CompTox Chemicals Dashboard Version 3/2019

http://comptox.epa.gov/dashboard

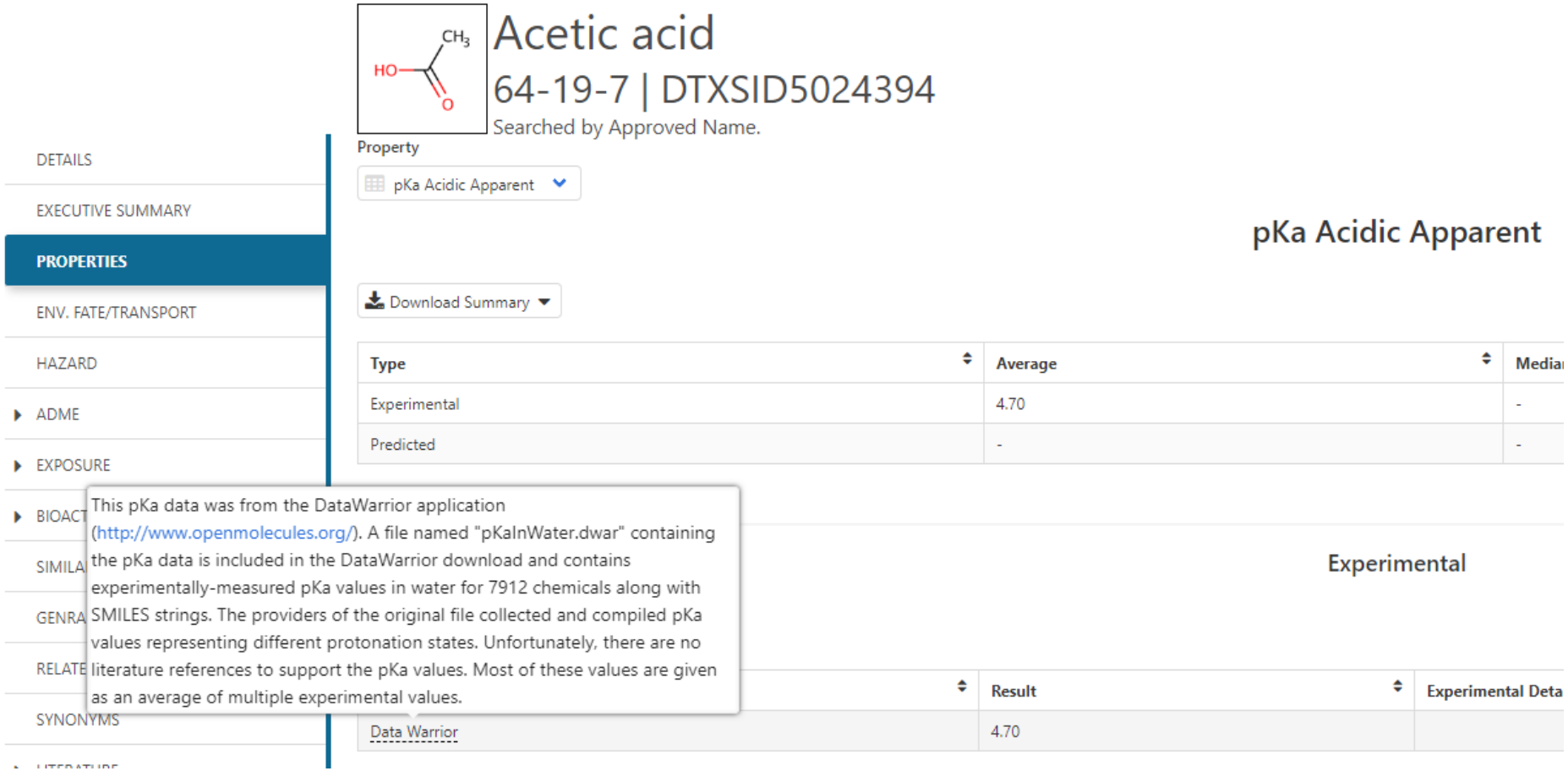
Antony Williams
National Center for Computational Toxicology

Overview of changes since August 2018 release

- Data
  - 875k chemicals total. An additional 110k chemical substances added
  - *InvitroDBv3.1* – including updated assay descriptions
  - ToxVal v7 data integrated – includes enormous curation effort
  - New OPERA predictions

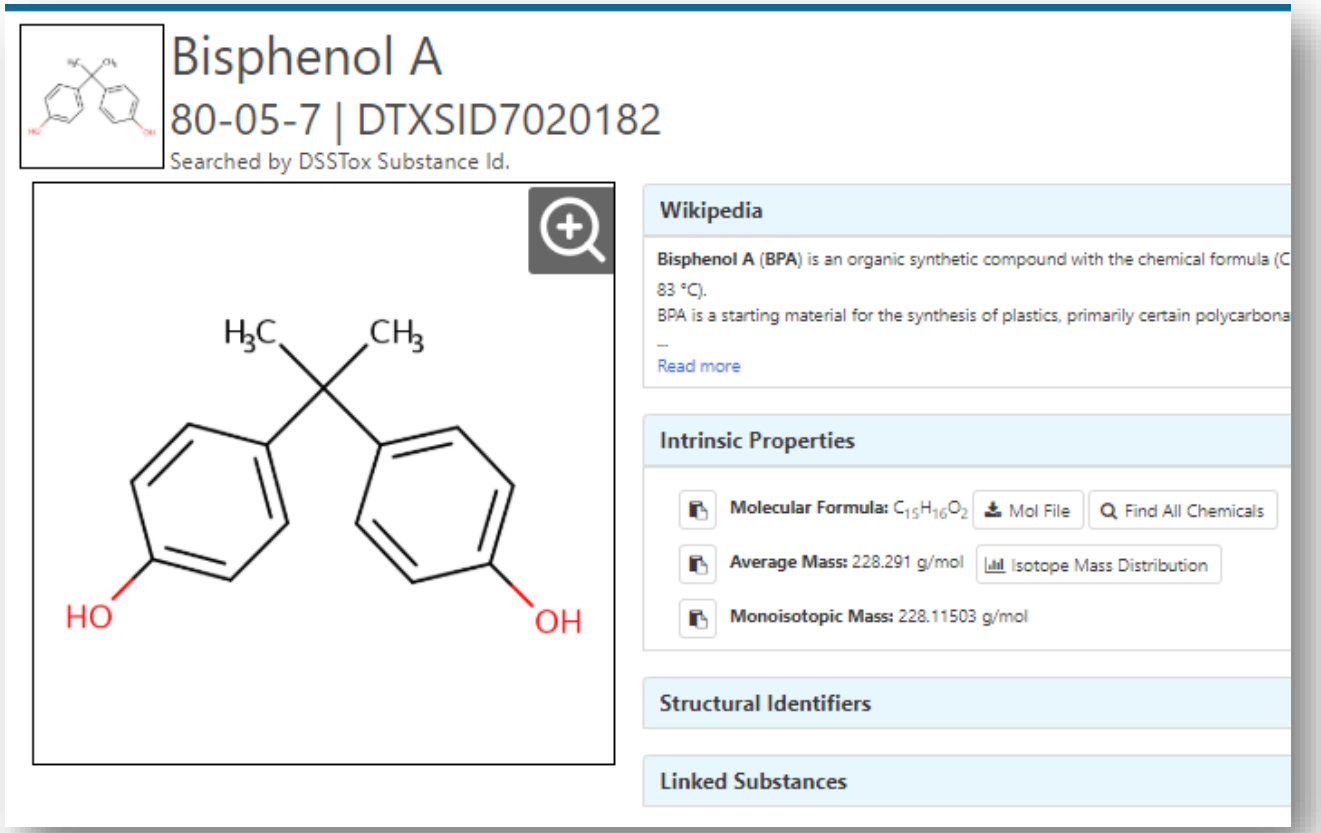
- New User Interface elements
  - Reworked tables across the application
  - Reworked multiple chemical results page
  - Navigating concentration response plots for all AEIDs in *invitroDB_v3* data, not just the EDSP21 assays
  - Enhanced batch search capabilities

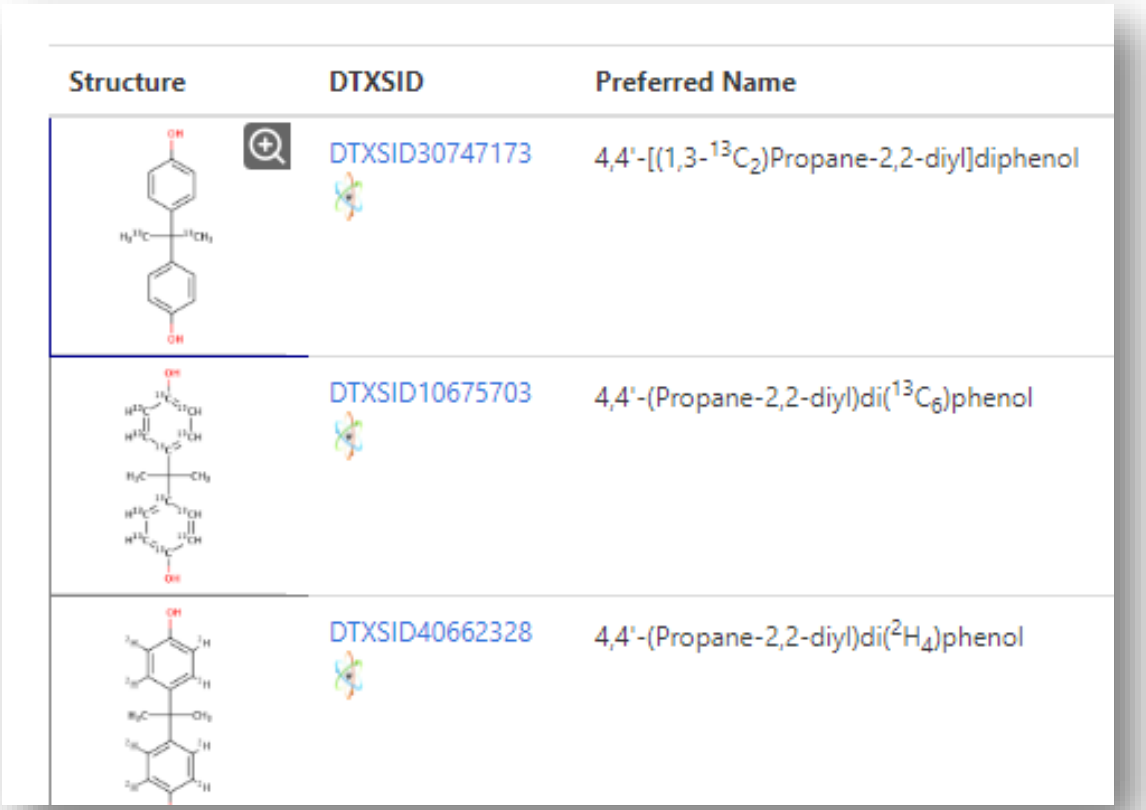
pKa experimental data added – no predictions



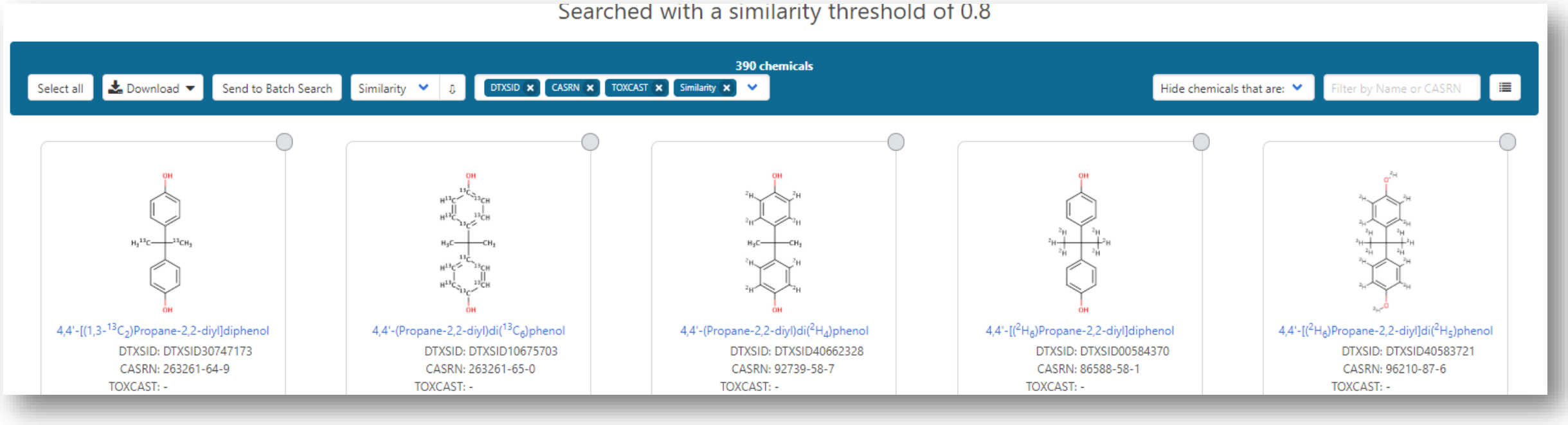
A new “Structure Zoom”

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



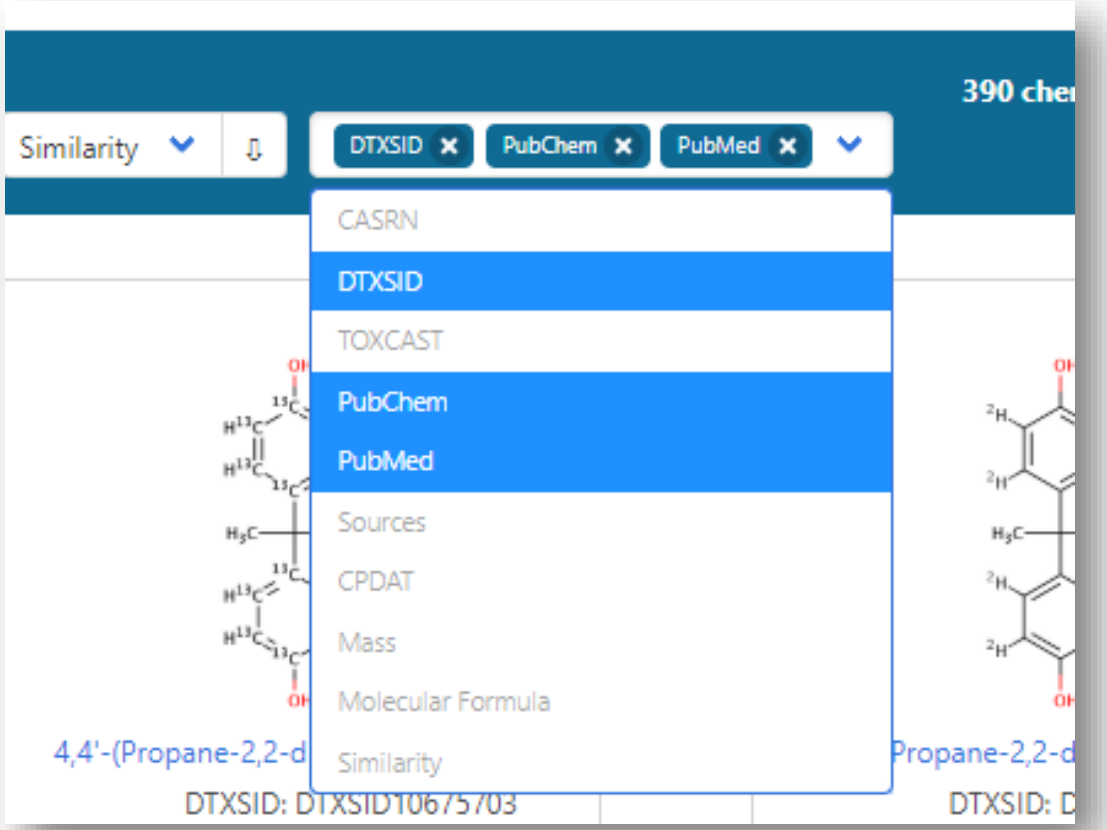


Reworked multiple results page



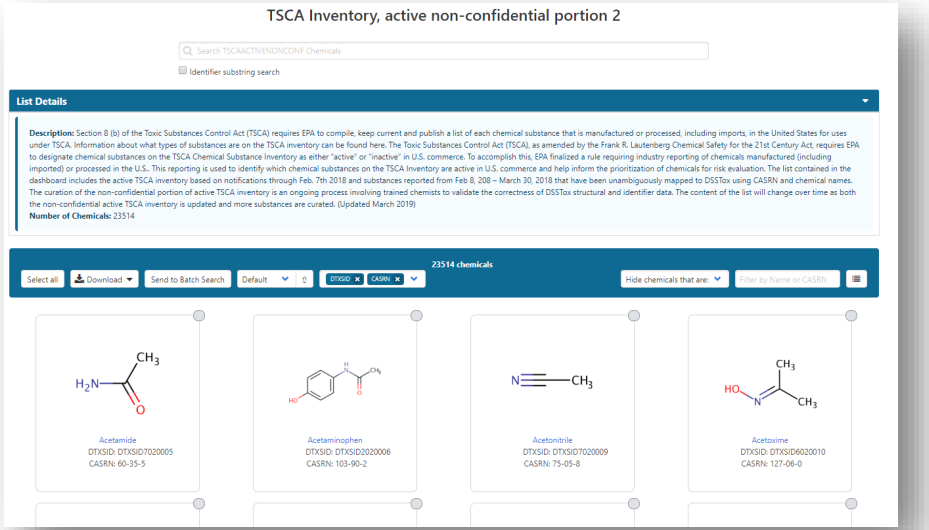
Reworked multiple results page

- Use Ctrl to select multiple display

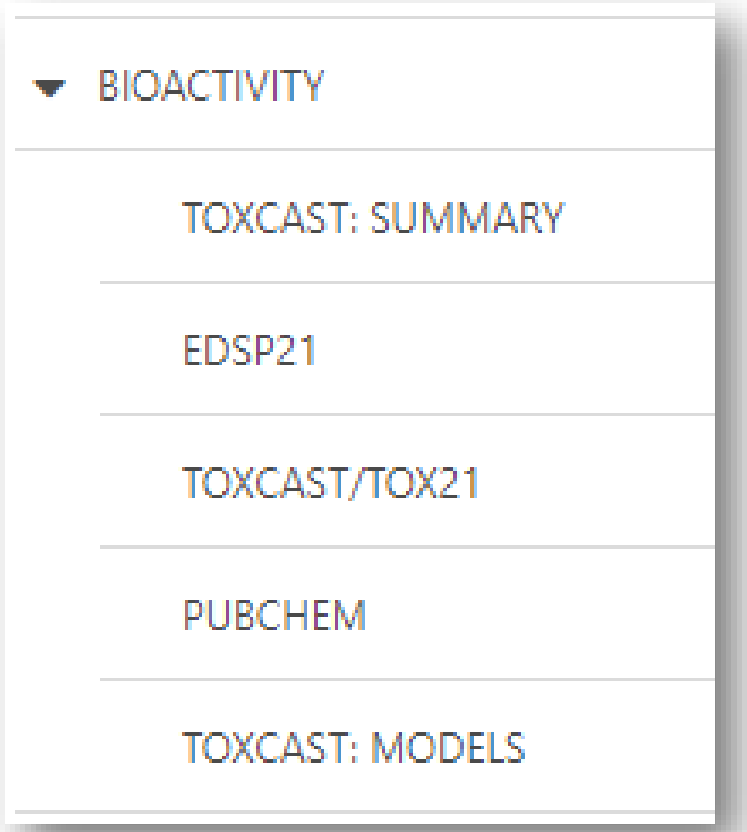


- Improved visual cues for loading large lists of chemicals

- Loading of Large lists RETAINS ordering



Bioactivity Data

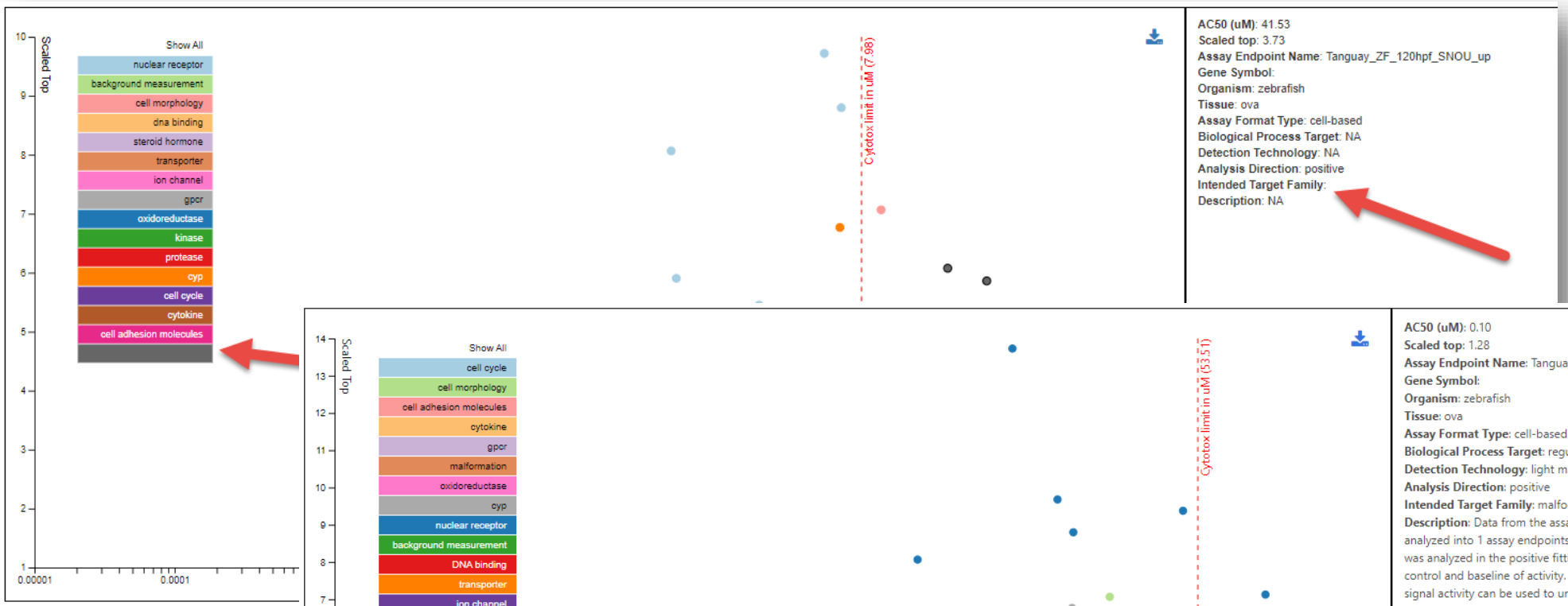


- Summary data now has “enhanced tables”
- EDSP21 subset of assays has grown
- Toxcast/Tox21 “all data” has been integrated
- PubChem data widget – no change
- Subset of ToxCast ”Models” – extended to include “COMPARA” data

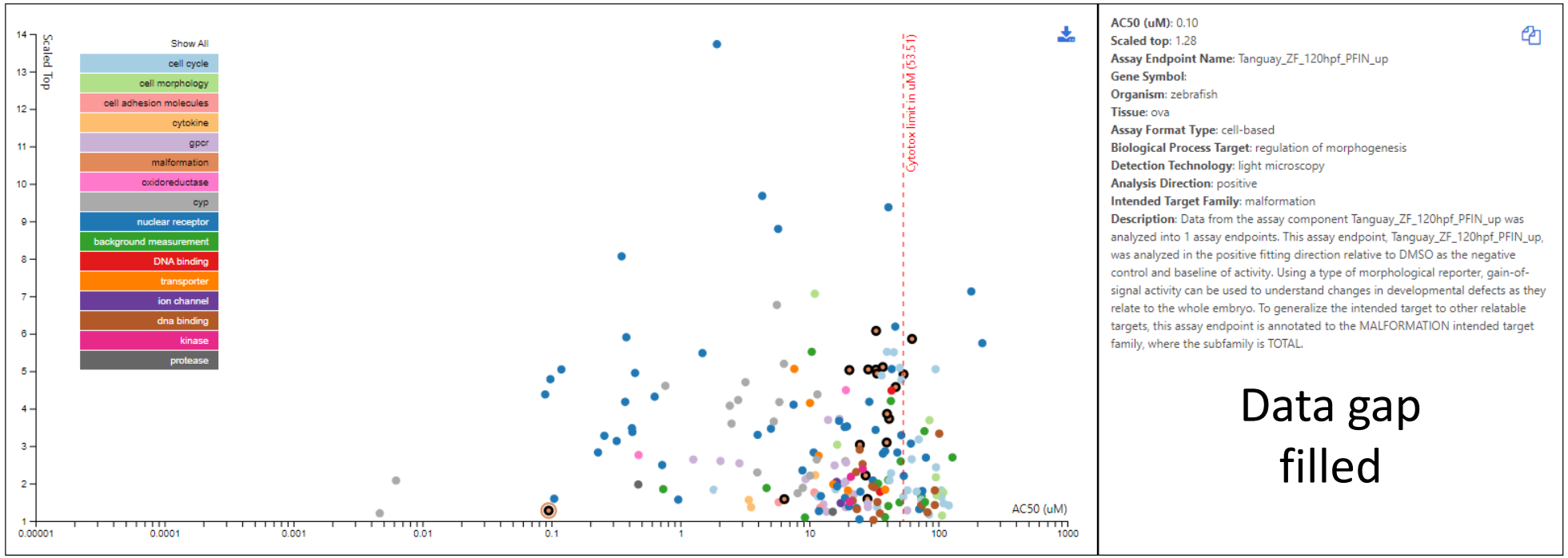
Tables Reworked – Column Selection

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

Assay Annotations Filled a Lot of Gaps!

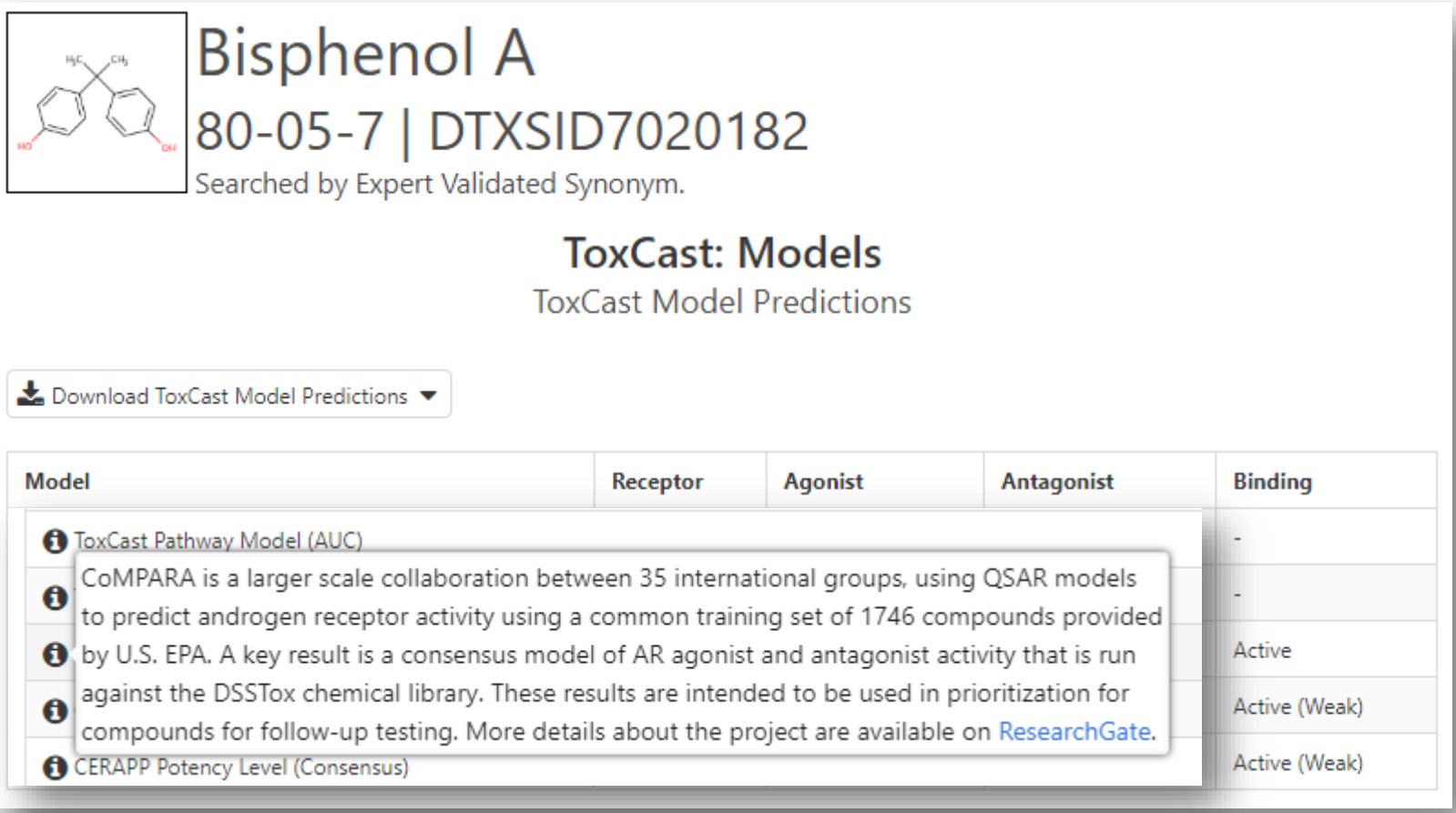


Previous data gaps



Data gap filled

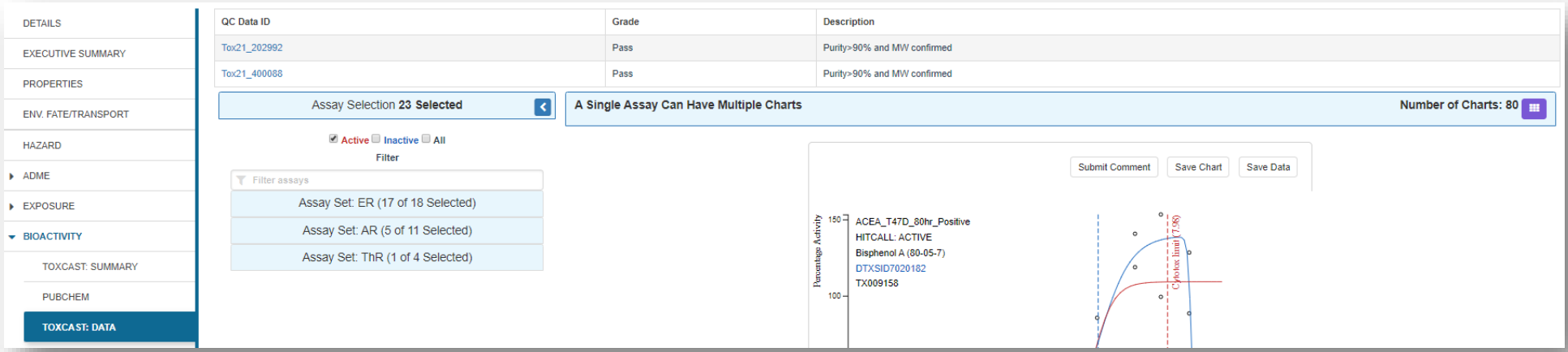
Toxcast: Models – COMPARA added



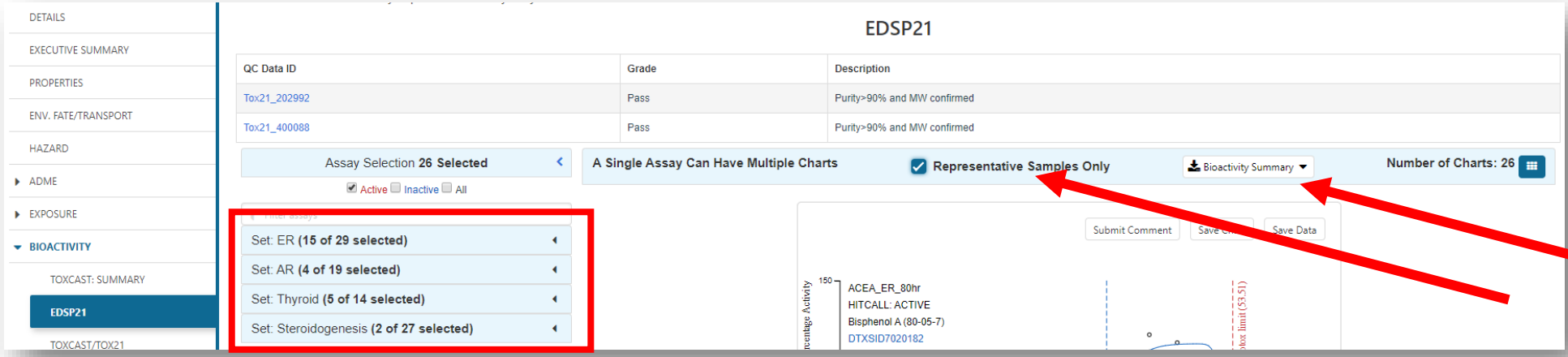
“EDSP Subset”

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

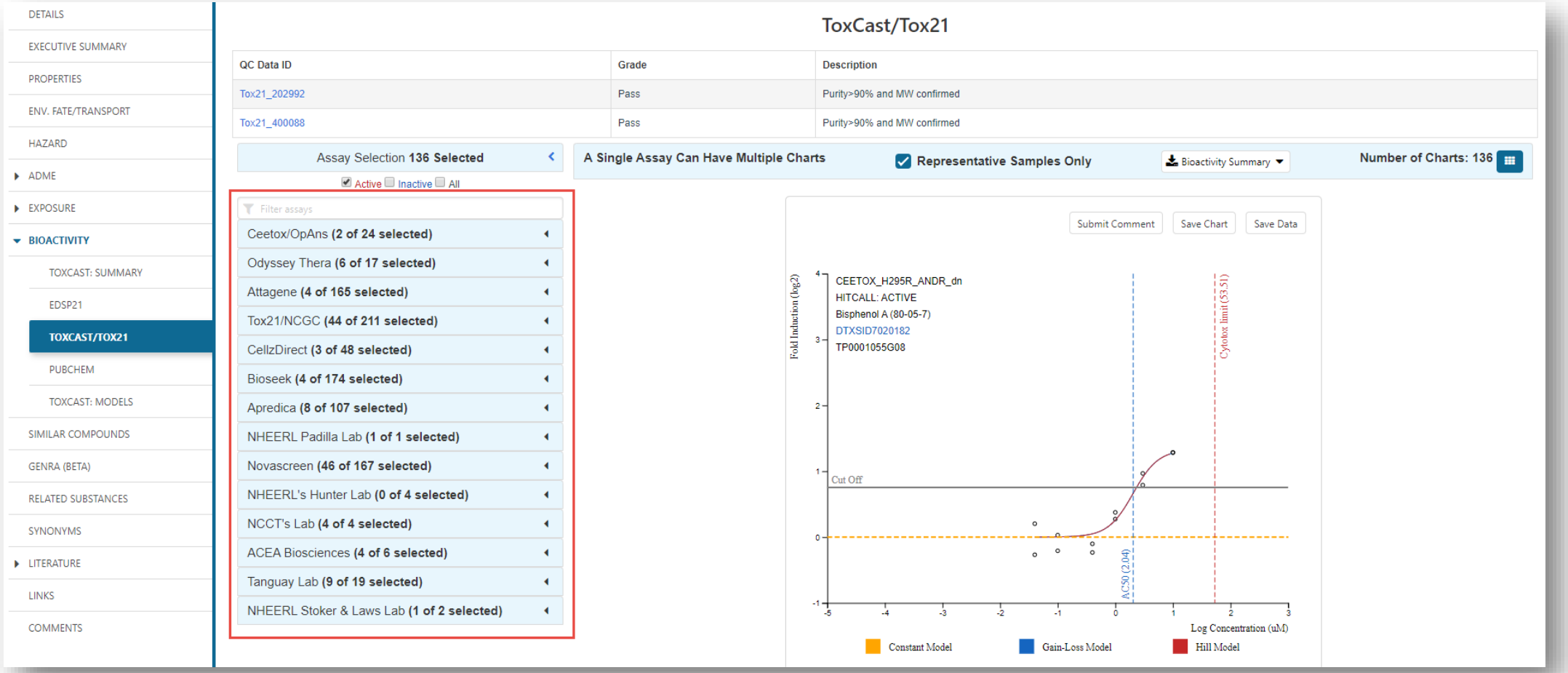
- Previous



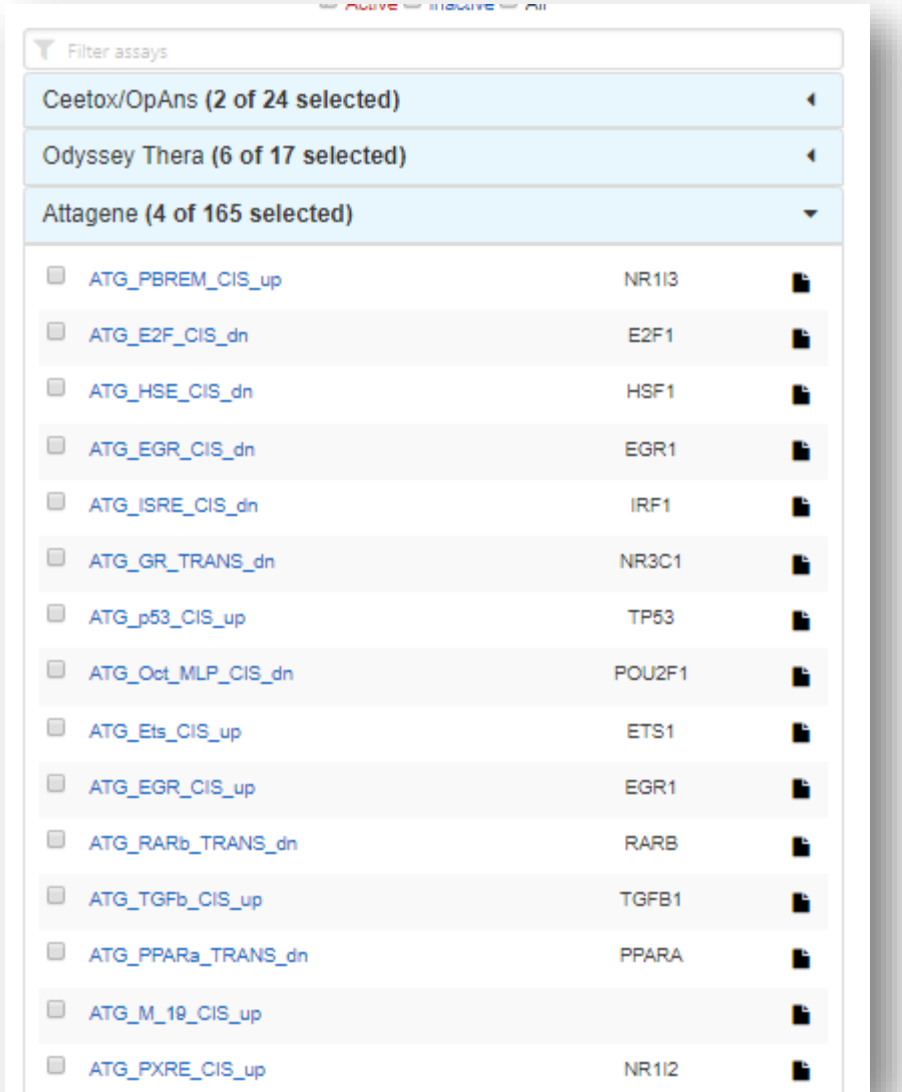
- Update

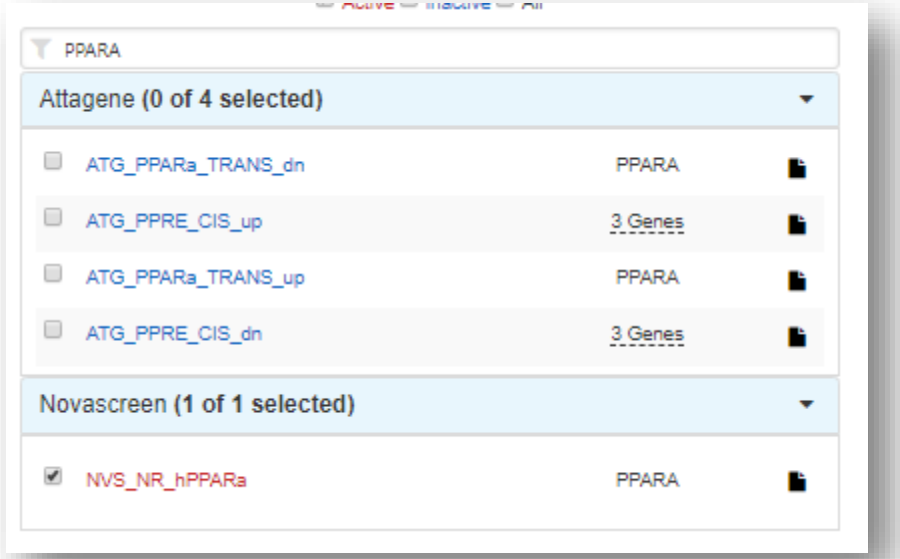


ToxCast/Tox21 Data – All data from invitroDBv3

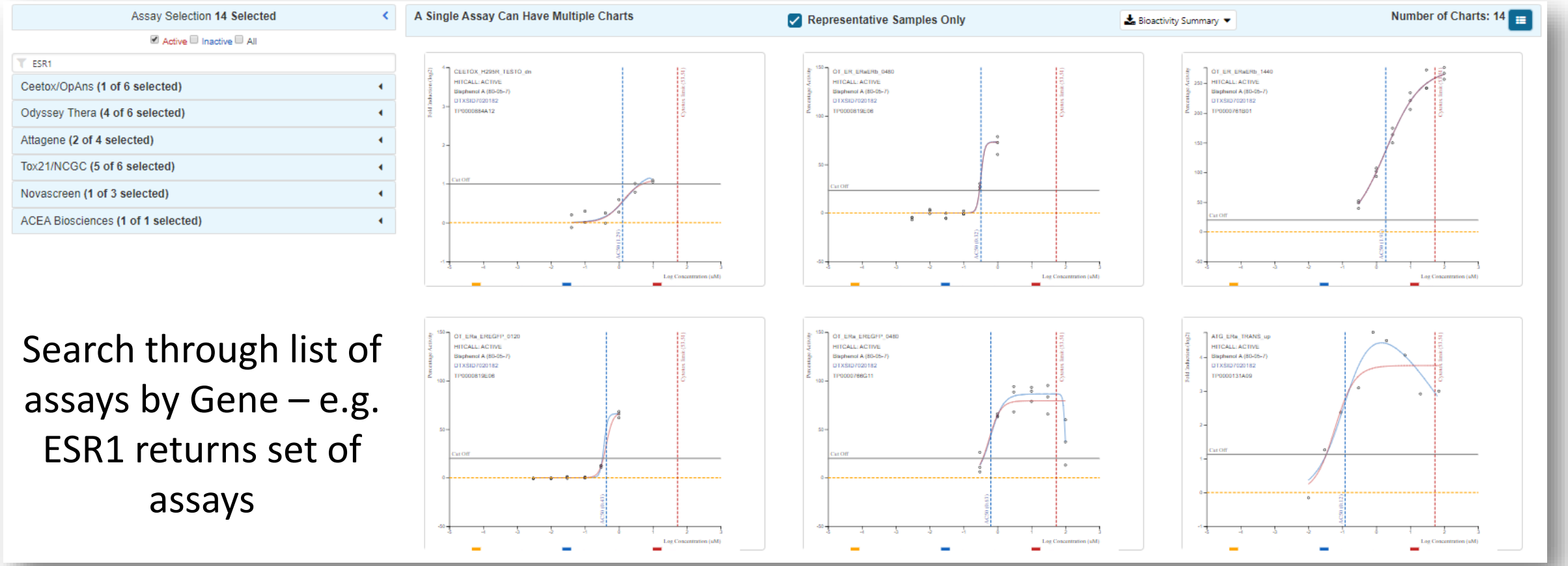


Filtering – Gene annotation added





Filtering



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

Lists of Chemicals/Lists of Assays

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

Lists of Chemicals

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

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

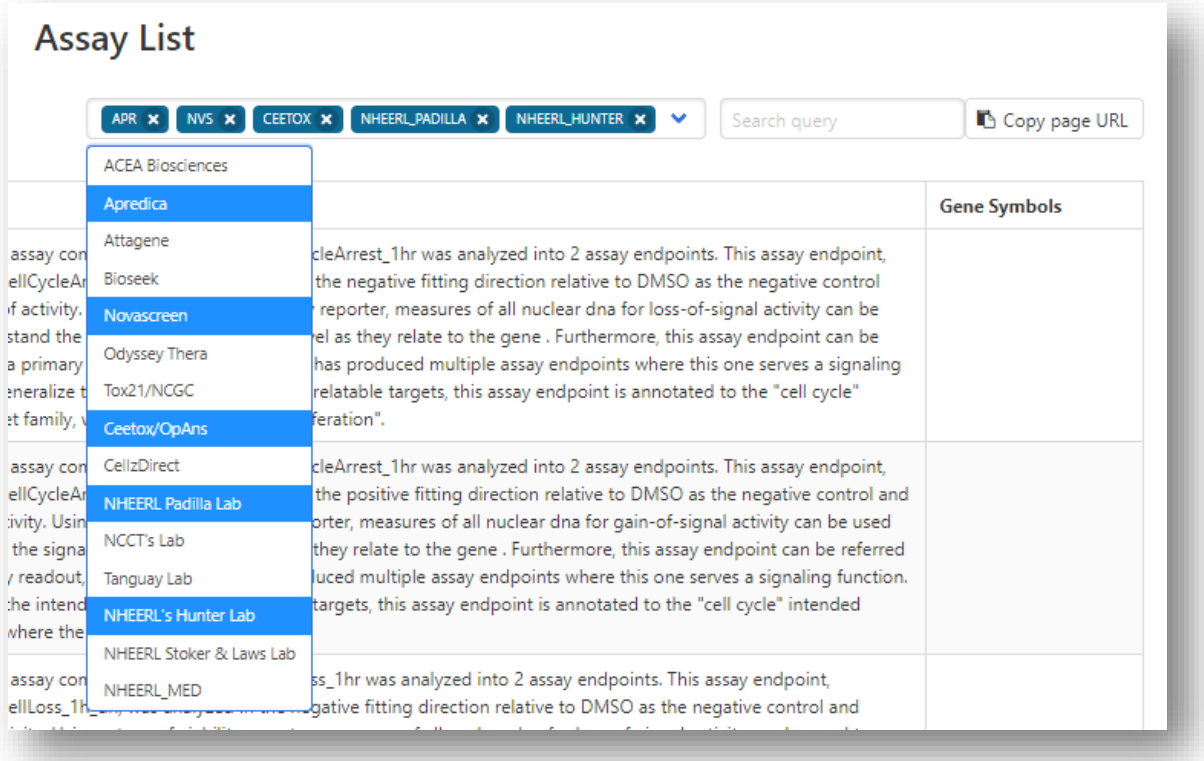
Select List

Download | Columns | NORMAN | Copy Filtered Lists URL

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

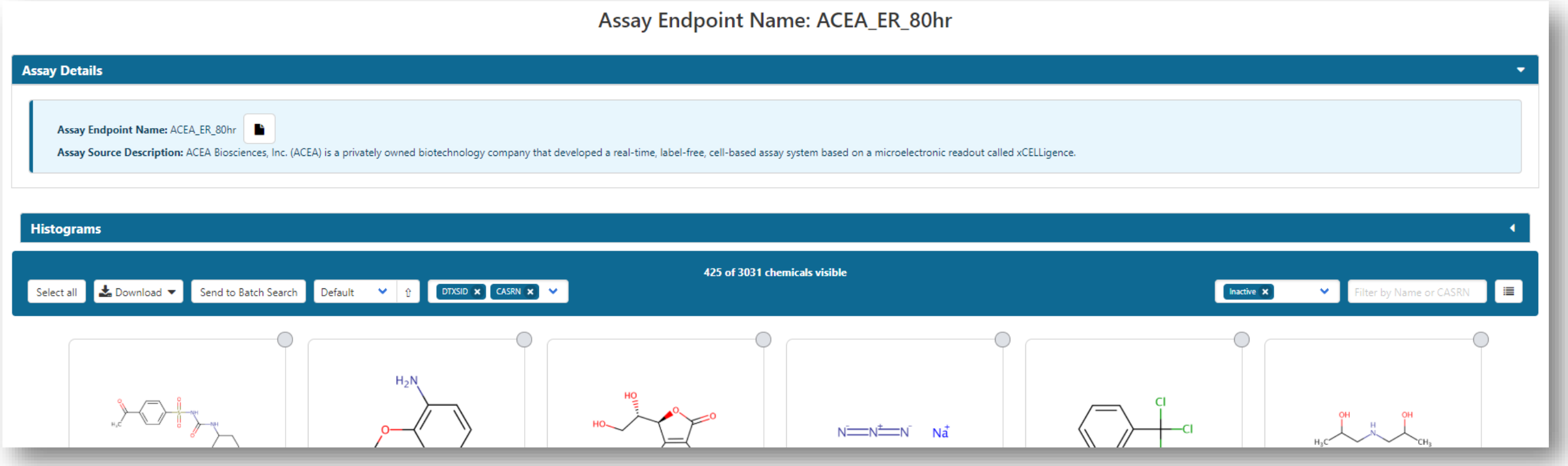
List of Assays

- Download list of all assays (Excel or TSV)
- Filter by Vendor or Multiple Vendors
- Subset of lists from query based on substring search e.g. http://comptox.epa.gov/dashboard/assay_endpoints/?search=ESR1



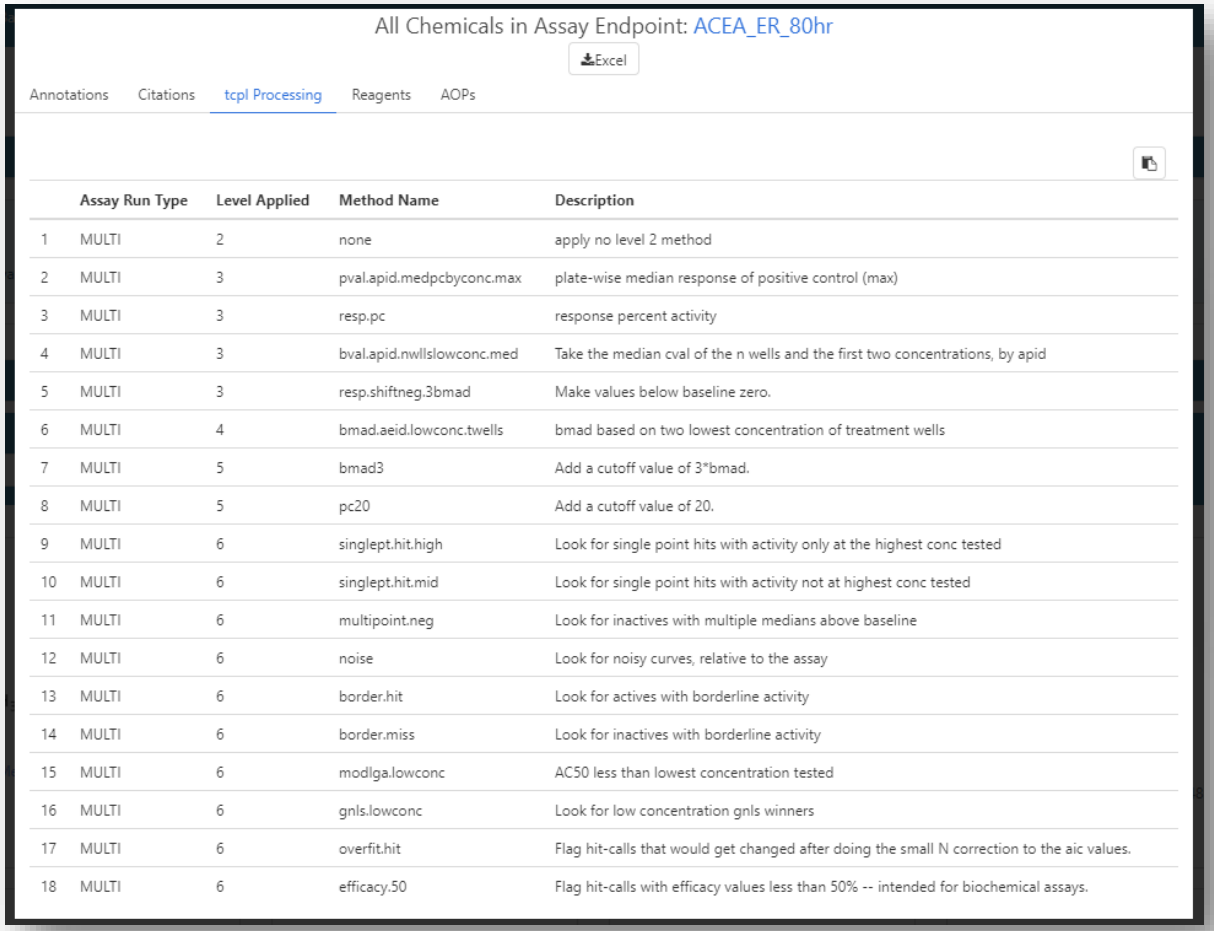
For a Specific Assay List

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



Specific Assay List

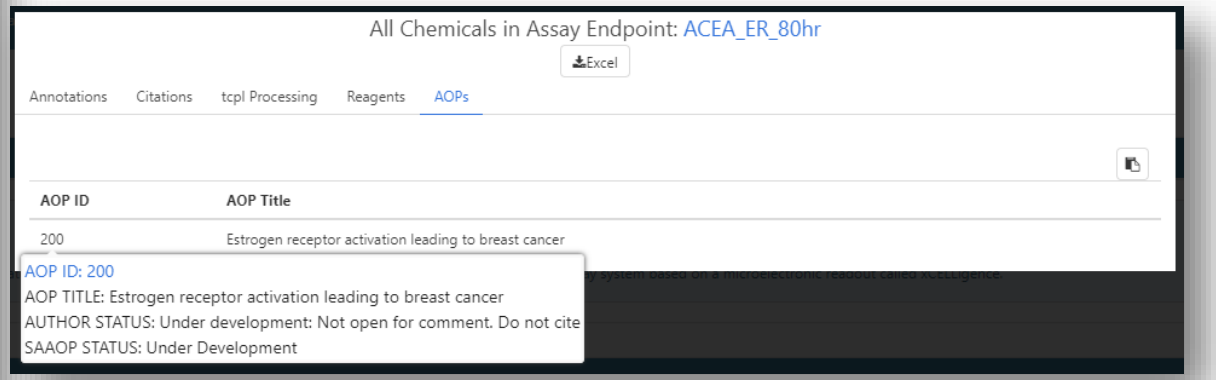
- Reworked assay table – more details available including AOP Wiki link


All Chemicals in Assay Endpoint: ACEA_ER_80hr

Excel

Annotations | Citations | tcpl Processing | Reagents | AOPs

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


All Chemicals in Assay Endpoint: ACEA_ER_80hr

Excel

Annotations | Citations | tcpl Processing | Reagents | AOPs

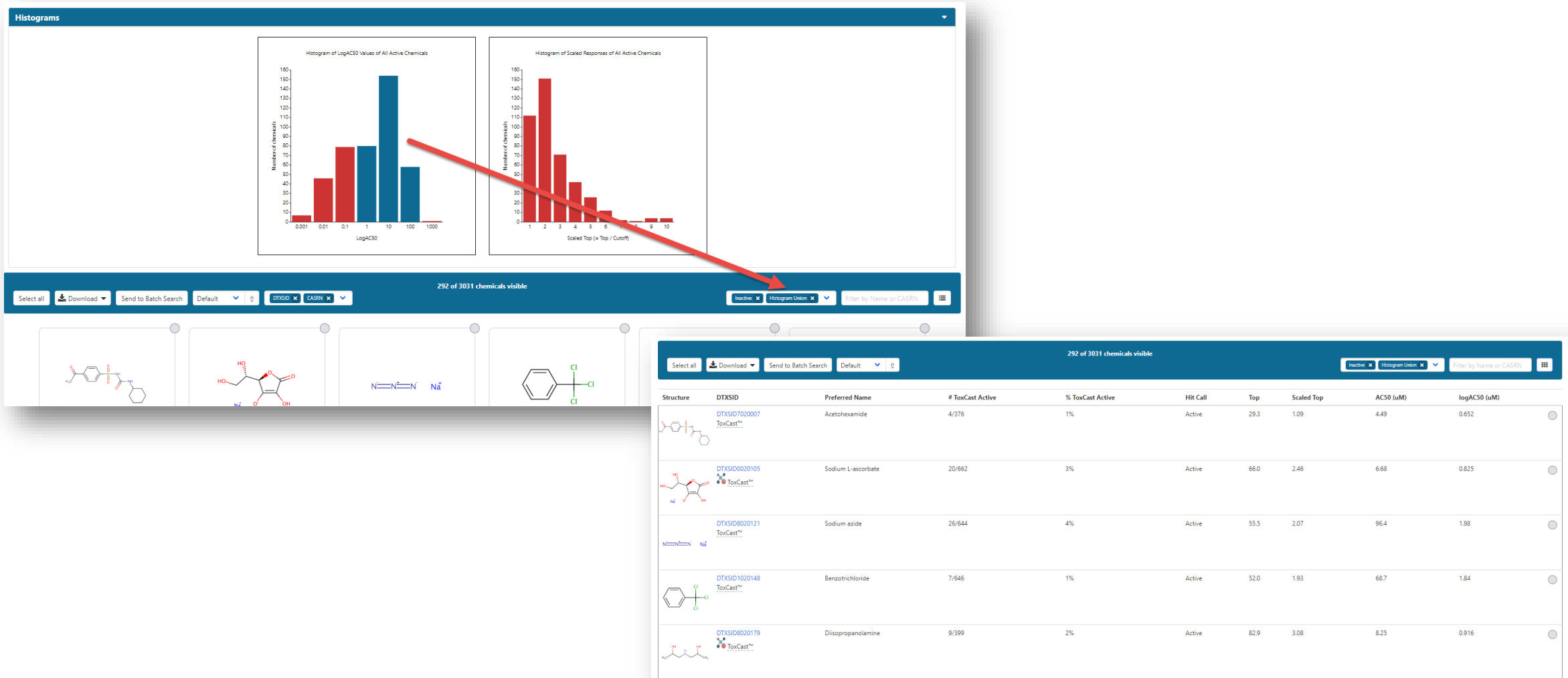
AOP ID	AOP Title
200	Estrogen receptor activation leading to breast cancer

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

Specific Assay List – Histogram summary view

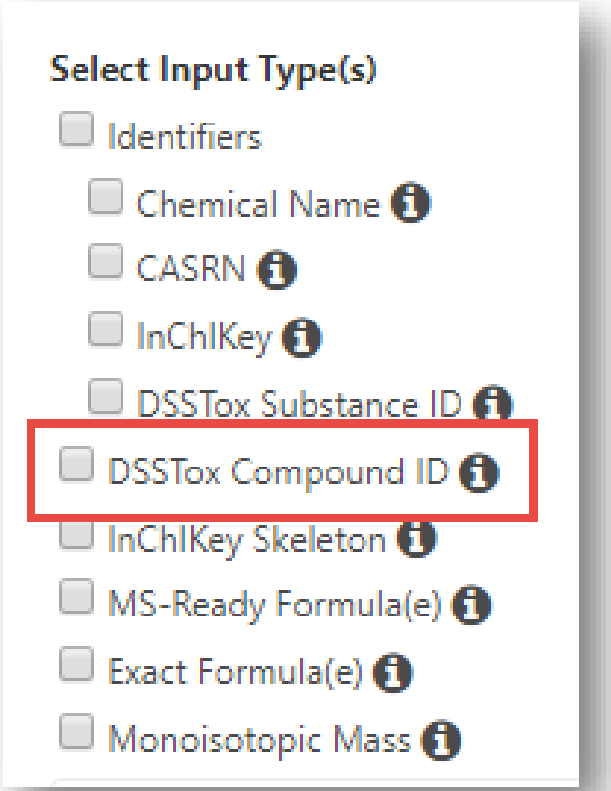
Specific Assay List – Histogram summary view

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

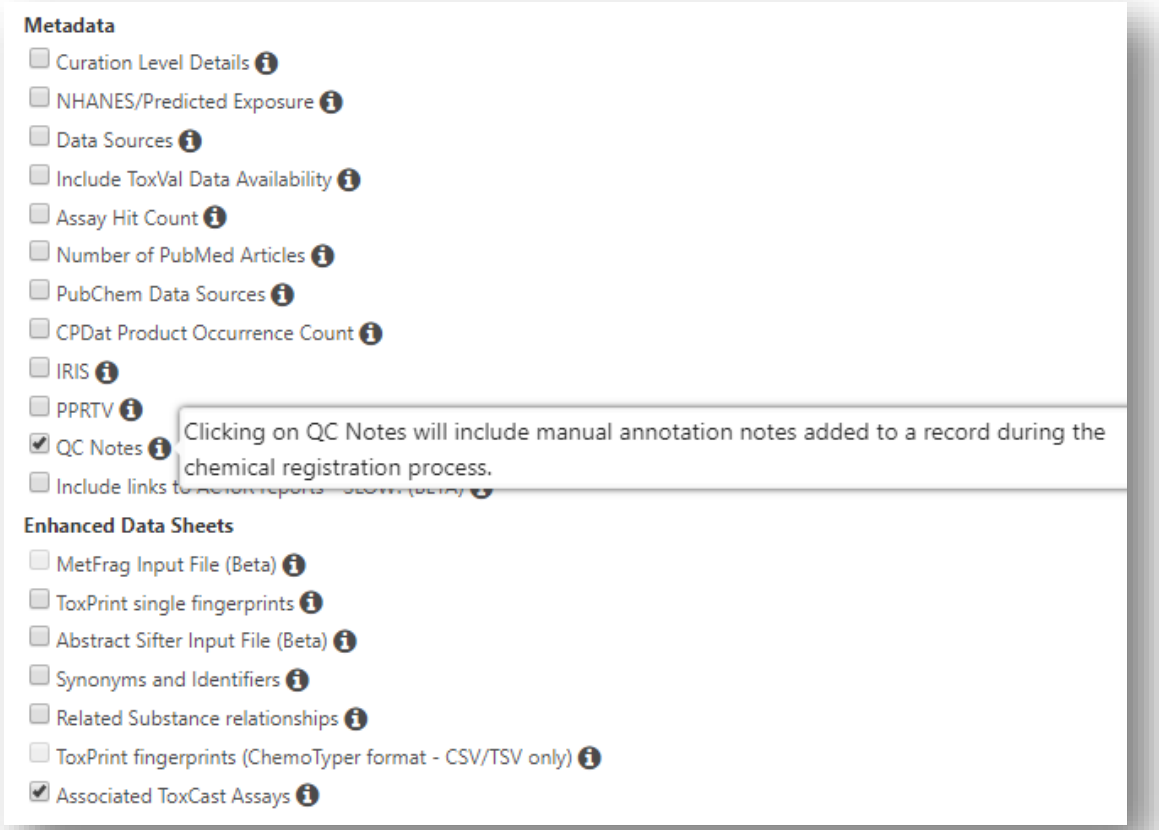


Batch Search

- New Search input - DTXCID



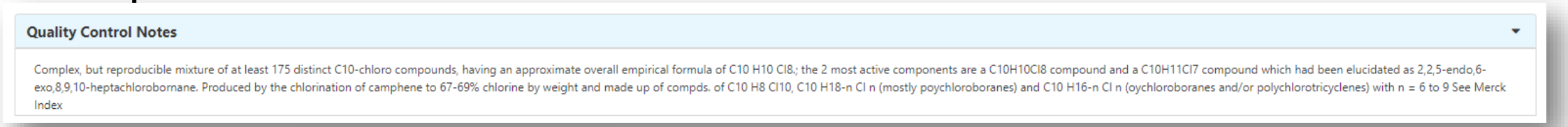
- New Search Outputs



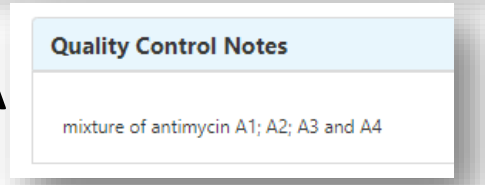
What are QC Notes?

Examples

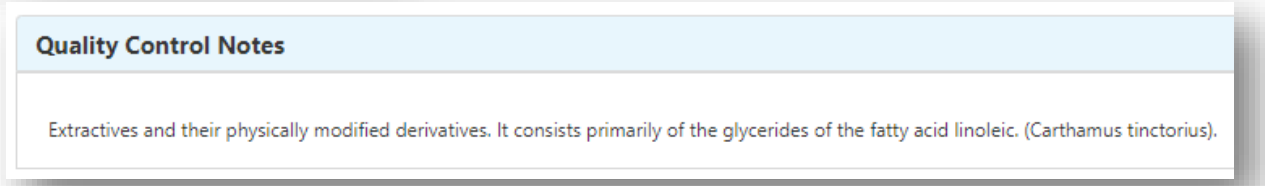
- Toxaphene



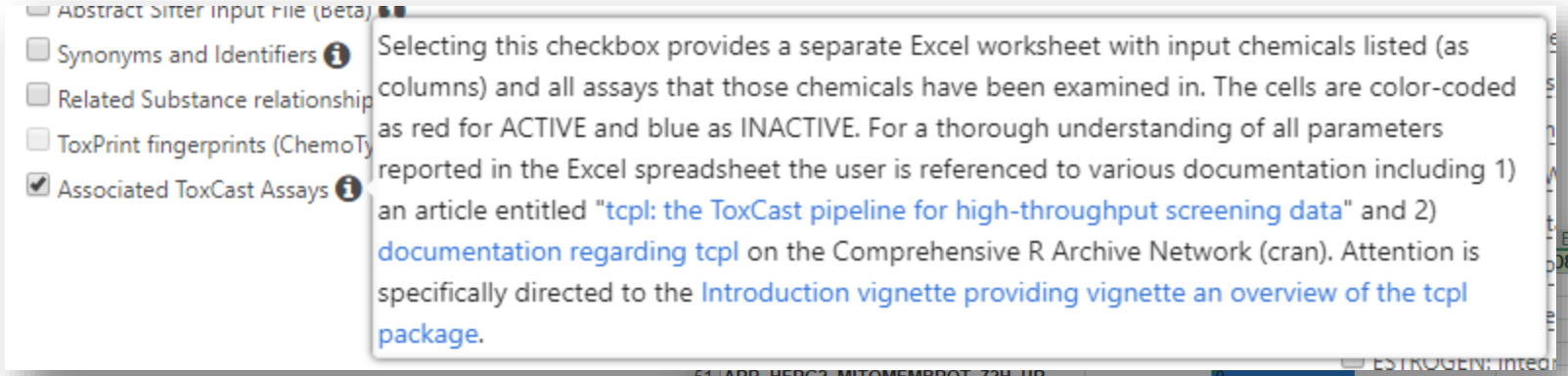
- Antimycin A

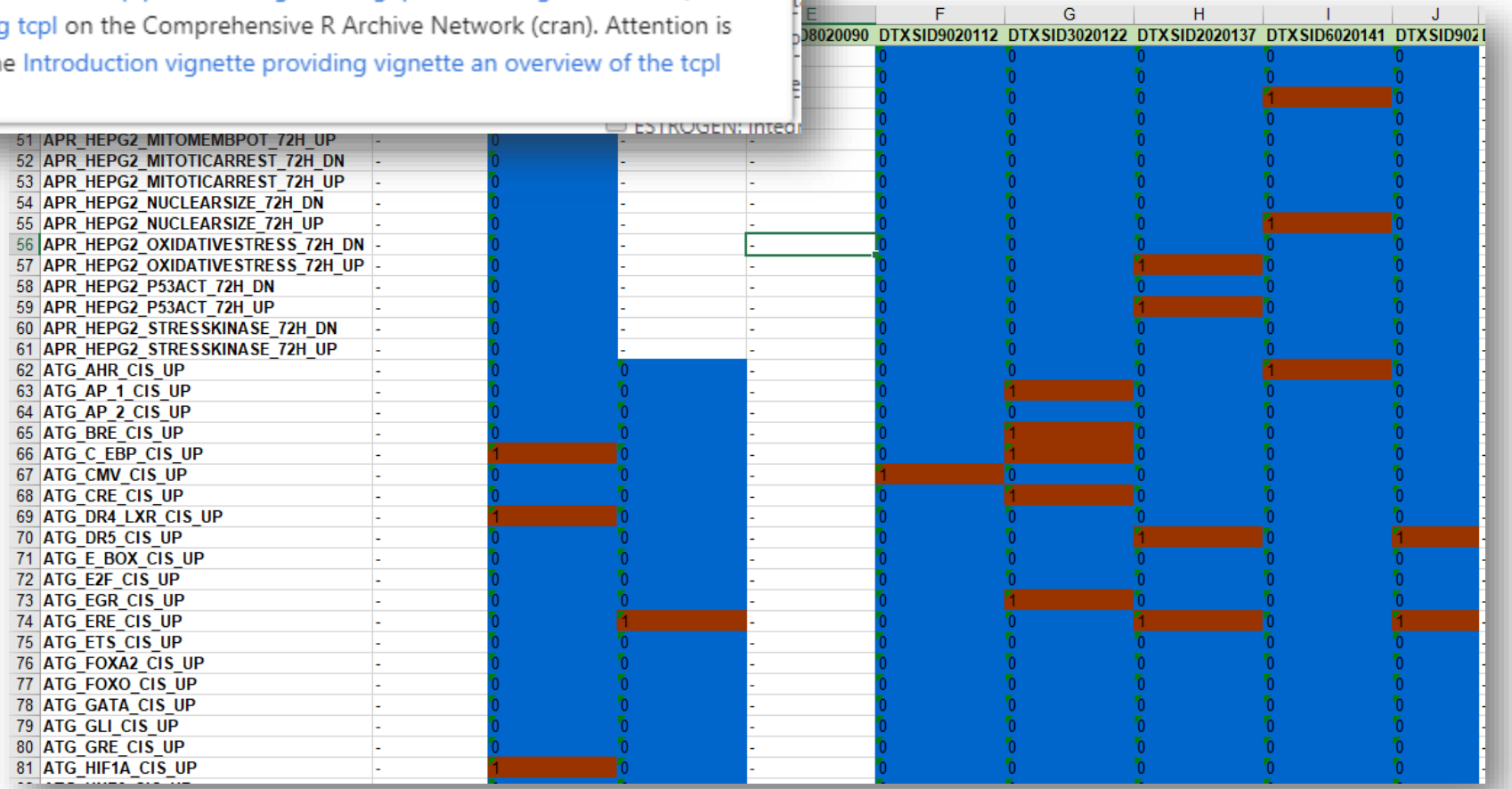


- Safflower Oil

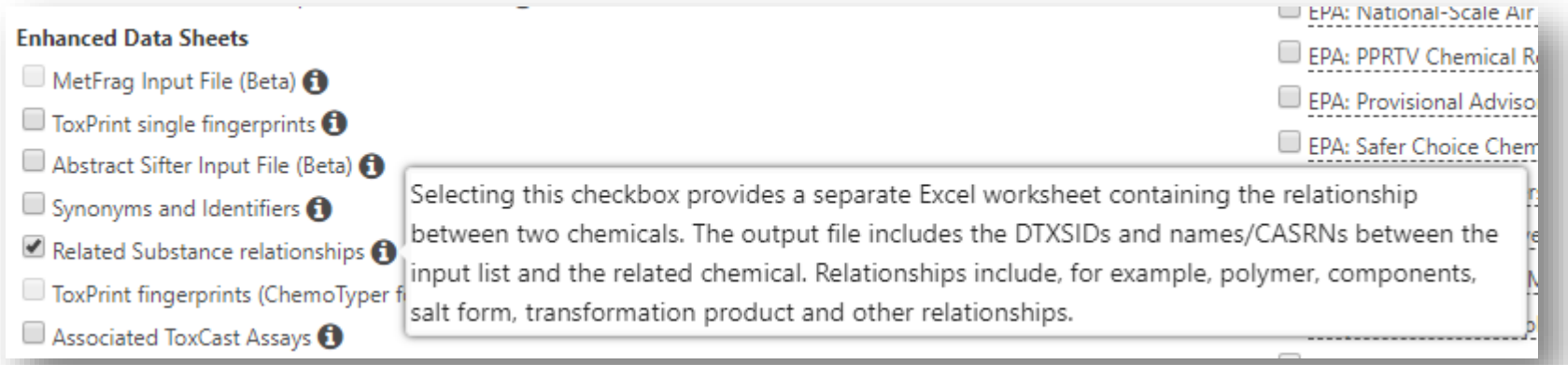


Associated ToxCast assays for chemicals





Related Substance Relationships



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

Work in Progress

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

Feedback welcome

williams.antony@epa.gov