DrugMap

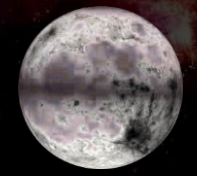
DRUGBANK

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

Grouped in 3 categories

Approved drugs

Withdrawn drugs



Drugs in development

PFASMap

Chemical dashboard

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

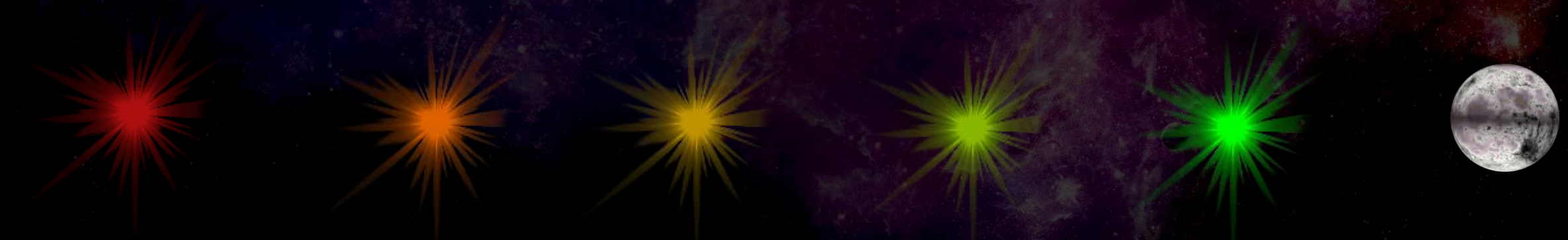
Grouped by Globally Harmonized System (GHS)

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)



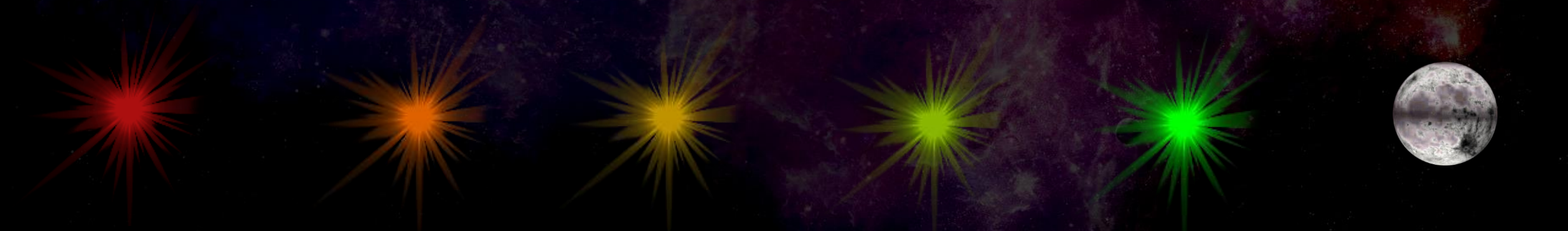
GHS=1 GHS=2 GHS=3 GHS=4 GHS=5 No GHS reported

DSSToxMap

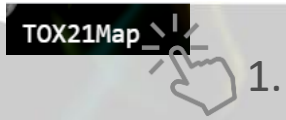
883,000 chemicals available on the EPA chemical dashboard, each navigation map included 10,000 chemicals center on the user choice chemical.

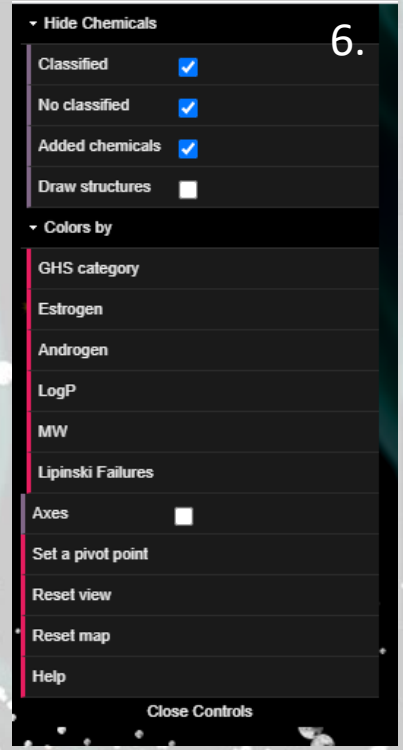
Chemical dashboard

Grouped by Globally Harmonized System (GHS)



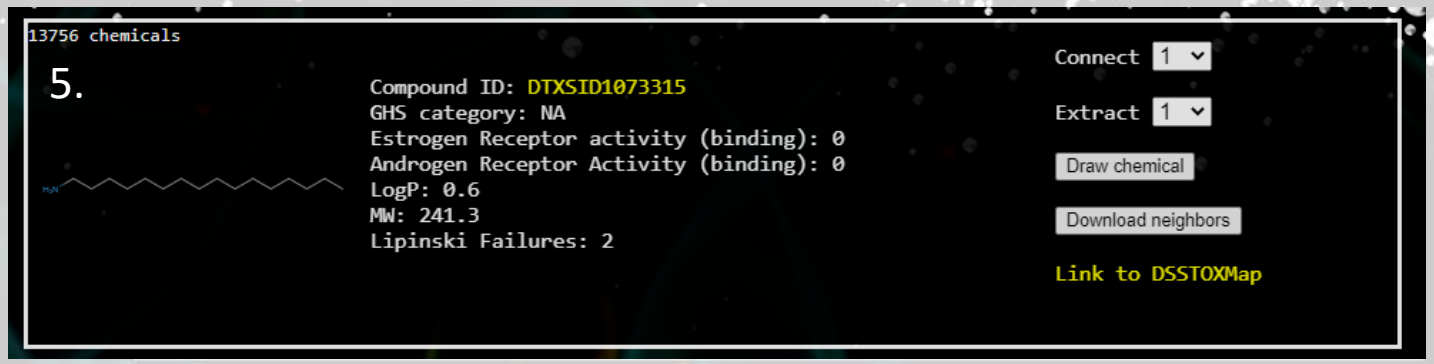
GHS=1 GHS=2 GHS=3 GHS=4 GHS=5 No GHS reported



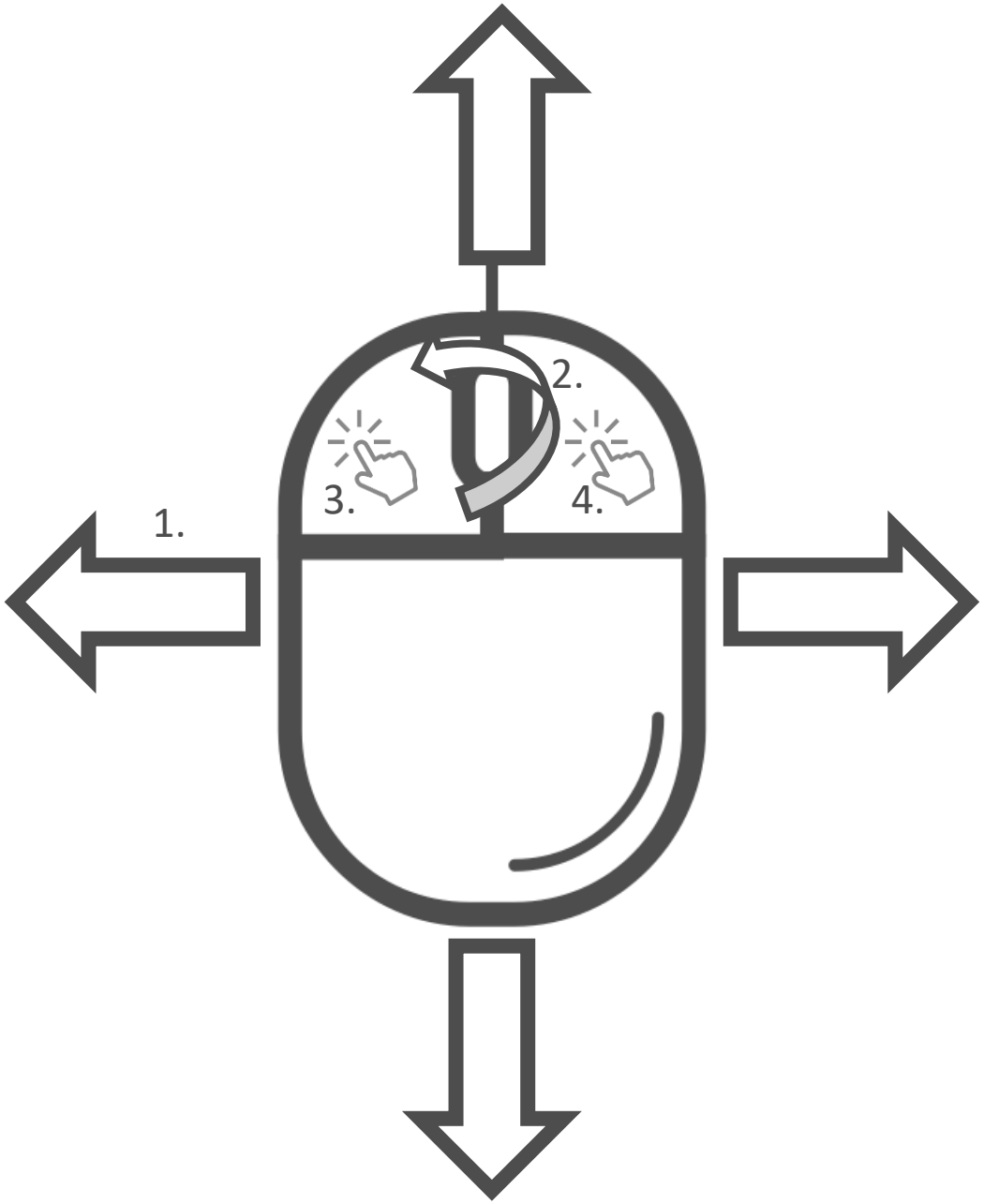


View blocked

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

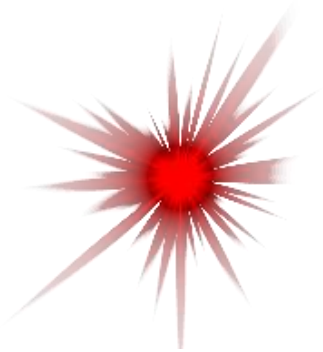


Mouse-based navigation

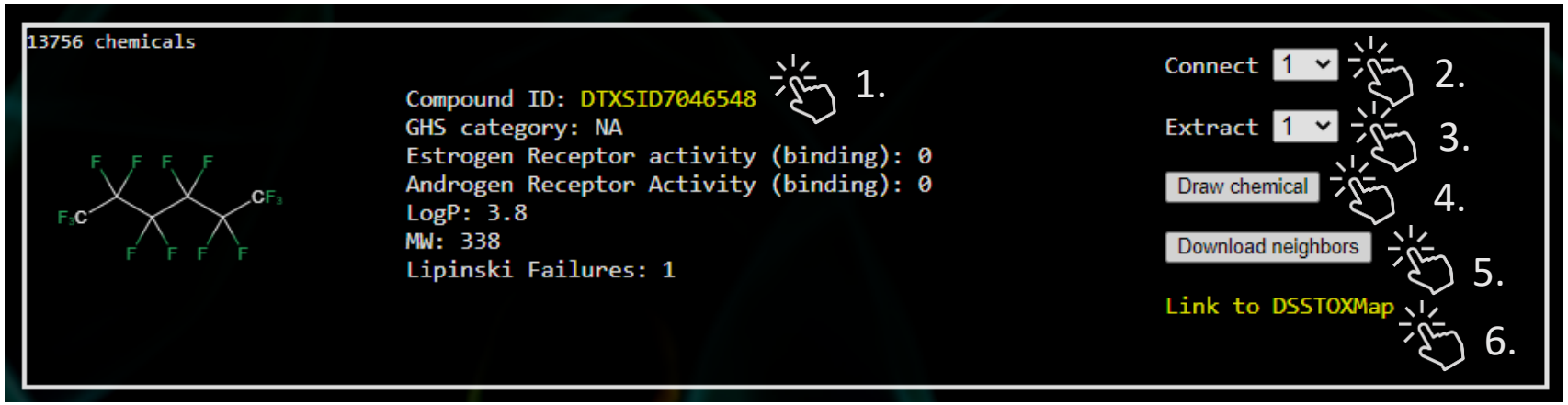


1. navigate on map
2. zoom in / zoom out
3. rotate the map
4. moved the map

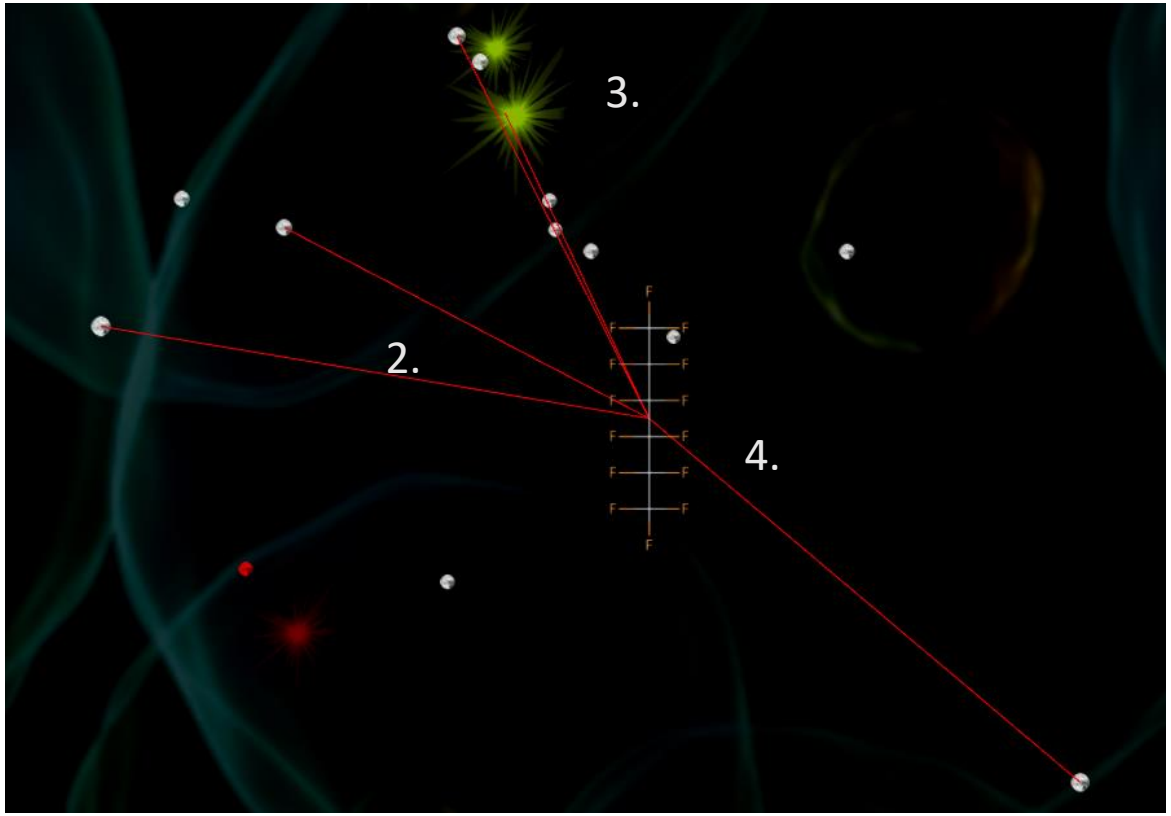
Interactive chemical panel



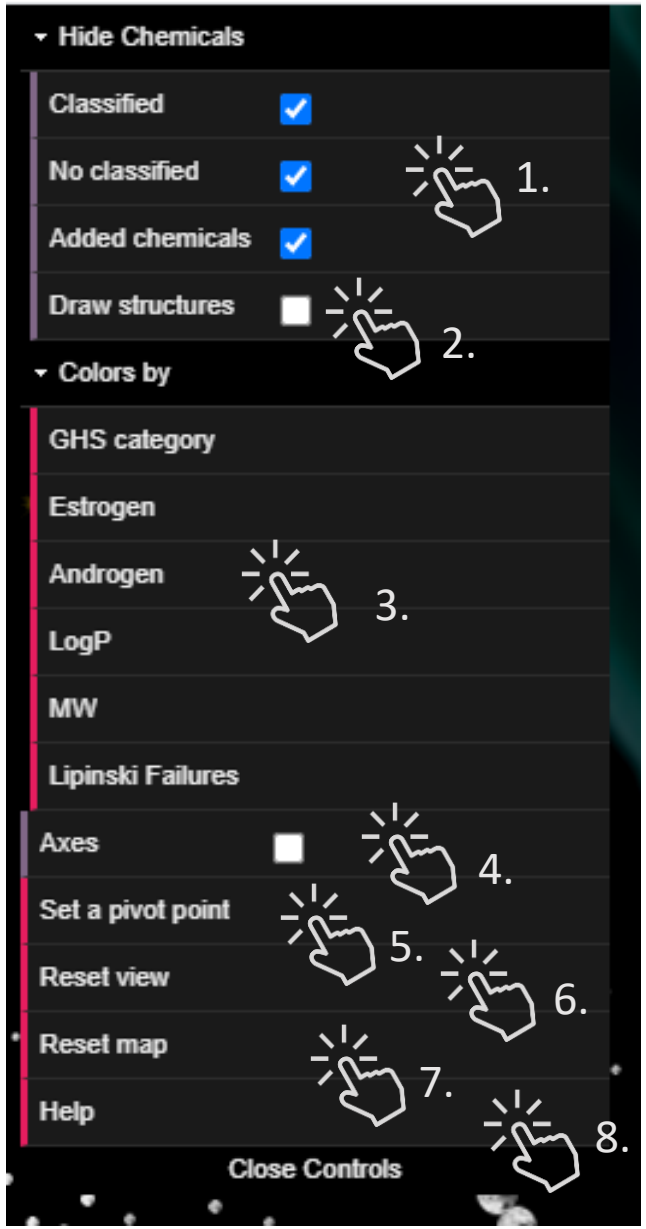
Selected chemical is in red on the map



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



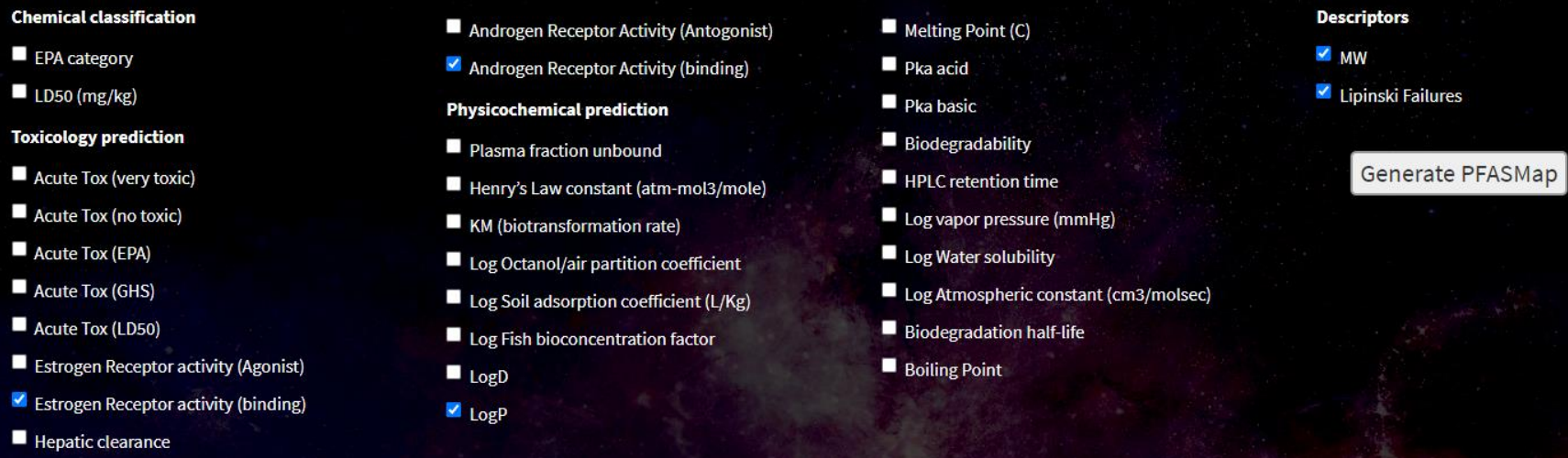
Control panel



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:



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

OPERA
OPEn (q)saR App

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)N1CCCCC1
CCCCNC1CCCCC1
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=CC=1
CC(N)CC(C)(C)N
 4-diallylaminophenyl ester
CC(C)C1C=CC(CO)=CC=1
N#CC1C(Cl)=C(Cl)C(Cl)=C(C#N)C=1Cl
DTXSID8064226
CCN(CC)C1C=CC(C=O)=CC=1
11-dihydro-5-(3-(4-morpholinyl)-1-oxopropyl)-5H-dibenz(b
.alpha.
1135-66-6
111-14-8
DTXSID4068082
COP(=O)(OC(Br)C(Br)(Br)Br)OC
CC(Cl)(Cl)C(O)=O
CCC(CC)C(=O)OCCOCCOCCOC(=O)C(CC)CC
COC(C1CCCCC1N1CCCCC1)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)OCC1CCCO1
DTXSID20191040
CC1=CC=C(Cl)C(NC2C=CC=CC=2C(=O)OCOCC)=C1Cl
```

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

1. Compute molecular descriptors

Create QSAR ready structures from input chemicals

Compute molecular descriptors

Descriptor computation

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

Descriptor

ID	Descriptor
1	OK
2	OK
3	OK
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 (Antogonist)

Physicochemical prediction

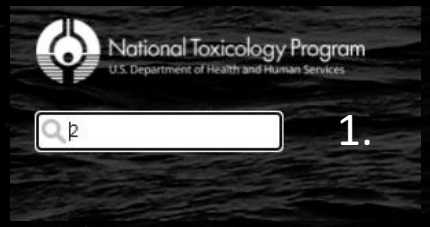
- [x] Androgen Receptor Activity (binding)
- [ ] Plasma fraction unbound
- [ ] Henry's Law constant (atm-mol3/mole)
- [ ] KM (biotransformation rate)
- [ ] Log Octanol/air partition coefficient
- [ ] Log Soil adsorption coefficient (L/Kg)
- [ ] Log Fish bioconcentration factor
- [ ] LogD
- [ ] Melting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

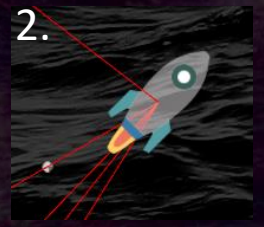
Descriptors

- [x] MW
- [x] Lipinski Failures

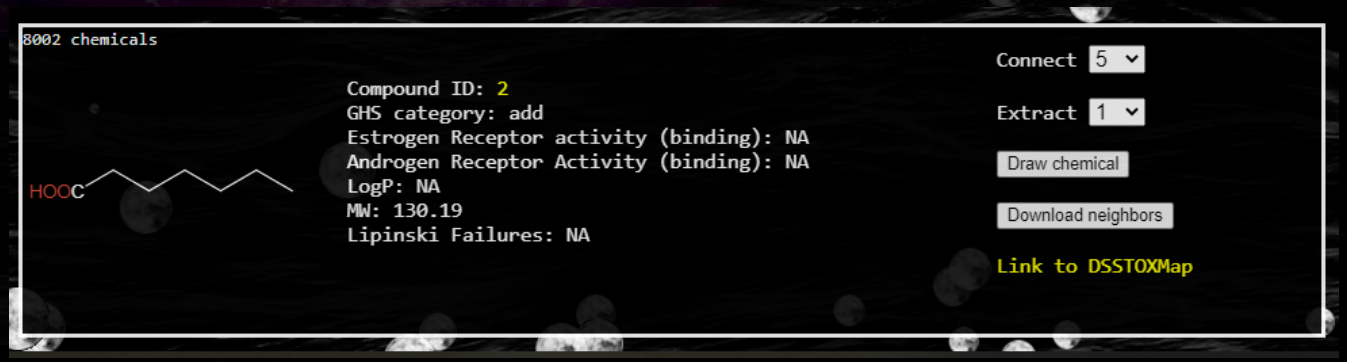
Generate PFASMap

Map with user chemicals





1. Search added chemicals by ID
2. Rocket represented added chemicals
3. Updated information about user chemical in the panel



Project the Tox21 assay results

Integrated Chemical Environment

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

Tox21

Projection on the Tox21Map:

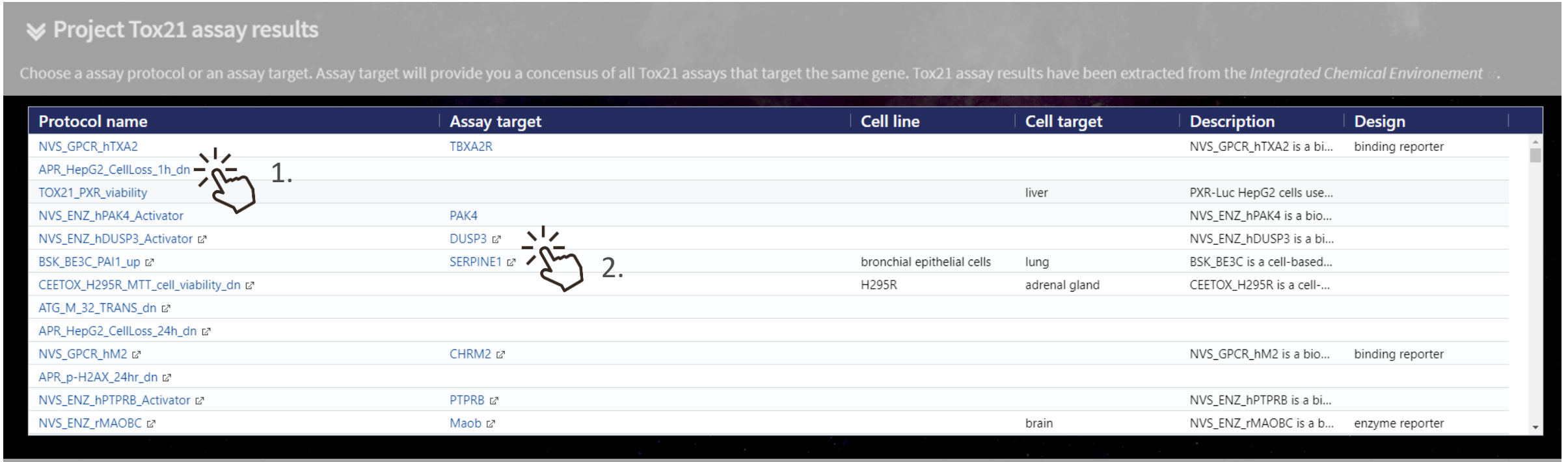
8,947 unique substance comprising the screening library for the Tox21 program, a multi-federal agency collaborative among the US EPA, NEHS/NTP, NIH/NCATS, and the US FDA.

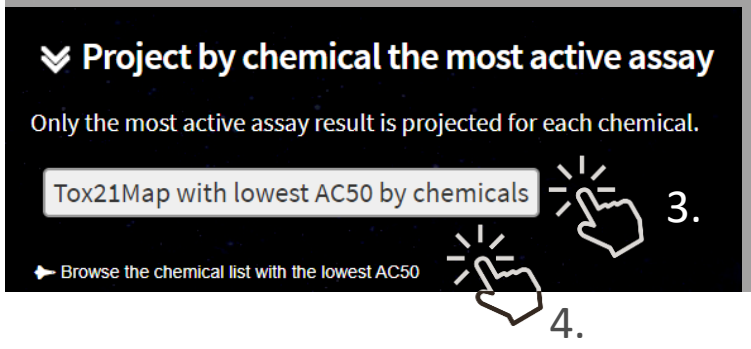
Active chemical

Inactive chemical

Inconclusive or no tested chemical

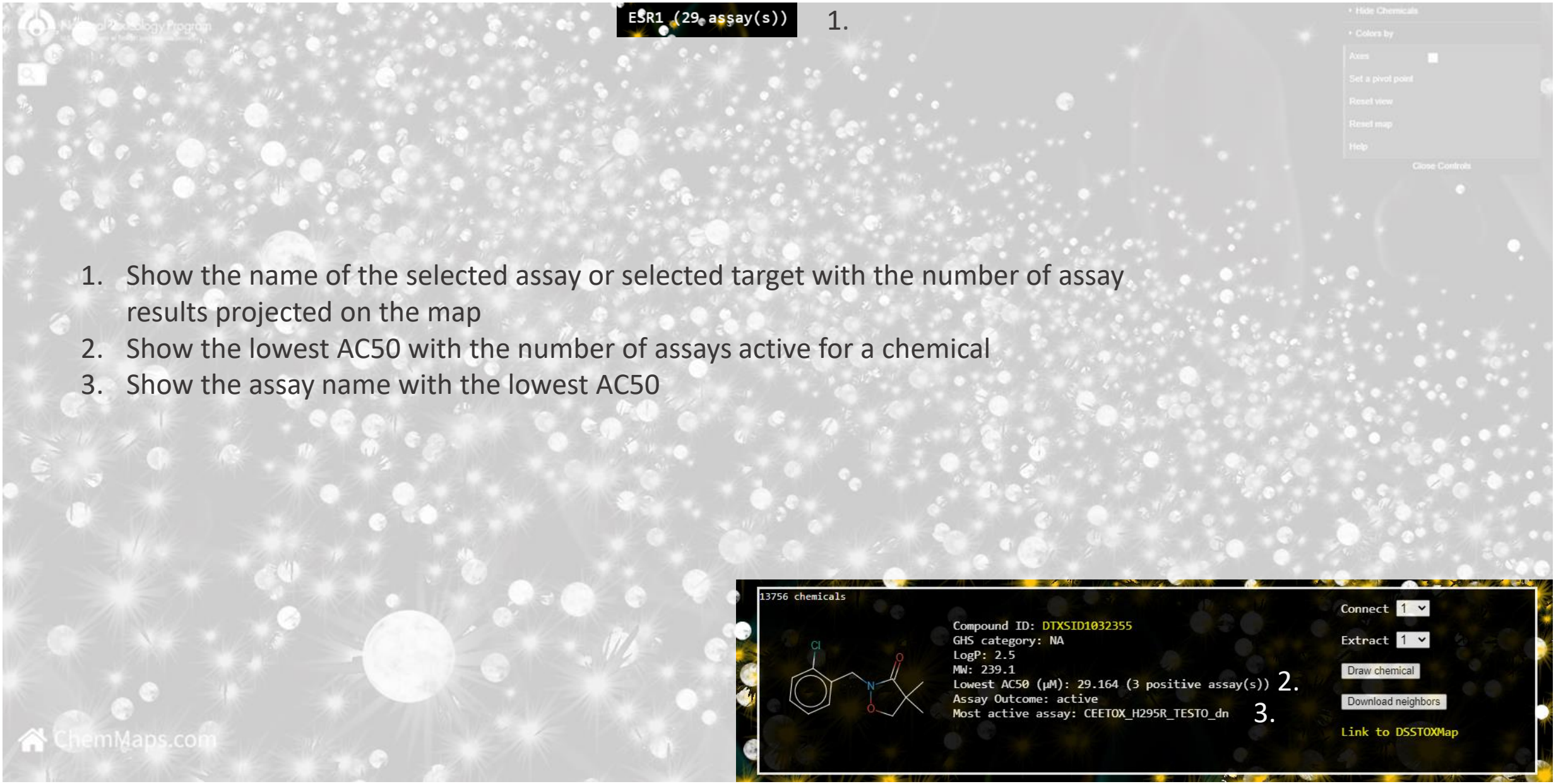
Select data to project





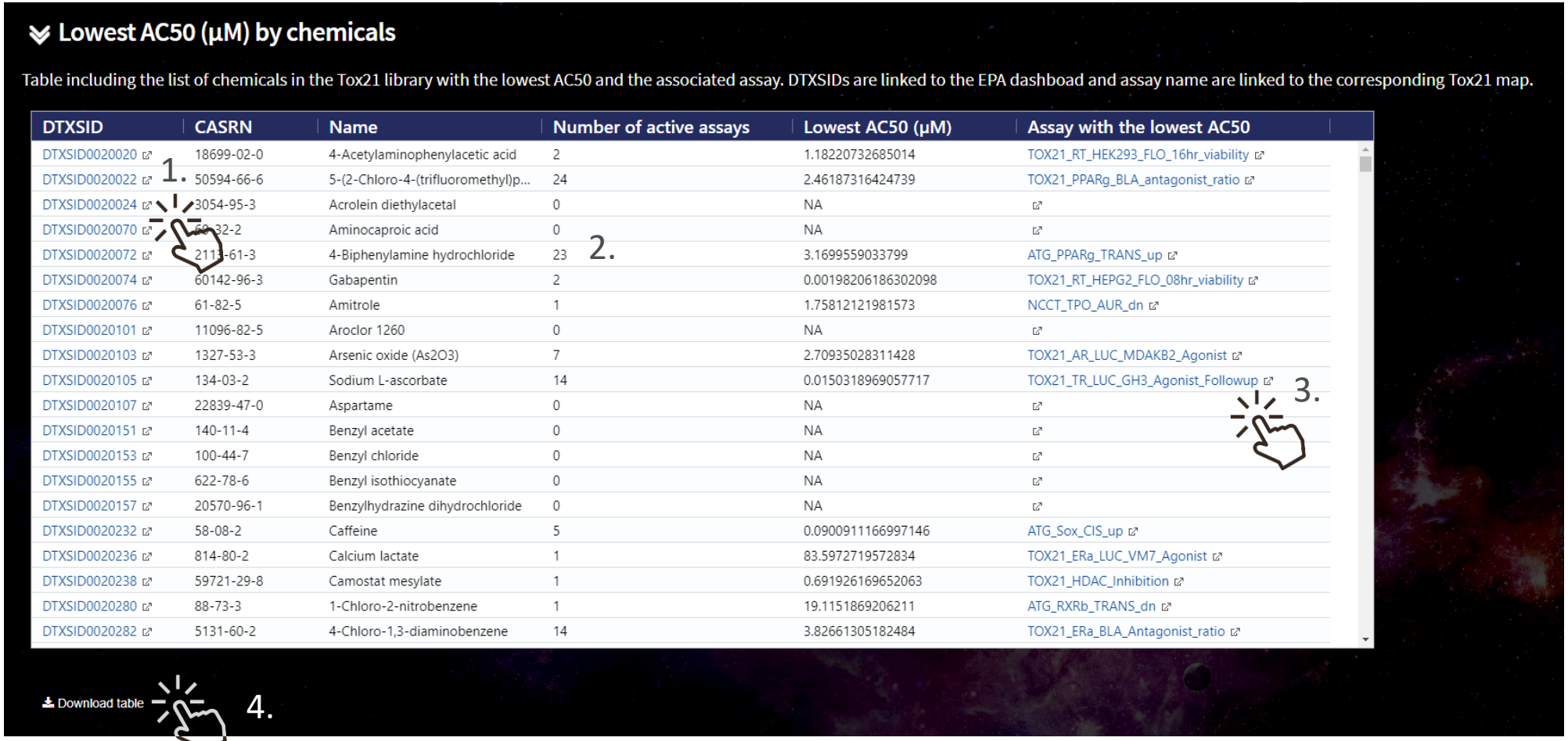
1. Project a unique assay results
2. Assay results for one target (combining several assays)
3. Project the lowest AC50 by chemicals
4. Browse chemical list with the lowest AC50

Assay results



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



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 dashboad 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-Acetylaminophenylacetic acid	2	1.18220732685014	TOX21_RT_HEK293_FLO_16hr_viability
DTXSID0020022	50594-66-6	5-(2-Chloro-4-(trifluoromethyl)p...	24	2.46187316424739	TOX21_PPARg_BLA_antagonist_ratio
DTXSID0020024	3054-95-3	Acrolein diethylacetal	0	NA	
DTXSID0020070	60-32-2	Aminocaproic acid	0	NA	
DTXSID0020072	2113-61-3	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 (As2O3)	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