

CompTox Chemicals Dashboard

Version 3/2019

<http://comptox.epa.gov/dashboard>

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Overview of changes since August 2018 release

- Data
 - 875k chemicals total. An additional 110k chemical substances added
 - *InvitroDBv3.1* – including updated assay descriptions
 - ToxVal v7 data integrated – includes enormous curation effort
 - New OPERA predictions
- New User Interface elements
 - Reworked tables across the application
 - Reworked multiple chemical results page
 - Navigating concentration response plots for all AEIDs in *invitroDB_v3* data, not just the EDSP21 assays
 - Enhanced batch search capabilities

pKa experimental data added – no predictions

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

▶ ADME

▶ EXPOSURE

▶ BIOACT

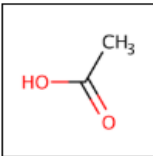
SIMILAR

GENRA

RELATE

SYNONYMS

LITERATURE



Acetic acid
64-19-7 | DTXSID5024394
Searched by Approved Name.

Property

pKa Acidic Apparent

▼

Download Summary

▼

Type	Average	Media
Experimental	4.70	-
Predicted	-	-

Experimental

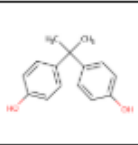
Result	Experimental Data
4.70	

This pKa data was from the DataWarrior application (<http://www.openmolecules.org/>). A file named "pKaInWater.dwar" containing the pKa data is included in the DataWarrior download and contains experimentally-measured pKa values in water for 7912 chemicals along with SMILES strings. The providers of the original file collected and compiled pKa values representing different protonation states. Unfortunately, there are no literature references to support the pKa values. Most of these values are given as an average of multiple experimental values.

Data Warrior

A new “Structure Zoom”

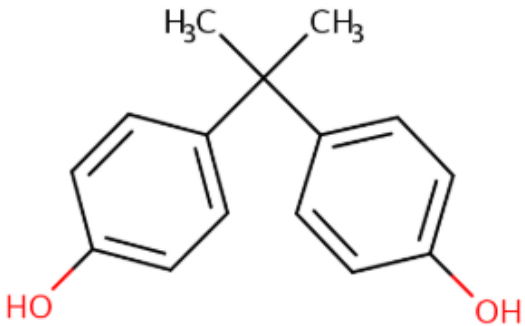

- On-click hover all over the dashboard as well as structure thumbnail



Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.








Wikipedia


Bisphenol A (BPA) is an organic synthetic compound with the chemical formula (C₁₅H₁₆O₂). BPA is a starting material for the synthesis of plastics, primarily certain polycarbonates.

[Read more](#)

Intrinsic Properties

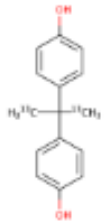


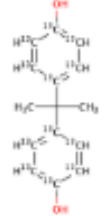


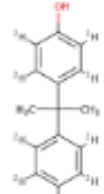


 **Molecular Formula:** C₁₅H₁₆O₂  Mol File  Find All Chemicals

 **Average Mass:** 228.291 g/mol  Isotope Mass Distribution

 **Monoisotopic Mass:** 228.11503 g/mol

Structural Identifiers

Linked Substances

Structure	DTXSID	Preferred Name
	 DTXSID30747173 	4,4'-[(1,3- ¹³ C ₂)Propane-2,2-diyl]diphenol
	 DTXSID10675703 	4,4'-(Propane-2,2-diyl)di(¹³ C ₆)phenol
	 DTXSID40662328 	4,4'-(Propane-2,2-diyl)di(² H ₄)phenol

Reworked multiple results page

Searched with a similarity threshold of 0.8

390 chemicals

Select all

Download

Send to Batch Search

Similarity



DTXSID

CASRN

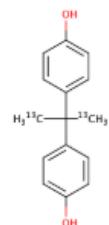
TOXCAST

Similarity



Hide chemicals that are:

Filter by Name or CASRN

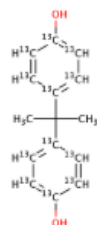


4,4'-[(1,3-¹³C₂)Propane-2,2-diyl]diphenol

DTXSID: DTXSID30747173

CASRN: 263261-64-9

TOXCAST: -

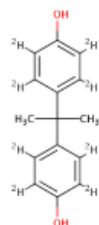


4,4'-(Propane-2,2-diyl)di(¹³C₆)phenol

DTXSID: DTXSID10675703

CASRN: 263261-65-0

TOXCAST: -

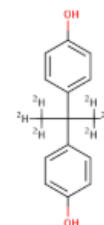


4,4'-(Propane-2,2-diyl)di(²H₄)phenol

DTXSID: DTXSID40662328

CASRN: 92739-58-7

TOXCAST: -

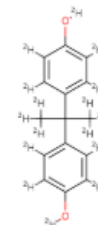


4,4'-[(²H₆)Propane-2,2-diyl]diphenol

DTXSID: DTXSID00584370

CASRN: 86588-58-1

TOXCAST: -



4,4'-[(²H₆)Propane-2,2-diyl]di(²H₅)phenol

DTXSID: DTXSID40583721

CASRN: 96210-87-6

TOXCAST: -

Reworked multiple results page

- Use Ctrl to select multiple display
- Improved visual cues for loading large lists of chemicals

The screenshot shows a web interface for chemical data. At the top, there's a header with "Similarity" and a dropdown arrow. Below it, a row of tabs includes "DTXSID", "PubChem", and "PubMed", each with a close button. A dropdown menu is open, listing options: "CASRN", "DTXSID", "TOXCAST", "PubChem", "PubMed", "Sources", "CPDAT", "Mass", "Molecular Formula", and "Similarity". The "DTXSID" option is highlighted in blue. In the background, chemical structures are visible, including one labeled "4,4'-(Propane-2,2-d)" and another labeled "Propane-2,2-d". At the bottom, "DTXSID: DTXSID10675703" is displayed.

The screenshot shows a dark blue navigation bar. On the right, it says "2000 of 23514 chemicals loaded" with a red arrow pointing to a progress bar. Below this, there are buttons for "Select all", "Download", "Send to Batch Search", "Default", and a dropdown menu showing "DTXSID" and "CASRN". A "Hide" button is on the far right.

- Loading of Large lists RETAINS ordering

The screenshot shows a page titled "TSCA Inventory, active non-confidential portion 2". It has a search bar and a "List Details" section. Below the search bar, there's a table of chemicals. The first row shows "Acetamide" with its chemical structure, DTXSID: DTXSID0702005, and CASRN: 60-35-5. The second row shows "Acetaminophen" with its chemical structure, DTXSID: DTXSID020006, and CASRN: 103-90-2. The third row shows "Acetonitrile" with its chemical structure, DTXSID: DTXSID0702009, and CASRN: 75-05-8. The fourth row shows "Acetoxime" with its chemical structure, DTXSID: DTXSID0602010, and CASRN: 127-06-9. At the bottom, it says "23514 chemicals".

Bioactivity Data

▼ BIOACTIVITY
TOXCAST: SUMMARY
EDSP21
TOXCAST/TOX21
PUBCHEM
TOXCAST: MODELS

- Summary data now has “enhanced tables”
- EDSP21 subset of assays has grown
- Toxcast/Tox21 “all data” has been integrated
- PubChem data widget – no change
- Subset of ToxCast “Models” – extended to include “COMPARA” data

Tables Reworked – Column Selection

- Ability to select columns to show added for tables –Bioactivity most important – Pick your own preferred display

185 active of 839 assays

Download Columns 10

Search query Show Inactive Show Background

Name	Modal	Description	SeqaPASS	Gene Name	AOP	Event	Hit Call	Top	AC50	logAC50	MaxMed	Cutoff	ModlAcc	Intended Target Family
ACEA_ER_80hr		2	NP_000116.2	ESR1	200	1181	ACTIVE	112	0.373	-0.428	113	26.9	-0.686	nuclear receptor
APR_HepG2_Cell		-	-	-	-	-	ACTIVE	1.20	106	2.02	1.20	0.663	2.04	cell cycle
APR_HepG2_Mitc		-	-	-	-	-	ACTIVE	0.874	109	2.04	0.867	0.496	2.05	cell morphology
APR_HepG2_Mitc		-	-	-	-	-	ACTIVE	5.92	11.0	1.04	6.45	0.838	0.813	cell morphology
APR_HepG2_Oxic		-	-	-	-	-	ACTIVE	1.20	110	2.04	1.19	0.819	2.08	cell cycle
APR_HepG2_Cell		-	-	-	-	-	ACTIVE	4.49	95.2	1.98	4.43	0.889	1.75	cell cycle
APR_HepG2_Mitc		-	-	-	-	-	ACTIVE	2.71	85.3	1.93	2.26	0.733	1.70	cell morphology
APR_HepG2_Mitc		-	-	-	-	-	ACTIVE	1.66	84.7	1.93	1.44	1.42	2.29	cell cycle
APR_HepG2_Oxic		-	-	-	-	-	ACTIVE	1.80	106	2.02	1.60	1.10	2.08	cell cycle
ATG_Ahr_CIS_up		-	NP_001612.1	AHR	150	18	ACTIVE	1.31	23.4	1.37	1.28	0.994	1.56	dna binding

First << < 1 2 3 4 5 6 7 8 9 10 > >> Last

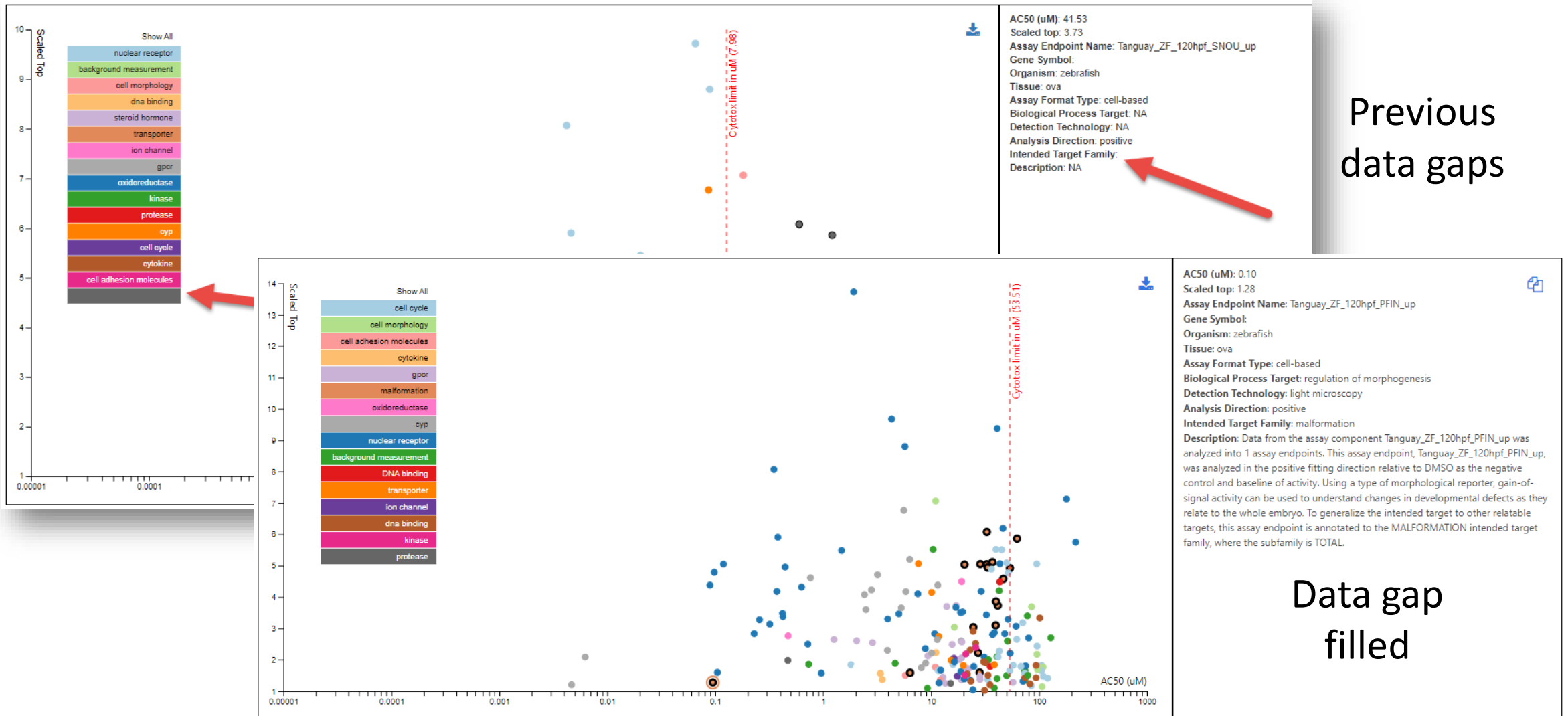
Showing 1 to 10 of 185 records

Discover. Connect. Ask.

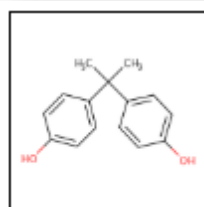
Column Selection Menu:

- ☒ Name
- ☒ Modal
- ☒ Description
- ☒ SeqaPASS
- ☒ Gene Name
- ☒ AOP
- ☒ Event
- ☒ Hit Call
- ☒ Top
- ☐ Scaled Top
- ☒ AC50
- ☒ logAC50
- ☐ Bmad
- ☒ MaxMed
- ☐ MaxMedConc
- ☒ Cutoff
- ☐ Flags
- ☒ ModlAcc
- ☐ ModlAc10
- ☐ ModlAcb
- ☐ Stock Concentration
- ☒ Intended Target Family

Assay Annotations Filled a Lot of Gaps!



Toxcast: Models – COMPARA added




Bisphenol A




80-05-7 | DTXSID7020182

Searched by Expert Validated Synonym.

ToxCast: Models

ToxCast Model Predictions

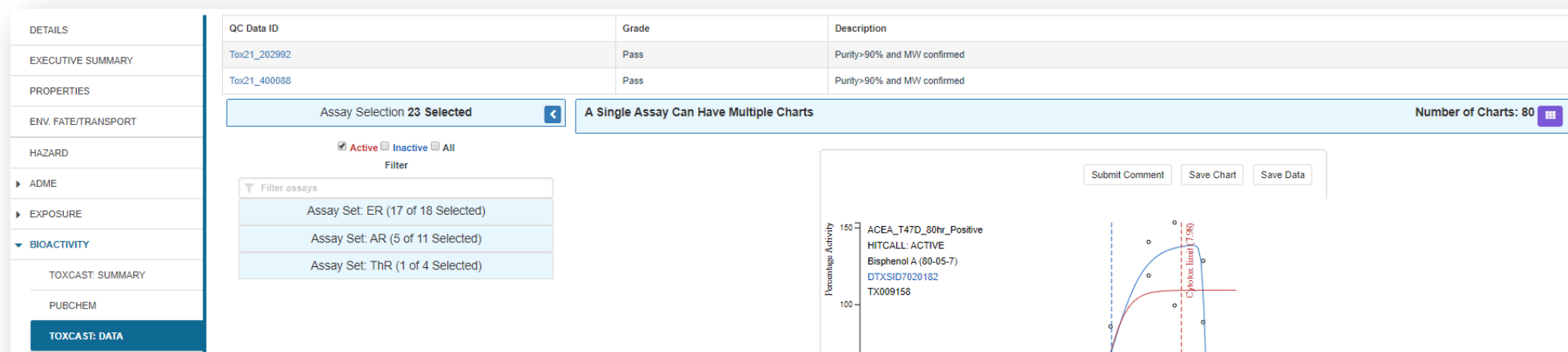
 Download ToxCast Model Predictions ▼

Model	Receptor	Agonist	Antagonist	Binding
 ToxCast Pathway Model (AUC)				-
 CoMPARA is a larger scale collaboration between 35 international groups, using QSAR models to predict androgen receptor activity using a common training set of 1746 compounds provided by U.S. EPA. A key result is a consensus model of AR agonist and antagonist activity that is run against the DSSTox chemical library. These results are intended to be used in prioritization for compounds for follow-up testing. More details about the project are available on ResearchGate .				-
 CERAPP Potency Level (Consensus)				Active
				Active (Weak)
				Active (Weak)

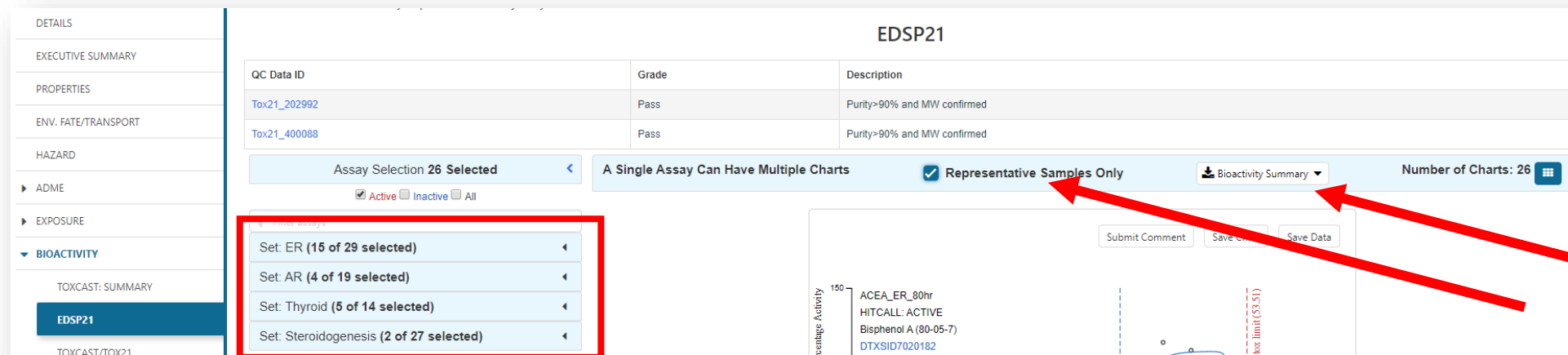
“EDSP Subset”

- New assays added – expanded all subsets. New set of steroidogenesis assays – including CEETOX data

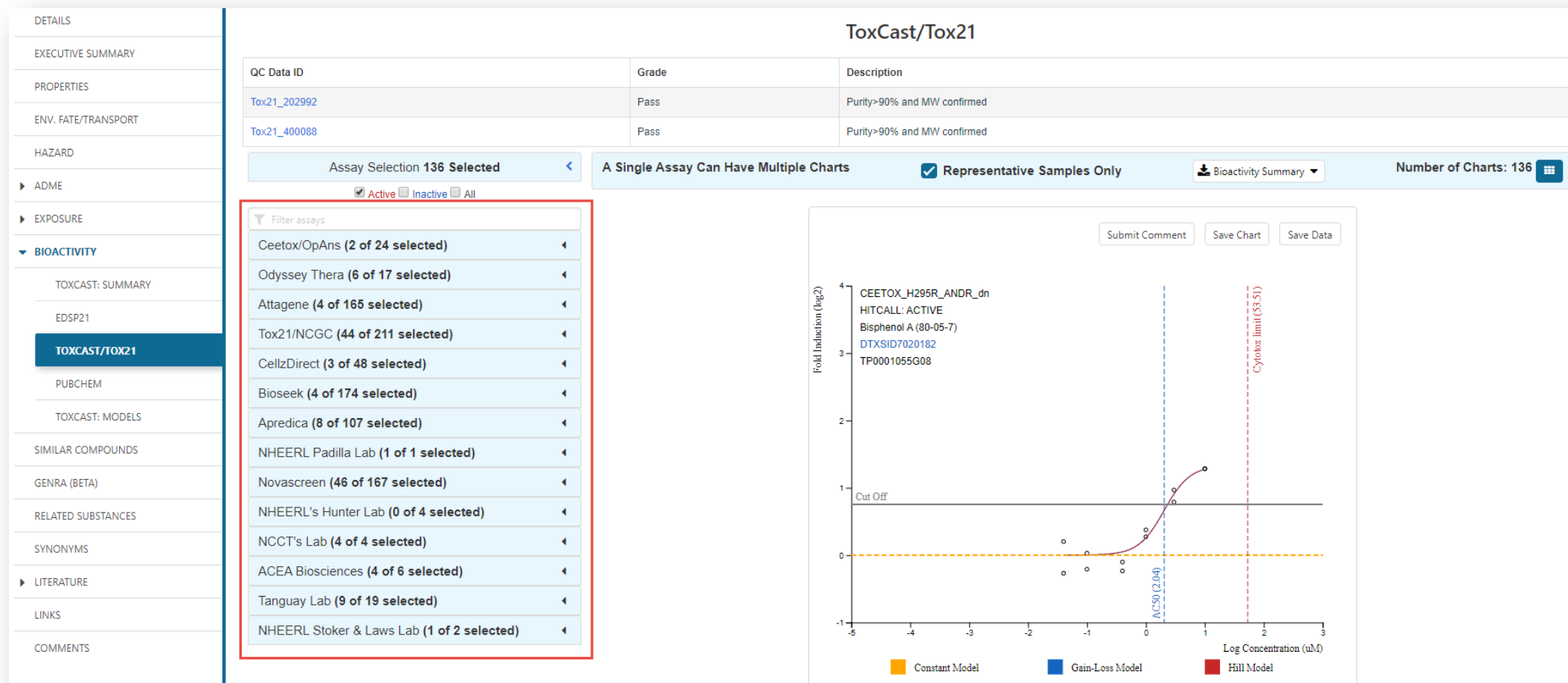
- Previous



- Update



ToxCast/Tox21 Data – All data from invitroDBv3



Filtering – Gene annotation added

Filter assays

Ceetox/OpAns (2 of 24 selected)

Odyssey Thera (6 of 17 selected)

Attagene (4 of 165 selected)

<input type="checkbox"/>	ATG_PBREM_CIS_up	NR1I3	
<input type="checkbox"/>	ATG_E2F_CIS_dn	E2F1	
<input type="checkbox"/>	ATG_HSE_CIS_dn	HSF1	
<input type="checkbox"/>	ATG_EGR_CIS_dn	EGR1	
<input type="checkbox"/>	ATG_ISRE_CIS_dn	IRF1	
<input type="checkbox"/>	ATG_GR_TRANS_dn	NR3C1	
<input type="checkbox"/>	ATG_p53_CIS_up	TP53	
<input type="checkbox"/>	ATG_Oct_MLP_CIS_dn	POU2F1	
<input type="checkbox"/>	ATG_Ets_CIS_up	ETS1	
<input type="checkbox"/>	ATG_EGR_CIS_up	EGR1	
<input type="checkbox"/>	ATG_RARb_TRANS_dn	RARB	
<input type="checkbox"/>	ATG_TGFB_CIS_up	TGFB1	
<input type="checkbox"/>	ATG_PPARG_TRANS_dn	PPARG	
<input type="checkbox"/>	ATG_M_10_CIS_up		
<input type="checkbox"/>	ATG_PXRE_CIS_up	NR1I2	

PPARG

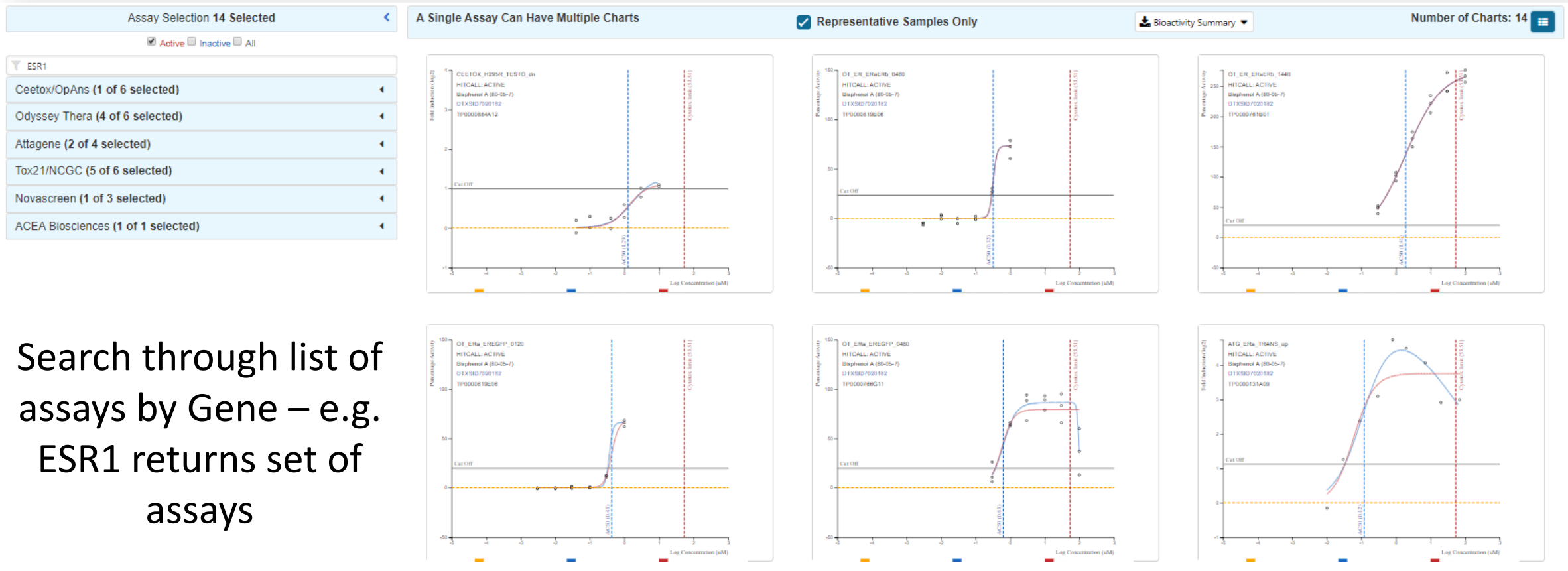
Attagene (0 of 4 selected)

<input type="checkbox"/>	ATG_PPARG_TRANS_dn	PPARG	
<input type="checkbox"/>	ATG_PPARG_CIS_up	3 Genes	
<input type="checkbox"/>	ATG_PPARG_TRANS_up	PPARG	
<input type="checkbox"/>	ATG_PPARG_CIS_dn	3 Genes	

Novascreen (1 of 1 selected)

<input checked="" type="checkbox"/>	NVS_NR_hPPARG	PPARG	
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Filtering



Lists of Chemicals/Lists of Assays

- Reworked Chemical List page – lots of lists added including segregation
 - LIST: Algal Toxins, Amino Acids, Bisphenol Compounds, PAHs, Synthetic Cannabinoids and Psychoactives, Vitamins, PCBs, PBDEs, Hair Dyes
 - WIKILIST: Additives in Cigarettes, Extremely Hazardous Substances
 - EPA: PALs, HPV list, Chemical Contaminants, PPRTV Reports etc, Pesticides Chemical Search
- Helps cluster in the batch search and as a query on the lists page (see figure)
- invitroDbv3 assays added to assay list



Lists of Chemicals

- Download the “list of lists” as Excel or TSV
- Subset of lists from query – “what are all Norman Network lists?”

http://comptox-prod.epa.gov/dashboard/chemical_lists/?search=NORMAN

Select List

Download Columns

NORMAN

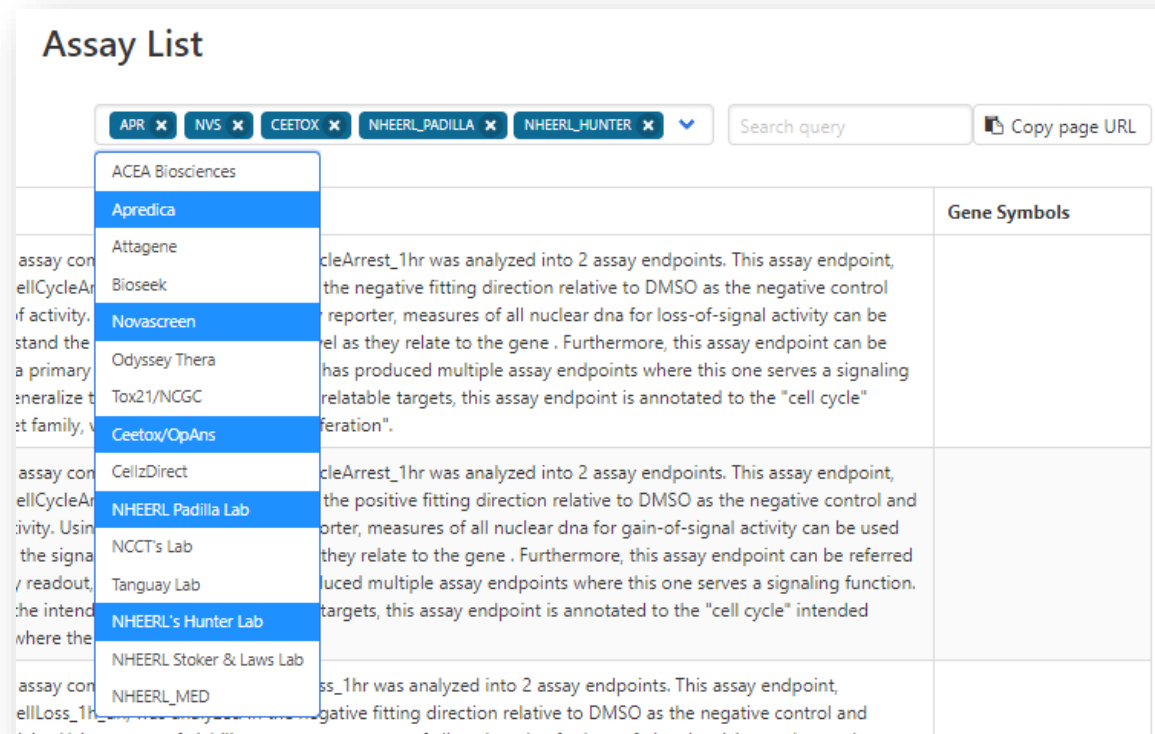
Copy Filtered Lists URL

List Acronym	List Name	Last Updated	Number of Chemicals	List Description
EUBIOCIDES	NORMAN: Biocides from the NORMAN Priority List	2018-07-26	160	List of compounds currently used in the EU as biocides or compounds recently banned as biocides from the 2015 NORMAN priority list, prioritized and assessed for exposure by NORMAN using data from ECHA and other sources.
EUCOSMETICS	NORMAN: Combined 2000/2006 EU Cosmetic Ingredients Inventory	2017-07-14	2878	EUCOSMETICS contains the Combined Inventory of Ingredients Employed in Cosmetic Products (2000, SCCNFP/0389/00 Final) and Revised Inventory (2006, Decision 2006/257/EC), prepared for NORMAN by P. von der Ohe (UBA) and R. Aalizadeh (Uni. Athens).
FRENCHLIST	NORMAN WATER: French Monitoring List	2017-07-14	1171	FRENCHLIST contains substances for prospective monitoring activities in France, developed in cooperation with the NORMAN Network Working Group 1 on Prioritization. Provided by Valeria Dulio, INERIS, France. Further details on the website.
KEMIMARKET	NORMAN: KEMI List of Substances on the Market	2017-07-13	30418	The KEMI Market List contains chemicals expected to be on the market. Compiled by Stellan Fischer, KEMI (Swedish Chemicals Agency) from various regulatory databases, including hazard and exposure scores to support the identification of unknowns.
NORMANCT15	NORMAN: Collaborative Trial 20215 Target and Suspects	2017-07-14	732	NORMANCT15 is a compilation of all target and suspect substances reported by participants in the NORMAN Collaborative Trial on Non-target Screening, run by the NORMAN Network and described in Schymanski et al 2015, DOI: 10.1007/s00216-015-8681-7

List of Assays

- Download list of all assays (Excel or TSV)
- Filter by Vendor or Multiple Vendors
- Subset of lists from query based on substring search e.g.

http://comptox.epa.gov/dashboard/assay_endpoints/?search=ESR1



The screenshot shows the 'Assay List' interface. At the top, there are several vendor filters: APR, NVS, CEETOX, NHEERL_PADILLA, and NHEERL_HUNTER. A search query box and a 'Copy page URL' button are also present. A dropdown menu is open, displaying a list of vendors: ACEA Biosciences, Apredica, Attagene, Bioseek, Novascreen, Odyssey Thera, Tox21/NCGC, Ceetox/OpAns, CellzDirect, NHEERL Padilla Lab, NCCT's Lab, Tanguay Lab, NHEERL's Hunter Lab, NHEERL Stoker & Laws Lab, and NHEERL_MED. The table below the dropdown has columns for assay details and 'Gene Symbols'.


	Gene Symbols
Assay con...	
ellCycleAr...	
of activity...	
stand the...	
a primary...	
eneralize t...	
st family, v...	
Assay con...	
ellCycleAr...	
ivity. Usin...	
the signa...	
/ readout...	
the intend...	
where the...	
Assay con...	
ellLoss_1h...	

For a Specific Assay List

- All the advantages of the new “Multiple Results Page” plus...

Assay Endpoint Name: ACEA_ER_80hr

Assay Details

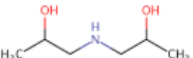
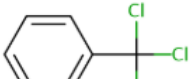

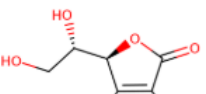
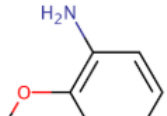
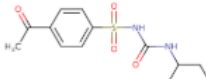
Assay Endpoint Name: ACEA_ER_80hr 

Assay Source Description: ACEA Biosciences, Inc. (ACEA) is a privately owned biotechnology company that developed a real-time, label-free, cell-based assay system based on a microelectronic readout called xCELLigence.

Histograms

425 of 3031 chemicals visible

Select all Download Send to Batch Search Default DTXSID CASRN Inactive Filter by Name or CASRN



Specific Assay List

- Reworked assay table – more details available including AOP Wiki link

All Chemicals in Assay Endpoint: [ACEA_ER_80hr](#)

[Annotations](#) [Citations](#) [tcpl Processing](#) [Reagents](#) [AOPs](#) [Excel](#)

	Assay Run Type	Level Applied	Method Name	Description
1	MULTI	2	none	apply no level 2 method
2	MULTI	3	pval.apid.medpcbyconc.max	plate-wise median response of positive control (max)
3	MULTI	3	resp.pc	response percent activity
4	MULTI	3	bval.apid.nwllslowconc.med	Take the median cval of the n wells and the first two concentrations, by apid
5	MULTI	3	resp.shiftneg.3bmad	Make values below baseline zero.
6	MULTI	4	bmad.aeid.lowconc.twells	bmad based on two lowest concentration of treatment wells
7	MULTI	5	bmad3	Add a cutoff value of 3*bmad.
8	MULTI	5	pc20	Add a cutoff value of 20.
9	MULTI	6	singlept.hit.high	Look for single point hits with activity only at the highest conc tested
10	MULTI	6	singlept.hit.mid	Look for single point hits with activity not at highest conc tested
11	MULTI	6	multipoint.neg	Look for inactives with multiple medians above baseline
12	MULTI	6	noise	Look for noisy curves, relative to the assay
13	MULTI	6	border.hit	Look for actives with borderline activity
14	MULTI	6	border.miss	Look for inactives with borderline activity
15	MULTI	6	modlga.lowconc	AC50 less than lowest concentration tested
16	MULTI	6	gnls.lowconc	Look for low concentration gnls winners
17	MULTI	6	overfit.hit	Flag hit-calls that would get changed after doing the small N correction to the aic values.
18	MULTI	6	efficacy.50	Flag hit-calls with efficacy values less than 50% -- intended for biochemical assays.

All Chemicals in Assay Endpoint: [ACEA_ER_80hr](#)

[Annotations](#) [Citations](#) [tcpl Processing](#) [Reagents](#) [AOPs](#) [Excel](#)

AOP ID	AOP Title
200	Estrogen receptor activation leading to breast cancer

[AOP ID: 200](#)
AOP TITLE: Estrogen receptor activation leading to breast cancer
AUTHOR STATUS: Under development: Not open for comment. Do not cite
SAAOP STATUS: Under Development

Specific Assay List – Histogram summary view








Specific Assay List – Histogram summary view

- Display specific subset of data from histogram – switch to Table Mode



292 of 3031 chemicals visible

Select all Download Send to Batch Search Default DTXSID CASRN Inactive Histogram Union Filter by Name or CASRN

Structure	DTXSID	Preferred Name	# ToxCast Active	% ToxCast Active	Hit Call	Top	Scaled Top	AC50 (uM)	logAC50 (uM)
	DTXSID7020007 ToxCast™	Acetohexamide	4/376	1%	Active	29.3	1.09	4.49	0.652
	DTXSID00020105 ToxCast™	Sodium L-ascorbate	20/662	3%	Active	66.0	2.46	6.68	0.825
	DTXSID8020121 ToxCast™	Sodium azide	26/644	4%	Active	55.5	2.07	96.4	1.98
	DTXSID1020148 ToxCast™	Benzotrichloride	7/646	1%	Active	52.0	1.93	68.7	1.84
	DTXSID8020179 ToxCast™	Diisopropanolamine	9/399	2%	Active	82.9	3.08	8.25	0.916

Batch Search

- New Search input - DTXCID

Select Input Type(s)

- ☐ Identifiers
 - ☐ Chemical Name
 - ☐ CASRN
 - ☐ InChIKey
 - ☐ DSSTox Substance ID
 - ☒ **DSSTox Compound ID**
- ☐ InChIKey Skeleton
- ☐ MS-Ready Formula(e)
- ☐ Exact Formula(e)
- ☐ Monoisotopic Mass

- New Search Outputs

Metadata

- ☐ Curation Level Details
- ☐ NHANES/Predicted Exposure
- ☐ Data Sources
- ☐ Include ToxVal Data Availability
- ☐ Assay Hit Count
- ☐ Number of PubMed Articles
- ☐ PubChem Data Sources
- ☐ CPDat Product Occurrence Count
- ☐ IRIS
- ☐ PPRTV
- ☒ **QC Notes** Clicking on QC Notes will include manual annotation notes added to a record during the chemical registration process.
- ☐ Include links to Action Reports

Enhanced Data Sheets

- ☐ MetFrag Input File (Beta)
- ☐ ToxPrint single fingerprints
- ☐ Abstract Sifter Input File (Beta)
- ☐ Synonyms and Identifiers
- ☐ Related Substance relationships
- ☐ ToxPrint fingerprints (ChemoTyper format - CSV/TSV only)
- ☒ **Associated ToxCast Assays**

What are QC Notes?

Examples

- Toxaphene

Quality Control Notes

Complex, but reproducible mixture of at least 175 distinct C₁₀-chloro compounds, having an approximate overall empirical formula of C₁₀H₁₀Cl₈; the 2 most active components are a C₁₀H₁₀Cl₈ compound and a C₁₀H₁₁Cl₇ compound which had been elucidated as 2,2,5-endo,6-exo,8,9,10-heptachlorobornane. Produced by the chlorination of camphene to 67-69% chlorine by weight and made up of compds. of C₁₀H₈Cl₁₀, C₁₀H₁₈-n Cl_n (mostly polychlorobornanes) and C₁₀H₁₆-n Cl_n (polychlorobornanes and/or polychlorotricyclenes) with n = 6 to 9 See Merck Index

- Antimycin A

Quality Control Notes

mixture of antimycin A1; A2; A3 and A4

- Safflower Oil

Quality Control Notes

Extractives and their physically modified derivatives. It consists primarily of the glycerides of the fatty acid linoleic. (*Carthamus tinctorius*).

Associated ToxCast assays for chemicals

☐ Abstract Sitter Input File (Beta)

☐ Synonyms and Identifiers

☐ Related Substance relationship

☐ ToxPrint fingerprints (ChemoTy

☒ Associated ToxCast Assays

Selecting this checkbox provides a separate Excel worksheet with input chemicals listed (as columns) and all assays that those chemicals have been examined in. The cells are color-coded as red for ACTIVE and blue as INACTIVE. For a thorough understanding of all parameters reported in the Excel spreadsheet the user is referenced to various documentation including 1) an article entitled "[tcpl: the ToxCast pipeline for high-throughput screening data](#)" and 2) [documentation regarding tcpl on the Comprehensive R Archive Network \(cran\)](#). Attention is specifically directed to the [Introduction vignette providing vignette an overview of the tcpl package](#).

		DTXSID9020112	DTXSID3020122	DTXSID2020137	DTXSID6020141
51	APR_HEPG2_MITOMEMBROT_72H_UP	0	0	0	0
52	APR_HEPG2_MITOTICARREST_72H_DN	0	0	0	0
53	APR_HEPG2_MITOTICARREST_72H_UP	0	0	0	0
54	APR_HEPG2_NUCLEARSIZE_72H_DN	0	0	0	0
55	APR_HEPG2_NUCLEARSIZE_72H_UP	0	0	0	0
56	APR_HEPG2_OXIDATIVESTRESS_72H_DN	0	0	0	0
57	APR_HEPG2_OXIDATIVESTRESS_72H_UP	0	0	0	0
58	APR_HEPG2_P53ACT_72H_DN	0	0	0	0
59	APR_HEPG2_P53ACT_72H_UP	0	0	0	0
60	APR_HEPG2_STRESSKINASE_72H_DN	0	0	0	0
61	APR_HEPG2_STRESSKINASE_72H_UP	0	0	0	0
62	ATG_AHR_CIS_UP	0	0	0	0
63	ATG_AP_1_CIS_UP	0	0	0	0
64	ATG_AP_2_CIS_UP	0	0	0	0
65	ATG_BRE_CIS_UP	0	0	0	0
66	ATG_C_EBP_CIS_UP	0	0	0	0
67	ATG_CMV_CIS_UP	0	0	0	0
68	ATG_CRE_CIS_UP	0	0	0	0
69	ATG_DR4_LXR_CIS_UP	0	0	0	0
70	ATG_DR5_CIS_UP	0	0	0	0
71	ATG_E_BOX_CIS_UP	0	0	0	0
72	ATG_E2F_CIS_UP	0	0	0	0
73	ATG_EGR_CIS_UP	0	0	0	0
74	ATG_ERE_CIS_UP	0	0	0	0
75	ATG_ETS_CIS_UP	0	0	0	0
76	ATG_FOXA2_CIS_UP	0	0	0	0
77	ATG_FOXP1_CIS_UP	0	0	0	0
78	ATG_GATA_CIS_UP	0	0	0	0
79	ATG_GLI_CIS_UP	0	0	0	0
80	ATG_GRE_CIS_UP	0	0	0	0
81	ATG_HIF1A_CIS_UP	0	0	0	0

Related Substance Relationships

Enhanced Data Sheets

☐ MetFrag Input File (Beta)

☐ ToxPrint single fingerprints

☐ Abstract Sifter Input File (Beta)

☐ Synonyms and Identifiers

☒ Related Substance relationships

☐ ToxPrint fingerprints (ChemoTyper f

☐ Associated ToxCast Assays

☐ EPA: National-Scale Air

☐ EPA: PPRTV Chemical R

☐ EPA: Provisional Adviso

☐ EPA: Safer Choice Chem

Selecting this checkbox provides a separate Excel worksheet containing the relationship between two chemicals. The output file includes the DTXSIDs and names/CASRN between the input list and the related chemical. Relationships include, for example, polymer, components, salt form, transformation product and other relationships.

	A	B	C	D	E	F	G	H
1	INPUT	DTXSID	PREFERRED_NAME	HAS_RELATIONSHIP_WITH	RELATED_DTXSID	RELATED_PREFERRED_NAME	RELATED_CASRN	
2	xylenes	DTXSID2021446	Xylenes	Transformation Product	DTXSID40176394	N-Benzoylalanine	2198-64-3	
3	xylenes	DTXSID2021446	Xylenes	Component	DTXSID6026298	m-Xylene	108-38-3	
4	xylenes	DTXSID2021446	Xylenes	Component	DTXSID3021807	o-Xylene	95-47-6	
5	xylenes	DTXSID2021446	Xylenes	Component	DTXSID2021868	p-Xylene	106-42-3	
6	xylenes	DTXSID2021446	Xylenes	Predecessor: Component	DTXSID9021421	Xylenes; defined mixture 1	NOCAS_21421	
7	xylenes	DTXSID2021446	Xylenes	Predecessor: Component	DTXSID7021447	Xylenes; defined mixture 2	NOCAS_21447	
8	xylenes	DTXSID2021446	Xylenes	Predecessor: Component	DTXSID30891529	Total Petroleum Hydrocarbons (TPH)	NOCAS_891529	
9	xylenes	DTXSID2021446	Xylenes	Markush Child	DTXSID3021807	o-Xylene	95-47-6	
10	xylenes	DTXSID2021446	Xylenes	Markush Child	DTXSID6026298	m-Xylene	108-38-3	
11	xylenes	DTXSID2021446	Xylenes	Markush Child	DTXSID2021868	p-Xylene	106-42-3	

Work in Progress

- New manual in development
- Training “videos” will be posted to YouTube in the future
- New lists are in preparation to add to the lists page

Feedback welcome

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