National Institute of Environmental Health Sciences
Division of Translational Toxicology

ChemMaps.com v2.0
Exploring the environmental chemical space

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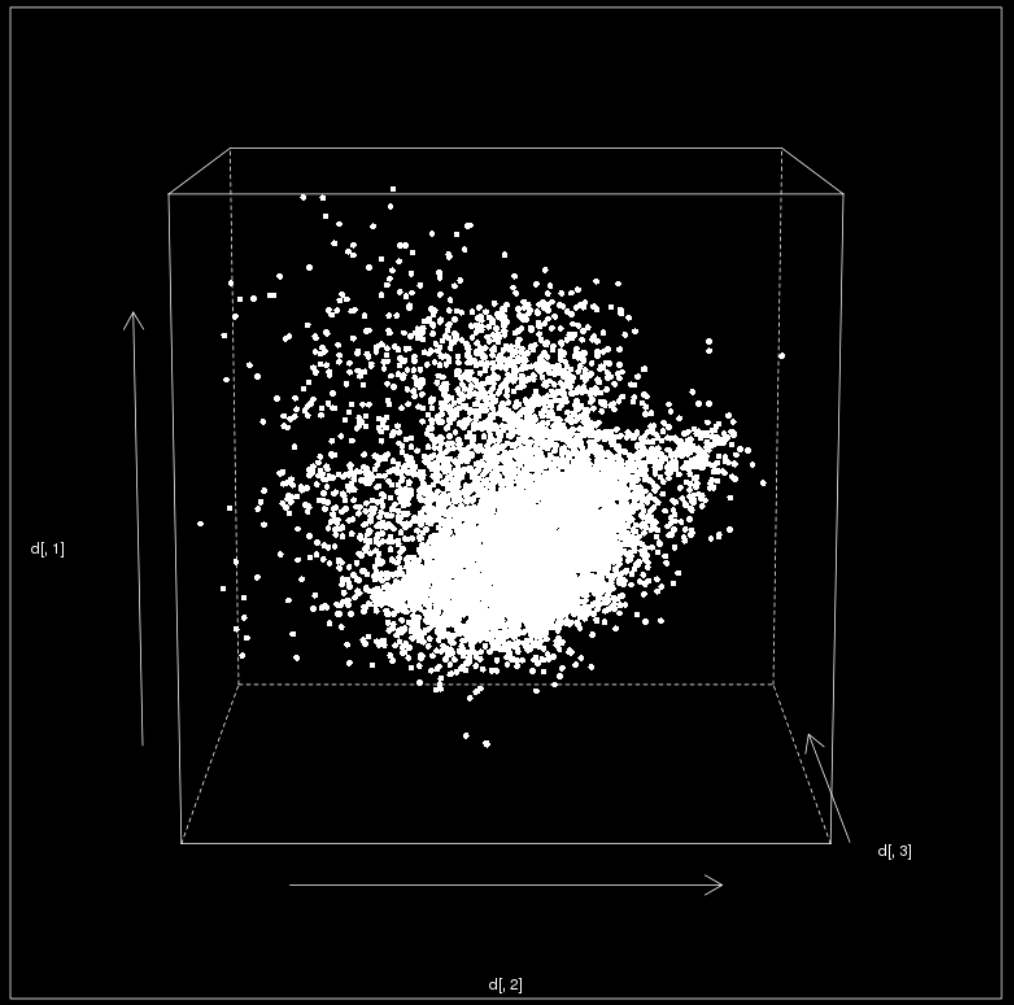
SACATM meeting

September 21-22, 2023 | NIEHS

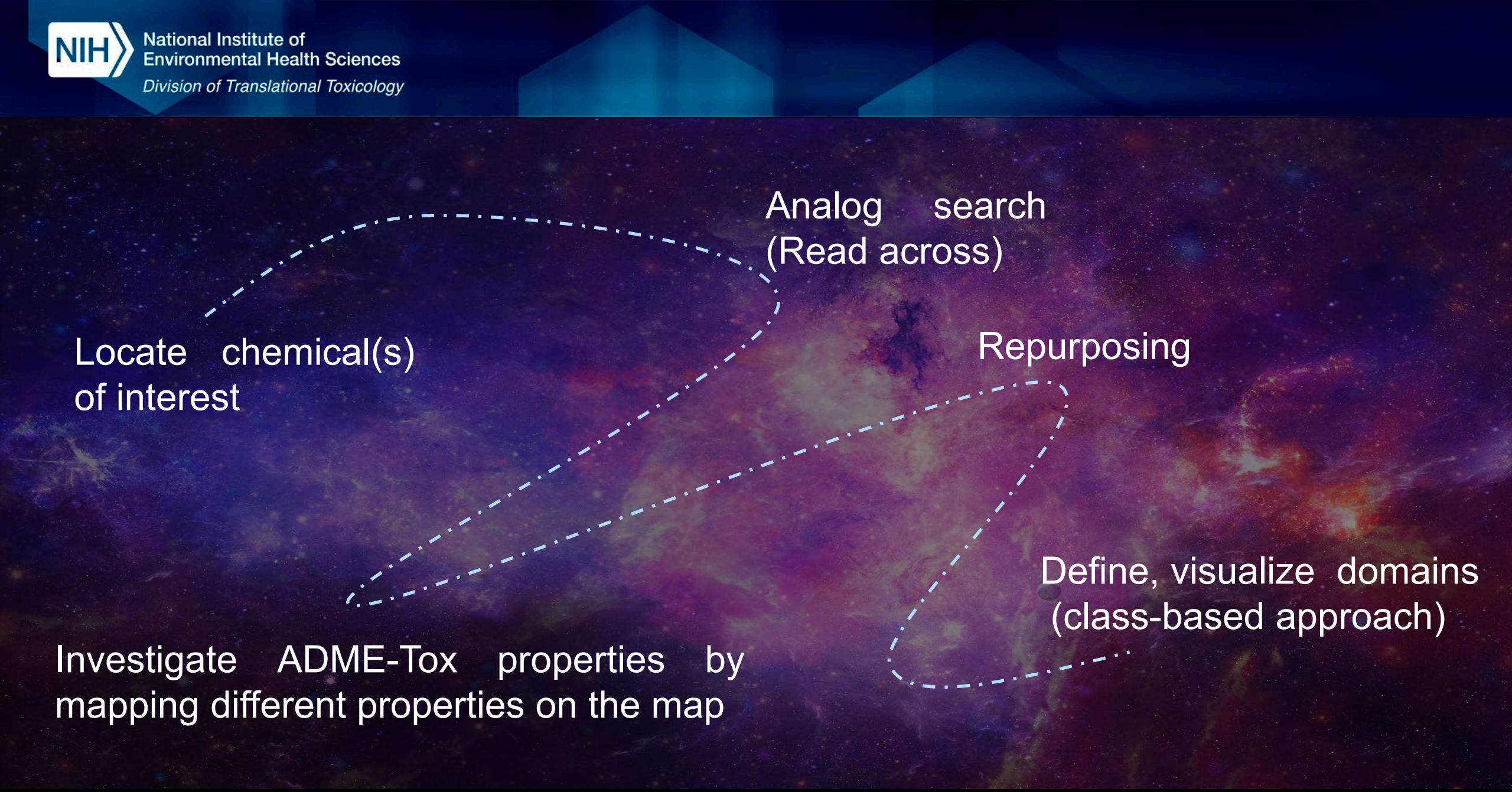
Chemical space: "…*Chemical space' is a term often used in place of '**multi- dimensional descriptor space**': it is a region defined by a particular choice of descriptors…*"

Dobson CM (2004) Nature 432:824–828



3D space computed on:

- Similarity metric (FP or/and molecular descriptors)
- Projection methods (PCA, UMAP, MDS …)


Analog search (Read across)
Locate chemical(s) of interest
Repurposing
Define, visualize domains (class-based approach)
Investigate ADME-Tox properties by mapping different properties on the map

Efficient tool of navigation

ChemMaps.com

ChemMaps.com V.1.0

- ~80,000 unique users since March 2018 (ACS - New Orleans)
- Limited to TSCA inventory and DrugBank (50k chemicals)

ChemMaps.com V2.0

New!

- Chemical database updates (from 800k to 1.1 M chemicals)
- Tox21/ToxCast assays results mapped on the map
- Interactive table to navigate Tox21/ToxCast results
- Ability to upload user chemicals, represented on the space by a rocket
- Redesigned spaces for PFAS, Tox21 chemicals and drugs

Live Demo

Future development

- Standalone version
- Training material
- Completely customizable map
- Linked ChemMaps.com in ICE
- Add other sources of bioactivities

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Acknowledgments

The NICEATM Group

NIEHS/DTT Contributors

UNITED STATES ICCVAM
Advancing Alternatives to Animal Testing

https://ntp.niehs.nih.gov/go/2021iccvamreport

Subscribe to NICEATM Newsemail list
https://ntp.niehs.nih.gov/go/niceatm

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

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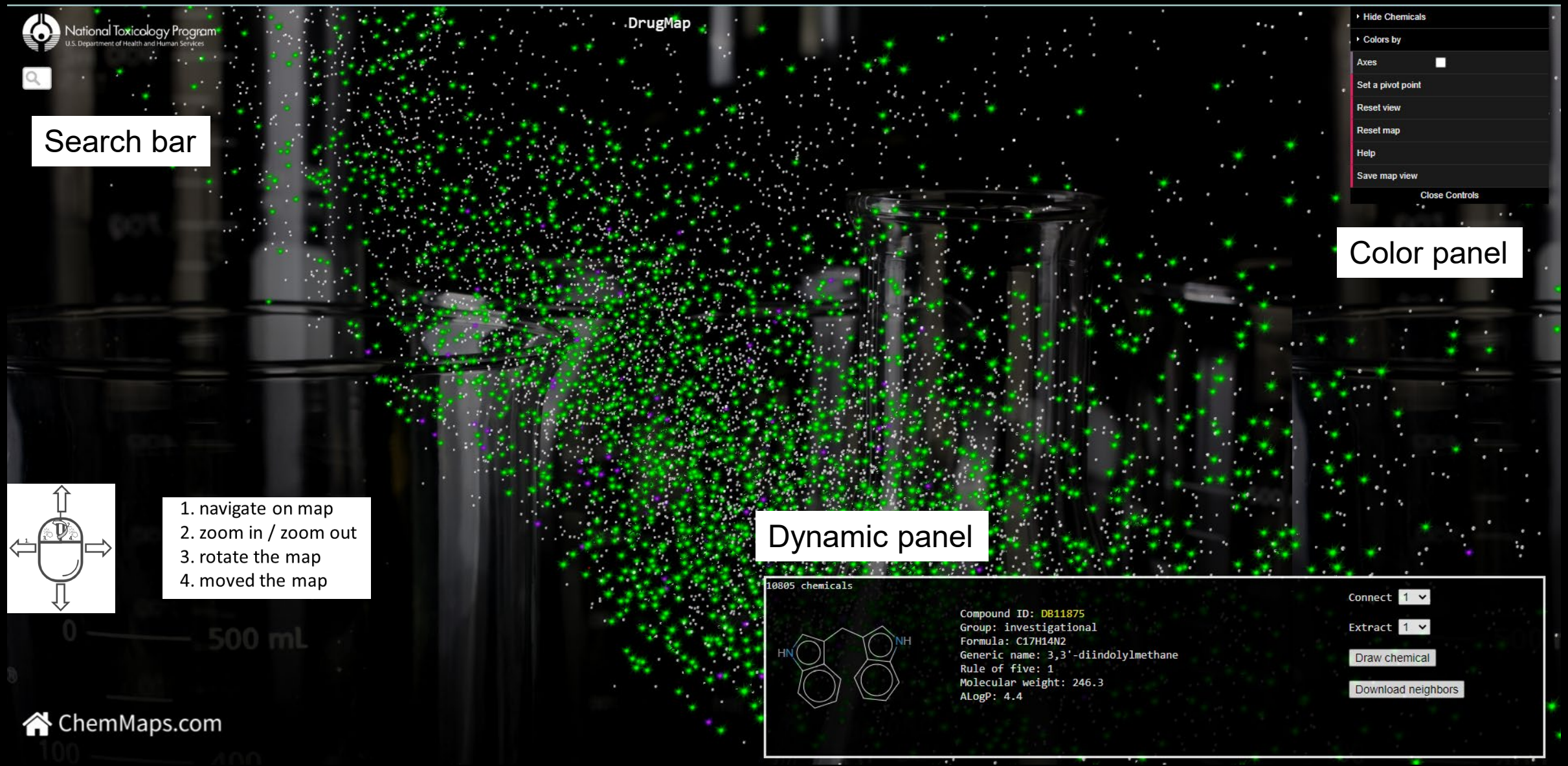
Annexe


National Toxicology Program
U.S. Department of Health and Human Services
DrugMap
Search bar
Hide Chemicals
Colors by
Axes
Set a pivot point
Reset view
Reset map
Help
Save map view
Close Controls
Color panel
1. navigate on map
2. zoom in / zoom out
3. rotate the map
4. moved the map
Dynamic panel
10805 chemicals
Compound ID: DB11875
Group: investigational
Formula: C17H14N2
Generic name: 3,3'-diindolylmethane
Rule of five: 1
Molecular weight: 246.3
ALogP: 4.4
Connect 1
Extract 1
Draw chemical
Download neighbors
ChemMaps.com

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 (Antogonist)
- 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

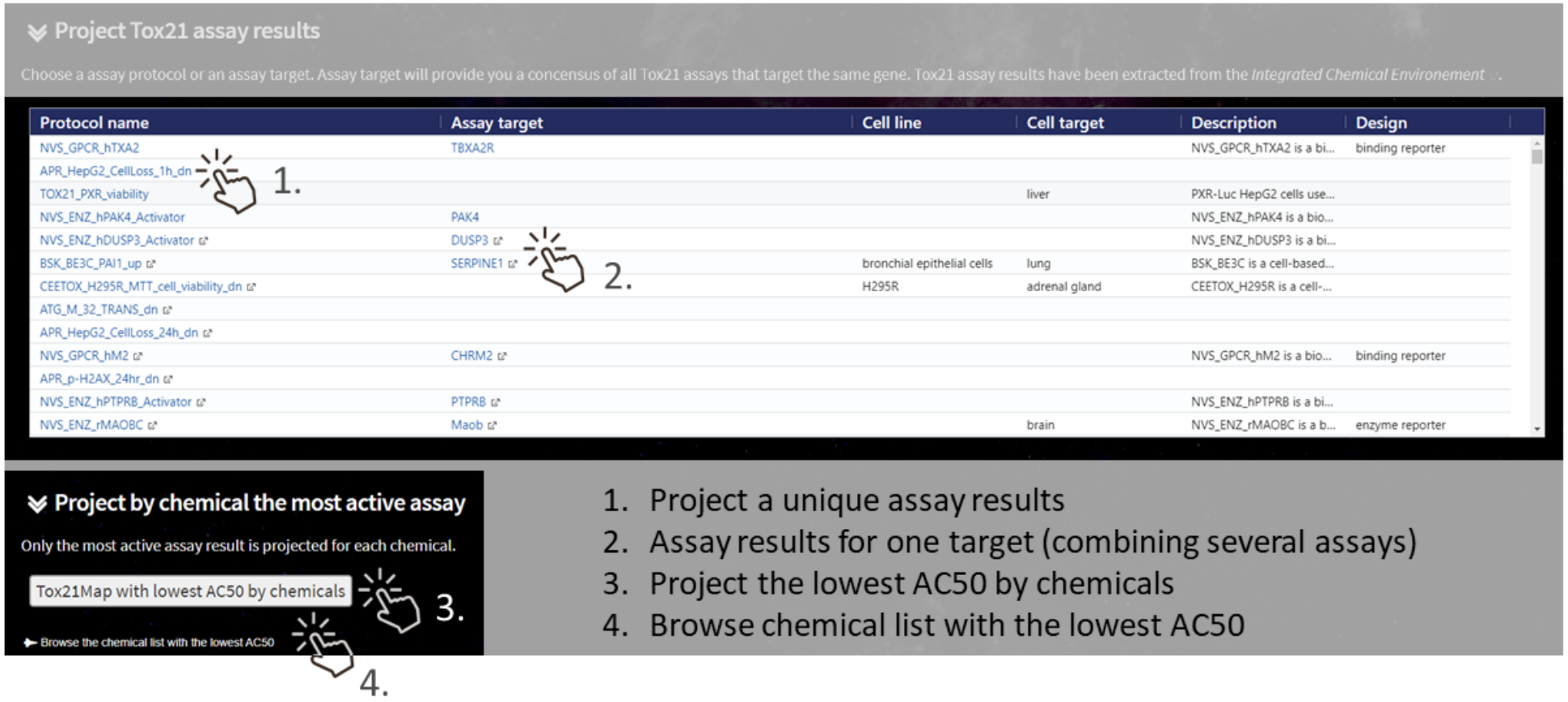
Mapping properties on map

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

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