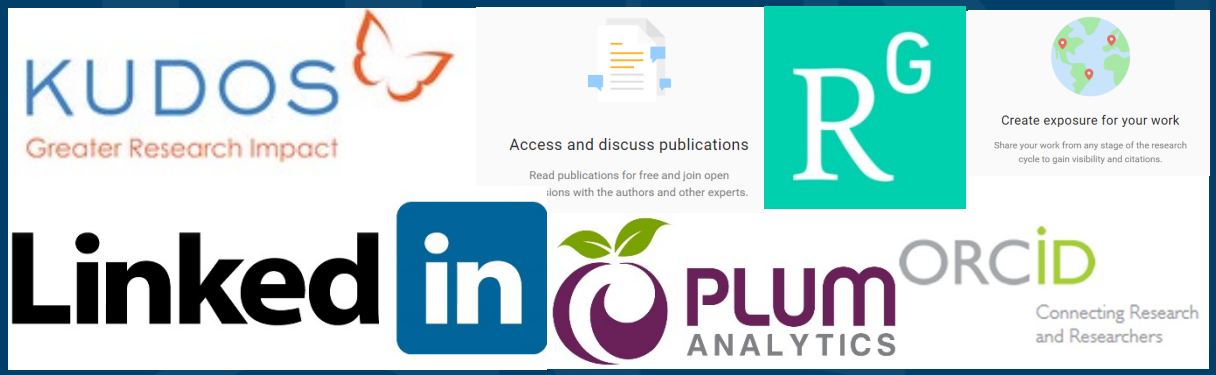
EPA United States Environmental Protection Agency

ORCID 0000-0002-2668-4821

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



Antony Williams
Center for Computational Toxicology and Exposure,
Office of Research and Development, US EPA

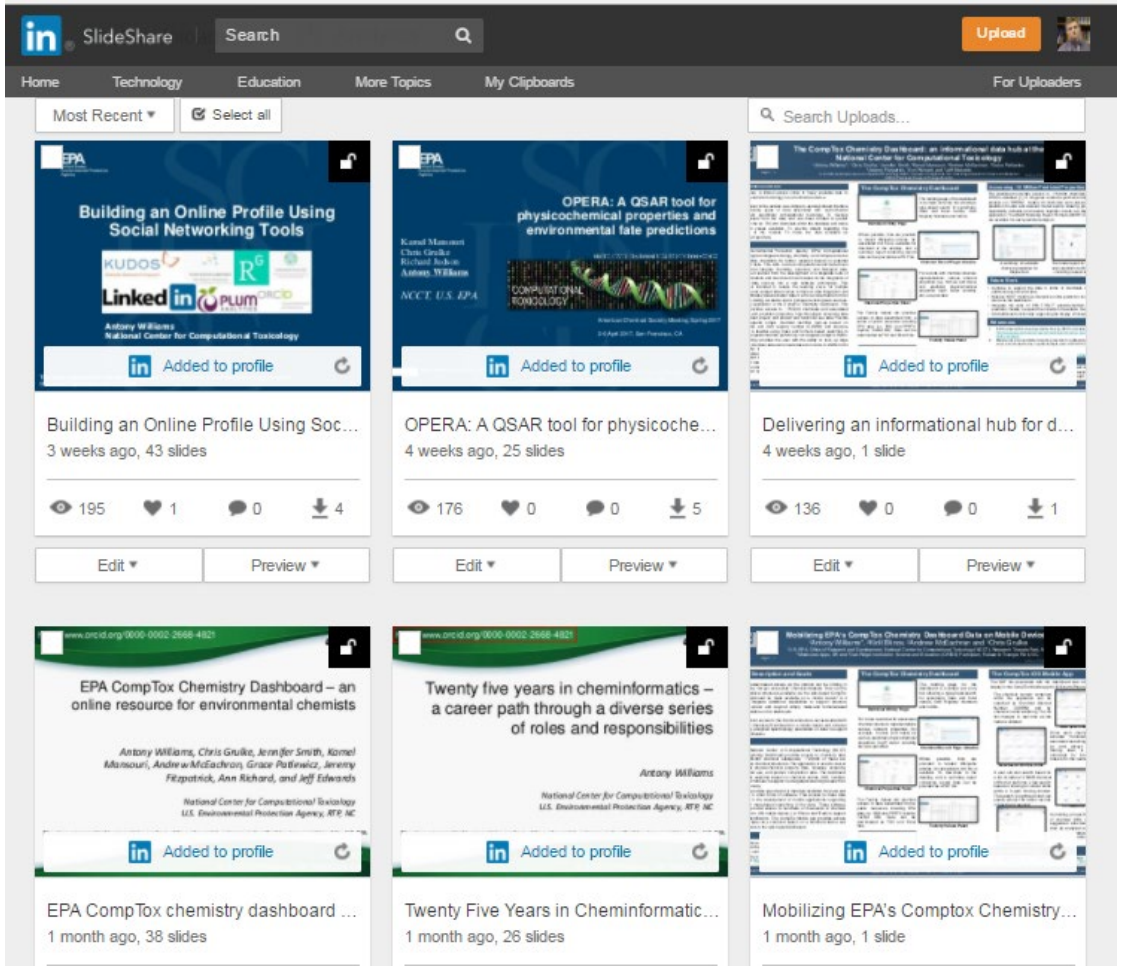
EPA United States Environmental Protection Agency

Feel free to take notes but..

- All slides will be made available later
- Contact me directly if I can help – williams.antony@epa.gov

Various Versions of This Talk

www.slideshare.net/AntonyWilliams



A related publication…

F1000Research F1000Research 2017, 6:1315 Last updated: 19 DEC 2018

Check for updates

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]

[1]National Center for Computational Toxicology, Environmental Protection Agency, Durham, NC, 27711, USA
[2]Lou Peck Consulting, Swansea, SA4 3JQ, UK
[3]Collaborations Pharmaceuticals, Inc., Raleigh, NC, 27606, USA

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Some Questions for you…

- Show of hands please…
  - How many of you have an ORCID?
  - How many of you have LinkedIn?
  - How many of you have SlideShare?
  - How many of you have published >3 papers?
  - How many of you share your work online?

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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

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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….

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ORCID – The Scientists SSN

ORCID

Connecting Research and Researchers

Antony Williams

ORCID ID

orcid.org/0000-0002-2668-4821

What's the value of ORCID?

- ORCIDs are now expected for many publications

- Single click through to your ORCID page – how rich is your ORCID biography??? See

https://orcid.org/0000-0002-2668-4821

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Publishers Requiring ORCIDs…

https://orcid.org/content/mandating-orcid-publication-workflows-open-letter

Requiring ORCID in Publication Workflows: Open Letter

Major publishers have committed to requiring ORCID iDs in the publishing process for their journals and invite other publishers to do the same.

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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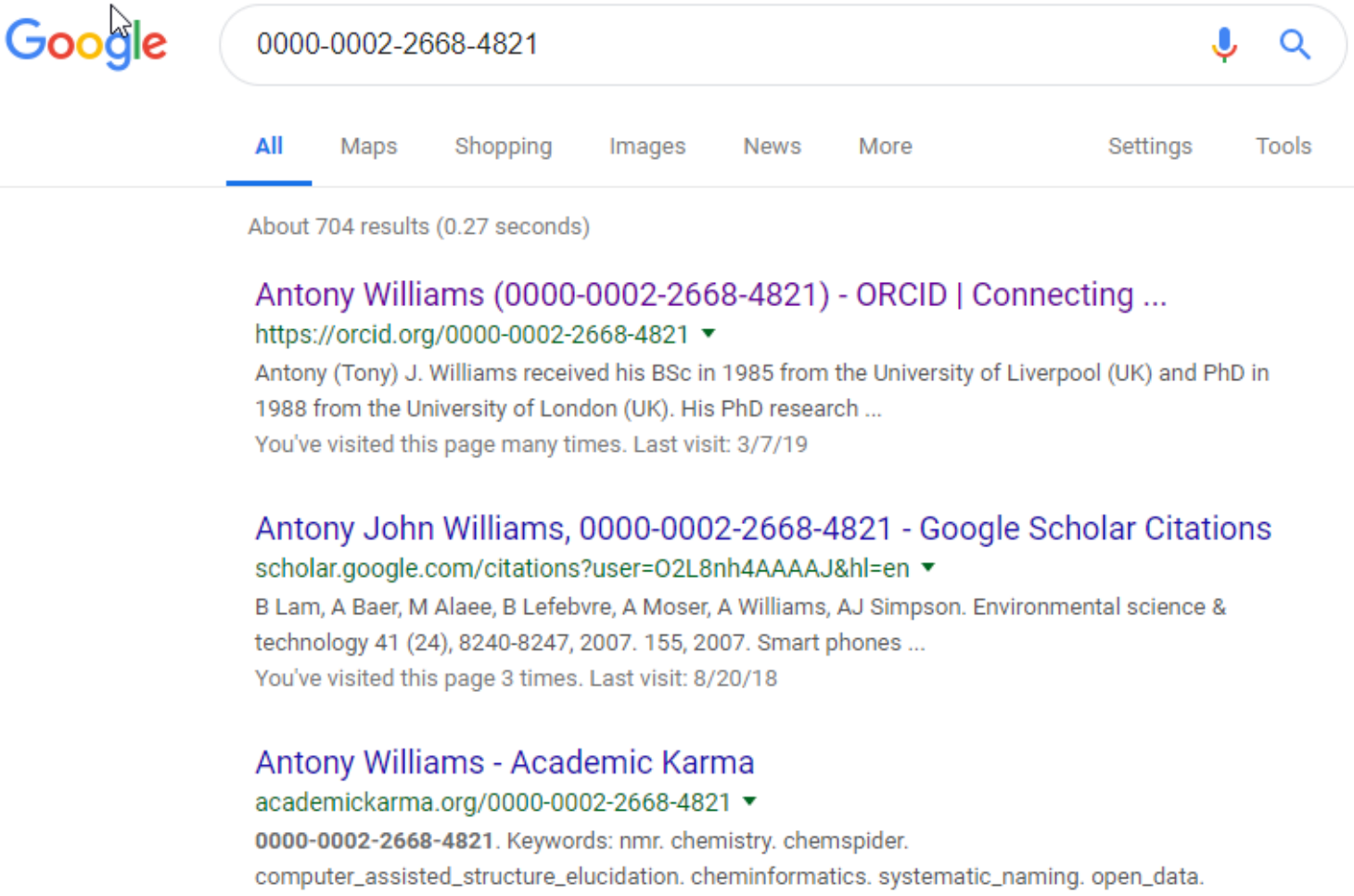
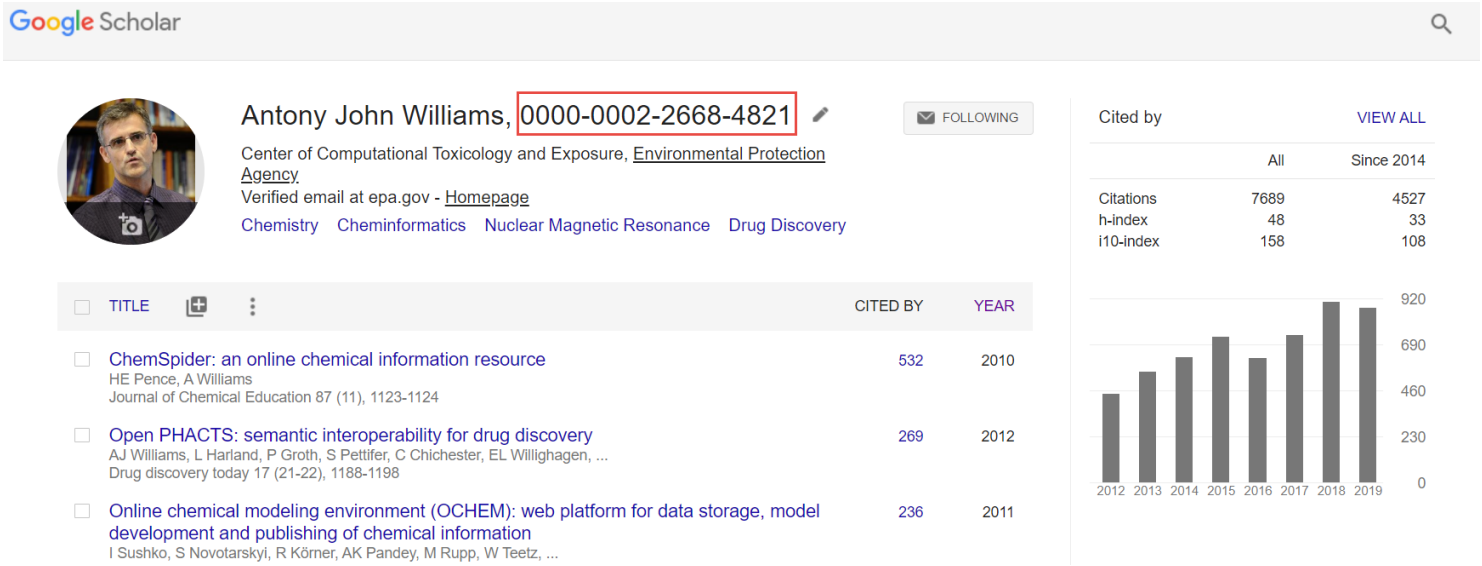
It's a Scientists SSN – use it in various places

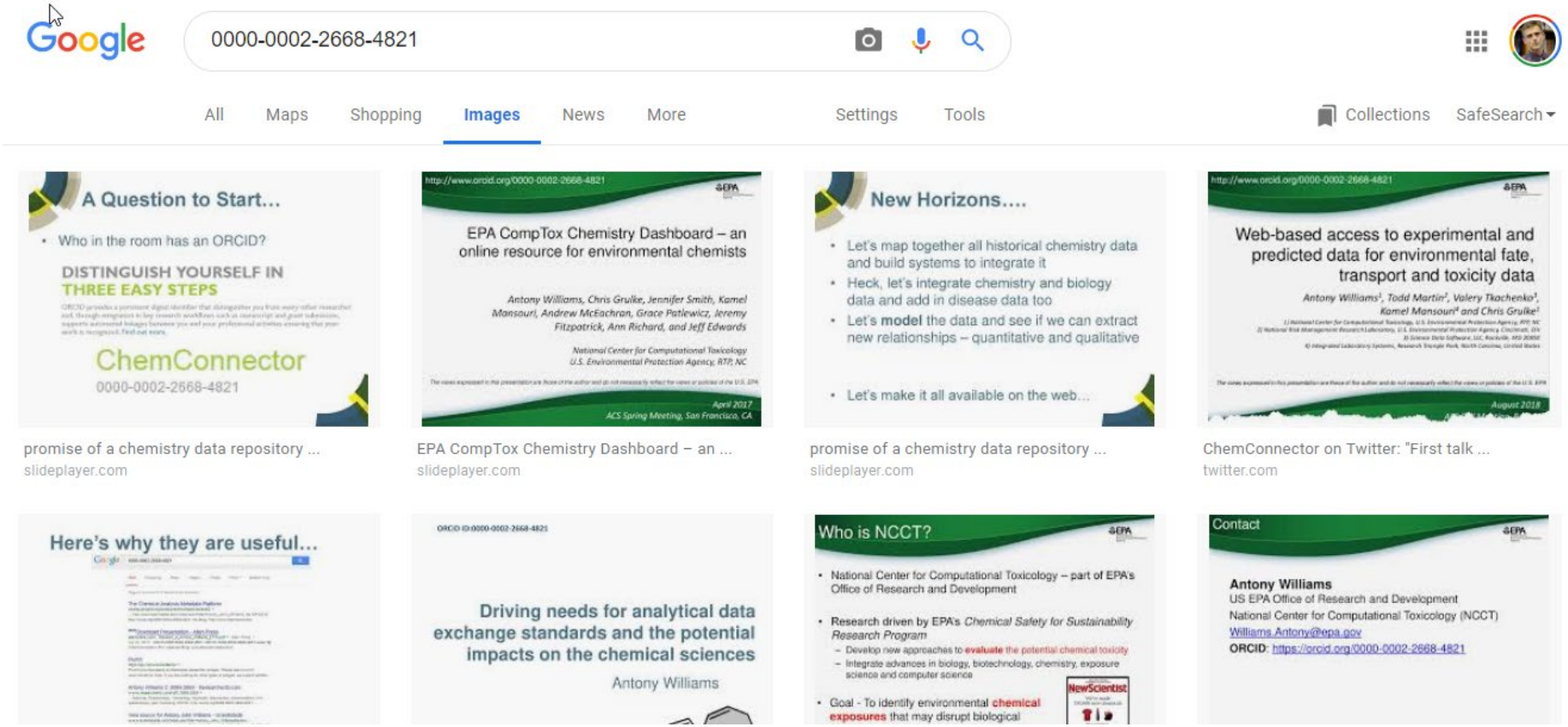


Use ORCID on all products

- Use your ORCID on everything you produce that will be indexed:
  - Presentations
  - Posters
  - Your profiles



Google will index all of your works…even if ORCID doesn't



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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???

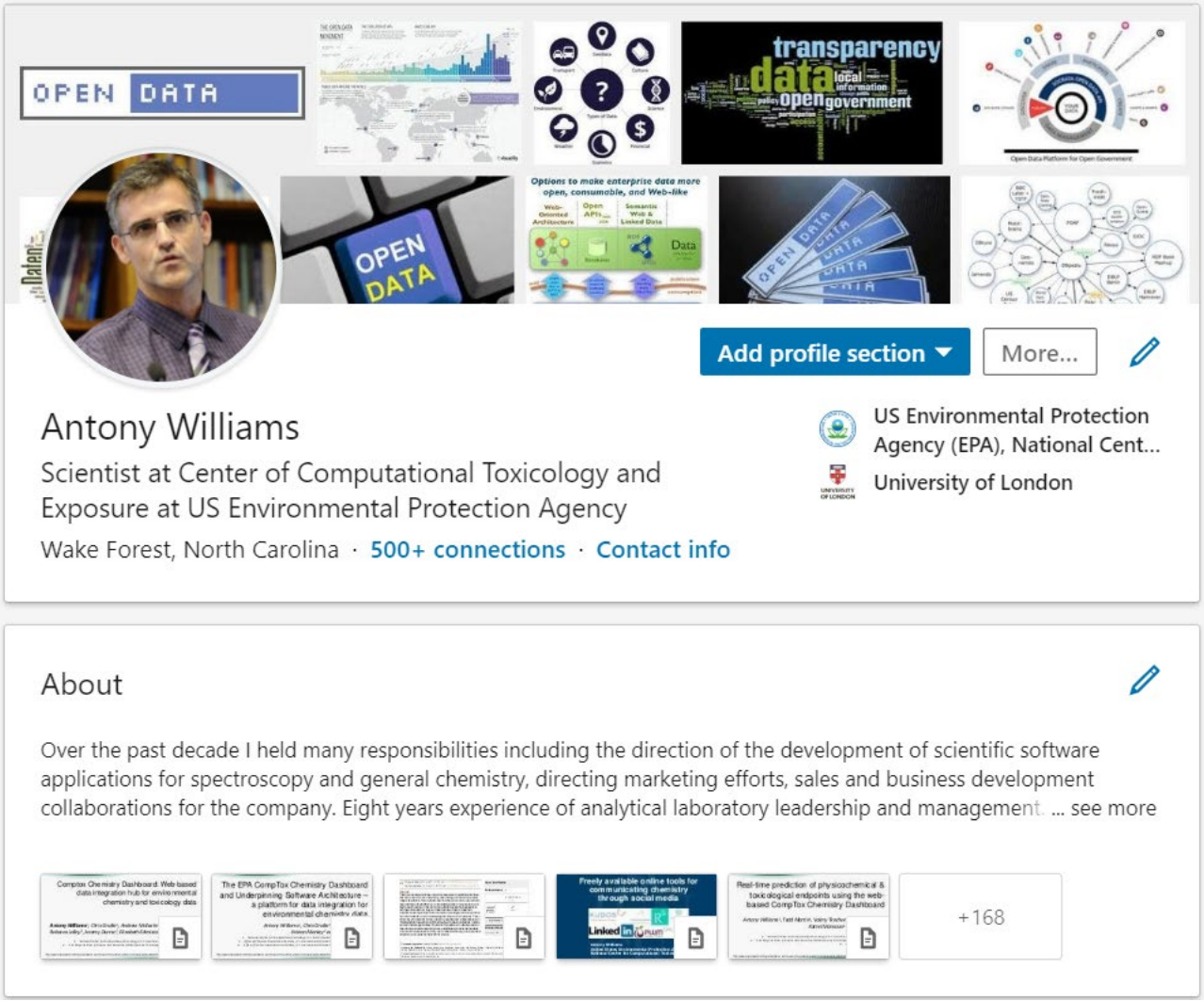
- Shouldn't **YOU** and your **CO-AUTHORS** invest some time in getting it out to the network???

- 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"

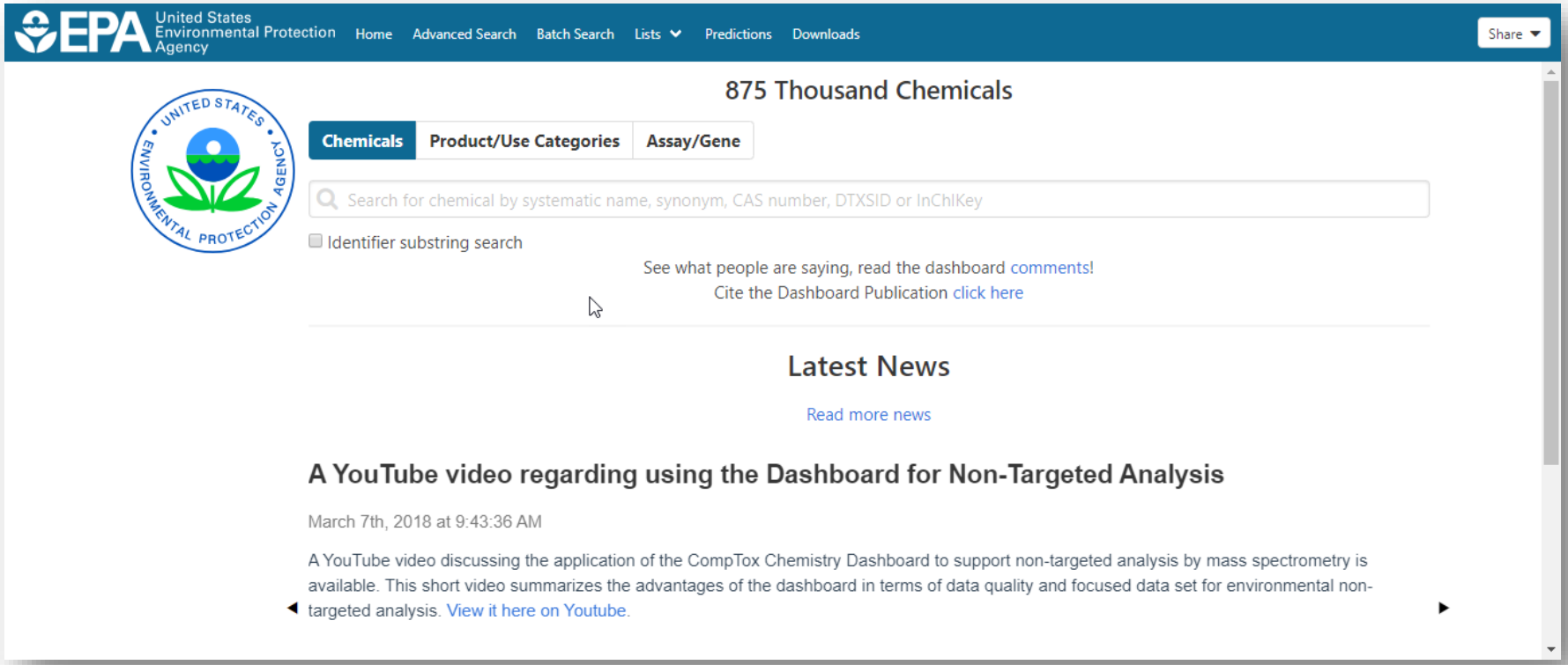
- Research datasets
- Scientific software
- Publications – peer-reviewed and many others
- Posters and presentations at conferences
- Electronic theses and dissertations
- Performances in film and audio
- Other forms of research
- **CAVEAT: Make sure you are *allowed* to share**

LinkedIn
The MOST BASIC Career Networking Tool



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

My primary project at present…



Ability to Highlight Projects

7 Projects

The CompTox Chemicals Dashboard
Dec 2015 – Present

The CompTox Chemicals Dashboard is an integration hub for chemistry and biology data of interest to environmental scientists and toxicologists. The dashboard was released as a beta on April 1st 2016 and formally as version 1 to the community in August 2016. The dashboard is free to use and presently provides access to data for ~875,000 chemicals.

The definitive article regarding the development of the dashboard is published in the Journal of Cheminformatics as https://jcheminf.biomedcentral.com/articles/10.1186/s13321-017-0247-6.

There are a number of derivative and related articles that have come from the related research and application development. These include:
1) OPERA models for predicting physicochemical properties and environmental fate endpoints - https://jcheminf.biomedcentral.com/articles/10.1186/s13321-018-0263-1
2) An automated curation procedure for addressing chemical errors and inconsistencies in public datasets used in QSAR modelling https://doi.org/10.1080/1062936X.2016.1253611
3) Generalized Read-Across (GenRA): A workflow implemented into the EPA CompTox Chemicals Dashboard https://www.altex.org/index.php/altex/article/view/1202
4) A Chemical Category-Based Prioritization Approach for Selecting 75 Per-and Polyfluoroalkyl Substances (PFAS) for Tiered Toxicity and Toxicokinetic Testing https://ehp.niehs.nih.gov/doi/10.1289/EHP4555

Other creators

Manage Articles Here Too…

64 Publications

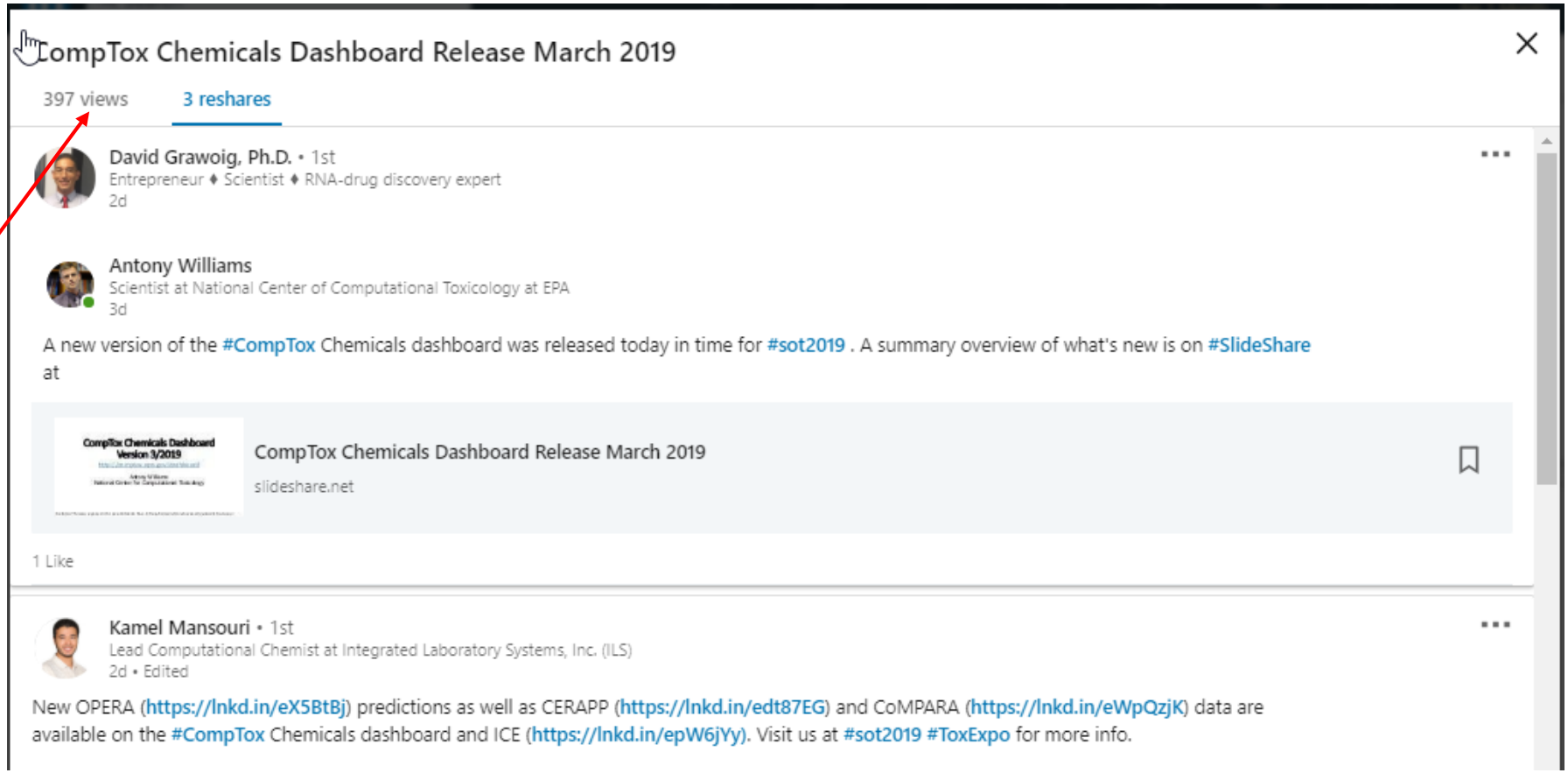
Generalized Read-Across (GenRA): A workflow implemented into the EPA CompTox Chemicals Dashboard

Feb 4, 2019 • ALTEX-Alternatives to animal experimentation

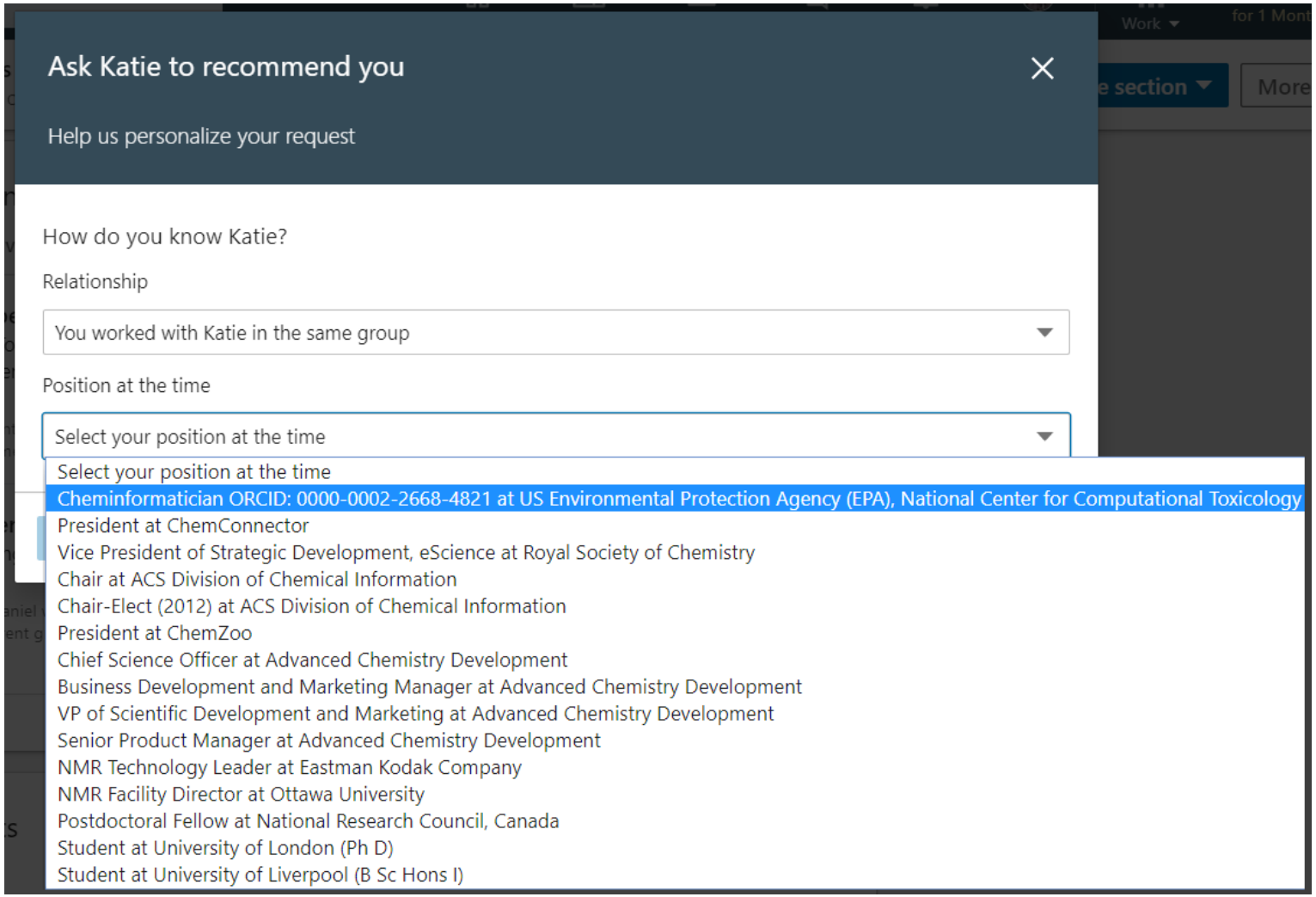
Generalized Read-Across (GenRA) is a data driven approach which makes read-across predictions on the basis of a similarity weighted activity of source analogues (nearest neighbors). GenRA has been described in more detail in the literature (Shah et al., 2016; Helman et al., 2018). Here we present its implementation within the EPA's CompTox Chemicals Dashboard to provide public access to a GenRA module structured as a read-across workflow. GenRA assists researchers in identifying source analogues, evaluating their validity and making predictions of in vivo toxicity effects for a target substance. Predictions are presented as binary outcomes reflecting presence or absence of toxicity together with quantitative measures of uncertainty. The approach allows users to identify analogues in different ways, quickly assess the availability of relevant in vivo data for those analogues and visualize these in a data matrix to evaluate the consistency and concordance of the available experimental data for those analogues before making a GenRA prediction. Predictions can be exported into a tab-separated value (TSV) or Excel file for additional review and analysis (e.g., doses of analogues associated with production of toxic effects). GenRA offers a new capability of making reproducible read-across predictions in an easy-to use-interface.

Other authors

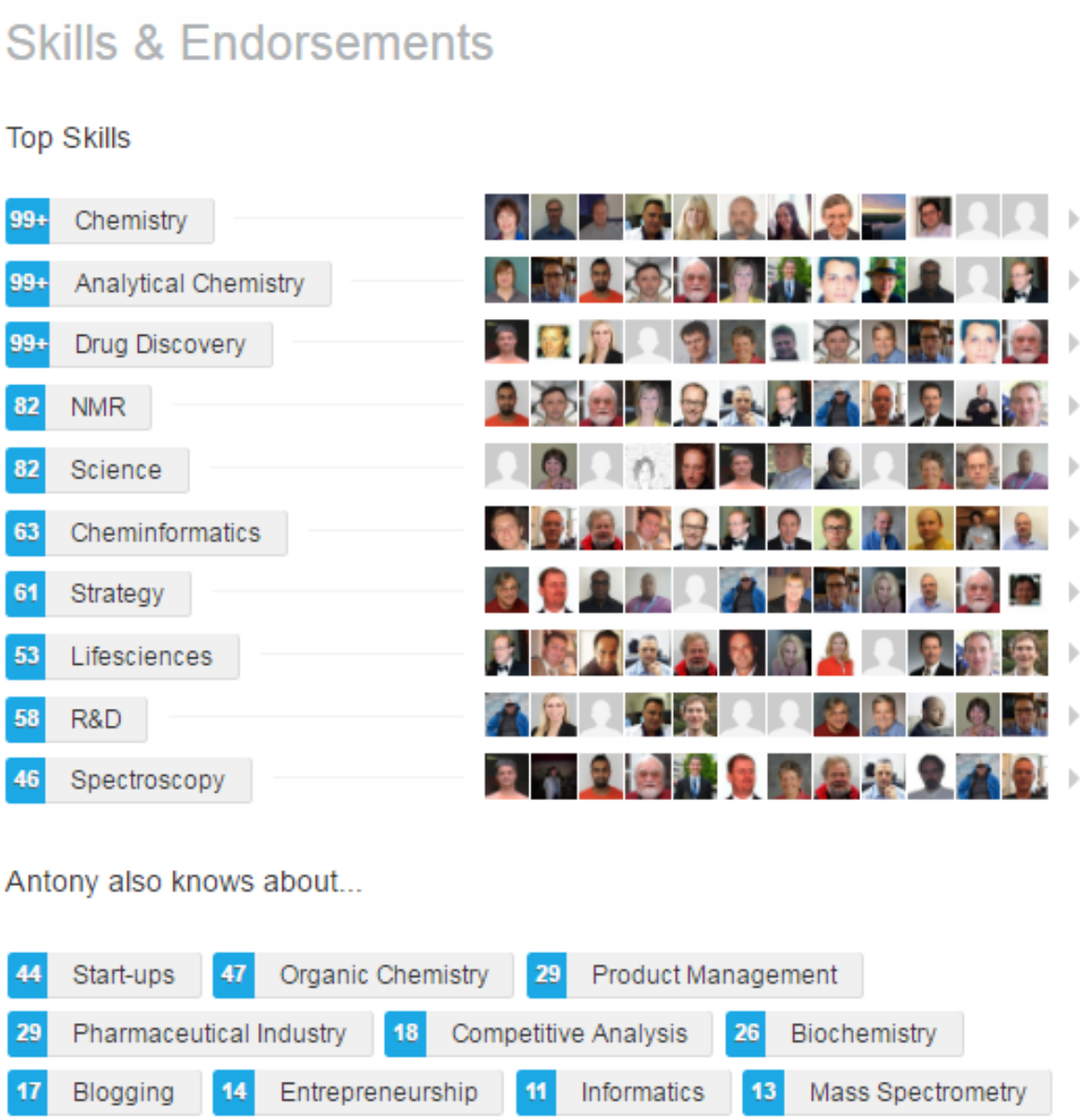
Your Postings Get Networked



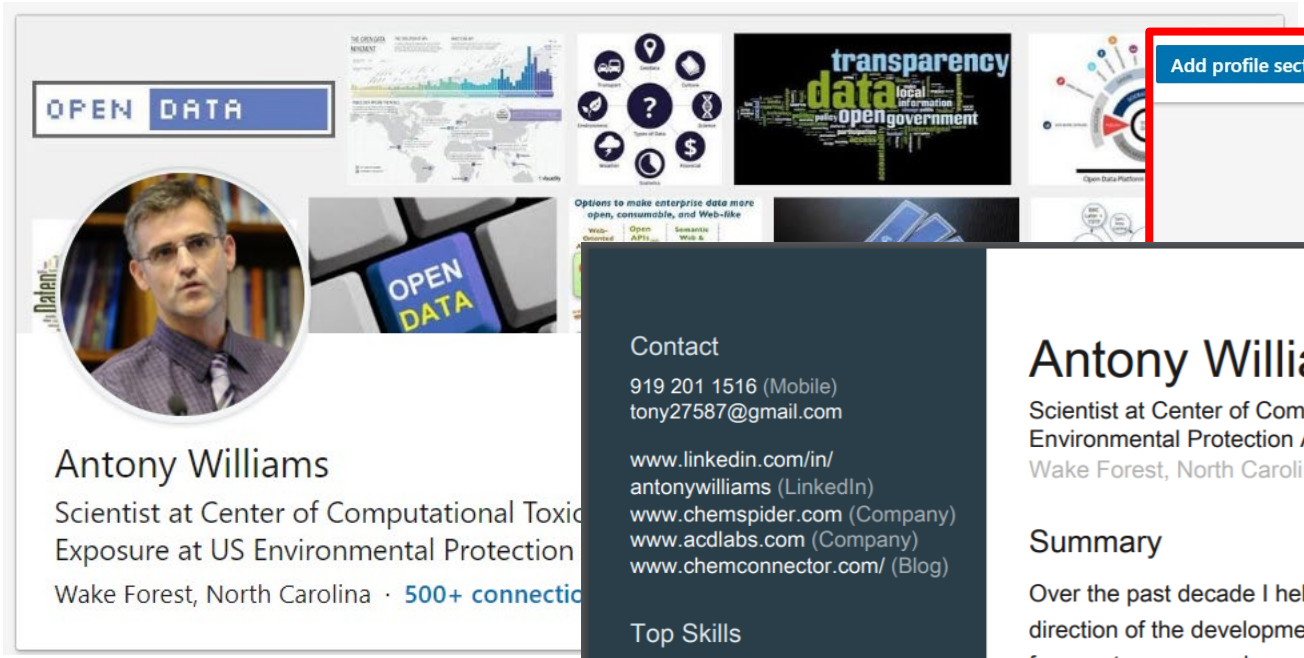
Ask for Recommendations

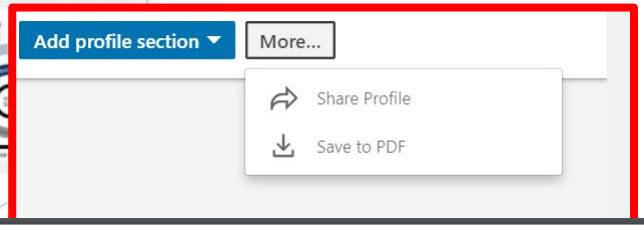


Ask for “Endorsements”,



Instant Summary as a PDF





Contact

919 201 1516 (Mobile)
tony27587@gmail.com

www.linkedin.com/in/antonywilliams (LinkedIn)
www.chemspider.com (Company)
www.acdlabs.com (Company)
www.chemconnector.com/ (Blog)

Top Skills

Chemistry
Analytical Chemistry
Drug Discovery

Languages

English

Certifications

Verified Peer Reviewer

Honors-Awards

North Carolina ACS Distinguished Lecturer of the Year 2016

Antony Williams

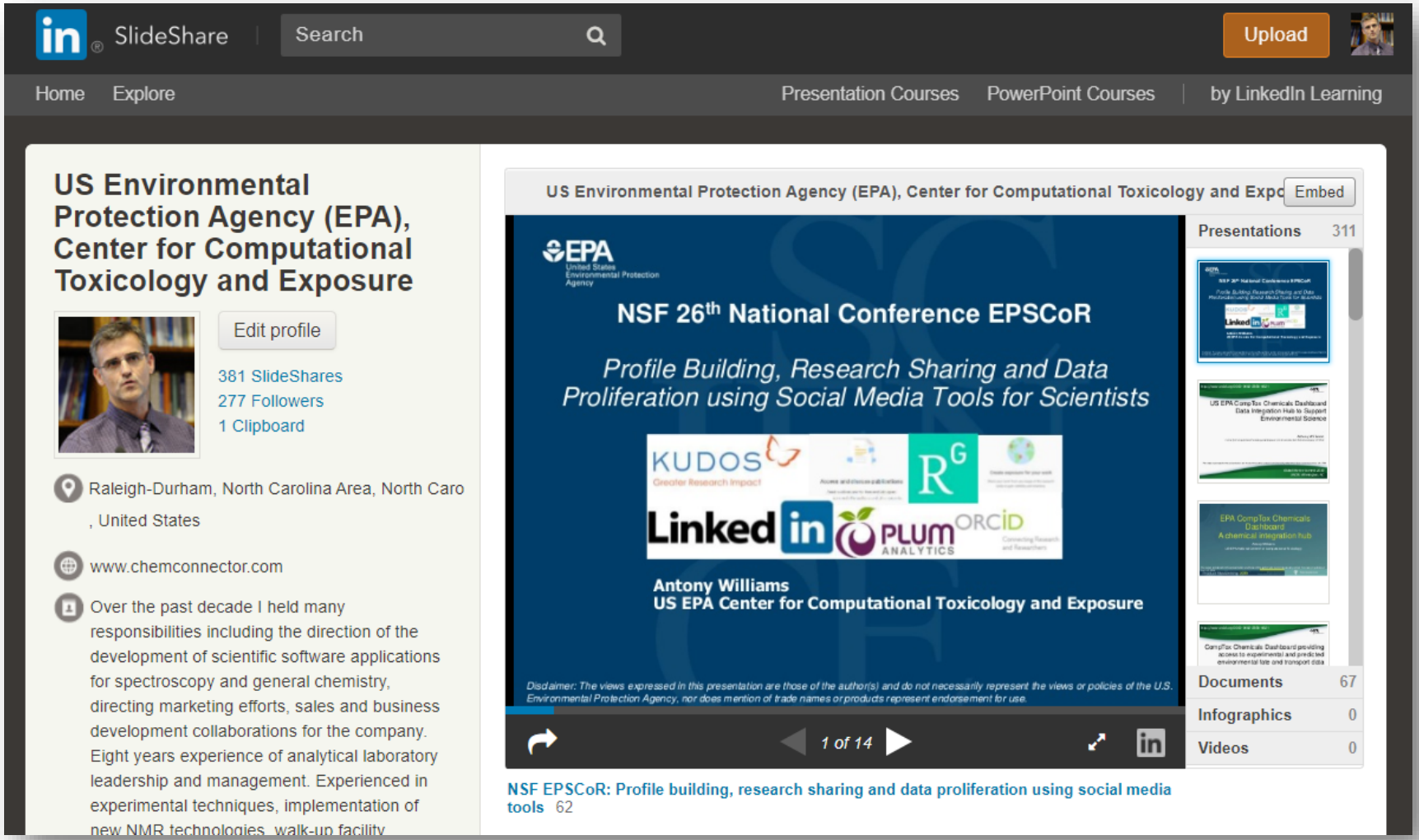
Scientist at Center of Computational Toxicology and Exposure at US Environmental Protection Agency
Wake Forest, North Carolina

Summary

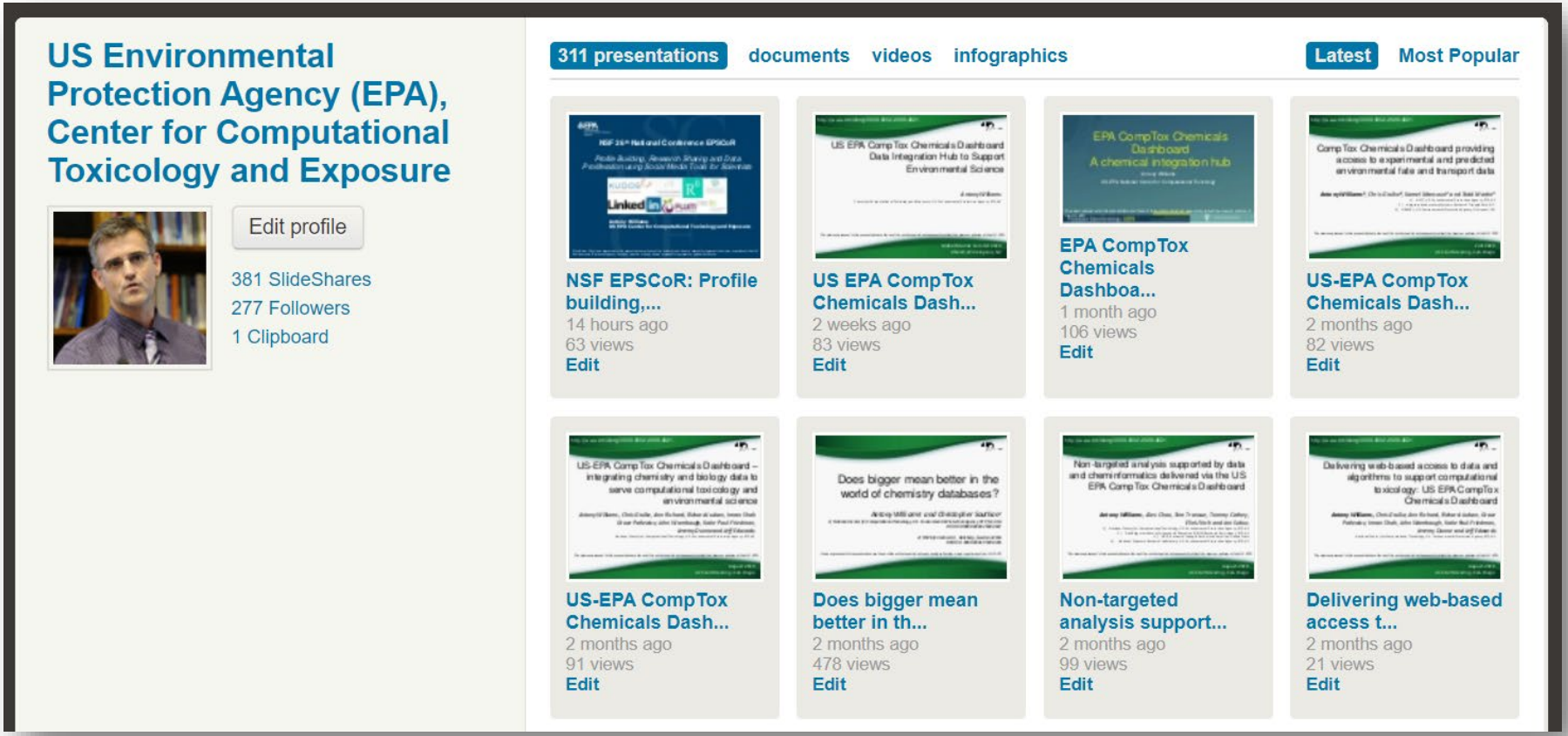
Over the past decade I held many responsibilities including the direction of the development of scientific software applications for spectroscopy and general chemistry, directing marketing efforts, sales and business development collaborations for the company. Eight years experience of analytical laboratory 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 scientific publications, 3 patents and many public presentations.

I am one of the Founders of ChemZoo Inc., the developers of the ChemSpider website (www.chemspider.com). ChemSpider is an

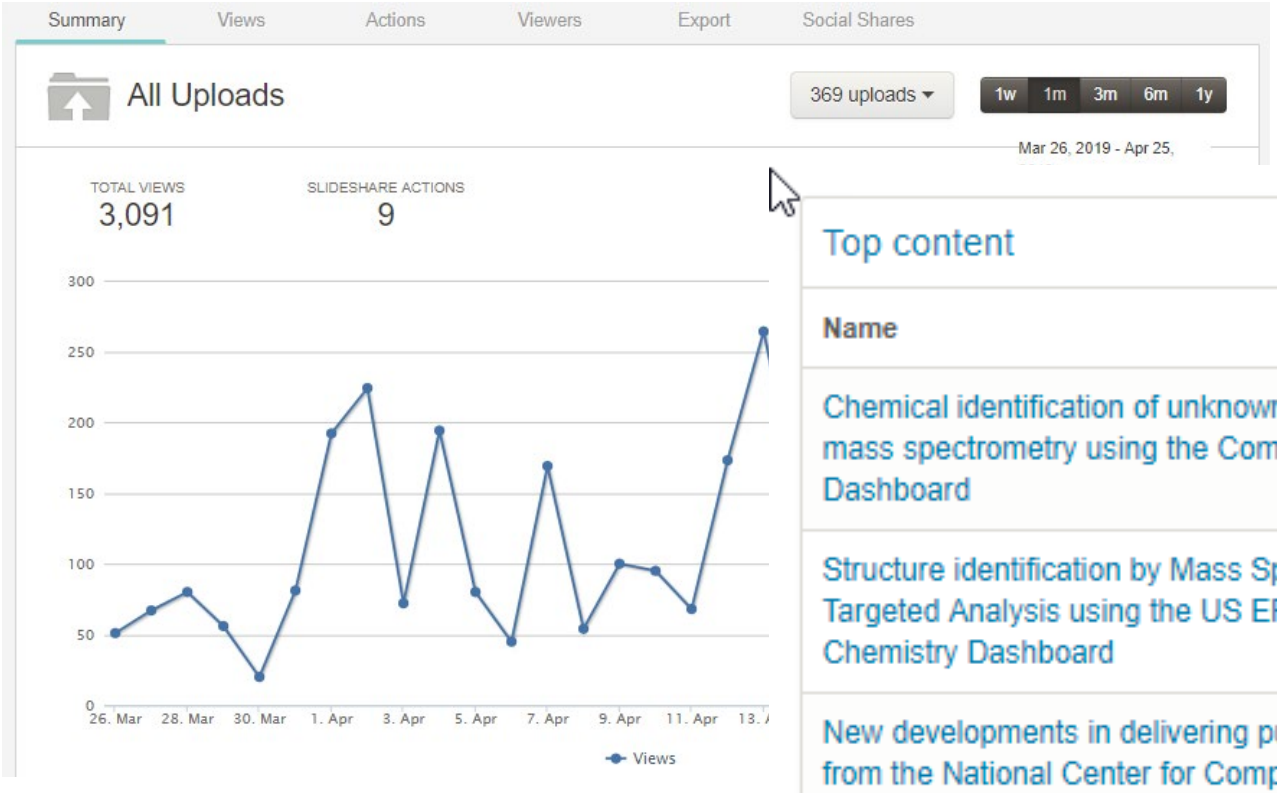
Presentations



Sharing your works online – can get 1000s of views



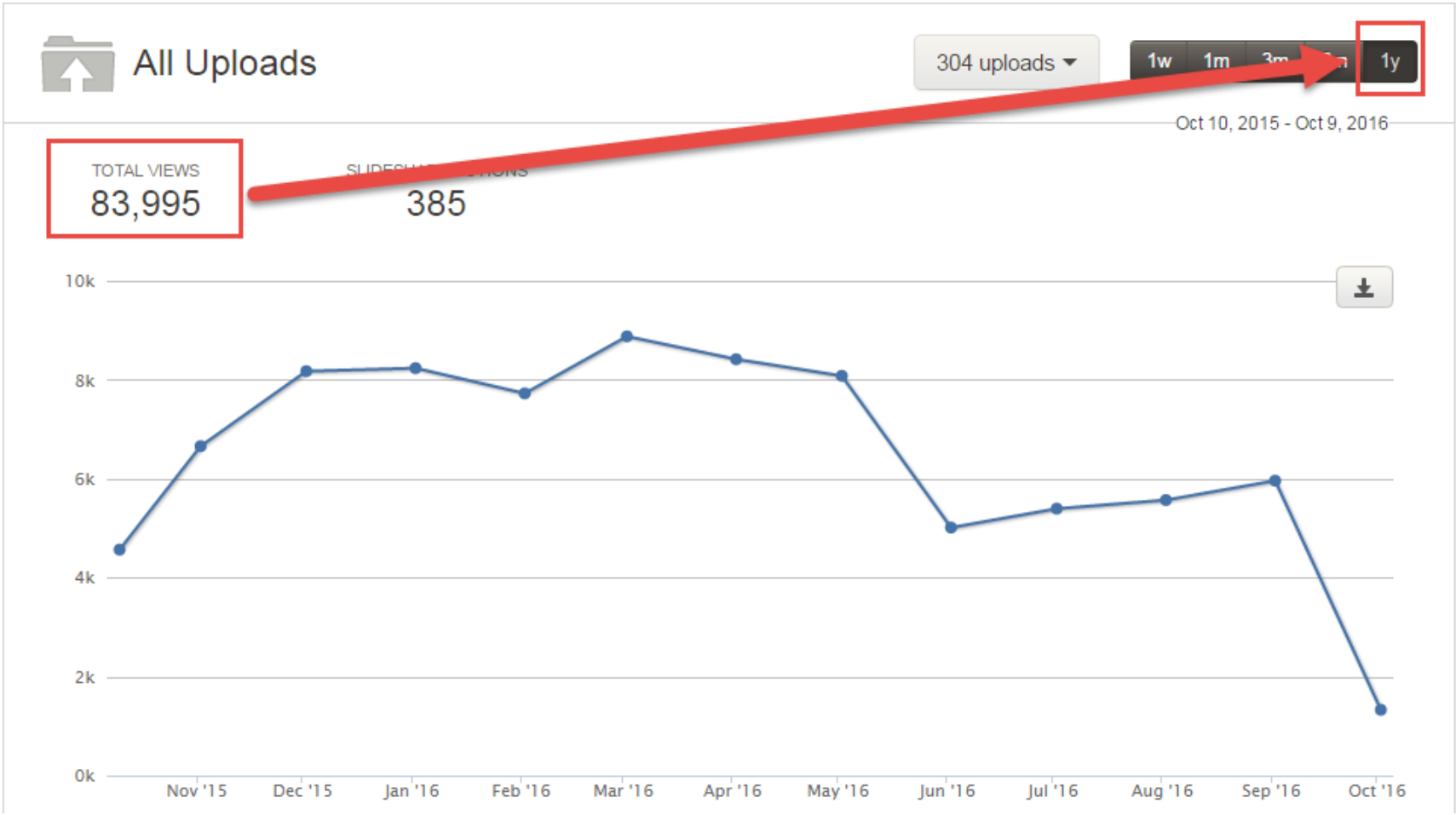
Analytics



Top content

Name	Views
Chemical identification of unknowns in high resolution mass spectrometry using the CompTox Chemicals Dashboard	240
Structure identification by Mass Spectrometry Non-Targeted Analysis using the US EPA's CompTox Chemistry Dashboard	189
New developments in delivering public access to data from the National Center for Computational Toxicology at the EPA	189
US EPA CompTox Chemistry Dashboard as a source of data to fill data gaps for chemical sources of risk	185
Development of a Tool for Systematic Integration of Traditional and New Approach Methods for Prioritizing Chemical Lists	183

Slideshare – Highly Accessed



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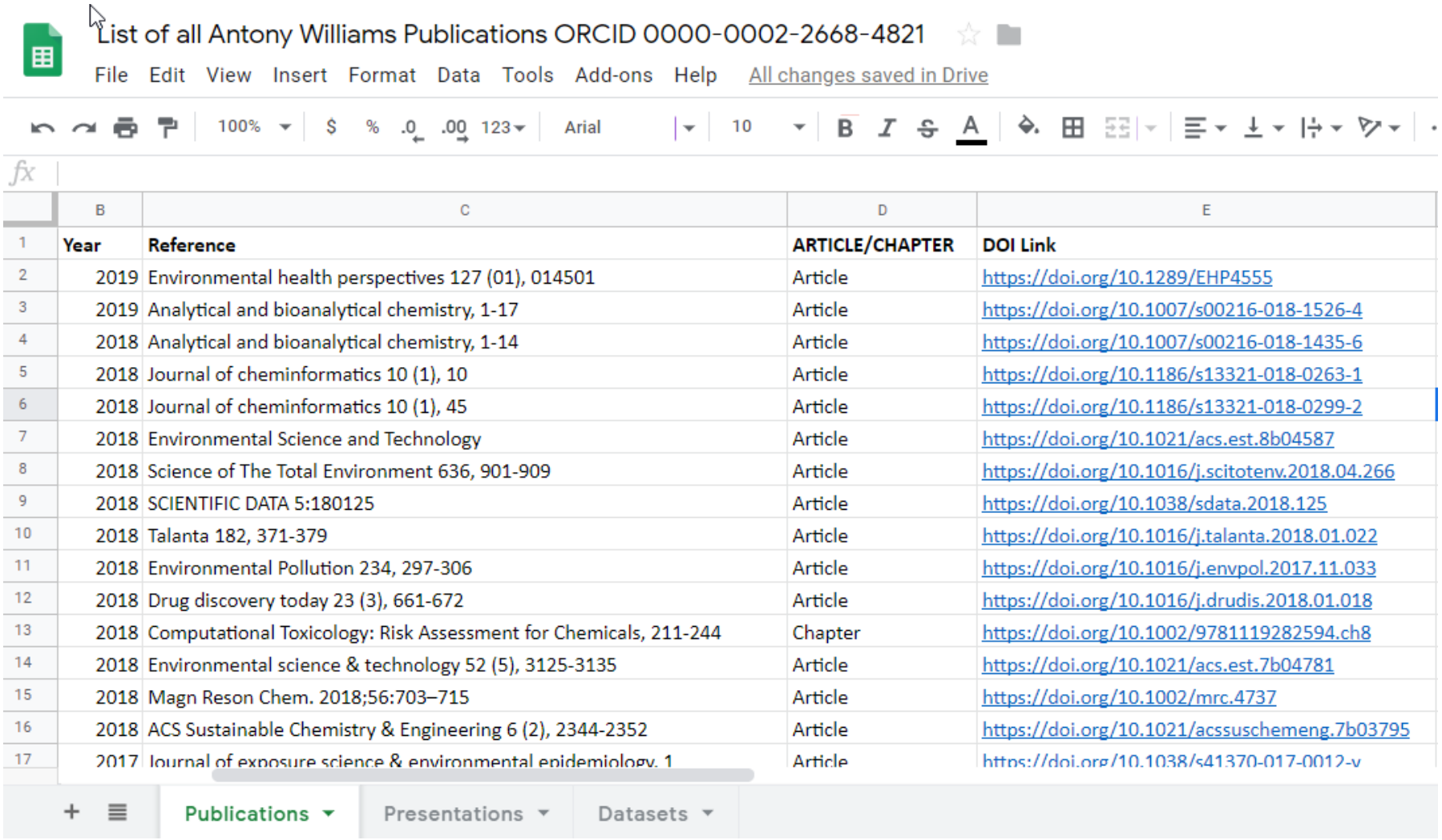

List of all Antony Williams Publications ORCID 0000-0002-2668-4821

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	B	C	D	E
1	**Year**	**Reference**	**ARTICLE/CHAPTER**	**DOI Link**
2	2019	Environmental health perspectives 127 (01), 014501	Article	https://doi.org/10.1289/EHP4555
3	2019	Analytical and bioanalytical chemistry, 1-17	Article	https://doi.org/10.1007/s00216-018-1526-4
4	2018	Analytical and bioanalytical chemistry, 1-14	Article	https://doi.org/10.1007/s00216-018-1435-6
5	2018	Journal of cheminformatics 10 (1), 10	Article	https://doi.org/10.1186/s13321-018-0263-1
6	2018	Journal of cheminformatics 10 (1), 45	Article	https://doi.org/10.1186/s13321-018-0299-2
7	2018	Environmental Science and Technology	Article	https://doi.org/10.1021/acs.est.8b04587
8	2018	Science of The Total Environment 636, 901-909	Article	https://doi.org/10.1016/j.scitotenv.2018.04.266
9	2018	SCIENTIFIC DATA 5:180125	Article	https://doi.org/10.1038/sdata.2018.125
10	2018	Talanta 182, 371-379	Article	https://doi.org/10.1016/j.talanta.2018.01.022
11	2018	Environmental Pollution 234, 297-306	Article	https://doi.org/10.1016/j.envpol.2017.11.033
12	2018	Drug discovery today 23 (3), 661-672	Article	https://doi.org/10.1016/j.drudis.2018.01.018
13	2018	Computational Toxicology: Risk Assessment for Chemicals, 211-244	Chapter	https://doi.org/10.1002/9781119282594.ch8
14	2018	Environmental science & technology 52 (5), 3125-3135	Article	https://doi.org/10.1021/acs.est.7b04781
15	2018	Magn Reson Chem. 2018;56:703–715	Article	https://doi.org/10.1002/mrc.4737
16	2018	ACS Sustainable Chemistry & Engineering 6 (2), 2344-2352	Article	https://doi.org/10.1021/acssuschemeng.7b03795
17	2017	Journal of exposure science & environmental epidemiology, 1	Article	https://doi.org/10.1038/s41370-017-0012-y

Publications Presentations Datasets

ResearchGate for Networking

Antony John Williams

45.21 · PhD · Edit

Add new research

Overview | Research | Info | Stats | Scores | Research you follow

Introduction

Edit

I am presently a Computational Chemist at the Center for Computational Toxicology and Exposure 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) Edit

Medicinal and Pharmaceutical Chemistry | Spectroscopy | Analytical Chemistry | Drug Discovery

Stats overview

View all

3,771
Total Research Interest

6,048
Citations

Affiliation

Edit

United States Environmental Protection Agency

Location
United States

Department
Center for Computational Toxicology and Exposure

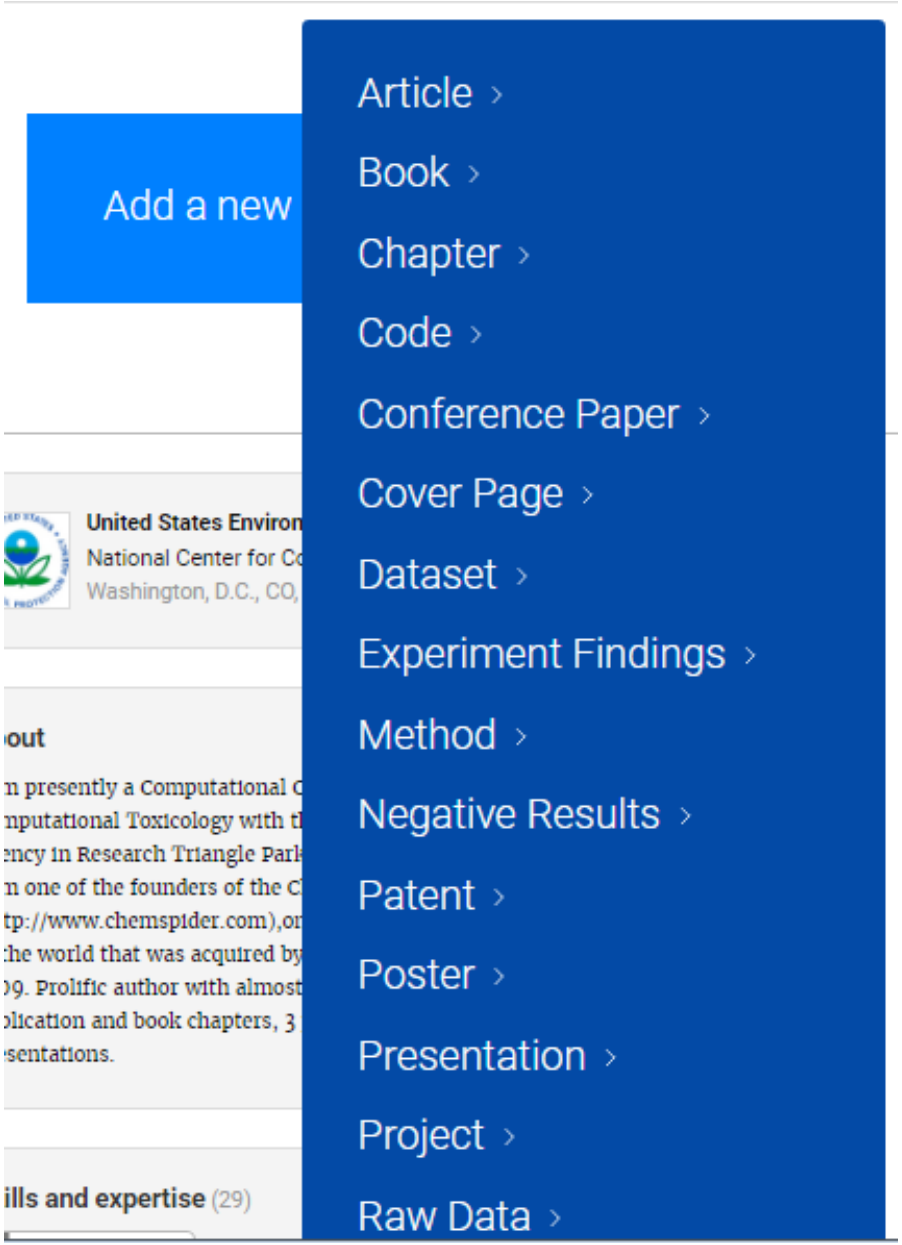
Position
Computational Chemist

National Center for Computational Toxicology

Lab head
Russell Scott Thomas

Lab members (18)

Add MANY Flavors of Research



ResearchGate for Sharing a PROJECT

United States Environmental Protection Agency

Home Questions Jobs Funding Beta Search for researchers, publications, and r

Project

The CompTox Chemicals Dashboard

Antony John Williams · Christopher M Grulke · Mansouri Ka

Goal: The CompTox Chemicals Dashboard is a web-based application tl chemistry and biology data of different types including experimental an and fate and transport data, in vivo and in vitro toxicity data, real time pr across approaches. The dashboard, available at https://comptox.epa.gc data for 875,000 chemicals as of March 2019

Date: 30 March 2016

Lab: Russell Scott Thomas's Lab

You
added an **update**

New update to CompTox Chemicals Dashboard rel March 2019

An update to the dashboard has been released in March 2019 to coincide with t of Toxicology and American Chemical Society Spring meetings. Six months of e resulted in the addition of 110,000 new chemical substances being added (brin total of chemical substances to 876k), improved support for Toxcast bioassay d (integrating data from the invitroDB_v3 release), the addition of multiple chemic new user interface enhancements across the application. A list of release notes available for review at https://comptox.epa.gov/dashboard/comptox_release_n

comptox_release_notes.pdf · 48.41 KB

Comment Share

You
added **2 research items**

Dec 26, 2018

EPA's non-targeted analysis collaborative trial (ENTACT): genesis, design, and initial findings

Article Dec 2018

Elin M Ulrich · Jon R. Sobus · Christopher M Grulke · [...] · Antony John Williams

In August 2015, the US Environmental Protection Agency (EPA) convened a workshop entitled "Advancing non-targeted analyses of xenobiotic chemicals in environmental and biological media." The purpose of the workshop was to bring...

Upload full-text 1 Recommendation · 80 Reads · 3 Citations

"MS-Ready" structures for non-targeted high-resolution mass spectrometry screening studies

Source

Article Dec 2018

Andrew McEachran · Mansouri Kamel · Christopher M Grulke · [...] · Antony John Williams

Chemical database searching has become a fixture in many non-targeted identification workflows based on high-resolution mass spectrometry (HRMS). However, the form of a chemical structure...

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ResearchGate for Networking

Stats overview

3,382	5,573	94	33,878
Research Interest	Citations	Recommendations	Reads
More details	View	Show breakdown	Show breakdown

Reads	33,878
Project reads	290
Question reads	11
Answer reads	693
Publication reads	32,884

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Oak Ridge National Laboratory
Knoxville, Tennessee, United States

Principal Scientist, Cancer Biology

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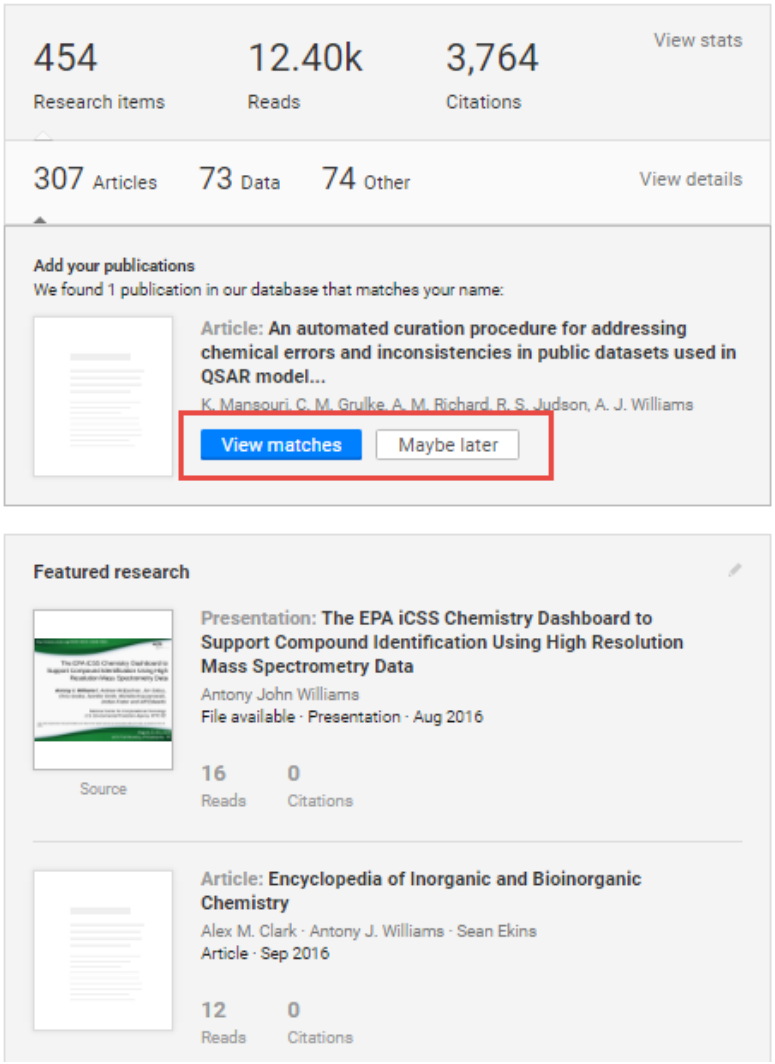
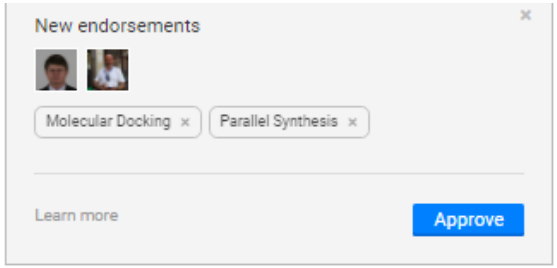
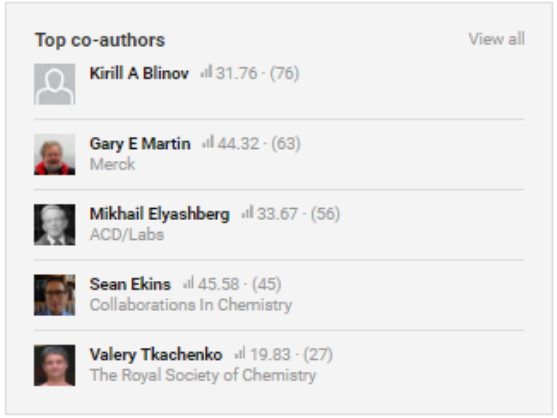
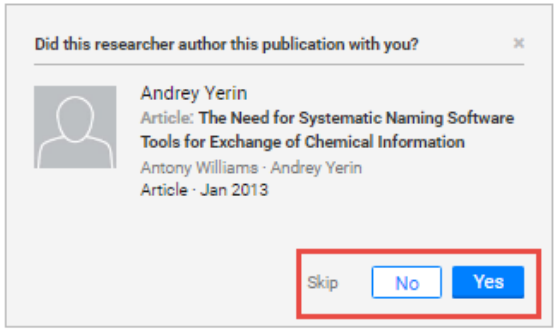


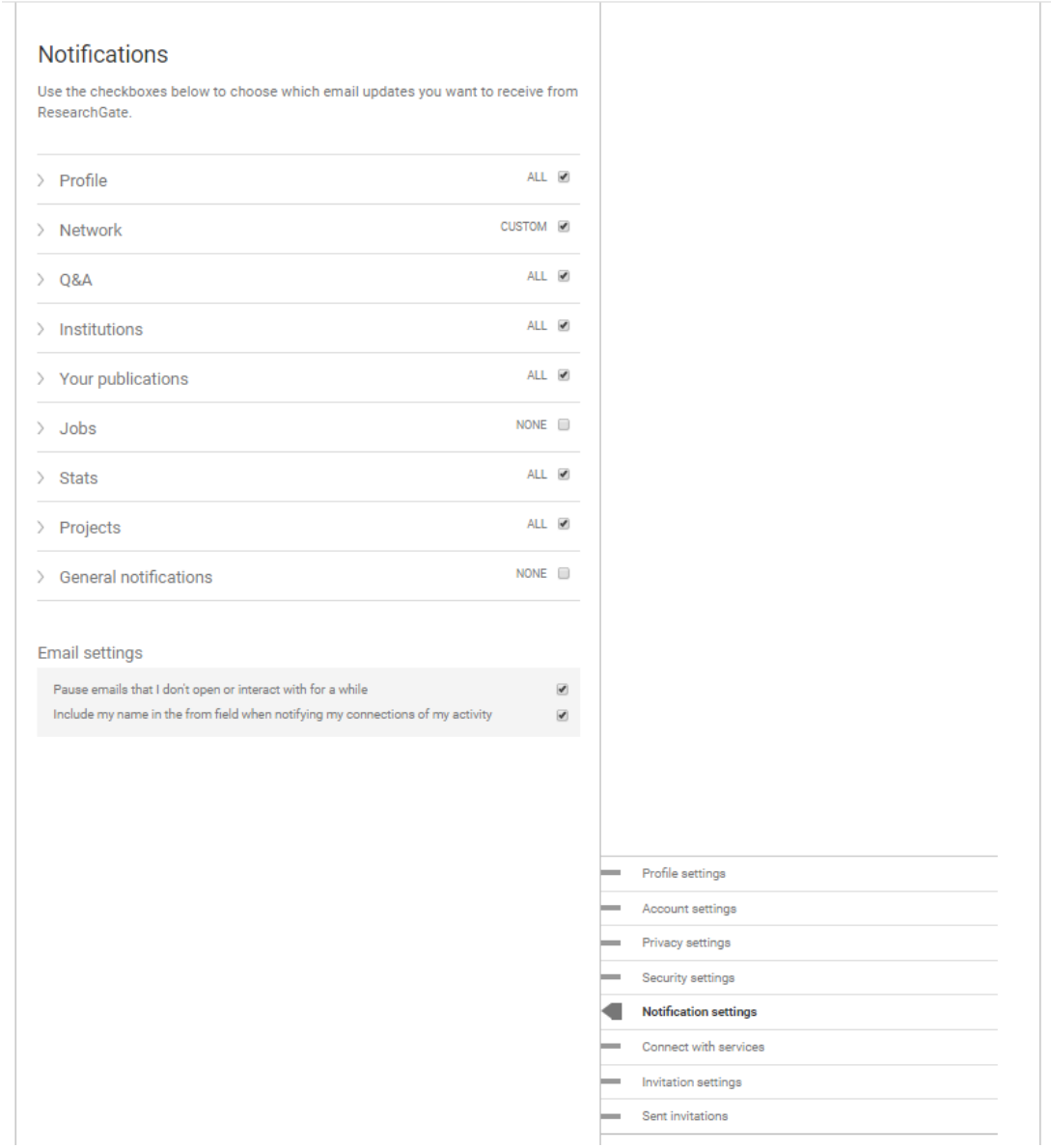




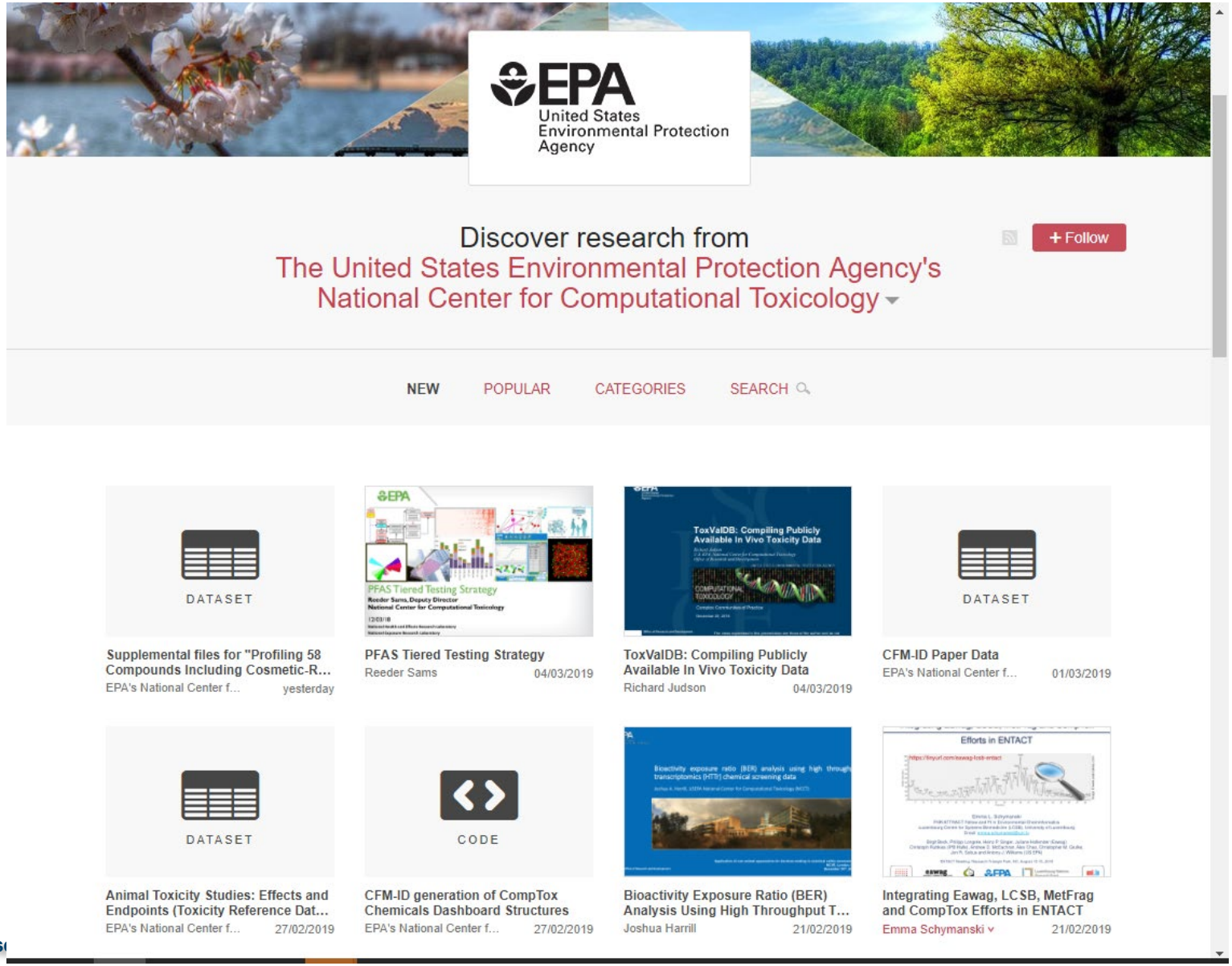


“I won’t use it I get too many emails”

https://www.researchgate.net/account.AccountNotificationSettings.html



What about “Data Sharing”?



Supplementary Data Access

Download (284.06 MB) Share Cite Embed + Collect

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

17.02.2017, 11:27 by Antony Williams

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

REFERENCES

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

203 views | 34 downloads | 0 citations

3

CATEGORIES

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

KEYWORD(S)

Chemistry | Mass Spectrometry | Cheminformatics

LICENCE

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"Personal Data Sharing"?

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Computational Chemist, Center for Computational Toxicology and Exposure, 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

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Co-workers & collaborators

Chris Grulke

Valery Tkachenko

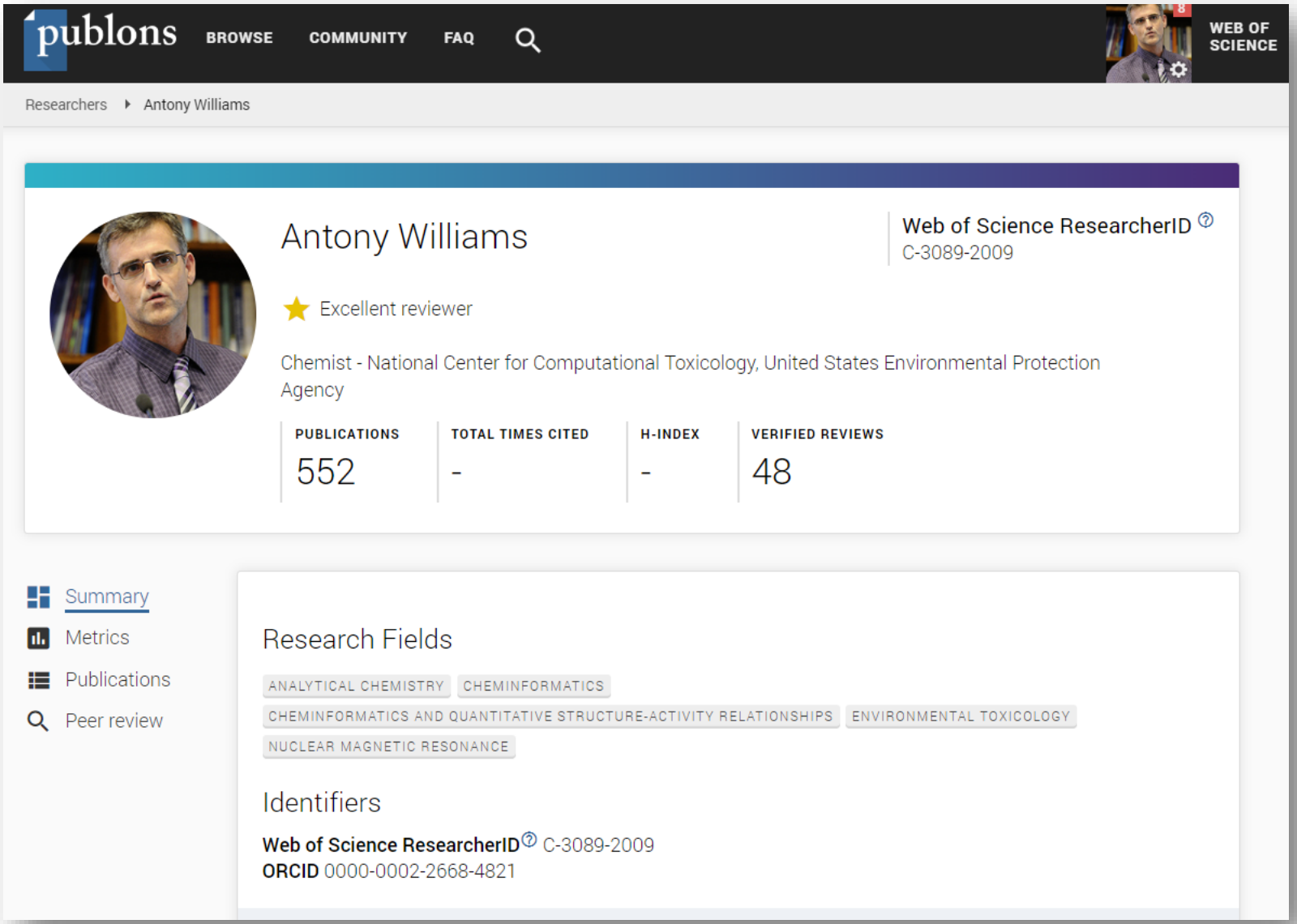
Andrew McEachran
ORISE Postdoctoral Fellow
Research Triangle Park, NC

Sean Ekins
senior consultant
Fuquay Varina, NC, USA

Jon Sobus

Jeff Edwards

Credit for Reviewing Papers?



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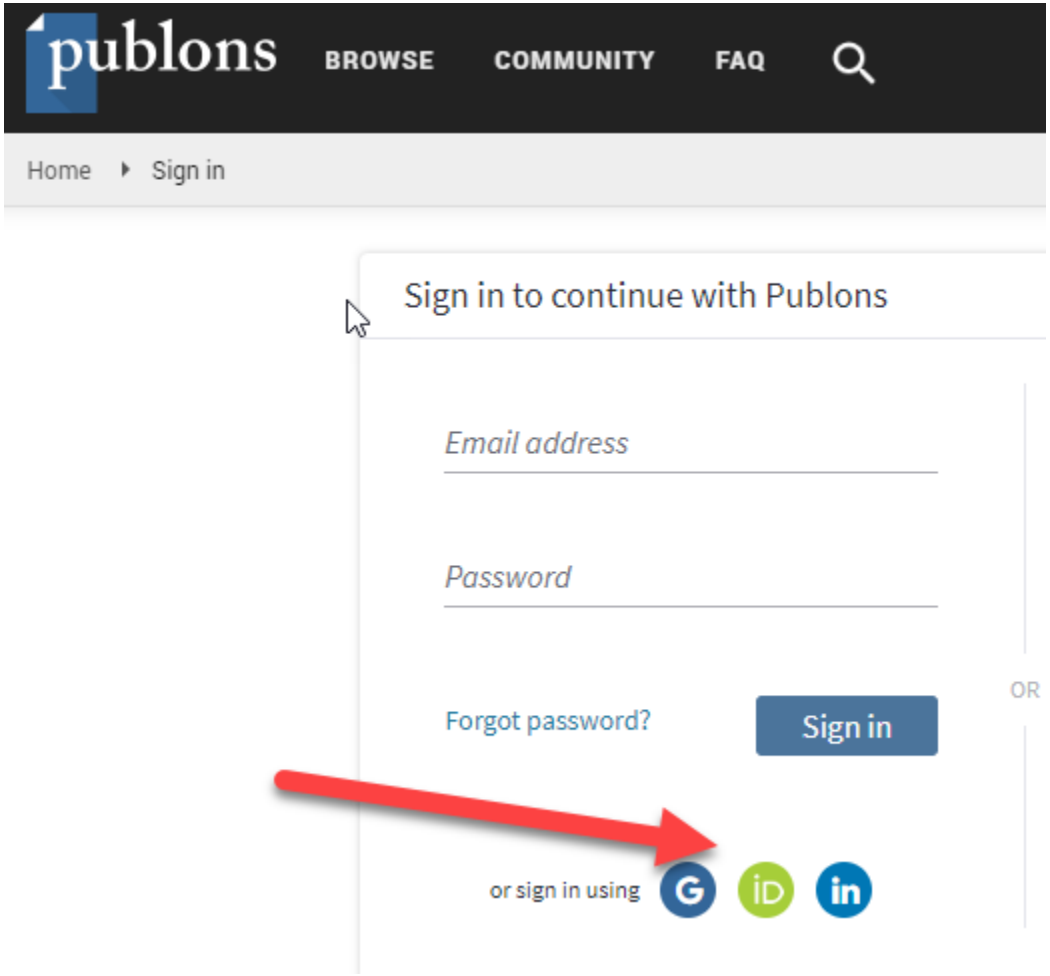

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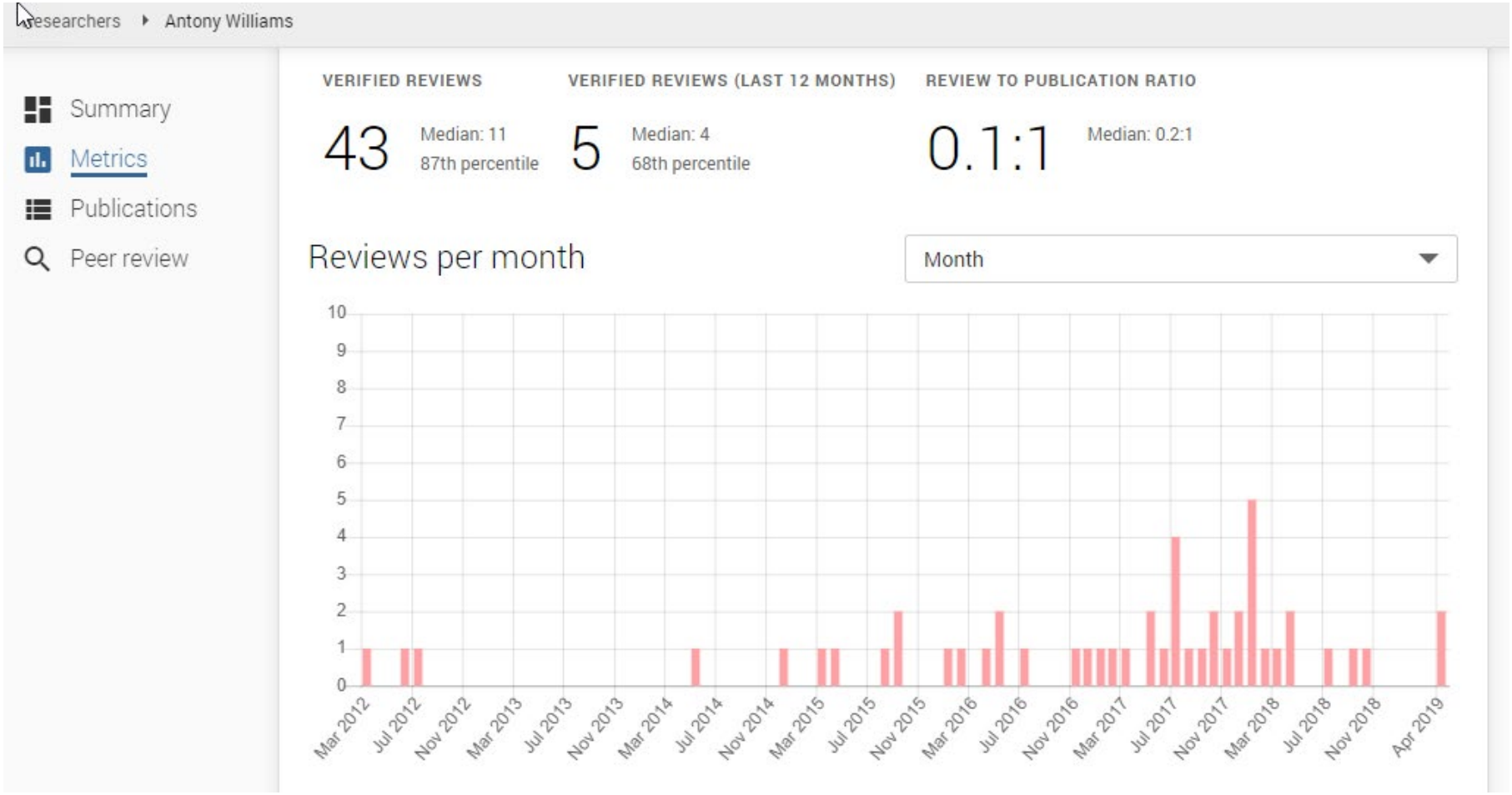

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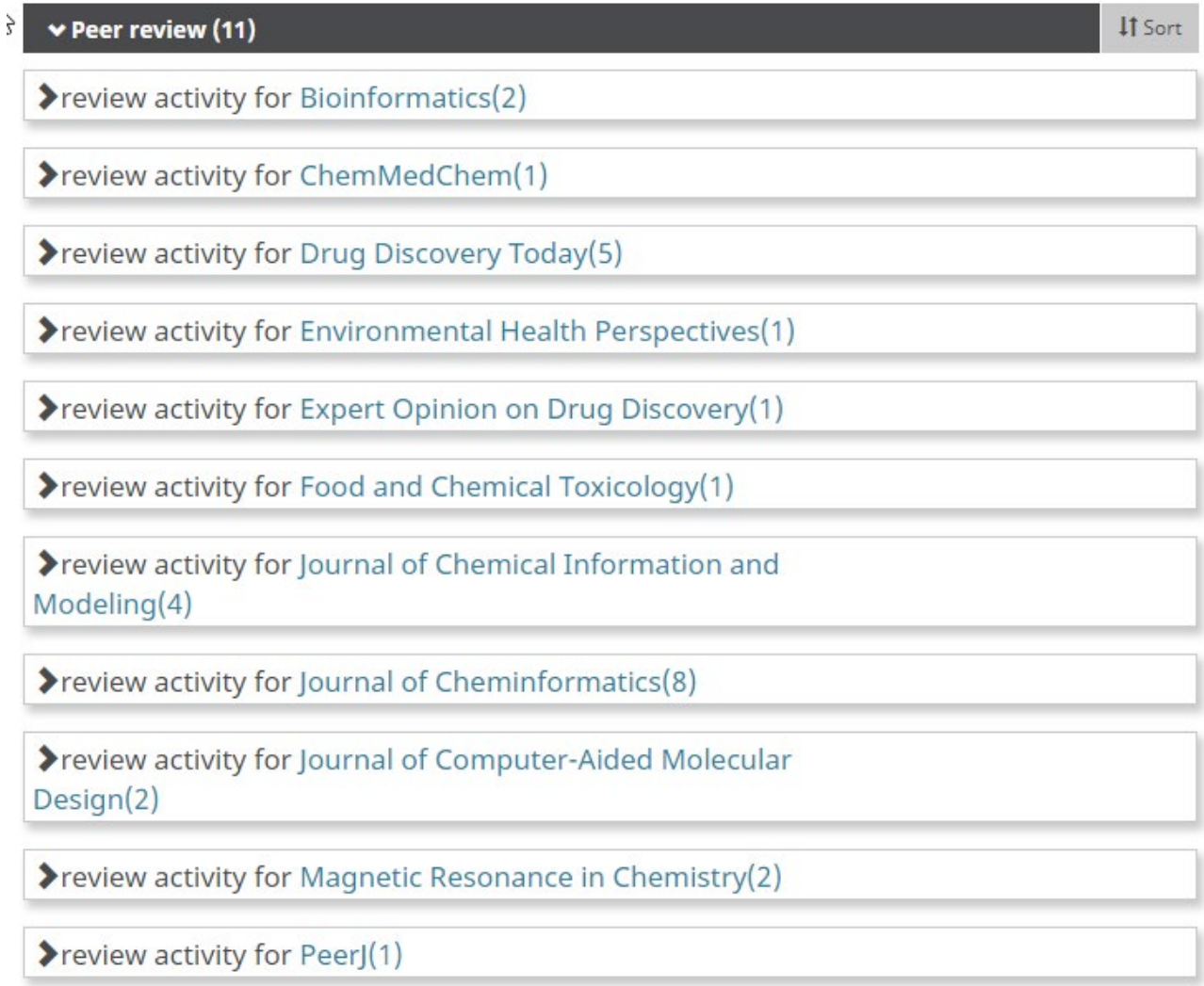

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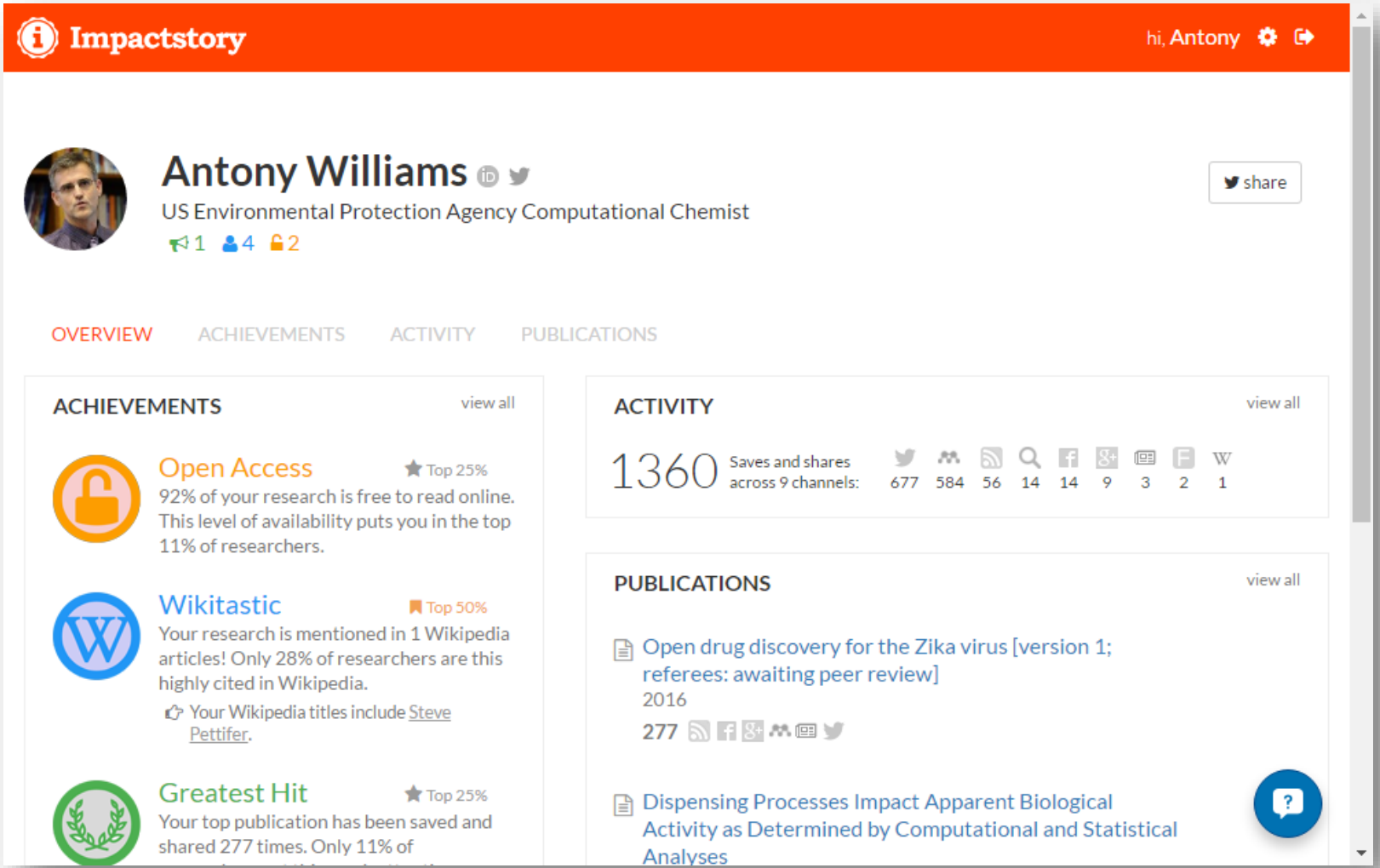

Antony Williams

US Environmental Protection Agency Computational Chemist

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Parallel Worlds of Public and Commercial Bioactive Chemistry Data [full text]
2015 *J. Med. Chem.*
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Coauthors

Egon Willighagen
Niklas Blomberg
Christopher Southan
Steve Pettifer
Christopher Lipinski
Jeremy Frey

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Sean Ekins, Joe Olechno, Antony J. Williams, Alexandre G. de Brevern
2013 PLoS ONE

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Analytical and Bioanalytical Chemistry
March 2017, Volume 409, Issue 7, pp 1729–1735

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

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First Online: 16 December 2016
DOI: 10.1007/s00216-016-0139-z

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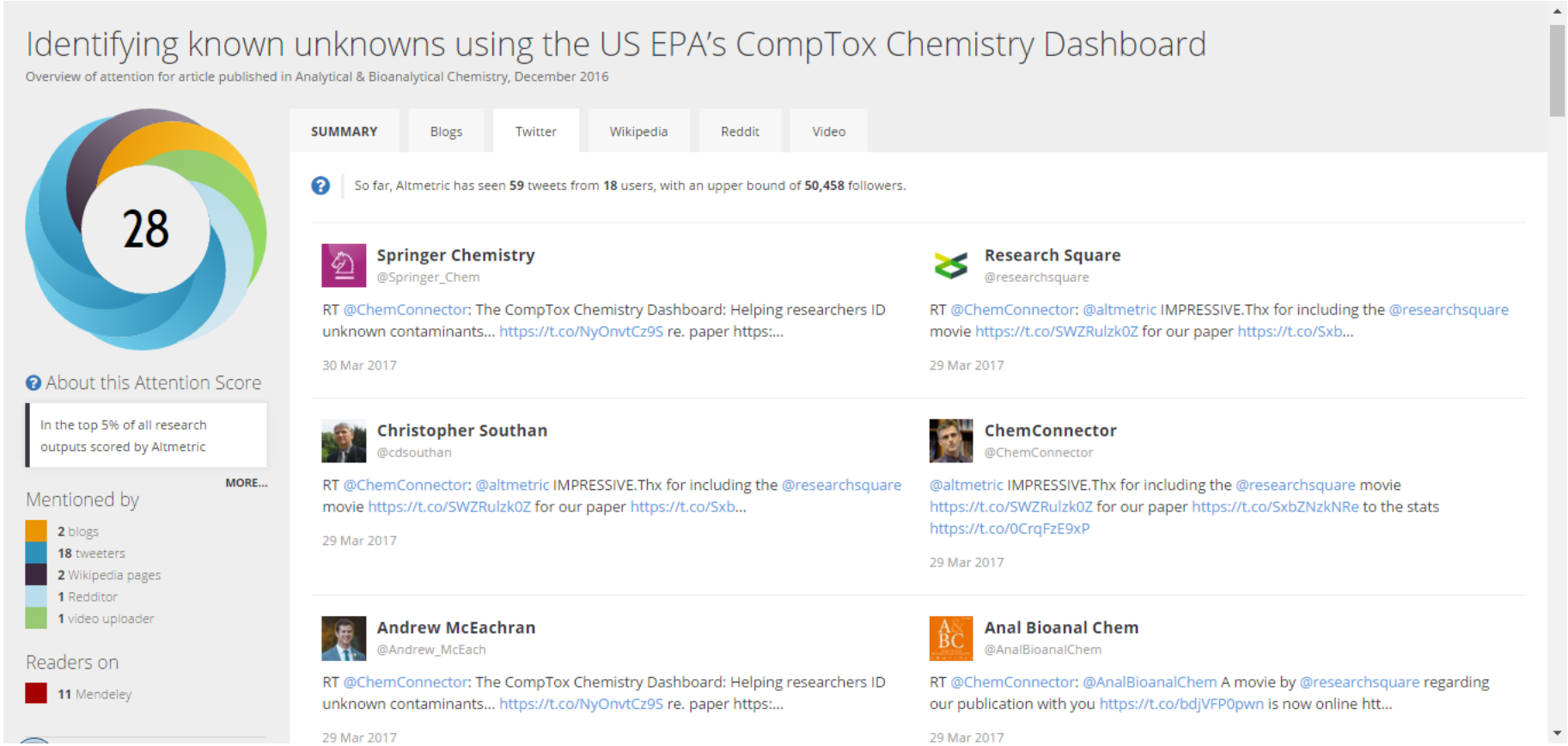

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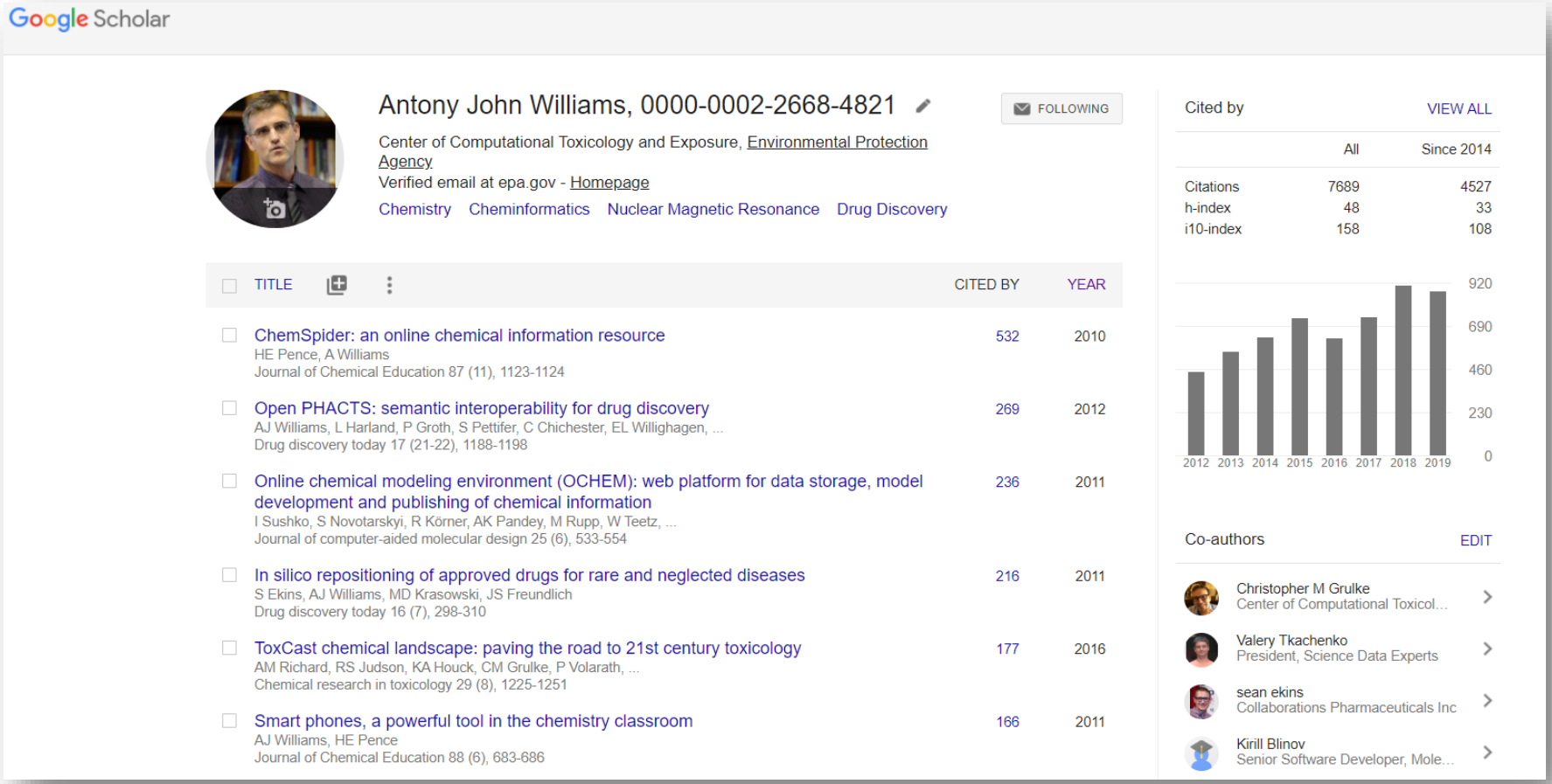

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EXPERIENCE WITH NASAL POSITIVE AIRWAY PRESSURE IN SLEEP-APNEA AJ WILLIAMS, S SANTIAGO, E PRESCOTT CLINICAL RESEARCH 33 (1), A83-A83			1985
COMPARISON OF LUNG-FUNCTION IN IDENTICAL-TWINS DISCORDANT FOR SMOKING AJ WILLIAMS, J CHOU, J KINNEY CLINICAL RESEARCH 32 (2), A438-A438			1984
OBSTRUCTIVE AIRWAYS DISEASE IN RHEUMATOID-ARTHRITIS (RA) AJ WILLIAMS, T PIETUCK, R CONSTANZ, J CHOU, J KINNEY CLINICAL RESEARCH 30 (2), A439-A439			1982
Analysis of the energy resources and demand of Western Europe. Final technical report, Jun 1974--Mar 1975 JF Schneider, KD Dance, RC Lind, RB Ryan, AR Williams Science Applications, Inc., McLean, Va.(USA)			1975
An investigation into the motions of ships at sea AJ Williams Trans. INA 95, 70		12	1953
Miscellanies in Prose and Verse A Williams, S Johnson T. Davies		12	1766

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☐	Computer-assisted structure verification and elucidation tools in NMR-based structure elucidation ME Elyashberg, AJ Williams, GE Martin Progress in Nuclear Magnetic Resonance Spectroscopy 53 (1), 1-104	86	2008
☐	Improved baseline recognition and modeling of FT NMR spectra S Golotvin, A Williams Journal of Magnetic Resonance 146 (1), 122-125	76	2000
☐	Internet-based tools for communication and collaboration in chemistry AJ Williams Drug discovery today 13 (11), 502-506	73	2008
☐	Sleep health New South Wales: chronic sleep restriction and daytime sleepiness DJ Bartlett, NS Marshall, A Williams, RR Grunstein Internal medicine journal 38 (1), 24-31	67	2008
☐	Carbon-carbon double-bond formation reductive coupling promoted by a monc Preparation and characterization of two R Duchateau, AJ Williams, S Gambarotta, MY Inorganic Chemistry 30 (25), 4863–4866		
☐	Public chemical compound databases AJ Williams Current Opinion in Drug Discovery and Develo		
☐	The use of NMR to study sodium dodec DD Miller, W Lenhart, BJ Antalek, AJ Williams, Langmuir 10 (1), 68-71		

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Antony John Williams, 0000-0002-2668-4821

Sleep health New South Wales: chronic sleep restriction and daytime sleepiness

Authors	DJ Bartlett, NS Marshall, A Williams, RR Grunstein
Publication date	2008/1/1
Journal	Internal medicine journal
Volume	38
Issue	1

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	For example: Patterson, David; Lamport, Leslie
Publication date	2016/11/25
	For example, 2008, 2008/12 or 2008/12/31.
Journal	SAR and QSAR in Environmental Research
Volume	27
Issue	11
Pages	911-937
Publisher	Taylor and Francis

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- 140 characters to connect and communicate
- Use a “brand name” on Twitter
- Greatest value for **me** – leading people into information I wish to share including my presentations and publications
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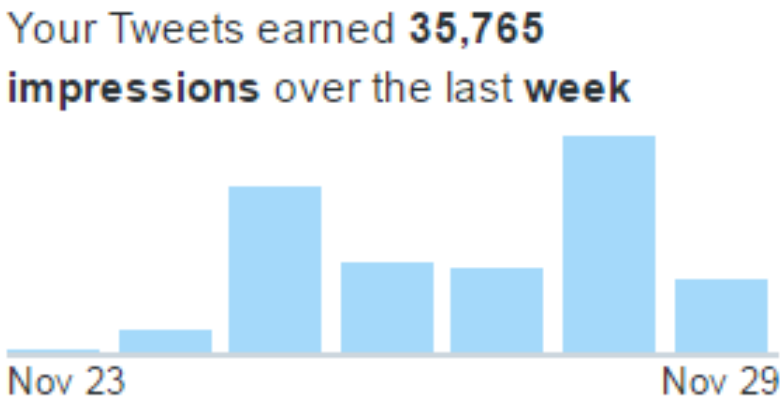

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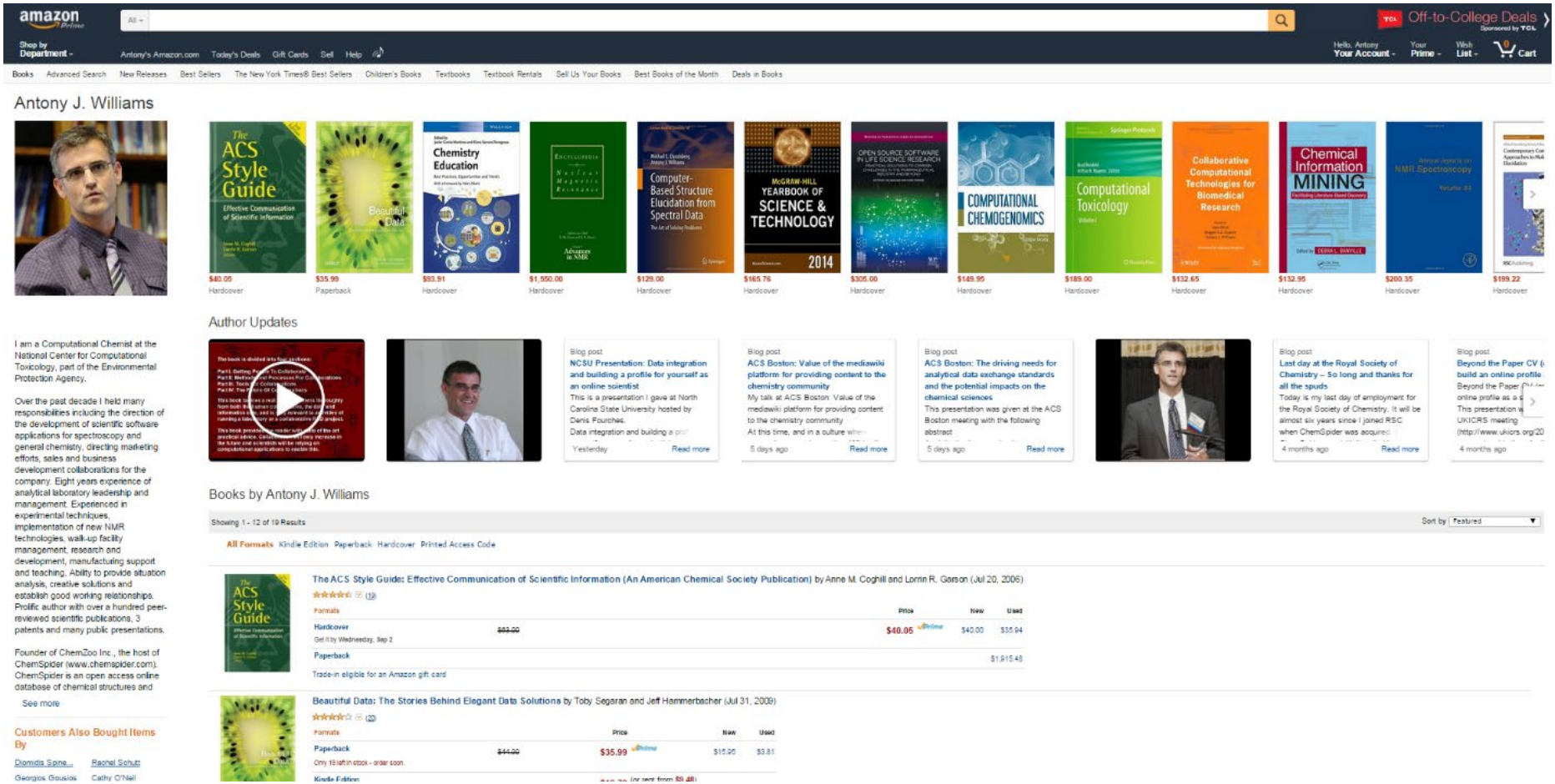
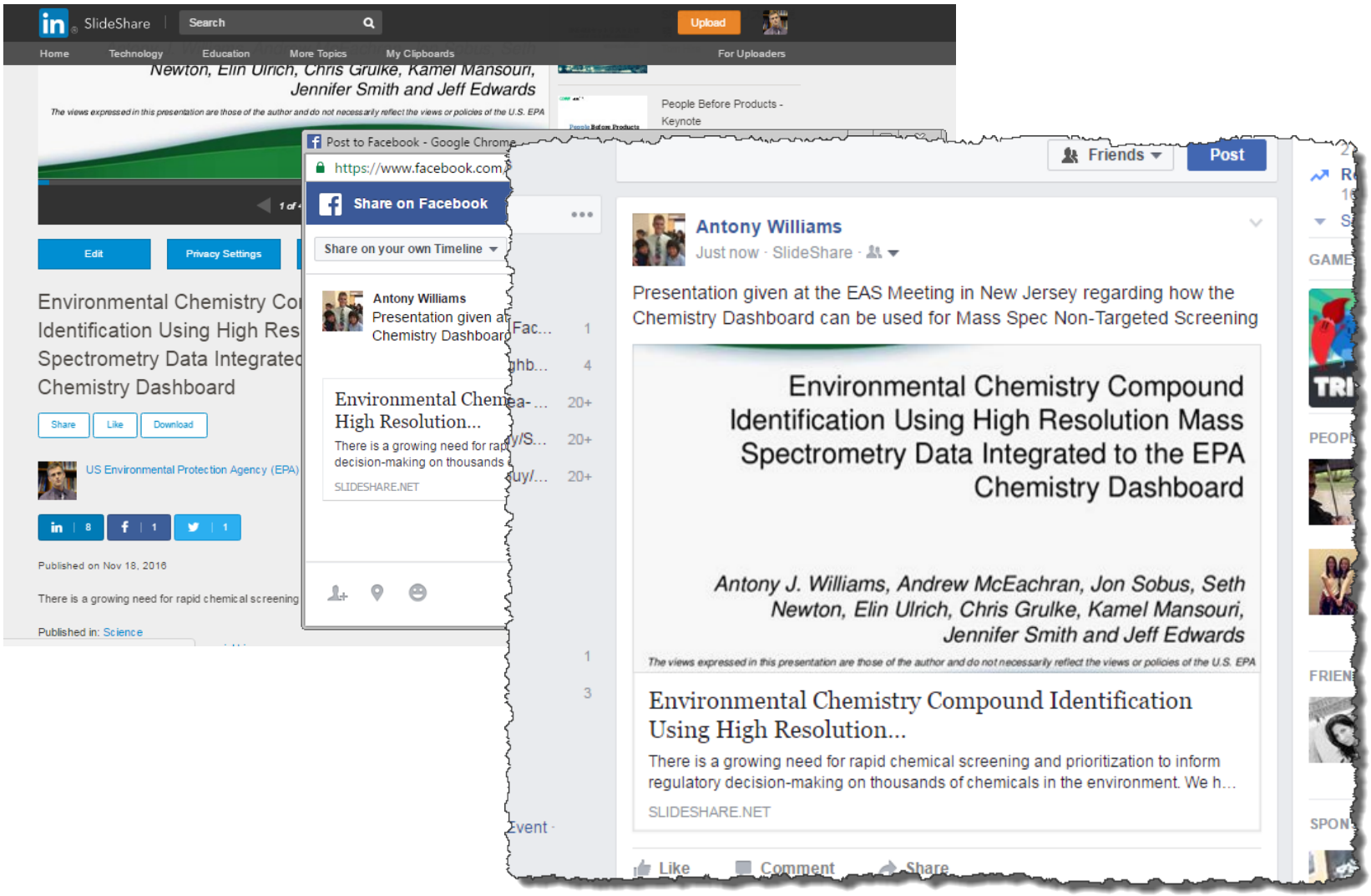


Facebook

- I personally use Facebook for “friends and family” – but since many of my friends are scientists…
  - I share my blog posts
  - I share links to my papers
  - I share my presentations directly from SlideShare

Facebook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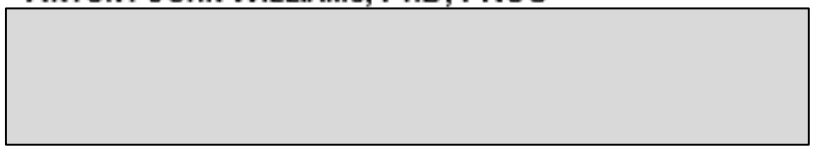

Blog: http://www.chemconnector.com

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SUMMARY SCIENTIST, ONLINE CHEMISTRY EVANGELIST AND SENIOR EXECUTIVE

- Experienced in senior leadership and management
- Expert at bridging science and community
- Thought leader and evangelist for "Open Access Chemistry"

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What Next?
My Recommendations

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

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

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What I said…

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

Email: williams.antony@epa.gov