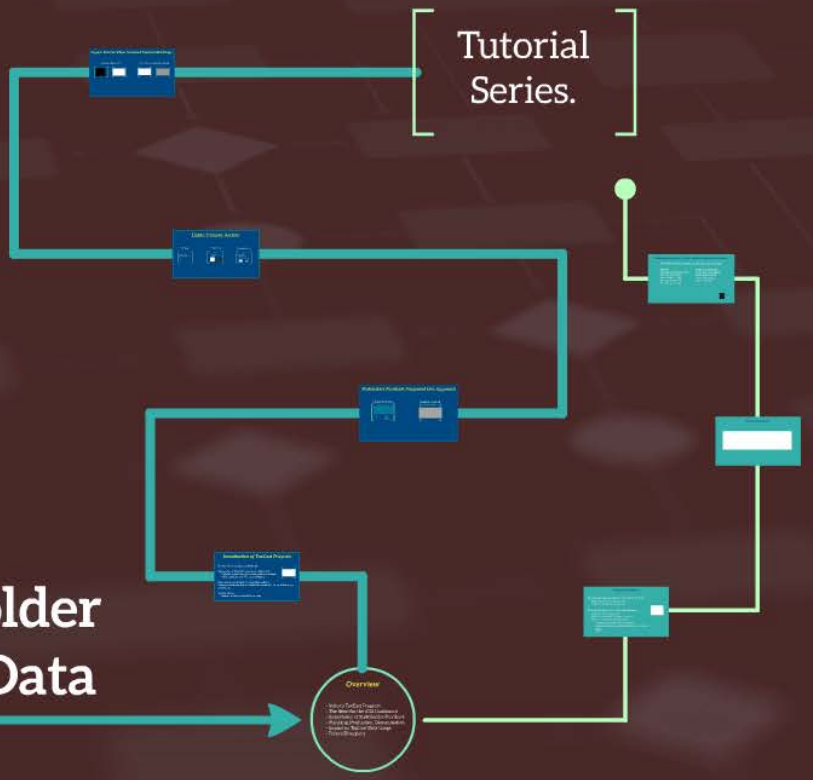
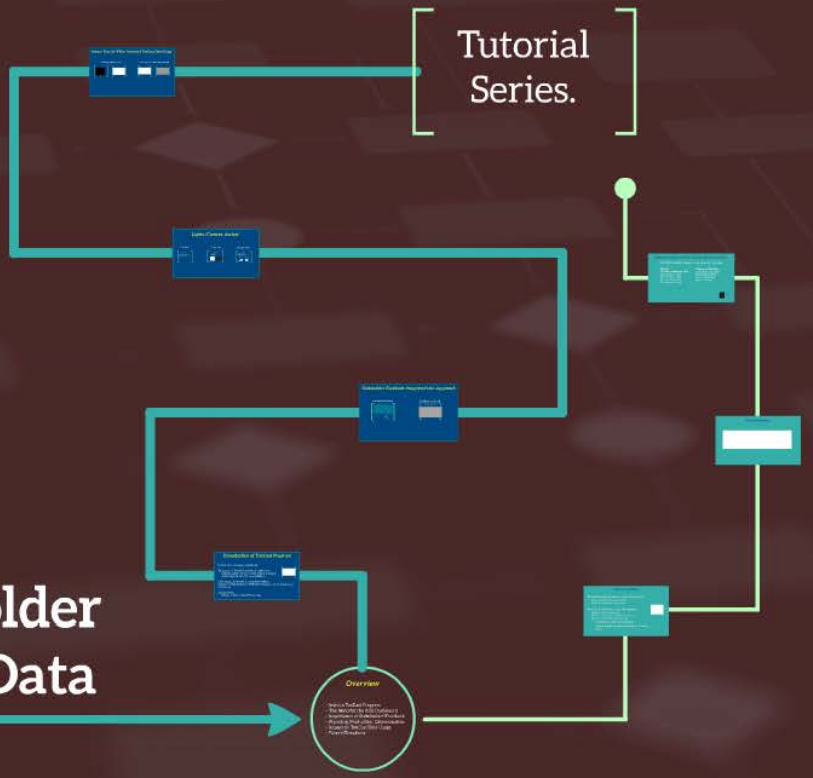


Tutorial Video Series: Using Stakeholder Feedback Increased Use of ToxCast Data

Christina Baghdikian
ASPPH Fellow
US EPA
SETAC EU, May 2015

Prezi

Tutorial Video Series: Using Stakeholder Feedback Increased Use of ToxCast Data



Christina Baghdikian
ASPPH Fellow
US EPA
SETAC EU, May 2015

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The views expressed in this presentation are those of the author and do not necessarily reflect the views or policies of the U.S. Environmental Protection Agency.

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Overview

- Intro to ToxCast Program
- The Need for the iCSS Dashboard
- Importance of Stakeholder Feedback
- Planning, Production, Dissemination
- Impact on ToxCast Data Usage
- Future Directions

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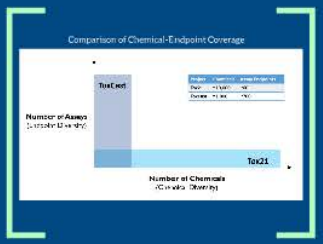
Introduction of ToxCast Program

Problem: Many chemicals and little data



ToxCast part of Tox21 US Government collaboration

- High-throughput chemical screening for prioritization
- ~1800 chemicals and ~700 assay endpoints

Early recognition of need for stakeholder feedback
Necessary to educate diverse stakeholder community for use of data usage and analysis

iCSS Dashboard

- Interactive tool to explore ToxCast data

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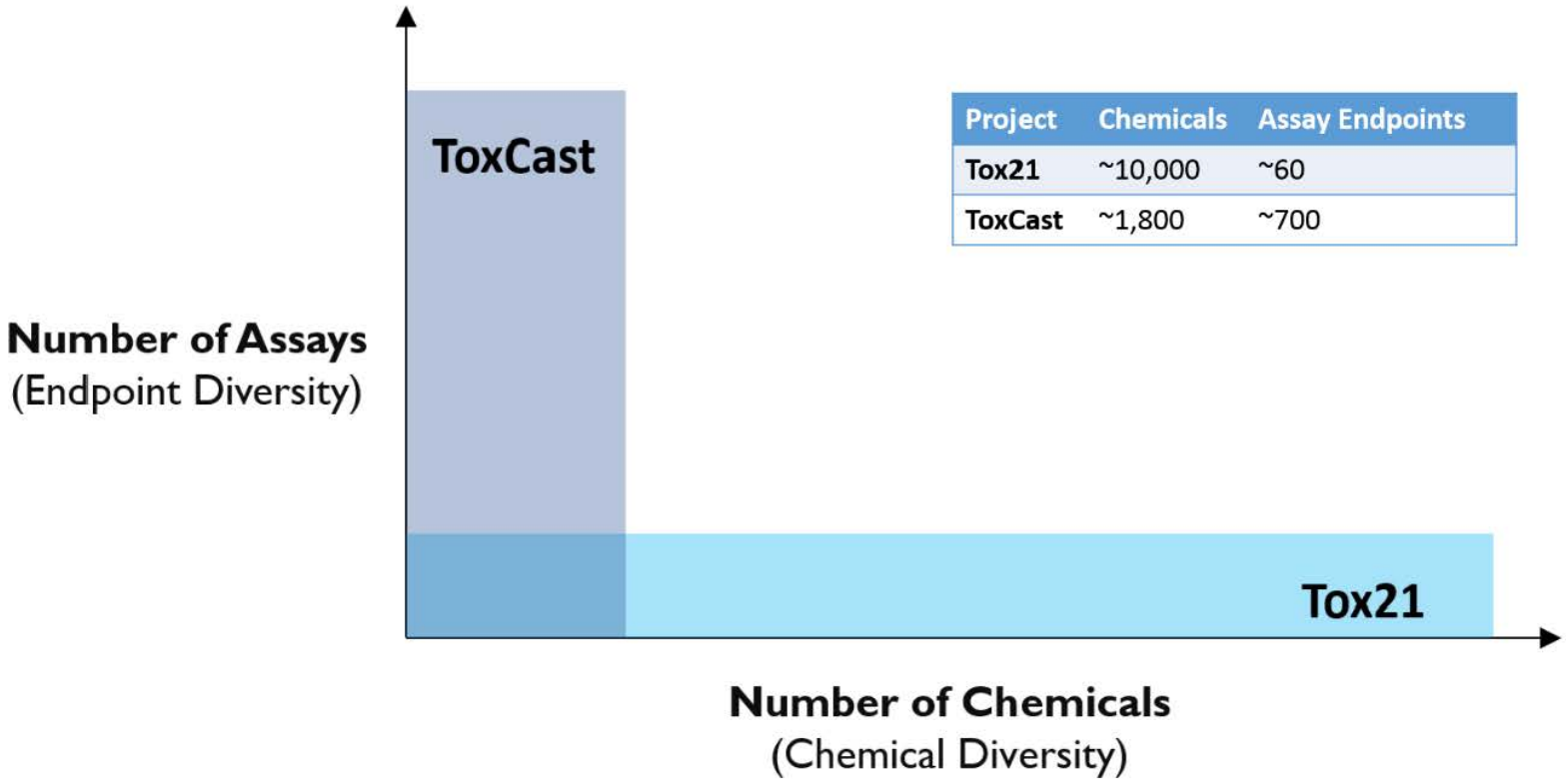
Comparison of Chemical-Endpoint Coverage



Project	Chemicals	Assay Endpoints
Tox21	~10,000	~60
ToxCast	~1,800	~700

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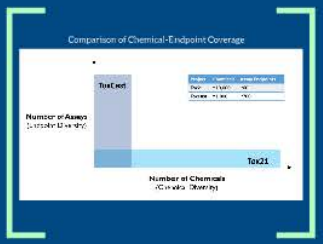
Introduction of ToxCast Program

Problem: Many chemicals and little data



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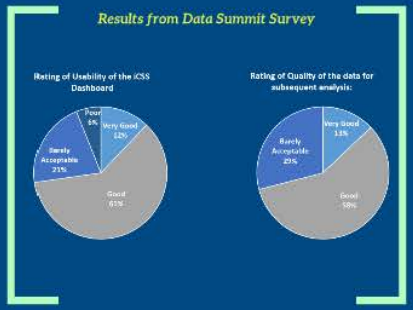
Stakeholder Feedback Integrated into Approach

Stakeholder Events

Feedback Collected



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Timeline of Stakeholder Events

Events and # of Participants

Workshops:
- January 85
- April 277

Data Summit:
- September 304

Diverse Participant Group

Academia
Consultant/Contractor
EPA Program Office
EPA Researchers
Other US Government
Industry
International Government
Media
Non-Governmental Organizations
State Environmental Agencies

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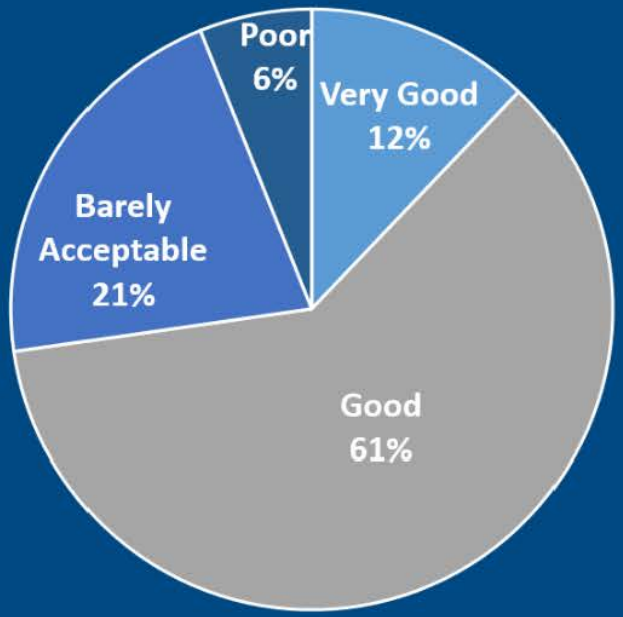
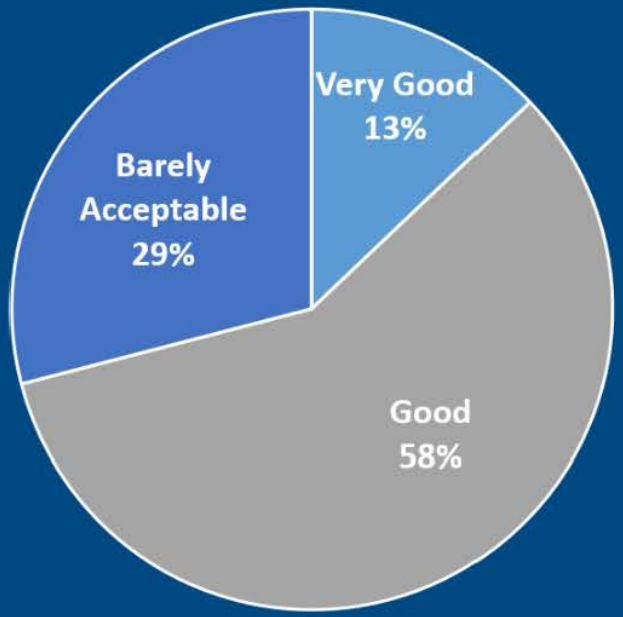
Results from Data Summit Survey

Rating of Usability of the iCSS Dashboard



Rating of Quality of the data for subsequent analysis:



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Lights, Camera, Action!

Planning

Planning

- Gather Stakeholder feedback from Workshop and Data Summit Surveys
- Draft Plan for Tutorial Series
- Draft Script for Video 1: iCSS Dashboard Tutorial

Production

Production

- Record draft of video
- Receive and incorporate feedback from users
- Produce final version

Dissemination

Dissemination

- Post to EPA YouTube and add link to iCSS Dashboard
- Announce and promote video
  - Communities of Practice webinars
  - Other communications efforts
    - Briefings to smaller scientific groups (e.g. ACC)
    - EPA websites (e.g.CompTox webpage, Data Download Page)
    - National/International scientific meetings (e.g. SOT, SETAC

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Planning

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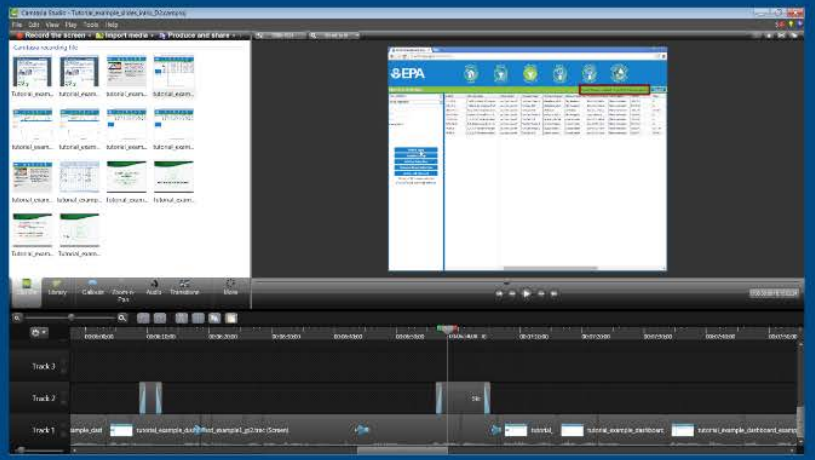
Production

- Record draft of video
- Receive and incorporate feedback from users
- Produce final version

Production Task	Production Tools
Screencasting and Editing Software	Camtasia Version 8
Graphics	Adobe Illustrator, Photoshop
Audio Recording and Narration	Rode Microphone



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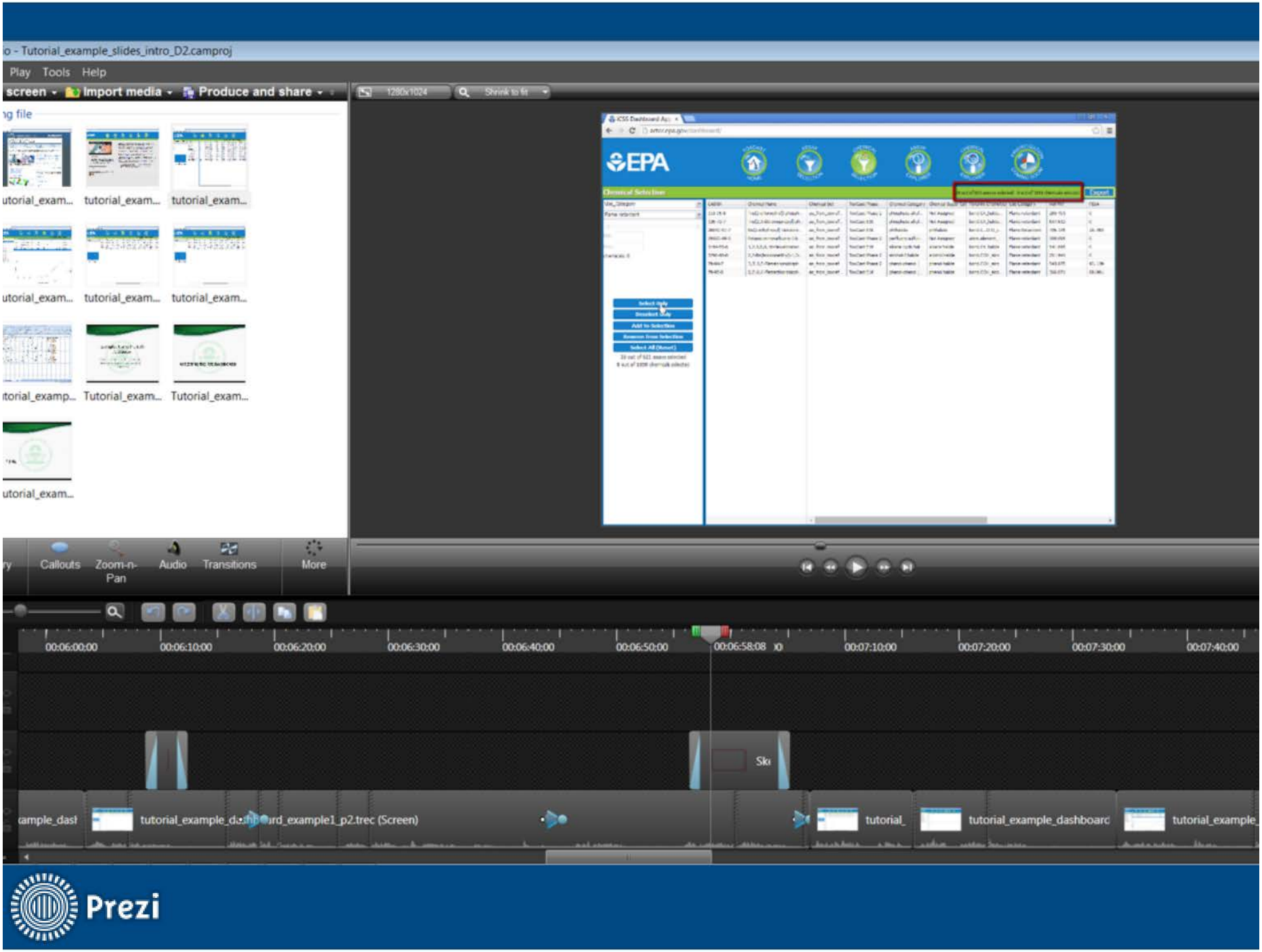
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Play Tools Help
Import media
Produce and share
Callouts
Zoom-n-Pan
Audio
Transitions
More
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Dissemination

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actor.epa.gov/dashboard/

EPA

TOXCAST HOME | ASSAY SELECTION | CHEMICAL SELECTION | ASSAY EXPLORER | CHEMICAL EXPLORER | PRIORITIZATION COMING SOON!

eholder Opportunities to Learn & Explore the Data

- Stakeholder Workshops & Data Summit

Cast Data Use Considerations

- The activity of a chemical in a specific assay does not necessarily mean that it will cause toxicity or an adverse health outcome. There are many factors that determine whether a chemical will cause a specific adverse health outcome. Careful review is required to determine the use of the data in a particular decision context.
- Interpretation of ToxCast data is expected to change over time as both the science and analytical methods improve.

et the best possible experience using the CSS Dashboard application we recommend using lla Firefox or Google Chrome.

EPA has released the first beta version (version 0.5) of the **Interactive Chemical Safety for Sustainability (iCSS) Dashboard**. The beta version of the iCSS Dashboard provides an interactive tool to explore rapid, automated (or in vitro high-throughput) chemical screening data generated by the Toxicity Forecaster (ToxCast) project and the federal Toxicity Testing in the 21st century (Tox21) collaboration.

The iCSS Dashboard contains the results from more than 800 Assay Endpoints (High-Throughput Screening-HTS Data) across over 1,800 chemicals from seven primary HTS assay sources. The release of the iCSS Dashboard coincides with the release of the ToxCast Phase II data. All of the ToxCast Phase II data (including assay summary activity files, assay description files, effect and endpoint data files from animal toxicity studies, concentration response data files & chemical library and structure files) are available on the ToxCast Data Download Page.

Users of the iCSS Dashboard v0.5 can perform basic data and chemical selection, as well as simple data exploration in a seamless environment. EPA will continuously add functionality and improve overall usability and performance. The initial release conveys the conceptual framework and design of the iCSS web application.

Please watch the video tutorial below that shows how to use the iCSS Dashboard through two examples.

Please email the Dashboards Team to provide feedback on ways to improve the Dashboard or to be added to a mailing list to receive status updates. The intent is to use stakeholder feedback to develop updated versions of the iCSS Dashboard and to add more Dashboards.

The vision is for the Dashboard to evolve into an iCSS web application which will become the portal to access all EPA computational toxicology research data and studies including:

- Rapid, automated (or in vitro high-throughput) chemical screening data generated by the EPA's Toxicity Forecaster (ToxCast) project and the federal Toxicity Testing in the 21st century (Tox21) collaboration.

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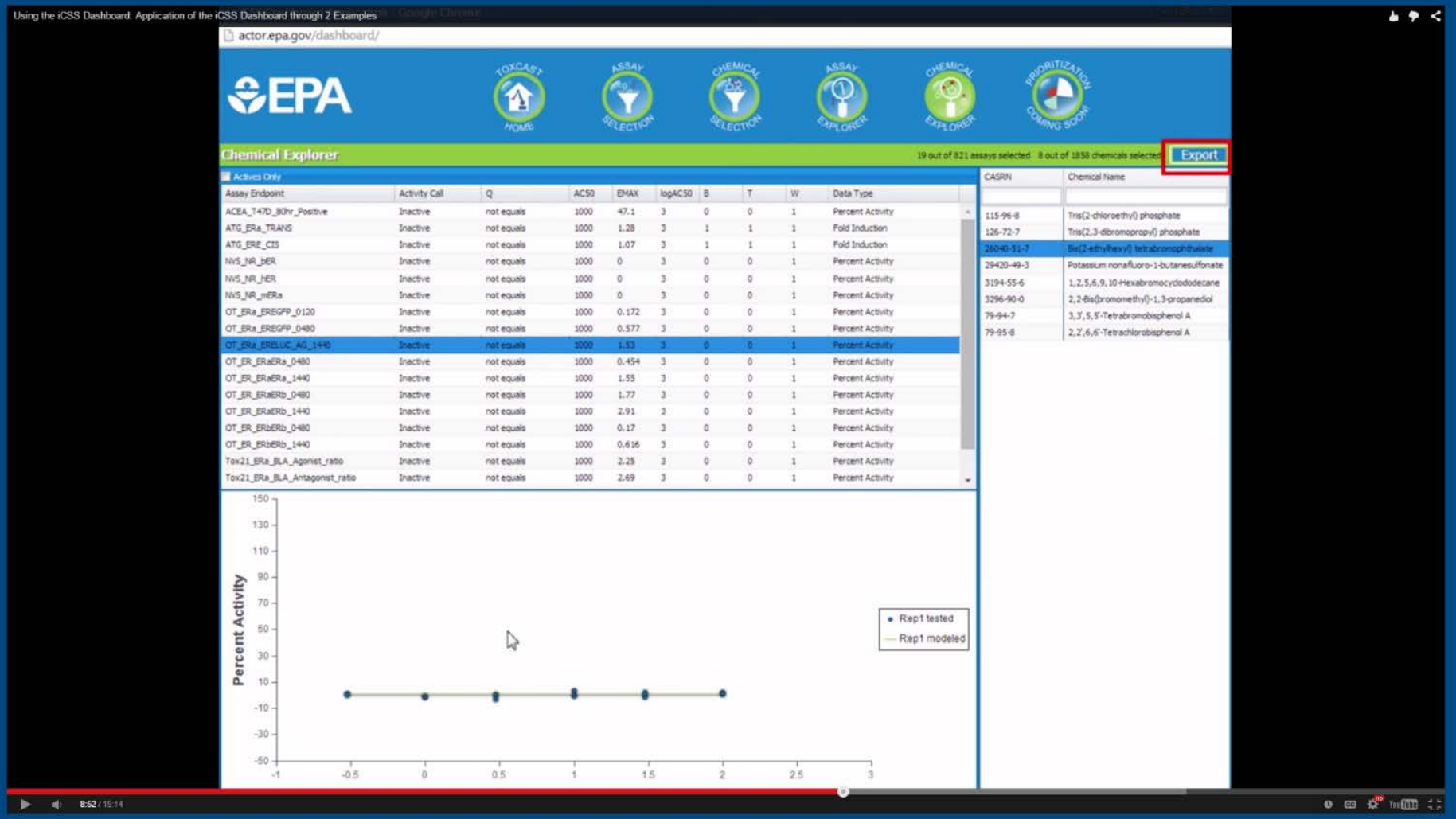
Using the iCSS Dashboard: Application of the iCSS Dashboard through 2 Examples
actor.epa.gov/dashboard/
EPA
TOXCAST HOME
ASSAY SELECTION
CHEMICAL SELECTION
ASSAY EXPLORER
CHEMICAL EXPLORER
PRIORITIZATION COMING SOON
Chemical Explorer
19 out of 821 assays selected 8 out of 1858 chemicals selected
Export
Actives Only
Assay Endpoint | Activity Call | Q | AC50 | EMAX | logAC50 | B | T | W | Data Type
ACEA_T47D_80hr_Positive | Inactive | not equals | 1000 | 47.1 | 3 | 0 | 0 | 1 | Percent Activity
ATG_ERa_TRANS | Inactive | not equals | 1000 | 1.28 | 3 | 1 | 1 | 1 | Fold Induction
ATG_ERE_CIS | Inactive | not equals | 1000 | 1.07 | 3 | 1 | 1 | 1 | Fold Induction
NVS_NR_bER | Inactive | not equals | 1000 | 0 | 3 | 0 | 0 | 1 | Percent Activity
NVS_NR_hER | Inactive | not equals | 1000 | 0 | 3 | 0 | 0 | 1 | Percent Activity
NVS_NR_mERa | Inactive | not equals | 1000 | 0 | 3 | 0 | 0 | 1 | Percent Activity
OT_ERa_EREGFP_0120 | Inactive | not equals | 1000 | 0.172 | 3 | 0 | 0 | 1 | Percent Activity
OT_ERa_EREGFP_0480 | Inactive | not equals | 1000 | 0.577 | 3 | 0 | 0 | 1 | Percent Activity
OT_ERa_ERELUC_AG_1440 | Inactive | not equals | 1000 | 1.53 | 3 | 0 | 0 | 1 | Percent Activity
OT_ER_ERaERa_0480 | Inactive | not equals | 1000 | 0.454 | 3 | 0 | 0 | 1 | Percent Activity
OT_ER_ERaERa_1440 | Inactive | not equals | 1000 | 1.55 | 3 | 0 | 0 | 1 | Percent Activity
OT_ER_ERaERb_0480 | Inactive | not equals | 1000 | 1.77 | 3 | 0 | 0 | 1 | Percent Activity
OT_ER_ERaERb_1440 | Inactive | not equals | 1000 | 2.91 | 3 | 0 | 0 | 1 | Percent Activity
OT_ER_ERbERb_0480 | Inactive | not equals | 1000 | 0.17 | 3 | 0 | 0 | 1 | Percent Activity
OT_ER_ERbERb_1440 | Inactive | not equals | 1000 | 0.616 | 3 | 0 | 0 | 1 | Percent Activity
Tox21_ERa_BLA_Agonist_ratio | Inactive | not equals | 1000 | 2.25 | 3 | 0 | 0 | 1 | Percent Activity
Tox21_ERa_BLA_Antagonist_ratio | Inactive | not equals | 1000 | 2.69 | 3 | 0 | 0 | 1 | Percent Activity
CASRN | Chemical Name
115-96-8 | Tris(2-chloroethyl) phosphate
126-72-7 | Tris(2,3-dibromopropyl) phosphate
26040-51-7 | Bis(2-ethylhexyl) tetrabromophthalate
29420-49-3 | Potassium nonafluoro-1-butanesulfonate
3194-55-6 | 1,2,5,6,9,10-Hexabromocyclododecane
3296-90-0 | 2,2-Bis(bromomethyl)-1,3-propanediol
79-94-7 | 3,3',5,5'-Tetrabromobisphenol A
79-95-8 | 2,2',6,6'-Tetrachlorobisphenol A
Percent Activity
150
130
110
90
70
50
30
10
-10
-30
-50
-1
-0.5
0
0.5
1
1.5
2
2.5
3
Rep1 tested
Rep1 modeled
8:52 / 15:14

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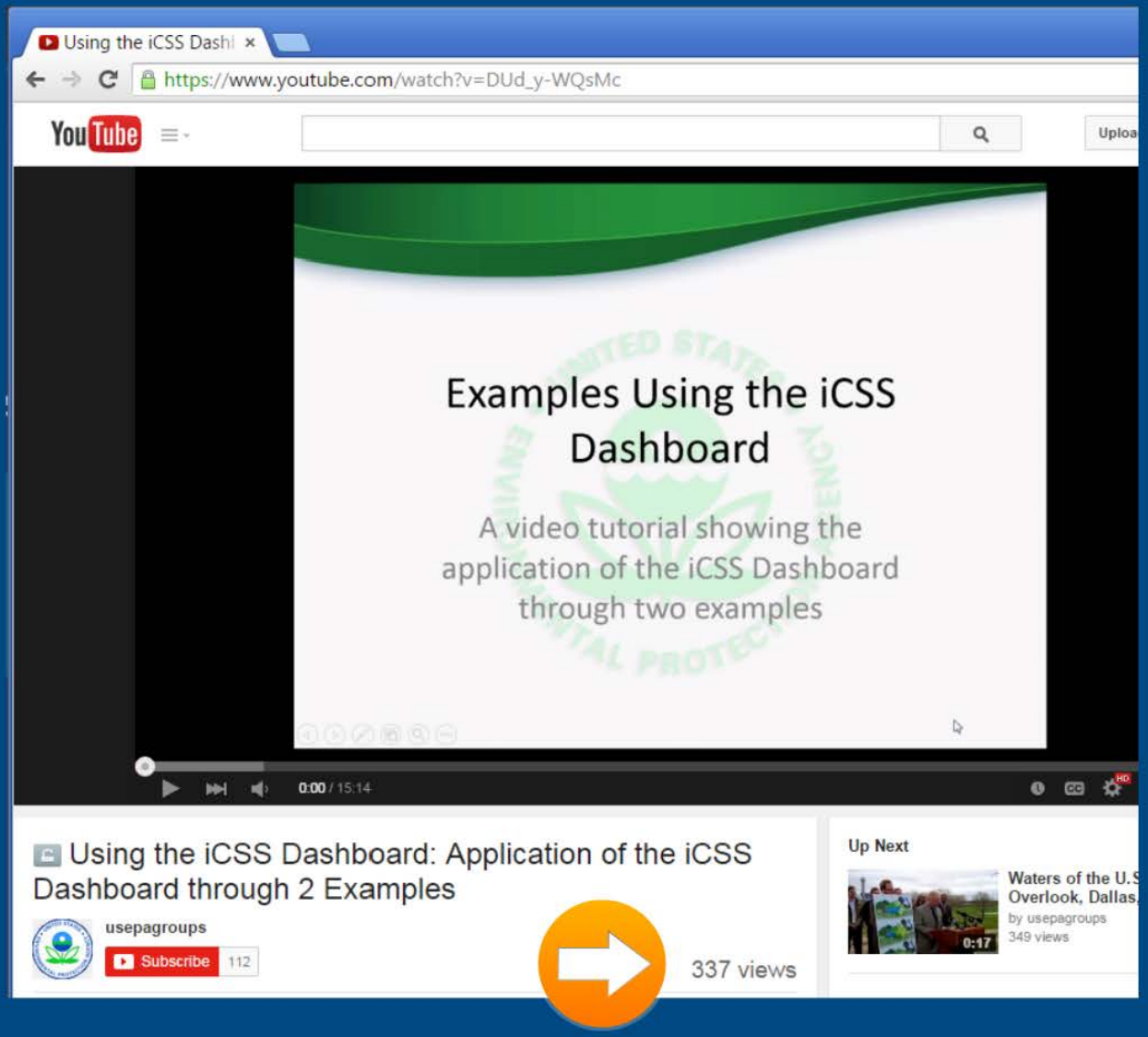
Impact: Tutorial Video Increased ToxCast Data Usage

Measuring impact of Video

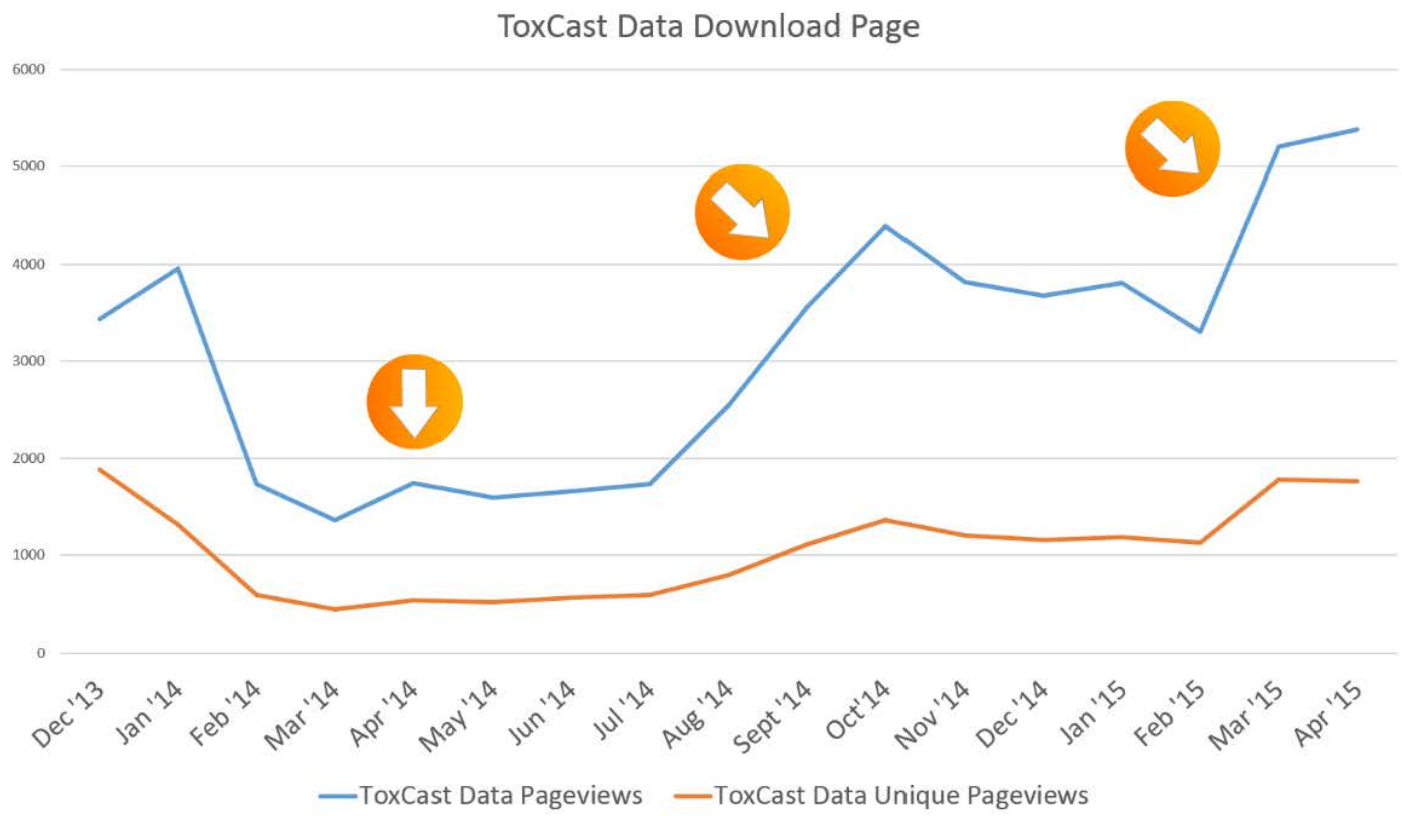
Further impact of stakeholder feedback

Prezi

Number of views as of April 26



Peaks in use around stakeholder events and video release



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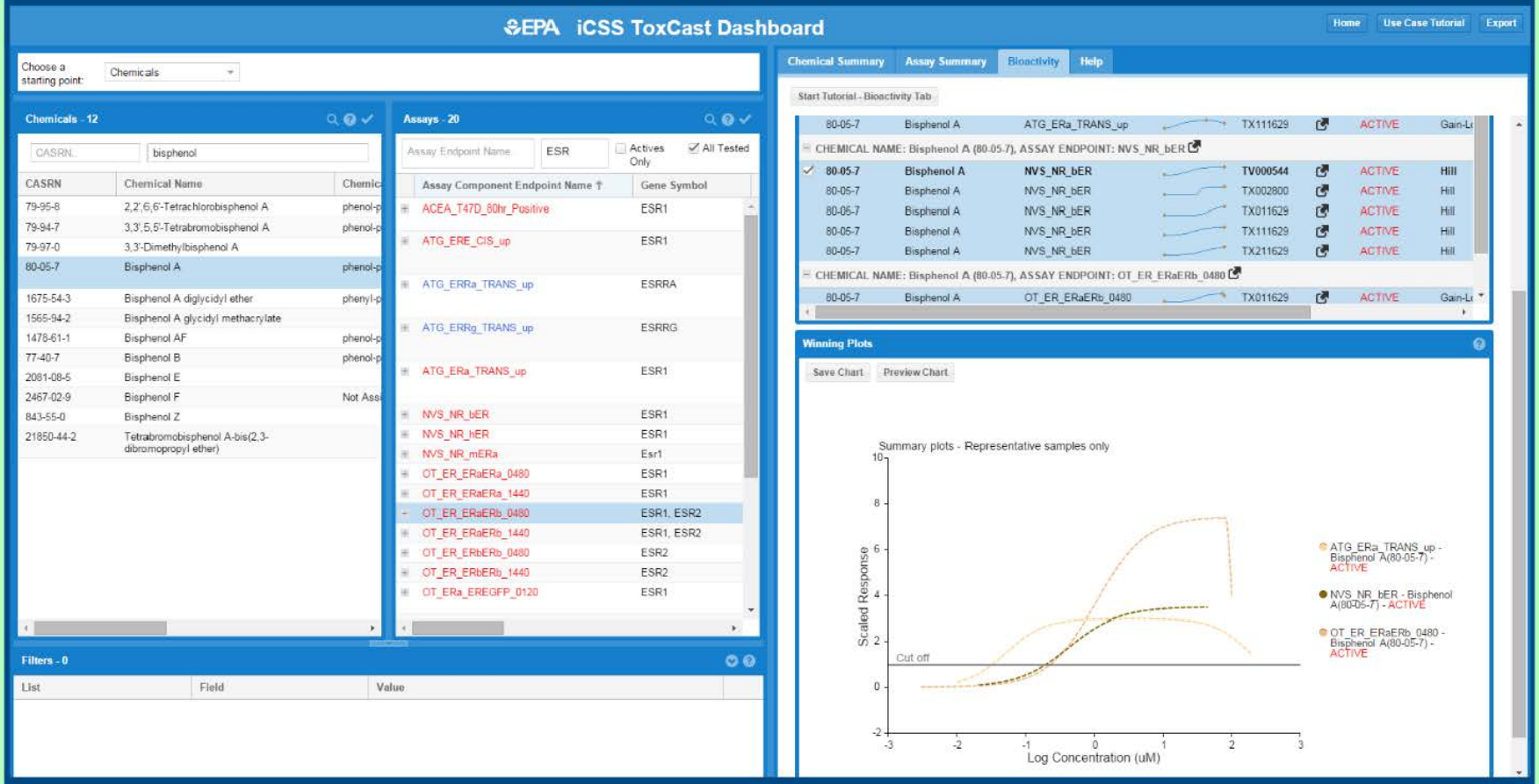
Impact: Tutorial Video Increased ToxCast Data Usage

Measuring impact of Video

Further impact of stakeholder feedback

Prezi

New Dashboard incorporates stakeholder feedback



Second tutorial video addresses stakeholder questions on CompTox tools

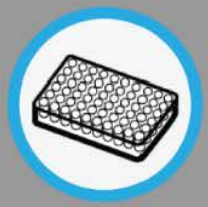
EPA's Computational Toxicology Tools

DSSTox Database

A resource for high quality chemical structures and chemical annotation in association with toxicity data

ToxCast and Tox21 chemical information management and cheminformatics foundation platform

www.epa.gov/ncct/dsstox



ToxCast Data Download

Download high-throughput data on all ToxCast chemicals, assays, genes, pathways, and endpoints

Data on over 1,800 chemicals and 500 assays

www.epa.gov/ncct/toxcast/data.html

CPCat Database

Contains data that maps over 43,000 chemicals to a set of terms categorizing their usage or function

User can search for chemicals by chemical name, CASRN, or CPCat terms (i.e. category names) associated with chemicals

actor.epa.gov/cpcat

ACToR Database

Warehouse of all publicly available chemical toxicity data

Aggregates data from over 1,000 public sources on over 500,000 environmental chemicals

Searchable by chemical name, structure and other identifiers

www.actor.epa.gov/actor

iCSS Dashboard

An easy to use interface that facilitates the navigation through millions of in-vitro data points included in the ToxCast data

User can export the subset of data of interest

actor.epa.gov/dashboard

Exposure Database

Consolidates observational human exposure data

Links to health related data, and also to ACToR data like: toxicity data, environmental fate data, and chemical manufacture information

actor.epa.gov/actor/faces/ExpoCastDB/Home.jsp

EDSP21 Dashboard

Explore data on over 1,800 chemicals that were tested in 11 androgen, 18 estrogen, and 4 thyroid assays

Integrates data from: DSSTox, ACToR, CPCat, ToxCast, and high-throughput exposure information

actor.epa.gov/edsp21

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Future Directions

iCSS Dashboard and Data are constantly evolving

- Improvement of data analysis
- Addition of chemicals/assays

New dashboard to be released this summer

- Addition of functionality
- Built in tutorials, FAQs and Glossary
- Plans for feedback and training
  - Internal and external user testing
  - Demos, webinars, and workshops for training
  - Ideas?

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EPA iCSS ToxCast Dashboard

Chemical Summary | Assay Summary | Bioactivity | Help

Glossary

Commonly used Abbreviations

Assay & Bioactivity descriptors

- AC50: chemical concentration (in uM) where 50% of the maximum response is achieved
- ACEA: assay vendor ACEA
- APR: assay vendor Apredica
- ATG: assay vendor Attagene
- BSK: assay vendor Bioseek
- Burst assay: set of assays used to estimate Cytotox limit per chemical
- CR: concentration-response
- CYP: cytochrome P450 enzymes
- Cytotox limit: estimate of concentration at which significant cytotoxicity occurs
- GPCR: G-protein coupled receptors
- Intended target family: biological grouping of assays (e.g., GPCR, Nuclear Receptor)
- Fold change: factor by which the chemical-mediated response differs from control
- NVS: assay vendor NovaScreen
- OT: assay vendor Odyssey Thera
- Representative sample: the sample chosen from replicates based on majority activity call and the minimum AC50.
- Top of curve (aka. Top): maximum response achieved by the modeled CR curve
- Tox21: assays run as part of the Tox21 collaboration
- Winning plots: Showing only the CR curve for the representative sample

Chemical descriptors

FAQ

What is can the iCSS ToxCast Dashboard be used for ?

The ToxCast Dashboard- for targeted users to **facilitate data distribution** and use of chemical screening data from the Toxicity Forecaster (ToxCast) project and the f

- Target user: industry, academia, researchers, state and federal agencies, NGO's, etc
- F a interactive tool to facilitate data exploration and visualization
- Functionality to export a subset of the user's data of interest

Future Directions

	Outline of Planned Videos	Release Date
1	iCSS Dashboard: Example Using iCSS Dashboard	Released 9/14
2	Overview of CompTox Tools	Expected Release 6/15
3	Data Download Page: Description of Files and Accessing Data	Expected Release 8/15
4	EDSP21 Dashboard	Expected Release 10/15
5	Detailed ToxCast Assay Data and Information	2016
6	Animal Toxicity Studies File	2016
7	Chemical List and Annotation Files	2016

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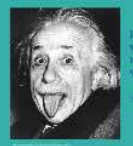
Collaborative effort, which would be impossible without...

The US EPA's National Center for Computational Toxicology

Mentors
Monica Linnenbrink, EPA
John Cowden, EPA
Kevin Crofton, EPA
Rusty Thomas, EPA
Tina Bahadori, EPA

Fellows and Post-Docs
Agnes Karmaus, ORISE
Jill Franzosa, ORISE
Sean Watford, SSC
Kamel Mansouri



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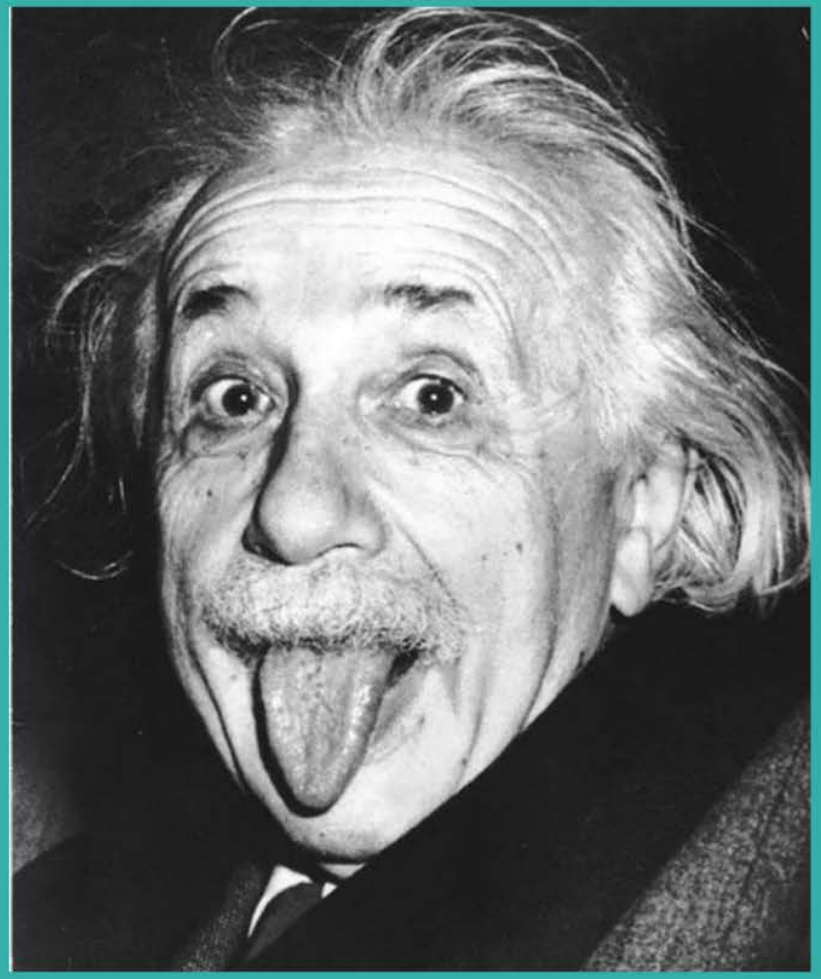

Photo courtesy of mentalfloss.com

If we knew what it was we were doing, it would not be called research, would it?

-Albert Einstein

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Tutorial Series.

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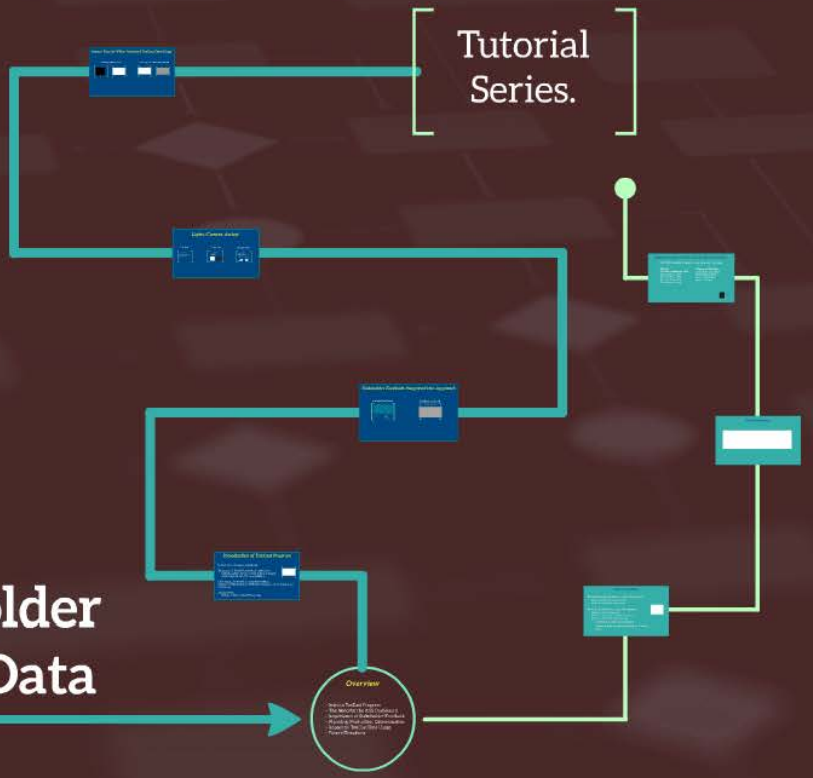
Tutorial Video Series: Using Stakeholder Feedback Increased Use of ToxCast Data



Christina Baghdikian
ASPPH Fellow
US EPA
SETAC EU, May 2015

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