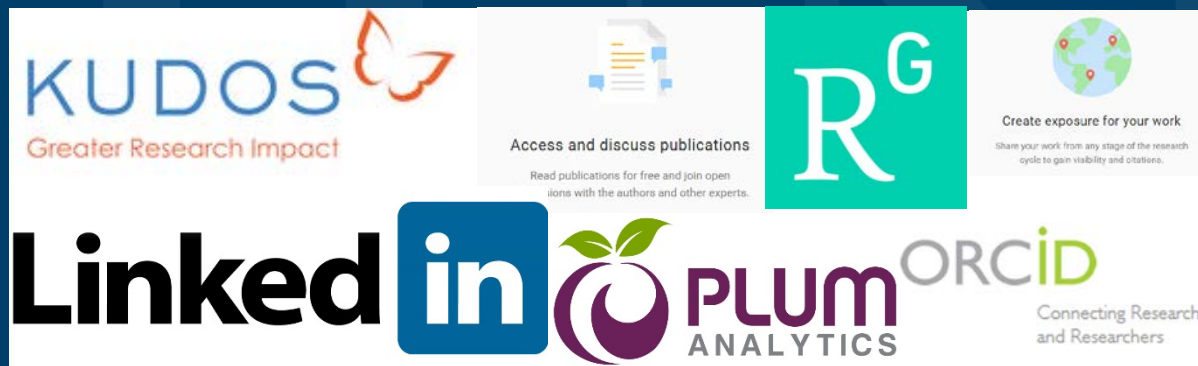


# Freely available online tools for communicating chemistry through social media



**Antony Williams**  
United States Environmental Protection Agency  
National Center for Computational Toxicology

# 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”

# 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”
- **Consider yourself as the most appropriate “marketer” for your science – your papers, your presentations, your data and your overall public presence**

# 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
- 
- Who informs the community of availability???

# 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???

# 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 Primary CV is my Blog

Helping to Create Connections in Chemistry

## ChemConnector Blog

Home Curriculum Vitae Presentations Publications RTP Cheminformatics Group

### Open Science for Identifying "Known Unknown" Chemicals

<http://dx.doi.org/10.1021/acs.est.7b01908>

Posted by [tony](#) in [MS Structure Identification](#), [Open Access Publishing](#), [Open Science..all its forms](#), [Publications and Presentations](#) on May 7, 2017

I am happy to announce the publishing of an article regarding "Open Science for Identifying "Known Unknown" Chemicals" at <http://dx.doi.org/10.1021/acs.est.7b01908>. I have been involved with two other articles about the identification of "Known Unknowns".

The first one was a ChemSpider article: "Identification of "known unknowns" utilizing accurate mass data and ChemSpider". *Journal of The American Society for Mass Spectrometry*. **23**: 179-185. [doi:10.1007/s13361-011-0265-y](https://doi.org/10.1007/s13361-011-0265-y)."

The second one was a recent article from the EPA: "Identifying known unknowns using the US EPA's CompTox Chemistry Dashboard". *Analytical and Bioanalytical Chemistry*. **409**: 1729-1735. [doi:10.1007/s00216-016-0139-z](https://doi.org/10.1007/s00216-016-0139-z)."

The most recent publication was a collaboration with [Emma Schymanski from Eawag](#) and it was a real pleasure to write this together. If you are interested in how Open Science can contribute to the challenges associated with the identification of known unknowns check out our latest publication!



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MY PLUM ANALYTICS

 **Antony J. Williams**  
Connections in Chemistry

Artifact Summary

 Lecture / Presentation:  Research Artifact: 5

# Blogging was VERY Important

- The blog was very important in building reputation for my projects
- Networks can take a long time to build...
- With an established network it is easier to move a message across multiple channels
- There is no one channel everyone uses!  
Spread the message
- I use blogging a lot less now...



# Twitter – fast messaging to bigger content



**ChemConnector**  
@ChemConnector

ORCID: 0000-0002-2668-4821 I'm the ChemConnector - connecting chemists and curating data across the internet. ALL CONTENT IS UNOFFICIAL AND NOT RELATED TO EPA

Tweets **10.5K** Following **1,256** Followers **3,160** Likes **2,001** Lists **2** Moments **0** [Edit profile](#)

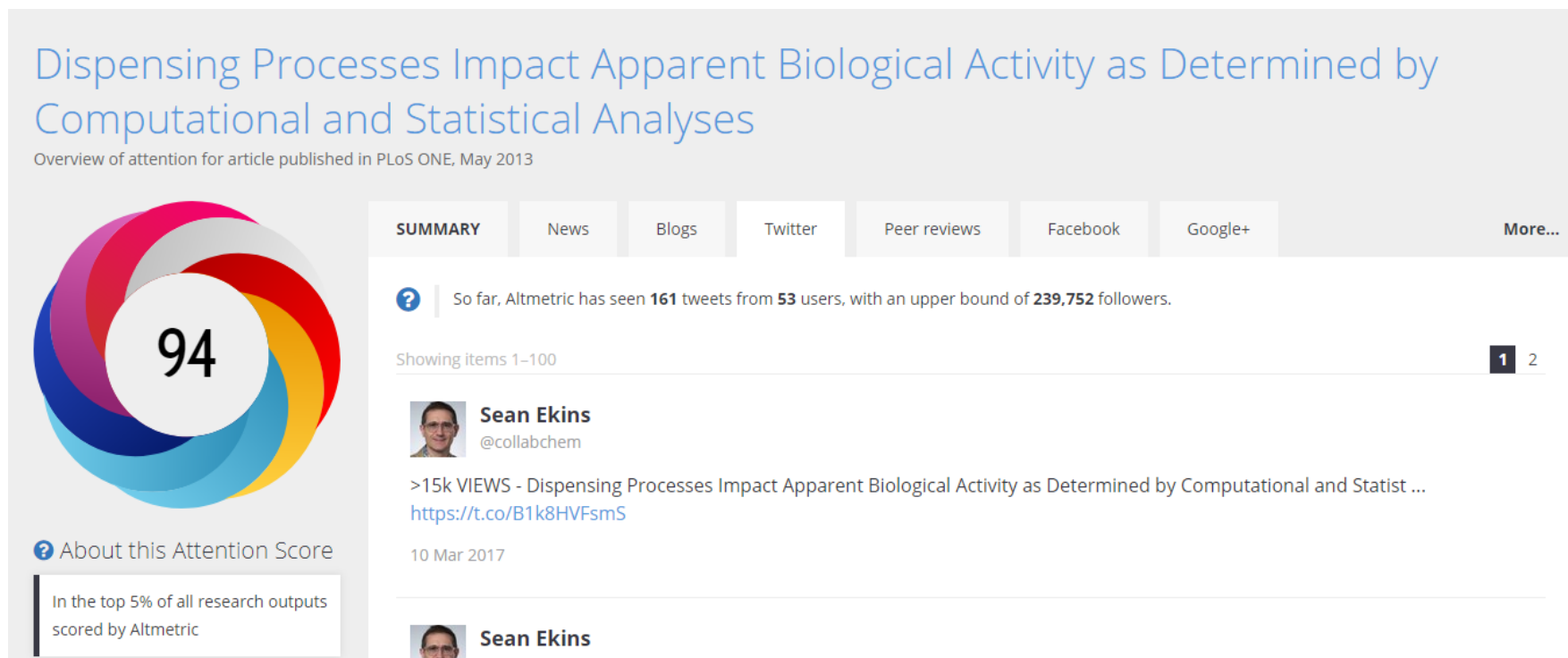
**Tweets** **Tweets & replies** **Media**

**ChemConnector** @ChemConnector · 9h  
Two comments on our article and still awaiting peer review. We'd appreciate other public feedback if possible?? [f1000research.com/articles/6-131...](https://f1000research.com/articles/6-131...)

**Your Tweet activity**  
Your Tweets earned **1,198 impressions** over the last **24 hours**


# Twitter for Marketing


- Use Twitter to point to your publications
- Altmetric shows its of value! More later...



# I have a YouTube Channel

<https://www.youtube.com/user/ChemSpiderMan/videos>


Antony Williams
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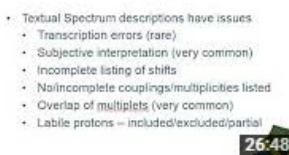


Providing Access to a Million NMR Spectra Online...

28:05

Our dire need to mandate data standards and expectations for...

60 views • 2 years ago



Textual Spectrum descriptions have issues

- Transcription errors (rare)
- Subjective interpretation (very common)
- Incomplete listing of shifts
- Nail/incomplete couplings/multiplicities listed
- Overlap of multiplets (very common)
- Labile protons – included/excluded/partial

26:48

Providing Access to a Million Spectra Online

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Give me kudos for taking responsibility for self-marketing...

22:27



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www.labfolder.com

37:48



Scilligence ELN Demo

47:30



RSPACE Demo March 4 2015

52:42



Dotmatics Demo

1:00:03



Open PHACTS

38:52



Delivering on the promise of a chemistry data repository for th...

12:19



Jean-Claude Bradley – a Visionary in the field of Open Science

Antony Williams

6:47



Data Repository

24:14



Data Repository

44:14



The Next XXX Years at RSC for Cheminformatics

22:08



Give me KUDOS for my Publications

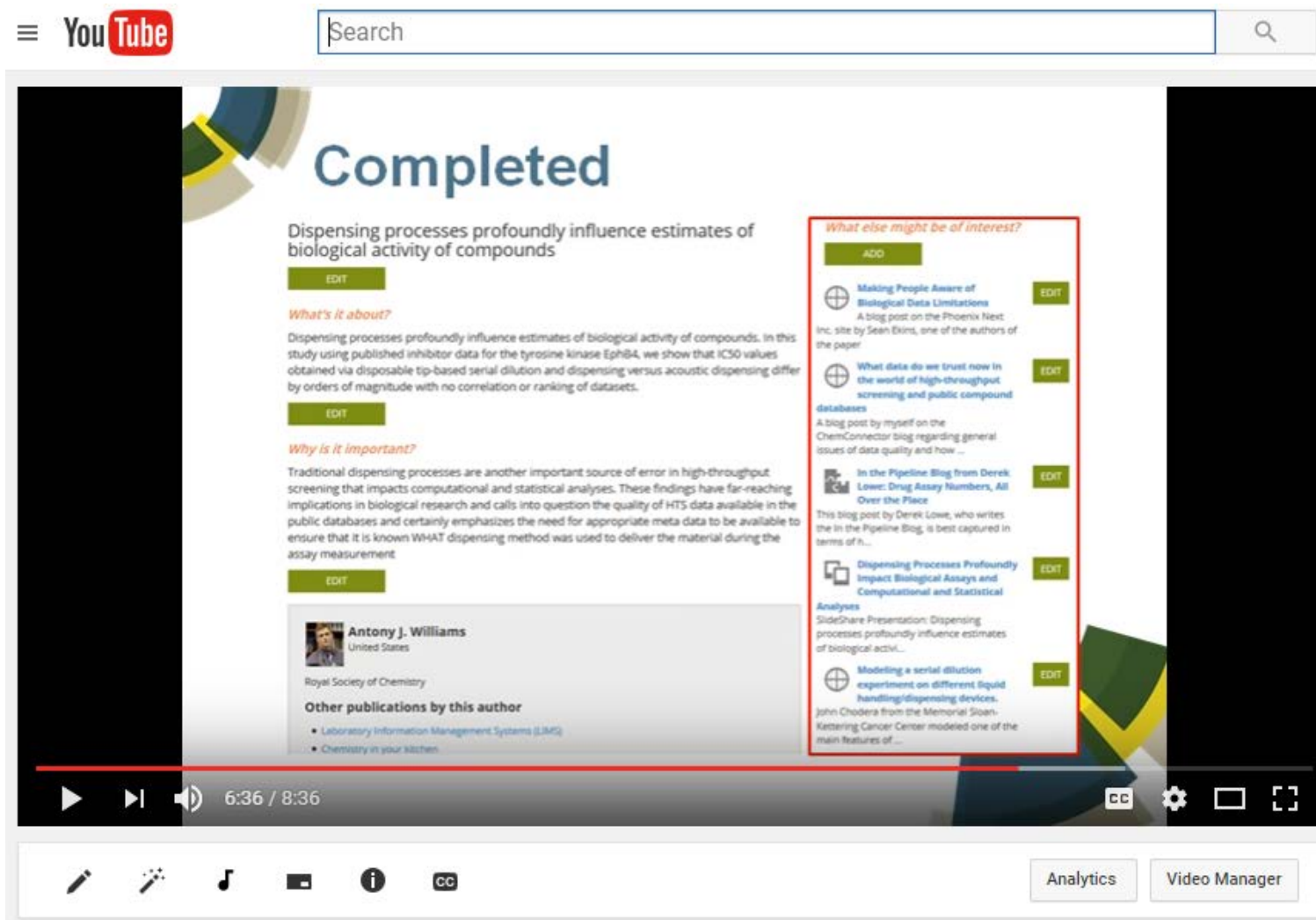
8:37



The Chemist Online and How to Expose Your Science to the World

22:42

# YouTube Sharing



The screenshot shows a YouTube video player interface. At the top, there is a search bar and a menu icon. The video player itself displays a presentation slide titled "Completed". The slide content includes a title, a description, and a list of other publications by the author, Antony J. Williams. The video player controls at the bottom show the video is at 6:36 / 8:36. Below the video player, there are icons for editing, sharing, and other functions, along with buttons for "Analytics" and "Video Manager".

**Completed**

Dispensing processes profoundly influence estimates of biological activity of compounds

*What's it about?*

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

*Why is it important?*

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

**Antony J. Williams**  
United States  
Royal Society of Chemistry

**Other publications by this author**

- Laboratory Information Management Systems (LIMS)
- Chemistry in your kitchen

*What else might be of interest?*

**ADD**

- Making People Aware of Biological Data Limitations** **EDIT**  
A blog post on the Phoenix Next, Inc. site by Sean Exlins, one of the authors of the paper
- What data do we trust now in the world of high-throughput screening and public compound databases** **EDIT**  
A blog post by myself on the ChemConnector blog regarding general issues of data quality and how ...
- In the Pipeline Blog from Derek Lowe: Drug Assay Numbers, All Over the Place** **EDIT**  
This blog post by Derek Lowe, who writes the In the Pipeline Blog, is best captured in terms of ...
- Dispensing Processes Profoundly Impact Biological Assays and Computational and Statistical Analyses** **EDIT**  
SlideShare Presentation: Dispensing processes profoundly influence estimates of biological activi...
- Modeling a serial dilution experiment on different liquid handling/dispensing devices.** **EDIT**  
John Chodera from the Memorial Sloan-Kettering Cancer Center modeled one of the main features of ...

6:36 / 8:36

Analytics Video Manager



# The 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),<br>ChemConnector                   |
| Previous  | Royal Society of Chemistry, ACS Division of Chemical<br>Information, ChemZoo |
| Education | University of London   |

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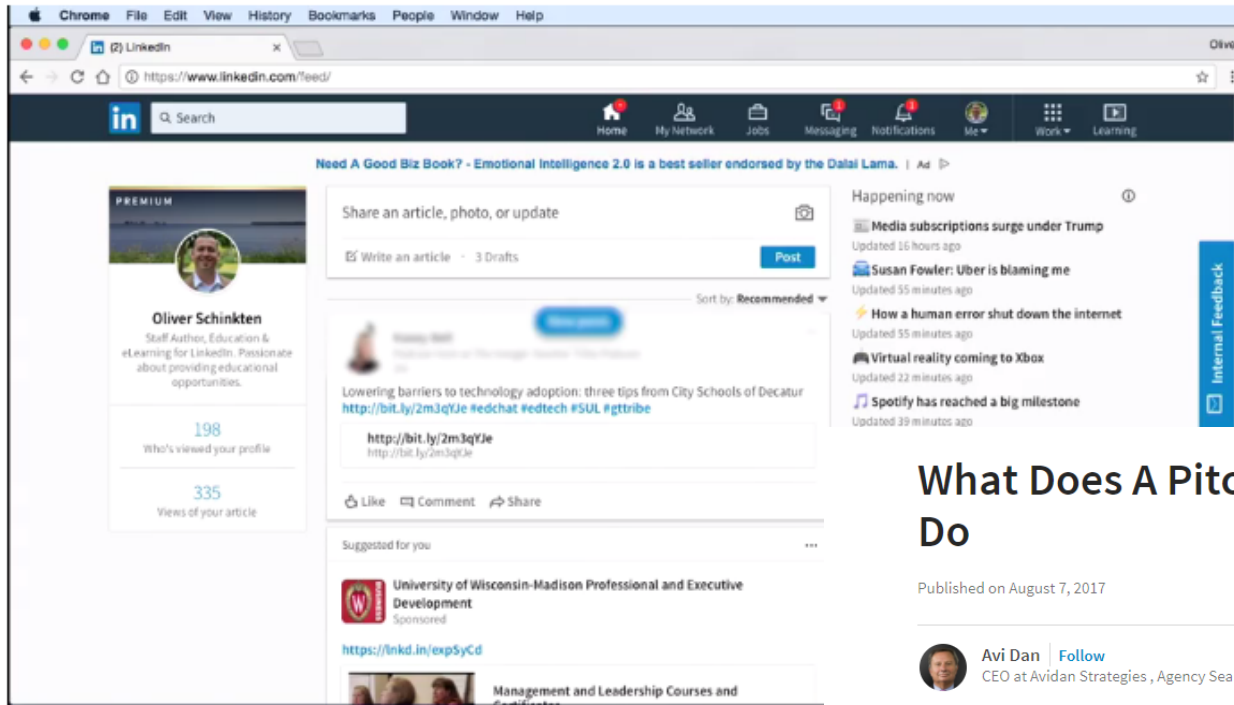
 <https://www.linkedin.com/in/antonywilliams>

 Contact Info

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

# as a publishing platform

## Publishing Articles on LinkedIn - Overview



## What Does A Pitch Consultant Actually Do

Published on August 7, 2017



Avi Dan | Follow  
CEO at Avidan Strategies, Agency Search and Compensation Con...



We're always looking for new ways for members to contribute professional insights. The platform allows members, in addition to Influencers, to publish articles at

A CMO who spends well over \$1 billion on advertising told me a couple of years ago, "When it comes to choosing a creative agency I manage the pitch myself. Only when it comes to picking a media agency or a digital agency, areas that I don't feel as comfortable with, I hire a pitch consultant." Eighteen months later he called my pitch consulting firm and confided: "I'm going to fire the creative agency that I hired last year. We need to talk." The main reason for the divorce was an irreconcilable culture clash.

Hiring an agency is one of the most important and challenging tasks for

# Your Postings Get Networked



**Antony Williams**

Scientist at National Center of Computational Toxicology at EPA

18h

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

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

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

Like • Comment • Share • 4

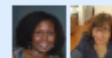
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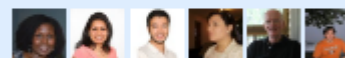
Todor Antonijevic, Heather King, Ellen Berg and Sine ...

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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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United States

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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)

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### 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.

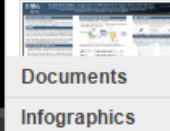
August 21-25, 2016  
ACS Fall Meeting, Philadelphia, PA



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National Center for Computational Toxicology  
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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 Grulke, Jennifer Smith, Michelle Krzyzanowski, Jordan Foster and Jeff Edwards

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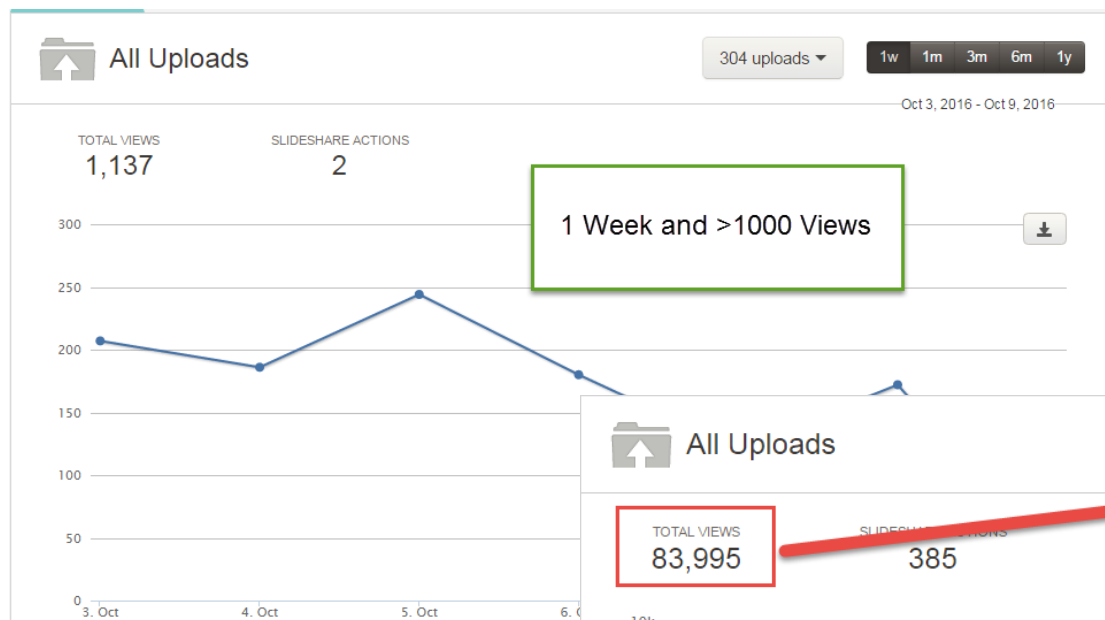
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Antony John Williams  42.06

PhD

Scientist

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United States Environmental Protection Agency  
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Corvallis, NC, United States

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

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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# Academia.edu

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



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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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**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

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## Antony J. Williams



### Author Updates

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

See more



Blog post  
NCSU Presentation: Data integration and building a profile for yourself as an online scientist.  
This is a presentation I gave at North Carolina State University hosted by Denis Fournier.  
Data integration and building a profile  
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My talk at ACS Boston: Value of the mediawiki platform for providing content to the chemistry community  
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Blog post  
ACS Boston: The driving needs for analytical data exchange standards and the potential impacts on the chemical sciences  
This presentation was given at the ACS Boston meeting with the following abstract  
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Blog post  
Last day at the Royal Society of Chemistry - So long and thanks for all the spuds  
Today is my last day of employment for the Royal Society of Chemistry. It will be almost six years since I joined RSC when ChemSpider was acquired.  
4 months ago [Read more](#)

Blog post  
Beyond the Paper CV (i) build an online profile as a scientist  
This presentation was given at the UNICRS meeting (http://www.unicrs.org/2010/09/04/)  
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4.5 (19)

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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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ensing processes profoundly influence estimates of biological activity of compounds

### Tell readers what your publication is about

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

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

### Tell readers the significance of your publication

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

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

# A publication as a point-in-time

- From a publication how do you cite forward?
  - to errata?
  - to your later publications?
  - to electronic notebook pages?
  - to blog posts about your work?
  - to other peoples related publications?
  - to reinterpreted data you don't publish?

# The Article...




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Full Paper

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

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

First published: 2 December 2014 [Full publication history](#)

DOI: 10.1002/chem.201404877 [View/save citation](#)

# Claimed...

## Single Molecule Microscopy and Properties of Olympicene: Olympic Rings at the molecular level



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

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

Published in: Chemistry - A European Journal

Publication date: December 2014

Publisher: Wiley

DOI: <http://dx.doi.org/10.1002/chem.201404877>

Report a data issue 

# Enriched...

## Resources

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



### In Celebration of Chemistry in Sports. Introducing Olympicene.

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



### Olympicene on ChemSpider

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



### Photo finish for Olympicene in Chemistry World

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



### 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.

# Alt-Metrics Manifesto

# Impact



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**Antony Williams**  

US Environmental Protection Agency Computational Chemist

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
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52. K. Blinov, M. Elyashberg, E. R. Martirosian, S. G. Molodtsov, **A. J. Williams**, M. H. M. Sharaf, P. L. Schiff, Jr., R. C. Crouch, G. E. Martin, C. E. Hadden, and J. E. Guido, Quindolinocryptotackeine: The Elucidation of a Novel Indoloquinoline Alkaloid Structure through the Use of Computer-Assisted Structure Elucidation and 2D-NMR, *Magn. Reson. Chem.*, 41, 577-584 (2003). [Link](#)

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

 Antony J. Williams <sup>1</sup>, Lou Peck <sup>2</sup>, Sean Ekins <sup>3</sup>

 Author details

 Grant information



METRICS

875

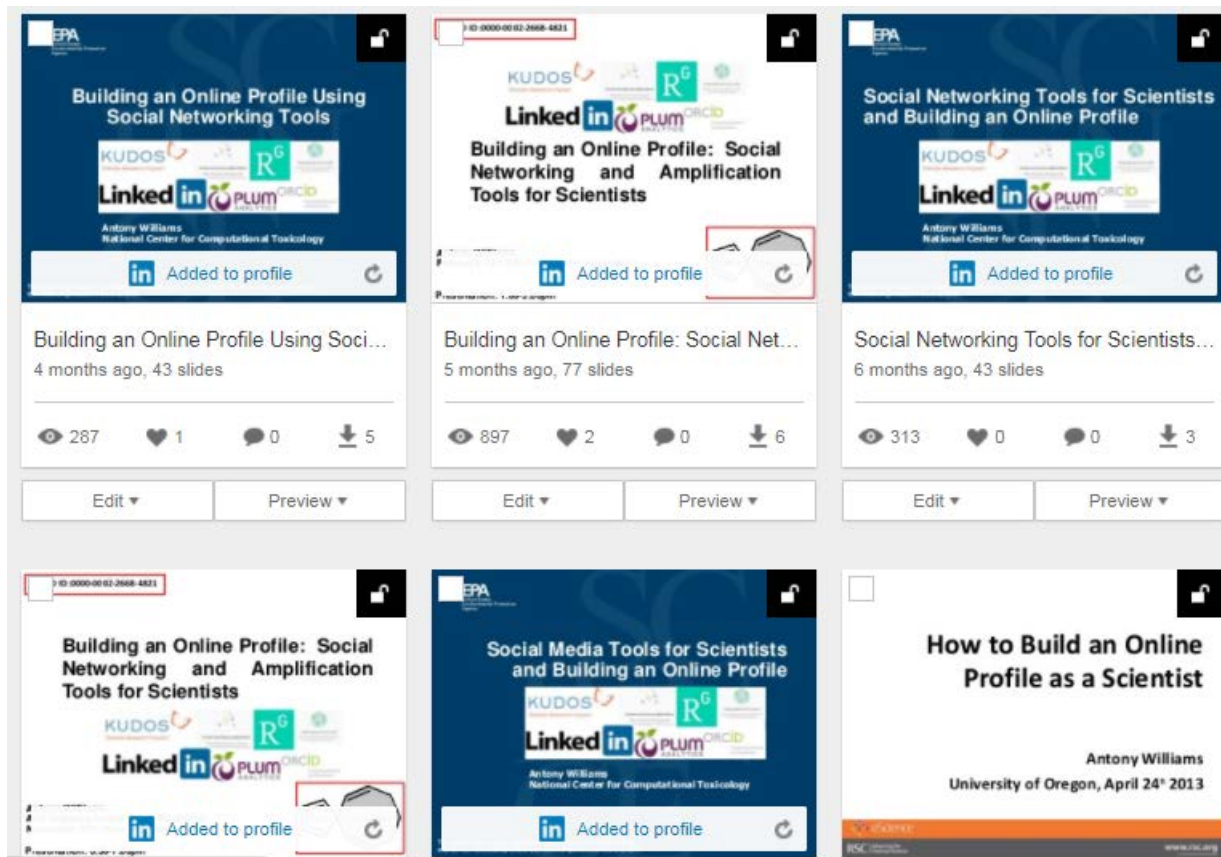
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[www.slideshare.net/AntonyWilliams](http://www.slideshare.net/AntonyWilliams)



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

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