scikit-chem Documentation

Release 0.0.6

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Contents

scikit-chem provides a high level, *Pythonic* interface to the rdkit library, with wrappers for other popular cheminformatics tools.

For a brief introduction to the ideas behind the package, please read the *introductory notes*. Installation info may be found on the *installation page*. To get started straight away, try the *quick start guide*. For a more in depth understanding, check out the *tutorial* and the *API reference*.

To read the code, submit feature requests, report a bug or contribute to the project, please visit the projects github repository.

CHAPTER 1

An introduction to scikit-chem

scikit-chem is a high level cheminformatics library built on rdkit that aims to integrate with the Scientific Python Stack by promoting interoperativity with libraries such as pandas and scikit-learn, and emulating similar patterns and APIs as found in those libraries.

Some notable features include:

- *Pythonic* core API
- **Consistent, declarative interfaces for many cheminformatics tasks, including:**
  - Reading file formats
  - Chemical standardization
  - Conformer generation
  - Filtering
  - Feature calculation
  - Pipelining
- A simple interface for chemical datasets
- Structure visualization
- Interactivity in Jupyter Notebooks

scikit-chem should be thought of as a simple complement to the excellent rdkit - **scikit-chem** objects are subclasses of rdkit objects, and as such, the two libraries can usually be used together easily when the advanced functionality of rdkit is required.

CHAPTER 2

What's New

New features, improvements and bug-fixes by release.

2.1 v0.0.7 (ongoing)

This is a minor release in the unstable 0.0.x series, with breaking API changes.

2.1.1 API changes

2.1.2 New features

0187d92: Improvements to the rdkit abstraction views (`Mol.atoms`, `Mol.bonds`, `{Mol,Atom,Bond}.props`).

2.1.3 Changes

2.1.4 Bug fixes

2.2 v0.0.6 (August 2016)

This is a minor release in the unstable 0.0.x series, with breaking API changes.

Highlights include a refactor of base classes to provide a more consistent and extensible API, the construction of this documentation and incremental improvements to the continuous integration.

2.2.1 API changes

Objects no longer take pandas dataframes as input directly, but instead require molecules to be passed as a Series, with their data as a supplemental series or dataframe (this may be reverted in a patch).

2.2.2 New features

Base classes were established for `Transformer`, `Filter`, `TransformFilter`. Verbosity options were added, allowing progress bars for most objects. Dataset support was added.

2.2.3 Changes

2.2.4 Bug fixes

CHAPTER 3

Quickstart

We will be working on a mutagenicity dataset, released by Kazius et al.. 4337 compounds, provided as the file `mols.sdf`, were subjected to the AMES test. The results are given in `labels.csv`. We will clean the molecules, perform a brief chemical space analysis before finally assessing potential predictive models built on the data.

3.1 Imports

scikit-chem imports all subpackages with the main package, so all we need to do is import the main package, `skchem`. We will also need `pandas`.

```
In [3]: import skchem
        import pandas as pd
```

3.2 Loading the data

We can use `skchem.read_sdf` to import the sdf file:

```
In [4]: ms_raw = skchem.read_sdf('mols.sdf'); ms_raw
```

```
Out[4]: batch
        1728-95-6     <Mol: COc1ccc(-c2nc(-c3ccccc3)c(-c3ccccc3)[nH]...
        91-08-7                              <Mol: Cc1c(N=C=O)cccc1N=C=O>
        89786-04-9      <Mol: CC1(Cn2ccnn2)C(C(=O)O)N2C(=O)CC2S1(=O)=O>
        2439-35-2                                 <Mol: C=CC(=O)OCCN(C)C>
        95-94-3                                <Mol: Clc1cc(Cl)c(Cl)cc1Cl>
                                               ...
        89930-60-9    <Mol: CCCn1cc2c3c(cccc31)C1C=C(C)CN(C)C1C2.O=C...
        9002-92-0             <Mol: CCCCCCCCCCCCCOCCOCCOCCOCCOCCOCCOCCO>
        90597-22-1               <Mol: Nc1ccn(C2C=C(CO)C(O)C2O)c(=O)n1>
        924-43-6                                        <Mol: CCC(C)ON=O>
        97534-21-9              <Mol: O=C1NC(=S)NC(=O)C1C(=O)Nc1ccccc1>
        Name: structure, dtype: object
```

And pandas to import the labels.

```
In [5]: y_raw = pd.read_csv('labels.csv').set_index('name').squeeze(); y_raw
```

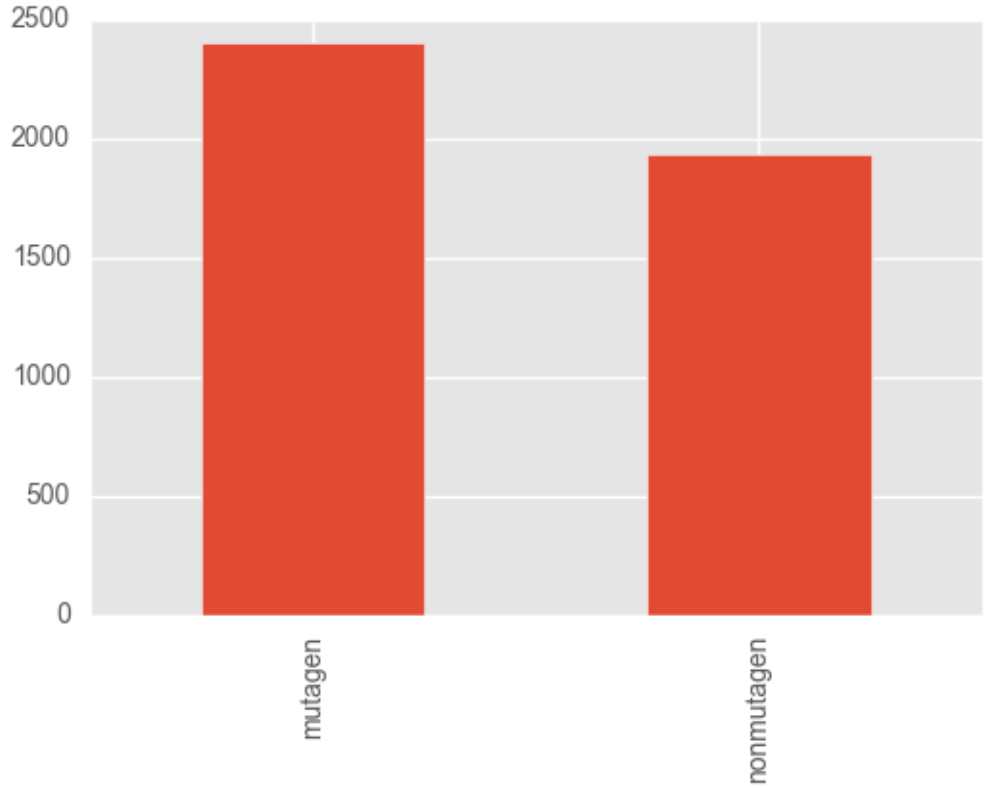
```
Out[5]: name
        1728-95-6        mutagen
        91-08-7          mutagen
```

```
89786-04-9    nonmutagen
2439-35-2     nonmutagen
95-94-3       nonmutagen
                  ...
89930-60-9       mutagen
9002-92-0     nonmutagen
90597-22-1    nonmutagen
924-43-6         mutagen
97534-21-9    nonmutagen
Name: Ames test categorisation, dtype: object
```

Quickly check the class balance:

```
In [9]: y_raw.value_counts().plot.bar()
```

```
Out[9]: <matplotlib.axes._subplots.AxesSubplot at 0x121204278>
```



And binarize them:

```
In [8]: y_bin = (y_raw == 'mutagen').astype(np.uint8); y_bin
```

```
Out[8]: name
        1728-95-6     1
        91-08-7       1
        89786-04-9    0
        2439-35-2     0
        95-94-3       0
                     ..
        89930-60-9    1
        9002-92-0     0
        90597-22-1    0
```

```
924-43-6      1
97534-21-9    0
Name: Ames test categorisation, dtype: uint8
```

The classes are (mercifully) quite balanced.

3.3 Cleaning

The data is unlikely to be canonicalized, and potentially contain broken or difficult molecules, so we will now clean it.

3.3.1 Standardization

The first step is to apply a `Transformer` to canonicalize the representations. Specifically, we will use the ChemAxon Standardizer wrapper. Some compounds are likely to fail this procedure, however they are likely to still be valid structures, so we will use the `keep_failed` configuration option on the object to keep these, rather than returning a None, or raising an error.

Tip: `Transformer` s implement the `transform` method, which converts `Mol` s into *something else*. This can either be another `Mol`, such as in this case, or into a vector or even a number. The result will be packaged as a `pandas` data structure of appropriate dimensionality.

```
In [8]: std = skchem.standardizers.ChemAxonStandardizer(keep_failed=True)

In [9]: ms = std.transform(ms_raw); ms

ChemAxonStandardizer: 100% (4337 of 4337) |####################################| Elapsed Ti

Out[9]: batch
        1728-95-6     <Mol: COc1ccc(-c2nc(-c3ccccc3)c(-c3ccccc3)[nH]...
        91-08-7                              <Mol: Cc1c(N=C=O)cccc1N=C=O>
        89786-04-9      <Mol: CC1(Cn2ccnn2)C(C(=O)O)N2C(=O)CC2S1(=O)=O>
        2439-35-2                                 <Mol: C=CC(=O)OCCN(C)C>
        95-94-3                                <Mol: Clc1cc(Cl)c(Cl)cc1Cl>
                                               ...
        89930-60-9          <Mol: CCCn1cc2c3c(cccc31)C1C=C(C)CN(C)C1C2>
        9002-92-0             <Mol: CCCCCCCCCCCCCOCCOCCOCCOCCOCCOCCOCCO>
        90597-22-1               <Mol: Nc1ccn(C2C=C(CO)C(O)C2O)c(=O)n1>
        924-43-6                                        <Mol: CCC(C)ON=O>
        97534-21-9             <Mol: O=C(Nc1ccccc1)c1c(O)nc(=S)[nH]c1O>
        Name: structure, dtype: object
```

Tip: This pattern is the typical way to handle all operations while using **scikit-chem**. The available configuration options for all classes may be found in the class's docstring, available in the *documentation* or using the builtin `help` function.

3.3.2 Filter undesirable molecules

Next, we will remove molecules that are likely to not work well with the circular descriptors that we will use. These are usually *large* or *inorganic* molecules.

To do this, we will use some `Filters`, which implement the `filter` method.

Tip: `Filter` s drop compounds that fail a predicicate. The results of the predicate can be found by using `transform` - that's right, each `Filter` is also a `Transformer` ! Labels with similar index can be passed in as a second argument, and will also be filtered and returned as a second return value.

```
In [10]: of = skchem.filters.OrganicFilter()

         ms, y = of.filter(ms, y)

OrganicFilter: 100% (4337 of 4337) |##########################################| Elapsed Ti

In [11]: mf = skchem.filters.MassFilter(above=100, below=900)

         ms, y = mf.filter(ms, y)

MassFilter: 100% (4337 of 4337) |##############################################| Elapsed Ti

In [12]: nf = skchem.filters.AtomNumberFilter(above=5, below=100, include_hydrogens=True)

         ms, y = nf.filter(ms, y)

AtomNumberFilter: 100% (4068 of 4068) |########################################| Elapsed Ti
```

3.3.3 Optimize Geometry

We would like to calculate some features that require three dimensional coordinates, so we will next calculate three dimensional conformers using the Universal Force Field. Additionally, some compounds may be unfeasible - these should be dropped from the dataset. In order to do this, we will use the `transform_filter` method:

```
In [13]: uff = skchem.forcefields.UFF()

         ms, y = uff.transform_filter(ms, y)

/Users/rich/projects/scikit-chem/skchem/forcefields/base.py:54: UserWarning: Failed to Embe
  warnings.warn(msg)
/Users/rich/projects/scikit-chem/skchem/forcefields/base.py:54: UserWarning: Failed to Embe
  warnings.warn(msg)
/Users/rich/projects/scikit-chem/skchem/forcefields/base.py:54: UserWarning: Failed to Embe
  warnings.warn(msg)
UFF: 100% (4046 of 4046) |#####################################################| Elapsed Ti

In [14]: len(ms)

Out[14]: 4043
```

As we can see, we get a warning that 3 molecules failed to embed, have been dropped. If we didn't care about the warnings, we could have set the `warn_on_fail` property to `False` (or set it using a keyword argument at initialization). Conversely, if we *really* cared about failures, we could have set `error_on_fail` to True, which would raise an Error if any `Mol`s failed to embed.

Tip: `TransformFilter` s implement the `transform_filter` method. This is a combination of `transform` and `filter` , which converts `Mol` s into *something else* **and** drops instances that fail the predicate. The `ChemAxonStandardizer` object is also a `TransformFilter`, as it can drop `Mol` s that fail to standardize.

3.3.4 Visualize Chemical Space

scikit-chem adds a custom `mol` accessor to `pandas.Series`, which provides a shorthand for calling methods on all `Mol`s in the collection. This is analogous to the `str` accessor:

```
In [15]: y_raw.str.get_dummies()
```

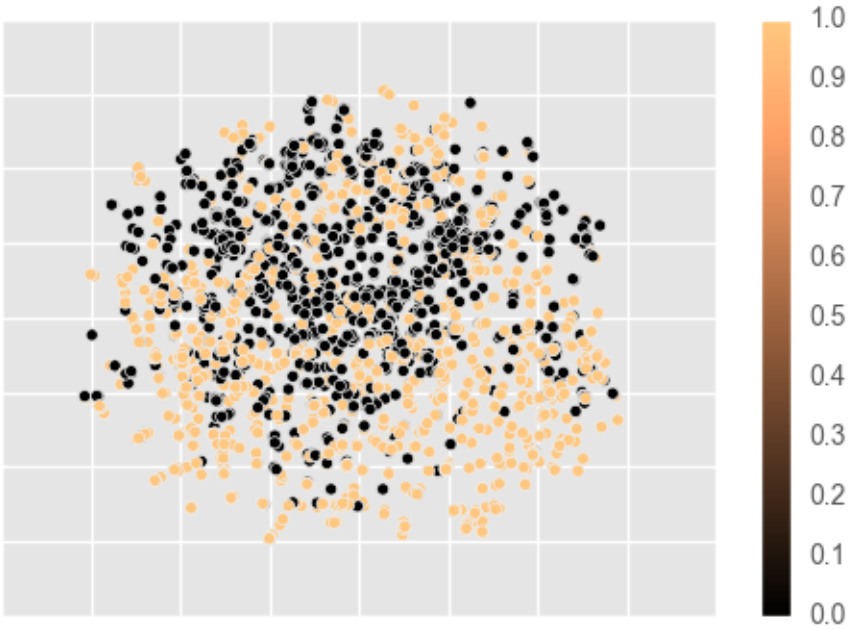
```
Out[15]: mutagen  nonmutagen
         name
         1728-95-6         1           0
         91-08-7           1           0
         89786-04-9        0           1
         2439-35-2         0           1
         95-94-3           0           1
         ...             ...         ...
         89930-60-9        1           0
         9002-92-0         0           1
         90597-22-1        0           1
         924-43-6          1           0
         97534-21-9        0           1

         [4043 rows x 2 columns]
```

We will use this function to binarize the labels:

```
In [16]: y = y.str.get_dummies()['mutagen']
```

Amongst other options, it is provides access to chemical space plotting functionality. This will featurize the molecules using a passed featurizer (or a string shortcut), and a dimensionality reduction technique to reduce the feature space to two dimensions, which are then plotted. In this example, we use circular Morgan fingerprints, reduced by t-SNE to visualize structural diversity in the dataset.

```
In [17]: ms.mol.visualize(fper='morgan',
                          dim_red='tsne', dim_red_kw={'method': 'exact'},
                          c=y,
                          cmap='copper')
```



The data appears to be reasonably separable in structural space, so we may suspect that Morgan fingerprints will be a good representation for modelling the data.

3.4 Featurizing the data

As previously noted, Morgan fingerprints would be a good fit for this data. To calculate them, we will use the `MorganFeaturizer` class, which is a `Transformer`.

```
In [18]: mf = skchem.descriptors.MorganFeaturizer()

         X, y = mf.transform(ms, y); X

MorganFeaturizer: 100% (4043 of 4043) |########################################| Elapsed Ti
```

Out[18]:

morgan_fp_idx	0	1	2	3	4	...	2043	2044	2045	2046	\
batch						...					
1728-95-6	0	0	0	0	0	...	0	0	0	0	
91-08-7	0	0	0	0	0	...	0	0	0	0	
89786-04-9	0	0	0	0	0	...	0	0	0	0	
2439-35-2	0	0	0	0	0	...	0	0	0	0	
95-94-3	0	0	0	0	0	...	0	0	0	0	
...	...	...	...	...	...	...	...	...	...	...	
89930-60-9	0	0	0	0	0	...	0	0	0	0	
9002-92-0	0	0	0	0	0	...	1	0	1	0	
90597-22-1	0	0	0	0	0	...	0	0	0	0	
924-43-6	0	0	0	0	0	...	0	0	0	0	
97534-21-9	0	0	0	0	0	...	0	0	0	0	

morgan_fp_idx	2047
batch	
1728-95-6	0
91-08-7	0

```
89786-04-9       0
2439-35-2        0
95-94-3          0
...            ...
89930-60-9       0
9002-92-0        0
90597-22-1       0
924-43-6         0
97534-21-9       0

[4043 rows x 2048 columns]
```

3.5 Pipelining

If this process appeared unnecessarily laborious (as it should!), **scikit-chem** provides a `Pipeline` class that will sequentially apply objects passed to it. For this example, we could have simply performed:

```
In [35]: pipeline = skchem.pipeline.Pipeline([
                 skchem.standardizers.ChemAxonStandardizer(keep_failed=True),
                 skchem.forcefields.UFF(),
                 skchem.filters.OrganicFilter(),
                 skchem.filters.MassFilter(above=100, below=1000),
                 skchem.filters.AtomNumberFilter(above=5, below=100),
                 skchem.descriptors.MorganFeaturizer()
         ])

         X, y = pipeline.transform_filter(ms_raw, y_raw)
```

```
ChemAxonStandardizer: 100% (4337 of 4337) |####################################| Elapsed Ti
/Users/rich/projects/scikit-chem/skchem/forcefields/base.py:54: UserWarning: Failed to Embe
  warnings.warn(msg)
/Users/rich/projects/scikit-chem/skchem/forcefields/base.py:54: UserWarning: Failed to Embe
  warnings.warn(msg)
/Users/rich/projects/scikit-chem/skchem/forcefields/base.py:54: UserWarning: Failed to Embe
  warnings.warn(msg)
/Users/rich/projects/scikit-chem/skchem/forcefields/base.py:54: UserWarning: Failed to Embe
  warnings.warn(msg)
/Users/rich/projects/scikit-chem/skchem/forcefields/base.py:54: UserWarning: Failed to Embe
  warnings.warn(msg)
/Users/rich/projects/scikit-chem/skchem/forcefields/base.py:54: UserWarning: Failed to Embe
  warnings.warn(msg)
/Users/rich/projects/scikit-chem/skchem/forcefields/base.py:54: UserWarning: Failed to Embe
  warnings.warn(msg)
UFF: 100% (4337 of 4337) |#####################################################| Elapsed Ti
OrganicFilter: 100% (4330 of 4330) |###########################################| Elapsed Ti
MassFilter: 100% (4330 of 4330) |##############################################| Elapsed Ti
AtomNumberFilter: 100% (4070 of 4070) |########################################| Elapsed Ti
MorganFeaturizer: 100% (4047 of 4047) |########################################| Elapsed Ti
```

3.6 Modelling the data

In this section, we will try building some basic scikit-learn models on the data.

3.6.1 Partitioning the data

To decide on the best model to use, we should perform some model selection. This will require comparing the relative performance of a selection of candidate molecules each trained on the same **train** set, and evaluated on a **validation** set.

In *cheminformatics*, partitioning datasets usually requires some thought, as chemical datasets usually vastly overrepresent certain *scaffolds*, and underrepresent others. In order to get as unbiased an estimate of performance as possible, one can either downsample compounds in a region of high density, or artifically favor splits that pool in the same split molecules that are too close in chemical space.

scikit-chem provides this functionality in the `SimThresholdSplit` class, which applies single link heirachical clustering to produce a large number of clusters consisting of highly similar compounds. These clusters are then randomly assigned to the desired splits, such that no split contains compounds that are more similar to compounds in any other split than the clustering threshold.

```
In [37]: cv = skchem.cross_validation.SimThresholdSplit(fper=None, n_jobs=4).fit(X)
         train, valid, test = cv.split((60, 20, 20))
         X_train, X_valid, X_test = X[train], X[valid], X[test]
         y_train, y_valid, y_test = y[train], y[valid], y[test]
```

3.6.2 Model selection

```
In [21]: import sklearn.ensemble
         import sklearn.linear_model
         import sklearn.naive_bayes
```

```
In [38]: rf = sklearn.ensemble.RandomForestClassifier(n_estimators=100)
         nb = sklearn.naive_bayes.BernoulliNB()
         lr = sklearn.linear_model.LogisticRegression()
```

```
In [39]: X_train.shape, y_train.shape
```

```
Out[39]: ((2428, 2048), (2428,))
```

```
In [42]: rf_score = rf.fit(X_train, y_train).score(X_valid, y_valid)
         nb_score = nb.fit(X_train, y_train).score(X_valid, y_valid)
         lr_score = lr.fit(X_train, y_train).score(X_valid, y_valid)

         print(rf_score, nb_score, lr_score)
```

```
0.843016069221 0.812113720643 0.796044499382
```

Random Forests appear to work best (although we should have chosen hyperparameters using Random or Grid search).

3.6.3 Assessing the Final performance

```
In [43]: rf.fit(X_train.append(X_valid), y_train.append(y_valid)).score(X_test, y_test)
```

```
Out[43]: 0.83580246913580247
```

CHAPTER 4

Installation and Getting Started

`scikit-chem` is easy to install and configure. Detailed instructions are listed below. The quickest way to get everything installed is by *using conda*.

4.1 Installation

`scikit-chem` is tested on Python 2.7 and 3.5. It depends on rdkit, most of the core Scientific Python Stack, as well as several smaller pure *Python* libraries.

4.1.1 Dependencies

The full list of dependencies is:

- rdkit
- numpy
- scipy
- matplotlib
- scikit-learn
- pandas
- h5py
- fuel
- ipywidgets
- progressbar2

The package and these dependencies are available through two different *Python* package managers, conda and pip. It is recommended to use conda.

4.1.2 Using conda

conda is a cross-platform, Python-agnostic package and environment manager developed by Continuum Analytics. It provides packages as prebuilt binary files, allowing for straightforward installation of Python packages, even those with complex C/C++ extensions. It is installed as part of the Anaconda Scientific Python distribution, or as the lightweight miniconda.

The package and all dependencies for `scikit-chem` are available through the defaults or richlewis conda channel. To install:

```
conda install -c richlewis scikit-chem
```

This will install `scikit-chem` with all its dependencies from the author's anaconda repository as `conda` packages.

Attention: For Windows, you will need to install a dependency, fuel, separately. This will be made available via conda in the future.

4.1.3 Using pip

pip is the standard Python package manager. The package is available via PyPI, although the dependencies may require compilation or at worst may not work at all.

```
pip install scikit-chem
```

This will install `scikit-chem` with all available dependencies as regular `pip` controlled packages.

Attention: A key dependency, rdkit, is not installable using pip, and will need to be installed by other means, such as conda, apt-get on Linux or Homebrew on Mac, or compiled from source (not recommended!!).

4.2 Configuration

4.2.1 scikit-chem

Currently, scikit-chem cannot be configured in a config file. This feature is planned to be added in future releases. To request this feature as a priority, please mention it in the appropriate github issue

4.2.2 Fuel

To use the *data* functionality, you will need to set up fuel. This involves configuring the .fuelrc. An example .fuelrc might be as follows:

```
data_path: ~/datasets
extra_downloaders:
- skchem.data.downloaders
extra_converters:
- skchem.data.converters
```

This adds the location for fuel datasets, and adds the `scikit-chem` data downloaders and converters to the fuel command line tools.

CHAPTER 5

Tutorial

This tutorial is written as a series of Jupyter Notebooks. These may be downloaded from documentation section of the GitHub page..

5.1 The Package

To start using **scikit-chem**, the package to import is `skchem`:

```
In [1]: import skchem
```

The different functionalities are arranged in subpackages:

```
In [2]: skchem.__all__
```

```
Out[2]: ['core',
         'filters',
         'data',
         'descriptors',
         'io',
         'vis',
         'cross_validation',
         'standardizers',
         'interact',
         'pipeline']
```

These are all imported as soon as the base package is imported, so everything is ready to use right away:

```
In [3]: skchem.core.Mol()
```

```
Out[3]: <Mol name="None" formula="" at 0x11d01d538>
```

5.2 Molecules in scikit-chem

scikit-chem is first and formost a wrapper around **rdkit** to make it more *Pythonic*, and more intuitive to a user familiar with other libraries in the Scientific Python Stack. The package implements a core `Mol` class, physically representing a molecule. It is a direct subclass of the `rdkit.Mol` class:

```
In [1]: import rdkit.Chem
        issubclass(skchem.Mol, rdkit.Chem.Mol)
```

```
Out[1]: True
```

As such, it has all the methods available that an `rdkit.Mol` class has, for example:

```
In [2]: hasattr(skchem.Mol, 'GetAromaticAtoms')
```

```
Out[2]: True
```

5.2.1 Initializing new molecules

Constructors are provided as classmethods on the `skchem.Mol` object, in the same fashion as **pandas** objects are constructed. For example, to make a `pandas.DataFrame` from a dictionary, you call:

```
In [3]: df = pd.DataFrame.from_dict({'a': [10, 20], 'b': [20, 40]}); df
```

```
Out[3]: a   b
        0  10  20
        1  20  40
```

Analogously, to make a `skchem.Mol` from a smiles string, you call;

```
In [4]: mol = skchem.Mol.from_smiles('CC(=O)Cl'); mol
```

```
Out[4]: <Mol name="None" formula="C2H3ClO" at 0x11dc8f490>
```

The available methods are:

```
In [5]: [method for method in skchem.Mol.__dict__ if method.startswith('from_')]
```

```
Out[5]: ['from_tplblock',
         'from_molblock',
         'from_molfile',
         'from_binary',
         'from_tplfile',
         'from_mol2block',
         'from_pdbfile',
         'from_pdbblock',
         'from_smiles',
         'from_smarts',
         'from_mol2file',
         'from_inchi']
```

When a molecule fails to parse, a `ValueError` is raised:

```
In [6]: skchem.Mol.from_smiles('NOTSMILES')
```

```
---------------------------------------------------------------------------
ValueError                                Traceback (most recent call last)
<ipython-input-6-99e03ef822e7> in <module>()
----> 1 skchem.Mol.from_smiles('NOTSMILES')

/Users/rich/projects/scikit-chem/skchem/core/mol.py in constructor(_, in_arg, name, *args,
    419             m = getattr(rdkit.Chem, 'MolFrom' + constructor_name)(in_arg, *args, **kwa
    420             if m is None:
--> 421                 raise ValueError('Failed to parse molecule, '.format(in_arg))
    422             m = Mol.from_super(m)
    423             m.name = name

ValueError: Failed to parse molecule, NOTSMILES
```

5.2.2 Molecule accessors

Atoms and **bonds** are accessible as a property:

```
In [7]: mol.atoms
```

```
Out[7]: <AtomView values="['C', 'C', 'O', 'Cl']" at 0x11dc9ac88>
```

```
In [8]: mol.bonds
```

```
Out[8]: <BondView values="['C-C', 'C=O', 'C-Cl']" at 0x11dc9abe0>
```

These are iterable:

```
In [9]: [a for a in mol.atoms]
```

```
Out[9]: [<Atom element="C" at 0x11dcfe8a0>,
         <Atom element="C" at 0x11dcfe9e0>,
         <Atom element="O" at 0x11dcfed00>,
         <Atom element="Cl" at 0x11dcfedf0>]
```

subscriptable:

```
In [10]: mol.atoms[3]
```

```
Out[10]: <Atom element="Cl" at 0x11dcfef30>
```

sliceable:

```
In [11]: mol.atoms[:3]
```

```
Out[11]: [<Atom element="C" at 0x11dcfebc0>,
          <Atom element="C" at 0x11de690d0>,
          <Atom element="O" at 0x11de693f0>]
```

indexable:

```
In [19]: mol.atoms[[1, 3]]
```

```
Out[19]: [<Atom element="C" at 0x11de74760>, <Atom element="Cl" at 0x11de7fe40>]
```

and maskable:

```
In [18]: mol.atoms[[True, False, True, False]]
```

```
Out[18]: [<Atom element="C" at 0x11de74ad0>, <Atom element="O" at 0x11de74f30>]
```

Properties on the rdkit objects are accessible through the `props` property:

```
In [11]: mol.props['is_reactive'] = 'very!'
```

```
In [12]: mol.atoms[1].props['kind'] = 'electrophilic'
         mol.atoms[3].props['leaving group'] = 1
         mol.bonds[2].props['bond strength'] = 'strong'
```

These are using the `rdkit` property functionality internally:

```
In [13]: mol.GetProp('is_reactive')
```

```
Out[13]: 'very!'
```

Note: RDKit properties can only store `str` s, `int` s and `float` s. Any other type will be coerced to a string before storage.

The properties of atoms and bonds are accessible molecule wide:

```
In [14]: mol.atoms.props
```

```
Out[14]: <MolPropertyView values="{'leaving group': [nan, nan, nan, 1.0], 'kind': [None, 'e
```

```
In [15]: mol.bonds.props
```

```
Out[15]: <MolPropertyView values="{'bond strength': [None, None, 'strong']}" at 0x11daf80f0
```

These can be exported as pandas objects:

```
In [16]: mol.atoms.props.to_frame()
```

```
Out[16]: kind  leaving group
         atom_idx
         0                  None            NaN
         1         electrophilic            NaN
         2                  None            NaN
         3                  None            1.0
```

5.2.3 Export and Serialization

Molecules are exported and/or serialized in a very similar way in which they are constructed, again with an inspiration from `pandas`.

```
In [17]: df.to_csv()
```

```
Out[17]: ',a,b\n0,10,20\n1,20,40\n'
```

```
In [18]: mol.to_inchi_key()
```

```
Out[18]: 'WETWJCDKMRHUPV-UHFFFAOYSA-N'
```

The total available formats are:

```
In [19]: [method for method in skchem.Mol.__dict__ if method.startswith('to_')]
```

```
Out[19]: ['to_inchi',
          'to_json',
          'to_smiles',
          'to_smarts',
          'to_inchi_key',
          'to_binary',
          'to_dict',
          'to_molblock',
          'to_tplfile',
          'to_formula',
          'to_molfile',
          'to_pdbblock',
          'to_tplblock']
```

5.3 Input/Output

Pandas objects are the main data structures used for collections of molecules. **scikit-chem** provides convenience functions to load objects into `pandas.DataFrames` from common file formats in cheminformatics.

5.3.1 Reading files

The **scikit-chem** functionality is modelled after the `pandas` API. To load an csv file using `pandas` you would call:

```
In [1]: df = pd.read_csv('https://archive.org/download/scikit-chem_example_files/iris.csv',
                         header=None); df
```

```
Out[1]: 0    1    2    3            4
        0  5.1  3.5  1.4  0.2  Iris-setosa
        1  4.9  3.0  1.4  0.2  Iris-setosa
        2  4.7  3.2  1.3  0.2  Iris-setosa
        3  4.6  3.1  1.5  0.2  Iris-setosa
        4  5.0  3.6  1.4  0.2  Iris-setosa
```

Analogously with **scikit-chem**:

```
In [2]: smi = skchem.read_smiles('https://archive.org/download/scikit-chem_example_files/ex
```

Currently available:

```
In [3]: [method for method in skchem.io.__dict__ if method.startswith('read_')]
```

```
Out[3]: ['read_sdf', 'read_smiles']
```

scikit-chem also adds convenience methods onto `pandas.DataFrame` objects.

```
In [4]: pd.DataFrame.from_smiles('https://archive.org/download/scikit-chem_example_files/ex
```

```
Out[4]: structure                1
        0                 <Mol: CC>          ethane
        1                <Mol: CCC>         propane
        2          <Mol: c1ccccc1>         benzene
        3  <Mol: CC(=O)[O-].[Na+]>  sodium acetate
        4      <Mol: NC(CO)C(=O)O>          serine
```

Note: Currently, only `read_smiles` can read files over a network connection. This functionality is planned to be added in future for all file types.

5.3.2 Writing files

Again, this is analogous to `pandas`:

```
In [5]: from io import StringIO
        sio = StringIO()
        df.to_csv(sio)
        sio.seek(0)
        print(sio.read())
```

```
,0,1,2,3,4
0,5.1,3.5,1.4,0.2,Iris-setosa
1,4.9,3.0,1.4,0.2,Iris-setosa
2,4.7,3.2,1.3,0.2,Iris-setosa
3,4.6,3.1,1.5,0.2,Iris-setosa
4,5.0,3.6,1.4,0.2,Iris-setosa
```

```
In [6]: sio = StringIO()
        smi.iloc[:2].to_sdf(sio) # don't write too many!
```

```
        sio.seek(0)
        print(sio.read())
```

```
0
     RDKit

  2  1  0  0  0  0  0  0  0  0999 V2000
    0.0000    0.0000    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.0000    0.0000    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  1  2  1  0
M  END
>  <1>  (1)
ethane

$$$$
1
     RDKit

  3  2  0  0  0  0  0  0  0  0999 V2000
    0.0000    0.0000    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.0000    0.0000    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.0000    0.0000    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  1  2  1  0
  2  3  1  0
M  END
>  <1>  (2)
propane

$$$$
```

5.4 Transforming

Operations on compounds are implemented as `Transformers` in **scikit-chem**, which are analoguous to `Transformer` objects in **scikit-learn**. These objects define a 1:1 mapping between input and output objects in a collection (i.e. the length of the collection remains the same during a transform). These mappings can be very varied, but the three main types currently implemented in `scikit-chem` are `Standardizers`, `Forcefields` and `Featurizers`.

5.4.1 Standardizers

Chemical data curation is a difficult concept, and data may be formatted differently depending on the source, or even the habits of the curator.

For example, **solvents** or **salts** might be included the representation, which might be considered an unnecessary detail to a modeller, or even irrelevant to an experimentalist, if the compound is solvated is a standard solvent during the protocol.

Even the structure of molecules that would be considered the 'same', can often be drawn very differently. For example, tautomers are arguably the same molecule in different conditions, and mesomers might be considered different aspects of the same molecule.

Often, it is sensible to canonicalize these compounds in a process called **Standardization**.

In `scikit-chem`, the *standardizers* package provides this functionality. `Standardizer` objects transform `Mol` objects into other `Mol` objects, which have their representation canonicalized (or into `None` if the protocol fails). The details of the canonicalization may be configured at object initialization, or by altering properties.

Tip: Currently, the only available *Standardizer* is a wrapper of the ChemAxon Standardizer. This requires the ChemAxon JChem software suite to be installed and licensed (free academic licenses are available from the website). We hope to implement an open source *Standardizer* in future.

As an example, we will standardize the sodium acetate:

```
In [3]: mol = skchem.Mol.from_smiles('CC(=O)[O-].[Na+]', name='sodium acetate'); mol.to_smi

Out[3]: 'CC(=O)[O-].[Na+]'
```

A `Standardizer` object is initialized:

```
In [43]: std = skchem.standardizers.ChemAxonStandardizer()
```

Calling transform on sodium acetate yields the conjugate 'canonical' acid, acetic acid.

```
In [44]: mol_std = std.transform(mol); mol_std.to_smiles()

Out[44]: 'CC(=O)O'
```

The standardization of a collection of `Mol`s can be achieved by calling `transform` on a `pandas.Series`:

```
In [45]: mols = skchem.read_smiles('https://archive.org/download/scikit-chem_example_files/
                                   name_column=1); mols

Out[45]: name
         ethane                          <Mol: CC>
         propane                        <Mol: CCC>
         benzene                     <Mol: c1ccccc1>
         sodium acetate     <Mol: CC(=O)[O-].[Na+]>
         serine                 <Mol: NC(CO)C(=O)O>
         Name: structure, dtype: object

In [46]: std.transform(mols)

ChemAxonStandardizer: 100% (5 of 5) |##########################################| Elapsed Ti

Out[46]: name
         ethane                       <Mol: CC>
         propane                     <Mol: CCC>
         benzene                  <Mol: c1ccccc1>
         sodium acetate            <Mol: CC(=O)O>
         serine               <Mol: NC(CO)C(=O)O>
         Name: structure, dtype: object
```

A loading bar is provided by default, although this can be disabled by lowering the verbosity:

```
In [47]: std.verbose = 0
         std.transform(mols)

Out[47]: name
         ethane                       <Mol: CC>
         propane                     <Mol: CCC>
         benzene                  <Mol: c1ccccc1>
         sodium acetate            <Mol: CC(=O)O>
         serine               <Mol: NC(CO)C(=O)O>
         Name: structure, dtype: object
```

5.4.2 Forcefields

Often the three dimensional structure of a compound is of relevance, but many chemical formats, such as SMILES do not encode this information (and often even in formats which serialize geometry only coordinates in two dimensions are provided).

To produce a reasonable three dimensional **conformer**, a compound must be roughly embedded in three dimensions according to local geometrical constraints, and forcefields used to optimize the geometry of a compound.

In `scikit-chem`, the *forcefields* package provides access to this functionality. Two forcefields, the Universal Force Field (UFF) and the Merck Molecular Force Field (MMFF) are currently provided. We will use the UFF:

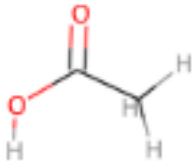
```
In [23]: uff = skchem.forcefields.UFF()
         mol = uff.transform(mol_std)

In [25]: mol.atoms

Out[25]: <AtomView values="['C', 'C', 'O', 'O', 'H', 'H', 'H', 'H']" at 0x12102b6a0>
```

This uses the forcefield to generate a reasonable three dimensional structure. In `rdkit` (and thus `scikit-chem`, conformers are separate entities). The forcefield creates a new conformer on the object:

```
In [27]: mol.conformers[0].atom_positions

Out[27]: [<Point3D coords="(1.22, -0.48, 0.10)" at 0x1214de3d8>,
          <Point3D coords="(0.00, 0.10, -0.54)" at 0x1214de098>,
          <Point3D coords="(0.06, 1.22, -1.11)" at 0x1214de168>,
          <Point3D coords="(-1.20, -0.60, -0.53)" at 0x1214de100>,
          <Point3D coords="(1.02, -0.64, 1.18)" at 0x1214de238>,
          <Point3D coords="(1.47, -1.45, -0.37)" at 0x1214de1d0>,
          <Point3D coords="(2.08, 0.21, -0.00)" at 0x1214de2a0>,
          <Point3D coords="(-1.27, -1.51, -0.08)" at 0x1214de308>]
```

The molecule can be visualized by drawing it:

```
In [35]: skchem.vis.draw(mol)

Out[35]: <matplotlib.image.AxesImage at 0x1236c6978>
```



5.4.3 Featurizers (fingerprint and descriptor generators)

Chemical representation is not by itself very amenable to data analysis and mining techniques. Often, a fixed length vector representation is required. This is achieved by calculating **features** from the chemical representation.

In **scikit-chem**, this is provided by the `descriptors` package. A selection of features are available:

```
In [11]: skchem.descriptors.__all__
```

```
Out[11]: ['PhysicochemicalFeaturizer',
          'AtomFeaturizer',
          'AtomPairFeaturizer',
          'MorganFeaturizer',
          'MACCSFeaturizer',
          'TopologicalTorsionFeaturizer',
          'RDKFeaturizer',
          'ErGFeaturizer',
          'ConnectivityInvariantsFeaturizer',
          'FeatureInvariantsFeaturizer',
          'ChemAxonNMRPredictor',
          'ChemAxonFeaturizer',
          'ChemAxonAtomFeaturizer',
          'GraphDistanceTransformer',
          'SpacialDistanceTransformer']
```

Circular fingerprints (of which Morgan fingerprints are an example) are often considered the most consistently well performing descriptor across a wide variety of compounds.

```
In [12]: mf = skchem.descriptors.MorganFeaturizer()
         mf.transform(mol)
```

```
Out[12]: morgan_fp_idx
         0            0
```

```
1       0
2       0
3       0
4       0
       ..
2043    0
2044    0
2045    0
2046    0
2047    0
Name: MorganFeaturizer, dtype: uint8
```

We can also call the standardizer on a series of `Mol`s:

```
In [13]: mf.transform(mols.structure)
```

```
MorganFeaturizer: 100% (5 of 5) |############################################| Elapsed Ti
```

```
Out[13]: morgan_fp_idx  0     1     2     3     4     ...   2043  2044  2045  2046  \
         0                 0     0     0     0     0  ...      0     0     0     0
         1                 0     0     0     0     0  ...      0     0     0     0
         2                 0     0     0     0     0  ...      0     0     0     0
         3                 0     0     0     0     0  ...      0     0     0     0
         4                 0     1     0     0     0  ...      0     0     0     0

         morgan_fp_idx  2047
         0                 0
         1                 0
         2                 0
         3                 0
         4                 0

         [5 rows x 2048 columns]
```

Note: Note that Morgan fingerprints are **1D**, and thus when we use a single `Mol` as input, we get the features in a **1D** `pandas.Series` . When we use a collection of `Mol` s, the features are returned in a `pandas.DataFrame` , which is one higher dimension than a `pandas.Series`, as a collection of `Mol` s are a dimension higher than a `Mol` by itself.

Some descriptors, such as the `AtomFeaturizer` , will yield **2D** features when used on a `Mol`, and thus will yield the **3D** `pandas.Panel` when used on a collection of `Mol` s.

5.5 Filtering

Operations looking to remove compounds from a collection are implemented as `Filters` in **scikit-chem**. These are implemented in the `skchem.filters` packages:

```
In [19]: skchem.filters.__all__
```

```
Out[19]: ['ChiralFilter',
          'SMARTSFilter',
          'PAINSFilter',
          'ElementFilter',
          'OrganicFilter',
```

```
          'AtomNumberFilter',
          'MassFilter',
          'Filter']
```

They are used very much like `Transformers`:

```
In [20]: of = skchem.filters.OrganicFilter()
```

```
In [21]: benzene = skchem.Mol.from_smiles('c1ccccc1', name='benzene')
         ferrocene = skchem.Mol.from_smiles('[cH-]1cccc1.[cH-]1cccc1.[Fe+2]', name='ferroce
         norbornane = skchem.Mol.from_smiles('C12CCC(C2)CC1', name='norbornane')
         dicyclopentadiene = skchem.Mol.from_smiles('C1C=CC2C1C3CC2C=C3')
         ms = [benzene, ferrocene, norbornane, dicyclopentadiene]
```

```
In [22]: of.filter(ms)
```

```
OrganicFilter: 100% (4 of 4) |################################################| Elapsed Ti
```

```
Out[22]: benzene                   <Mol: c1ccccc1>
         norbornane              <Mol: C1CC2CCC1C2>
         3             <Mol: C1=CC2C3C=CC(C3)C2C1>
         Name: structure, dtype: object
```

`Filters` essentially use a *predicate* function to decide whether to keep or remove instances. The result of this function can be returned using `transform`:

```
In [23]: of.transform(ms)
```

```
OrganicFilter: 100% (4 of 4) |################################################| Elapsed Ti
```

```
Out[23]: benzene        True
         ferrocene     False
         norbornane     True
         3              True
         dtype: bool
```

5.5.1 Filters are Transformers

As `Filters` have a transform method, they are themselves `Transformers`, that transform a molecule into the result of the predicate!

```
In [24]: issubclass(skchem.filters.Filter, skchem.base.Transformer)
```

```
Out[24]: True
```

The predicate functions should return `None`, `False` or `np.nan` for negative results, and anything else for positive results

Creating your own Filter

You can create your own filter by passing a predicate function to the `Filter` class. For example, perhaps you only wanted compounds to keep compounds that had a name:

```
In [25]: is_named = skchem.filters.Filter(lambda m: m.name is not None)
```

We carelessly did not set dicyclopentadiene's name previously, so we want this to get filtered out:

```
In [26]: is_named.filter(ms)
```

```
Filter: 100% (4 of 4) |################################################| Elapsed Ti
```

```
Out[26]: benzene                                  <Mol: c1ccccc1>
         ferrocene     <Mol: [Fe+2].c1cc[cH-]c1.c1cc[cH-]c1>
         norbornane                          <Mol: C1CC2CCC1C2>
         Name: structure, dtype: object
```

It worked!

Transforming and Filtering

A common functionality in cheminformatics is to convert a molecule into *something else*, and if the conversion fails, to just remove the compound. An example of this is **standardization**, where one might want to throw away compounds that fail to standardize, or **geometry optimization** where one might throw away molecules that fail to converge.

This functionality is similar to but crucially **different from simply ‘‘filtering‘‘**, as filtering returns the original compounds, rather than the transformed compounds. Instead, there are special `Filters`, called `TransformFilters`, that can perform this task in a single method call. To give an example of the functionality, we will use the `UFF` class:

```
In [27]: issubclass(skchem.forcefields.UFF, skchem.filters.base.TransformFilter)
```

```
Out[27]: True
```

They are instanciated the same way as normal `Transformers` and `Filters`:

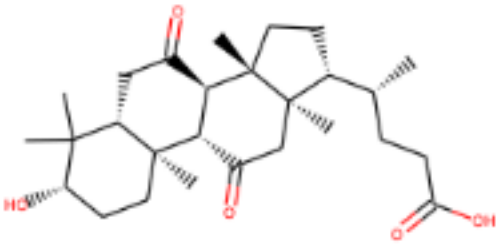
```
In [28]: uff = skchem.forcefields.UFF()
```

An example molecule that fails is taken from the NCI DTP Diversity set III:

```
In [29]: mol_that_fails = skchem.Mol.from_smiles('C[C@H](CCC(=O)O)[C@H]1CC[C@@]2(C)[C@@H]3C
                                                  name='7524')
```

```
In [30]: skchem.vis.draw(mol_that_fails)
```

```
Out[30]: <matplotlib.image.AxesImage at 0x121561eb8>
```



```
In [31]: ms.append(mol_that_fails)
```

```
In [32]: res = uff.filter(ms); res
```

```
/Users/rich/projects/scikit-chem/skchem/forcefields/base.py:54: UserWarning: Failed to Embe
  warnings.warn(msg)
UFF: 100% (5 of 5) |############################################################| Elapsed Ti
```

```
Out[32]: benzene                              <Mol: c1ccccc1>
         ferrocene     <Mol: [Fe+2].c1cc[cH-]c1.c1cc[cH-]c1>
         norbornane                        <Mol: C1CC2CCC1C2>
         3                        <Mol: C1=CC2C3C=CC(C3)C2C1>
         Name: structure, dtype: object
```

Note: *filter* returns the *original* molecules, which have **not** been optimized:

```
In [33]: skchem.vis.draw(res.ix[3])
```

```
Out[33]: <matplotlib.image.AxesImage at 0x12174c198>
```

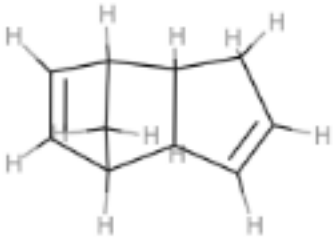
```
In [34]: res = uff.transform_filter(ms); res
```

```
/Users/rich/projects/scikit-chem/skchem/forcefields/base.py:54: UserWarning: Failed to Embe
  warnings.warn(msg)
UFF: 100% (5 of 5) |############################################################| Elapsed Ti
```

```
Out[34]: benzene                 <Mol: [H]c1c([H])c([H])c([H])c([H])c1[H]>
         ferrocene     <Mol: [Fe+2].[H]c1c([H])c([H])[c-]([H])c1[H].[...
         norbornane    <Mol: [H]C1([H])C([H])([H])C2([H])C([H])([H])C...
         3             <Mol: [H]C1=C([H])C2([H])C3([H])C([H])=C([H])C...
         Name: structure, dtype: object
```

```
In [35]: skchem.vis.draw(res.ix[3])
```

```
Out[35]: <matplotlib.image.AxesImage at 0x121925390>
```



5.6 Pipelining

scikit-chem expands on the scikit-learn `Pipeline` object to support filtering. It is initialized using a list of Transformer objects.

```
In [10]: pipeline = skchem.pipeline.Pipeline([
                 skchem.standardizers.ChemAxonStandardizer(keep_failed=True),
                 skchem.forcefields.UFF(),
                 skchem.filters.OrganicFilter(),
                 skchem.descriptors.MorganFeaturizer()])
```

The pipeline will apply each in turn to objects, using the the highest priority function that each object implements, according to the order `transform_filter` > `filter` > `transform`.

For example, our pipeline can transform sodium acetate all the way to fingerprints:

```
In [11]: mol = skchem.Mol.from_smiles('CC(=O)[O-].[Na+]')

In [4]: pipeline.transform_filter(mol)

Out[4]: morgan_fp_idx
        0       0
        1       0
        2       0
        3       0
        4       0
               ..
        2043    0
        2044    0
        2045    0
        2046    0
        2047    0
        Name: MorganFeaturizer, dtype: uint8
```

It also works on collections of molecules:

```
In [12]: mols = skchem.read_smiles('https://archive.org/download/scikit-chem_example_files/
```

```
Out[12]: batch
         ethane                          <Mol: CC>
         propane                        <Mol: CCC>
         benzene                  <Mol: c1ccccc1>
         sodium acetate    <Mol: CC(=O)[O-].[Na+]>
         serine                <Mol: NC(CO)C(=O)O>
         Name: structure, dtype: object
```

```
In [16]: pipeline.transform_filter(mols)
```

```
ChemAxonStandardizer: 100% (5 of 5) |##########################################| Elapsed Ti
UFF: 100% (5 of 5) |##########################################################| Elapsed Ti
OrganicFilter: 100% (5 of 5) |################################################| Elapsed Ti
MorganFeaturizer: 100% (5 of 5) |#############################################| Elapsed Ti
```

```
Out[16]: morgan_fp_idx   0     1     2     3     4     ...   2043  2044  2045  2046  \
         batch                                          ...
         ethane              0     0     0     0     0  ...      0     0     0     0
         propane             0     0     0     0     0  ...      0     0     0     0
         benzene             0     0     0     0     0  ...      0     0     0     0
         sodium acetate      0     0     0     0     0  ...      0     0     0     0
         serine              0     0     0     0     0  ...      0     0     1     0

         morgan_fp_idx   2047
         batch
         ethane             0
         propane            0
         benzene            0
         sodium acetate     0
         serine             0

         [5 rows x 2048 columns]
```

```
In [ ]:
```

5.7 Data

scikit-chem provides a simple interface to chemical datasets, and a framework for constructing these datasets. The data module uses fuel to make complex out of memory iterative functionality straightforward (see the fuel documentation). It also offers an abstraction to allow easy loading of smaller datasets, that can fit in memory.

5.7.1 In memory datasets

Datasets consist of **sets** and **sources**. Simply put, sets are collections of molecules in the dataset, and sources are types of data relating to these molecules.

For demonstration purposes, we will use the Bursi Ames dataset. This has 3 sets:

```
In [31]: skchem.data.BursiAmes.available_sets()
```

```
Out[31]: ('train', 'valid', 'test')
```

And many sources:

```
In [32]: skchem.data.BursiAmes.available_sources()
```

```
Out[32]: ('G', 'A', 'y', 'A_cx', 'G_d', 'X_morg', 'X_cx', 'X_pc')
```

Note: Currently, the nature of the sources are not alway well documented, but as a guide, **X** are moleccular features, **y** are target variables, **A** are atom features, **G** are distances. When available, they will be detailed in the docstring of the dataset, accessible with `help`.

For this example, we will load the X_morg and the y **sources** for all the **sets**. These are circular fingerprints, and the target labels (in this case, whether the molecule was a mutagen).

We can load the data for requested sets and sources using the in memory API:

```
In [33]: kws = {'sets': ('train', 'valid', 'test'), 'sources':('X_morg', 'y')}

         (X_train, y_train), (X_valid, y_valid), (X_test, y_test) = skchem.data.BursiAmes.l
```

The requested data is loaded as nested tuples, sorted first by **set**, and then by **source**, which can easily be unpacked as above.

```
In [34]: print('train shapes:', X_train.shape, y_train.shape)
         print('valid shapes:', X_valid.shape, y_valid.shape)
         print('test shapes:', X_test.shape, y_test.shape)
```

```
train shapes: (3007, 2048) (3007,)
valid shapes: (645, 2048) (645,)
test shapes: (645, 2048) (645,)
```

The raw data is loaded as numpy arrays:

```
In [35]: X_train
```

```
Out[35]: array([[0, 0, 0, ..., 0, 0, 0],
                [0, 0, 0, ..., 0, 0, 0],
                [0, 0, 0, ..., 0, 0, 0],
                ...,
                [0, 0, 0, ..., 0, 0, 0],
                [0, 0, 0, ..., 0, 0, 0],
                [0, 0, 0, ..., 0, 0, 0]])
```

```
In [36]: y_train
```

```
Out[36]: array([1, 1, 1, ..., 0, 1, 1], dtype=uint8)
```

Which should be ready to use as fuel for modelling!

5.7.2 Data as pandas objects

The data is originally saved as pandas objects, and can be retrieved as such using the `read_frame` class method.

Features are available under the 'feats' namespace:

```
In [37]: skchem.data.BursiAmes.read_frame('feats/X_morg')
```

```
Out[37]: morgan_fp_idx  0     1     2     3     4     ...   2043  2044  2045  2046  \
         batch                                      ...
         1728-95-6         0     0     0     0     0  ...      0     0     0     0
         74550-97-3        0     0     0     0     0  ...      0     0     0     0
```

```
16757-83-8         0     0     0     0     0  ...       0     0     0     0
553-97-9           0     0     0     0     0  ...       0     0     0     0
115-39-9           0     0     0     0     0  ...       0     0     0     0
...              ...   ...   ...   ...   ...  ...     ...   ...   ...   ...
874-60-2           0     0     0     0     0  ...       0     0     0     0
92-66-0            0     0     0     0     0  ...       0     0     0     0
594-71-8           0     0     0     0     0  ...       0     0     0     0
55792-21-7         0     0     0     0     0  ...       0     0     0     0
84987-77-9         0     0     0     0     0  ...       0     0     0     0

morgan_fp_idx  2047
batch
1728-95-6         0
74550-97-3        0
16757-83-8        0
553-97-9          0
115-39-9          0
...              ...
874-60-2          0
92-66-0           0
594-71-8          0
55792-21-7        0
84987-77-9        0

[4297 rows x 2048 columns]
```

Target variables under 'targets':

```
In [39]: skchem.data.BursiAmes.read_frame('targets/y')
```

```
Out[39]: batch
         1728-95-6     1
         74550-97-3    1
         16757-83-8    1
         553-97-9      0
         115-39-9      0
                      ..
         874-60-2      1
         92-66-0       0
         594-71-8      1
         55792-21-7    0
         84987-77-9    1
         Name: is_mutagen, dtype: uint8
```

Set membership masks under 'indices':

```
In [40]: skchem.data.BursiAmes.read_frame('indices/train')
```

```
Out[40]: batch
         1728-95-6      True
         74550-97-3     True
         16757-83-8     True
         553-97-9       True
         115-39-9       True
                       ...
         874-60-2      False
         92-66-0       False
```

```
594-71-8      False
55792-21-7    False
84987-77-9    False
Name: split, dtype: bool
```

Finally, molecules are accessible via 'structure':

```
In [42]: skchem.data.BursiAmes.read_frame('structure')
```

```
Out[42]: batch
         1728-95-6      <Mol: [H]c1c([H])c([H])c(-c2nc(-c3c([H])c([H])...
         119-34-6       <Mol: [H]Oc1c([H])c([H])c(N([H])[H])c([H])c1[N...
         371-40-4           <Mol: [H]c1c([H])c(N([H])[H])c([H])c([H])c1F>
         2319-96-2      <Mol: [H]c1c([H])c([H])c2c([H])c3c(c([H])c(C([...
         1822-51-1         <Mol: [H]c1nc([H])c([H])c(C([H])([H])Cl)c1[H]>
                                                  ...
         84-64-0        <Mol: [H]c1c([H])c([H])c(C(=O)OC2([H])C([H])([...
         121808-62-6    <Mol: [H]OC(=O)C1([H])N(C(=O)C2([H])N([H])C(=O...
         134-20-3       <Mol: [H]c1c([H])c([H])c(N([H])[H])c(C(=O)OC([...
         6441-91-4      <Mol: [H]Oc1c([H])c(S(=O)(=O)O[H])c([H])c2c([H...
         97534-21-9     <Mol: [H]Oc1nc(=S)n([H])c(O[H])c1C(=O)N([H])c1...
         Name: structure, dtype: object
```

Note: The dataset building functionality is likely to undergo a large change in future so is not documented here. Please look at the example datasets to understand the format required to build the datasets directly.

CHAPTER 6

API

The API documentation, autogenerated from the docstrings.

6.1 skchem package

6.1.1 Subpackages

skchem.core package

Submodules

skchem.core.atom module

skchem.core.atom

Defining atoms in scikit-chem.

class skchem.core.atom.**Atom**
Bases: rdkit.Chem.rdchem.Atom, *skchem.core.base.ChemicalObject*

Object representing an Atom in scikit-chem.

atomic_mass
float – the atomic mass of the atom in u.

atomic_number
int – the atomic number of the atom.

bonds
tuple<skchem.Bonds> – the bonds to this *Atom*.

cahn_ingold_prelog
The Cahn Ingold Prelog chirality indicator.

chiral_tag
int – the chiral tag.

covalent_radius
float – the covalent radius in angstroms.

degree
int – the degree of the atom.

depleted_degree
int – the degree of the atom in the h depleted molecular graph.

electron_affinity
float – the first electron affinity in eV.

explicit_valence
int – the explicit valence.

formal_charge
int – the formal charge.

full_degree
int – the full degree of the atom in the h full molecular graph.

hexcode
The hexcode to use as a color for the atom.

hybridization_state
str – the hybridization state.

implicit_valence
int – the implicit valence.

index
int – the index of the atom.

intrinsic_state
float – the intrinsic state of the atom.

ionisation_energy
float – the first ionisation energy in eV.

is_aromatic
bool – whether the atom is aromatic.

is_in_ring
bool – whether the atom is in a ring.

is_terminal
bool – whether the atom is terminal.

kier_hall_alpha_contrib
float – the covalent radius in angstroms.

kier_hall_electronegativity
float – the hall-keir electronegativity.

mcgowan_parameter
float – the mcgowan volume parameter

n_explicit_hs
int – the number of explicit hydrogens.

n_hs
int – the instanced, implicit and explicit number of hydrogens

n_implicit_hs
int – the number of implicit hydrogens.

n_instanced_hs
int – The number of instanced hydrogens.

n_lone_pairs
int – the number of lone pairs.

n_pi_electrons
int – the number of pi electrons.

n_total_hs
int – the total number of hydrogens (according to rdkit).

n_val_electrons
int – the number of valence electrons.

neighbours()
tuple<Atom>: the neighbours of the atom.

owner
skchem.Mol – the owning molecule.

> **Warning:** This will seg fault if the atom is created manually.

pauling_electronegativity
float – the pauling electronegativity on Pauling scale.

polarisability
float – the atomic polarisability in 10^{-20} m^3.

principal_quantum_number
int – the principle quantum number.

props
PropertyView – rdkit properties of the atom.

sanderson_electronegativity
float – the sanderson electronegativity on Pauling scale.

symbol
str – the element symbol of the atom.

valence
int – the valence.

valence_degree
int – the valence degree.

$$ delta_i^v = Z_i^v - h_i $$

Where $ Z_i^v $ is the number of valence electrons and $ h_i $ is the number of hydrogens.

van_der_waals_radius
float – the Van der Waals radius in angstroms.

van_der_waals_volume
float –

the van der waals volume in angstroms^3.

$

rac{4}{3} pi r_v^3 $

class skchem.core.atom.**AtomView**(*owner*)
Bases: *skchem.core.base.ChemicalObjectView*

adjacency_matrix(*bond_orders=False*, *force=True*)
The vertex adjacency matrix.

Parameters

- **bond_orders** (*bool*) – Whether to use bond orders.
- **force** (*bool*) – Whether to recalculate or used rdkit cached value.

Returns np.array[int]

atomic_mass
np.array<float> – the atomic mass of the atoms in view

atomic_number
np.array<int> – the atomic number of the atoms in view

cahn_ingold_prelog
np.array<str> – the CIP string representation of atoms in view.

chiral_tag
np.array<str> – the chiral tag of the atoms in view.

covalent_radius
np.array<float> – the covalent radius of the atoms in the view.

degree
np.array<int> – the degree of the atoms in view, according to rdkit.

depleted_degree
np.array<int> – the degree of the atoms in the view in the h-depleted molecular graph.

distance_matrix(*bond_orders=False*, *force=True*)
The vertex distance matrix.

Parameters

- **bond_orders** (*bool*) – Whether to use bond orders.
- **force** (*bool*) – Whether to recalculate or used rdkit cached value.

Returns np.array[int]

electron_affinity
np.array<float> – the electron affinity of the atoms in the view.

explicit_valence
np.array<int> – the explicit valence of the atoms in view..

formal_charge
np.array<int> – the formal charge on the atoms in view

full_degree
np.array<int> – the degree of the atoms in the view in the h-filled molecular graph.

hexcode
The hexcode to use as a color for the atoms in the view.

hybridization_state
np.array<str> – the hybridization state of the atoms in view.

One of 'SP', 'SP2', 'SP3', 'SP3D', 'SP3D2', 'UNSPECIFIED', 'OTHER'

implicit_valence
np.array<int> – the explicit valence of the atoms in view.

index
pd.Index – an index for the atoms in the view.

intrinsic_state
np.ndarray<float> – the intrinsic state of the atoms in the view.

ionisation_energy
np.array<float> – the first ionisation energy of the atoms in the view.

is_aromatic
np.array<bool> – whether the atoms in the view are aromatic.

is_in_ring
np.array<bool> – whether the atoms in the view are in a ring.

is_terminal
np.array<bool> – whether the atoms in the view are terminal.

kier_hall_alpha_contrib
np.array<float> – the contribution to the kier hall alpha for each atom in the view.

kier_hall_electronegativity
np.array<float> – the hall kier electronegativity of the atoms in the view.

mcgowan_parameter
np.array<float> – the mcgowan parameter of the atoms in the iew.

n_explicit_hs
np.array<int> – the number of explicit hydrogens bonded to atoms in view, according to rdkit.

n_hs
np.array<int> – the number of hydrogens bonded to atoms in view.

n_implicit_hs
np.array<int> – the number of implicit hydrogens bonded to atoms in view, according to rdkit.

n_instanced_hs
np.array<int> – the number of instanced hydrogens bonded to atoms in view.

In this case, instanced means the number hs explicitly initialized as atoms.

n_lone_pairs
np.array<int> – the number of lone pairs on atoms in view.

n_pi_electrons
np.array<int> – the number of pi electrons on atoms in view.

n_total_hs
np.array<int> – the number of total hydrogens bonded to atoms in view, according to rdkit.

n_val_electrons
np.array<int> – the number of valence electrons bonded to atoms in view.

pauling_electronegativity
np.array<float> – the pauling electronegativity of the atoms in the view.

polarisability
np.array<float> – the atomic polarisability of the atoms in the view.

principal_quantum_number
np.array<float> – the principal quantum number of the atoms in the view.

sanderson_electronegativity
np.array<float> – the sanderson electronegativity of the atoms in the view.

symbol
np.array<str> – the symbols of the atoms in view

valence
np.array<int> – the valence of the atoms in view.

valence_degree
np.array<int> – the valence degree of the atoms in the view.

van_der_waals_radius
np.array<float> – the Van der Waals radius of the atoms in the view.

van_der_waals_volume
np.array<float> – the Van der Waals volume of the atoms in the view.

skchem.core.base module

skchem.core.base

Define base classes for scikit chem objects

class skchem.core.base.**ChemicalObject**
Bases: object

A mixin for each chemical object in scikit-chem.

classmethod from_super(*obj*)
Converts the class of an object to this class.

class skchem.core.base.**ChemicalObjectIterator**(*view*)
Bases: object

Iterator for chemical object views.

next()

class skchem.core.base.**ChemicalObjectView**(*owner*)
Bases: object

Abstract iterable view of chemical objects.

Concrete classes inheriting from it should implement *__getitem__* and *__len__*.

props
Return a property view of the objects in the view.

to_list()
Return a list of objects in the view.

class skchem.core.base.**MolPropertyView**(*obj_view*)
Bases: *skchem.core.base.View*

Mol property wrapper.

This provides properties for the atom and bond views.

get(*key*, *default=None*)

keys()
The available property keys on the object.

to_dict()
Return a dict of the properties of the view's objects.

to_frame()
Return a DataFrame of the properties of the view's objects.

class skchem.core.base.**PropertyView**(*owner*)
Bases: *skchem.core.base.View*

Property object wrapper.

This provides properties for rdkit objects.

keys()
The available property keys on the object.

class skchem.core.base.**View**
Bases: object

View wrapper interface. Conforms to the dictionary interface.

Objects inheriting from this should implement the *keys*, *getitem*, *setitem* and *delitem* methods.

clear()
Remove all properties from the object.

get(*index*, *default=None*)

items()
Return an iterable of key, value pairs.

keys()

pop(*index*, *default=None*)

remove(*key*)
Remove a property from the object.

to_dict()
Return a dict of the properties on the object.

to_series()
Return a pd.Series of the properties on the object.

skchem.core.bond module

skchem.core.bond

Defining chemical bonds in scikit-chem.

class skchem.core.bond.**Atom**
Bases: rdkit.Chem.rdchem.Atom, *skchem.core.base.ChemicalObject*

Object representing an Atom in scikit-chem.

atomic_mass
float – the atomic mass of the atom in u.

atomic_number
int – the atomic number of the atom.

bonds
tuple<skchem.Bonds> – the bonds to this *Atom*.

cahn_ingold_prelog
The Cahn Ingold Prelog chirality indicator.

chiral_tag
int – the chiral tag.

covalent_radius
float – the covalent radius in angstroms.

degree
int – the degree of the atom.

depleted_degree
int – the degree of the atom in the h depleted molecular graph.

electron_affinity
float – the first electron affinity in eV.

explicit_valence
int – the explicit valence.

formal_charge
int – the formal charge.

full_degree
int – the full degree of the atom in the h full molecular graph.

hexcode
The hexcode to use as a color for the atom.

hybridization_state
str – the hybridization state.

implicit_valence
int – the implicit valence.

index
int – the index of the atom.

intrinsic_state
float – the intrinsic state of the atom.

ionisation_energy
float – the first ionisation energy in eV.

is_aromatic
bool – whether the atom is aromatic.

is_in_ring
bool – whether the atom is in a ring.

is_terminal
bool – whether the atom is terminal.

kier_hall_alpha_contrib
float – the covalent radius in angstroms.

kier_hall_electronegativity
float – the hall-keir electronegativity.

mcgowan_parameter
float – the mcgowan volume parameter

n_explicit_hs
int – the number of explicit hydrogens.

n_hs
int – the instanced, implicit and explicit number of hydrogens

n_implicit_hs
int – the number of implicit hydrogens.

n_instanced_hs
int – The number of instanced hydrogens.

n_lone_pairs
int – the number of lone pairs.

n_pi_electrons
int – the number of pi electrons.

n_total_hs
int – the total number of hydrogens (according to rdkit).

n_val_electrons
int – the number of valence electrons.

neighbours()
tuple<Atom>: the neighbours of the atom.

owner
skchem.Mol – the owning molecule.

> **Warning:** This will seg fault if the atom is created manually.

pauling_electronegativity
float – the pauling electronegativity on Pauling scale.

polarisability
float – the atomic polarisability in 10^{-20} m^3.

principal_quantum_number
int – the principle quantum number.

props
PropertyView – rdkit properties of the atom.

sanderson_electronegativity
float – the sanderson electronegativity on Pauling scale.

symbol
str – the element symbol of the atom.

valence
int – the valence.

valence_degree
int – the valence degree.

$$ delta_i^v = Z_i^v - h_i $$

Where $ Z_i^v $ is the number of valence electrons and $ h_i $ is the number of hydrogens.

van_der_waals_radius
float – the Van der Waals radius in angstroms.

van_der_waals_volume
float –

the van der waals volume in angstroms^3.

$

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skchem.core.conformer module

skchem.core.conformer

Defining conformers in scikit-chem.

class skchem.core.conformer.**Conformer**
Bases: rdkit.Chem.rdchem.Conformer, *skchem.core.base.ChemicalObject*

Class representing a Conformer in scikit-chem.

align_with_principal_axes()
Align the reference frame with the principal axes of inertia.

canonicalize()
Center the reference frame at the centre of mass and

centre_of_mass
np.array – the centre of mass of the comformer.

centre_representation(*centre_of_mass=True*)
Centre representation to the center of mass.

Parameters **centre_of_mass** (*bool*) – Whether to use the masses of atoms to calculate the centre of mass, or just use the mean position coordinate.

Returns Conformer

geometric_centre
np.array – the geometric centre of the conformer.

id
The ID of the conformer.

is_3d
bool – whether the conformer is three dimensional.

owner
skchem.Mol – the owning molecule.

positions
np.ndarray – the atom positions in the conformer.

Note: This is a copy of the data, not the data itself. You cannot allocate to a slice of this.

class skchem.core.conformer.**ConformerIterator**(*view*)
Bases: object

Iterator for chemical object views.

next()

class skchem.core.conformer.**ConformerView**(*owner*)
Bases: *skchem.core.base.ChemicalObjectView*

append(*value*)

append_2d(***kwargs*)
Append a 2D conformer.

append_3d(*n_conformers=1*, ***kwargs*)
Append (a) 3D conformer(s), roughly embedded but not optimized.

Parameters

- **n_conformers** (*int*) – The number of conformers to append.
- **kwargs are passed to EmbedMultipleConfs.** (*Further*) –

id

is_3d

positions

skchem.core.mol module

skchem.core.mol

Defining molecules in scikit-chem.

class skchem.core.mol.**Mol**(**args*, ***kwargs*)
Bases: rdkit.Chem.rdchem.Mol, *skchem.core.base.ChemicalObject*

Class representing a Molecule in scikit-chem.

Mol objects inherit directly from rdkit Mol objects. Therefore, they contain atom and bond information, and may also include properties and atom bookmarks.

Example

Constructors are implemented as class methods with the *from_* prefix.

```
>>> import skchem
>>> m = skchem.Mol.from_smiles('CC(=O)Cl'); m
<Mol name="None" formula="C2H3ClO" at ...>
```

This is an rdkit Mol:

```
>>> from rdkit.Chem import Mol as RDKMol
>>> isinstance(m, RDKMol)
True
```

A name can be given at initialization: >>> m = skchem.Mol.from_smiles('CC(=O)Cl', name='acetyl chloride'); m # doctest: +ELLIPSIS <Mol name="acetyl chloride" formula="C2H3ClO" at ...>

```
>>> m.name
'acetyl chloride'
```

Serializers are implemented as instance methods with the *to_* prefix.

```
>>> m.to_smiles()
'CC(=O)Cl'
```

```
>>> m.to_inchi()
'InChI=1S/C2H3ClO/c1-2(3)4/h1H3'
```

```
>>> m.to_inchi_key()
'WETWJCDKMRHUPV-UHFFFAOYSA-N'
```

RDKit properties are accessible through the *props* property:

```
>>> m.SetProp('example_key', 'example_value') # set prop with rdkit directly
>>> m.props['example_key']
'example_value'
```

```
>>> m.SetIntProp('float_key', 42) # set int prop with rdkit directly
>>> m.props['float_key']
42
```

They can be set too:

```
>>> m.props['example_set'] = 'set_value'
>>> m.GetProp('example_set') # getting with rdkit directly
'set_value'
```

We can export the properties into a dict or a pandas series:

```
>>> m.props.to_series()
example_key    example_value
example_set        set_value
float_key                  42
dtype: object
```

Atoms and bonds are provided in views:

```
>>> m.atoms
<AtomView values="['C', 'C', 'O', 'Cl']" at ...>
```

```
>>> m.bonds
<BondView values="['C-C', 'C=O', 'C-Cl']" at ...>
```

These are iterable: >>> [a.symbol for a in m.atoms] ['C', 'C', 'O', 'Cl']

The view provides shorthands for some attributes to get these:

```
>>> m.atoms.symbol
array(['C', 'C', 'O', 'Cl'], dtype=...)
```

Atom and bond props can also be set:

```
>>> m.atoms[0].props['atom_key'] = 'atom_value'
>>> m.atoms[0].props['atom_key']
'atom_value'
```

The properties for atoms on the whole molecule can be accessed like so:

```
>>> m.atoms.props
<MolPropertyView values="{'atom_key': ['atom_value', None, None, None]}" at ...>
```

The properties can be exported as a pandas dataframe >>> m.atoms.props.to_frame()

atom_key

atom_idx 0 atom_value 1 None 2 None 3 None

add_hs(*inplace=False*, *add_coords=True*, *explicit_only=False*, *only_on_atoms=False*)
Add hydrogens to self.

Parameters

- **inplace** (*bool*) – Whether to add Hs to *Mol*, or return a new *Mol*.
- **add_coords** (*bool*) – Whether to set 3D coordinate for added Hs.
- **explicit_only** (*bool*) – Whether to add only explicit Hs, or also implicit ones.
- **only_on_atoms** (*iterable<bool>*) – An iterable specifying the atoms to add Hs.

Returns *Mol* with Hs added.

Return type skchem.Mol

atoms
List[skchem.Atom] – An iterable over the atoms of the molecule.

bonds
List[skchem.Bond] – An iterable over the bonds of the molecule.

conformers
List[Conformer] – conformers of the molecule.

copy()
Return a copy of the molecule.

classmethod from_binary(*binary*)
Decode a molecule from a binary serialization.

Parameters **binary** – The bytes string to decode.

Returns The molecule encoded in the binary.

Return type skchem.Mol

classmethod from_inchi(*_*, *in_arg*, *name=None*, **args*, ***kwargs*)
The constructor to be bound.

classmethod from_mol2block(*_*, *in_arg*, *name=None*, **args*, ***kwargs*)
The constructor to be bound.

classmethod from_mol2file(*_*, *in_arg*, *name=None*, **args*, ***kwargs*)
The constructor to be bound.

classmethod from_molblock(*_*, *in_arg*, *name=None*, **args*, ***kwargs*)
The constructor to be bound.

classmethod from_molfile(*_*, *in_arg*, *name=None*, **args*, ***kwargs*)
The constructor to be bound.

classmethod from_pdbblock(*_*, *in_arg*, *name=None*, **args*, ***kwargs*)
The constructor to be bound.

classmethod from_pdbfile(*_*, *in_arg*, *name=None*, **args*, ***kwargs*)
The constructor to be bound.

classmethod from_smarts(*_*, *in_arg*, *name=None*, **args*, ***kwargs*)
The constructor to be bound.

classmethod from_smiles(*_*, *in_arg*, *name=None*, **args*, ***kwargs*)
The constructor to be bound.

classmethod **from_tplblock**(*_*, *in_arg*, *name=None*, **args*, ***kwargs*)
The constructor to be bound.

classmethod **from_tplfile**(*_*, *in_arg*, *name=None*, **args*, ***kwargs*)
The constructor to be bound.

mass
float – the mass of the molecule.

name
str – The name of the molecule.

Raises KeyError

props
PropertyView – A dictionary of the properties of the molecule.

remove_hs(*inplace=False*, *sanitize=True*, *update_explicit=False*, *implicit_only=False*)
Remove hydrogens from self.

Parameters

- **inplace** (*bool*) – Whether to add Hs to *Mol*, or return a new *Mol*.
- **sanitize** (*bool*) – Whether to sanitize after Hs are removed.
- **update_explicit** (*bool*) – Whether to update explicit count after the removal.
- **implicit_only** (*bool*) – Whether to remove explict and implicit Hs, or Hs only.

Returns *Mol* with Hs removed.

Return type skchem.Mol

to_binary()
Serialize the molecule to binary encoding.

Returns the molecule in bytes.

Return type bytes

Notes

Due to limitations in RDKit, not all data is serialized. Notably, properties are not, so e.g. compound names are not saved.

to_dict(*kind='chemdoodle'*, *conformer_id=-1*)
A dictionary representation of the molecule.

Parameters **kind** (*str*) – The type of representation to use. Only *chemdoodle* is currently supported.

Returns dictionary representation of the molecule.

Return type dict

to_formula()
str: the chemical formula of the molecule.

Raises RuntimeError

to_inchi(**args*, ***kwargs*)
The serializer to be bound.

to_inchi_key()
The InChI key of the molecule.

Returns the InChI key.

Return type str

Raises RuntimeError

to_json(*kind='chemdoodle'*)
Serialize a molecule using JSON.

Parameters **kind** (*str*) – The type of serialization to use. Only *chemdoodle* is currently supported.

Returns the json string.

Return type str

to_molblock(**args*, ***kwargs*)
The serializer to be bound.

to_molfile(**args*, ***kwargs*)
The serializer to be bound.

to_pdbblock(**args*, ***kwargs*)
The serializer to be bound.

to_smarts(**args*, ***kwargs*)
The serializer to be bound.

to_smiles(**args*, ***kwargs*)
The serializer to be bound.

to_tplblock(**args*, ***kwargs*)
The serializer to be bound.

to_tplfile(**args*, ***kwargs*)
The serializer to be bound.

skchem.core.mol.**bind_constructor**(*constructor_name*, *name_to_bind=None*)
Bind an (rdkit) constructor to the class

skchem.core.mol.**bind_serializer**(*serializer_name*, *name_to_bind=None*)
Bind an (rdkit) serializer to the class

skchem.core.point module

Module contents

skchem.core

Module defining chemical types used in scikit-chem.

class skchem.core.**Atom**
Bases: rdkit.Chem.rdchem.Atom, *skchem.core.base.ChemicalObject*

Object representing an Atom in scikit-chem.

atomic_mass
float – the atomic mass of the atom in u.

atomic_number
int – the atomic number of the atom.

bonds
tuple<skchem.Bonds> – the bonds to this *Atom*.

cahn_ingold_prelog
The Cahn Ingold Prelog chirality indicator.

chiral_tag
int – the chiral tag.

covalent_radius
float – the covalent radius in angstroms.

degree
int – the degree of the atom.

depleted_degree
int – the degree of the atom in the h depleted molecular graph.

electron_affinity
float – the first electron affinity in eV.

explicit_valence
int – the explicit valence.

formal_charge
int – the formal charge.

full_degree
int – the full degree of the atom in the h full molecular graph.

hexcode
The hexcode to use as a color for the atom.

hybridization_state
str – the hybridization state.

implicit_valence
int – the implicit valence.

index
int – the index of the atom.

intrinsic_state
float – the intrinsic state of the atom.

ionisation_energy
float – the first ionisation energy in eV.

is_aromatic
bool – whether the atom is aromatic.

is_in_ring
bool – whether the atom is in a ring.

is_terminal
bool – whether the atom is terminal.

kier_hall_alpha_contrib
float – the covalent radius in angstroms.

kier_hall_electronegativity
float – the hall-keir electronegativity.

mcgowan_parameter
float – the mcgowan volume parameter

n_explicit_hs
int – the number of explicit hydrogens.

n_hs
int – the instanced, implicit and explicit number of hydrogens

n_implicit_hs
int – the number of implicit hydrogens.

n_instanced_hs
int – The number of instanced hydrogens.

n_lone_pairs
int – the number of lone pairs.

n_pi_electrons
int – the number of pi electrons.

n_total_hs
int – the total number of hydrogens (according to rdkit).

n_val_electrons
int – the number of valence electrons.

neighbours()
tuple<Atom>: the neighbours of the atom.

owner
skchem.Mol – the owning molecule.

> **Warning:** This will seg fault if the atom is created manually.

pauling_electronegativity
float – the pauling electronegativity on Pauling scale.

polarisability
float – the atomic polarisability in 10^{-20} m^3.

principal_quantum_number
int – the principle quantum number.

props
PropertyView – rdkit properties of the atom.

sanderson_electronegativity
float – the sanderson electronegativity on Pauling scale.

symbol
str – the element symbol of the atom.

valence
int – the valence.

valence_degree
int – the valence degree.

$$ delta_i^v = Z_i^v - h_i $$

Where $ Z_i^v $ is the number of valence electrons and $ h_i $ is the number of hydrogens.

van_der_waals_radius
float – the Van der Waals radius in angstroms.

van_der_waals_volume
float –

the van der waals volume in angstroms^3.

$

rac{4}{3} pi r_v^3 $

class skchem.core.**Bond**
Bases: rdkit.Chem.rdchem.Bond, *skchem.core.base.ChemicalObject*

Class representing a chemical bond in scikit-chem.

atom_idxs
tuple[int] – list of atom indexes involved in the bond.

atoms
tuple[Atom] – list of atoms involved in the bond.

draw()
str: Draw the bond in ascii.

index
int – the index of the bond in the atom.

is_aromatic
bool – whether the bond is aromatic.

is_conjugated
bool – whether the bond is conjugated.

is_in_ring
bool – whether the bond is in a ring.

order
int – the order of the bond.

owner
skchem.Mol – the molecule this bond is a part of.

props
PropertyView – rdkit properties of the atom.

stereo_symbol
str – the stereo label of the bond ('Z', 'E', 'ANY', 'NONE')

to_dict()
dict: Convert to a dictionary representation.

class skchem.core.**Conformer**
Bases: rdkit.Chem.rdchem.Conformer, *skchem.core.base.ChemicalObject*

Class representing a Conformer in scikit-chem.

align_with_principal_axes()
Align the reference frame with the principal axes of inertia.

canonicalize()
Center the reference frame at the centre of mass and

centre_of_mass
np.array – the centre of mass of the comformer.

centre_representation(*centre_of_mass=True*)
Centre representation to the center of mass.

Parameters **centre_of_mass** (*bool*) – Whether to use the masses of atoms to calculate the centre of mass, or just use the mean position coordinate.

Returns Conformer

geometric_centre
np.array – the geometric centre of the conformer.

id
The ID of the conformer.

is_3d
bool – whether the conformer is three dimensional.

owner
skchem.Mol – the owning molecule.

positions
np.ndarray – the atom positions in the conformer.

Note: This is a copy of the data, not the data itself. You cannot allocate to a slice of this.

class skchem.core.**Mol**(**args*, ***kwargs*)
Bases: rdkit.Chem.rdchem.Mol, *skchem.core.base.ChemicalObject*

Class representing a Molecule in scikit-chem.

Mol objects inherit directly from rdkit Mol objects. Therefore, they contain atom and bond information, and may also include properties and atom bookmarks.

Example

Constructors are implemented as class methods with the *from_* prefix.

```
>>> import skchem
>>> m = skchem.Mol.from_smiles('CC(=O)Cl'); m
<Mol name="None" formula="C2H3ClO" at ...>
```

This is an rdkit Mol:

```
>>> from rdkit.Chem import Mol as RDKMol
>>> isinstance(m, RDKMol)
True
```

A name can be given at initialization: >>> m = skchem.Mol.from_smiles('CC(=O)Cl', name='acetyl chloride'); m # doctest: +ELLIPSIS <Mol name="acetyl chloride" formula="C2H3ClO" at ...>

```
>>> m.name
'acetyl chloride'
```

Serializers are implemented as instance methods with the *to_* prefix.

```
>>> m.to_smiles()
'CC(=O)Cl'
```

```
>>> m.to_inchi()
'InChI=1S/C2H3ClO/c1-2(3)4/h1H3'
```

```
>>> m.to_inchi_key()
'WETWJCDKMRHUPV-UHFFFAOYSA-N'
```

RDKit properties are accessible through the *props* property:

```
>>> m.SetProp('example_key', 'example_value') # set prop with rdkit directly
>>> m.props['example_key']
'example_value'
```

```
>>> m.SetIntProp('float_key', 42) # set int prop with rdkit directly
>>> m.props['float_key']
42
```

They can be set too:

```
>>> m.props['example_set'] = 'set_value'
>>> m.GetProp('example_set') # getting with rdkit directly
'set_value'
```

We can export the properties into a dict or a pandas series:

```
>>> m.props.to_series()
example_key    example_value
example_set        set_value
float_key                  42
dtype: object
```

Atoms and bonds are provided in views:

```
>>> m.atoms
<AtomView values="['C', 'C', 'O', 'Cl']" at ...>
```

```
>>> m.bonds
<BondView values="['C-C', 'C=O', 'C-Cl']" at ...>
```

These are iterable: >>> [a.symbol for a in m.atoms] ['C', 'C', 'O', 'Cl']

The view provides shorthands for some attributes to get these:

```
>>> m.atoms.symbol
array(['C', 'C', 'O', 'Cl'], dtype=...)
```

Atom and bond props can also be set:

```
>>> m.atoms[0].props['atom_key'] = 'atom_value'
>>> m.atoms[0].props['atom_key']
'atom_value'
```

The properties for atoms on the whole molecule can be accessed like so:

```
>>> m.atoms.props
<MolPropertyView values="{'atom_key': ['atom_value', None, None, None]}" at ...>
```

The properties can be exported as a pandas dataframe >>> m.atoms.props.to_frame()

atom_key

atom_idx 0 atom_value 1 None 2 None 3 None

add_hs(*inplace=False*, *add_coords=True*, *explicit_only=False*, *only_on_atoms=False*)
Add hydrogens to self.

Parameters

- **inplace** (*bool*) – Whether to add Hs to *Mol*, or return a new *Mol*.
- **add_coords** (*bool*) – Whether to set 3D coordinate for added Hs.
- **explicit_only** (*bool*) – Whether to add only explicit Hs, or also implicit ones.
- **only_on_atoms** (*iterable<bool>*) – An iterable specifying the atoms to add Hs.

Returns *Mol* with Hs added.

Return type skchem.Mol

atoms
List[skchem.Atom] – An iterable over the atoms of the molecule.

bonds
List[skchem.Bond] – An iterable over the bonds of the molecule.

conformers
List[Conformer] – conformers of the molecule.

copy()
Return a copy of the molecule.

classmethod from_binary(*binary*)
Decode a molecule from a binary serialization.

Parameters **binary** – The bytes string to decode.

Returns The molecule encoded in the binary.

Return type skchem.Mol

classmethod from_inchi(*_*, *in_arg*, *name=None*, **args*, ***kwargs*)
The constructor to be bound.

classmethod from_mol2block(*_*, *in_arg*, *name=None*, **args*, ***kwargs*)
The constructor to be bound.

classmethod from_mol2file(*_*, *in_arg*, *name=None*, **args*, ***kwargs*)
The constructor to be bound.

classmethod from_molblock(*_*, *in_arg*, *name=None*, **args*, ***kwargs*)
The constructor to be bound.

classmethod from_molfile(*_*, *in_arg*, *name=None*, **args*, ***kwargs*)
The constructor to be bound.

classmethod from_pdbblock(*_*, *in_arg*, *name=None*, **args*, ***kwargs*)
The constructor to be bound.

classmethod **from_pdbfile**(*_*, *in_arg*, *name=None*, **args*, ***kwargs*)
The constructor to be bound.

classmethod **from_smarts**(*_*, *in_arg*, *name=None*, **args*, ***kwargs*)
The constructor to be bound.

classmethod **from_smiles**(*_*, *in_arg*, *name=None*, **args*, ***kwargs*)
The constructor to be bound.

classmethod **from_tplblock**(*_*, *in_arg*, *name=None*, **args*, ***kwargs*)
The constructor to be bound.

classmethod **from_tplfile**(*_*, *in_arg*, *name=None*, **args*, ***kwargs*)
The constructor to be bound.

mass
float – the mass of the molecule.

name
str – The name of the molecule.

Raises `KeyError`

props
PropertyView – A dictionary of the properties of the molecule.

remove_hs(*inplace=False*, *sanitize=True*, *update_explicit=False*, *implicit_only=False*)
Remove hydrogens from self.

Parameters

- **inplace** (*bool*) – Whether to add Hs to *Mol*, or return a new *Mol*.
- **sanitize** (*bool*) – Whether to sanitize after Hs are removed.
- **update_explicit** (*bool*) – Whether to update explicit count after the removal.
- **implicit_only** (*bool*) – Whether to remove explict and implicit Hs, or Hs only.

Returns *Mol* with Hs removed.

Return type skchem.Mol

to_binary()
Serialize the molecule to binary encoding.

Returns the molecule in bytes.

Return type bytes

Notes

Due to limitations in RDKit, not all data is serialized. Notably, properties are not, so e.g. compound names are not saved.

to_dict(*kind='chemdoodle'*, *conformer_id=-1*)
A dictionary representation of the molecule.

Parameters **kind** (*str*) – The type of representation to use. Only *chemdoodle* is currently supported.

Returns dictionary representation of the molecule.

Return type dict

to_formula()
str: the chemical formula of the molecule.

Raises RuntimeError

to_inchi(**args*, ***kwargs*)
The serializer to be bound.

to_inchi_key()
The InChI key of the molecule.

Returns the InChI key.

Return type str

Raises RuntimeError

to_json(*kind='chemdoodle'*)
Serialize a molecule using JSON.

Parameters **kind** (*str*) – The type of serialization to use. Only *chemdoodle* is currently supported.

Returns the json string.

Return type str

to_molblock(**args*, ***kwargs*)
The serializer to be bound.

to_molfile(**args*, ***kwargs*)
The serializer to be bound.

to_pdbblock(**args*, ***kwargs*)
The serializer to be bound.

to_smarts(**args*, ***kwargs*)
The serializer to be bound.

to_smiles(**args*, ***kwargs*)
The serializer to be bound.

to_tplblock(**args*, ***kwargs*)
The serializer to be bound.

to_tplfile(**args*, ***kwargs*)
The serializer to be bound.

skchem.cross_validation package

Submodules

skchem.cross_validation.similarity_threshold module

skchem.cross_validation.similarity_threshold

Similarity threshold dataset partitioning functionality.

class skchem.cross_validation.similarity_threshold.**SimThresholdSplit**(*min_threshold=0.45*, *largest_cluster_fraction=0.1*, *fper='morgan'*, *similarity_metric='jaccard'*, *memory_optimized=True*, *n_jobs=1*, *block_width=1000*, *verbose=False*)

Bases: object

block_width
The width of the subsets of features.

Note: Only used in parallelized.

fit(*inp*, *pairs=None*)
Fit the cross validator to the data. :param inp:

- *pd.Series* of *Mol* instances
- *pd.DataFrame* with *Mol* instances as a *structure* row.
- *pd.DataFrame* of fingerprints if *fper* is *None*
- *pd.DataFrame* of sim matrix if *similarity_metric* is *None*
- *np.array* of sim matrix if *similarity_metric* is *None*

k_fold(*n_folds*)
Returns k-fold cross-validated folds with thresholded similarity.

Parameters **n_folds** (*int*) – The number of folds to provide.

Returns **generator[** – The splits in series.

Return type pd.Series, pd.Series

n_instances_
The number of instances that were used to fit the object.

n_jobs
The number of processes to use to calculate the distance matrix.

-1 for all available.

split(*ratio*)
Return splits of the data with thresholded similarity according to a specified ratio.

Parameters **ratio** (*tuple[ints]*) – the ratio to use.

Returns Generator of boolean split masks for the reqested splits.

Return type generator[pd.Series]

Example

```
>>> ms = skchem.data.Diversity.read_frame('structure')
>>> st = SimThresholdSplit(fper='morgan',
...                        similarity_metric='jaccard')
>>> st.fit(ms)
>>> train, valid, test = st.split(ratio=(70, 15, 15))
```

visualize_similarities(*subsample=5000*, *ax=None*)
Plot a histogram of similarities, with the threshold plotted.

Parameters

- **subsample** (*int*) – For a large dataset, subsample the number of compounds to consider.
- **ax** (*matplotlib.axis*) – Axis to make the plot on.

Returns matplotlib.axes

visualize_space(*dim_reducer='tsne'*, *dim_red_kw=None*, *subsample=5000*, *ax=None*, *plt_kw=None*)
Plot chemical space using a transformer

Parameters

- **dim_reducer** (*str or sklearn object*) – Technique to use to reduce fingerprint space.
- **dim_red_kw** (*dict*) – Keyword args to pass to dim_reducer.
- **subsample** (*int*) – for a large dataset, subsample the number of compounds to consider.
- **ax** (*matplotlib.axis*) – Axis to make the plot on.
- **plt_kw** (*dict*) – Keyword args to pass to the plot.

Returns matplotlib.axes

skchem.cross_validation.similarity_threshold.**returns_pairs**(*func*)
Wraps a function that returns a ((i, j), sim) list to return a dataframe.

Module contents

skchem.cross_validation

Module implementing cross validation routines useful for chemical data.

class skchem.cross_validation.**SimThresholdSplit**(*min_threshold=0.45*, *largest_cluster_fraction=0.1*, *fper='morgan'*, *similarity_metric='jaccard'*, *memory_optimized=True*, *n_jobs=1*, *block_width=1000*, *verbose=False*)
Bases: object

block_width
The width of the subsets of features.

Note: Only used in parallelized.

fit (*inp*, *pairs=None*)
Fit the cross validator to the data. :param inp:

- *pd.Series* of *Mol* instances
- *pd.DataFrame* with *Mol* instances as a *structure* row.
- *pd.DataFrame* of fingerprints if *fper* is *None*
- *pd.DataFrame* of sim matrix if *similarity_metric* is *None*
- *np.array* of sim matrix if *similarity_metric* is *None*

k_fold (*n_folds*)
Returns k-fold cross-validated folds with thresholded similarity.

Parameters **n_folds** (*int*) – The number of folds to provide.

Returns **generator[** – The splits in series.

Return type pd.Series, pd.Series

n_instances_
The number of instances that were used to fit the object.

n_jobs
The number of processes to use to calculate the distance matrix.

-1 for all available.

split (*ratio*)
Return splits of the data with thresholded similarity according to a specified ratio.

Parameters **ratio** (*tuple[ints]*) – the ratio to use.

Returns Generator of boolean split masks for the reqested splits.

Return type generator[pd.Series]

Example

```
>>> ms = skchem.data.Diversity.read_frame('structure')
>>> st = SimThresholdSplit(fper='morgan',
...                        similarity_metric='jaccard')
>>> st.fit(ms)
>>> train, valid, test = st.split(ratio=(70, 15, 15))
```

visualize_similarities (*subsample=5000*, *ax=None*)
Plot a histogram of similarities, with the threshold plotted.

Parameters

- **subsample** (*int*) – For a large dataset, subsample the number of compounds to consider.
- **ax** (*matplotlib.axis*) – Axis to make the plot on.

Returns matplotlib.axes

visualize_space(*dim_reducer='tsne'*, *dim_red_kw=None*, *subsample=5000*, *ax=None*, *plt_kw=None*)

Plot chemical space using a transformer

Parameters

- **dim_reducer** (*str or sklearn object*) – Technique to use to reduce fingerprint space.
- **dim_red_kw** (*dict*) – Keyword args to pass to dim_reducer.
- **subsample** (*int*) – for a large dataset, subsample the number of compounds to consider.
- **ax** (*matplotlib.axis*) – Axis to make the plot on.
- **plt_kw** (*dict*) – Keyword args to pass to the plot.

Returns matplotlib.axes

skchem.data package

Subpackages

skchem.data.converters package

Submodules

skchem.data.converters.base module

skchem.data.converters.base

Defines the base converter class.

class skchem.data.converters.base.**Converter**(*directory*, *output_directory*, *output_filename='default.h5'*)

Bases: object

Create a fuel dataset from molecules and targets.

classmethod convert(***kwargs*)

create_file(*path*)

classmethod fill_subparser(*subparser*)

run(*ms*, *y*, *output_path*, *splits=None*, *features=None*, *pytables_kws={'complib': 'bzip2', 'complevel': 9}*)

Args:

ms (pd.Series): The molecules of the dataset.

ys (pd.Series or pd.DataFrame): The target labels of the dataset.

output_path (str): The path to which the dataset should be saved.

features (list[Feature]): The features to calculate. Defaults are used if *None*.

splits (iterable<(name, split)>): An iterable of name, split tuples. Splits are provided as boolean arrays of the whole data.

save_features(*ms*)
Save all features for the dataset.

save_frame(*data*, *name*, *prefix='targets'*)
Save the a frame to the data file.

save_molecules(*mols*)
Save the molecules to the data file.

save_splits()
Save the splits to the data file.

save_targets(*y*)

source_names

split_names

class skchem.data.converters.base.**Feature**(*fper*, *key*, *axis_names*)
Bases: tuple

axis_names
Alias for field number 2

fper
Alias for field number 0

key
Alias for field number 1

class skchem.data.converters.base.**Split**(*mask*, *name*, *converter*)
Bases: object

contiguous

indices

ref

save()

to_dict()

skchem.data.converters.base.**contiguous_order**(*to_order*, *splits*)
Determine a contiguous order from non-overlapping splits, and put data in that order.

Parameters

- **to_order** (*iterable<pd.Series, pd.DataFrame, pd.Panel>*) – The pandas objects to put in contiguous order.
- **splits** (*iterable<pd.Series>*) – The non-overlapping splits, as boolean masks.

Returns The data in contiguous order.

Return type iterable<pd.Series, pd.DataFrame, pd.Panel>

skchem.data.converters.base.**default_features**()

skchem.data.converters.base.**default_pipeline**()
Return a default pipeline to be used for general datasets.

skchem.data.converters.bradley_open_mp module

class skchem.data.converters.bradley_open_mp.**BradleyOpenMPConverter**(*directory*, *output_directory*, *output_filename='bradley_open_mp.h5'*)

Bases: *skchem.data.converters.base.Converter*

static filter_bad(*data*)

static fix_mp(*data*)

static parse_data(*path*)

skchem.data.converters.bursi_ames module

class skchem.data.converters.bursi_ames.**BursiAmesConverter**(*directory*, *output_directory*, *output_filename='bursi_ames.h5'*)

Bases: *skchem.data.converters.base.Converter*

skchem.data.converters.diversity_set module

skchem.data.coverters.example

Formatter for the example dataset.

class skchem.data.converters.diversity_set.**DiversityConverter**(*directory*, *output_directory*, *output_filename='diversity.h5'*)

Bases: *skchem.data.converters.base.Converter*

Example Converter, using the NCI DTP Diversity Set III.

parse_file(*path*)

synthetic_targets(*index*)

skchem.data.converters.muller_ames module

class skchem.data.converters.muller_ames.**MullerAmesConverter**(*directory*, *output_directory*, *output_filename='muller_ames.h5'*)

Bases: *skchem.data.converters.base.Converter*

create_split_dict(*splits*, *name*)

drop_indices(*splits*, *indices*)

parse_splits(*f_path*)

patch_data(*data*, *patches*)

Patch smiles in a DataFrame with rewritten ones that specify diazo groups in rdkit friendly way.

skchem.data.converters.nmrshiftdb2 module

class skchem.data.converters.nmrshiftdb2.**NMRShiftDB2Converter**(*directory*, *output_directory*, *output_filename='nmrshiftdb2.h5'*)

Bases: *skchem.data.converters.base.Converter*

static combine_duplicates(*data*)
Collect duplicate spectra into one dictionary. All shifts are collected into lists.

static extract_duplicates(*data*, *kind='13c'*)
Get all 13c duplicates.

static get_spectra(*data*)
Retrieves spectra from raw data.

static log_dists(*data*)

log_duplicates(*data*)

static parse_data(*filepath*)
Reads the raw datafile.

static process_spectra(*data*)
Turn the string representations found in sdf file into a dictionary.

static squash_duplicates(*data*)
Take the mean of all the duplicates. This is where we could do a bit more checking.

static to_frame(*data*)
Convert a series of dictionaries to a dataframe.

skchem.data.converters.physprop module

class skchem.data.converters.physprop.**PhysPropConverter**(*directory*, *output_directory*, *output_filename='physprop.h5'*)

Bases: *skchem.data.converters.base.Converter*

drop_inconsistencies(*data*)

extract(*directory*)

static fix_temp(*s*, *mean_range=5*)

process_bp(*data*)

process_logP(*data*)

process_logS(*data*)

process_mp(*data*)

process_sdf(*path*)

process_targets(*data*)

process_txt(*path*)

skchem.data.converters.tox21 module

skchem.data.transformers.tox21

Module defining transformation techniques for tox21.

class skchem.data.converters.tox21.**Tox21Converter**(*directory*, *output_directory*, *output_filename='tox21.h5'*)

Bases: *skchem.data.converters.base.Converter*

Class to build tox21 dataset.

extract(*directory*)

static fix_assay_name(*s*)

static fix_id(*s*)

static patch_test(*test*)

read_test(*test*, *test_data*)

read_train(*train*)

read_valid(*valid*)

Module contents

class skchem.data.converters.**DiversityConverter**(*directory*, *output_directory*, *output_filename='diversity.h5'*)

Bases: *skchem.data.converters.base.Converter*

Example Converter, using the NCI DTP Diversity Set III.

parse_file(*path*)

synthetic_targets(*index*)

class skchem.data.converters.**BursiAmesConverter**(*directory*, *output_directory*, *output_filename='bursi_ames.h5'*)

Bases: *skchem.data.converters.base.Converter*

class skchem.data.converters.**MullerAmesConverter**(*directory*, *output_directory*, *output_filename='muller_ames.h5'*)

Bases: *skchem.data.converters.base.Converter*

create_split_dict(*splits*, *name*)

drop_indices(*splits*, *indices*)

parse_splits(*f_path*)

patch_data(*data*, *patches*)

Patch smiles in a DataFrame with rewritten ones that specify diazo groups in rdkit friendly way.

class skchem.data.converters.**PhysPropConverter**(*directory*, *output_directory*, *output_filename='physprop.h5'*)

Bases: *skchem.data.converters.base.Converter*

drop_inconsistencies(*data*)

extract(*directory*)

static fix_temp(*s*, *mean_range=5*)

process_bp(*data*)

process_logP(*data*)

process_logS(*data*)

process_mp(*data*)

process_sdf(*path*)

process_targets(*data*)

process_txt(*path*)

class skchem.data.converters.**BradleyOpenMPConverter**(*directory*, *output_directory*, *output_filename='bradley_open_mp.h5'*)

Bases: *skchem.data.converters.base.Converter*

static filter_bad(*data*)

static fix_mp(*data*)

static parse_data(*path*)

class skchem.data.converters.**NMRShiftDB2Converter**(*directory*, *output_directory*, *output_filename='nmrshiftdb2.h5'*)

Bases: *skchem.data.converters.base.Converter*

static combine_duplicates(*data*)
Collect duplicate spectra into one dictionary. All shifts are collected into lists.

static extract_duplicates(*data*, *kind='13c'*)
Get all 13c duplicates.

static get_spectra(*data*)
Retrieves spectra from raw data.

static log_dists(*data*)

log_duplicates(*data*)

static parse_data(*filepath*)
Reads the raw datafile.

static process_spectra(*data*)
Turn the string representations found in sdf file into a dictionary.

static squash_duplicates(*data*)
Take the mean of all the duplicates. This is where we could do a bit more checking.

static to_frame(*data*)
Convert a series of dictionaries to a dataframe.

class skchem.data.converters.**Tox21Converter**(*directory*, *output_directory*, *output_filename='tox21.h5'*)

Bases: *skchem.data.converters.base.Converter*

Class to build tox21 dataset.

extract(*directory*)

static fix_assay_name(*s*)

static fix_id(*s*)

static patch_test(*test*)

read_test(*test*, *test_data*)

read_train(*train*)

read_valid(*valid*)

class skchem.data.converters.**ChEMBLConverter**(*directory*, *output_directory*, *output_filename='chembl.h5'*)
Bases: *skchem.data.converters.base.Converter*

Converter for the ChEMBL dataset.

parse_infile(*filename*)

skchem.data.datasets package

Submodules

skchem.data.datasets.base module

class skchem.data.datasets.base.**Dataset**(***kwargs*)
Bases: fuel.datasets.hdf5.H5PYDataset

Abstract base class providing an interface to the skchem data format.

classmethod available_sets()

classmethod available_sources()

classmethod download(*output_directory=None*, *download_directory=None*)
Download the dataset and convert it.

Parameters

- **output_directory** (*str*) – The directory to save the data to. Defaults to the first directory in the fuel data path.
- **download_directory** (*str*) – The directory to save the raw files to. Defaults to a temporary directory.

Returns The path of the downloaded and processed dataset.

Return type str

classmethod load_data(*sets=()*, *sources=()*)
Load a set of sources.

Parameters

- **sets** (*tuple[str]*) – The sets to return data for.
- **sources** – The sources to return data for.

Example

(X_train, y_train), (X_test, y_test) = Dataset.load_data(sets=('train', 'test'), sources=('X', 'y'))

classmethod load_set(*set_name*, *sources=()*)
Load the sources for a single set.

Parameters

- **set_name** (*str*) – The set name.
- **sources** (*tuple[str]*) – The sources to return data for.

Returns

tuple[np.array] The requested sources for the requested set.

classmethod read_frame(*key*, **args*, ***kwargs*)
Load a set of features from the dataset as a pandas object.

Parameters **key** (*str*) – The HDF5 key for required data. Typically, this will be one of

- structure: for the raw molecules
- smiles: for the smiles
- features/{feat_name}: for the features
- targets/{targ_name}: for the targets

Returns

pd.Series or pd.DataFrame or pd.Panel The data as a dataframe.

skchem.data.datasets.bradley_open_mp module

class skchem.data.datasets.bradley_open_mp.**BradleyOpenMP**(***kwargs*)
Bases: *skchem.data.datasets.base.Dataset*

converter
alias of BradleyOpenMPConverter

downloader
alias of BradleyOpenMPDownloader

filename = 'bradley_open_mp.h5'

skchem.data.datasets.bursi_ames module

class skchem.data.datasets.bursi_ames.**BursiAmes**(***kwargs*)
Bases: *skchem.data.datasets.base.Dataset*

converter
alias of BursiAmesConverter

downloader
alias of BursiAmesDownloader

filename = 'bursi_ames.h5'

skchem.data.datasets.diversity_set module

file title

Description

class skchem.data.datasets.diversity_set.**Diversity**(***kwargs*)
Bases: *skchem.data.datasets.base.Dataset*

Example dataset, the NCI DTP Diversity Set III.

converter
alias of DiversityConverter

downloader
alias of DiversityDownloader

filename = 'diversity.h5'

skchem.data.datasets.muller_ames module

class skchem.data.datasets.muller_ames.**MullerAmes**(**kwargs)
Bases: *skchem.data.datasets.base.Dataset*

converter
alias of MullerAmesConverter

downloader
alias of MullerAmesDownloader

filename = 'muller_ames.h5'

skchem.data.datasets.nmrshiftdb2 module

class skchem.data.datasets.nmrshiftdb2.**NMRShiftDB2**(**kwargs)
Bases: *skchem.data.datasets.base.Dataset*

converter
alias of NMRShiftDB2Converter

downloader
alias of NMRShiftDB2Downloader

filename = 'nmrshiftdb2.h5'

skchem.data.datasets.physprop module

class skchem.data.datasets.physprop.**PhysProp**(**kwargs)
Bases: *skchem.data.datasets.base.Dataset*

converter
alias of PhysPropConverter

downloader
alias of PhysPropDownloader

filename = 'physprop.h5'

skchem.data.datasets.tox21 module

class skchem.data.datasets.tox21.**Tox21**(**kwargs)
Bases: *skchem.data.datasets.base.Dataset*

converter
alias of Tox21Converter

downloader
alias of Tox21Downloader

filename = 'tox21.h5'

Module contents

skchem.data.datasets

Module defining skchem datasets.

class skchem.data.datasets.**Diversity**(***kwargs*)
Bases: *skchem.data.datasets.base.Dataset*

Example dataset, the NCI DTP Diversity Set III.

converter
alias of DiversityConverter

downloader
alias of DiversityDownloader

filename = 'diversity.h5'

class skchem.data.datasets.**BursiAmes**(***kwargs*)
Bases: *skchem.data.datasets.base.Dataset*

converter
alias of BursiAmesConverter

downloader
alias of BursiAmesDownloader

filename = 'bursi_ames.h5'

class skchem.data.datasets.**MullerAmes**(***kwargs*)
Bases: *skchem.data.datasets.base.Dataset*

converter
alias of MullerAmesConverter

downloader
alias of MullerAmesDownloader

filename = 'muller_ames.h5'

class skchem.data.datasets.**PhysProp**(***kwargs*)
Bases: *skchem.data.datasets.base.Dataset*

converter
alias of PhysPropConverter

downloader
alias of PhysPropDownloader

filename = 'physprop.h5'

class skchem.data.datasets.**BradleyOpenMP**(***kwargs*)
Bases: *skchem.data.datasets.base.Dataset*

converter
alias of BradleyOpenMPConverter

downloader
alias of BradleyOpenMPDownloader

filename = 'bradley_open_mp.h5'

class skchem.data.datasets.**NMRShiftDB2**(***kwargs*)
Bases: *skchem.data.datasets.base.Dataset*

converter
alias of NMRShiftDB2Converter

downloader
alias of NMRShiftDB2Downloader

filename = 'nmrshiftdb2.h5'

class skchem.data.datasets.**Tox21**(***kwargs*)
Bases: *skchem.data.datasets.base.Dataset*

converter
alias of Tox21Converter

downloader
alias of Tox21Downloader

filename = 'tox21.h5'

class skchem.data.datasets.**ChEMBL**(***kwargs*)
Bases: *skchem.data.datasets.base.Dataset*

converter
alias of ChEMBLConverter

downloader
alias of ChEMBLDownloader

filename = 'chembl.h5'

skchem.data.downloaders package

Submodules

skchem.data.downloaders.base module

class skchem.data.downloaders.base.**Downloader**
Bases: object

classmethod download(*directory=None*)

filenames = []

classmethod fill_subparser(*subparser*)

urls = []

skchem.data.downloaders.bradley_open_mp module

class skchem.data.downloaders.bradley_open_mp.**BradleyOpenMPDownloader**
Bases: *skchem.data.downloaders.base.Downloader*

filenames = ['bradley_melting_point_dataset.xlsx']

urls = ['https://ndownloader.figshare.com/files/1503990']

skchem.data.downloaders.bursi_ames module

class skchem.data.downloaders.bursi_ames.**BursiAmesDownloader**
Bases: *skchem.data.downloaders.base.Downloader*

filenames = ['cas_4337.zip']

urls = ['http://cheminformatics.org/datasets/bursi/cas_4337.zip']

skchem.data.downloaders.diversity module

file title

Description

class skchem.data.downloaders.diversity.**DiversityDownloader**
Bases: *skchem.data.downloaders.base.Downloader*

filenames = ['structures.sdf']

urls = ['https://wiki.nci.nih.gov/download/attachments/160989212/Div3_2DStructures_Oct2014.sdf']

skchem.data.downloaders.muller_ames module

class skchem.data.downloaders.muller_ames.**MullerAmesDownloader**
Bases: *skchem.data.downloaders.base.Downloader*

filenames = ['ci900161g_si_001.zip']

urls = ['https://ndownloader.figshare.com/files/4523278']

skchem.data.downloaders.nmrshiftdb2 module

class skchem.data.downloaders.nmrshiftdb2.**NMRShiftDB2Downloader**
Bases: *skchem.data.downloaders.base.Downloader*

filenames = ['nmrshiftdb2.sdf']

urls = ['https://sourceforge.net/p/nmrshiftdb2/code/HEAD/tree/trunk/snapshots/nmrshiftdb2withsignals.sd?format=raw

skchem.data.downloaders.physprop module

class skchem.data.downloaders.physprop.**PhysPropDownloader**
Bases: *skchem.data.downloaders.base.Downloader*

filenames = ['phys_sdf.zip', 'phys_txt.zip']

urls = ['http://esc.syrres.com/interkow/Download/phys_sdf.zip', 'http://esc.syrres.com/interkow/Download/phys_txt.zip'

skchem.data.downloaders.tox21 module

class skchem.data.downloaders.tox21.**Tox21Downloader**
Bases: *skchem.data.downloaders.base.Downloader*

filenames = ['train.sdf.zip', 'valid.sdf.zip', 'test.sdf.zip', 'test.txt']

urls = ['https://tripod.nih.gov/tox21/challenge/download?id=tox21_10k_data_allsdf', 'https://tripod.nih.gov/tox21/challe

Module contents

class skchem.data.downloaders.**DiversityDownloader**
Bases: *skchem.data.downloaders.base.Downloader*

filenames = ['structures.sdf']

urls = ['https://wiki.nci.nih.gov/download/attachments/160989212/Div3_2DStructures_Oct2014.sdf']

class skchem.data.downloaders.**ChEMBLDownloader**
Bases: *skchem.data.downloaders.base.Downloader*

filenames = ['chembl_raw.h5']

urls = []

class skchem.data.downloaders.**BursiAmesDownloader**
Bases: *skchem.data.downloaders.base.Downloader*

filenames = ['cas_4337.zip']

urls = ['http://cheminformatics.org/datasets/bursi/cas_4337.zip']

class skchem.data.downloaders.**MullerAmesDownloader**
Bases: *skchem.data.downloaders.base.Downloader*

filenames = ['ci900161g_si_001.zip']

urls = ['https://ndownloader.figshare.com/files/4523278']

class skchem.data.downloaders.**Tox21Downloader**
Bases: *skchem.data.downloaders.base.Downloader*

filenames = ['train.sdf.zip', 'valid.sdf.zip', 'test.sdf.zip', 'test.txt']

urls = ['https://tripod.nih.gov/tox21/challenge/download?id=tox21_10k_data_allsdf', 'https://tripod.nih.gov/tox21/challe

class skchem.data.downloaders.**NMRShiftDB2Downloader**
Bases: *skchem.data.downloaders.base.Downloader*

filenames = ['nmrshiftdb2.sdf']

urls = ['https://sourceforge.net/p/nmrshiftdb2/code/HEAD/tree/trunk/snapshots/nmrshiftdb2withsignals.sd?format=raw

class skchem.data.downloaders.**PhysPropDownloader**
Bases: *skchem.data.downloaders.base.Downloader*

filenames = ['phys_sdf.zip', 'phys_txt.zip']

urls = ['http://esc.syrres.com/interkow/Download/phys_sdf.zip', 'http://esc.syrres.com/interkow/Download/phys_txt.zip'

class skchem.data.downloaders.**BradleyOpenMPDownloader**
Bases: *skchem.data.downloaders.base.Downloader*

filenames = ['bradley_melting_point_dataset.xlsx']

urls = ['https://ndownloader.figshare.com/files/1503990']

Module contents

skchem.data

Module for handling data. Data can be accessed using the resource function.

class skchem.data.**Diversity**(***kwargs*)
Bases: *skchem.data.datasets.base.Dataset*

Example dataset, the NCI DTP Diversity Set III.

converter
alias of DiversityConverter

downloader
alias of DiversityDownloader

filename = 'diversity.h5'

class skchem.data.**BursiAmes**(***kwargs*)
Bases: *skchem.data.datasets.base.Dataset*

converter
alias of BursiAmesConverter

downloader
alias of BursiAmesDownloader

filename = 'bursi_ames.h5'

class skchem.data.**MullerAmes**(***kwargs*)
Bases: *skchem.data.datasets.base.Dataset*

converter
alias of MullerAmesConverter

downloader
alias of MullerAmesDownloader

filename = 'muller_ames.h5'

class skchem.data.**PhysProp**(***kwargs*)
Bases: *skchem.data.datasets.base.Dataset*

converter
alias of PhysPropConverter

downloader
alias of PhysPropDownloader

filename = 'physprop.h5'

class skchem.data.**BradleyOpenMP**(***kwargs*)
Bases: *skchem.data.datasets.base.Dataset*

converter
alias of BradleyOpenMPConverter

downloader
alias of BradleyOpenMPDownloader

filename = 'bradley_open_mp.h5'

class skchem.data.**NMRShiftDB2**(***kwargs*)
Bases: *skchem.data.datasets.base.Dataset*

converter
alias of NMRShiftDB2Converter

downloader
alias of NMRShiftDB2Downloader

filename = 'nmrshiftdb2.h5'

class skchem.data.**Tox21**(**kwargs)
Bases: *skchem.data.datasets.base.Dataset*

converter
alias of Tox21Converter

downloader
alias of Tox21Downloader

filename = 'tox21.h5'

class skchem.data.**ChEMBL**(**kwargs)
Bases: *skchem.data.datasets.base.Dataset*

converter
alias of ChEMBLConverter

downloader
alias of ChEMBLDownloader

filename = 'chembl.h5'

skchem.descriptors package

Submodules

skchem.descriptors.atom module

skchem.descriptors.chemaxon module

skchem.descriptors.fingerprints module

skchem.descriptors.moe module

skchem.descriptors.physicochemical module

Module contents

skchem.filters package

Submodules

skchem.filters.base module

skchem.filters

Chemical filters are defined.

class skchem.filters.base.**BaseFilter**(*agg='any'*, ***kwargs*)
Bases: *skchem.base.BaseTransformer*

The base Filter class.

agg
callable – The aggregate function to use. String aliases for *'any'*, *'not any'*, 'all', *'not all'* are available.

axes_names()

columns
pd.Index – The column index to use.

filter(*mols*, *y=None*, *neg=False*)

transform(*mols*, *agg=True*, ***kwargs*)

class skchem.filters.base.**Filter**(*func=None*, *agg='any'*, *n_jobs=1*, *verbose=True*)
Bases: *skchem.filters.base.BaseFilter*, *skchem.base.Transformer*

Filter base class.

Examples

```
>>> import skchem
```

Initialize the filter with a function: >>> is_named = skchem.filters.Filter(lambda m: m.name is not None)

Filter results can be found with *transform*: >>> ethane = skchem.Mol.from_smiles('CC', name='ethane') >>> is_named.transform(ethane) True

```
>>> anonymous = skchem.Mol.from_smiles('c1ccccc1')
>>> is_named.transform(anonymous)
False
```

Can take a series or dataframe: >>> mols = pd.Series({'anonymous': anonymous, 'ethane': ethane}) >>> is_named.transform(mols) anonymous False ethane True Name: Filter, dtype: bool

Using *filter* will drop out molecules that fail the test: >>> is_named.filter(mols) ethane <Mol: CC> dtype: object

Only failed are retained with the *neg* keyword argument: >>> is_named.filter(mols, neg=True) anonymous <Mol: c1ccccc1> dtype: object

class skchem.filters.base.**TransformFilter**(*agg='any'*, ***kwargs*)
Bases: *skchem.filters.base.BaseFilter*

Transform Filter object.

Implements *transform_filter*, which allows a transform, then a filter step returning the transformed values that are not *False*, *None* or *np.nan*.

transform_filter(*mols*, *y=None*, *neg=False*)

skchem.filters.base.**identity**(*x*)
The identity

skchem.filters.base.**not_all**(*x*)
Not all x

skchem.filters.base.**not_any**(*x*)
Not any x

skchem.filters.simple module

skchem.filters.simple

Simple filters for compounds.

class skchem.filters.simple.**AtomNumberFilter**(*above=3*, *below=60*, *include_hydrogens=False*, *n_jobs=1*, *verbose=True*)

Bases: *skchem.filters.base.Filter*

Filter whether the number of atoms in a Mol falls in a defined interval.

above <= *n_atoms* < *below*

Examples

```
>>> import skchem
```

```
>>> data = [
...         skchem.Mol.from_smiles('CC', name='ethane'),
...         skchem.Mol.from_smiles('CCCC', name='butane'),
...         skchem.Mol.from_smiles('NC(C)C(=O)O', name='alanine'),
...         skchem.Mol.from_smiles('C12C=CC(C=C2)C=C1', name='barrelene')
... ]
```

```
>>> af = skchem.filters.AtomNumberFilter(above=3, below=7)
```

```
>>> af.transform(data)
ethane       False
butane        True
alanine       True
barrelene    False
Name: num_atoms_in_range, dtype: bool
```

```
>>> af.filter(data)
butane            <Mol: CCCC>
alanine    <Mol: CC(N)C(=O)O>
Name: structure, dtype: object
```

```
>>> af = skchem.filters.AtomNumberFilter(above=5, below=15, include_
↪hydrogens=True)
```

```
>>> af.transform(data)
ethane        True
butane        True
alanine       True
barrelene    False
Name: num_atoms_in_range, dtype: bool
```

columns

class skchem.filters.simple.**ElementFilter**(*elements=None*, *as_bits=False*, *agg='any'*, *n_jobs=1*, *verbose=True*)

Bases: *skchem.filters.base.Filter*

Filter by elements.

Examples

Basic usage on molecules:

```
>>> import skchem
>>> hal_f = skchem.filters.ElementFilter(['F', 'Cl', 'Br', 'I'])
```

Molecules with one of the atoms transform to *True*.

```
>>> m1 = skchem.Mol.from_smiles('ClC(Cl)Cl', name='chloroform')
>>> hal_f.transform(m1)
True
```

Molecules with none of the atoms transform to *False*.

```
>>> m2 = skchem.Mol.from_smiles('CC', name='ethane')
>>> hal_f.transform(m2)
False
```

Can see the atom breakdown by passing *agg* == *False*: >>> hal_f.transform(m1, agg=False) has_element F 0 Cl 3 Br 0 I 0 Name: ElementFilter, dtype: int64

Can transform series.

```
>>> ms = [m1, m2]
>>> hal_f.transform(ms)
chloroform     True
ethane        False
dtype: bool
```

```
>>> hal_f.transform(ms, agg=False)
has_element  F  Cl  Br  I
chloroform   0   3   0  0
ethane       0   0   0  0
```

Can also filter series:

```
>>> hal_f.filter(ms)
chloroform    <Mol: ClC(Cl)Cl>
Name: structure, dtype: object
```

```
>>> hal_f.filter(ms, neg=True)
ethane    <Mol: CC>
Name: structure, dtype: object
```

columns

elements

class skchem.filters.simple.**MassFilter**(*above=3*, *below=900*, *n_jobs=1*, *verbose=True*)
Bases: *skchem.filters.base.Filter*

Filter whether the molecular weight of a molecule is outside a range.

above <= *mass* < *below*

Examples

```
>>> import skchem
```

```
>>> data = [
...          skchem.Mol.from_smiles('CC', name='ethane'),
...          skchem.Mol.from_smiles('CCCC', name='butane'),
...          skchem.Mol.from_smiles('NC(C)C(=O)O', name='alanine'),
...          skchem.Mol.from_smiles('C12C=CC(C=C2)C=C1', name='barrelene')
... ]
```

```
>>> mf = skchem.filters.MassFilter(above=31, below=100)
```

```
>>> mf.transform(data)
ethane       False
butane        True
alanine       True
barrelene    False
Name: mass_in_range, dtype: bool
```

```
>>> mf.filter(data)
butane             <Mol: CCCC>
alanine    <Mol: CC(N)C(=O)O>
Name: structure, dtype: object
```

columns

class skchem.filters.simple.**OrganicFilter**(*n_jobs=1*, *verbose=True*)

Bases: *skchem.filters.simple.ElementFilter*

Whether a molecule is organic.

For the purpose of this function, an organic molecule is defined as having atoms with elements only in the set H, B, C, N, O, F, P, S, Cl, Br, I.

Examples

Basic usage as a function on molecules: >>> import skchem >>> of = skchem.filters.OrganicFilter() >>> benzene = skchem.Mol.from_smiles('c1ccccc1', name='benzene')

```
>>> of.transform(benzene)
True
```

```
>>> ferrocene = skchem.Mol.from_smiles('[cH-]1cccc1.[cH-]1cccc1.[Fe+2]',
...                                    name='ferrocene')
>>> of.transform(ferrocene)
False
```

More useful on collections:

```
>>> sa = skchem.Mol.from_smiles('CC(=O)[O-].[Na+]', name='sodium acetate')
>>> norbornane = skchem.Mol.from_smiles('C12CCC(C2)CC1', name='norbornane')
```

```
>>> data = [benzene, ferrocene, norbornane, sa]
>>> of.transform(data)
benzene            True
ferrocene         False
norbornane         True
sodium acetate    False
dtype: bool
```

```
>>> of.filter(data)
benzene          <Mol: c1ccccc1>
norbornane    <Mol: C1CC2CCC1C2>
Name: structure, dtype: object
```

```
>>> of.filter(data, neg=True)
ferrocene         <Mol: [Fe+2].c1cc[cH-]c1.c1cc[cH-]c1>
sodium acetate                  <Mol: CC(=O)[O-].[Na+]>
Name: structure, dtype: object
```

skchem.filters.simple.**mass**(*mol*, *above=10*, *below=900*)

Whether a the molecular weight of a molecule is lower than a threshold.

above <= *mass* < *below*

Parameters

- **mol** – (skchem.Mol): The molecule to be tested.
- **above** (*float*) – The lower threshold on the mass. Defaults to None.
- **below** (*float*) – The higher threshold on the mass. Defaults to None.

Returns Whether the mass of the molecule is lower than the threshold.

Return type bool

Examples

Basic usage as a function on molecules:

```
>>> import skchem
>>> m = skchem.Mol.from_smiles('c1ccccc1') # benzene has M_r = 78.
>>> skchem.filters.mass(m, above=70)
True
>>> skchem.filters.mass(m, above=80)
False
>>> skchem.filters.mass(m, below=80)
True
>>> skchem.filters.mass(m, below=70)
False
>>> skchem.filters.mass(m, above=70, below=80)
True
```

skchem.filters.simple.**n_atoms**(*mol*, *above=2*, *below=75*, *include_hydrogens=False*)

Whether the number of atoms in a molecule falls in a defined interval.

```
above <= n_atoms < below
```

Parameters

- **mol** – (skchem.Mol): The molecule to be tested.
- **above** (*int*) – The lower threshold number of atoms (exclusive).
- **below** (*int*) – The higher threshold number of atoms (inclusive).
- **include_hydrogens** (*bool*) – Whether to consider hydrogens in the atom count.

Returns Whether the molecule has more atoms than the threshold.

Return type bool

Examples

Basic usage as a function on molecules:

```
>>> import skchem
>>> m = skchem.Mol.from_smiles('c1ccccc1') # benzene has 6 atoms.
```

Lower threshold:

```
>>> skchem.filters.n_atoms(m, above=3)
True
>>> skchem.filters.n_atoms(m, above=8)
False
```

Higher threshold:

```
>>> skchem.filters.n_atoms(m, below=8)
True
>>> skchem.filters.n_atoms(m, below=3)
False
```

Bounds work like Python slices - inclusive lower, exclusive upper:

```
>>> skchem.filters.n_atoms(m, above=6)
True
>>> skchem.filters.n_atoms(m, below=6)
False
```

Both can be used at once:

```
>>> skchem.filters.n_atoms(m, above=3, below=8)
True
```

Can include hydrogens:

```
>>> skchem.filters.n_atoms(m, above=3, below=8, include_hydrogens=True)
False
>>> skchem.filters.n_atoms(m, above=9, below=14, include_hydrogens=True)
True
```

skchem.filters.smarts module

skchem.filters.smarts

Module defines SMARTS filters.

class skchem.filters.smarts.**PAINSFilter**(*n_jobs=1*, *verbose=True*)

Bases: *skchem.filters.smarts.SMARTSFilter*

Whether a molecule passes the Pan Assay INterference (PAINS) filters.

These are supplied with RDKit, and were originally proposed by Baell et al.

_pains

pd.Series – a series of smarts template molecules.

References

[The original paper](http://dx.doi.org/10.1021/jm901137j)

Examples

Basic usage as a function on molecules:

```
>>> import skchem
>>> benzene = skchem.Mol.from_smiles('c1ccccc1', name='benzene')
>>> pf = skchem.filters.PAINSFilter()
>>> pf.transform(benzene)
True
>>> catechol = skchem.Mol.from_smiles('Oc1c(O)cccc1', name='catechol')
>>> pf.transform(catechol)
False
```

```
>>> res = pf.transform(catechol, agg=False)
>>> res[res]
names
catechol_A(92)    True
Name: PAINSFilter, dtype: bool
```

More useful in combination with pandas DataFrames:

```
>>> data = [benzene, catechol]
>>> pf.transform(data)
benzene      True
catechol    False
dtype: bool
```

```
>>> pf.filter(data)
benzene    <Mol: c1ccccc1>
Name: structure, dtype: object
```

class skchem.filters.smarts.**SMARTSFilter**(*smarts*, *agg='any'*, *merge_hs=True*, *n_jobs=1*, *verbose=True*)

Bases: *skchem.filters.base.Filter*

Filter a molecule based on smarts.

Examples

```
>>> import skchem
```

```
>>> data = [
...         skchem.Mol.from_smiles('CC', name='ethane'),
...         skchem.Mol.from_smiles('c1ccccc1', name='benzene'),
...         skchem.Mol.from_smiles('c1ccccc1-c2c(C=O)ccnc2', name='bg')
... ]
```

```
>>> f = skchem.filters.SMARTSFilter({'benzene': 'c1ccccc1',
...                                  'pyridine': 'c1ccccn1',
...                                  'acetyl': 'C=O'})
>>> f.transform(data, agg=False)
        acetyl benzene pyridine
ethane   False   False    False
benzene  False    True    False
bg        True    True     True
```

```
>>> f.transform(data)
ethane     False
benzene     True
bg          True
dtype: bool
```

```
>>> f.filter(data)
benzene                 <Mol: c1ccccc1>
bg         <Mol: O=Cc1ccncc1-c1ccccc1>
Name: structure, dtype: object
```

```
>>> f.agg = all
>>> f.filter(data)
bg    <Mol: O=Cc1ccncc1-c1ccccc1>
Name: structure, dtype: object
```

columns

skchem.filters.stereo module

skchem.filters.stereo

Stereo filters for scikit-chem.

class skchem.filters.stereo.**ChiralFilter**(*check_meso=True*, *n_jobs=1*, *verbose=True*)

Bases: *skchem.filters.base.Filter*

Filter chiral compounds.

Examples

```
>>> import skchem
>>> cf = skchem.filters.ChiralFilter()
>>> ms = [
...     skchem.Mol.from_smiles('F[C@@H](F)[C@H](F)F', name='achiral'),
...     skchem.Mol.from_smiles('F[C@@H](Br)[C@H](Br)F', name='chiral'),
...     skchem.Mol.from_smiles('F[C@H](Br)[C@H](Br)F', name='meso'),
```

```
...     skchem.Mol.from_smiles('FC(Br)C(Br)F', name='racemic')
... ]
>>> cf.transform(ms)
achiral     False
chiral       True
meso        False
racemic     False
Name: is_chiral, dtype: bool
```

columns

static is_meso(*mol*)

Determines whether the molecule is meso.

Meso compounds have chiral centres, but has a mirror plane allowing superposition.

Examples

```
>>> import skchem
```

```
>>> cf = skchem.filters.ChiralFilter()
```

```
>>> meso = skchem.Mol.from_smiles('F[C@H](Br)[C@H](Br)F')
```

```
>>> cf.is_meso(meso)
True
```

```
>>> non_meso = skchem.Mol.from_smiles('F[C@H](Br)[C@@H](Br)F')
>>> cf.is_meso(non_meso)
False
```

Module contents

skchem.filters

Molecule filters for scikit-chem.

class skchem.filters.**ChiralFilter**(*check_meso=True*, *n_jobs=1*, *verbose=True*)

Bases: *skchem.filters.base.Filter*

Filter chiral compounds.

Examples

```
>>> import skchem
>>> cf = skchem.filters.ChiralFilter()
>>> ms = [
...     skchem.Mol.from_smiles('F[C@@H](F)[C@H](F)F', name='achiral'),
...     skchem.Mol.from_smiles('F[C@@H](Br)[C@H](Br)F', name='chiral'),
...     skchem.Mol.from_smiles('F[C@H](Br)[C@H](Br)F', name='meso'),
...     skchem.Mol.from_smiles('FC(Br)C(Br)F', name='racemic')
... ]
```

```
>>> cf.transform(ms)
achiral    False
chiral      True
meso       False
racemic    False
Name: is_chiral, dtype: bool
```

columns

static is_meso (*mol*)

Determines whether the molecule is meso.

Meso compounds have chiral centres, but has a mirror plane allowing superposition.

Examples

```
>>> import skchem
```

```
>>> cf = skchem.filters.ChiralFilter()
```

```
>>> meso = skchem.Mol.from_smiles('F[C@H](Br)[C@H](Br)F')
```

```
>>> cf.is_meso(meso)
True
```

```
>>> non_meso = skchem.Mol.from_smiles('F[C@H](Br)[C@@H](Br)F')
>>> cf.is_meso(non_meso)
False
```

class skchem.filters.**SMARTSFilter** (*smarts*, *agg='any'*, *merge_hs=True*, *n_jobs=1*, *verbose=True*)

Bases: *skchem.filters.base.Filter*

Filter a molecule based on smarts.

Examples

```
>>> import skchem
```

```
>>> data = [
...          skchem.Mol.from_smiles('CC', name='ethane'),
...          skchem.Mol.from_smiles('c1ccccc1', name='benzene'),
...          skchem.Mol.from_smiles('c1ccccc1-c2c(C=O)ccnc2', name='bg')
... ]
```

```
>>> f = skchem.filters.SMARTSFilter({'benzene': 'c1ccccc1',
...                                  'pyridine': 'c1ccccn1',
...                                  'acetyl': 'C=O'})
>>> f.transform(data, agg=False)
        acetyl benzene pyridine
ethane   False   False    False
benzene  False    True    False
bg        True    True     True
```

```
>>> f.transform(data)
ethane     False
benzene     True
bg          True
dtype: bool
```

```
>>> f.filter(data)
benzene                 <Mol: c1ccccc1>
bg         <Mol: O=Cc1ccncc1-c1ccccc1>
Name: structure, dtype: object
```

```
>>> f.agg = all
>>> f.filter(data)
bg    <Mol: O=Cc1ccncc1-c1ccccc1>
Name: structure, dtype: object
```

columns

class skchem.filters.**PAINSFilter**(*n_jobs=1*, *verbose=True*)

Bases: *skchem.filters.smarts.SMARTSFilter*

Whether a molecule passes the Pan Assay INterference (PAINS) filters.

These are supplied with RDKit, and were originally proposed by Baell et al.

_pains

pd.Series – a series of smarts template molecules.

References

[The original paper](http://dx.doi.org/10.1021/jm901137j)

Examples

Basic usage as a function on molecules:

```
>>> import skchem
>>> benzene = skchem.Mol.from_smiles('c1ccccc1', name='benzene')
>>> pf = skchem.filters.PAINSFilter()
>>> pf.transform(benzene)
True
>>> catechol = skchem.Mol.from_smiles('Oc1c(O)cccc1', name='catechol')
>>> pf.transform(catechol)
False
```

```
>>> res = pf.transform(catechol, agg=False)
>>> res[res]
names
catechol_A(92)    True
Name: PAINSFilter, dtype: bool
```

More useful in combination with pandas DataFrames:

```
>>> data = [benzene, catechol]
>>> pf.transform(data)
```

```
benzene      True
catechol    False
dtype: bool
```

```
>>> pf.filter(data)
benzene    <Mol: c1ccccc1>
Name: structure, dtype: object
```

class skchem.filters.**ElementFilter**(*elements=None*, *as_bits=False*, *agg='any'*, *n_jobs=1*, *verbose=True*)

Bases: *skchem.filters.base.Filter*

Filter by elements.

Examples

Basic usage on molecules:

```
>>> import skchem
>>> hal_f = skchem.filters.ElementFilter(['F', 'Cl', 'Br', 'I'])
```

Molecules with one of the atoms transform to *True*.

```
>>> m1 = skchem.Mol.from_smiles('ClC(Cl)Cl', name='chloroform')
>>> hal_f.transform(m1)
True
```

Molecules with none of the atoms transform to *False*.

```
>>> m2 = skchem.Mol.from_smiles('CC', name='ethane')
>>> hal_f.transform(m2)
False
```

Can see the atom breakdown by passing *agg* == *False*: >>> hal_f.transform(m1, agg=False) has_element F 0 Cl 3 Br 0 I 0 Name: ElementFilter, dtype: int64

Can transform series.

```
>>> ms = [m1, m2]
>>> hal_f.transform(ms)
chloroform     True
ethane        False
dtype: bool
```

```
>>> hal_f.transform(ms, agg=False)
has_element  F  Cl  Br  I
chloroform   0   3   0  0
ethane       0   0   0  0
```

Can also filter series:

```
>>> hal_f.filter(ms)
chloroform    <Mol: ClC(Cl)Cl>
Name: structure, dtype: object
```

```
>>> hal_f.filter(ms, neg=True)
ethane    <Mol: CC>
Name: structure, dtype: object
```

columns

elements

class skchem.filters.**OrganicFilter**(*n_jobs=1*, *verbose=True*)
Bases: *skchem.filters.simple.ElementFilter*

Whether a molecule is organic.

For the purpose of this function, an organic molecule is defined as having atoms with elements only in the set H, B, C, N, O, F, P, S, Cl, Br, I.

Examples

Basic usage as a function on molecules: >>> import skchem >>> of = skchem.filters.OrganicFilter() >>> benzene = skchem.Mol.from_smiles('c1ccccc1', name='benzene')

```
>>> of.transform(benzene)
True
```

```
>>> ferrocene = skchem.Mol.from_smiles('[cH-]1cccc1.[cH-]1cccc1.[Fe+2]',
...                                    name='ferrocene')
>>> of.transform(ferrocene)
False
```

More useful on collections:

```
>>> sa = skchem.Mol.from_smiles('CC(=O)[O-].[Na+]', name='sodium acetate')
>>> norbornane = skchem.Mol.from_smiles('C12CCC(C2)CC1', name='norbornane')
```

```
>>> data = [benzene, ferrocene, norbornane, sa]
>>> of.transform(data)
benzene            True
ferrocene         False
norbornane         True
sodium acetate    False
dtype: bool
```

```
>>> of.filter(data)
benzene          <Mol: c1ccccc1>
norbornane    <Mol: C1CC2CCC1C2>
Name: structure, dtype: object
```

```
>>> of.filter(data, neg=True)
ferrocene         <Mol: [Fe+2].c1cc[cH-]c1.c1cc[cH-]c1>
sodium acetate                 <Mol: CC(=O)[O-].[Na+]>
Name: structure, dtype: object
```

class skchem.filters.**AtomNumberFilter**(*above=3*, *below=60*, *include_hydrogens=False*, *n_jobs=1*, *verbose=True*)
Bases: *skchem.filters.base.Filter*

Filter whether the number of atoms in a Mol falls in a defined interval.

above <= *n_atoms* < *below*

Examples

```
>>> import skchem
```

```
>>> data = [
...          skchem.Mol.from_smiles('CC', name='ethane'),
...          skchem.Mol.from_smiles('CCCC', name='butane'),
...          skchem.Mol.from_smiles('NC(C)C(=O)O', name='alanine'),
...          skchem.Mol.from_smiles('C12C=CC(C=C2)C=C1', name='barrelene')
... ]
```

```
>>> af = skchem.filters.AtomNumberFilter(above=3, below=7)
```

```
>>> af.transform(data)
ethane       False
butane        True
alanine       True
barrelene    False
Name: num_atoms_in_range, dtype: bool
```

```
>>> af.filter(data)
butane             <Mol: CCCC>
alanine    <Mol: CC(N)C(=O)O>
Name: structure, dtype: object
```

```
>>> af = skchem.filters.AtomNumberFilter(above=5, below=15, include_
↪hydrogens=True)
```

```
>>> af.transform(data)
ethane        True
butane        True
alanine       True
barrelene    False
Name: num_atoms_in_range, dtype: bool
```

columns

class skchem.filters.**MassFilter**(*above=3*, *below=900*, *n_jobs=1*, *verbose=True*)

Bases: *skchem.filters.base.Filter*

Filter whether the molecular weight of a molecule is outside a range.

above <= *mass* < *below*

Examples

```
>>> import skchem
```

```
>>> data = [
...          skchem.Mol.from_smiles('CC', name='ethane'),
...          skchem.Mol.from_smiles('CCCC', name='butane'),
```

```
...         skchem.Mol.from_smiles('NC(C)C(=O)O', name='alanine'),
...         skchem.Mol.from_smiles('C12C=CC(C=C2)C=C1', name='barrelene')
... ]
```

```
>>> mf = skchem.filters.MassFilter(above=31, below=100)
```

```
>>> mf.transform(data)
ethane       False
butane        True
alanine       True
barrelene    False
Name: mass_in_range, dtype: bool
```

```
>>> mf.filter(data)
butane             <Mol: CCCC>
alanine    <Mol: CC(N)C(=O)O>
Name: structure, dtype: object
```

columns

class skchem.filters.**Filter**(*func=None*, *agg='any'*, *n_jobs=1*, *verbose=True*)

Bases: *skchem.filters.base.BaseFilter*, *skchem.base.Transformer*

Filter base class.

Examples

```
>>> import skchem
```

Initialize the filter with a function: >>> is_named = skchem.filters.Filter(lambda m: m.name is not None)

Filter results can be found with *transform*: >>> ethane = skchem.Mol.from_smiles('CC', name='ethane') >>> is_named.transform(ethane) True

```
>>> anonymous = skchem.Mol.from_smiles('c1ccccc1')
>>> is_named.transform(anonymous)
False
```

Can take a series or dataframe: >>> mols = pd.Series({'anonymous': anonymous, 'ethane': ethane}) >>> is_named.transform(mols) anonymous False ethane True Name: Filter, dtype: bool

Using *filter* will drop out molecules that fail the test: >>> is_named.filter(mols) ethane <Mol: CC> dtype: object

Only failed are retained with the *neg* keyword argument: >>> is_named.filter(mols, neg=True) anonymous <Mol: c1ccccc1> dtype: object

skchem.forcefields package

Submodules

skchem.forcefields.base module

skchem.forcefields.base

Module specifying base class for forcefields.

class skchem.forcefields.base.**ForceField**(*preembed=True*, *warn_on_fail=True*, *error_on_fail=False*, *add_hs=True*, *n_jobs=1*, *verbose=True*)

Bases: *skchem.base.Transformer*, *skchem.filters.base.TransformFilter*

Base forcefield class.

Filter drops those that fail to be optimized.

columns

embed(*mol*)

class skchem.forcefields.base.**RoughEmbedding**(*preembed=True*, *warn_on_fail=True*, *error_on_fail=False*, *add_hs=True*, *n_jobs=1*, *verbose=True*)

Bases: *skchem.forcefields.base.ForceField*

skchem.forcefields.mmff module

skchem.forcefields.mmff

Module specifying the Merck Molecular Force Field.

class skchem.forcefields.mmff.**MMFF**(*preembed=True*, *warn_on_fail=True*, *error_on_fail=False*, *add_hs=True*, *n_jobs=1*, *verbose=True*)

Bases: *skchem.forcefields.base.ForceField*

Merck Molecular Force Field transformer.

skchem.forcefields.uff module

skchem.forcefields.uff

Module specifying the universal force field.

class skchem.forcefields.uff.**UFF**(*preembed=True*, *warn_on_fail=True*, *error_on_fail=False*, *add_hs=True*, *n_jobs=1*, *verbose=True*)

Bases: *skchem.forcefields.base.ForceField*

Universal Force Field transformer.

Module contents

skchem.forcefields

Module specifying forcefields.

class skchem.forcefields.**MMFF**(*preembed=True*, *warn_on_fail=True*, *error_on_fail=False*, *add_hs=True*, *n_jobs=1*, *verbose=True*)

Bases: *skchem.forcefields.base.ForceField*

Merck Molecular Force Field transformer.

class skchem.forcefields.**UFF**(*preembed=True*, *warn_on_fail=True*, *error_on_fail=False*, *add_hs=True*, *n_jobs=1*, *verbose=True*)

Bases: *skchem.forcefields.base.ForceField*

Universal Force Field transformer.

class skchem.forcefields.**RoughEmbedding**(*preembed=True*, *warn_on_fail=True*, *error_on_fail=False*, *add_hs=True*, *n_jobs=1*, *verbose=True*)
Bases: *skchem.forcefields.base.ForceField*

skchem.interact package

Submodules

skchem.interact.desc_vis module

class skchem.interact.desc_vis.**Visualizer**(*fper='morgan'*, *smiles='c1ccccc1O'*, *dpi=200*)
Bases: object

calculate()

current_bit

current_smiles

display()

dpi

static initialize_ipython()

mol

plot(_)

typing(_)

update_dropdown()

update_smiles(_)

Module contents

skchem.interact

Tools for use in the JuPyteR notebook for scikit-chem.

class skchem.interact.**Visualizer**(*fper='morgan'*, *smiles='c1ccccc1O'*, *dpi=200*)
Bases: object

calculate()

current_bit

current_smiles

display()

dpi

static initialize_ipython()

mol

plot(_)

typing(_)

update_dropdown()

update_smiles(_)

skchem.io package

Submodules

skchem.io.sdf module

skchem.io.sdf

Defining input and output operations for sdf files.

skchem.io.sdf.**read_sdf**(*sdf*, *error_bad_mol=False*, *warn_bad_mol=True*, *nmols=None*, *skipmols=None*, *skipfooter=None*, *read_props=True*, *mol_props=False*, **args*, ***kwargs*)

Read an sdf file into a *pd.DataFrame*.

The function wraps the RDKit *ForwardSDMolSupplier* object.

Parameters

- **sdf** (*str or file-like*) – The location of data to load as a file path, or a file-like object.
- **error_bad_mol** (*bool*) – Whether an error should be raised if a molecule fails to parse. Default is False.
- **warn_bad_mol** (*bool*) – Whether a warning should be output if a molecule fails to parse. Default is True.
- **nmols** (*int*) – The number of molecules to read. If *None*, read all molecules. Default is *None*.
- **skipmols** (*int*) – The number of molecules to skip at start. Default is *0*.
- **skipfooter** (*int*) – The number of molecules to skip from the end. Default is *0*.
- **read_props** (*bool*) – Whether to read the properties into the data frame. Default is *True*.
- **mol_props** (*bool*) – Whether to keep properties in the molecule dictionary after they are extracted to the DataFrame. Default is *False*.
- **kwargs** (*args,*) – Arguments will be passed to RDKit ForwardSDMolSupplier.

Returns The loaded data frame, with Mols supplied in the *structure* field.

Return type pandas.DataFrame

See also:

rdkit.Chem.SDForwardMolSupplier skchem.read_smiles

skchem.io.sdf.**write_sdf**(*data*, *sdf*, *write_cols=True*, *index_as_name=True*, *mol_props=False*, **args*, ***kwargs*)

Write an sdf file from a dataframe.

Parameters

- **data** (*pandas.Series or pandas.DataFrame*) – Pandas data structure with a *structure* column containing compounds to serialize.

- **sdf** (*str or file-like*) – A file path or file-like object specifying where to write the compound data.
- **write_cols** (*bool*) – Whether columns should be written as props. Default *True*.
- **index_as_name** (*bool*) – Whether to use index as the header, or the molecule's name. Default is *True*.
- **mol_props** (*bool*) – Whether to write properties in the Mol dictionary in addition to fields in the frame.

Warn: This function will change the names of the compounds if the *index_as_name* argument is *True*, and will delete all properties in the molecule dictionary if *mol_props* is *False*.

skchem.io.smiles module

skchem.io.smiles

Defining input and output operations for smiles files.

skchem.io.smiles.**read_smiles**(*smiles_file*, *smiles_column=0*, *name_column=None*, *delimiter='\t'*, *title_line=False*, *error_bad_mol=False*, *warn_bad_mol=True*, *drop_bad_mol=True*, **args*, ***kwargs*)

Read a smiles file into a pandas dataframe.

The class wraps the pandas read_csv function.

smiles_file (str, file-like): Location of data to load, specified as a string or passed directly as a file-like object. URLs may also be used, see the pandas.read_csv documentation.

smiles_column (int): The column index at which SMILES are provided. Defaults to *0*.

name_column (int): The column index at which compound names are provided, for use as the index in the DataFrame. If None, use the default index. Defaults to *None*.

delimiter (str): The delimiter used. Defaults to *t*.

title_line (bool): Whether a title line is provided, to use as column titles. Defaults to *False*.

error_bad_mol (bool): Whether an error should be raised when a molecule fails to parse. Defaults to *False*.

warn_bad_mol (bool): Whether a warning should be raised when a molecule fails to parse. Defaults to *True*.

drop_bad_mol (bool): If true, drop any column with smiles that failed to parse. Otherwise, the field is None. Defaults to *True*.

args, kwargs: Arguments will be passed to pandas read_csv arguments.

Returns The loaded data frame, with Mols supplied in the *structure* field.

Return type pandas.DataFrame

See also:

pandas.read_csv skchem.Mol.from_smiles skchem.io.sdf

skchem.io.smiles.**write_smiles**(*data*, *smiles_path*)

Write a dataframe to a smiles file.

Parameters

- **data** (*pd.Series or pd.DataFrame*) – The dataframe to write.
- **smiles_path** (*str*) – The path to write the dataframe to.

Module contents

skchem.io

Module defining input and output methods in scikit-chem.

skchem.io.**read_sdf**(*sdf*, *error_bad_mol=False*, *warn_bad_mol=True*, *nmols=None*, *skipmols=None*, *skipfooter=None*, *read_props=True*, *mol_props=False*, **args*, ***kwargs*)

Read an sdf file into a *pd.DataFrame*.

The function wraps the RDKit *ForwardSDMolSupplier* object.

Parameters

- **sdf** (*str or file-like*) – The location of data to load as a file path, or a file-like object.
- **error_bad_mol** (*bool*) – Whether an error should be raised if a molecule fails to parse. Default is False.
- **warn_bad_mol** (*bool*) – Whether a warning should be output if a molecule fails to parse. Default is True.
- **nmols** (*int*) – The number of molecules to read. If *None*, read all molecules. Default is *None*.
- **skipmols** (*int*) – The number of molecules to skip at start. Default is *0*.
- **skipfooter** (*int*) – The number of molecules to skip from the end. Default is *0*.
- **read_props** (*bool*) – Whether to read the properties into the data frame. Default is *True*.
- **mol_props** (*bool*) – Whether to keep properties in the molecule dictionary after they are extracted to the DataFrame. Default is *False*.
- **kwargs** (*args,*) – Arguments will be passed to RDKit ForwardSDMolSupplier.

Returns The loaded data frame, with Mols supplied in the *structure* field.

Return type pandas.DataFrame

See also:

rdkit.Chem.SDForwardMolSupplier skchem.read_smiles

skchem.io.**write_sdf**(*data*, *sdf*, *write_cols=True*, *index_as_name=True*, *mol_props=False*, **args*, ***kwargs*)

Write an sdf file from a dataframe.

Parameters

- **data** (*pandas.Series or pandas.DataFrame*) – Pandas data structure with a *structure* column containing compounds to serialize.
- **sdf** (*str or file-like*) – A file path or file-like object specifying where to write the compound data.
- **write_cols** (*bool*) – Whether columns should be written as props. Default *True*.
- **index_as_name** (*bool*) – Whether to use index as the header, or the molecule's name. Default is *True*.
- **mol_props** (*bool*) – Whether to write properties in the Mol dictionary in addition to fields in the frame.

Warn: This function will change the names of the compounds if the *index_as_name* argument is *True*, and will delete all properties in the molecule dictionary if *mol_props* is *False*.

skchem.io.**read_smiles**(*smiles_file*, *smiles_column=0*, *name_column=None*, *delimiter='\t'*, *title_line=False*, *error_bad_mol=False*, *warn_bad_mol=True*, *drop_bad_mol=True*, **args*, ***kwargs*)

Read a smiles file into a pandas dataframe.

The class wraps the pandas read_csv function.

smiles_file (str, file-like): Location of data to load, specified as a string or passed directly as a file-like object. URLs may also be used, see the pandas.read_csv documentation.

smiles_column (int): The column index at which SMILES are provided. Defaults to *0*.

name_column (int): The column index at which compound names are provided, for use as the index in the DataFrame. If None, use the default index. Defaults to *None*.

delimiter (str): The delimiter used. Defaults to *t*.

title_line (bool): Whether a title line is provided, to use as column titles. Defaults to *False*.

error_bad_mol (bool): Whether an error should be raised when a molecule fails to parse. Defaults to *False*.

warn_bad_mol (bool): Whether a warning should be raised when a molecule fails to parse. Defaults to *True*.

drop_bad_mol (bool): If true, drop any column with smiles that failed to parse. Otherwise, the field is None. Defaults to *True*.

args, kwargs: Arguments will be passed to pandas read_csv arguments.

Returns The loaded data frame, with Mols supplied in the *structure* field.

Return type pandas.DataFrame

See also:

pandas.read_csv skchem.Mol.from_smiles skchem.io.sdf

skchem.io.**write_smiles**(*data*, *smiles_path*)

Write a dataframe to a smiles file.

Parameters

- **data** (*pd.Series or pd.DataFrame*) – The dataframe to write.
- **smiles_path** (*str*) – The path to write the dataframe to.

skchem.io.**read_config**(*conf*)

Deserialize an object from a config dict.

Parameters **conf** (*dict*) – The config dict to deseriailize.

Returns object

Note: *config* is different from *params*, in that it specifies the class. The *params* dict is a subdict in *config*.

---

skchem.io.**write_config**(*obj*)

Serialize an object to a config dict.

skchem.io.**read_yaml**(*conf*)

Deserialize an object from a yaml file, filename or str.

Parameters **yaml** (*str or filelike*) – The yaml file to deserialize.

Returns object

skchem.io.**write_yaml**(*obj*, *target=None*)
Serialize a scikit-chem object to yaml.

skchem.io.**read_json**(*conf*)
Deserialize an object from a json file, filename or str.

Parameters **json** (*str or filelike*) – The json file to deserialize.

Returns object

skchem.io.**write_json**(*obj*, *target=None*)
Serialize a scikit-chem object as json.

skchem.pandas_ext package

Submodules

skchem.pandas_ext.structure_methods module

skchem.pandas.structure_methods

Tools for adding a default attribute to pandas objects.

class skchem.pandas_ext.structure_methods.**StructureAccessorMixin**
Bases: object

Mixin to bind chemical methods to objects.

mol
alias of *StructureMethods*

class skchem.pandas_ext.structure_methods.**StructureMethods**(*data*)
Bases: pandas.core.base.NoNewAttributesMixin

Accessor for calling chemical methods on series of molecules.

add_hs(***kwargs*)

atoms

remove_hs(***kwargs*)

visualize(*fper='morgan'*, *dim_red='tsne'*, *dim_red_kw=None*, ***kwargs*)

skchem.pandas_ext.structure_methods.**only_contains_mols**(*ser*)

Module contents

skchem.pandas_ext

Tools for better integration with pandas.

skchem.pipeline package

Submodules

skchem.pipeline.pipeline module

skchem.pipeline.pipeline

Module implementing pipelines.

class skchem.pipeline.pipeline.**Pipeline**(*objects*)
Bases: object

Pipeline object. Applies filters and transformers in sequence.

copy()
Return a copy of this object.

classmethod from_params(*params*)
Create a instance from a params dictionary.

get_params()

to_dict()
Return a dictionary representation of the object.

to_json(*target=None*)
Serialize the object as JSON.

Parameters

- **target** (*str or file-like*) – A file or filepath to serialize the object to. If *None*, return the JSON as a string.
- **Returns** – None or str

to_yaml(*target=None*)
Serialize the object as YAML.

Parameters

- **target** (*str or file-like*) – A file or filepath to serialize the object to. If *None*, return the YAML as a string.
- **Returns** – None or str

transform_filter(*mols*, *y=None*)

skchem.pipeline.pipeline.**is_filter**(*obj*)
Whether an object is a Filter (by duck typing).

skchem.pipeline.pipeline.**is_transform_filter**(*obj*)
Whether an object is a TransformFilter (by duck typing).

skchem.pipeline.pipeline.**is_transformer**(*obj*)
Whether an object is a Transformer (by duck typing).

Module contents

skchem.pipeline

Package implementing pipelines.

class skchem.pipeline.**Pipeline**(*objects*)
Bases: object

Pipeline object. Applies filters and transformers in sequence.

copy()
Return a copy of this object.

classmethod from_params(*params*)
Create a instance from a params dictionary.

get_params()

to_dict()
Return a dictionary representation of the object.

to_json(*target=None*)
Serialize the object as JSON.

Parameters

- **target** (*str or file-like*) – A file or filepath to serialize the object to. If *None*, return the JSON as a string.
- **Returns** – None or str

to_yaml(*target=None*)
Serialize the object as YAML.

Parameters

- **target** (*str or file-like*) – A file or filepath to serialize the object to. If *None*, return the YAML as a string.
- **Returns** – None or str

transform_filter(*mols*, *y=None*)

skchem.resource package

Module contents

skchem.resource.**resource**(**args*)
passes a file path for a data resource specified

skchem.standardizers package

Submodules

skchem.standardizers.chemaxon module

skchem.standardizers.chemaxon

Module wrapping ChemAxon Standardizer. Must have standardizer installed and license activated.

class skchem.standardizers.chemaxon.**ChemAxonStandardizer**(*config_path=None*, *keep_failed=False*, ***kwargs*)
Bases: *skchem.base.CLIWrapper*, *skchem.base.BatchTransformer*, *skchem.base.Transformer*, *skchem.filters.base.TransformFilter*

ChemAxon Standardizer Wrapper.

Parameters **config_path** (*str*) – The path of the config_file. If None, use the default one.

Notes

ChemAxon Standardizer must be installed and accessible as *standardize* from the shell launching the program.

Warning: Must use a unique index (see #31).

Examples

```
>>> import skchem
>>> std = skchem.standardizers.ChemAxonStandardizer()
>>> m = skchem.Mol.from_smiles('CC.CCC')
>>> print(std.transform(m))
<Mol: CCC>
```

```
>>> data = [m, skchem.Mol.from_smiles('C=CO'), skchem.Mol.from_smiles('C[O-]')]
>>> std.transform(data)
0     <Mol: CCC>
1    <Mol: CC=O>
2      <Mol: CO>
Name: structure, dtype: object
```

```
>>> will_fail = mol = '''932-97-8
...      RDKit          3D
...
...   9  9  0  0  0  0  0  0  0  0999 V2000
...    -0.9646    0.0000    0.0032 C   0  0  0  0  0  0  0  0  0  0  0  0
...    -0.2894   -1.2163    0.0020 C   0  0  0  0  0  0  0  0  0  0  0  0
...    -0.2894    1.2163    0.0025 C   0  0  0  0  0  0  0  0  0  0  0  0
...    -2.2146    0.0000   -0.0004 N   0  0  0  0  0  0  0  0  0  0  0  0
...     1.0710   -1.2610    0.0002 C   0  0  0  0  0  0  0  0  0  0  0  0
...     1.0710    1.2610    0.0007 C   0  0  0  0  0  0  0  0  0  0  0  0
...    -3.3386    0.0000   -0.0037 N   0  0  0  0  0  0  0  0  0  0  0  0
...     1.8248    0.0000   -0.0005 C   0  0  0  0  0  0  0  0  0  0  0  0
...     3.0435    0.0000   -0.0026 O   0  0  0  0  0  0  0  0  0  0  0  0
...   1  2  1  0
...   1  3  1  0
...   1  4  2  3
...   2  5  2  0
...   3  6  2  0
...   4  7  2  0
...   5  8  1  0
...   8  9  2  0
...   6  8  1  0
... M  CHG  2   4   1   7  -1
... M  END
... '''
```

```
>>> will_fail = skchem.Mol.from_molblock(will_fail)
>>> std.transform(will_fail)
nan
```

```
>>> data = [will_fail] + data
```

```
>>> std.transform(data)
0           None
1     <Mol: CCC>
2    <Mol: CC=O>
3      <Mol: CO>
Name: structure, dtype: object
```

```
>>> std.transform_filter(data)
1     <Mol: CCC>
2    <Mol: CC=O>
3      <Mol: CO>
Name: structure, dtype: object
```

```
>>> std.keep_failed = True
>>> std.transform(data)
0    <Mol: [N-]=[N+]=C1C=CC(=O)C=C1>
1                        <Mol: CCC>
2                       <Mol: CC=O>
3                         <Mol: CO>
Name: structure, dtype: object
```

DEFAULT_CONFIG = '/home/docs/checkouts/readthedocs.org/user_builds/scikit-chem/checkouts/latest/skchem/standardiz

columns

filter(**args*, ***kwargs*)

install_hint = ' Install ChemAxon from https://www.chemaxon.com. It requires a license,\n which can be freely obtai

monitor_progress(*filename*)

static validate_install()
Check if we can call cxcalc.

Module contents

class skchem.standardizers.**ChemAxonStandardizer**(*config_path=None*, *keep_failed=False*, ***kwargs*)

Bases: *skchem.base.CLIWrapper*, *skchem.base.BatchTransformer*, *skchem.base.Transformer*, *skchem.filters.base.TransformFilter*

ChemAxon Standardizer Wrapper.

Parameters **config_path** (*str*) – The path of the config_file. If None, use the default one.

Notes

ChemAxon Standardizer must be installed and accessible as *standardize* from the shell launching the program.

Warning: Must use a unique index (see #31).

Examples

```
>>> import skchem
>>> std = skchem.standardizers.ChemAxonStandardizer()
>>> m = skchem.Mol.from_smiles('CC.CCC')
>>> print(std.transform(m))
<Mol: CCC>
```

```
>>> data = [m, skchem.Mol.from_smiles('C=CO'), skchem.Mol.from_smiles('C[O-]')]
>>> std.transform(data)
0     <Mol: CCC>
1    <Mol: CC=O>
2      <Mol: CO>
Name: structure, dtype: object
```

```
>>> will_fail = mol = '''932-97-8
...      RDKit           3D
...
...   9  9  0  0  0  0  0  0  0  0999 V2000
...    -0.9646    0.0000    0.0032 C   0  0  0  0  0  0  0  0  0  0  0  0
...    -0.2894   -1.2163    0.0020 C   0  0  0  0  0  0  0  0  0  0  0  0
...    -0.2894    1.2163    0.0025 C   0  0  0  0  0  0  0  0  0  0  0  0
...    -2.2146    0.0000   -0.0004 N   0  0  0  0  0  0  0  0  0  0  0  0
...     1.0710   -1.2610    0.0002 C   0  0  0  0  0  0  0  0  0  0  0  0
...     1.0710    1.2610    0.0007 C   0  0  0  0  0  0  0  0  0  0  0  0
...    -3.3386    0.0000   -0.0037 N   0  0  0  0  0  0  0  0  0  0  0  0
...     1.8248    0.0000   -0.0005 C   0  0  0  0  0  0  0  0  0  0  0  0
...     3.0435    0.0000   -0.0026 O   0  0  0  0  0  0  0  0  0  0  0  0
...   1  2  1  0
...   1  3  1  0
...   1  4  2  3
...   2  5  2  0
...   3  6  2  0
...   4  7  2  0
...   5  8  1  0
...   8  9  2  0
...   6  8  1  0
... M  CHG  2   4   1   7  -1
... M  END
... '''
```

```
>>> will_fail = skchem.Mol.from_molblock(will_fail)
>>> std.transform(will_fail)
nan
```

```
>>> data = [will_fail] + data
```

```
>>> std.transform(data)
0          None
1     <Mol: CCC>
2    <Mol: CC=O>
```

```
3      <Mol: CO>
Name: structure, dtype: object
```

```
>>> std.transform_filter(data)
1     <Mol: CCC>
2    <Mol: CC=O>
3      <Mol: CO>
Name: structure, dtype: object
```

```
>>> std.keep_failed = True
>>> std.transform(data)
0    <Mol: [N-]=[N+]=C1C=CC(=O)C=C1>
1                          <Mol: CCC>
2                         <Mol: CC=O>
3                           <Mol: CO>
Name: structure, dtype: object
```

DEFAULT_CONFIG = '/home/docs/checkouts/readthedocs.org/user_builds/scikit-chem/checkouts/latest/skchem/standardiz

columns

filter(**args*, ***kwargs*)

install_hint = ' Install ChemAxon from https://www.chemaxon.com. It requires a license,\n which can be freely obtai

monitor_progress(*filename*)

static validate_install()
Check if we can call cxcalc.

skchem.test package

Subpackages

skchem.test.test_cross_validation package

Submodules

skchem.test.test_cross_validation.test_similarity_threshold module

skchem.tests.test_cross_validation.test_similarity_threshold

Tests for similarity threshold dataset partitioning functionality.

skchem.test.test_cross_validation.test_similarity_threshold.**cv**(*x*)

skchem.test.test_cross_validation.test_similarity_threshold.**test_k_fold**(*cv*, *x*)

skchem.test.test_cross_validation.test_similarity_threshold.**test_split**(*cv*, *x*)

skchem.test.test_cross_validation.test_similarity_threshold.**x**()

Module contents

skchem.test.test_cross_validation

Tests for cross validation functionality.

skchem.test.test_data package

Submodules

skchem.test.test_data.test_data module

Tests for data functions

skchem.test.test_data.test_data.**test_resource**()
Does resource target the the methane smiles test file?

Module contents

skchem.test.test_filters package

Submodules

skchem.test.test_filters.test_filters module

skchem.test.test_filters.test_filters.**f**()

skchem.test.test_filters.test_filters.**m**()

skchem.test.test_filters.test_filters.**ms**()

skchem.test.test_filters.test_filters.**test_filter**(*ms*, *f*)

skchem.test.test_filters.test_filters.**test_takes_dict**(*m*, *f*)

skchem.test.test_filters.test_filters.**test_takes_list**(*m*, *f*)

skchem.test.test_filters.test_filters.**test_takes_mol**(*m*, *f*)

skchem.test.test_filters.test_filters.**test_takes_mol_transform**(*m*, *f*)

skchem.test.test_filters.test_filters.**test_takes_ser**(*m*, *f*)

Module contents

skchem.test.test_io package

Submodules

skchem.test.test_io.test_sdf module

Tests for sdf io functionality

class skchem.test.test_io.test_sdf.**TestSDF**
Bases: object

Test class for sdf file parser

test_arg_forwarding()
Check that kwargs can still be parsed to the rdkit object

test_bad_structure()
Does it throw an error if bad structures are given?

test_file_correct_structure()
When opened with a file-like object, is the structure correct? Done by checking atom number (should be one, as rdkit ignores Hs by default

test_multi_diff_properties()
if there are properties not common for all, are they all detected?

test_multi_index_correct()
is it the right index?

test_multi_index_detected()
Is index set?

test_multi_parsed()
Do we find right number of molecules?

test_opening_with_file()
Can an sdf file be opened with a file-like object?

test_opening_with_path()
Do we find a molecule in example file?

test_path_correct_structure()
When opened with a path, is the structure correct?

test_single_index_correct()
is name correct?

test_single_index_detected()
Does molecule have a name set to index?

test_single_properties_correct()
Are they the right properties?

test_single_properties_detected()
Does the dataframe have properties?

skchem.test.test_io.test_smiles module

Tests for smiles io functionality

class skchem.test.test_io.test_smiles.**TestSmiles**
Bases: object

Test smiles io functionality

test_bad_chemistry()
Does it throw an error without force?

test_bad_chemistry_force()
Can we force the parse?

test_bad_smiles()
Does it throw an error for an improper smiles code?

test_change_smiles_column()
Does it work with smiles at different positions

test_configure_header()
Can you pass header directly through to pandas?

test_header_correct()
Is the header line correctly set?

test_multiple_parsed()
Do we find the exact number of molecules expected in a multi molecule smiles file?

test_name_column()
Can it set the index?

test_properties()
Can we read other properties?

test_single_parsed()
Do we find a molecule in a single smiles file

test_title_line()
Test parsing a smiles file with a header.

Module contents

skchem.test.test_standardizers package

Submodules

skchem.test.test_standardizers.test_chemaxon module

skchem.test.test_standardizers.test_chemaxon.**m**()

skchem.test.test_standardizers.test_chemaxon.**s**()

skchem.test.test_standardizers.test_chemaxon.**test_on_mol**(*s*, *m*)

skchem.test.test_standardizers.test_chemaxon.**test_on_series**(*s*, *m*)

Module contents

Submodules

skchem.test.test_featurizers module

skchem.test.test_featurizers.**a**(*m*)

skchem.test.test_featurizers.**af**()

skchem.test.test_featurizers.**m**()

skchem.test.test_featurizers.**s**(*m*)

skchem.test.test_featurizers.**test_af**(*af*)

skchem.test.test_featurizers.**test_on_a**(*af*, *a*)

skchem.test.test_featurizers.**test_on_m**(*af*, *m*)

skchem.test.test_featurizers.**test_on_ser**(*af*, *s*)

Module contents

skchem.test

Tests for scikit-chem

class skchem.test.**FakeConfig**
Bases: object

getoption(*arg*)

skchem.utils package

Submodules

skchem.utils.decorators module

skchem.utils.helpers module

skchem.utils.helpers

Module providing helper functions for scikit-chem

class skchem.utils.helpers.**Defaults**(*defaults*)
Bases: object

get(*val*)

skchem.utils.helpers.**iterable_to_series**(*mols*)

skchem.utils.helpers.**nanarray**(*shape*)
Produce an array of NaN in provided shape.

Parameters **shape** (*tuple*) – The shape of the nan array to produce.

Returns np.array

skchem.utils.helpers.**optional_second_method**(*func*)

skchem.utils.helpers.**squeeze**(*data*, *axis=None*)
Squeeze dimension for length 1 arrays.

Parameters

- **data** (*pd.Series or pd.DataFrame or pd.Panel*) – The pandas object to squeeze.
- **axis** (*int or tuple*) – The axes along which to squeeze.

Returns pd.Series or pd.DataFrame

skchem.utils.io module

skchem.utils.io

IO helper functions for skchem.

skchem.utils.io.**json_dump**(*obj*, *target=None*)
Write object as json to file or stream, or return as string.

skchem.utils.io.**line_count**(*filename*)
Quickly count the number of lines in a file.

Adapted from http://stackoverflow.com/questions/845058/how-to-get-line-count-cheaply-in-python

Parameters **filename** (*str*) – The name of the file to count for.

skchem.utils.io.**sdf_count**(*filename*)
Efficiently count molecules in an sdf file.

Specifically, the function counts the number of times '$$$$' occurs at the start of lines in the file.

Parameters **filename** (*str*) – The filename of the sdf file.

Returns the number of molecules in the file.

Return type int

skchem.utils.io.**yaml_dump**(*obj*, *target=None*)
Write object as yaml to file or stream, or return as string.

skchem.utils.progress module

skchem.utils.progress

Module implementing progress bars.

class skchem.utils.progress.**DummyProgressBar**(**args*, ***kwargs*)
Bases: object

finish()

update(*val*)

class skchem.utils.progress.**NamedProgressBar**(*name=None*, ***kwargs*)
Bases: progressbar.bar.ProgressBar

default_widgets()

skchem.utils.string module

skchem.utils.string.**camel_to_snail**(*s*)
Convert CamelCase to snail_case.

skchem.utils.string.**free_to_snail**(*s*)
Convert Free Case to snail_case.

skchem.utils.suppress module

skchem.utils.suppress

Class for suppressing C extensions output.

class skchem.utils.suppress.**Suppressor**
Bases: object

A context manager for doing a "deep suppression" of stdout and stderr.

It will suppress all print, even if the print originates in a compiled C/Fortran sub-function.

This will not suppress raised exceptions, since exceptions are printed to stderr just before a script exits, and after the context manager has exited (at least, I think that is why it lets exceptions through).

null_fds = [4, 5]

Module contents

skchem.utils

Module providing utility functions for scikit-chem

class skchem.utils.**Suppressor**
Bases: object

A context manager for doing a "deep suppression" of stdout and stderr.

It will suppress all print, even if the print originates in a compiled C/Fortran sub-function.

This will not suppress raised exceptions, since exceptions are printed to stderr just before a script exits, and after the context manager has exited (at least, I think that is why it lets exceptions through).

null_fds = [4, 5]

skchem.utils.**camel_to_snail**(*s*)
Convert CamelCase to snail_case.

skchem.utils.**free_to_snail**(*s*)
Convert Free Case to snail_case.

class skchem.utils.**NamedProgressBar**(*name=None*, ***kwargs*)
Bases: progressbar.bar.ProgressBar

default_widgets()

class skchem.utils.**DummyProgressBar**(**args*, ***kwargs*)
Bases: object

finish()

update(*val*)

skchem.utils.**json_dump**(*obj*, *target=None*)
Write object as json to file or stream, or return as string.

skchem.utils.**yaml_dump**(*obj*, *target=None*)
Write object as yaml to file or stream, or return as string.

skchem.utils.**line_count**(*filename*)
Quickly count the number of lines in a file.

Adapted from http://stackoverflow.com/questions/845058/how-to-get-line-count-cheaply-in-python

Parameters **filename** (*str*) – The name of the file to count for.

skchem.utils.**sdf_count**(*filename*)
Efficiently count molecules in an sdf file.

Specifically, the function counts the number of times '$$$$' occurs at the start of lines in the file.

Parameters **filename** (*str*) – The filename of the sdf file.

Returns the number of molecules in the file.

Return type int

skchem.utils.**iterable_to_series**(*mols*)

skchem.utils.**nanarray**(*shape*)
Produce an array of NaN in provided shape.

Parameters **shape** (*tuple*) – The shape of the nan array to produce.

Returns np.array

skchem.utils.**squeeze**(*data*, *axis=None*)
Squeeze dimension for length 1 arrays.

Parameters

- **data** (*pd.Series or pd.DataFrame or pd.Panel*) – The pandas object to squeeze.
- **axis** (*int or tuple*) – The axes along which to squeeze.

Returns pd.Series or pd.DataFrame

skchem.utils.**optional_second_method**(*func*)

class skchem.utils.**Defaults**(*defaults*)
Bases: object

get(*val*)

skchem.vis package

Submodules

skchem.vis.atom module

skchem.vis.atom

Module for atom contribution visualization.

skchem.vis.atom.**plot_weights**(*mol*, *weights*, *quality=1*, *l=0.4*, *step=50*, *levels=20*, *contour_opacity=0.5*, *cmap='RdBu'*, *ax=None*, ***kwargs*)
Plot weights as a sum of gaussians across a structure image.

Parameters

- **mol** (*skchem.Mol*) – Molecule to visualize weights for.
- **weights** (*iterable<float>*) – Array of weights in atom index order.
- **l** (*float*) – Lengthscale of gaussians to visualize as a multiple of bond length.
- **step** (*int*) – Size of grid edge to calculate the gaussians.

- **levels** (*int*) – Number of contours to plot.
- **contour_opacity** (*float*) – Alpha applied to the contour layer.
- **ax** (*plt.axis*) – Axis to apply the plot to. Defaults to current axis.
- **cmap** (*plt.cm*) – Colormap to use for the contour.
- ****kwargs** – Passed to contourf function.

Returns The plot.

Return type matplotlib.AxesSubplot

skchem.vis.mol module

skchem.vis.mol

Module for drawing molecules.

skchem.vis.mol.**draw**(*mol*, *quality=1*, *ax=None*)
Draw a molecule on a matplotlib axis.

Parameters

- **mol** (*skchem.Mol*) – The molecule to be drawn.
- **quality** (*int*) – The level of quality. Higher quality takes more time, but will look better (so long as matplotlib's savefig.dpi is high enough).
- **ax** (*plt.Axes or None*) – An existing axis on which to draw the molecule.

Returns A matplotlib AxesImage object with the molecule drawn.

Return type plt.AxesImage

skchem.vis.mol.**draw_3d**(*m*, *conformer_id=-1*, *label_atoms=None*)
Draw a molecule in three dimensions.

Parameters

- **conformer_id** (*int*) – The id of the conformer to draw.
- **label_atoms** (*bool*) – Whether to label the atoms (this can be toggled in interactive mode):

Returns plt.figure

Note: This works great in the notebook with *%matplotlib notebook*.

Module contents

skchem.vis

Module for plotting images of molecules.

skchem.vis.**draw**(*mol*, *quality=1*, *ax=None*)
Draw a molecule on a matplotlib axis.

Parameters

- **mol** (*skchem.Mol*) – The molecule to be drawn.

- **quality** (*int*) – The level of quality. Higher quality takes more time, but will look better (so long as matplotlib's savefig.dpi is high enough).
- **ax** (*plt.Axes or None*) – An existing axis on which to draw the molecule.

Returns A matplotlib AxesImage object with the molecule drawn.

Return type plt.AxesImage

skchem.vis.**draw_3d**(*m*, *conformer_id=-1*, *label_atoms=None*)

Draw a molecule in three dimensions.

Parameters

- **conformer_id** (*int*) – The id of the conformer to draw.
- **label_atoms** (*bool*) – Whether to label the atoms (this can be toggled in interactive mode):

Returns plt.figure

Note: This works great in the notebook with *%matplotlib notebook*.

---

skchem.vis.**plot_weights**(*mol*, *weights*, *quality=1*, *l=0.4*, *step=50*, *levels=20*, *contour_opacity=0.5*, *cmap='RdBu'*, *ax=None*, ***kwargs*)

Plot weights as a sum of gaussians across a structure image.

Parameters

- **mol** (*skchem.Mol*) – Molecule to visualize weights for.
- **weights** (*iterable<float>*) – Array of weights in atom index order.
- **l** (*float*) – Lengthscale of gaussians to visualize as a multiple of bond length.
- **step** (*int*) – Size of grid edge to calculate the gaussians.
- **levels** (*int*) – Number of contours to plot.
- **contour_opacity** (*float*) – Alpha applied to the contour layer.
- **ax** (*plt.axis*) – Axis to apply the plot to. Defaults to current axis.
- **cmap** (*plt.cm*) – Colormap to use for the contour.
- ****kwargs** – Passed to contourf function.

Returns The plot.

Return type matplotlib.AxesSubplot

6.1.2 Submodules

6.1.3 skchem.base module

skchem.base

Base classes for scikit-chem objects.

class skchem.base.**AtomTransformer**(*max_atoms=100*, ***kwargs*)

Bases: *skchem.base.BaseTransformer*

Transformer that will produce a Panel.

Concrete classes inheriting from this should implement *_transform_atom*, *_transform_mol* and *minor_axis*.

See also:

Transformer

axes_names
tuple – The names of the axes.

minor_axis
pd.Index – Minor axis of transformed values.

transform(*mols*)
Transform objects according to the objects transform protocol.

Parameters **mols** (*skchem.Mol or pd.Series or iterable*) – The mol objects to transform.

Returns pd.Series or pd.DataFrame

class skchem.base.**BaseTransformer**(*n_jobs=1*, *verbose=True*)
Bases: object

Transformer Base Class.

Specific Base Transformer classes inherit from this class and implement *transform* and *axis_names*.

axes_names
tuple – The names of the axes.

copy()
Return a copy of this object.

classmethod **from_params**(*params*)
Create a instance from a params dictionary.

get_params()
Get a dictionary of the parameters of this object.

n_jobs

optional_bar(***kwargs*)

to_dict()
Return a dictionary representation of the object.

to_json(*target=None*)
Serialize the object as JSON.

Parameters

- **target** (*str or file-like*) – A file or filepath to serialize the object to. If *None*, return the JSON as a string.
- **Returns** – None or str

to_yaml(*target=None*)
Serialize the object as YAML.

Parameters

- **target** (*str or file-like*) – A file or filepath to serialize the object to. If *None*, return the YAML as a string.
- **Returns** – None or str

transform(*mols*)
Transform objects according to the objects transform protocol.

Parameters **mols** (*skchem.Mol or pd.Series or iterable*) – The mol objects to transform.

Returns pd.Series or pd.DataFrame

class skchem.base.**BatchTransformer**(*n_jobs=1*, *verbose=True*)
Bases: *skchem.base.BaseTransformer*

Mixin for which transforms on multiple molecules save overhead.

Implement *_transform_series* with the transformation rather than *_transform_mol*. Must occur before *Transformer* or *AtomTransformer* in method resolution order.

See also:

Transformer, AtomTransformer.

class skchem.base.**CLIWrapper**(*error_on_fail=False*, *warn_on_fail=True*, ***kwargs*)
Bases: *skchem.base.External*, *skchem.base.BaseTransformer*

CLI wrapper.

Concrete classes inheriting from this must implement *_cli_args*, *monitor_progress*, *_parse_outfile*, *_parse_errors*.

monitor_progress(*filename*)
Report the progress.

n_jobs

class skchem.base.**External**(***kwargs*)
Bases: object

Mixin for wrappers of external CLI tools.

Concrete classes must implement *validate_install*.

install_hint
str – an explanation of how to install external tool.

install_hint = ''

static validate_install()
Determine if the external tool is available.

validated
bool – whether the external tool is installed and active.

class skchem.base.**Featurizer**
Bases: object

Base class for m -> data transforms, such as Fingerprinting etc.

Concrete subclasses should implement *name*, returning a string uniquely identifying the featurizer.

class skchem.base.**Transformer**(*n_jobs=1*, *verbose=True*)
Bases: *skchem.base.BaseTransformer*

Molecular based Transformer Base class.

Concrete Transformers inherit from this class and must implement *_transform_mol* and *_columns*.

See also:

AtomTransformer.

axes_names
tuple – The names of the axes.

columns
pd.Index – The column index to use.

transform(*mols*, ***kwargs*)
Transform objects according to the objects transform protocol.

Parameters **mols** (*skchem.Mol or pd.Series or iterable*) – The mol objects to transform.

Returns pd.Series or pd.DataFrame

6.1.4 skchem.metrics module

skchem.metrics.**bedroc_score**(*y_true*, *y_pred*, *decreasing=True*, *alpha=20.0*)
BEDROC metric implemented according to Truchon and Bayley.

The Boltzmann Enhanced Descrimination of the Receiver Operator Characteristic (BEDROC) score is a modification of the Receiver Operator Characteristic (ROC) score that allows for a factor of *early recognition*.

References

The original paper by Truchon et al. is located at 10.1021/ci600426e.

Parameters

- **y_true** (*array_like*) – Binary class labels. 1 for positive class, 0 otherwise.
- **y_pred** (*array_like*) – Prediction values.
- **decreasing** (*bool*) – True if high values of y_pred correlates to positive class.
- **alpha** (*float*) – Early recognition parameter.

Returns Value in interval [0, 1] indicating degree to which the predictive technique employed detects (early) the positive class.

Return type float

6.1.5 Module contents

A cheminformatics library to integrate with the Scientific Python Stack

CHAPTER 7

Developing

Development occurs on GitHub. We gladly accept pull requests !

7.1 Development Requirements

To start developing features for the package, you will need the core runtime dependencies, shown in *installing*, in addition to the below:

7.1.1 Testing

- py.test
- pytest-cov
- coverage

7.1.2 Linting

- pylint

7.1.3 Documentation

- sphinx >= 1.4
- sphinx_bootstrap_theme
- nbsphinx

These are all installable with pip.

7.2 Continuous Integration

Pull requests and commits are automatically built and tested on Travis.

7.3 Running the Tests

Tests may be run locally through py.test. This can be invoked using either `py.test` or `python setup.py test` in the project root. Command line extensions are not tested by default - these can be tested also, by using the appropriate flag, such as `python setup.py test --with-chemaxon`.

7.4 Test Coverage

Test coverage is assessed using `coverage`. This is run locally as part of the pytest command. It is set up to run as part of the CI, and can be viewed on Scrutinzer. Test coverage has suffered as features were rapidly developed in response to needs for the author's PhD, and will be improved once the PhD is submitted!

7.5 Code Quality

scikit-chem conforms to pep8. PyLint is used to assess code quality locally, and can be run using `pylint skchem` from the root of the project. Scrutinzer is also set up to run as part of the CI. As with test coverage, code quality has slipped due to time demands, and will be fixed once the PhD is submitted!

7.6 Documentation

This documentation is built using Sphinx, and Bootstrap using the Bootswatch Flatly theme. The documentation is hosted on Github Pages. To build the html documentation locally, run `make html`. To serve it, run `make livehtml`.

Warning: **scikit-chem** is currently in pre-alpha. The basic API may change between releases as we develop and optimise the library. Please read the *what's new* page when updating to stay on top of changes.

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Symbols

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