

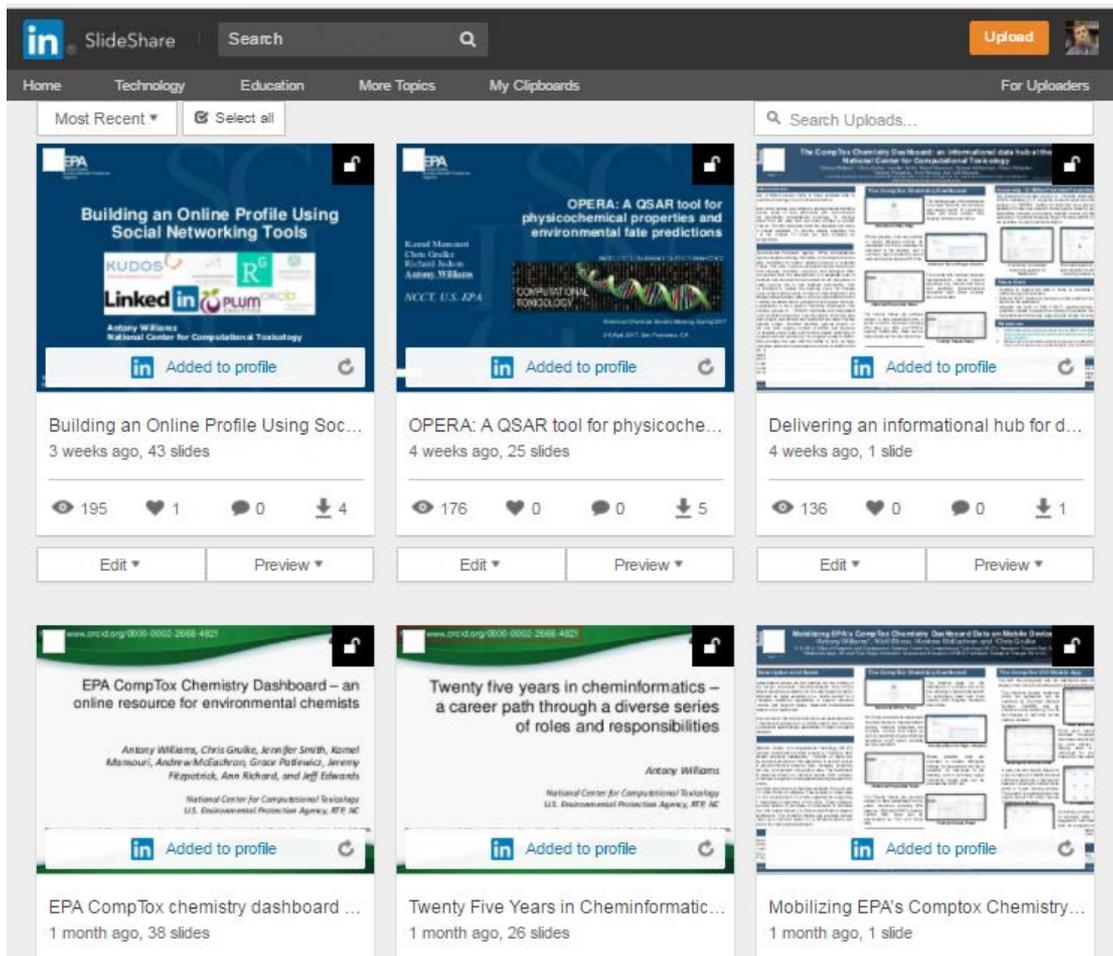
Profile Building, Research Sharing and Data Proliferation using Social Media Tools for Scientists



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 member of the National Center for Computational Toxicology at the EPA. The profile features a grid of six presentations:

- Building an Online Profile Using Social Networking Tools**: 43 slides, 195 views, 1 like, 0 comments, 4 downloads. Added to profile 3 weeks ago.
- OPERA: A QSAR tool for physicochemical properties and environmental fate predictions**: 25 slides, 176 views, 0 likes, 0 comments, 5 downloads. Added to profile 4 weeks ago.
- The CompTox Chemistry Dashboard: an informational data hub at the National Center for Computational Toxicology**: 1 slide, 136 views, 0 likes, 0 comments, 1 download. Added to profile 4 weeks ago.
- EPA CompTox Chemistry Dashboard – an online resource for environmental chemists**: 38 slides, 1 month ago.
- Twenty five years in cheminformatics – a career path through a diverse series of roles and responsibilities**: 26 slides, 1 month ago.
- Mobilizing EPA's CompTox Chemistry Dashboard Data on Mobile Devices**: 1 slide, 1 month ago.

You have help here...

Your NIEHS Library staff are available to assist with questions about ORCID, altmetrics, and other scholarly communication tools.

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**
 - You will claim an **ORCiD**
 - You will invest ~2 hours per month on your profile
 - You have a bigger “Impact” online....

**Think now of something
to share!**

**A Paper
A Report
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
My profile is public

Edit Follow

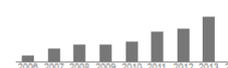
Change photo

Title	Add	More	1-20	Cited by	Year
<input type="checkbox"/> ChemSpider: an online chemical information resource				104	2010
HE Pence, 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
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
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
AJ Williams Drug discovery today 13 (11), 502-506					

Google Scholar

Citation indices

	All	Since 2009
Citations	2939	2010
h-index	32	24
i10-index	92	87



Co-authors Edit...

Kirill Blinov

Sean Ekins

Mikhail Elyashberg

Gary E. Martin

Valery Tkachenko

Yann R. Smeuninx

PLUMX

Antony Williams

Connections in Chemistry



Artifact Summary

Presentation: 266	Data Set: 4
Article: 127	Unknown: 3
Paper: 38	Poster: 3
Video: 28	Patent: 2
Figure: 11	Media: 2
Book: 9	Web Page: 1
Chapter: 7	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**

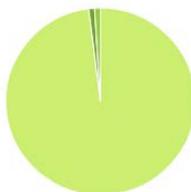
40.36

RG Score

A new way to measure scientific reputation.

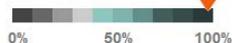
The RG Score takes all your research and turns it into a source of reputation.

- 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

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

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

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Notifications

4 people like your update, "The work done by the..." Phenotypic screening of... 5h

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

2 people like your update, Identification of... 9h

Chantel Nicolas and Dr. Rachelle J. Bienstock

6 people like your update, "Our latest paper..." An automated curation... 9h

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

4 people like your update, "ON KUDOS: Does data..." https://goo.gl/hpU181 10h

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

 Rima HAJJO
likes your update, "I just added a SlideShare to my..." Automatic vs 16h

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

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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

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

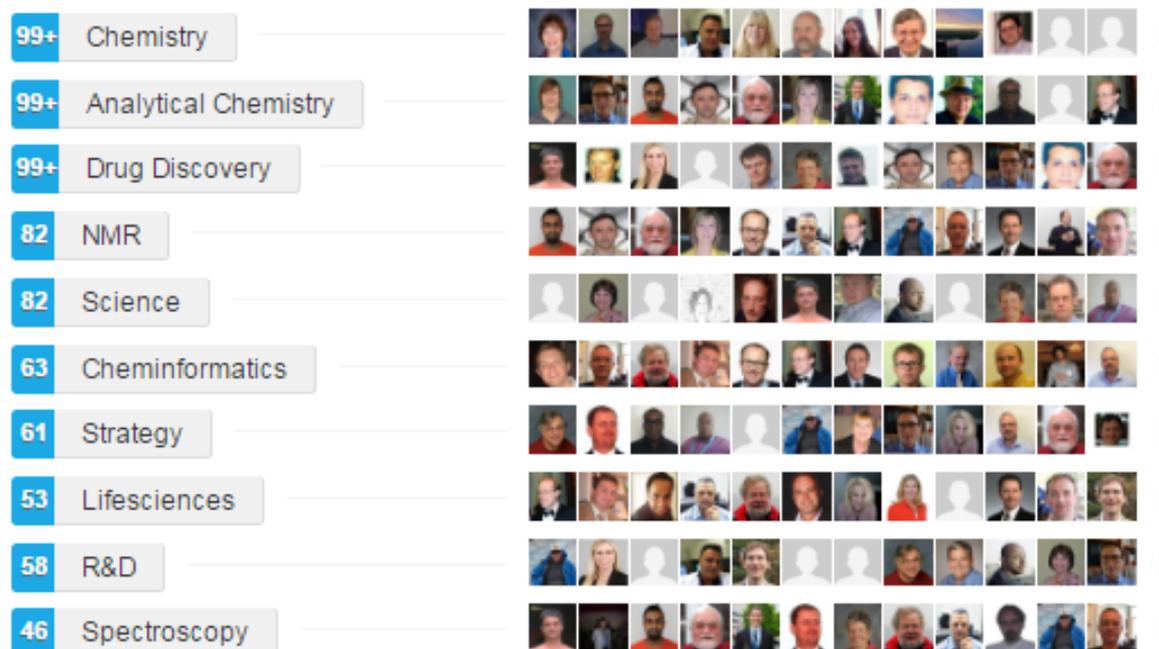
Subject:

Can you recommend me?

Ask for “Endorsements”,

Skills & Endorsements

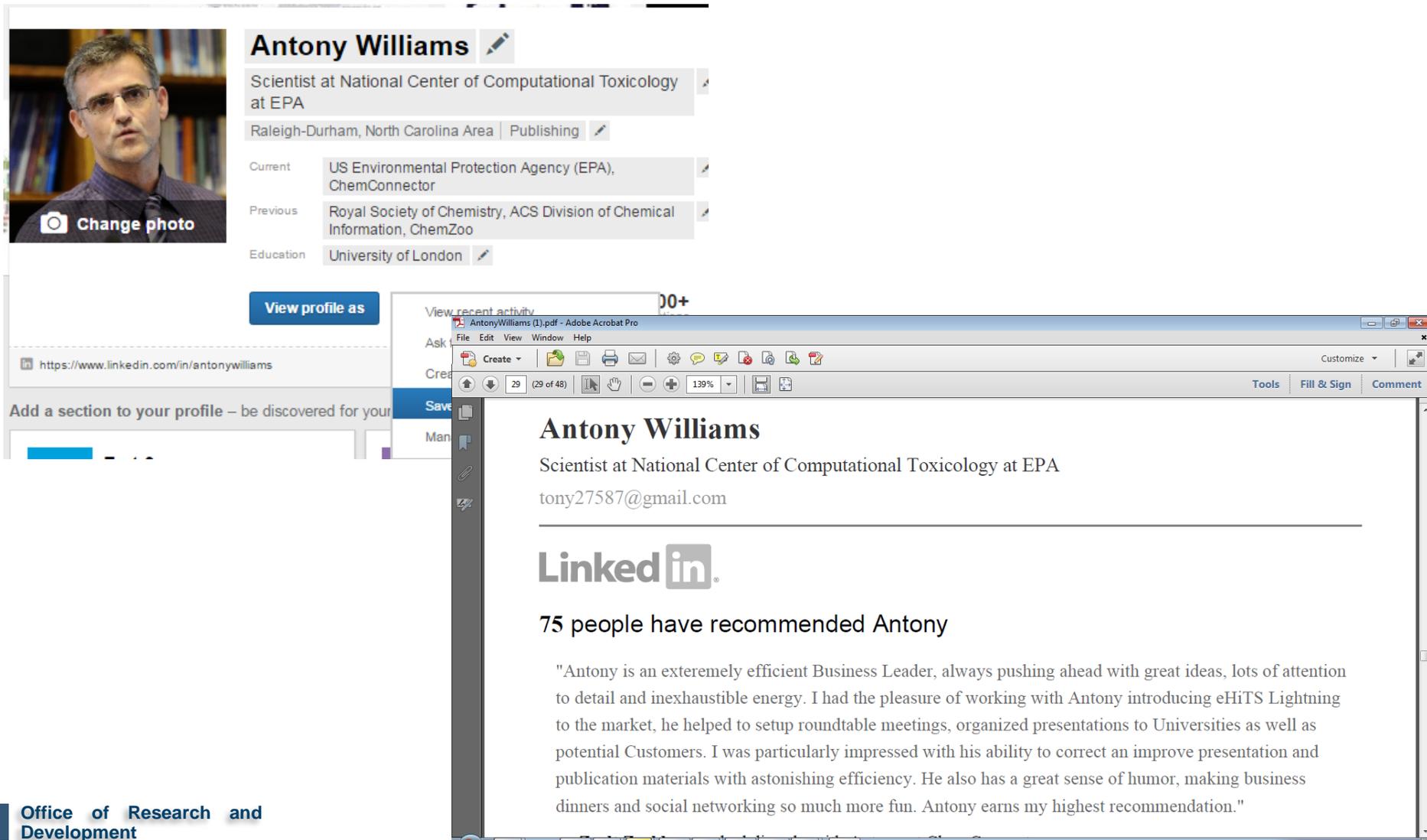
Top Skills



Antony also knows about...



Instant Summary as a PDF



The image shows a LinkedIn profile for Antony Williams, a Scientist at the National Center of Computational Toxicology at EPA. The profile includes a photo, a 'Change photo' button, and a 'View profile as' button. The profile details are as follows:

- Name:** Antony Williams
- Current Position:** Scientist at National Center of Computational Toxicology at EPA
- Location:** Raleigh-Durham, North Carolina Area
- Industry:** Publishing
- Current Organization:** US Environmental Protection Agency (EPA), ChemConnector
- Previous Organization:** Royal Society of Chemistry, ACS Division of Chemical Information, ChemZoo
- Education:** University of London

The profile URL is <https://www.linkedin.com/in/antonywilliams>. A blue button below the profile says "Add a section to your profile – be discovered for your".

Overlaid on the profile is a screenshot of the PDF summary generated in Adobe Acrobat Pro. The PDF content is as follows:

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."



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

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US Environmental Protection Agency (EPA)



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

www.chemconnector.com

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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

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

Anthony 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.

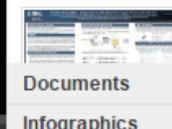
August 21-25, 2016
ACS Fall Meeting, Philadelphia, PA



1 of 34



Presentations 235



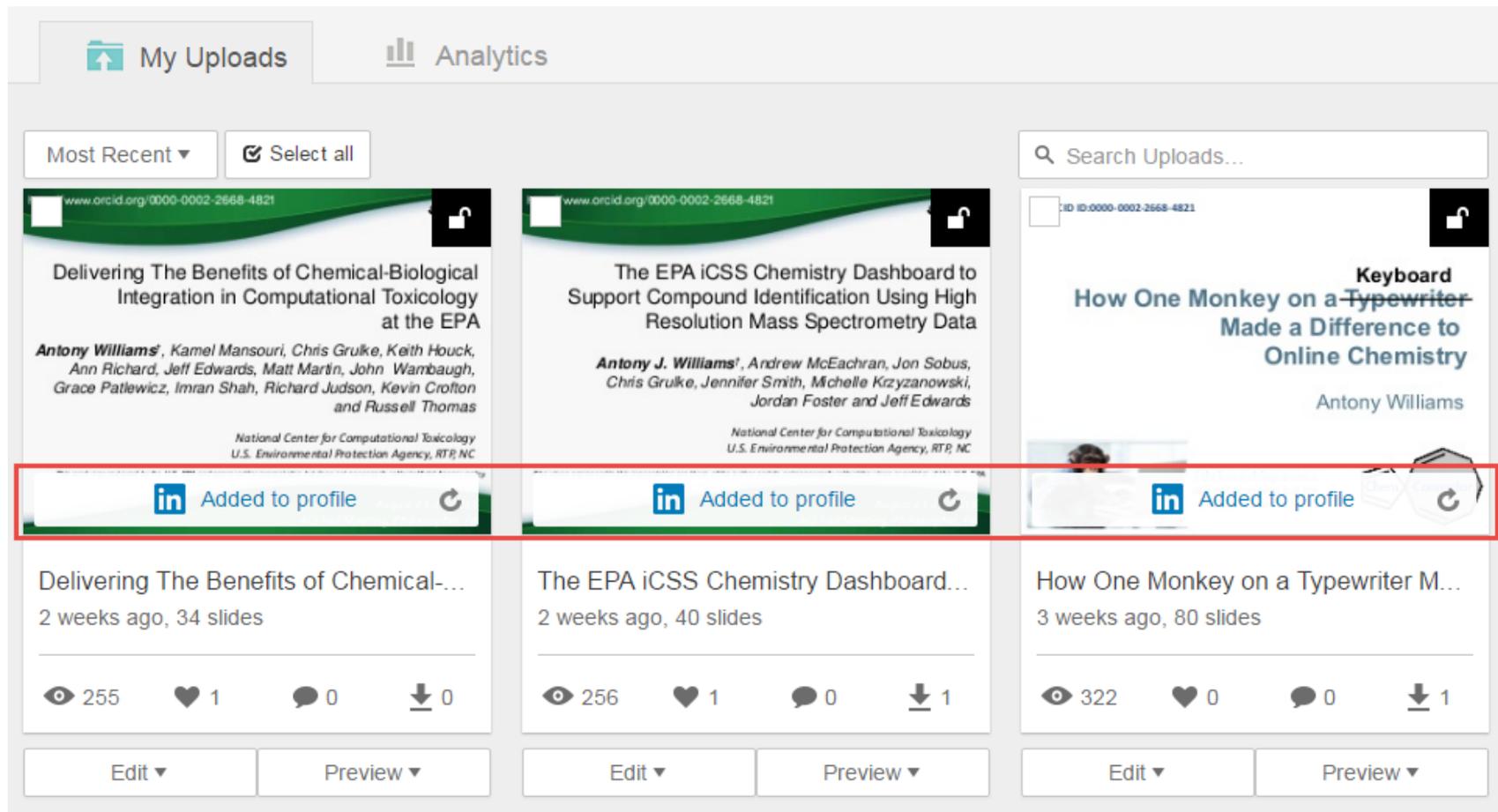
Documents 66

Infographics 0

Videos 0

[Delivering The Benefits of Chemical-Biological Integration in Computational Toxicology at the EPA](#) 255

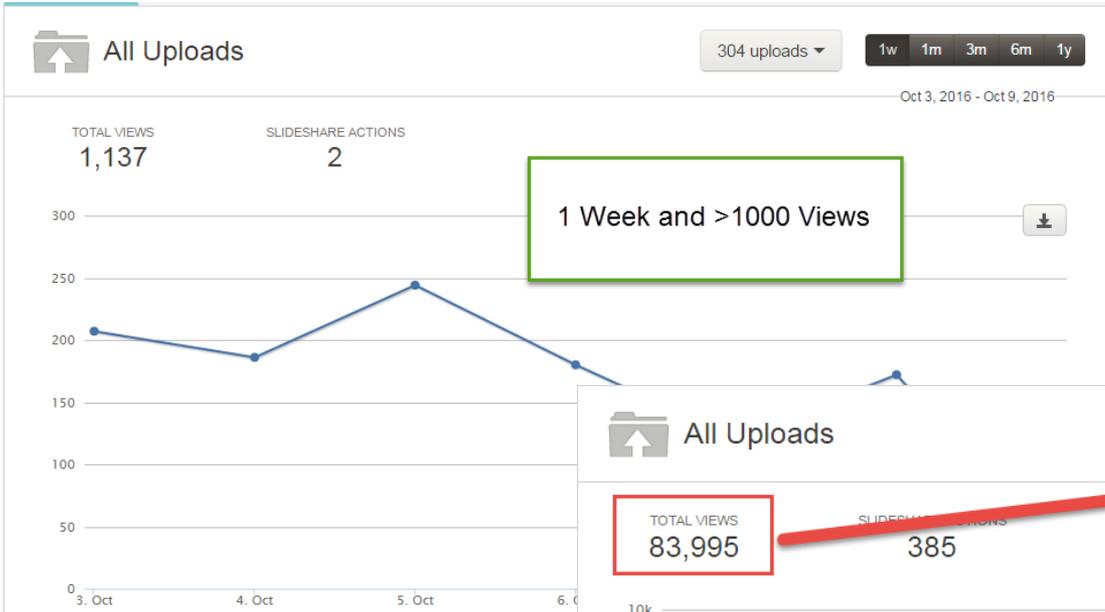
Sharing your works online



The screenshot shows the 'My Uploads' interface with three presentations. Each presentation card includes a title, author list, and engagement metrics. A red box highlights the LinkedIn sharing buttons for each presentation.

Presentation Title	Author(s)	Engagement (Views, Likes, Comments, Downloads)
Delivering The Benefits of Chemical-Biological Integration in Computational Toxicology at the EPA	Antony Williams [†] , Kamel Mansouri, Chris Gruke, Keith Houck, Ann Richard, Jeff Edwards, Matt Martin, John Wambaugh, Grace Patlewicz, Imran Shah, Richard Judson, Kevin Croton and Russell Thomas	255 Views, 1 Like, 0 Comments, 0 Downloads
The EPA iCSS Chemistry Dashboard to Support Compound Identification Using High Resolution Mass Spectrometry Data	Antony J. Williams [†] , Andrew McEachran, Jon Sobus, Chris Gruke, Jennifer Smith, Michelle Krzyzanowski, Jordan Foster and Jeff Edwards	256 Views, 1 Like, 0 Comments, 1 Download
Keyboard How One Monkey on a Typewriter Made a Difference to Online Chemistry	Antony Williams	322 Views, 0 Likes, 0 Comments, 1 Download

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Slideshare – NOT Just Slides

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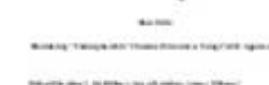


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Antony John Williams 42.06

PhD

Scientist

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

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OVERVIEW

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INFO

STATS

RG SCORE

347

PUBLICATIONS

34k

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15,695

Downloads

2,400

Citations

518.42

Impact Points

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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

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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,

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

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 **Gary E Martin** 41 44.32 · (63)
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 **Mikhail Elyashberg** 41 33.67 · (56)
ACD/Labs

 **Sean Ekins** 41 45.58 · (45)
Collaborations In Chemistry

 **Valery Tkachenko** 41 19.83 · (27)
The Royal Society of Chemistry

Featured research ✎



Presentation: The EPA iCSS Chemistry Dashboard to Support Compound Identification Using High Resolution Mass Spectrometry Data
Antony John Williams
File available · Presentation · Aug 2016

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Article: Encyclopedia of Inorganic and Bioinorganic Chemistry
Alex M. Clark · Antony J. Williams · Sean Ekins
Article · Sep 2016

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 **Andrey Yerin**
Article: **The Need for Systematic Naming Software Tools for Exchange of Chemical Information**
Antony Williams · Andrey Yerin
Article · Jan 2013

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Pause emails that I don't open or interact with for a while	<input checked="" type="checkbox"/>
Include my name in the from field when notifying my connections of my activity	<input checked="" type="checkbox"/>

- Profile settings
- Account settings
- Privacy settings
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- Notification settings**
- Connect with services
- Invitation settings
- Sent invitations



Antony John Williams 43.02
PhD
Computational Chemist
United States Environmental Pr..., Washington, D.C. · Natio...

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Antony John Williams
shared an update

3s ago

Overview Contributions Timeline Info Stats Scores

The interactive Chemical Safety for Sustainability Dashboard 50 Total reads
6 Updates · 3 Collaborators 6 Total followers
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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.

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 Identif...](#)
[Comment](#)

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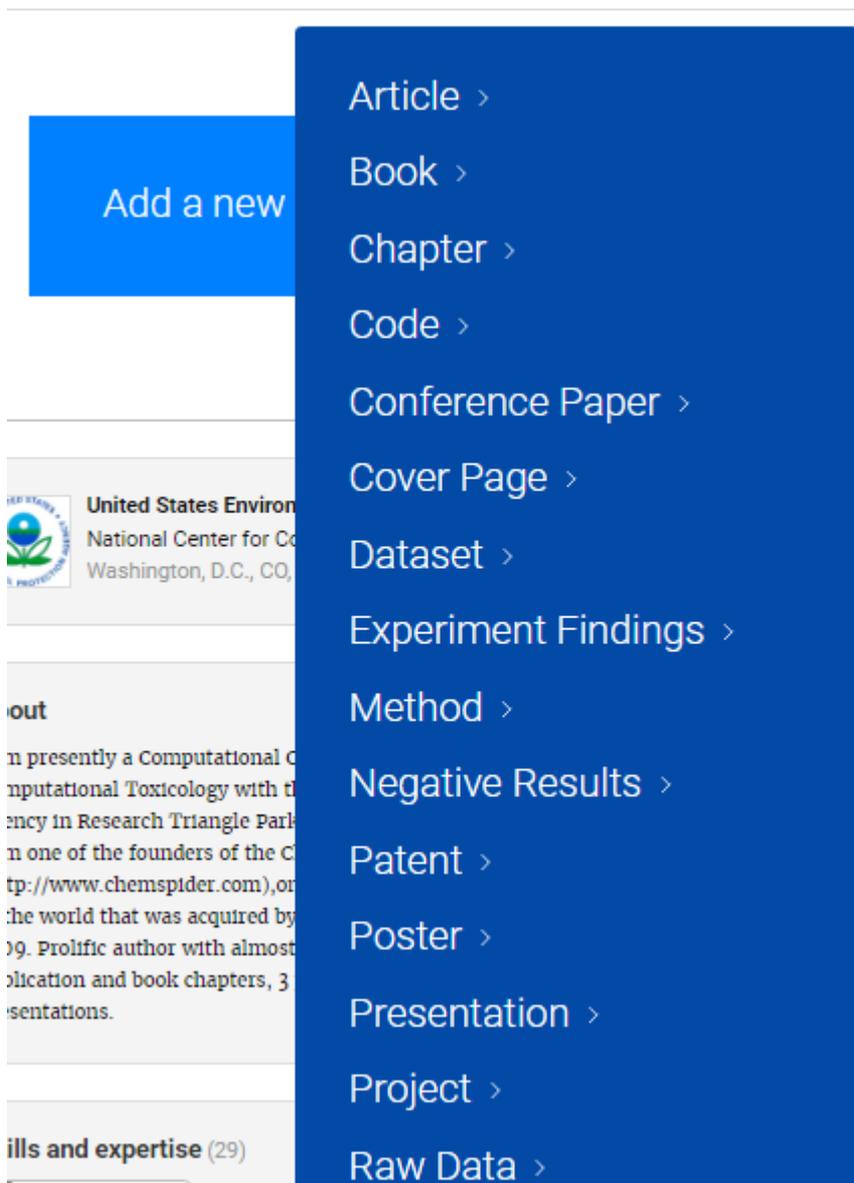
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Skills and expertise (29)
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13 Cheminformatics

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The interactive Chemical Safety for Sustainability Dashboard
[See all followers](#)

Add MANY Flavors of Your Research



The screenshot shows a web interface for adding research. A blue button labeled "Add a new" is visible. Below it, a dropdown menu is open, listing various research types with right-pointing chevrons. The background shows a profile card for a researcher at the United States Environmental Protection Agency, National Center for Computational Toxicology.

- Article >
- Book >
- Chapter >
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- Conference Paper >
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- Method >
- Negative Results >
- Patent >
- Poster >
- Presentation >
- Project >
- Raw Data >

Academia.edu

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



About

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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...
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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](#)



What about “Data Sharing”?



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Antony Williams



Antony Williams

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

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

 United States



63978
item views

11215
item downloads

1
citations

Co-workers & collaborators



Valery Tkachenko



Sean Ekins

senior consultant, Fuquay Varina, NC, USA



Kirill Blinov



Alexey Pshenichnov



Ken Karapetyan



Mikhail Elyashberg

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

Download (284.06 MB)

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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



CATEGORIES

- [Cheminformatics](#)
- [Cheminformatics and Quantitative Structure-Activity Relationships](#)
- [Analytical Spectrometry](#)

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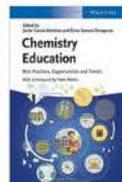
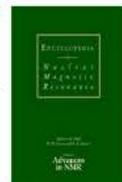
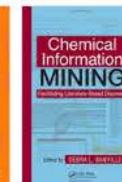
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I am a Computational Chemist at the National Center for Computational Toxicology, part of the Environmental Protection Agency.

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

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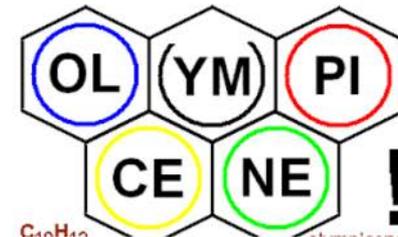
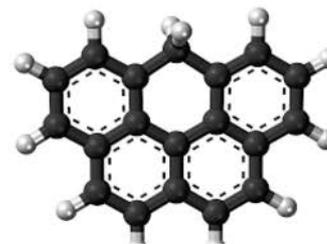
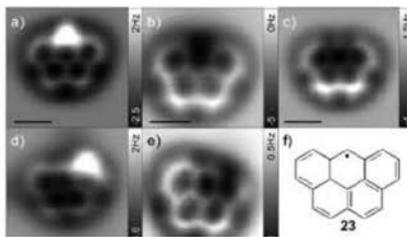
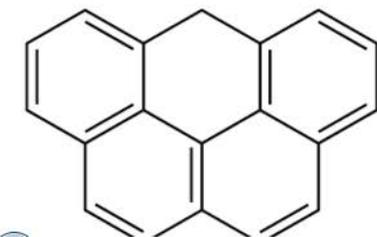
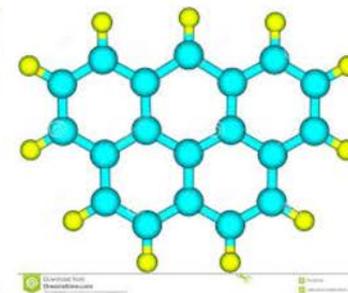
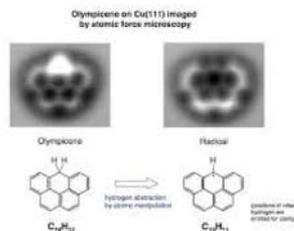
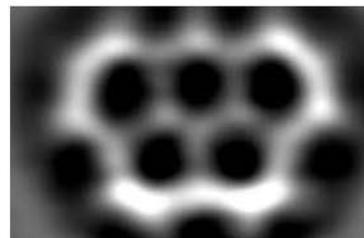
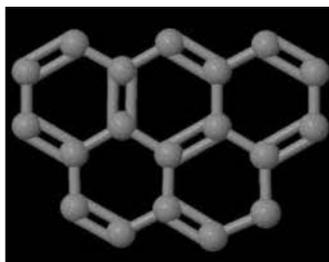
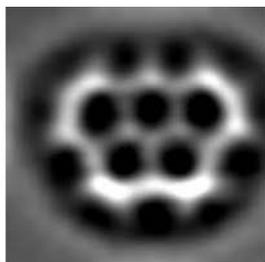
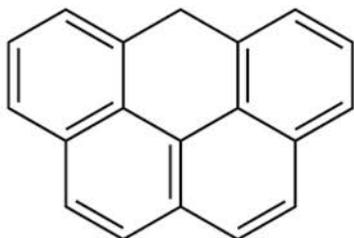
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A crazy idea to celebrate sports: Olympicene



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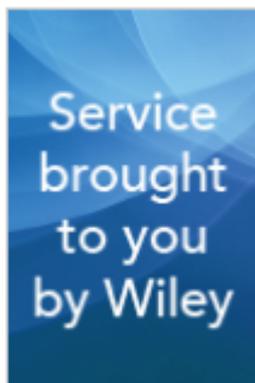
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[In Celebration of Chemistry in Sports. Introducing Olympicine.](#)

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

[Olympicine on ChemSpider](#)

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

[Photo finish for Olympicine in Chemistry World](#)

Chemistry World article about olympicine "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."

[Olympicine on the Chemistry Periodic Table of Videos](#)

Olympicine 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 Olympicine from Concept to Completion on the ChemConnector blog](#)

The story of Olympicine, 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 Olympicine

[An entry about olympicine in Wiktionary](#)

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

[Theoretical Prediction of the Structures and Energies of Olympicine and its Isomers](#)

This paper offers the first theoretical study of the kinetic stability of olympicine 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 olympicine's isomers may be separated into aromatic and diradical isomers. The olympicine molecule has the potential to complement pentacene as an organic semiconductor.

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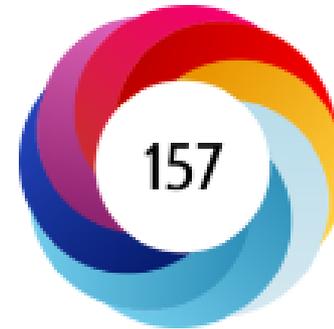
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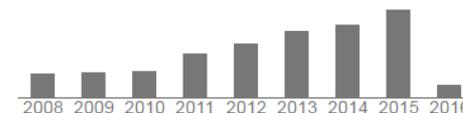
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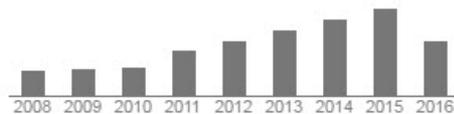
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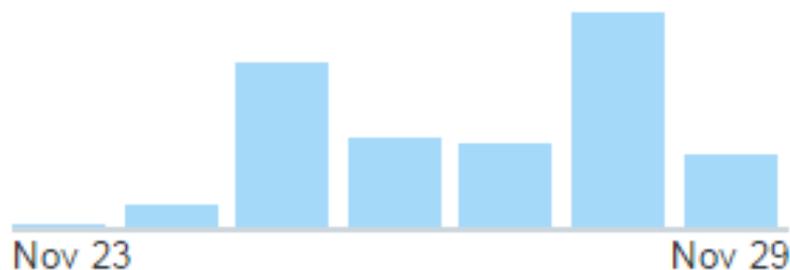
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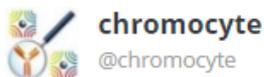
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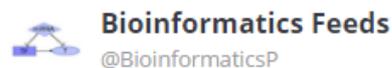
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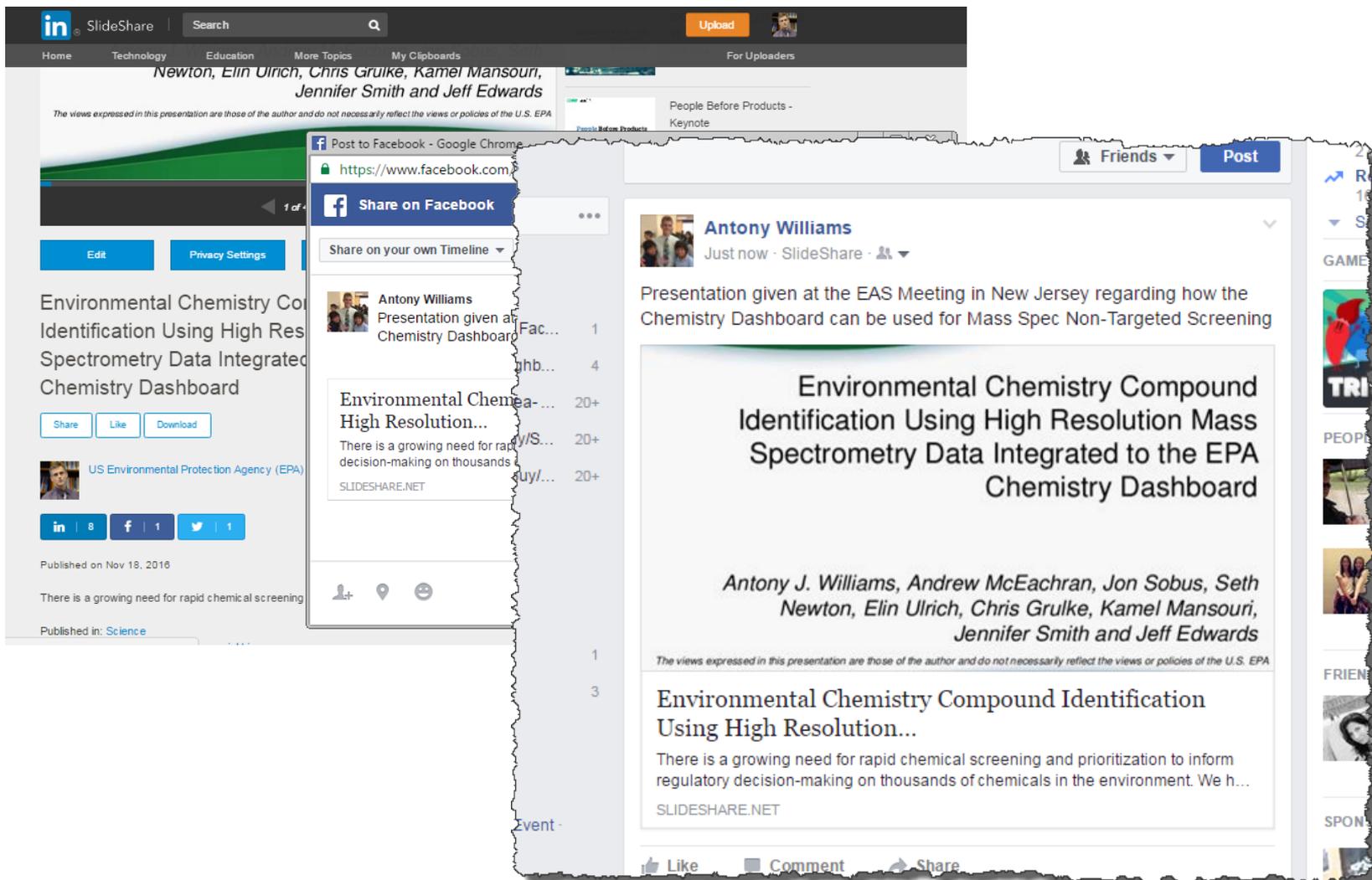
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In November, 2015, a group of publishers asked ORCID to help facilitate communications about their plans to require authors to use an ORCID iD, including hosting this open letter explaining their rationale, developing best practices for using iDs in publishing, and maintaining the signatory list. The publishers' goal is to encourage others to join them in supporting the adoption of ORCID. Publishers signing this open letter are committing to requiring ORCID iDs during 2016 following specific implementation standards.

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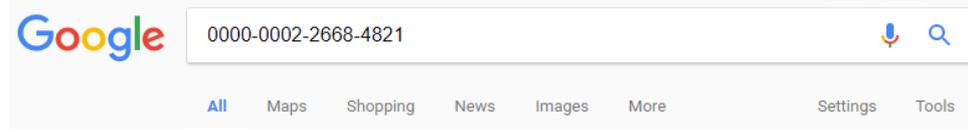
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Antony (Tony) J. Williams received his BSc in 1985 from the University of Liverpool (UK) and PhD in 1988 from the University of London (UK). His PhD research ...

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OPINION ARTICLE

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

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

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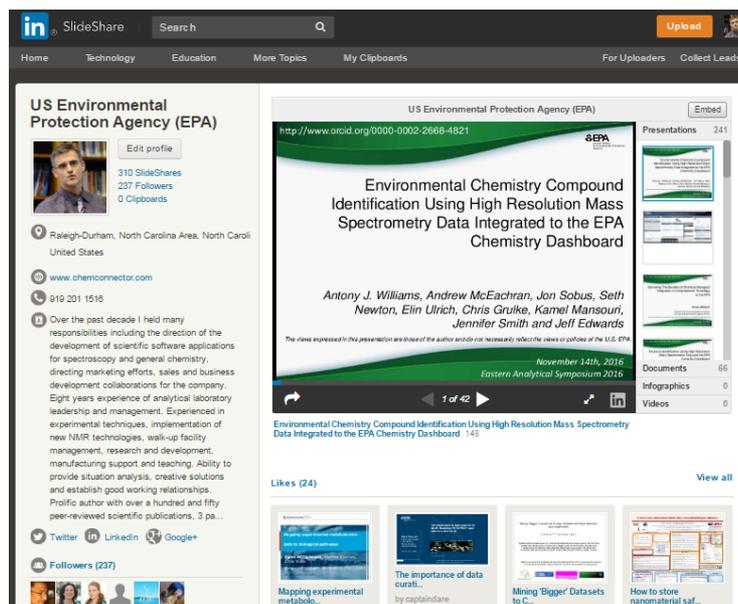
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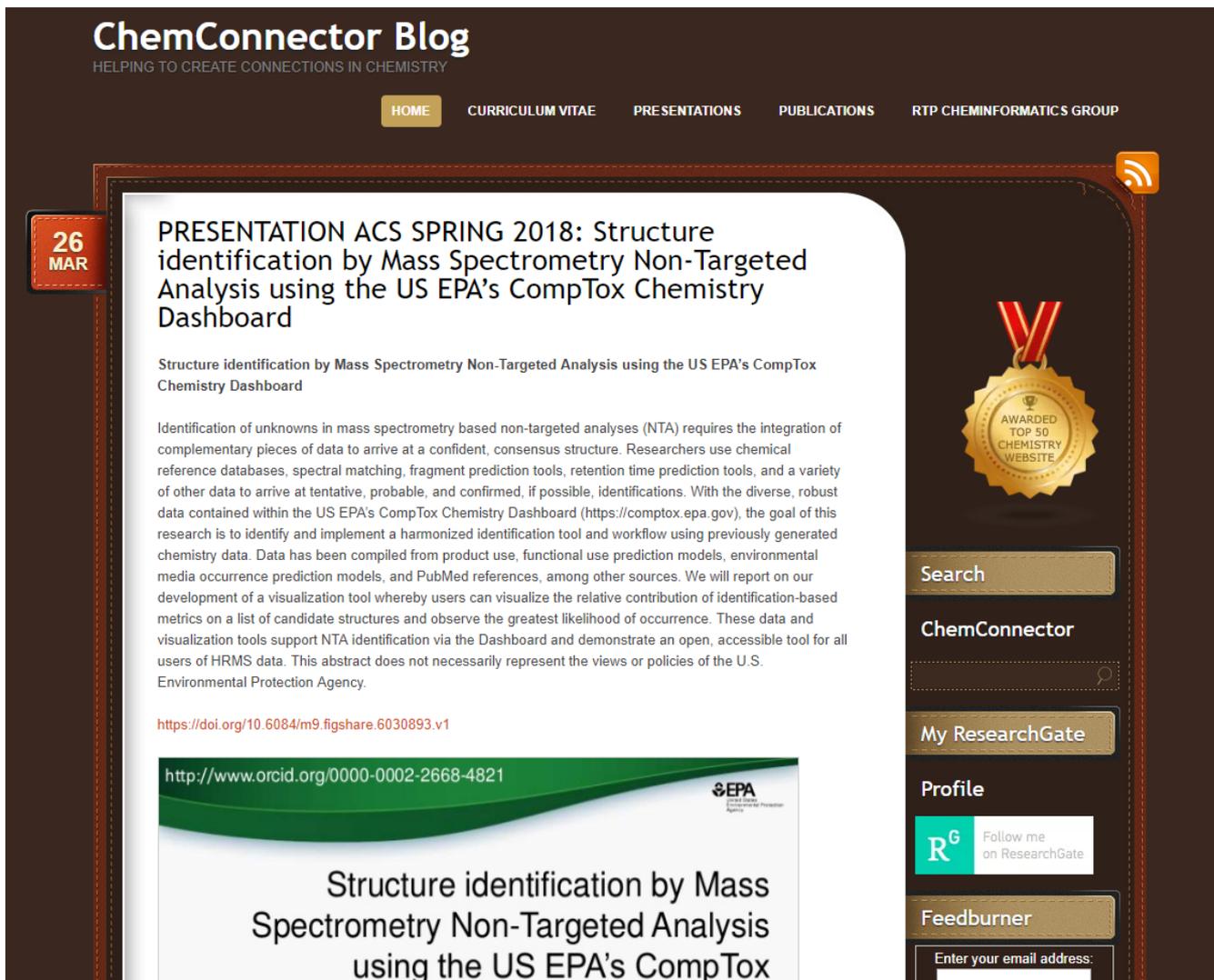
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Structure identification by Mass Spectrometry Non-Targeted Analysis using the US EPA's CompTox Chemistry Dashboard

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

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