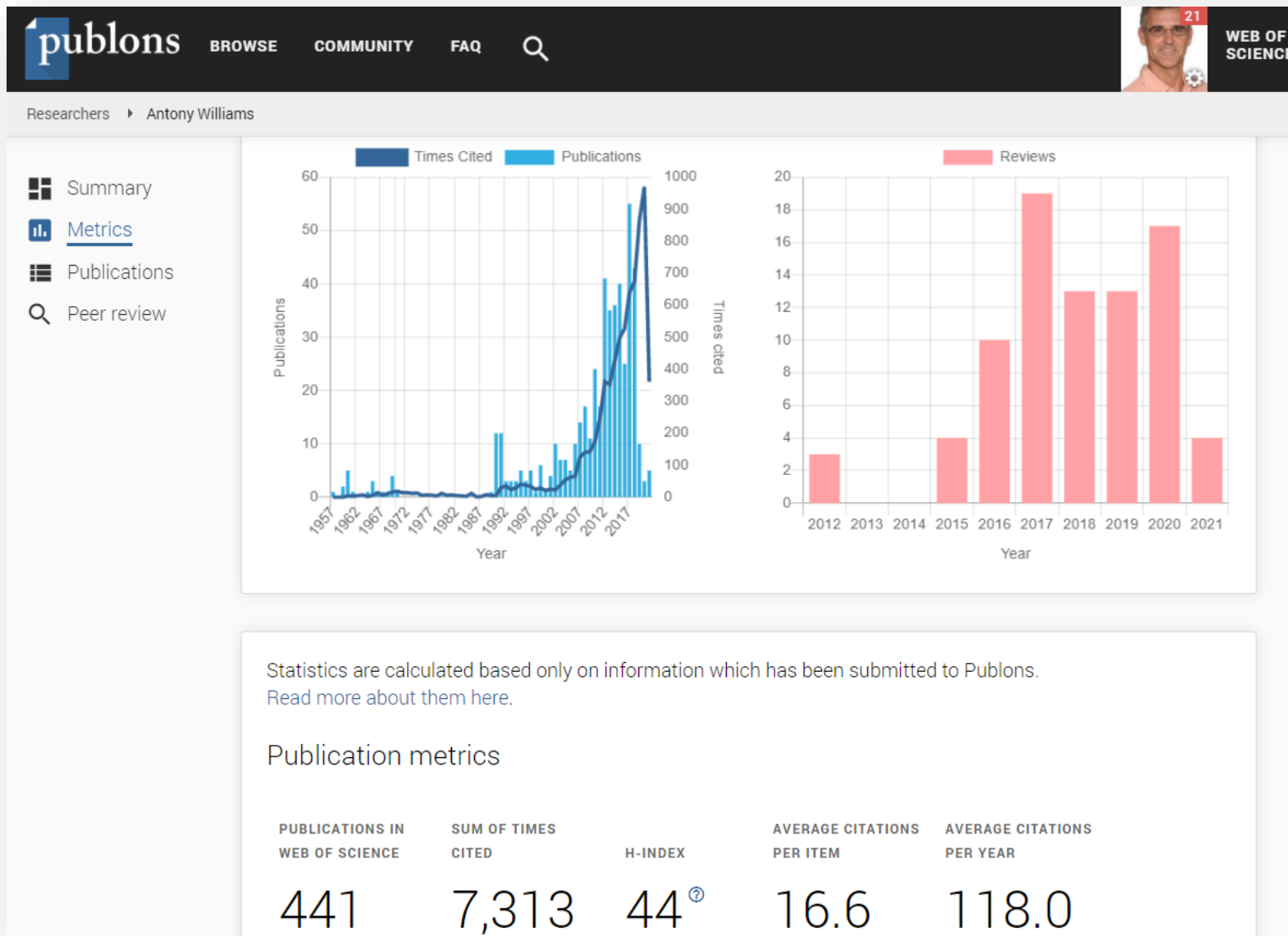
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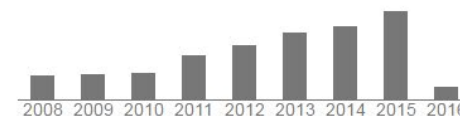
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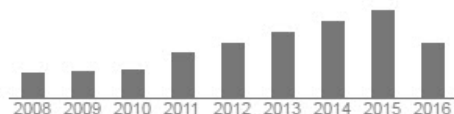
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Gary Martin is an [American chemist](#) and expert in the fields of both [NMR spectroscopy](#) and [medicinal chemistry](#). He is a distinguished fellow at the [Merck Research Laboratories](#). He is also a photographer specializing in the capture of images of lighthouses, especially under conditions of extreme weather.^{[1][2]}

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Career [\[edit \]](#)

Martin holds a B.S. in Pharmacy from the University of Pittsburgh and a Ph.D. degree in Medicinal Chemistry/Pharmaceutical Sciences from the [University of Kentucky](#).^[3] He was a Professor of Medicinal Chemistry at the University of Houston from 1975–1989 and the director of the University of Houston [NMR Facility](#) between 1984–1989. He moved to the pharmaceutical industry in 1989 and worked at a number of pharmaceutical companies as described below. He has published more than 275 papers, invited reviews, and chapters and is a frequently invited lecturer at national and international NMR meetings.

Between 1989 and 1995 he worked at [Burroughs Wellcome](#) (later [GlaxoSmithKline](#)) (see reference 3) and worked on the development of new one- and two-dimensional NMR experiments for the solution of complex structural and spectral assignment problems. He developed new methods for the acquisition of submicromole and sub-nanomole NMR data for molecular structure characterization, especially work involving inverse-detected heteronuclear shift correlation techniques. These efforts led to collaborative development with Nalorac Cryogenics Corp. to develop micro inverse detection probes which facilitated the acquisition of [HMQC](#) spectra on samples to the level of 0.05 μmole for small (200-500 Da) molecule NMR.^[4]

Gary Martin

Born

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Nationality

[United States](#)

Alma mater

[University of Kentucky](#)
[University of Pittsburgh](#)

Known for

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Doctoral advisor

[George A. Digenis](#)

Google shaved him...

Gary E. Martin

American chemist



Gary Martin is an American chemist and expert in the fields of both NMR spectroscopy and medicinal chemistry. He is a distinguished fellow at the Merck Research Laboratories. He is also a photographer specializing in the capture of images of lighthouses, especially under conditions of extreme weather.

[Wikipedia](#)

Born: October 1949 (age 71 years), [Wilksburg, PA](#)

Doctoral advisor: [George A. Digenis](#)

Education: [University of Pittsburgh](#), [University of Kentucky](#), [University of Kentucky College of Pharmacy](#)

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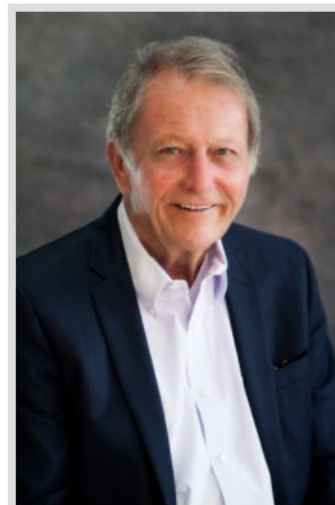
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Author Updates

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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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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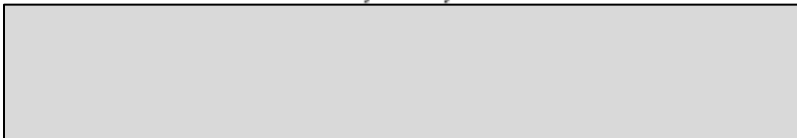
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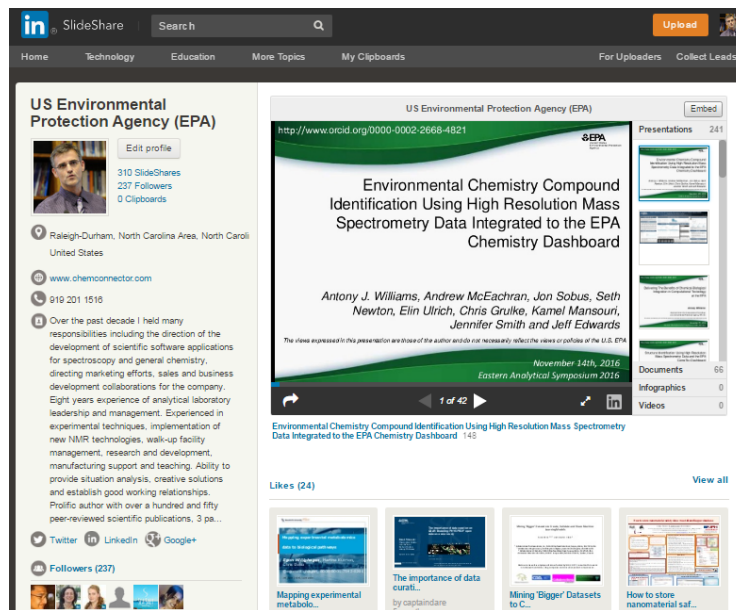
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Various Versions of This Talk

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