

# 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

The image shows a screenshot of the EPA website's CompTox portal. At the top left is the EPA logo with the text "United States Environmental Protection Agency". A blue navigation bar contains the links "Environmental Topics", "Laws & Regulations", and "About EPA", along with a search bar labeled "Search EPA.gov". Below the navigation bar are six featured tiles, each with a background image and text:

- CompTox Chemicals Dashboard**: A screenshot of the dashboard interface.
- Aggregated Publicly Available Chemical Data ACToR**: A screenshot of the ACToR data collection interface.
- ToxCast Dashboard High-throughput screening data**: A photograph of a scientist in a lab coat and gloves working with a high-throughput screening machine.
- EDSP21 Dashboard High-throughput screening and exposure estimates for evaluating chemicals for potential endocrine activity**: A photograph of a woman smiling and holding a baby in a field.
- RapidTox Decision support workflows to integrate chemistry, toxicity, and exposure information**: A photograph of various household cleaning products on a counter.
- Downloadable Data**: A 3D graphic of a DNA double helix against a background of binary code.

# Two legacy dashboards to be discontinued

The image shows a screenshot of the EPA website's dashboard. At the top left is the EPA logo and the text "United States Environmental Protection Agency". Below this is a blue navigation bar with the following links: "Environmental Topics", "Laws & Regulations", and "About EPA". To the right of the navigation bar is a search box labeled "Search EPA.gov" with a magnifying glass icon.

The main content area contains six dashboard tiles, each with a blue border and rounded corners:

- CompTox Chemicals Dashboard**: Shows a screenshot of the dashboard interface with chemical structures.
- Aggregated Publicly Available Chemical Data ACToR**: Shows a screenshot of the ACToR data collection interface.
- ToxCast Dashboard**: Features a photo of a scientist in a lab coat and purple gloves working with a high-throughput screening machine. Text: "ToxCast Dashboard High-throughput screening data". This tile is highlighted with a red border.
- EDSP21 Dashboard**: Features a photo of a woman holding a baby in a field. Text: "EDSP21 Dashboard High-throughput screening and exposure estimates for evaluating chemicals for potential endocrine activity". This tile is highlighted with a red border.
- RapidTox**: Features a photo of various household cleaning products. Text: "RapidTox Decision support workflows to integrate chemistry, toxicity, and exposure information".
- Downloadable Data**: Features a 3D rendering of a DNA double helix against a background of binary code.

# *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

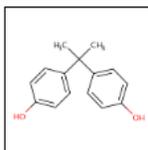
TOXCAST: MODELS

- 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

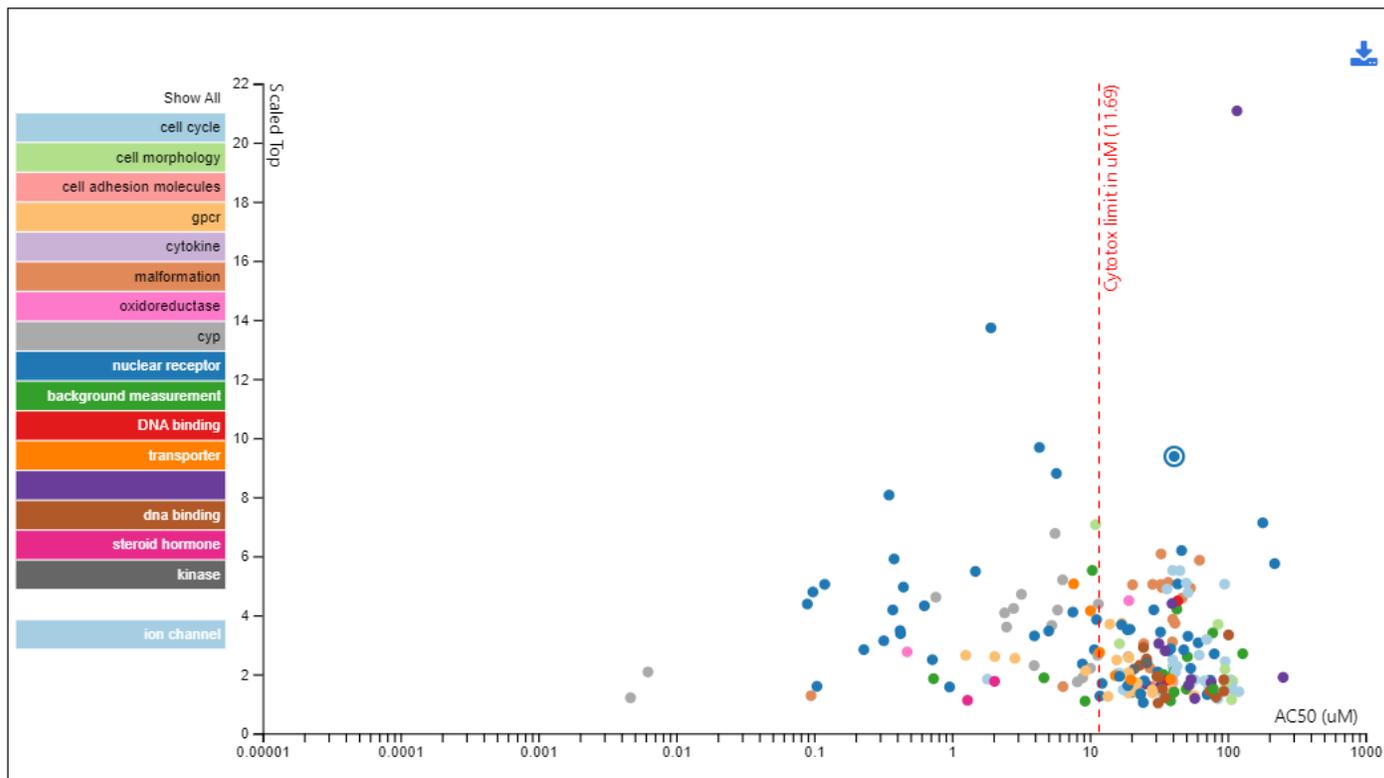
GENRA (BETA)

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

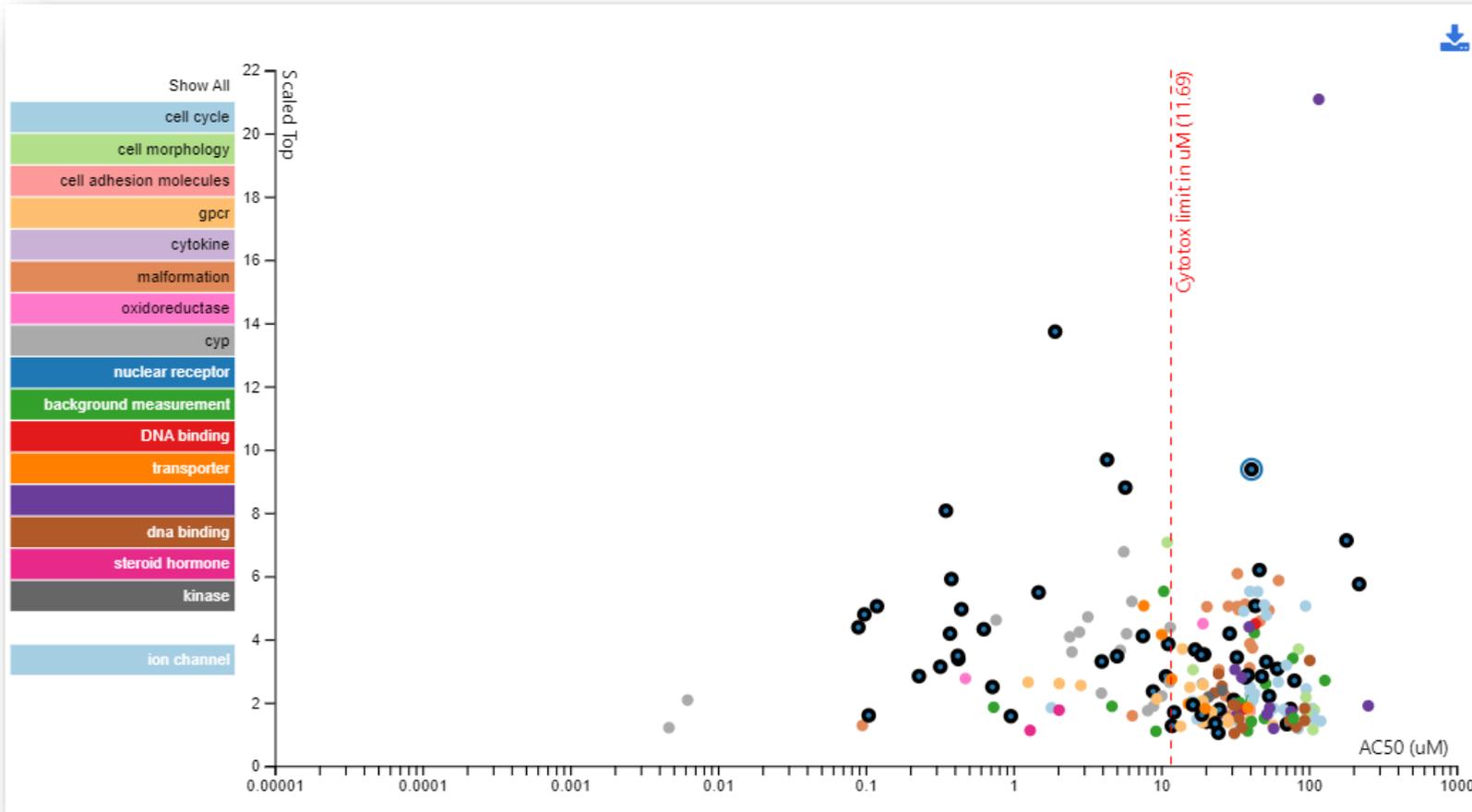
Chemical Activity Summary 

 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               |       | <a href="#">EAW52902.1</a>  | <a href="#">NTRK1</a>  | -   | -     | ACTIVE   | 43.6  | 21.0    | 1.32    | 20.0   | 1.28    | kinase                  |
| BSK_hDFCGF_CollagenIII_down |       | <a href="#">NP_000081.1</a> | <a href="#">COL3A1</a> | -   | -     | ACTIVE   | 0.254 | 40.0    | 1.60    | 0.144  | 1.60    | cell adhesion molecules |
| ACEA_ER_80hr                |       | <a href="#">NP_000116.2</a> | <a href="#">ESR1</a>   | 200 | 1181  | ACTIVE   | 112   | 0.373   | -0.428  | 26.9   | -0.686  | nuclear receptor        |
| ATG_ERE_CIS_up              |       | <a href="#">NP_000116.2</a> | <a href="#">ESR1</a>   | 200 | 1181  | ACTIVE   | 2.41  | 9.81e-2 | -1.01   | 0.503  | -1.32   | nuclear receptor        |
| ATG_ERa_TRANS_up            |       | <a href="#">NP_000116.2</a> | <a href="#">ESR1</a>   | 200 | 1181  | ACTIVE   | 5.70  | 0.119   | -0.923  | 1.13   | -1.49   | nuclear receptor        |
| NVS_NR_hER                  |       | <a href="#">NP_000116.2</a> | <a href="#">ESR1</a>   | 200 | 1181  | ACTIVE   | 69.2  | 0.230   | -0.639  | 24.4   | -0.805  | nuclear receptor        |
| OT_ER_ERaERa_0480           |       | <a href="#">NP_000116.2</a> | <a href="#">ESR1</a>   | 200 | 1181  | ACTIVE   | 176   | 5.73    | 0.758   | 20.0   | 7.33e-2 | nuclear receptor        |
| OT_ER_ERaERa_1440           |       | <a href="#">NP_000116.2</a> | <a href="#">ESR1</a>   | 200 | 1181  | ACTIVE   | 194   | 4.31    | 0.635   | 20.0   | 2.15e-2 | nuclear receptor        |
| OT_ERa_EREgFP_0120          |       | <a href="#">NP_000116.2</a> | <a href="#">ESR1</a>   | 200 | 1181  | ACTIVE   | 67.5  | 0.424   | -0.372  | 20.0   | -0.458  | nuclear receptor        |
| OT_ERa_EREgFP_0480          |       | <a href="#">NP_000116.2</a> | <a href="#">ESR1</a>   | 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

- 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

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
- ModlAcc
- ModlAr10

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

Info : Chemical concentration (in  $\mu\text{M}$ ) 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               |       | LAW52902.1  | 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](#)



[Annotations](#) Citations tcpl Processing Reagents AOPs

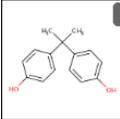
Five individual sub-tabs describing an individual assay

|                               |  |
|-------------------------------|--|
| 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 an 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

 **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

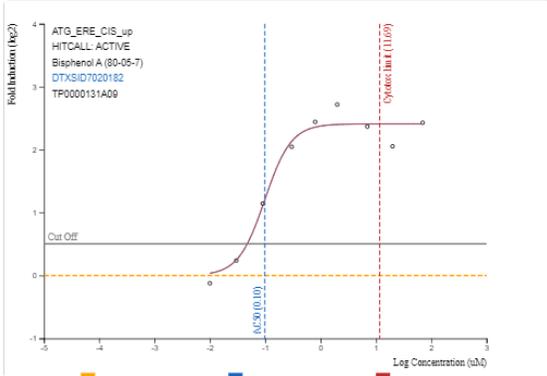
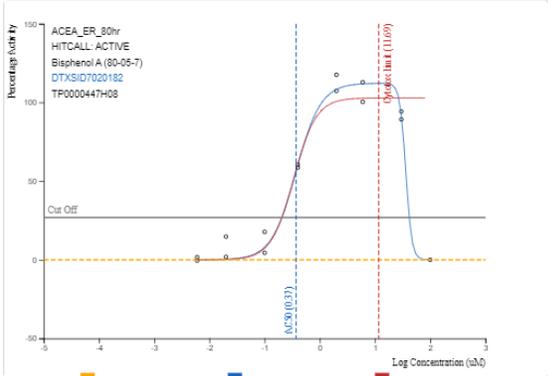
Filter assays

Set: ER (5 of 28 selected)

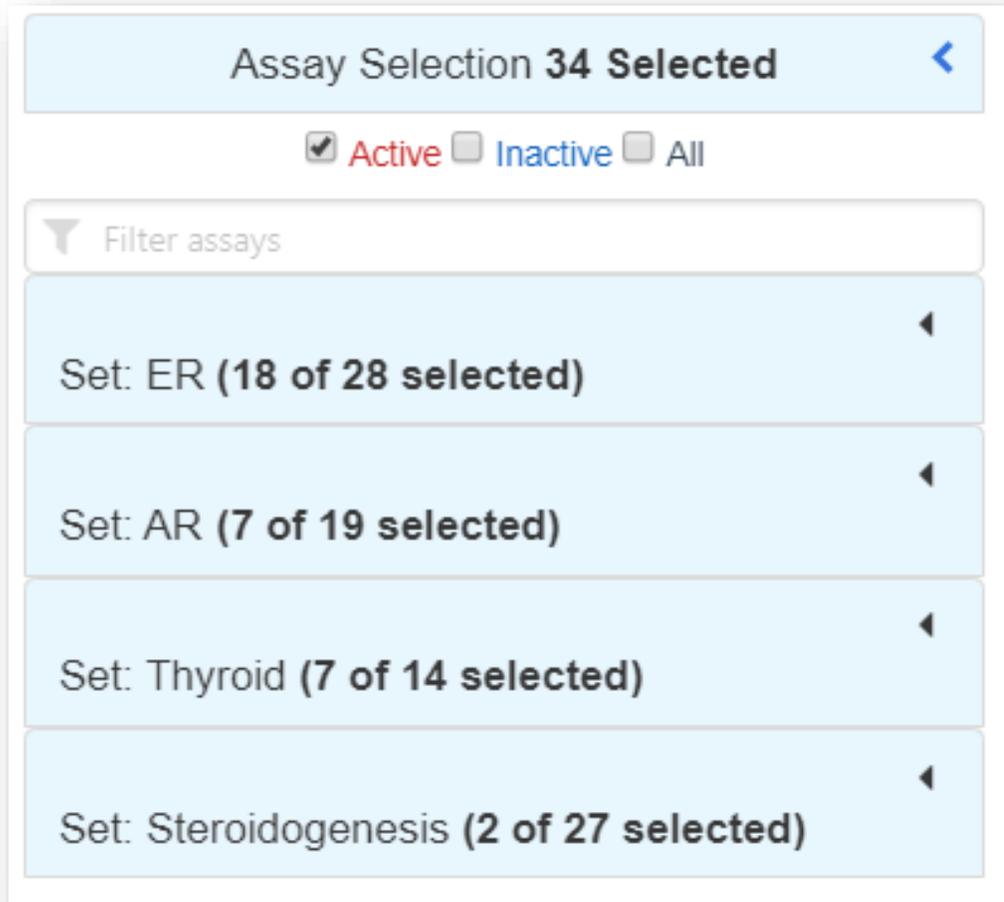
- ACEA\_ER\_80hr
- ATG\_ERE\_CIS\_up
- ATG\_ERa\_TRANS\_up
- NVS\_NR\_bER
- NVS\_NR\_hER
- OT\_ER\_ERaERa\_0480
- OT\_ER\_ERaERa\_1440
- OT\_ER\_ERbERb\_0480
- OT\_ER\_ERbERb\_1440

**EDSP21**

A Single Assay Can Have Multiple Charts  Representative Samples Only  Number of Charts: 5



# EDSP21 Subset of Assays



Assay Selection **34 Selected** <

Active  Inactive  All

Filter assays

Set: ER (18 of 28 selected) ◀

Set: AR (7 of 19 selected) ◀

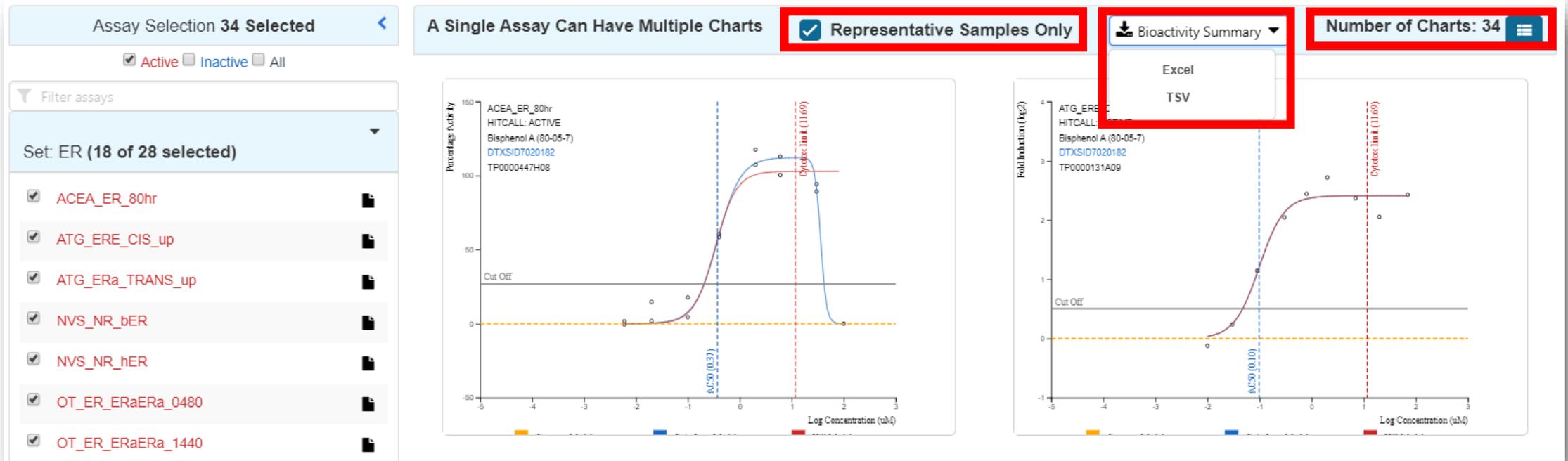
Set: Thyroid (7 of 14 selected) ◀

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

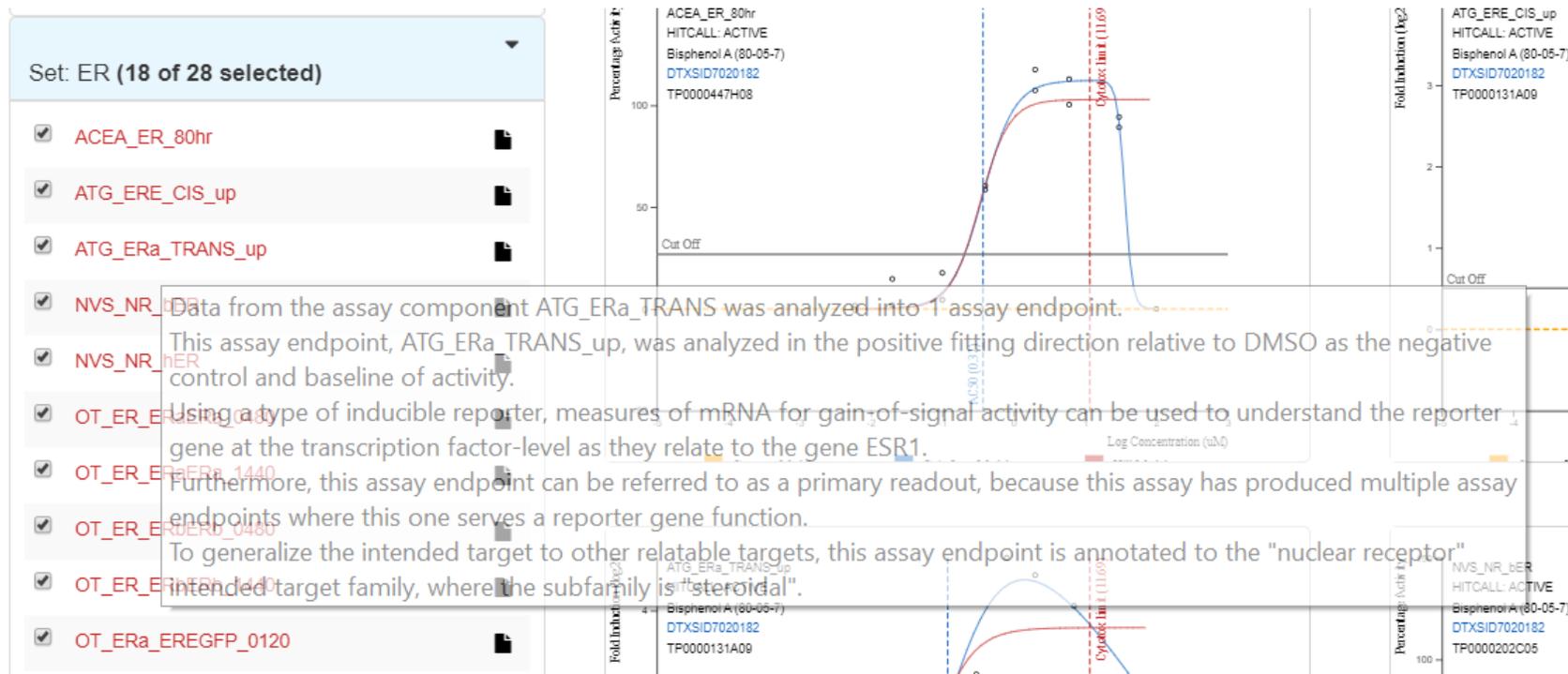
- Display bioactivity plots associated with an assay – default is “**Representative Samples Only**” – one chart per assay. Deselect to see all charts for an assay.
- Select  to switch between multiple chart or single chart view
- Download a summary of bioactivity for a chemical as Excel or TSV



The screenshot displays the EDSP21 bioactivity interface. At the top, it shows "Assay Selection 34 Selected" and a filter for "Active" assays. A list of 18 selected assays is shown, including ACEA\_ER\_80hr, ATG\_ERE\_CIS\_up, ATG\_ERa\_TRANS\_up, NVS\_NR\_bER, NVS\_NR\_hER, OT\_ER\_ERaERa\_0480, and OT\_ER\_ERaERa\_1440. The interface includes a header for "A Single Assay Can Have Multiple Charts" with a "Representative Samples Only" checkbox checked. A "Bioactivity Summary" dropdown menu is open, showing options for "Excel" and "TSV". The number of charts is set to 34. Two representative bioactivity plots are shown side-by-side. The left plot is for ACEA\_ER\_80hr (HitCall: ACTIVE) with Bisphenol A (80-05-7) and TP0000447H08. The right plot is for ATG\_ERE\_CIS\_up (HitCall: INACTIVE) with Bisphenol A (80-05-7) and TP0000131A09. Both plots show Percentage Activity vs. Log Concentration (uM) with a sigmoidal fit curve, a blue vertical line for AC50 (0.37) and a red vertical line for Cytotoxic limit (11.09).

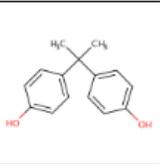
# EDSP21 Subset of Assays

- 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                 |
|------------------------------|-------|-----------------------------|
| <a href="#">Tox21_202992</a> | Pass  | Purity>90% and MW confirmed |
| <a href="#">Tox21_400088</a> | 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 

Active  Inactive  All

Filter assays

dir ty <sup>150</sup> ACEA\_ER\_80hr  
HITCALL: ACTIVE (1,69)

(log) <sup>4</sup> ATG\_ERE\_CIS\_up  
HITCALL: ACTIVE (1,69)

# 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)

### ToxCast/Tox21

| 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)

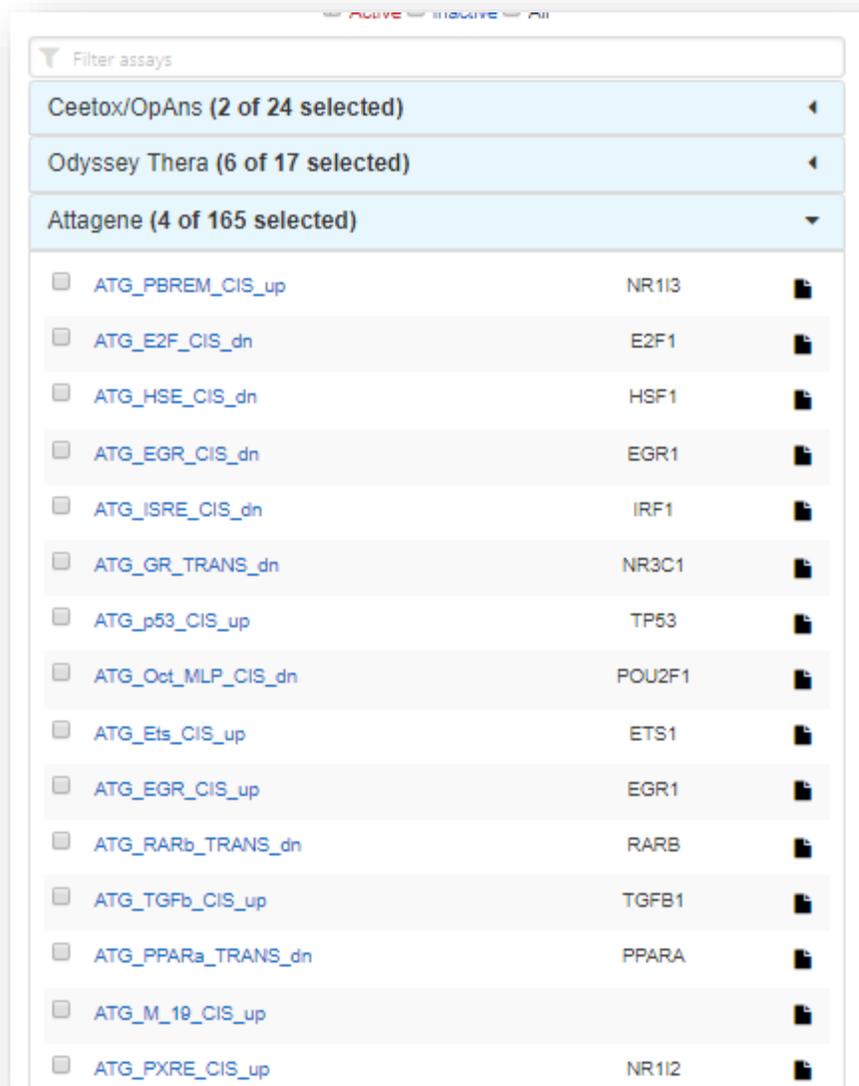
NHEERL Padilla Lab (1 of 1 selected)

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



Filter assays

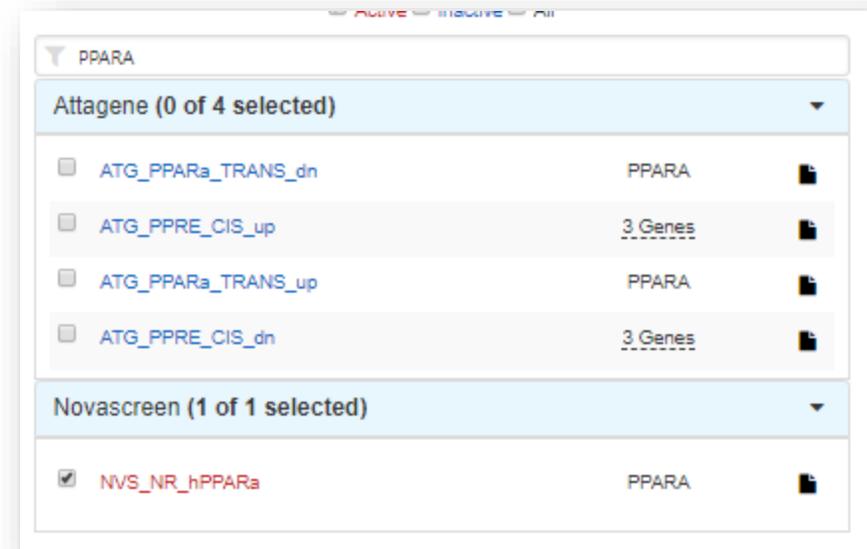
Ceetox/OpAns (2 of 24 selected)

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_PPARGa_TRANS_dn | PPARG  |  |
| <input type="checkbox"/> | ATG_M_10_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)



PPARG

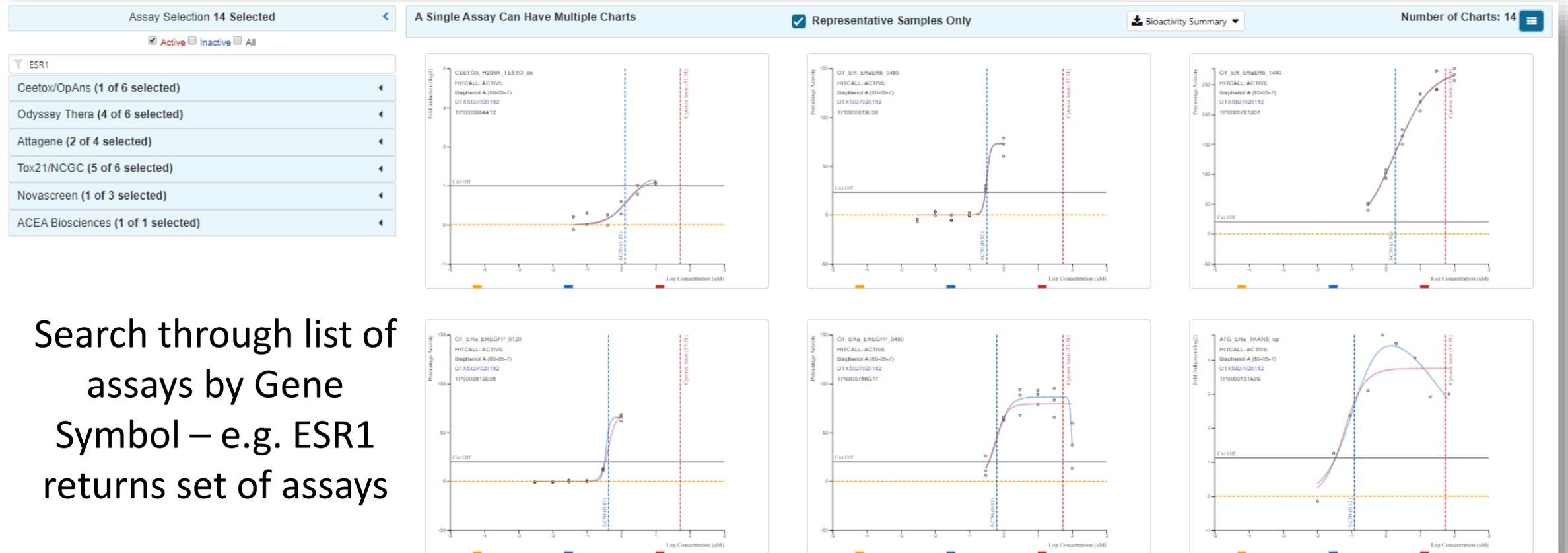
Attagene (0 of 4 selected)

|                          |                     |         |  |
|--------------------------|---------------------|---------|--|
| <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 |  |

Novascreen (1 of 1 selected)

|                                     |                |       |  |
|-------------------------------------|----------------|-------|--|
| <input checked="" type="checkbox"/> | NVS_NR_hPPARGa | PPARG |  |
|-------------------------------------|----------------|-------|--|

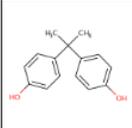
# Filtering



# PubChem

## Sub-Tab

# PubChem – integrated view of bioassay data



**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, $\mu\text{M}$ | 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            | <a href="#">Chain A, Crystal Structure Of Human Estrogen-Related Receptor Gamma Ligand Binding Domain Complex With Bisphenol A (human)</a> | Experimentally measured binding affinity data (Kd) for protein-ligand complexes derived from PDB   | 977611       | 87557090      |
| Active       | 0.0055                        | Kd            | <a href="#">ESRRG - estrogen related receptor gamma (human)</a>  | Binding affinity to human ERR gamma  | 1121409      | 103308477     |
| Inconclusive | 0.0126                        | Potency       | <a href="#">THRB - thyroid hormone receptor beta (human)</a>   | 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 $\delta$ ) 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

**Bisphenol A**  
80-05-7 | DTXSID7020182  
Searched by Expert Validated Synonym.

**ToxCast: Models**  
ToxCast Model Predictions

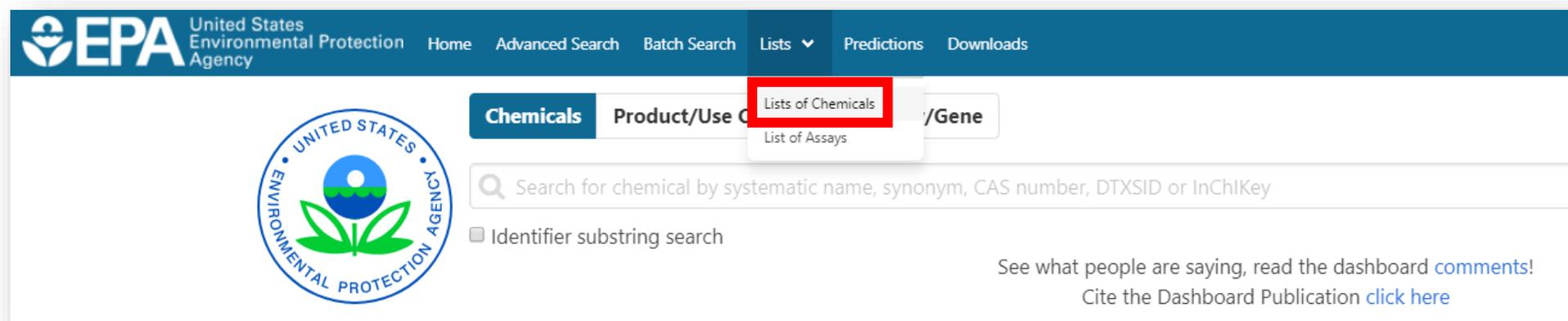
Download ToxCast Model Predictions ▼ **Download all model data**

| 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  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

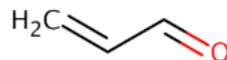


Acetonitrile

DTXSID: DTXSID7020009

CASRN: 75-05-8

TOXCST: 3/210

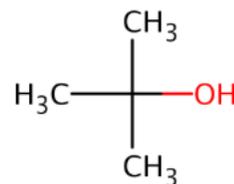


Acrolein

DTXSID: DTXSID5020023

CASRN: 107-02-8

TOXCST: 2/211

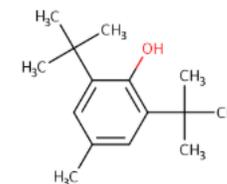


tert-Butyl alcohol

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 |
|---|---|---------------------|--|--|--------------|
| <a href="#">NVS_ADME_hCYP19A1</a>           |    | 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      |
| <a href="#">NVS_ADME_hCYP19A1_Activator</a> |    | 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      |
| <a href="#">NVS_ADME_hCYP1A1</a>            |  | 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       |

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    | <a href="#">DTXSID9022526</a> | 9.68 | 29.0 | ACTIVE   | 79.8    |
| tert-Butylbenzene              | 98-06-6    | <a href="#">DTXSID3047138</a> | 9.68 | 29.0 | ACTIVE   | 60.4    |
| 1,2,4,5-Tetrachlorobenzene     | 95-94-3    | <a href="#">DTXSID7024320</a> | 9.68 | 29.0 | ACTIVE   | 36.8    |
| Sodium dodecylbenzenesulfonate | 25155-30-0 | <a href="#">DTXSID7025219</a> | 9.68 | 29.0 | ACTIVE   | 62.7    |
| Octabenzene                    | 1843-05-6  | <a href="#">DTXSID9027441</a> | 9.68 | 29.0 | ACTIVE   | 33.9    |
| Methyl 2-aminobenzoate         | 134-20-3   | <a href="#">DTXSID6025567</a> | 9.68 | 29.0 | ACTIVE   | 36.4    |
| 1,2-Dichlorobenzene            | 95-50-1    | <a href="#">DTXSID6020430</a> | 9.68 | 29.0 | ACTIVE   | 29.5    |
| 1-Benzylquinolinium chloride   | 15619-48-4 | <a href="#">DTXSID8044593</a> | 9.68 | 29.0 | INACTIVE | -0.803  |
| Dodecylbenzene                 | 123-01-3   | <a href="#">DTXSID7026994</a> | 9.68 | 29.0 | INACTIVE | -3.05   |
| Benzoin                        | 119-53-9   | <a href="#">DTXSID1020144</a> | 9.68 | 29.0 | INACTIVE | 1.13    |

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

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

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

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

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

**Diethyls**  
DTXSID:  
CASRN:  
TOXCAST:

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

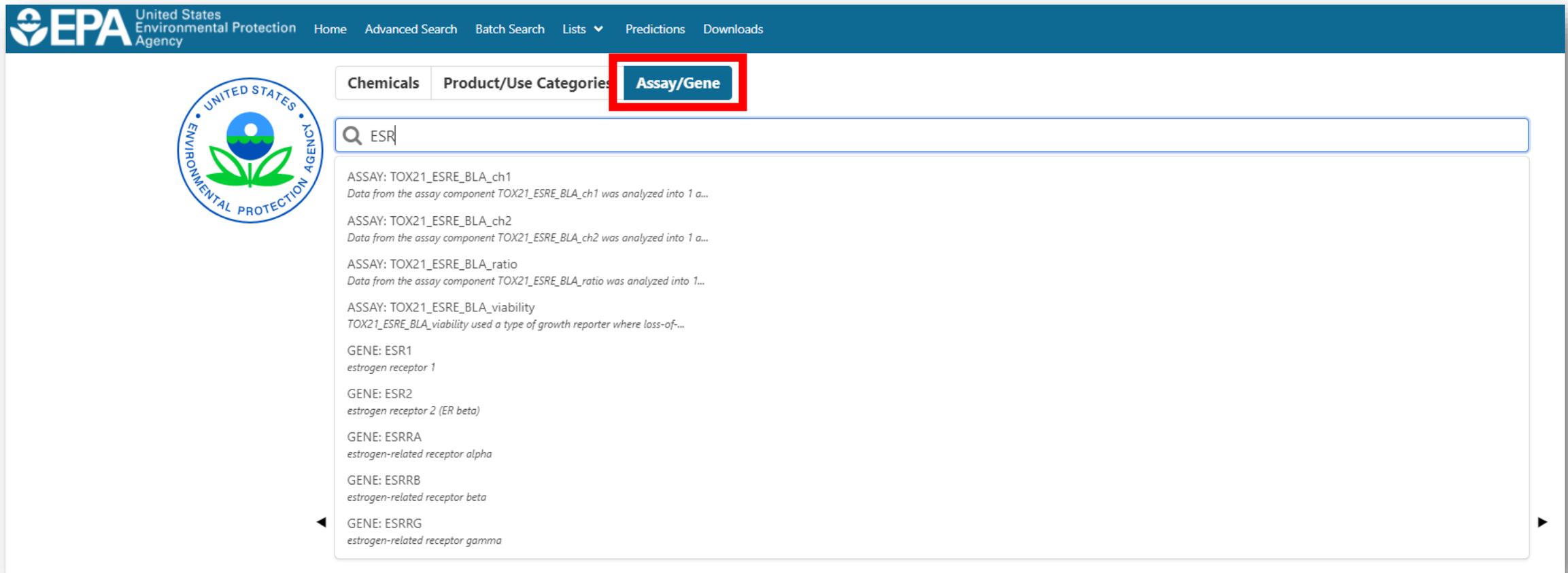


# New Search Capability

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 the navigation bar, there are three tabs: 'Chemicals', 'Product/Use Categories', and 'Assay/Gene', with the 'Assay/Gene' tab highlighted by a red box. A search bar contains the text 'ESR'. Below the search bar, a list of search results is displayed, including assays and genes related to ESR.

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

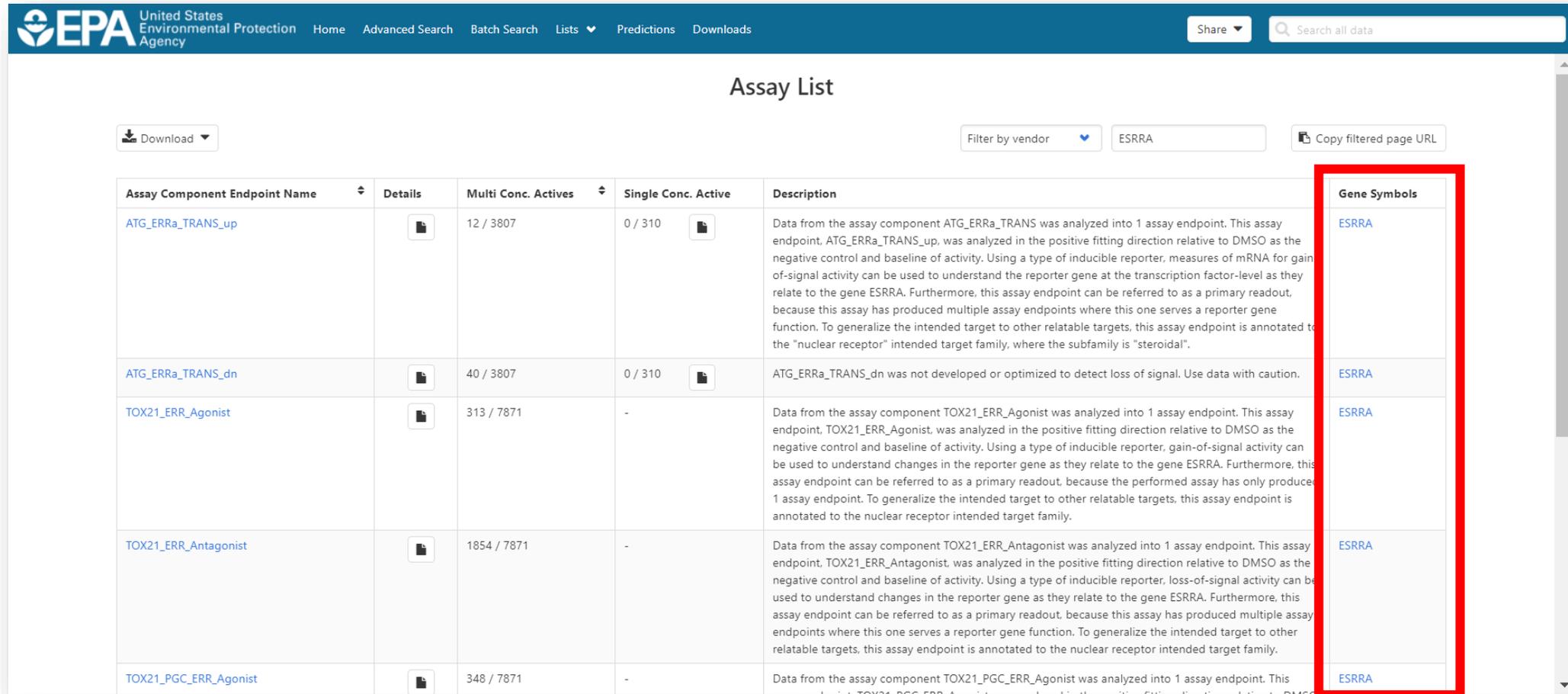
**2-Amino-5-azotoluene**  
DTXSID: DTXSID1020069  
CASRN: 97-56-3  
TOXCAST: 252/709

**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



The screenshot displays the EPA Assay List interface. At the top, the EPA logo and navigation menu are visible. The main content area is titled "Assay List" and includes a "Download" button, a "Filter by vendor" dropdown set to "ESRRA", and a "Copy filtered page URL" button. The table below lists assay endpoints with columns for name, details, multi-concentration active counts, single concentration active counts, and descriptions. A red box highlights the "Gene Symbols" column, which lists "ESRRA" for all entries.

| Assay Component Endpoint Name         | Details   | Multi Conc. Actives | Single Conc. Active   | Description   | Gene Symbols          |
|---------------------------------------|---|---------------------|---|---|-----------------------|
| <a href="#">ATG_ERRa_TRANS_up</a>     |    | 12 / 3807           | 0 / 310  | Data from the assay component ATG_ERRa_TRANS was analyzed into 1 assay endpoint. This assay endpoint, ATG_ERRa_TRANS_up, was analyzed in the positive fitting direction relative to DMSO as the negative control and baseline of activity. Using a type of inducible reporter, measures of mRNA for gain-of-signal activity can be used to understand the reporter gene at the transcription factor-level as they relate to the gene ESRRA. 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 reporter gene 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". | <a href="#">ESRRA</a> |
| <a href="#">ATG_ERRa_TRANS_dn</a>     |    | 40 / 3807           | 0 / 310  | ATG_ERRa_TRANS_dn was not developed or optimized to detect loss of signal. Use data with caution.   | <a href="#">ESRRA</a> |
| <a href="#">TOX21_ERR_Agonist</a>     |    | 313 / 7871          | -   | Data from the assay component TOX21_ERR_Agonist was analyzed into 1 assay endpoint. This assay endpoint, TOX21_ERR_Agonist, was analyzed in the positive fitting direction relative to DMSO as the negative control and baseline of activity. Using a type of inducible reporter, gain-of-signal activity can be used to understand changes in the reporter gene as they relate to the gene ESRRA. 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.   | <a href="#">ESRRA</a> |
| <a href="#">TOX21_ERR_Antagonist</a>  |  | 1854 / 7871         | -   | Data from the assay component TOX21_ERR_Antagonist was analyzed into 1 assay endpoint. This assay endpoint, TOX21_ERR_Antagonist, was analyzed in the positive fitting direction relative to DMSO as the negative control and baseline of activity. Using a type of inducible reporter, loss-of-signal activity can be used to understand changes in the reporter gene as they relate to the gene ESRRA. 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 reporter gene function. To generalize the intended target to other relatable targets, this assay endpoint is annotated to the nuclear receptor intended target family.  | <a href="#">ESRRA</a> |
| <a href="#">TOX21_PGC_ERR_Agonist</a> |  | 348 / 7871          | -   | Data from the assay component TOX21_PGC_ERR_Agonist was analyzed into 1 assay endpoint. This assay endpoint, TOX21_PGC_ERR_Agonist, was analyzed in the positive fitting direction relative to DMSO as the negative control and baseline of activity. Using a type of inducible reporter, gain-of-signal activity can be used to understand changes in the reporter gene as they relate to the gene ESRRA. 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.   | <a href="#">ESRRA</a> |

# Future CompTox Portal



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# Feedback Welcomed

- Send comments to us via the web page at [http://comptox.epa.gov/dashboard/contact\\_us](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.

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Subject

Message

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