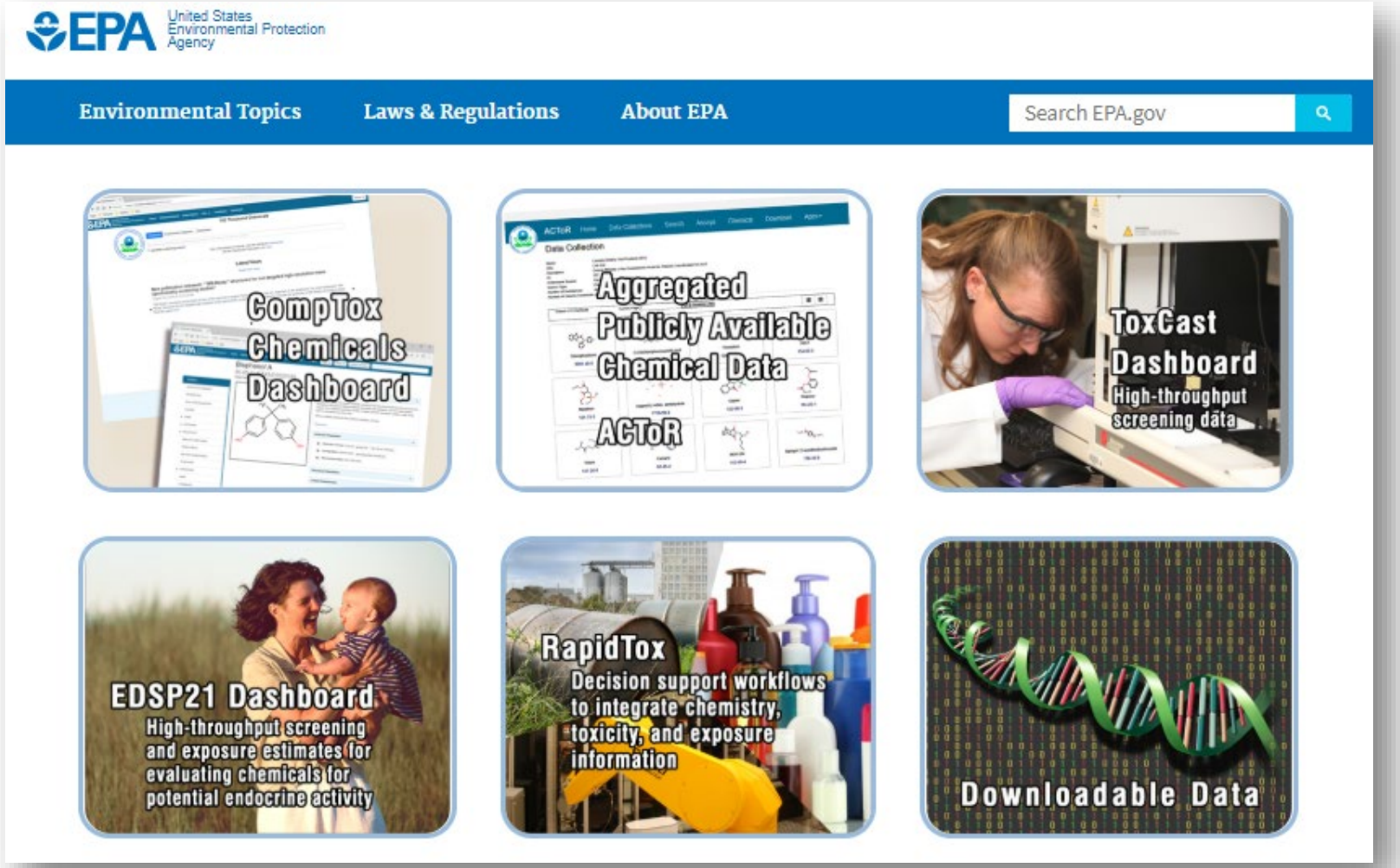
ANNOUNCEMENT

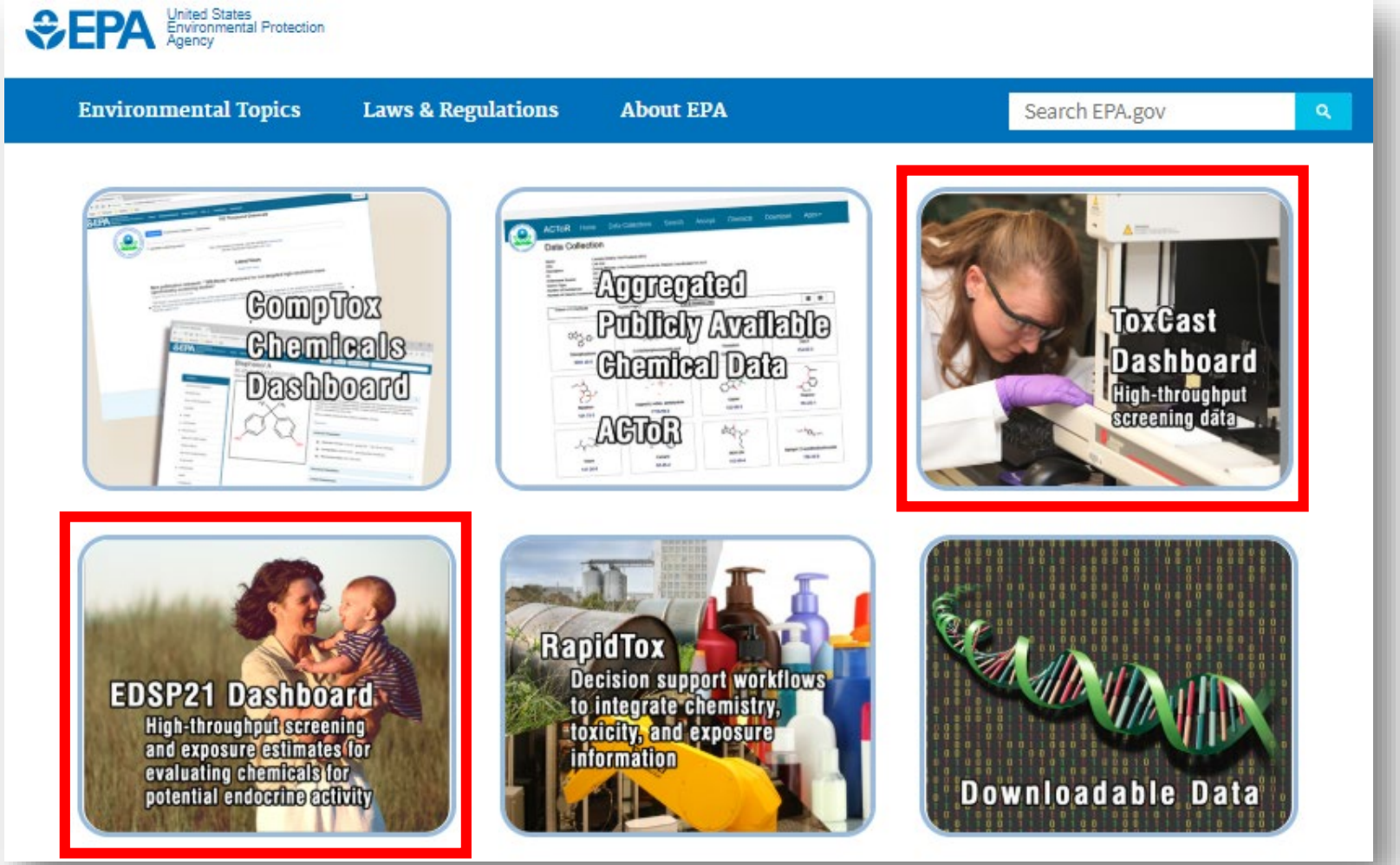
EDSP21 and ToxCast Dashboards To Be Discontinued

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**

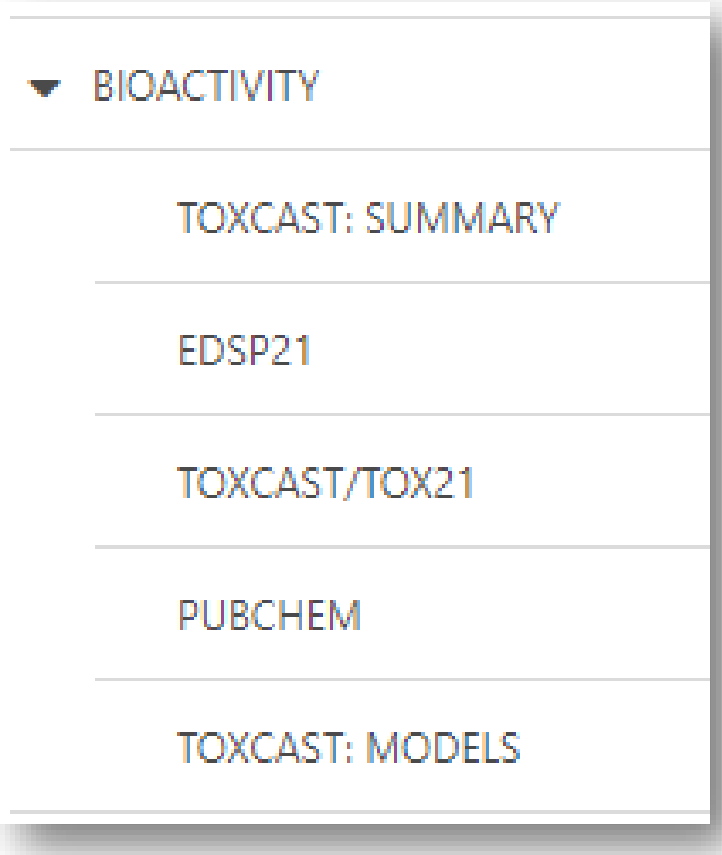
- New functionality supporting the bioactivity data associated with ToxCast, Tox21 and EDSP is available at https://comptox.epa.gov/dashboard

- This presentation provides an overview of bioactivity data in the dashboard

Bioactivity Sub-Tabs

Segregation of data

Bioactivity Data

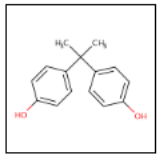


- Summary view of data – tabular and graphical
- Navigate to the EDSP21 subset of assays
- Navigate to all Toxcast/Tox21 data
- Navigate to PubChem data widget
- ToxCast ”Models” – now includes “COMPARA” data

ToxCast:Summary

Sub-Tab

ToxCast Summary Plot



Bisphenol A

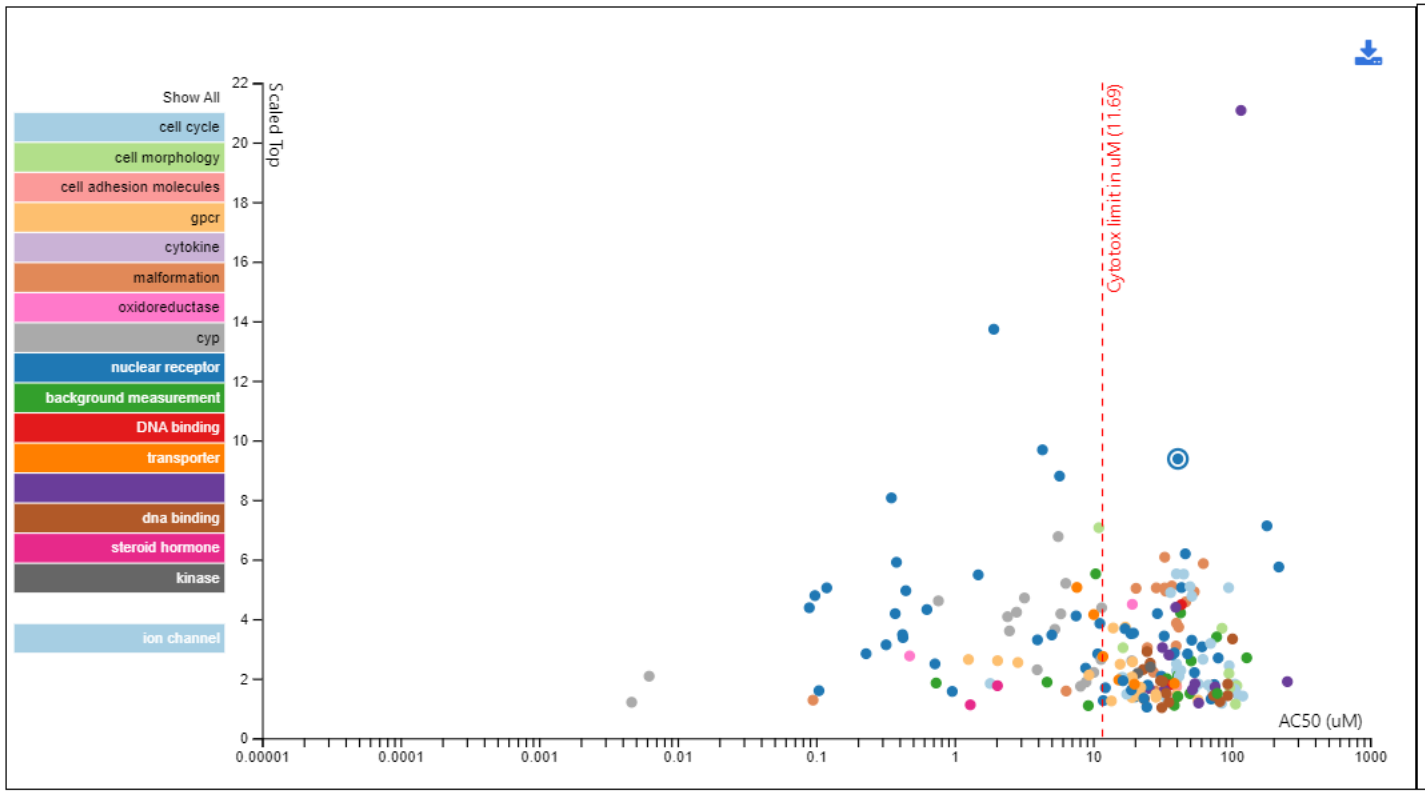
80-05-7 | DTXSID7020182

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

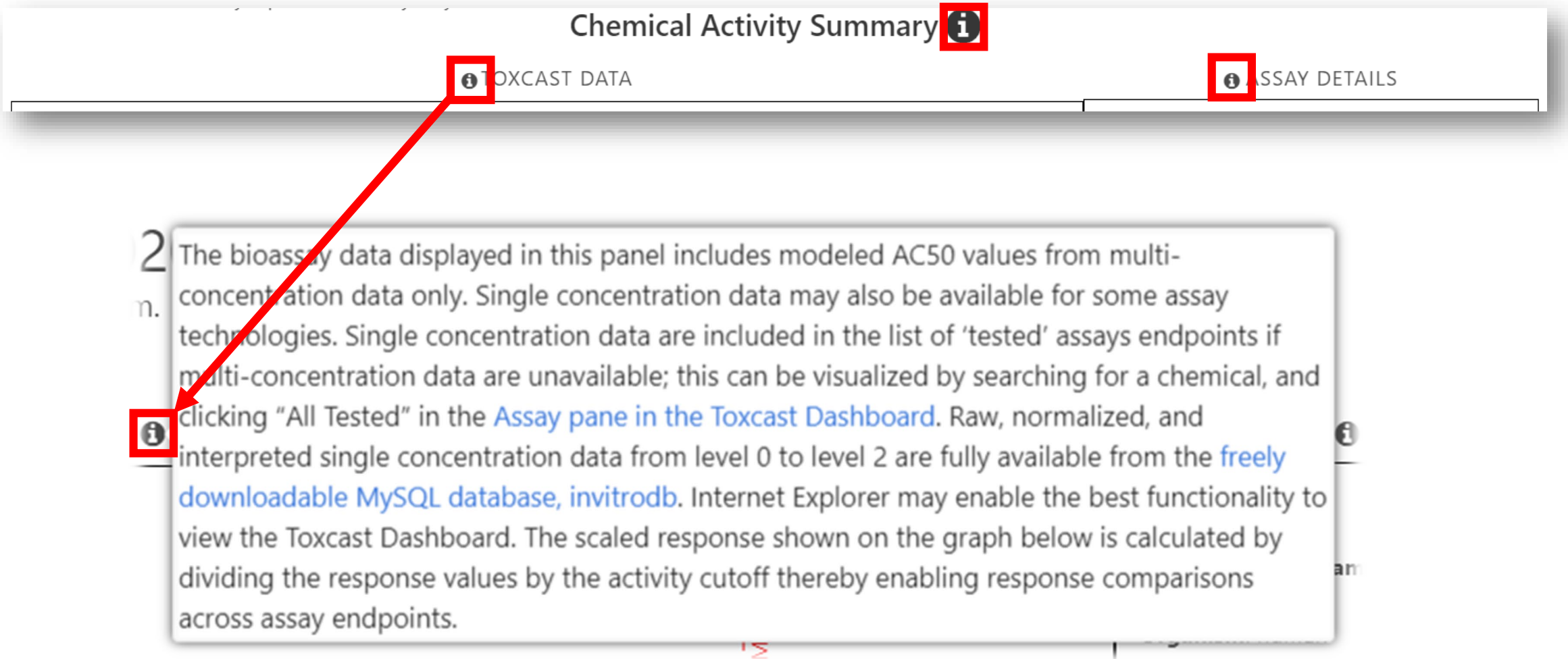
TOXCAST DATA



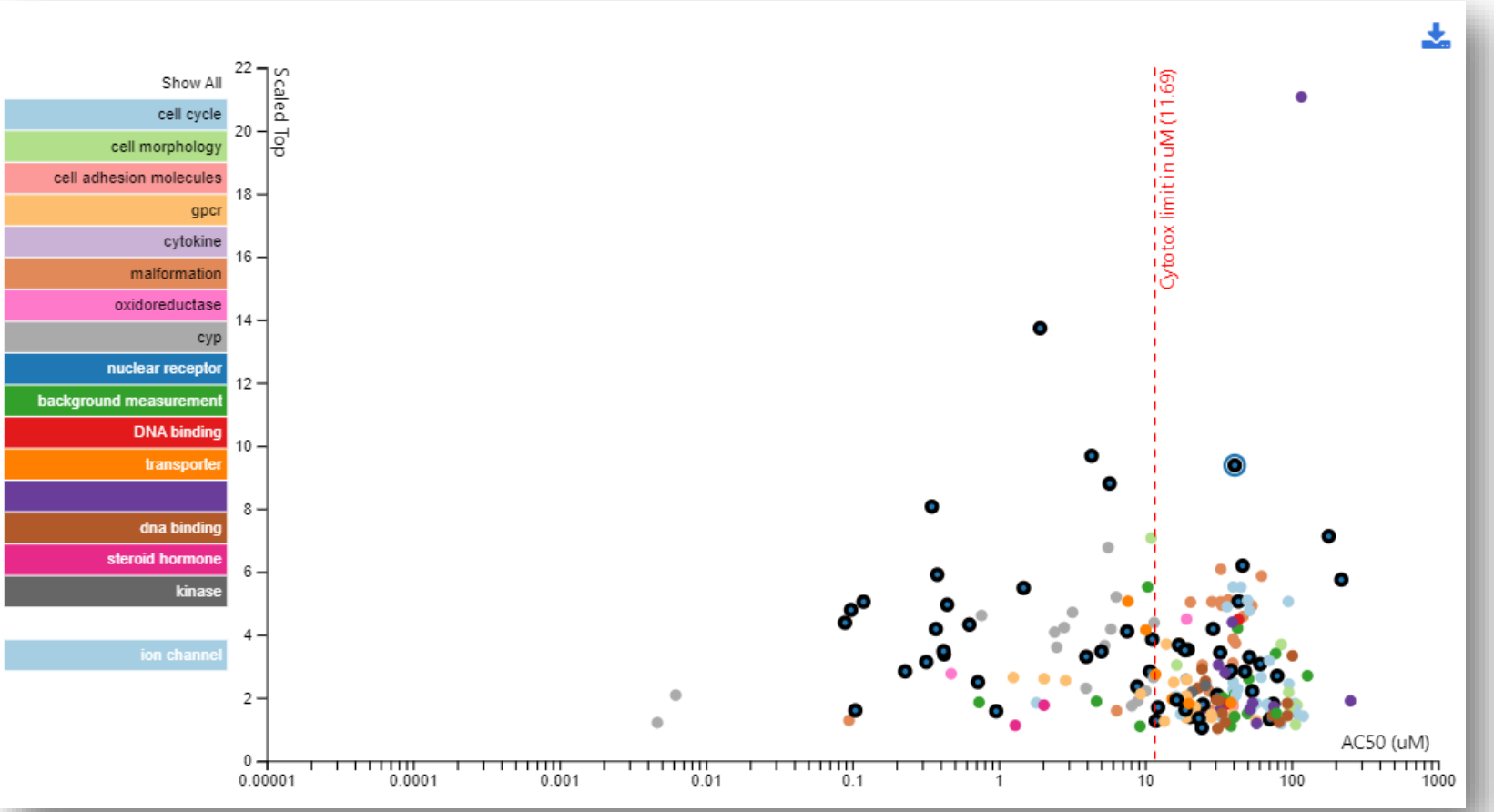
ASSAY DETAILS

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



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

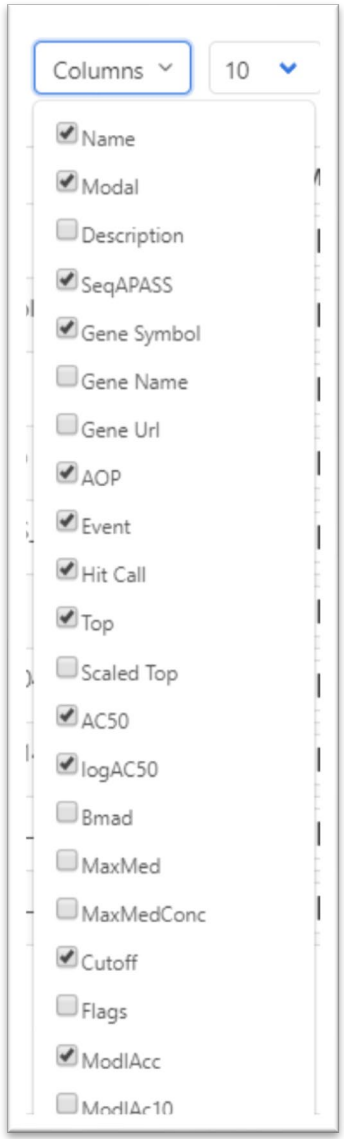
Download | Columns | 10 | Search query | Show Inactive | Show Background

Name	Modal	SeqAPASS	Gene Symbol	AOP	Event	Hit Call	Top	AC50	logAC50	Cutoff	ModlAcc	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



- 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	ModlAcc	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

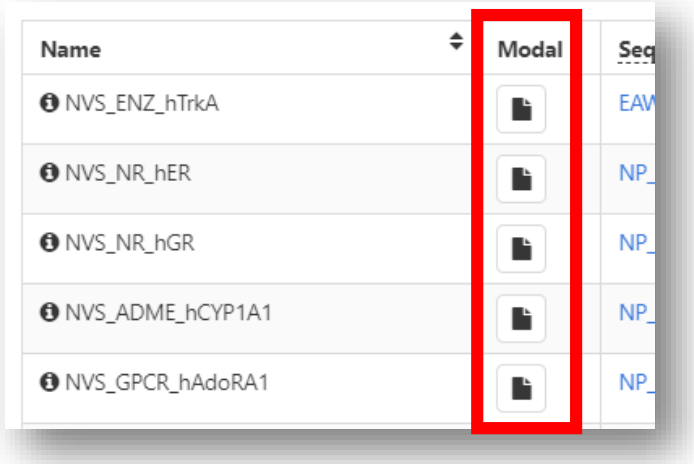
Insert query text to filter table

Switch to show all INACTIVE hit calls

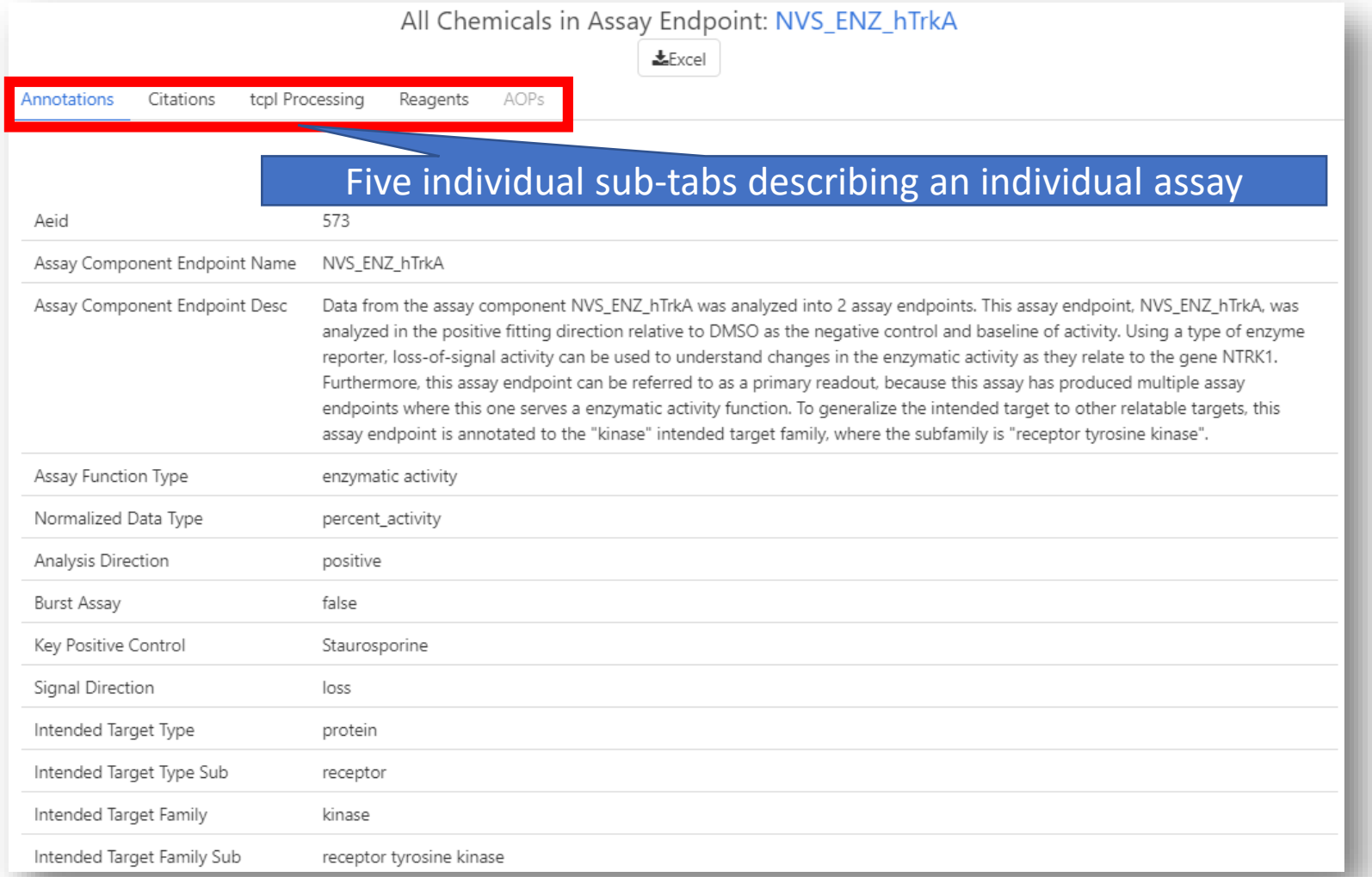
Download | Columns | 10 | NVS | Show Inactive | Show Background

Name	Modal	SeqAPASS	Gene Symbol	AOP	Event	Hit Call	Top	AC50	logAC50	Cutoff	ModlAcc	Intended Target Family
NVS_ENZ_hTrkA		AAW52902.1	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



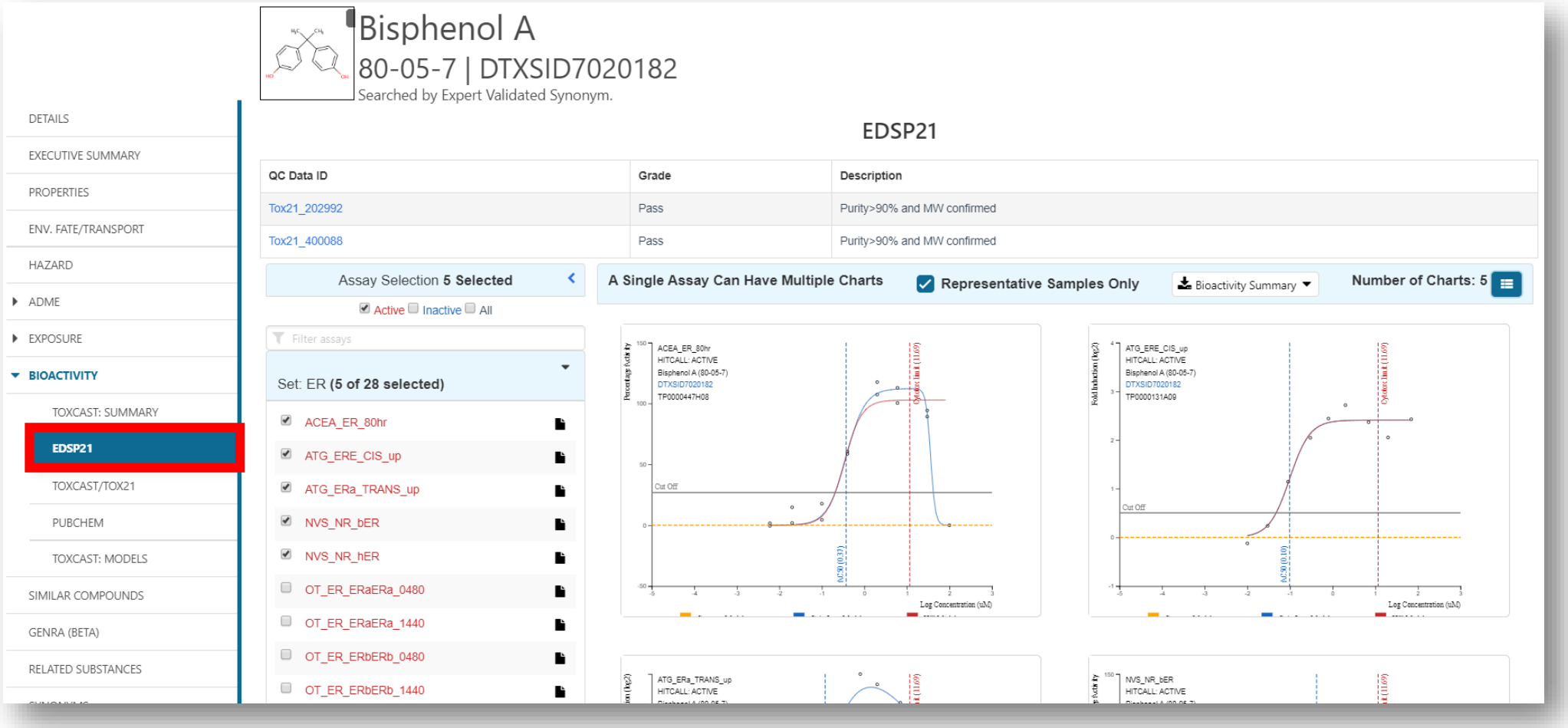
- Select modal icon to display assay details
  - Assay annotations
  - Citations re. the assay
  - tcpl processing details
  - Reagents used in assay
  - Links to Adverse Outcome Pathways



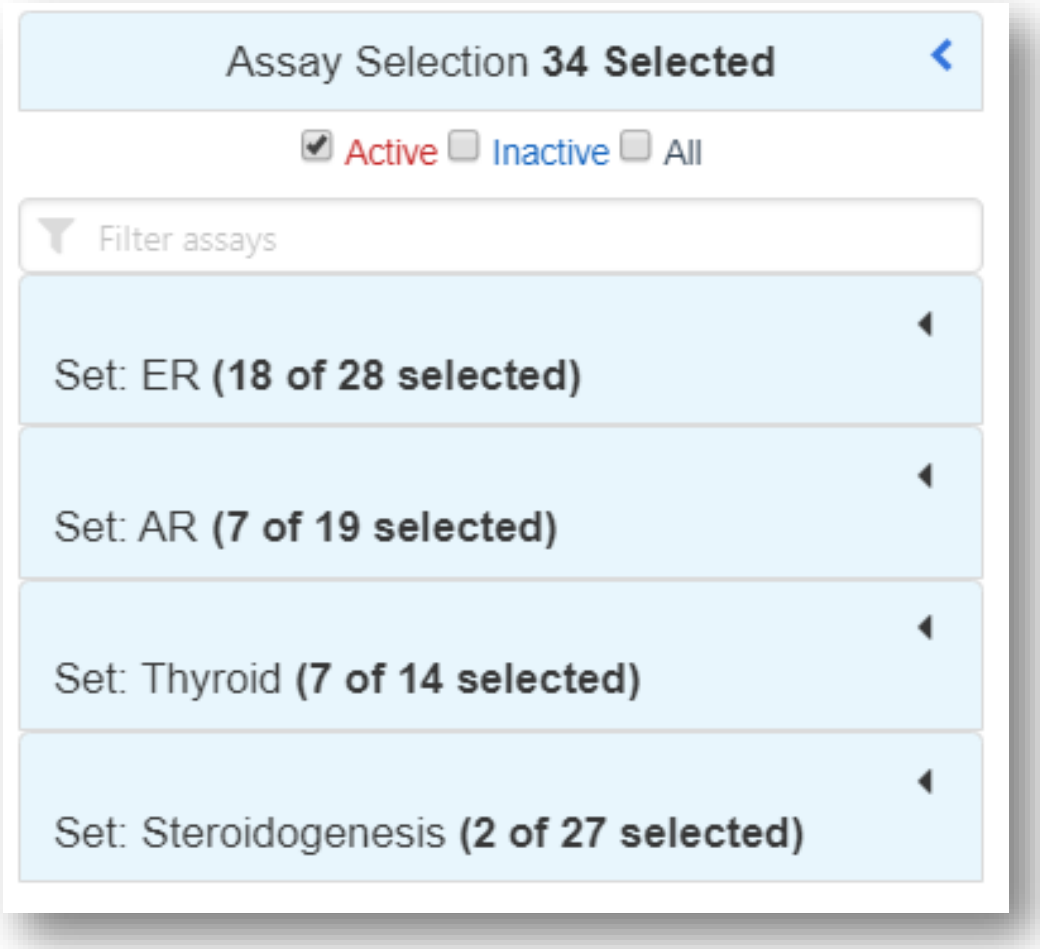
Endocrine Disruptor Screening Program (EDSP)

Sub-Tab

EDSP21 Subset of Assays



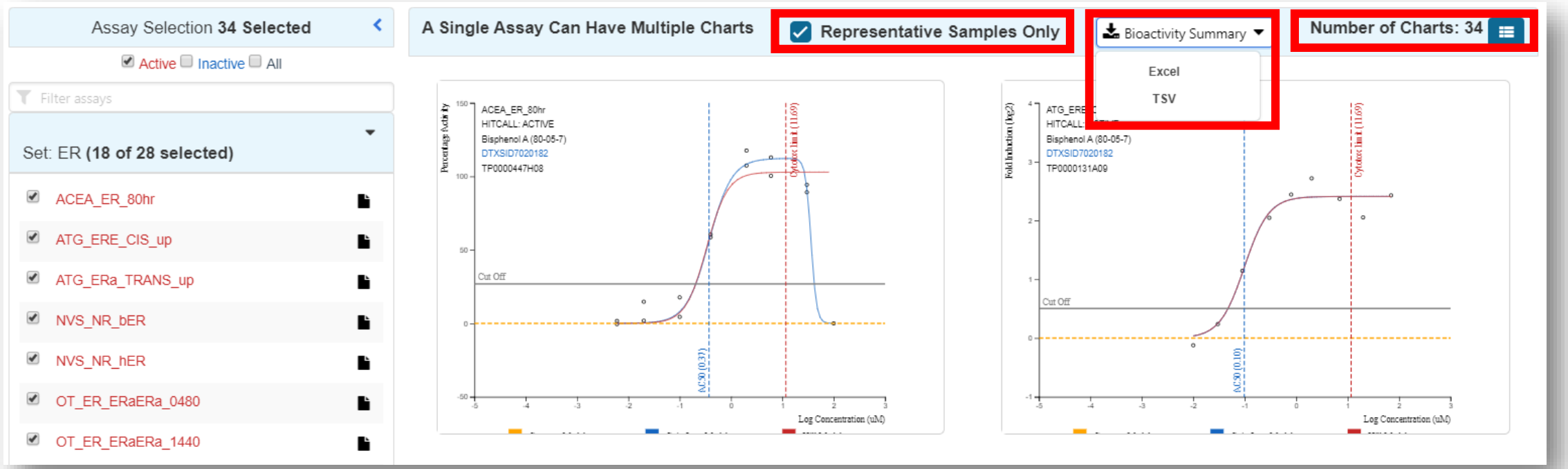
EDSP21 Subset of Assays



- 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

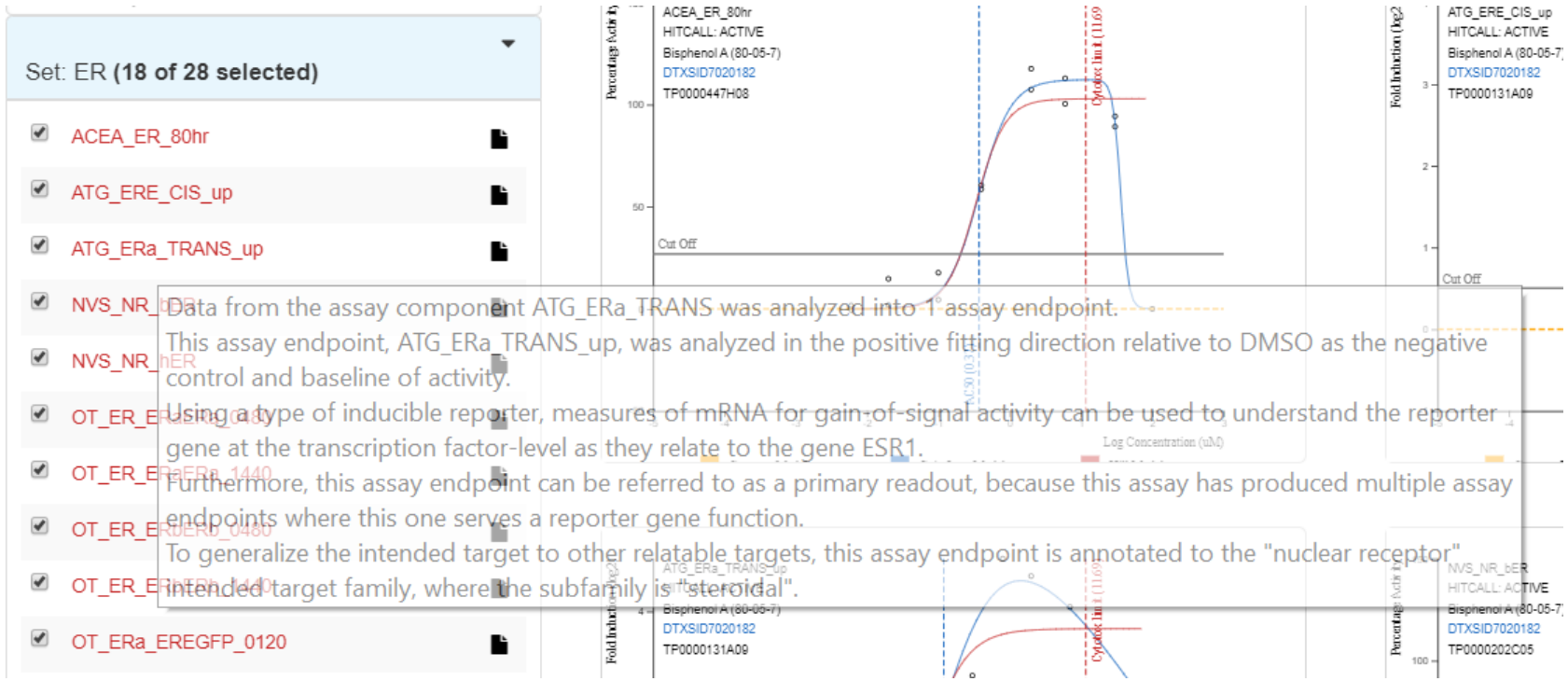
EDSP21 Subset of Assays

- 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



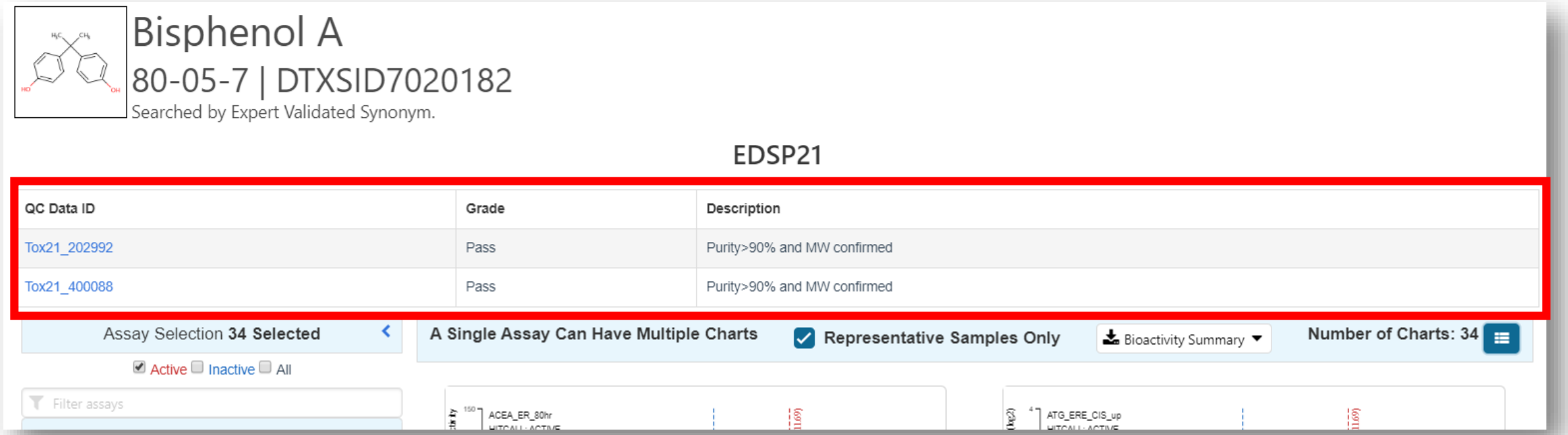
EDSP21 Subset of Assays

- 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

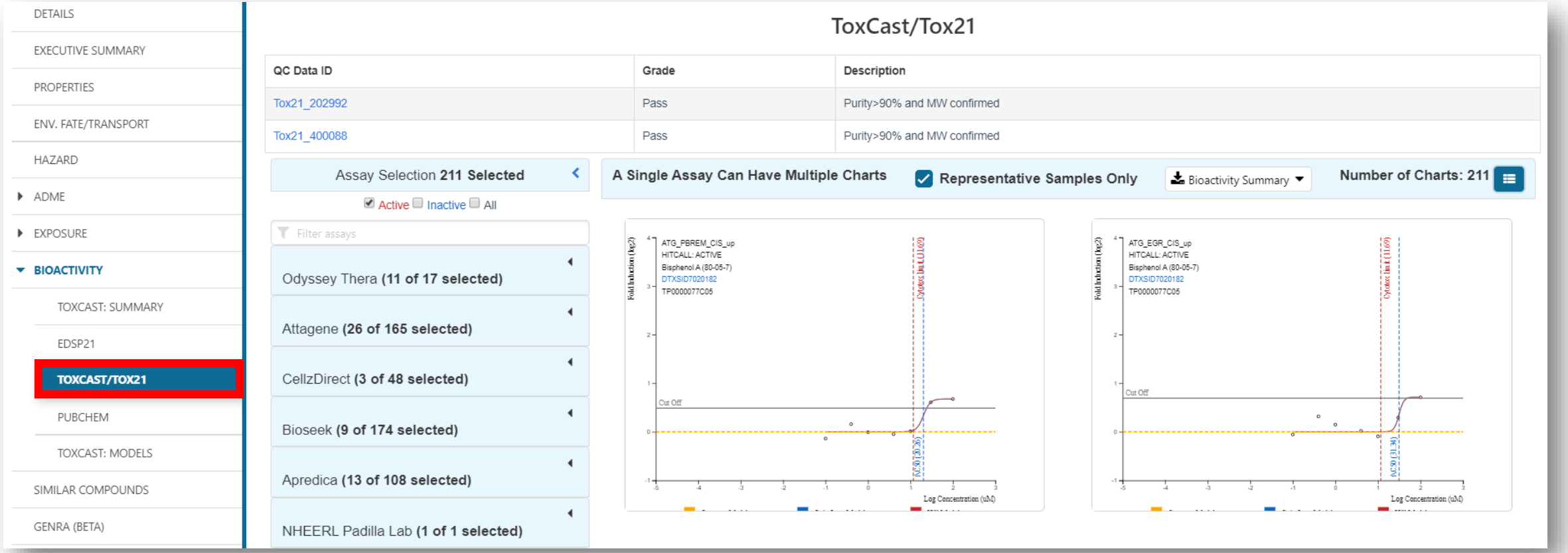


ToxCast/Tox21

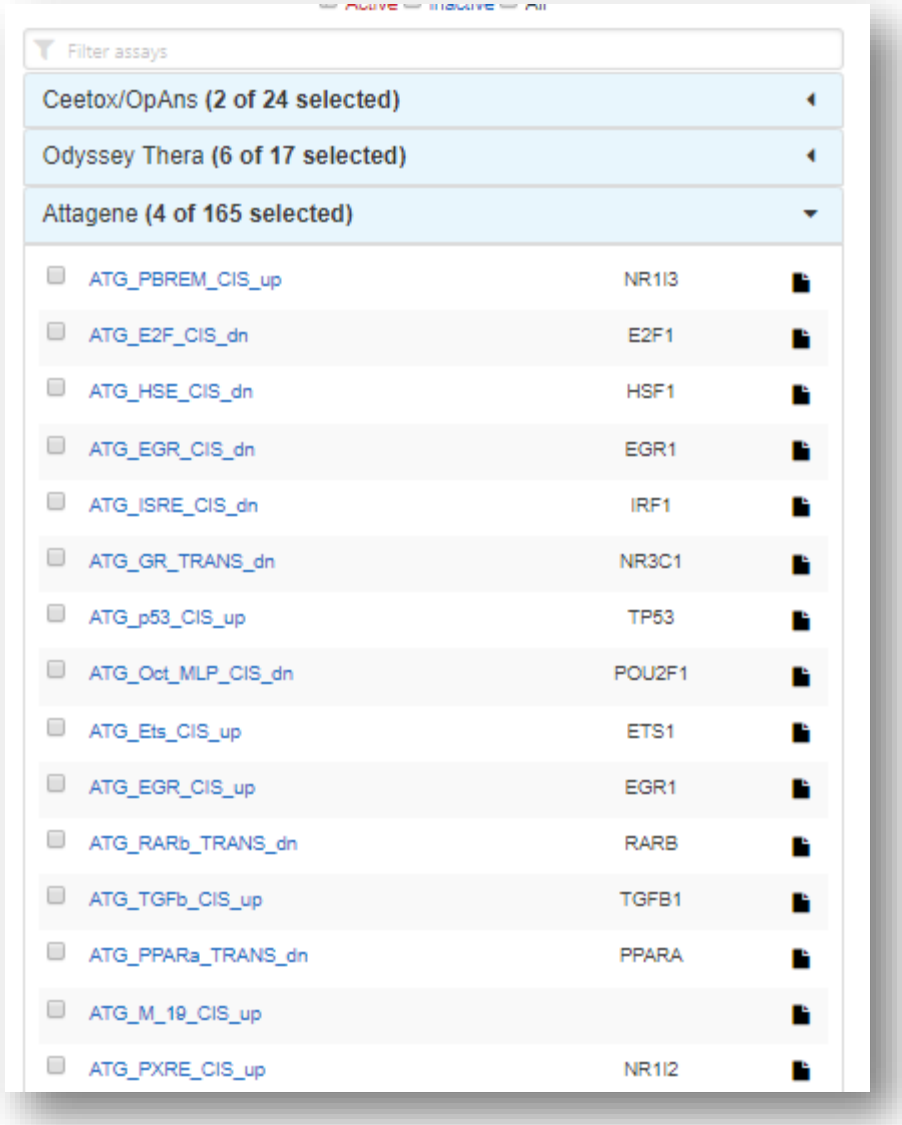
Sub-Tab

ToxCast/Tox21 data

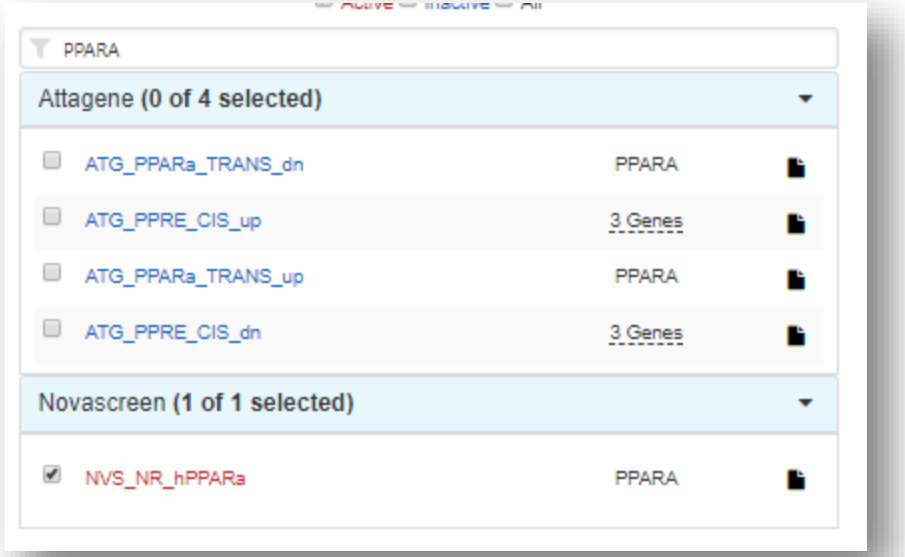
- Navigation of data under this sub-tab parallels the capabilities of the EDSP21 sub-tab except data are organized based on “assay vendor”



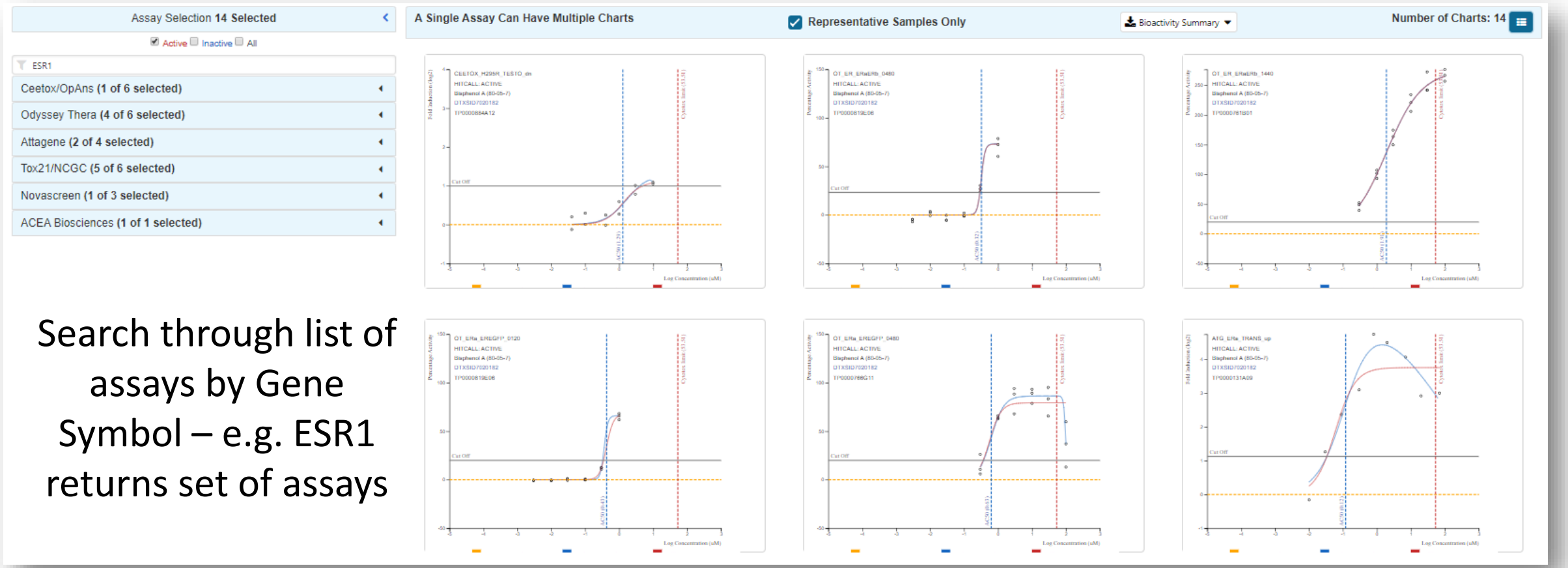
Filtering – Gene annotation added



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



Filtering

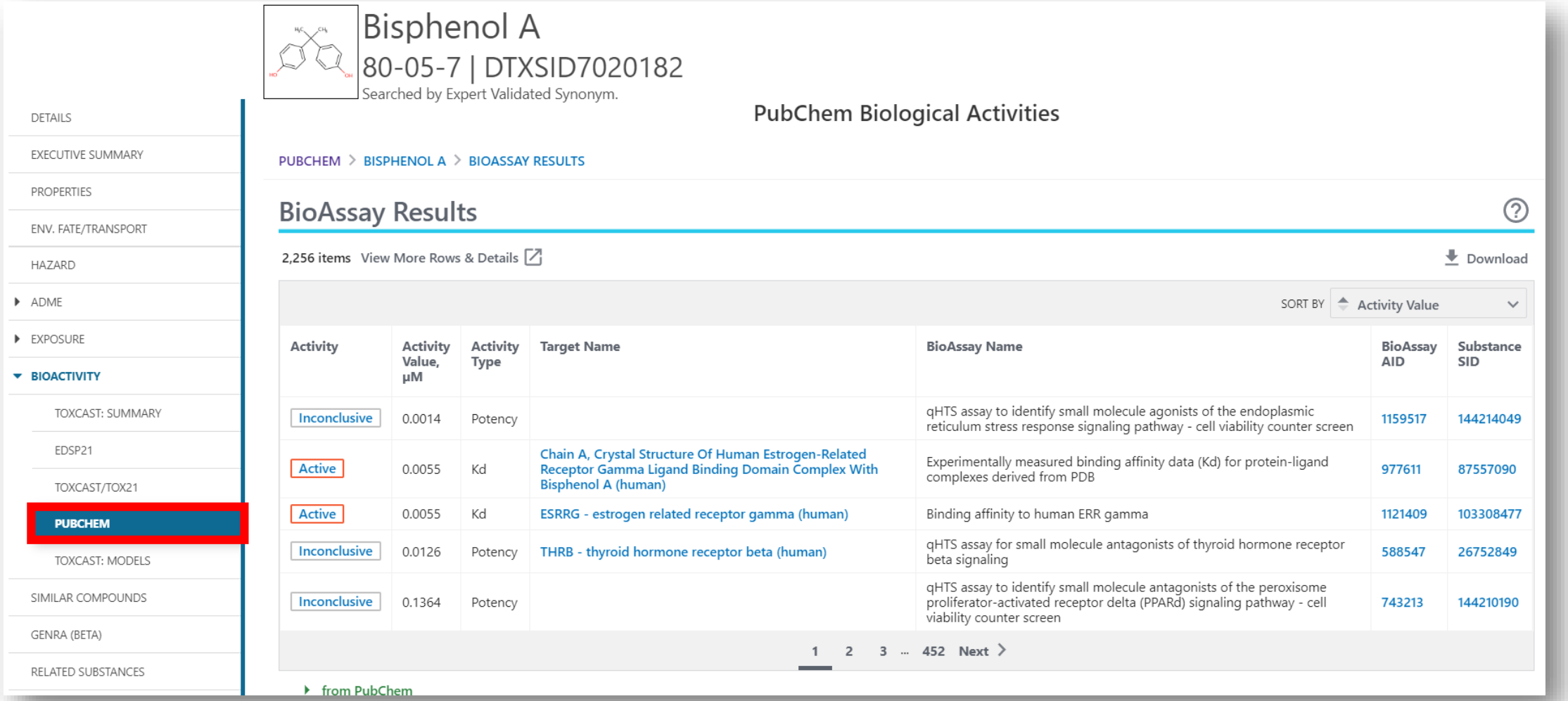


Search through list of assays by Gene Symbol – e.g. ESR1 returns set of assays

PubChem

Sub-Tab

PubChem – integrated view of bioassay data

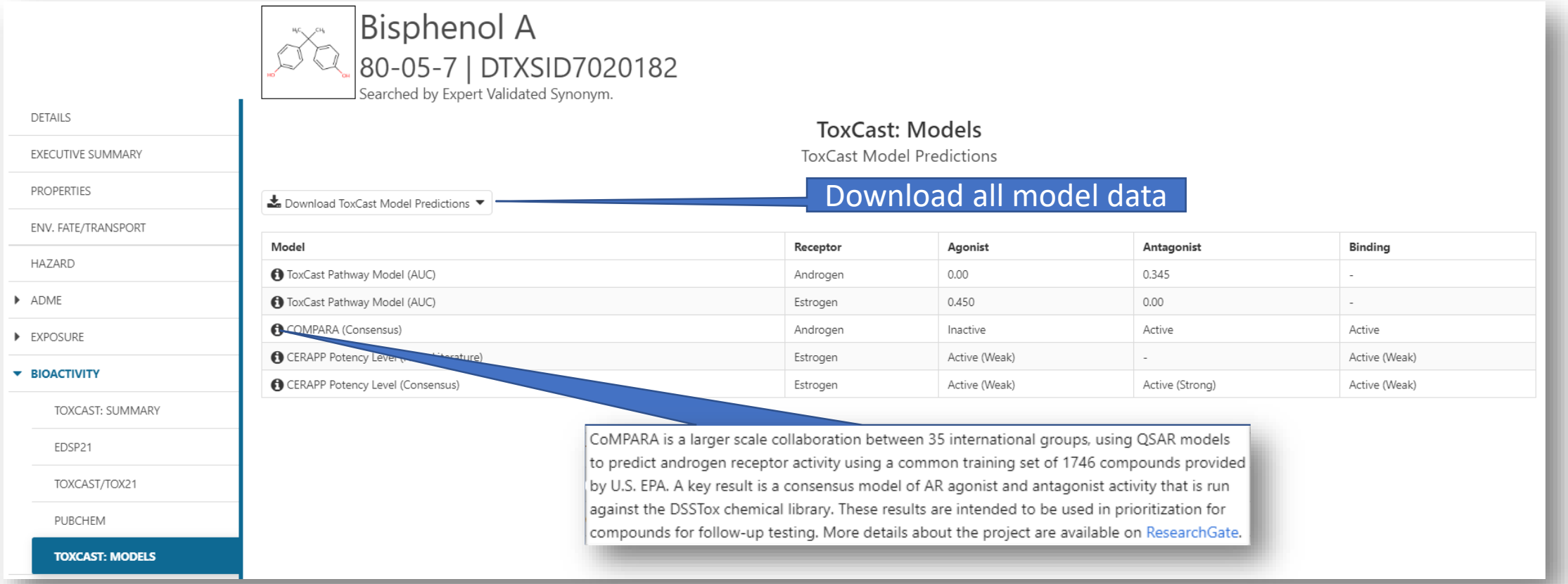


ToxCast Models

Sub-Tab

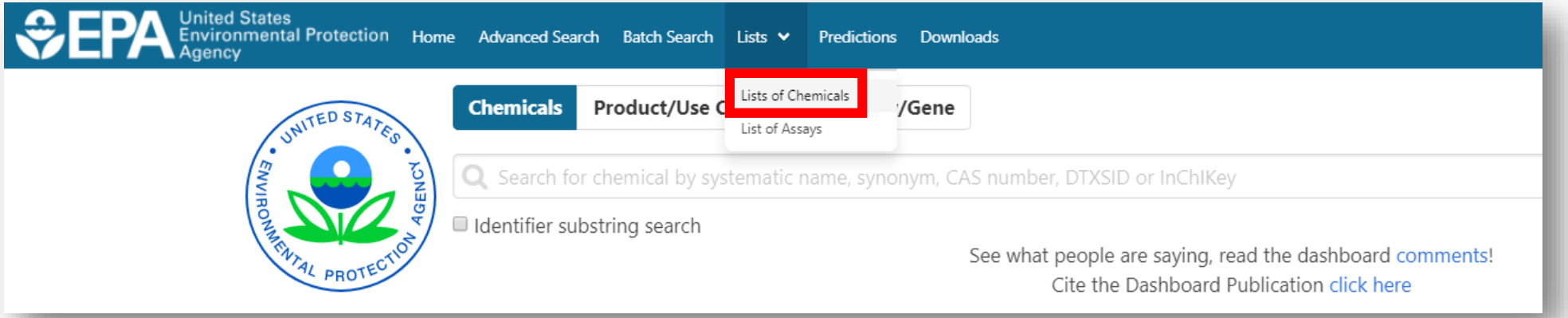
PubChem – integrated view of bioassay data

- 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



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

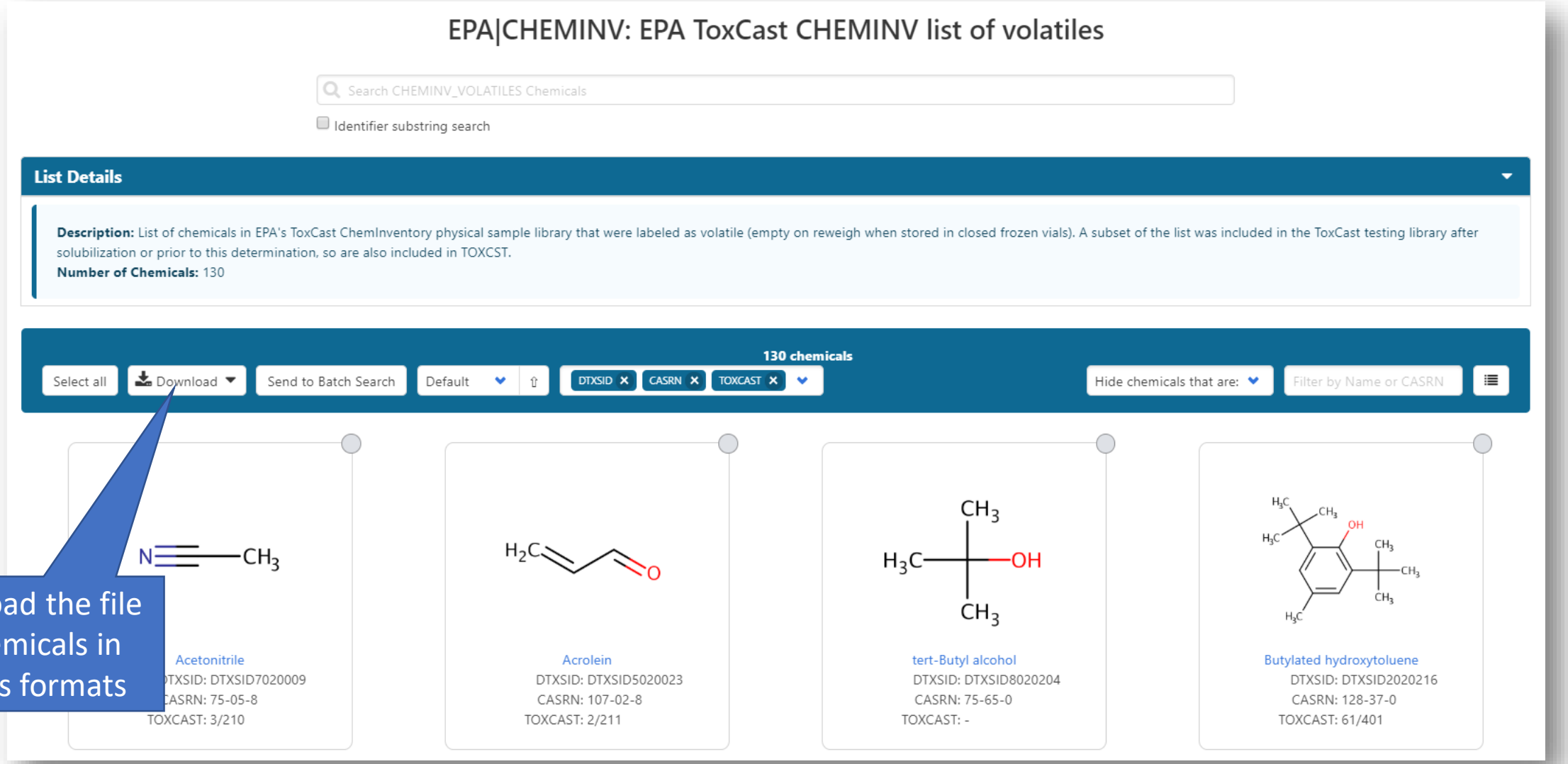
Download | Columns | 10 | ToxCast | Copy Filtered Lists URL

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

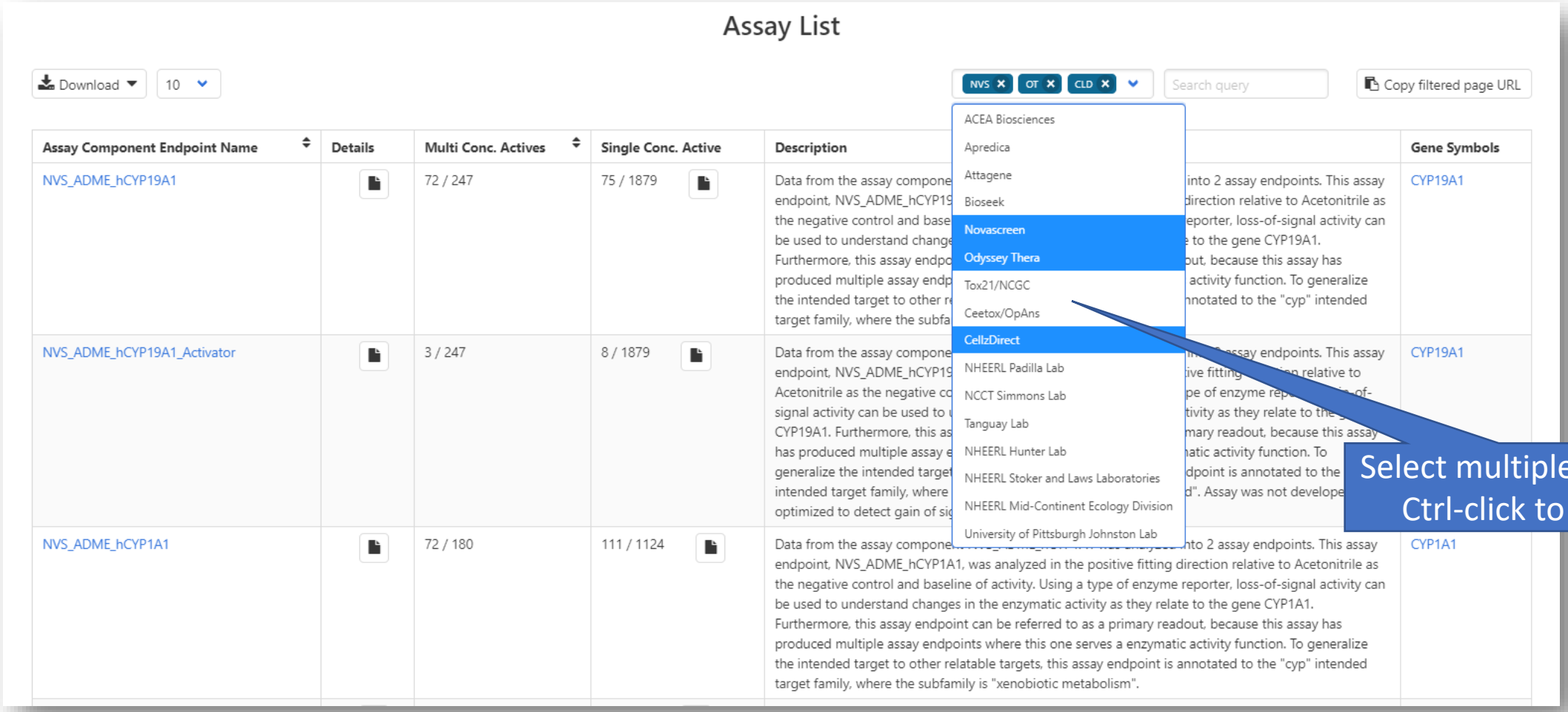


Download the file of chemicals in various formats

Lists of Assays

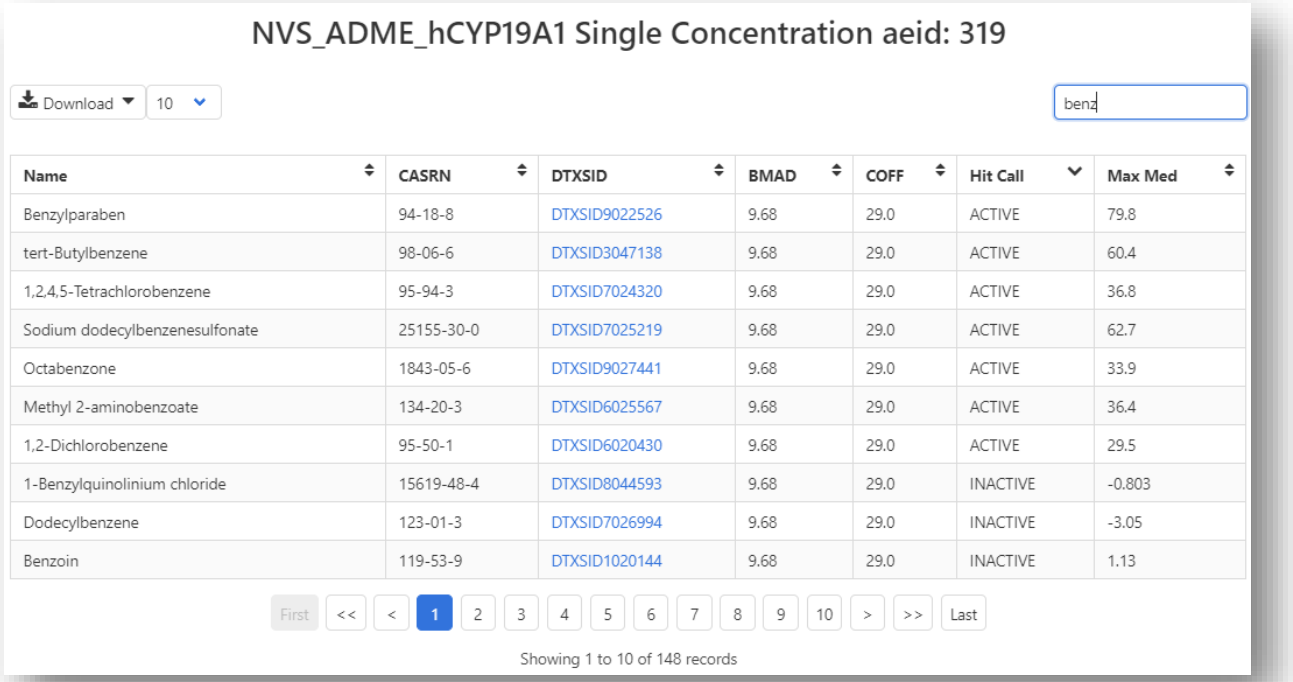
List of Assays - Filter by Vendor

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



Single Concentration Data (August 2019 release)

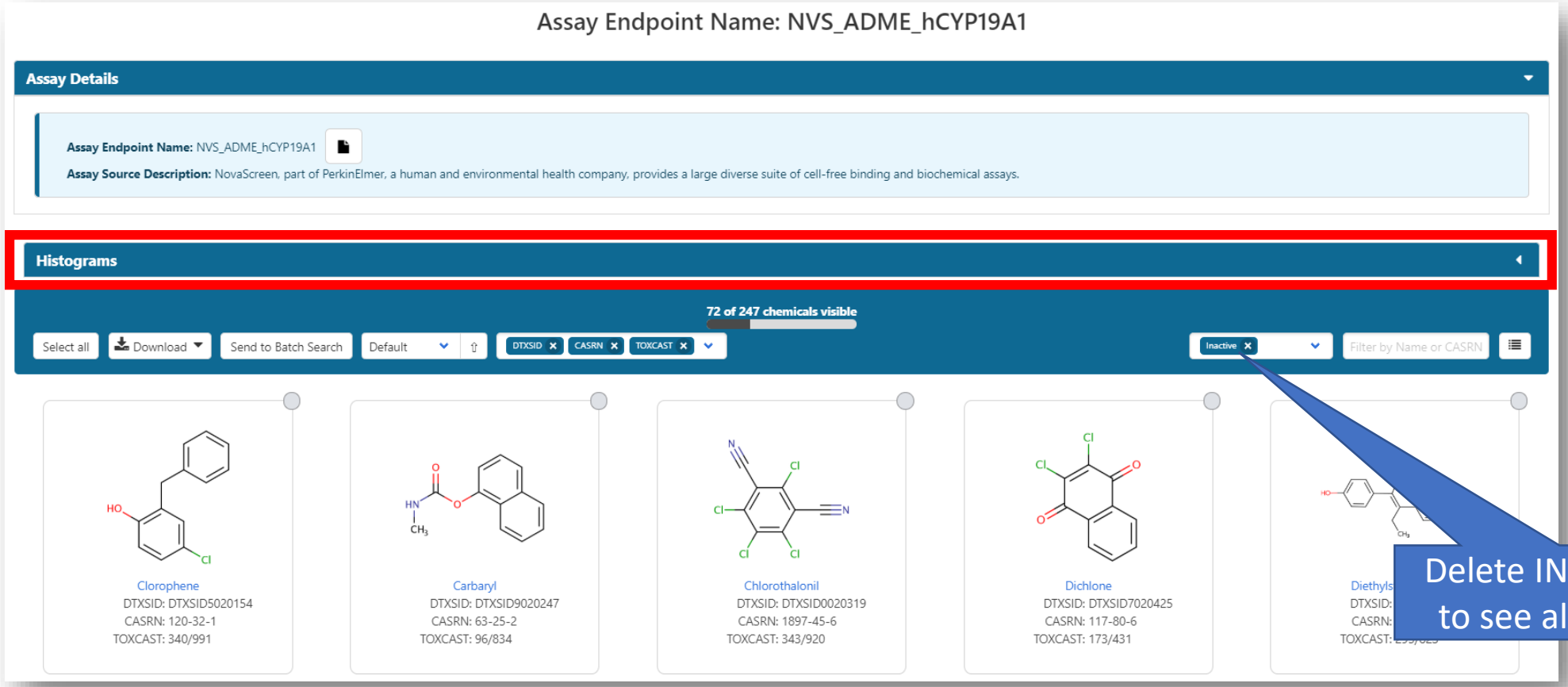
- Some assays have single concentration screening data. Select modal to view data



- 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

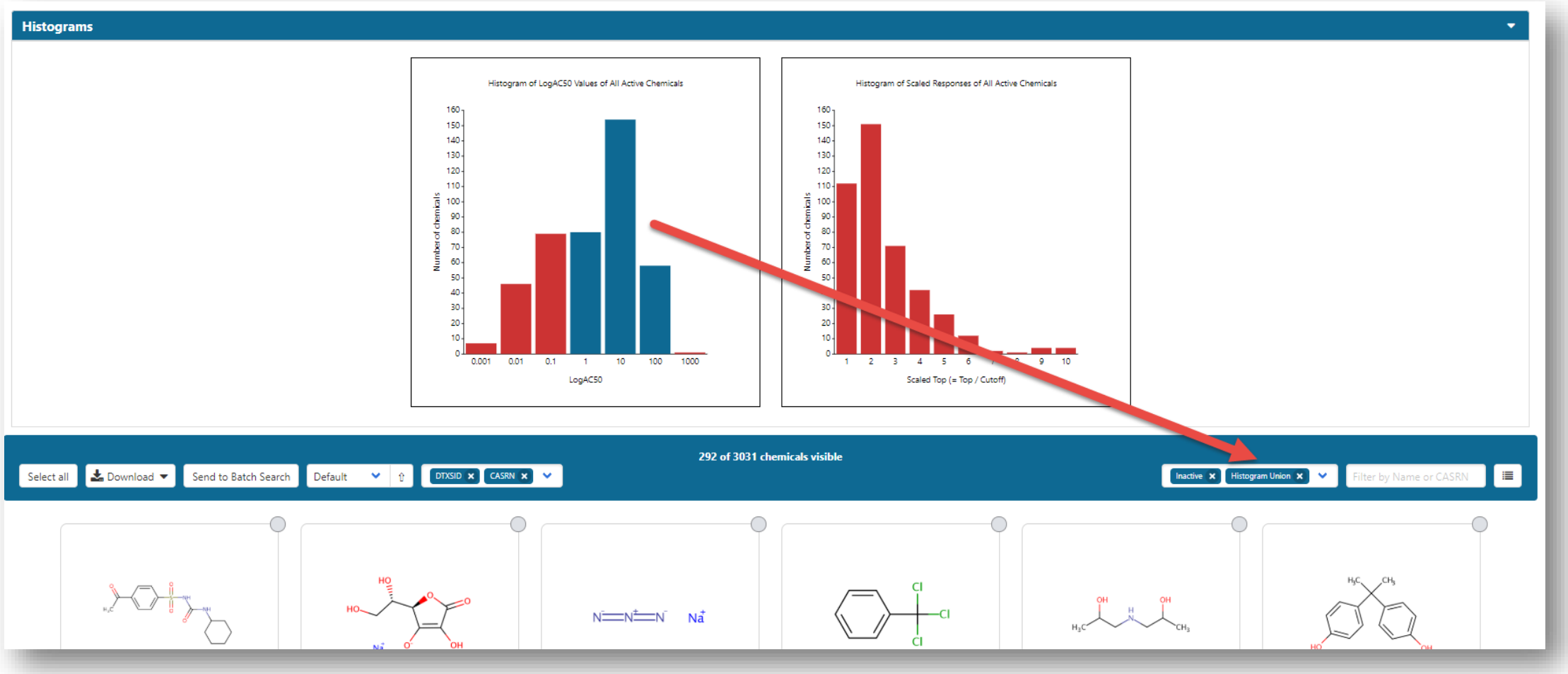
- The modal icon opens up details regarding the individual assay
- ACTIVE hits shown by default. Delete INACTIVE filter to see all data



Interactive histogram summary view

Interactive histogram summary view

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

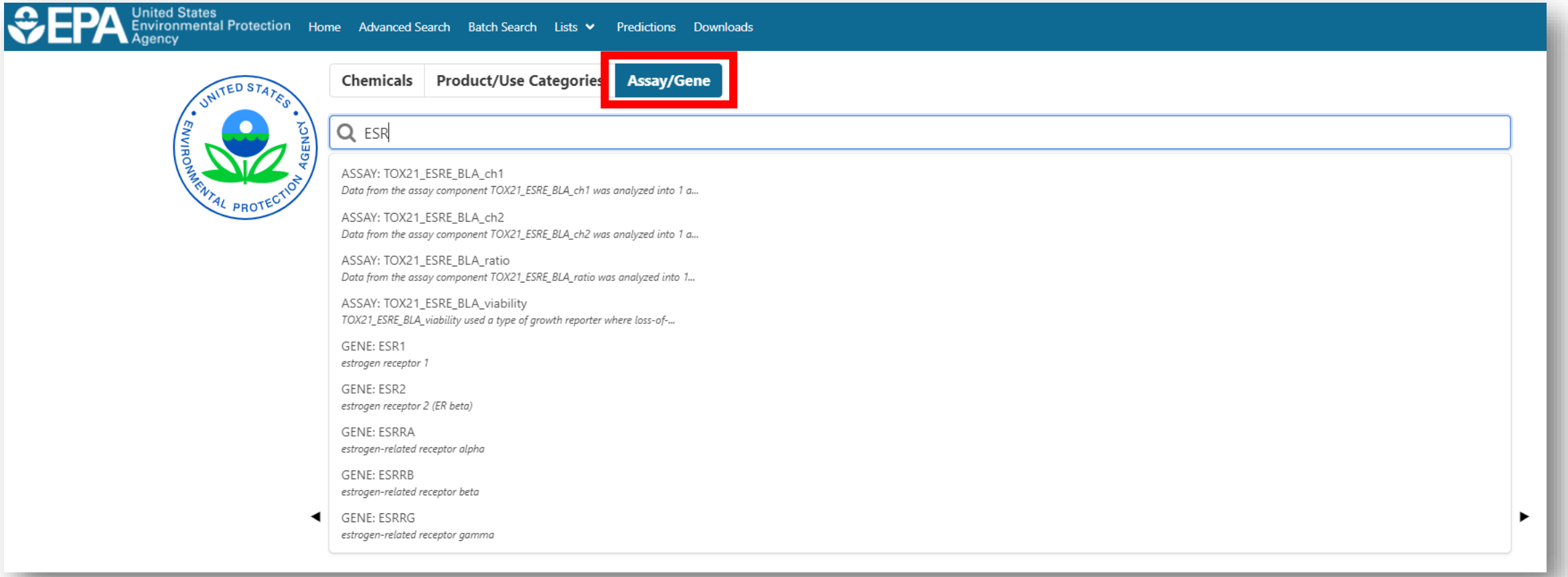


New Search Capability

Search Assay or Gene from Home Page

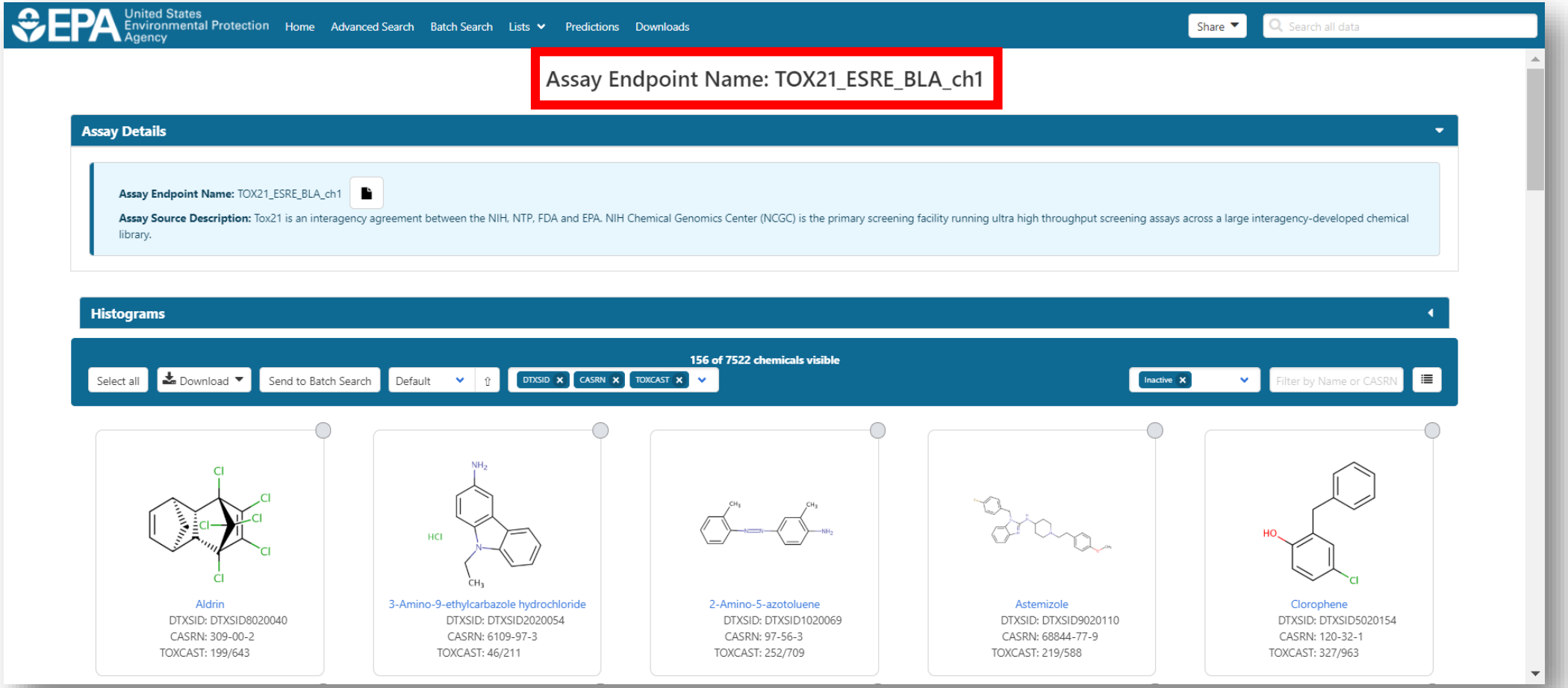
Searching Gene or Assay from the Home Page

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



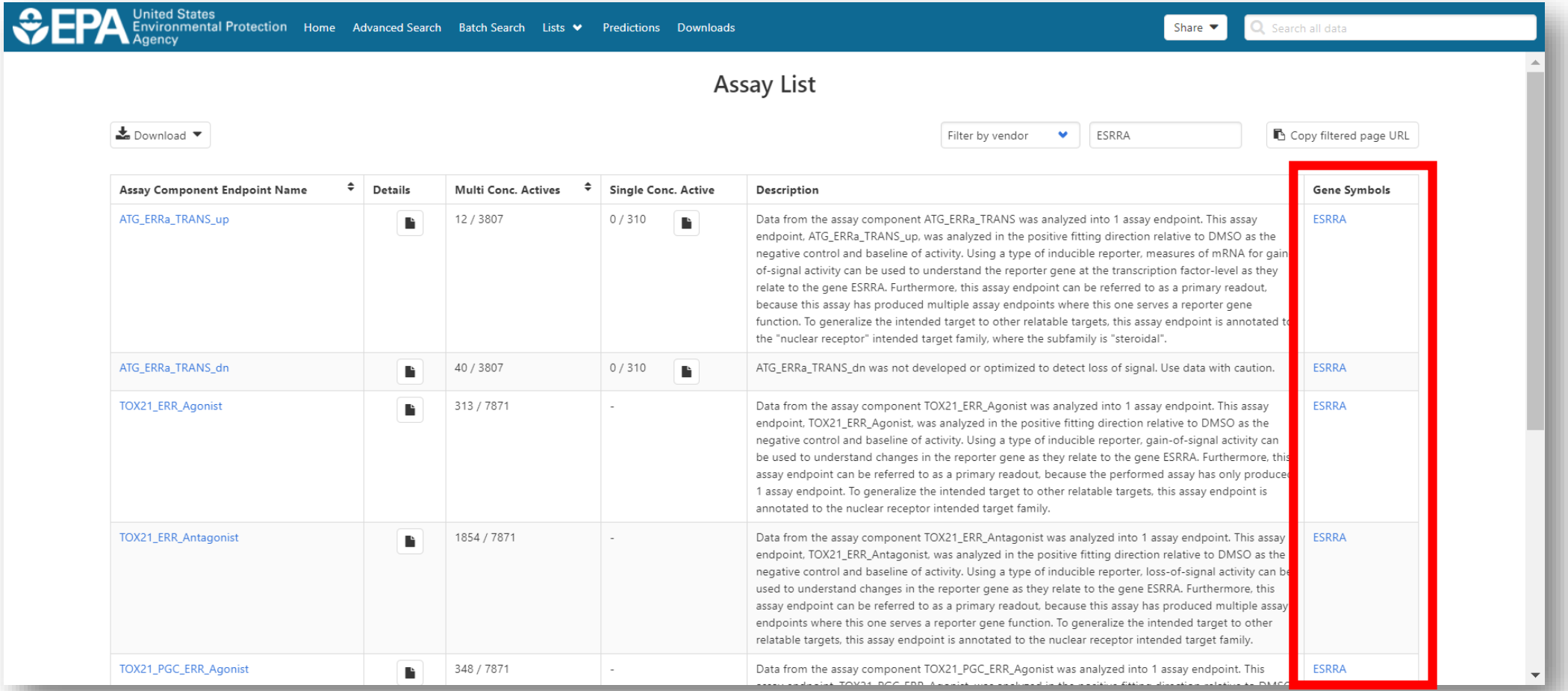
Select hit based on **Assay**

Opens associated list of chemicals for an assay

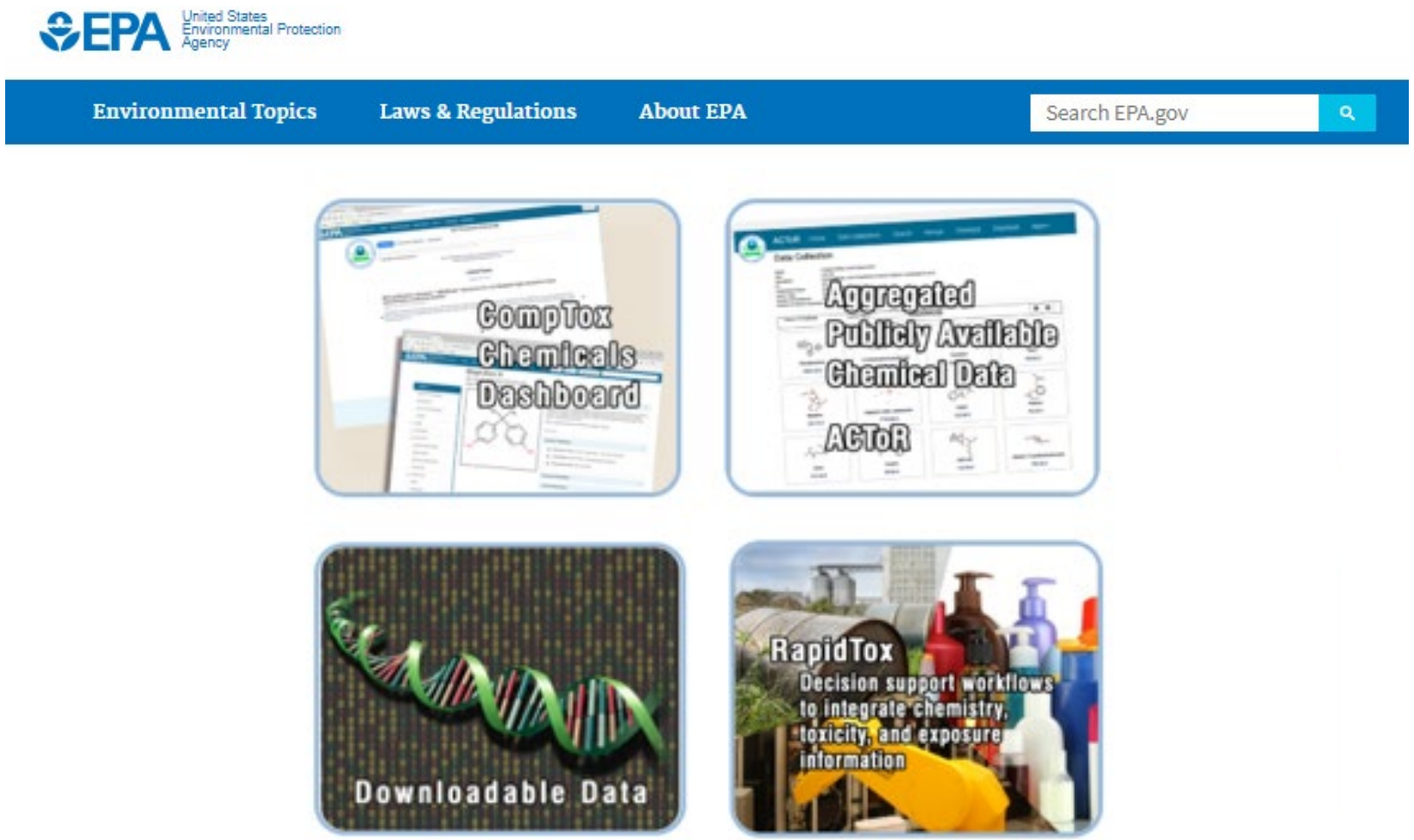


Select hit based on **Gene Symbol**

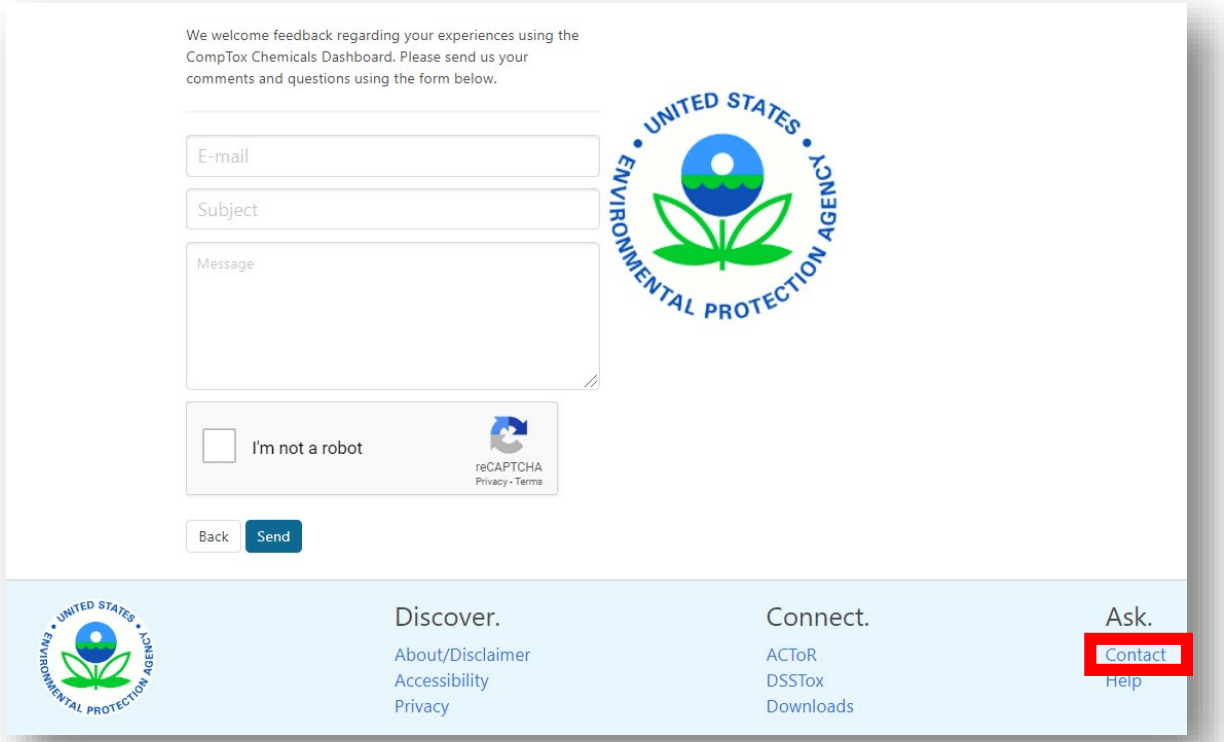
Opens list of assays associated with that Gene



Future CompTox Portal



Feedback Welcomed

- Send comments to us via the web page at

  http://comptox.epa.gov/dashboard/contact_us