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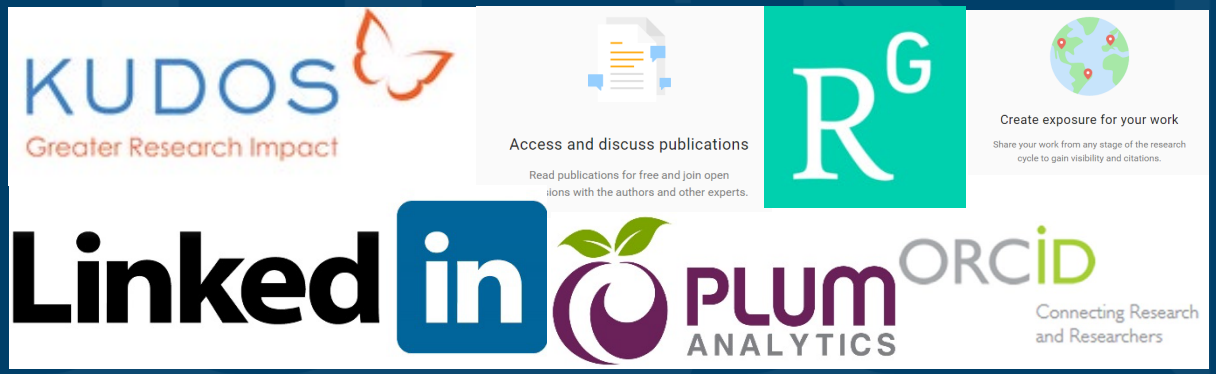
ORCID 0000-0002-2668-4821

Sharing Yourself and Your Science using Social Media Tools for Scientists



Antony Williams
Center for Computational Toxicology and Exposure

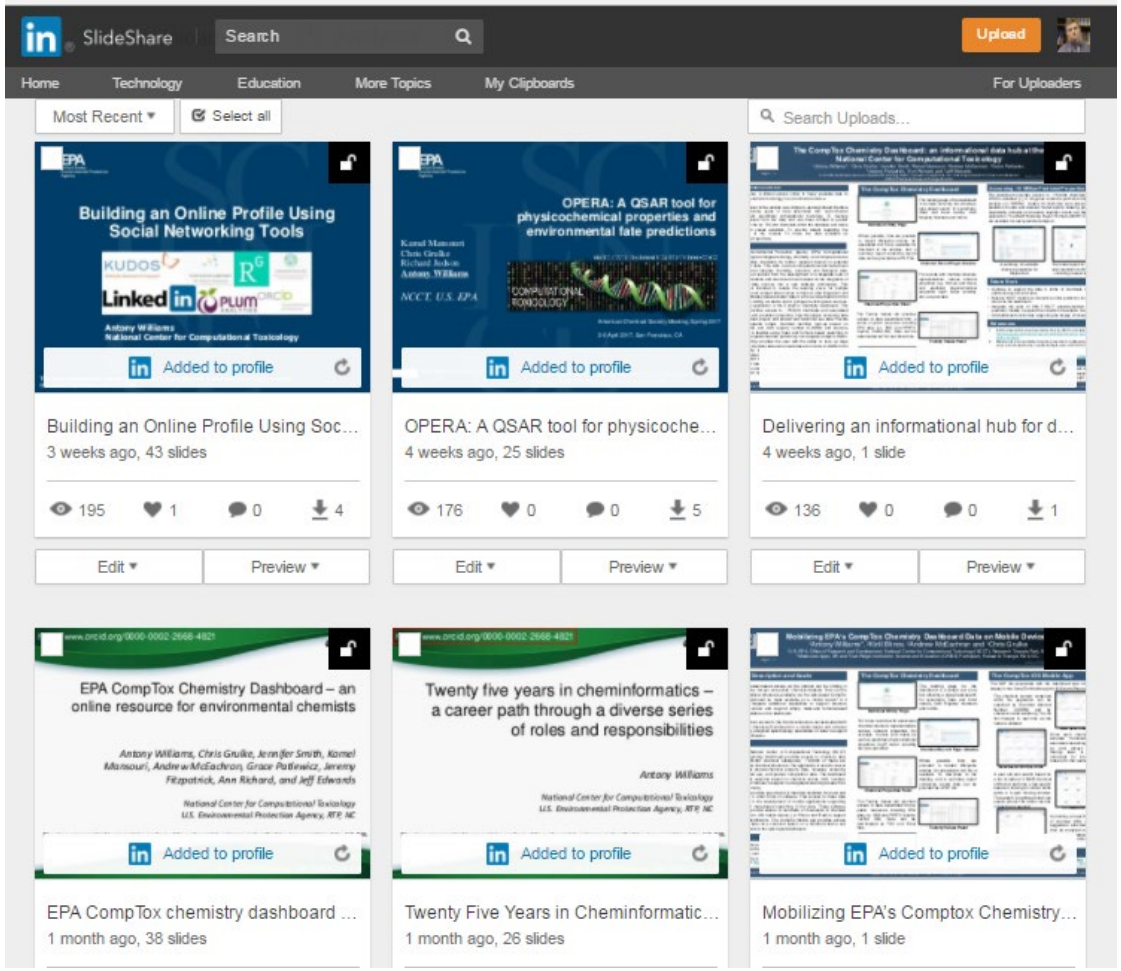
EPA United States Environmental Protection Agency

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…

- Consider…
  - 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?

- Maybe after this it will change…

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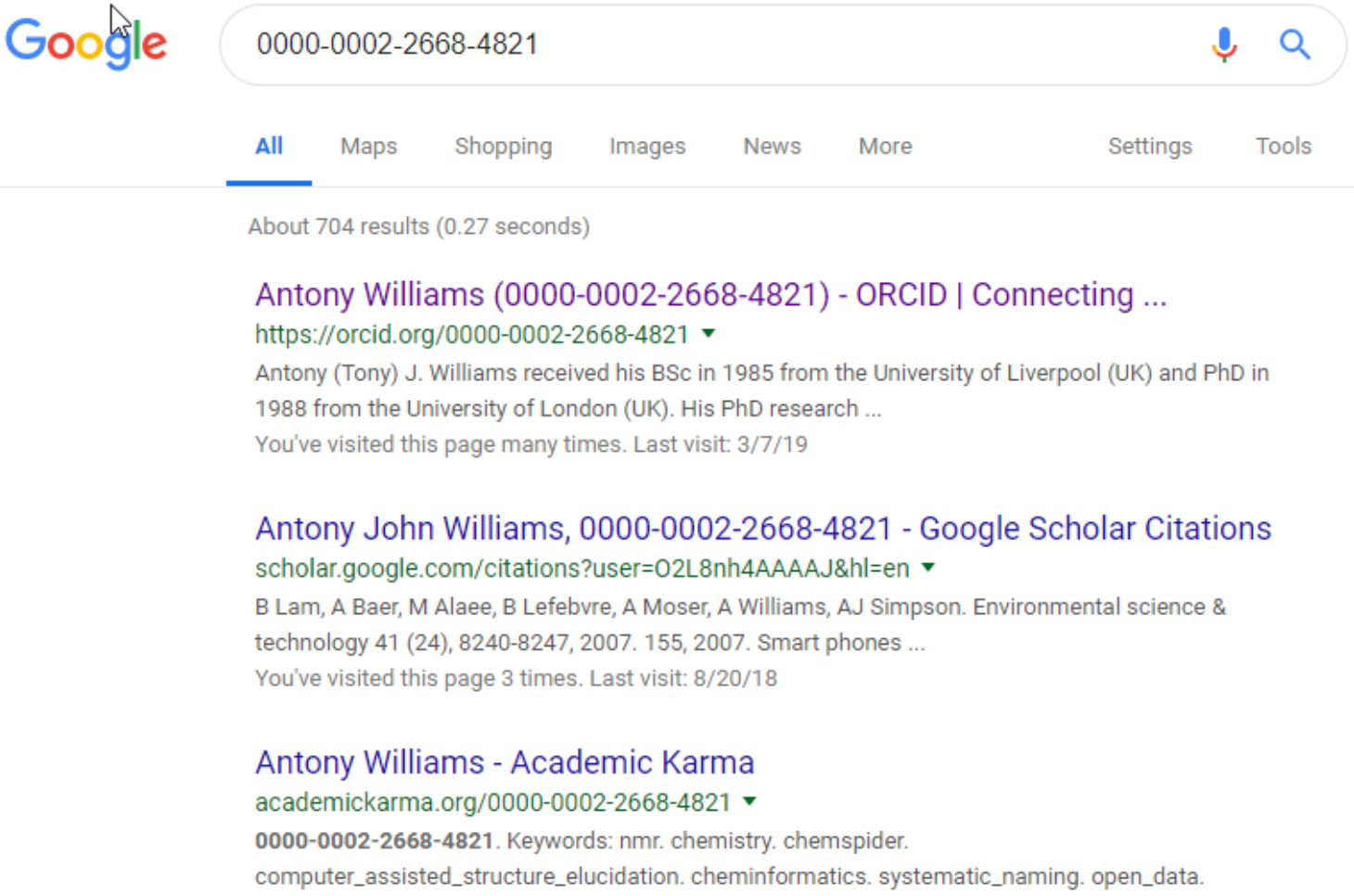
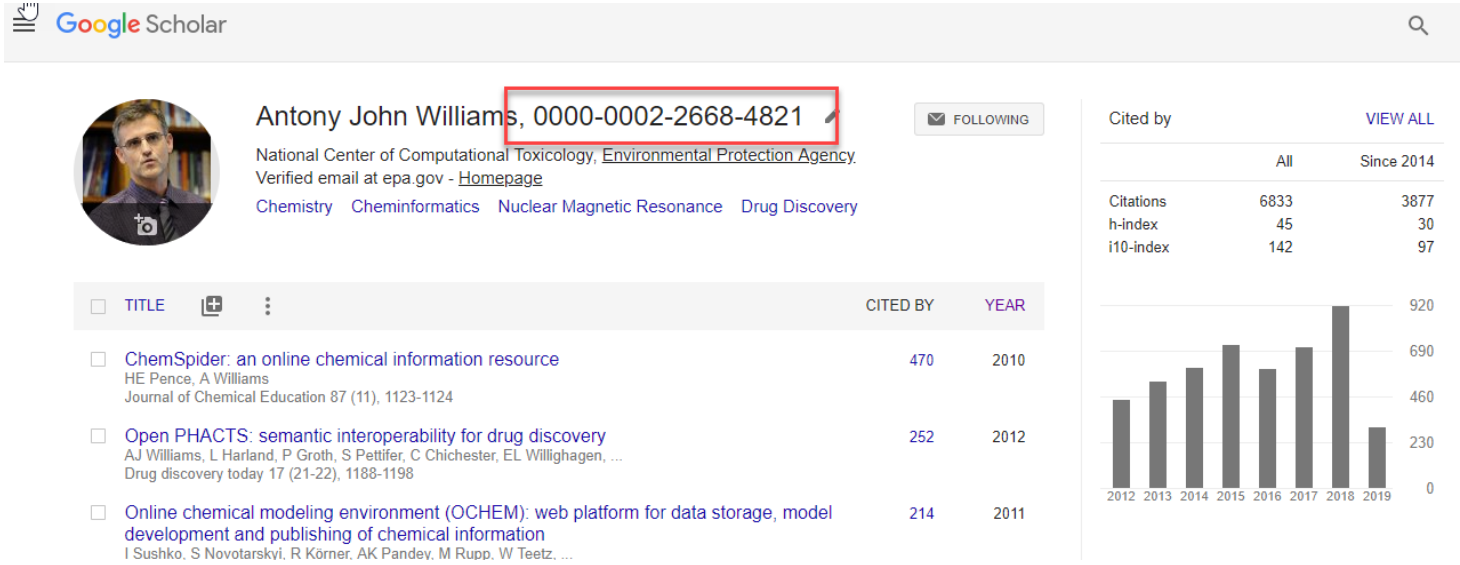
It's a Scientists SSN – use it in various places

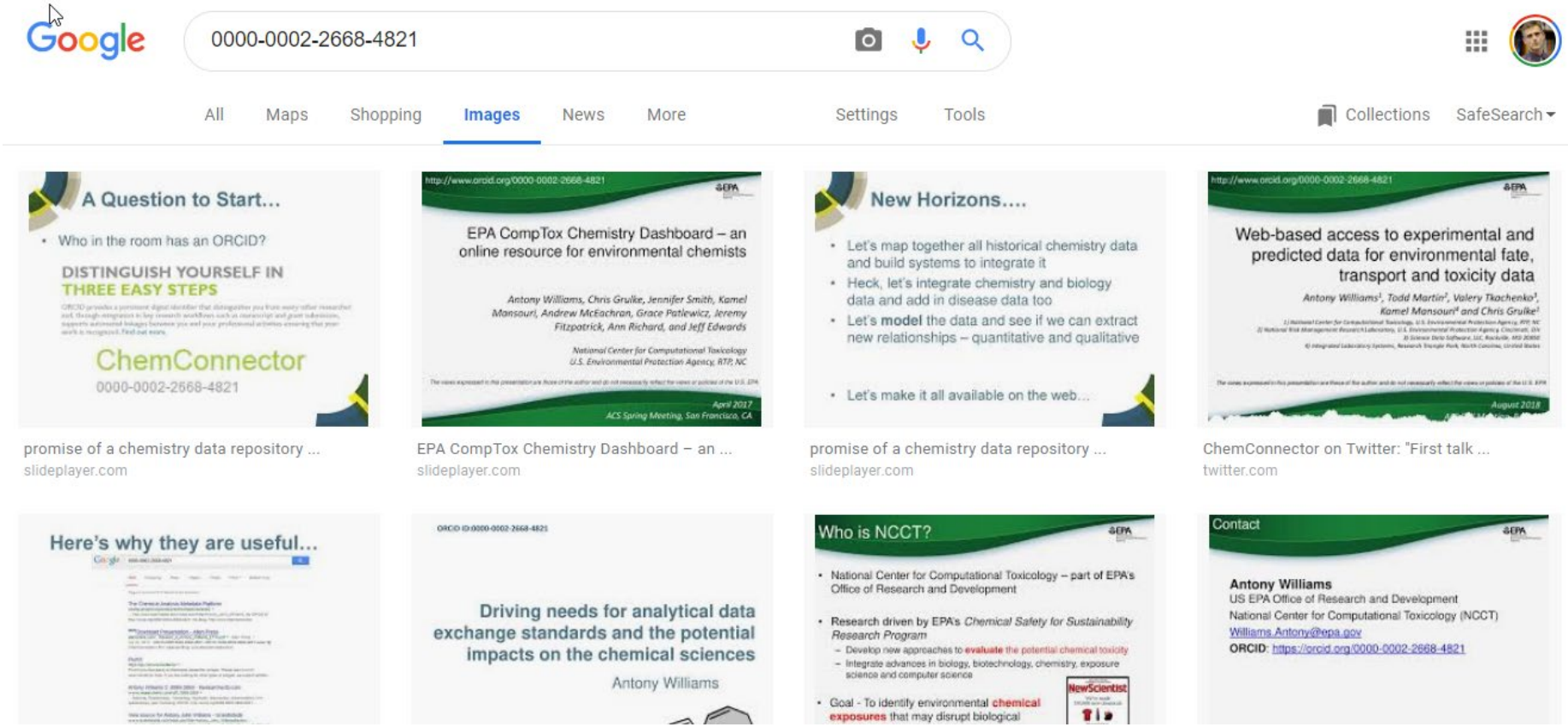


Use ORCID on all products

- 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.

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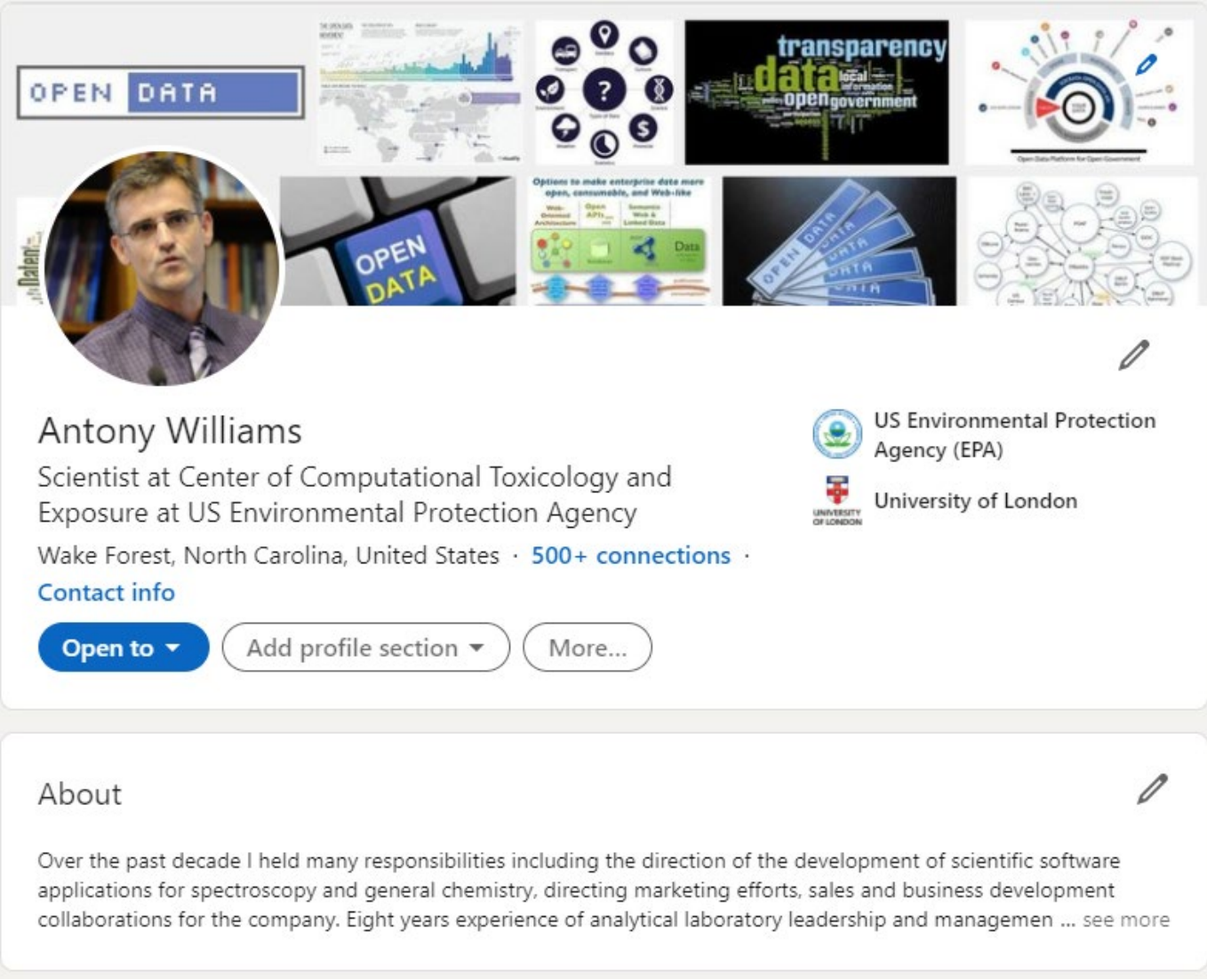
Scientists are Evaluated: "Statistics"

- 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: Career Networking Tool



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

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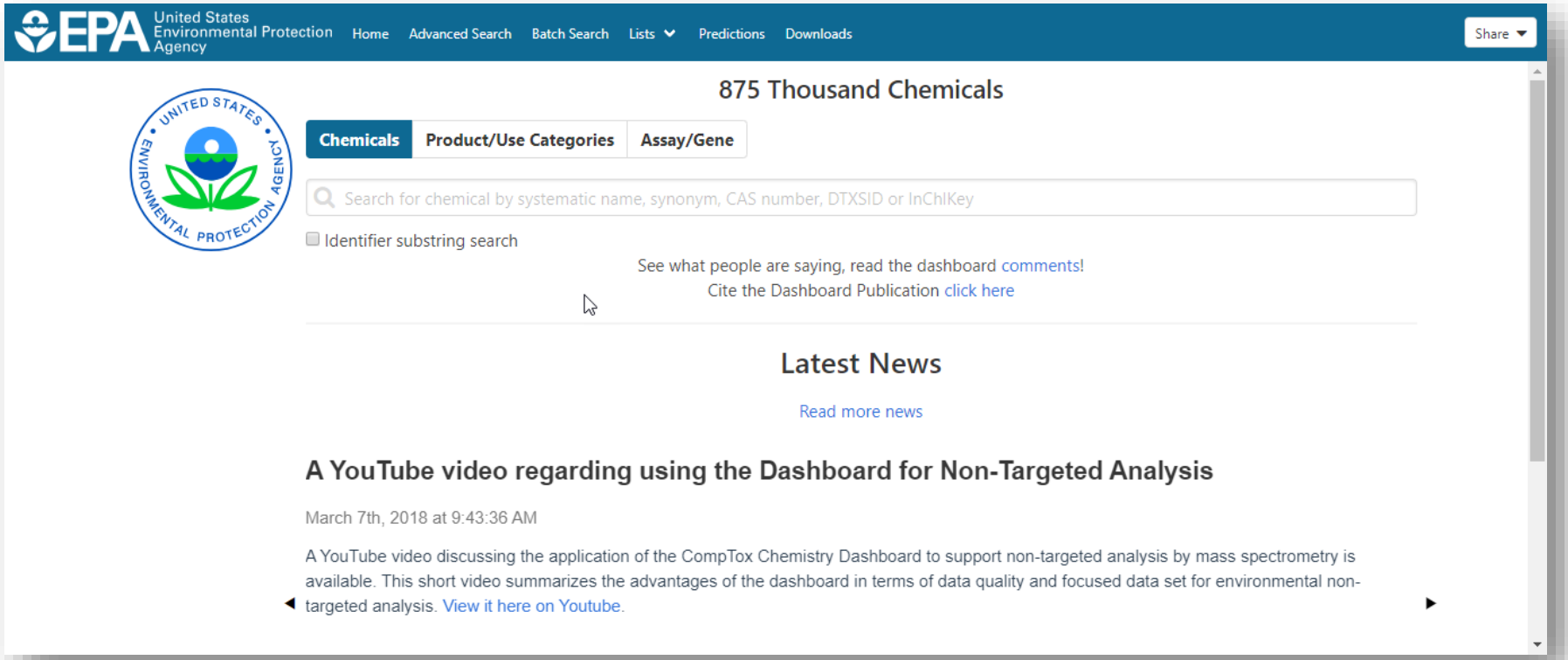
Something I worked on…



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

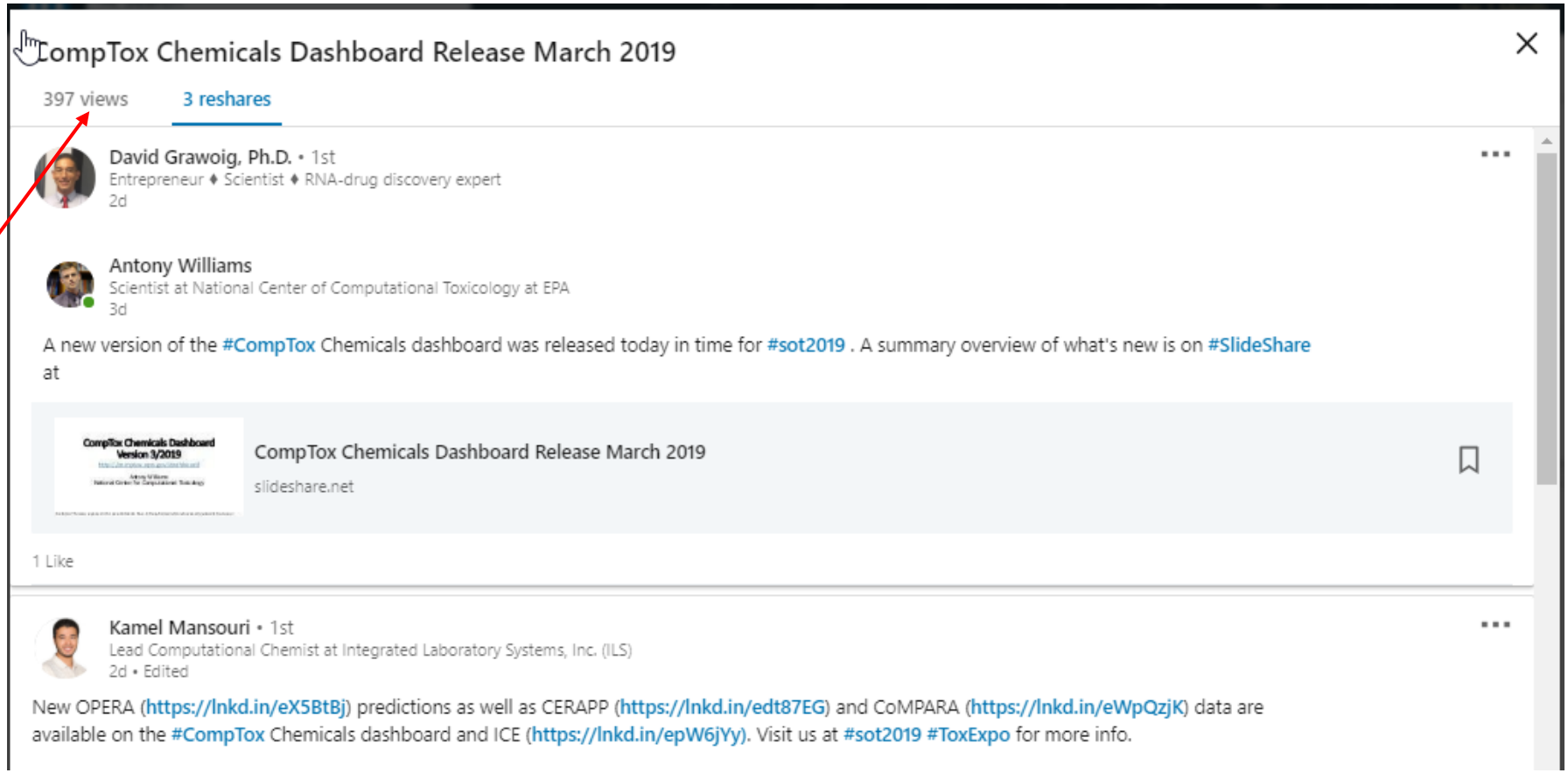
Generalized Read-Across (GenRA): A workflow implemented into the EPA CompTox Chemicals Dashboard

Feb 4, 2019 • ALTEX-Alternatives to animal experimentation

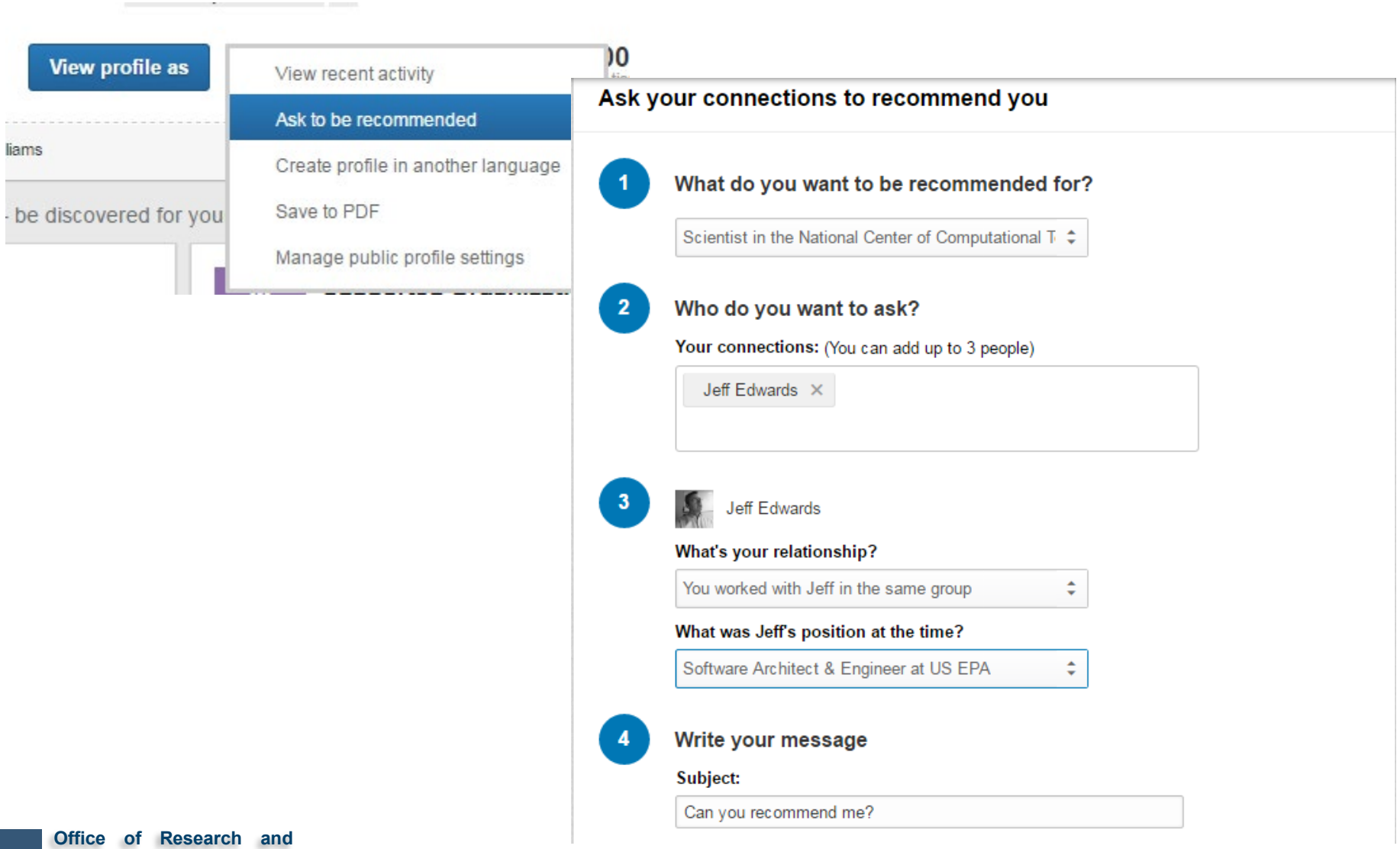
Generalized Read-Across (GenRA) is a data driven approach which makes read-across predictions on the basis of a similarity weighted activity of source analogues (nearest neighbors). GenRA has been described in more detail in the literature (Shah et al., 2016; Helman et al., 2018). Here we present its 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

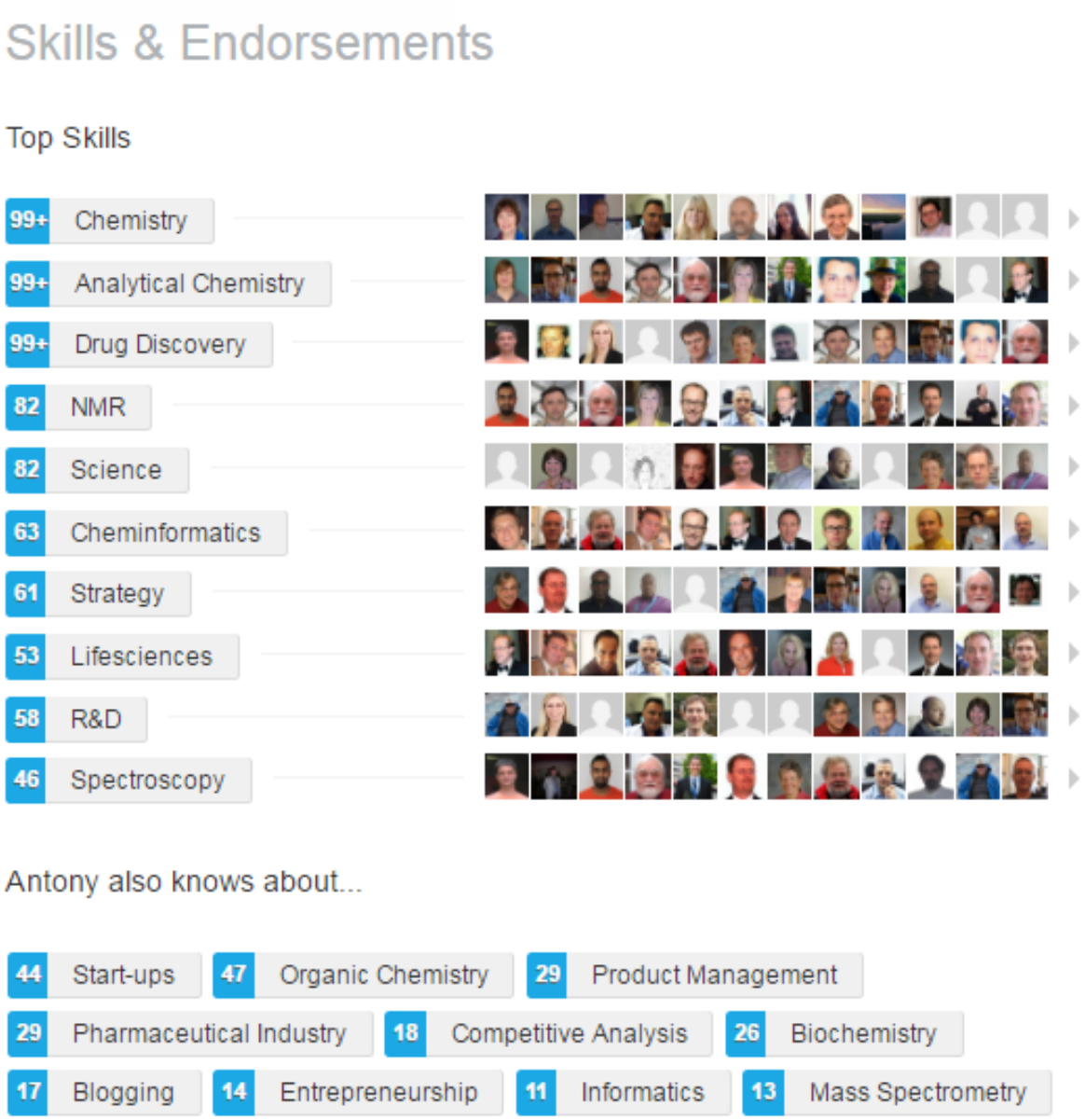
Your Postings Get Networked



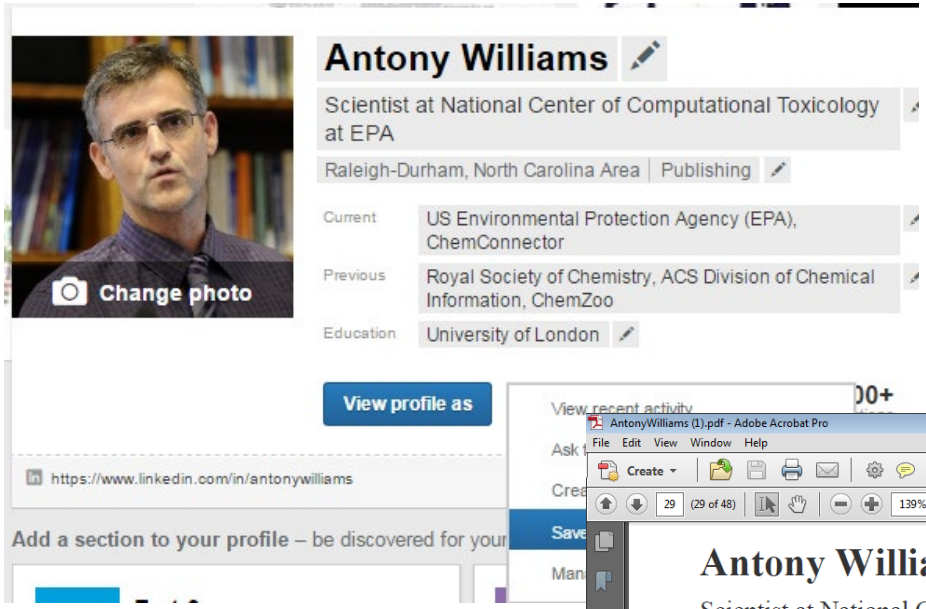
Ask for Recommendations

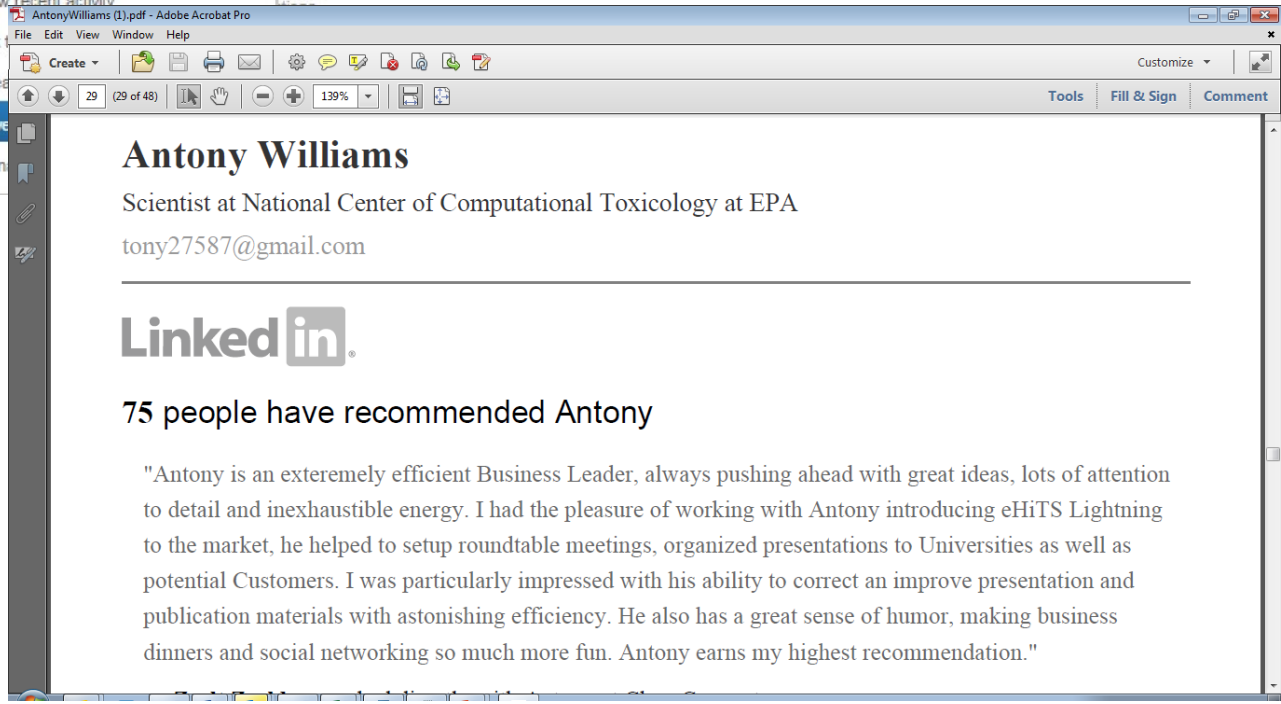


Ask for “Endorsements”,

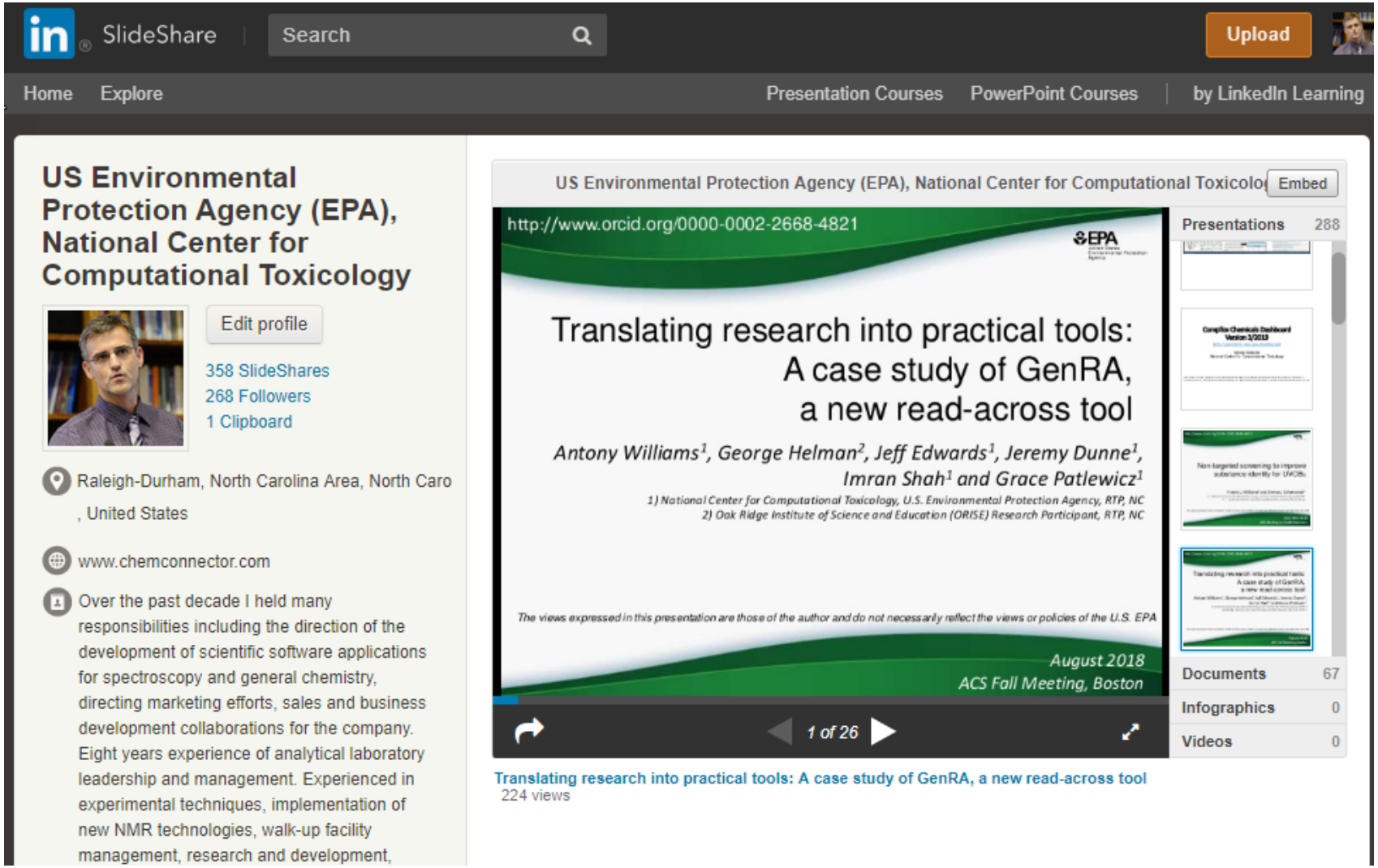


Instant Summary as a PDF

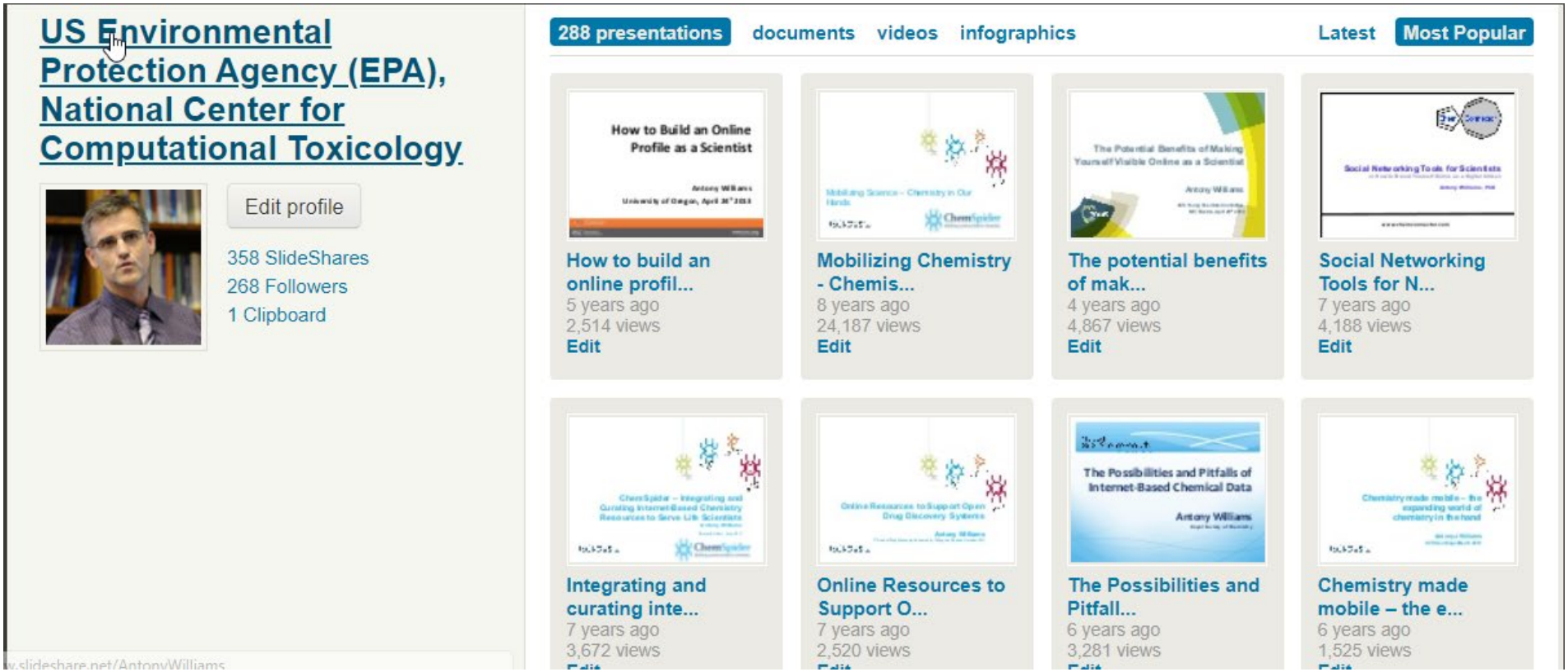




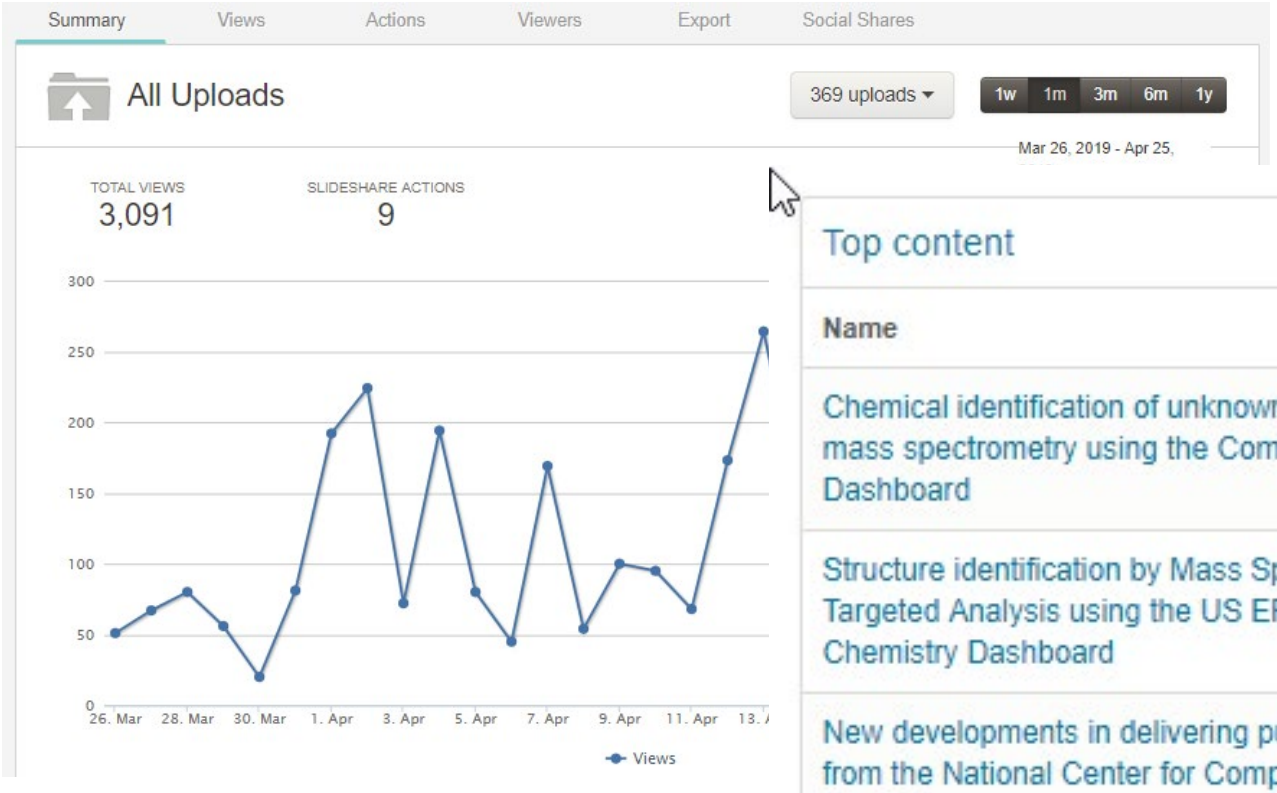
Presentations



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

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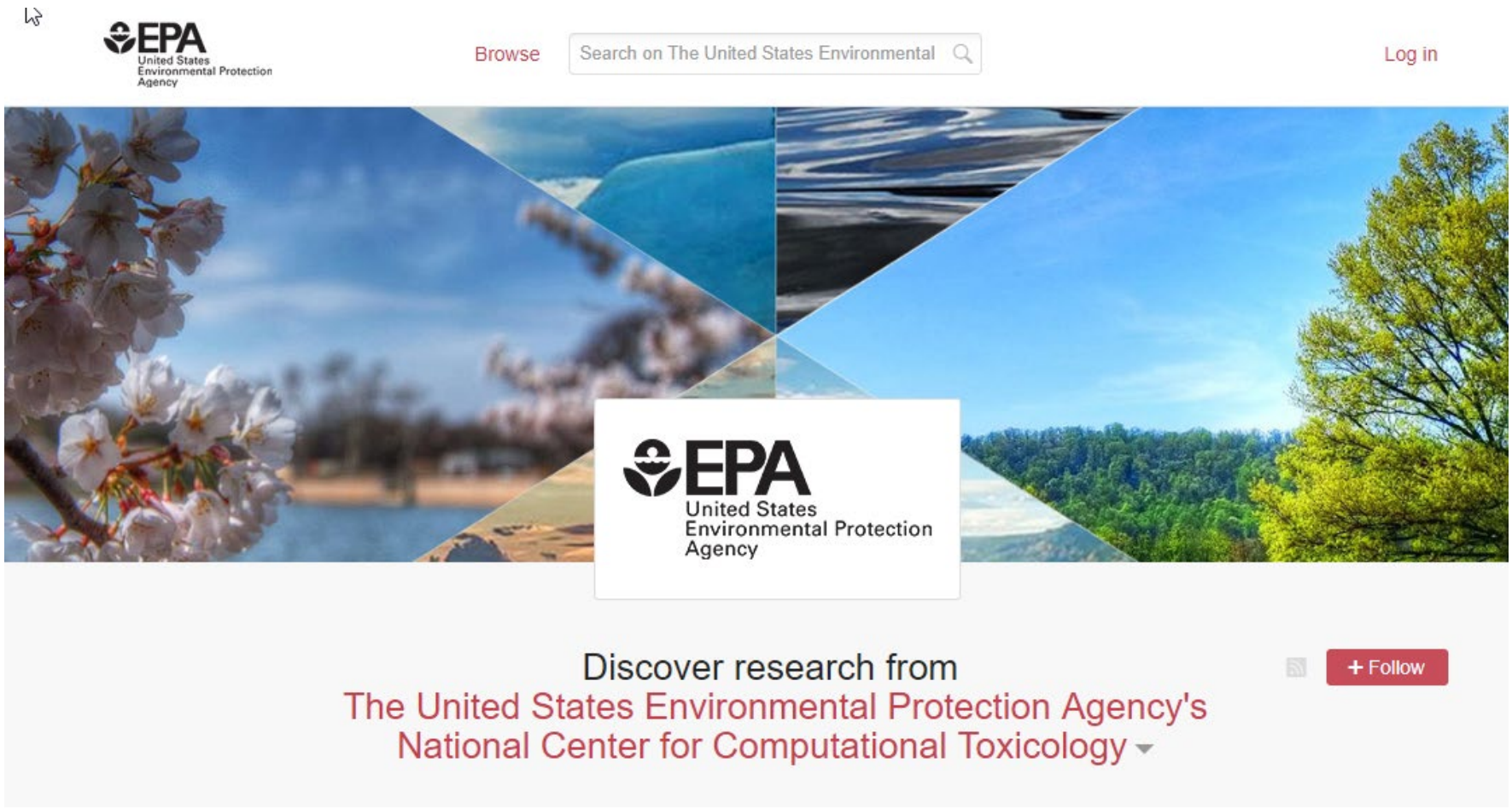

Presentations and Datasets

United States Environmental Protection Agency

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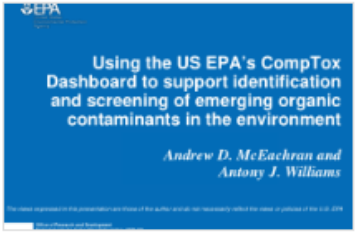
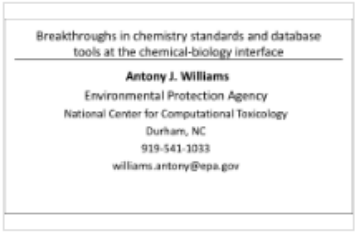
DSSTox: The Open Environmental Chemistry Data underlying the Co...
Chris Grulke 06/06/2018



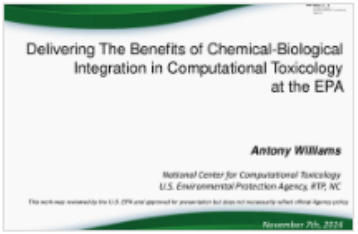
Using the US EPA's CompTox Dashboard to support identificatio...
Antony Williams 30/06/2017

Building an Online Profile Using Social Networking Tools
Antony Williams 30/05/2018

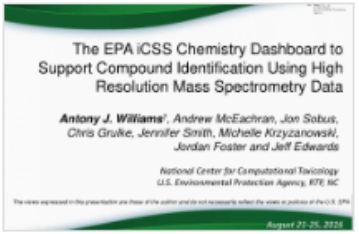


Breakthroughs in chemistry standards and database tools at th...
Antony Williams 30/06/2017

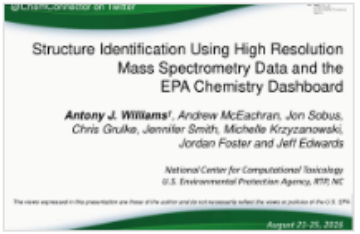
Influence of data curation on QSAR Modeling – examining issues of qu...



Delivering The Benefits of Chemical-Biological Integration in ...

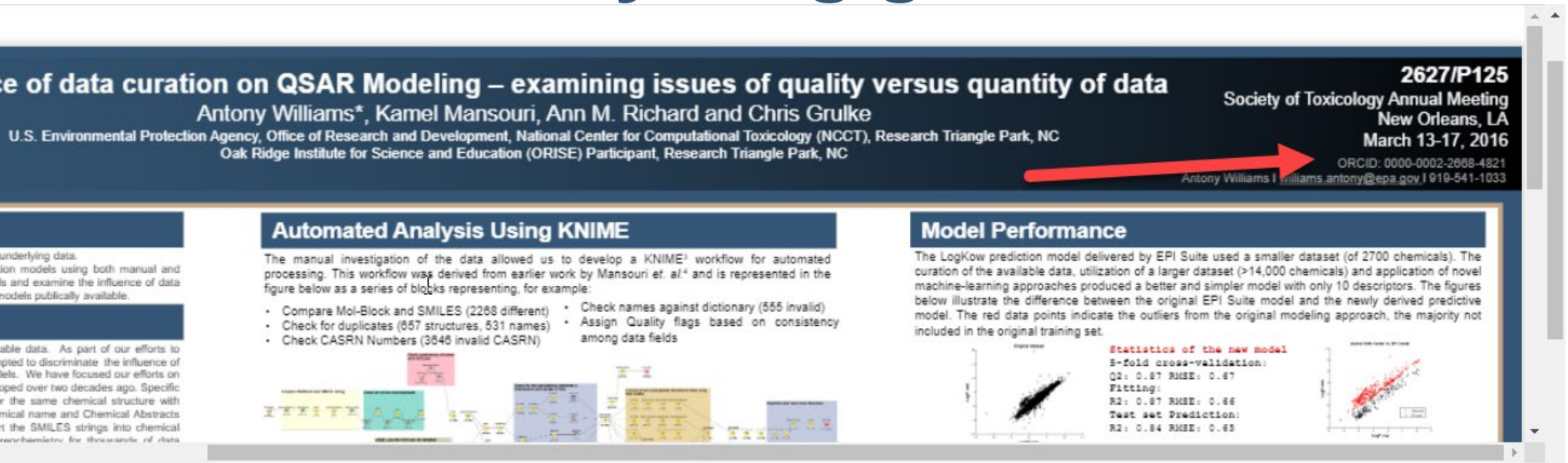


The EPA iCSS Chemistry Dashboard to Support Compound Identificatio...



Structure Identification Using High Resolution Mass Spectrometry Dat...

Including all Posters… everything gets DOI'ed



ms Quality Poster 0307_2016_fin….pdf (699.07 kB)

MD5: 684b9db8c33b6b26d4f2740161573329

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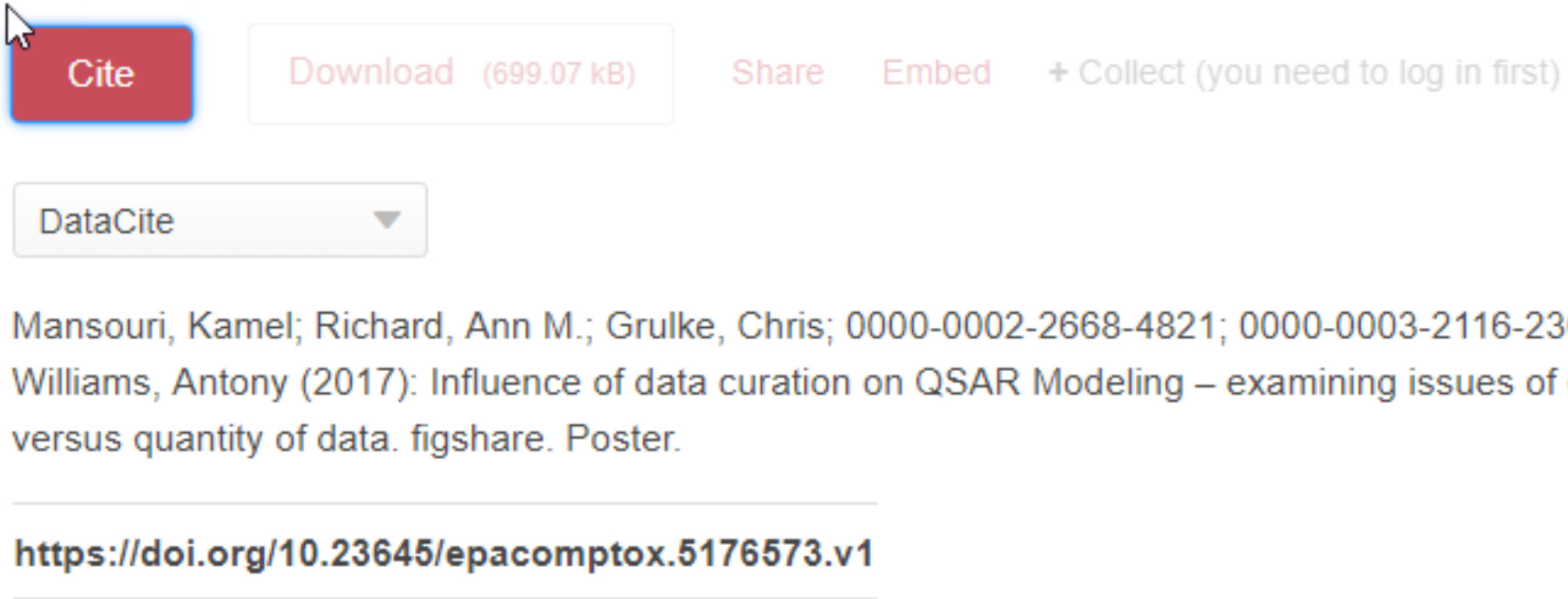
Influence of data curation on QSAR Modeling – examining issues of quality versus quantity of data

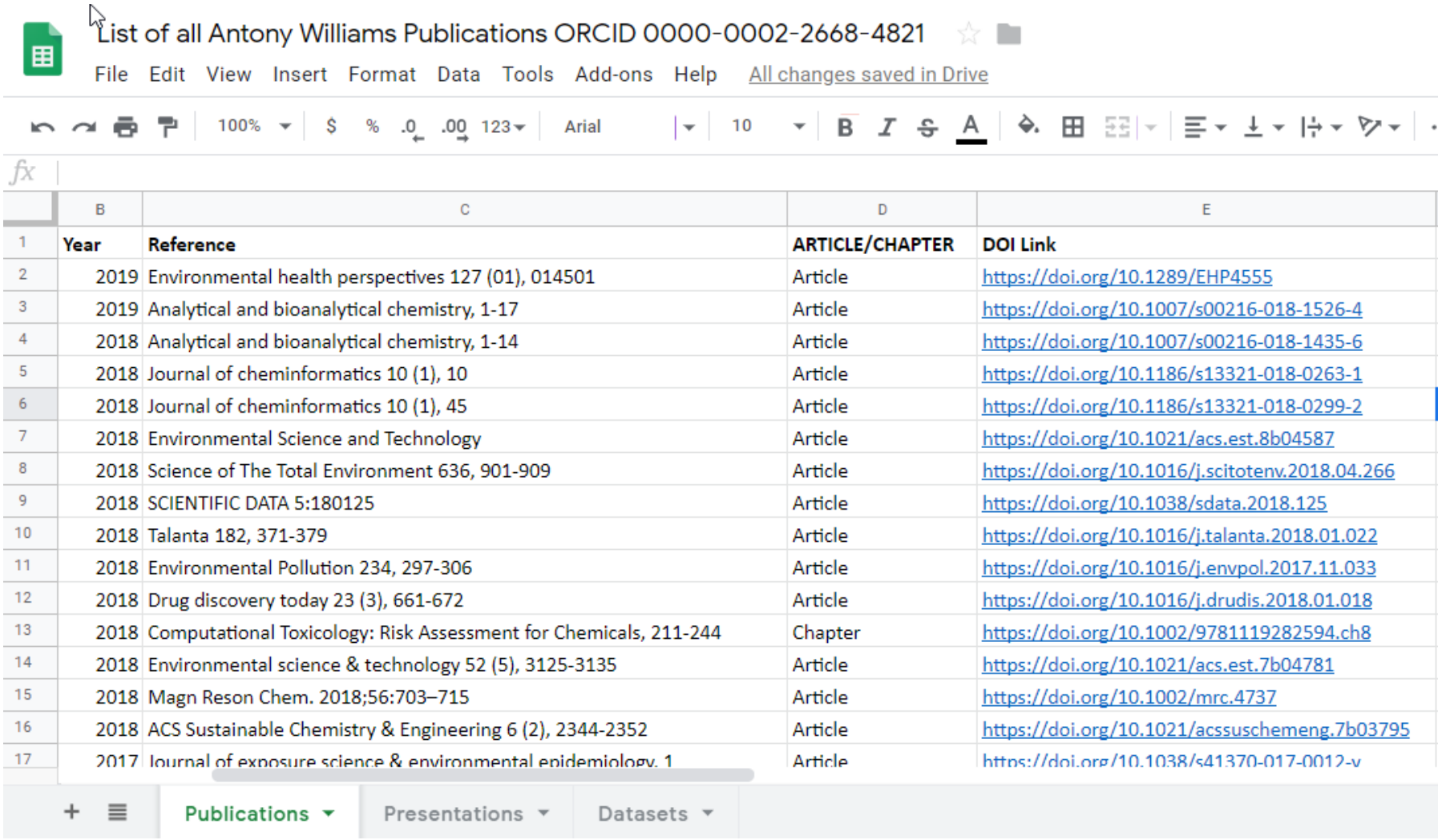
114 views | 34 downloads | 0 citations

Poster posted on 24.07.2017, 11:18 by Kamel Mansouri, Ann M. Richard, Chris Grulke, 0000-0002-2668-4821, 0000-0003-2116-2300, Antony Williams

DOI everything if you can



DOI your research outputs and put online… Don't Wait!



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

File Edit View Insert Format Data Tools Add-ons Help All changes saved in Drive

	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

45.02 · PhD · Edit

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Introduction

Edit

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) Edit

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

Stats overview

View all

3,373 Total Research Interest	5,570 Citations
92 Recommendations	33,618 Reads

Affiliation

Edit

United States Environmental Protection Agency

Location
United States

Department
National Center for Computational Toxicology

Position
Computational Chemist

Russell Scott Thomas's Lab

Lab head
Russell Scott Thomas

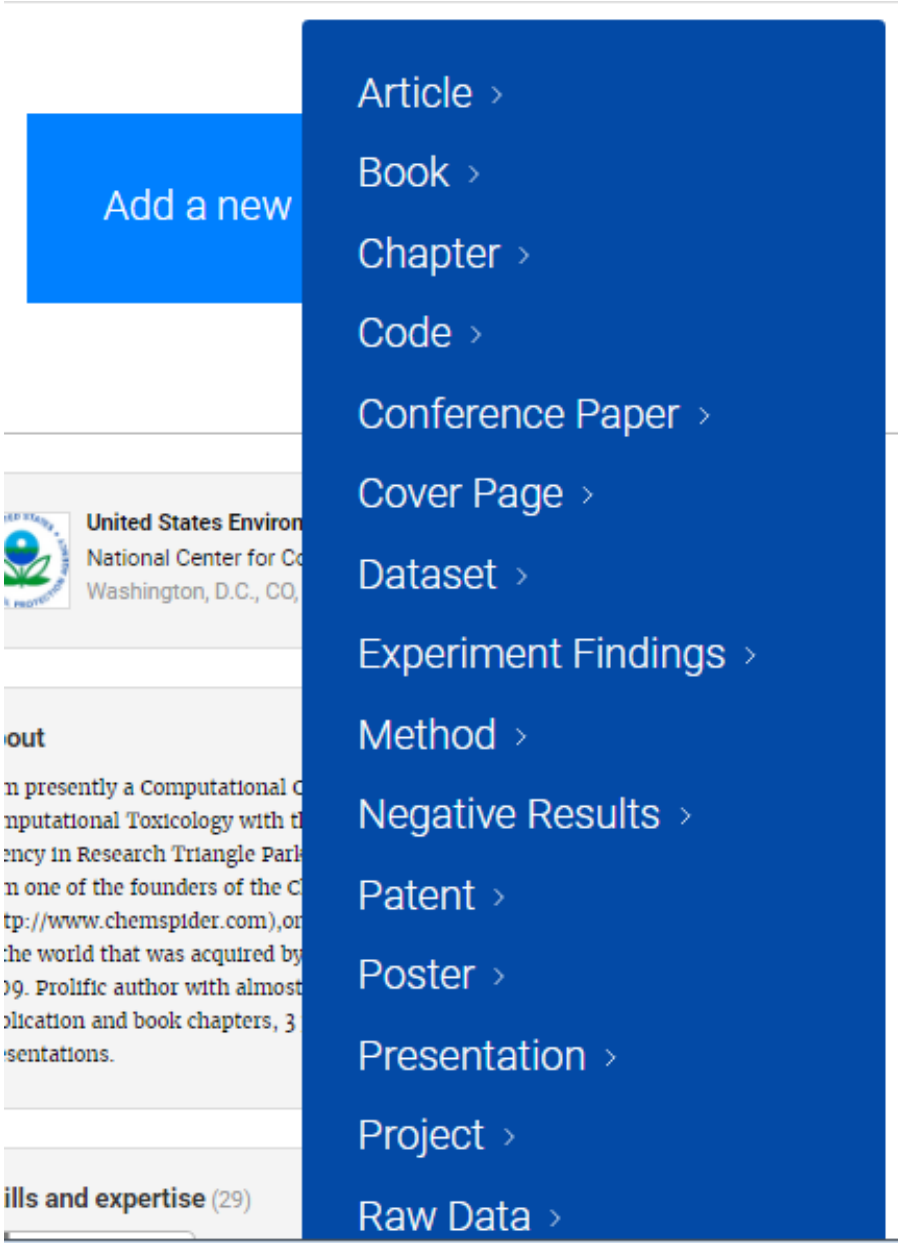
Lab members (6)

View lab Edit

Awarded grants (0)

Office of Developmer

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…

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"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
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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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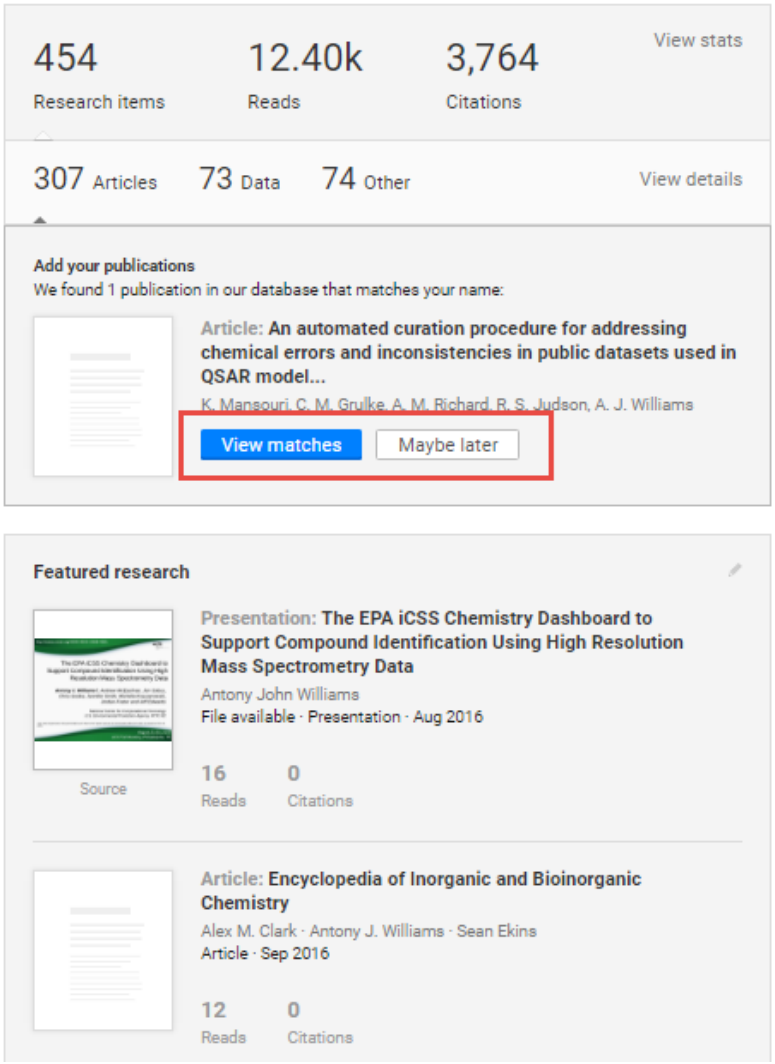

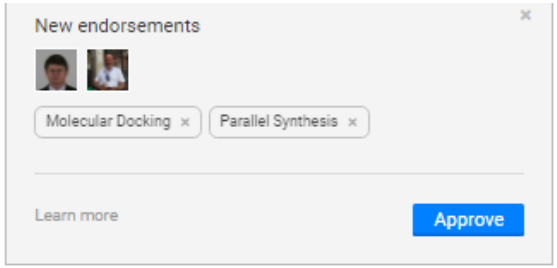

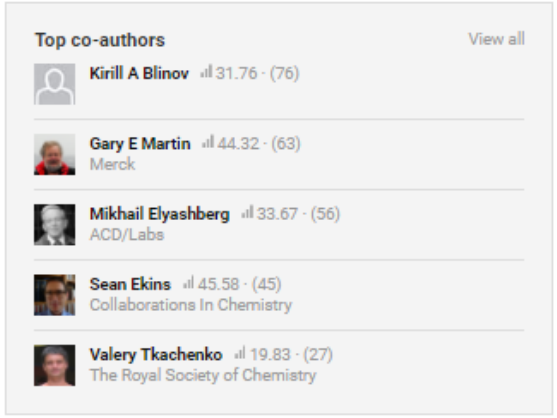

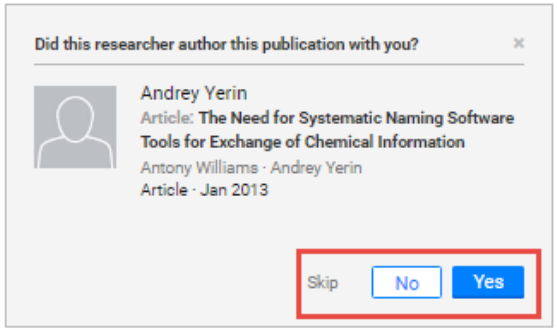

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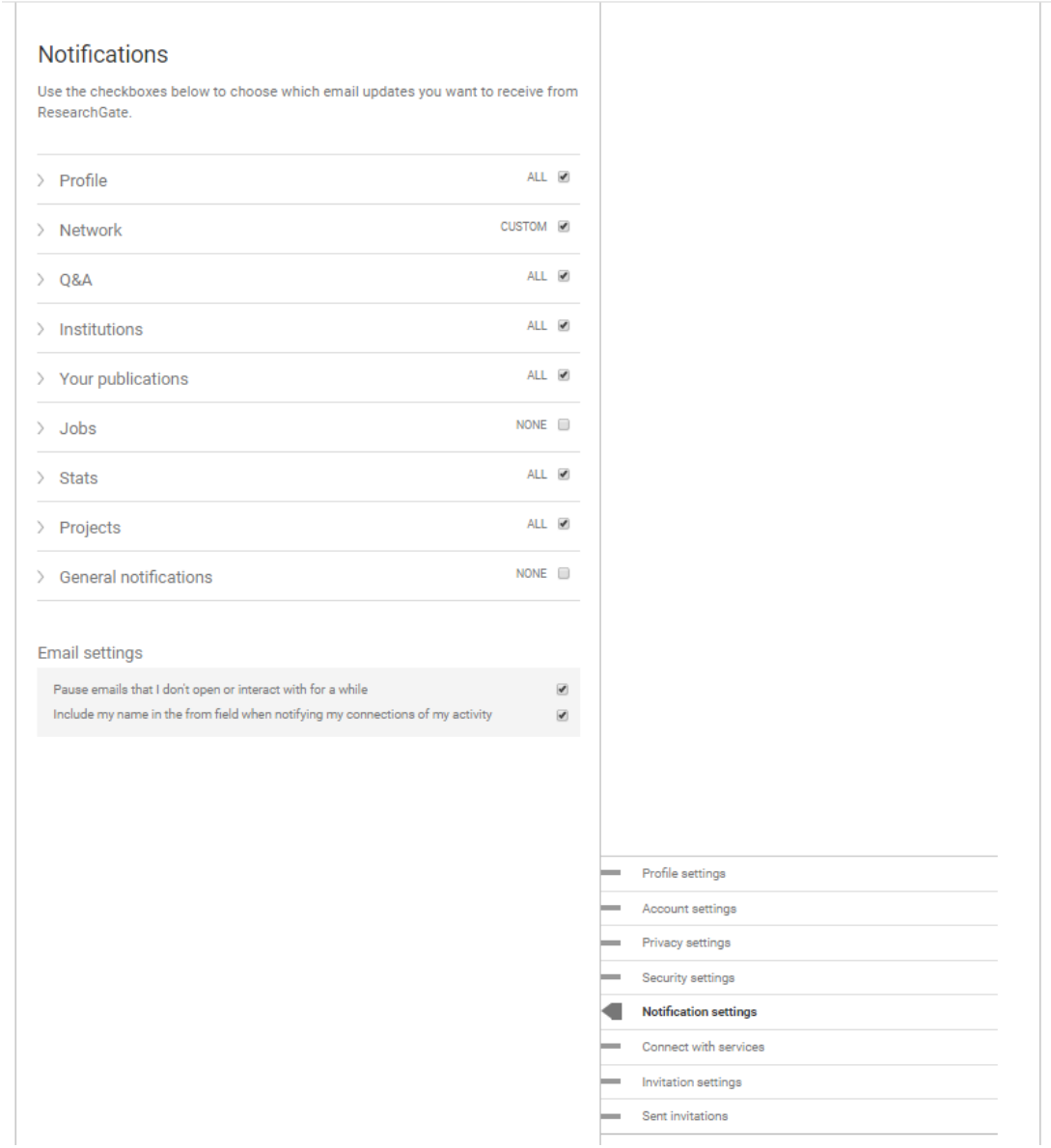

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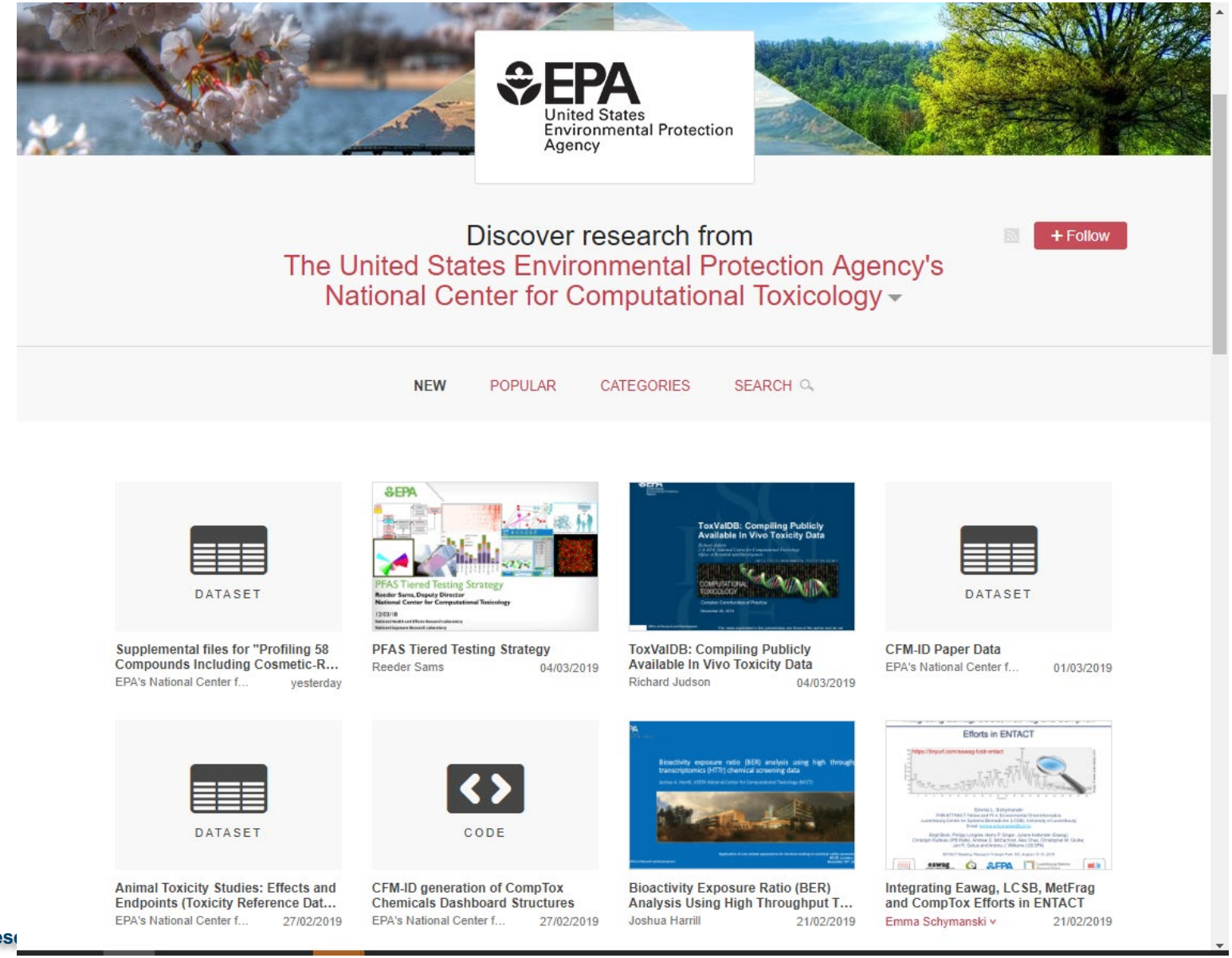

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17.02.2017, 11:27 by Antony Williams

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REFERENCES

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

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- Cheminformatics
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Computational Chemist, National Center for Computational Toxicology, US-EPA (Chemistry)

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

Co-workers & collaborators

- Chris Grulke
- Valery Tkachenko
- Andrew McEachran
  ORISE Postdoctoral Fellow
  Research Triangle Park, NC
- Sean Ekins
  senior consultant
  Fuquay Varina, NC, USA
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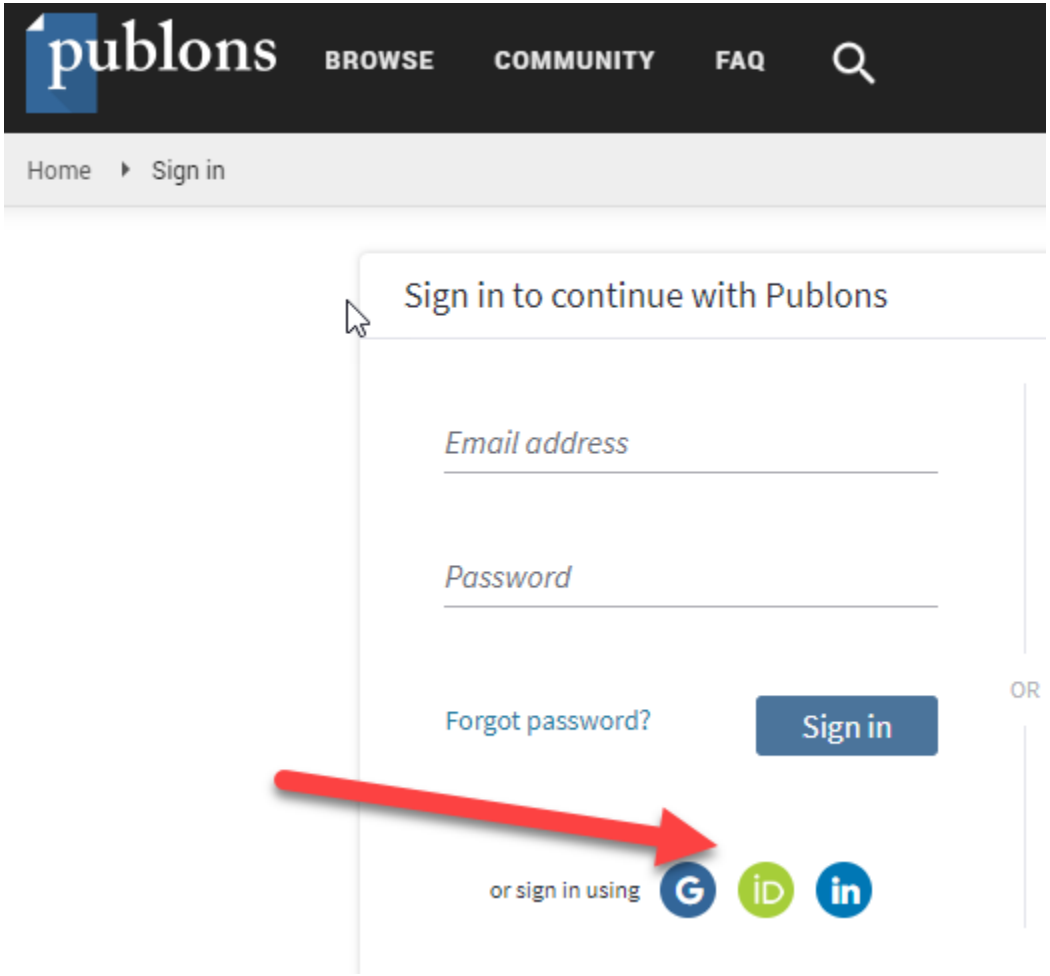

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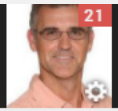

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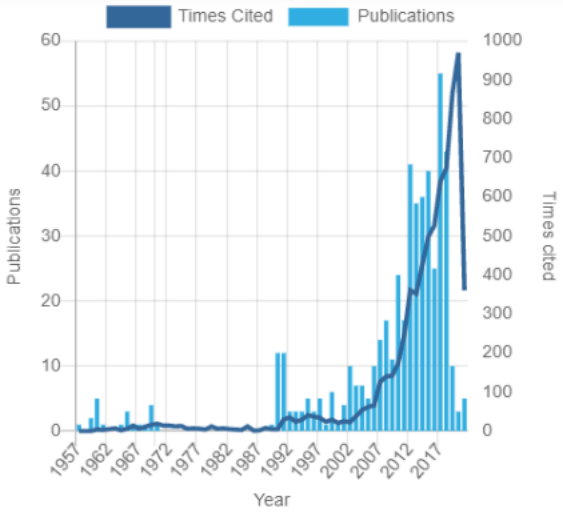

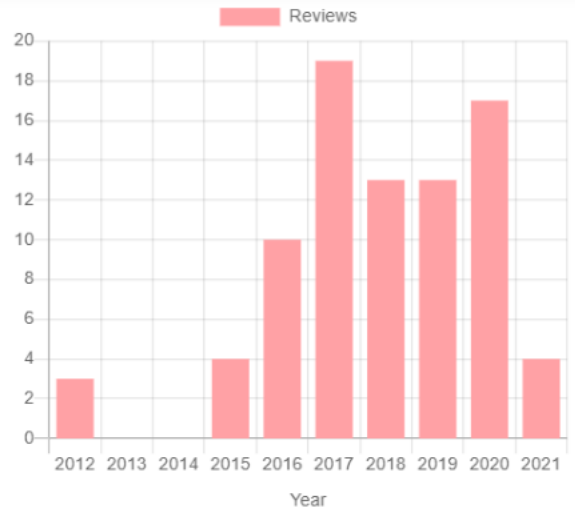

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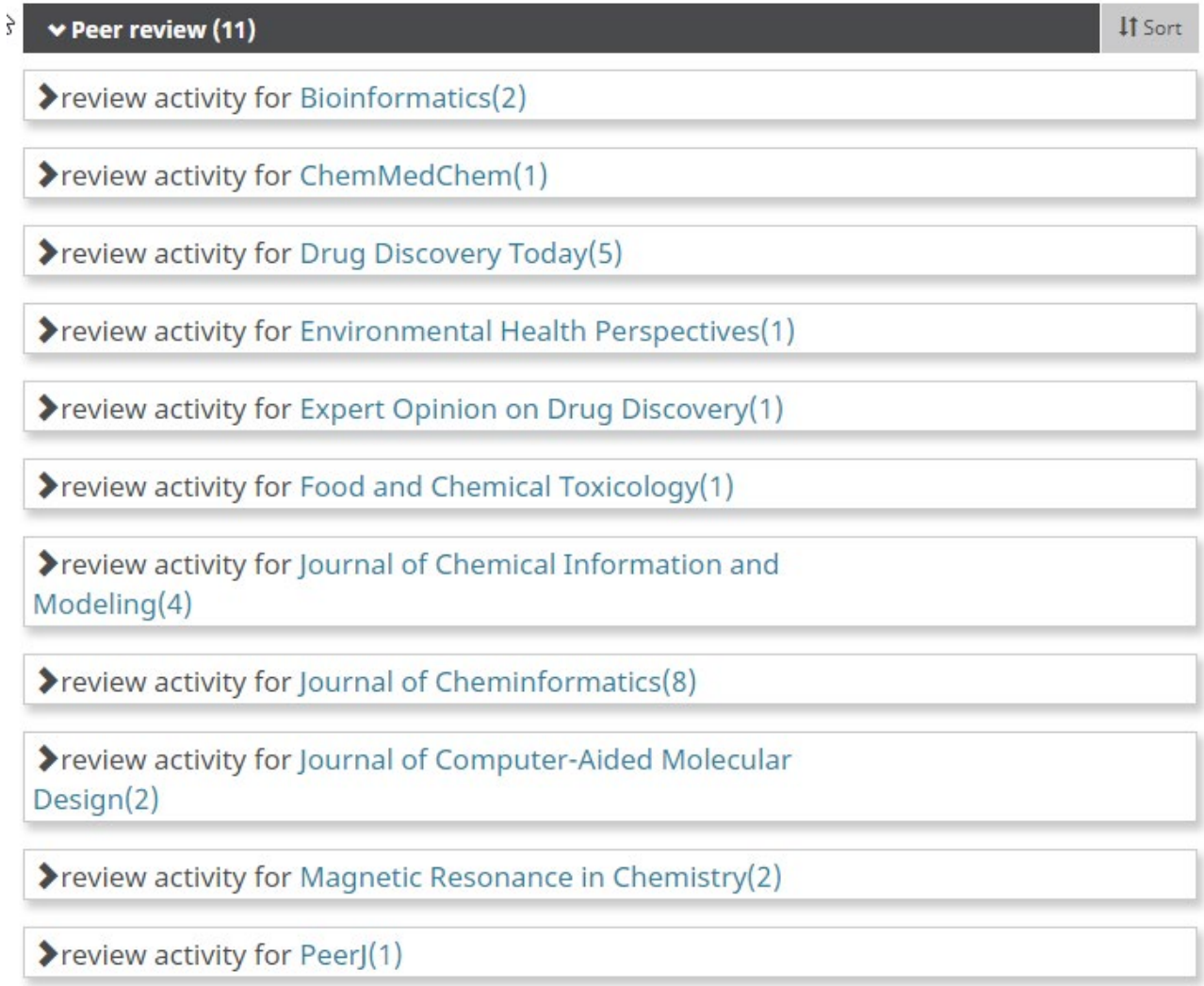

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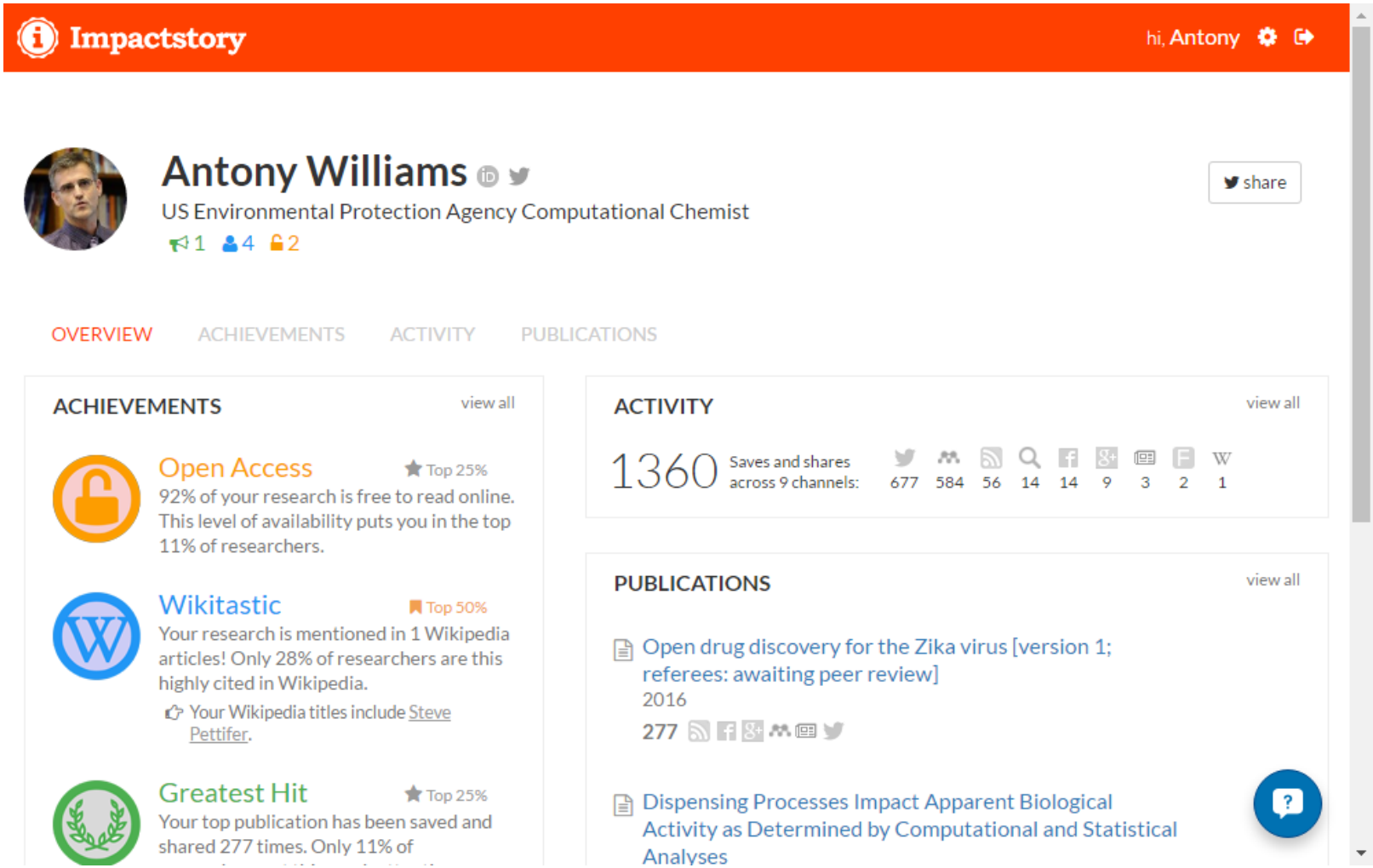

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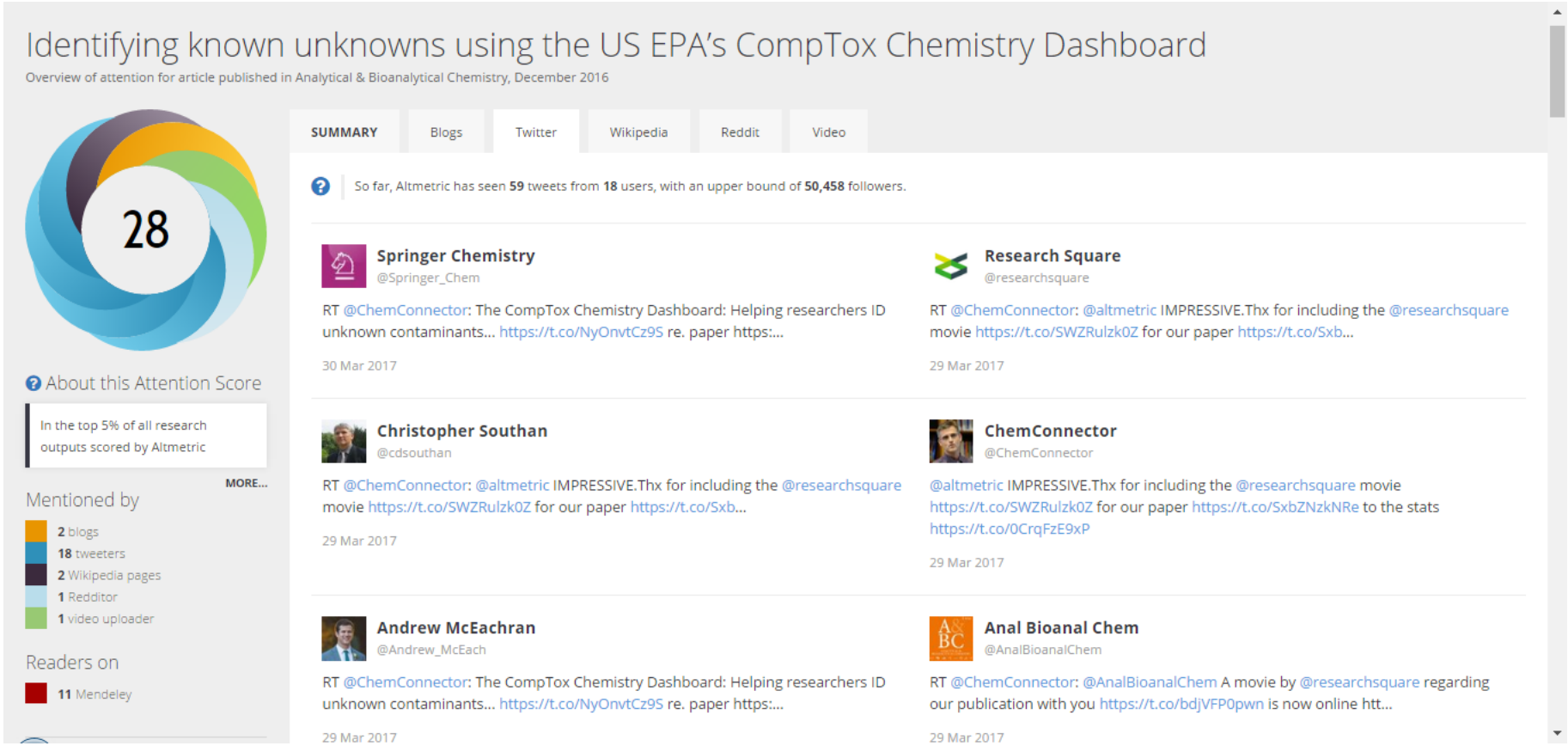

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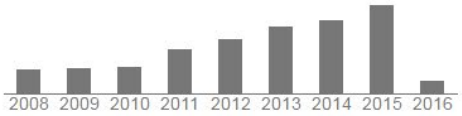

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Co-authors Edit...

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Alex M. Clark
Carole Goble
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☐	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		
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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
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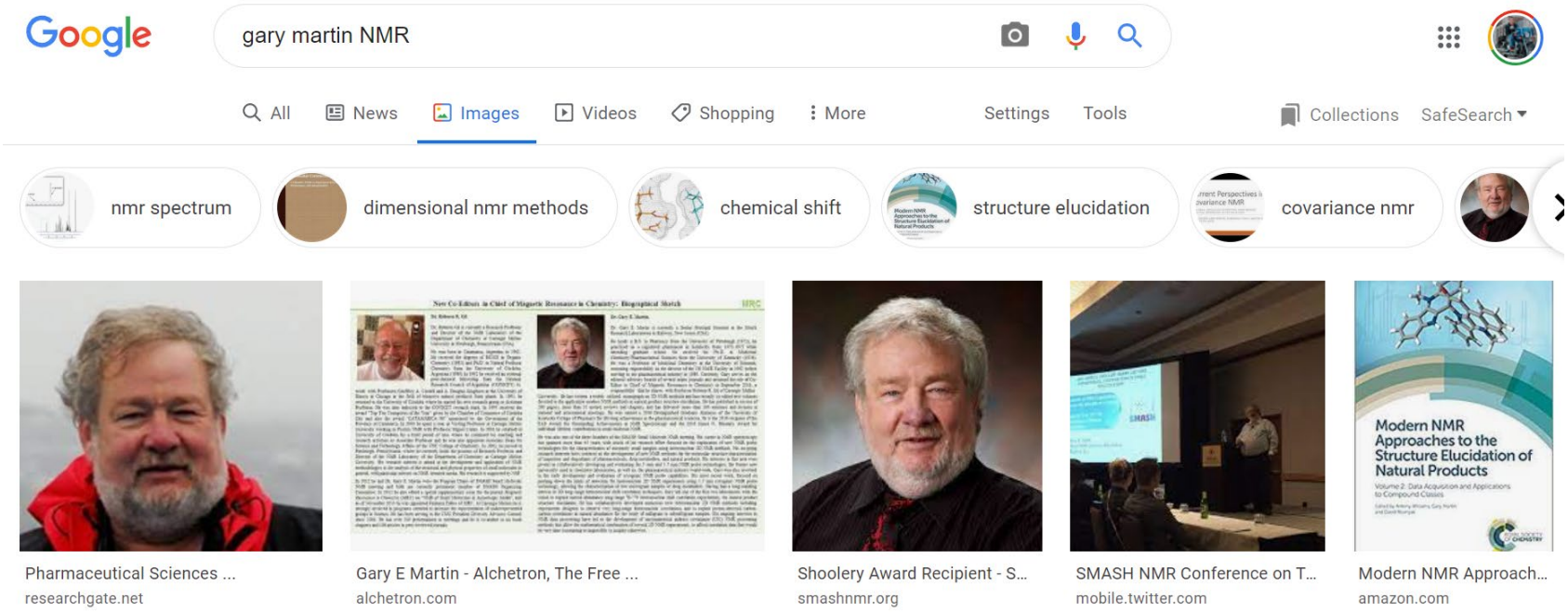

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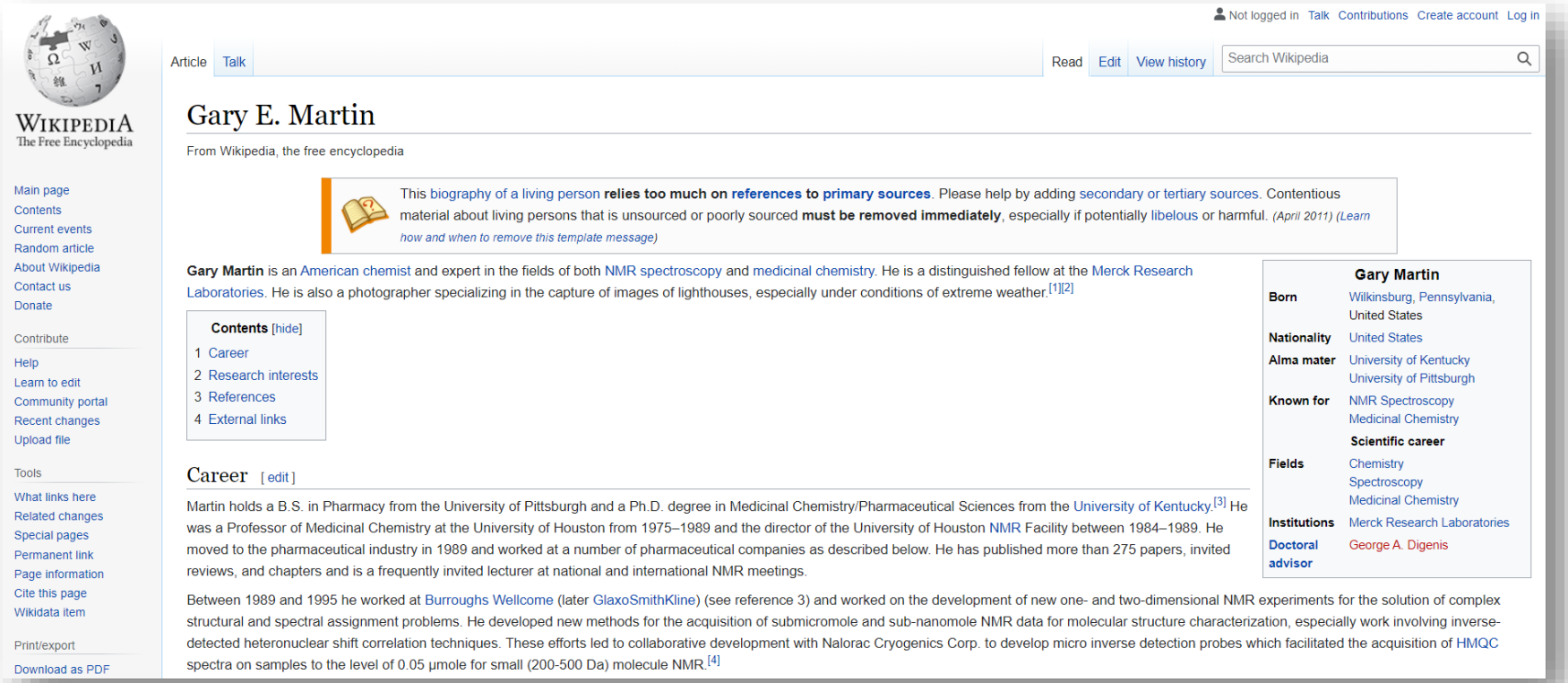

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Gary Martin is an American chemist and expert in the fields of both NMR spectroscopy and medicinal chemistry. He is a distinguished fellow at the Merck Research Laboratories. He is also a photographer specializing in the capture of images of lighthouses, especially under conditions of extreme weather.[1][2]

Contents [hide]
1 Career
2 Research interests
3 References
4 External links

Gary Martin

Born	Wilkinsburg, Pennsylvania, United States
Nationality	United States
Alma mater	University of Kentucky University of Pittsburgh
Known for	NMR Spectroscopy Medicinal Chemistry
Scientific career	
Fields	Chemistry Spectroscopy Medicinal Chemistry
Institutions	Merck Research Laboratories
Doctoral advisor	George A. Digenis

Career [edit]

Martin holds a B.S. in Pharmacy from the University of Pittsburgh and a Ph.D. degree in Medicinal Chemistry/Pharmaceutical Sciences from the University of Kentucky.[3] He was a Professor of Medicinal Chemistry at the University of Houston from 1975–1989 and the director of the University of Houston NMR Facility between 1984–1989. He moved to the pharmaceutical industry in 1989 and worked at a number of pharmaceutical companies as described below. He has published more than 275 papers, invited reviews, and chapters and is a frequently invited lecturer at national and international NMR meetings.

Between 1989 and 1995 he worked at Burroughs Wellcome (later GlaxoSmithKline) (see reference 3) and worked on the development of new one- and two-dimensional NMR experiments for the solution of complex structural and spectral assignment problems. He developed new methods for the acquisition of submicromole and sub-nanomole NMR data for molecular structure characterization, especially work involving inverse-detected heteronuclear shift correlation techniques. These efforts led to collaborative development with Nalorac Cryogenics Corp. to develop micro inverse detection probes which facilitated the acquisition of HMQC spectra on samples to the level of 0.05 µmole for small (200-500 Da) molecule NMR.[4]

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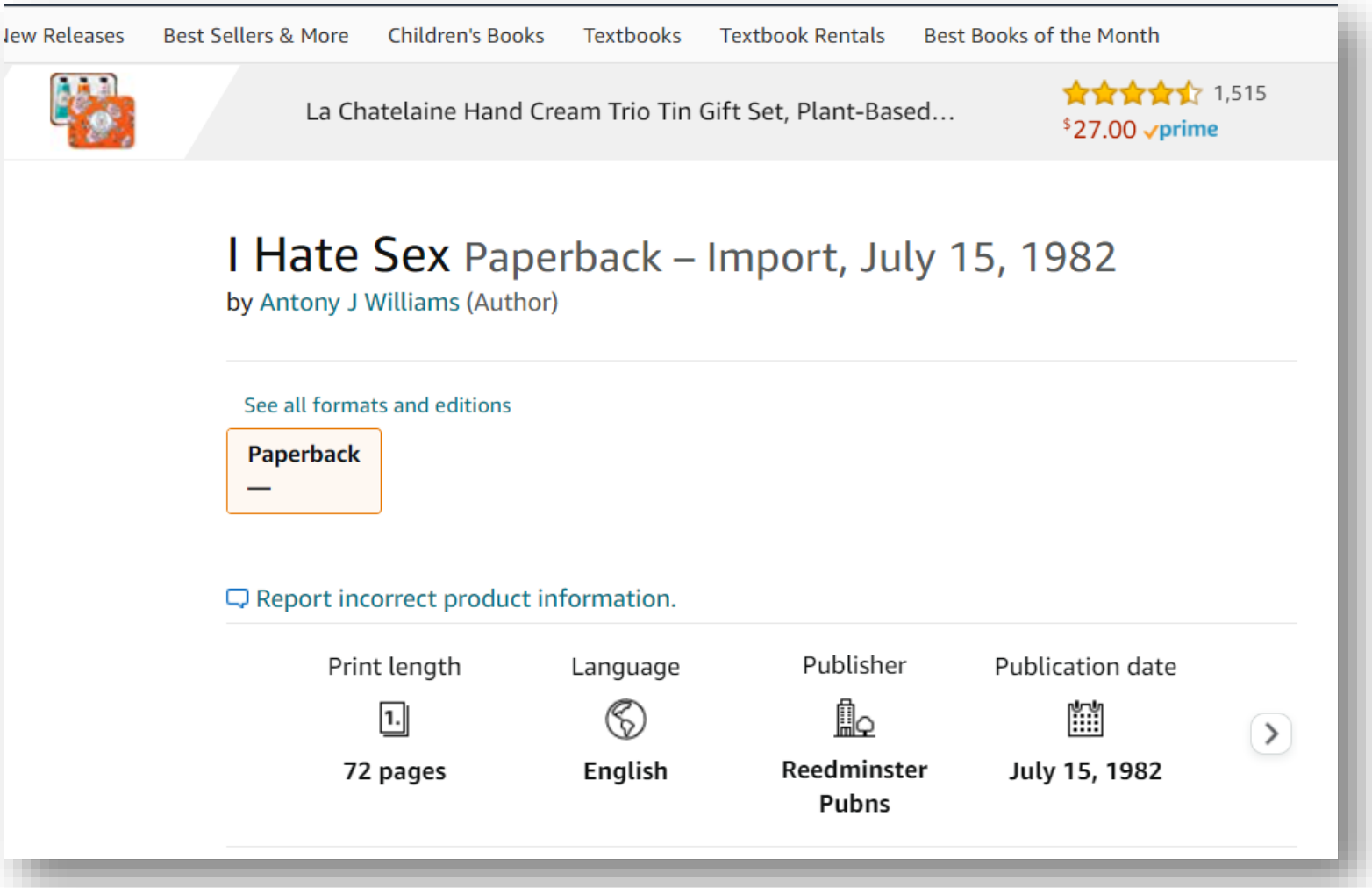

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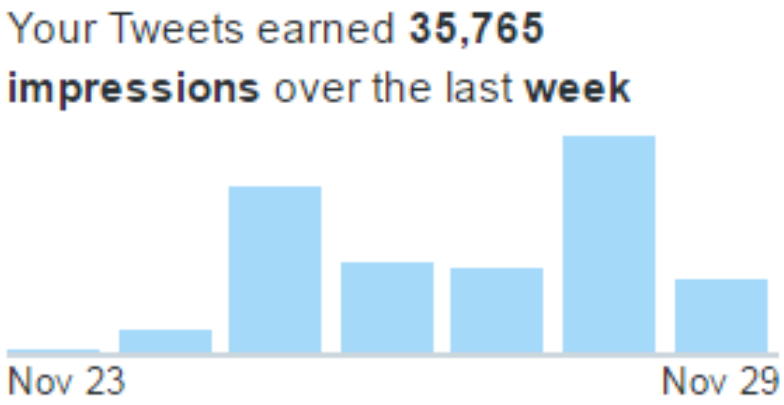

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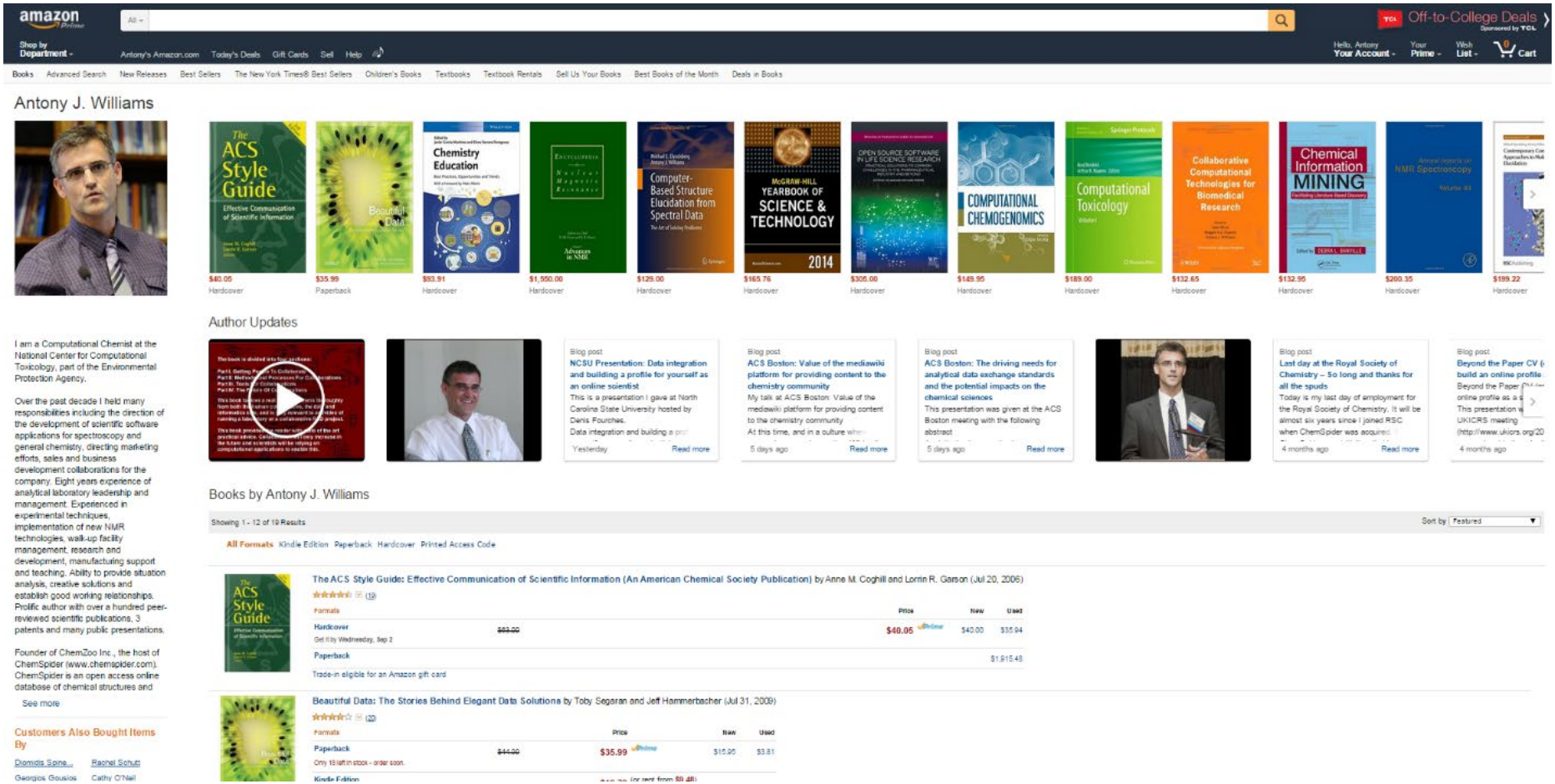

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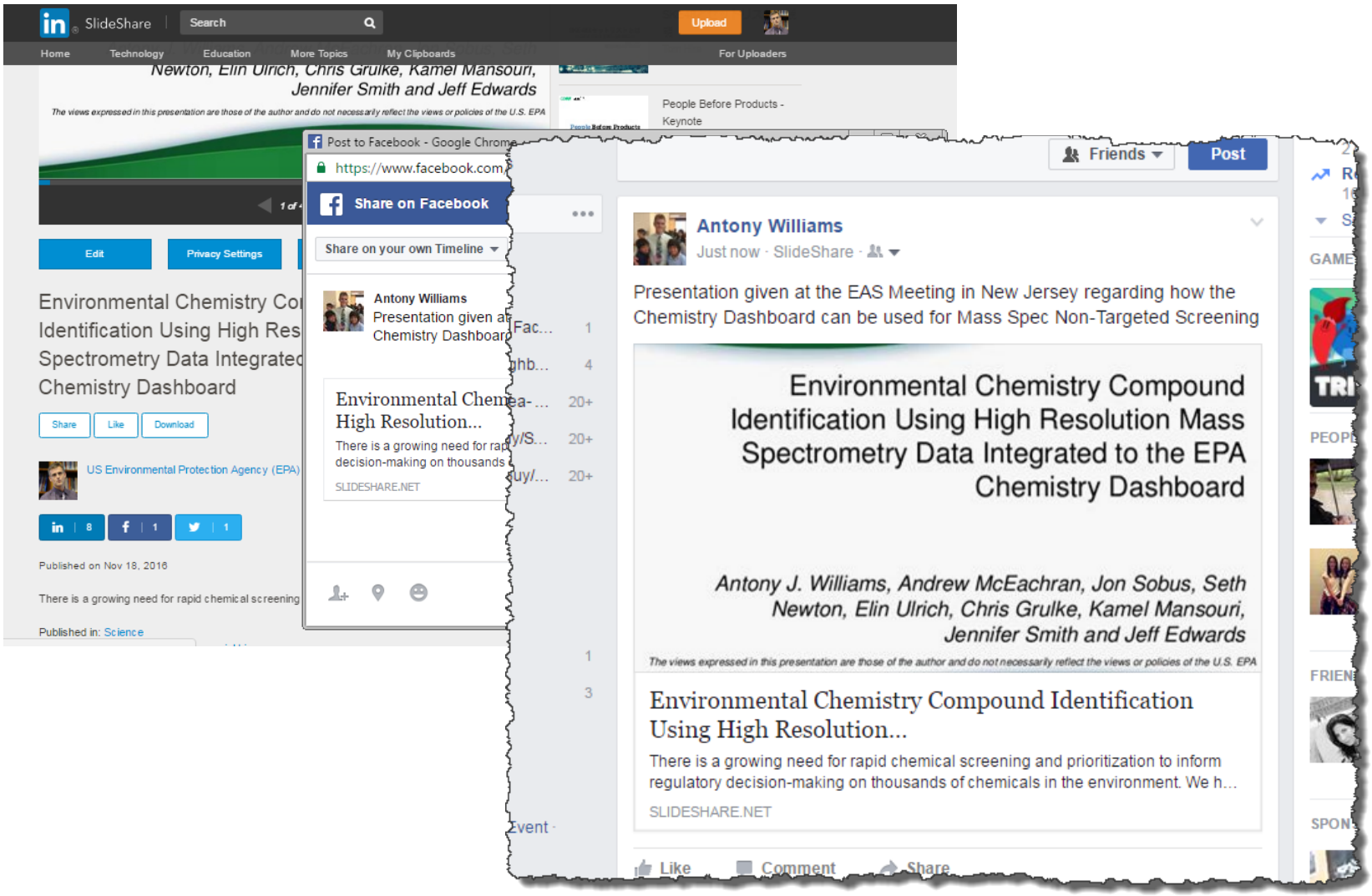
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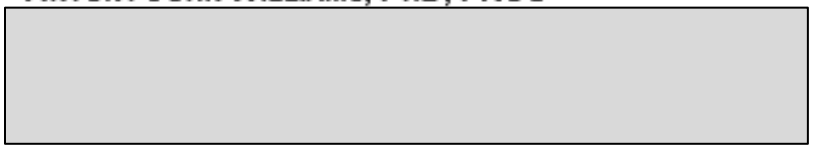

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What Next?
My Recommendations

- 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

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