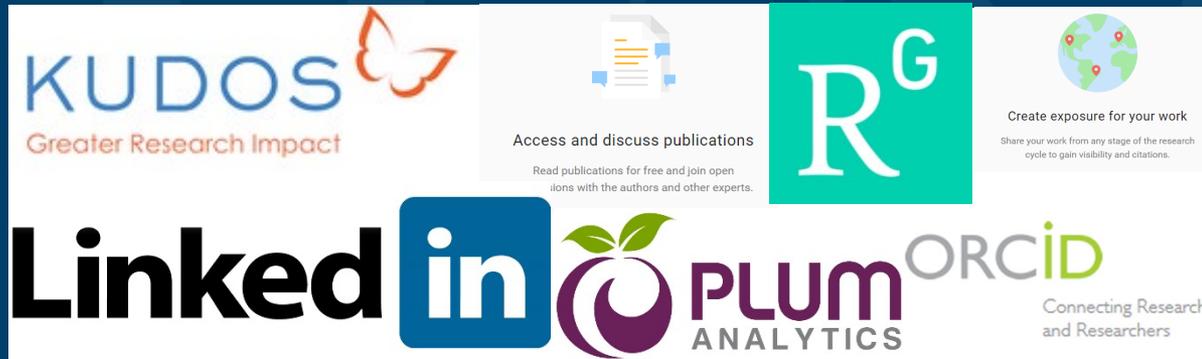




Profile Building, Research Sharing and Data Proliferation using Social Media Tools for Scientists



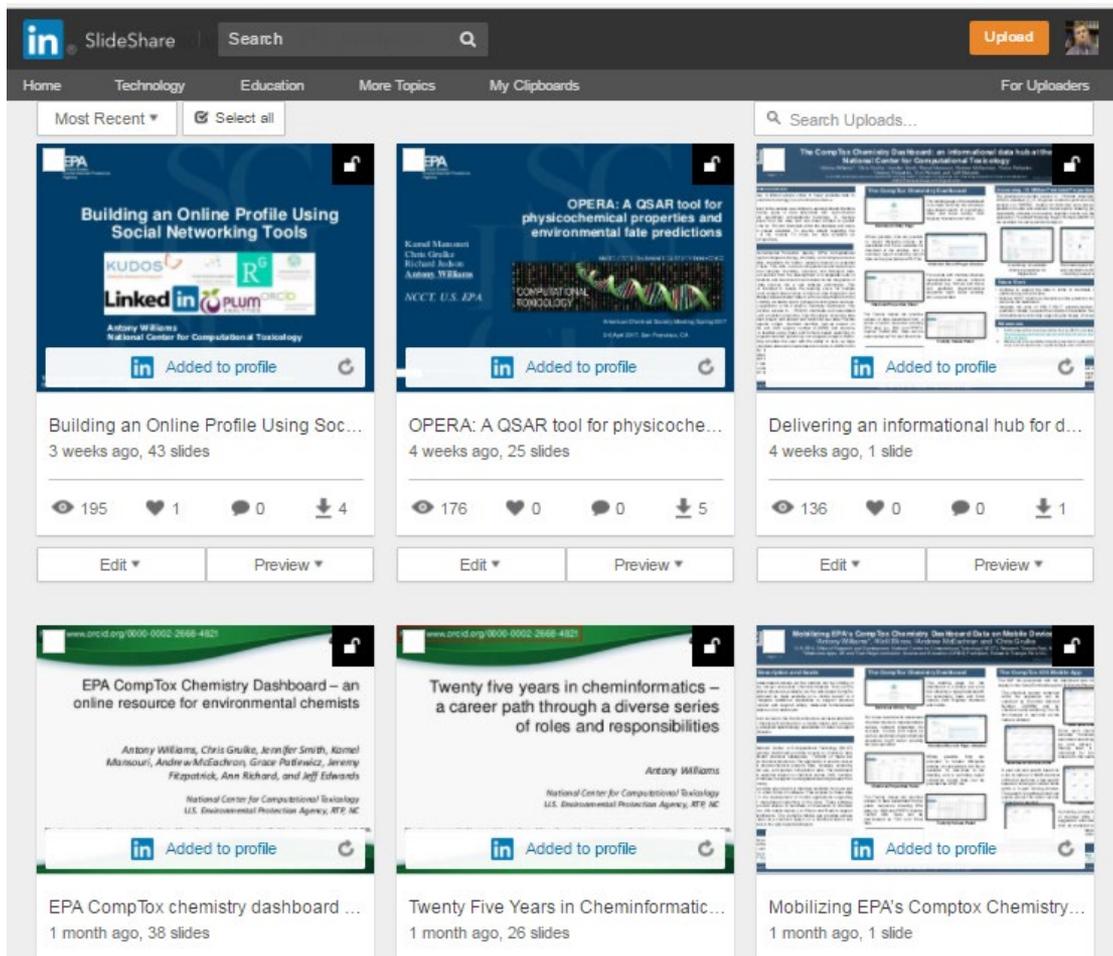
Antony Williams
Center for Computational Toxicology and Exposure,
Office of Research and Development, US EPA

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 a grid of six presentations:

- Building an Online Profile Using Social Networking Tools** (3 weeks ago, 43 slides, 195 views, 1 like)
- OPERA: A QSAR tool for physicochemical properties and environmental fate predictions** (4 weeks ago, 25 slides, 176 views, 0 likes)
- The CompTox Chemistry Dashboard: an informational data hub at the National Center for Computational Toxicology** (4 weeks ago, 1 slide, 136 views, 0 likes)
- 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 Dashboard Data on Mobile Devices** (1 month ago, 1 slide)

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?

- ORCID's 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???

<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



0000-0002-2668-4821



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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

academickarma.org/0000-0002-2668-4821 ▼

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

computer_assisted_structure_elucidation. cheminformatics. systematic_naming. open_data.

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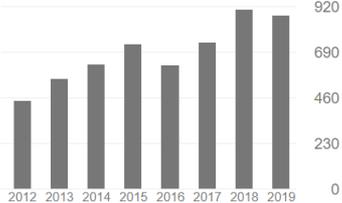
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<input type="checkbox"/> Open PHACTS: semantic interoperability for drug discovery AJ Williams, L Harland, P Groth, S Pettifer, C Chichester, EL Willighagen, ... Drug discovery today 17 (21-22), 1188-1198	269	2012
<input type="checkbox"/> Online chemical modeling environment (OCHEM): web platform for data storage, model development and publishing of chemical information I Sushko, S Novotarskiy, R Körner, AK Pandey, M Rupp, W Teetz, ...	236	2011

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



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A Question to Start...

- Who in the room has an ORCID?

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ORCID provides a permanent digital identifier that distinguishes you from every other researcher out there. Integration to key research workflows such as manuscript and grant submission, grants and automated ledgers between you and your professional activities ensuring that your work is recognized. Read the story.

ChemConnector

0000-0002-2668-4821

promise of a chemistry data repository ...
slideplayer.com

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

EPA CompTox Chemistry Dashboard – an online resource for environmental chemists

Antony Williams, Chris Gruke, Jennifer Smith, Kamel Mansouri, Andrew McEachran, Grace Patlewicz, Jeremy Fitzpatrick, Ann Richard, and Jeff Edwards

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

April 2017
ACS Spring Meeting, San Francisco, CA

EPA CompTox Chemistry Dashboard – an ...
slideplayer.com

New Horizons....

- Let's map together all historical chemistry data and build systems to integrate it
- Heck, let's integrate chemistry and biology data and add in disease data too
- Let's **model** the data and see if we can extract new relationships – quantitative and qualitative
- Let's make it all available on the web...

promise of a chemistry data repository ...
slideplayer.com

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

Web-based access to experimental and predicted data for environmental fate, transport and toxicity data

Antony Williams¹, Todd Martin², Valery Tkachenko³, Kamel Mansouri⁴ and Chris Gruke¹

¹ National Center for Computational Toxicology, U.S. Environmental Protection Agency, RTP, NC
² Working Risk Management Research Laboratory, U.S. Environmental Protection Agency, Cincinnati, OH
³ Science Data Software, LLC, Rockville, MD 20850
⁴ Integrated Laboratory Systems, Research Triangle Park, North Carolina, United States

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August 2018

ChemConnector on Twitter: "First talk ...
twitter.com

Here's why they are useful...

Google Scholar

The Chemical Analysis Methods Platform

ORCID

Antony Williams (ORCID: 0000-0002-2668-4821)

View Source For Antony Williams (ORCID: 0000-0002-2668-4821)

ORCID ID: 0000-0002-2668-4821

Driving needs for analytical data exchange standards and the potential impacts on the chemical sciences

Antony Williams

Who is NCCT?

- National Center for Computational Toxicology – part of EPA's Office of Research and Development
- Research driven by EPA's **Chemical Safety for Sustainability Research Program**
 - Develop new approaches to **evaluate** the potential chemical toxicity
 - Integrate advances in biology, biotechnology, chemistry, exposure science and computer science
- Goal - To identify environmental **chemical exposures** that may disrupt biological

NewsScientist

Contact

Antony Williams
US EPA Office of Research and Development
National Center for Computational Toxicology (NCCT)
Williams.Antony@epa.gov
ORCID: <https://orcid.org/0000-0002-2668-4821>

Think about it...

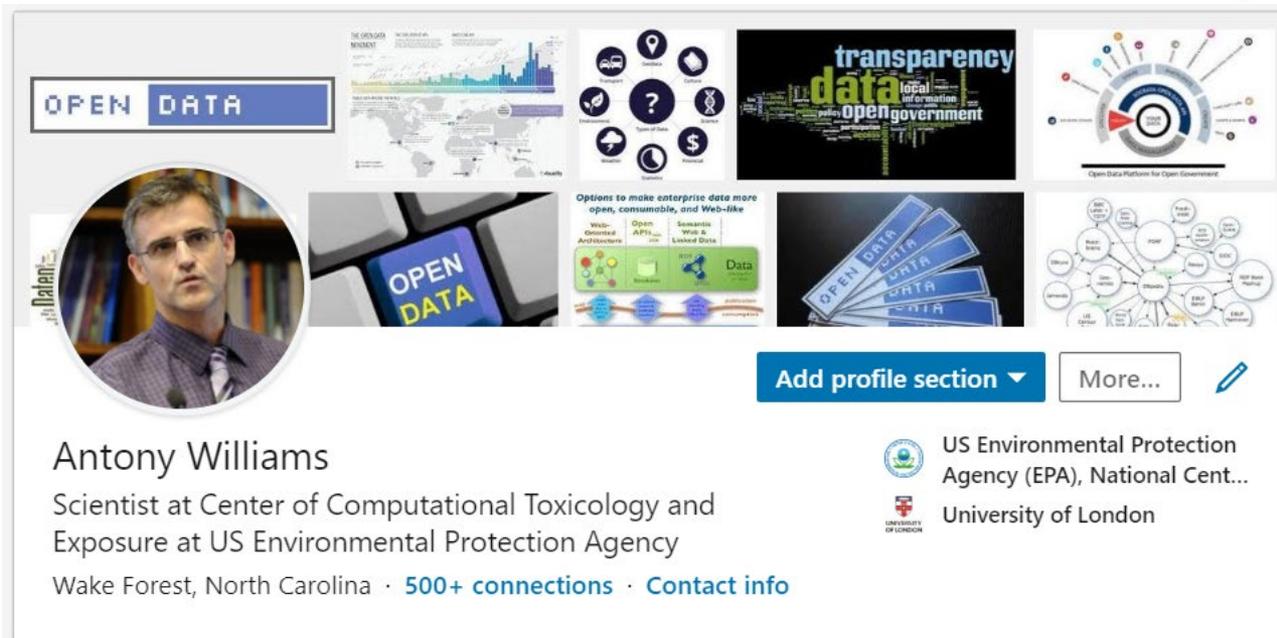
- 100s if not 1000s of hours of research behind a paper. How much work is the PUBLISHER going to do to make sure people find out about your article?? How do you find out about an article???
- Shouldn't **YOU** and your **CO-AUTHORS** invest some time in getting it out to the network???
- A presentation 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**

LinkedIn

The MOST BASIC Career Networking Tool



OPEN DATA

transparency data local information open government

Options to make enterprise data more open, consumable, and Web-like

Web-Generated Architecture Open APIs Linked Data Semantic Web & Linked Data

OPEN DATA DATA DATA DATA DATA

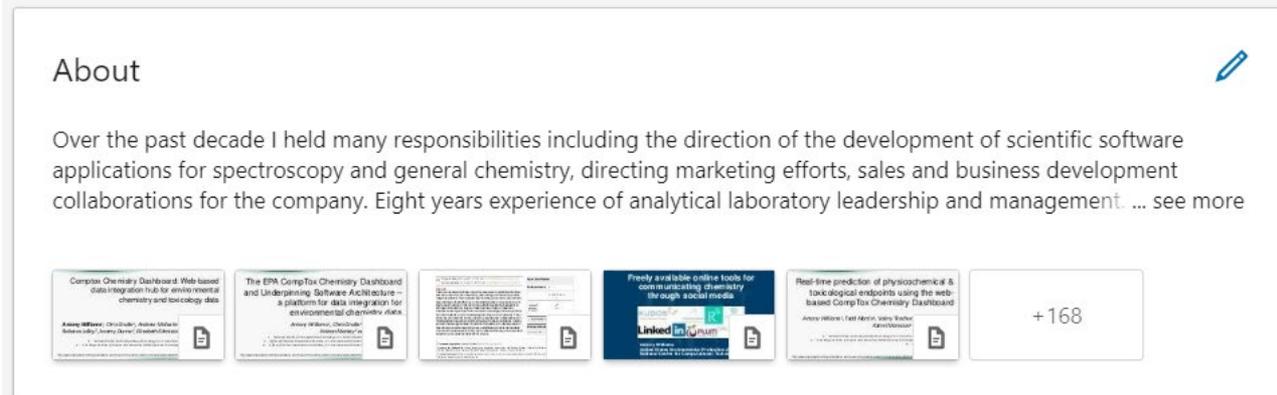
ADD profile section More...

Antony Williams
 Scientist at Center of Computational Toxicology and Exposure at US Environmental Protection Agency
 Wake Forest, North Carolina · 500+ connections · Contact info

US Environmental Protection Agency (EPA), National Cent...
 University of London

About

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. ... see more



Complex Chemistry Dashboard: Web-based data integration hub for environmental chemistry and toxicology data

The EPA CompTox Chemistry Dashboard and Underlying Software Architecture - a platform for data integration for environmental chemistry data

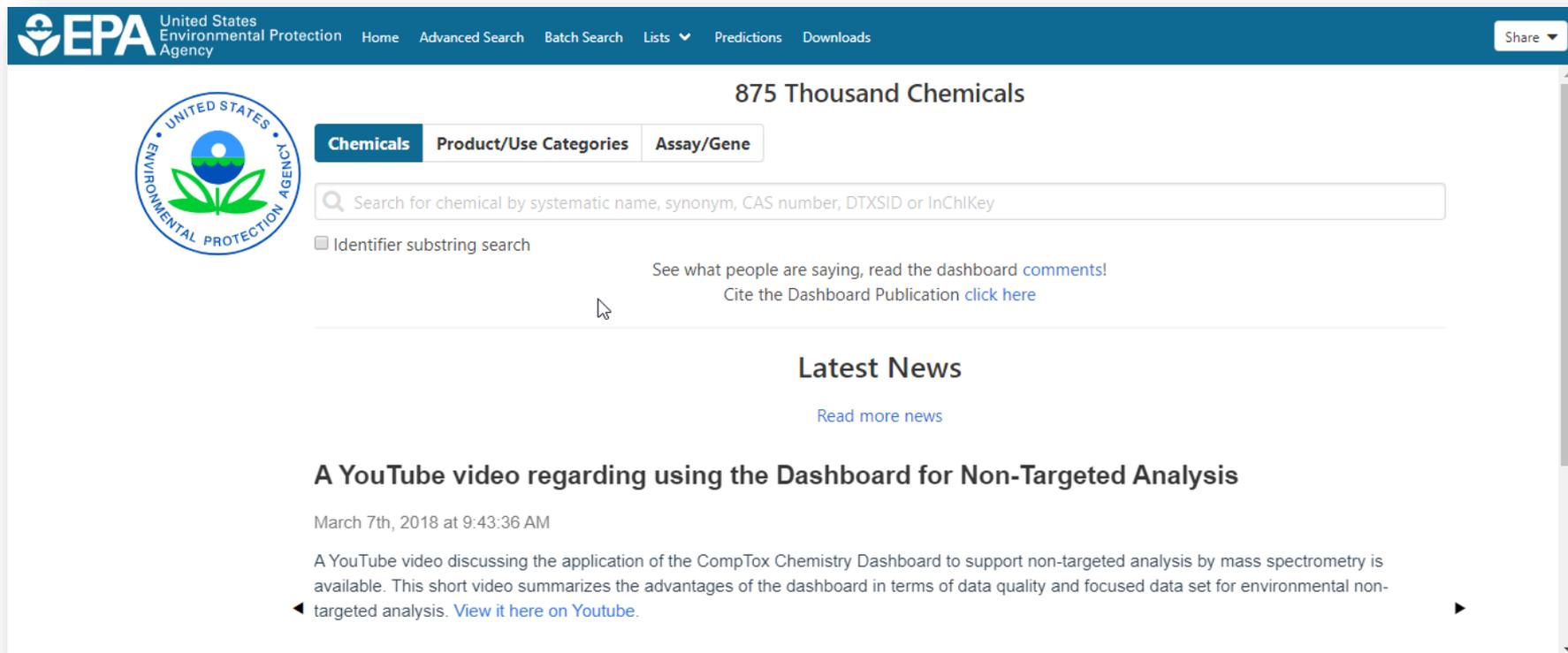
Freely available online tools for communicating chemistry through a social media

Real-time prediction of physicochemical & toxicological endpoints using the web-based CompTox Chemistry Dashboard

+168

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

My primary project at present...



The screenshot shows the EPA CompTox Chemistry Dashboard. At the top, the EPA logo and navigation menu are visible. The main heading is "875 Thousand Chemicals". Below this, there are three tabs: "Chemicals", "Product/Use Categories", and "Assay/Gene". A search bar is present with the placeholder text "Search for chemical by systematic name, synonym, CAS number, DTXSID or InChIKey". There is a checkbox for "Identifier substring search". Below the search bar, there are links for "See what people are saying, read the dashboard comments!" and "Cite the Dashboard Publication click here". The "Latest 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

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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

Identifier substring search

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

Latest News

[Read more news](#)

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

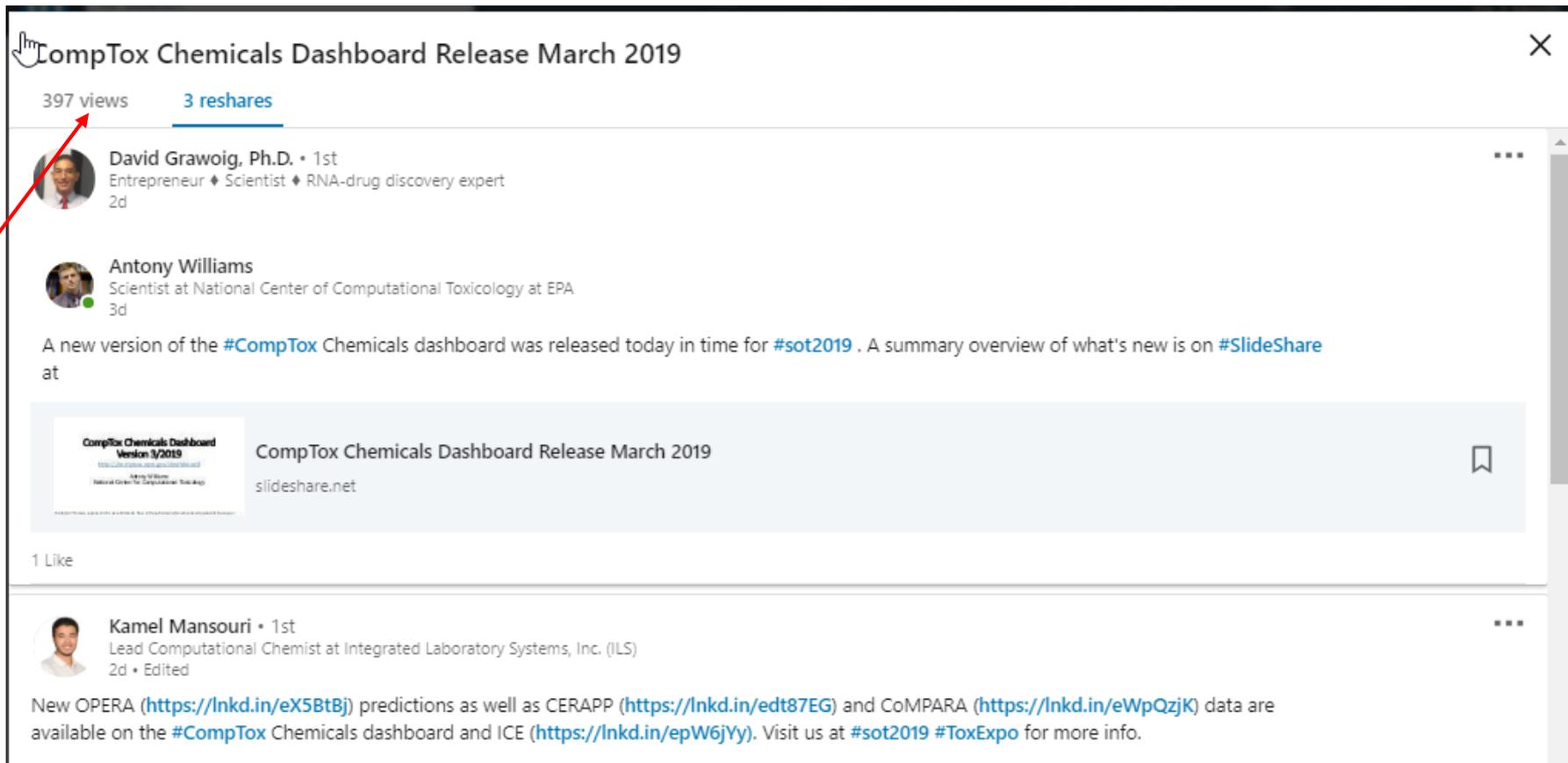
Feb 4, 2019 • ALTEX-Alternatives to animal experimentation

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 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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You worked with Katie in the same group

Position at the time

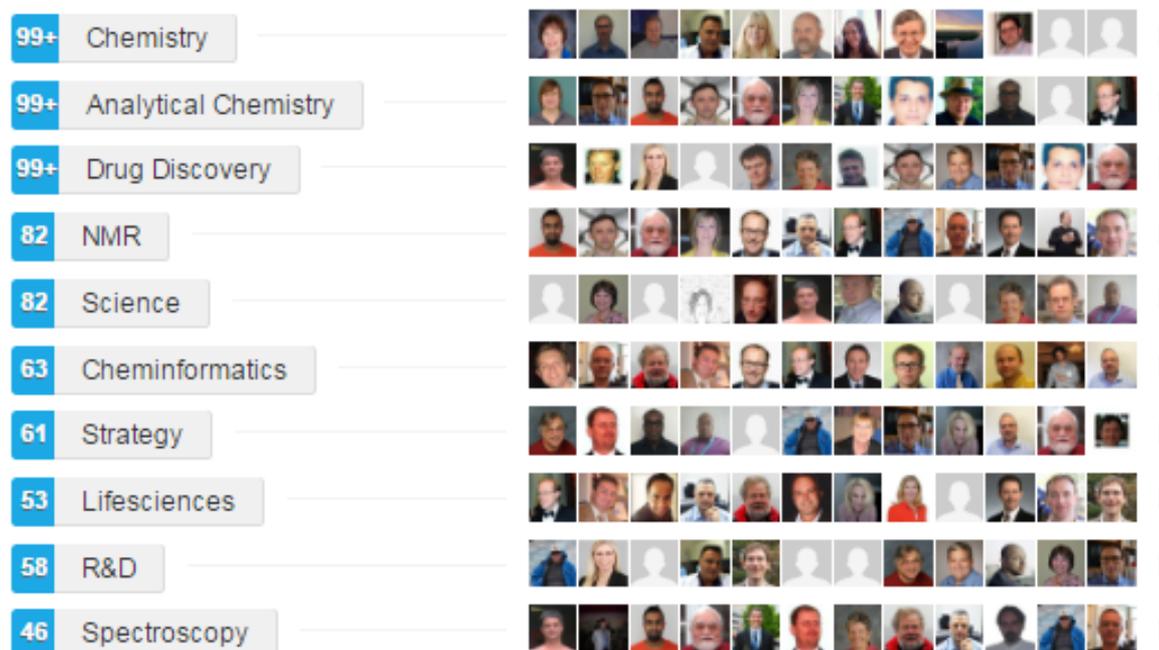
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- Select your position at the time
- Cheminformatician ORCID: 0000-0002-2668-4821 at US Environmental Protection Agency (EPA), National Center for Computational Toxicology**
- President at ChemConnector
- Vice President of Strategic Development, eScience at Royal Society of Chemistry
- Chair at ACS Division of Chemical Information
- Chair-Elect (2012) at ACS Division of Chemical Information
- President at ChemZoo
- Chief Science Officer at Advanced Chemistry Development
- Business Development and Marketing Manager at Advanced Chemistry Development
- VP of Scientific Development and Marketing at Advanced Chemistry Development
- Senior Product Manager at Advanced Chemistry Development
- NMR Technology Leader at Eastman Kodak Company
- NMR Facility Director at Ottawa University
- Postdoctoral Fellow at National Research Council, Canada
- Student at University of London (Ph D)
- Student at University of Liverpool (B Sc Hons I)

Ask for “Endorsements”,

Skills & Endorsements

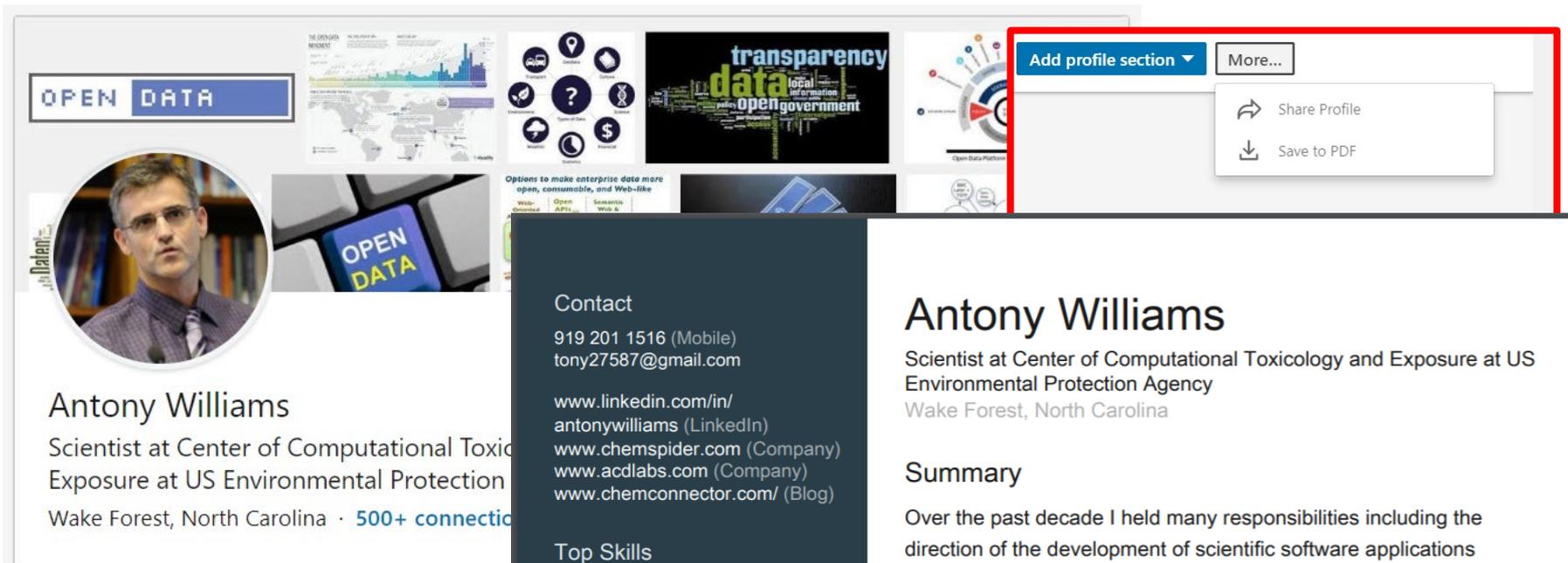
Top Skills



Antony also knows about...



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Antony Williams

Scientist at Center of Computational Toxicology and Exposure at US Environmental Protection Agency
Wake Forest, North Carolina · 500+ connections

Contact

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tony27587@gmail.com

www.linkedin.com/in/antonywilliams (LinkedIn)
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Top Skills

Chemistry
Analytical Chemistry
Drug Discovery

Languages

English

Certifications

Verified Peer Reviewer

Honors-Awards

North Carolina ACS Distinguished Lecturer of the Year 2016

Antony Williams

Scientist at Center of Computational Toxicology and Exposure at US Environmental Protection Agency
Wake Forest, North Carolina

Summary

Over the past decade I held many responsibilities including the direction of the development of scientific software applications for spectroscopy and general chemistry, directing marketing efforts, sales and business development collaborations for the company. Eight years experience of analytical laboratory leadership and management. Experienced in experimental techniques, implementation of new NMR technologies, walk-up facility management, research and development, manufacturing support and teaching. Ability to provide situation analysis, creative solutions and establish good working relationships. Prolific author with over a hundred and fifty peer-reviewed scientific publications, 3 patents and many public presentations.

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 Raleigh-Durham, North Carolina Area, North Carolina, United States

 www.chemconnector.com

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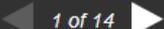
Profile Building, Research Sharing and Data Proliferation using Social Media Tools for Scientists






Antony Williams
US EPA Center for Computational Toxicology and Exposure

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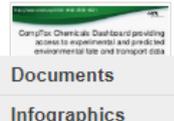
NSF EPSCoR: Profile building, research sharing and data proliferation using social media tools 62

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



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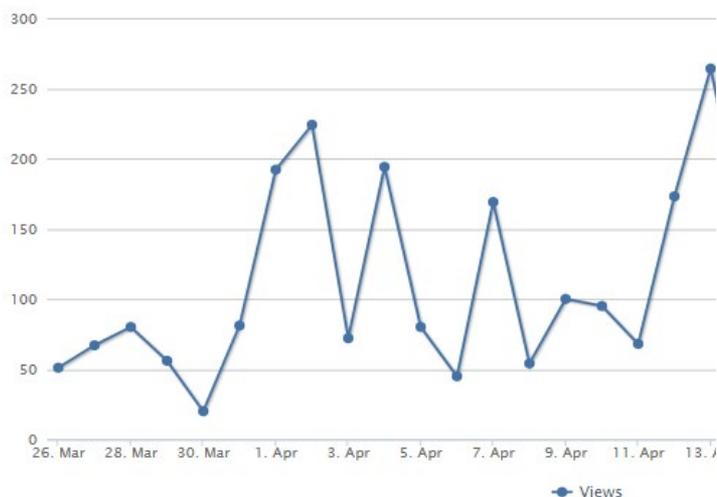
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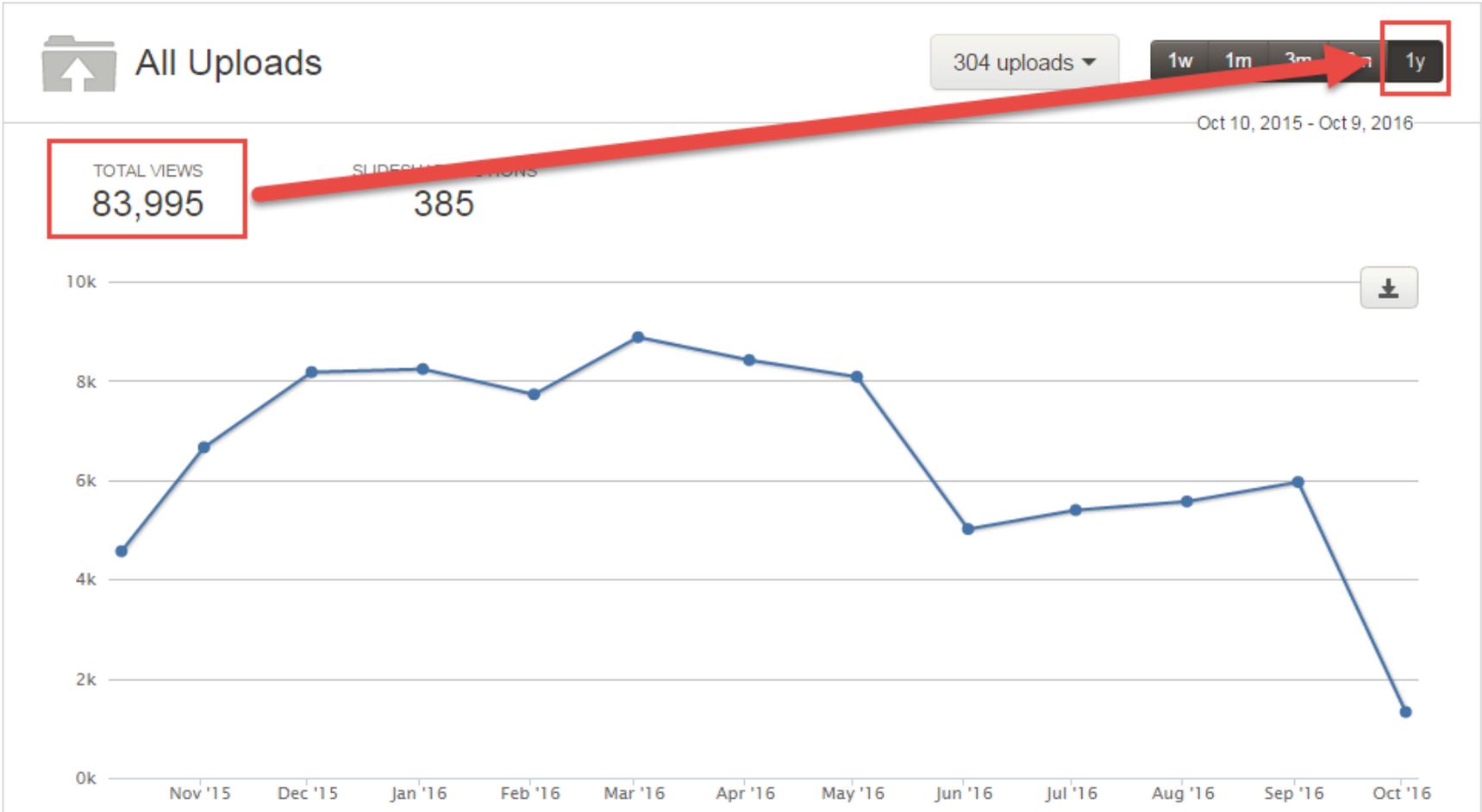
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New developments in delivering public access to data from the National Center for Computational Toxicology at the EPA	189
US EPA CompTox Chemistry Dashboard as a source of data to fill data gaps for chemical sources of risk	185
Development of a Tool for Systematic Integration of Traditional and New Approach Methods for Prioritizing Chemical Lists	183

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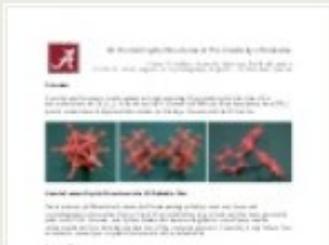
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1	Year	Reference	ARTICLE/CHAPTER	DOI Link
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3	2019	Analytical and bioanalytical chemistry, 1-17	Article	https://doi.org/10.1007/s00216-018-1526-4
4	2018	Analytical and bioanalytical chemistry, 1-14	Article	https://doi.org/10.1007/s00216-018-1435-6
5	2018	Journal of cheminformatics 10 (1), 10	Article	https://doi.org/10.1186/s13321-018-0263-1
6	2018	Journal of cheminformatics 10 (1), 45	Article	https://doi.org/10.1186/s13321-018-0299-2
7	2018	Environmental Science and Technology	Article	https://doi.org/10.1021/acs.est.8b04587
8	2018	Science of The Total Environment 636, 901-909	Article	https://doi.org/10.1016/j.scitotenv.2018.04.266
9	2018	SCIENTIFIC DATA 5:180125	Article	https://doi.org/10.1038/sdata.2018.125
10	2018	Talanta 182, 371-379	Article	https://doi.org/10.1016/j.talanta.2018.01.022
11	2018	Environmental Pollution 234, 297-306	Article	https://doi.org/10.1016/j.envpol.2017.11.033
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
15	2018	Magn Reson Chem. 2018;56:703-715	Article	https://doi.org/10.1002/mrc.4737
16	2018	ACS Sustainable Chemistry & Engineering 6 (2), 2344-2352	Article	https://doi.org/10.1021/acssuschemeng.7b03795
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Introduction

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I am presently a Computational Chemist at the Center for Computational Toxicology and Exposure 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.

Skills and expertise (29)

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Position

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**National Center for Computational
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Lab head



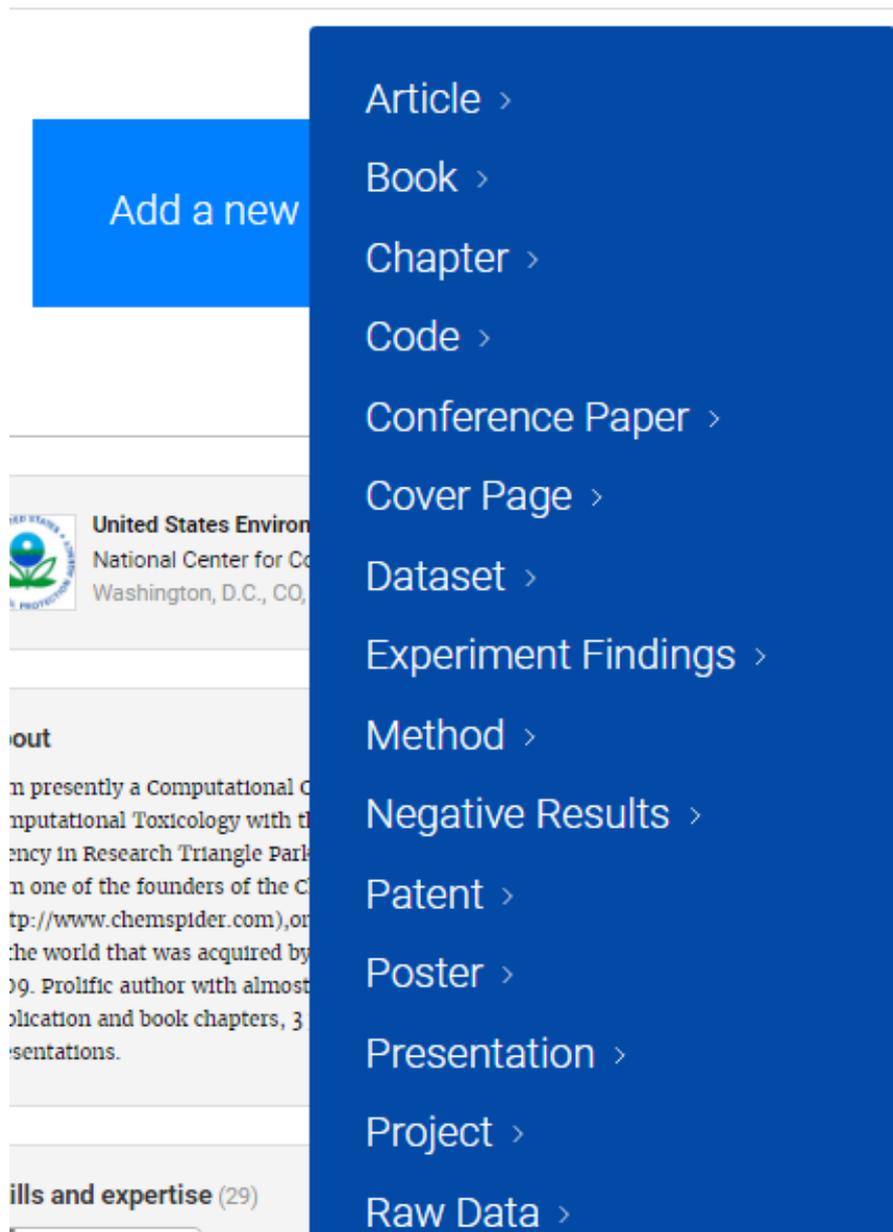
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n presently a Computational Computational Toxicology with the Agency in Research Triangle Park n one of the founders of the Center for Computational Toxicology (<http://www.chemspider.com>), or the world that was acquired by 09. Prolific author with almost 100 publications and book chapters, 3 presentations.

Skills and expertise (29)



Project

The CompTox Chemicals Dashboard

 Antony John Williams ·  Christopher M Grulke ·  Mansouri Ka

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

Date: 30 March 2016

Lab: [Russell Scott Thomas's Lab](#)



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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 the 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

 [comptox_release_notes.pdf](#) · 48.41 KB

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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

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Article Dec 2018

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

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Presentation: The EPA iCSS Chemistry Dashboard to Support Compound Identification Using High Resolution Mass Spectrometry Data
Antony John Williams
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analysis using high throughput
Toxicogenomics (HTT) chemical screening data
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Efforts in ENACT
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Integrating Eawag, LCSB, MetFrag
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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

Co-workers & collaborators



Chris Grulke



Valery Tkachenko



Andrew McEachran

ORISE Postdoctoral Fellow
Research Triangle Park, NC



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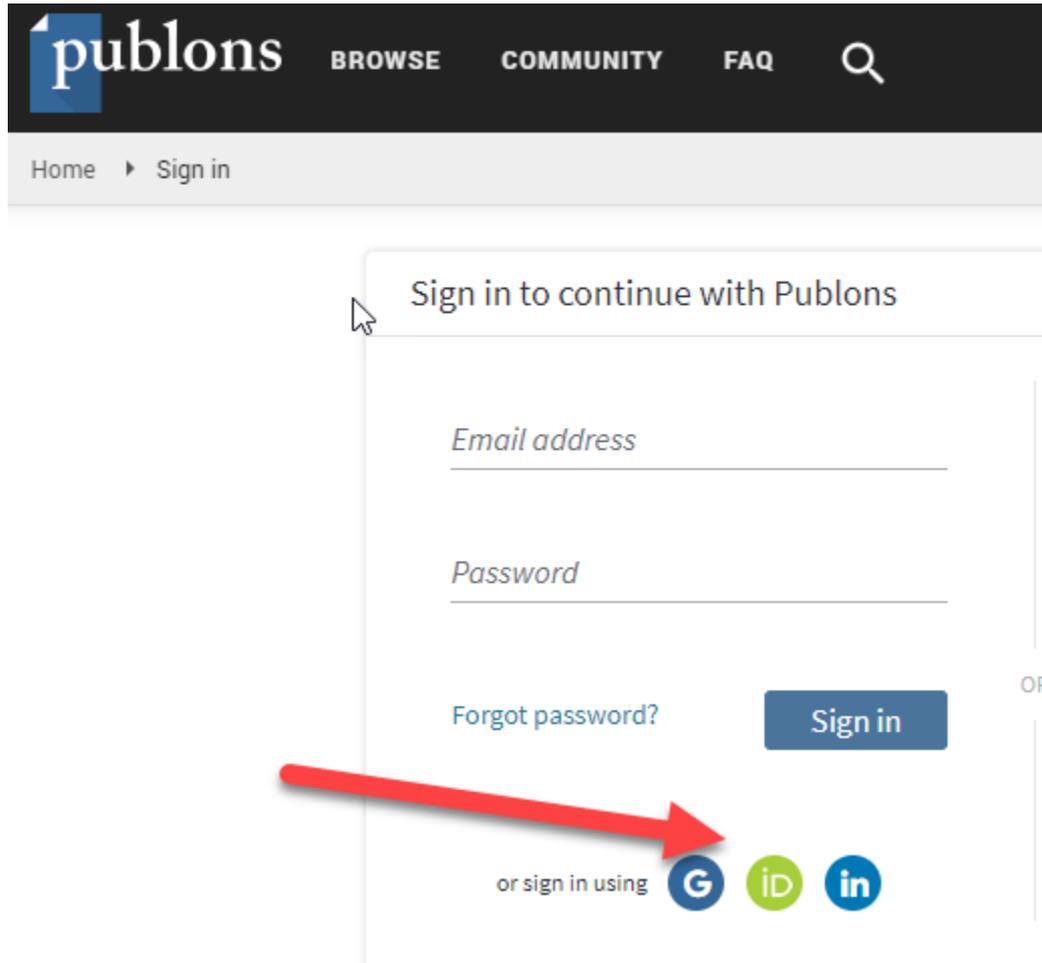
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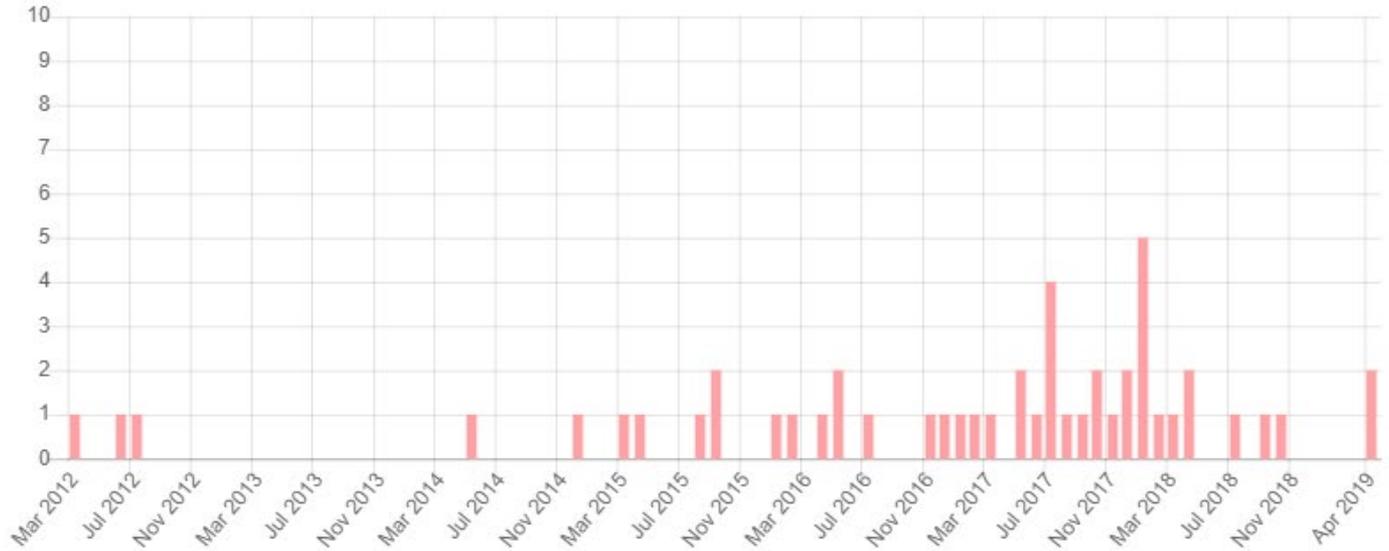
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Identifying known unknowns using the US EPA's CompTox Chemistry Dashboard

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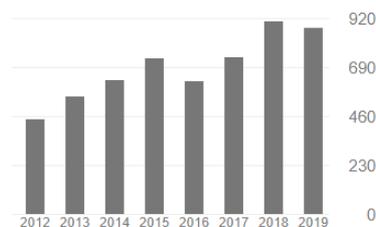
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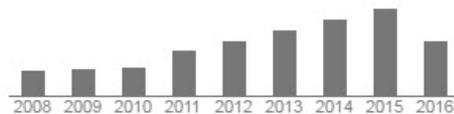
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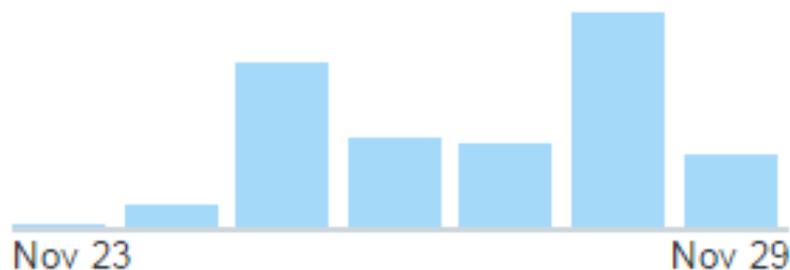
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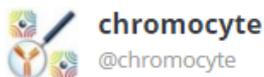
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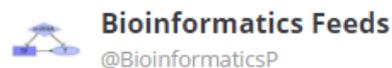
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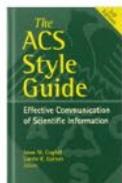
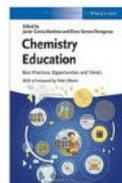
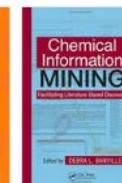
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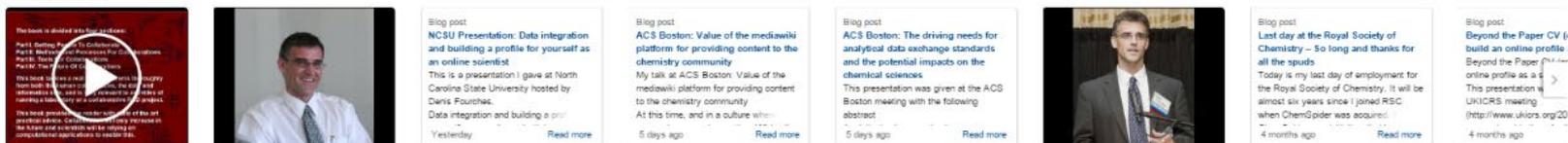
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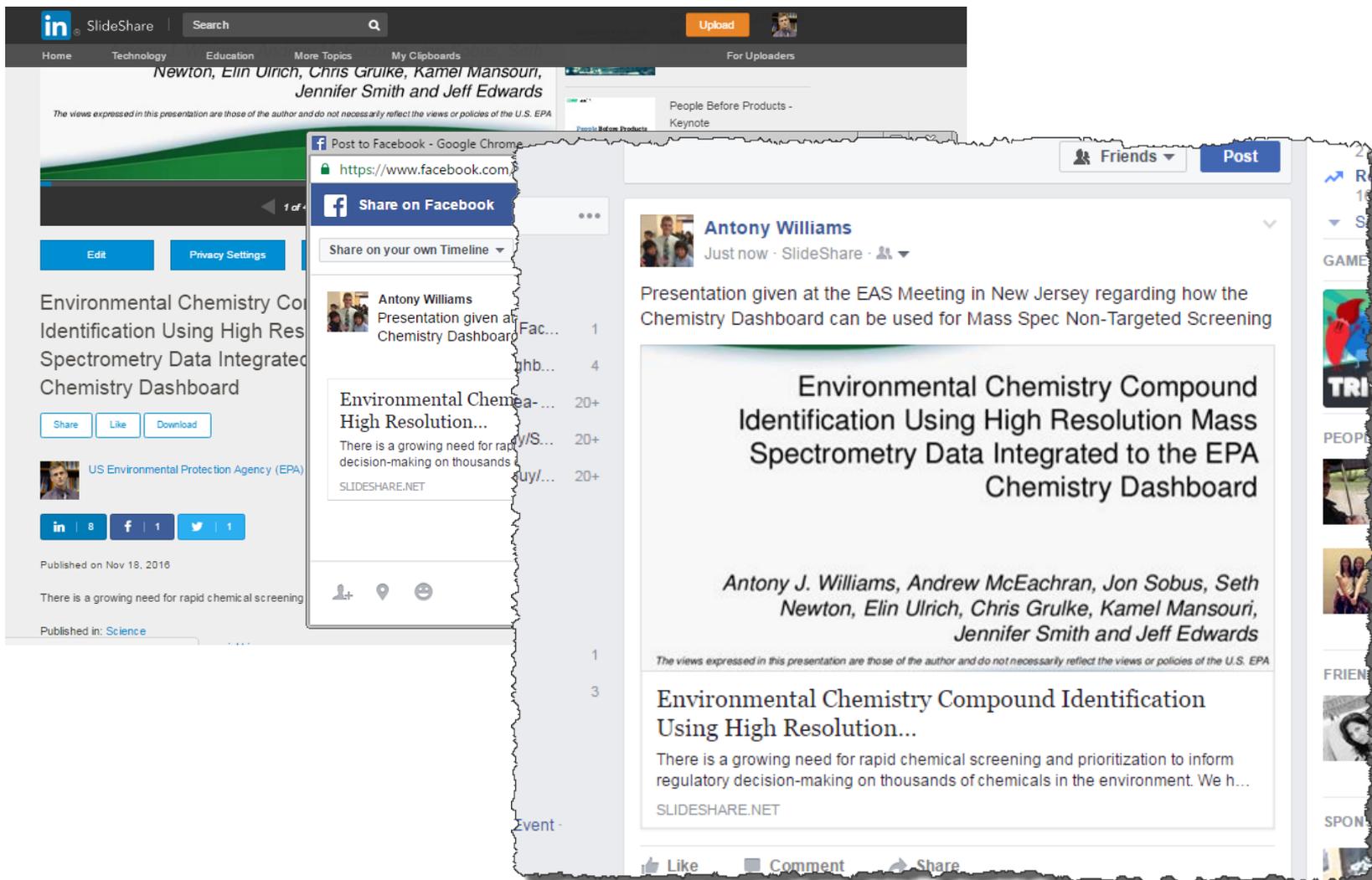
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PRESENTATION ACS SPRING 2018: Structure identification by Mass Spectrometry Non-Targeted Analysis using the US EPA's CompTox Chemistry Dashboard

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.

<https://doi.org/10.6084/m9.figshare.6030893.v1>

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

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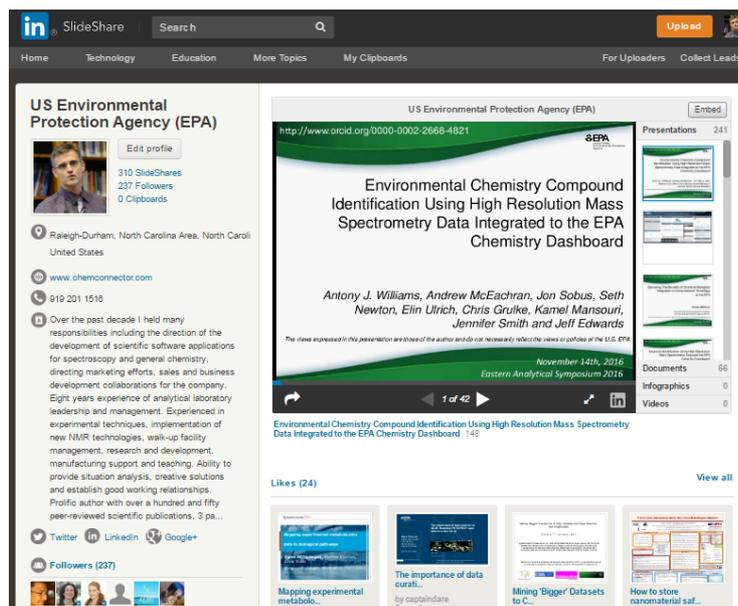
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...choose **two or three** social-media platforms, invest the time to get them set up, and then spend perhaps **two hours a month** keeping them current. If nothing else, he says, build a **LinkedIn** profile as an online CV, claim and update an **ORCID ID**, and log peer-review activities on **Publons.com**.

...a research paper is itself the end product of an extraordinary investment of time and energy. It takes thousands of hours of research, data analysis, writing and peer review, he says. “**Shouldn't you** put at least 10 to 20 hours of work into making sure that you can **get the message out to relevant people?**”

Various Versions of This Talk

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The image shows a screenshot of 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 information for Antony Williams, including his location (Raleigh-Durham, North Carolina Area), website (www.chemconnector.com), and a bio. Below the bio are social media links for Twitter, LinkedIn, and Google+. The profile also shows a list of presentations, with the top one being "Environmental Chemistry Compound Identification Using High Resolution Mass Spectrometry Data Integrated to the EPA Chemistry Dashboard" by Antony J. Williams and others. The slide itself is titled "Environmental Chemistry Compound Identification Using High Resolution Mass Spectrometry Data Integrated to the EPA Chemistry Dashboard" and lists the authors: Antony J. Williams, Andrew McEachran, Jon Sobus, Seth Newton, Elin Ulrich, Chris Grukke, Kamel Mansouri, Jennifer Smith, and Jeff Edwards. The slide is dated November 14th, 2016, and was presented at the Eastern Analytical Symposium 2016.

Email: williams.antony@epa.gov