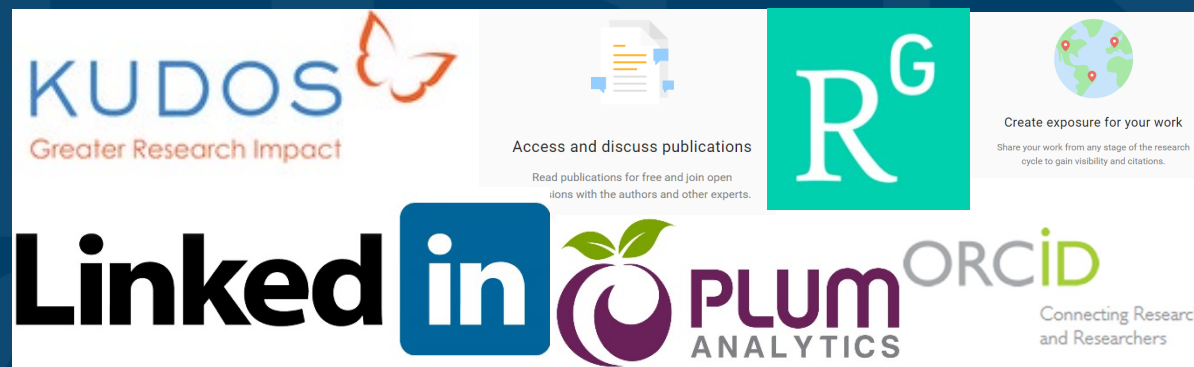


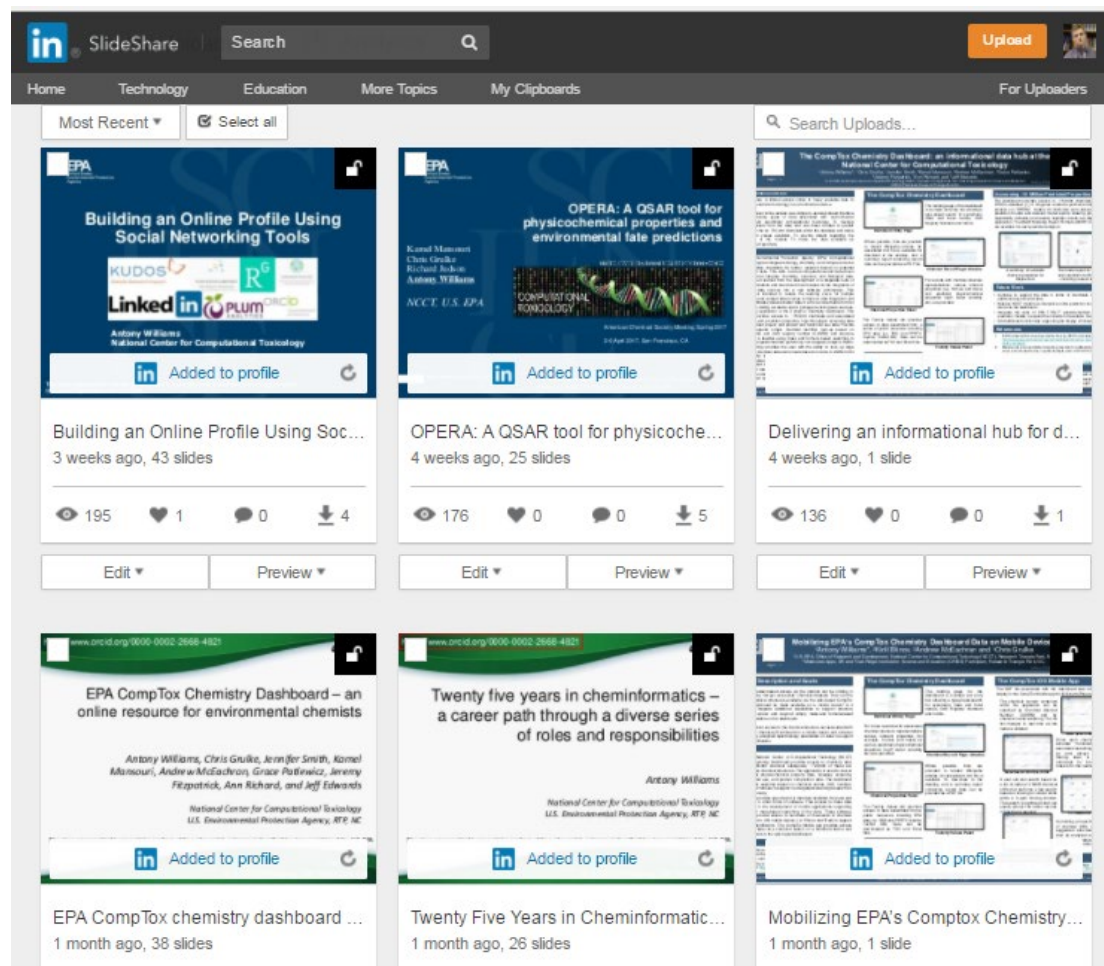
# Using free social media online tools to communicate scientific activities, distribute data and enhance scientific articles post-publication



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

# Various Versions of This Talk

## [www.slideshare.net/AntonyWilliams](http://www.slideshare.net/AntonyWilliams)



The screenshot displays a SlideShare profile for Antony Williams, a National Center for Computational Toxicology (NCCT) scientist at the U.S. Environmental Protection Agency (EPA). The profile features a grid of six presentations:

- Building an Online Profile Using Social Networking Tools**: 43 slides, posted 3 weeks ago, with 195 views and 1 like.
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- Delivering an informational hub for d...**: 1 slide, posted 4 weeks ago, with 136 views and 0 likes.
- EPA CompTox Chemistry Dashboard – an online resource for environmental chemists**: 38 slides, posted 1 month ago, with 136 views and 0 likes.
- Twenty five years in cheminformatics – a career path through a diverse series of roles and responsibilities**: 26 slides, posted 1 month ago, with 136 views and 0 likes.
- Mobilizing EPA's CompTox Chemistry...**: 1 slide, posted 1 month ago, with 136 views and 0 likes.

Each presentation card includes a thumbnail image, a title, a brief description, the number of slides, the upload date, view counts, and like counts. The presentations are primarily related to EPA's CompTox Chemistry Dashboard and the OPERA QSAR tool.

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- **“It's not the job of researchers to become experts in public relations — that's why universities have press offices, says Matt Shipman, research communications lead at North Carolina State University in Raleigh. But he recommends scientists toot their own horns as well.”**

- <http://www.nature.com/news/kudos-promises-to-help-scientists-promote-their-papers-to-new-audiences-1.20346>

# Think about it...


- 100s if not 1000s of hours of research behind a paper. How much work is the PUBLISHER going to do to make sure people find out about your article?? How do you find out about an article???
- Shouldn't **YOU** and your **CO-AUTHORS** invest some time in getting it out to the network???
- A presentation given to a small room of people has a lifetime of “20-30 mins”. A presentation shared online for all to see lives a lot longer. An article shared in the network has a much wider audience.


# Scientists are Evaluated: “Statistics”


- Research datasets
- Scientific software
- Publications – peer-reviewed and many others
- Posters and presentations at conferences
- Electronic theses and dissertations
- Performances in film and audio
- Other forms of research
- **CAVEAT: Make sure you are *allowed* to share**

# How do you share your works?

- There are many tools to share – this talk gives examples
- More examples in this paper: <https://doi.org/10.12688/f1000research.12185.1>


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

 Author details


 Grant information




This article is included in the [Science Policy Research](#) gateway.

**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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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)

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

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

**Antony Williams<sup>†</sup>, 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

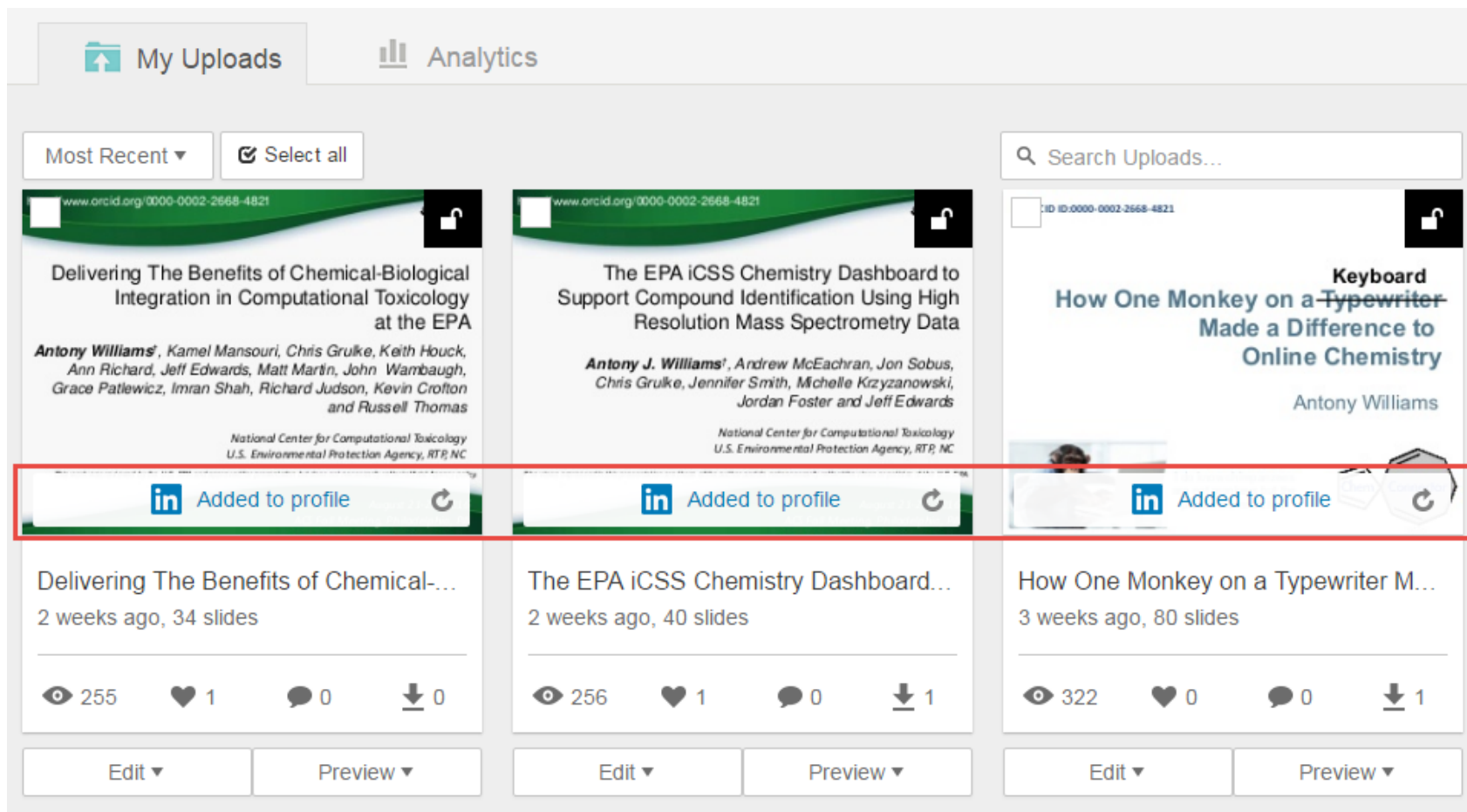
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National Center for Computational Toxicology  
U.S. Environmental Protection Agency, RTP, NC

**The EPA iCSS Chemistry Dashboard to Support Compound Identification Using High Resolution Mass Spectrometry Data**  
Antony J. Williams<sup>†</sup>, Andrew McEachran, Jon Sobus, Chris Grukke, Jennifer Smith, Michelle Krzyzanowski, Jordan Foster and Jeff Edwards  
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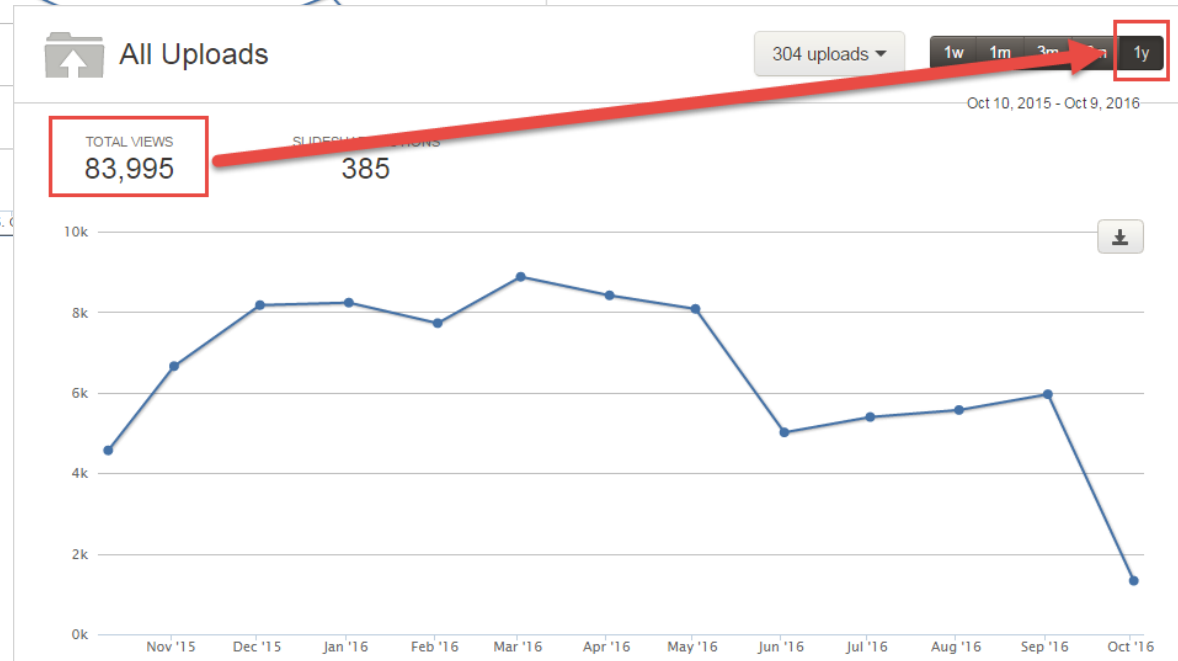
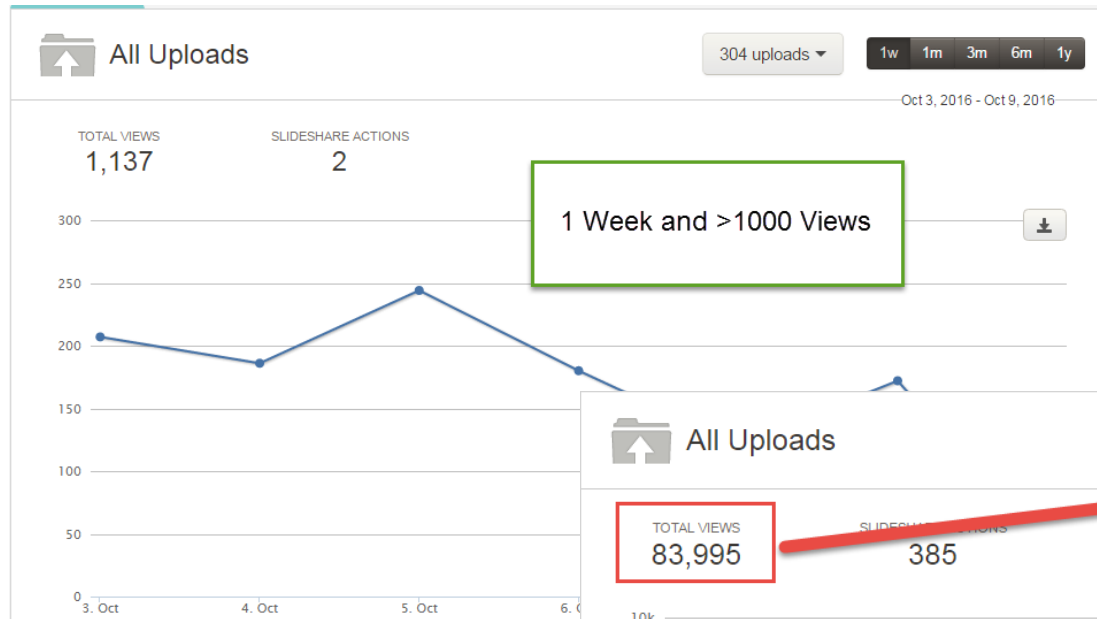
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## Introduction

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I am presently a Computational Chemist at the National Center for Computational Toxicology with the US Environmental Protection Agency in Research Triangle Park, North Carolina. I am one of the founders of the ChemSpider database (<http://www.chemspider.com>), one of the top chemistry databases in the world that was acquired by the Royal Society of Chemistry in 2009. Prolific author with almost 200 peer-reviewed scientific publication and book chapters, 3 patents and 100s of public presentations.

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Agency**



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



**United States Environmental Protection Agency**

National Center for Computational Toxicology

Washington, D.C., CQ, United States


**About**

I am presently a Computational Chemist at the National Center for Computational Toxicology with the US Environmental Protection Agency in Research Triangle Park, North Carolina. I am one of the founders of the chemSpider database (<http://www.chemspider.com>), one of the top chemistry databases in the world that was acquired by the Royal Society of Chemistry in 2009. Prolific author with almost 200 peer-reviewed scientific publication and book chapters, 3 patents and 100s of public presentations.

**Skills and expertise** (29)

15 Cheminformatics

13 Cheminformatics and Computational Chemistry

 **Antony John Williams** shared an update 3s ago

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:

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

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## EPA Comptox Chemistry Dashboard "MS-Ready" File of Structures

17.02.2017, 11:27 by [Antony Williams](#)

The EPA CompTox Chemistry Dashboard (at <https://comptox.epa.gov>) can be used by mass spectrometrists for the purpose of structure identification. A normal formula search would search the exact formula associated with any chemical, whether it include solvents of hydration, salts or multiple components. However, mass spectrometry detects ionized chemical structures and molecular formulae searches should be based on desalted, and desolvated structures with stereochemistry removed. We refer to these as "MS ready structures" and the MS-ready mappings are delivered as Excel Spreadsheets containing the Preferred Name, CAS-RN, DTXSID, Formula, Formula of the MS-ready structure and associated masses, SMILES and InChI Strings/Keys.

### REFERENCES

- <http://link.springer.com/article/10.1007/s00216-016-0139-z>

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## Antony Williams

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

 United States



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

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### Co-workers & collaborators



Chris Grulke



Valery Tkachenko



**Andrew McEachran**  
ORISE Postdoctoral Fellow  
Research Triangle Park, NC



**Sean Ekins**  
senior consultant  
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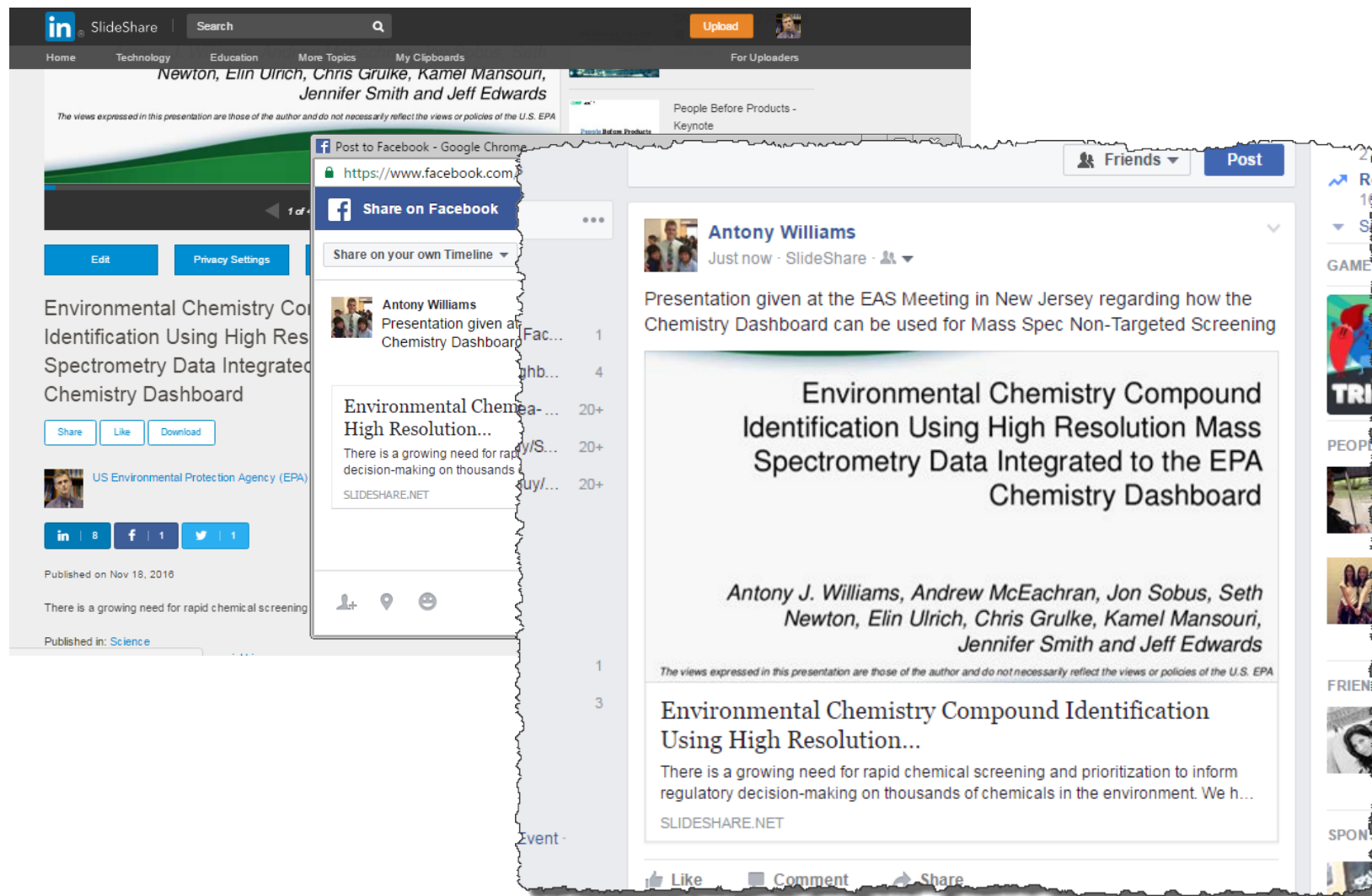
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Newton, Elin Ulrich, Chris Grulke, Kamel Mansouri, Jennifer Smith and Jeff Edwards

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Published on Nov 18, 2016

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Presentation given at the EAS Meeting in New Jersey regarding how the Chemistry Dashboard can be used for Mass Spec Non-Targeted Screening

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

Antony J. Williams, Andrew McEachran, Jon Sobus, Seth Newton, Elin Ulrich, Chris Grulke, Kamel Mansouri, Jennifer Smith and Jeff Edwards

The views expressed in this presentation are those of the author and do not necessarily reflect the views or policies of the U.S. EPA

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## Antony J. Williams



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

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

Founder of ChemZoo Inc., the host of ChemSpider (www.chemspider.com). ChemSpider is an open access online database of chemical structures and

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Beautiful Data: The Stories Behind Elegant Data Solutions by Toby Segaran and Jeff Hammerbacher (Jul 31, 2009)

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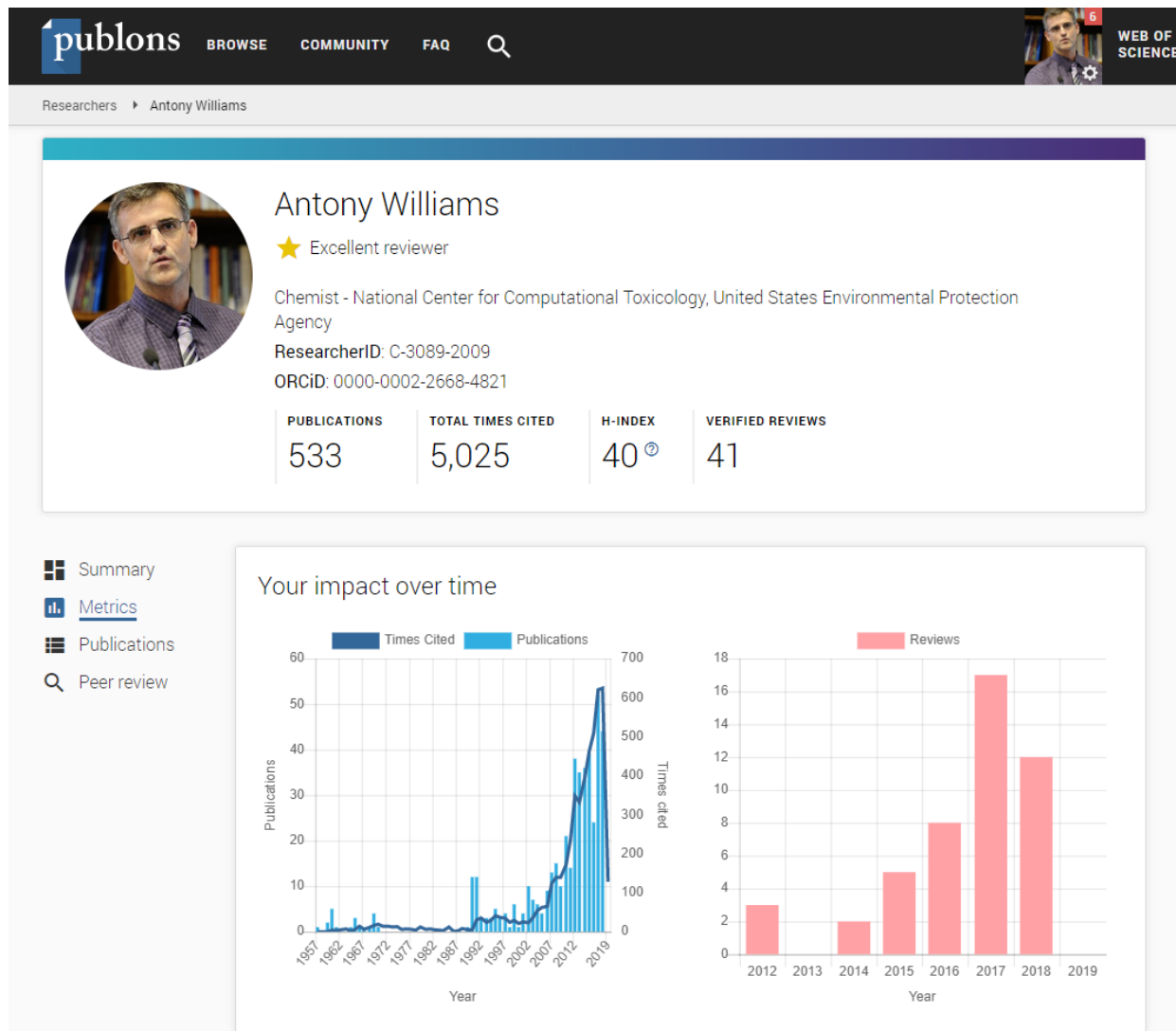
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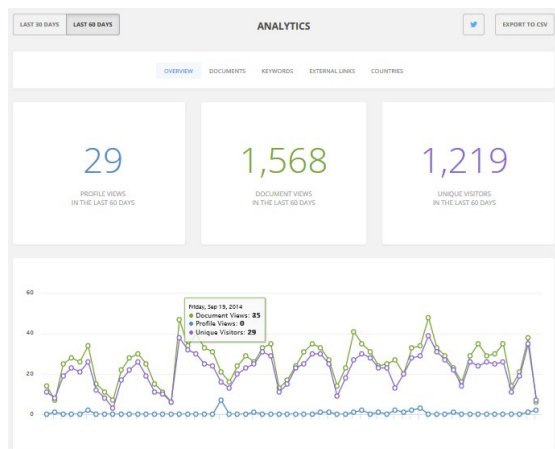
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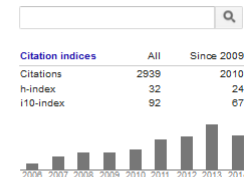
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S Ekins, AJ Williams, MD Krasovski, JS Freundlich Drug discovery today 16 (7), 298-310					
<input type="checkbox"/> <b>Open PHACTS: semantic interoperability for drug discovery</b>				72	2012
AJ Williams, L Harland, P Groth, S Pettifer, C Chichester, EL Willighagen, ... Drug discovery today 17 (21), 1188-1198					
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[Kirill Blinov](#)

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- 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

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**Antony John Williams**  
PhD  
VP Strategic Development  
The Royal Society of Chemistry · Chemistry

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Antony John Williams, 0000-0002-2668-4821

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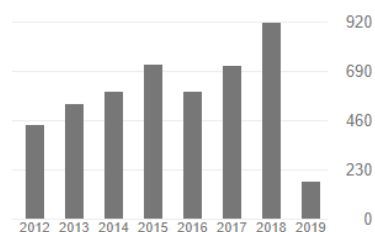
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<input type="checkbox"/>	<a href="#">In silico repositioning of approved drugs for rare and neglected diseases</a> S Ekins, AJ Williams, MD Krasowski, JS Freundlich Drug discovery today 16 (7), 298-310		205	2011
<input type="checkbox"/>	<a href="#">Online chemical modeling environment (OCHEM): web platform for data storage, model development and publishing of chemical information</a> I Sushko, S Novotarskyi, R Körner, AK Pandey, M Rupp, W Teetz, ... Journal of computer-aided molecular design 25 (6), 533-554		202	2011
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<input type="checkbox"/>	<a href="#">Computer-assisted structure verification and elucidation tools in NMR-based structure elucidation</a> ME Elyashberg, AJ Williams, GE Martin Progress in Nuclear Magnetic Resonance Spectroscopy 53 (1-2), 1-104		116	2008
<input type="checkbox"/>	<a href="#">Identification of "Known Unknowns" Utilizing Accurate Mass Data and ChemSpider</a> APVT James L. Little, Antony J. Williams Journal of the American Society of Mass Spectrometry 23 (1), 179-85		113	2012

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# Alt-Metrics Manifesto





Antony Williams

US Environmental Protection Agency Computational Chemist

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[Analytical and Bioanalytical Chemistry](#)

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

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

Authors

[Authors and affiliations](#)

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

Rapid Communication

First Online: 16 December 2016

DOI: 10.1007/s00216-016-0139-z

Cite this article as:

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

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



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16 Sep 2017




**Egon Willighagen**  
@egonwillighagen

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10 Sep 2017



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# 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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# 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**

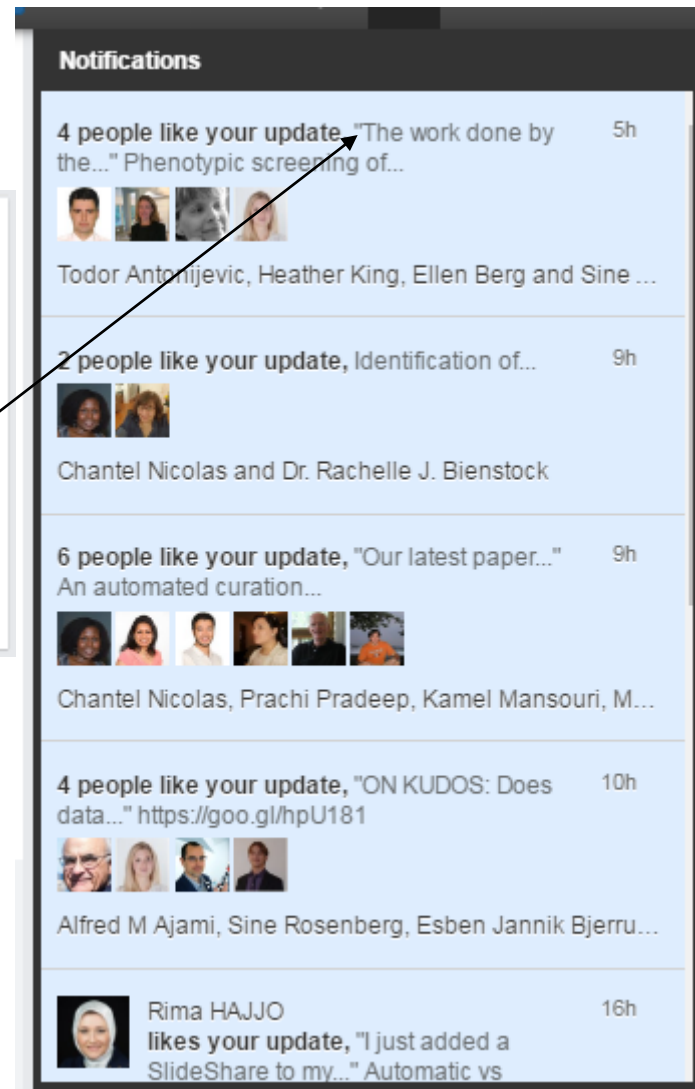
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Founder and CEO at Collaborations ...

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**ORCID ID**  
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United States  
**Keywords**  
NMR, Computer-assisted Structure  
Elucidation, Chemistry, ChemSpider,  
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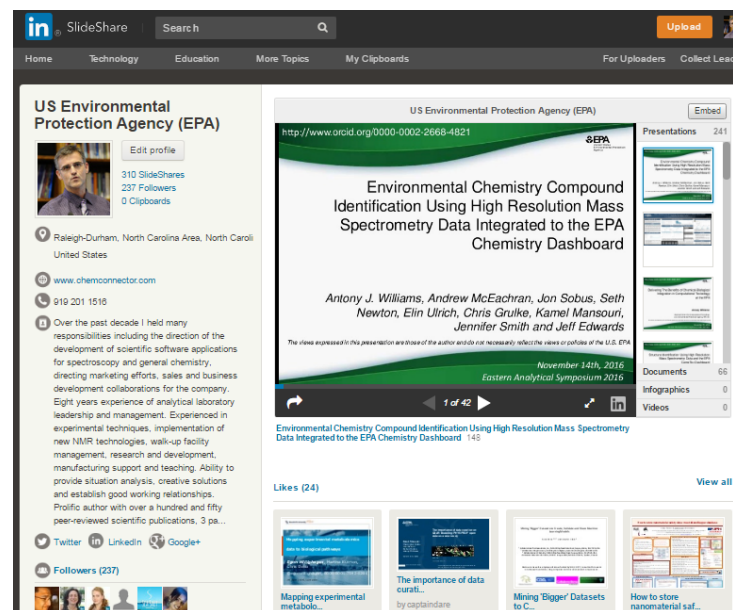
<http://www.nature.com/news/kudos-promises-to-help-scientists-promote-their-papers-to-new-audiences-1.20346>

...choose **two or three** social-media platforms, invest the time to get them set up, and then spend perhaps **two hours a month** keeping them current. If nothing else, he says, build a **LinkedIn** profile as an online CV, claim and update an **ORCID ID**, and log peer-review activities on **Publons.com**.

...a research paper is itself the end product of an extraordinary investment of time and energy. It takes thousands of hours of research, data analysis, writing and peer review, he says. “**Shouldn't you** put at least 10 to 20 hours of work into making sure that you can **get the message out to relevant people?**”

# Various Versions of This Talk

[www.slideshare.net/AntonyWilliams](http://www.slideshare.net/AntonyWilliams)



Email: [williams.antony@epa.gov](mailto:williams.antony@epa.gov)