http://www.orcid.org/0000-0002-2668-4821

Delivering access to chemistry and bioassay data from the National Center for Computational Toxicology at the EPA

Antony Williams

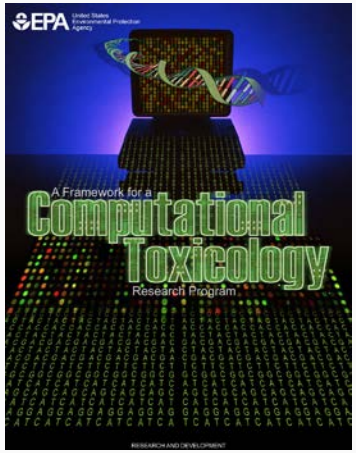
National Center for Computational Toxicology, U.S. Environmental Protection Agency, RTP, NC

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

June 12th 2018

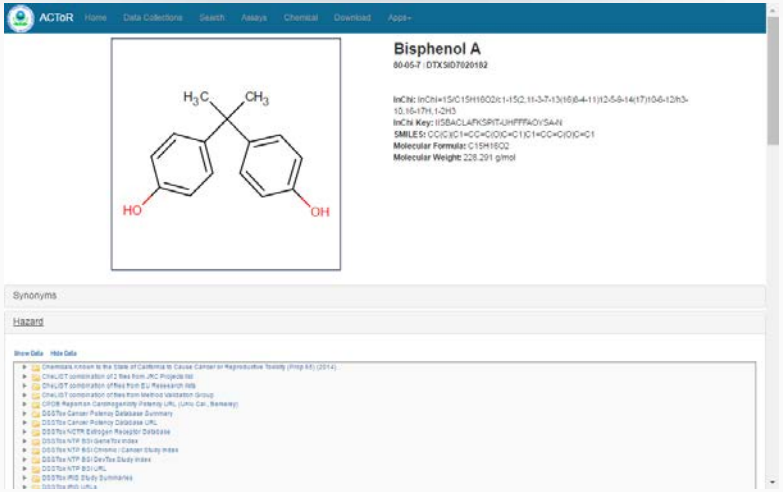
RTP Regional Seminar – Collaboration and Your Research Data

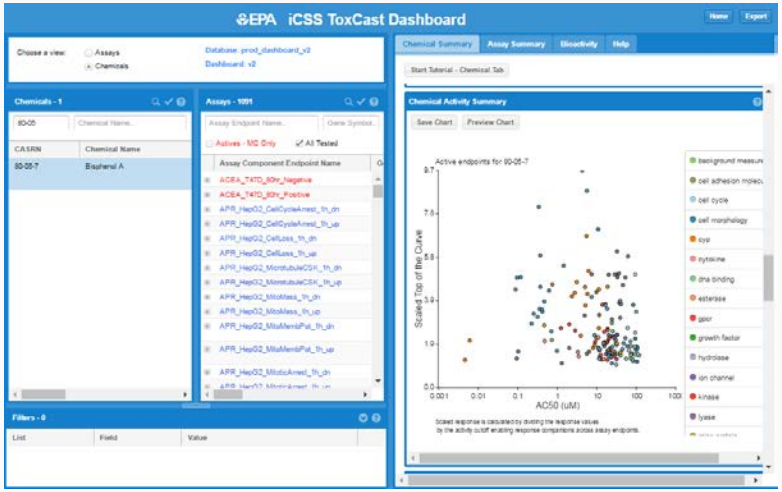
National Center for Computational Toxicology

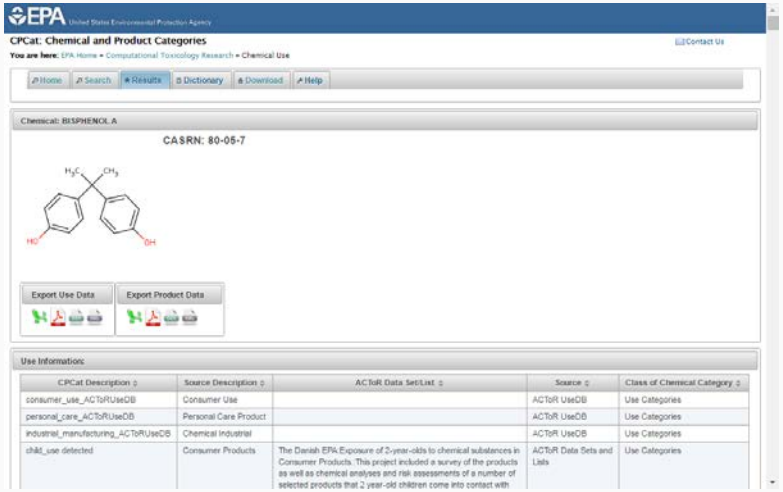


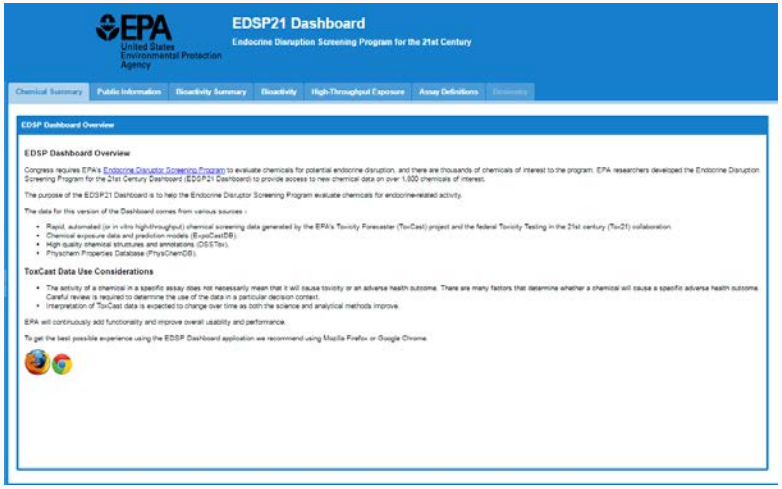
- National Center for Computational Toxicology established in 2005 to integrate:
  - High-throughput and high-content technologies
  - Modern molecular biology
  - Data mining and statistical modeling
  - Computational biology and chemistry
- Outputs: a lot of data, models, algorithms and software applications
- Open Data – we want scientists to interrogate it, learn from it, develop understanding

Early Dashboard Applications









Earlier Dashboards

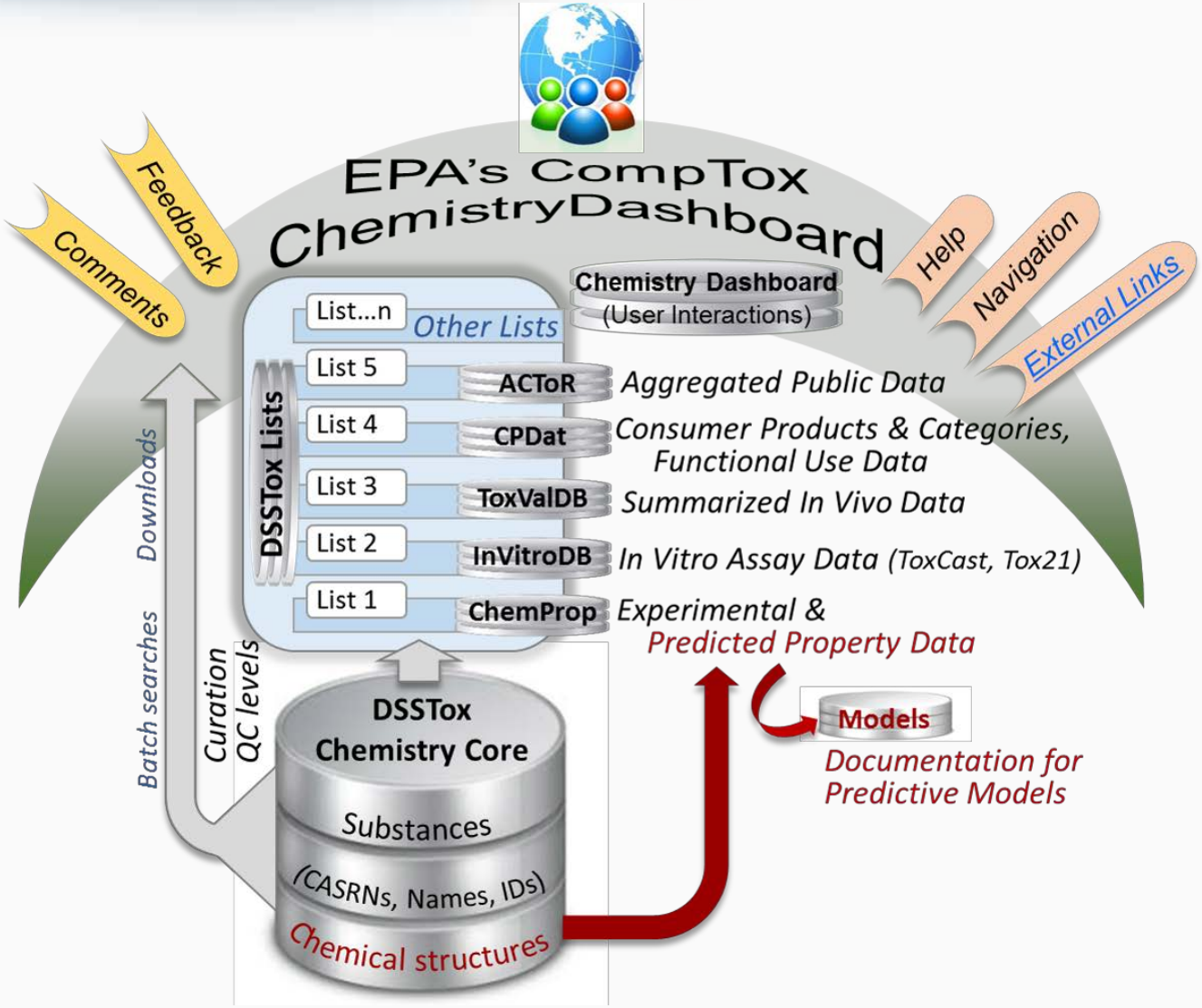
- Chemistry data mashed together based on CAS Number/Names
- Chemistry data quality issues
- Multiple applications requiring maintenance

- April 2016 – beta release of the CompTox Chemistry Dashboard as an integration hub

The CompTox Chemistry Dashboard

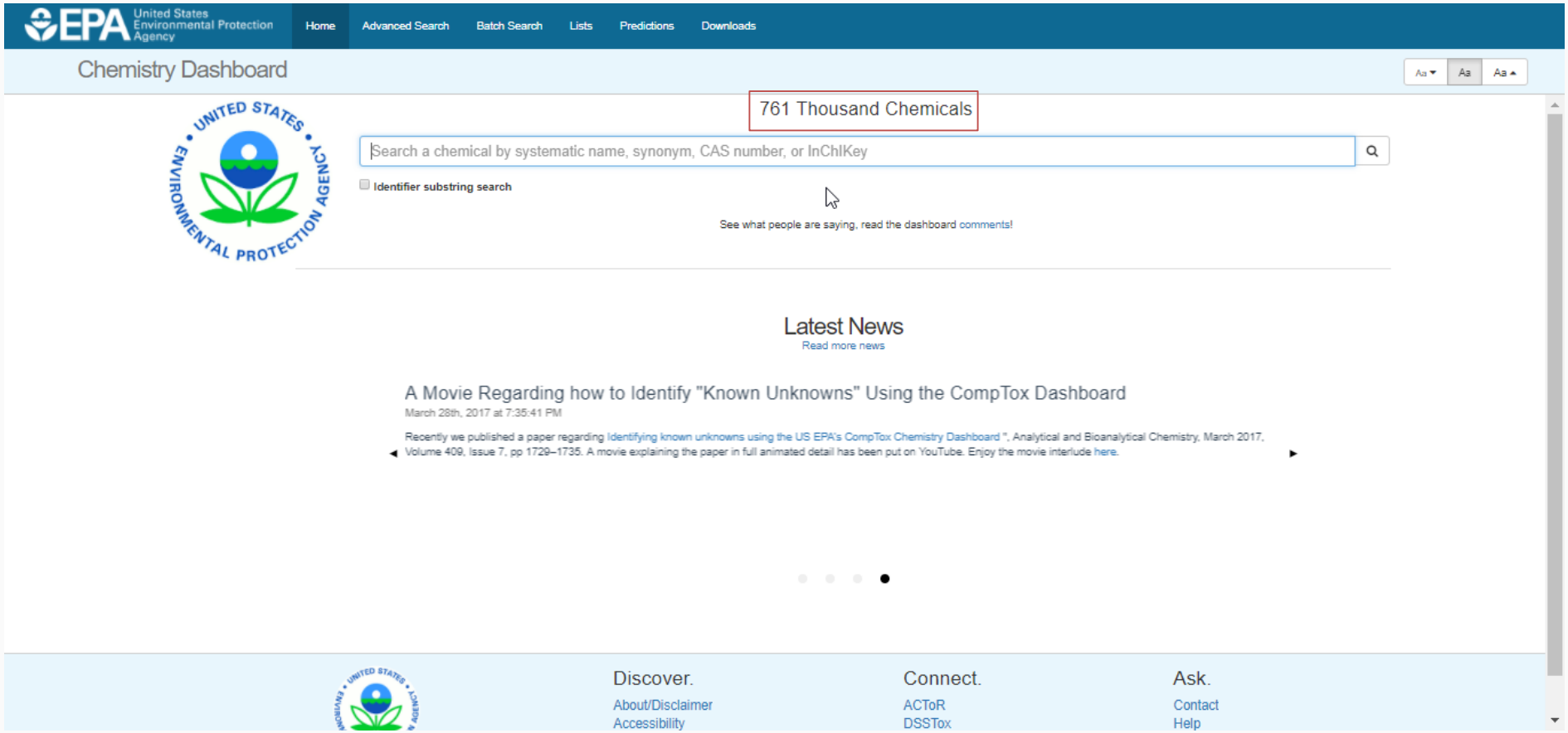
- A **publicly accessible website** delivering access:
  - ~760,000 chemicals with related property data
  - Experimental and predicted physicochemical property data
  - Integration to “biological assay data” for 1000s of chemicals
  - Information regarding consumer products containing chemicals
  - Links to other agency websites and public data resources
  - “Literature” searches for chemicals using public resources
  - “Batch searching” for thousands of chemicals
  - **DOWNLOADABLE Open Data for reuse and repurposing**

The CompTox Chemistry Dashboard



CompTox Chemistry Dashboard

https://comptox.epa.gov/dashboard



Detailed Chemical Pages

EPA United States Environmental Protection Agency

EPA United States Environmental Protection Agency | Home | Advanced Search | Batch Search | Lists | Predictions | Downloads | Search All Data

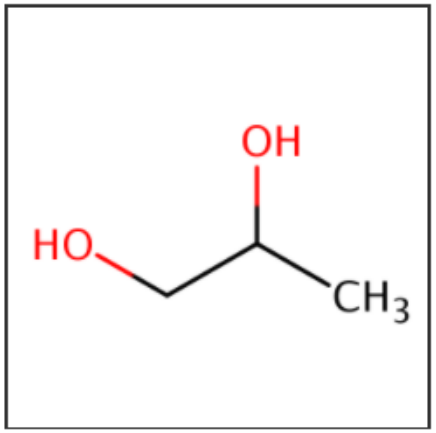
Chemistry Dashboard | EPAHFR

Submit Comment | Copy | Aa | Aa | Aa

1,2-Propylene glycol

57-55-6 | DTXSID0021206

Searched by DSSTox_Substance_Id: Found 1 result for 'DTXSID0021206'.



Wikipedia

Propylene glycol (IUPAC name: propane-1,2-diol) is a synthetic organic compound with the chemical formula C3H8O2. It is a viscous colorless liquid which is nearly odorless but possesses a faintly sweet taste. Chemically it is classed as a diol and is miscible with a broad range of solvents, including water, acetone, and chloroform. It is produced on a large scale and is primarily used in the production of polymers, but also sees use in food...Read more

- Intrinsic Properties
- Structural Identifiers
- Linked Substances
- Presence in Lists
- Record Information
- Quality Control Notes

Chemical Properties | Env. Fate/Transport | Hazard | ADME (Beta) | Exposure | Bioassays | Similar Compounds | Related Substances | Synonyms | Literature | Links | Comments

Access to Chemical Hazard Data

EPA United States Environmental Protection Agency

EPA United States Environmental Protection Agency | Home | Advanced Search | Batch Search | Lists | Predictions | Downloads | Search All Data

Chemistry Dashboard | EPAHFR

Submit Comment | Copy | Aa | Aa | Aa

Chemical Properties | Env. Fate/Transport | Hazard | ADME (Beta) | Exposure | Bioassays | Similar Compounds | Related Substances | Synonyms | Literature | Links | Comments

- Exposure Limit
- Lethality Effect Level
- **Point of Departure**
- Toxicity Value

Download table as: TSV | Excel | Human | Eco

	Priority	Type	Subtype	Risk Assessment Class	Values	Units	Study Type	Exposure Route	Species	Subsource	Source
+	8	NOEL	Cardiova...	subchronic	5000.0	mg/kg-day	subchronic	oral	rat	Vaille et ...	PPRTV (...
+	8	NOEL	Endocrine	subchronic	5000.0	mg/kg-day	subchronic	oral	rat	Vaille et ...	PPRTV (...
+	8	LOEL	Hematol...	subchronic	2500.0	mg/kg-day	subchronic	oral	rat	Vaille et ...	PPRTV (...
+	8	LOEL	Hepatic	subchronic	2500.0	mg/kg-day	subchronic	oral	rat	Vaille et ...	PPRTV (...
+	8	NOEL	Immune	immunot...	5000.0	mg/kg-day	subchronic	oral	rat	Vaille et ...	PPRTV (...
+	8	NOEL	Renal	subchronic	5000.0	mg/kg-day	subchronic	oral	rat	Vaille et ...	PPRTV (...
+	8	LOEL	Systemic	subchronic	2500.0	mg/kg-day	subchronic	oral	rat	Vaille et ...	PPRTV (...
+	8	NOEL	Hematol...	subchronic	1500.0	mg/kg-day	subchronic	oral	rabbit	Vaille et ...	PPRTV (...
+	8	NOEL	Systemic	subchronic	1500.0	mg/kg-day	subchronic	oral	rabbit	Vaille et ...	PPRTV (...

In Vitro Bioassay Screening

ToxCast and Tox21

EPA United States Environmental Protection Agency

EPA United States Environmental Protection Agency | Home | Advanced Search | Batch Search | Lists | Predictions | Downloads | Search All Data

Chemistry Dashboard | EPAHFR

Submit Comment | Copy | Aa | Aa | Aa

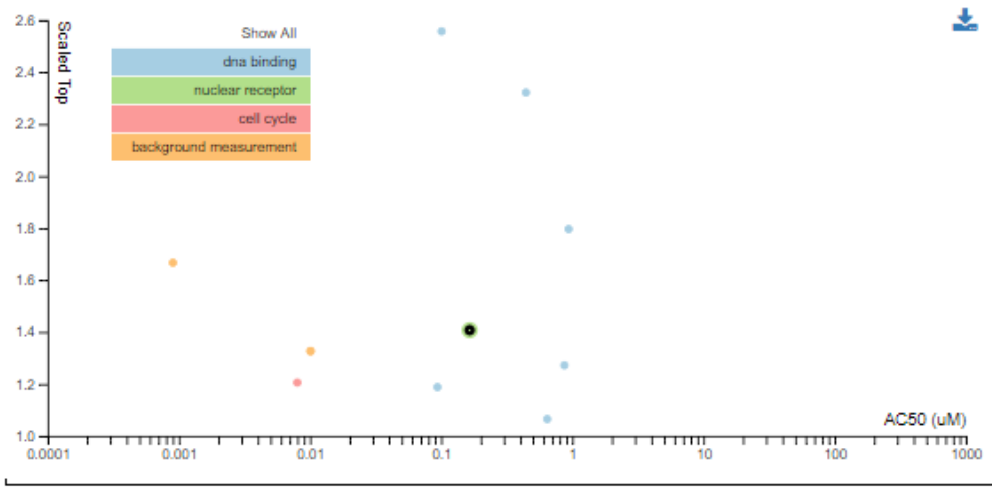
Chemical Properties | Env. Fate/Transport | Hazard | ADME (Beta) | Exposure | Bioassays | Similar Compounds | Related Substances | Synonyms | Literature | Links | Comments

ToxCast: Summary

PubChem

Chemical Activity Summary

ToxCast Data



Assay Details

AC50 (uM): 0.16
Scaled top: 1.41
Assay Name: NVS_NR_hFXR_Antagonist
Assay Description: 716
Gene Symbol: NR1H4
Organism: human
Tissue: NA
Assay Format Type: biochemical
Biological Process Target: receptor binding
Detection Technology: TR-FRET
Analysis Direction: positive
Intended Target Family: nuclear receptor
Description: Data from the assay component NVS_NR_hFXR_Antagonist was analyzed into 1 assay endpoint. This assay endpoint, NVS_NR_hFXR_Antagonist, was analyzed in the positive fitting direction relative to DMSO as the negative control and baseline of activity. Using a type of binding reporter, loss-of-signal activity can be used to understand changes in the binding as they relate to the gene NR1H4.

Download as: TSV | Excel Show: Inactive | Background

Assay Name	Assa...	SeqA...	AOP Link	AOP Eve...	Hit Call	T...	Scale...	...	log ...	Target Family

Sources of Exposure to Chemicals

EPA United States Environmental Protection Agency

Product & Use Categories

Chemical Weight Fraction

Chemical Functional Use

Monitoring Data

Exposure Predictions

Production Volume

osure | Bioassays | Similar Compounds | Related Substances | Synonyms | Literature | Links | Comments

Product & Use Categories (PUCs)

Categorization type	Number of Unique Products
PUC	288
PUC	206
PUC	117
PUC	107
PUC	107
PUC	101
PUC	101
PUC	90
PUC	89

Identifiers to Support Searches

Chemical Properties | Env. Fate/Transport | Hazard | ADME (Beta) | Exposure | Bioassays | Similar Compounds | Related Substances | Synonyms

Found 78 synonyms

Legend: **Valid Synonyms** *Good Synonyms* Other Synonyms Copy all Synonyms

1,2-Propylene glycol

Propane-1,2-diol

1,2-Propanediol

57-55-6 Active CAS-RN

alpha-Propylene glycol

(+/-) 1,2-Propanediol

(RS)-1,2-Propanediol

dl-Propylene glycol

3-01-00-02142 Beilstein Registry Number

1,2-Propanediol

(.+-.)-1,2-Propanediol

(.+-.)-Propylene glycol

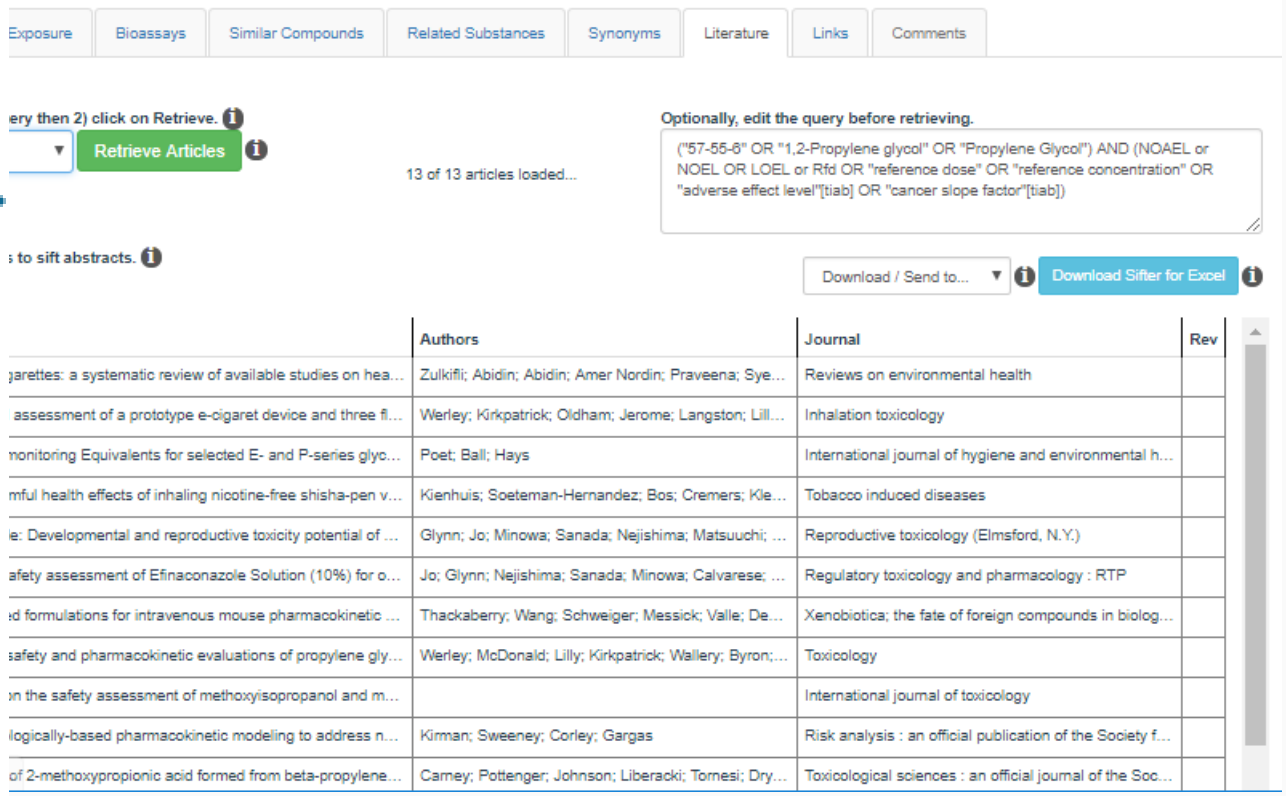
1,2-(RS)-Propanediol

1,2-DIHYDROXYPROPANE

1,2-PROPANDIOL

Literature Searches and Links

- Google Scholar
- **PubMed Abstract Sifter**
- PubChem Articles
- PubChem Patents
- PPRTV
- IRIS



External Links to Data and Services

EPA United States Environmental Protection Agency

Chemical Properties | Env. Fate/Transport | Hazard | ADME (Beta) | Exposure | Bioassays | Similar Compounds | Related Substances | Synonyms | Literature | Links

General

- EPA Substance Registry ...
- Household Products Data...
- PubChem
- CPCat
- DrugBank
- Wikipedia
- MSDS Lookup
- ChEMBL
- Chemical Vendors
- NIOSH Chemical Safety ...
- ToxPlanet
- ACS Reagent Chemicals
- Wikidata
- ChemHat: Hazards and A...
- Wolfram Alpha

Toxicology

- ACToR
- DrugPortal
- CCRIS
- ChemView
- CTD
- eChemPortal
- Gene-Tox
- HSDB
- ToxCast Dashboard 2
- LactMed
- International Toxicity Esti...
- ATSDR Toxic Substances...
- ACToR PDF Report
- CREST

Publications

- Toxline
- Environmental Health Per...
- NIEHS
- National Toxicology Progr...
- Google Books
- Google Scholar
- Google Patents
- PPRTVWEB
- PubMed
- IRIS Assessments
- EPA HERO
- RSC Publications
- BioCaddie DataMed
- Springer Materials
- Federal Register

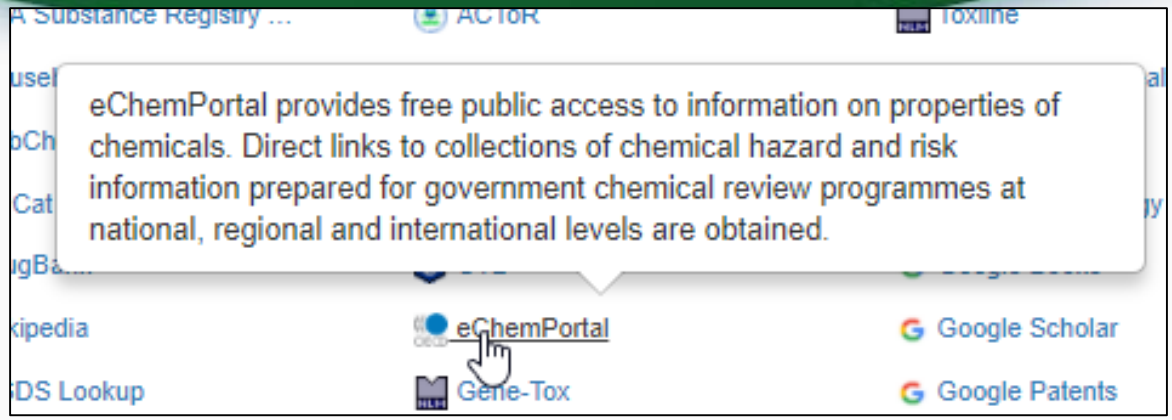
Analytical

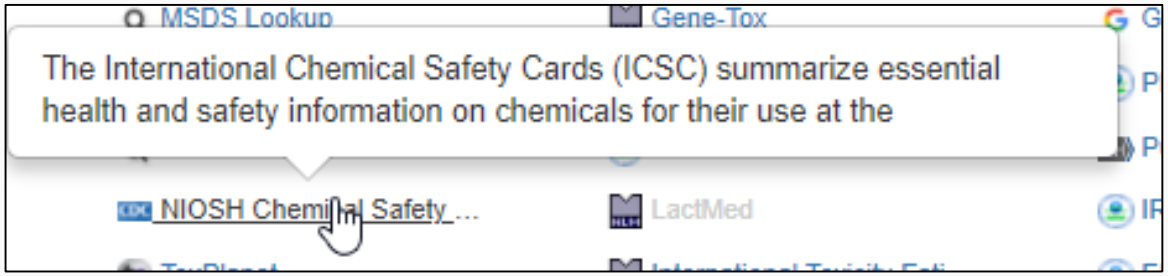
- RSC Analytical Abstracts
- Tox21 Analytical Data
- MONA: MassBank North ...
- NIST IR Spectrum
- NIST MS Spectrum

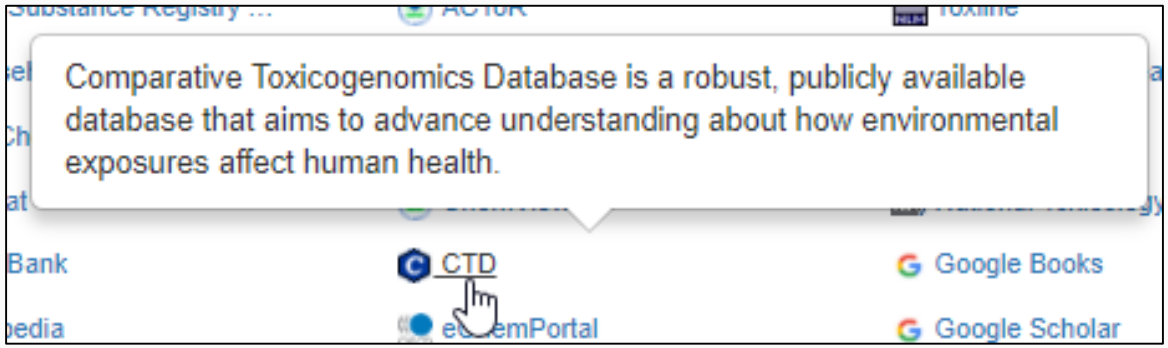
Prediction

- 2D NMR HSQC/HMBC Pr...
- Carbon-13 NMR Prediction
- Proton NMR Prediction
- ChemRTP Predictor
- LSERD

Integrated Linkouts







Integrated Linkouts

Comparative Toxicogenomics DB

EPA United States Environmental Protection Agency

ctd *Illuminating how chemicals affect human health.*

Comparative Toxicogenomics Database

YOUR QUERIES | CONTACT US

Chemicals | Name, CAS RN, ID | Search

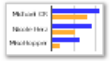
Home | Search | Analyze | Download | Help

Propylene Glycol

Basics | Gene Interactions | Genes | Diseases | Phenotypes | Comps | Pathways | GO | Exposure Studies | Exposure Details | References

These diseases are associated with *Propylene Glycol* or its descendants. Each association is *curated* (M *marker/mechanism* and/or T *therapeutic*) and/or *inferred* (via a curated gene interaction).

Disease categories [Show chart]



Filter by Disease category: ALL | Association type: ALL | Filter

1–50 of 240 results.

First | Previous | 1 | 2 | 3 | 4 | 5 | Next | Last

	Chemical	Disease	Direct Evidence	Enrichment Analysis	Inference Network	Inference Score	References
1.	Propylene Glycol	Drug-Related Side Effects and Adverse Reactions	M	GO	*2 genes:* ABCC2 | ABCC4	4.09	5
2.	Propylene Glycol	Acute Kidney Injury	M	GO	*2 genes:* IL6 | TGFB1	3.78	3
3.	Propylene Glycol	Chemical and Drug Induced Liver Injury	M	GO	*2 genes:* ABCC2 | IL6	2.82	5
4.	Propylene Glycol	Kidney Diseases	M		*1 gene:* TGFB1	2.54	4

Advanced Searches

Advanced Search

Mass Search

± | Min/Max

M

Mass Da ± Error Da ppm Search

Molecular Formula Search

Molecular Formula

MS Ready Formula

Exact Formula

Search

Generate Molecular Formula(e)

± | Min/Max

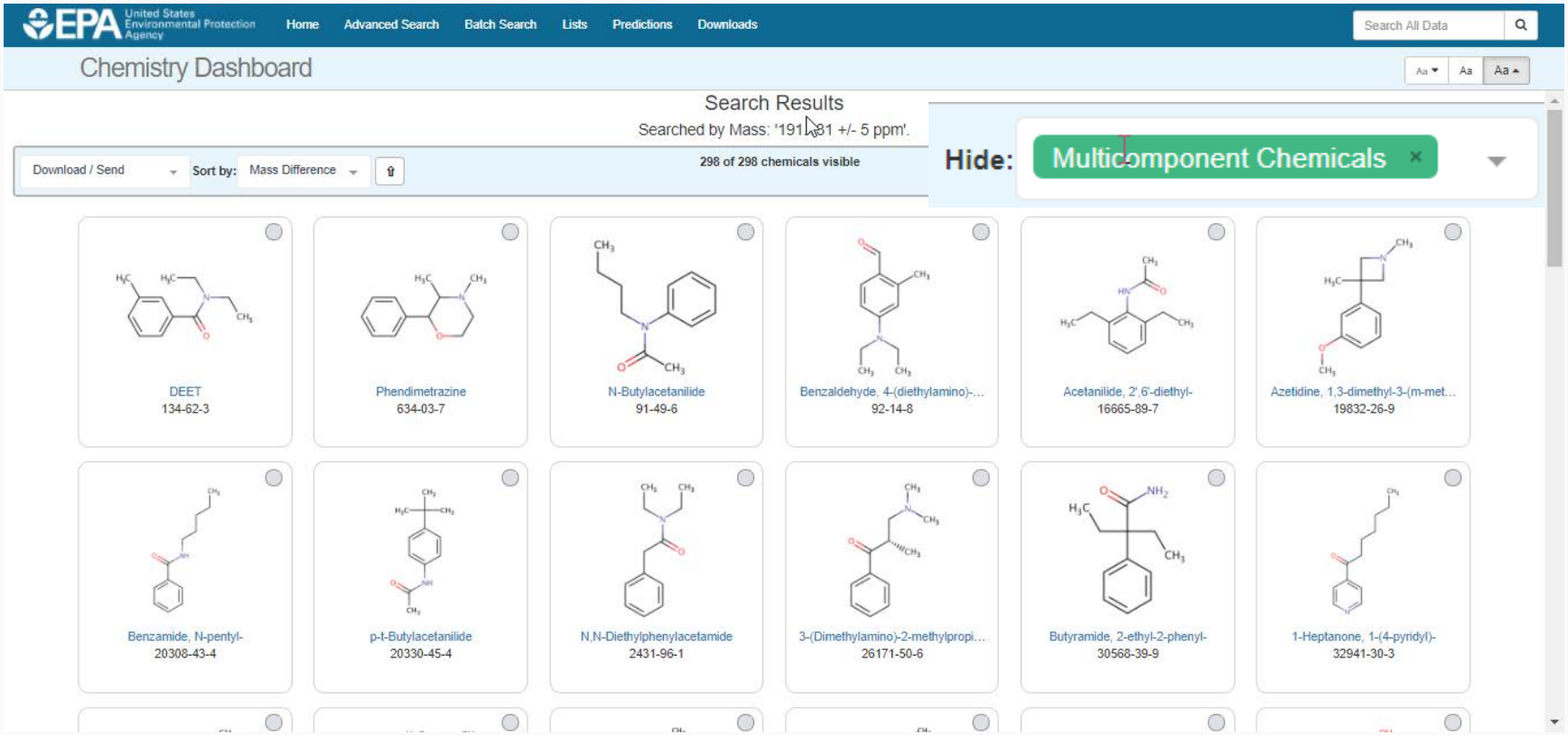
Mass Da ± Error Da ppm Search

Default Options: C[1-50] H[0-100] O[0-20] N[0-20] P[0-20] S[0-10]

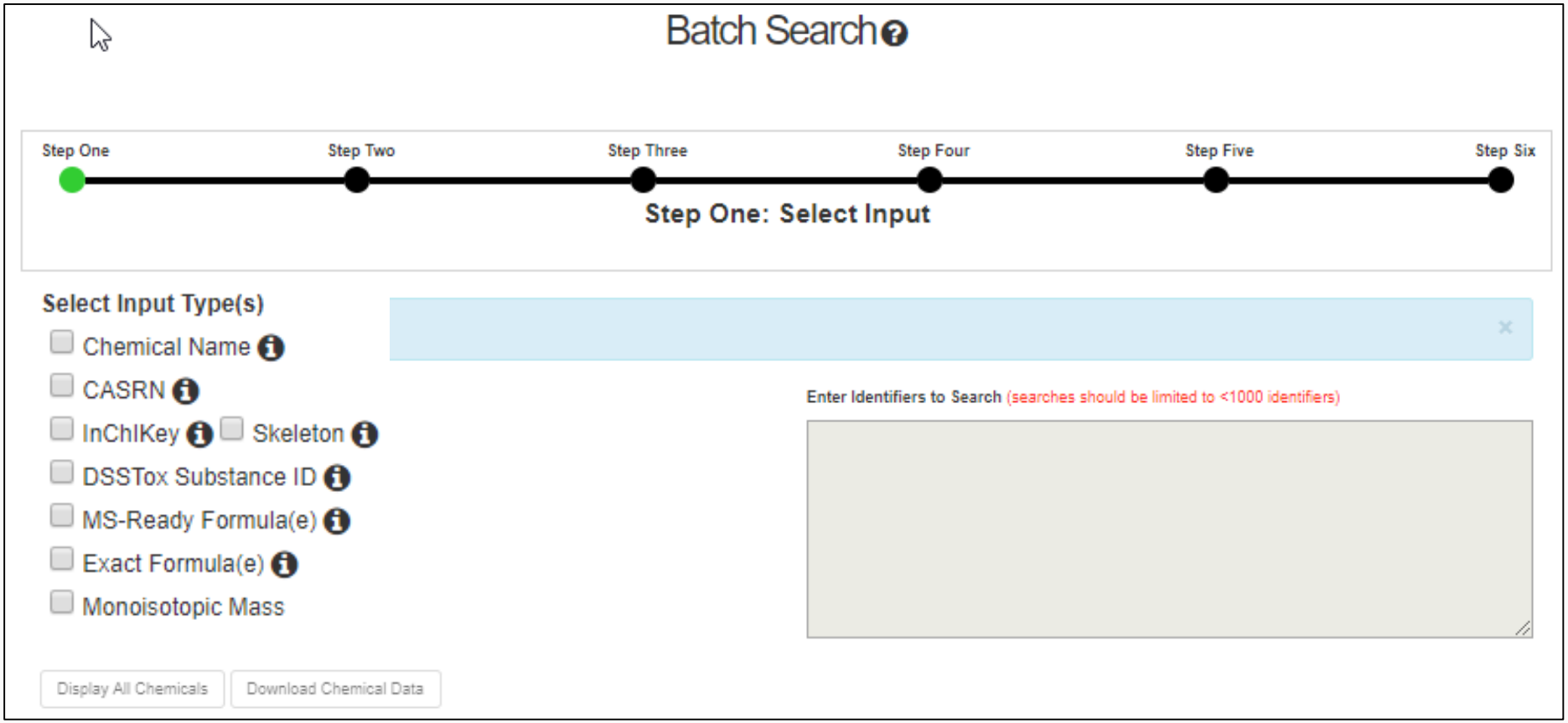
Include Halogens: F[0-20] Cl[0-20] Br[0-20] I[0-20]

Options

Advanced Searches



Batch Searches



Batch Search

Select Input Type(s)

- [ ] Chemical Name
- [ ] CASRN
- [ ] InChIKey
- [ ] Skeleton
- [ ] DSSTox Substance ID
- [x] MS-Ready Formula(e)
- [ ] Exact Formula(e)
- [ ] Monoisotopic Mass

Enter Identifiers to Search (searches should be limited to <1000 identifiers)

C6H12O3
C7H7N3
C8H11NO
C7H5NOS
C9H15NO
C11H12O
C9H8O3
C6H12O5
C9H15NO2

Metadata

- [ ] Curation Level Details
- [x] Data Sources
- [x] Assay Hit Count
- [ ] Include links to ACToR reports - SLOW! (BETA)
- [x] NHANES/Predicted Exposure
- [x] Include ToxVal Data Availability
- [x] Number of PubMed Articles
- [ ] Abstract Sifter Input File (Beta)
- [ ] MetFrag Input File(Beta)
- [x] IRIS
- [x] PPRTV
- [x] PubChem Data Sources
- [ ] ToxPrint fingerprints

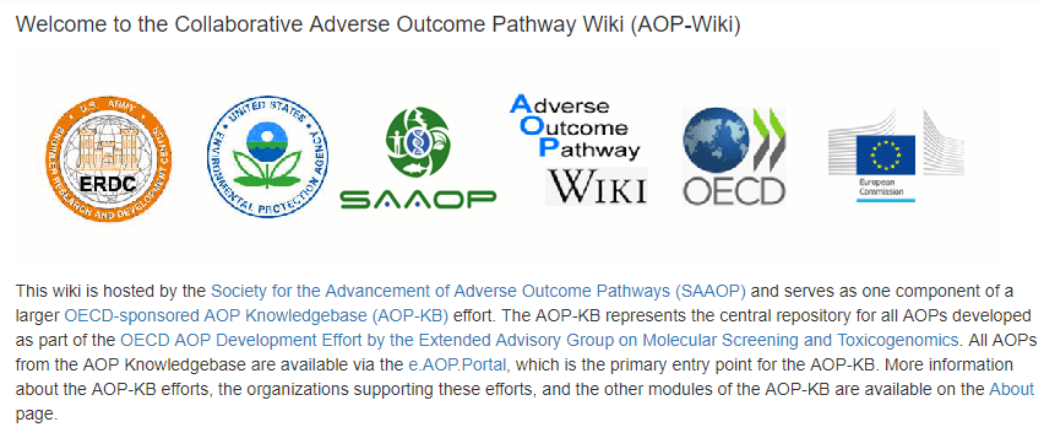
- [ ] NIOSH IDLH Values
- [ ] NIOSH International Chemical Safety Cards
- [ ] NIOSH Pocket Guide to Chemical Hazards
- [ ] NIOSH Skin Notation Profiles
- [ ] NORMAN Collaborative Trial 2015 Targets and Suspects
- [ ] Norman Network PFAS (KEMI Report)
- [ ] NORMAN Network Priority List
- [ ] NormaNEWS: Norman Early Warning System
- [ ] PFAS list provided by X.Trier et al
- [ ] Pharmaceutical List with EU, Swiss and US Consumption Data
- [ ] Provisional Peer Reviewed Toxicity Values
- [ ] Stockholm Convention on Organic Pollutants
- [x] STOFF-IDENT Database of Water-Relevant Substances
- [ ] Superfund Chemical Data Matrix
- [x] Surfactant List Screened in Swiss Wastewater (2014)

Excel Output

INPUT	FOUND_BY	DTXCID_IN	DATA_SOU	TOXVAL_D	TOXCAST_	TOXCAST_	NUMBER_C	PUBCHEM_	STO
C6H12O3	MS Ready	DTXCID701	91	Y	0.36	2/562	24	83	Y
C6H12O3	MS Ready	DTXCID003	67	Y	0.36	1/276	376	80	Y
C6H12O3	MS Ready	DTXCID106	65	Y	4.42	5/113	6	77	Y
C6H12O3	MS Ready	DTXCID105	45	Y	0.0	0/163	3	94	-
C6H12O3	MS Ready	DTXCID901	38	Y	-	-	14	110	Y
C6H12O3	MS Ready	DTXCID402	34	Y	0.0	0/113	-	53	Y
C6H12O3	MS Ready	DTXCID202	31	Y	-	-	-	36	Y
C6H12O3	MS Ready	DTXCID202	30	-	2.54	7/276	-	54	-
C6H12O3	MS Ready	DTXCID109	26	Y	-	-	-	46	-
C6H12O3	MS Ready	DTXCID202	24	Y	0.0	0/113	-	47	-
C6H12O3	MS Ready	DTXCID303	22	Y	-	-	-	89	-
C6H12O3	MS Ready	DTXCID302	20	Y	-	-	2	25	Y
C6H12O3	MS Ready	DTXCID407	19	Y	-	-	12	62	-
C6H12O3	MS Ready	DTXCID704	17	Y	-	-	-	64	-
C6H12O3	MS Ready	DTXCID704	16	Y	-	-	3	49	-

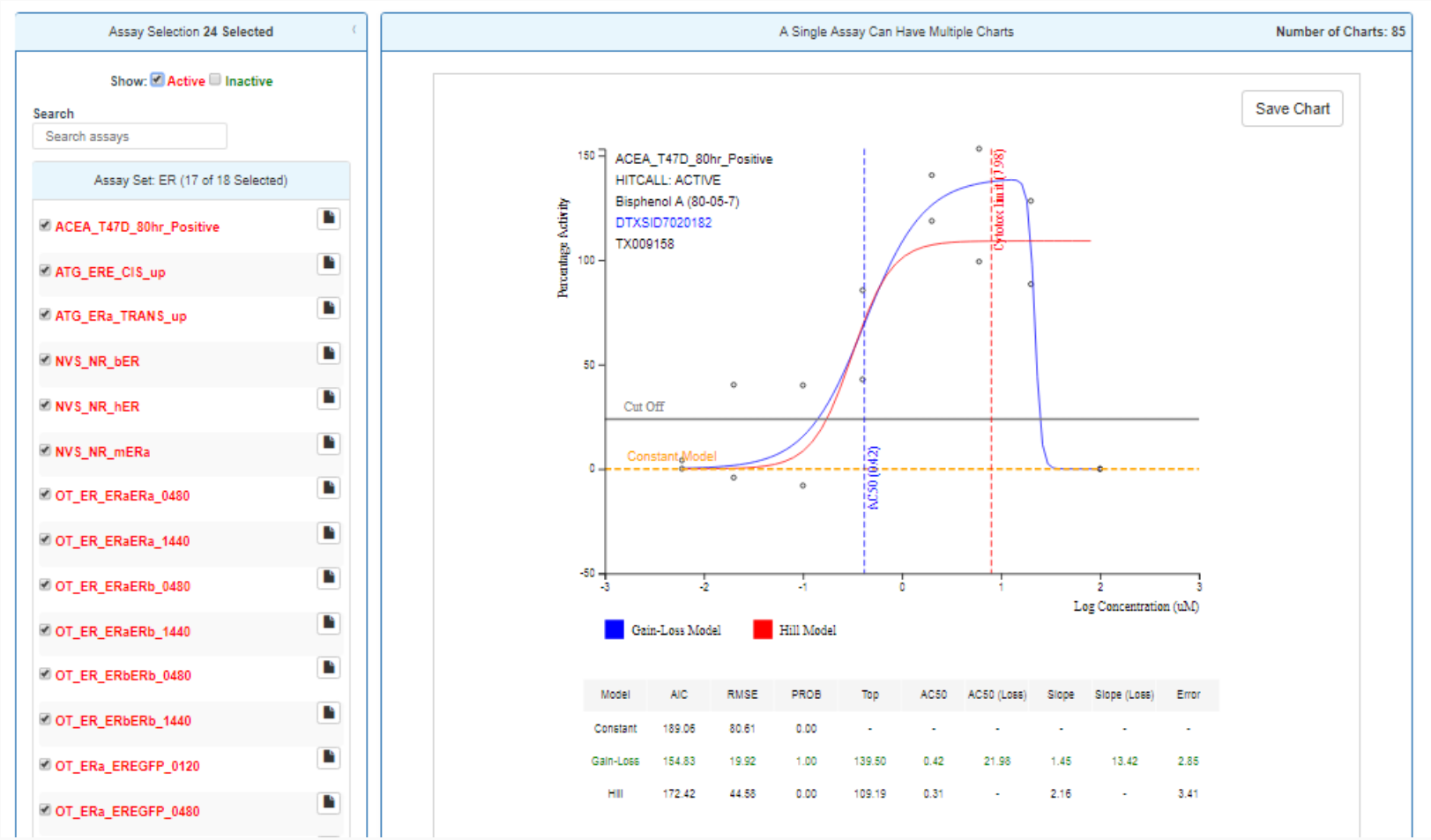
Work in Progress (August release)

- Migrating ToxCast dashboard supporting bioactivity curve display, gene searching, assay searching
- Integration to the Adverse Outcome Pathway Wiki



Presently in Development

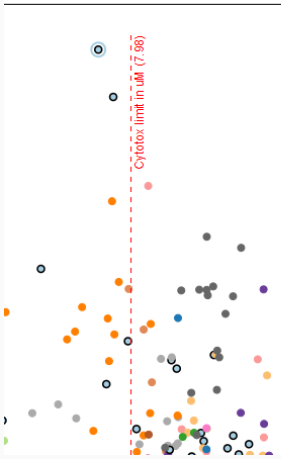
- Bioactivity Curve display



Model	AIC	RMSE	PROB	Top	AC50	AC50 (Loss)	Slope	Slope (Loss)	Error
Constant	189.06	80.61	0.00	-	-	-	-	-	-
Gain-Loss	154.83	19.92	1.00	139.50	0.42	21.98	1.45	13.42	2.85
Hill	172.42	44.58	0.00	109.19	0.31	-	2.16	-	3.41

Linkages to Detailed Assay Descriptions

Chemical Activity Summary



Assay Details

AC50 (uM): 4.33
Scaled top: 9.72
Assay Endpoint Name: OT_ER_ERaERa_1440
Assay Description: 743
Gene Symbol: ESR1
Organism: human
Tissue: kidney
Assay Format Type: cell-based
Biological Process Target: protein stabilization
Detection Technology: Protein-fragment Complementation
Analysis Direction: positive
Intended Target Family: nuclear receptor
Description: Data from the assay component OT_ER_ERaERa_1440 was analyzed into 1 assay endpoint. This assay endpoint, OT_ER_ERaERa_1440, was analyzed in the positive fitting direction relative to DMSO as the negative control and baseline of activity. Using a type of binding reporter, measures of receptor for gain-of-signal activity can be used to understand the binding at the pathway-level as they relate to the gene ESR1. Furthermore, this assay endpoint can be referred to as a primary readout, because the performed assay has only produced 1 assay endpoint. To generalize the intended target to other relatable targets, this assay endpoint is annotated to the 'nuclear receptor' intended target family, where the subfamily is 'steroidal'.

Assay Endpoint Name	Assay Description	SeqAPASS
NVS_ENZ_hTrkA	-	EAW52902.1
BSK_hDFCGF_CollagenIII_down	-	NP_000081.1
ACEA_T47D_80hr_Positive	2	NP_000116.2
ATG_ERE_CIS_up	75	NP_000116.2
ATG_ERa_TRANS_up	117	NP_000116.2
NVS_NR_hER	714	NP_000116.2

ACEA_T47D_80hr_Positive

Assay Title: ACEA 80-hr T47-D Human Breast Cell Proliferation Assay

1. Assay Descriptions

1.1. Overview

Assay Summary:

One possible effect of endocrine disrupting chemicals is increased cell growth through perturbation of pathways linked to cell cycle regulation. Activation of the estrogen receptor (ER) signaling pathway, for example, is one possible mechanism that underlies cell proliferation in hormonally sensitive tissues such as mammary and endometrial tissue. The role of steroid hormones in the regulation of some mammary tumors has been well established (Russo and Russo 2006, Yager and Davidson 2006) and has motivated the development of estrogen pathway-based chemotherapeutics. This assay was designed to identify those chemicals in the ToxCast chemical library with the potential to affect cell growth by activating the estrogen receptor-mediated cell proliferation pathway. These impacts were observed by monitoring changes in electrical impedance on the surface of an electronic cell culture growth plate (E-plates) following 80-hour incubation with test chemicals.

1.2. Assay Definition

Assay Throughput:

The assay is conducted on 96-well plates with each plate containing positive controls for proliferation (17β-estradiol) and cytotoxicity (MG132), negative controls (assay media, RPMI 1640), and two concentrations (0.5% and 0.125%) of DMSO solvent controls. Following a 24-hour incubation period, the cells are exposed to test chemicals for 80 hours and response is monitored no less than once per hour.

Experimental System:

T-47D human breast carcinoma ductal cell line, originally derived in 1974 from pleural effusion of a 57-year-old patient, which exhibits epithelial-like morphology (Horwitz et al. 1978, Keydar et al. 1979).

Xenobiotic Biotransformation Potential:

T-47D cells contain specific high affinity receptors for estradiol, progesterone, glucocorticoid and androgen (Horwitz et al. 1978). Some potential for P450 mediated metabolism is present, e.g. CYP1A1, CYP1A2, CYP1B1 (Angus et al. 1999, Hevir et al. 2011, MacPherson and Matthews 2010, Spink et al. 2002, Spink et al. 1998), CYP2B6 (Lo et al. 2010), CYP3A4 (Nagaoka et al. 2006) and CYP2C8(Mitra et al. 2011), as well as some experimental evidence for the capacity to retain expression of some phase II metabolizing enzymes, e.g., UGTs (Harrington et al. 2006, Hevir et al. 2011), GSTs (Hevir et al. 2011) and sulphotransferases (e.g., SULT1A3(Miki et al. 2006), SULT1E1, SULT2B1 (Hevir et al. 2011)).

Basic Procedure:

Materials

	Product	Source	Cat. No.
Cells	T-47D	ATCC	HTB-133
Growth media	RPMI1640	Hyclone	SH30027FS
Growth media serum	10% FBS	Hyclone	SH3007103
Test media	RPMI 1640	Gibco.	11835030
Test media serum	10% charcoal stripped FBS	Hyclone	SH3006803HI

Presently in Development

- Integrate Modal for assay details, tcpl processing, linkages to AOPs etc

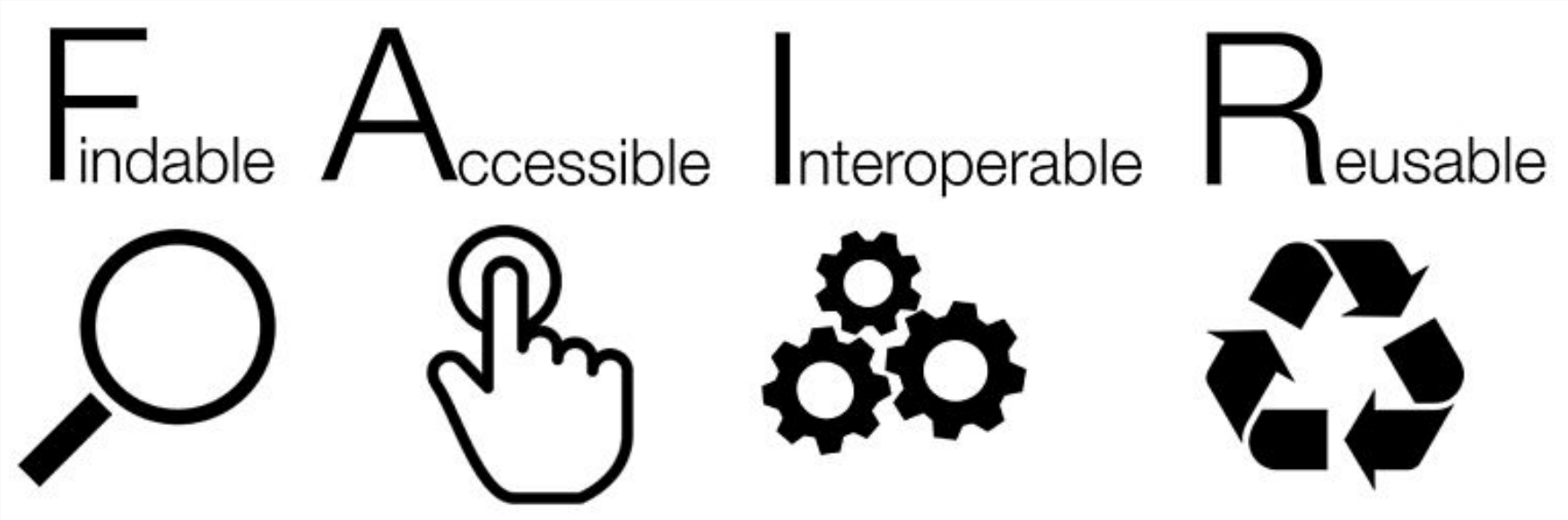
Annotations | Citations | TCPL Processing | Reagents | AOPs

Excel

	Assay Run Type	Level Applied	Method Name	Description
1	MULTI	level2	none	apply no level 2 method
2	MULTI	level3	bval.apid.nwllslowconc.med	Take the median cval of the n wells and the first two concentrations, by apid
3	MULTI	level3	pval.apid.medpcbyconc.min	plate-wise median response of positive control (min)
4	MULTI	level3	resp.pc	response percent activity
5	MULTI	level3	resp.blineshift.50.repi	Do baseline correction by repi, with a window of 50
6	MULTI	level5	bmad3	Add a cutoff value of 3*bmad.
7	MULTI	level5	pc20	Add a cutoff value of 20.
8	MULTI	level5	bmad6	Add a cutoff value of 6*bmad.
9	SINGLE	level1	bval.apid.tn.med	Take the median cval of the t and n wells, by apid
10	SINGLE	level1	pval.apid.or.aeid.pwlls.med	calculates pval first based on p wells by plate and then for any plates missing p wells it calculates a pval by median of pval for all other plates
11	SINGLE	level1	resp.pc	response percent activity
12	SINGLE	level2	pc30orbmad3	Add a cutoff value of either 30 or 3*bmad, whichever is less.

NVS_NR_hER 714 NP_000116.2 200 1181 ACTIVE 69.2 2.85 0.230 -0.639 nuclear

Our support for FAIR Data



Downloadable Data

EPA United States Environmental Protection Agency

EPA United States Environmental Protection Agency | Home | Advanced Search | Batch Search | Lists | Predictions | Downloads | Search All Data

Chemistry Dashboard

Downloads

DSSTox Identifier to PubChem Identifier Mapping File — Posted: 11/14/2016

The DSSTox to PubChem Identifiers mapping file is in TXT format and includes the PubChem SID, PubChem CID and DSSTox substance identifier (DTXSID).

```
SID        CID        DTXSID
316388891  20404      DTXSID30873143
316388890  10142816   DTXSID70873142
316388889  50742127   DTXSID40873139
316388888  19073841   DTXSID20873137
316388887  11505215   DTXSID00873135
316388886  25021861   DTXSID80873133
316388885  2784427    DTXSID60873131
316388884  6731       DTXSID00873130
```

DSSTox identifiers mapped to CAS Numbers and Names File — Posted: 11/14/2016

The DSSTox Identifiers file is in Excel format and includes the CAS Number, DSSTox substance identifier (DTXSID) and the Preferred Name.

1	casrn	dsstox_substance_id	preferred_name
2	26148-68-5	DTXSID7020001	A-alpha-C
3	107-29-9	DTXSID2020004	Acetaldehyde oxime
4	60-35-5	DTXSID7020005	Acetamide
5	103-90-2	DTXSID2020006	Acetaminophen
6	968-81-0	DTXSID7020007	Acetohexamide
7	18523-69-8	DTXSID2020008	Acetone[4-(5-nitro-2-furyl)-2-thiazolyl] hydrazone
8	75-05-8	DTXSID7020009	Acetonitrile
9	127-06-0	DTXSID6020010	Acetoxime
10	65734-38-5	DTXSID6020012	N'-Acetyl-4-(hydroxymethyl) phenylhydrazine

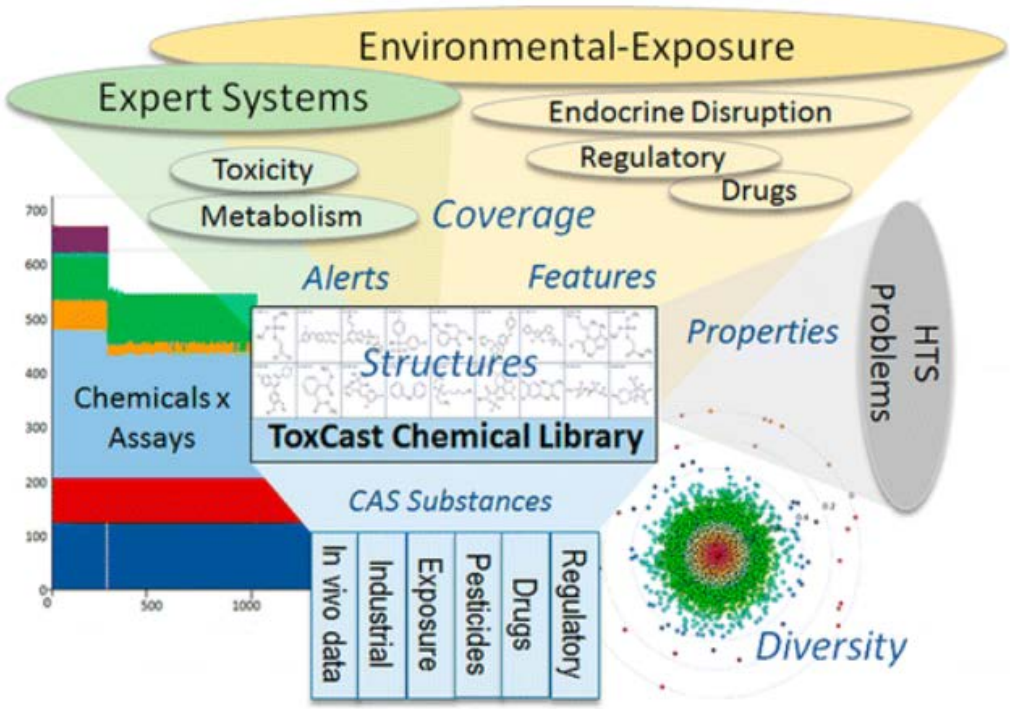
The ToxCast Chemical Landscape

https://pubs.acs.org/doi/abs/10.1021/acs.chemrestox.6b00135

Chemical Research in Toxicology

ToxCast Chemical Landscape: Paving the Road to 21st Century Toxicology

Ann M. Richard[*†], Richard S. Judson[†], Keith A. Houck[†], Christopher M. Grulke[†], Patra Volarath[‡], Inthirany Thillainadarajah[§], Chihae Yang[∥⊥], James Rathman[⊥#], Matthew T. Martin[†], John F. Wambaugh[†], Thomas B. Knudsen[†], Jayaram Kancherla[▽], Kamel Mansouri[▽], Grace Patlewicz[†], Antony J. Williams[†], Stephen B. Little[†], Kevin M. Crofton[†], and Russell S. Thomas[†]



New ToxCast Users Manual

https://www.epa.gov/chemical-research/toxcast-owners-manual-guidance-exploring-data

EPA United States Environmental Protection Agency

ToxCast Owner's Manual – Guidance for Exploring Data

ToxCast is a multi-year effort launched in 2007 that uses automated chemical screening technologies called high-throughput screening assays to expose living cells, isolated proteins, or other biological molecules to chemicals. The cells or proteins are then screened for changes in biological activity that may suggest potential toxic effects.

These innovative methods have the potential to limit the number of required laboratory animal-based toxicity tests while quickly and efficiently screening thousands of chemicals for potential health effects.

Resources

- ToxCast Owner's Manual PDF
- Toxicity Forecaster (ToxCast) Fact Sheet
- ToxCast Publications
- About ToxCast

Generating ToxCast Data

- Chemicals
- Assays
- Results Processing and Analysis
- Publicly Available Data

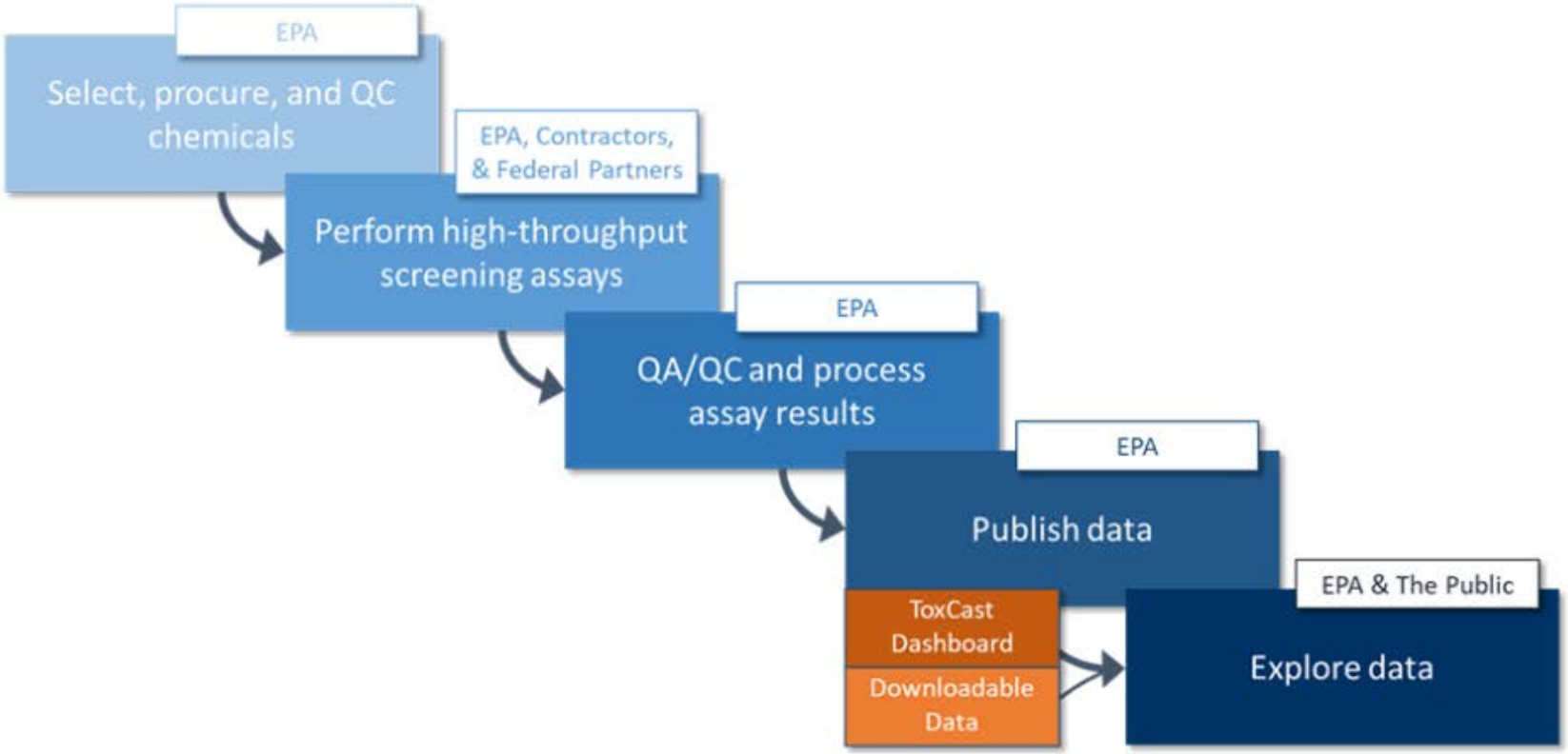
Exploring ToxCast Data

- ToxCast Data
- Accessing ToxCast Data and Scenarios for Exploring Data
- Citations for ToxCast Data

New ToxCast Users Manual

https://www.epa.gov/chemical-research/toxcast-owners-manual-guidance-exploring-data

Click on the boxes in the figure below to link to more information.



Future Search Possibilities

EPA United States Environmental Protection Agency

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Chemistry Dashboard

Aa | Aa | Aa

761 Thousand Chemicals

Chemical | Assay | Gene | Product

Search Assay Endpoint Name

Identifier substring search

Latest News

Read more news

An article regarding an Excel Version of the Abstract Sifter is published.

March 7th, 2018 at 9:21:27 AM

The abstract sifter that is integrated into the Dashboard (for example here for Atrazine) is available as an Excel add-in. Our recent article on the Abstract Sifter for Excel has been published.

Conclusion

- The CompTox Chemistry Dashboard provides access to data for ~760,000 chemicals
- High quality data from ongoing curation efforts
- An integration hub for multiple “modules”
  - Experimental and predicted properties
  - Human and Ecological Hazard data
  - Exposure data – products, data in the environment
  - *In vitro* bioassay data – ToxCast/Tox21
  - Literature searching – Google Scholar and PubMed
  - Specialized searches – mass/formula for analytical support
  - Batch searching and Real Time Predictions
- The primary architecture for NCCT data

Acknowledgments

- The NCCT CompTox Chemistry Dashboard Development Team
- NERL scientists (Jon Sobus, Elin Ulrich) – Mass Spectrometry
- Kamel Mansouri – OPERA models
- Todd Martin – TEST predictions
- Nancy Baker – Abstract Sifter

Contact

Antony Williams

US EPA Office of Research and Development

National Center for Computational Toxicology (NCCT)

Williams.Antony@epa.gov

ORCID: https://orcid.org/0000-0002-2668-4821