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

Five years of helping chemists to create an online presence using freely available resources

Antony Williams

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

August 2017
ACS Fall Meeting, Washington, DC

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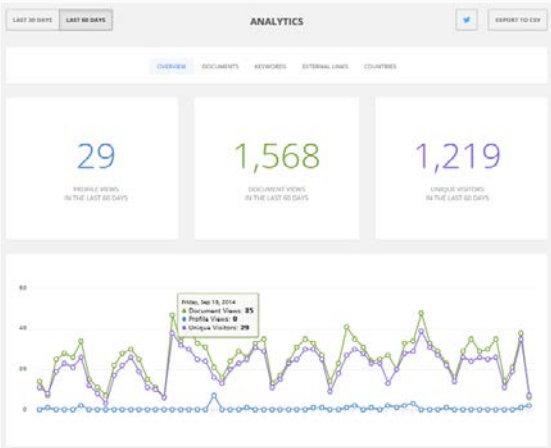
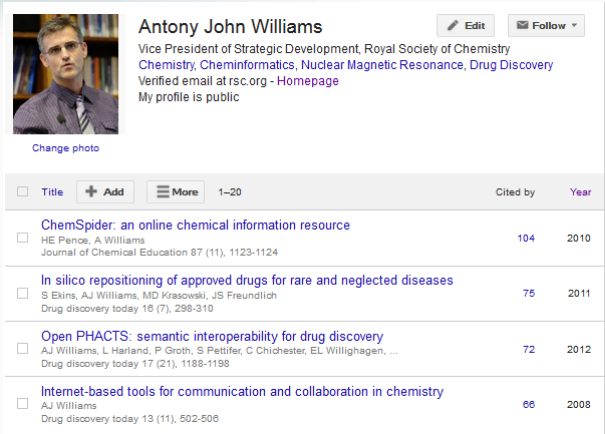
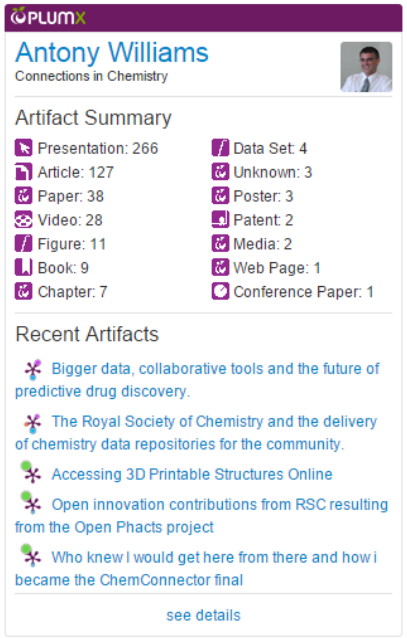
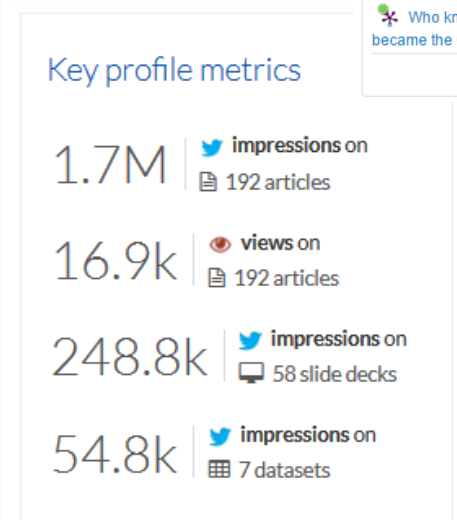








Published two weeks ago

https://f1000research.com/articles/6-1315/v1

Check for updates

OPINION ARTICLE

The new alchemy: Online networking, data sharing and research activity distribution tools for scientists [version 1; referees: awaiting peer review]

Antony J. Williams [1], Lou Peck [2], Sean Ekins [3]

Author details

Grant information

METRICS

875

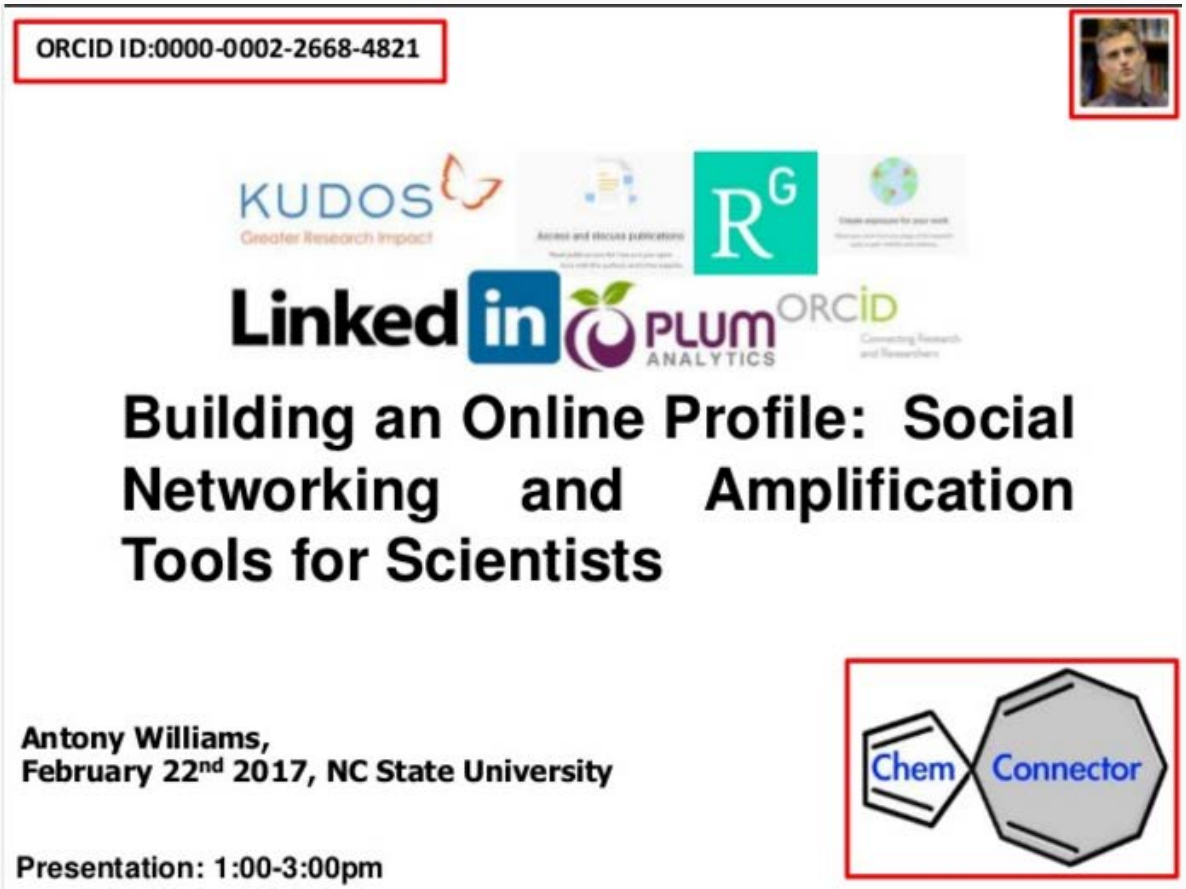
VIEWS

181

DOWNLOADS

Maybe of use…

- **https://www.slideshare.net/AntonyWilliams**/building-an-online-profile-social-networking-and-amplification-tools-for-scientists



Five Years, ~100 Talks

- Encouraging the “era of participation”
- Providing an overview of some tools available
- Sharing stories, statistics and strategies
- Encouraging “sharing for the sake of community/science as well as for yourself”

- **OUTCOMES**
- Lots of people have claimed **ORCiDs**
- People have been building profiles and benefiting
- I HOPE they are now having an “Impact” online….

You can be evaluated based on these contributions…

- 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
- CONNECT THEM to your **ORCiD**

ORCID – The Scientists SSN

ORCID

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Antony Williams

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ORCID

Connecting Research and Researchers

3,418,420 ORCID iDs and counting. See more...

Antony Williams

ORCID ID

orcid.org/0000-0002-2668-4821

Also known as

ChemConnector, ChemSpiderman, Tony Williams

Country

United States

Keywords

NMR, Computer-assisted Structure Elucidation, Chemistry, ChemSpider, Cheminformatics, Open PHACTS, PharmaSea, Open Science, Computational Toxicology

Other IDs

Scopus Author ID: 55258539900

Works (511) Sort

Open Science for Identifying "Known Unknown" Chemicals
Environmental Science & Technology
2017-05-16 | journal-article
DOI: 10.1021/acs.est.7b01908
Source: Crossref — Preferred source

Laboratory Information Management Systems (LIMS)
Encyclopedia of Spectroscopy and Spectrometry
2017 | other
DOI: 10.1016/b978-0-12-803224-4.00070-4
Source: CrossRef Metadata Search — Preferred source

Weaver's historic accessible collection of synthetic dyes: a cheminformatics analysis
Chem. Sci.
2017 | journal-article
DOI: 10.1039/C7SC00567A
Source: Crossref — Preferred source

Mobile Apps for Green Chemistry
Encyclopedia of Inorganic and Bioinorganic Chemistry
2016-09 | other
DOI: 10.1002/9781119951438.eibc2413
Source: CrossRef Metadata Search — Preferred source

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

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

Contact Info

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

Can Also Function as an Electronic CV

EPA United States Environmental Protection Agency

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 в 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

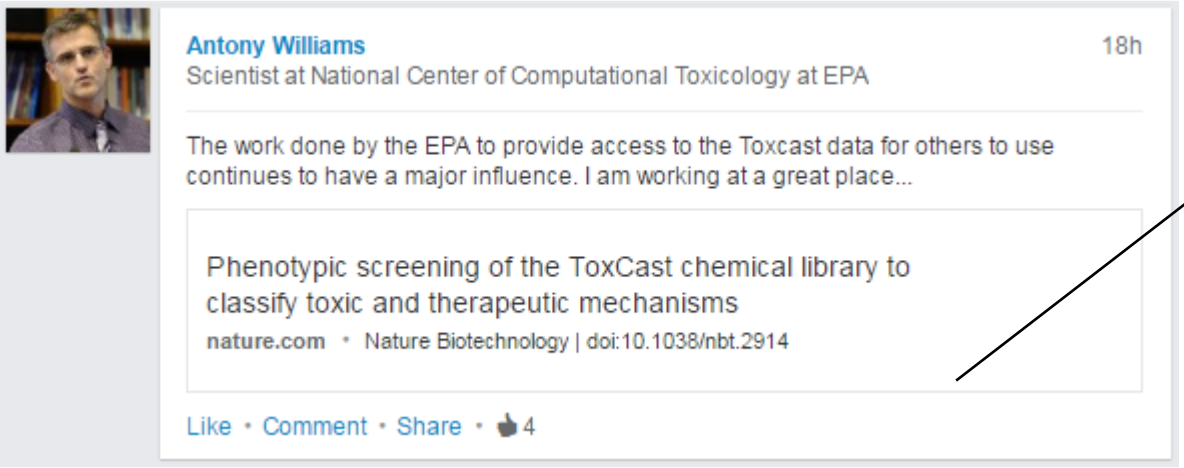
Neglected infectious diseases such as tuberculosis (TB) and malaria kill millions of people annually and the oral drugs used are subject to resistance requiring the urgent development of new therapeutics. Several groups, including pharmaceutical companies, have made large sets of antimalarial screening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

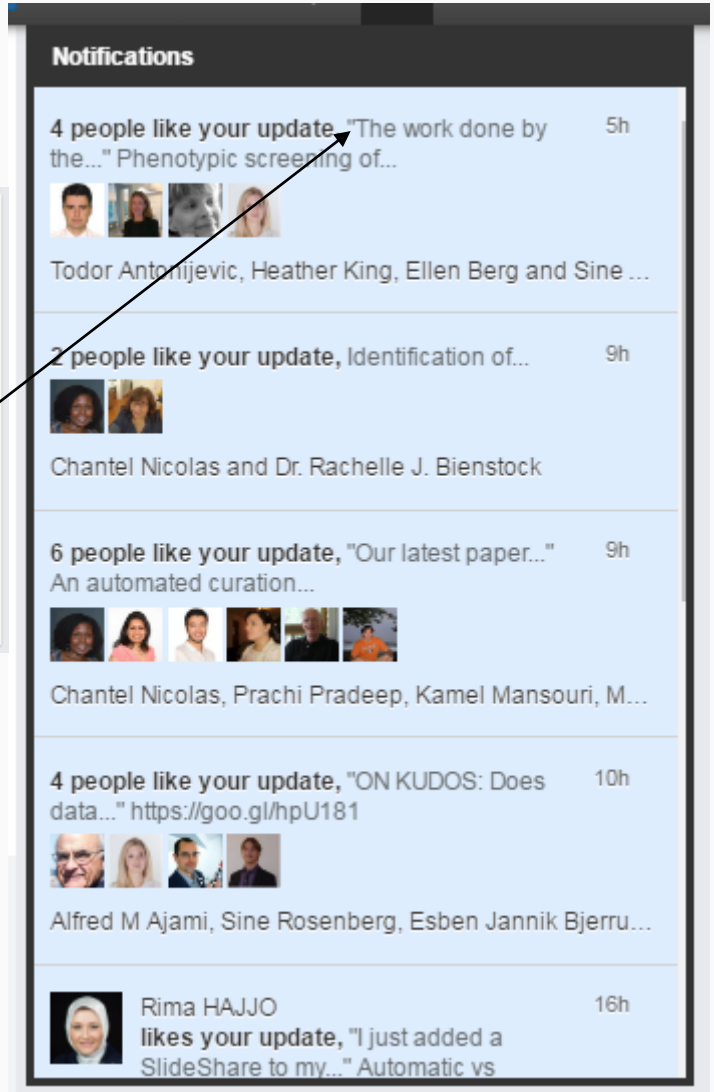
2 authors

Antony Williams
VP Strategic Development, Head of ...

Sean Ekins
Founder and CEO at Collaborations ...

Your Postings Get Networked





It's All Networking, Networking……..

Ask for “Endorsements”, or get them…

Skills & Endorsements

Top Skills

- 99+ Chemistry
- 99+ Analytical Chemistry
- 99+ Drug Discovery
- 82 NMR
- 82 Science
- 63 Cheminformatics
- 61 Strategy
- 53 Lifesciences
- 58 R&D
- 46 Spectroscopy

Antony also knows about...

- 44 Start-ups
- 47 Organic Chemistry
- 29 Product Management
- 29 Pharmaceutical Industry
- 18 Competitive Analysis
- 26 Biochemistry
- 17 Blogging
- 14 Entrepreneurship
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Presentations

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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

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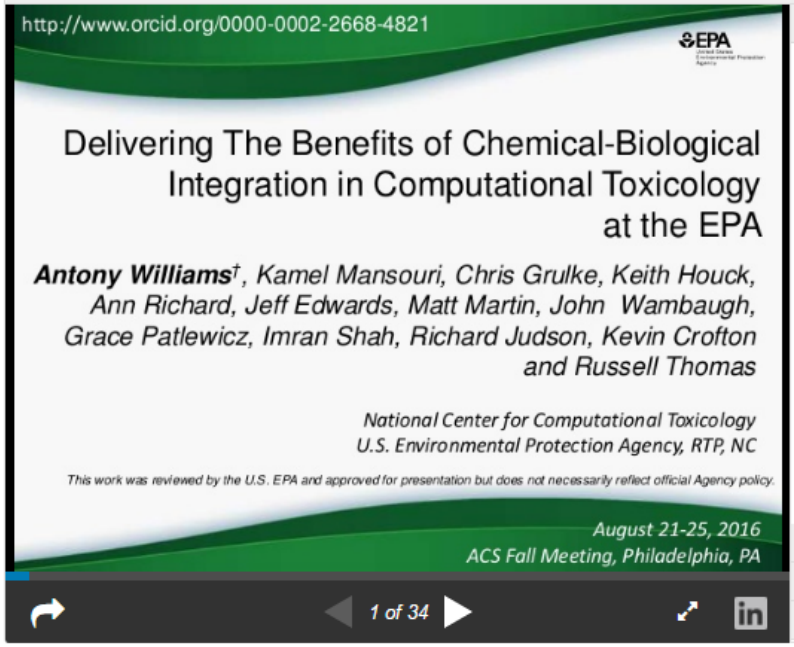


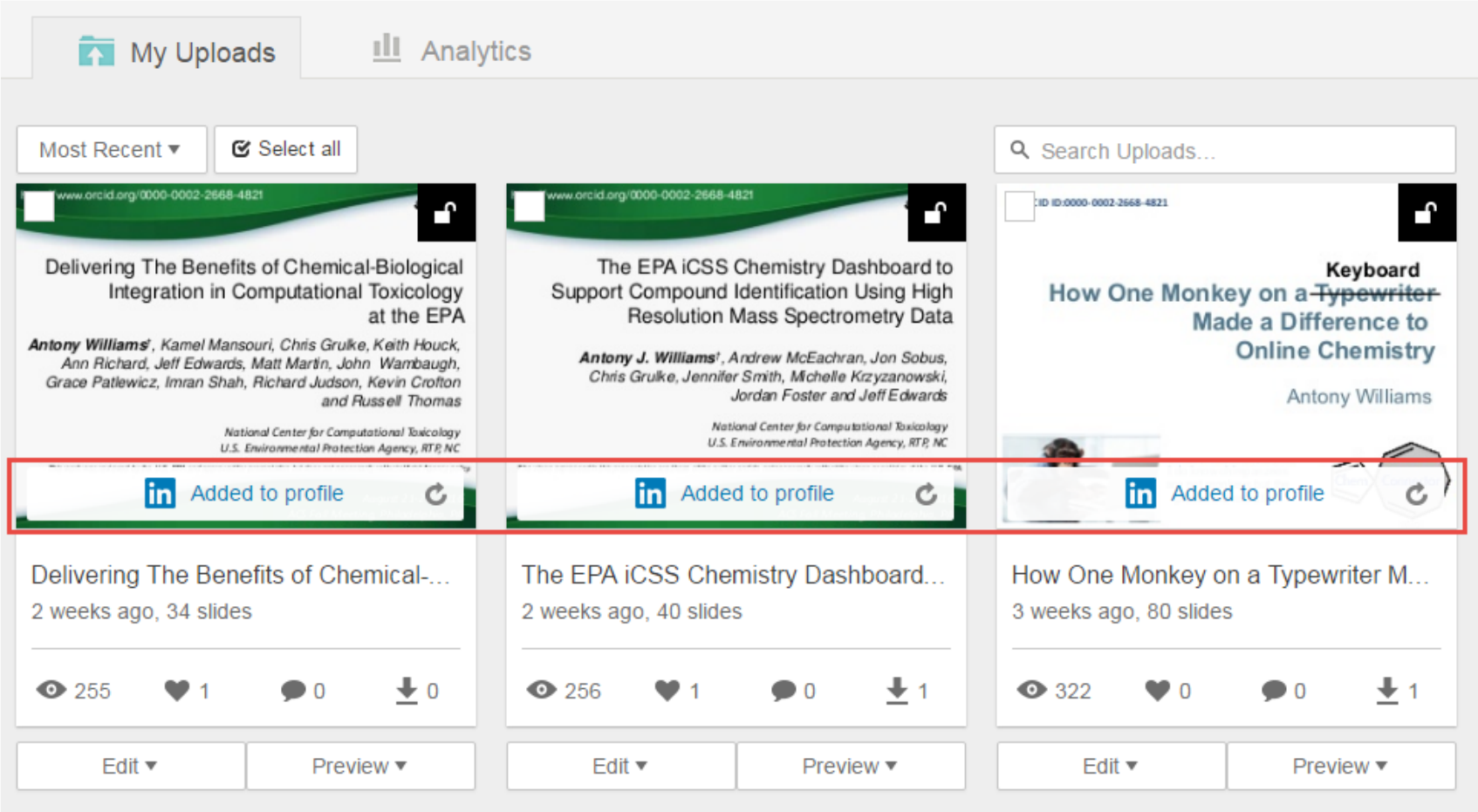
Presentations	235
Documents	66
Infographics	0
Videos	0

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

Think about it…

- 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.

Sharing your works online



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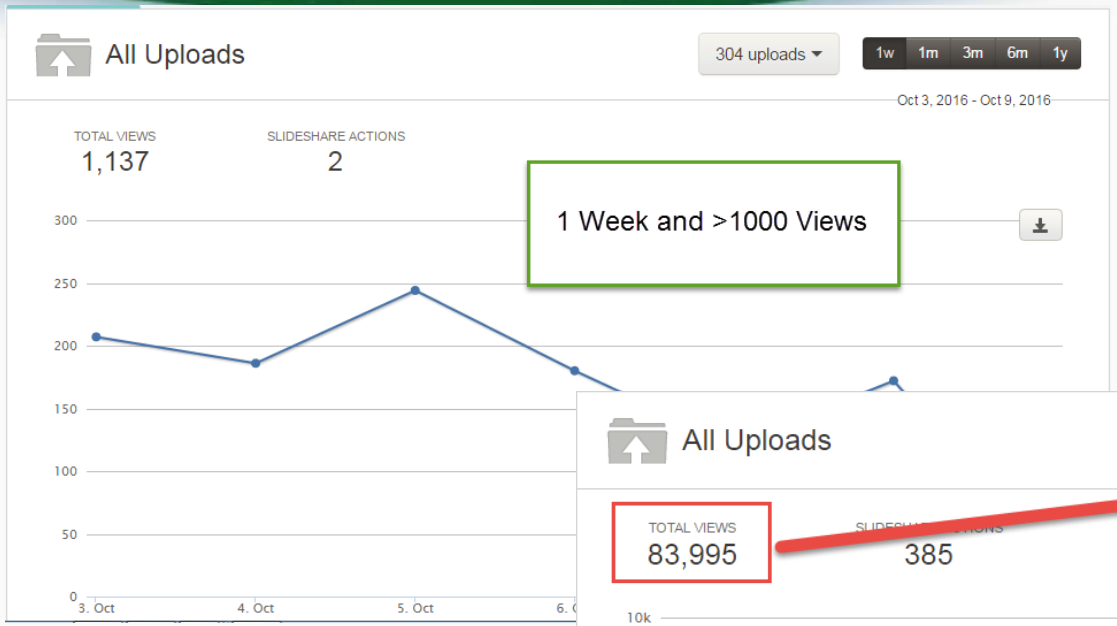

Slideshare – NOT Just Slides

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Title	Cited by	Year
ChemSpider: an online chemical information resource HE Pence, A Williams Journal of Chemical Education 87 (11), 1123-1124	186	2010
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
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
Major structural components in freshwater dissolved organic matter B Lam, A Baer, M Alaee, B Lefebvre, A Moser, A Williams, AJ Simpson Environmental science & technology 41 (24), 8240-8247	93	2007
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
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), 179-185	82 *	2012

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Citations	4071	2688
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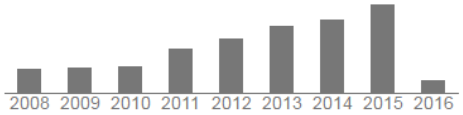

Co-authors Edit...

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- 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
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- Tatiana Churanova

http://scholar.google.com/citations?user=O2L8nh4AAAAJ

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Antony John Williams 42.06

PhD

Scientist

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

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347	34k	15,695	2,400	518.42	
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United States Environmental Protection Agency
National Center for Computational Toxicology
Corvallis, NC, United States

FEATURED PUBLICATIONS

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

Antony John Williams

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Views	Downloads	Citations

Source

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	

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https://rsc.academia.edu/AntonyWilliams

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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... more

Edit

About

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ensing processes profoundly influence estimates of biological activity of compounds

Tell readers what your publication is about

Adding a simple, non-technical explanation of your publication will make it easier to find, and more accessible to a broader audience. Learn more.

Dispensing processes profoundly influence estimates of biological activity of compounds. In this study using published inhibitor data for the tyrosine kinase EphB4, we show that IC50 values obtained via disposable tip-based serial dilution and dispensing versus acoustic dispensing differ by orders of magnitude with no correlation or ranking of datasets.

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Adding an explanation of what is most unique and/or timely about your work, and the difference it might make, will help increase readership. Learn more.

Traditional dispensing processes are another important source of error in high-throughput screening that impacts computational and statistical analyses. These findings have far-reaching implications in biological research and calls into question the quality of HTS data available in the public databases and certainly emphasizes the need for appropriate meta data to be available to ensure that it

The Article…

CHEMISTRY
A European Journal

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Full Paper

The Synthesis and STM/AFM Imaging of 'Olympicene' Benzo[*cd*]pyrenes

Anish Mistry, Ben Moreton, Dr. Bruno Schuler, Dr. Fabian Mohn, Dr. Gerhard Meyer, Dr. Leo Gross, Dr. Antony Williams, Prof. Peter Scott, Dr. Giovanni Costantini, Dr. David J. Fox

First published: 2 December 2014 Full publication history

DOI: 10.1002/chem.201404877 View/save citation

Enriched…

EPA United States Environmental Protection Agency

Olympicene on the Chemistry Periodic Table of Videos

Olympicene is a gimmicky but clever molecule based on a famous set of rings - yet they are not linked!!! A discussion with Martin Poliakoff in a video.

The Story of Olympicene from Concept to Completion on the ChemConnector blog

The story of Olympicene, and our intention to try and get it synthesized and analyzed, was first reported in August 2011. The original conversation was between Prof Graham Richards and I over a drink in Belgium at the RSC Editors Symposium in March 2010. The concept of having someone synthesize a small organic molecule that would be a molecular representation of a famous symbol of sport was a fascinating challenge. This blog post summarizes the project.

Stunning image of smallest possible five rings

Press release from the University of Warwick

Resources

External resources such as presentations, videos, interviews, figures, data-sets or related publications

In Celebration of Chemistry in Sports. Introducing Olympicene.

The initial introduction to the Olympicene project as announced on the ChemConnector website

Olympicene on ChemSpider

The ChemSpider record for Olympicene with the initial structure registered and related data including proton NMR spectrum.

Photo finish for Olympicene in Chemistry World

Chemistry World article about olympicene "UK chemists have synthesised and imaged a molecule that closely resembles the Olympic rings. While the molecule shows promise for applications in electronics, the project was undertaken principally as a means to celebrate the Olympics coming to London in 2012, as well as encouraging online sharing of synthetic chemistry procedures."

Gold medal! Scientists create smallest-ever version of Olympics logo - a single molecule with five familiar 'rings'

A story by the Daily Mail about Olympicene

An entry about olympicene in Wiktionary

How many compounds get an entry in the Wiktionary???

Theoretical Prediction of the Structures and Energies of Olympicene and its Isomers

This paper offers the first theoretical study of the kinetic stability of olympicene and its isomers. We use the parametric two-electron reduced density matrix (2-RDM) method, which takes the 2-RDM as the basic variable in lieu of the traditional wave function in calculations . Our calculations demonstrate that olympicene's isomers may be separated into aromatic and diradical isomers. The olympicene molecule has the potential to complement pentacene as an organic semiconductor.

What about “Data Sharing”?

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Antony Williams

0000-0002-2668-4821

Computational Chemist, National Center for Computational Toxicology, US-EPA in Chemistry

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Co-workers & collaborators

Valery Tkachenko

Sean Ekins
senior consultant, Fuquay Varina, NC, USA

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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

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

203 views | 34 downloads | 0 citations

3

CATEGORIES

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

KEYWORD(S)

Chemistry | Mass Spectrometry | Cheminformatics

LICENCE

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Alt-Metrics Manifesto

http://altmetrics.org/manifesto/

ImpactStory.

https://impactstory.org/u/0000-0002-2668-4821

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Impactstory

hi, Antony

Antony Williams

US Environmental Protection Agency Computational Chemist

1 4 2

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

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
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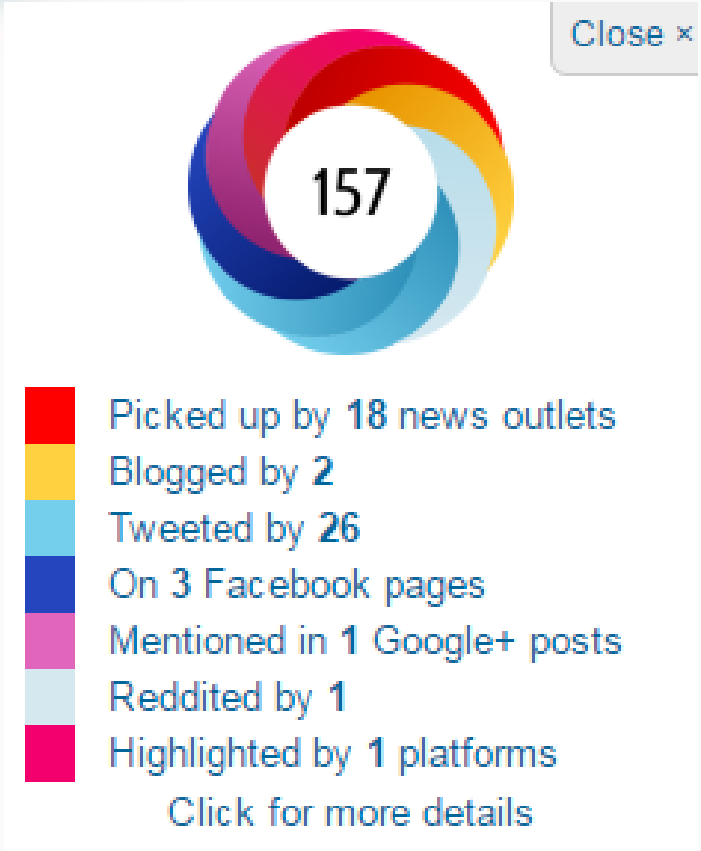
AltMetric Scores and “Donuts”

Metrics

Article accesses: 258

Citations: 0 more information

Altmetric score: 49



AltMetricIt Bookmarklet

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

EPA United States Environmental Protection Agency

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

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

28

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:...

30 Mar 2017

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Christopher Southan
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Andrew McEachran
@Andrew_McEach

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What Next?
My Recommendations

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

- Participate building your profile – share data, papers, presentations, etc..

Various Versions of This Talk

www.slideshare.net/AntonyWilliams

Email: williams.antony@epa.gov