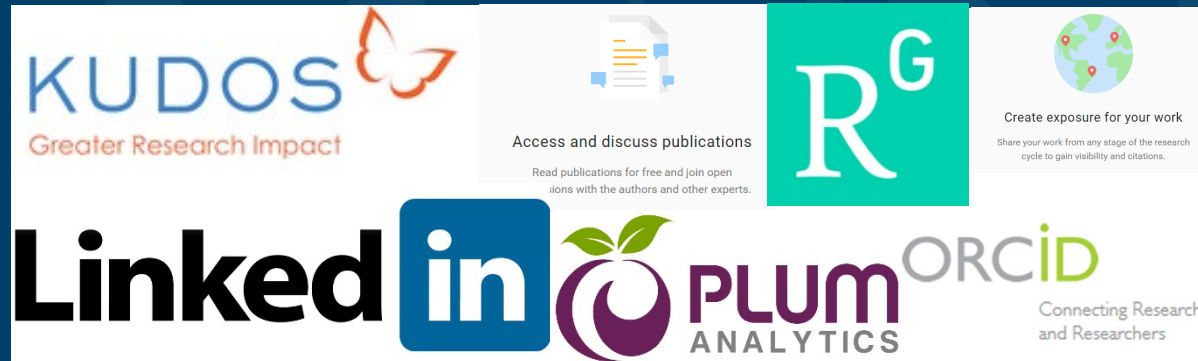


# Profile Building, Research Sharing and Data Proliferation using Social Media Tools for Scientists



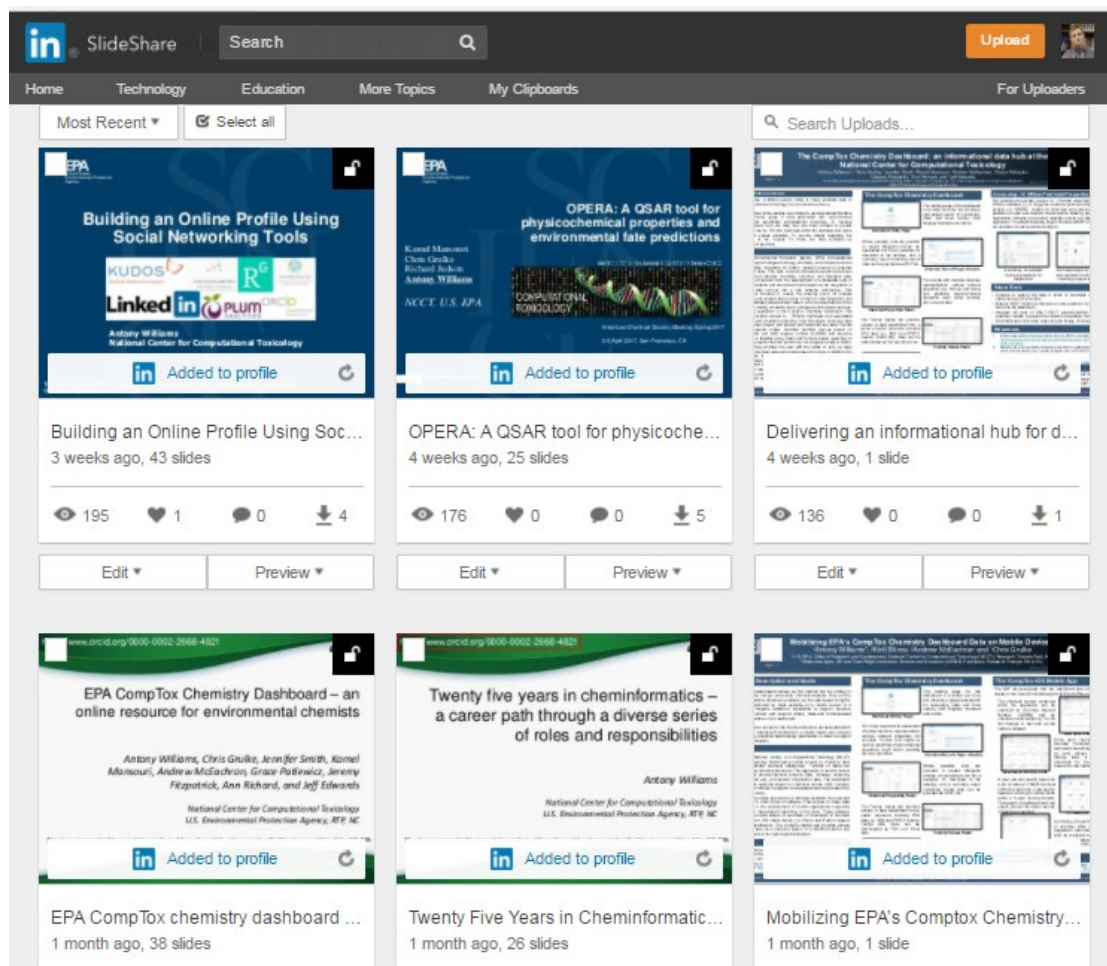
**Antony Williams**  
**National Center for Computational Toxicology**

# Feel free to take notes but..

- All slides will be made available later
- Contact me directly if I can help –  
[williams.antony@epa.gov](mailto:williams.antony@epa.gov)

# Various Versions of This Talk

[www.slideshare.net/AntonyWilliams](http://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 related to EPA initiatives, computational toxicology tools like OPERA and the CompTox Chemistry Dashboard, and professional development topics.

# 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 <sup>1</sup>, Lou Peck <sup>2</sup>, Sean Ekins <sup>3</sup>

<sup>1</sup>National Center for Computational Toxicology, Environmental Protection Agency, Durham, NC, 27711, USA

<sup>2</sup>Lou Peck Consulting, Swansea, SA4 3JQ, UK

<sup>3</sup>Collaborations 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
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# ORCID – The Scientists SSN

ORCID

Connecting Research  
and Researchers

---

**Antony Williams**

**ORCID ID**



[orcid.org/0000-0002-2668-4821](https://orcid.org/0000-0002-2668-4821)



# What's the value of ORCID?

- ORCIDs are now expected for many publications

 Antony J. Williams <sup>1</sup>, Lou Peck <sup>2</sup>, Sean Ekins <sup>3</sup>

- 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



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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## Antony John Williams, 0000-0002-2668-4821 - Google Scholar Citations

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## Antony Williams - Academic Karma



[academickarma.org/0000-0002-2668-4821](https://academickarma.org/0000-0002-2668-4821) ▼


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


computer\_assisted\_structure\_elucidation. cheminformatics. systematic\_naming. open\_data.

# Use ORCID on all products

- Use your ORCID on everything you produce that will be indexed:
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  - Posters
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**Antony John Williams, 0000-0002-2668-4821** 

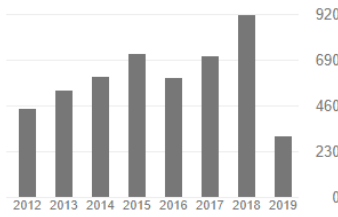
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<input type="checkbox"/> <a href="#">Online chemical modeling environment (OCHEM): web platform for data storage, model development and publishing of chemical information</a> I Sushko, S Novotarskyi, R Körner, AK Pandey, M Rupp, W Teetz, ...	214	2011

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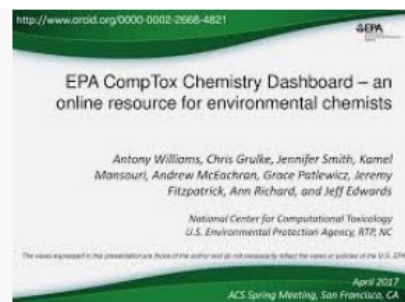


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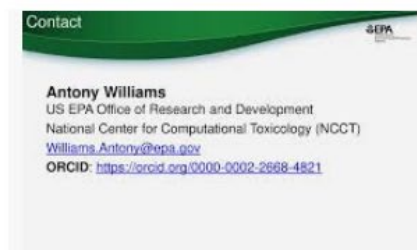
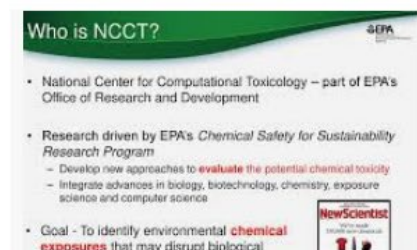
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promise of a chemistry data repository ...  
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ChemConnector on Twitter: "First talk ...  
twitter.com



# 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**







# My primary project at present...



United States  
Environmental Protection  
Agency

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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**  
Version 3/2019  
[https://compd.in/compd3/2019](#)  
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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Scientist in the National Center of Computational T

2

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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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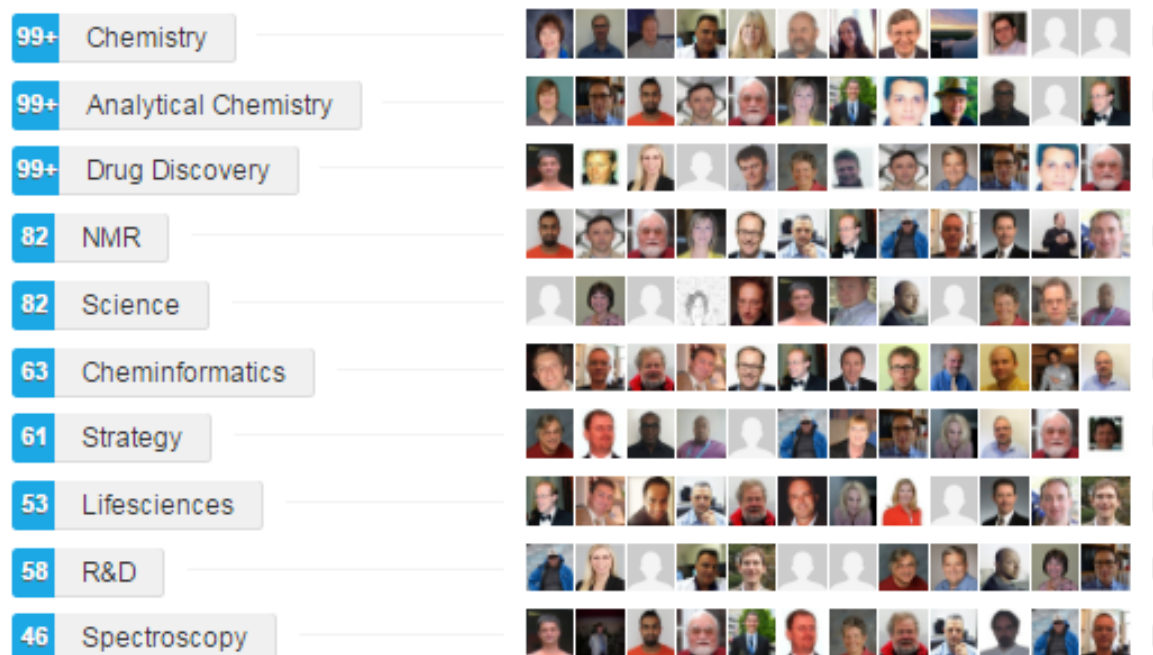
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## Skills & Endorsements

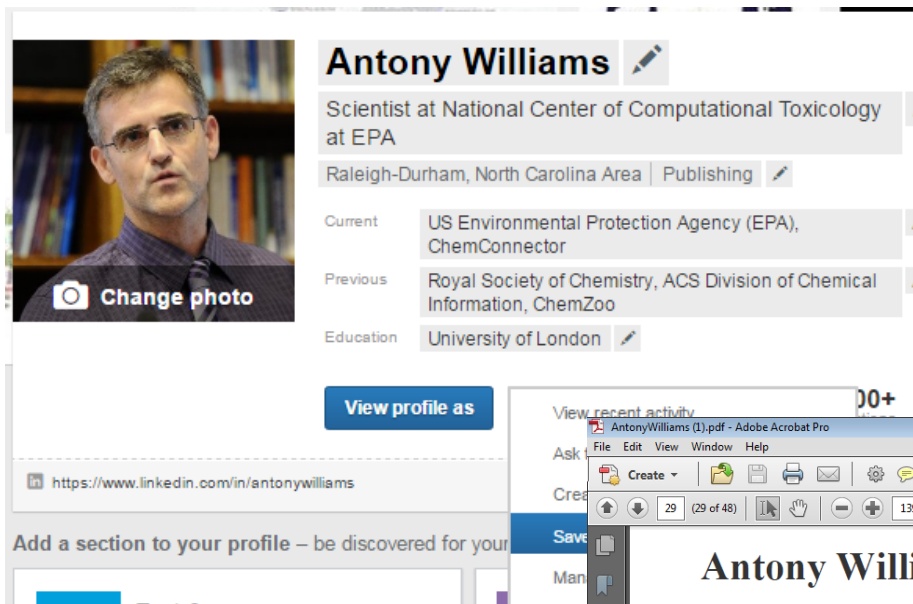
### Top Skills




### Antony also knows about...




# Instant Summary as a PDF




**Antony Williams** 

Scientist at National Center of Computational Toxicology at EPA

Raleigh-Durham, North Carolina Area | Publishing 

Current US Environmental Protection Agency (EPA), ChemConnector

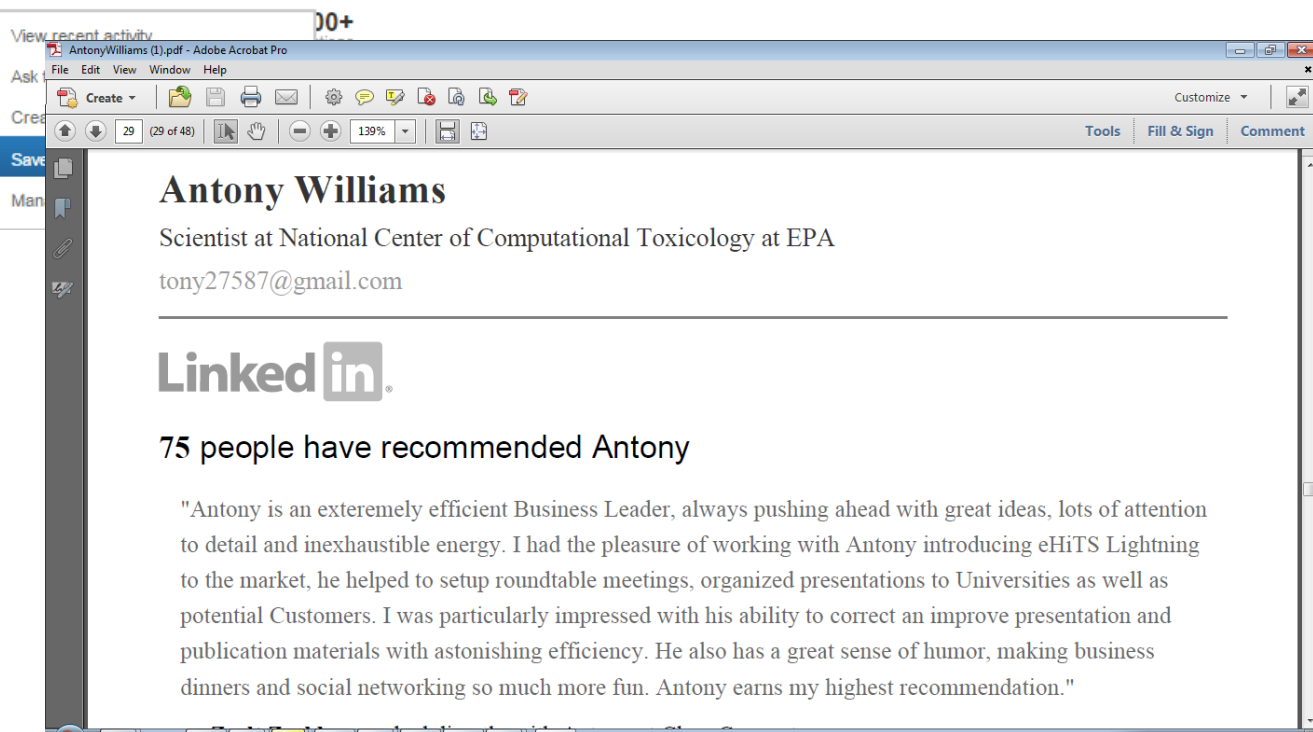
Previous Royal Society of Chemistry, ACS Division of Chemical Information, ChemZoo

Education University of London 

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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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Over the past decade I held many responsibilities including the direction of the development of scientific software applications for spectroscopy and general chemistry, directing marketing efforts, sales and business development collaborations for the company. Eight years experience of analytical laboratory leadership and management. Experienced in experimental techniques, implementation of new NMR technologies, walk-up facility management, research and development,

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

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



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

Antony Williams<sup>1</sup>, George Helman<sup>2</sup>, Jeff Edwards<sup>1</sup>, Jeremy Dunne<sup>1</sup>,  
Imran Shah<sup>1</sup> and Grace Patlewicz<sup>1</sup>

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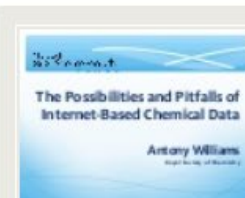
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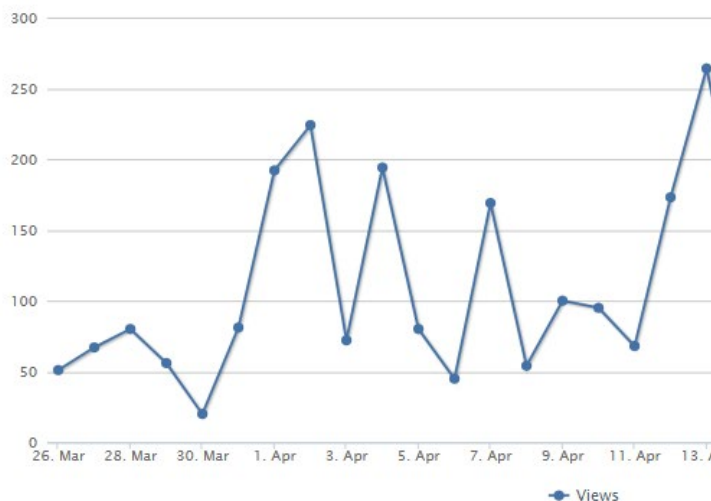
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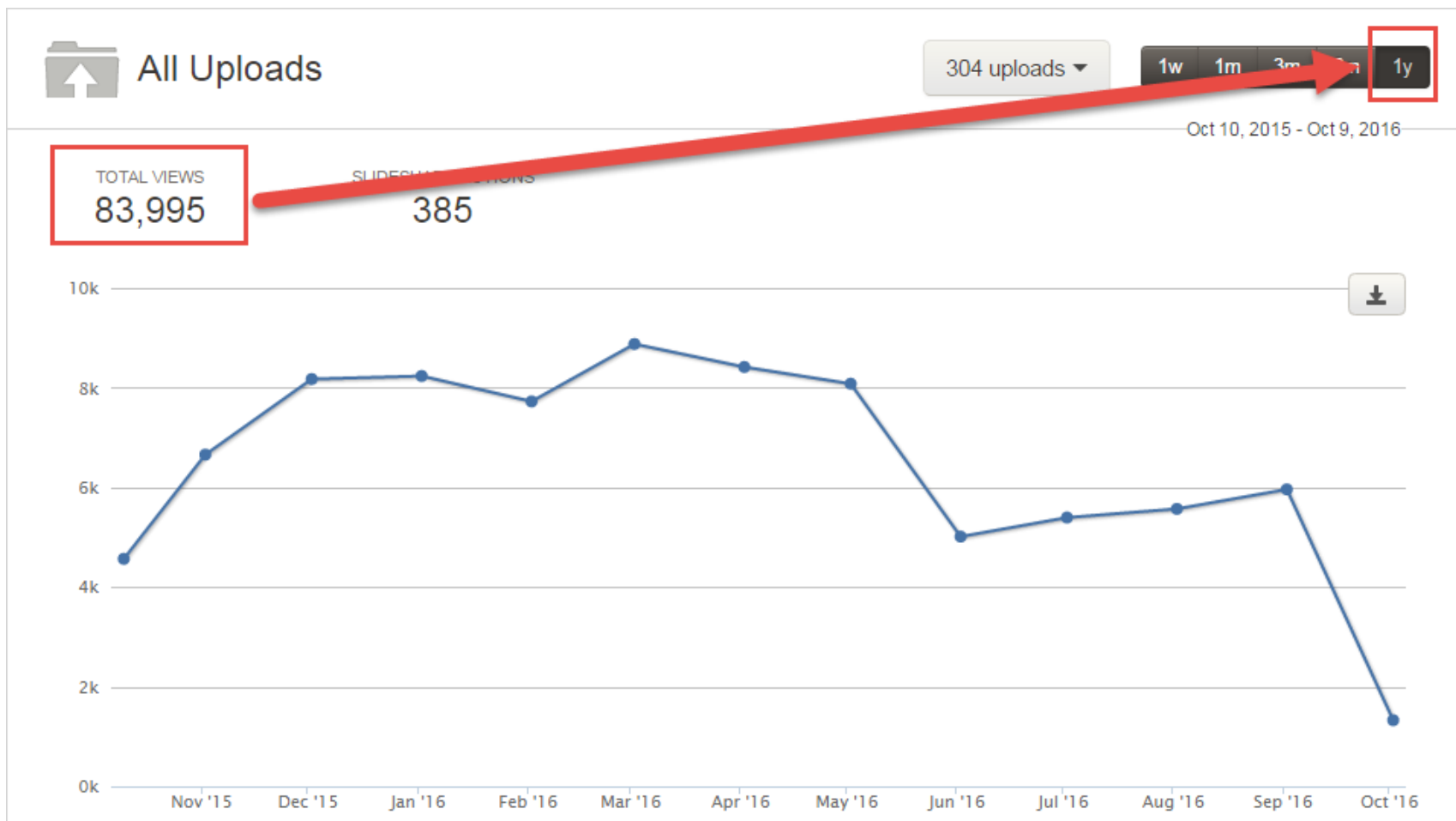
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New developments in delivering public access to data from the National Center for Computational Toxicology at the EPA	189
US EPA CompTox Chemistry Dashboard as a source of data to fill data gaps for chemical sources of risk	185
Development of a Tool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

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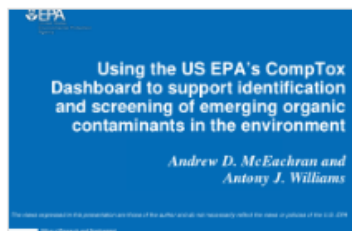
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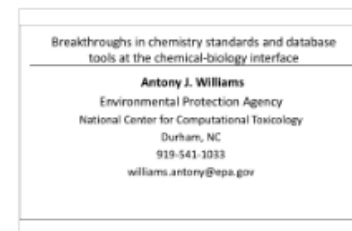
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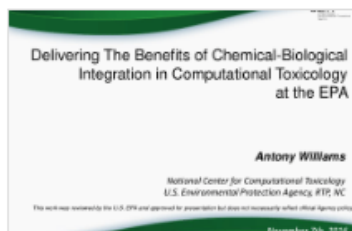
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Antony Williams ▾ 30/05/2018



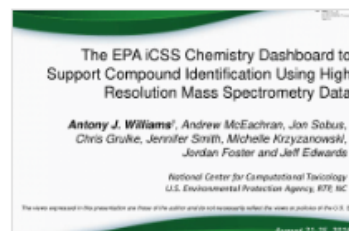
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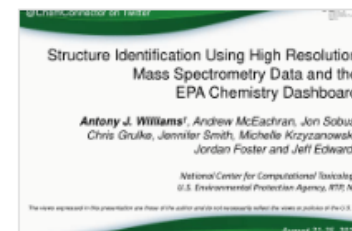
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# Including all Posters... everything gets DOI'd

## 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](mailto:williams.antony@epa.gov) | 919-541-1033

### Automated Analysis Using KNIME

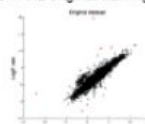
The manual investigation of the data allowed us to develop a KNIME<sup>3</sup> workflow for automated processing. This workflow was derived from earlier work by Mansouri et. al.<sup>4</sup> and is represented in the figure below as a series of blocks representing, for example:

- 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

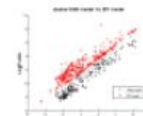


### Model Performance

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

Poster posted on 24.07.2017, 11:18 by Kamel Mansouri, Ann M. Richard, Chris Grulke, 0000-0002-2668-4821 0000-0003-2116-2300 Antony Williams

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Mansouri, Kamel; Richard, Ann M.; Grulke, Chris; 0000-0002-2668-4821; 0000-0003-2116-2300;  
Williams, Antony (2017): Influence of data curation on QSAR Modeling – examining issues of quality  
versus quantity of data. figshare. Poster.

---

<https://doi.org/10.23645/epacomptox.5176573.v1>

---



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1	Year	Reference	ARTICLE/CHAPTER	DOI Link
2	2019	Environmental health perspectives 127 (01), 014501	Article	<a href="https://doi.org/10.1289/EHP4555">https://doi.org/10.1289/EHP4555</a>
3	2019	Analytical and bioanalytical chemistry, 1-17	Article	<a href="https://doi.org/10.1007/s00216-018-1526-4">https://doi.org/10.1007/s00216-018-1526-4</a>
4	2018	Analytical and bioanalytical chemistry, 1-14	Article	<a href="https://doi.org/10.1007/s00216-018-1435-6">https://doi.org/10.1007/s00216-018-1435-6</a>
5	2018	Journal of cheminformatics 10 (1), 10	Article	<a href="https://doi.org/10.1186/s13321-018-0263-1">https://doi.org/10.1186/s13321-018-0263-1</a>
6	2018	Journal of cheminformatics 10 (1), 45	Article	<a href="https://doi.org/10.1186/s13321-018-0299-2">https://doi.org/10.1186/s13321-018-0299-2</a>
7	2018	Environmental Science and Technology	Article	<a href="https://doi.org/10.1021/acs.est.8b04587">https://doi.org/10.1021/acs.est.8b04587</a>
8	2018	Science of The Total Environment 636, 901-909	Article	<a href="https://doi.org/10.1016/j.scitotenv.2018.04.266">https://doi.org/10.1016/j.scitotenv.2018.04.266</a>
9	2018	SCIENTIFIC DATA 5:180125	Article	<a href="https://doi.org/10.1038/sdata.2018.125">https://doi.org/10.1038/sdata.2018.125</a>
10	2018	Talanta 182, 371-379	Article	<a href="https://doi.org/10.1016/j.talanta.2018.01.022">https://doi.org/10.1016/j.talanta.2018.01.022</a>
11	2018	Environmental Pollution 234, 297-306	Article	<a href="https://doi.org/10.1016/j.envpol.2017.11.033">https://doi.org/10.1016/j.envpol.2017.11.033</a>
12	2018	Drug discovery today 23 (3), 661-672	Article	<a href="https://doi.org/10.1016/j.drudis.2018.01.018">https://doi.org/10.1016/j.drudis.2018.01.018</a>
13	2018	Computational Toxicology: Risk Assessment for Chemicals, 211-244	Chapter	<a href="https://doi.org/10.1002/9781119282594.ch8">https://doi.org/10.1002/9781119282594.ch8</a>
14	2018	Environmental science & technology 52 (5), 3125-3135	Article	<a href="https://doi.org/10.1021/acs.est.7b04781">https://doi.org/10.1021/acs.est.7b04781</a>
15	2018	Magn Reson Chem. 2018;56:703-715	Article	<a href="https://doi.org/10.1002/mrc.4737">https://doi.org/10.1002/mrc.4737</a>
16	2018	ACS Sustainable Chemistry & Engineering 6 (2), 2344-2352	Article	<a href="https://doi.org/10.1021/acssuschemeng.7b03795">https://doi.org/10.1021/acssuschemeng.7b03795</a>
17	2017	Journal of exposure science & environmental epidemiology. 1	Article	<a href="https://doi.org/10.1038/s41370-017-0012-v">https://doi.org/10.1038/s41370-017-0012-v</a>



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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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**United States  
Environmental Protection  
Agency**



Location  
United States

Department  
National Center for Computational  
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Position  
Computational Chemist

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Lab head



Russell Scott Thomas

Lab members (6)



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## The CompTox Chemicals Dashboard

Antony John Williams · Christopher M Grulke · Mansouri Ka

Goal: The CompTox Chemicals Dashboard is a web-based application that integrates chemistry and biology data of different types including experimental and computational data, in vivo and in vitro toxicity data, real time predictions, and fate and transport 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

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



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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 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 structure types, and 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](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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**Presentation: The EPA iCSS Chemistry Dashboard to Support Compound Identification Using High Resolution Mass Spectrometry Data**

Antony John Williams

File available · Presentation · Aug 2016


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**Article: Encyclopedia of Inorganic and Bioinorganic Chemistry**

Alex M. Clark · Antony J. Williams · Sean Ekins

Article · Sep 2016



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**Sean Ekins**

45.58 · (45)

Collaborations In Chemistry

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**Valery Tkachenko**

19.83 · (27)

The Royal Society of Chemistry

**Did this researcher author this publication with you?**



**Andrey Yerin**

Article: **The Need for Systematic Naming Software Tools for Exchange of Chemical Information**

Antony Williams · Andrey Yerin

Article · Jan 2013

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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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Antony joined the department National Center of Computational Toxicology, 4 months ago

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Supplemental files for "Profiling 58  
Compounds Including Cosmetic-R...

EPA's National Center f... yesterday



PFAS Tiered Testing Strategy  
Reeder Sams, Deputy Director  
National Center for Computational Toxicology  
November 26, 2019

PFAS Tiered Testing Strategy

Reeder Sams 04/03/2019



ToxValDB: Compiling Publicly  
Available In Vivo Toxicity Data  
Richard Judson  
November 26, 2019

ToxValDB: Compiling Publicly  
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Animal Toxicity Studies: Effects and  
Endpoints (Toxicity Reference Dat...

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CODE

CFM-ID generation of CompTox  
Chemicals Dashboard Structures


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Bioactivity exposure ratio (BER) analysis using high throughput  
transcriptomics (HT) chemical screening data  
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November 26, 2019

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Joshua Harrill 21/02/2019



Efforts in ENTACT  
Emma Schymanski  
November 26, 2019

Integrating Eawag, LCSB, MetFrag  
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Emma Schymanski ▾ 21/02/2019

# Supplementary Data Access

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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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### CATEGORIES

- Cheminformatics
- Cheminformatics and Quantitative Structure-Activity Relationships
- Analytical Spectrometry

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Chemistry

Mass Spectrometry

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## Antony Williams

 [0000-0002-2668-4821](#) 



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■ Computational Chemist, National Center for Computational Toxicology, US-EPA ([Chemistry](#))

📍 United States



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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### Co-workers & collaborators



Chris Grulke



Valery Tkachenko



Andrew McEachran

ORISE Postdoctoral Fellow  
Research Triangle Park, NC



Sean Ekins

senior consultant  
Fuquay Varina, NC, USA




Jon Sobus



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## Antony Williams

★ Excellent reviewer

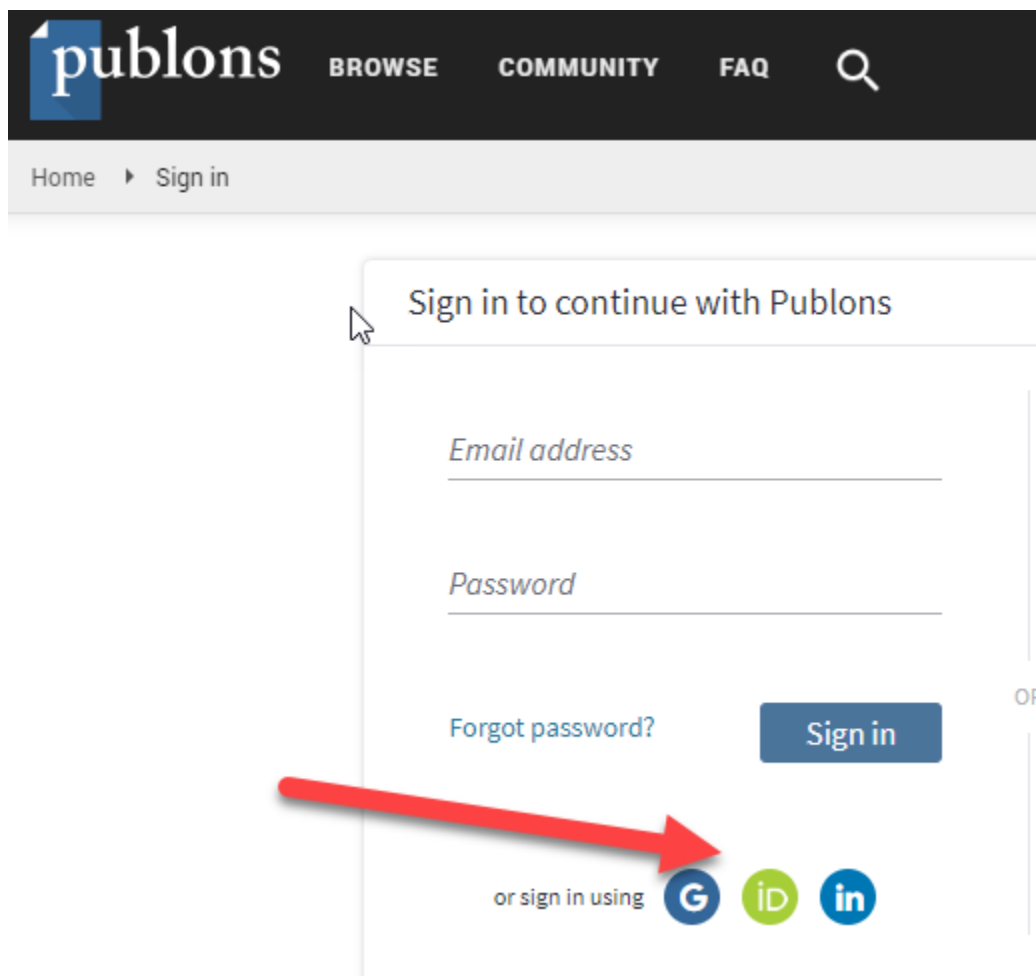
Chemist - National Center for Computational Toxicology, United States Environmental Protection Agency

ORCID: 0000-0002-2668-4821

PUBLICATIONS	TOTAL TIMES CITED	H-INDEX	VERIFIED REVIEWS
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**43** Median: 11  
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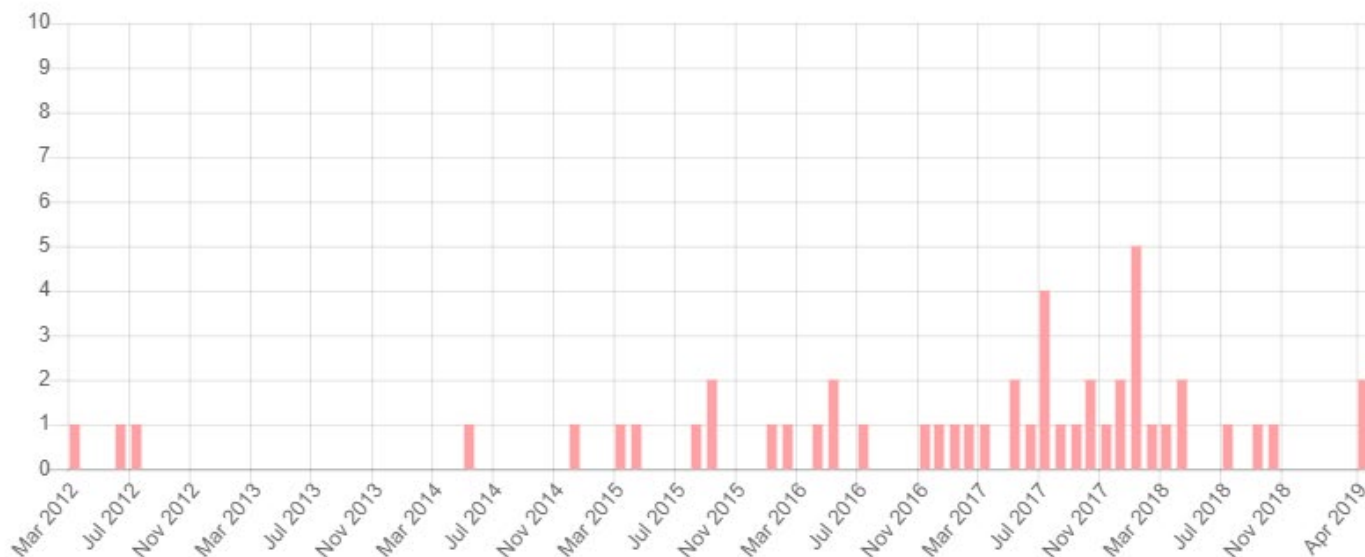
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Month





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US Environmental Protection Agency Computational Chemist

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Determined by Computational and Statistical Analyses

2013 *PLoS ONE*

262      

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Chemistry Data

2015 *J. Med. Chem.*

131      


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## Coauthors

Egon Willighagen

Niklas Blomberg

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# Dispensing Processes Impact Apparent Biological Activity as Determined by Computational and Statistical Analyses

Sean Ekins, Joe Olechno, Antony J. Williams, Alexandre G. de Brevern  
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[Analytical and Bioanalytical Chemistry](#)

..... March 2017, Volume 409, [Issue 7](#), pp 1729-1735

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

Authors

[Authors and affiliations](#)

Andrew D. McEachran , Jon R. Sobus, Antony J. Williams 

Rapid Communication

First Online: [16 December 2016](#)

DOI: [10.1007/s00216-016-0139-z](#)

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Overview of attention for article published in Analytical & Bioanalytical Chemistry, December 2016



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**Andrew McEachran**

@Andrew\_McEach

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29 Mar 2017



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29 Mar 2017



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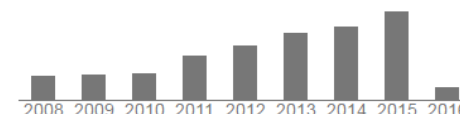
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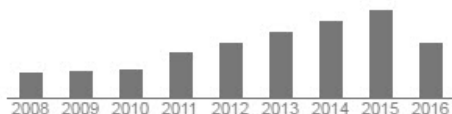
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**Sleep health New South Wales: chronic sleep restriction and daytime sleepiness**

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## Antony J. Williams



### 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.

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

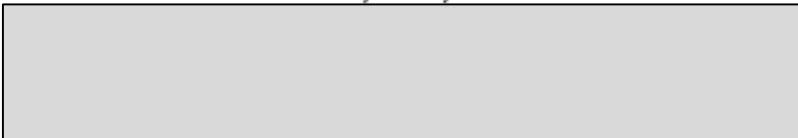
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### Structure identification by Mass Spectrometry Non-Targeted Analysis using the US EPA's CompTox



# But the top of my CV...

ANTONY JOHN WILLIAMS, PhD, FRSC



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

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

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## SUMMARY SCIENTIST, ONLINE CHEMISTRY EVANGELIST AND SENIOR EXECUTIVE

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

# What Next?

## My Recommendations

- Register for an ORCID ID
- **Enhance** your LinkedIn profile
- Use Google Scholar Citations and **curate**
- **Choose:** ResearchGate **or** Academia.edu
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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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