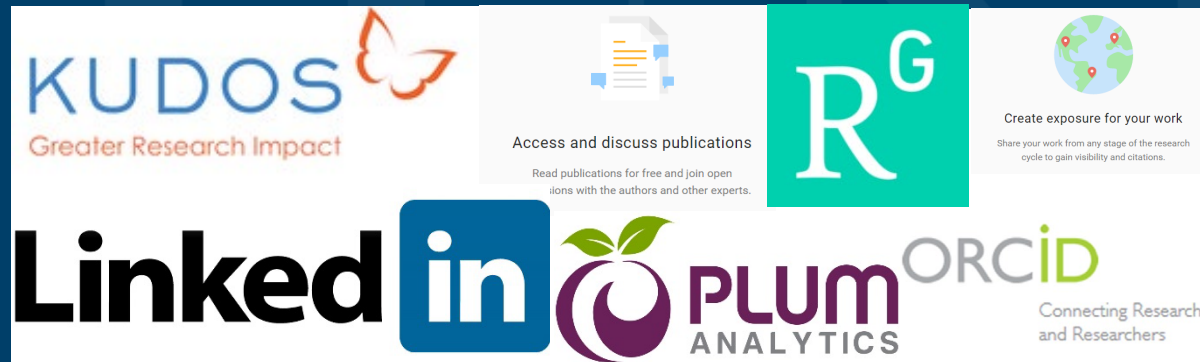


Profile Building, Research Sharing and Data Proliferation using Social Media Tools for Scientists



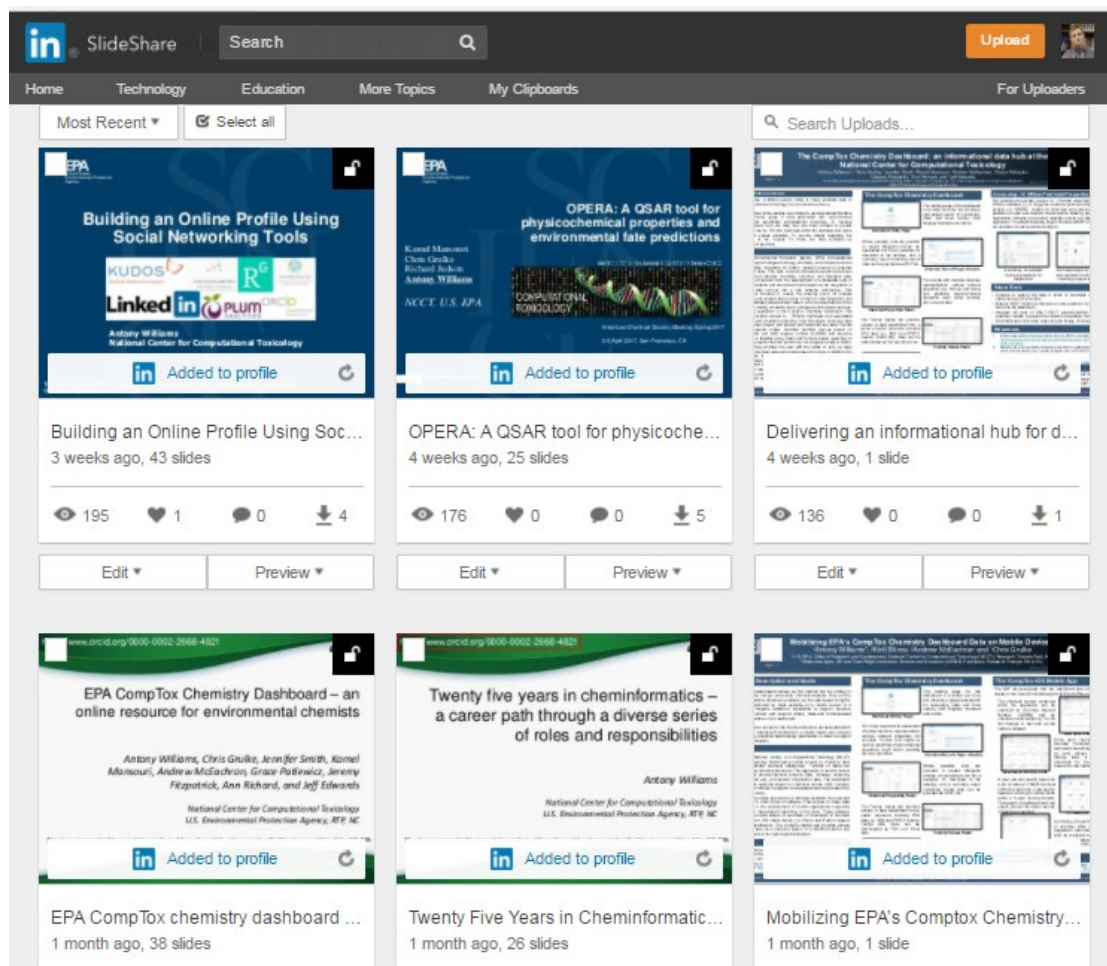
Antony Williams
Center for Computational Toxicology and Exposure

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 a SlideShare profile for Antony Williams, a National Center for Computational Toxicology researcher at the EPA. The profile features six presentations:

- 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)
- Twenty five years in cheminformatics – a career path through a diverse series of roles and responsibilities** (1 month ago, 26 slides)
- Mobilizing EPA's Comptox Chemistry...** (1 month ago, 1 slide)

Each presentation card includes a thumbnail image, a title, a brief description, and engagement metrics (views, likes, comments, downloads). The presentations are primarily related to EPA's computational toxicology efforts, including the development of the OPERA tool and the CompTox Chemistry Dashboard.

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...

- Show of hands please...
 - 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?

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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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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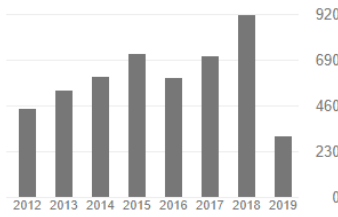
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<input type="checkbox"/> Open PHACTS: semantic interoperability for drug discovery AJ Williams, L Harland, P Groth, S Pattifer, C Chichester, EL Willighagen, ... Drug discovery today 17 (21-22), 1188-1198	252	2012
<input type="checkbox"/> Online chemical 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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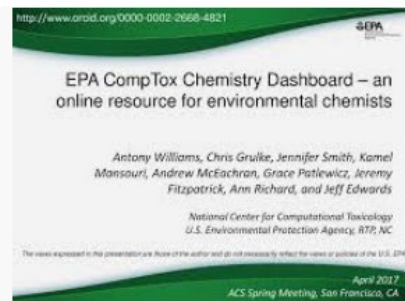


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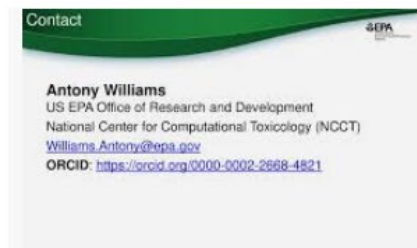
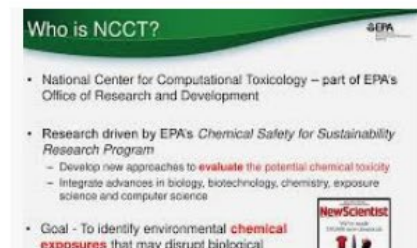
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Think about it...


- 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
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- Performances in film and audio
- Other forms of research
- **CAVEAT: Make sure you are *allowed* to share**



My primary project at present...



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875 Thousand Chemicals

Chemicals Product/Use Categories Assay/Gene

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

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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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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
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)
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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1

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Scientist in the National Center of Computational T

2

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Jeff Edwards X

3



Jeff Edwards

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What was Jeff's position at the time?

Software Architect & Engineer at US EPA

4

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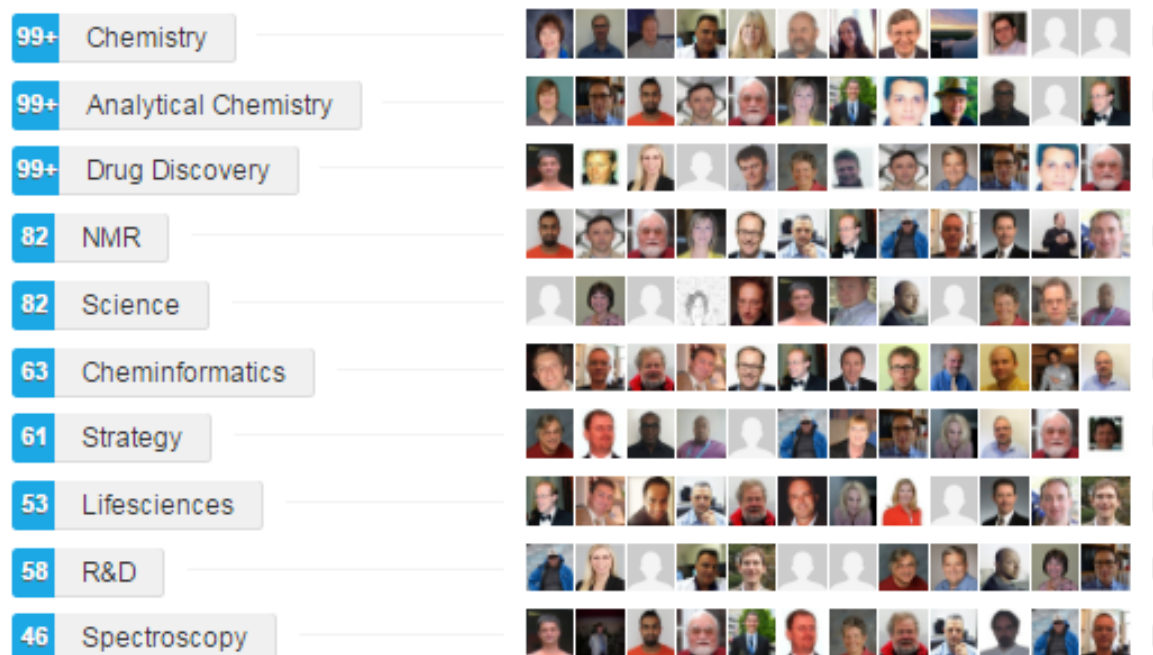
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Skills & Endorsements

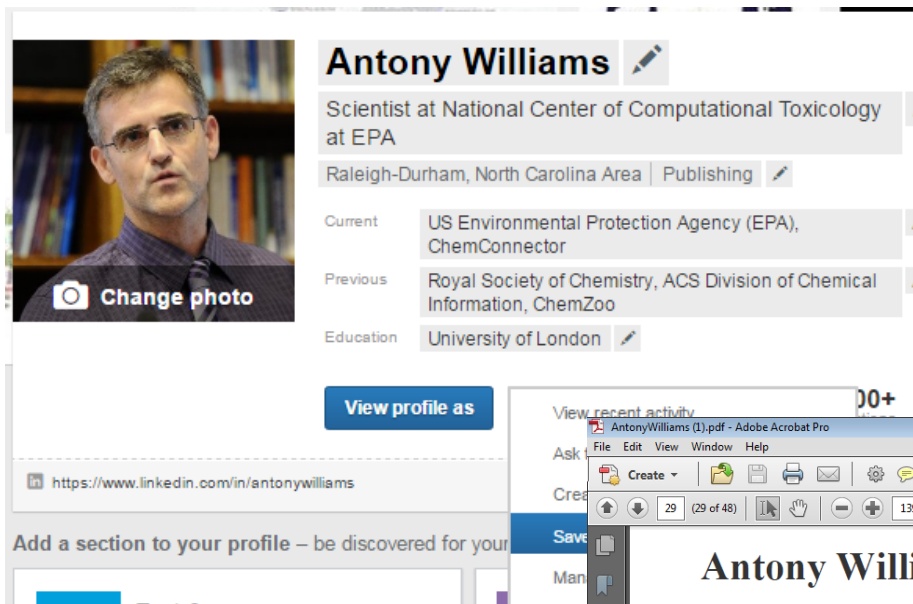
Top Skills




Antony also knows about...




Instant Summary as a PDF




Antony Williams 

Scientist at National Center of Computational Toxicology at EPA

Raleigh-Durham, North Carolina Area | Publishing 

Current US Environmental Protection Agency (EPA), ChemConnector

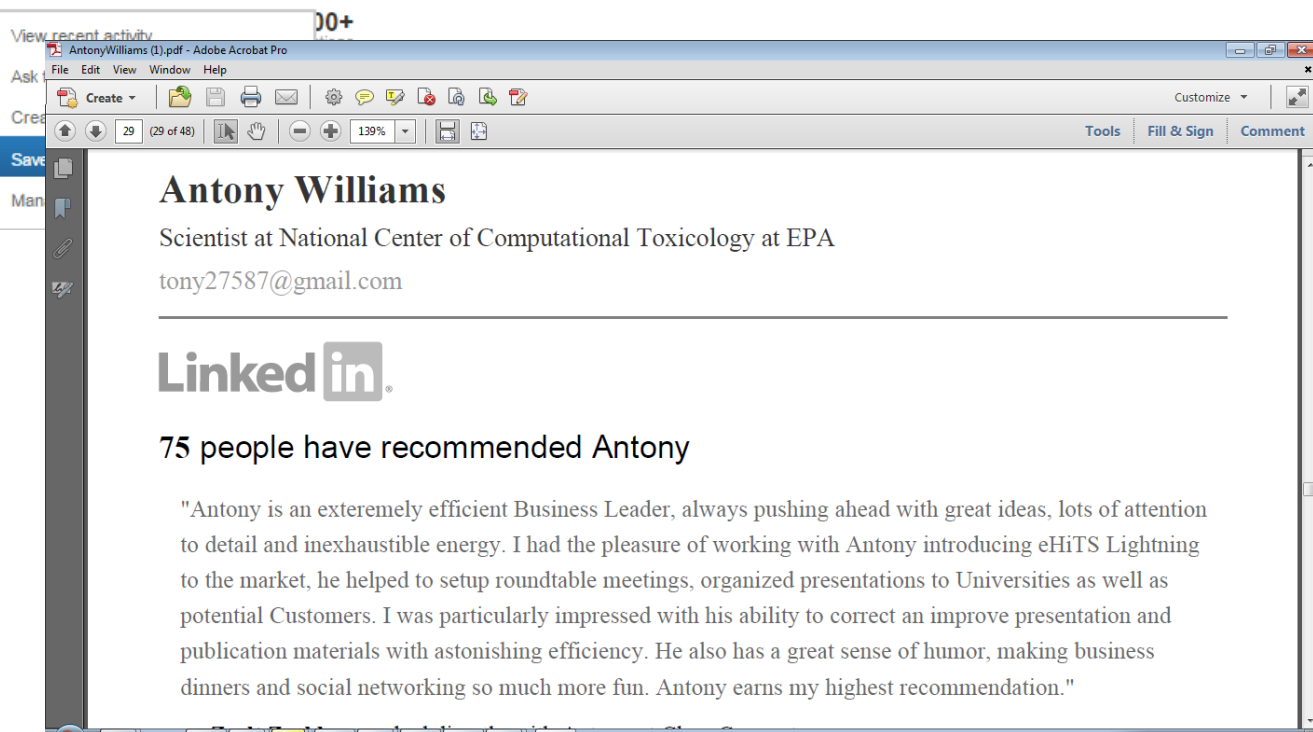
Previous Royal Society of Chemistry, ACS Division of Chemical Information, ChemZoo

Education University of London 

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























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Antony Williams

Scientist at National Center of Computational Toxicology at EPA

tony27587@gmail.com

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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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- www.chemconnector.com
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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

August 2018
ACS Fall Meeting, Boston

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Version 3/2018

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substance identity for UVCBs

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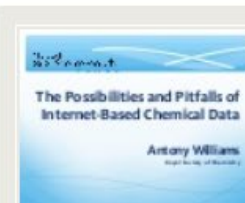
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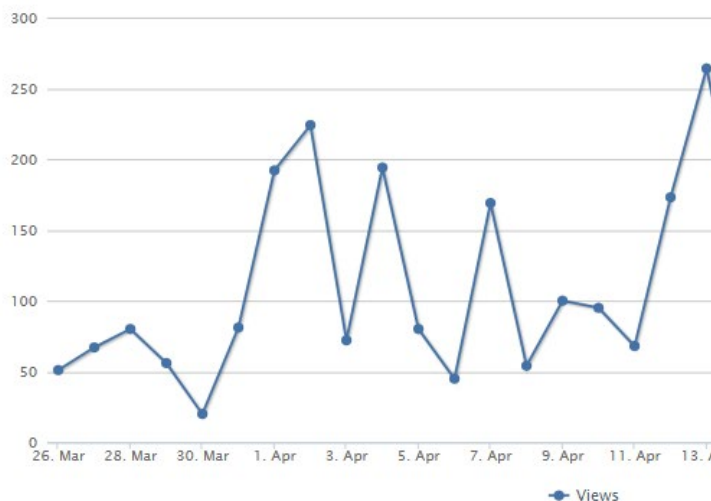
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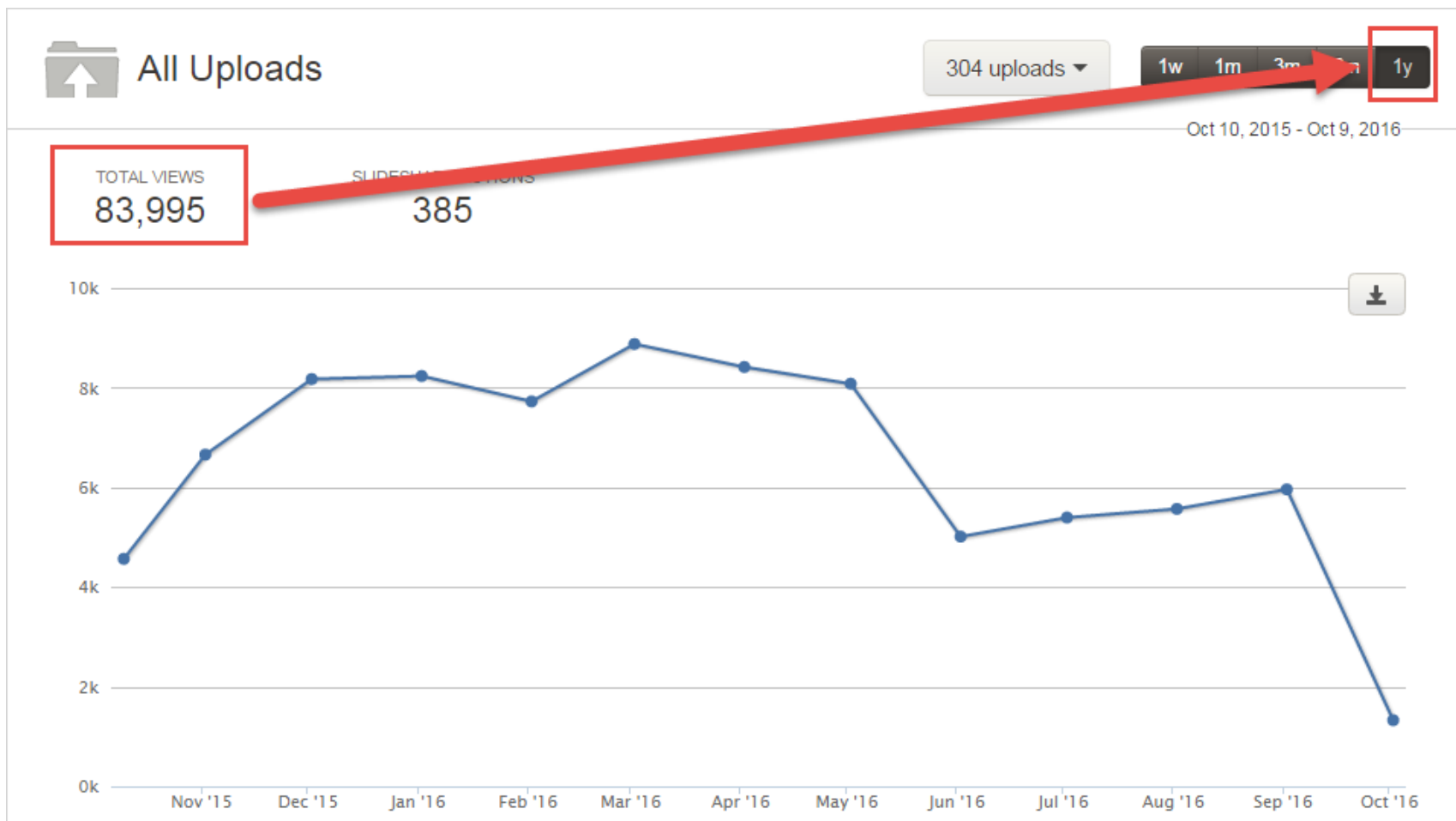
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US EPA CompTox Chemistry Dashboard as a source of data to fill data gaps for chemical sources of risk	185
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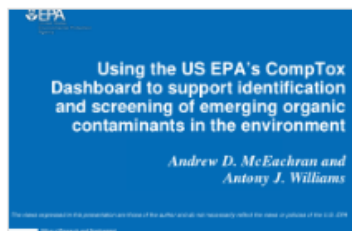
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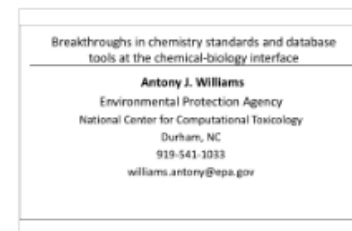
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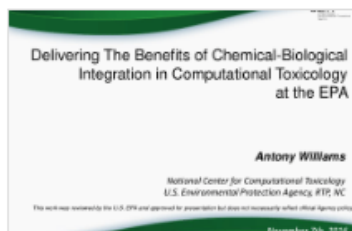
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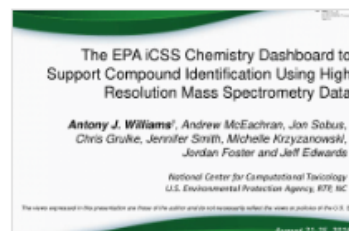
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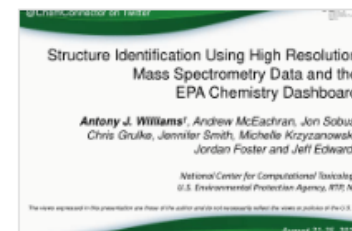
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Antony Williams*, Kamel Mansouri, Ann M. Richard and Chris Grulke

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

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New Orleans, LA
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ORCID: 0000-0002-2668-4821

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

Automated Analysis Using KNIME

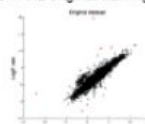
The manual investigation of the data allowed us to develop a KNIME³ workflow for automated processing. This workflow was derived from earlier work by Mansouri et. al.⁴ and is represented in the figure below as a series of blocks representing, for example:

- 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

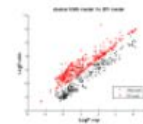


Model Performance

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
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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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The CompTox Chemicals Dashboard

Antony John Williams · Christopher M Grulke · Mansouri Ka

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

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

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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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Antony J Williams

United States Environmental Protection Agency, National Center of Computational Toxicology,
Faculty Member [edit](#)

Research Interests: Chemistry, Nuclear Magnetic Resonance, Cheminformatics, Drug discovery and Cheminformatics, Collaborative Design, Analytical Chemistry, and E Science

About:

My passion is connecting people to chemistry. Over the past decade I held many jobs and responsibilities including th...
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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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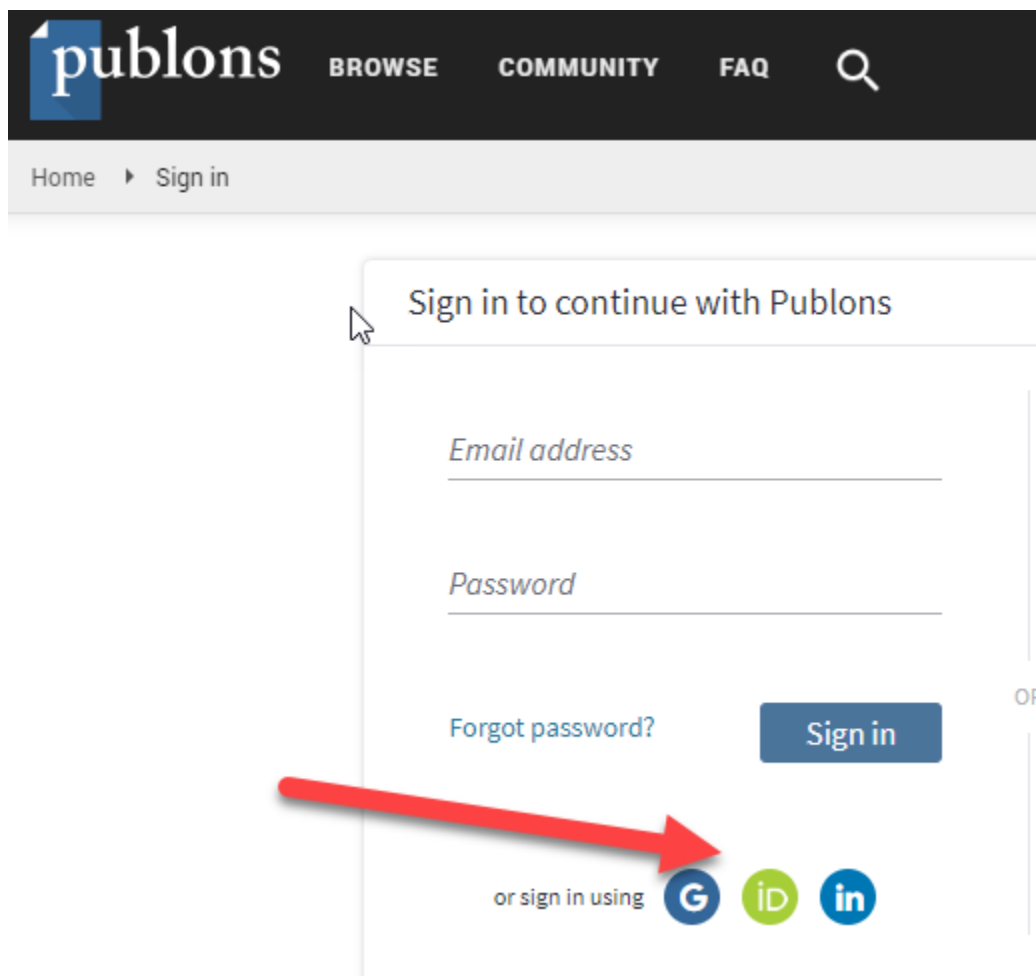
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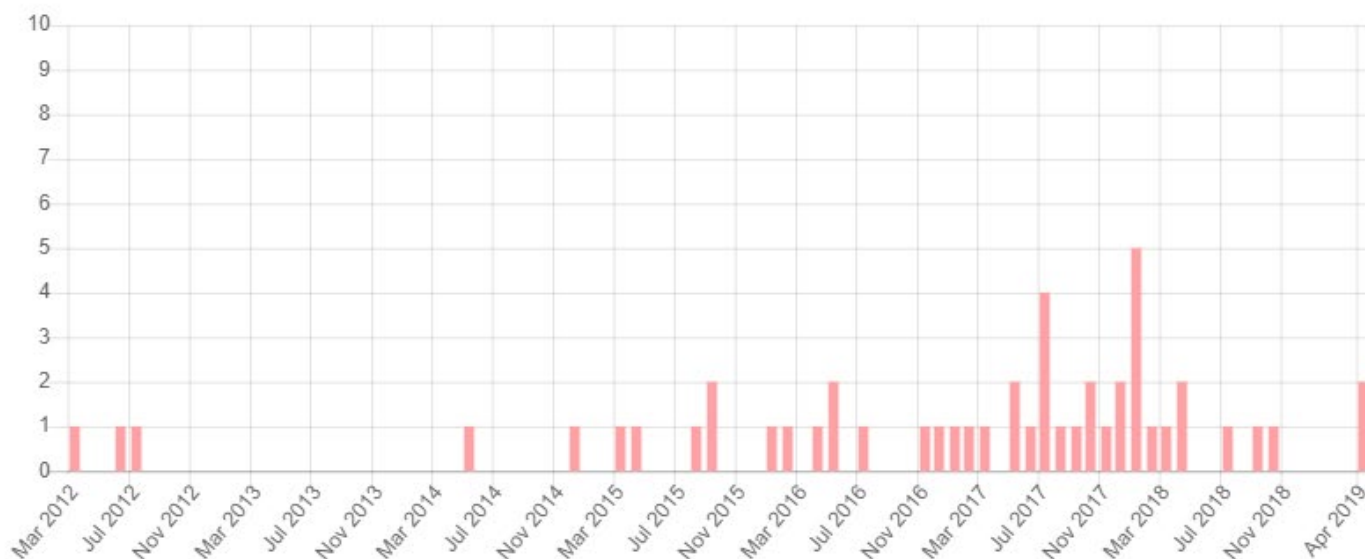
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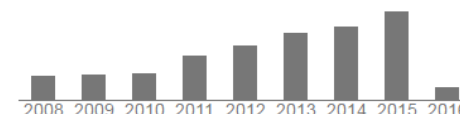
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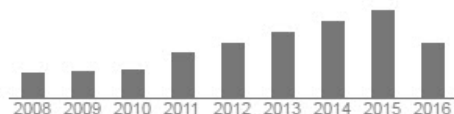
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Author Updates

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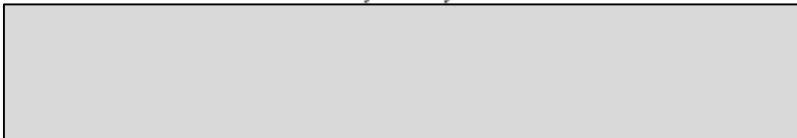
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Structure identification by Mass Spectrometry Non-Targeted Analysis using the US EPA's CompTox



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ANTONY JOHN WILLIAMS, PhD, FRSC



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

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

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Positions

Computational Chemist, [National Center for Computational Toxicology](#), [Office of Research and Development](#), [Environmental Protection Agency](#).

Expertise

NMR spectroscopist

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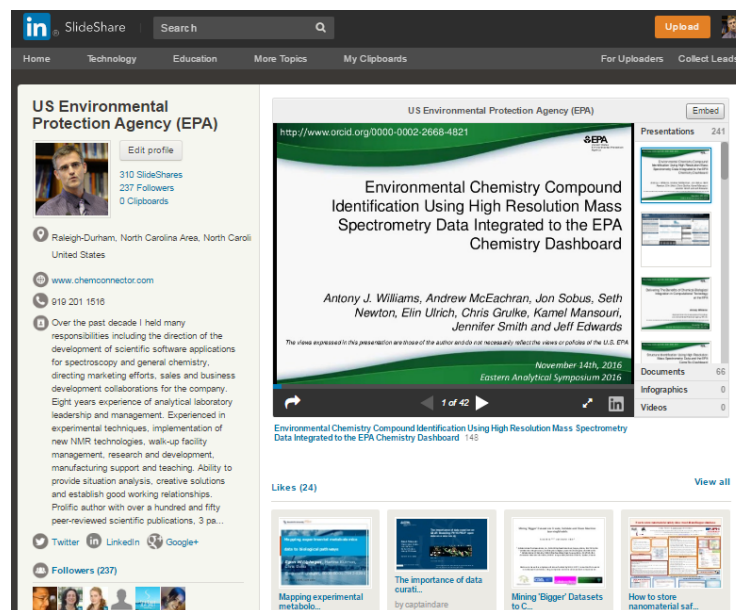
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