

DrugMap



11,886 drug-like molecules from the DRUGBANK database (2020)

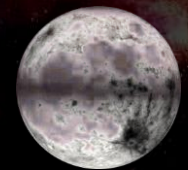
Grouped in 3 categories



Approved drugs



Withdrawn drugs



Drugs in development

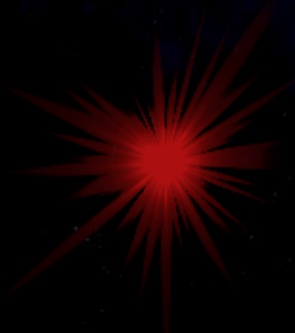
PFASMap



9,252 structures polyfluoroalkyl substances extracted from the EPA chemical dashboard (PFAS master list)



Grouped by Globally Harmonized System (GHS)



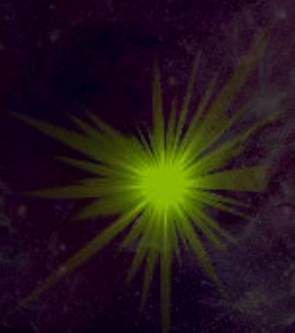
GHS=1



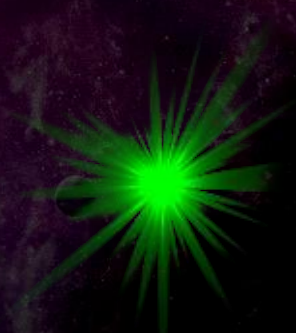
GHS=2



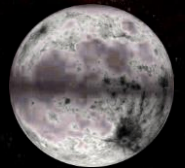
GHS=3



GHS=4



GHS=5



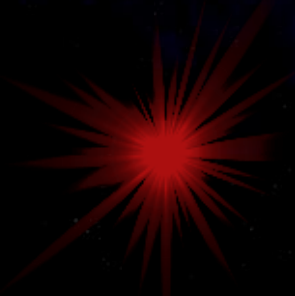
No GHS reported

Tox21Map

13,756 unique substances (8,947 unique) comprising the screening library for the Tox21 program, a multi-federal agency collaborative among the US EPA, NEHS/NTP, NIH/NCATS, and the US FDA.



Grouped by Globally Harmonized System (GHS)



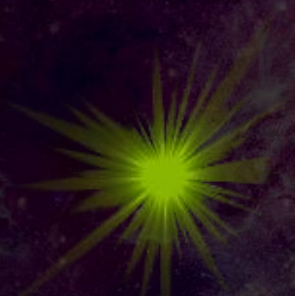
GHS=1



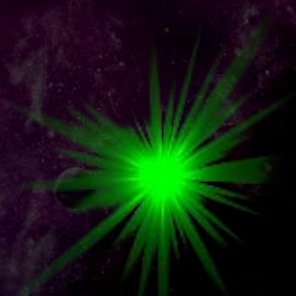
GHS=2



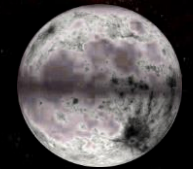
GHS=3



GHS=4



GHS=5



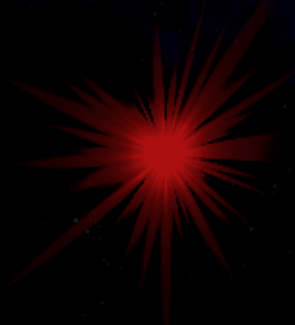
No GHS reported

DSSToxMap

883,000 chemicals available on the EPA chemical dashboard, each navigation map included 10,000 chemicals center on the user choice chemical.



Grouped by Globally Harmonized System (GHS)



GHS=1



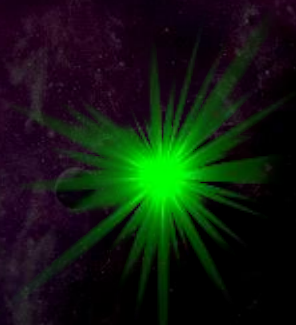
GHS=2



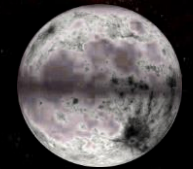
GHS=3



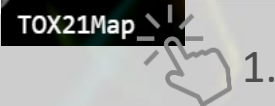
GHS=4



GHS=5



No GHS reported



6.

Hide Chemicals

- Classified
- No classified
- Added chemicals
- Draw structures

Colors by

- GHS category
- Estrogen
- Androgen
- LogP
- MW
- Lipinski Failures
- Axes
- Set a pivot point
- Reset view
- Reset map
- Help

Close Controls

1. Link to the map
2. Link to the NTP website
3. Search bar (using DSSTOX ID or Drugbank ID)
4. Link to the home page
5. Interactive chemical panel
6. Control panel
7. Block the view with double click



13756 chemicals

5.

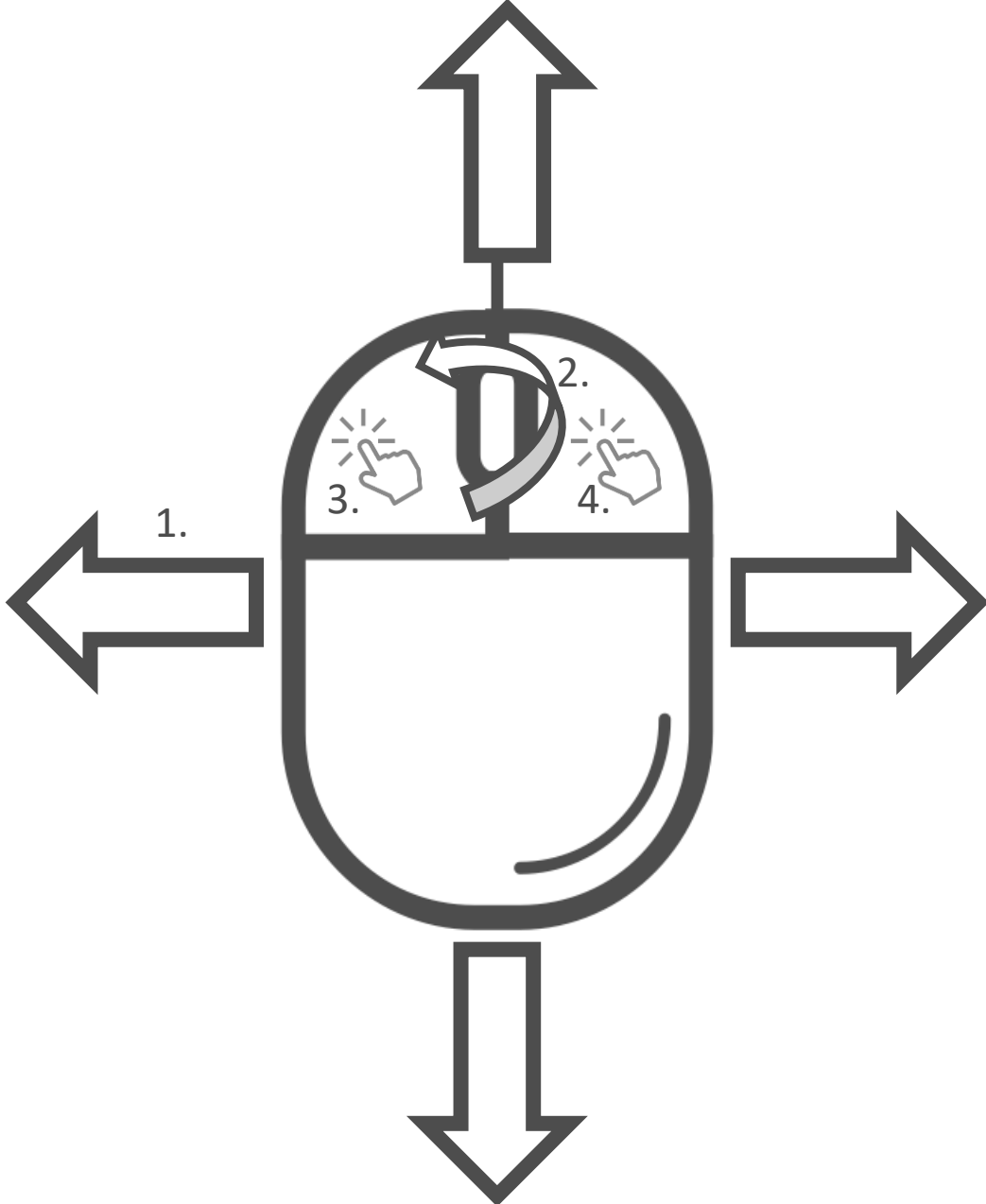
Compound ID: **DTXSID1073315**
GHS category: NA
Estrogen Receptor activity (binding): 0
Androgen Receptor Activity (binding): 0
LogP: 0.6
MW: 241.3
Lipinski Failures: 2

Connect 1
Extract 1

Draw chemical
Download neighbors

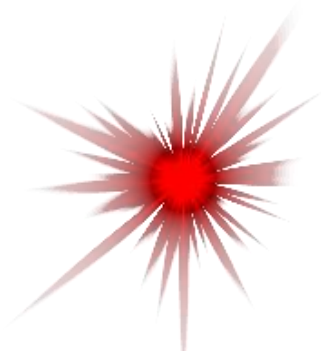
[Link to DSSTOXMap](#)

Mouse-based navigation



- 1. navigate on map
- 2. zoom in / zoom out
- 3. rotate the map
- 4. moved the map

Interactive chemical panel



Selected chemical is in red on the map

13756 chemicals

Compound ID: **DTXSID7046548** 1.

GHS category: NA

Estrogen Receptor activity (binding): 0

Androgen Receptor Activity (binding): 0

LogP: 3.8

MW: 338

Lipinski Failures: 1

Connect 1 2.

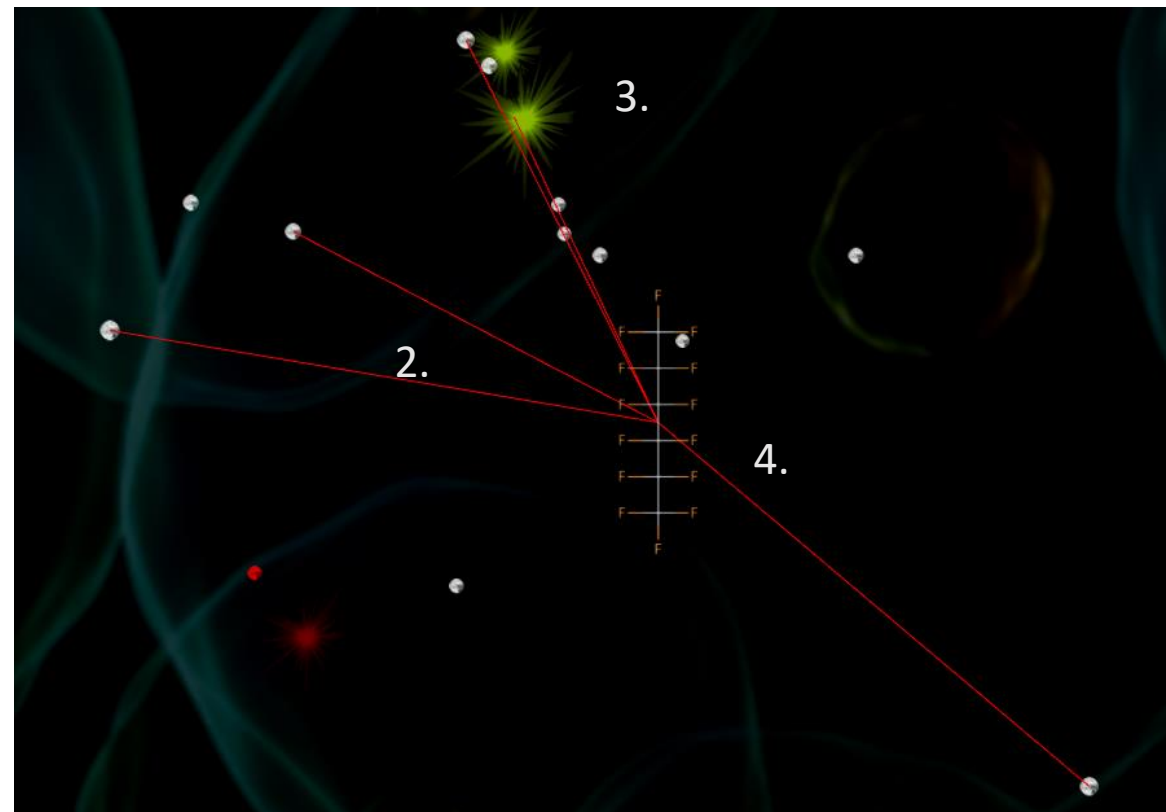
Extract 1 3.

Draw chemical 4.

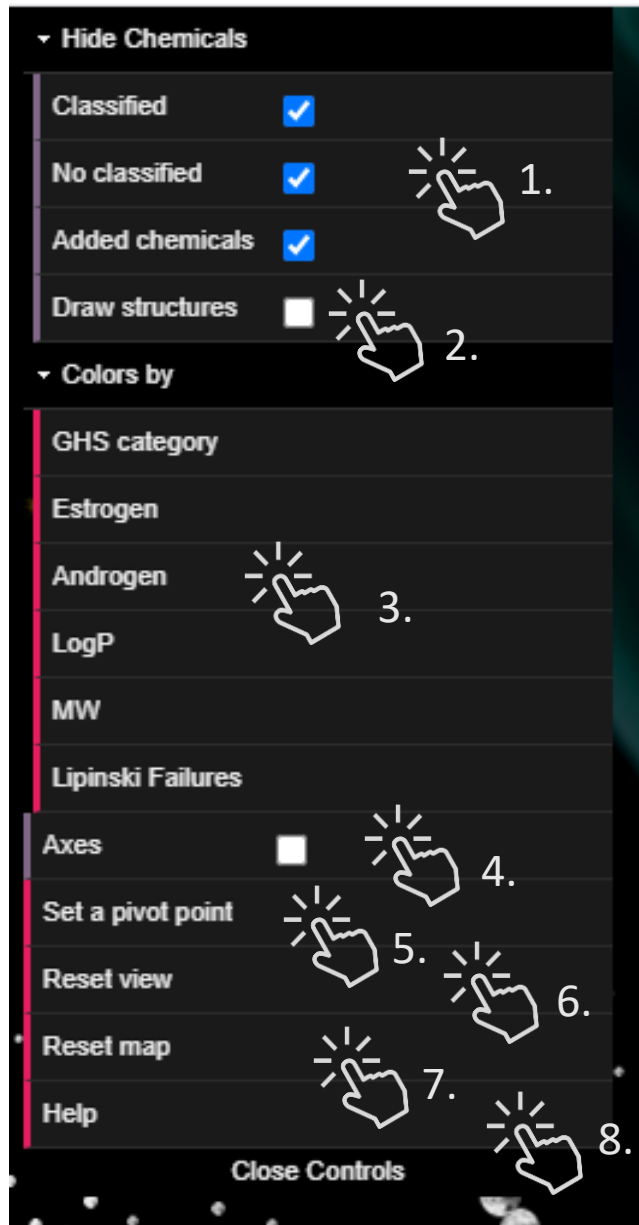
Download neighbors 5.

Link to DSSTOxMap 6.

1. Link to EPA chemical dashboard
2. Connect neighbor chemicals on the maps
3. Focus the map on 1 to 20 chemical neighbors
4. Draw chemical selected on the map
5. Download a text file with 20 chemical neighbors including chemical descriptions and relative distance on map from the centered chemical
6. Link with the DSSToxMap



Control panel



1. Select chemical by class, chemicals with GHS index, chemicals without GHS index or added chemicals. On the Tox21Map you can select chemicals with an AC50 reported and on the Drugmap you can select approved, withdrawn or in development drugs
2. Draw all chemical structures on the map (up to 50 chemicals)
3. Color panel, change the chemical color based on the selected properties on the map
4. Draw the axes from the origin
5. Move the map to be centered on the selected chemical, the view needs to be blocked to set a new pivot point
6. Reset the view in the origin
7. Reload the map
8. Link to the help page

Personalized map

Select up to 5 features you would like put on the map:

Chemical classification

- EPA category
- LD50 (mg/kg)

Toxicology prediction

- Acute Tox (very toxic)
- Acute Tox (no toxic)
- Acute Tox (EPA)
- Acute Tox (GHS)
- Acute Tox (LD50)
- Estrogen Receptor activity (Agonist)
- Estrogen Receptor activity (binding)
- Hepatic clearance

- Androgen Receptor Activity (Antagonist)
- Androgen Receptor Activity (binding)

Physicochemical prediction

- Plasma fraction unbound
- Henry's Law constant (atm-mol³/mole)
- KM (biotransformation rate)
- Log Octanol/air partition coefficient
- Log Soil adsorption coefficient (L/Kg)
- Log Fish bioconcentration factor
- LogD
- LogP

- Melting Point (C)
- Pka acid
- Pka basic
- Biodegradability
- HPLC retention time
- Log vapor pressure (mmHg)
- Log Water solubility
- Log Atmospheric constant (cm³/molsec)
- Biodegradation half-life
- Boiling Point

Descriptors

- MW
- Lipinski Failures

Generate PFASMap

Project on the map up to 5 features including toxicology predictions, physicochemical predictions from OPERA and molecular descriptors from RDKit.



Add user chemicals

Upload your list of chemicals (< 100 chemicals)

From a list including SMILES, DrugBankID, DTXSID or CAS (not recommended):

```
CCCCO
111-14-8
DTXSID4068082
DB00316
```

1.

Submit chemicals



2.

From a file:

Choose File No file chosen

Upload list of chemicals

3.

Example of input: *Test input*

4.

```
DTXSID60200549
NC(=O)C1(CCN(CCC(C#N)(C2C=CC=CC=2)C2C=CC=CC=2)CC1)N1CCCC1
CCCCNC1CCCC1
CCOP(=S)(OC1C=CC(=CC=1)[N+]([O-])=O)OCC
DTXSID8060246
CC(C)NCC(O)C1=CC=C(O)C(O)=C1
OS(=O)(=O)C1C=C2C=CC=CC2=C1
CC(N)CC(C)C)N
4-diallylaminophenyl ester
CC(C)C1C=CC(CO)=CC=1
N#CC1C(C1)=C(C1)C(C1)=C(C#N)C=1C1
DTXSID8064226
CCN(CC)C1C=CC(C=O)=CC=1
11-dihydro-5-(3-(4-morpholinyl)-1-oxopropyl)-5H-dibenz(b
.alpha.
1135-06-6
111-14-8
DTXSID4068082
COP(=O)(OC(Br)C(Br)Br)OC
CC(C1)(C1)C(O)=O
CCC(CC)C(=O)OCCOCCOCC(=O)C(CC)CC
COC(C1CCCC1N1CCCC1)C1C=CC(=CC=1)OC
C1=CC=CC=C1OP(OC1C=CC=CC=1)OC1C=CC=CC=1
CC(CCO)CO
2'-1
CC(=C)C(=O)OCC1CCCC1
DTXSID20191040
CC1=CC=C(C1)C(NC2C=CC=CC=2C(=O)OCOC)=C1C1
```

1. Add your chemicals manually in SMILES format or using CARSN, DTXSID or DrugBank ID
2. Submit to prepare your chemicals
3. Upload a list of chemicals in txt format
4. Click to see an example of a list of chemicals

Prepare your chemicals

☑️ QSAR-ready SMILES

Inputs	
ID	Input
1	CCCCO
2	111-14-8
3	DTXSID4068082
4	DB00316

QSAR-ready SMILES	
ID	SMILES
1	CCCCO ✓
2	CCCCCCC(=O)O ✓
3	CCCCC(=O)c1ccc(N)cc1 ✓
4	CC(=O)Nc1ccc(O)cc1 ✓

Resubmit Chemicals

Compute descriptors 

1. Compute molecular descriptors

Create QSAR ready structures from input chemicals

Compute molecular descriptors

Descriptor computation

Inputs		QSAR-ready SMILES		Descriptor	
ID	Input	ID	SMILES	ID	Descriptor
1	CCCCO	1	CCCCO	1	OK
2	111-14-8	2	CCCCCCC(=O)O	2	OK
3	DTXSID4068082	3	CCCCC(=O)c1ccc(N)cc1	3	OK
4	DB00316	4	CC(=O)Nc1ccc(O)cc1	4	OK

[Download 2D descriptor table](#)
[Download 3D descriptor table](#)

1. Download 1D-2D descriptors
2. Download 3D descriptors
3. Select features to add on the map
4. Generate the map with the user chemicals

Generate the PfasMap

Select up to 5 features you would like put on the map

Chemical classification

- EPA category
- LD50 (mg/kg)

Toxicology prediction

- Acute Tox (very toxic)
- Acute Tox (no toxic)
- Acute Tox (EPA)
- Acute Tox (GHS)
- Acute Tox (LD50)
- Estrogen Receptor activity (Agonist)

- Androgen Receptor Activity (Antagonist)

Physicochemical prediction

- Androgen Receptor Activity (binding)
- Plasma fraction unbound
- Henry's Law constant (atm-mol3/mole)
- KM (biotransformation rate)
- Log Octanol/air partition coefficient
- Log Soil adsorption coefficient (L/Kg)
- Log Fish bioconcentration factor
- LogD

- Melting Point (C)

- Pka acid
- Pka basic
- Biodegradability
- HPLC retention time
- Log vapor pressure (mmHg)
- Log Water solubility
- Log Atmospheric constant (cm3/molsec)
- Biodegradation half-life
- Boiling Point

Descriptors

- MW
- Lipinski Failures

Generate PFASMap

3.

4.

Map with user chemicals

The image shows a screenshot of the PFASMap web application. The interface includes a search bar at the top left with the text '1.' next to it. The main map area displays a dark background with a grid of circular markers. A red rocket icon is positioned over one of the markers, with the number '2.' next to it. A red line connects the rocket to a red circular marker on the map, with the number '3.' next to it. In the bottom right corner, a detailed information panel for a chemical is shown, containing a chemical structure, various properties, and interactive buttons. The panel is titled '8002 chemicals' and includes a 'Connect' dropdown set to '5', an 'Extract' dropdown set to '1', and buttons for 'Draw chemical', 'Download neighbors', and 'Link to DSSTOXMap'. The National Toxicology Program logo and 'chemMaps.com' are also visible.

1. Search added chemicals by ID

2. Rocket represented added chemicals

3. Updated information about user chemical in the panel

8002 chemicals

Compound ID: 2
GHS category: add
Estrogen Receptor activity (binding): NA
Androgen Receptor Activity (binding): NA
LogP: NA
MW: 130.19
Lipinski Failures: NA

Connect 5
Extract 1
Draw chemical
Download neighbors
Link to DSSTOXMap

Project the Tox21 assay results

Project Tox21/ToxCast assays results available in inVitroDB v3, data are available on the ICE platform (<https://ice.ntp.niehs.nih.gov/>)

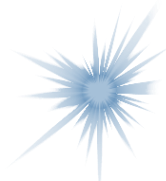
- 1,337 assays available
- 394 assay targets identified

Projection on the Tox21Map:

8,947 unique substance comprising the screening library for the Tox21 program, a multi-federal agency collaborative among the US EPA, NEHS/NTP, NIH/NCATS, and the US FDA.



Active chemical



Inactive chemical



Inconclusive or no tested chemical



Integrated
Chemical
Environment



Select data to project

Project Tox21 assay results

Choose a assay protocol or an assay target. Assay target will provide you a consensus of all Tox21 assays that target the same gene. Tox21 assay results have been extracted from the *Integrated Chemical Environment*.

Protocol name	Assay target	Cell line	Cell target	Description	Design
NVS_GPCR_hTXA2	TBXA2R			NVS_GPCR_hTXA2 is a bi...	binding reporter
APR_HepG2_CellLoss_1h_dn					
TOX21_PXR_viability			liver	PXR-Luc HepG2 cells use...	
NVS_ENZ_hPAK4_Activator	PAK4			NVS_ENZ_hPAK4 is a bio...	
NVS_ENZ_hDUSP3_Activator	DUSP3			NVS_ENZ_hDUSP3 is a bi...	
BSK_BE3C_PA11_up	SERPINE1	bronchial epithelial cells	lung	BSK_BE3C is a cell-based...	
CEETOX_H295R_MTT_cell_viability_dn		H295R	adrenal gland	CEETOX_H295R is a cell-...	
ATG_M_32_TRANS_dn					
APR_HepG2_CellLoss_24h_dn					
NVS_GPCR_hM2	CHRM2			NVS_GPCR_hM2 is a bio...	binding reporter
APR_p-H2AX_24hr_dn					
NVS_ENZ_hPTPRB_Activator	PTPRB			NVS_ENZ_hPTPRB is a bi...	
NVS_ENZ_rMAOBC	Maob		brain	NVS_ENZ_rMAOBC is a b...	enzyme reporter

Project by chemical the most active assay

Only the most active assay result is projected for each chemical.

Tox21Map with lowest AC50 by chemicals

► Browse the chemical list with the lowest AC50

1. Project a unique assay results
2. Assay results for one target (combining several assays)
3. Project the lowest AC50 by chemicals
4. Browse chemical list with the lowest AC50

Assay results

The screenshot shows the ChemMaps.com interface. At the top, a black box displays "ESR1 (29 assay(s))" and "1.". The map area is filled with numerous small, glowing chemical nodes. A tooltip window is open in the bottom right, showing the chemical structure of a compound and its associated assay data. The tooltip includes the following information:

- 13756 chemicals
- Compound ID: DTXSID1032355
- GHS category: NA
- LogP: 2.5
- MW: 239.1
- Lowest AC50 (μM): 29.164 (3 positive assay(s))
- Assay Outcome: active
- Most active assay: CEETOX_H295R_TESTO_dn

On the right side of the tooltip, there are controls for "Connect" (set to 1), "Extract" (set to 1), "Draw chemical", "Download neighbors", and "Link to DSSTOXMap".

1. Show the name of the selected assay or selected target with the number of assay results projected on the map
2. Show the lowest AC50 with the number of assays active for a chemical
3. Show the assay name with the lowest AC50

Chemical list with the lowest AC50



Chemical dashboard

Lowest AC50 (μM) by chemicals

Table including the list of chemicals in the Tox21 library with the lowest AC50 and the associated assay. DTXSIDs are linked to the EPA dashboard and assay name are linked to the corresponding Tox21 map.

DTXSID	CASRN	Name	Number of active assays	Lowest AC50 (μM)	Assay with the lowest AC50
DTXSID0020020	18699-02-0	4-Acetylamino-phenylacetic acid	2	1.18220732685014	TOX21_RT_HEK293_FLO_16hr_viability
DTXSID0020022	50594-66-6	5-(2-Chloro-4-(trifluoromethyl)phenoxy)benzoic acid	24	2.46187316424739	TOX21_PPARg_BLA_antagonist_ratio
DTXSID0020024	3054-95-3	Acrolein diethylacetal	0	NA	
DTXSID0020070	50-32-2	Aminocaproic acid	0	NA	
DTXSID0020072	2111-61-3	4-Biphenylamine hydrochloride	23	3.1699559033799	ATG_PPARg_TRANS_up
DTXSID0020074	60142-96-3	Gabapentin	2	0.00198206186302098	TOX21_RT_HEPG2_FLO_08hr_viability
DTXSID0020076	61-82-5	Amitrole	1	1.75812121981573	NCCT_TPO_AUR_dn
DTXSID0020101	11096-82-5	Aroclor 1260	0	NA	
DTXSID0020103	1327-53-3	Arsenic oxide (As ₂ O ₃)	7	2.70935028311428	TOX21_AR_LUC_MDAKB2_Agonist
DTXSID0020105	134-03-2	Sodium L-ascorbate	14	0.0150318969057717	TOX21_TR_LUC_GH3_Agonist_Followup
DTXSID0020107	22839-47-0	Aspartame	0	NA	
DTXSID0020151	140-11-4	Benzyl acetate	0	NA	
DTXSID0020153	100-44-7	Benzyl chloride	0	NA	
DTXSID0020155	622-78-6	Benzyl isothiocyanate	0	NA	
DTXSID0020157	20570-96-1	Benzylhydrazine dihydrochloride	0	NA	
DTXSID0020232	58-08-2	Caffeine	5	0.0900911166997146	ATG_Sox_CIS_up
DTXSID0020236	814-80-2	Calcium lactate	1	83.5972719572834	TOX21_ERa_LUC_VM7_Agonist
DTXSID0020238	59721-29-8	Camostat mesylate	1	0.691926169652063	TOX21_HDAC_Inhibition
DTXSID0020280	88-73-3	1-Chloro-2-nitrobenzene	1	19.1151869206211	ATG_RXRb_TRANS_dn
DTXSID0020282	5131-60-2	4-Chloro-1,3-diaminobenzene	14	3.82661305182484	TOX21_ERa_BLA_Antagonist_ratio

Download table

1. Link to the EPA chemical dashboard on the bioactivity page
2. Number of assay where the chemical has a AC50 value
3. Link to the Tox21Map with the most active assay results
4. Link to download this table in .csv format