National Institute of Environmental Health Sciences
Division of Translational Toxicology

ChemMaps.com V2 – Exploring the Environmental Chemical Universe

A. Borrel[1], A. Unnikrishnan[1], D.G. Allen[1], N. Kleinstreuer[2]

[1]Inotiv, RTP, NC, USA; [2]NIH/NIEHS/DTT/NICEATM, RTP, NC, USA

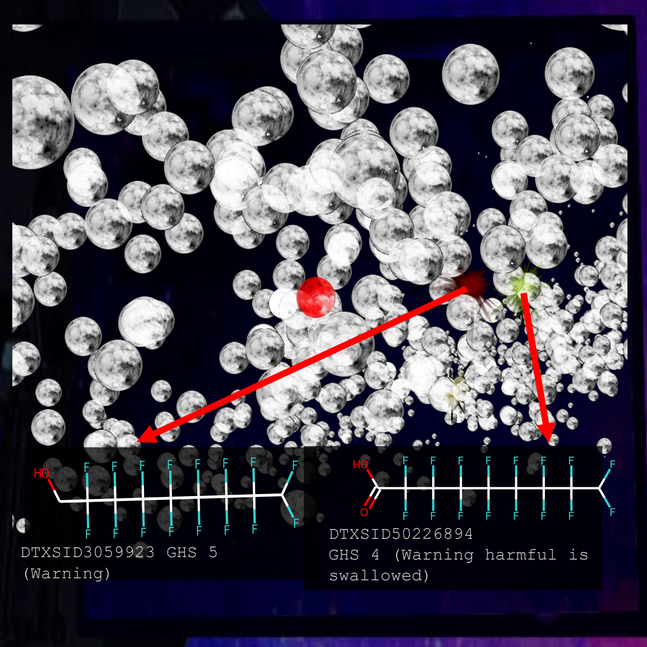
Journey through chemical space with ChemMaps.com, an interactive application that uses chemical descriptors to explore chemical properties and relationships.

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.

5. See PFOA on the per- and polyfluoroalkyl substances (PFAS) space and identify closest PFAS chemicals with acute tox data.

The PFAS space is defined using 7998 PFAS structures.

For many PFAS no information is available; those are represented by planets other by stars.



PFAS

PFAS

PFAS

PFAS

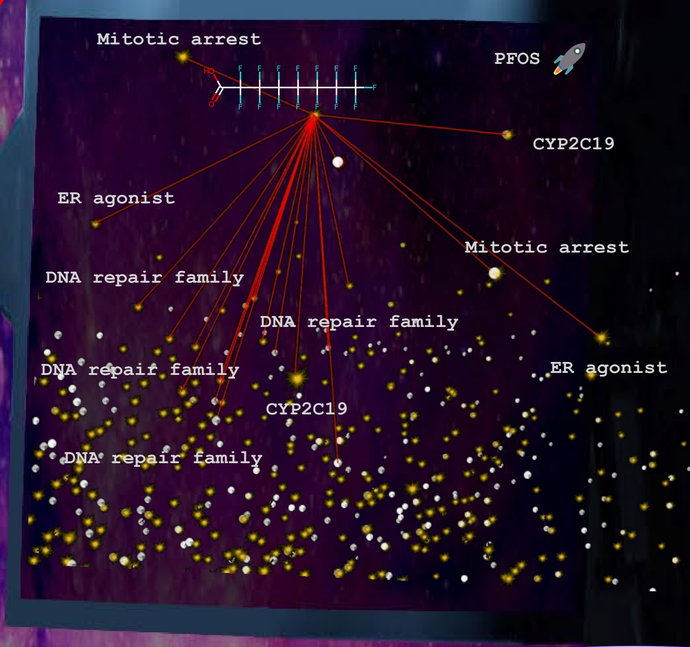
PFAS

PFAS

Perfluoro-4,4-dimethylhexanoic acid
DTXSID40896601
Molecular weight: 414
LogP: 3.9

Perfluoro-4-methylheptanoic acid
DTXSID10896597
Molecular weight: 414
LogP: 3.8

6. Make a detour to identify active assays in the neighborhood of PFOA.



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

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

10. Identify user-uploaded PFOS on the space.

3. Navigate space using your mouse.

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

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

Updates

New!

- 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
- Redesigned spaces for PFAS, Tox21 chemical and drugs
- Added screenshot option
- Added measurement of relative space between two chemicals on the map

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

Mouse-based navigation

Chemical search: Perfluorooctanoic acid

Chemical upload: (up to 100) Perfluorooctanesulfonic acid (PFOS)

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

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 which shown a poorly characterized area.

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

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

Features panel

Predicted physicochemical
- Plasma fraction bound
- Henry's law constant
- KM (biotransformation rate)
- Log octanol/air partition
- Log soil adsorption coefficient
- Log fish bioconcentration factor
- LogD
- LogP
- Pka acid
- Melting point
- Pka basic
- Log vapor pressure
- Log water solubility
- Log atmospheric constant
- Boiling point
- Biodegradation half-time

Chemical identification
- Product name
- Formula
- Generic name
- Brand name
- IUPAC

Molecular descriptors
- Molecular weight
- Polar surface
- Rotatable bond
- Failure Lipinski rules
- Failure Veber rules
- Failure Ghose rules

Toxicity prediction
- Acute Tox (very toxic)
- Acute Tox (no toxic)
- LD50 acute tox
- Estrogen receptor agonist
- Estrogen receptor binding
- Hepatic clearance
- Androgen receptor antagonist
- Androgen receptor binding

Toxicity identification
- Acute Tox (EPA classification)
- Acute Tox (GHS classification)

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 class, GHS predicted, Molecular weight, ER agonist, LogP, AR antagonist

Book your next journey:

https://sandbox.ntp.niehs.nih.gov/chemmaps/