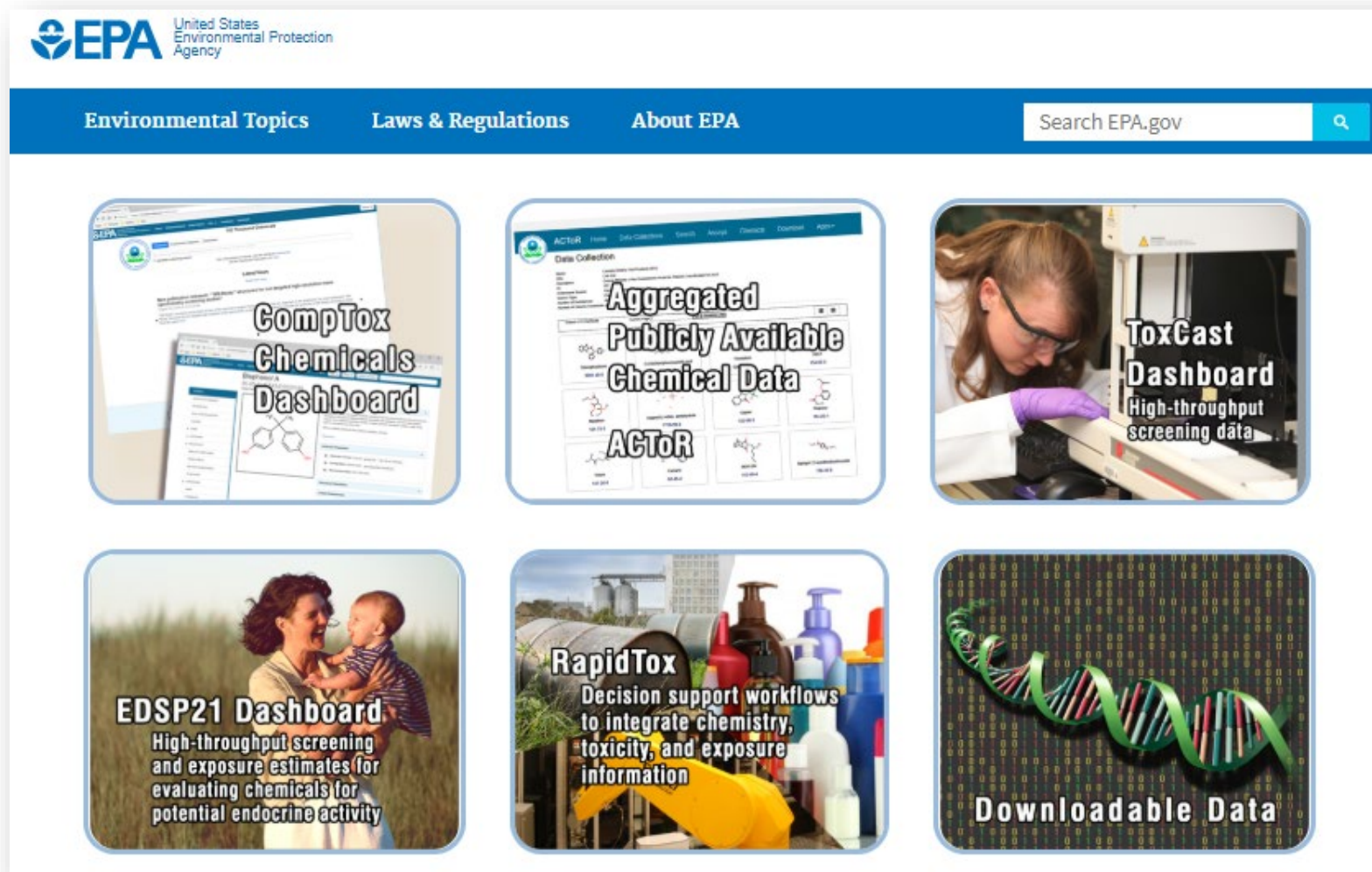


ANNOUNCEMENT

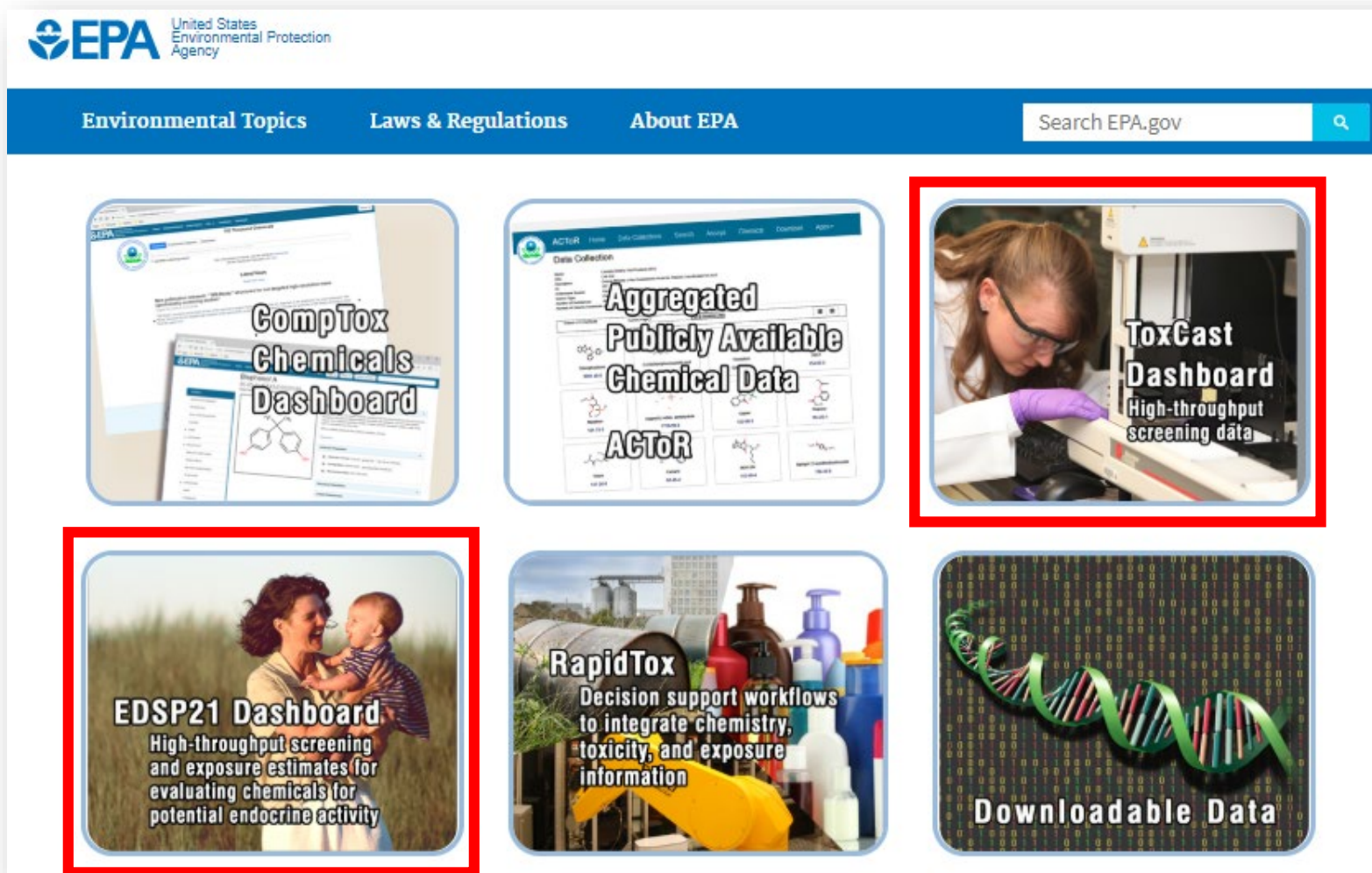
EDSP21 and ToxCast Dashboards To Be Discontinued

Disclaimer: The views expressed in this presentation are those of the author(s) and do not necessarily represent the views or policies of the U.S. Environmental Protection Agency, nor does mention of trade names or products represent endorsement for use.

The Existing CompTox Portal



Two legacy dashboards to be discontinued



invitrodb version 3 data release

- When *invitrodb* version 3 data were released access was provided to the data via the CompTox Chemicals Dashboard only
- Legacy EDSP21 and ToxCast dashboards were **not** updated with new data and **will be retired from service by end of August 2019**
- New functionality supporting the bioactivity data associated with ToxCast, Tox21 and EDSP is available at <https://comptox.epa.gov/dashboard>
- This presentation provides an overview of bioactivity data in the dashboard

Bioactivity Sub-Tabs

Segregation of data

Bioactivity Data

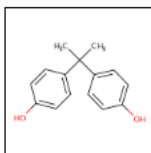
▼ BIOACTIVITY
TOXCAST: SUMMARY
EDSP21
TOXCAST/TOX21
PUBCHEM
TOXCAST: MODELS

- Summary view of data – tabular and graphical
- Navigate to the EDSP21 subset of assays
- Navigate to all Toxcast/Tox21 data
- Navigate to PubChem data widget
- ToxCast "Models" – now includes "COMPARA" data

ToxCast:Summary

Sub-Tab

ToxCast Summary Plot



Bisphenol A

80-05-7 | DTXSID7020182

Searched by Expert Validated Synonym.

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

▶ ADME

▶ EXPOSURE

▼ BIOACTIVITY

TOXCAST: SUMMARY

EDSP21

TOXCAST/TOX21

PUBCHEM

TOXCAST: MODELS

SIMILAR COMPOUNDS

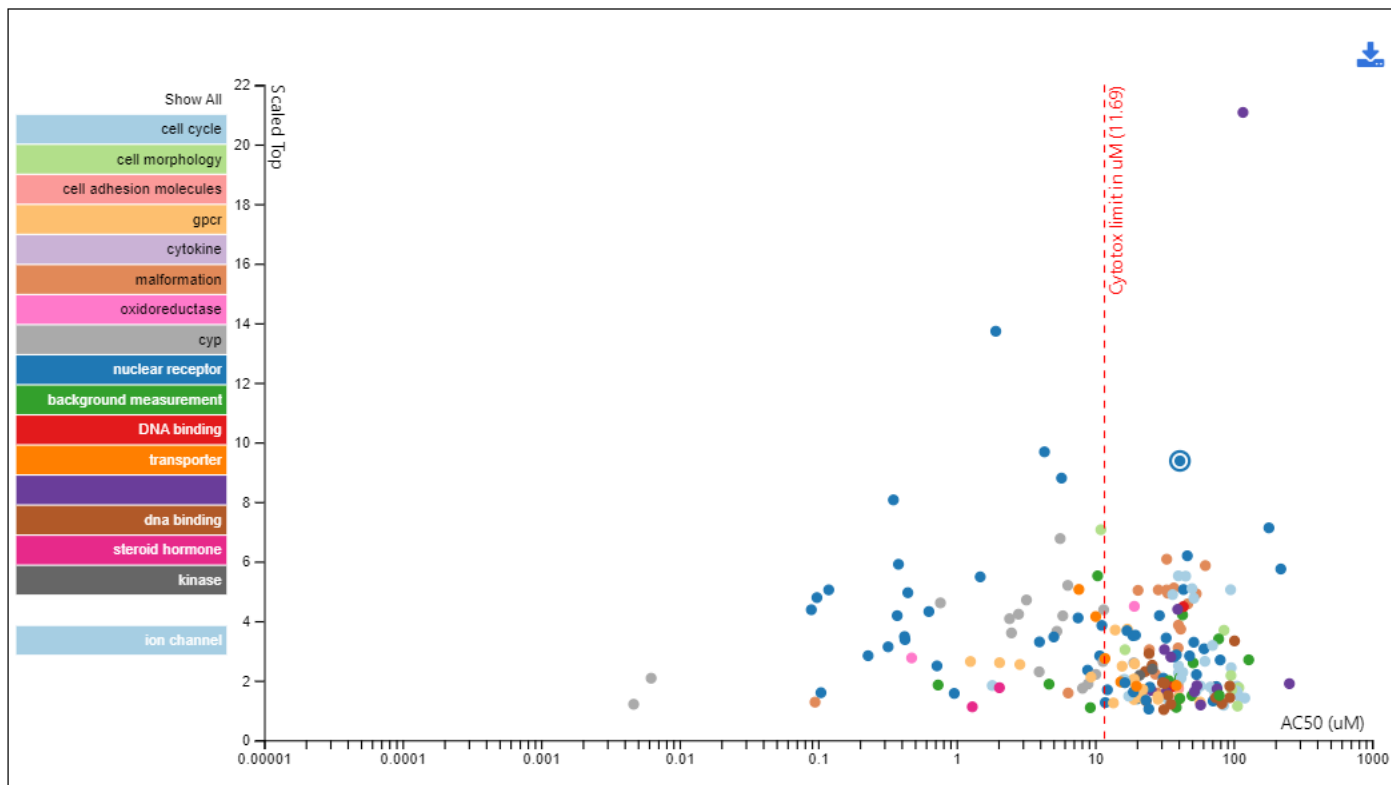
GENRA (BETA)

RELATED SUBSTANCES

Chemical Activity Summary i

i TOXCAST DATA

i ASSAY DETAILS



AC50 (uM): 40.99

Scaled top: 9.38

Assay Endpoint Name: ACEA_AR_antagonist_80hr

Gene Symbol: AR

Organism: human

Tissue: prostate

Assay Format Type: cell-based

Biological Process Target: cell proliferation

Detection Technology: RT-CES

Analysis Direction: NA

Intended Target Family: nuclear receptor

Description: Data from the assay component ACEA_AR_agonist_80hr was analyzed in the positive fitting direction relative to DMSO as the negative control and baseline of activity. Using a type of growth reporter, measures of the cells for gain-of-signal activity can be used to understand the signaling at the pathway-level as they relate to the gene AR. Furthermore, this assay endpoint can be referred to as a primary readout, because this assay has produced multiple assay endpoints where this one serves a signaling function. 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".

Hover over Informational Icons for help

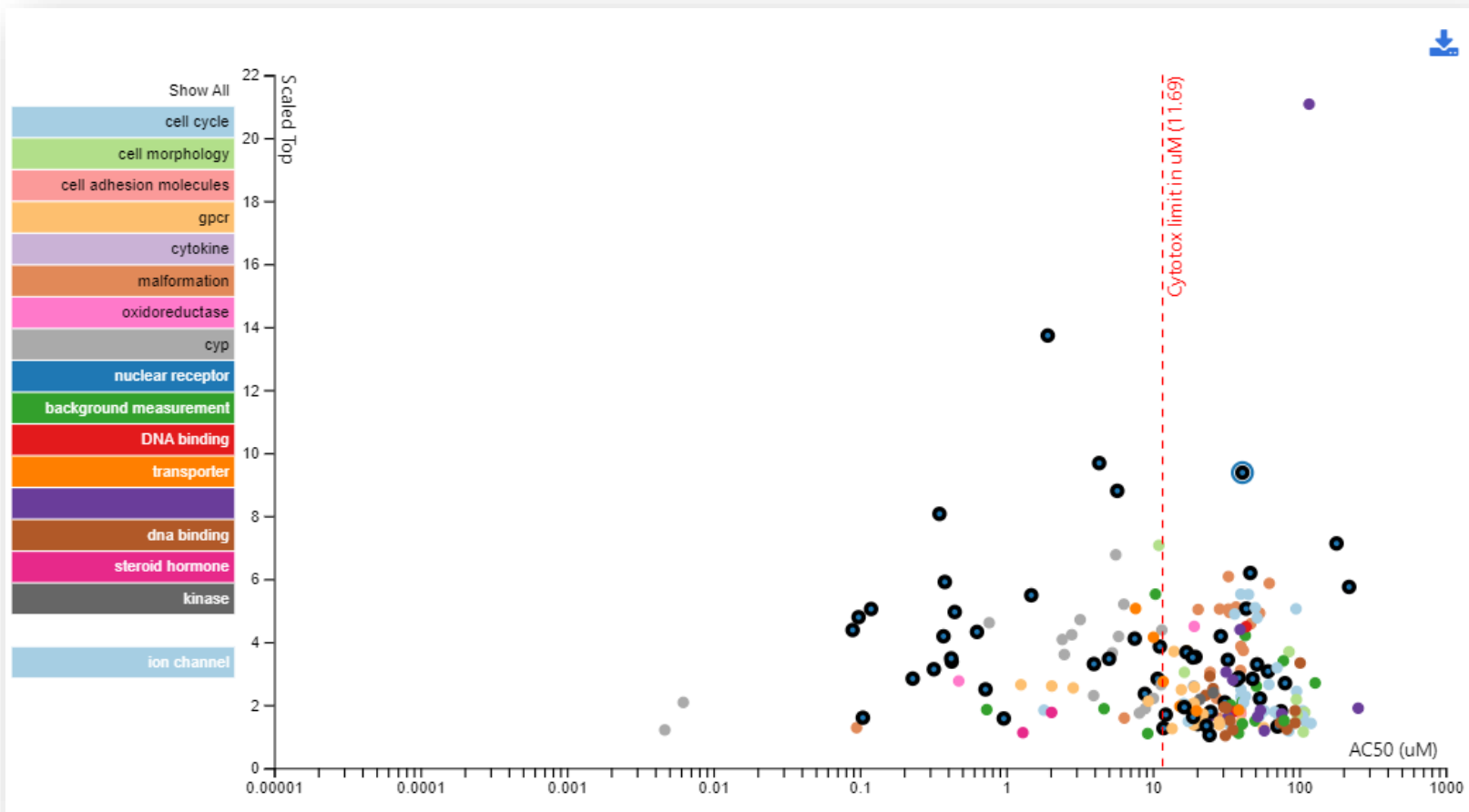
Chemical Activity Summary 


 TOXCAST DATA

 ASSAY DETAILS

2 The bioassay data displayed in this panel includes modeled AC50 values from multi-concentration data only. Single concentration data may also be available for some assay technologies. Single concentration data are included in the list of 'tested' assays endpoints if multi-concentration data are unavailable; this can be visualized by searching for a chemical, and clicking "All Tested" in the [Assay pane in the Toxcast Dashboard](#). Raw, normalized, and interpreted single concentration data from level 0 to level 2 are fully available from the [freely downloadable MySQL database, invitrodb](#). Internet Explorer may enable the best functionality to view the Toxcast Dashboard. The scaled response shown on the graph below is calculated by dividing the response values by the activity cutoff thereby enabling response comparisons across assay endpoints.

ToxCast Summary Plot



- Hover over target type and associated data points will “pulse”
- Click on target type to switch off all data points. Click again to switch them on.
- Download a copy of the Summary Plot by clicking on 

ToxCast Summary Table

211 active of 989 assays

Download

Columns

10

Search query



Show Inactive



Show Background

Name	Modal	SeqAPASS	Gene Symbol	AOP	Event	Hit Call	Top	AC50	logAC50	Cutoff	ModIAcc	Intended Target Family
NVS_ENZ_hTrkA		EAW52902.1	NTRK1	-	-	ACTIVE	43.6	21.0	1.32	20.0	1.28	kinase
BSK_hDFCGF_CollagenIII_down		NP_000081.1	COL3A1	-	-	ACTIVE	0.254	40.0	1.60	0.144	1.60	cell adhesion molecules
ACEA_ER_80hr		NP_000116.2	ESR1	200	1181	ACTIVE	112	0.373	-0.428	26.9	-0.686	nuclear receptor
ATG_ERE_CIS_up		NP_000116.2	ESR1	200	1181	ACTIVE	2.41	9.81e-2	-1.01	0.503	-1.32	nuclear receptor
ATG_ERa_TRANS_up		NP_000116.2	ESR1	200	1181	ACTIVE	5.70	0.119	-0.923	1.13	-1.49	nuclear receptor
NVS_NR_hER		NP_000116.2	ESR1	200	1181	ACTIVE	69.2	0.230	-0.639	24.4	-0.805	nuclear receptor
OT_ER_ERaERa_0480		NP_000116.2	ESR1	200	1181	ACTIVE	176	5.73	0.758	20.0	7.33e-2	nuclear receptor
OT_ER_ERaERa_1440		NP_000116.2	ESR1	200	1181	ACTIVE	194	4.31	0.635	20.0	2.15e-2	nuclear receptor
OT_ERa_EREGFP_0120		NP_000116.2	ESR1	200	1181	ACTIVE	67.5	0.424	-0.372	20.0	-0.458	nuclear receptor
OT_ERa_EREGFP_0480		NP_000116.2	ESR1	200	1181	ACTIVE	86.4	0.631	-0.200	20.0	-0.423	nuclear receptor

First

<<

<

1

2

3

4

5

6

7

8

9

10

>

>>

Last











Showing 1 to 10 of 211 records

ToxCast Summary Table

Columns ▾ 10 ▾

- ☒ Name
- ☒ Modal
- ☐ Description
- ☒ SeqAPASS
- ☒ Gene Symbol
- ☐ Gene Name
- ☐ Gene Url
- ☒ AOP
- ☒ Event
- ☒ Hit Call
- ☒ Top
- ☐ Scaled Top
- ☒ AC50
- ☒ logAC50
- ☐ Bmad
- ☐ MaxMed
- ☐ MaxMedConc
- ☒ Cutoff
- ☐ Flags
- ☒ ModIAcc
- ☐ ModIAcc10

- Select/change columns of data displayed in the table
- In the table hover over some column-headings for details
- Sort columns using up/down arrows
- Blue hyperlinks either download files or link out

SeqAPASS ^	Gene Symbol ↕	AOP ↕	Event ↕	Hit Call ↕	Top ↕	AC50 ↕	logAC50 ↕	Cutoff ↕	ModIAcc ↕	Intended Target Family ↕
EAW52902.1 	NTRK1			ACTIVE	43.6	21.0	1.32	20.0	1.28	kinase
NP_000081.1 	COL3A1									
NP_000116.2 	ESR1	200	1181	ACTIVE	112	0.373	-0.428	26.9	-0.686	nuclear receptor
NP_000116.2 	ESR1	200	1181	ACTIVE	2.41	9.81e-2	-1.01	0.503	-1.32	nuclear receptor
NP_000116.2 	ESR1	200	1181	ACTIVE	5.70	0.119	-0.923	1.13	-1.49	nuclear receptor
NP_000116.2 	ESR1	200	1181	ACTIVE	69.2	0.230	-0.639	24.4	-0.805	nuclear receptor
NP_000116.2 	ESR1	200	1181	ACTIVE	176	5.73	0.758	20.0	7.33e-2	nuclear receptor
NP_000116.2 	ESR1	200	1181	ACTIVE	194	4.31	0.635	20.0	2.15e-2	nuclear receptor
NP_000116.2 	ESR1	200	1181	ACTIVE	67.5	0.424	-0.372	20.0	-0.458	nuclear receptor
NP_000116.2 	ESR1	200	1181	ACTIVE	86.4	0.631	-0.200	20.0	-0.423	nuclear receptor

Info : Chemical concentration (in μM) where 50% of the maximum response is achieved. For BSK assays, the value listed here as an AC50 is actually a LOEC and not from a fitted curve. This is work in progress. For more information, contact us

ToxCast Summary Table

Insert query text
to filter table






Switch to show all
INACTIVE hit calls


Download Columns 10


NVS ☐ Show Inactive ☒ Show Background

Name	Modal	SeqAPASS	Gene Symbol	AOP	Event	Hit Call	Top	AC50	logAC50	Cutoff	ModIAcc	Intended Target Family
NVS_ENZ_hTrkA		LAWS2902.1	NTRK1	-	-	ACTIVE	43.6	21.0	1.32	20.0	1.28	kinase
NVS_NR_hER		NP_000116.2	ESR1	200	1181	ACTIVE	69.2	0.230	-0.639	24.4	-0.805	nuclear receptor
NVS_NR_hGR		NP_000167.1	NR3C1	66	654	ACTIVE	100	5.04	0.702	28.9	0.286	nuclear receptor
NVS_ADME_hCYP1A1		NP_000490.1	CYP1A1	-	-	ACTIVE	83.5	5.85	0.767	20.0	0.252	cyp
NVS_GPCR_hAdoRA1		NP_000665.1	ADORA1	-	-	ACTIVE	76.2	2.04	0.311	29.3	-0.146	gpcr
NVS_GPCR_hAdrb1		NP_000675.1	ADRB1	-	-	ACTIVE	28.0	22.2	1.35	20.0	1.67	gpcr
NVS_ADME_hCYP2B6		NP_000758.1	CYP2B6	-	-	ACTIVE	87.6	11.5	1.06	20.0	0.880	cyp
NVS_ADME_hCYP2C19_Activator		NP_000760.1	CYP2C19	-	-	ACTIVE	135	5.60	0.748	20.0	-8.01e-2	cyp
NVS_ADME_hCYP2C9		NP_000762.2	CYP2C9	-	-	ACTIVE	72.0	2.49	0.396	20.0	0.211	cyp
NVS_ADME_hCYP2C18		NP_000763.1	CYP2C18	-	-	ACTIVE	104	6.35	0.803	20.0	0.569	cyp

ToxCast Summary Table – Display Assay Modal

Name	Modal	Seq
NVS_ENZ_hTrkA		EAV
NVS_NR_hER		NP
NVS_NR_hGR		NP
NVS_ADME_hCYP1A1		NP
NVS_GPCR_hAdoRA1		NP

- Select modal icon  to display assay details
 - Assay annotations
 - Citations re. the assay
 - tcpl processing details
 - Reagents used in assay
 - Links to Adverse Outcome Pathways

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

<div>Annotations Citations tcpl Processing Reagents AOPs</div>	
Five individual sub-tabs describing an individual assay	
Aeid	573
Assay Component Endpoint Name	NVS_ENZ_hTrkA
Assay Component Endpoint Desc	Data from the assay component NVS_ENZ_hTrkA was analyzed into 2 assay endpoints. This assay endpoint, NVS_ENZ_hTrkA, was analyzed in the positive fitting direction relative to DMSO as the negative control and baseline of activity. Using a type of enzyme reporter, loss-of-signal activity can be used to understand changes in the enzymatic activity as they relate to the gene NTRK1. Furthermore, this assay endpoint can be referred to as a primary readout, because this assay has produced multiple assay endpoints where this one serves a enzymatic activity function. To generalize the intended target to other relatable targets, this assay endpoint is annotated to the "kinase" intended target family, where the subfamily is "receptor tyrosine kinase".
Assay Function Type	enzymatic activity
Normalized Data Type	percent_activity
Analysis Direction	positive
Burst Assay	false
Key Positive Control	Staurosporine
Signal Direction	loss
Intended Target Type	protein
Intended Target Type Sub	receptor
Intended Target Family	kinase
Intended Target Family Sub	receptor tyrosine kinase

Endocrine Disruptor Screening Program (EDSP)

Sub-Tab

EDSP21 Subset of Assays

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

ADME

EXPOSURE

BIOACTIVITY

TOXCAST: SUMMARY

TOXCAST/TOX21


PUBCHEM

TOXCAST: MODELS

SIMILAR COMPOUNDS

GENRA (BETA)

RELATED SUBSTANCES



Bisphenol A

80-05-7 | DTXSID7020182

Searched by Expert Validated Synonym.

EDSP21

QC Data ID	Grade	Description
Tox21_202992	Pass	Purity>90% and MW confirmed
Tox21_400088	Pass	Purity>90% and MW confirmed

Assay Selection **5 Selected**

☒ Active ☐ Inactive ☐ All

A Single Assay Can Have Multiple Charts

☒ Representative Samples Only

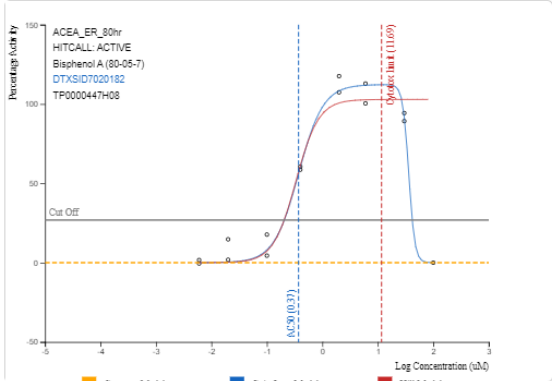
[Bioactivity Summary](#)

Number of Charts: **5**

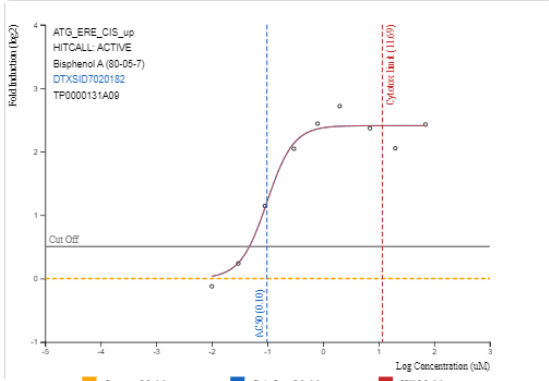
Filter assays

Set: ER (5 of 28 selected)

- ☒ ACEA_ER_80hr
- ☒ ATG_ERE_CIS_up
- ☒ ATG_ERa_TRANS_up
- ☒ NVS_NR_bER
- ☒ NVS_NR_hER
- ☐ OT_ER_ERaERa_0480
- ☐ OT_ER_ERaERa_1440
- ☐ OT_ER_ERbERb_0480
- ☐ OT_ER_ERbERb_1440

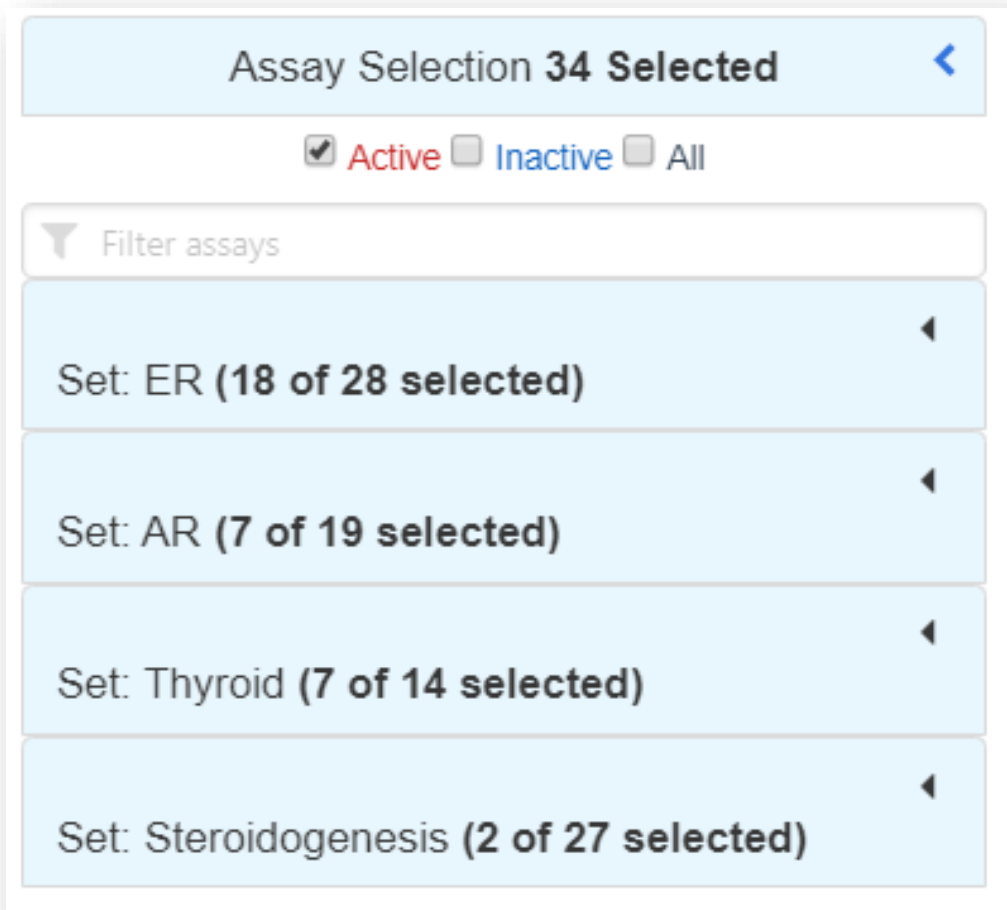


ACEA_ER_80hr
HITCALL: ACTIVE
Bisphenol A (80-05-7)
DTXSID7020182
TP0000447H08



ATG_ERE_CIS_up
HITCALL: ACTIVE
Bisphenol A (80-05-7)
DTXSID7020182
TP0000131A09

EDSP21 Subset of Assays



The screenshot shows a web interface for selecting assays. At the top, a blue header bar displays 'Assay Selection 34 Selected' with a left-pointing arrow. Below this, there are three radio buttons: 'Active' (checked), 'Inactive', and 'All'. Underneath is a search bar labeled 'Filter assays' with a funnel icon. Below the search bar are four light blue selection boxes, each with a left-pointing arrow on the right side. The boxes contain the following text: 'Set: ER (18 of 28 selected)', 'Set: AR (7 of 19 selected)', 'Set: Thyroid (7 of 14 selected)', and 'Set: Steroidogenesis (2 of 27 selected)'.

Assay Selection 34 Selected

☒ Active ☐ Inactive ☐ All

Filter assays

Set: ER (18 of 28 selected)


Set: AR (7 of 19 selected)

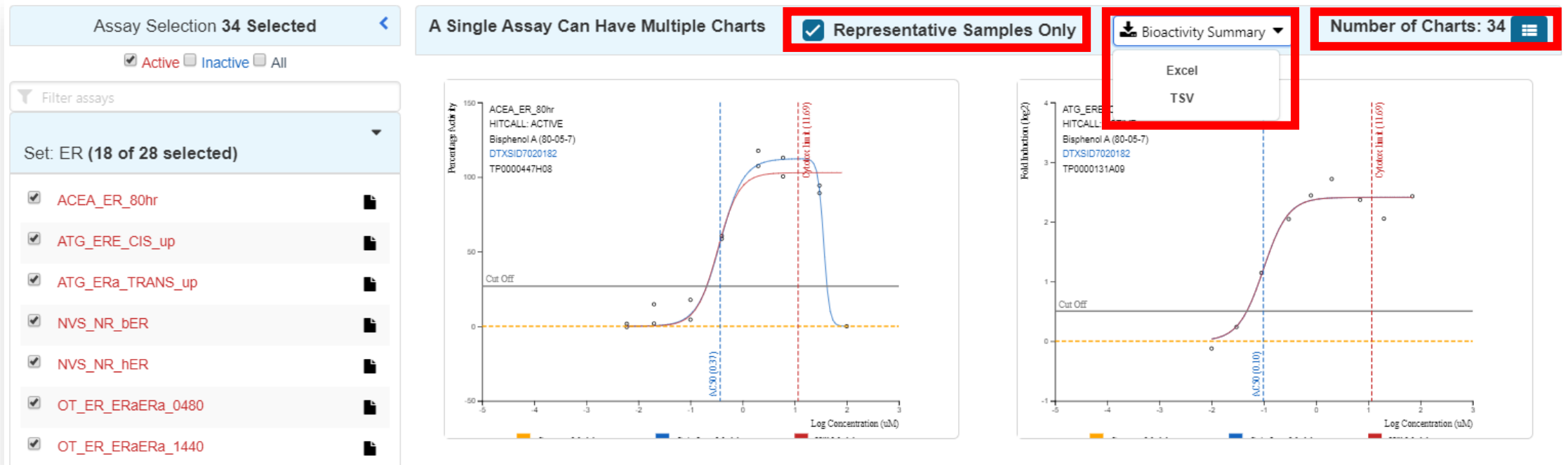
Set: Thyroid (7 of 14 selected)

Set: Steroidogenesis (2 of 27 selected)


- The EDSP21 assays are segregated into ER (Estrogen Receptor), AR (Androgen Receptor), Thyroid and Steroidogenesis
- Selecting the Active subset of hit calls displays all associated bioactivity curves
- Use Filter Assays to filter by text string

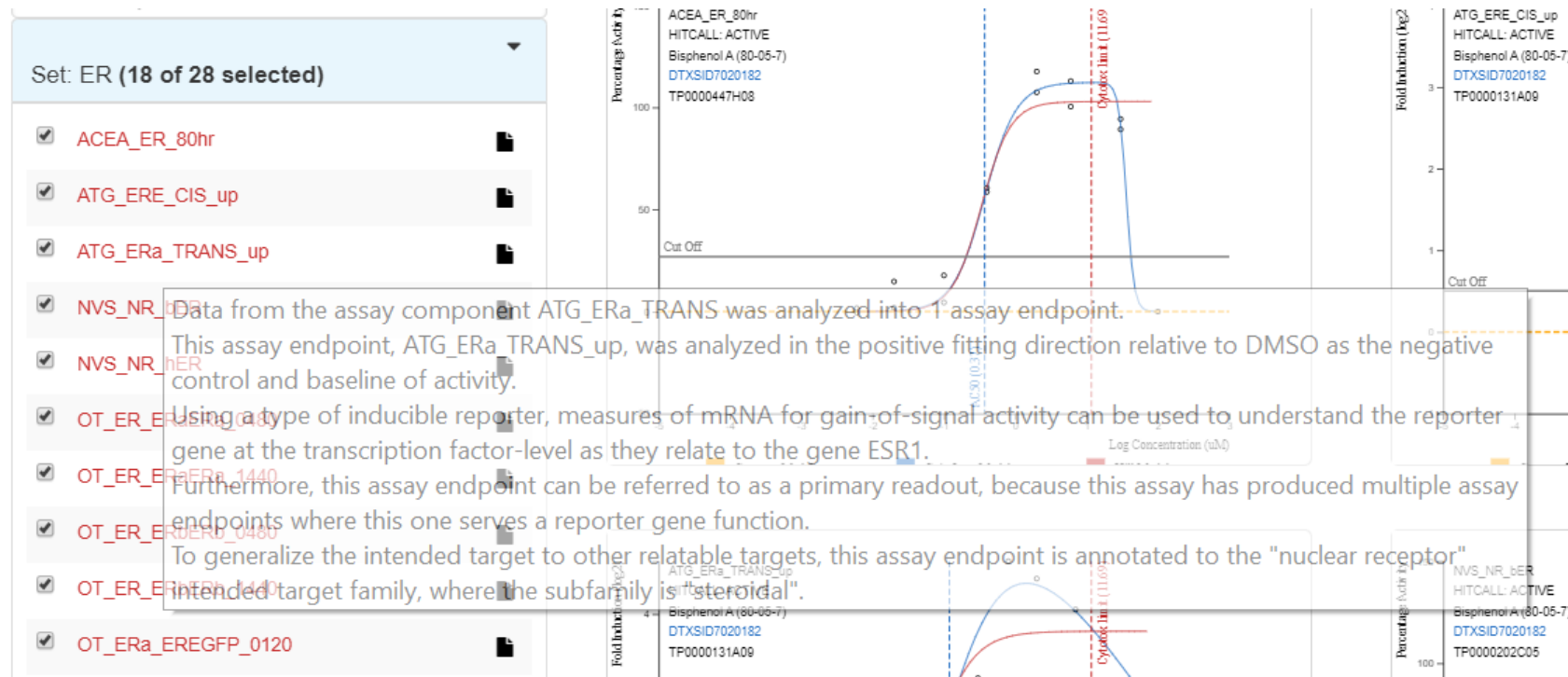
EDSP21 Subset of Assays

- Display bioactivity plots associated with an assay – default is “**Representative Samples Only**” – one chart per assay. Deselect to see all charts for an assay.
- Select  to switch between multiple chart or single chart view
- Download a summary of bioactivity for a chemical as Excel or TSV



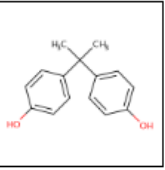
EDSP21 Subset of Assays

- For a summary description of an assay hover over the assay name
- For full assay details select the associated assay modal icon 



Associated Analytical QC data

- When analytical quality control data is available the Pass/Fail grade with purity information and annotations are displayed above the bioactivity charts
- The Analytical QC data are hyperlinked to the relevant data files



Bisphenol A

80-05-7 | DTXSID7020182

Searched by Expert Validated Synonym.

EDSP21

QC Data ID	Grade	Description
Tox21_202992	Pass	Purity>90% and MW confirmed
Tox21_400088	Pass	Purity>90% and MW confirmed

Assay Selection 34 Selected

A Single Assay Can Have Multiple Charts

☒ Representative Samples Only

Bioactivity Summary

Number of Charts: 34

Filter assays

ACEA_ER_80hr
HITCALL: ACTIVE

ATG_ERE_CIS_up
HITCALL: ACTIVE

ToxCast/Tox21

Sub-Tab

ToxCast/Tox21 data

- Navigation of data under this sub-tab parallels the capabilities of the EDSP21 sub-tab except data are organized based on “assay vendor”

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

▶ ADME

▶ EXPOSURE

▼ BIOACTIVITY

TOXCAST: SUMMARY

EDSP21

TOXCAST/TOX21

PUBCHEM

TOXCAST: MODELS

SIMILAR COMPOUNDS

GENRA (BETA)

QC Data ID

Grade

Description

Tox21_202992	Pass	Purity>90% and MW confirmed
Tox21_400088	Pass	Purity>90% and MW confirmed

Assay Selection 211 Selected

☒ Active ☐ Inactive ☐ All

Filter assays

Odyssey Thera (11 of 17 selected)

Attagene (26 of 165 selected)

CellzDirect (3 of 48 selected)

Bioseek (9 of 174 selected)

Apredica (13 of 108 selected)

NHEERL Padilla Lab (1 of 1 selected)

A Single Assay Can Have Multiple Charts

☒ Representative Samples Only

Bioactivity Summary

Number of Charts: 211

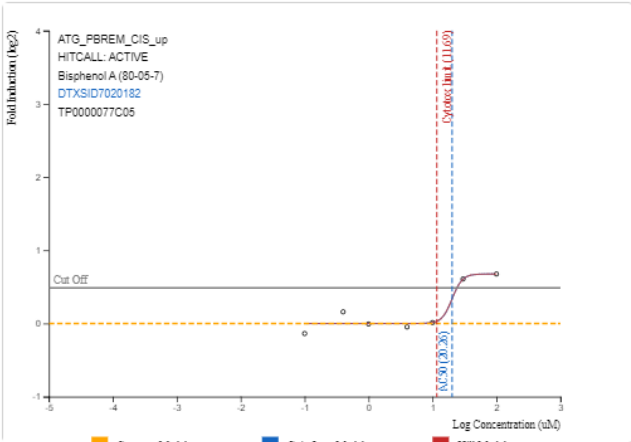
ATG_PBREM_CIS_up

HITCALL: ACTIVE

Bisphenol A (80-05-7)

DTXSID7020182

TP0000077C05



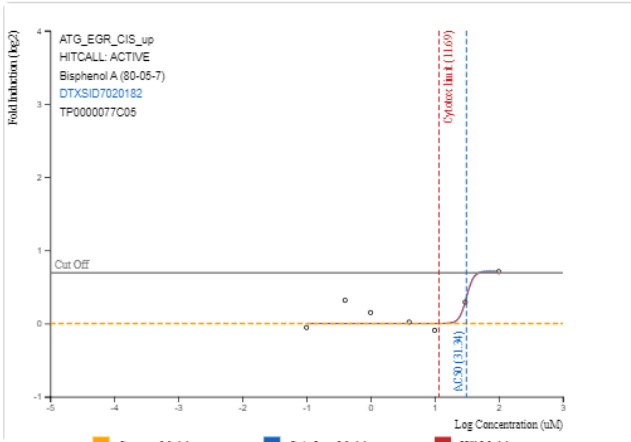
ATG_EGR_CIS_up

HITCALL: ACTIVE

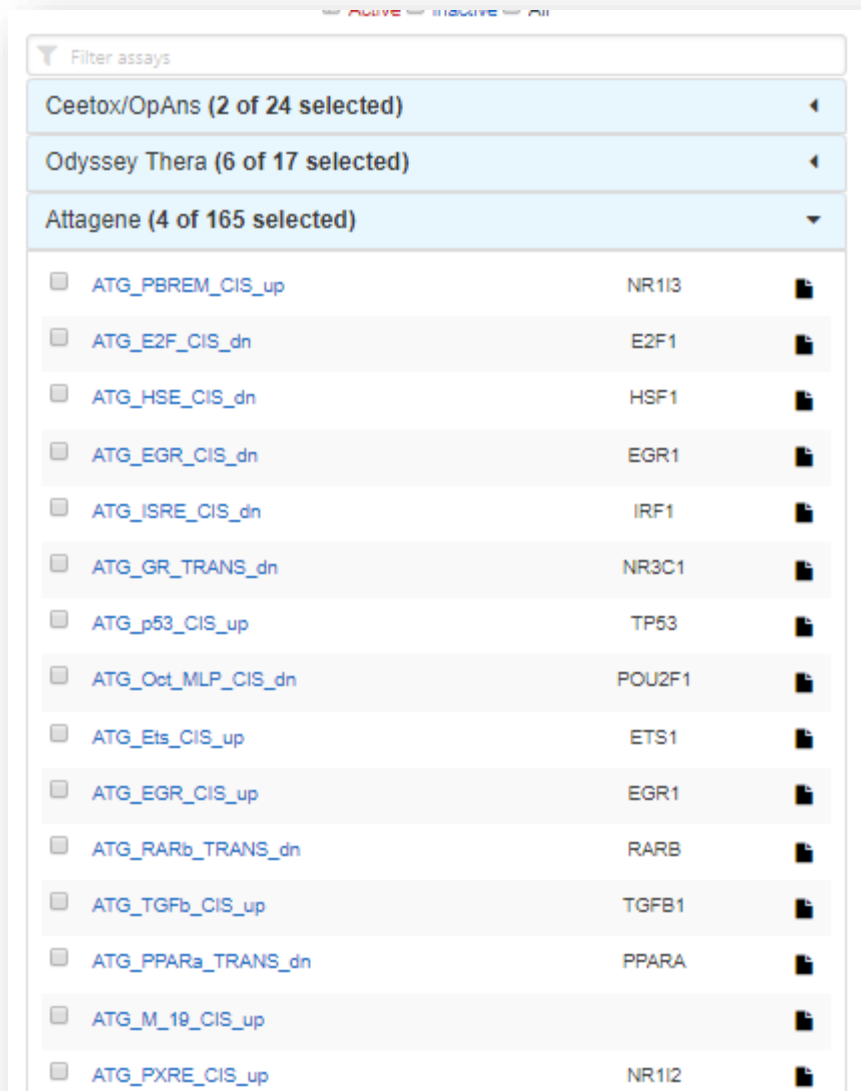
Bisphenol A (80-05-7)

DTXSID7020182

TP0000077C05



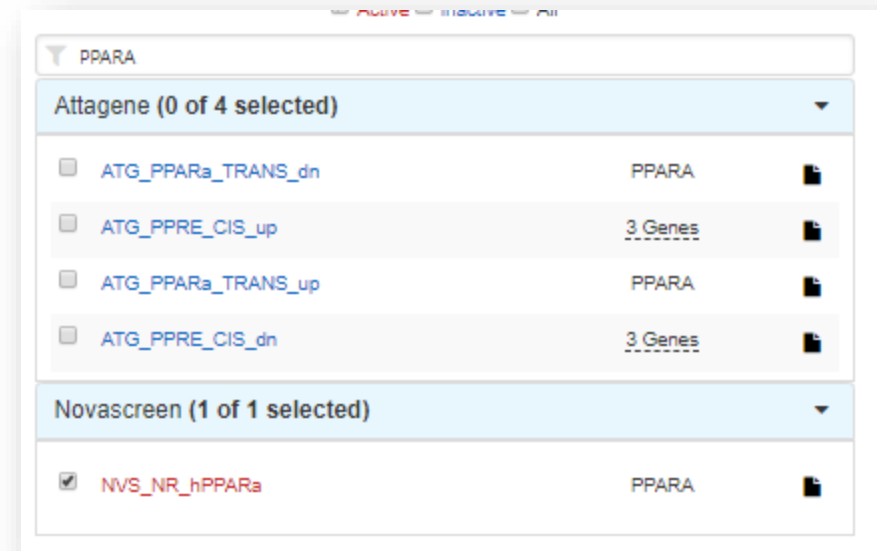
Filtering – Gene annotation added



The screenshot shows a web interface with a 'Filter assays' dropdown menu. The 'Attagene (4 of 165 selected)' option is expanded, displaying a list of assays. Each row includes a checkbox, an assay name, a gene symbol, and a document icon.

Assay	Gene
<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_TGFB1_CIS_up	TGFB1
<input type="checkbox"/> ATG_PPARGa_TRANS_dn	PPARG
<input type="checkbox"/> ATG_M_19_CIS_up	
<input type="checkbox"/> ATG_PXRE_CIS_up	NR1I2

- Using the filter assay box it is possible to find all assays associated with a particular gene. The example below shows filtering based on PPARG (PPAR-alpha)



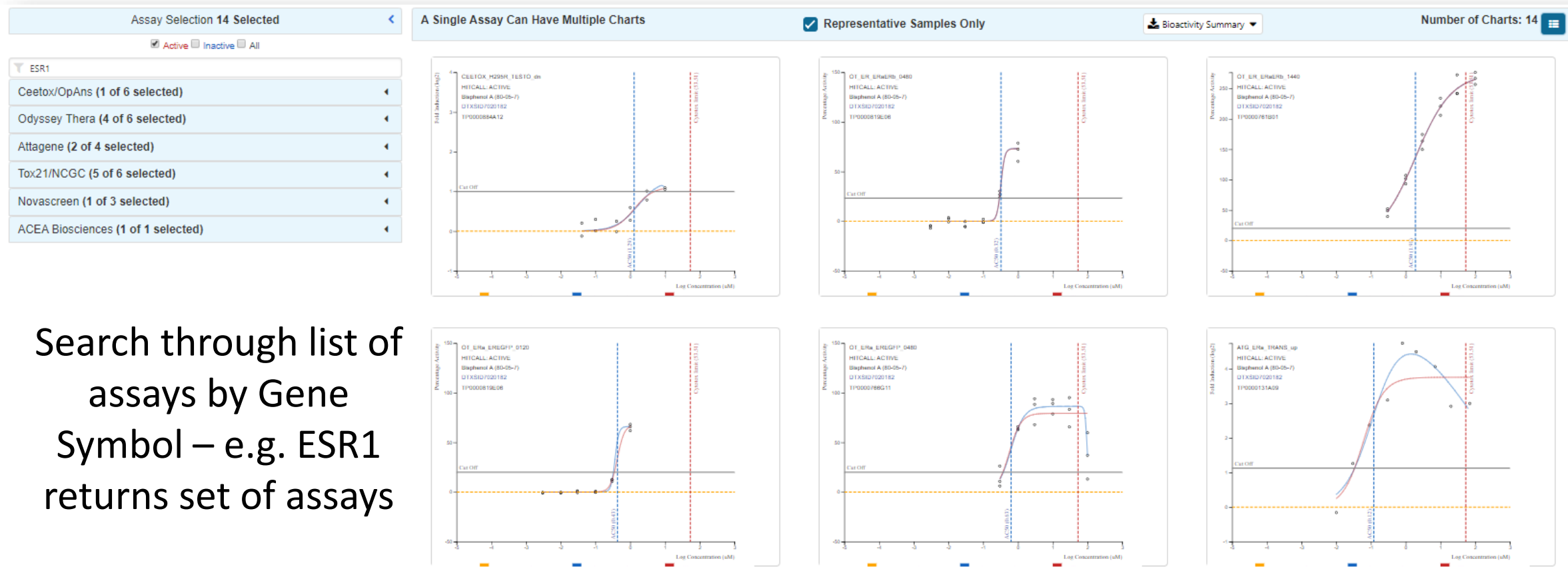
The screenshot shows the same web interface with the 'Filter assays' dropdown menu set to 'PPARG'. The 'Attagene (0 of 4 selected)' option is expanded, displaying a list of assays. Each row includes a checkbox, an assay name, a gene symbol, and a document icon.

Assay	Gene
<input type="checkbox"/> ATG_PPARGa_TRANS_dn	PPARG
<input type="checkbox"/> ATG_PPARG_CIS_up	3 Genes
<input type="checkbox"/> ATG_PPARGa_TRANS_up	PPARG
<input type="checkbox"/> ATG_PPARG_CIS_dn	3 Genes

Below the 'Attagene' section, the 'Novascreen (1 of 1 selected)' option is expanded, displaying a list of assays.

Assay	Gene
<input checked="" type="checkbox"/> NVS_NR_hPPARGa	PPARG

Filtering



PubChem

Sub-Tab

PubChem – integrated view of bioassay data

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

ADME

EXPOSURE

BIOACTIVITY

TOXCAST: SUMMARY

EDSP21

TOXCAST/TOX21

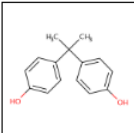
PUBCHEM

TOXCAST: MODELS

SIMILAR COMPOUNDS

GENRA (BETA)

RELATED SUBSTANCES



Bisphenol A

80-05-7 | DTXSID7020182

Searched by Expert Validated Synonym.

PubChem Biological Activities

PUBCHEM > BISPHENOL A > BIOASSAY RESULTS

BioAssay Results

2,256 items View More Rows & Details

Download

SORT BY

Activity Value

Activity	Activity Value, μ M	Activity Type	Target Name	BioAssay Name	BioAssay AID	Substance SID
Inconclusive	0.0014	Potency		qHTS assay to identify small molecule agonists of the endoplasmic reticulum stress response signaling pathway - cell viability counter screen	1159517	144214049
Active	0.0055	Kd	Chain A, Crystal Structure Of Human Estrogen-Related Receptor Gamma Ligand Binding Domain Complex With Bisphenol A (human)	Experimentally measured binding affinity data (Kd) for protein-ligand complexes derived from PDB	977611	87557090
Active	0.0055	Kd	ESRRG - estrogen related receptor gamma (human)	Binding affinity to human ERR gamma	1121409	103308477
Inconclusive	0.0126	Potency	THRB - thyroid hormone receptor beta (human)	qHTS assay for small molecule antagonists of thyroid hormone receptor beta signaling	588547	26752849
Inconclusive	0.1364	Potency		qHTS assay to identify small molecule antagonists of the peroxisome proliferator-activated receptor delta (PPAR δ) signaling pathway - cell viability counter screen	743213	144210190

1 2 3 ... 452 Next >

from PubChem

ToxCast Models

Sub-Tab

PubChem – integrated view of bioassay data

- Prediction models associated with bioactivity are all assembled under the ToxCast:Models sub-tab - the Estrogen and Androgen Pathway Models and the CERAPP and COMPARA QSAR models.
- For Model details and links to papers etc. hover over the help icon

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

ADME

EXPOSURE

BIOACTIVITY

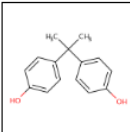
TOXCAST: SUMMARY

EDSP21

TOXCAST/TOX21

PUBCHEM

TOXCAST: MODELS



Bisphenol A

80-05-7 | DTXSID7020182






Searched by Expert Validated Synonym.

ToxCast: Models

ToxCast Model Predictions

Download ToxCast Model Predictions

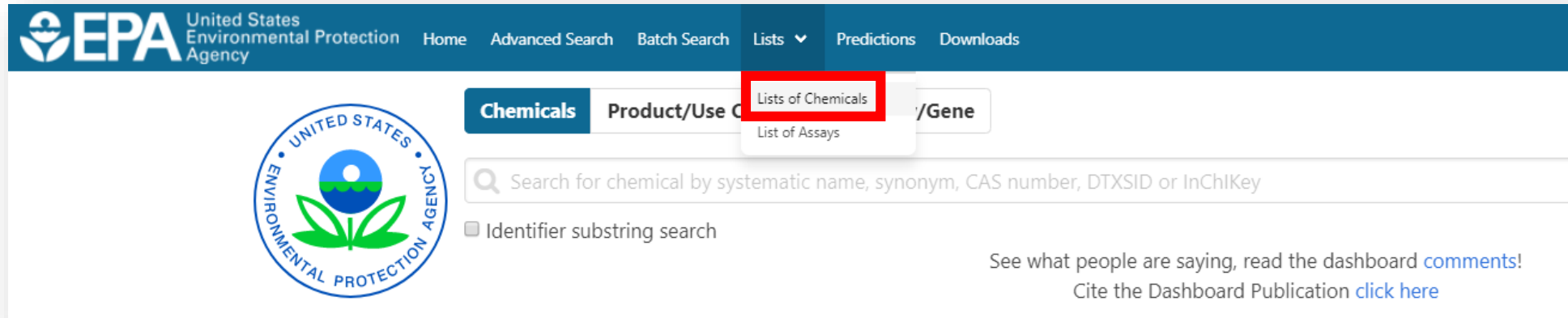
Download all model data

Model	Receptor	Agonist	Antagonist	Binding
 ToxCast Pathway Model (AUC)	Androgen	0.00	0.345	-
 ToxCast Pathway Model (AUC)	Estrogen	0.450	0.00	-
 COMPARA (Consensus)	Androgen	Inactive	Active	Active
 CERAPP Potency Level (Literature)	Estrogen	Active (Weak)	-	Active (Weak)
 CERAPP Potency Level (Consensus)	Estrogen	Active (Weak)	Active (Strong)	Active (Weak)

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](#).

Lists of Chemicals

Lists of Chemicals



- Chemical List page – lots of lists added including segregation
 - LIST: Algal Toxins, Amino Acids, Bisphenol Compounds, PAHs, Synthetic Cannabinoids and Psychoactives, Vitamins, PCBs
 - WIKILIST: Additives in Cigarettes, Extremely Hazardous Substances
 - EPA: Chemical Contaminants, Pesticides Chemical Search
 - **TOXCAST related chemicals lists**

Lists of Chemicals

- Filter lists using text string – “what are all ToxCast lists?”

Select List

Download

Columns

10

ToxCast

Copy Filtered Lists URL

List Acronym	List Name	Last Updated	Number of Chemicals	List Description
CHEMINV	EPA CHEMINV: EPA Chemical Inventory for ToxCast	2017-02-23	5231	CHEMINV is full list of unique DSSTox substances mapped to historical chemical inventory of physical samples registered by EPA's ToxCast Chemical Contractor (Evotec) since launch of ToxCast program in 2007.
CHEMINV_DMSOINSOLUBLES	EPA CHEMINV: EPA ToxCast Cheminventory DMSO Insolubles	2016-02-10	558	Chemicals in EPA's ToxCast physical sample library CHEMINV insoluble in DMSO
CHEMINV_REACTIVES	EPA CHEMINV: EPA ToxCast Cheminventory List of Reactives	2016-02-10	24	ToxCast Chemical inventory (CHEMINV) physical sample library list of chemicals that were deemed too reactive to include in HTS testing.
CHEMINV_STABILITY	EPA CHEMINV: EPA ToxCast Cheminventory chemicals with stability problems	2016-02-10	34	ToxCast chemical inventory (CHEMINV) physical sample library list of chemicals that were determined to have stability problems such that they decompose over time in DMSO.
CHEMINV_VOLATILES	EPA CHEMINV: EPA ToxCast CHEMINV list of volatiles	2016-02-10	130	List of volatile chemicals in EPA ToxCast chemical inventory physical sample library, CHEMINV
EPACHEMINV_AVAIL	EPA CHEMINV: ToxCast/Tox21 Chemical inventory available as DMSO solutions (20181123)	2018-11-21	6408	EPACHEMINV_AVAIL is list of unique DSSTox substances available as DMSO solutions for ToxCast and Tox21 partner projects, managed by EPA Chemical Contract Services.
EPAPFASINSOL	PFAS EPA: Chemical Inventory Insoluble in DMSO	2018-06-29	43	PFAS chemicals included in EPA's expanded ToxCast chemical inventory found to be insoluble in DMSO above 5mM.
EPAPFASINV	PFAS EPA: ToxCast Chemical Inventory	2018-06-29	430	PFAS chemicals included in EPA's expanded ToxCast chemical inventory and available for testing.
TOXCAST	TOXCAST: EPA ToxCast Screening Library	2017-04-11	4746	TOXCAST is the complete list of chemicals having undergone some level of screening in EPA's ToxCast research program since 2007 (last updated 4/11/2017); sublists included.
TOXCAST_E1K	TOXCAST_e1k - EPA ToxCast Screening Library (e1k Subset)	2016-01-25	799	TOXCAST_e1k is the e1k subset of TOXCAST, selected for screening in endocrine-related assays.

<<

<

1

2

>

>>

Showing 1 to 10 of 17 records

Individual chemical lists with details

EPA|CHEMINV: EPA ToxCast CHEMINV list of volatiles

Search CHEMINV_VOLATILES Chemicals

☐ Identifier substring search

List Details

Description: List of chemicals in EPA's ToxCast ChemInventory physical sample library that were labeled as volatile (empty on reweigh when stored in closed frozen vials). A subset of the list was included in the ToxCast testing library after solubilization or prior to this determination, so are also included in TOXCST.

Number of Chemicals: 130

130 chemicals

Select all

Download

Send to Batch Search

Default



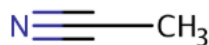
DTXSID

CASRN

TOXCST

Hide chemicals that are:

Filter by Name or CASRN

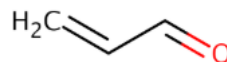


Acetonitrile

DTXSID: DTXSID7020009

CASRN: 75-05-8

TOXCST: 3/210

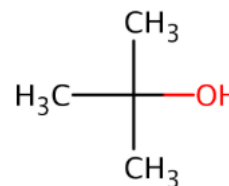


Acrolein

DTXSID: DTXSID5020023

CASRN: 107-02-8

TOXCST: 2/211

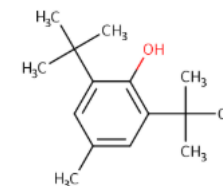


tert-Butyl alcohol

DTXSID: DTXSID8020204

CASRN: 75-65-0

TOXCST: -



Butylated hydroxytoluene

DTXSID: DTXSID2020216


CASRN: 128-37-0

TOXCST: 61/401



Download the file
of chemicals in
various formats



Lists of Assays







List of Assays - Filter by Vendor

- The modal icon  opens up details regarding the individual assay
- The list of assays, or selected assays, can be downloaded as a file

Assay List

Download  10 

NVS x OT x CLD x  Search query  Copy filtered page URL

Assay Component Endpoint Name	Details	Multi Conc. Actives	Single Conc. Active	Description	Gene Symbols
NVS_ADME_hCYP19A1		72 / 247	75 / 1879 	Data from the assay component endpoint, NVS_ADME_hCYP19A1, was analyzed in the positive fitting direction relative to Acetonitrile as the negative control and baseline of activity. Using a type of enzyme reporter, loss-of-signal activity can be used to understand changes in the enzymatic activity as they relate to the gene CYP19A1. Furthermore, this assay endpoint can be referred to as a primary readout, because this assay has produced multiple assay endpoints where this one serves an enzymatic activity function. To generalize the intended target to other relatable targets, this assay endpoint is annotated to the "cyp" intended target family, where the subfamily is "xenobiotic metabolism".	CYP19A1
NVS_ADME_hCYP19A1_Activator		3 / 247	8 / 1879 	Data from the assay component endpoint, NVS_ADME_hCYP19A1, was analyzed in the positive fitting direction relative to Acetonitrile as the negative control and baseline of activity. Using a type of enzyme reporter, loss-of-signal activity can be used to understand changes in the enzymatic activity as they relate to the gene CYP19A1. Furthermore, this assay endpoint can be referred to as a primary readout, because this assay has produced multiple assay endpoints where this one serves an enzymatic activity function. To generalize the intended target to other relatable targets, this assay endpoint is annotated to the "cyp" intended target family, where the subfamily is "xenobiotic metabolism".	CYP19A1
NVS_ADME_hCYP1A1		72 / 180	111 / 1124 	Data from the assay component endpoint, NVS_ADME_hCYP1A1, was analyzed in the positive fitting direction relative to Acetonitrile as the negative control and baseline of activity. Using a type of enzyme reporter, loss-of-signal activity can be used to understand changes in the enzymatic activity as they relate to the gene CYP1A1. Furthermore, this assay endpoint can be referred to as a primary readout, because this assay has produced multiple assay endpoints where this one serves an enzymatic activity function. To generalize the intended target to other relatable targets, this assay endpoint is annotated to the "cyp" intended target family, where the subfamily is "xenobiotic metabolism".	CYP1A1

ACEA Biosciences

Apredica

Attagene

Bioseek

Novascreen

Odyssey Thera

Tox21/NCGC

Ceetox/OpAns

CellzDirect

NHEERL Padilla Lab

NCCT Simmons Lab

Tanguay Lab

NHEERL Hunter Lab

NHEERL Stoker and Laws Laboratories

NHEERL Mid-Continent Ecology Division

University of Pittsburgh Johnston Lab

Select multiple vendors
Ctrl-click to select

Single Concentration Data (August 2019 release)

- Some assays have single concentration screening data. Select modal to view data

Multi Conc. Actives	Single Conc. Active	Description
72 / 247	75 / 1879 	Data from the a endpoint, NVS

NVS_ADME_hCYP19A1 Single Concentration aeid: 319

Download 10 benz


Name	CASRN	DTXSID	BMAD	COFF	Hit Call	Max Med
Benzylparaben	94-18-8	DTXSID9022526	9.68	29.0	ACTIVE	79.8
tert-Butylbenzene	98-06-6	DTXSID3047138	9.68	29.0	ACTIVE	60.4
1,2,4,5-Tetrachlorobenzene	95-94-3	DTXSID7024320	9.68	29.0	ACTIVE	36.8
Sodium dodecylbenzenesulfonate	25155-30-0	DTXSID7025219	9.68	29.0	ACTIVE	62.7
Octabenzene	1843-05-6	DTXSID9027441	9.68	29.0	ACTIVE	33.9
Methyl 2-aminobenzoate	134-20-3	DTXSID6025567	9.68	29.0	ACTIVE	36.4
1,2-Dichlorobenzene	95-50-1	DTXSID6020430	9.68	29.0	ACTIVE	29.5
1-Benzylquinolinium chloride	15619-48-4	DTXSID8044593	9.68	29.0	INACTIVE	-0.803
Dodecylbenzene	123-01-3	DTXSID7026994	9.68	29.0	INACTIVE	-3.05
Benzoin	119-53-9	DTXSID1020144	9.68	29.0	INACTIVE	1.13

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

Showing 1 to 10 of 148 records


- Sort data based on various parameters
- Filter through the data using name substrings
- Download the data as a file

Histogram Views of Data for Assays

- The modal icon  opens up details regarding the individual assay
- ACTIVE hits shown by default. Delete INACTIVE filter to see all data

Assay Endpoint Name: NVS_ADME_hCYP19A1

Assay Details

Assay Endpoint Name: NVS_ADME_hCYP19A1 

Assay Source Description: NovaScreen, part of PerkinElmer, a human and environmental health company, provides a large diverse suite of cell-free binding and biochemical assays.

Histograms

72 of 247 chemicals visible

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

Oc1ccc(cc1Cc2ccccc2)Cl

Clorophene
DTXSID: DTXSID5020154
CASRN: 120-32-1
TOXCAST: 340/991

CC(=O)Nc1ccc2ccccc2o1

Carbaryl
DTXSID: DTXSID9020247
CASRN: 63-25-2
TOXCAST: 96/834

N#Cc1c(Cl)c(Cl)c(Cl)c1C#N

Chlorothalonil
DTXSID: DTXSID0020319
CASRN: 1897-45-6
TOXCAST: 343/920

O=C1C(=O)c2ccccc2C1=CCl

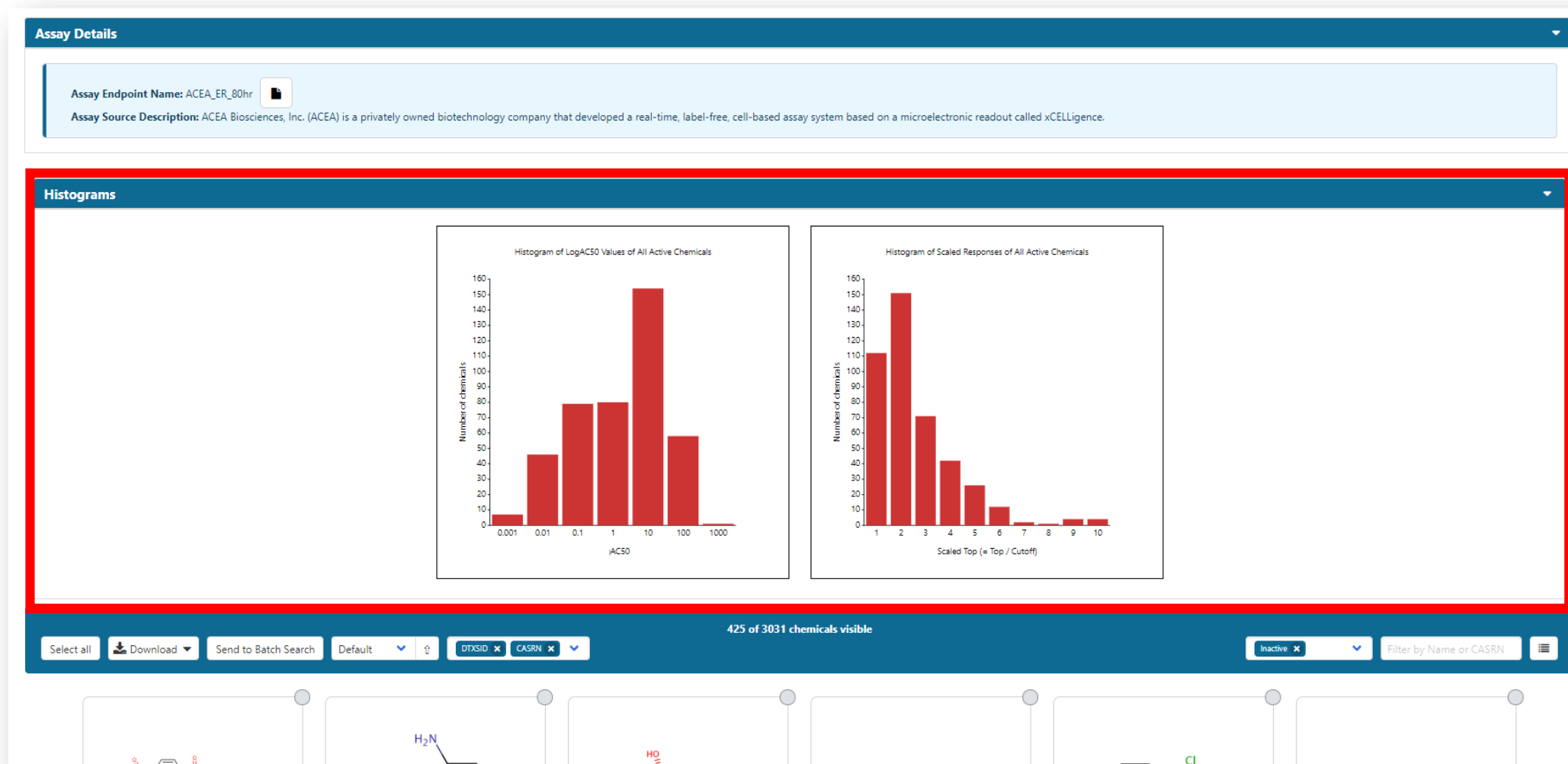
Dichlorone
DTXSID: DTXSID7020425
CASRN: 117-80-6
TOXCAST: 173/431

CC1=CC=C(C=C1)/C=C/c2ccc(O)cc2

Diethylstilbestrol
DTXSID: DTXSID5020154
CASRN: 118-04-6
TOXCAST: 173/431

Delete INACTIVE filter
to see all data in set

Interactive histogram summary view



Interactive histogram summary view

- Display specific subset of data from histogram by selecting individual bars

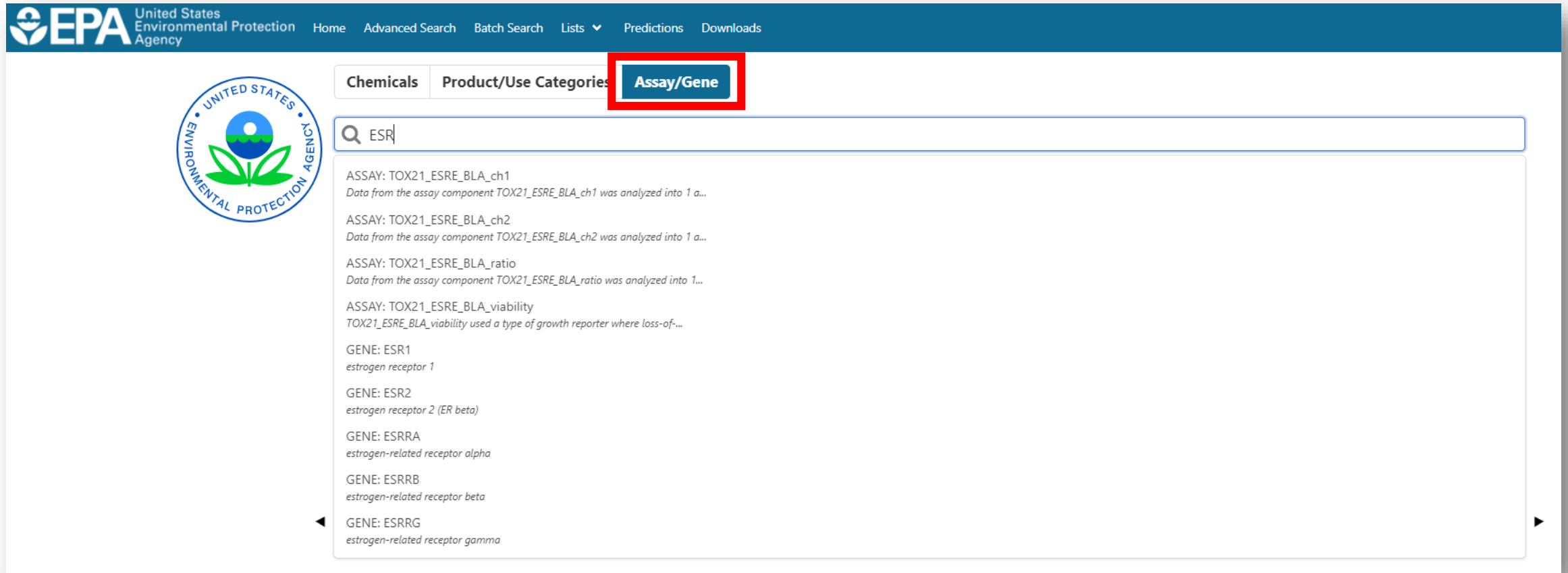


New Search Capability

Search Assay or Gene from Home Page

Searching Gene or Assay from the Home Page

- Switch to Assay/Gene Search tab and use the type-ahead search



The screenshot displays the EPA website's search interface. The top navigation bar includes the EPA logo and links for Home, Advanced Search, Batch Search, Lists, Predictions, and Downloads. Below this, a tabbed interface shows 'Chemicals', 'Product/Use Categories', and 'Assay/Gene', with the latter highlighted by a red box. A search bar on the left contains the text 'ESR'. To the right of the search bar, a list of search results is displayed, including assays and genes related to estrogen receptors. The EPA logo is visible on the left side of the page.

United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

Chemicals Product/Use Categories **Assay/Gene**

Q ESR

ASSAY: TOX21_ESRE_BLA_ch1
Data from the assay component TOX21_ESRE_BLA_ch1 was analyzed into 1 a...

ASSAY: TOX21_ESRE_BLA_ch2
Data from the assay component TOX21_ESRE_BLA_ch2 was analyzed into 1 a...

ASSAY: TOX21_ESRE_BLA_ratio
Data from the assay component TOX21_ESRE_BLA_ratio was analyzed into 1...

ASSAY: TOX21_ESRE_BLA_viability
TOX21_ESRE_BLA_viability used a type of growth reporter where loss-of-...

GENE: ESR1
estrogen receptor 1

GENE: ESR2
estrogen receptor 2 (ER beta)

GENE: ESRRA
estrogen-related receptor alpha

GENE: ESRRB
estrogen-related receptor beta

GENE: ESRRG
estrogen-related receptor gamma

Select hit based on Assay

Opens associated list of chemicals for an assay

EPA United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

Share Search all data

Assay Endpoint Name: TOX21_ESRE_BLA_ch1

Assay Details

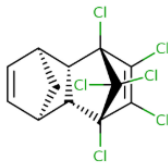
Assay Endpoint Name: TOX21_ESRE_BLA_ch1

Assay Source Description: Tox21 is an interagency agreement between the NIH, NTP, FDA and EPA. NIH Chemical Genomics Center (NCGC) is the primary screening facility running ultra high throughput screening assays across a large interagency-developed chemical library.

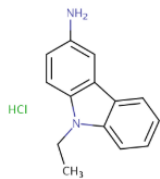
Histograms

156 of 7522 chemicals visible

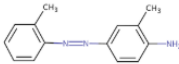
Select all Download Send to Batch Search Default DTXSID CASRN TOXCAST Inactive Filter by Name or CASRN



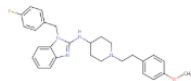
Aldrin
DTXSID: DTXSID8020040
CASRN: 309-00-2
TOXCAST: 199/643



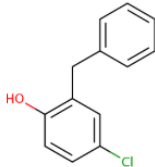
3-Amino-9-ethylcarbazole hydrochloride
DTXSID: DTXSID2020054
CASRN: 6109-97-3
TOXCAST: 46/211



2-Amino-5-azotoluene
DTXSID: DTXSID1020069
CASRN: 97-56-3
TOXCAST: 252/709




Astemizole
DTXSID: DTXSID9020110
CASRN: 68844-77-9
TOXCAST: 219/588



Clorophene
DTXSID: DTXSID5020154
CASRN: 120-32-1
TOXCAST: 327/963

Select hit based on Gene Symbol

Opens list of assays associated with that Gene



United States
Environmental Protection
Agency

HomeAdvanced SearchBatch SearchLists ▼PredictionsDownloads

Share

Search all data

Assay List

Download

Filter by vendor

ESRRA

Copy filtered page URL

Future CompTox Portal



Environmental Topics

Laws & Regulations

About EPA

Search EPA.gov



Feedback Welcomed


- Send comments to us via the web page at http://comptox.epa.gov/dashboard/contact_us

We welcome feedback regarding your experiences using the CompTox Chemicals Dashboard. Please send us your comments and questions using the form below.


E-mail


Subject

Message

☐ I'm not a robot  reCAPTCHA
Privacy - Terms

Back Send

 UNITED STATES • ENVIRONMENTAL PROTECTION AGENCY

 UNITED STATES • ENVIRONMENTAL PROTECTION AGENCY

Discover.
[About/Disclaimer](#)
[Accessibility](#)
[Privacy](#)

Connect.
[ACToR](#)
[DSSTox](#)
[Downloads](#)

Ask.
[Contact](#)
[Help](#)