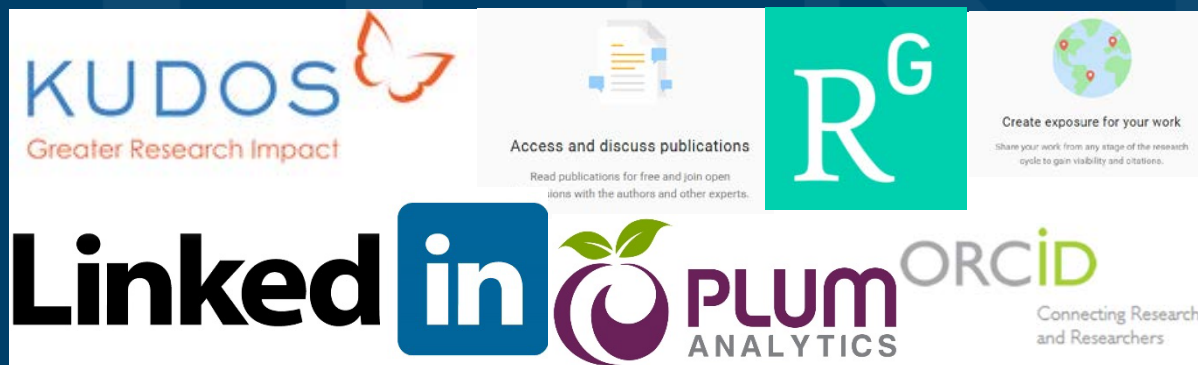


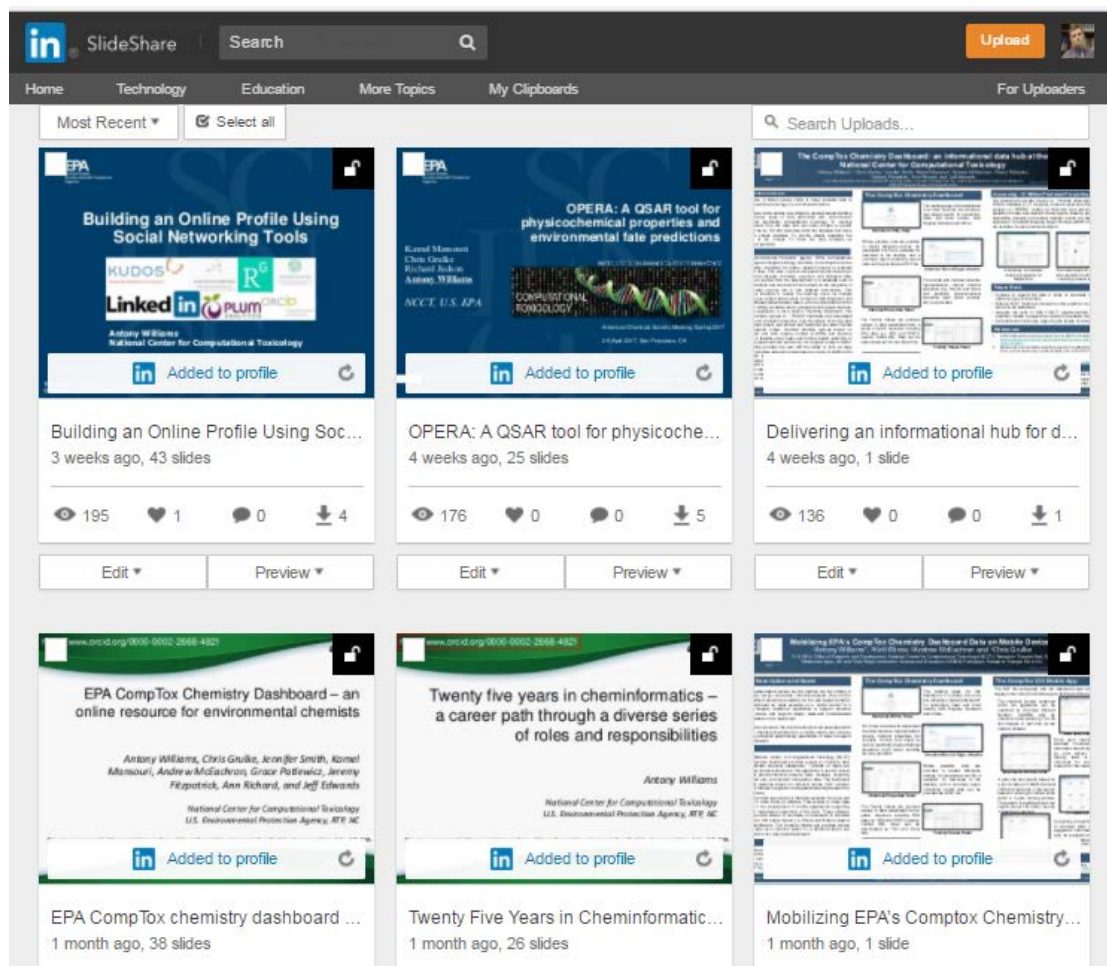
Profile Building, Research Sharing and Data Proliferation using Social Media Tools for Scientists



Antony Williams
National Center for Computational Toxicology

Various Versions of This Talk

www.slideshare.net/AntonyWilliams



The screenshot displays a SlideShare profile for Antony Williams, a National Center for Computational Toxicology (NCCT) scientist at the U.S. EPA. The profile features a header with the SlideShare logo, a search bar, and navigation links. Below the header, there are tabs for 'Most Recent' and 'Select all'. The main content area shows six presentations, each with a thumbnail, title, description, and engagement metrics (views, likes, comments, downloads). The presentations are:

- 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, 136 views, 0 likes, 0 comments, 1 download.
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Contact Erin Knight for further details.

You Will Choose...

Self-marketing vs. Narcissism

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



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**
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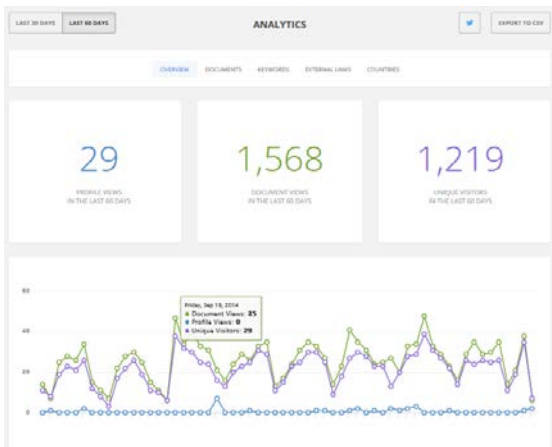
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to share!**

**A Paper
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Some Data
A Presentation**

It MUST already be Public!



How to Measure Impact

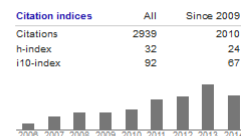


Antony John Williams

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

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Co-authors Edit...

Kirill Blinov

Sean Ekins

Mikhail Elyashberg

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Antony Williams

Connections in Chemistry



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<input type="checkbox"/> Book: 9	<input type="checkbox"/> Web Page: 1
<input type="checkbox"/> Chapter: 7	<input 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

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40.36

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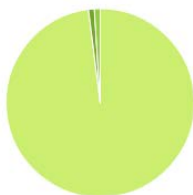
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- Other forms of research

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 |

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 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



--

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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

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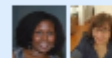
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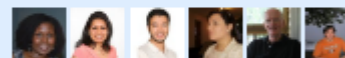
Todor Antonijevic, Heather King, Ellen Berg and Sine ...

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...

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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

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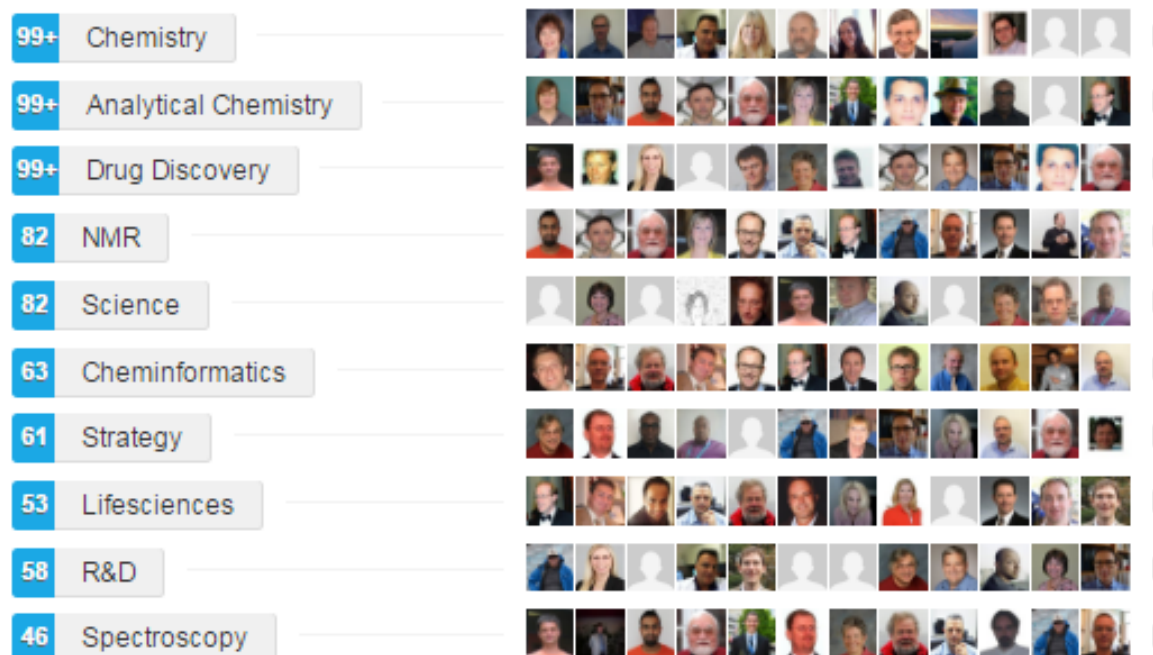
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Ask for “Endorsements”,

Skills & Endorsements

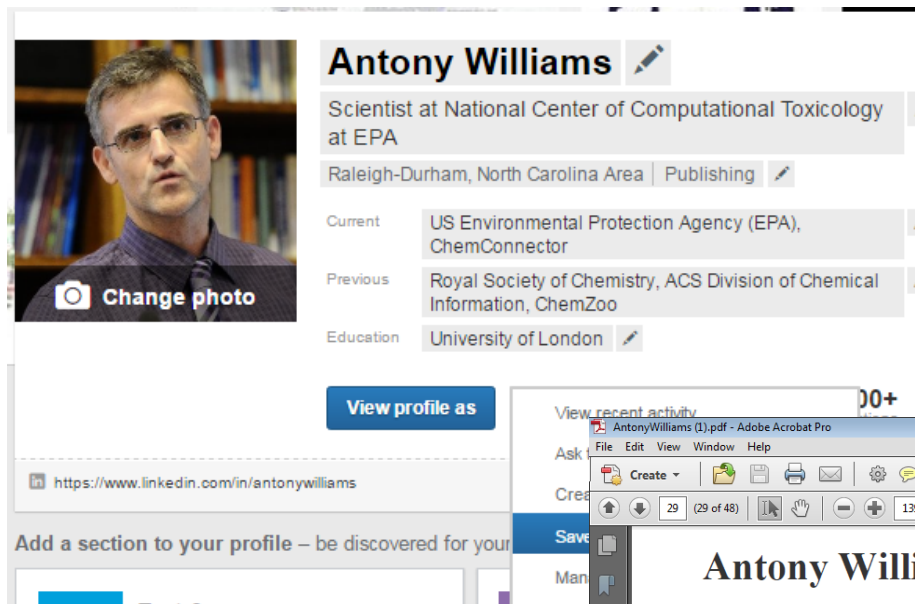
Top Skills




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

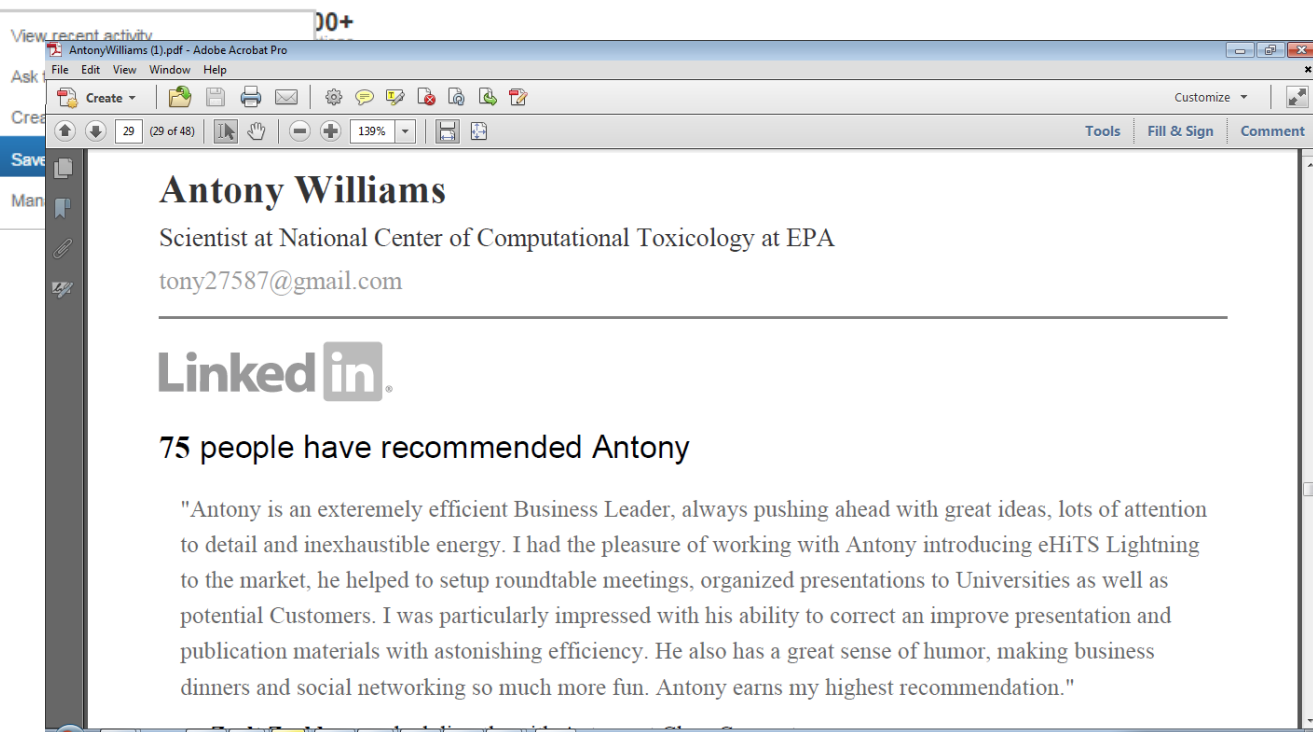
Previous Royal Society of Chemistry, ACS Division of Chemical Information, ChemZoo

Education University of London 

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Antony Williams

Scientist at National Center of Computational Toxicology at EPA

tony27587@gmail.com

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75 people have recommended Antony

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



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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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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.

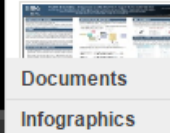
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The EPA iCSS Chemistry Dashboard to Support Compound Identification Using High Resolution Mass Spectrometry Data

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

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Antony Williams

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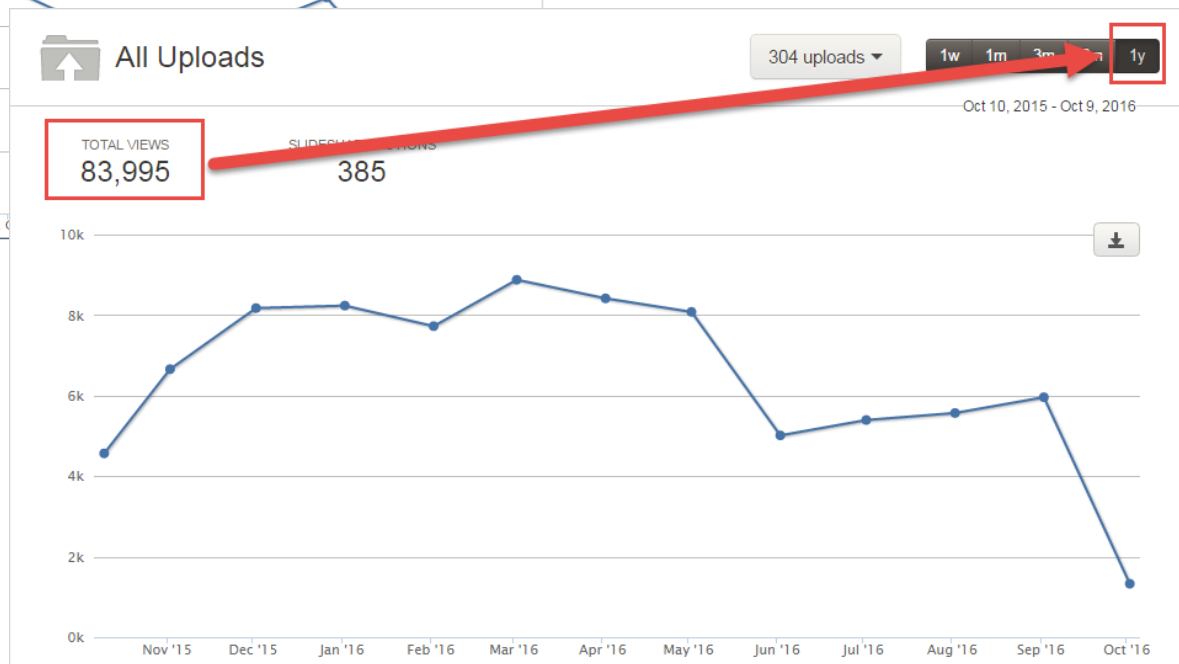
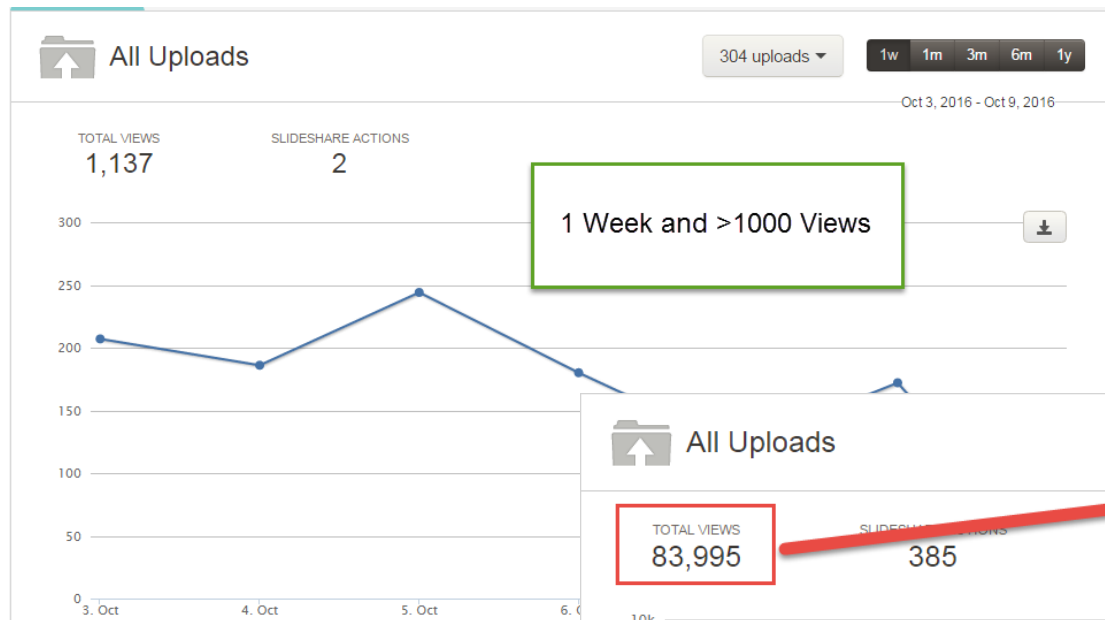
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Antony John Williams  42.06

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Antony John Williams

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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,

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Valery Tkachenko

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The Royal Society of Chemistry

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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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Antony John Williams 43.02

PhD
Computational Chemist
United States Environmental Protection Agency, Washington, D.C. · National Center for Environmental Health Sciences

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United States Environmental Protection Agency
National Center for Environmental Health Sciences
Washington, D.C., DC

About

I am presently a Computational Computational Toxicology with Agency in Research Triangle Park. I am one of the founders of the (http://www.chemspider.com), in the world that was acquired in 2009. Prolific author with almost 1000 publications and book chapters, presentations.

Skills and expertise (29)

15 Cheminformatics
13 Cheminformatics

444

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Presentation: The EPA iCSS Chemistry Dashboard to Support Compound Identification Using High Resolution

By the end of this year we will release a lot of new functionality to support Non-Targeted Analysis by Mass Spectrometry. The next release of the CompTox Chemistry Dashboard will have batch searching based on formulae that will be particularly useful, data source ranking and a number of specific searches of value to Mass Spectrometrists. See this presentation given at EAS for more detail:

[Presentation: The EPA iCSS Chemistry Dashboard to Support Compound Identification](#)

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nputational Toxicology with t
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ills and expertise (29)

Academia.edu

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Antony J Williams

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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

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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.

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Author Updates

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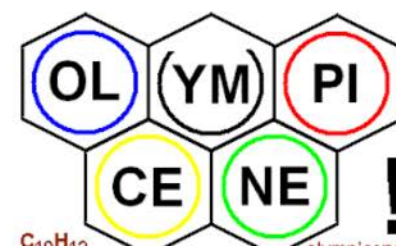
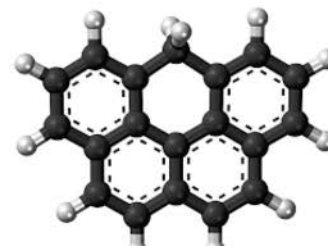
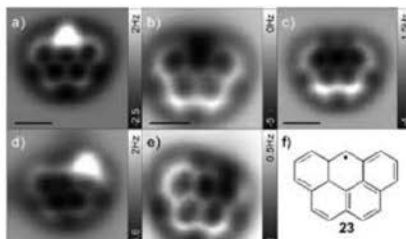
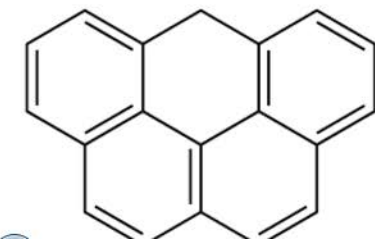
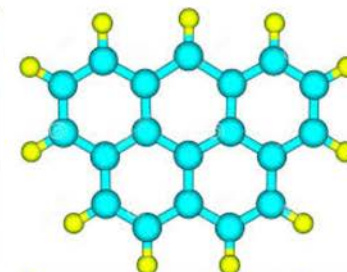
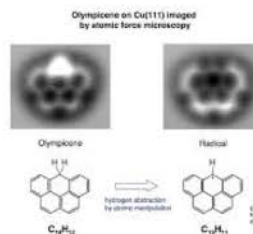
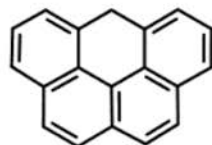
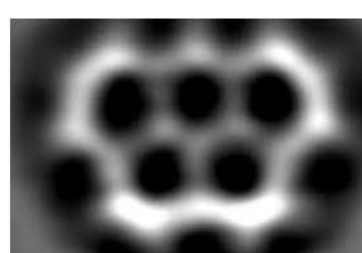
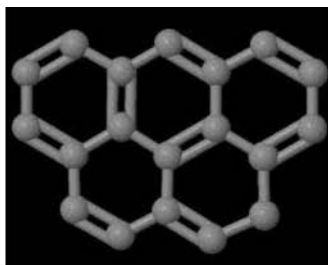
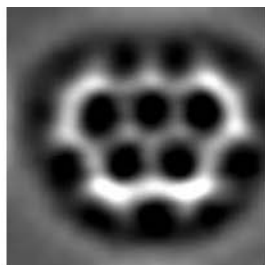
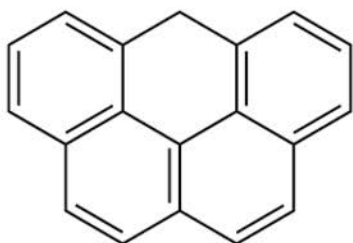
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A crazy idea to celebrate sports: Olympicene



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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."



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



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.

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
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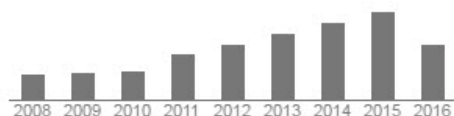
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Environmental Chemistry Compound Identification Using High Resolution Mass Spectrometry Data Integrated to the EPA Chemistry Dashboard

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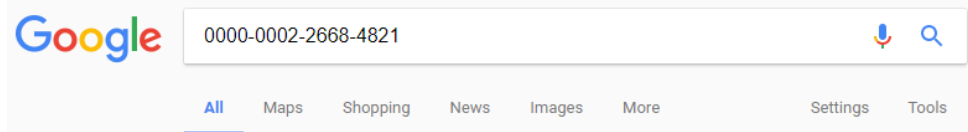
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The new alchemy: Online networking, data sharing and research activity distribution tools for scientists [version 1; referees: 2 approved, 1 approved with reservations]

✉ [Antony J. Williams](#) ¹, [Lou Peck](#) ², [Sean Ekins](#) ³

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Abstract

There is an abundance of free online tools accessible to scientists and others that can be used for online networking, data sharing and measuring research impact. Despite this, few scientists know how these tools can be used or fail to take advantage of using them as an integrated pipeline to raise awareness of their research outputs. In this article, the authors describe their experiences with these tools and how they can make best use of them to make their scientific research generally

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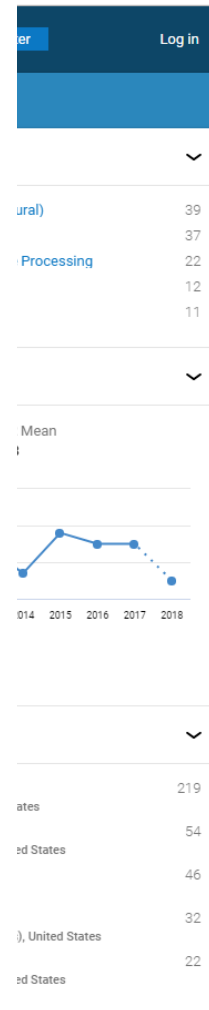
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Structure identification by Mass Spectrometry Non-Targeted Analysis using the US EPA's CompTox Chemistry Dashboard

Identification of unknowns in mass spectrometry based non-targeted analyses (NTA) requires the integration of complementary pieces of data to arrive at a confident, consensus structure. Researchers use chemical reference databases, spectral matching, fragment prediction tools, retention time prediction tools, and a variety of other data to arrive at tentative, probable, and confirmed, if possible, identifications. With the diverse, robust data contained within the US EPA's CompTox Chemistry Dashboard (<https://comptox.epa.gov>), the goal of this research is to identify and implement a harmonized identification tool and workflow using previously generated chemistry data. Data has been compiled from product use, functional use prediction models, environmental media occurrence prediction models, and PubMed references, among other sources. We will report on our development of a visualization tool whereby users can visualize the relative contribution of identification-based metrics on a list of candidate structures and observe the greatest likelihood of occurrence. These data and visualization tools support NTA identification via the Dashboard and demonstrate an open, accessible tool for all users of HRMS data. This abstract does not necessarily represent the views or policies of the U.S. Environmental Protection Agency.

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

