EPA
United States
Environmental Protection
Agency

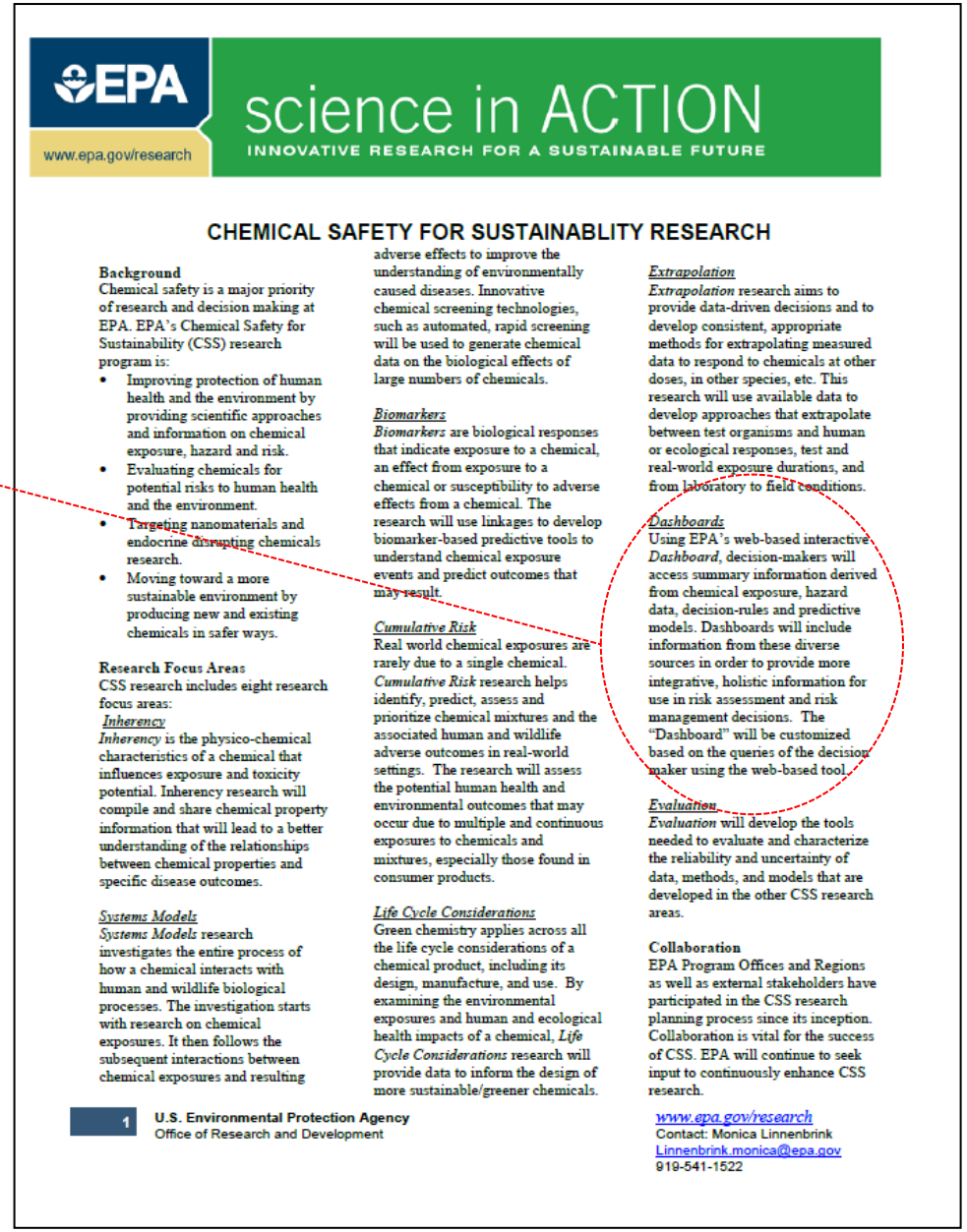
CSS DASHBOARD

United States Environmental Protection Agency

Dashboards

Using EPA's web-based interactive Dashboard, decision-makers will access summary information derived from chemical exposure, hazard data, decision-rules and predictive models. Dashboards will include information from these diverse sources in order to provide more integrative, holistic information for use in risk assessment and risk management decisions. The "Dashboard" will be customized based on the queries of the decision maker using the web-based tool.

More information available at:
http://css.epa.gov/



EPA science in ACTION
www.epa.gov/research
INNOVATIVE RESEARCH FOR A SUSTAINABLE FUTURE

CHEMICAL SAFETY FOR SUSTAINABLITY RESEARCH

Background
Chemical safety is a major priority of research and decision making at EPA. EPA's Chemical Safety for Sustainability (CSS) research program is:

- Improving protection of human health and the environment by providing scientific approaches and information on chemical exposure, hazard and risk.
- Evaluating chemicals for potential risks to human health and the environment.
- Targeting nanomaterials and endocrine disrupting chemicals research.
- Moving toward a more sustainable environment by producing new and existing chemicals in safer ways.

Research Focus Areas
CSS research includes eight research focus areas:

Inherency
Inherency is the physico-chemical characteristics of a chemical that influences exposure and toxicity potential. Inherency research will compile and share chemical property information that will lead to a better understanding of the relationships between chemical properties and specific disease outcomes.

Systems Models
Systems Models research investigates the entire process of how a chemical interacts with human and wildlife biological processes. The investigation starts with research on chemical exposures. It then follows the subsequent interactions between chemical exposures and resulting adverse effects to improve the understanding of environmentally caused diseases. Innovative chemical screening technologies, such as automated, rapid screening will be used to generate chemical data on the biological effects of large numbers of chemicals.

Biomarkers
Biomarkers are biological responses that indicate exposure to a chemical, an effect from exposure to a chemical or susceptibility to adverse effects from a chemical. The research will use linkages to develop biomarker-based predictive tools to understand chemical exposure events and predict outcomes that may result.

Cumulative Risk
Real world chemical exposures are rarely due to a single chemical. *Cumulative Risk* research helps identify, predict, assess and prioritize chemical mixtures and the associated human and wildlife adverse outcomes in real-world settings. The research will assess the potential human health and environmental outcomes that may occur due to multiple and continuous exposures to chemicals and mixtures, especially those found in consumer products.

Life Cycle Considerations
Green chemistry applies across all the life cycle considerations of a chemical product, including its design, manufacture, and use. By examining the environmental exposures and human and ecological health impacts of a chemical, *Life Cycle Considerations* research will provide data to inform the design of more sustainable/greener chemicals.

Extrapolation
Extrapolation research aims to provide data-driven decisions and to develop consistent, appropriate methods for extrapolating measured data to respond to chemicals at other doses, in other species, etc. This research will use available data to develop approaches that extrapolate between test organisms and human or ecological responses, test and real-world exposure durations, and from laboratory to field conditions.

Dashboards
Using EPA's web-based interactive *Dashboard*, decision-makers will access summary information derived from chemical exposure, hazard data, decision-rules and predictive models. Dashboards will include information from these diverse sources in order to provide more integrative, holistic information for use in risk assessment and risk management decisions. The "Dashboard" will be customized based on the queries of the decision maker using the web-based tool.

Evaluation
Evaluation will develop the tools needed to evaluate and characterize the reliability and uncertainty of data, methods, and models that are developed in the other CSS research areas.

Collaboration
EPA Program Offices and Regions as well as external stakeholders have participated in the CSS research planning process since its inception. Collaboration is vital for the success of CSS. EPA will continue to seek input to continuously enhance CSS research.

1 U.S. Environmental Protection Agency
Office of Research and Development

www.epa.gov/research
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919-541-1522

Dashboards key concepts

- The purpose is to provide an interface that allows access to both ORD and PO research/tools and synthesis for integrated decision support

- User-driven design concepts
  - Transparent, retraceable, updatable, interactive, modular, flexible, secure

- Leveraging resources
  - Data: Integration of diverse databases that facilitates continued growth
  - Research: Access to computational tools and models
  - People: Smart design means that a focused team can have far-reaching effects
  - Communication: Distributed, shareable web interface (internal/external)

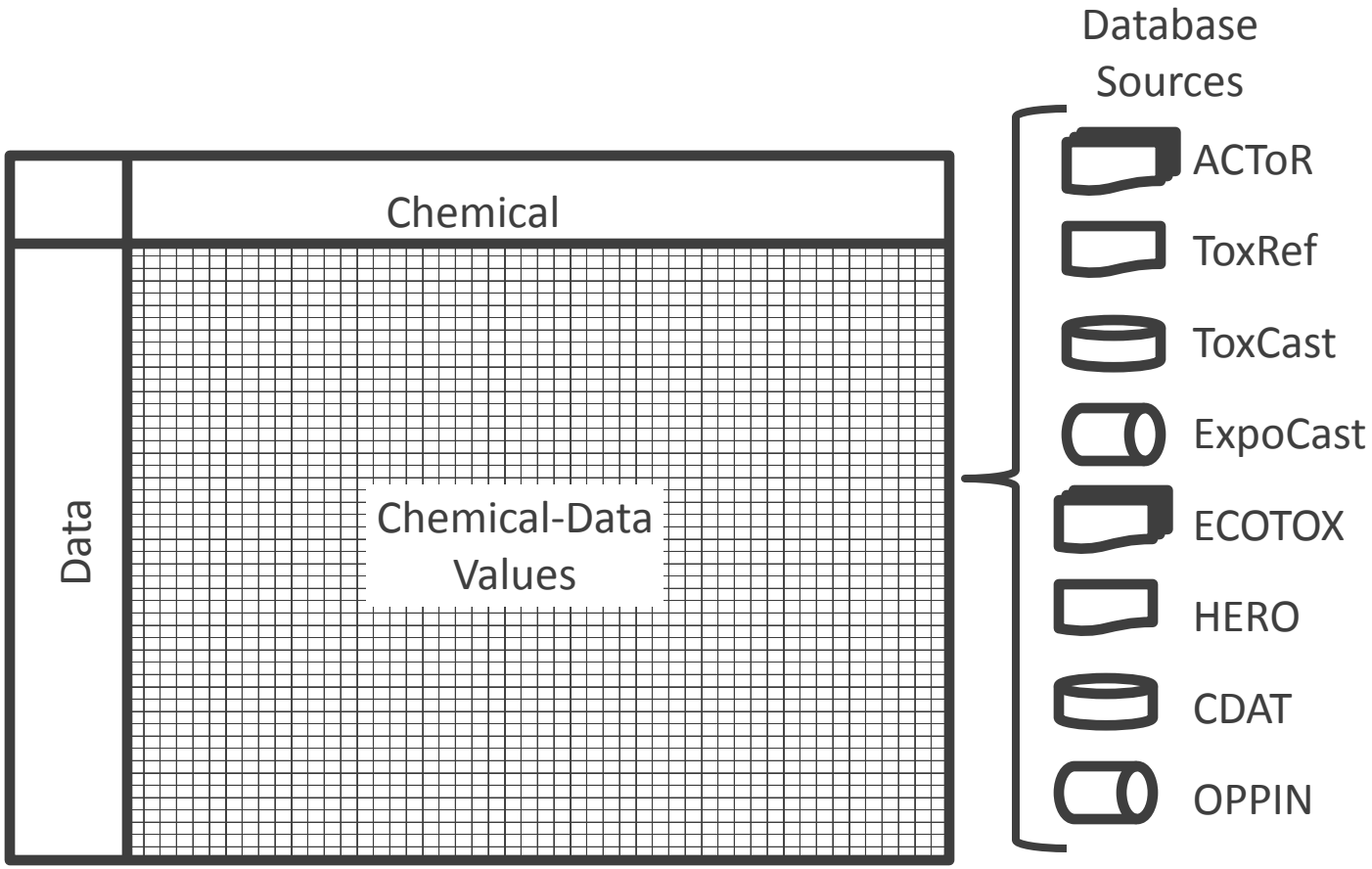
- Current Dashboard has 3 major interactive modes
  - Data Explorer: Selecting relevant data/models/chemicals
  - Chemical Explorer: Integrating evidence and scoring chemicals
  - Prioritization: Formalized, yet flexible, schemes for decision support

Near-term priorities & release schedule

- Near-term priorities:
  - Data Explorer: Provide interactivity to PO partners for “tagging” data
  - Chemical Explorer: Development and expansion of widget library
  - Prioritization: Development and expansion of widget library
  - Assure that development allows seamless transition to public-facing Dashboard
  - Explore incorporation of non-ORD data sources (e.g. PO databases)

- Release schedule for PO partners: OW21, EDSP21 & TSCA21 Dashboards
  - [Dec. 2012] Data source identification & Case study development
  - [March. 2013] PO-driven Data Explorer
    - Using Dashboard to further identify & evaluate data sources
    - Early beta testing of single Dashboard component (Data explorer)
    - Evaluation of case study success
  - [July 2012] Beta-testing of remaining Dashboard components
    Chemical explorer & Prioritization mode
  - [Sep. 2013] Internal/External (public) version of Dashboard released

pluto.epa.gov/dash/view/login.html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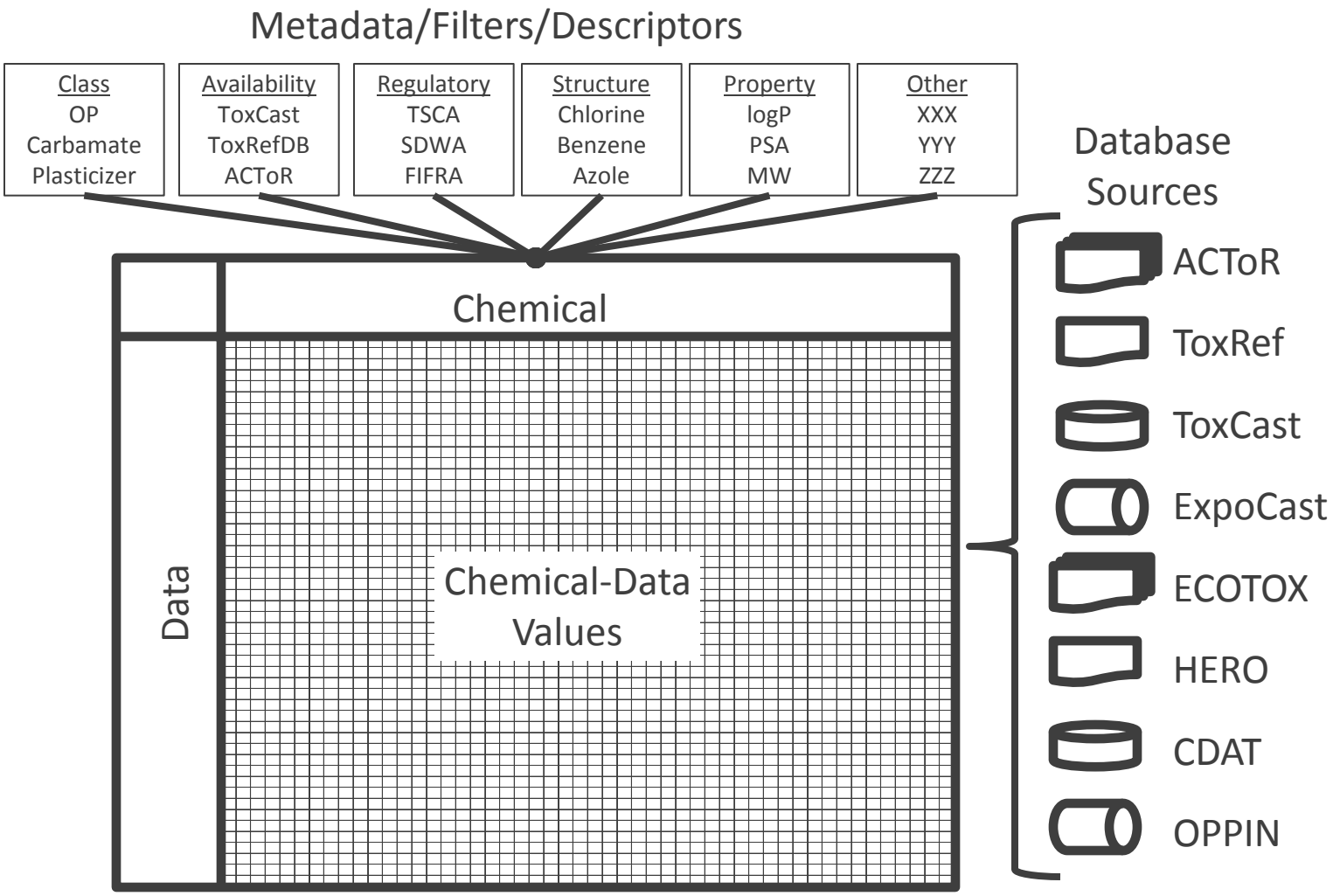
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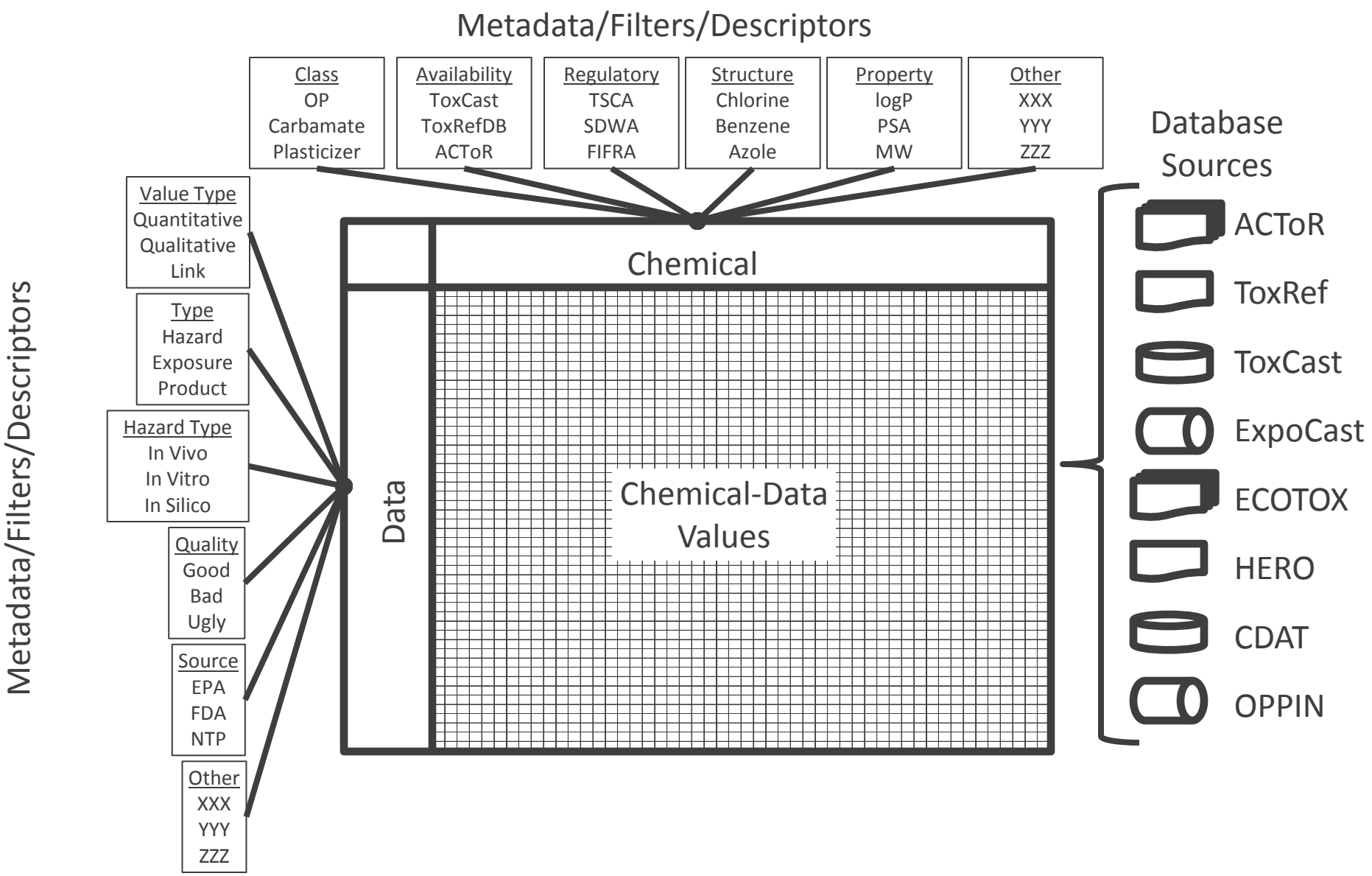
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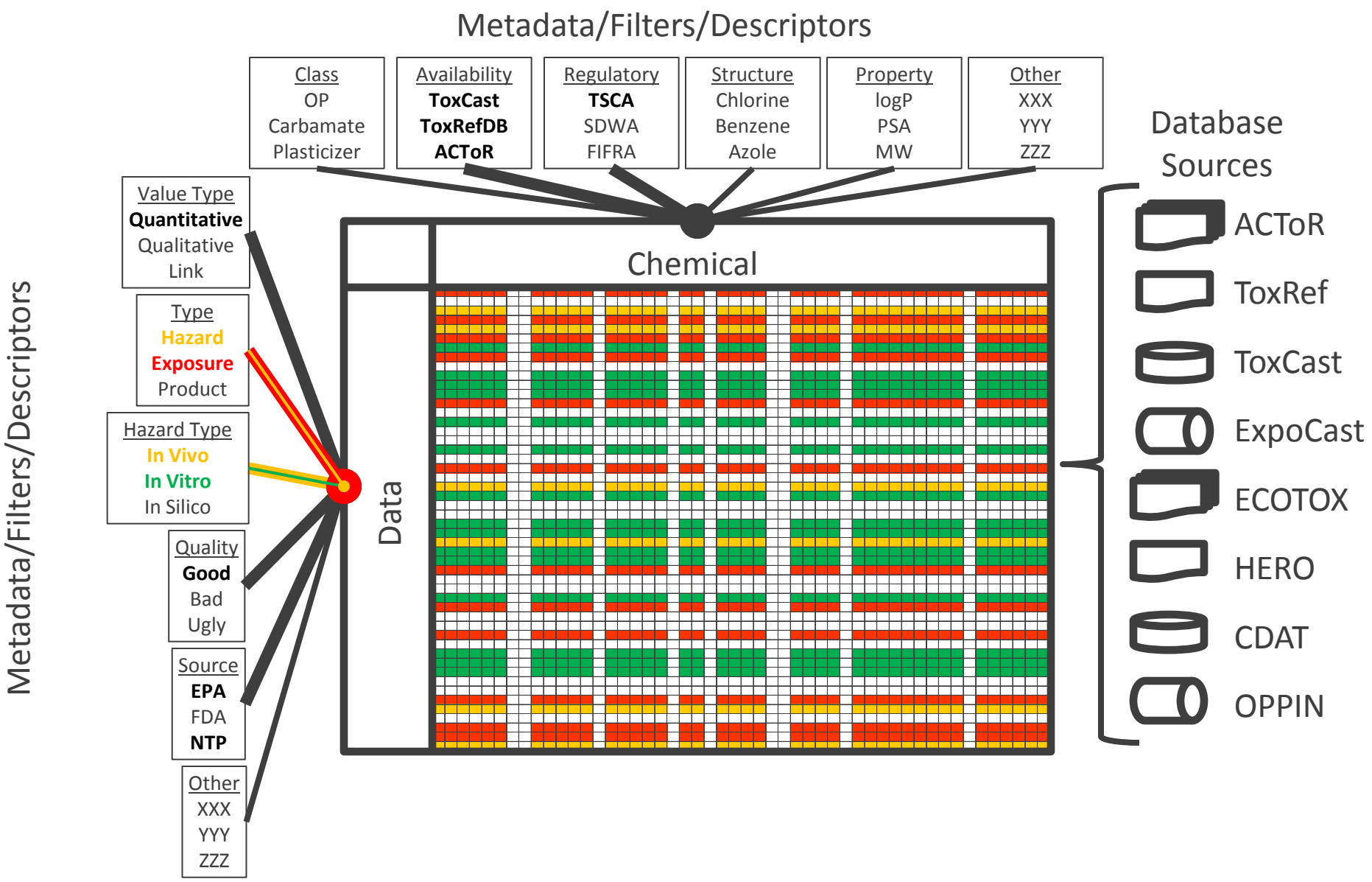
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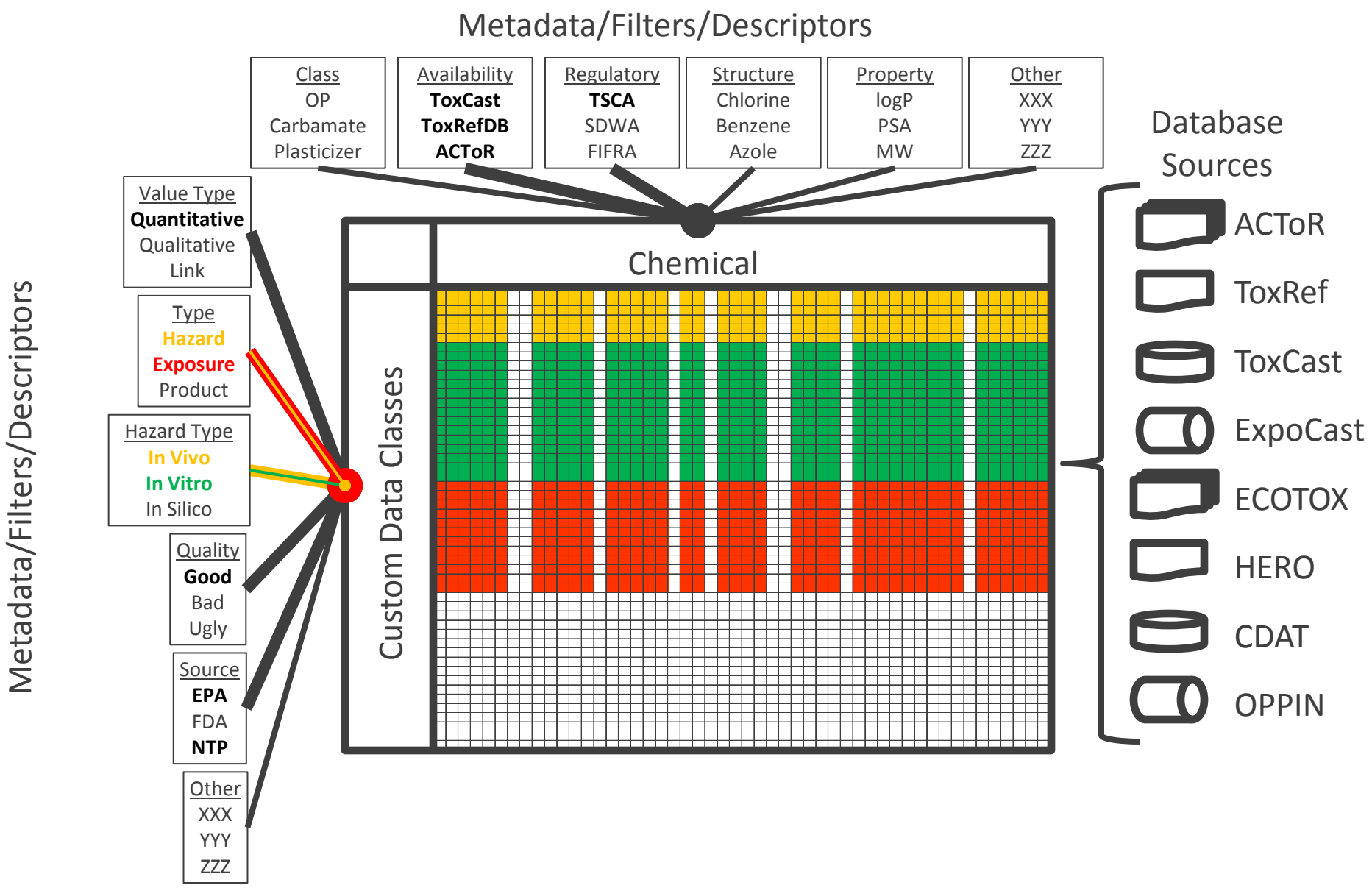
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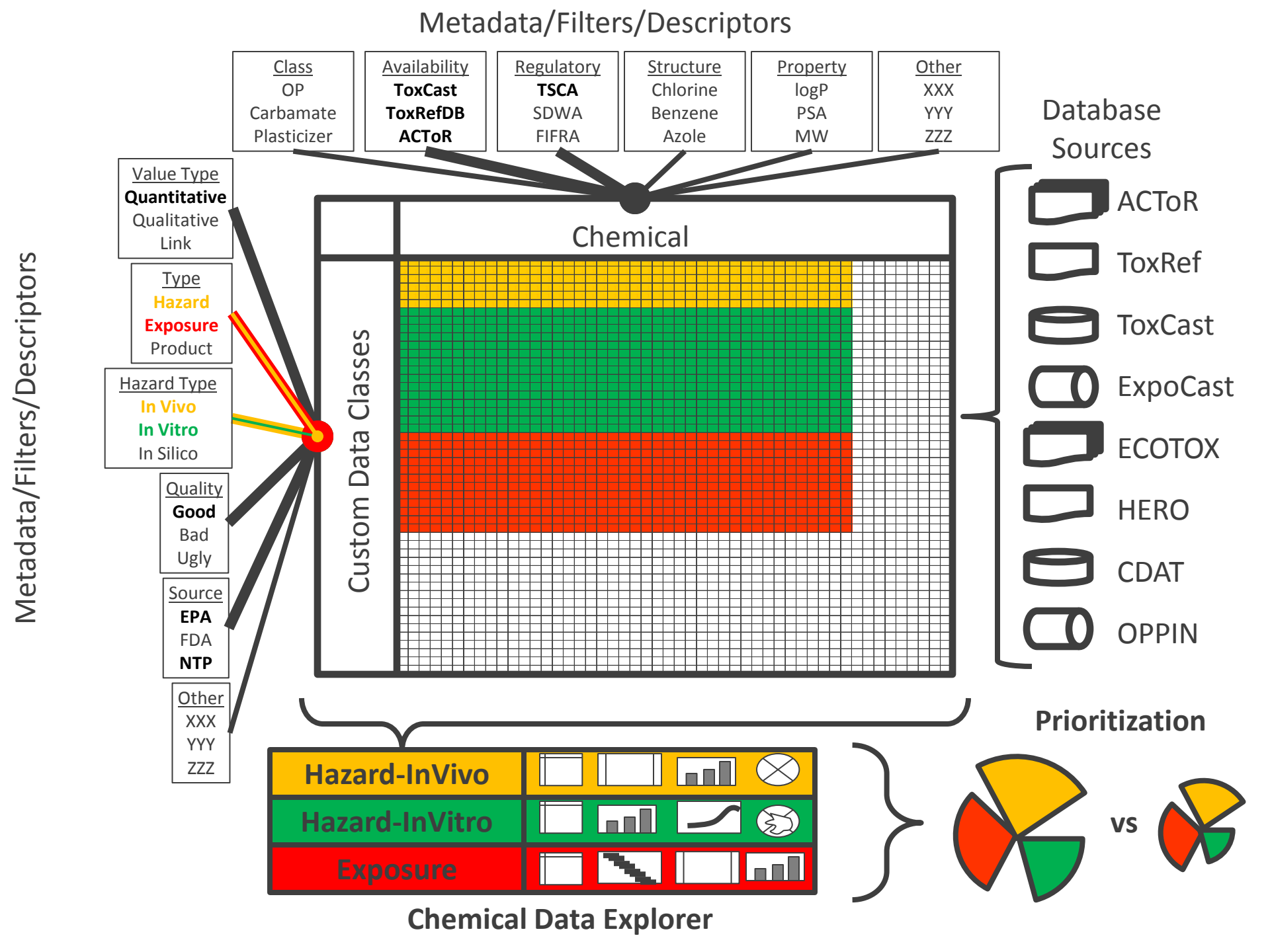
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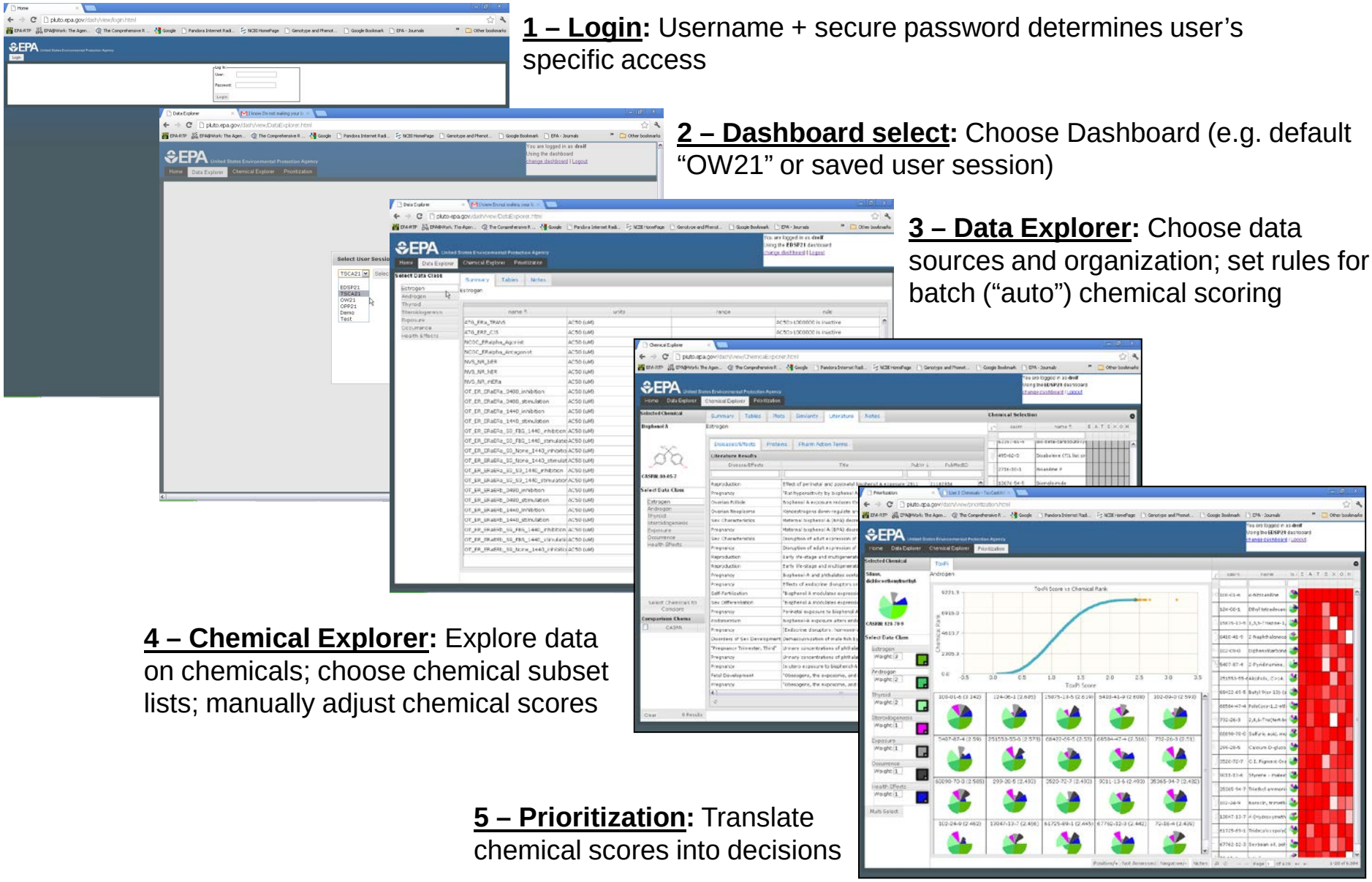
vs

Dashboards workflow:

Dynamic, Recordable, Reversible



1 – Login: Username + secure password determines user's specific access

2 – Dashboard select: Choose Dashboard (e.g. default "OW21" or saved user session)

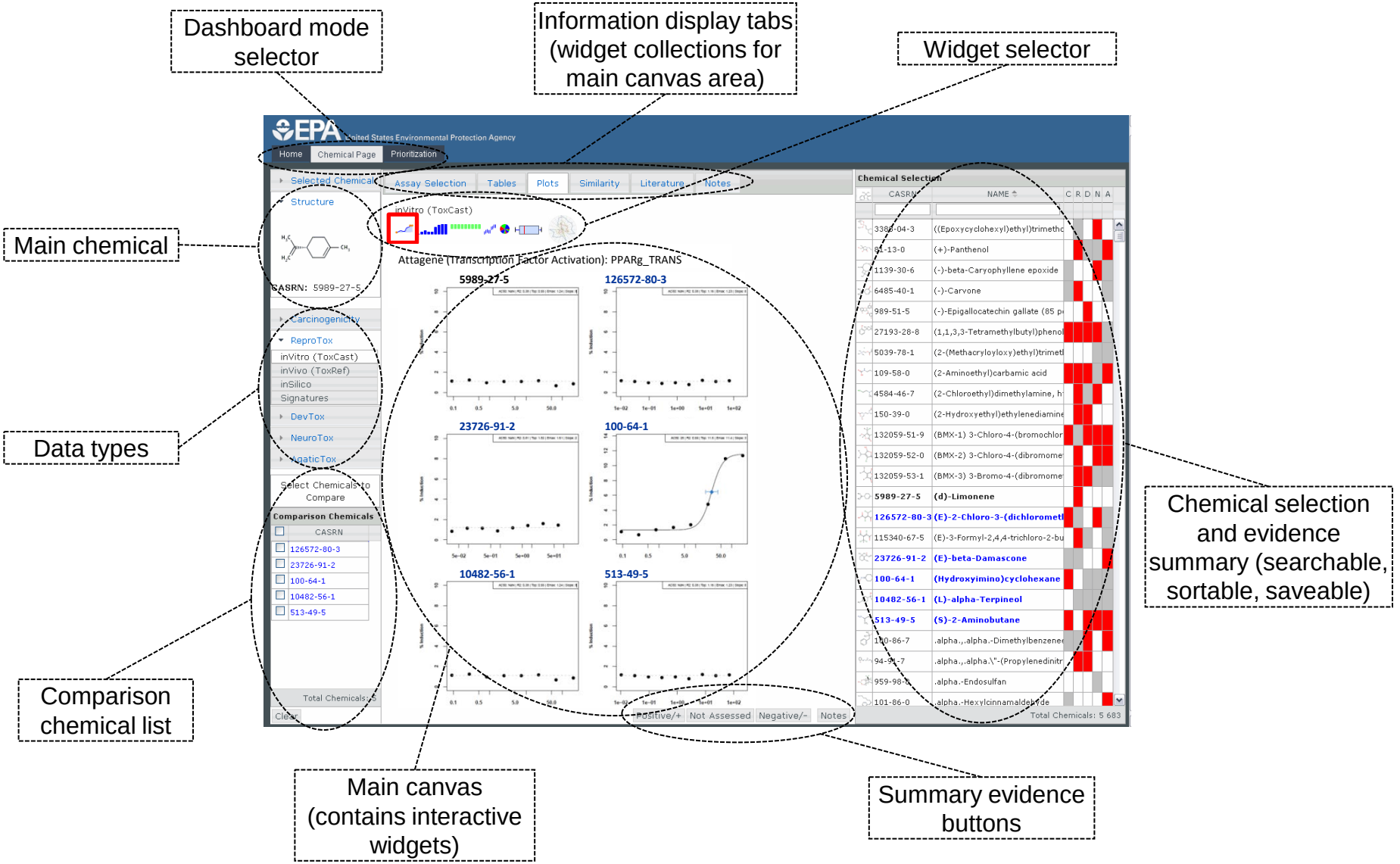
3 – Data Explorer: Choose data sources and organization; set rules for batch ("auto") chemical scoring

4 – Chemical Explorer: Explore data on chemicals; choose chemical subset lists; manually adjust chemical scores

5 – Prioritization: Translate chemical scores into decisions

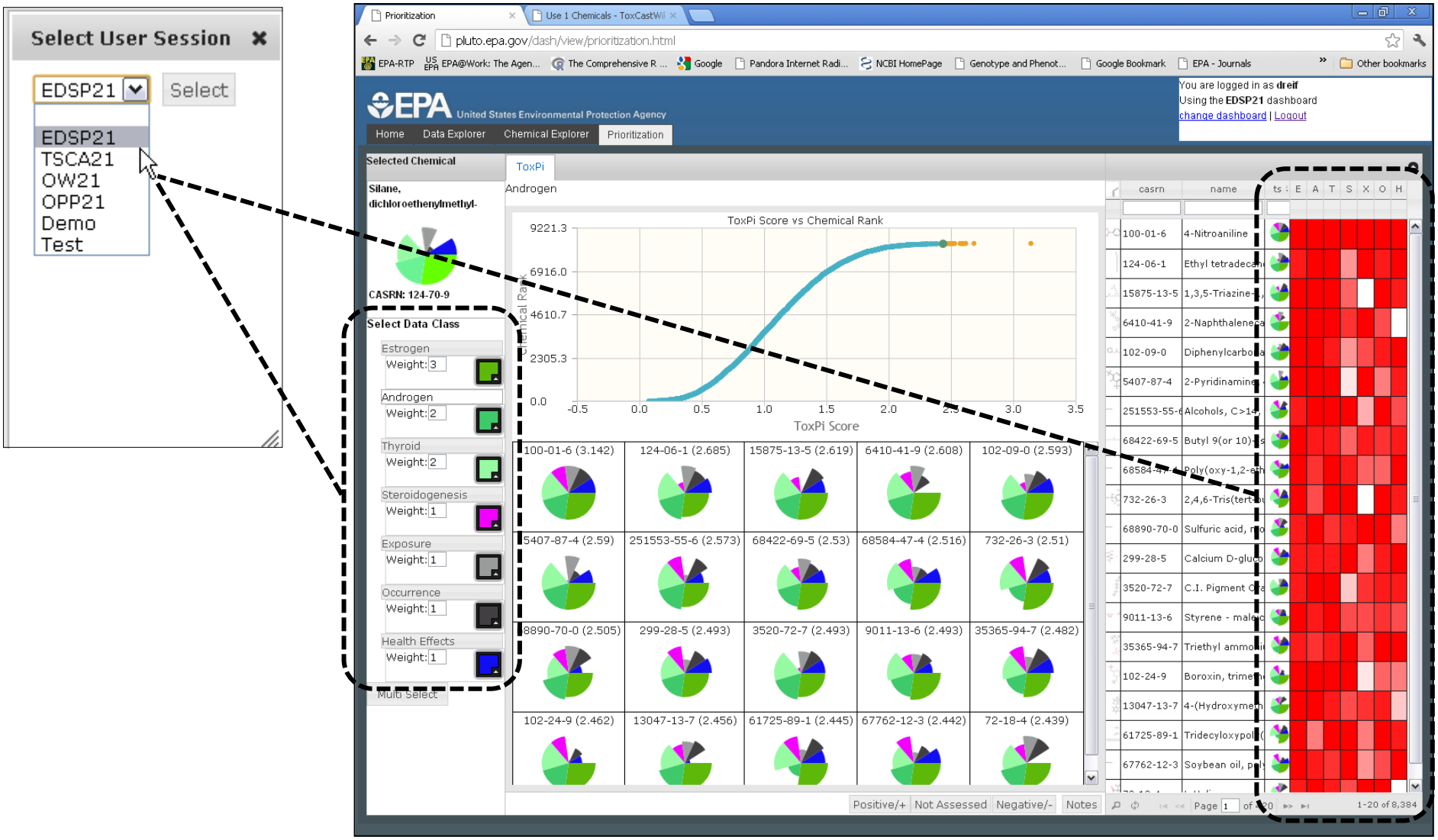
Dashboard components in the 'Chemical Explorer' mode

Modular design facilitates development: This includes new data types (e.g. ExpoCast), widget development (e.g. hazard banding or chemical profile read-across), alternate modes (e.g. HH Risk Assessment), evidence translation, etc.



Dashboard components in the 'Prioritization Mode': ToxPi widget

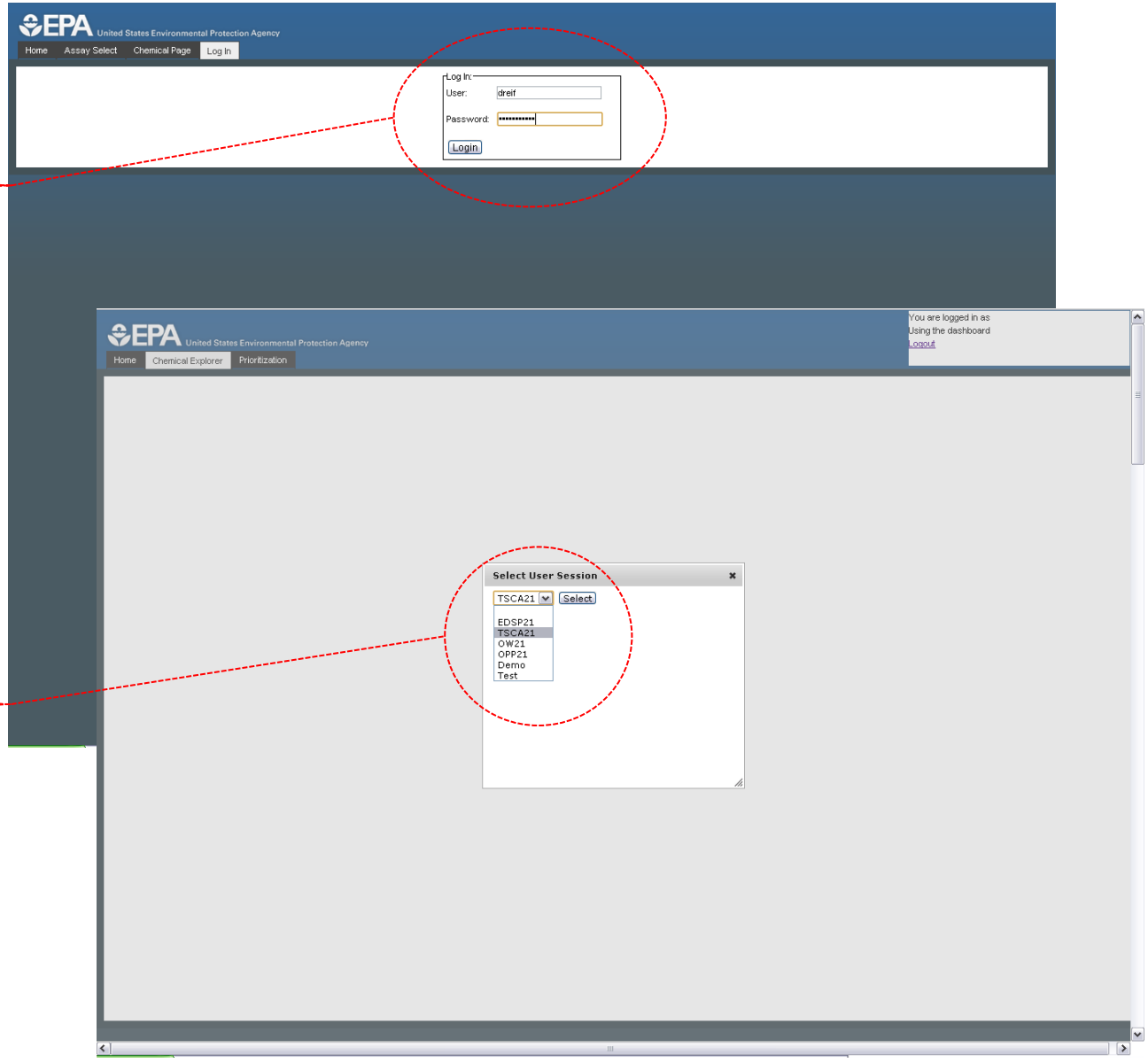
The organization of information is user-group specific (e.g. The Dashboard below has chemical information organized into endocrine-relevant data classes to support EDSP decisions)



Chemical Explorer mode: Exploring assay results *(Screenshot from prototype Dashboard)*

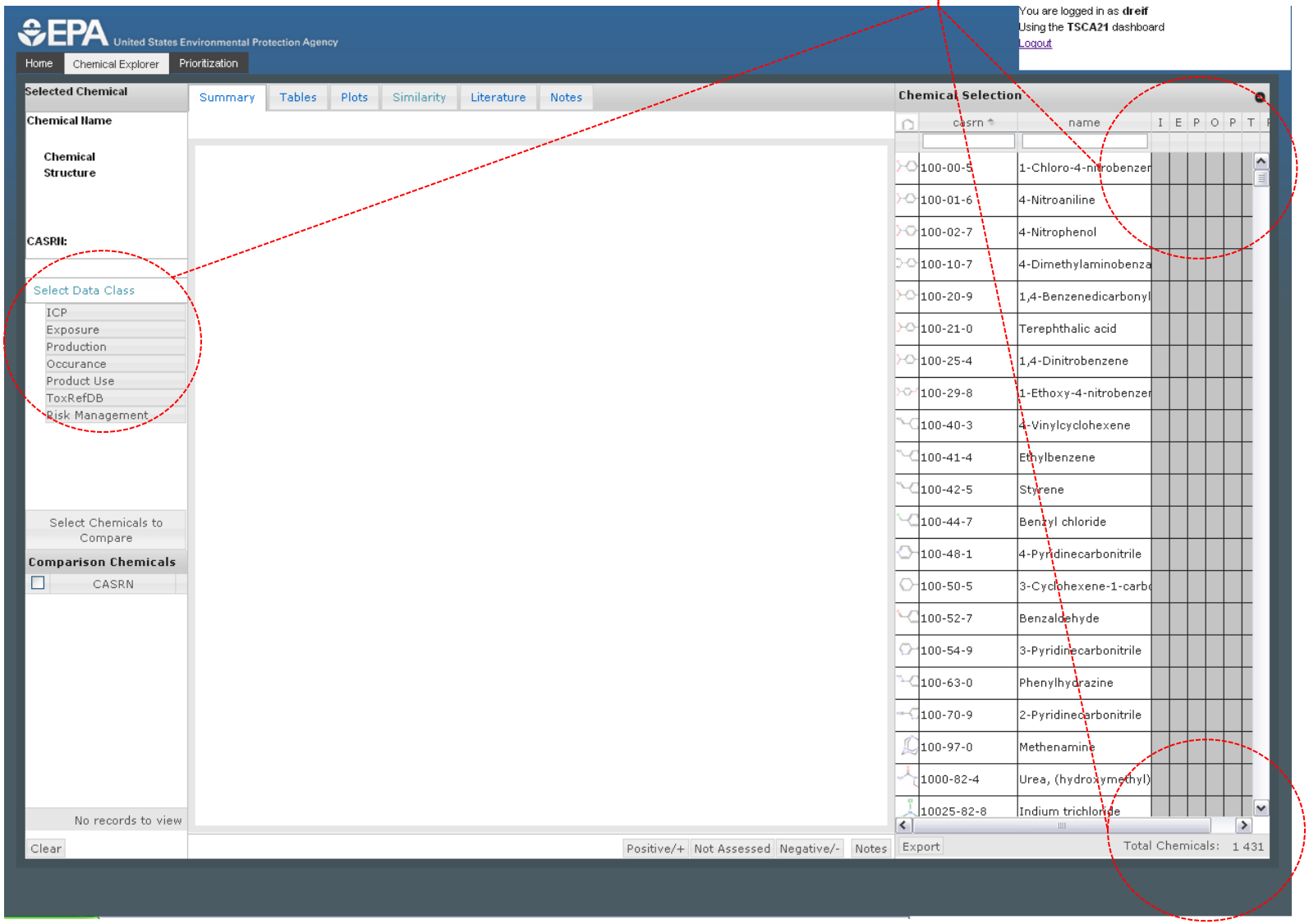
Users login to gain access to specific Dashboards. This allows control over protected information and setting of various roles (e.g. division manager, specific assessor) to facilitate oversight or sharing.

Login grants access to a menu of available Dashboards for that user.



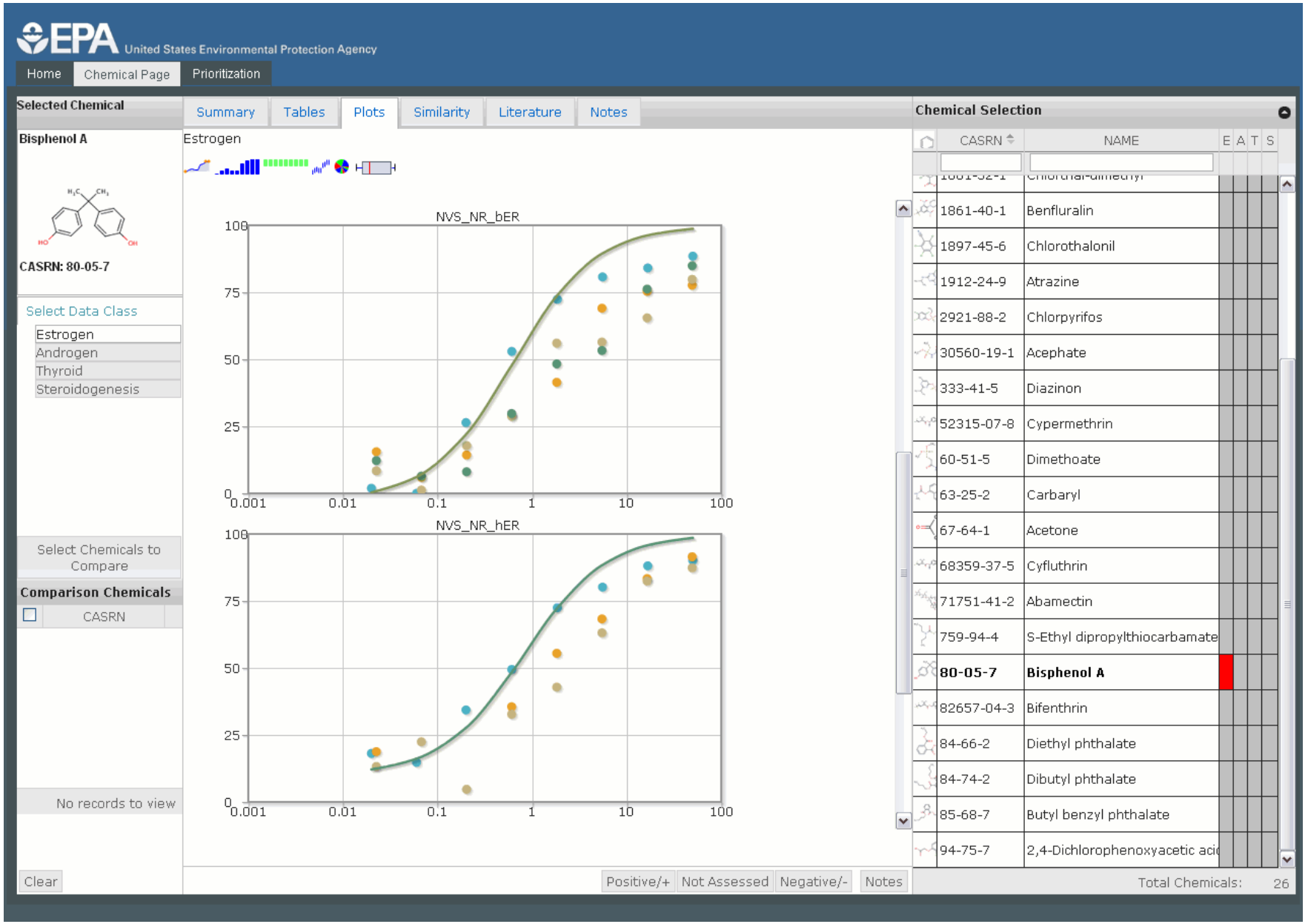
Chemical Explorer mode: Exploring assay results *(Screenshot from prototype Dashboard)*

The specific dashboard chosen affects the chemical set, organization of data classes, and defaults for the evidence table.



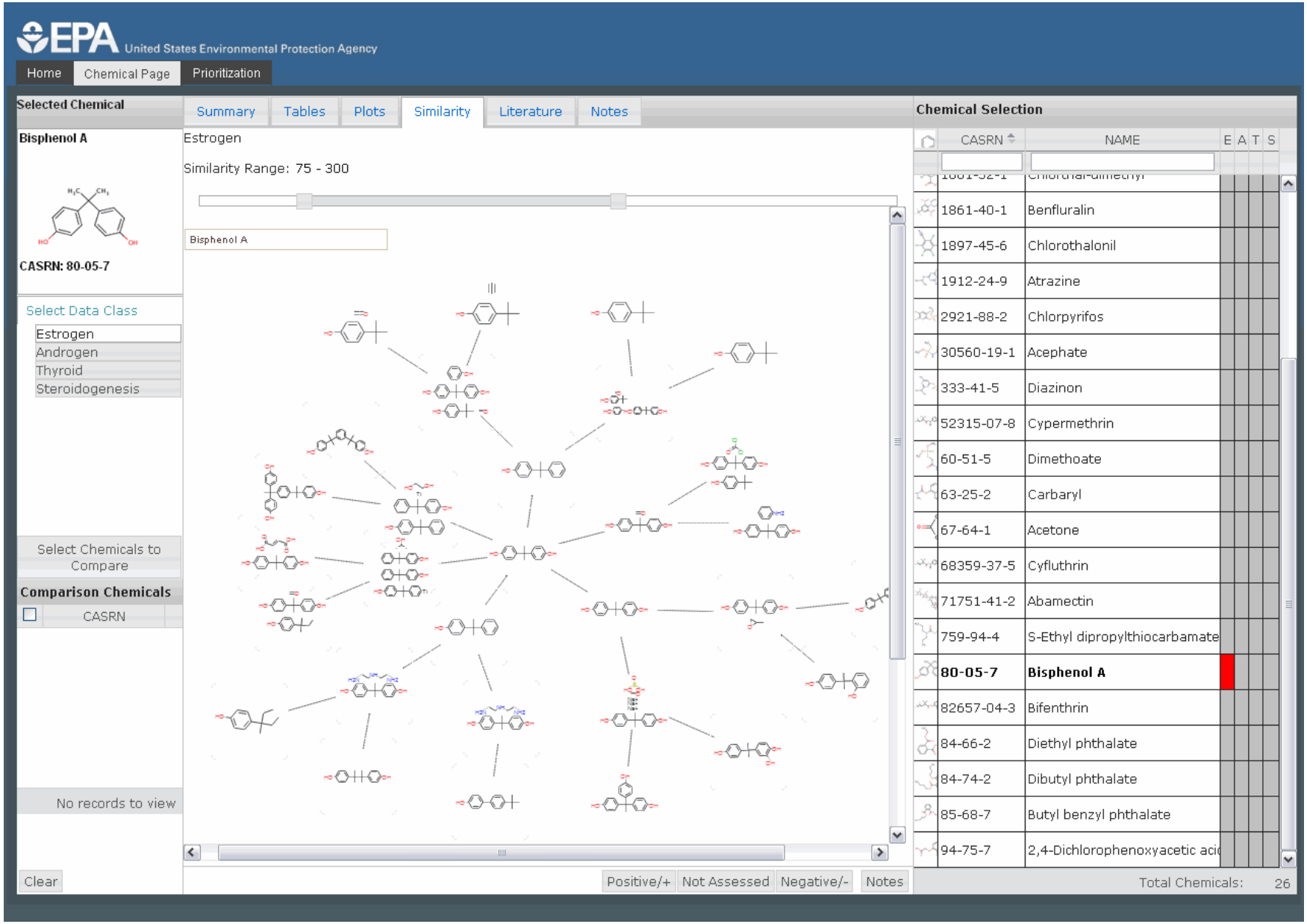
Chemical Explorer mode: Exploring assay results

(Screenshot from prototype EDSP Dashboard for a HTS assay probing Estrogen Receptor activity)



Chemical Explorer mode: Exploring structural similarity

(Screenshot from prototype EDSP Dashboard using a chemoinformatic model to find structurally similar chemicals)

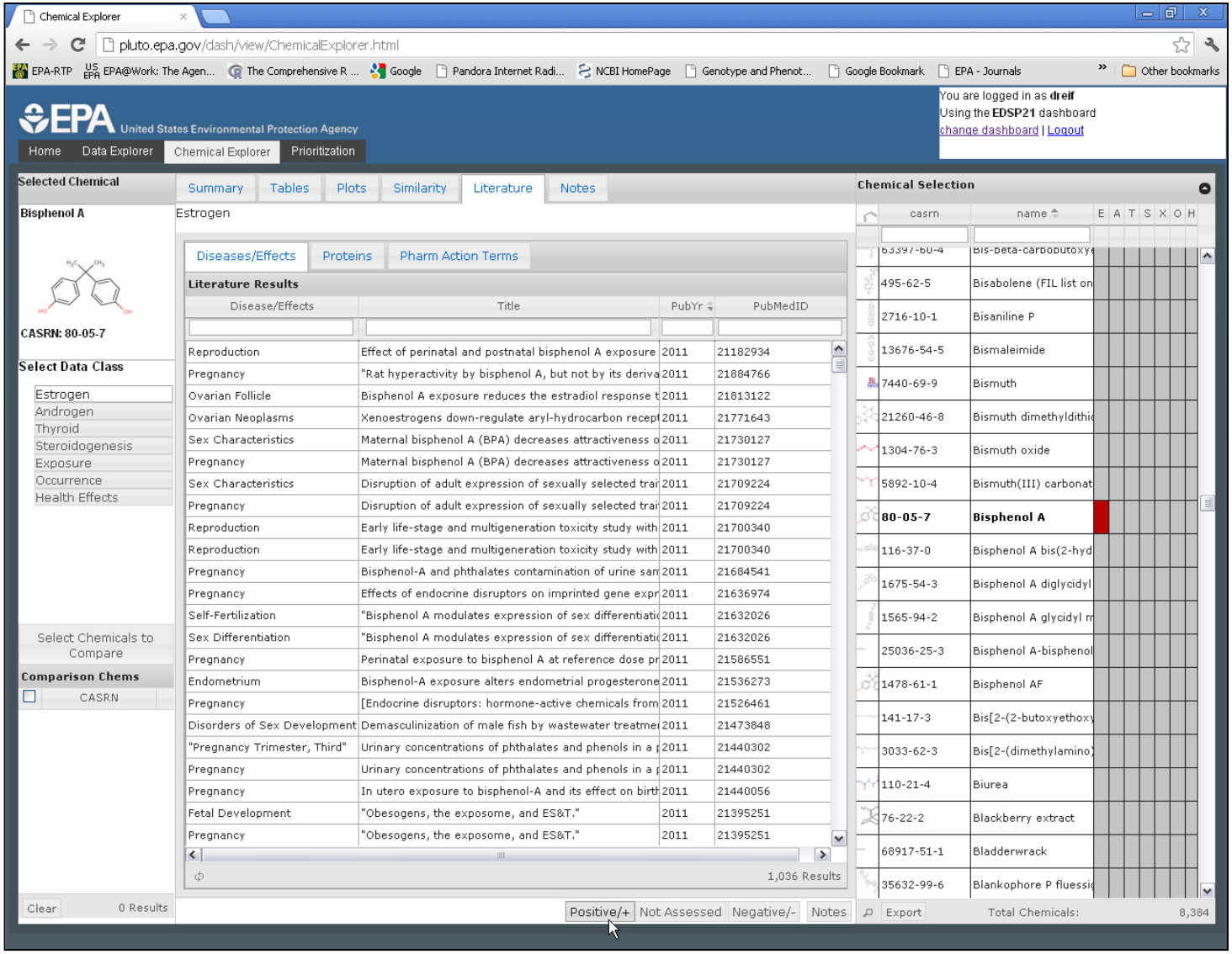


Integrating information into a web-enabled, interactive 'Dashboard': Literature mining

The Dashboard provides an interactive front-end for (re)organizing information from public databases and recording decisions

This interface was designed to integrate any number of information sources to let users make comprehensive decisions about chemicals

e.g. A user has assigned BPA as having positive evidence of estrogen-related effects in the table at right



Integrating information into a web-enabled, interactive 'Dashboard': ToxPi implementation

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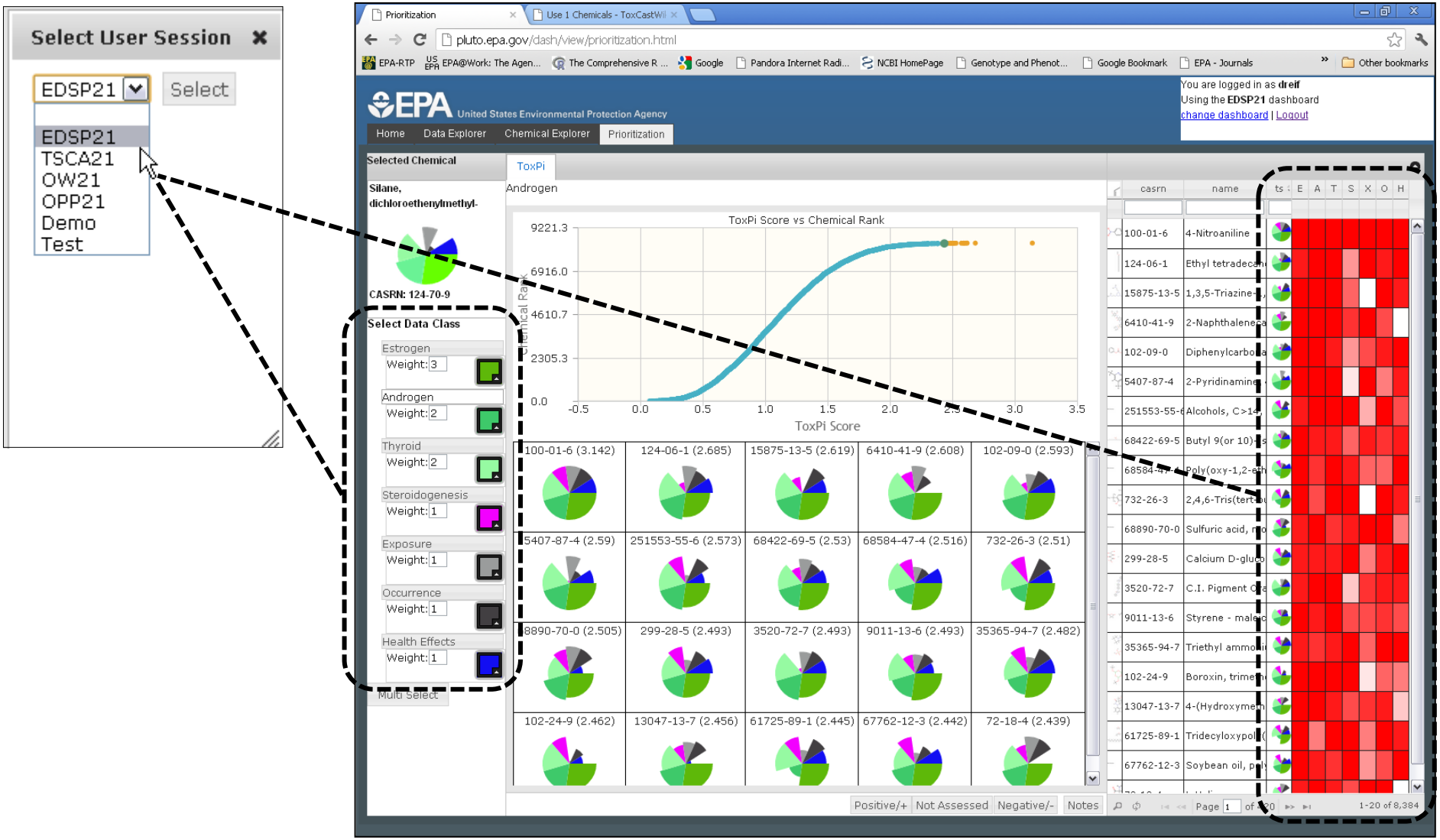
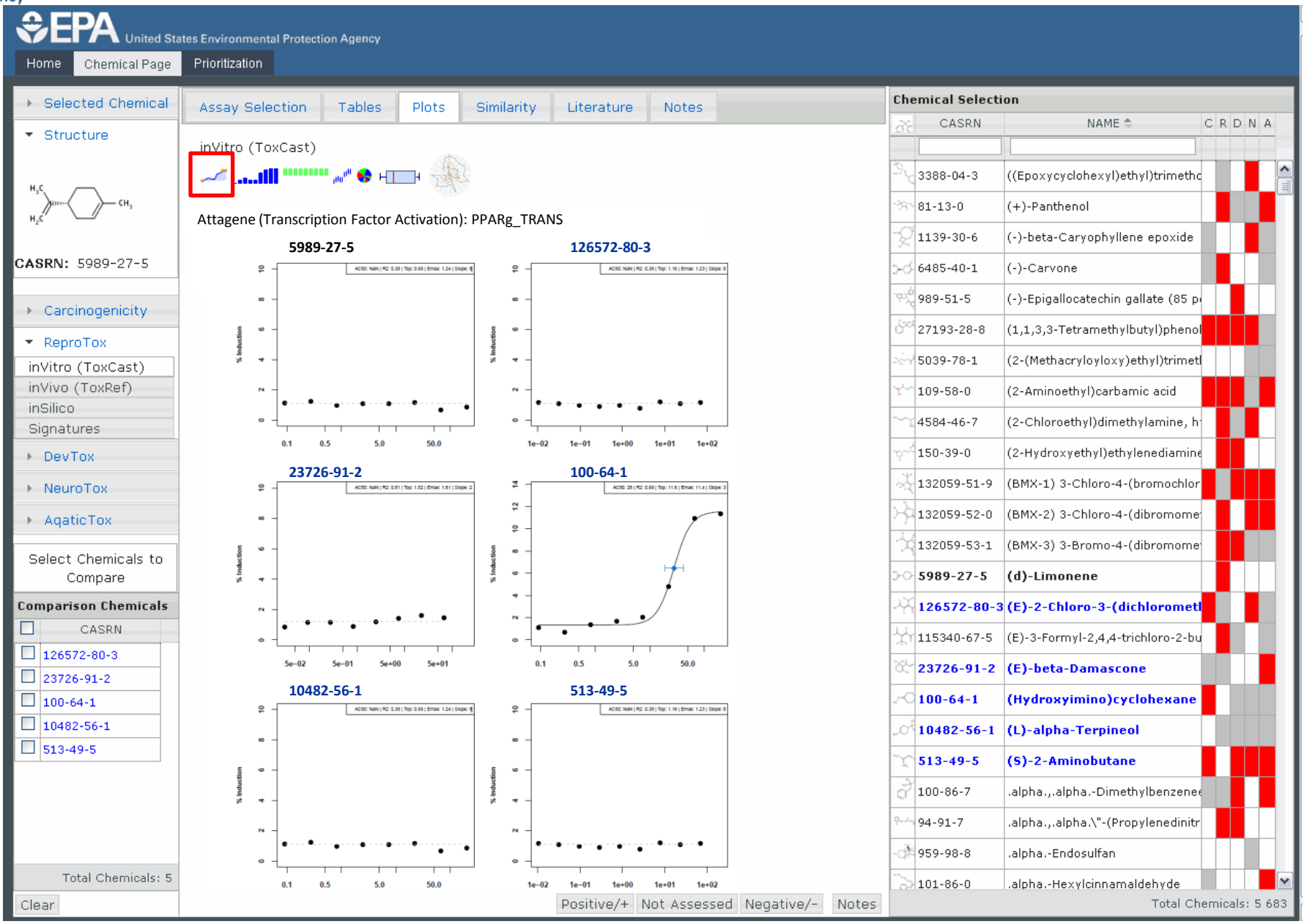


Dashboards provide interactive ways to explore and synthesize information (= “Translation”)

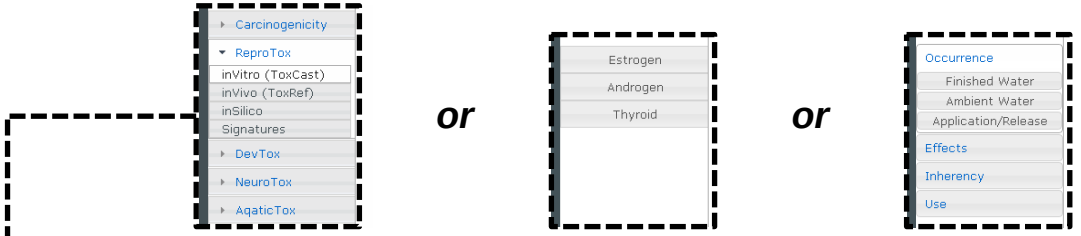


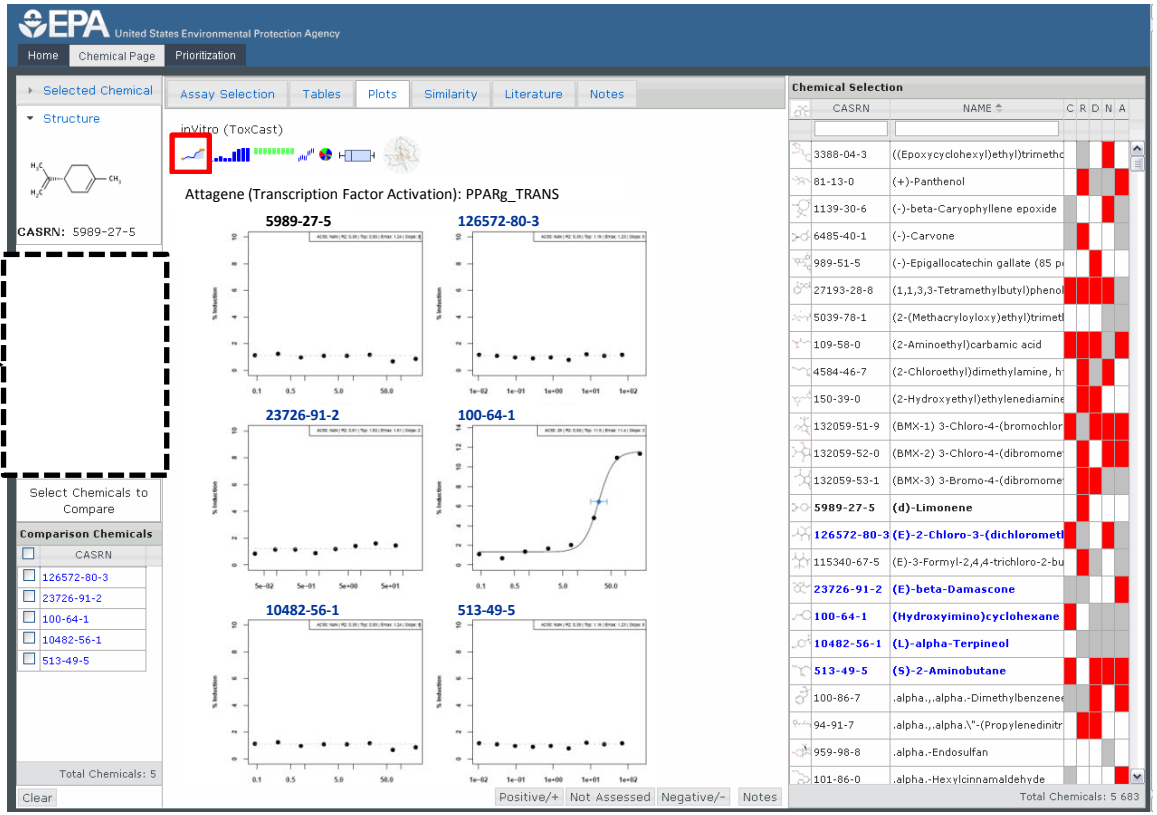
“Collaboration” means Dashboards are customized for particular needs

Leverage resources by repackaging the same data for custom uses

Components are modular, so the Dashboards infrastructure can be customized to translate data according to particular use cases

Single Source Database (e.g. ACToR)



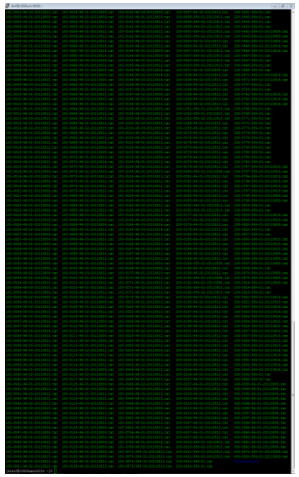


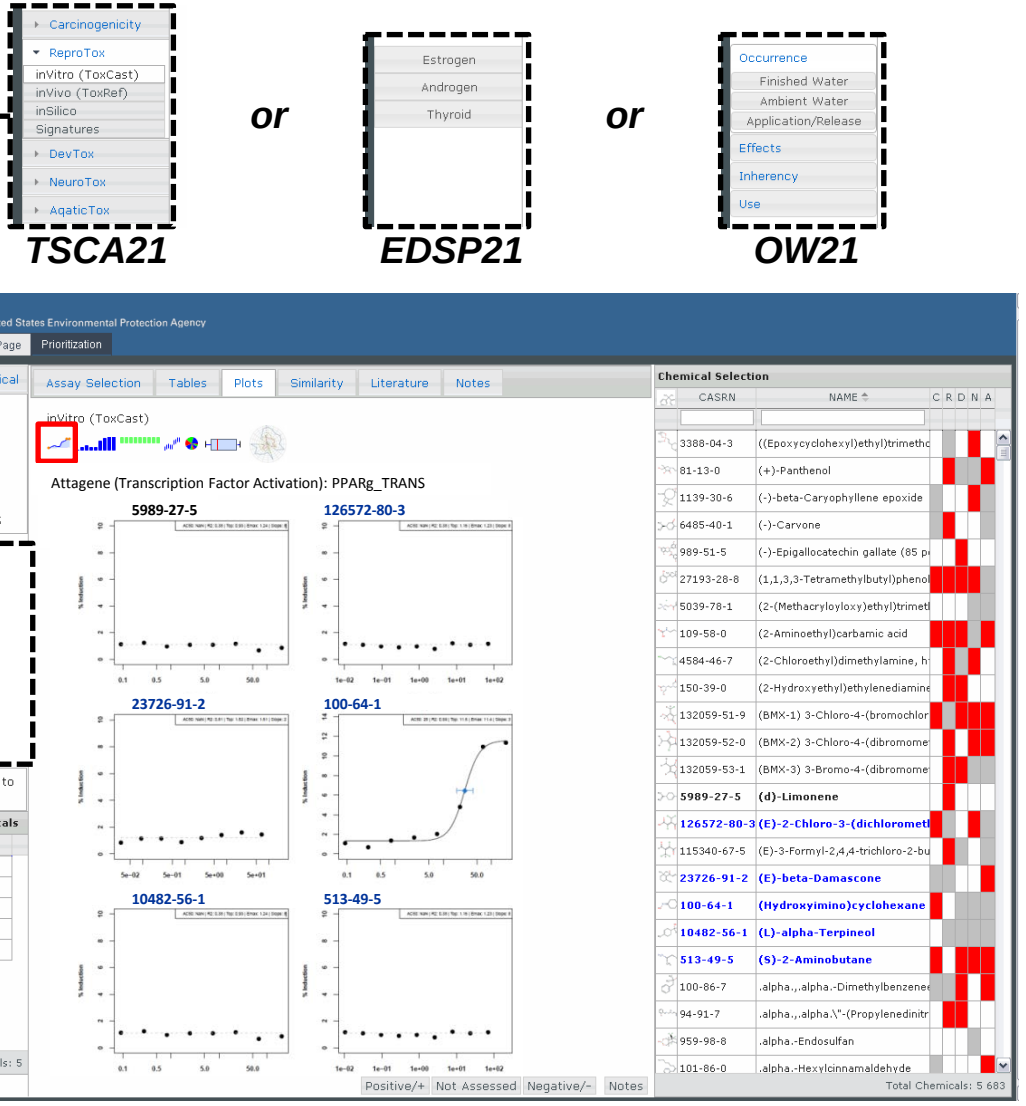
“Collaboration” means Dashboards are customized for particular needs

Specialized data may be needed for certain uses

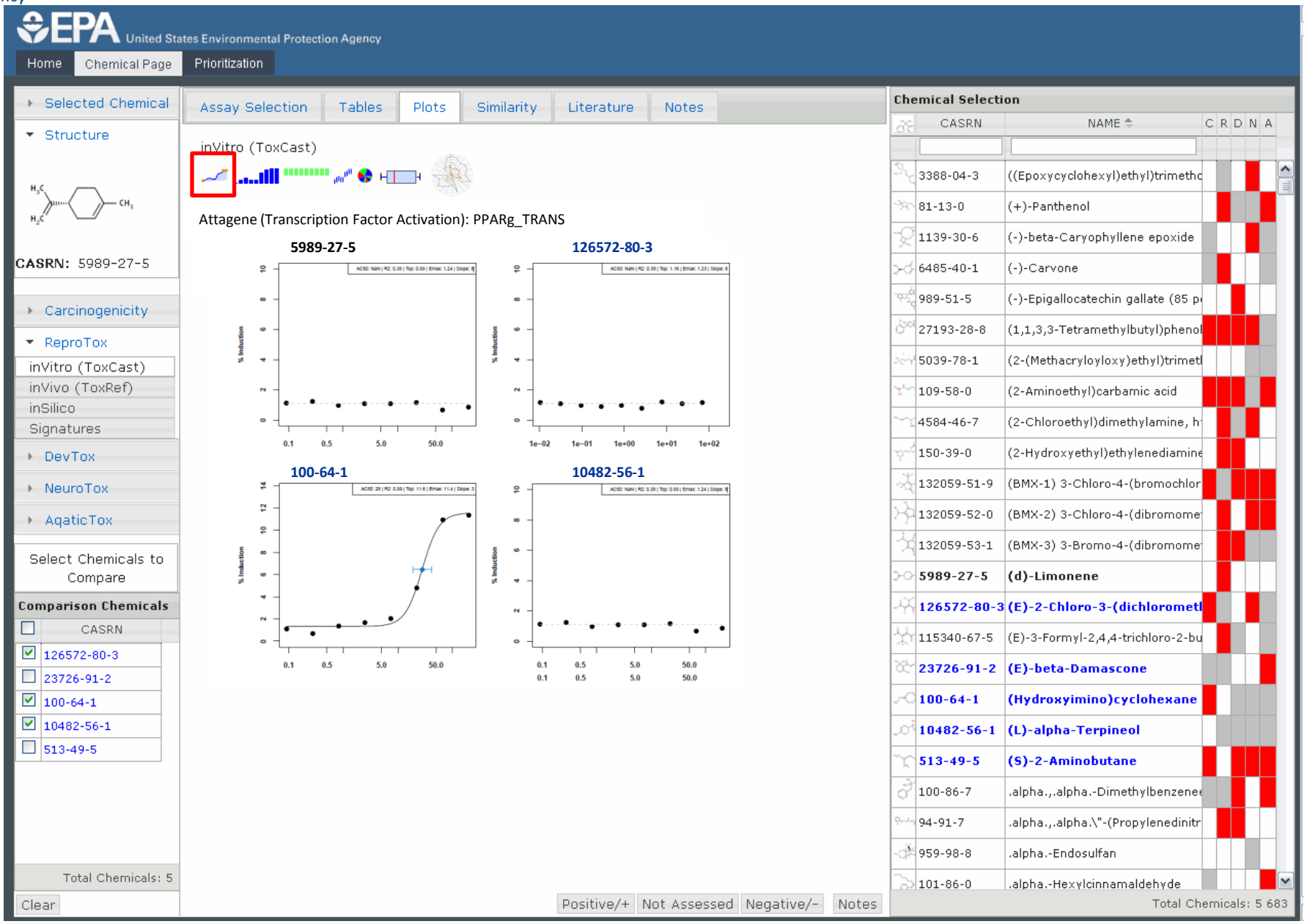
Components are modular, so the Dashboards infrastructure can be customized to translate data according to particular use cases

Multiple Source Databases (e.g. ACToR + PO-specific DB)





Dashboards provide interactive ways to explore and synthesize data (e.g. many chemicals by single data source)



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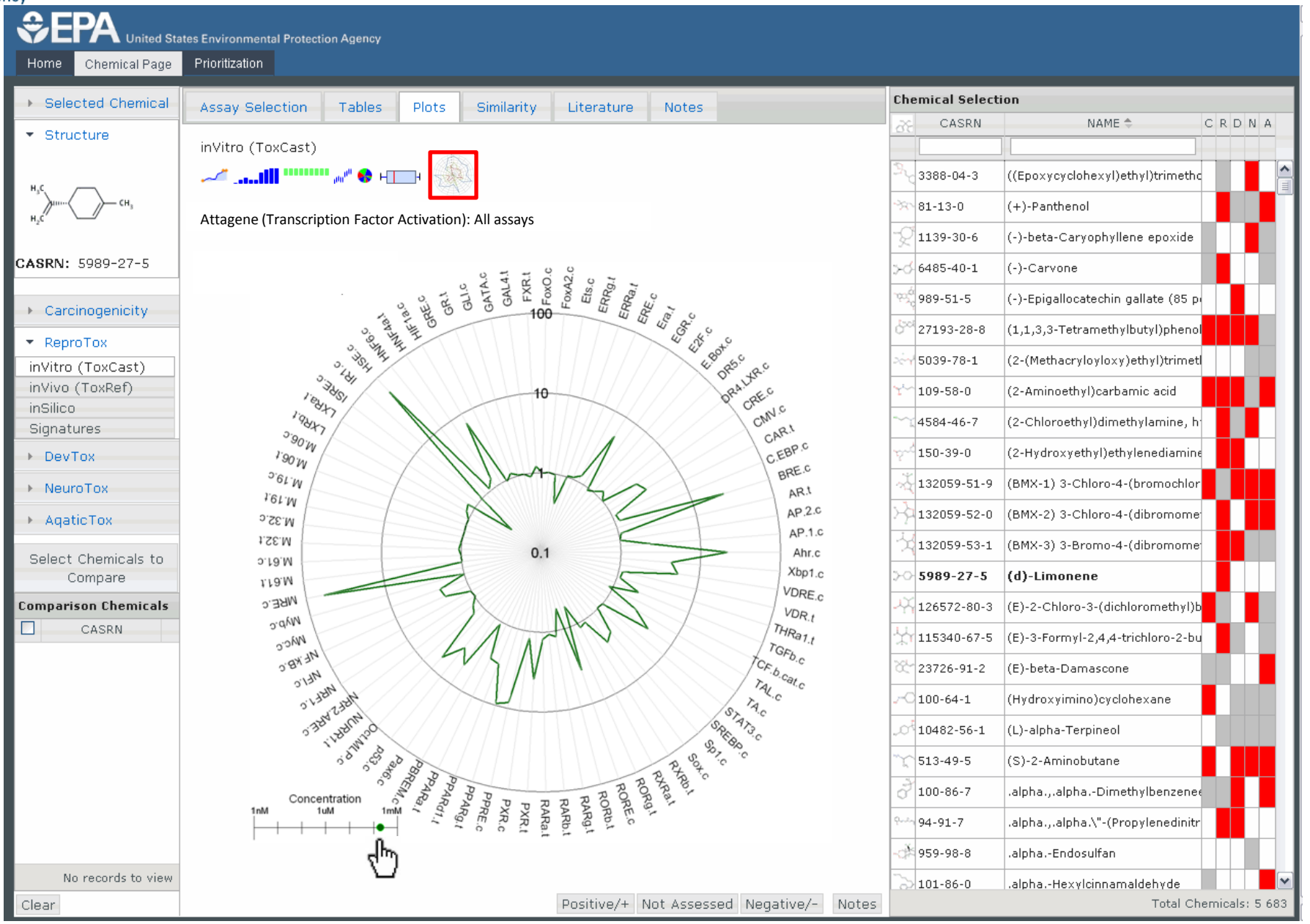

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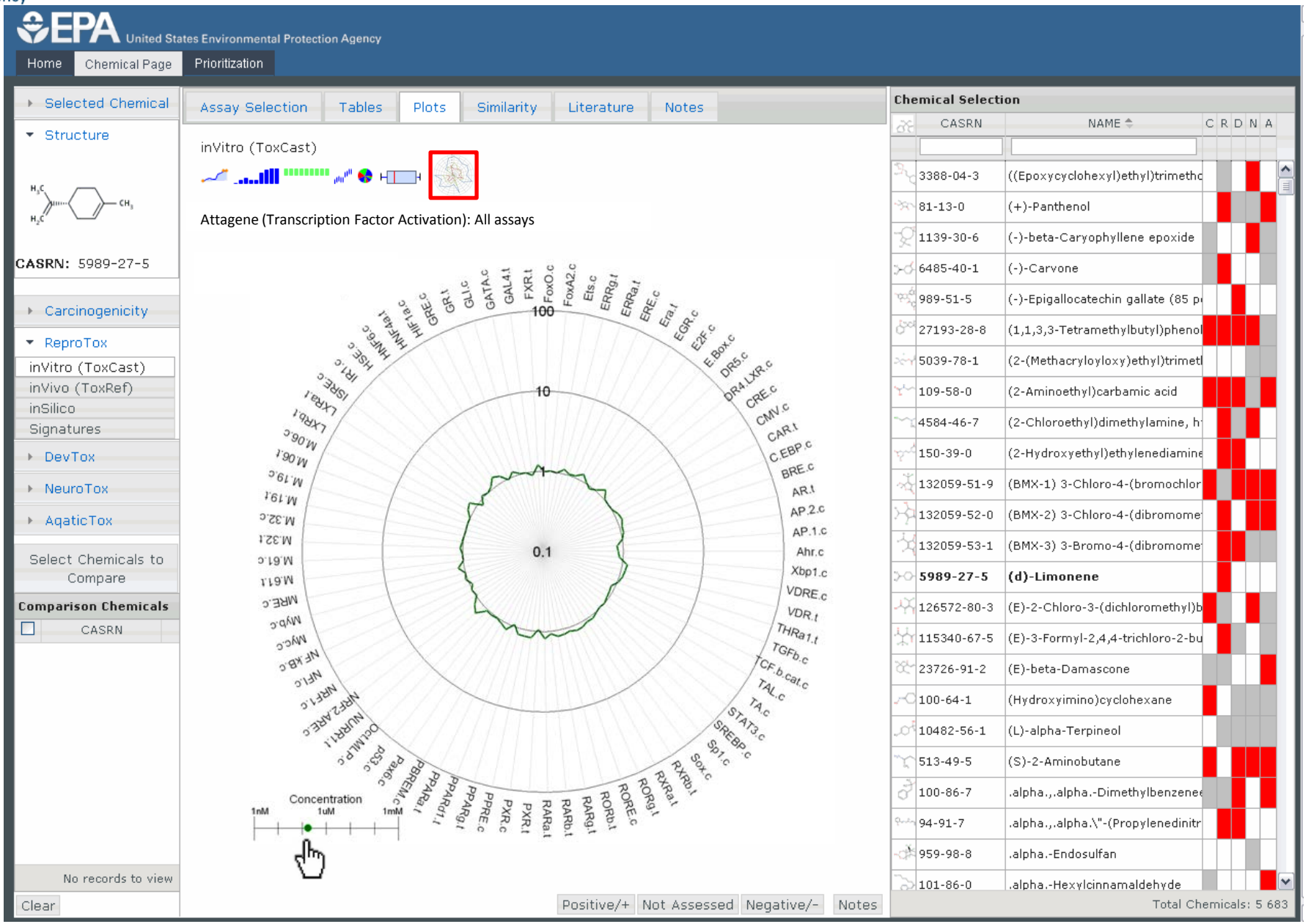
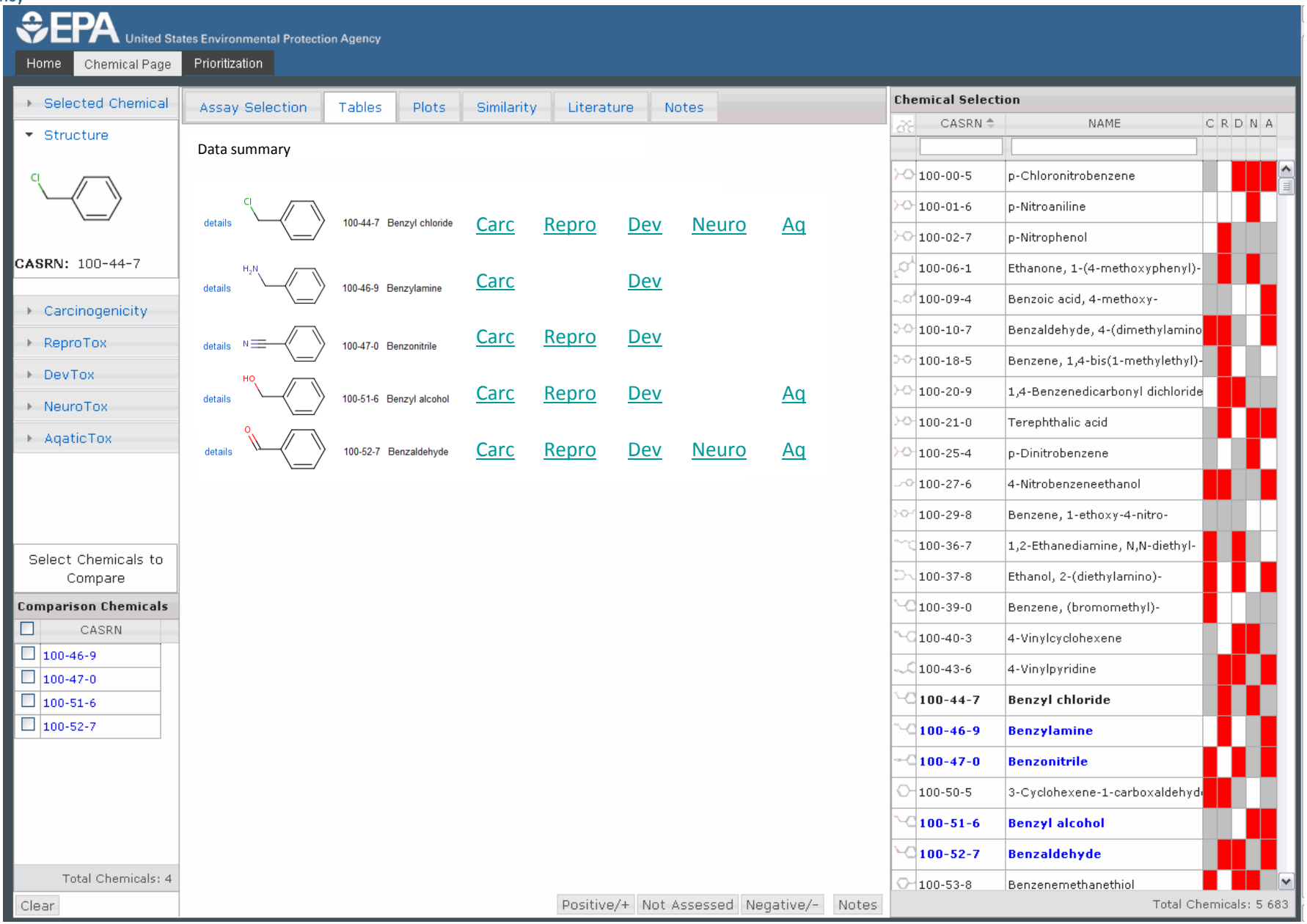
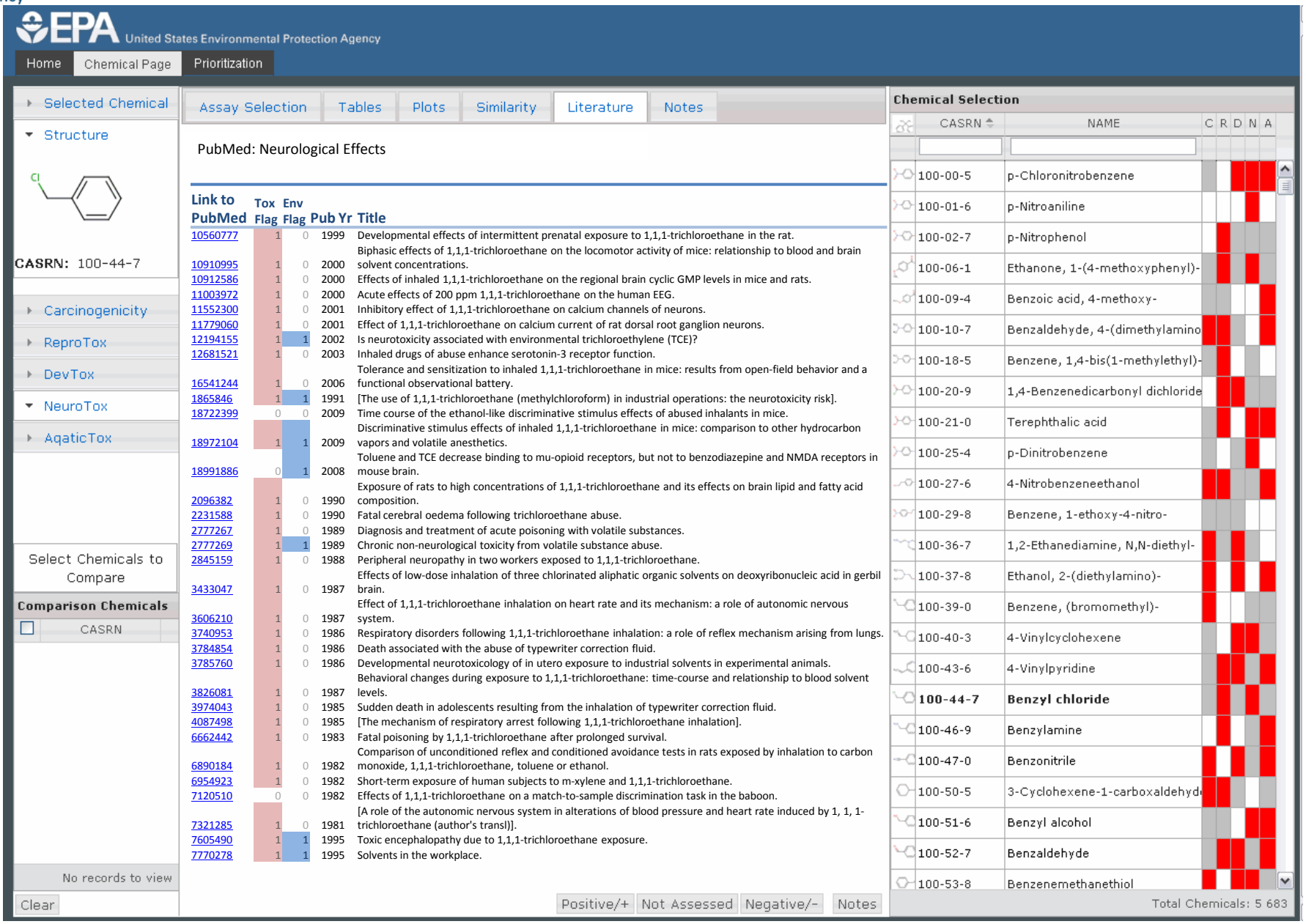


What kind of information is available for selected chemical sets?



Annotated literature searches for specific effects by chemical



Annotated literature searches for specific effects by chemical: interactive browsing

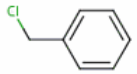
United States Environmental Protection Agency

EPA United States Environmental Protection Agency

Home | Chemical Page | Prioritization

Selected Chemical

Structure



CASRN: 100-44-7

Carcinogenicity

ReproTox

DevTox

NeuroTox

AqaticTox

Select Chemicals to Compare

Comparison Chemicals

CASRN

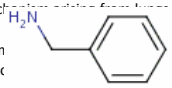
No records to view

Clear

Assay Selection | Tables | Plots | Similarity | Literature | Notes

PubMed: Neurological Effects

Link to PubMed	Tox Flag	Env Flag	Pub Yr	Title
10560777	1	0	1999	Developmental effects of intermittent prenatal exposure to 1,1,1-trichloroethane in the rat.
10910995	1	0	2000	Biphasic effects of 1,1,1-trichloroethane on the locomotor activity of mice: relationship to blood and brain solvent concentrations.
10912586	1	0	2000	Effects of inhaled 1,1,1-trichloroethane on the regional brain cyclic GMP levels in mice and rats.
11003972	1	0	2000	Acute effects of 200 ppm 1,1,1-trichloroethane on the human EEG.
11552300	1	0	2001	Inhibitory effect of 1,1,1-trichloroethane on calcium channels of neurons.
11779060	1	0	2001	Effect of 1,1,1-trichloroethane on calcium current of rat dorsal root ganglion neurons.
12194155	1	1	2002	Is neurotoxicity associated with environmental trichloroethylene (TCE)?
12681521	1	0	2003	Inhaled drugs of abuse enhance serotonin-3 receptor function.
16541244	1	0	2006	Tolerance and sensitization to inhaled 1,1,1-trichloroethane in mice: results from open-field behavior and a functional observational battery.
1865846	1	1	1991	[The use of 1,1,1-trichloroethane (methylchloroform) in industrial operations: the neurotoxicity risk].
18722399	0	0	2009	Time course of the ethanol-like discriminative stimulus effects of abused inhalants in mice.
18972104	1	1	2009	Discriminative stimulus effects of inhaled 1,1,1-trichloroethane in mice: comparison to other hydrocarbon vapors and volatile anesthetics.
18991886	0	1	2008	Toluene and TCE decrease binding to mu-opioid receptors, but not to benzodiazepine and NMDA receptors in mouse brain.
2096382	1	0	1990	Exposure of rats to high concentrations of 1,1,1-trichloroethane and its effects on brain lipid and fatty acid composition.
2231588	1	0	1990	Fatal cerebral oedema following trichloroethane abuse.
2777267	1	0	1989	Diagnosis and treatment of acute poisoning with volatile substances.
2777269	1	1	1989	Chronic non-neurological toxicity from volatile substance abuse.
2845159	1	0	1988	Peripheral neuropathy in two workers exposed to 1,1,1-trichloroethane.
3433047	1	0	1987	Effects of low-dose inhalation of three chlorinated aliphatic organic solvents on deoxyribonucleic acid in gerbil brain.
3606210	1	0	1987	Effect of 1,1,1-trichloroethane inhalation on heart rate and its mechanism: a role of autonomic nervous system.
3740953	1	0	1986	Respiratory disorders following 1,1,1-trichloroethane inhalation: a role of reflex mech
3784854	1	0	1986	Death associated with the abuse of typewriter correction fluid.
3785760	1	0	1986	Developmental neurotoxicology of in utero exposure to industrial solvents in experin
3826081	1	0	1987	Behavioral changes during exposure to 1,1,1-trichloroethane: time-course and relati levels.
3974043	1	0	1985	Sudden death in adolescents resulting from the inhalation of typewriter correction fluid.
4087498	1	0	1985	[The mechanism of respiratory arrest following 1,1,1-trichloroethane inhalation].
6662442	1	0	1983	Fatal poisoning by 1,1,1-trichloroethane after prolonged survival.
6890184	1	0	1982	Comparison of unconditioned reflex and conditioned avoidance tests in rats exposed by inhalation to carbon monoxide, 1,1,1-trichloroethane, toluene or ethanol.
6954923	1	0	1982	Short-term exposure of human subjects to m-xylene and 1,1,1-trichloroethane.
7120510	0	0	1982	Effects of 1,1,1-trichloroethane on a match-to-sample discrimination task in the baboon.
7321285	1	0	1981	[A role of the autonomic nervous system in alterations of blood pressure and heart rate induced by 1, 1, 1-trichloroethane (author's transl)].
7605490	1	1	1995	Toxic encephalopathy due to 1,1,1-trichloroethane exposure.
7770278	1	1	1995	Solvents in the workplace.



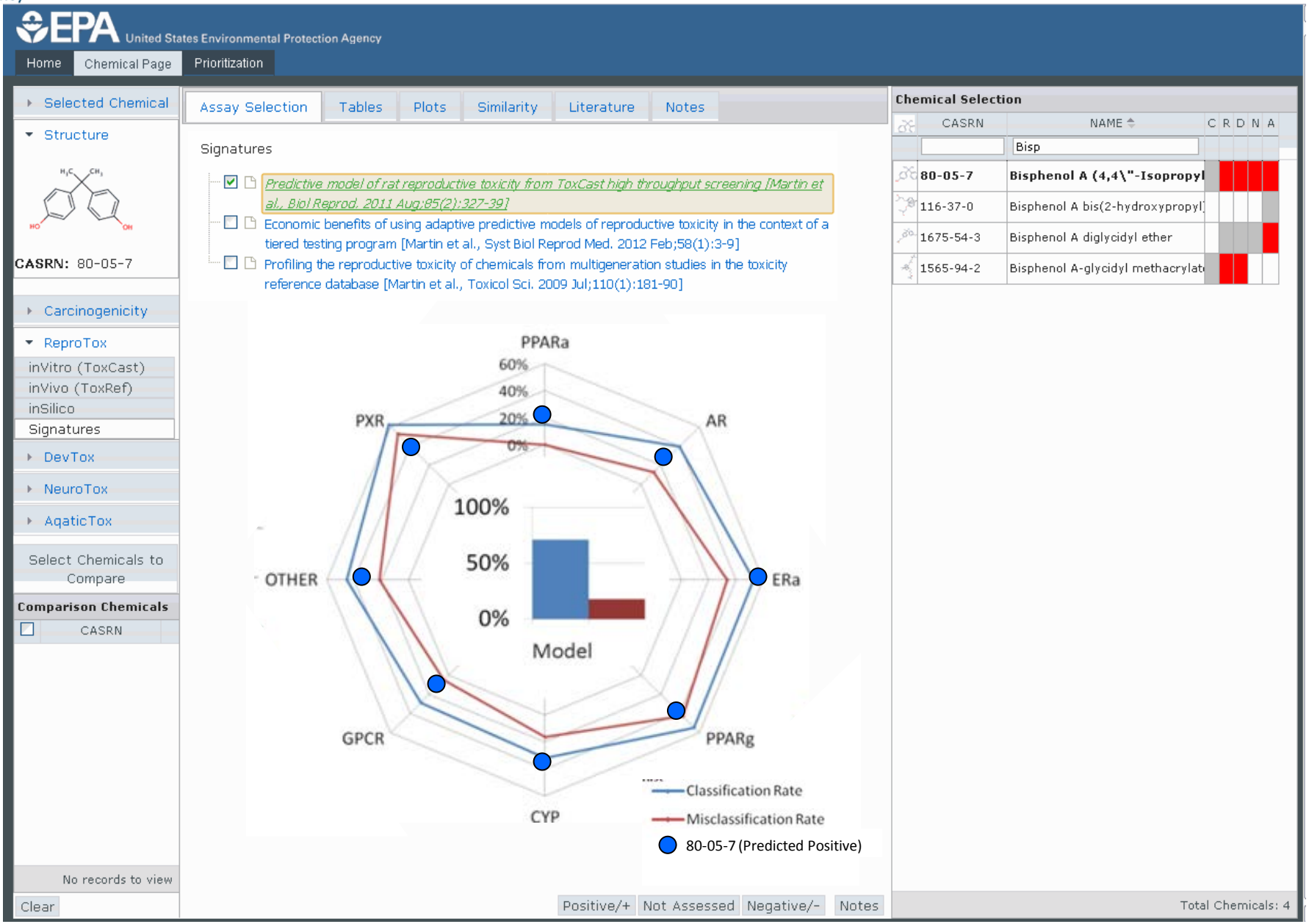
Positive/+ | Not Assessed | Negative/- | Notes

Chemical Selection

CASRN	NAME	C	R	D	N	A
100-00-5	p-Chloronitrobenzene					
100-01-6	p-Nitroaniline					
100-02-7	p-Nitrophenol					
100-06-1	Ethanone, 1-(4-methoxyphenyl)-					
100-09-4	Benzoic acid, 4-methoxy-					
100-10-7	Benzaldehyde, 4-(dimethylamino					
100-18-5	Benzene, 1,4-bis(1-methylethyl)-					
100-20-9	1,4-Benzenedicarbonyl dichloride					
100-21-0	Terephthalic acid					
100-25-4	p-Dinitrobenzene					
100-27-6	4-Nitrobenzeneethanol					
100-29-8	Benzene, 1-ethoxy-4-nitro-					
100-36-7	1,2-Ethanediamine, N,N-diethyl-					
100-37-8	Ethanol, 2-(diethylamino)-					
100-39-0	Benzene, (bromomethyl)-					
100-40-3	4-Vinylcyclohexene					
100-43-6	4-Vinylpyridine					
100-44-7	**Benzyl chloride**					
100-46-9	Benzylamine					
100-47-0	Benzonitrile					
100-50-5	3-Cyclohexene-1-carboxaldehyd					
100-51-6	Benzyl alcohol					
100-52-7	Benzaldehyde					
100-53-8	Benzenemethanethiol					

Total Chemicals: 5 683

Predictive signatures connect *in vitro* assays to *in vivo* endpoints



Dashboard/Workflow Conceptual Framework