

# Measuring Impact of EPA's Computational Toxicology Research

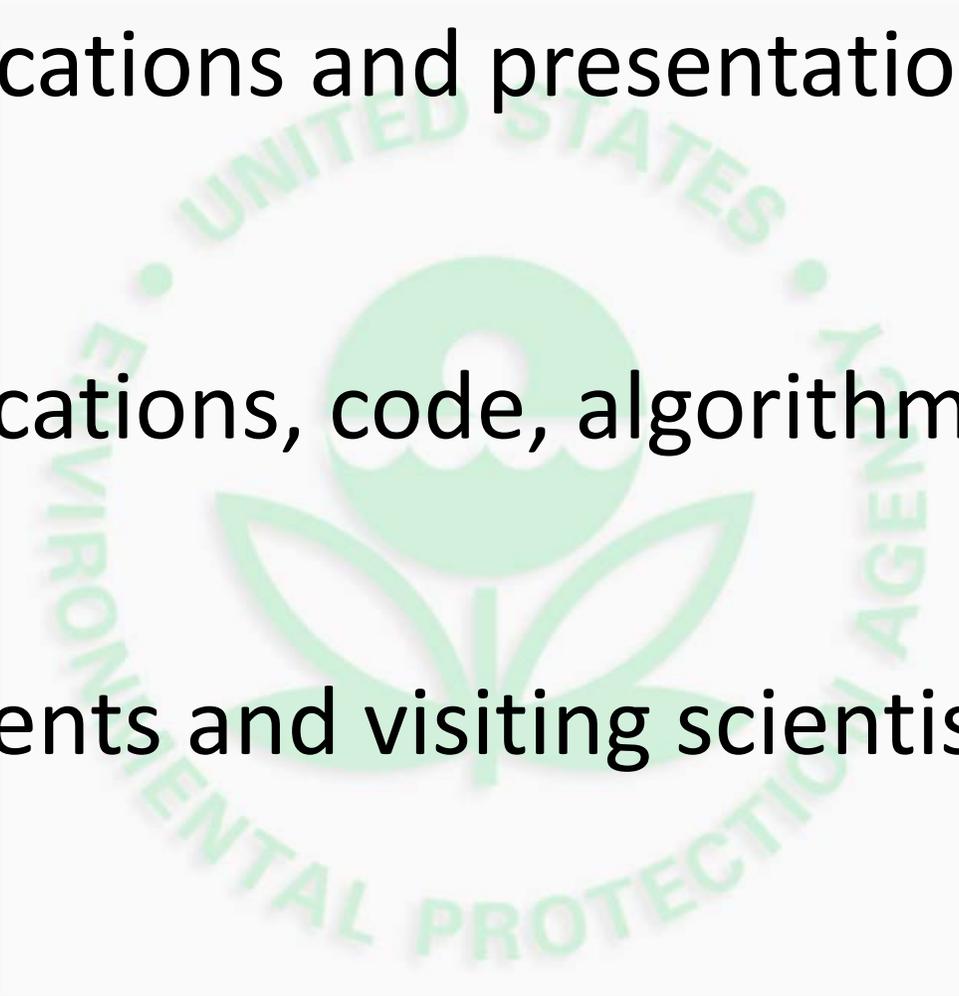
Presenter: Monica Linnenbrink  
EPA Office of Research and Development  
Strategic Stakeholder Engagement and Outreach

# Vision for CompTox Impact Site

- EPA CompTox Research
  - Transformative
  - Game-changing
  - Wide-spread interest
- Purpose: Track metric trends to showcase impact of research and evaluate usefulness of metric
- Learn from approach and broadly apply at multiple organizational levels (e.g., Chemical Safety for Sustainability Research Program)

# Computational Toxicology Research Products

- Scientific publications and presentations
- Research data
- Software applications, code, algorithms and models
- Trainings, students and visiting scientists



# What metrics should we track?

- **Classical metrics** – publications (How many, where published, how many times cited)
- **Alternative metrics**– publication and data downloads, views, (<http://altmetrics.org/manifesto/>)
- **Most important – usage of research**
  - Usage of research for decision-making
  - Presence of research or reference to it in influential documents such as budget or statutory language.



# Alternative Metric Sources

- Many Social and Altmetric platforms in recent years...

The collage displays five different altmetric and social platforms:

- Impactstory:** Profile for Antony Williams, US Environmental Protection Agency Computational Chemist. Shows achievements like 'Open Access' (84% free to read) and 'ACTIVITY' (1333 saves and shares).
- Publons:** Dashboard for Antony Williams, showing a 'REVIEW HISTORY' table with columns for DATE, MANUSCRIPT, and JOURNAL.
- ORCID:** Profile for Antony Williams, ORCID ID: 0000-0002-2668-4821. Includes a biography and a QR code for the ID.
- KUDOS:** Profile for Dr Antony John Williams, National Center of Computational Toxicology. Shows a 'Publications' section with a 'Read more' button.
- Altmetric:** Article page for 'Dispensing Processes Impact Apparent Biological Activity as Determined by Computational and Statistical Analyses'. Features an 'Attention Score' of 85 and a 'SUMMARY' section.

## EPA Computational Toxicology Impact

Chemical safety has been a major priority for EPA since it was established in 1970. As the number of chemicals entering the marketplace has increased, evaluating chemicals for potential health effects has become a formidable challenge. Today, some 80,000 chemicals are listed or registered under the Toxic Substance Control Act (TSCA), and hundreds of new chemicals are introduced every year. EPA's computational toxicology research has made a tremendous impact on this challenge by developing scientific approaches that can be used to evaluate thousands of chemicals for potential health effects. Approaches are faster, more efficient, and far less costly than traditional methods. Learn more about our impact by exploring our scientists, publications and data.



Scientists



Publications



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Impact



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## Our Scientists

Sorty By: Last Name



[Antony Williams](#)  
Chemist



[Thomas Knudsen](#)  
Developmental Systems  
Biologist



[Dustin Kapraun](#)  
Mathematical  
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[Richard Judson](#)  
Research Chemist



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Research Toxicologist



[Chris Grulke](#)  
Cheminformatician



[Danica DeGroot](#)  
Post-Doctoral Fellow



[Kevin Crofton](#)  
Deputy Director



Comptox Impact x ruelas-rivera...

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**Area of Expertise:**  
Dr. Williams' present focus at NCCT is as part of the Chemical Safety for Sustainability (CSS) Research Program to develop a cheminformatics architecture for the center. This work has already produced the publicly accessible website, the iCSS Chemistry Dashboard, providing access to chemistry related data for over 700,000 chemicals (<https://comptox.epa.gov/dashboard>).

**Education:**

- B.S., Liverpool University, Liverpool, UK; Chemistry, 1985
- Ph.D., University of London, London, UK; Chemistry, 1988

**Professional Experience:**

- North Carolina ACS Distinguished Lecturer, 2016
- Microsoft eScience Jim Gray Award, 2012
- Fellow of the Royal Society of Chemistry, 2009
- University of London Bourne Medal for best Chemistry Thesis, 1988

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### Publications

I.V. Tetko, D.M. Lowe and A.J. Williams. [The development of models to predict melting and pyrolysis point data associated with several hundred thousand compounds mined from PATENTS](#). Journal of Cheminformatics 2016 8:2. 

J. Sobus, J.E Rager, M.J Strynar, S. Liang, R.L McMahan, AM Richard, C.M Grulke, J.F Wambaugh, K.K Isaacs, R.J. Judson and A.J Williams. [Linking High Resolution Mass Spectrometry Data with Exposure and Toxicity Forecasts to Advance High-Throughput Environmental Monitoring](#). Environmental International, Volume 88, 2016, 269–280. 

S.A. Akhondi, S. Muresan, A.J. Williams and J.A. Kors. [Ambiguity of non-systematic chemical identifiers within and between small-molecule databases](#). Journal of Cheminformatics, 2015, 7:54. 

C. Lipinski, N. Litterman, C. Southan, A.J. Williams, A. Clark and S. Ekins. [The parallel worlds of chemistry data](#). Journal of Medicinal Chemistry, 58 (5), pp 2068–2076, 2015. 

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### Presentations

Williams, A., K. Mansouri, T. Martin, Chris Grulke, J. Wambaugh, R. Judson, G. Patlewicz, I. Shah, AND A. Richard. [Delivering The Benefits of Chemical-Biological Integration in Computational Toxicology at the EPA \(ACS Fall meeting\)](#). Presented at ACS Fall Meeting, Philadelphia, PA. August 21 - 25, 2016.

Richard, A., C. Grulke, I. Thillainadarajah, K. Mansouri, J. Kancherla, R. Judson, AND A. Williams. [EPAs DSSTox Chemical Database: A Resource for the Non-Targeted Testing Community \(EPA NTA workshop\)](#). Presented at Advancing Non-targeted Analyses of Xenobiotics in Environmental and Biological Media, RTP, NC. August 18 - 19, 2015.

<https://www.altmetric.com/details.php?domain=localhost...>

# Publications

Search NCCT Publications

Filter by:

2016

Rapid Exposure Dose  
High-throughput Tox Testing

Richard, A. Williams, A.  
Judson, R.

Publications Research Project Altmetric PlumX Kudos

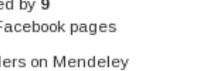
Rager, Julia E; Strynar, Mark; Liang, Shuang; McMahan, Rebecca L; Richard, Ann; Grukle, Christopher M.; Wambaugh, John; Isaacs, Kristin; Judson, Richard; Williams, Antony; Sobus, Jon. (2016). [Linking high resolution mass spectrometry data with exposure and toxicity forecasts to advance high-throughput environmental monitoring](#). Environment International Volume 88, 2016, Pages 269–280.

[Rapid Exposure and Dose](#)



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Judson, Richard; Houck, Keith; Martin, Matt; Richard, Ann; Knudsen, Thomas; Shah, Imran; Little, Stephen; Wambaugh, John; Setzer, Woodrow; Kothiya, Parth; Phuong, Jimmy; Filer, Dayne; Sipes, Doris; Reif, David; Rotroff, Daniel; Kleinstreuer, Nicole; Sipes, Nisha; Xia, Menghang; Huang, Crofton, Kevin; Thomas, Russell. (2016). [Editor's Highlight: Analysis of the Effects of Cell Stress on Cytotoxicity on In Vitro Assay Activity Across a Diverse Chemical and Assay Space](#). Toxicol. Sci. (2016) 152 (2): 323-339.



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[High-throughput Tox Testing](#)



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# Publications

Search NCCT Publications

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Publications      Research Project      Altmetric      PlumX      Kudos

Rager, Julia E; Strynar, Mark; Liang, Shuang; McMahan, Rebecca L; Richard, Ann; Grulke, Christopher M.; Wambaugh, John; Isaacs, Kristin; Judson, Richard; Williams, Antony; Sobus, Jon. (2016). [Linking high resolution mass spectrometry data with exposure and toxicity forecasts to advance high-throughput environmental monitoring](#). Environment International Volume 88, 2016, Pages 269–280.

[Rapid Exposure and Dose](#)

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Judson, Richard; Houck, Keith; Martin, Matt; Richard, Ann; Knudsen, Thomas; Shah, Imran; Little, Stephen; Wambaugh, John; Setzer, Woodrow; Kothiya, Parth; Phuong, Jimmy; Filer, Dayne; Smith, Doris; Reif, David; Rotroff, Daniel; Kleinstreuer, Nicole; Sipes, Nisha; Xia, Menghang; Huang, Ruili; Crofton, Kevin; Thomas, Russell. (2016). [Editor's Highlight Analysis of the Effects of Cell Stress and Cytotoxicity on In Vitro Assay Activity Across a Diverse Chemical and Assay Space](#). Toxicol. Sci. (2016) 152 (2): 323-339.

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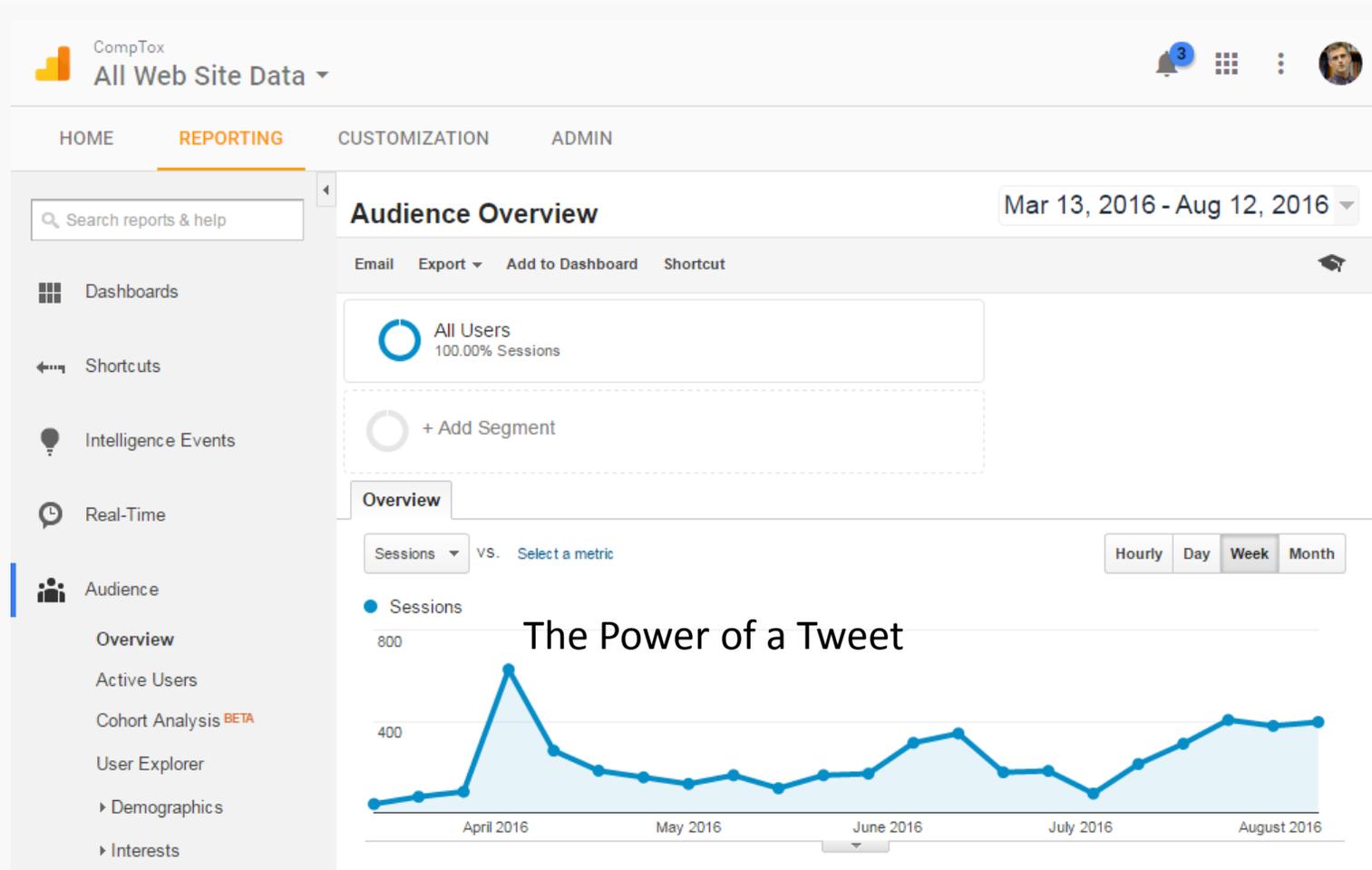


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[High-throughput Tox Testing](#)



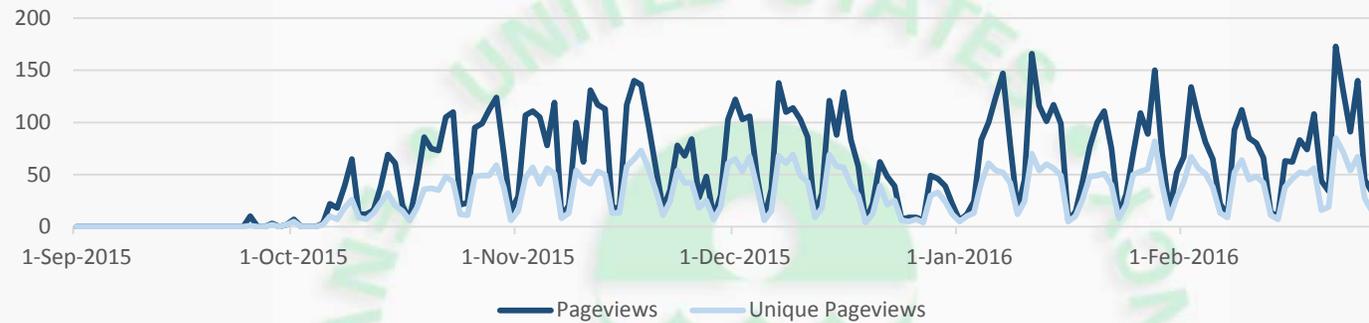
# In development: Online Apps Google Analytics



# In development: Data Download Google Analytics

## Data & Tools: ToxCast Data Download Web

ToxCast Data Download Webpage Traffic (Daily)



ToxCast Data Download Webpage Traffic (Monthly)

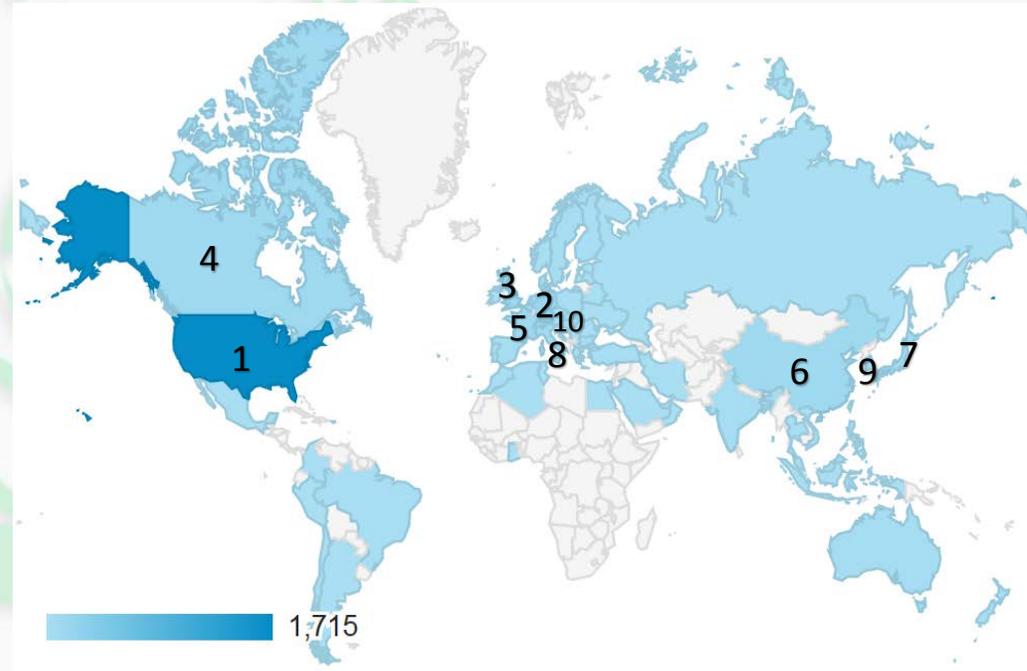


# In development: Google Analytics Demographics

Data & Tools: ToxCast Data Download Web Demographics

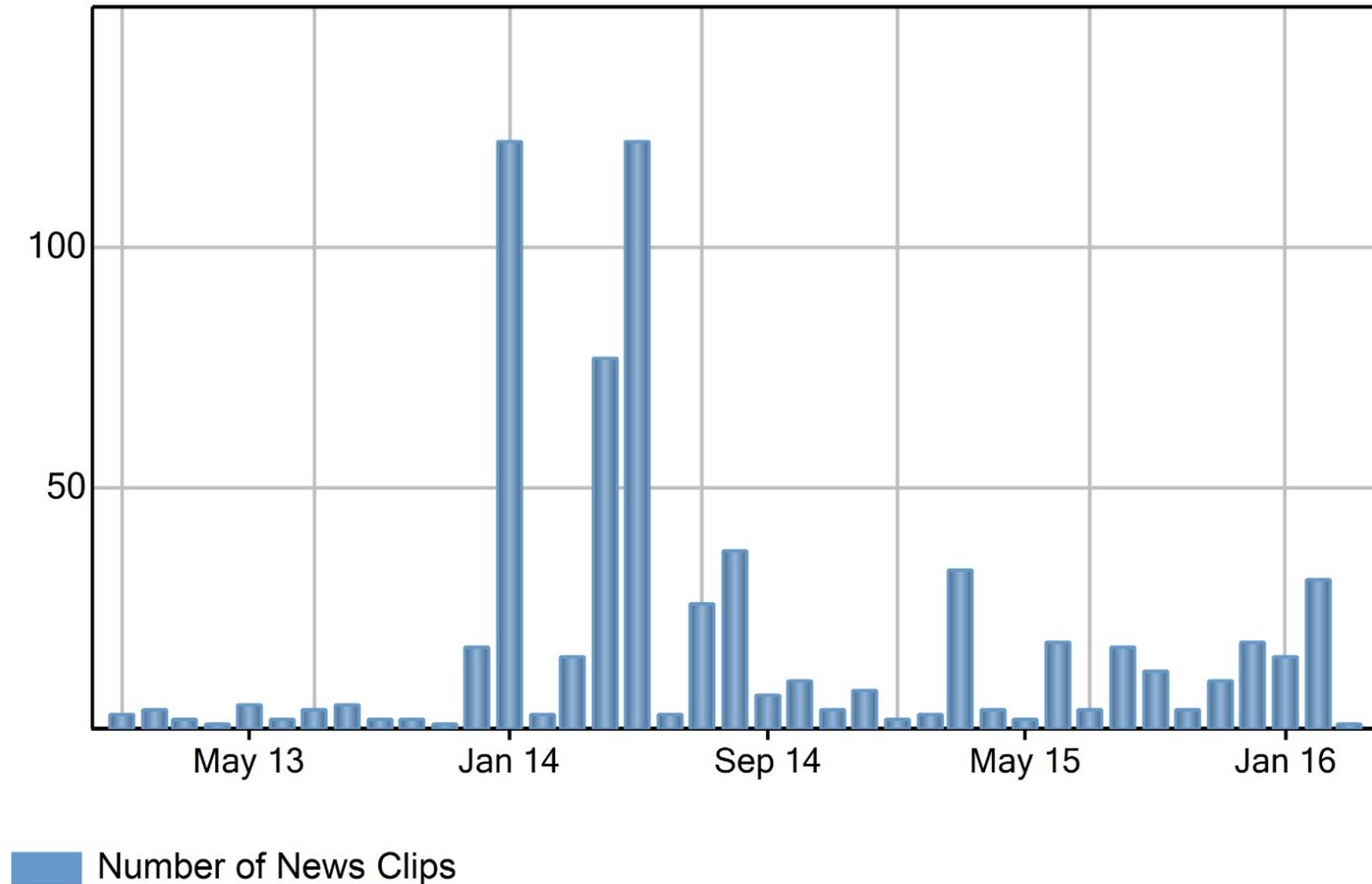
## Top Users by Country

1. United States	1,715
2. Germany	170
3. United Kingdom	148
4. Canada	120
5. France	119
6. China	117
7. Japan	84
8. Italy	78
9. South Korea	60
10. Switzerland	56



# In development: Media Coverage

## EPA Releases New Chemical Data Media Coverage



# Next Steps

- Investigate how to:
  - Consider relevance of the measures and evaluate other data to collect.
  - “Roll-up” scores to show institution wide scores.
  - Compare our scores to other similar research institutions.
  - Track when others use CompTox research for decision making.
  - Address challenges such as evaluating research usage in gray literature and changing ORD’s culture (scientific & technological)
  - Integrate into existing/in development EPA systems – e.g. EPA Science Inventory

# National Center for Computational Toxicology



**Russell Thomas**  
Director



**Kevin Crofton**  
Deputy Director



**Sandra Roberts**  
Associate Director



**John Cowden**  
Matrix Interface



**Monica Linnenbrink**  
Chemical Safety Research  
Communications Director



**David Murphy**  
Extramural  
Management Specialist



**Stephen Little**  
Quality Assurance  
Manager



**Temberly James**  
Administrative  
Officer



**Katherine Coutros**  
Program Analyst



**Joan Breeze**  
SEE Grantee



**Gisele Hamm**  
SEE Grantee



**Lynn Tudor**  
SEE Grantee



**Angelica Adrian**  
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**Todor Anton ijevic**  
ORISE Fellow



**Nancy Baker**  
Leidos  
Contractor



**John Bartlett**  
NSSC



**Audrey Bone**  
Toxicologist



**Cassandra Brinkman**  
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**Swapnil Chavan**  
ORISE Fellow



**Cameron Clark**  
NSSC



**Danica DeGroot**  
Toxicologist



**Chad Deisenroth**  
Research Biologist



**Jeffery Edwards**  
Computer Scientist



**Jeremy Fitzpatrick**  
Chemist



**Stacie Flood**  
NSSC



**Chris Grulke**  
Computational  
Chemist



**Joshua Harrill**  
Toxicologist



**Jason Harris**  
ORISE Fellow



**George Helman**  
ORISE Fellow



**Keith Houder**  
Toxicologist



**Richard Judson**  
Bioinformatician



**Dustin Kapraun**  
Mathematical  
Statistician



**Thomas Knudsen**  
Developmental  
Systems Biologist



**Kamel Mansouri**  
ORISE Fellow



**Matthew Martin**  
Biologist



**Andrew McEachran**  
ORISE Fellow



**Joshua McLane**  
ORISE Fellow



**Grace Patlewicz**  
Research Chemist



**Katie Paul-Friedman**  
Toxicologist



**Jacob Pearce**  
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**Robert Pearce**  
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**LyLy Pham**  
ORISE Fellow



**Prachi Pradeep**  
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**Ann Richard**  
Research Chemist



**Victor Ruelas-Rivera**  
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**Raymond Ruiz-Veve**  
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**Nathaniel Rush**  
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**Hayley Ryskoski**  
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**Kate Saili**  
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**Risa Sayre**  
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**R. Woodrow Setzer**  
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Statistician



**Imran Shah**  
Computational  
Systems Biologist



**Steven Simmons**  
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**Sean Watford**  
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Contractor



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**Antony Williams**  
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**Clinton Willis**  
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**Todd Zurlinde**  
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