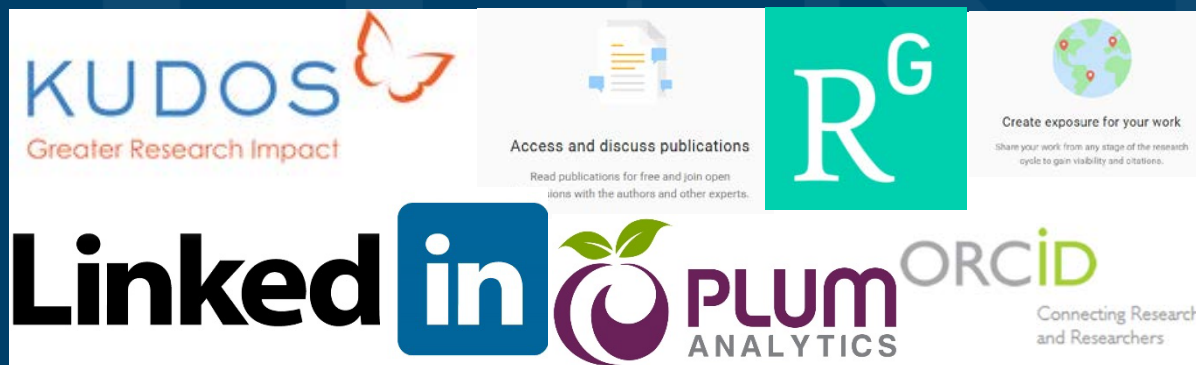


Building an Online Profile Using Social Networking Tools



Antony Williams
National Center for Computational Toxicology

Various Versions of This Talk

www.slideshare.net/AntonyWilliams



The screenshot shows a SlideShare profile for the US Environmental Protection Agency (EPA). The profile includes a header with the EPA logo and name, a search bar, and navigation links. The main content area displays the profile picture, name, location (Raleigh-Durham, North Carolina Area, North Caroli United States), and statistics (310 SlideShares, 237 Followers, 0 Clipboards). A bio section follows, detailing the user's experience in scientific software development and laboratory management. Social media links for Twitter, LinkedIn, and Google+ are provided, along with a 'Followers (237)' section. To the right, a presentation slide is displayed. The slide title is 'Environmental Chemistry Compound Identification Using High Resolution Mass Spectrometry Data Integrated to the EPA Chemistry Dashboard'. The authors listed are Antony J. Williams, Andrew McEachran, Jon Sobus, Seth Newton, Elin Ulrich, Chris Grukke, Kamel Mansouri, Jennifer Smith, and Jeff Edwards. The slide also mentions the Eastern Analytical Symposium 2016 and includes a disclaimer about the views expressed. Below the slide, there is a 'Likes (24)' section with a 'View all' link and a row of four smaller presentation thumbnails.

Email: williams.antony@epa.gov

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....

You Will Choose...

Self-marketing vs. Narcissism

Users, narcissism and control – tracking the impact of scholarly publications in the 21st century





Scientists are Constantly Evaluated Based on “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

Today, Scientists Can Easily Share Their Work...

- Once a scientific work(s) is public...
 - Share
 - Distribute
 - Enhance my connection network
 - “Advertise and market”

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>

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.

The MOST BASIC Career Networking Tool



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 |

View profile as



500+
connections



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



Contact Info

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

Can Also Function as an Electronic CV



Experience

Vice President of Strategic Development, ChemSpider

RSC | Advancing the
Chemical Sciences

Royal Society of Chemistry

May 2009 – Present (4 years 1 month) | Raleigh

As the VP of Strategic Development at RSC I am responsible for the eScience team within the organization. Our primary focus is on the development of cheminformatics solutions to serve the community and to support activities within our publishing business. These include our ChemSpider platform and related projects (e.g. ChemSpider Reactions and SyntheticPages). Our team also supports a number of grant-based projects including the Open PHACTS project (an Innovative Medicines Initiative project providing a semantic web solution to support drug discovery), PharmaSea, a European project to identify new natural products from the ocean and the National Chemical Database Service serving UK academics with a series of commercial databases and services and developing a national repository to host chemistry data.

- 5 projects
- 2 honors and awards
- ▾ 9 recommendations, including:



James Milne

Managing Director, Publishing at Royal S...

Tony is a highly creative and action based individual. His vision for developing innovative products and services make him... [View ↓](#)



David James

Executive Director, Strategic Innovation ...

Antony has extensive experience in leading and managing internationally distributed project teams working on a very broad... [View ↓](#)

[7 more recommendations ↓](#)

Ability to Highlight Projects



Projects

Open PHACTS ➤

Starting March 2012

What is Open PHACTS?

To reduce the barriers to drug discovery in industry, academia and for small businesses, the Open PHACTS consortium is building an Open Pharmacological Space (OPS). This will be a freely available platform, integrating pharmacological data from a variety of information resources and providing tools and services to question this integrated data to support pharmacological... [more](#)

► 9 team members, including:



Antony Williams

VP Strategic Development, Head of ...



Valery Tkachenko

Chief Technology Officer at Royal S...



Lee Harland

CEO SciBite Limited



Paul Groth

Disruptive Technology Director @ Els...

UK National Chemical Database ➤

Starting December 2012

The RSC will be operating the EPSRC National Chemical Database Service from 2013-2017. We intend to build the Service for the future - to develop a chemistry data repository for UK academia, and to build tools, models and services on this data store to increase the value and impact of researchers' funded work. We will continue to develop this data store through the lifetime of the contract period... [more](#)

► 6 team members, including:



Antony Williams

VP Strategic Development, Head of ...



Valery Tkachenko

Chief Technology Officer at Royal S...



Colin Batchelor

Senior Informatics Analyst



--

-

Manage Articles Here Too...

Structural revisions of natural products by Computer-Assisted Structure Elucidation (CASE) systems ➤

Natural Products Reports

July 2010

Computer-Aided Structure Elucidation (CASE) is a scientific area of investigation initiated over forty years ago and on the frontier between organic chemistry, molecular spectroscopy and computer science. As a result of the efforts of many researchers, a series of so-called expert systems (ES) intended for the purpose of molecular structure elucidation from spectral data have been developed.... [more](#)

3 authors



Antony Williams

VP Strategic Development, Head of ...



Mikhail Elyashberg

Senior Researcher & Advanced Che...



Kirill Blinov

Software Developer

Meta-analysis of molecular property patterns and filtering of public datasets of antimalarial “hits” and drugs ➤

Royal Society of Chemistry, Med. Chem. Commun, 2010, 1, 325-330

2010

Neglected infectious diseases such as tuberculosis (TB) and malaria kill millions of people annually and the oral drugs used are subject to resistance requiring the urgent development of new therapeutics. Several groups, including pharmaceutical companies, have made large sets of antimalarial screening hit compounds and the associated bioassay data available for the community to learn from and... [more](#)

2 authors



Antony Williams

VP Strategic Development, Head of ...



Sean Ekins

Founder and CEO at Collaborations ...

Your Postings Get Networked



Antony Williams

Scientist at National Center of Computational Toxicology at EPA

18h

The work done by the EPA to provide access to the Toxcast data for others to use continues to have a major influence. I am working at a great place...

Phenotypic screening of the ToxCast chemical library to classify toxic and therapeutic mechanisms

[nature.com](#) • [Nature Biotechnology](#) | doi:10.1038/nbt.2914

Like • Comment • Share • 4

Notifications

4 people like your update, "The work done by the..." Phenotypic screening of...



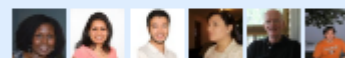
Todor Antonijevic, Heather King, Ellen Berg and Sine ...

2 people like your update, Identification of...



Chantel Nicolas and Dr. Rachelle J. Bienstock

6 people like your update, "Our latest paper..." An automated curation...



Chantel Nicolas, Prachi Pradeep, Kamel Mansouri, M...

4 people like your update, "ON KUDOS: Does data..." <https://goo.gl/hpU181>



Alfred M Ajami, Sine Rosenberg, Esben Jannik Bjerru...



Rima HAJJO
likes your update, "I just added a SlideShare to my..." Automatic vs

It's All Networking, Networking.....

Ask for Recommendations

View profile as

View recent activity

Ask to be recommended

Create profile in another language

Save to PDF

Manage public profile settings

10

Ask your connections to recommend you

1

What do you want to be recommended for?

Scientist in the National Center of Computational T

2

Who do you want to ask?

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

Jeff Edwards X

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

Write your message

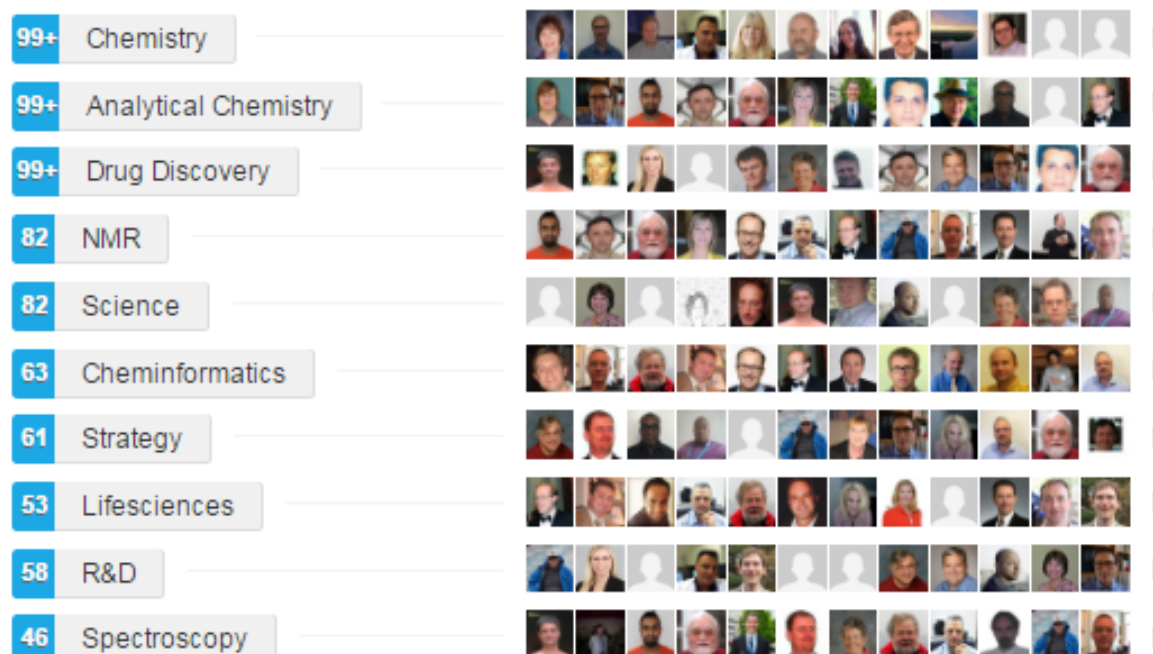
Subject:

Can you recommend me?

Ask for “Endorsements”,

Skills & Endorsements

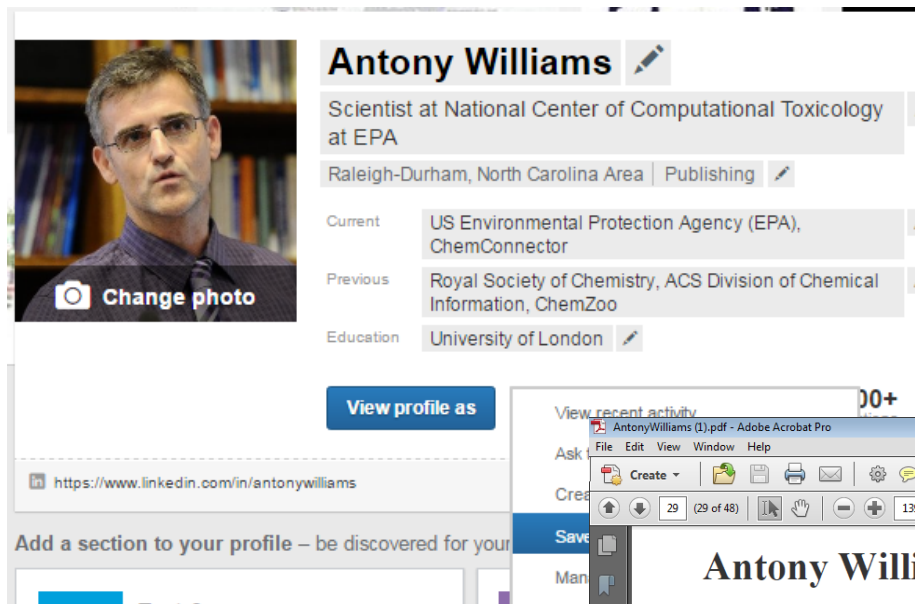
Top Skills



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 ✎

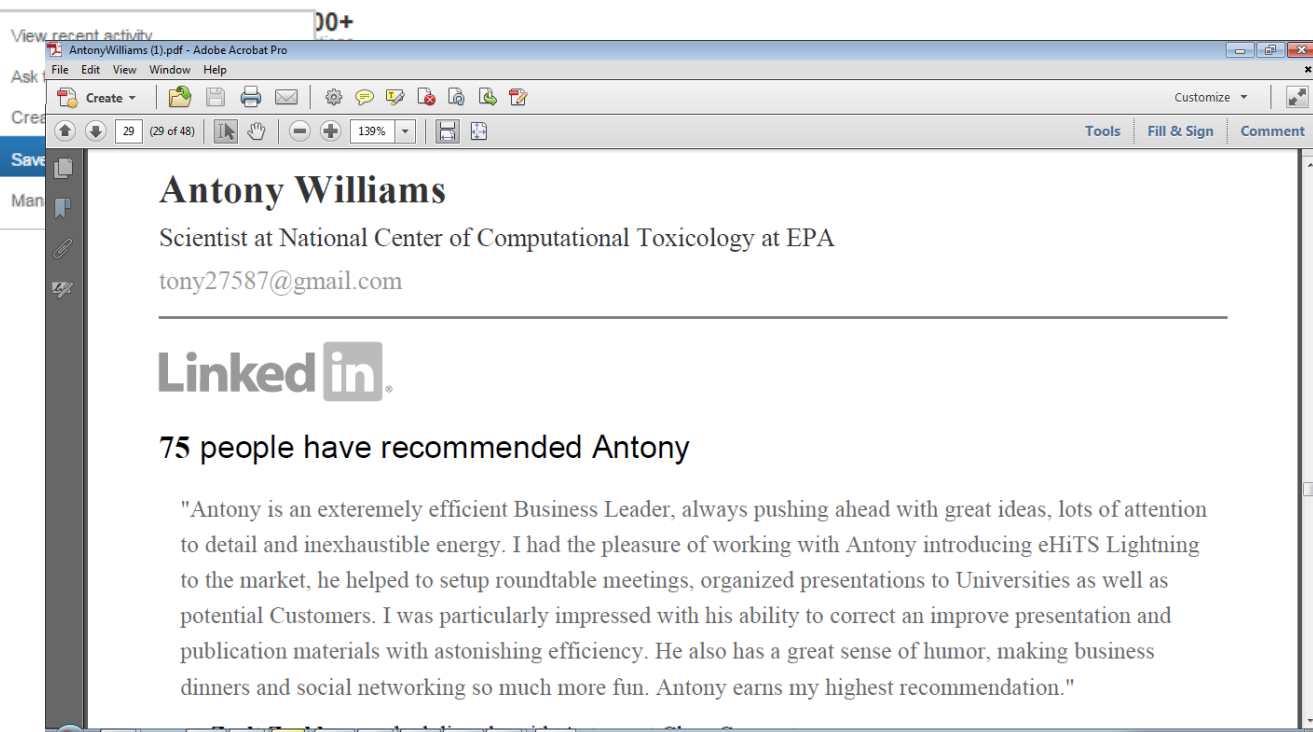
Previous Royal Society of Chemistry, ACS Division of Chemical Information, ChemZoo ✎

Education University of London ✎

[View profile as](#)

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

Add a section to your profile – be discovered for your expertise



View recent activity 00+

AntonyWilliams (1).pdf - Adobe Acrobat Pro

File Edit View Window Help

Create

29 (29 of 48) 139%

Tools Fill & Sign Comment

Antony Williams

Scientist at National Center of Computational Toxicology at EPA

tony27587@gmail.com

LinkedIn

75 people have recommended Antony

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



SlideShare

LinkedIn Acquires Professional Content Sharing Platform SlideShare For \$119M

Login Signup

Home

Collect Leads

US Environmental Protection Agency (EPA)



Follow

304 SlideShares
233 Followers
0 Clipboards

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

www.chemconnector.com

919 201 1516

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

US Environmental Protection Agency (EPA)

Embed

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



Delivering The Benefits of Chemical-Biological Integration in Computational Toxicology at the EPA

Antony Williams[†], Kamel Mansouri, Chris Grulke, Keith Houck, Ann Richard, Jeff Edwards, Matt Martin, John Wambaugh, Grace Patlewicz, Imran Shah, Richard Judson, Kevin Crofton and Russell Thomas

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

This work was reviewed by the U.S. EPA and approved for presentation but does not necessarily reflect official Agency policy.

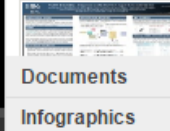
August 21-25, 2016
ACS Fall Meeting, Philadelphia, PA



1 of 34



Presentations 235



Documents 66

Infographics 0

Videos 0

Delivering The Benefits of Chemical-Biological Integration in Computational Toxicology at the EPA 255

Sharing your works online

My Uploads

Analytics

Most Recent ▾

Select all

Search Uploads...

www.orcid.org/0000-0002-2668-4821

Delivering The Benefits of Chemical-Biological Integration in Computational Toxicology at the EPA

Antony Williams[†], Kamel Mansouri, Chris Grulke, Keith Houck, Ann Richard, Jeff Edwards, Matt Martin, John Wambaugh, Grace Patlewicz, Imran Shah, Richard Judson, Kevin Crofton and Russell Thomas

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

Added to profile

Delivering The Benefits of Chemical-...

2 weeks ago, 34 slides

255

1

0

0

Edit ▾

Preview ▾

www.orcid.org/0000-0002-2668-4821

The EPA iCSS Chemistry Dashboard to Support Compound Identification Using High Resolution Mass Spectrometry Data

Antony J. Williams[†], Andrew McEachran, Jon Sobus, Chris Grulke, Jennifer Smith, Michelle Krzyzanowski, Jordan Foster and Jeff Edwards

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

Added to profile

The EPA iCSS Chemistry Dashboard...

2 weeks ago, 40 slides

256

1

0

1

Edit ▾

Preview ▾

ID:0000-0002-2668-4821

Keyboard
How One Monkey on a Typewriter Made a Difference to Online Chemistry

Antony Williams

Added to profile

How One Monkey on a Typewriter M...

3 weeks ago, 80 slides

322

0

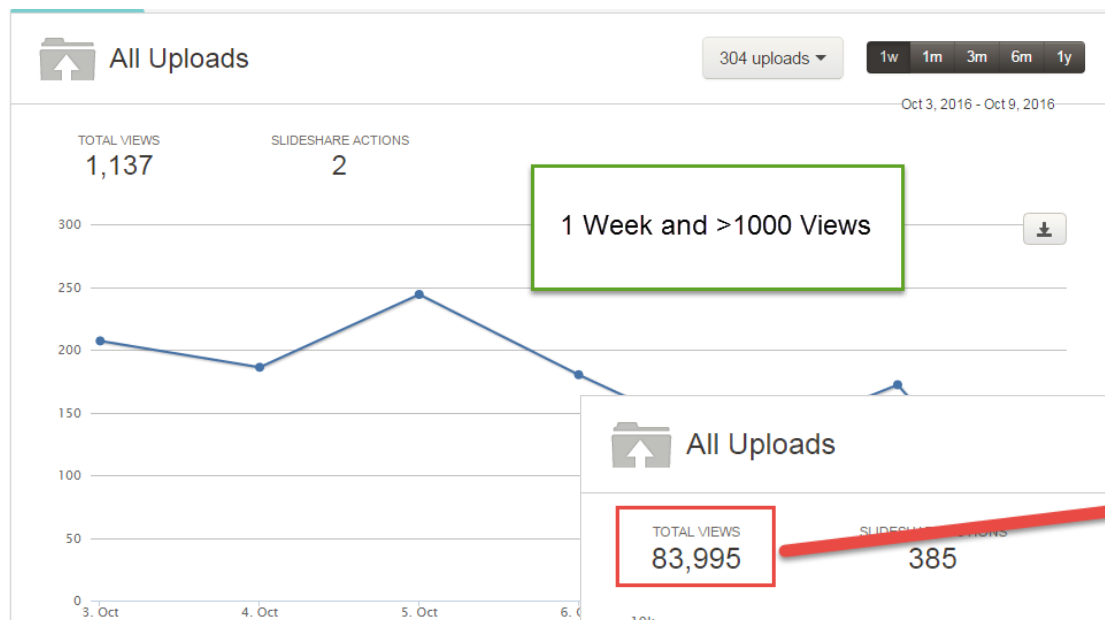
0

1

Edit ▾

Preview ▾

Slideshare – Highly Accessed



Slideshow – NOT Just Slides

Presentations

65 Documents

Videos

Infographics

Latest

Most viewed



3D printing crystal structure...

8 months ago,
1207 views

[Edit](#)



Why High-Throughput Screening...

9 months ago,
234 views

[Edit](#)



Dispensing Processes Impact A...

1 year ago,
406 views

[Edit](#)



ChemSpider as a hub for onlin...

2 years ago,
271 views

[Edit](#)



Revisiting the nmr assignment...

2 years ago,
328 views

[Edit](#)



Structure revision of asperji...

2 years ago,
119 views

[Edit](#)



Elucidating undecipherable ch...

2 years ago,
266 views

[Edit](#)




Using indirect covariance spe...

2 years ago,
182 views

[Edit](#)

ResearchGate is Another Tool for Networking and Citation Tracking



Antony John Williams  42.06

PhD 

Scientist 

United States Environmental Pr..., Corvallis · National Center for Computational Toxicology 

[Add your publications](#)

[Add unpublished work](#)

OVERVIEW

CONTRIBUTIONS

INFO

STATS

RG SCORE

347

PUBLICATIONS

34k

Views

15,695

Downloads

2,400

Citations

518.42

Impact Points

[View stats](#)



United States Environmental Protection Agency
National Center for Computational Toxicology
Corvallis, NC, United States

FEATURED PUBLICATIONS



Source

Research: Data integration and building a profile for yourself as an online scientist

Antony John Williams

0

Views

0

Downloads

0

Citations


I am a Computational Chemist in the National Center of Computational Toxicology at the Environmental Protection Agency in Research Triangle Park, North Carolina.

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,





ResearchGate

Personal stats	Total	Last week	
 Publication views	30k	266	See views by country / institution
 Citations	2k	13	See who cited your research
 Profile views	52k	39	See views by country / institution
 Question views	818	1	

[See your stats](#)

Congratulations 

With **452 new publication views**, you were the **most viewed** researcher from your department

ACHIEVED WEEK ENDING AUG 30TH ● ● ● ● ● ●



With **155 new downloads**, you were the **most downloaded** researcher from your department last week

Academia.edu

<https://rsc.academia.edu/AntonyWilliams>



Change photo

About

Papers 129

Books 4

Conference
Presentations 67

Book Chapters 10

Posters 3

Magazine Article 1

Non-conference
Presentations 8

+ Add Section

+ Add Post

CV

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...
[more](#)

[Edit](#)

PAPERS

+ Add Paper [Reorder](#)

Serving the medicinal chemistry community with Royal Society of Chemistry cheminformatics platforms [more](#)

138

[Download](#)

Dispensing Processes Impact Apparent Biological Activity as Determined by Computational and Statistical Analyses [more](#)

26

[Download](#)

Optimization of the Ugi reaction using parallel synthesis and automated liquid handling [more](#)

19

[Download](#)

top 0.5%
by 30-day views



21,689
total views

850
followers

48 Following



Recent Activity

Antony started following the work of Jon Weinberg. about a month ago

Antony added a conference presentation and a paper 4 months ago

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

[View more activity](#)

Credit for Reviewing Papers?



Search or Import 

BROWSE ▾


ABOUT ▾

ACTIONS ▾



Dashboard ▸ Researchers ▸ Antony Williams





 Edit your profile


 Verified reviewer

 21 Merit

 publons.com/a/306575/

 0000-0002-2668-4821

 Share on Twitter

 Add to LinkedIn

 PROFILE

 STATISTICS

RESEARCH FIELD

Pharmacology, Toxicology and Pharmaceuticals

Drug Discovery



Compare statistics to others in this field

REVIEWS

7
Median: 2
70th percentile

MERIT

21
Median: 6
72nd percentile

REVIEWS (LAST 12 MONTHS)

4
Median: 2
72nd percentile

OPENNESS

42.9%
Median: 0.0%
93rd percentile

Alt-Metrics Manifesto

Impact



usage

downloads
views



peer-review

expert opinion



citations



alt-metrics

storage
links
bookmarks
conversations

National Information Standards Organization and “Altmetrics”



NISO Altmetrics Standards Project White Paper
(Draft 4, June 6, 2014)



Altmetric



PlumTM Analytics
Measuring Research Impact

ImpactStory.

Share the full story of your
research impact.

ImpactStory is your impact profile on the web: we reveal the diverse impacts of your articles, datasets, software, and more.

- http://www.niso.org/apps/group_public/download.php/13809/Altmetrics_project_phase1_white_paper.pdf



Antony Williams  

US Environmental Protection Agency Computational Chemist

 1  4  2

 share

OVERVIEW

ACHIEVEMENTS

ACTIVITY

PUBLICATIONS

ACHIEVEMENTS

[view all](#)



Open Access

★ Top 25%


92% of your research is free to read online. This level of availability puts you in the top 11% of researchers.



Wikistatic

🏆 Top 50%

Your research is mentioned in 1 Wikipedia articles! Only 28% of researchers are this highly cited in Wikipedia.

 Your Wikipedia titles include [Steve Pettifer](#).



Greatest Hit

★ Top 25%

Your top publication has been saved and shared 277 times. Only 11% of

ACTIVITY

[view all](#)


1360

Saves and shares
across 9 channels:

 677  584  56  14  14  9  3  2  1

PUBLICATIONS

[view all](#)

 [Open drug discovery for the Zika virus \[version 1; referees: awaiting peer review\]](#)
2016

277      

 [Dispensing Processes Impact Apparent Biological Activity as Determined by Computational and Statistical Analyses](#)






Antony Williams  

US Environmental Protection Agency Computational Chemist

 1  4  2

 share

OVERVIEW








ACHIEVEMENTS

ACTIVITY








PUBLICATIONS

100 PUBLICATIONS

[+ Add publications](#)

 [Open drug discovery for the Zika virus \[version 1; referees: awaiting peer review\]](#) [\[full text\]](#)
2016
277      

 [Dispensing Processes Impact Apparent Biological Activity as Determined by Computational and Statistical Analyses](#) [\[full text\]](#)
2013 *PLoS ONE*
262      

 [Parallel Worlds of Public and Commercial Bioactive Chemistry Data](#) [\[full text\]](#)
2015 *J. Med. Chem.*
131      

impactstory.org/u/0000-0002-2668-4821/publications

Filter by genre

-  articles (25)
-  others (15)
-  undefineds (59)
-  book (1)

Coauthors

Egon Willighagen
Niklas Blomberg
Christopher Southan
Steve Pettifer
Christopher Lipinski
Jeremy Fry



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

Sean Ekins, Joe Olechno, Antony J. Williams, Alexandre G. de Brevern
2013 PLoS ONE


 Free fulltext available

SAVED AND SHARED 262 TIMES


 73 Mendeley saves

since this article's publication in 2013

Mendeley is a reference manager, like Endnote. For privacy reasons, they conceal identifiable timeline and user information. Some summary info is available on [Mendeley's website](#)

  3 tweets [click to show](#)

2 months ago









 Discover when your work is discussed & shared online - Raising Your Scholarly Profile - LibGuides at Duquesne University

5 months ago by Research Tools

 [Dispensing Processes Impact Apparent Biological Activity as Determined by...](#)

  2 tweets [click to show](#)

Filter by activity

-  Tweets (159)
-  Mendeley saves (73)
-  Blog posts (20)
-  Google+ posts (4)
-  News mentions (2)
-  Public peer reviews (2)
-  F1000 reviews (1)
-  Facebook pages (1)

AltMetric Scores and “Donuts”

Close ×



Metrics

Article accesses: 258

Citations: 0 [more information](#)

Altmetric score: 49



-  Picked up by 18 news outlets
 -  Blogged by 2
 -  Tweeted by 26
 -  On 3 Facebook pages
 -  Mentioned in 1 Google+ posts
 -  Reddited by 1
 -  Highlighted by 1 platforms
- [Click for more details](#)



AltMetric Scores and “Donuts”

<https://www.altmetric.com/about-our-data/the-donut-and-score/>

Instantly recognisable and easy to decipher

The Altmetric Attention Score and donut are designed to help you easily identify how much and what type of attention a research output has received. You might come across them on publisher article metrics pages, institutional repositories, or even individual researcher or lab publications pages.

You can always click on the donut to visit the details page for the research output, to see the original mentions and references that have contributed to the attention score.



Colors of the donut

The colors of the Altmetric donut each represent a different source of attention:

- | | |
|---------------------------------|------------------------|
| ● Policy documents | ● Google+ |
| ● News | ● LinkedIn |
| ● Blogs | ● Reddit |
| ● Twitter | ● Faculty1000 |
| ● Post-publication peer-reviews | ● Q&A (stack overflow) |
| ● Facebook | ● Youtube |
| ● Sina Weibo | ● Pinterest |
| ● Wikipedia | |

Does Social Media Work?

678 Downloads since Dec 16




[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](#)

Cite this article as:

McEachran, A.D., Sobus, J.R. & Williams, A.J. Anal Bioanal Chem (2017) 409: 1729. doi:10.1007/s00216-016-0139-z

66

Shares

678

Downloads



[Close x](#)

[Blogged by 2](#)

[Tweeted by 18](#)

[Referenced in 2 Wikipedia pages](#)

[Reddited by 1](#)

[On 1 videos](#)

[Click for more details](#)

AltMetric Bookmarklet

<https://www.altmetric.com/products/free-tools/bookmarklet/>

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

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



About this Attention Score

In the top 5% of all research outputs scored by Altmetric

MORE...

Mentioned by

- 2 blogs
- 18 tweeters
- 2 Wikipedia pages
- 1 Redditor
- 1 video uploader

Readers on

- 11 Mendeley

SUMMARY

Blogs

Twitter

Wikipedia

Reddit

Video

So far, Altmetric has seen 59 tweets from 18 users, with an upper bound of 50,458 followers.



Springer Chemistry

@Springer_Chem

RT @ChemConnector: The CompTox Chemistry Dashboard: Helping researchers ID unknown contaminants... <https://t.co/NyOnvtCz9S> re. paper <https://t.co/Sxb...>

30 Mar 2017



Research Square

@researchsquare

RT @ChemConnector: @altmetric IMPRESSIVE.Thx for including the @researchsquare movie <https://t.co/SWZRulzk0Z> for our paper <https://t.co/Sxb...>

29 Mar 2017



Christopher Southan

@cdsouthan

RT @ChemConnector: @altmetric IMPRESSIVE.Thx for including the @researchsquare movie <https://t.co/SWZRulzk0Z> for our paper <https://t.co/Sxb...>

29 Mar 2017



ChemConnector

@ChemConnector

@altmetric IMPRESSIVE.Thx for including the @researchsquare movie <https://t.co/SWZRulzk0Z> for our paper <https://t.co/SxbZNzkNRe> to the stats <https://t.co/0CqFzE9xP>

29 Mar 2017



Andrew McEachran

@Andrew_McEach

RT @ChemConnector: The CompTox Chemistry Dashboard: Helping researchers ID unknown contaminants... <https://t.co/NyOnvtCz9S> re. paper <https://t.co/Sxb...>

29 Mar 2017



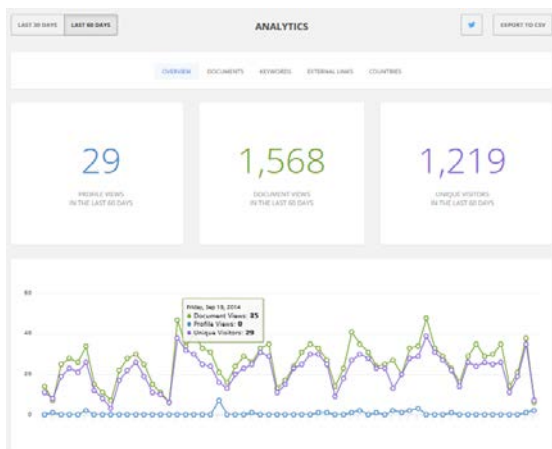
Anal Bioanal Chem

@AnalBioanalChem

RT @ChemConnector: @AnalBioanalChem A movie by @researchsquare regarding our publication with you <https://t.co/bdjVFP0pwn> is now online <https://t.co/bdjVFP0pwn>

29 Mar 2017

Tools to Track and Aggregate Altmetrics

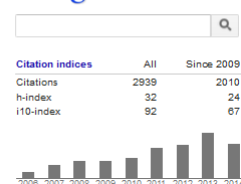


Antony John Williams

Vice President of Strategic Development, Royal Society of Chemistry
Chemistry, Cheminformatics, Nuclear Magnetic Resonance, Drug Discovery
Verified email at rsc.org - [Homepage](#)
My profile is public

Title	Add	More	1-20	Cited by	Year
<input type="checkbox"/> ChemSpider: an online chemical information resource				104	2010
<input type="checkbox"/> HE Penoe, A Williams Journal of Chemical Education 87 (11), 1123-1124					
<input type="checkbox"/> In silico repositioning of approved drugs for rare and neglected diseases				75	2011
<input type="checkbox"/> S Ekins, AJ Williams, MD Krasowski, JS Freundlich Drug discovery today 16 (7), 298-310					
<input type="checkbox"/> Open PHACTS: semantic interoperability for drug discovery				72	2012
<input type="checkbox"/> AJ Williams, L Harland, P Groth, S Pettifer, C Chichester, EL Willighagen, ... Drug discovery today 17 (21), 1188-1198					
<input type="checkbox"/> Internet-based tools for communication and collaboration in chemistry				66	2008
<input type="checkbox"/> AJ Williams Drug discovery today 13 (11), 502-506					

Google Scholar



Co-authors

Kirill Blinov
Sean Ekins
Mikhail Elyashberg
Gary E. Martin
Valery Tkachenko
Yann R. Smeets

PLUM

Antony Williams

Connections in Chemistry



Artifact Summary

<input checked="" type="checkbox"/> Presentation: 266	<input checked="" type="checkbox"/> Data Set: 4
<input checked="" type="checkbox"/> Article: 127	<input checked="" type="checkbox"/> Unknown: 3
<input checked="" type="checkbox"/> Paper: 38	<input checked="" type="checkbox"/> Poster: 3
<input checked="" type="checkbox"/> Video: 28	<input checked="" type="checkbox"/> Patent: 2
<input checked="" type="checkbox"/> Figure: 11	<input checked="" type="checkbox"/> Media: 2
<input checked="" type="checkbox"/> Book: 9	<input checked="" type="checkbox"/> Web Page: 1
<input checked="" type="checkbox"/> Chapter: 7	<input checked="" type="checkbox"/> Conference Paper: 1

Recent Artifacts

- ☒ Bigger data, collaborative tools and the future of predictive drug discovery.
- ☒ The Royal Society of Chemistry and the delivery of chemistry data repositories for the community.
- ☒ Accessing 3D Printable Structures Online
- ☒ Open innovation contributions from RSC resulting from the Open Phacts project
- ☒ Who knew I would get here from there and how I became the ChemConnector final

[see details](#)



Antony John Williams

PhD

VP Strategic Development
The Royal Society of Chemistry - Chemistry

Add your publications

40.36

OVERVIEW CONTRIBUTIONS INFO STATS RG SCORE

40.36

RG Score

A new way to measure scientific reputation.

The RG Score takes all your research and turns it into a source of reputation.

- PUBLICATIONS
- QUESTIONS
- ANSWERS
- FOLLOWERS



PERCENTILE

Your score is higher than 97.5% of ResearchGate members'.



Key profile metrics

1.7M impressions on
192 articles

16.9k views on
192 articles

248.8k impressions on
58 slide decks

54.8k impressions on
7 datasets

Google Scholar Tracks Publications and Citations



[Change photo](#)

Antony John Williams, 0000-0002-2668-4821

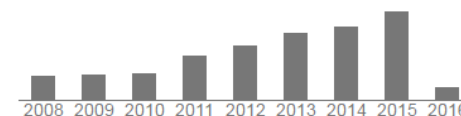
[Edit](#)

[Follow](#)

National Center of Computational Toxicology, [Environmental Protection Agency](#)
[Chemistry](#), [Cheminformatics](#), [Nuclear Magnetic Resonance](#), [Drug Discovery](#)
Verified email at [epa.gov](#) - [Homepage](#)
My profile is public

Google Scholar

Citation indices	All	Since 2011
Citations	4071	2688
h-index	35	27
i10-index	106	78



Co-authors [Edit...](#)

[Kirill Blinov](#)
[Sean Ekins](#)
[Mikhail Elyashberg](#)
[Valery Tkachenko](#)
[Gary E. Martin](#)
[Alex M. Clark](#)
[Carole Goble](#)
[Lee Harland](#)
[Egon Willighagen](#)
[Andrew SID Lang 0000-0002-9922-14...](#)
[Chris Evelo](#)
[Yegor Smurnyy](#)
[Paul Groth](#)
[Tatiana Churanova](#)

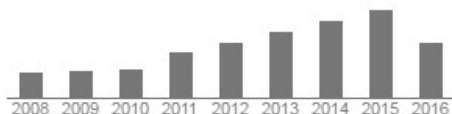
<input type="checkbox"/> Title	+ Add	More	1-20	Cited by	Year
<input type="checkbox"/> ChemSpider: an online chemical information resource			HE Pence, A Williams Journal of Chemical Education 87 (11), 1123-1124	186	2010
<input type="checkbox"/> Open PHACTS: semantic interoperability for drug discovery			AJ Williams, L Harland, P Groth, S Pettifer, C Chichester, EL Willighagen, ... Drug discovery today 17 (21), 1188-1198	146	2012
<input type="checkbox"/> In silico repositioning of approved drugs for rare and neglected diseases			S Ekins, AJ Williams, MD Krasowski, JS Freundlich Drug discovery today 16 (7), 298-310	118	2011
<input type="checkbox"/> Major structural components in freshwater dissolved organic matter			B Lam, A Baer, M Alaei, B Lefebvre, A Moser, A Williams, AJ Simpson Environmental science & technology 41 (24), 8240-8247	93	2007
<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, ... Journal of computer-aided molecular design 25 (6), 533-554	86	2011
<input type="checkbox"/> Identification of "Known Unknowns" Utilizing Accurate Mass Data and ChemSpider			J Little, A Williams, V Tkachenko, A Pshenichnov Journal of the American Society of Mass Spectrometry 23 (1), 170-185	82 *	2012

NOISE in Your Google Citations Profile

<http://tinyurl.com/hyz4aba>

Google Scholar

Citation indices	All	Since 2011
Citations	4684	3167
h-index	38	29
i10-index	120	87






Add co-authors

Dr Paul Jackson	+	×
Yuri Feldman	+	×
Jennie Brand-Miller	+	×
Peter Petocz	+	×
John MOHAN	+	×

<input type="checkbox"/>	EXPERIENCE WITH NASAL POSITIVE AIRWAY PRESSURE IN SLEEP-APNEA AJ WILLIAMS, S SANTIAGO, E PRESCOTT CLINICAL RESEARCH 33 (1), A83-A83	1985
<input type="checkbox"/>	COMPARISON OF LUNG-FUNCTION IN IDENTICAL-TWINS DISCORDANT FOR SMOKING AJ WILLIAMS, J CHOU, J KINNEY CLINICAL RESEARCH 32 (2), A438-A438	1984
<input type="checkbox"/>	OBSTRUCTIVE AIRWAYS DISEASE IN RHEUMATOID- ARTHRITIS (RA) AJ WILLIAMS, T PIETUCK, R CONSTANZ, J CHOU, J KINNEY CLINICAL RESEARCH 30 (2), A439-A439	1982
<input type="checkbox"/>	Analysis of the energy resources and demand of Western Europe. Final technical report, Jun 1974--Mar 1975 JF Schneider, KD Dance, RC Lind, RB Ryan, AR Williams Science Applications, Inc., McLean, Va.(USA)	1975
<input type="checkbox"/>	An investigation into the motions of ships at sea AJ Williams Trans. INA 95, 70	12 1953
<input type="checkbox"/>	Miscellanies in Prose and Verse A Williams, S Johnson T. Davies	12 1766

Check your profile data

<input type="checkbox"/>	Computer-assisted structure verification and elucidation tools in NMR-based structure elucidation ME Elyashberg, AJ Williams, GE Martin Progress in Nuclear Magnetic Resonance Spectroscopy 53 (1), 1-104	86	2008
<input type="checkbox"/>	Improved baseline recognition and modeling of FT NMR spectra S Golotvin, A Williams Journal of Magnetic Resonance 146 (1), 122-125	76	2000
<input type="checkbox"/>	Internet-based tools for communication and collaboration in chemistry AJ Williams Drug discovery today 13 (11), 502-506	73	2008
<input type="checkbox"/>	Sleep health New South Wales: chronic sleep restriction and daytime sleepiness DJ Bartlett, NS Marshall, A Williams, RR Grunstein Internal medicine journal 38 (1), 24-31	67	2008

<input type="checkbox"/> Carbon-carbon double-bond formation reductive coupling promoted by a mononuclear cobalt complex Preparation and characterization of two cobalt complexes R Duchateau, AJ Williams, S Gambarotta, MY Li Inorganic Chemistry 30 (25), 4863-4866		
<input type="checkbox"/> Public chemical compound databases AJ Williams Current Opinion in Drug Discovery and Development 10 (1), 1-10 <input type="checkbox"/> The use of NMR to study sodium dodecyl sulfate micelles DD Miller, W Lenhart, BJ Antalek, AJ Williams, Langmuir 10 (1), 68-71	<div data-bbox="647 863 1796 949">  <div> <input type="button" value="Previous"/> <input type="button" value="Edit"/> <input type="button" value="Delete"/> <input type="button" value="Export"/> </div> </div> <div data-bbox="647 949 1796 1255"> <div>  <p>Antony John Williams, 0000-0002-2668-4821</p> </div> <div> <p>Sleep health New South Wales: chronic sleep restriction and daytime sleepiness</p> <p>Authors DJ Bartlett, NS Marshall, A Williams, RR Grunstein</p> <p>Publication date 2008/1/1</p> <p>Journal Internal medicine journal</p> <p>Volume 38</p> <p>Issue 1</p> </div> </div>	

Add Articles that Are Missed

SAVE

Cancel

Journal

Conference

Chapter

Book

Thesis

Patent

Court case

Other

Title

An automated curation procedure for addressing chemical errors and inconsistencies in public datasets

Authors

K. Mansouri, C. Grulke, A. Richard, R. Judson and A.J. Williams

For example: Patterson, David; Lamport, Leslie

Publication date

2016/11/25

For example, 2008, 2008/12 or 2008/12/31.

Journal

SAR and QSAR in Environmental Research

Volume

27

Issue

11

Pages

911-937

Publisher

Taylor and Francis

SAVE

Cancel

ORCID – The Scientists SSN

ORCID

Connecting Research
and Researchers

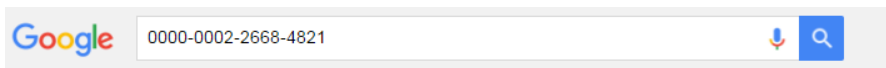
Antony Williams

ORCID ID



orcid.org/0000-0002-2668-4821

“Statistics” Based on an Open SSN



All Maps Shopping Images News More Search tools

About 826 results (0.53 seconds)

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

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

orcid.org/0000-0002-2668-4821. Also known as. ChemConnector, ChemSpiderman, Tony Williams. Country. United States. Keywords. NMR, Computer-assisted ...

Antony John Williams, 0000-0002-2668-4821 - Google ...

<https://scholar.google.com/citations?user...> Google Scholar

National Center of Computational Toxicology, Environmental Protection Agency - epa.gov

Antony John Williams, 0000-0002-2668-4821. National Center of Computational Toxicology, Environmental Protection Agency - Chemistry, Cheminformatics ...

You've visited this page 2 times. Last visit: 2/14/16

[PDF] williams quality poster 0307_2016_final_v4.pdf - EPA - US...

<https://cfpub.epa.gov/.../s...> United States Environmental Protection Agency

Mar 17, 2016 - Innovative Research for a Sustainable Future www.epa.gov/research. ORCID: 0000-0002-2668-4821. Antony Williams I ...

Welcome Antony Williams - Reviewer recognition - Elsevier

<https://www.reviewerrecognition.elsevier.com/recognition/index?key...>

tony27587@gmail.com. Royal Society of Chemistry 0000-0002-2668-4821. We thank you for your contributions to the peer review process. If you are interested ...

The Chemical Analysis Metadata Platform

champ-project.org/component/contact/contact/2

... http://www.scientistsdb.com/index.php?title=Antony_John_Williams. My ORCID ID:

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

Curriculum Vitae « ChemConnector Blog

www.chemconnector.com/antonywilliams_cv/

Publons Profile: <https://publons.com/author/306575/antony-williams>. Academic

Karma Profile: <http://academickarma.org/0000-0002-2668-4821> ...

You've visited this page 3 times. Last visit: 10/4/15

Wikipedia:ORCID/Items with ORCID identifiers - Wikipedia ...

https://en.wikipedia.org/wiki/.../Items_with_ORCID_identifiers Wikipedia

... Andy Mabbett.JPG. Antony John Williams - human - male - chemist, 0000-0002-2668-4821, 41556144, 0000 0001 1093 9159, Antony John Williams ...



EPA Science Inventory

You are here: EPA Home » Science Inventory » Search Results » The influence of data curation on QSAR Modeling - examining issues of quality versus quantity of data (SOT)

The influence of data curation on QSAR Modeling - examining issues of quality versus quantity of data (SOT)

Citation:

Williams, A., K. Mansouri, A. Richard, AND C. Grukke. The influence of data curation on QSAR Modeling - examining issues of quality versus quantity of data (SOT). Presented at Society of Toxicology, New Orleans, LA, March 13 - 17, 2016.

Description:

The construction of QSAR models is critically dependent on the quality of available data. As part of our efforts to develop public platforms to provide access to predictive models, we have attempted to discriminate the influence of the quality versus quantity of data available to develop and validate QSAR models. We have focused our efforts on the widely used EPISuite software that was initially developed over two decades ago. Specific examples of quality issues for the EPISuite data include multiple records for the same chemical structure with different measured property values, inconsistency between the structure, chemical name and CAS registry number for single records, the inability to convert the SMILES strings into chemical structures, hypervalency in the chemical structures and the absence of stereochemistry for thousands of data records. Relative to the era of EPISuite development, modern cheminformatics tools allow for more advanced capabilities in terms of chemical structure representation and storage, as well as enabling automated data validation and standardization approaches to examine data quality. This presentation will review both our manual and automated approaches to examining key datasets related to the EPISuite training and test data. This includes approaches to validate between chemical structure representations (e.g. molfile and SMILES) and identifiers (chemical names and registry numbers), as well as approaches to standardize the data into QSAR-consumable formats for modeling. We have quantified and segregated the data into various quality categories to allow us to thoroughly investigate the resulting models that can be developed from these data slices and to examine to what extent efforts into the development of large high-quality datasets have the expected pay-off in terms of prediction performance. This abstract does not reflect U.S. EPA policy.

Purpose/Objective:

Poster Presentation at Society of Toxicology 2016 meeting

URLs/Downloads:

[WILLIAMS QUALITY POSTER 0307_2016_FINAL_V4.PDF](#) (PDF, NA pp, 699.071 KB, [about PDF](#))

Record Details:

Record Type: DOCUMENT (PRESENTATION/POSTER)

Start Date: 03/16/2016

Completion Date: 03/16/2016

Record Last Revised: 03/18/2016

Record Created: 03/18/2016

Record Released: 03/18/2016

OMB Category: Other

Record ID: 311418

Organization:

U.S. ENVIRONMENTAL PROTECTION AGENCY

OFFICE OF RESEARCH AND DEVELOPMENT

NATIONAL CENTER FOR COMPUTATIONAL TOXICOLOGY

[Show Additional Record Data](#)

Upsides and Cautions

- UPSIDES

- Cleared products are public domain and can create awareness, traffic, and usage of ORD science
- Many of you are ALREADY using some of these tools
- Rapid and highly beneficial distribution of data/articles through social networks

- CAUTIONS

- Your “products” are cleared. Be cautious of reinterpretation and wording.
- Check and validate your profiles about once/month

Recommendations

- Register for an ORCID ID – then use it

Antony John Williams,
0000-0002-2668-4821

Edit

Follow

Vice President of Strategic Development, Royal Society of Chemistry
[Chemistry](#), [Cheminformatics](#), [Nuclear Magnetic Resonance](#), [Drug Discovery](#)
Verified email at rsc.org - [Homepage](#)
My profile is public

Google Scholar

Citation indices	All	Since 2010
Citations	3437	2273
h-index	33	25
i10-index	101	73

- Develop your LinkedIn profile
- Track Google Scholar Citations
- Choose: ResearchGate **or** Academia.edu
- **Participate** in building your profile