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PFAS-Map / not_submitting / README.md

🗂 **ansumdiub** slight modification   🕐 **History**

👥 **1 contributor**

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116 lines (75 sloc)   4.84 KB

🔗 PFAS-Map

- Installation
- How to Use PFAS-Map
  - Exploring the classification of PFASs
  - Classify an unknown (potential) PFAS
  - Show your own PFAS dataset including classification and property

Installation

1. Do not worry about operating systems as PFAS-Map has been tested on macOS Catalina, Linux (Ubuntu LTS 20.04), and Windows 10.

2. Install Anaconda for Python 3.7 if your computer do not have Anaconda for Python 3. https://www.anaconda.com/products/individual

3. Install JRE 8 if your computer do not have Java Runtime Environment. If you are not sure, skip this step and come back later if error occurs. https://www.oracle.com/java/technologies/javase-jre8-downloads.html

4. Open Terminal (or "cmd" for Windows), input:

```
conda create -c rdkit -n pfasmap rdkit python=3.7
```

This will setup a conda virtual environment "pfasmap" that you will use to run PFAS-Map

5. When the pfasmap environment is properly setup, input:

```
conda activate pfasmap
```

6. Now you are in the pfasmap virtual environment. Let's install the basic machine learning and visualization libraries:

```
conda install numpy pandas scikit-learn plotly xlrd
```

7. Two extra packages need to be installed using pip:

```
pip install padelpy streamlit
```

8. Then navigate to the path where you save the "PFAS-Map" package. For example, if you save the "PFAS-Map" package under "Documents/GitHub", input:

```
cd Documents/GitHub/PFAS-Map
```

9. Input the command below to start the PFAS-Map user interface:

```
streamlit run user_interface.py
```

10. Start exploring PFAS-Map! If there is any problem in the installation, please contact ansuzjut@outlook.com. If you want to skip the installation, you can still explore function 1 and 3 of PFAS-Map through the interactive graphs we provide in figshare files.

How to Use PFAS-Map

Exploring the classification of PFASs

1. Select the first function from the side bar

PFAS-Map

PFAS-Map is a database framework for the rapid screening of structure-function relationships in PFASs. You can explore the classification of PFASs from US EPA PFAS Master List, classify an unknown PFAS, or explore your experimental or machine-learning data of PFASs through PFAS-Map.

What would you like to do?

Explore the classification of PFASs ▾
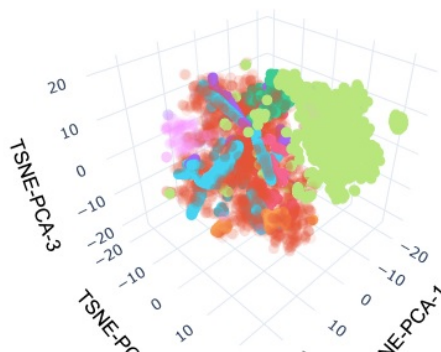
Explore the classification of PFASs   **STEP1**
Classify a potential PFAS
Explore your PFAS property data

Explore the classification of PFASs

Would you like to explore all PFASs or a specific class of PFAS?

All ▾

Legend:
- PFAS derivatives
- Non-PFAA perfluoroalkyl substances
- FASA-based PFAA precursors
- PFAAs
- PFASs containing Silicon
- Other aliphatic PFASs
- Perfluoroalkyl PFAA precursors
- Fluorotelomer-based PFAA precursors
- Side-chain fluorinated aromatic PFASs

2. Select "all classes" if you want to see the classification from the main class level; Select "a specific class" if you want to see the subclass of PFASs under a specific class.

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What would you like to do?

Explore the classification of PFASs ▾
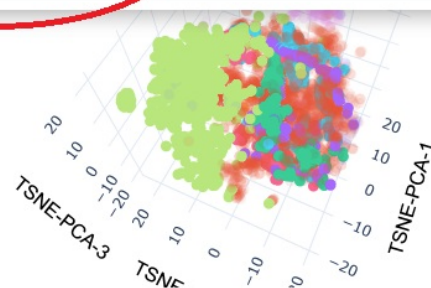
Explore the classification of PFASs

Would you like to explore all PFASs or a specific class of PFAS?

All ▾

All

A specific class

Legend:
- PFAS derivatives
- Non-PFAA perfluoroalkyl substances
- FASA-based PFAA precursors
- PFAAs
- PFASs containing Silicon
- Other aliphatic PFASs
- Perfluoroalkyl PFAA precursors
- Fluorotelomer-based PFAA precursors
- Side-chain fluorinated aromatic PFASs

If you selected "a specific class", you will need to select one of the classes you are interested in.

3. Hover the mouse cursor to the top right of the graph, click "full screen enter".

4. Start exploring the PFASs!
   ○ Feel free to rotate the graph to find the perspective you like.

- Hover the mouse cursor on any data point to see the value of components, SMILES, and class/subclass name.
- Single-click the class/subclass legend to mute the class/subclass. Click the legend again to bring it back.
- Double-click the class/subclass legend to only see this class/subclass.

Classify an unknown PFAS

1.
- Select the second function "classify a potential PFAS" from the side bar,
- Then input the SMILES of the PFAS to the box, and press "enter".

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What would you like to do?

Classify a potential PFAS ▾ **STEP 1-1**

Please input the SMILES of the PFAS you want to classify

C(C(C(C(C(F)(F)S(=O)(=O)O)(F)F)(F)F) **STEP 1-2**

Classify a Potential PFAS

Classification results:

Class: PFAAs

Subclass: PFSAs

Plotting the potential PFAS in PFAS-Map...(it may take several minutes)

Select the level of classification you would like to see

Classes ▾
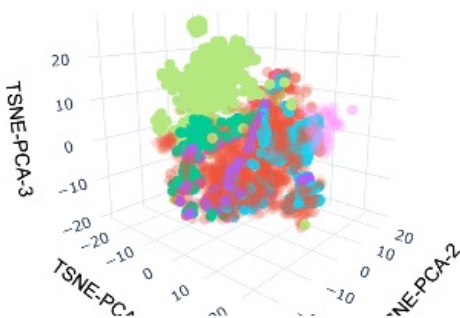
- PFAS derivatives
- Non-PFAA perfluoroalkyl substances
- FASA-based PFAA precursors
- PFAAs
- PFASs containing Silicon
- Other aliphatic PFASs
- Perfluoroalkyl PFAA precursors
- Fluorotelomer-based PFAA precursors
- Side-chain fluorinated aromatic PFASs
- The PFAS you input

2. o Wait for a few seconds and the classification results will show up.

   o Select to see the PFAS you input from "classes"---the view of all classes or "subclasses"---in the class the PFAS belongs to along with all other subclasses.

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What would you like to do?

Classify a potential PFAS

Please input the SMILES of the PFAS you want to classify

C(C(C(C(C(C(F)(F)S(=O)(=O)O)(F)F)(F)F)

Classify a Potential PFAS

Classification results:

Class: PFAAs

STEP 2-1

Subclass: PFSAs

Plotting the potential PFAS in PFAS-Map...(it may take several minutes)

Select the level of classification you would like to see

Classes

Classes   **STEP 2-2**

Subclasses

- PFAS derivatives
- Non-PFAA perfluoroalkyl substances
- FASA-based PFAA precursors
- PFAAs
- PFASs containing Silicon
- Other aliphatic PFASs
- Perfluoroalkyl PFAA precursors
- Fluorotelomer-based PFAA precursors
- Side-chain fluorinated aromatic PFASs
- The PFAS you input

3. - Go to full-screen graph and explore as instructed in step 3 and 4 of "Exploring the classification of PFASs".
    - The only difference will be the extra data point and its legend for the PFAS you input.

The PFAS you input

x: −6.896168
y: 12.96424
z: −8.573637
O=S(=O)(O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F

- PFSAs
- PFCAs
- PFSiAs
- PFECAs
- PFESAs
- PFPAs
- PFPiAs
- The PFAS you input

Show your own PFAS dataset including classification and property

1.
   - Select the third function "explore your PFAS property data".
   - Select the .csv file you would like to put on PFAS-Map. Make sure you follow the instruction to modify the corresponding column names. There are some sample datasets for you to test under the "test_data" folder.

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What would you like to do?

Explore your PFAS property data ▾ **STEP1-1**

Choose a csv file with PFAS property data, use 'NAME' as column name for compound's name, 'SMILES' as column name for compound's SMILES, and 'PROPERTY' as column name for compound's property data

Drag and drop file here
Limit 200MB per file • CSV **STEP1-2**

Browse files

2. ○ Wait for several minutes (the time depends on the size of your dataset).
   ○ After the graph shows up, go to the fullscreen mode as instructed.

PFAS-Map

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What would you like to do?

Explore your PFAS property data ▾

Choose a csv file with PFAS property data, use 'NAME' as column name for compound's name, 'SMILES' as column name for compound's SMILES, and 'PROPERTY' as column name for compound's property data

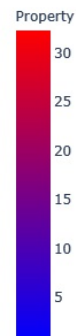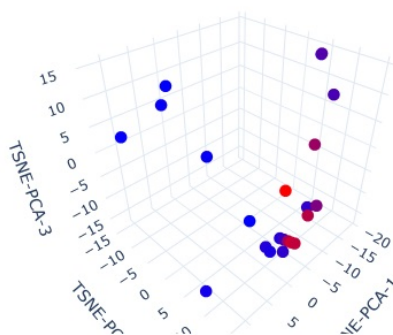Drag and drop file here
Limit 200MB per file • CSV

Browse files

⬜ 0803_updated_TOXCAS... ✕
2.4KB

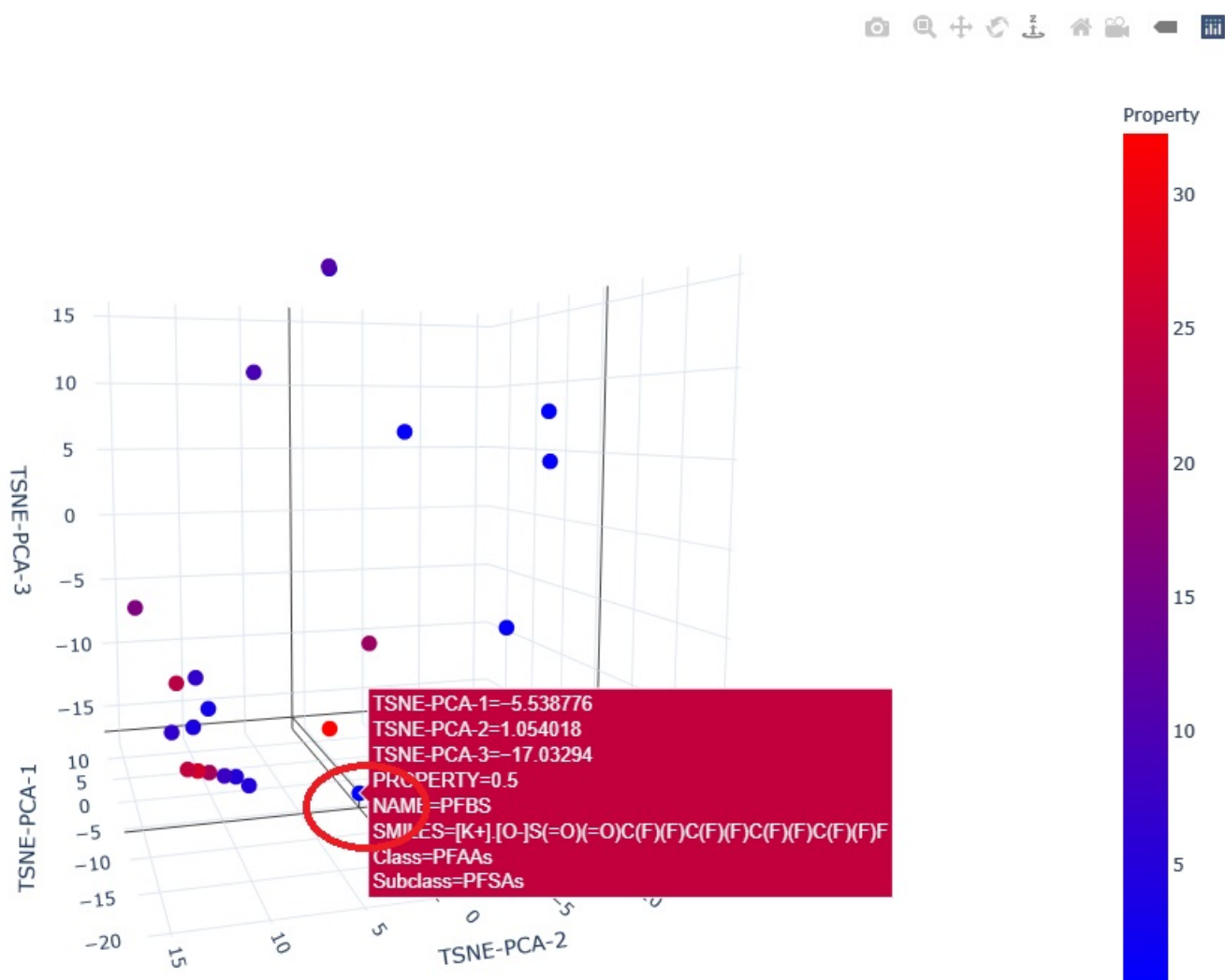# Explore your PFAS property data

Classifying your PFASs and plotting their property data in PFAS-Map...(it may take several minutes)

3. o Explore your PFAS dataset! The hover text shows the PC values, name, SMILES, property value, and classification results.

Authors

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