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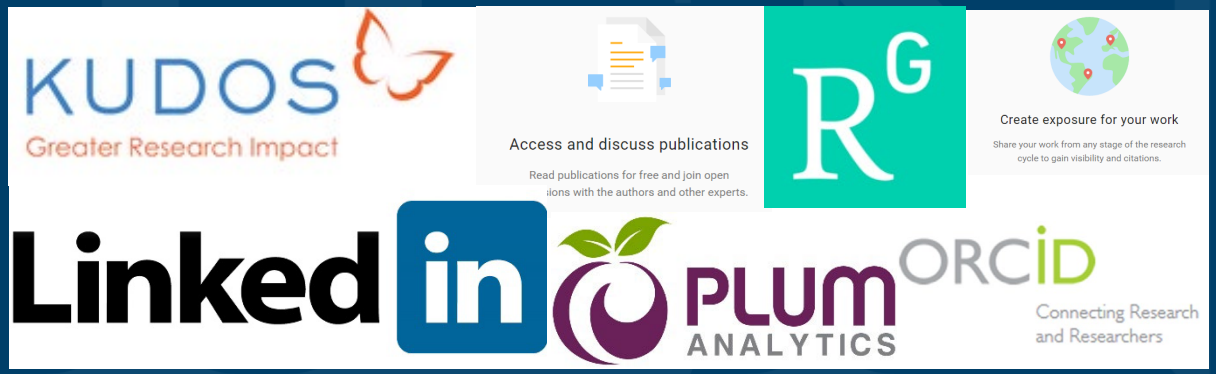
ORCID 0000-0002-2668-4821

Sharing Yourself and Your Science using Social Media Tools for Scientists

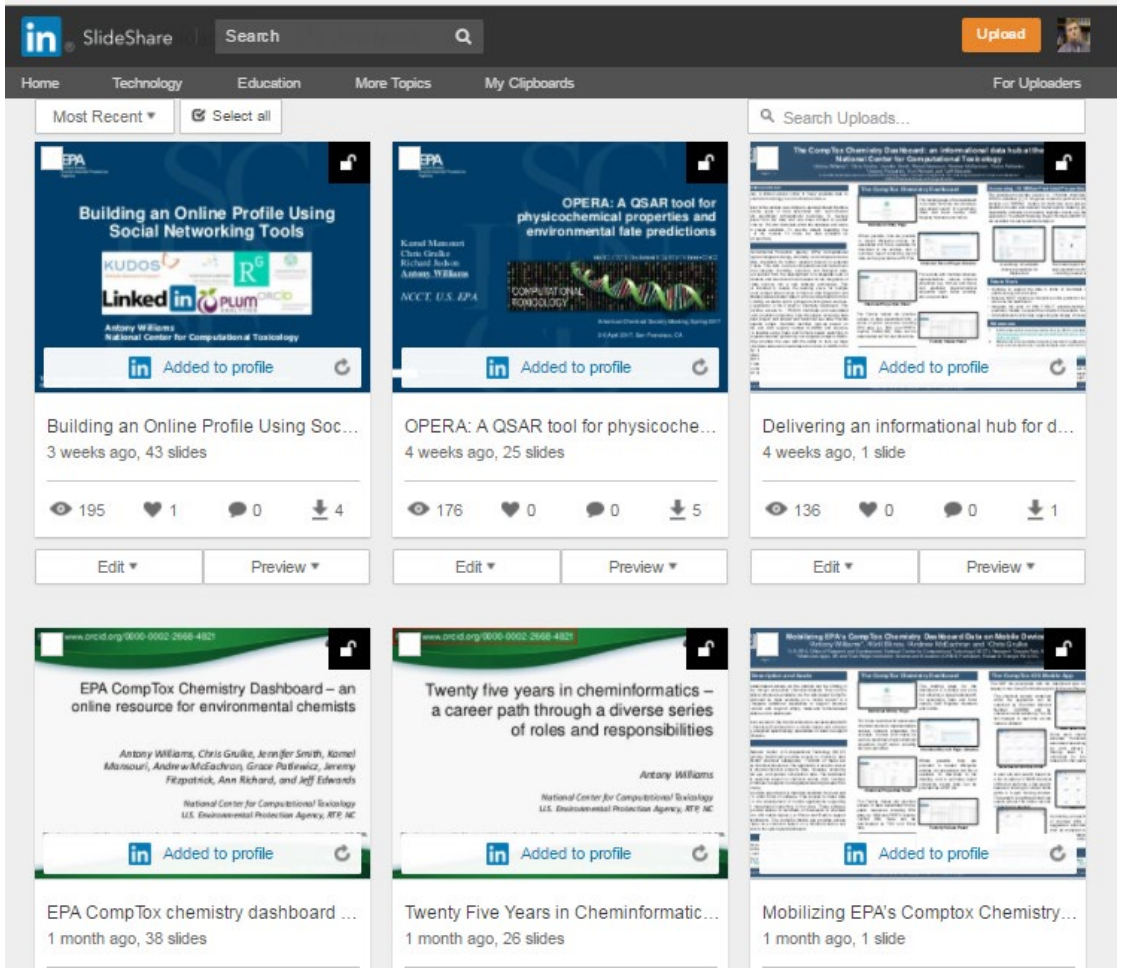


Antony Williams
Center for Computational Toxicology and Exposure

GREENELIT Webinar: "How to raise a research profile?"
24th January 2022

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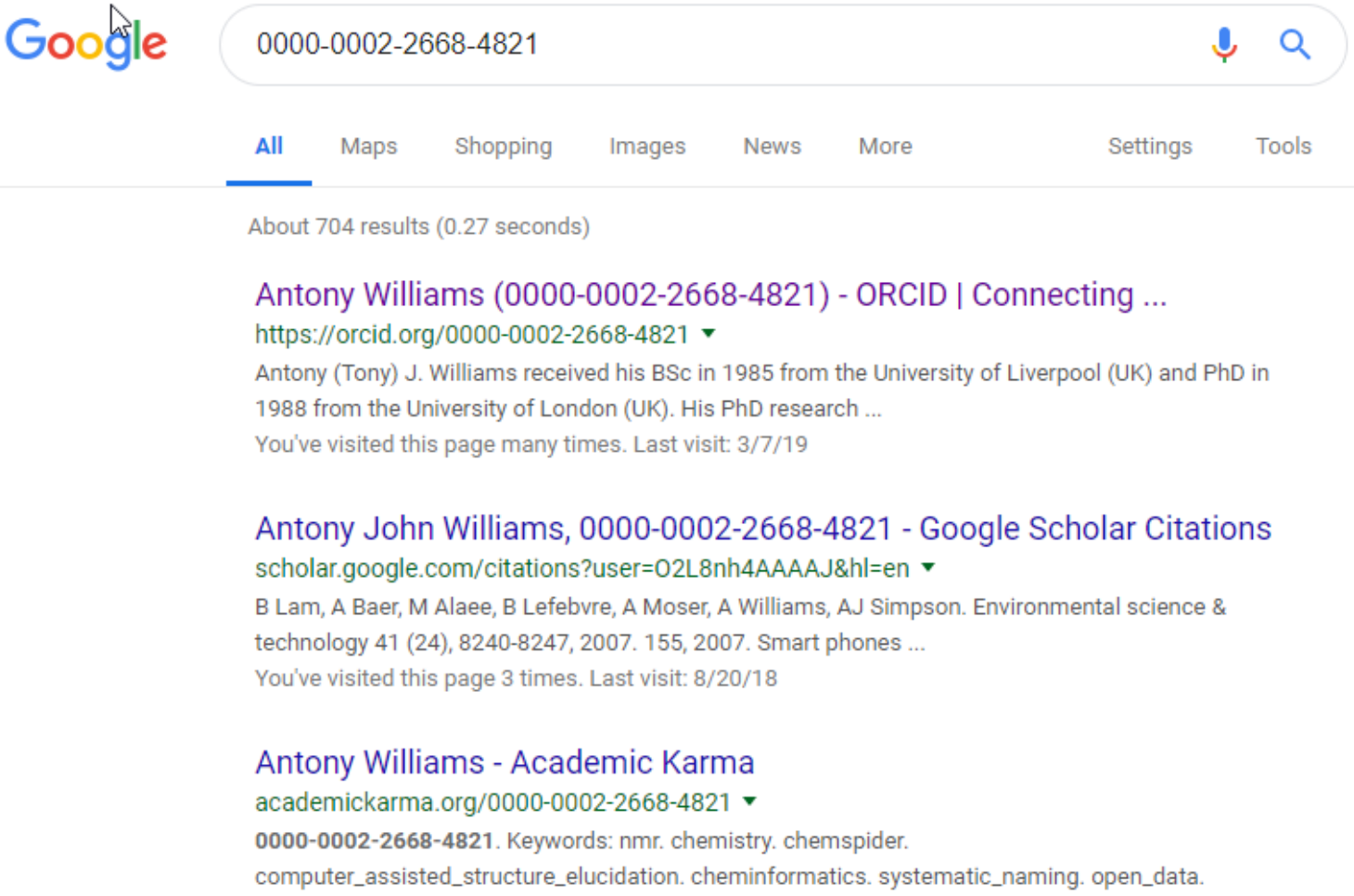
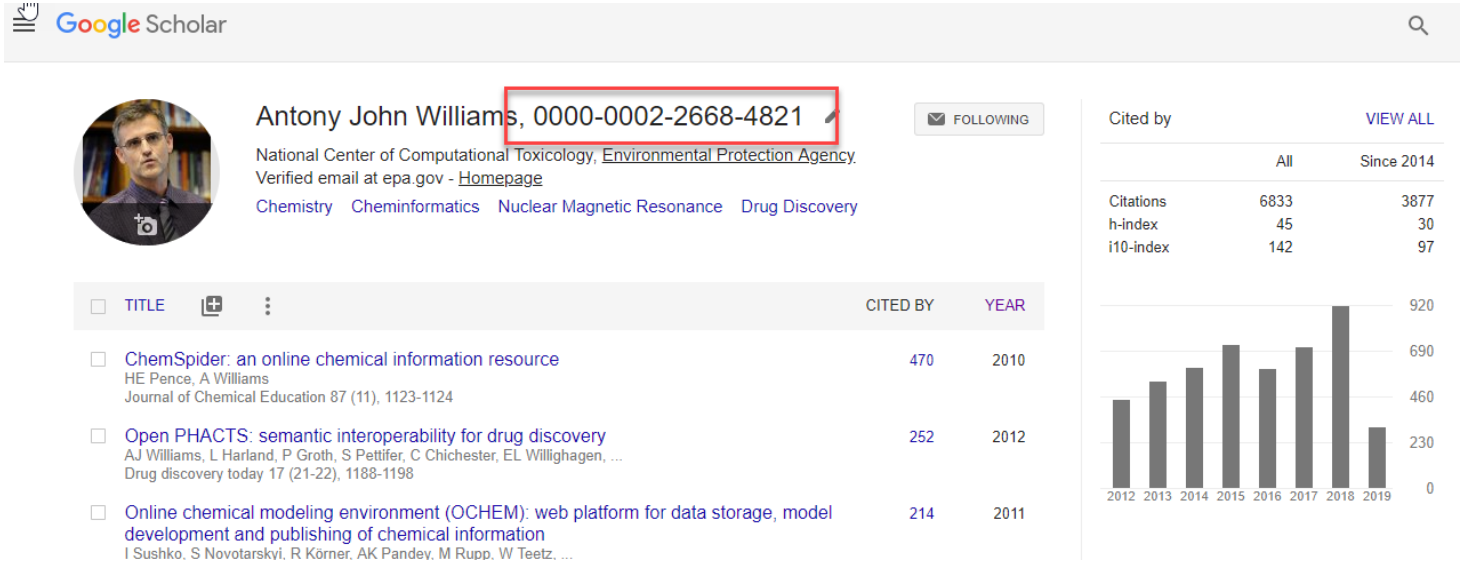
It's a Scientists SSN – use it in various places

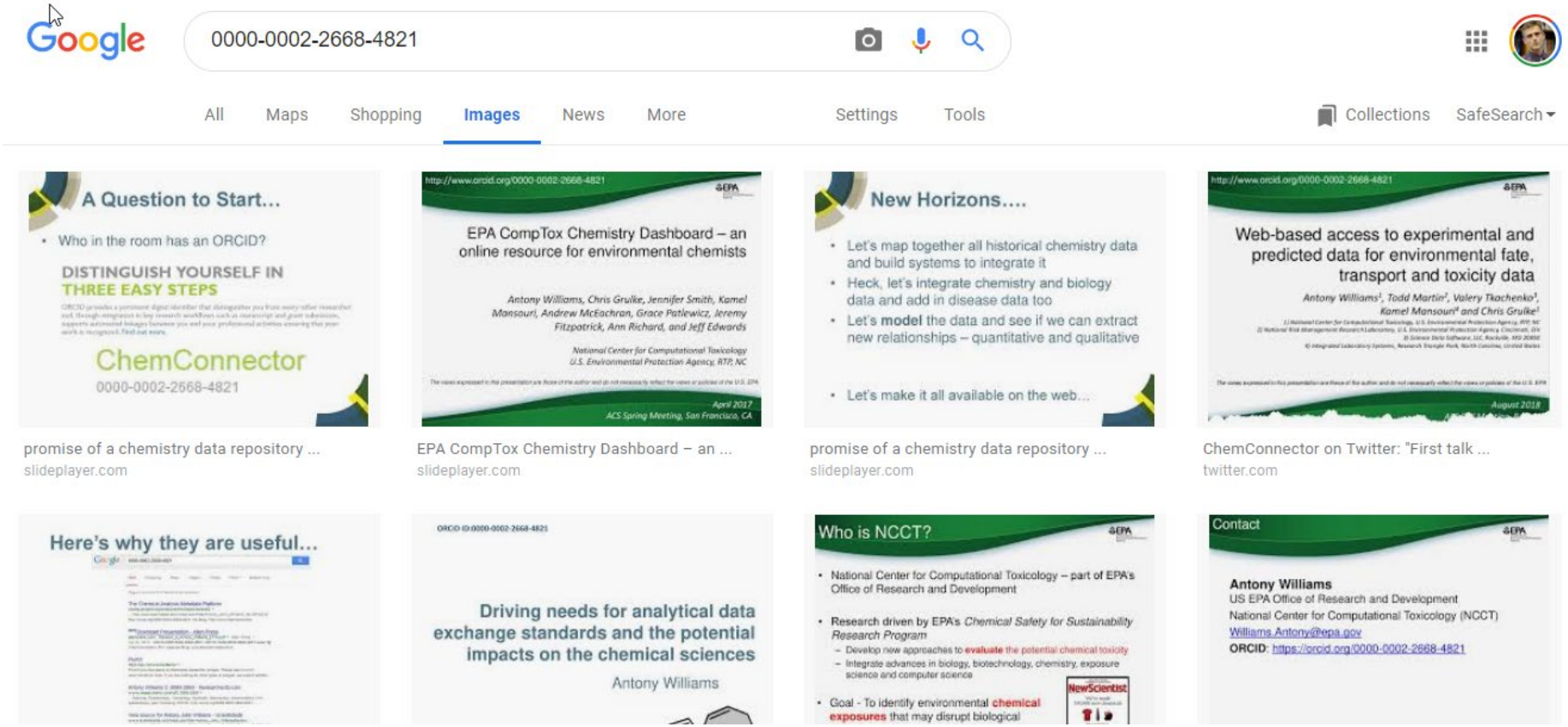


Use ORCID on all products

- 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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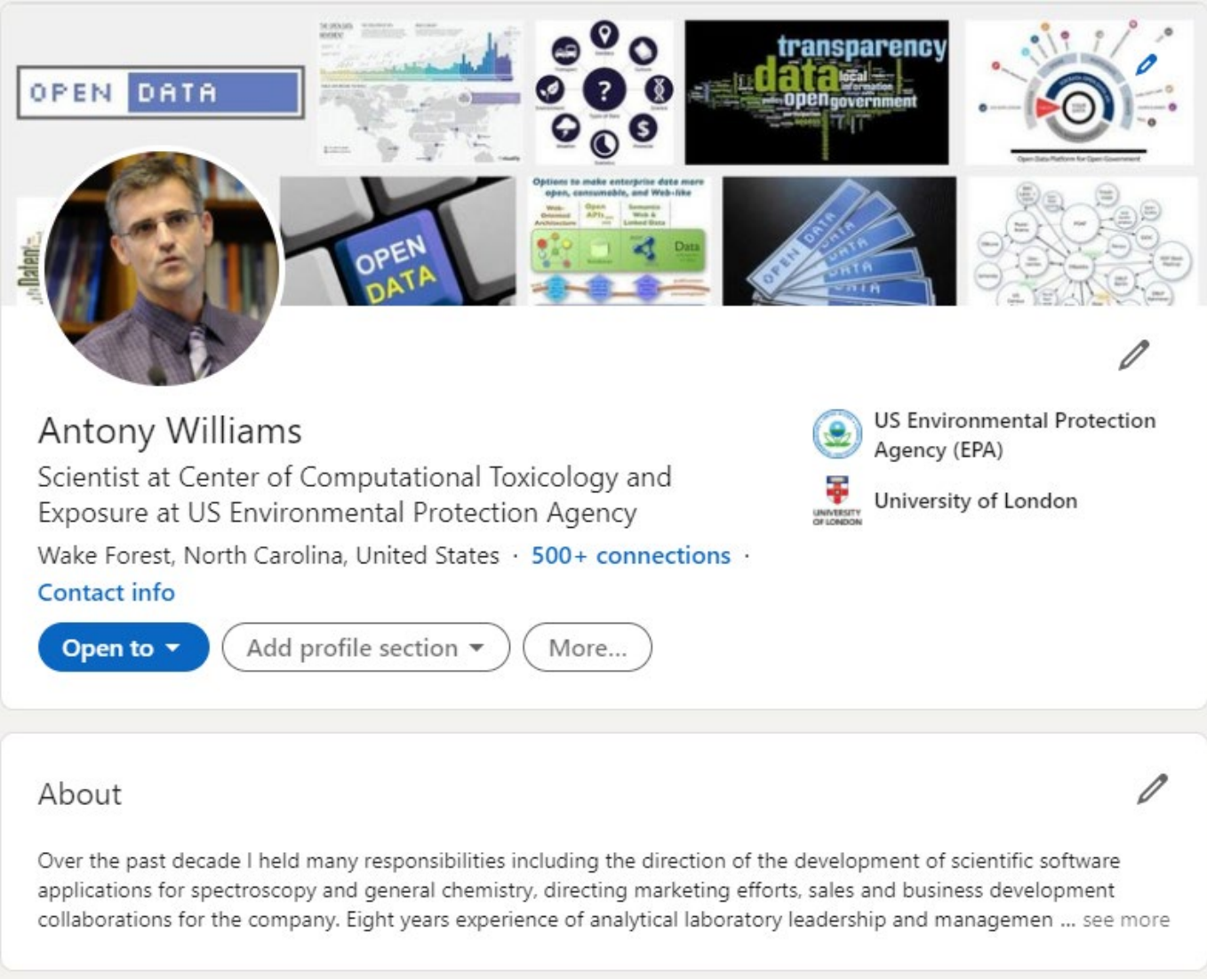
Scientists are Evaluated: "Statistics"

- 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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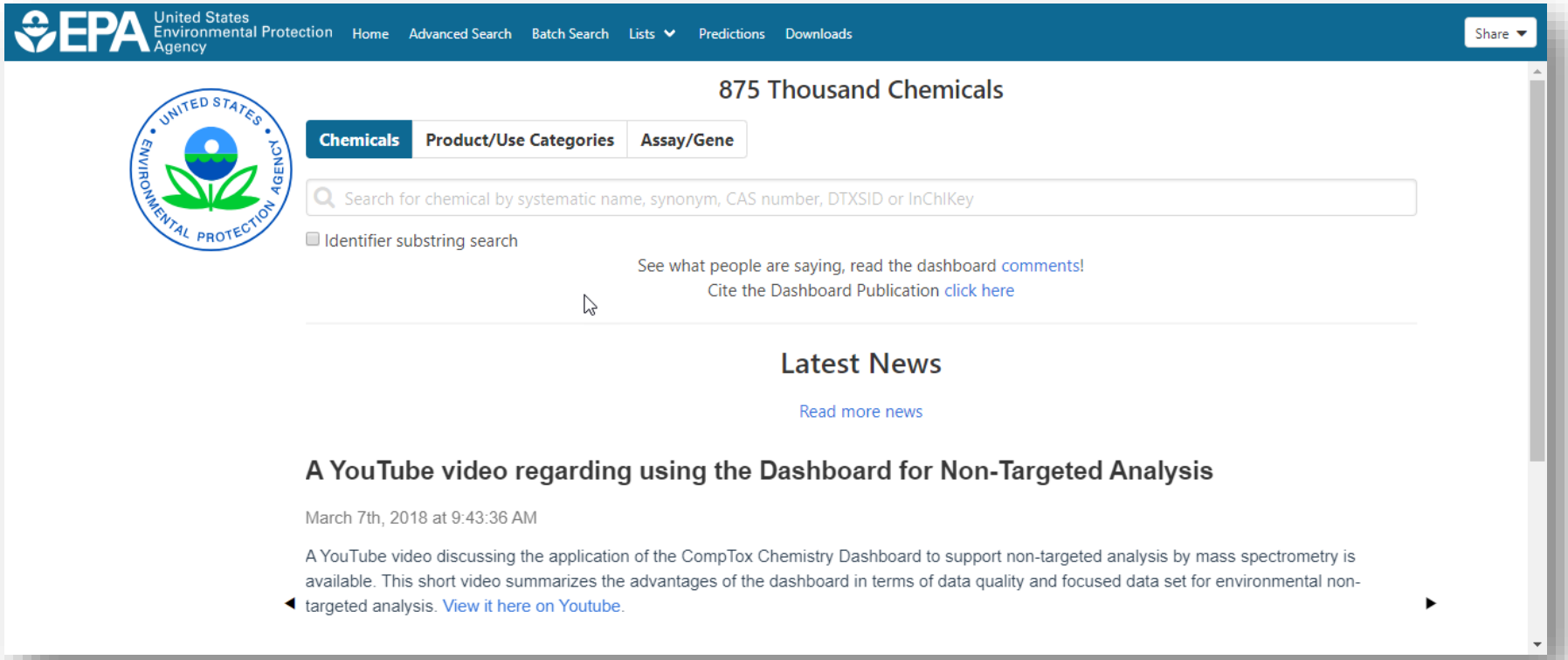
Something I worked on…



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

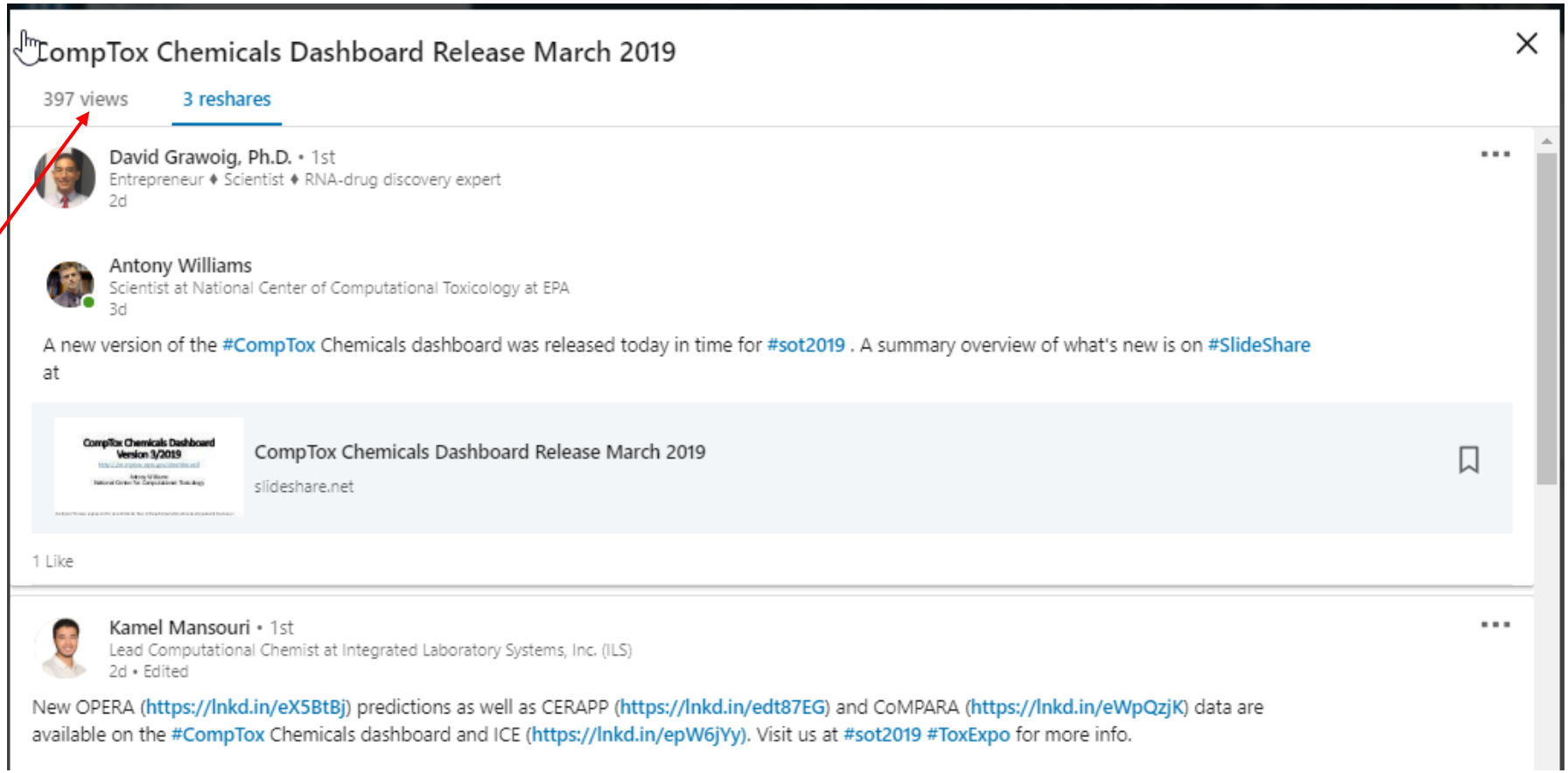
Generalized Read-Across (GenRA): A workflow implemented into the EPA CompTox Chemicals Dashboard

Feb 4, 2019 • ALTEX-Alternatives to animal experimentation

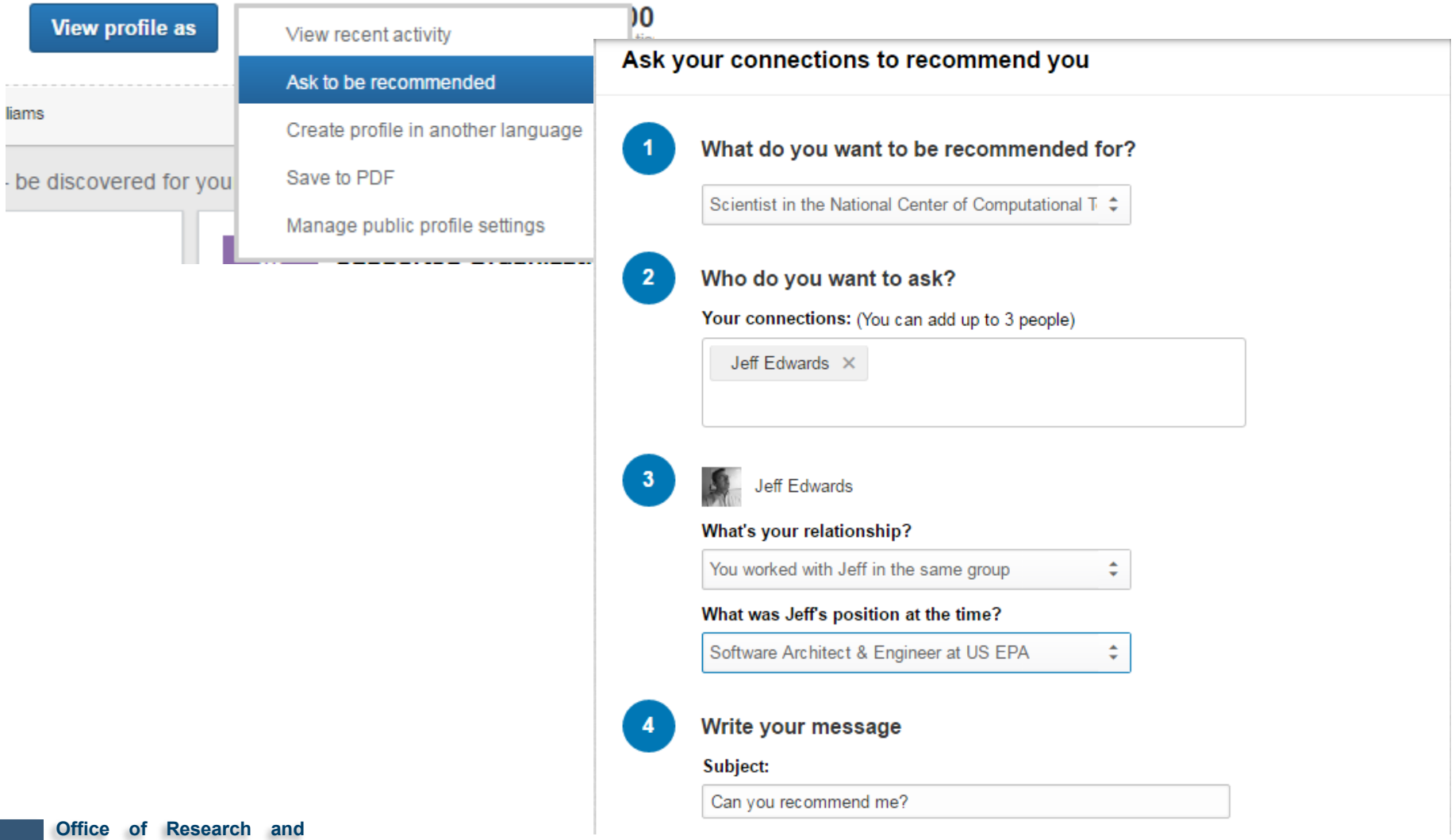
Generalized Read-Across (GenRA) is a data driven approach which makes read-across predictions on the basis of a similarity weighted activity of source analogues (nearest neighbors). GenRA has been described in more detail in the literature (Shah et al., 2016; Helman et al., 2018). Here we present its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

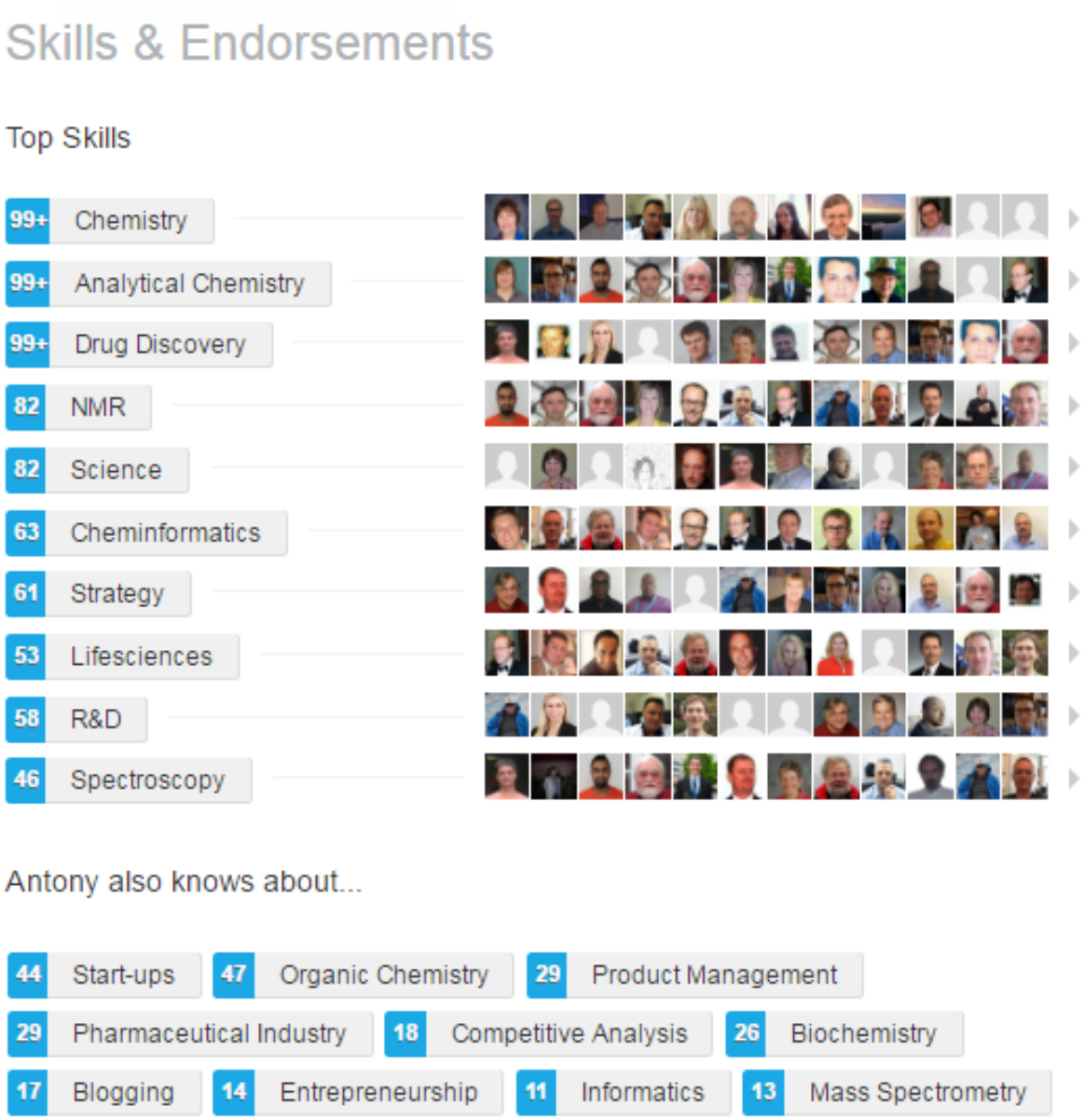
Your Postings Get Networked



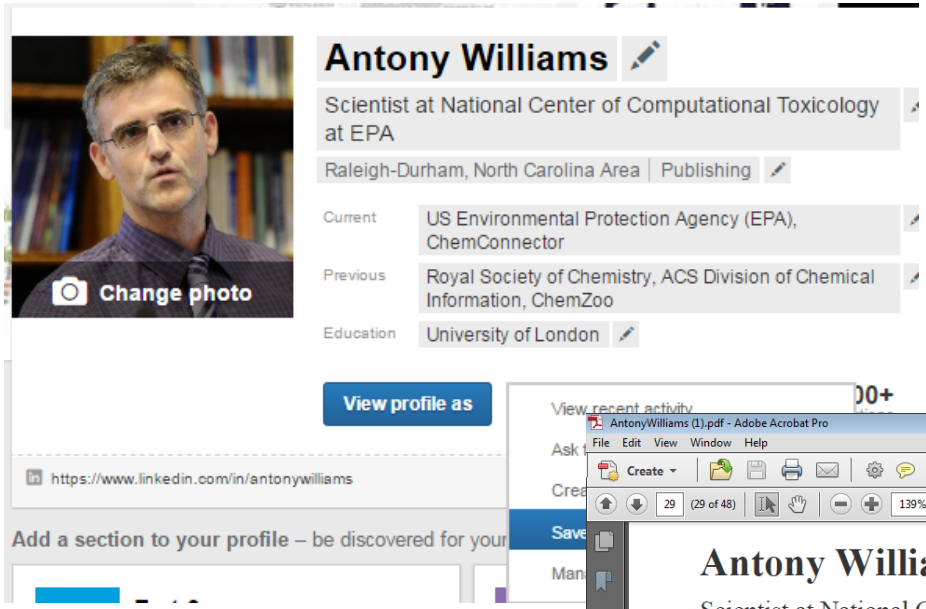
Ask for Recommendations

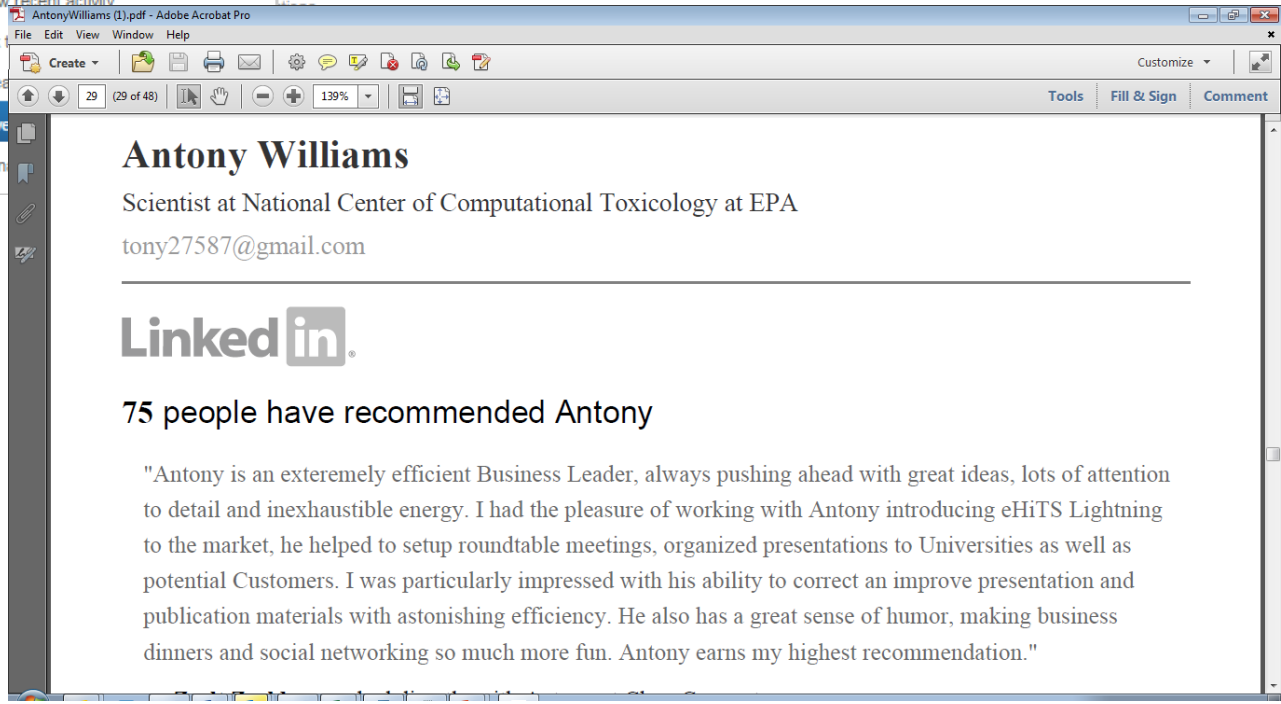


Ask for “Endorsements”,

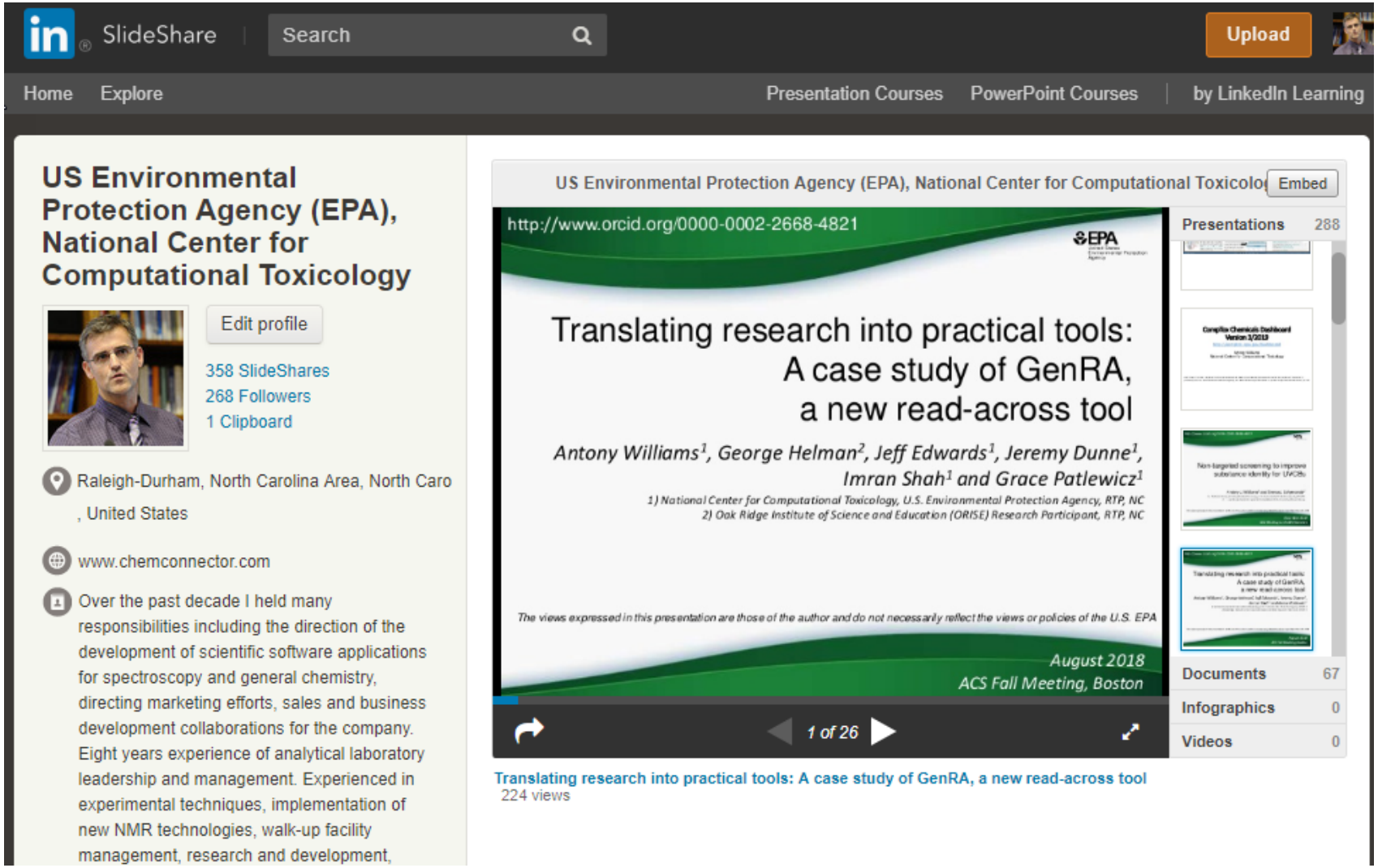


Instant Summary as a PDF

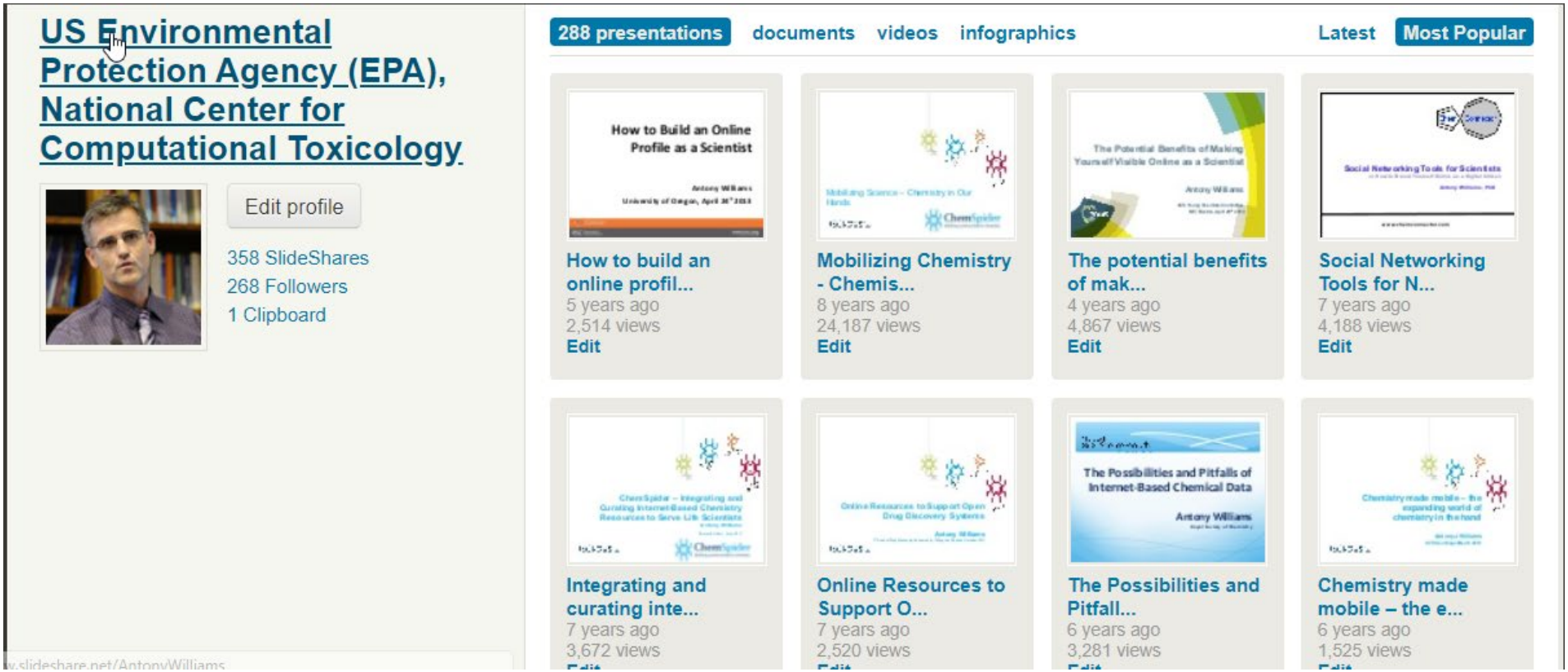




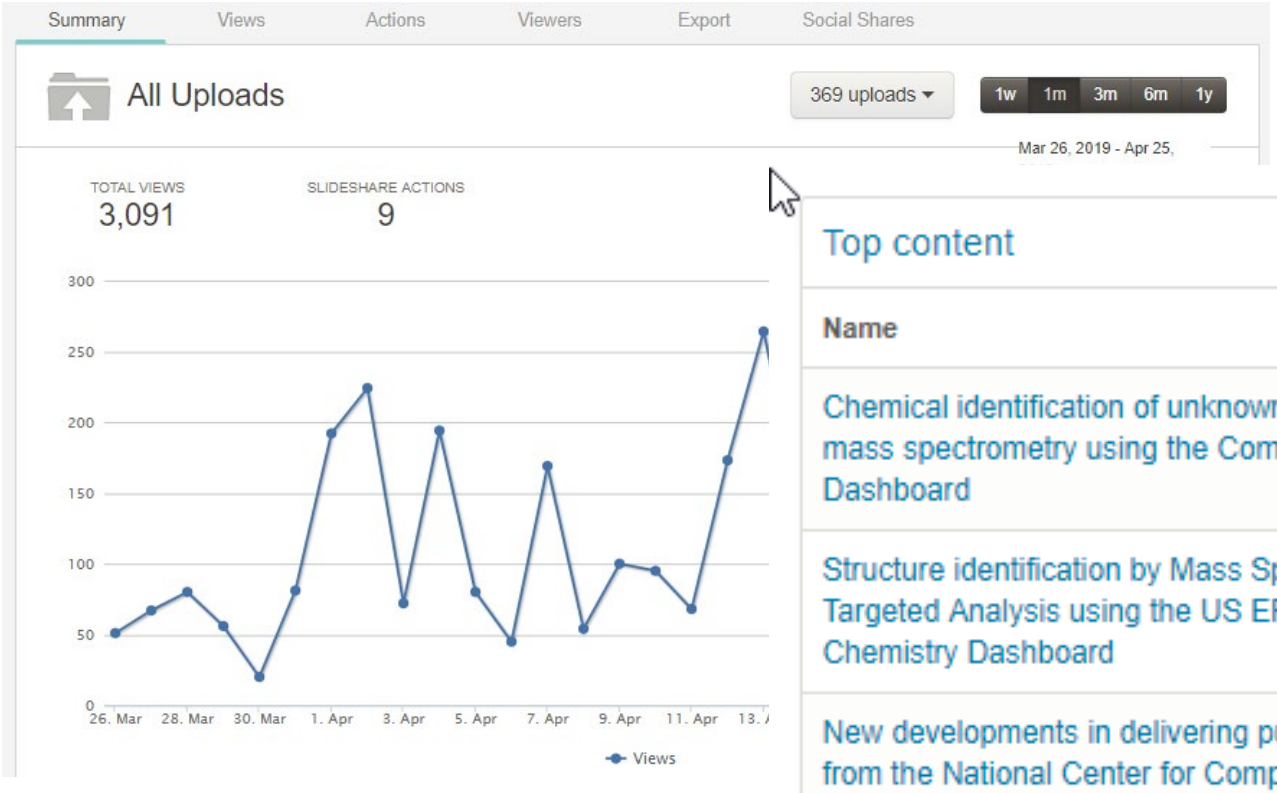
Presentations



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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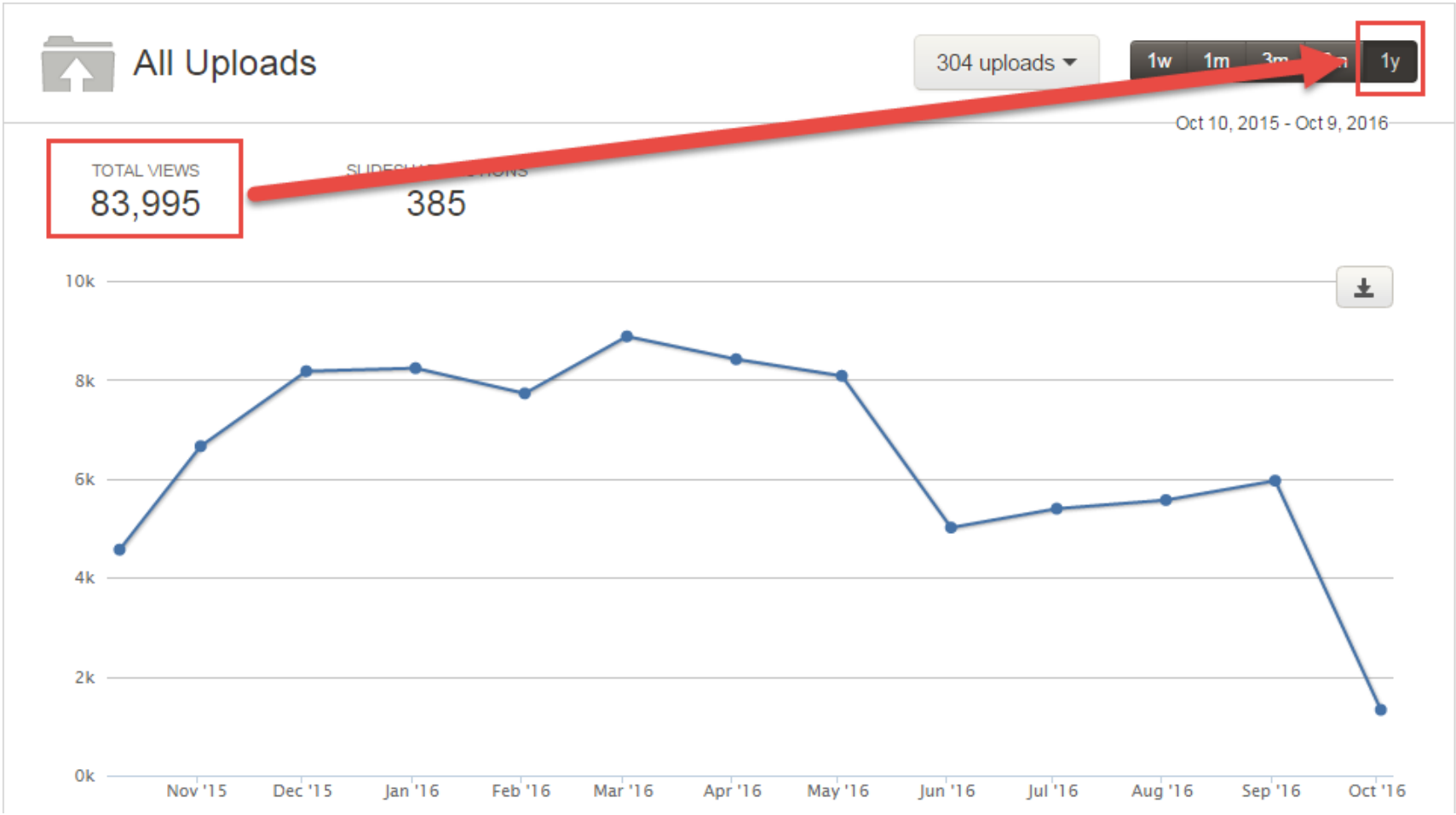

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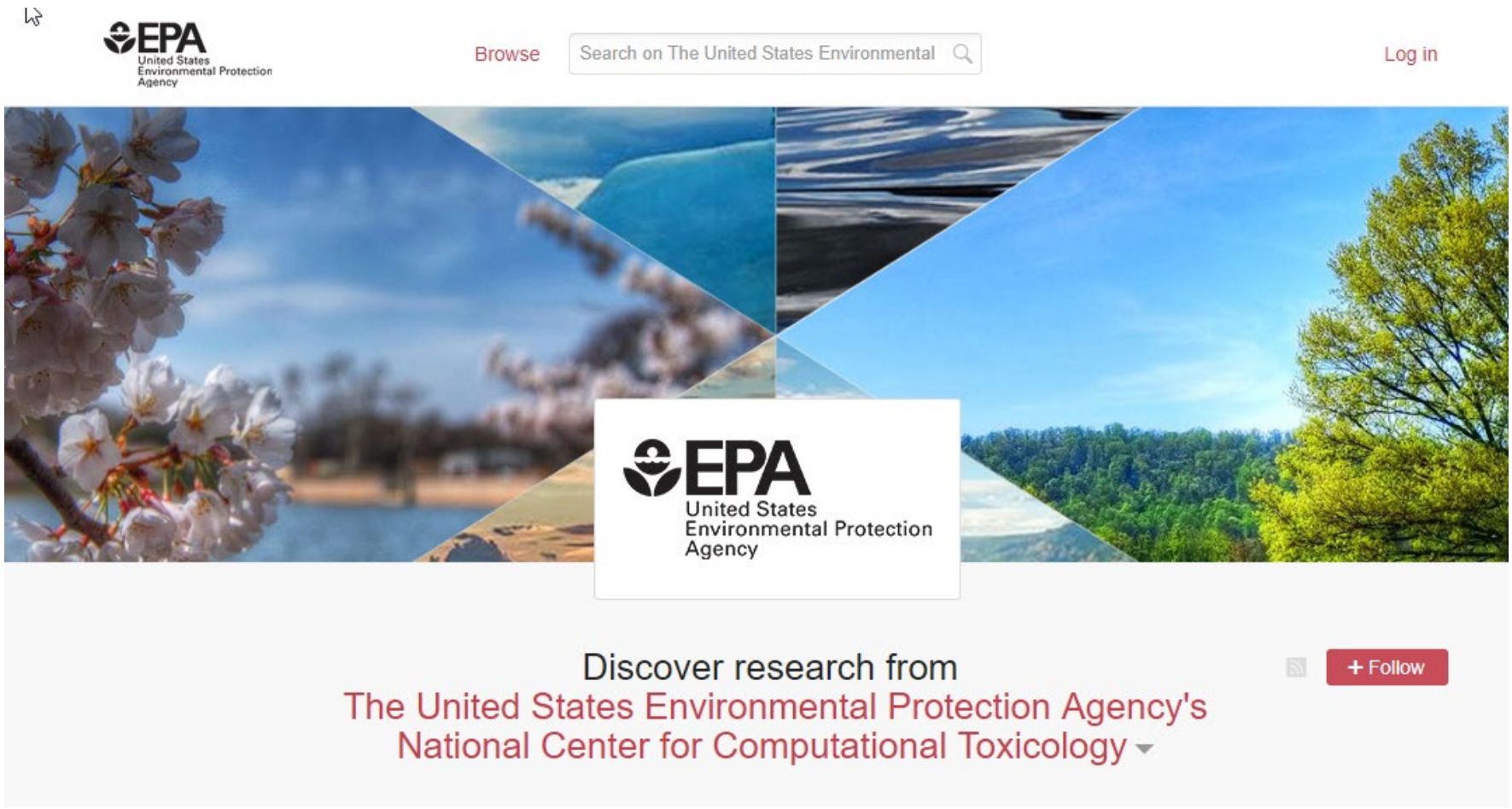

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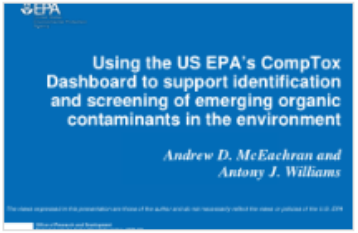
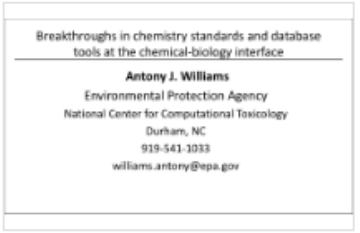
DSSTox: The Open Environmental Chemistry Data underlying the Co...
Chris Grulke 06/06/2018



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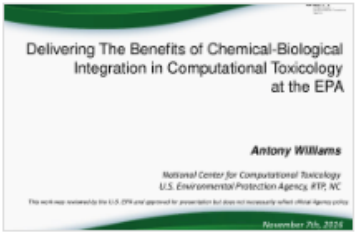
Influence of data curation on QSAR Modeling – examining issues of qu...



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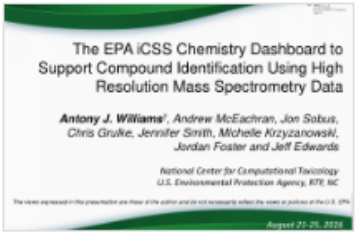
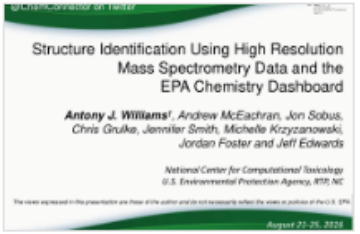
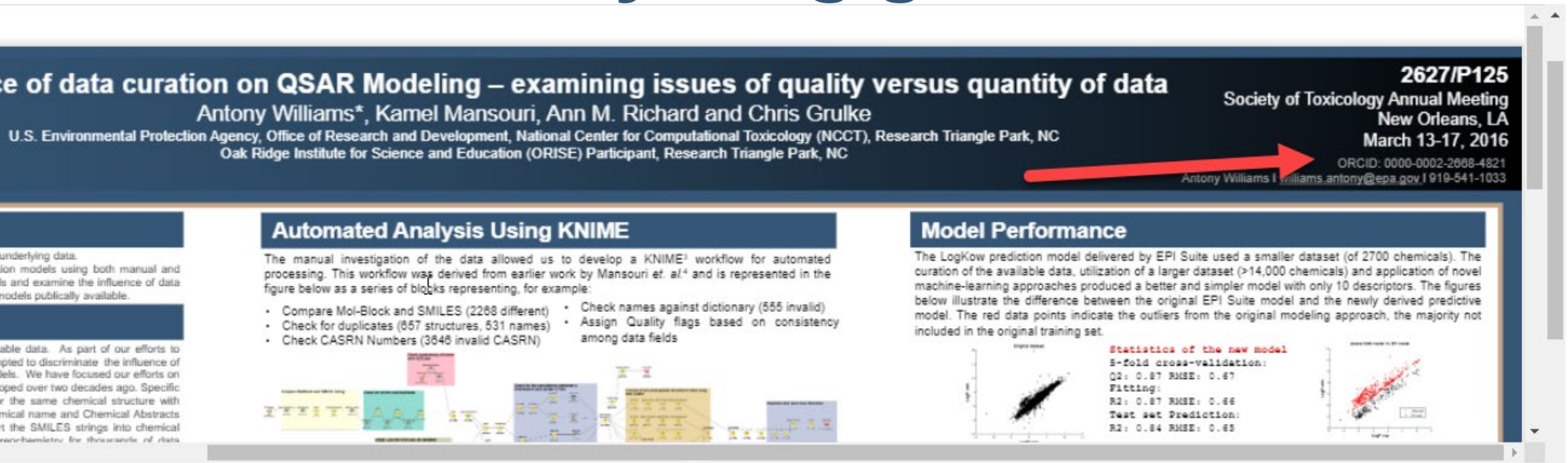


The EPA iCSS Chemistry Dashboard to Support Compound Identificatio...



Structure Identification Using High Resolution Mass Spectrometry Dat...

Including all Posters… everything gets DOI'ed



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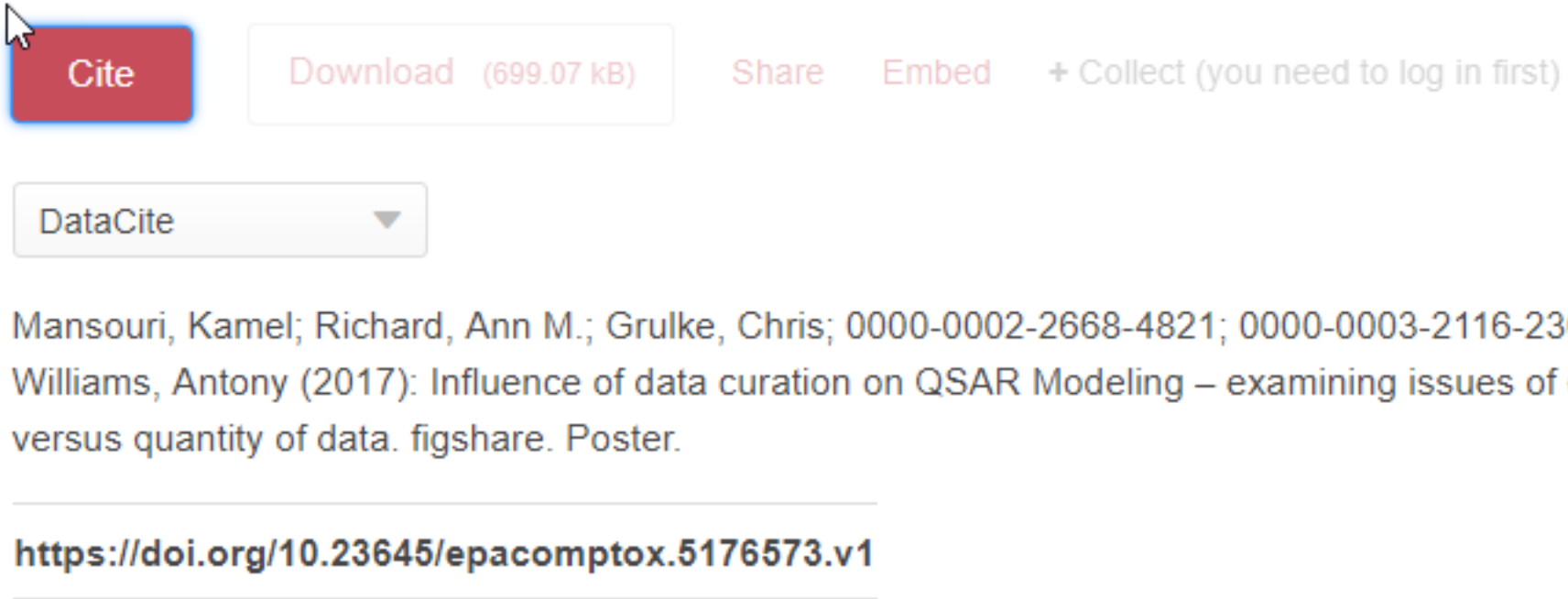
Influence of data curation on QSAR Modeling – examining issues of quality versus quantity of data

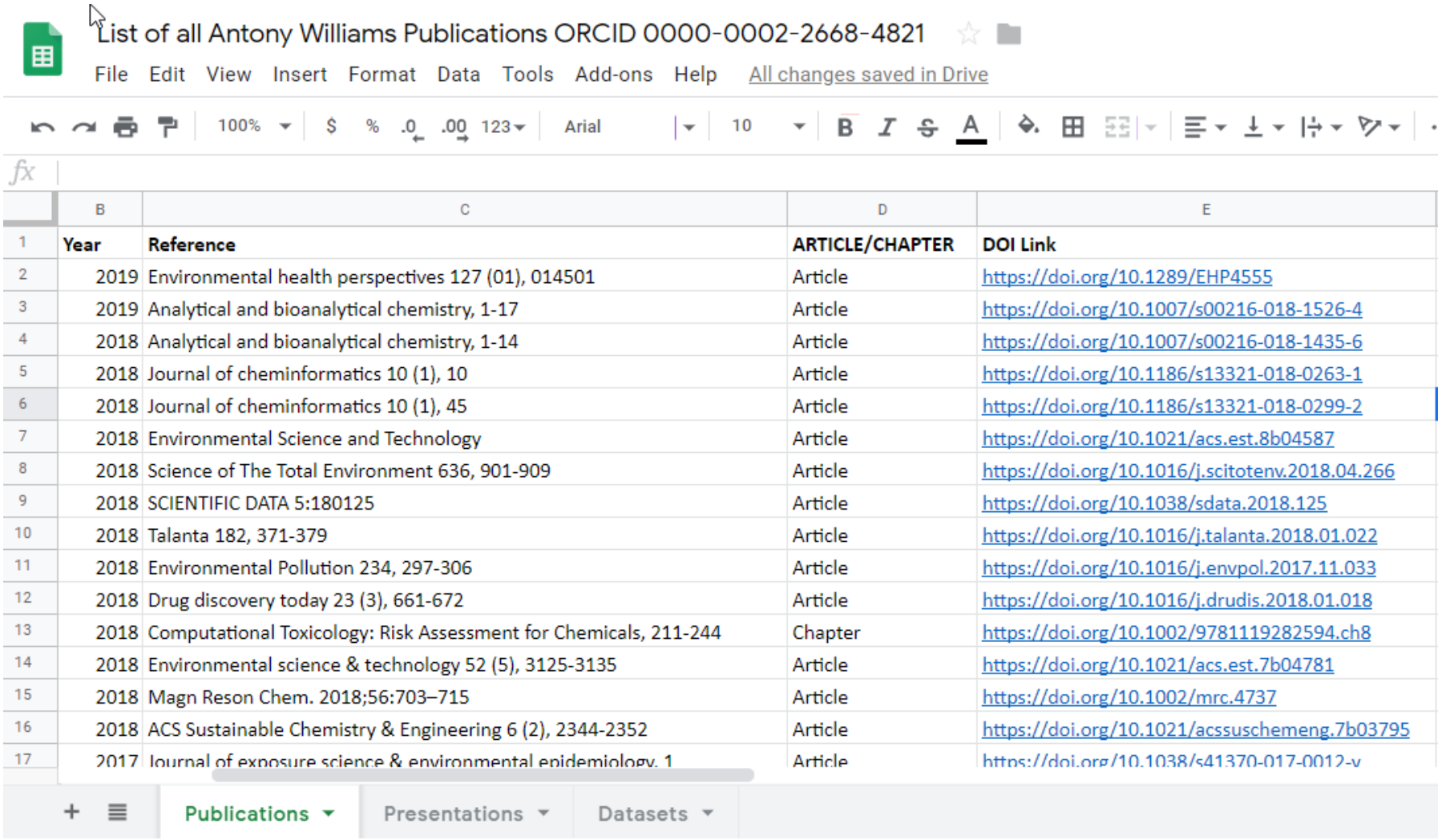
114 views | 34 downloads | 0 citations

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

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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

45.02 · 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

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View lab Edit

Awarded grants (0)

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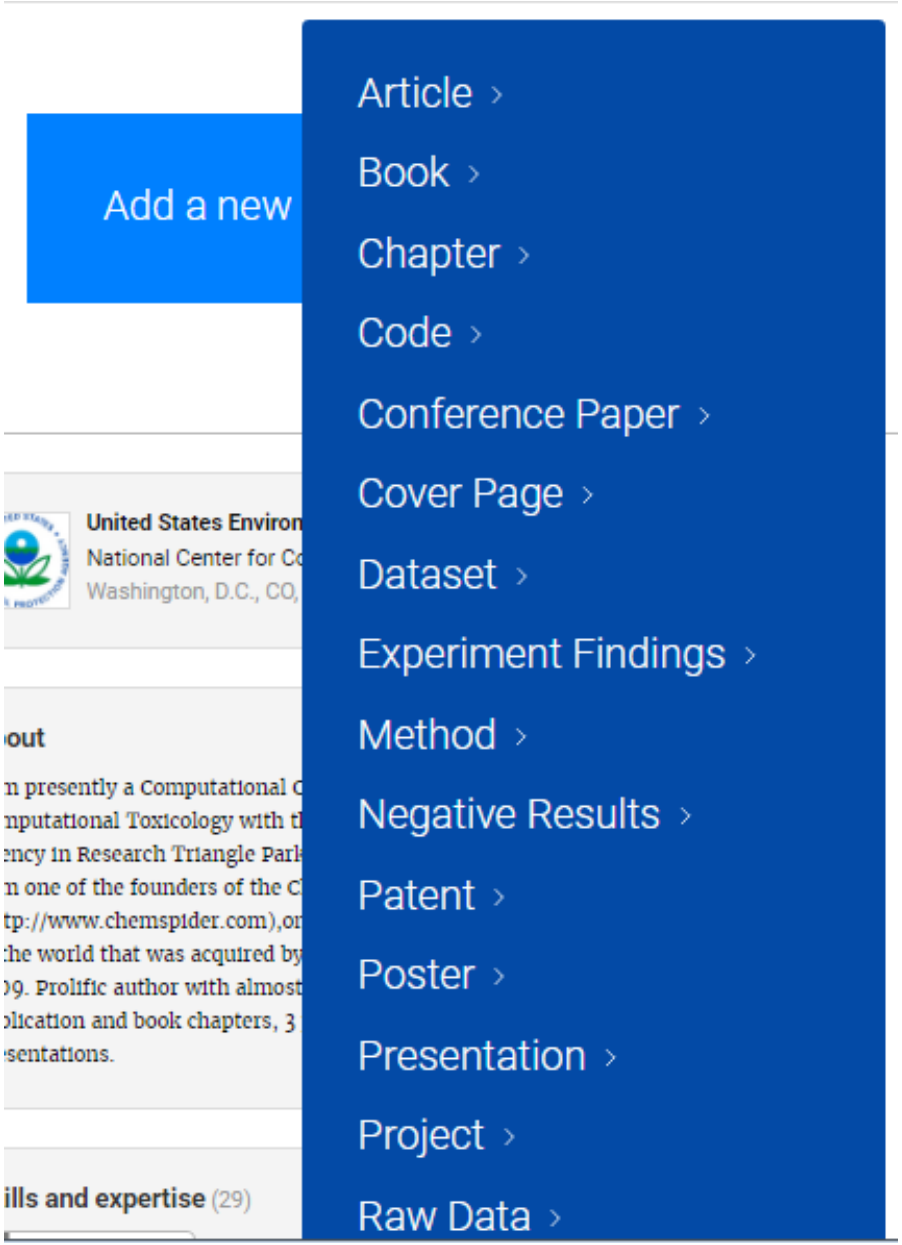

ResearchGate for Sharing a PROJECT

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

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Answer reads	693
Publication reads	32,884

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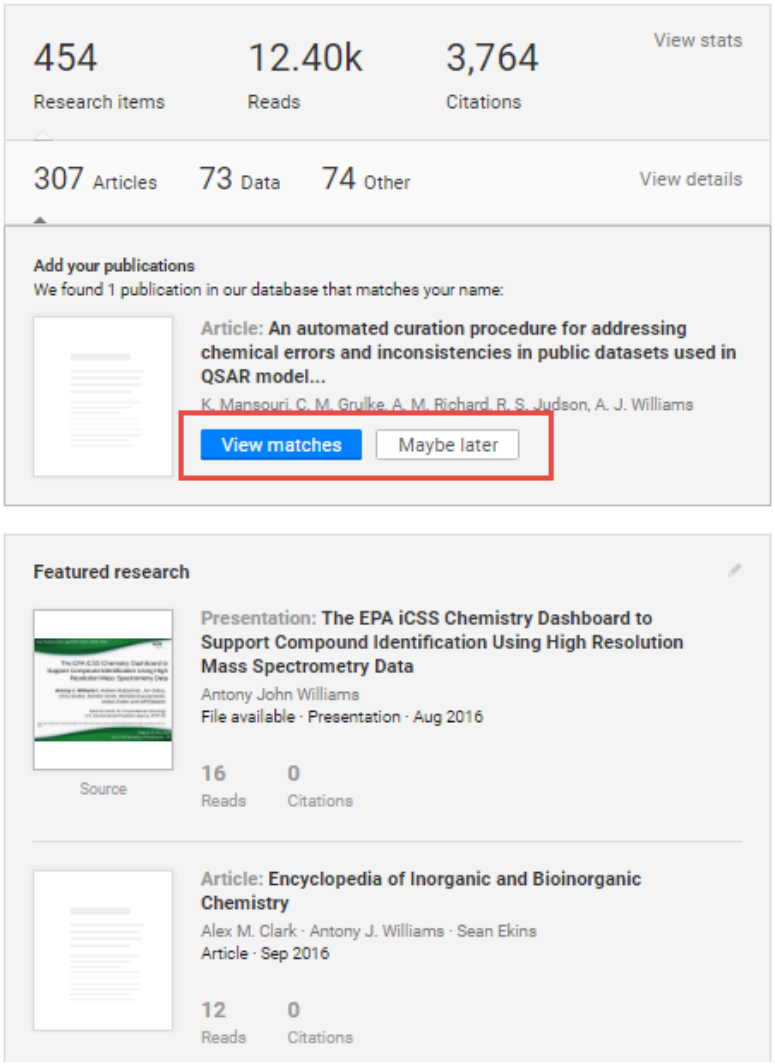

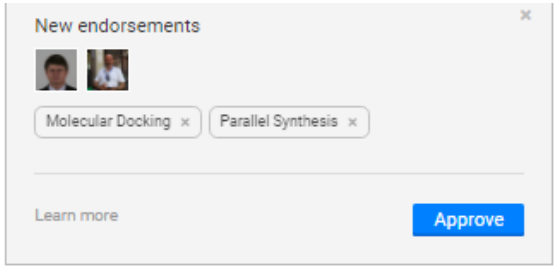

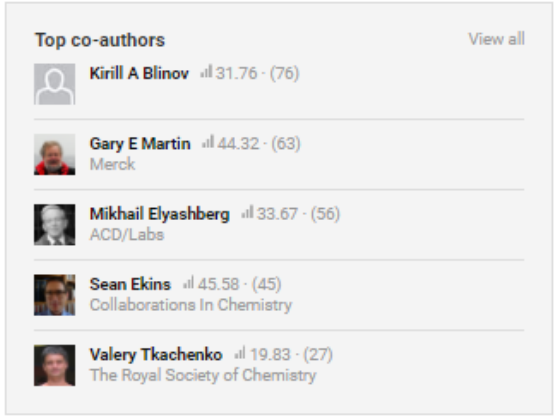

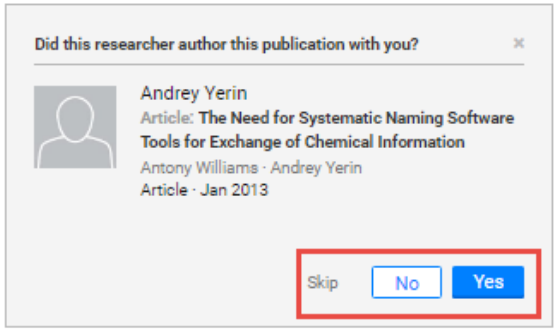

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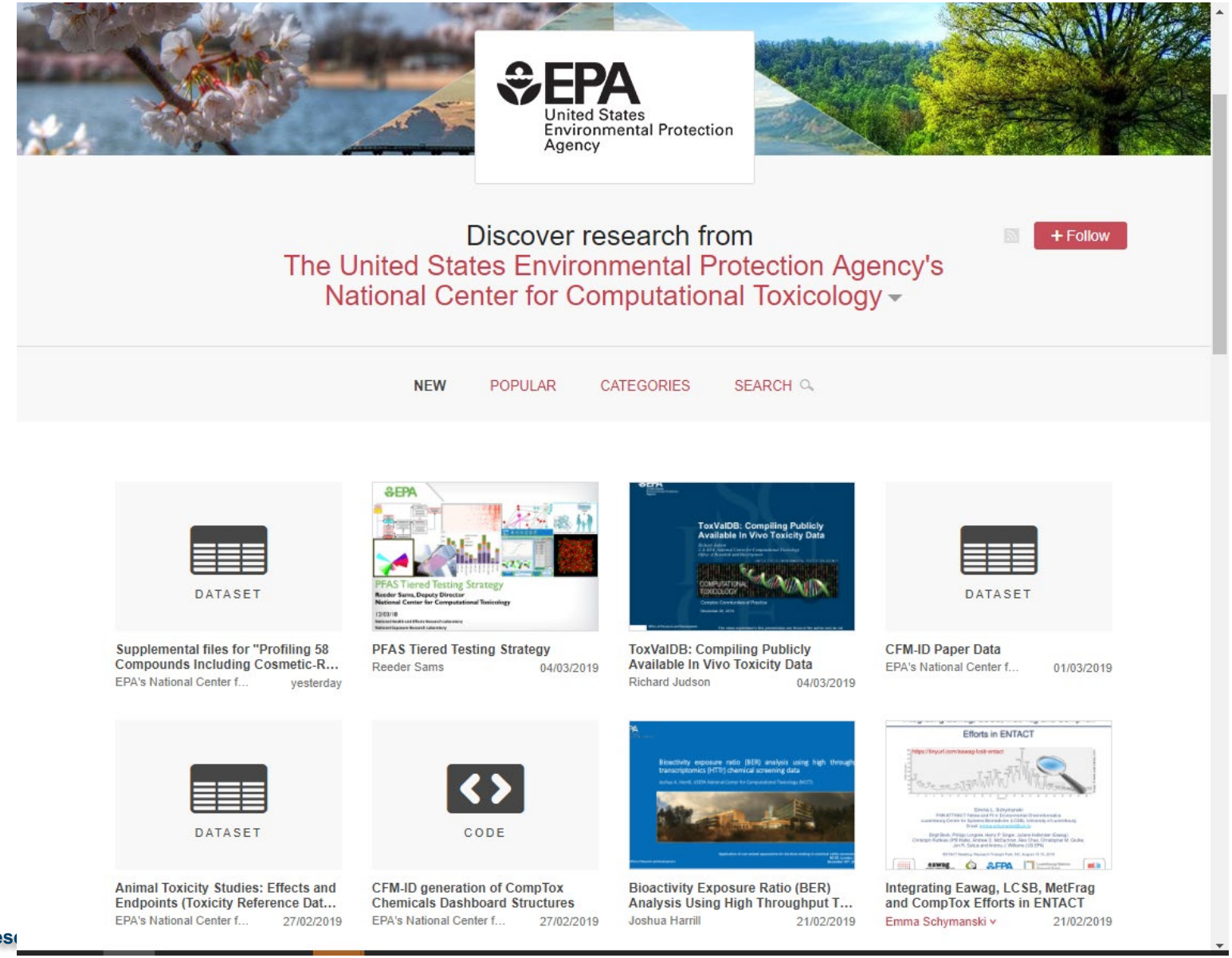

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17.02.2017, 11:27 by Antony Williams

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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

CATEGORIES

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

KEYWORD(S)

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Co-workers & collaborators

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- Valery Tkachenko
- Andrew McEachran
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  Research Triangle Park, NC
- Sean Ekins
  senior consultant
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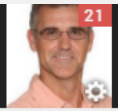

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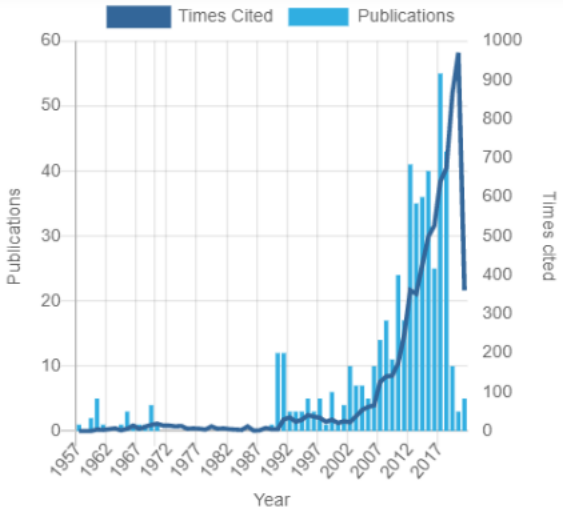

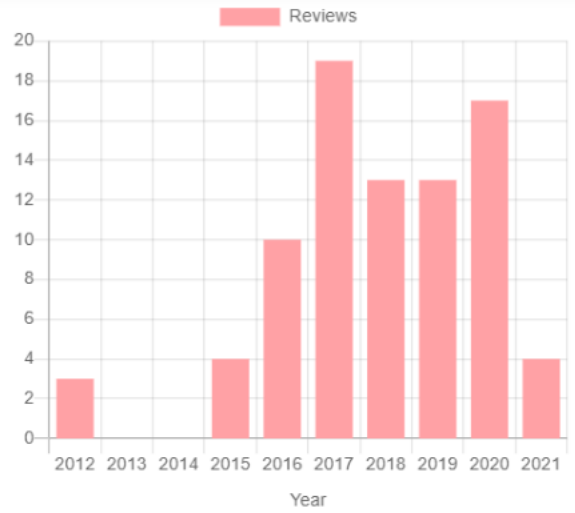

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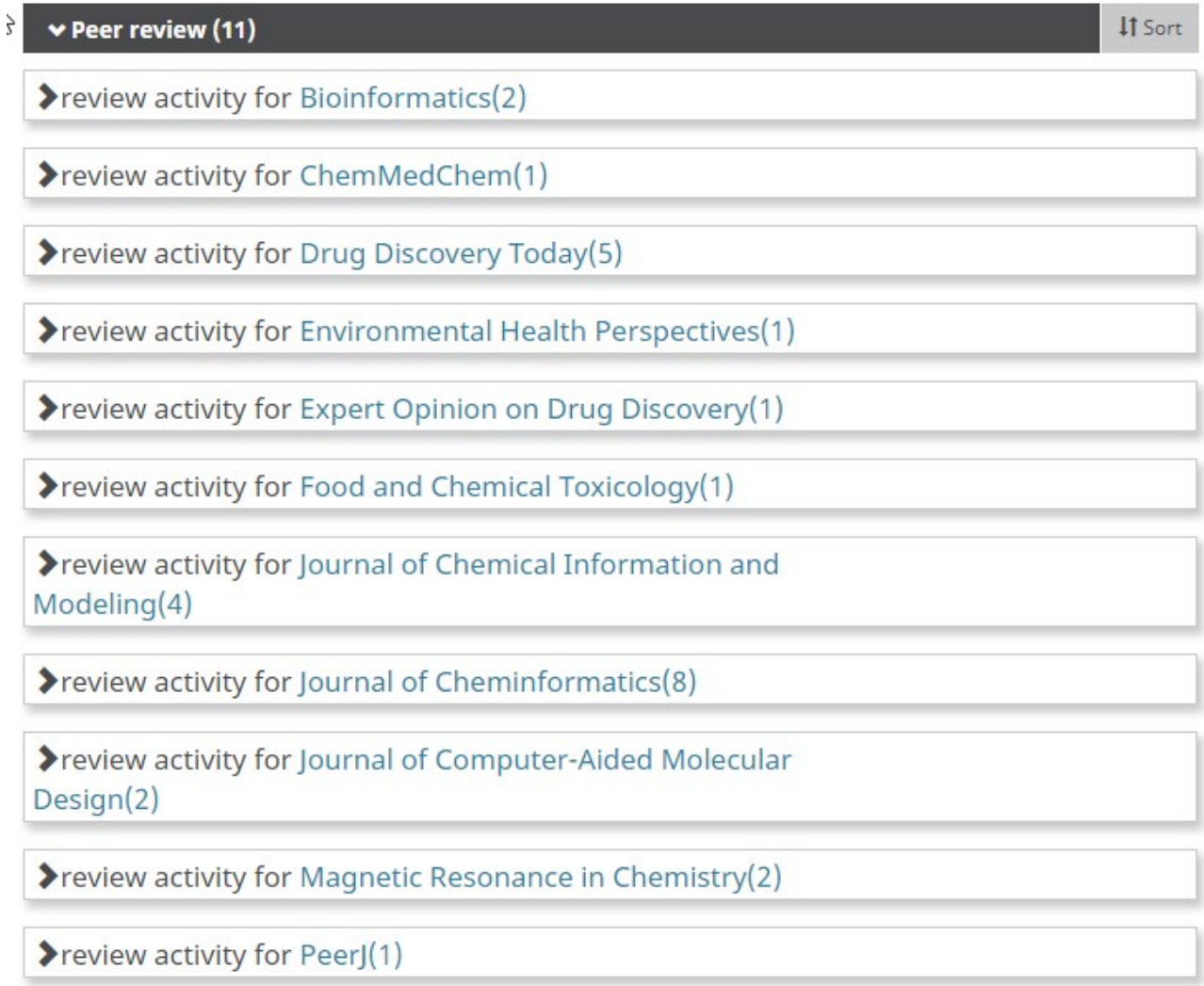

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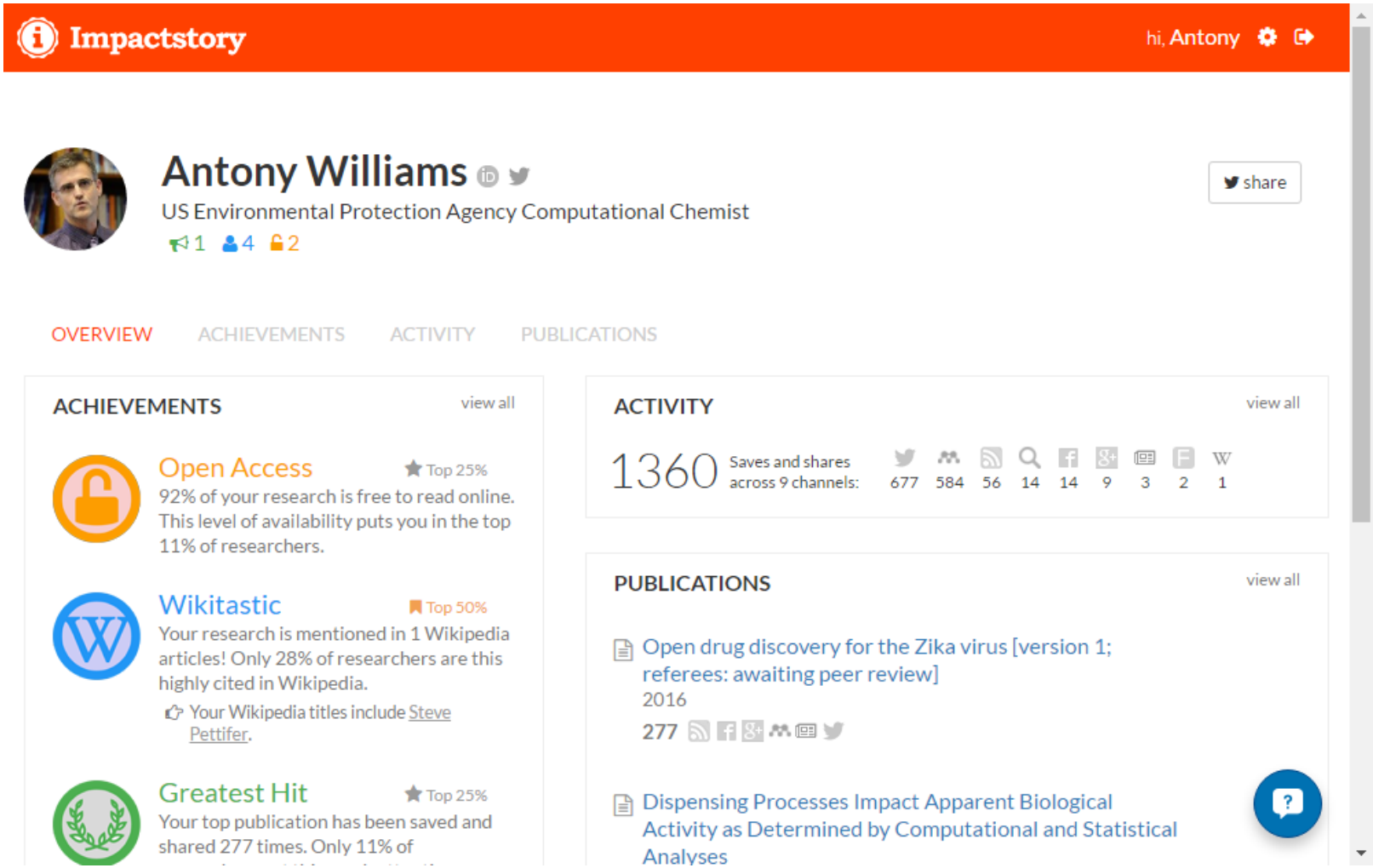

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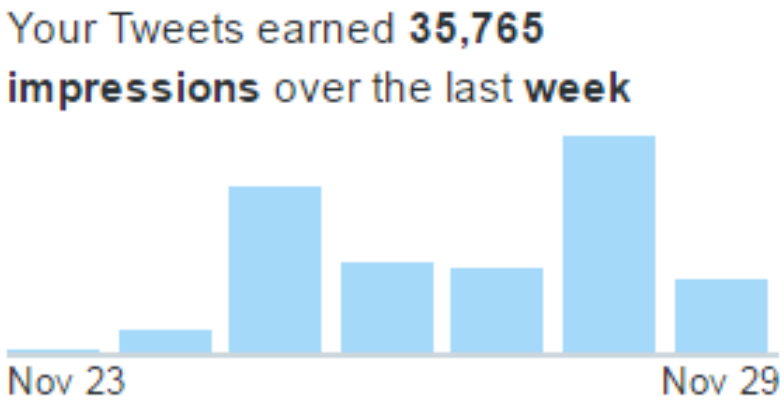

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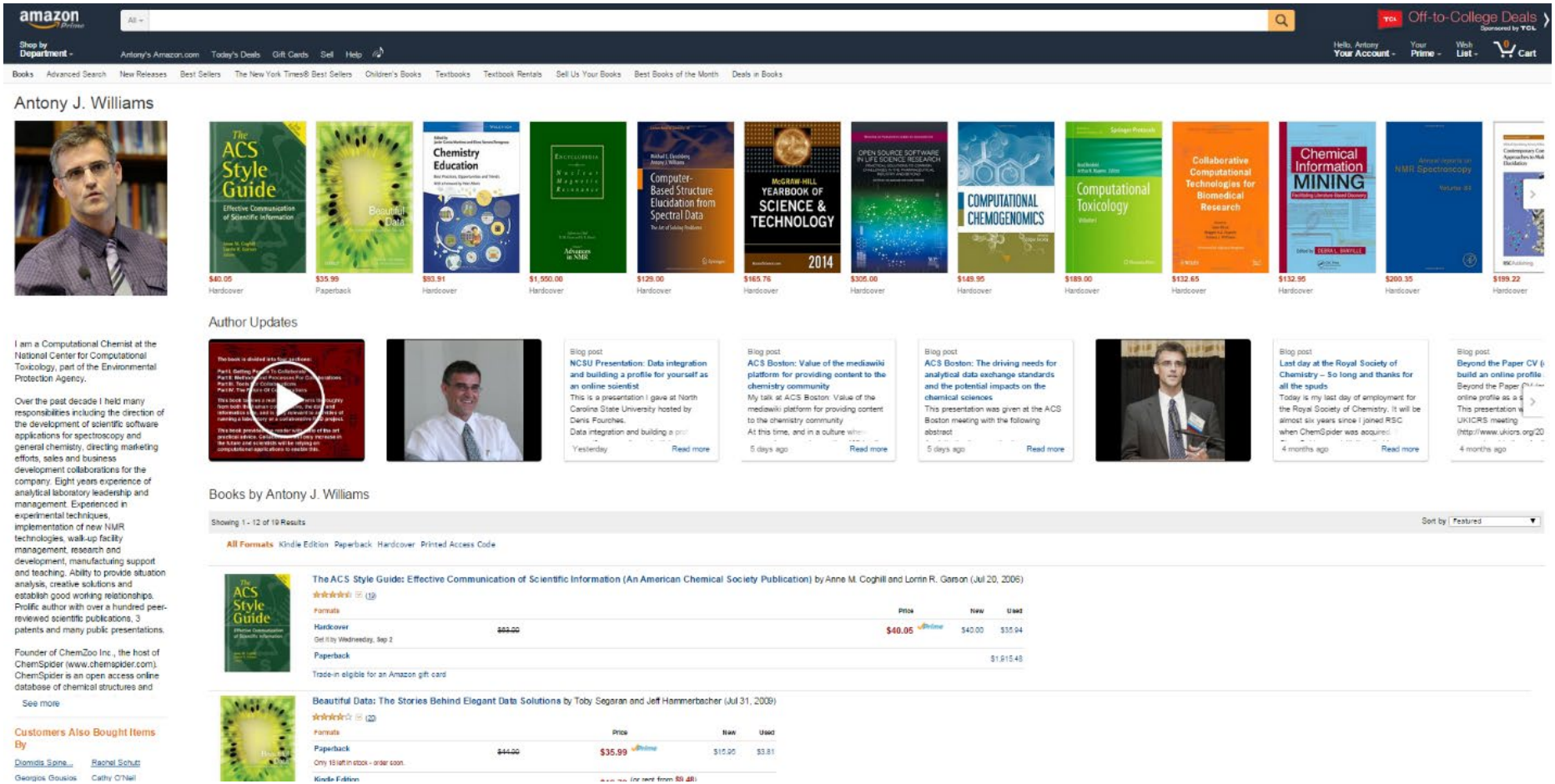

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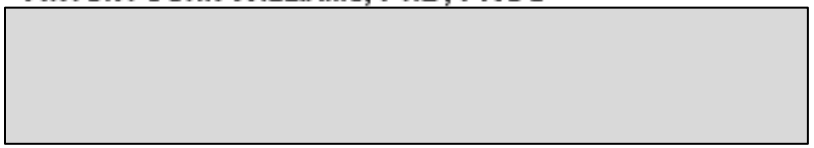

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