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In the last decades, Machine Learning (ML) applications have had a great impact on molecular and material science. However, every ML model requires a definition of its applicability domain. We developed a python package, Chemplot, that allows users to plot the chemical space of their datasets. Chemplot contains smart algorithms behind which uses both structural and tailored similarity. Moreover, it is easy to use even for non-experts. For details on the background of ChemPlot you can find here our paper.

This guide provides the user with the explanation of ChemPlot concepts and functionality.
1.1 Installing an official release

There are two different options you can follow to install ChemPlot.

1.1.1 Option 1: Use conda

You can install ChemPlot using conda. To install ChemPlot, at the command line, run:

~~~
$ conda install -c conda-forge chemplot
~~~

1.1.2 Option 2: Use pip

An alternative method is to install is using pip:

~~~
$ pip install chemplot
~~~

**Note:** ChemPlot requires RDKit, which cannot be installed using pip. The official RDKit documentation contains installation instructions for multiple platforms.

1.2 Verify Installation

You can verify that ChemPlot was installed on your local computer by running:

~~~
$ pip show chemplot
Name: chemplot
...
~~~

If instead of what is shown above your output is:

**WARNING:** Package(s) not found: chemplot

ChemPlot was not installed correctly or your system cannot find the path to it. If ChemPlot is installed correctly you can also test the package by running:
These will run all the library tests against your installation. For every official release from 1.2.0 you can use this command to verify that every function of your local installation of ChemPlot works as expected.
ChemPlot is a cheminformatics tool whose purpose is to visualize subsets of the chemical space in two dimensions. It uses the RDKit chemistry framework, the scikit-learn API and the umap-learn API.

### 2.1 Getting started

To demonstrate how to use the functions the library offers we will use a BBBP (blood-brain barrier penetration)\(^1\) molecular dataset. This is a set of molecules encoded as SMILES, which have been assigned a binary label according to their permeability properties. This dataset can be retrieved from the library as a pandas \(<https://pandas.pydata.org/pandas-docs/stable/index.html>\) DataFrame object.

```python
from chemplot import load_data
data_BBBP = load_data("BBBP")
```

To visualize the molecules in 2D according to their similarity it is first needed to construct a Plotter object. This is the class containing all the functions ChemPlot uses to produce the desired visualizations. A Plotter object can be constructed using classmethods, which differentiate between the type of input that is feed to the object. In our example we need to use the method from_smiles. We pass three parameters: the list of SMILES from the BBBP dataset, their target values (the binary labels) and the target type (in this case “C”, which stands for “Classification”).

```python
from chemplot import Plotter
cp = Plotter.from_smiles(data_BBBP["smiles"], target=data_BBBP["target"], target_type="C")
```

### 2.2 Plotting the results

When the Plotter object was constructed, descriptors for each SMILES were calculated, using the library mordred, and then selected based on the target values. We reduce the number of dimensions for each molecule from the number of descriptors selected to only 2. ChemPlot uses three different algorithms in order to achieve this. In this example we will first use t-SNE\(^2\).

```python
cp.tsne()
```

---

\(^1\) Martins, Ines Filipa, et al. (2012). A Bayesian approach to in silico blood-brain barrier penetration modeling. Journal of chemical information and modeling 52.6, 1686-1697

The output will be a dataframe containing the reduced dimensions and the target values.

<table>
<thead>
<tr>
<th>t-SNE-1</th>
<th>t-SNE-2</th>
<th>target</th>
</tr>
</thead>
<tbody>
<tr>
<td>-41.056122</td>
<td>0.355575</td>
<td>1</td>
</tr>
<tr>
<td>-35.535915</td>
<td>21.648867</td>
<td>1</td>
</tr>
<tr>
<td>23.771597</td>
<td>-14.438373</td>
<td>1</td>
</tr>
</tbody>
</table>

To now visualize the chemical space of the dataset we use `visualize_plot()`.

```python
import matplotlib.pyplot as plt

cp.visualize_plot()
```

![t-SNE plot](image)

The second figure shows the results obtained by reducing the dimensions of features Principal Component Analysis.
The third figure shows the results obtained by reducing the dimensions of features by UMAP\textsuperscript{4}.

\begin{verbatim}
cp.umap()
cp.visualize_plot()
\end{verbatim}


In each figure the molecules are coloured by class value.

References:
In this example we will use two molecular datasets: the BBBP (blood-brain barrier penetration) dataset\(^1\), already used in the previous section, and the BACE (-secretase inhibitors) dataset\(^2\). While the target values of the molecules collected by the BBBP dataset are binary, and therefore discrete, the target values of the molecules collected by the BACE dataset are continuous.

```python
from chemplot import Plotter, load_data

data_BBBP = load_data("BBBP")
data_BACE = load_data("BACE")
```

In order to plot a subset of the chemical space over a 2D graph it is necessary to define the metric according to which a certain molecule will be plotted on a certain location of the graph. What ChemPlot uses when deciding which molecules need to be plotted where is the concept of “molecular similarity”. Similar molecules will be displayed closer together, while molecules which are less similar will be displayed further apart.

ChemPlot distinguishes between two definitions of molecular similarity: structural and tailored\(^3\).

### 3.1 Structural

Structural similarity is defined as the number and dimensions of “fragments” different molecules share. Molecules are groups of atoms and bonds which a molecule can be divided into. The higher the number and dimensions of fragments two molecules share the more similar they are according to structural similarity. ChemPlot uses Extended-Connectivity Fingerprints (ECFPs)\(^4\) to define which fragments are present in each molecule. To create a `Plotter` object which visualizes the desired molecules according to structural similarity we need to pass the keyword “structural” as the `sim_type` parameter when constructing the object.

```python
cp_BBBP = Plotter.from_smiles(data_BBBP["smiles"], target=data_BBBP["target"], target_type="C", sim_type="structural")

cp_BACE = Plotter.from_smiles(data_BACE["smiles"], target=data_BACE["target"], target_type="R", sim_type="structural")
```

\(^1\) Martins, Ines Filipa, et al. (2012). A Bayesian approach to in silico blood-brain barrier penetration modeling. Journal of chemical information and modeling 52.6, 1686-1697


cp_BACE.tsne()
cp_BACE.visualize_plot()
3.2 Tailored

Tailored similarity is a similarity metric between molecules which takes into account the target property for determining if two molecules are similar or not. Indeed after a general set of descriptors is calculated for each molecule, a subset of those is selected by optimizing for the target property. Finally depending on the values of the subset ChemPlot can decide which molecules are more similar than others. To create a Plotter object which visualizes the desired molecules according to structural similarity, we need to pass the keyword “tailored” as the sim_type parameter when constructing the object. Since “tailored” is the default value of sim_type if a list of target values is passed in construction, in the following example we could have omitted the last parameter and still have got the same objects.

```python
cp_BBBP = Plotter.from_smiles(data_BBBP["smiles"], target=data_BBBP["target"], target_type="C", sim_type="tailored")

cp_BACE = Plotter.from_smiles(data_BACE["smiles"], target=data_BACE["target"], target_type="R", sim_type="tailored")
```

(continues on next page)
cp_BBBP.tsne()
cp_BBBP.visualize_plot()

t-SNE plot

0
1

t-SNE-2

t-SNE-1

cp_BACE.tsne()
cp_BACE.visualize_plot()
References:
CHAPTER
FOUR

DIMENSIONALITY REDUCTION

ChemPlot uses different machine learning techniques to reduce the number of dimensions, or features, of each molecule to only two in order to then create 2D graphs. These algorithms are: PCA\(^1\), t-SNE\(^2\) and UMAP\(^3\).

For the following examples we will use two molecular datasets, already mentioned in the previous section: the BBBP (blood-brain barrier penetration) dataset\(^4\) and the BACE (-secretase inhibitors) dataset\(^5\).

```python
from chemplot import Plotter, load_data
data_BBBP = load_data("BBBP")
data_BACE = load_data("BACE")
cp_BBBP = Plotter.from_smiles(data_BBBP["smiles"], target=data_BBBP["target"], target_type="C")
cp_BACE = Plotter.from_smiles(data_BACE["smiles"], target=data_BACE["target"], target_type="R")
```

4.1 PCA

ChemPlot uses PCA from the scikit-learn package to compute the two principal components of the molecular dataset. PCA allows for time efficient results and for a visualization which gives a global view of the data.

```python
cp_BBBP.pca()
cp_BBBP.visualize_plot()
```

---

\(^4\) Martins, Ines Filipa, et al. (2012). A Bayesian approach to in silico blood-brain barrier penetration modeling. Journal of chemical information and modeling 52.6, 1686-1697
PCA plot

0
1

PC-2 (8%)

PC-1 (10%)

cp_BACE.pca()
cp_BACE.visualize_plot()
ChemPlot uses t-SNE from the scikit-learn package to reduce to only 2 the number of features of the molecular dataset. t-SNE looks at local neighbourhoods of molecules when it is reducing their dimensions. In this way the local structure of the dataset is better preserved, while the global structure is mostly lost when plotting the results in a 2D graph. However because of the locality preservation that t-SNE offers it is possible to visualize well-defined clusters of similar molecules that exhibit similar properties.

```python
cp_BBBP.tsne()
cp_BBBP.visualize_plot()
```
Chapter 4. Dimensionality Reduction

cp_BACE.tsne()
cp_BACE.visualize_plot()
Two important parameters of the \texttt{tsne()} method are \texttt{perplexity} and \texttt{pca}. The former is a positive integer parameter which defines the size of the neighbourhoods the algorithm will look for when analyzing the dataset. The higher the value of \texttt{perplexity} the wider the analyzed neighbourhoods. The recommended values for \texttt{perplexity} range from 5 to 50. The \texttt{pca} parameter is a Boolean value which indicates if the data has to be preprocessed with PCA. Its value is taken into account when plotting according to structural similarities when each molecule is encoded with a long number of features. Since t-SNE is computationally expensive, preprocessing the data can save substantial amounts of time when generating plots, at the cost of losing some of the molecular structural information.
4.3 UMAP

ChemPlot uses UMAP from the umap-learn package to reduce to only 2 the number of features of the molecular dataset. As t-SNE, UMAP looks at local neighbourhoods of molecules when it is reducing their dimensions. While this also results in 2D clusters of locally similar molecules, compared to t-SNE, UMAP retains more of the global structure of the dataset. Compared to t-SNE, furthermore, UMAP is much more computationally efficient and faster.

```python
cp_BBBP.umap()
cp_BBBP.visualize_plot()
```

![UMAP plot](image)
Two important parameters of the `umap()` method are `n_neighbors`, `min_dist` and `pca`. The former is a positive integer parameter which constrains the size of the local neighbourhood the algorithm will look for when analyzing the dataset. Low values of `n_neighbors` will make ChemPlot visualize very local structures. The `min_dist` parameter is a value which ranges from 0.0 to 0.99. It provides the minimum distance apart that points are allowed to be in the 2D graph. The `pca` parameter is a Boolean value which indicates if the data has to be preprocessed with PCA.

References:

4.3. UMAP
VISUALIZE THE CHEMICAL SPACE

ChemPlot can generate two types of plots for a given chemical space: static and interactive. For the following examples we will use the BBBP (blood-brain barrier penetration) dataset¹.

```python
from chemplot import Plotter, load_data
data = load_data("BBBP")
cp = Plotter.from_smiles(data["smiles"], target=data["target"], target_type="C")
```

### 5.1 Static Plot

To generate a static plot first reduce the dimensions of the molecules used to initialize the Plotter instance. Then you can use `visualize_plot()` to generate a static visualization of the chemical space.

```python
import matplotlib.pyplot as plt
cp.tsne()
cp.visualize_plot()
```

¹ Martins, Ines Filipa, et al. (2012). A Bayesian approach to in silico blood-brain barrier penetration modeling. Journal of chemical information and modeling 52.6, 1686-1697
5.2 Interactive Plot

To generate an interactive plot first reduce the dimensions of the molecules used to initialize the Plotter instance. Then you can use `interactive_plot()` to generate an interactive visualization of the chemical space.

```
cp.interactive_plot(show_plot=True)
```

The interactive plot is generated using the library `bokeh`. You can interact with it by using the toolbar displayed on the top right of the visualization. You can navigate across the plot, select group of molecules, zoom in and out the visualization and save the plot as an image. Furthermore you can hover over the molecules to see their 2D image.

References:
ChemPlot allows you to identify different clusters in your data by making use of the KMeans\textsuperscript{1} algorithm as implemented in sklearn. To illustrate its implementation in ChemPlot, we will load the LOGP dataset\textsuperscript{2}, a dataset about Lipophilicity with continuous targets. Let’s load the sample dataset and create a Plotter object.

```python
from chemplot import Plotter, load_data

data = load_data("LOGP")

cp = Plotter.from_smiles(data["smiles"], target=data["target"], target_type="R")
```

Let’s then reduce the dimensions of the molecular descriptors.

```python
cp.umap(random_state=500)
```

Now that the dimensions are reduced, we can plot the image as shown in the previous chapters. We can also, however, identify some clusters in the data by calling this function:

```python
cp.cluster()
```

`cluster()` will identify the clusters in our reduced dataset by using KMeans. The function takes one parameter `n_clusters`, identifying the number of clusters we want to see. By default `n_clusters` is 5. Once we clustered the data, we can call `visualize_plot(clusters=True)` to see the plot. Notice how we need to pass a parameter `clusters` set to `True` in order to see the clusters in the resulting image.

```python
cp.visualize_plot(clusters=True)
```


\textsuperscript{2} Hersey, A. (2015) ChEMBL Deposited Data Set - AZ dataset
We can however also select a number of clusters we want to highlight. The parameter `clusters` in `visualize_plot()` can indeed also be a list of integers or an int itself. An integer represents one of the clusters identified in the previous steps. ChemPlot will either read the list or the single number passed as a parameter and highlight those clusters as selected.

```python
cp.visualize_plot(clusters=0)
```
cp.visualize_plot(clusters=[1,2,3])
We can also use `interactive_plot()` to visualize the clusters. In these cases, pass `clusters=True` to generate a Bokeh plot with two tabs. The first tab will contain the plot that would have been generated also without clustering. The second tab will contain a plot showing the different clusters. Click on the elements of the legend to mute a cluster’s data points.

```
cp.interactive_plot(clusters=True)
```

References:
ChemPlot offers additional features for chemical space visualization which can improve the understanding of the underlying similarities between the investigated molecules.

Using the `Plotter` object it is possible to create two different kind plots of the chemical space, aside from the scatterplots showed in the previous sections. These plots investigate the density distribution of the chemical space an are hexagonal bin plot and the kernel density estimate plot.

To show the before mentioned features we will use the BBBP (blood-brain barrier penetration) dataset\(^1\), already mentioned in the previous section:

```python
from chemplot import Plotter, load_data
data_BBBP = load_data("BBBP")
cp_BBBP = Plotter.from_smiles(data_BBBP["smiles"], target=data_BBBP["target"], target_type="C")
```

### 7.1 Hexagonal Bin Plot

In a hexagonal bin plot points are binned into hexagons, which in turn are coloured depending on the count of observations they cover. To create a hexagonal bin plot we need to pass the keyword “hex” as the `kind` parameter when visualizing the plot.

```python
cp_BBBP.tsne(random_state=0)
cp_BBBP.visualize_plot(kind="hex")
```

\(^1\) Martins, Ines Filipa, et al. (2012). A Bayesian approach to in silico blood-brain barrier penetration modeling. Journal of chemical information and modeling 52.6, 1686-1697
7.2 Kernel Density Estimate Plot

In a kernel density estimate plot, the data distribution is visualized by a continuous probability density curve which in our case is in 2 dimensions. To create a kernel density estimate plot we need to pass the keyword “kde” as the kind parameter when visualizing the plot.

```python
cp_BBBP.visualize_plot(kind="kde")
```
7.2. Kernel Density Estimate Plot
CHAPTER
EIGHT

SAMPLE DATASETS

ChemPlot provides some sample datasets that can be used to get started right away with exploring the libraries features. These datasets can be loaded with the following function:

```python
from chemplot import load_data

df = load_data("BBBP")
```

In these case we are loading the BBBP dataset, used in the previous sections of this manual. `load_data()` returns a pandas DataFrame built using the sample dataset provided as a parameter. Chemplot contains the following sample datasets:

<table>
<thead>
<tr>
<th>ID</th>
<th>Name</th>
<th>Type</th>
<th>Size</th>
</tr>
</thead>
<tbody>
<tr>
<td>C_1478_CLINTOX_2</td>
<td>Clintox (Toxicity)</td>
<td>Classification</td>
<td>1478</td>
</tr>
<tr>
<td>C_1513_BACE_2</td>
<td>BACE (Inhibitor)</td>
<td>Classification</td>
<td>1513</td>
</tr>
<tr>
<td>C_2039_BBBP_2</td>
<td>BBBP (Blood-brain barrier penetration)</td>
<td>Classification</td>
<td>2039</td>
</tr>
<tr>
<td>C_41127_HIV_3</td>
<td>HIV</td>
<td>Classification</td>
<td>41127</td>
</tr>
<tr>
<td>R_642_SAMPL</td>
<td>SAMPL (Hydration free energy)</td>
<td>Regression</td>
<td>642</td>
</tr>
<tr>
<td>R_1513_BACE</td>
<td>BACE (Binding affinity)</td>
<td>Regression</td>
<td>1513</td>
</tr>
<tr>
<td>R_4200_LOGP</td>
<td>LOGP (Lipophilicity)</td>
<td>Regression</td>
<td>4200</td>
</tr>
<tr>
<td>R_1291_LOGS</td>
<td>LOGS (Aqueous Solubility)</td>
<td>Regression</td>
<td>1291</td>
</tr>
<tr>
<td>R_9982_AQSOLDB</td>
<td>AQSOLDB (Aqueous Solubility)</td>
<td>Regression</td>
<td>9982</td>
</tr>
</tbody>
</table>

The datasets ID are constructed in the following way:

**Name Formatting:** type_size_name_num_of_classes.csv

4. Aggregate Analysis of ClinicalTrials.gov (AACT) Database.
7. AIDS Antiviral Screen Data.
• **type:** R->Numerical and C->Categorical
• **size:** Number of instances in the dataset
• **name:** Name of dataset
• **num_of_classes:** Number of classes (Categorical only)

You can retrieve the datasets by passing their ID to `load_data()`.

**Note:** The first 8 datasets in the table are edited versions of the MoleculeNet repository\(^{12}\).

You can print the available sample datasets to console with ChemPlot using the following function:

```python
from chemplot import info_data

df = info_data()
```

**References:**

The development environment is an installation of ChemPlot on your local computer which can be used for testing existing features or developing new ones in order to contribute to the library.

Start by making sure you have conda installed. This is needed since an important dependency of ChemPlot is RDKit, which can safely be installed only with conda.

Then clone your forked GitHub repository of ChemPlot on your local computer using either HTTPS:

```bash
~$ git clone https://github.com/<your-username>/ChemPlot.git
```

Or using SSH:

```bash
~$ git clone git@github.com:<your-username>/ChemPlot.git
```

Then from the terminal navigate to the ChemPlot repository you just created. From there create a new conda environment with all the dependencies needed to work with ChemPlot. Create the environment by running:

```bash
~/<PATH-TO-CLONE>/ChemPlot$ conda env create -f requirements_conda.yml
```

When conda finishes creating the environment, activate it by running:

```bash
~/<PATH-TO-CLONE>/ChemPlot$ conda activate chemplot_env
```

You can now install ChemPlot in editable mode. Editable mode will allow your code changes to be propagated through the library code without having to reinstall.

```bash
~/<PATH-TO-CLONE>/ChemPlot$ pip install -e .
```

You are now ready to develop ChemPlot!

### 9.1 Testing

To run the unit tests for ChemPlot use this command:

```bash
~$ python -m pytest --pyargs chemplot
```

On your cloned version of the ChemPlot repository you have two more tests, used to check performance of the library on your machine and to check the figures ChemPlot can generate. You can find these tests inside the performance_tests folder:
You can run these tests by navigating to the performance_test library:

```bash
~/ChemPlot$ cd performance_tests
~/ChemPlot/performance_tests$ python performanceTest.py
~/ChemPlot/performance_tests$ python visualplotsTest.py
```

If it doesn’t work you might have to change `python` with `python3` in the command. `performanceTest.py` will generate a `.csv` file containing all the times taken by ChemPlot to run all the dimensionality reduction methods on your machine. It will use the sample datasets provided with the library. `visualplotsTest.py` will instead create a multipage `.pdf` file containing different figures illustrating all plotting options for ChemPlot. These method as well will use the sample datasets included in the library.
ChemPlot principal class is `Plotter`. It receives a list of molecules as a parameter in order to then use different functions for plotting the data in two dimensions. All the main functions of ChemPlot are part of the `Plotter`. There are however two more functions outside of `Plotter`, which can be used to access the sample datasets.

### 10.1 chemplot.Plotter

**class** `chemplot.Plotter(encoding_list, target, target_type, sim_type, get_desc, get_fingerprints)`

A class used to plot the ECFP fingerprints of the molecules used to instantiate it.

**Parameters**

- `__sim_type (string)` – similarity type structural or tailored
- `__target_type (string)` – target type R (regression) or C (classification)
- `__target (list)` – list containing the target values. Is empty if a target does not exist
- `__mols (rdkit.Chem.rdchem.Mol)` – list of valid molecules that can be plotted
- `__df_descriptors (Dataframe)` – dataframe containing the descriptors representation of each molecule
- `__df_2_components (Dataframe)` – dataframe containing the two-dimensional representation of each molecule
- `__plot_title (string)` – title of the plot reflecting the dimensionality reduction algorithm used
- `__data (list)` – list of the scaled descriptors to which the dimensionality reduction algorithm is applied
- `pca_fit (sklearn.decomposition.TSNE)` – PCA object created when the corresponding algorithm is applied to the data
- `tsne_fit (sklearn.manifold.TSNE)` – t-SNE object created when the corresponding algorithm is applied to the data
- `umap_fit (umap.umap_.UMAP)` – UMAP object created when the corresponding algorithm is applied to the data
- `df_plot_xy (Dataframe)` – dataframe containing the coordinates that have been plotted

**classmethod** `from_smiles(smiles_list, target=[], target_type=None, sim_type=None)`

Class method to construct a Plotter object from a list of SMILES.

**Parameters**
• **smile_list** (list) – List of the SMILES representation of the molecules to plot.
• **target** (list) – target values
• **target_type** (string) – target type R (regression) or C (classification)
• **sim_type** (string) – similarity type structural or tailored

Returns A Plotter object for the molecules given as input.

Return type *Plotter*

classmethod **from_inchi**(inchi_list=[], target=[], target_type=None, sim_type=None)

Class method to construct a Plotter object from a list of InChi.

Parameters

• **inchi_list** (dict) – List of the InChi representation of the molecules to plot.
• **target** (dict) – target values
• **target_type** (string) – target type R (regression) or C (classification)
• **sim_type** (string) – similarity type structural or tailored

Returns A Plotter object for the molecules given as input.

Return type *Plotter*

**pca**(**kwargs**)

Calculates the first 2 PCA components of the molecular descriptors.

Parameters **kwargs** (key, value mappings) – Other keyword arguments are passed down to sklearn.decomposition.PCA

Returns The dataframe containing the PCA components.

Return type *Dataframe*

**tsne**(perplexity=None, pca=False, random_state=None, **kwargs**)

Calculates the first 2 t-SNE components of the molecular descriptors.

Parameters

• **perplexity** (int) – perplexity value for the t-SNE model
• **pca** (boolean) – indicates if the features must be preprocessed by PCA
• **random_state** (int) – random seed that can be passed as a parameter for reproducing the same results
• **kwargs** (key, value mappings) – Other keyword arguments are passed down to sklearn.manifold.TSNE

Returns The dataframe containing the t-SNE components.

Return type *Dataframe*

**umap**(n_neighbors=None, min_dist=None, pca=False, random_state=None, **kwargs**)

Calculates the first 2 UMAP components of the molecular descriptors.

Parameters

• **num_neighbors** (int) – Number of neighbours used in the UMAP model.
• **min_dist** (float) – Value between 0.0 and 0.99, indicates how close to each other the points can be displayed.
• `random_state` (int) – random seed that can be passed as a parameter for reproducing the same results
• `kwargs` (key, value mappings) – Other keyword arguments are passed down to umap.UMAP

**Returns** The dataframe containing the UMAP components.

**Return type** Dataframe

`cluster(n_clusters=5, **kwargs)`
Computes the clusters presents in the embedded chemical space.

**Parameters**
• `n_clusters` (int) – Number of clusters that will be computed
• `kwargs` (key, value mappings) – Other keyword arguments are passed down to sklearn.cluster.KMeans

**Returns** The dataframe containing the 2D embedding.

**Return type** Dataframe

`visualize_plot(size=20, kind='scatter', remove_outliers=False, is_colored=True, colorbar=False, clusters=False, filename=None, title=None)`
Generates a plot for the given molecules embedded in two dimensions.

**Parameters**
• `size` (int) – Size of the plot
• `kind` (string) – Type of plot
• `remove_outliers` (boolean) – Boolean value indicating if the outliers must be identified and removed
• `is_colored` (boolean) – Indicates if the points must be colored according to target
• `colorbar` (boolean) – Indicates if the plot legend must be represented as a colorbar. Only considered when the target_type is “R”.
• `clusters` (boolean or list or int) – If True the clusters are shown instead of possible targets. Pass a list or a int to only show selected clusters (indexed by int).
• `filename` (string) – Indicates the file where to save the plot
• `title` (string) – Title of the plot.

**Returns** The matplotlib axes containing the plot.

**Return type** Axes

`interactive_plot(size=700, kind='scatter', remove_outliers=False, is_colored=True, clusters=False, filename=None, show_plot=False, title=None)`
Generates an interactive Bokeh plot for the given molecules embedded in two dimensions.

**Parameters**
• `size` (int) – Size of the plot
• `kind` (string) – Type of plot
• `remove_outliers` (boolean) – Boolean value indicating if the outliers must be identified and removed
• `is_colored` (boolean) – Indicates if the points must be colored according to target
• **clusters** – Indicates if to add a tab with the clusters if these have been computed

• **filename** *(string)* – Indicates the file where to save the Bokeh plot

• **show_plot** *(boolean)* – Immediately display the current plot.

• **title** *(string)* – Title of the plot.

**Returns**  The bokeh figure containing the plot.

**Return type**  Figure

10.2 **Utils**

chemplot.load_data *(name)*

Returns one of the sample datasets.

**Parameters**  name *(string)* – Name of the sample dataset

**Returns**  The Dataframe of the sample dataset

**Return type**  Dataframe

chemplot.info_data()

Prints the metadata relative to the available sample datasets.
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