

# ChemMaps.com V2 – Exploring the Environmental Chemical Universe

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Journey through chemical space with ChemMaps.com, an interactive application that uses chemical descriptors to explore chemical properties and relationships.

5. See PFOA on the PFAS space and identify closest PFAS chemicals with acute tox data.

4. Visualize PFOA within the space defined by the DSSTox chemicals. Chemicals appear as stars if they have measured acute tox data or planets if not.

6. Make a detour to locate PFOA in the biological activity space and identify most active assays in the neighborhood.

7. Use info panel to see chemical properties (updated in real time navigation).

8. Navigate in sub-spaces with sets of up to 20 chemicals.

3. Navigate space using your mouse.

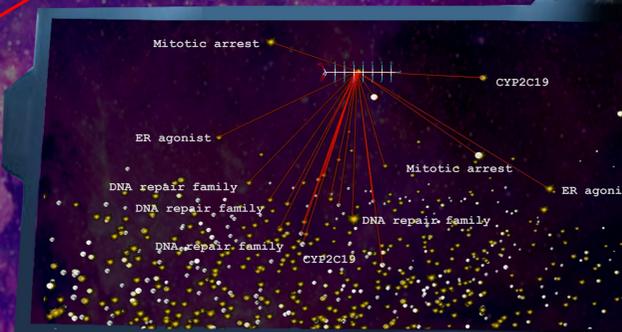
2. Use the search bar to set a course for PFOA and upload PFOS as user chemical.

1. Take a seat, follow the numbers and navigate the chemical space of perfluorooctanoic acid (PFOA) and perfluorooctane sulfonic acid (PFOS).

9. Refine your navigation by selecting features to project on the space (up to 5).

The PFAS space is defined using 7998 PFAS structures.

For many PFAS no information is available; those are represented by a planet.



ChemMaps.com uses Tox21/ToxCast assays to characterize biological activity.

PFOA is active in assays that measure interaction with the CYP2B6 metabolic enzyme.

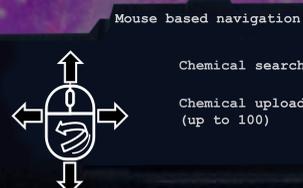
## Updates

- Chemical database updates (from 800k to 1.1 M chemicals)
- Tox21/ToxCast assays results mapped on chemicals including most active assay mapping and interactive table to navigate Tox21/ToxCast results
- Ability to upload user chemicals, represented on the space by a rocket
- Redesign spaces for PFAS, Tox21 chemical and drugs
- Added screenshot option
- Added measurement of the relative space distances between two chemicals on the map

## Features panel

- |  |  |   |
|--|--|---|
| <p><b>Chemical identification</b></p> <ul style="list-style-type: none"> <li>Product name</li> <li>Formula</li> <li>Generic name</li> <li>Brand name</li> <li>IUPAC</li> </ul> <p><b>Toxicity identification</b></p> <ul style="list-style-type: none"> <li>Acute Tox (EPA classification)</li> <li>Acute Tox (GHS classification)</li> </ul> <p><b>Toxicity prediction</b></p> <ul style="list-style-type: none"> <li>Acute Tox (very toxic)</li> <li>Acute Tox (no toxic)</li> <li>LD50 acute tox</li> <li>Estrogen receptor agonist</li> <li>Estrogen receptor binding</li> <li>Hepatic clearance</li> <li>Androgen receptor antagonist</li> <li>Androgen receptor binding</li> </ul> | <p><b>Predicted physicochemical properties</b></p> <ul style="list-style-type: none"> <li>Plasma fraction bound</li> <li>Henry's law constant</li> <li>KM (biotransformation rate)</li> <li>Log octanol/air partition</li> <li>Log soil adsorption coefficient</li> <li>Log fish bioconcentration factor</li> <li>LogD</li> <li>LogP</li> <li>Pka acid</li> <li>Melting point</li> <li>Pka basic</li> <li>Log vapor pressure</li> <li>Log water solubility</li> <li>Log atmospheric constant</li> <li>Boiling point</li> <li>Biodegradation half-time</li> </ul> | <p><b>Molecular descriptors</b></p> <ul style="list-style-type: none"> <li>Molecular weight</li> <li>Polar surface</li> <li>Rotable bond</li> <li>Failure Lipinski rules</li> <li>Failure Veber rules</li> <li>Failure Ghose rules</li> </ul> |
|--|--|---|

DTXSID40896601  
PFOS (user uploaded chemical)  
Molecular weight: 414  
LogP: 3.9



Chemical search:

Perfluorooctanoic acid

Chemical upload:

Perfluorooctanesulfonic acid (PFOS)

## Perfluorooctanoic acid (PFOA)

DTXSID8031865  
GHS: Not classified  
GHS predicted: 3  
ER agonist: predict not active  
AR antagonist: predict not active

Molecular Weight : 414 Da  
LogP: 3.1  
Lipinski Failure: 1

On the whole space PFOA is in a low-density area around other PFAS chemicals.

## Navigation panel

- Draw structure
- Reset view
- Hide chemicals without GHS classification
- Sub-space around selected chemical (up to 20 chemicals)
- Change color based on selected property
- Connect closest chemicals and compute distances
- GHS predicted
- ER agonist
- AR antagonist
- Molecular weight
- LogP

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