Datamol

Molecular Manipulation Made Easy

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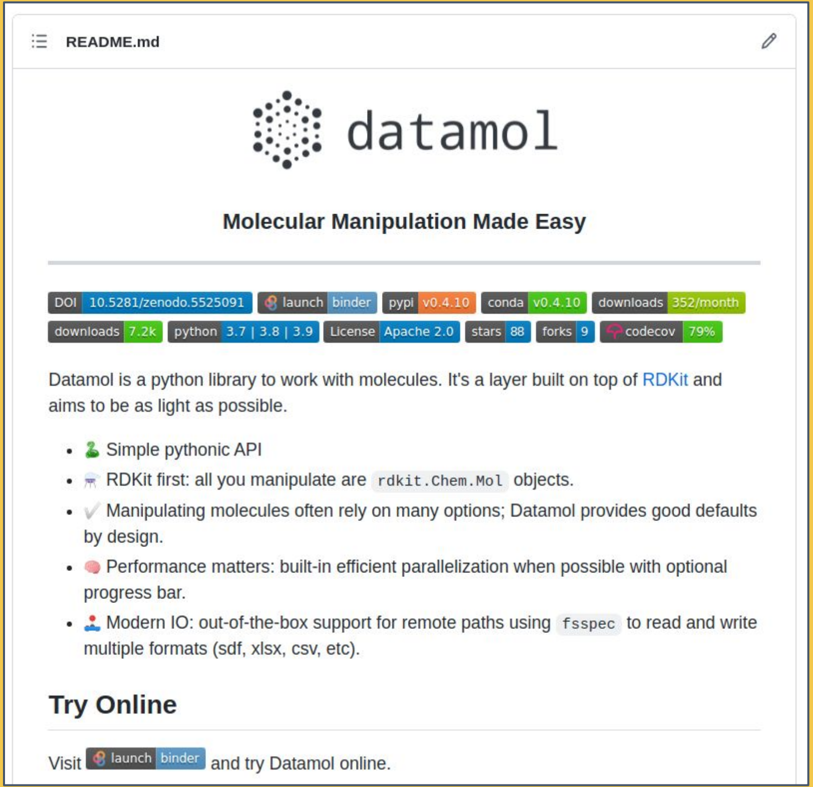
The Drug Design Company

What is Datamol?

“Datamol is an elegant, rdkit-powered python library to perform computational tasks on molecules.”



README.md

datamol

Molecular Manipulation Made Easy

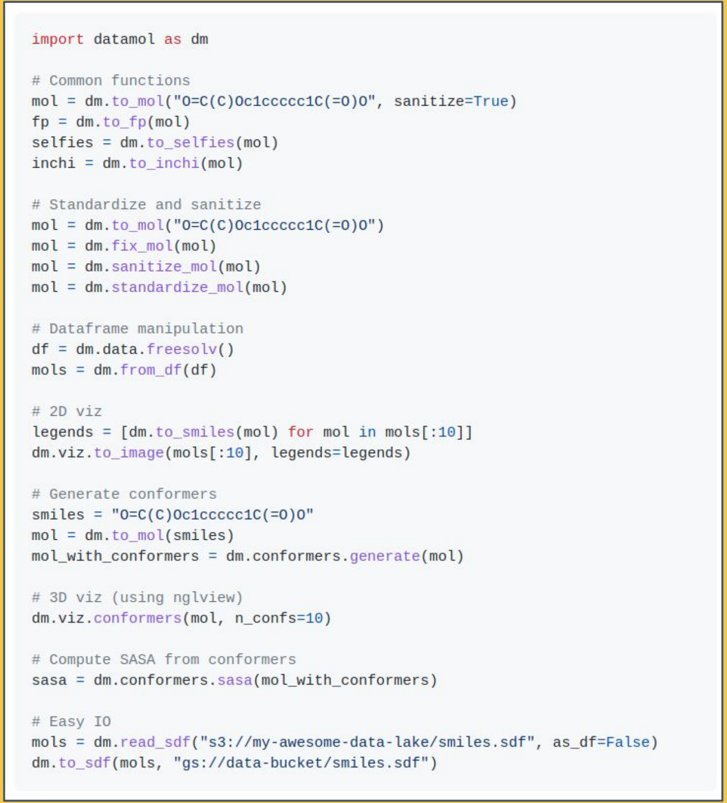
DOI 10.5281/zenodo.5525091 | launch binder | pypi v0.4.10 | conda v0.4.10 | downloads 352/month | downloads 7.2k | python 3.7 | 3.8 | 3.9 | License Apache 2.0 | stars 88 | forks 9 | codecov 79%

Datamol is a python library to work with molecules. It's a layer built on top of RDKit and aims to be as light as possible.

- Simple pythonic API
- RDKit first: all you manipulate are `rdkit.Chem.Mol` objects.
- Manipulating molecules often rely on many options; Datamol provides good defaults by design.
- Performance matters: built-in efficient parallelization when possible with optional progress bar.
- Modern IO: out-of-the-box support for remote paths using `fsspec` to read and write multiple formats (sdf, xlsx, csv, etc).

Try Online

Visit launch binder and try Datamol online.



```python
import datamol as dm

# Common functions
mol = dm.to_mol("O=C(C)Oc1ccccc1C(=O)O", sanitize=True)
fp = dm.to_fp(mol)
selfies = dm.to_selfies(mol)
inchi = dm.to_inchi(mol)

# Standardize and sanitize
mol = dm.to_mol("O=C(C)Oc1ccccc1C(=O)O")
mol = dm.fix_mol(mol)
mol = dm.sanitize_mol(mol)
mol = dm.standardize_mol(mol)

# Dataframe manipulation
df = dm.data.freesolv()
mols = dm.from_df(df)

# 2D viz
legends = [dm.to_smiles(mol) for mol in mols[:10]]
dm.viz.to_image(mols[:10], legends=legends)

# Generate conformers
smiles = "O=C(C)Oc1ccccc1C(=O)O"
mol = dm.to_mol(smiles)
mol_with_conformers = dm.conformers.generate(mol)

# 3D viz (using nglview)
dm.viz.conformers(mol, n_confs=10)

# Compute SASA from conformers
sasa = dm.conformers.sasa(mol_with_conformers)

# Easy IO
mols = dm.read_sdf("s3://my-awesome-data-lake/smiles.sdf", as_df=False)
dm.to_sdf(mols, "gs://data-bucket/smiles.sdf")
```

https://github.com/datamol-org/datamol

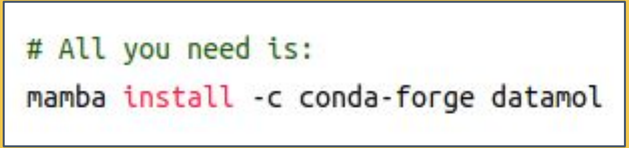
Why Datamol?

- Remove **code duplication** across Valence's codebase.
- Lower the **learning curve** for newcomers.
- **Standardized procedures** for common molecules manipulations.
- Reduce **"code surface area"** for potential bugs.

Audience:

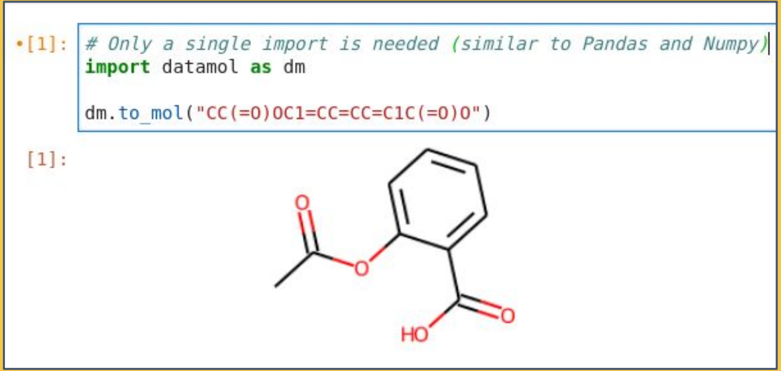
- **Newcomers** in chemoinformatics.
- **Experienced** chemoinformatics practitioners and existing **RDKit users**.

Datamol: a Python library



```
# All you need is:
mamba install -c conda-forge datamol
```

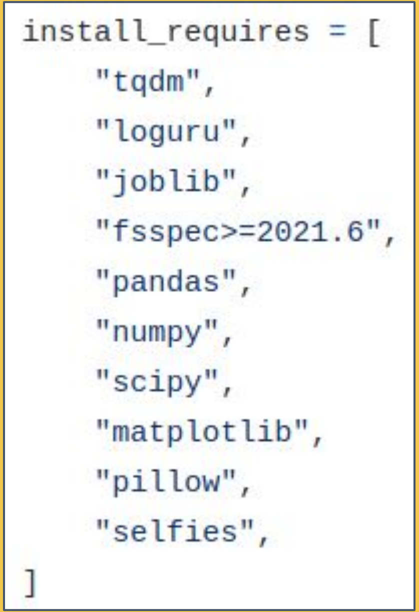
You can also install from `pip` or `conda`.



```
[1]: # Only a single import is needed (similar to Pandas and Numpy)
     import datamol as dm

     dm.to_mol("CC(=O)OC1=CC=CC=C1C(=O)O")
```

```
[1]:
```

Work with a single Python import.



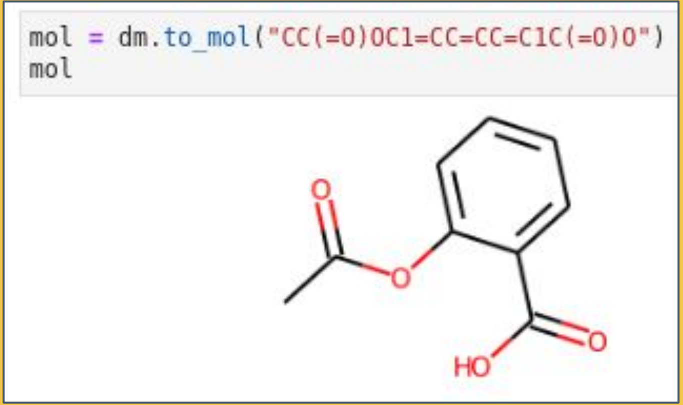
```
install_requires = [
    "tqdm",
    "loguru",
    "joblib",
    "fsspec>=2021.6",
    "pandas",
    "numpy",
    "scipy",
    "matplotlib",
    "pillow",
    "selfies",
]
```

Small list of direct dependencies.

All snippets presented are available at https://gist.github.com/hadim/634767d15f626c71735f0405bd13dc92

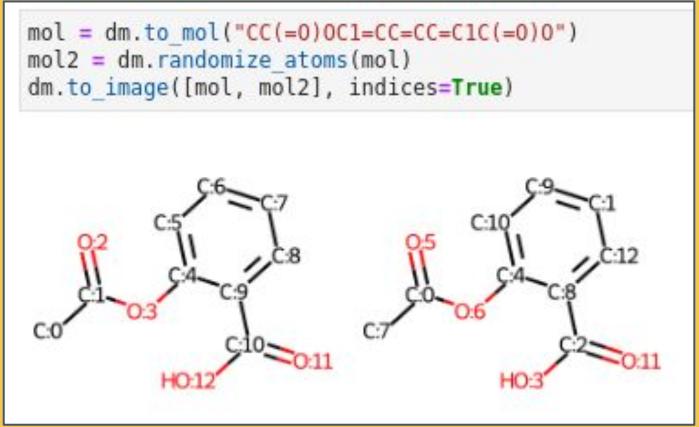
API Tour - Working with molecules

Convert a SMILES to a mol



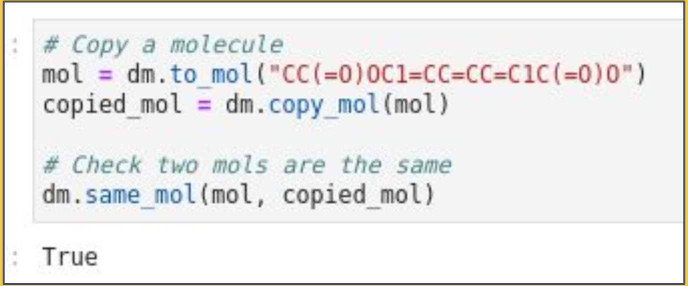
```
mol = dm.to_mol("CC(=O)OC1=CC=CC=C1C(=O)O")
mol
```

Randomize atoms



```
mol = dm.to_mol("CC(=O)OC1=CC=CC=C1C(=O)O")
mol2 = dm.randomize_atoms(mol)
dm.to_image([mol, mol2], indices=True)
```

Copy and check same molecules

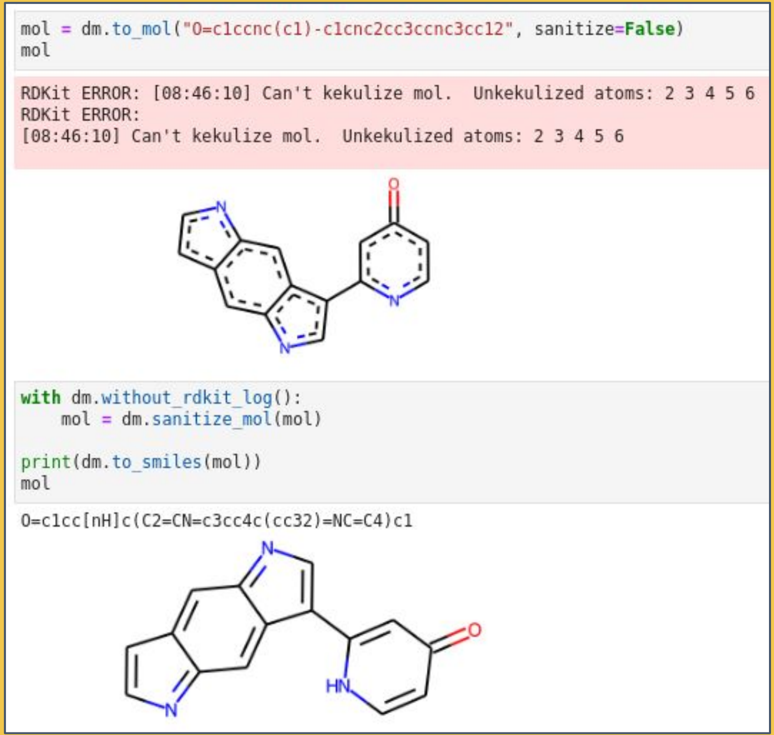


```
# Copy a molecule
mol = dm.to_mol("CC(=O)OC1=CC=CC=C1C(=O)O")
copied_mol = dm.copy_mol(mol)

# Check two mols are the same
dm.same_mol(mol, copied_mol)
```

```
True
```

API Tour - Working with molecules

Sanitize a molecule



```
mol = dm.to_mol("O=c1ccnc(c1)-c1cnc2cc3ccnc3cc12", sanitize=False)
mol
```

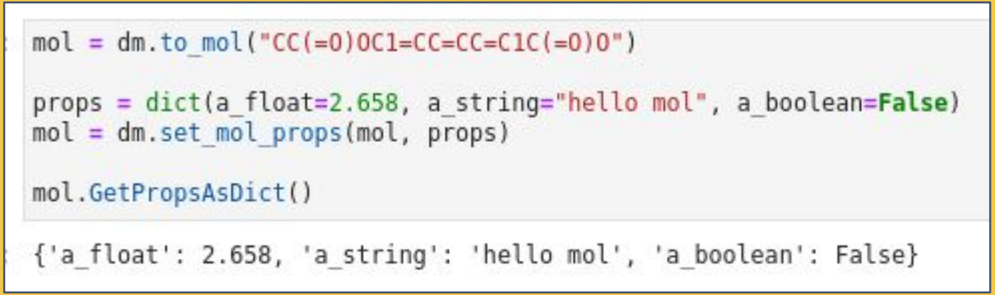
```
RDKit ERROR: [08:46:10] Can't kekulize mol.  Unkekulized atoms: 2 3 4 5 6
RDKit ERROR:
[08:46:10] Can't kekulize mol.  Unkekulized atoms: 2 3 4 5 6
```

```
with dm.without_rdkit_log():
    mol = dm.sanitize_mol(mol)

print(dm.to_smiles(mol))
mol
```

```
O=c1cc[nH]c(C2=CN=c3cc4c(cc32)=NC=C4)c1
```

API Tour - Working with molecules

Add properties from a dict directly

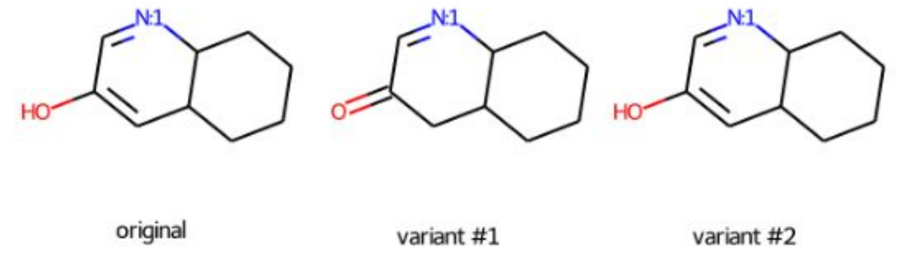


```python
mol = dm.to_mol("CC(=O)OC1=CC=CC=C1C(=O)O")

props = dict(a_float=2.658, a_string="hello mol", a_boolean=False)
mol = dm.set_mol_props(mol, props)

mol.GetPropsAsDict()
```

```
{'a_float': 2.658, 'a_string': 'hello mol', 'a_boolean': False}
```

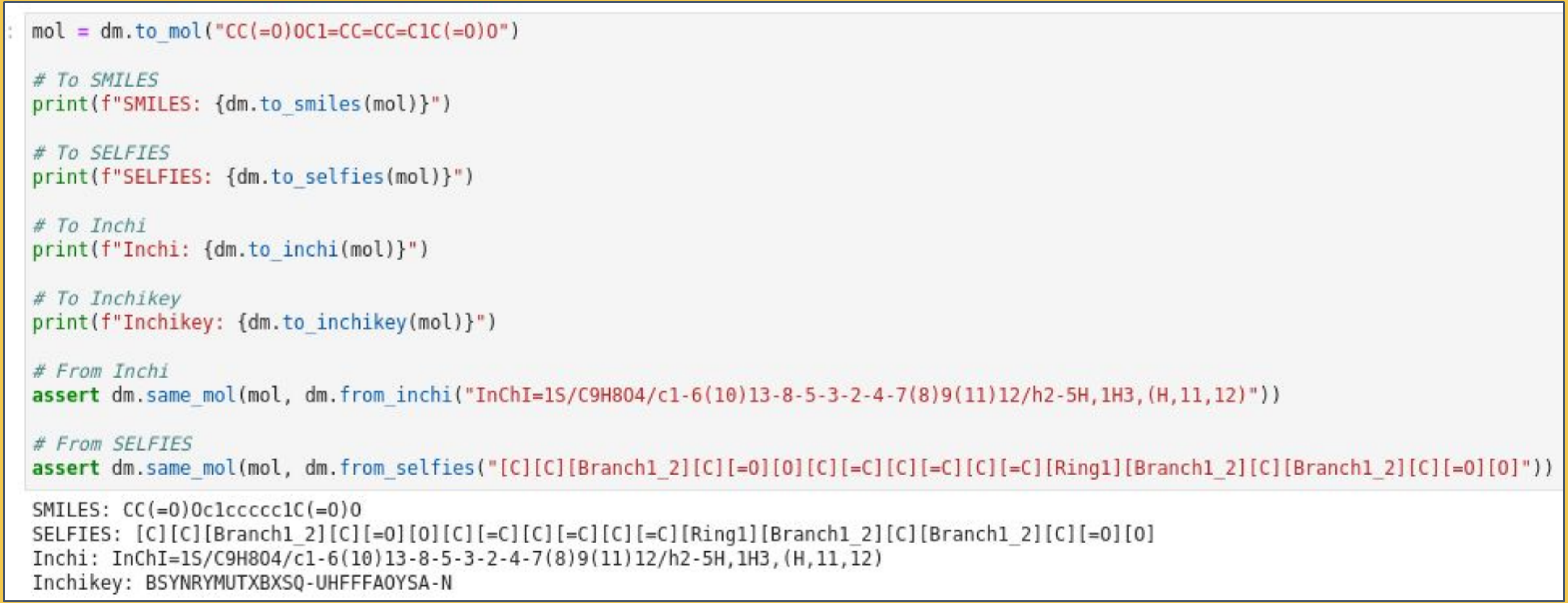
Enumerate tautomers

```python
mol = dm.to_mol("OC1=CC2CCCCC2[N:1]=C1")
variants = dm.enumerate_tautomers(mol, n_variants=10)

dm.to_image([mol] + variants, legends=["original", "variant #1", "variant #2"])
```



API Tour - Conversion

Convert **from** and **to** various molecule formats

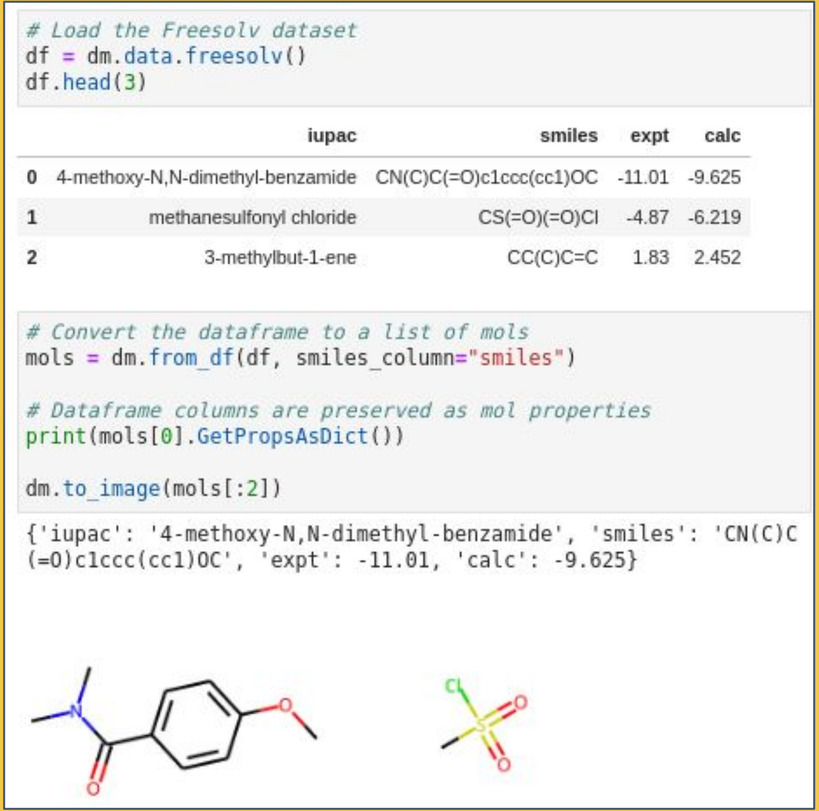


```
mol = dm.to_mol("CC(=O)OC1=CC=CC=C1C(=O)O")

# To SMILES
print(f"SMILES: {dm.to_smiles(mol)}")

# To SELFIES
print(f"SELFIES: {dm.to_selfies(mol)}")

# To Inchi
print(f"Inchi: {dm.to_inchi(mol)}")

# To Inchikey
print(f"Inchikey: {dm.to_inchikey(mol)}")

# From Inchi
assert dm.same_mol(mol, dm.from_inchi("InChI=1S/C9H8O4/c1-6(10)13-8-5-3-2-4-7(8)9(11)12/h2-5H,1H3,(H,11,12)"))

# From SELFIES
assert dm.same_mol(mol, dm.from_selfies("[C][C][Branch1_2][C][=O][O][C][=C][C][=C][C][=C][Ring1][Branch1_2][C][Branch1_2][C][=O][O]"))
```

```
SMILES: CC(=O)Oc1ccccc1C(=O)O
SELFIES: [C][C][Branch1_2][C][=O][O][C][=C][C][=C][C][=C][Ring1][Branch1_2][C][Branch1_2][C][=O][O]
Inchi: InChI=1S/C9H8O4/c1-6(10)13-8-5-3-2-4-7(8)9(11)12/h2-5H,1H3,(H,11,12)
Inchikey: BSYNRYMUTXBXSQ-UHFFFAOYSA-N
```

API Tour - Dataframe

Dataframe to a list of molecules

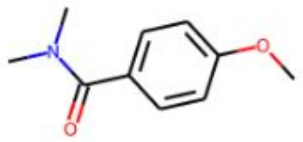
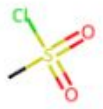


```python
# Load the Freesolv dataset
df = dm.data.freesolv()
df.head(3)
```

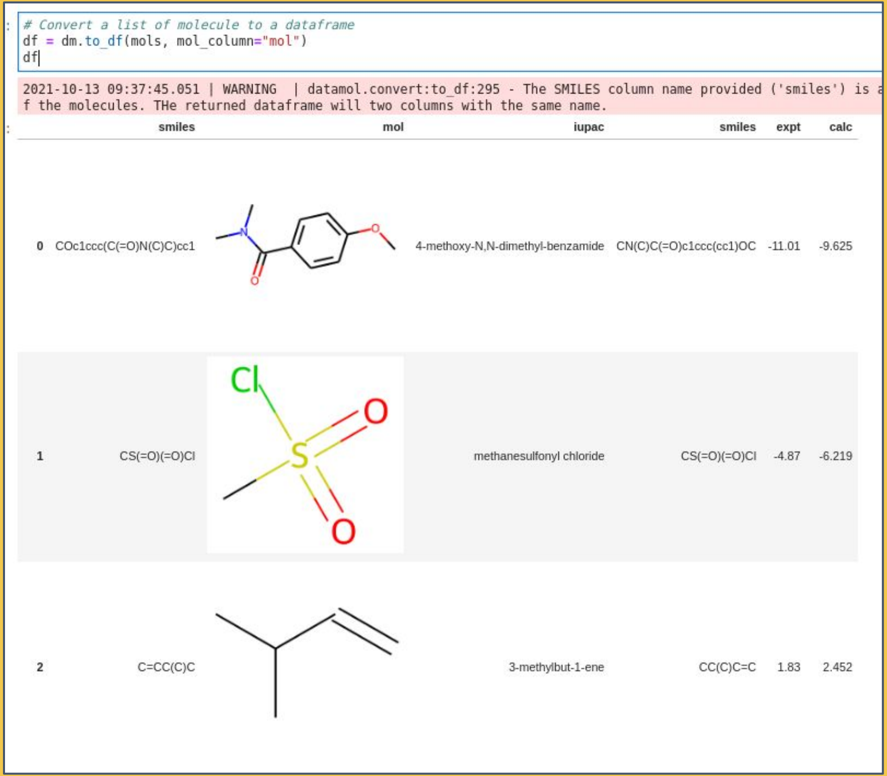
	iupac	smiles	expt	calc
0	4-methoxy-N,N-dimethyl-benzamide	CN(C)C(=O)c1ccc(cc1)OC	-11.01	-9.625
1	methanesulfonyl chloride	CS(=O)(=O)Cl	-4.87	-6.219
2	3-methylbut-1-ene	CC(C)C=C	1.83	2.452

```python
# Convert the dataframe to a list of mols
mols = dm.from_df(df, smiles_column="smiles")

# Dataframe columns are preserved as mol properties
print(mols[0].GetPropsAsDict())

dm.to_image(mols[:2])
```

```
{'iupac': '4-methoxy-N,N-dimethyl-benzamide', 'smiles': 'CN(C)C
(=O)c1ccc(cc1)OC', 'expt': -11.01, 'calc': -9.625}
```

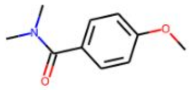
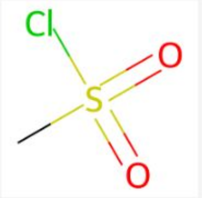
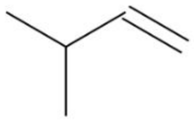



A list of molecules to a dataframe



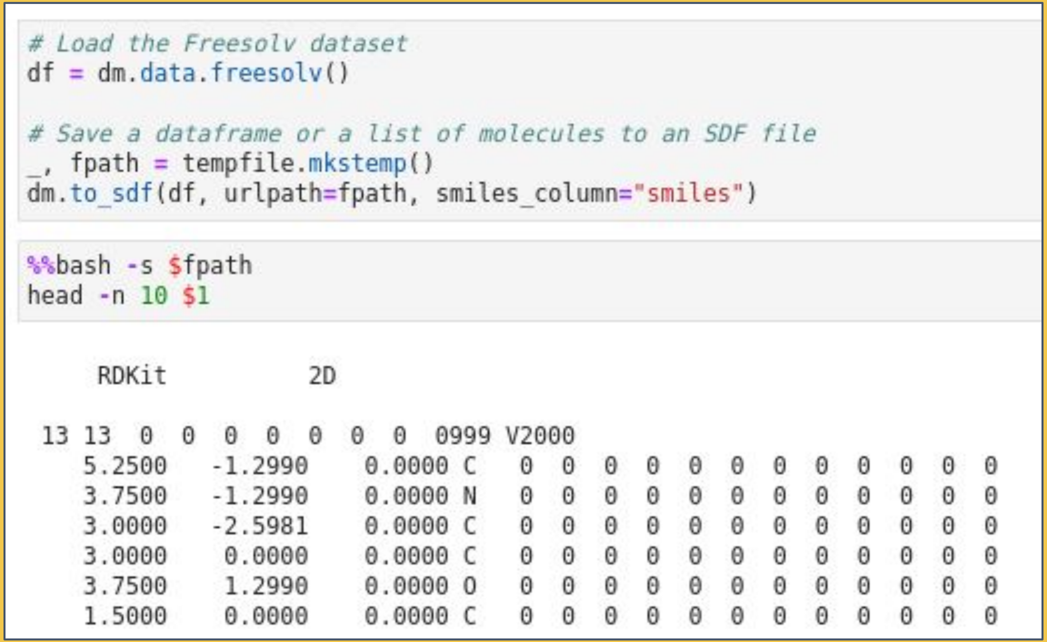
```python
# Convert a list of molecule to a dataframe
df = dm.to_df(mols, mol_column="mol")
df
```

```
2021-10-13 09:37:45.051 | WARNING  | datamol.convert:to_df:295 - The SMILES column name provided ('smiles') is a
f the molecules. THe returned dataframe will two columns with the same name.
```

	smiles	mol	iupac	smiles	expt	calc
0	COc1ccc(C(=O)N(C)C)cc1		4-methoxy-N,N-dimethyl-benzamide	CN(C)C(=O)c1ccc(cc1)OC	-11.01	-9.625
1	CS(=O)(=O)Cl		methanesulfonyl chloride	CS(=O)(=O)Cl	-4.87	-6.219
2	C=CC(C)C		3-methylbut-1-ene	CC(C)C=C	1.83	2.452

API Tour - Input/Output

Save molecules to an SDF file



```
# Load the Freesolv dataset
df = dm.data.freesolv()

# Save a dataframe or a list of molecules to an SDF file
_, fpath = tempfile.mkstemp()
dm.to_sdf(df, urlpath=fpath, smiles_column="smiles")
```

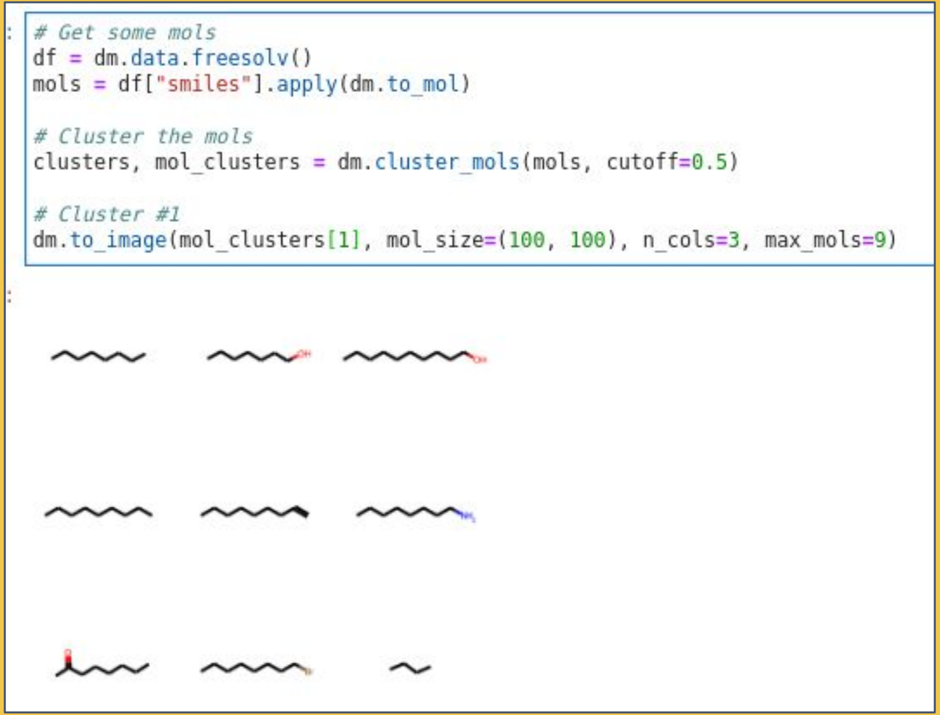
```
%%bash -s $fpath
head -n 10 $1
```

```

     RDKit          2D

 13 13  0  0  0  0  0  0  0  0999 V2000
    5.2500   -1.2990    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.7500   -1.2990    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
    3.0000   -2.5981    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.0000    0.0000    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.7500    1.2990    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
    1.5000    0.0000    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
```

- *Datamol can read and write from/to CSV, Excel, SDF and SMI.*
- *Both **local** and **remote** file paths are allowed.*

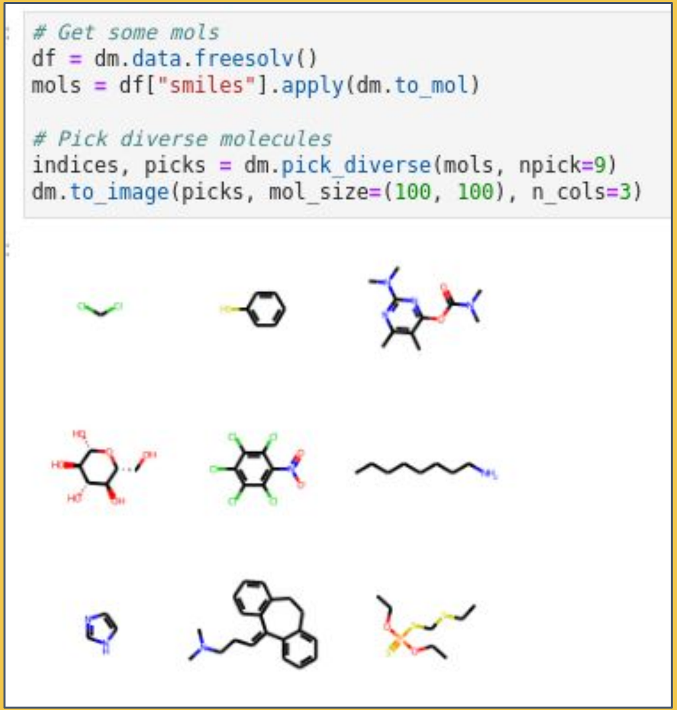
API Tour - Cluster

Cluster a list of molecules



```
# Get some mols
df = dm.data.freesolv()
mols = df["smiles"].apply(dm.to_mol)

# Cluster the mols
clusters, mol_clusters = dm.cluster_mols(mols, cutoff=0.5)

# Cluster #1
dm.to_image(mol_clusters[1], mol_size=(100, 100), n_cols=3, max_mols=9)
```

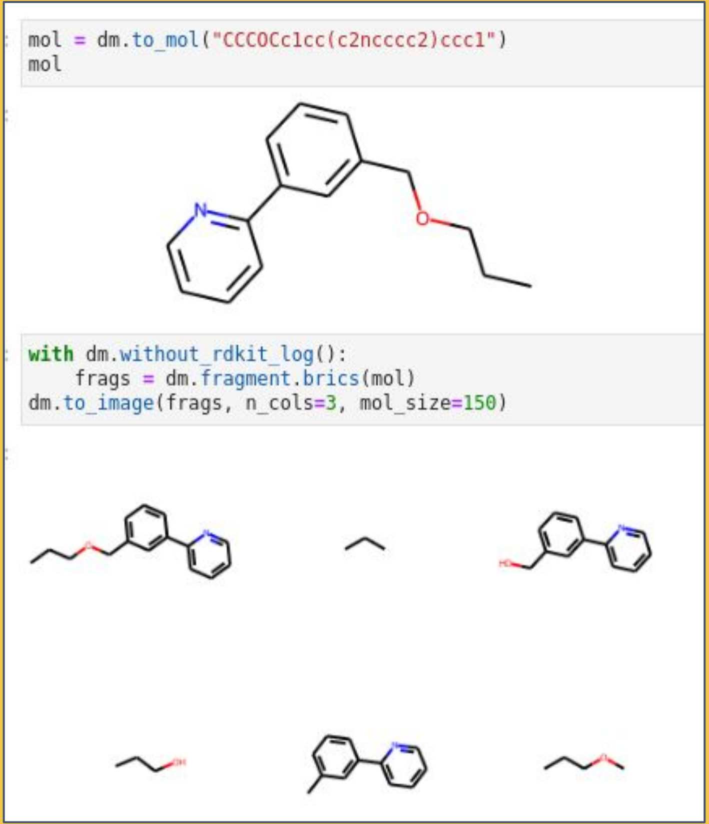
Pick diverse molecules from a list



```
# Get some mols
df = dm.data.freesolv()
mols = df["smiles"].apply(dm.to_mol)

# Pick diverse molecules
indices, picks = dm.pick_diverse(mols, npick=9)
dm.to_image(picks, mol_size=(100, 100), n_cols=3)
```

API Tour - Fragmentation and scaffolding

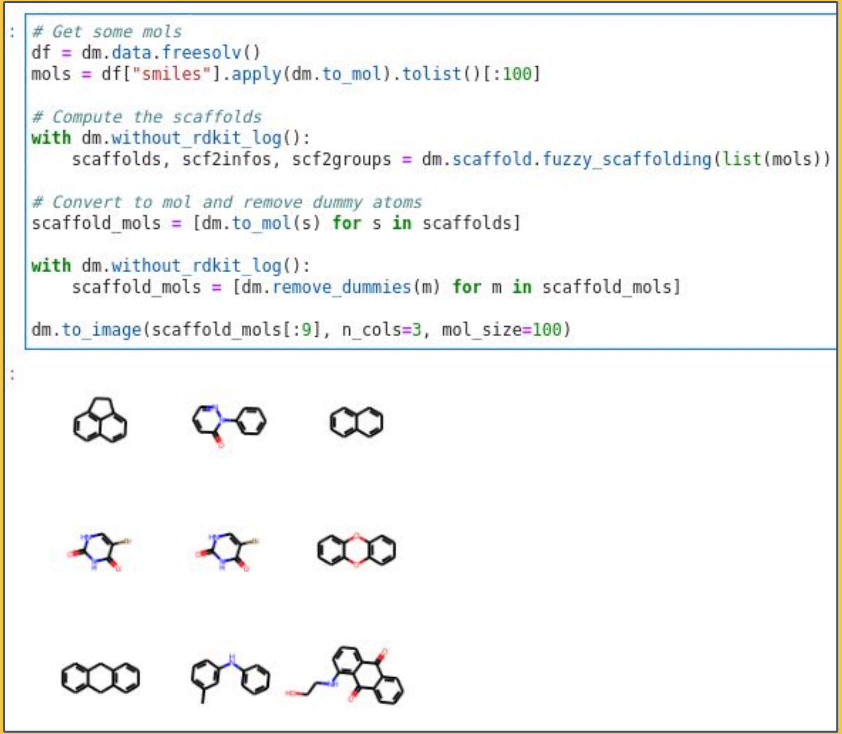
Fragment a molecule



```python
mol = dm.to_mol("CCCOCc1cc(c2ncccc2)ccc1")
mol
```

```python
with dm.without_rdkit_log():
    frags = dm.fragment.brics(mol)
dm.to_image(frags, n_cols=3, mol_size=150)
```

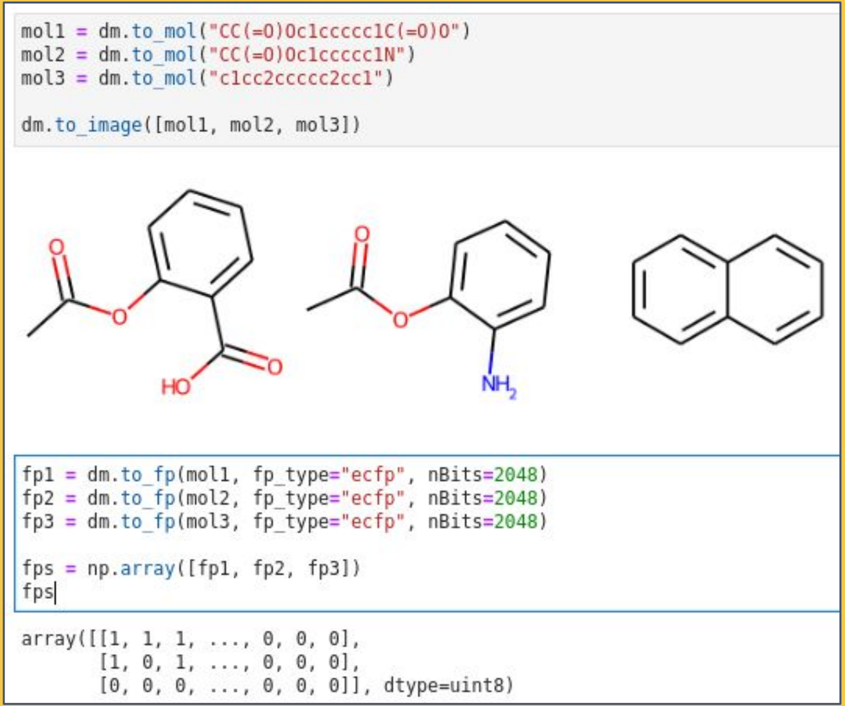
Extract the scaffolds from a list of molecules



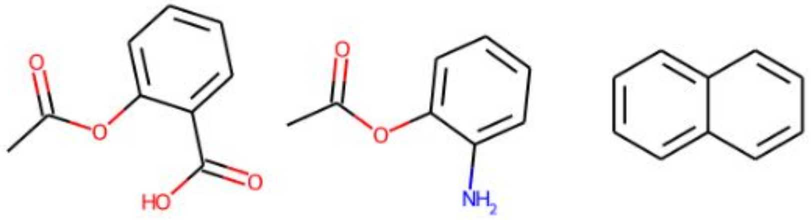
```python
# Get some mols
df = dm.data.freesolv()
mols = df["smiles"].apply(dm.to_mol).tolist()[:100]

# Compute the scaffolds
with dm.without_rdkit_log():
    scaffolds, scf2infos, scf2groups = dm.scaffold.fuzzy_scaffolding(list(mols))

# Convert to mol and remove dummy atoms
scaffold_mols = [dm.to_mol(s) for s in scaffolds]

with dm.without_rdkit_log():
    scaffold_mols = [dm.remove_dummies(m) for m in scaffold_mols]

dm.to_image(scaffold_mols[:9], n_cols=3, mol_size=100)
```

API Tour - Fingerprints and similarities

Compute fingerprints



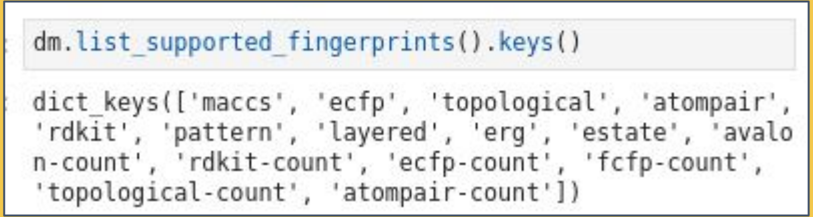
```
mol1 = dm.to_mol("CC(=O)Oc1ccccc1C(=O)O")
mol2 = dm.to_mol("CC(=O)Oc1ccccc1N")
mol3 = dm.to_mol("c1cc2ccccc2cc1")

dm.to_image([mol1, mol2, mol3])
```



```
fp1 = dm.to_fp(mol1, fp_type="ecfp", nBits=2048)
fp2 = dm.to_fp(mol2, fp_type="ecfp", nBits=2048)
fp3 = dm.to_fp(mol3, fp_type="ecfp", nBits=2048)

fps = np.array([fp1, fp2, fp3])
fps
```

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

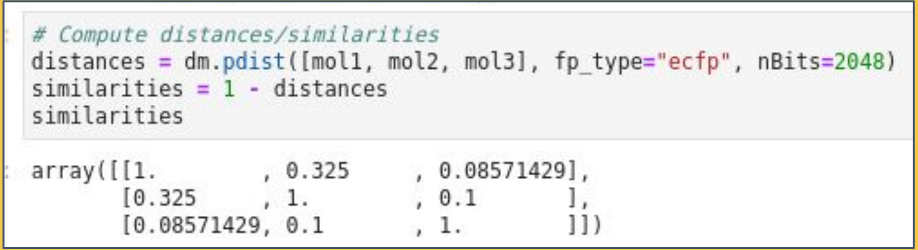
List of available fingerprints



```
dm.list_supported_fingerprints().keys()
```

```
dict_keys(['maccs', 'ecfp', 'topological', 'atompair',
'rdkit', 'pattern', 'layered', 'erg', 'estate', 'avalo
n-count', 'rdkit-count', 'ecfp-count', 'fcfp-count',
'topological-count', 'atompair-count'])
```

Compute distances and similarities

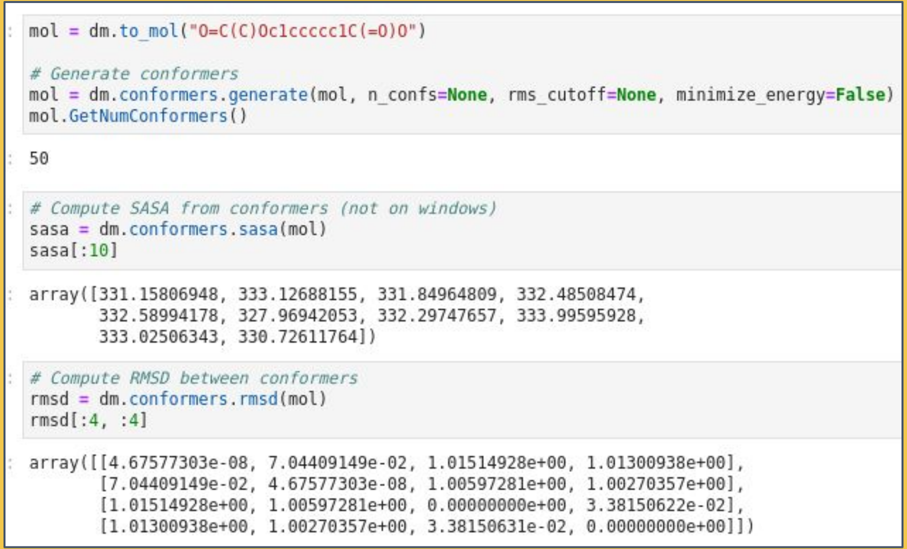


```
# Compute distances/similarities
distances = dm.pdist([mol1, mol2, mol3], fp_type="ecfp", nBits=2048)
similarities = 1 - distances
similarities
```

```
array([[1.        , 0.325     , 0.08571429],
       [0.325     , 1.        , 0.1       ],
       [0.08571429, 0.1       , 1.        ]])
```

API Tour - Conformers

Generate and work with conformers



```
mol = dm.to_mol("O=C(C)Oc1ccccc1C(=O)O")

# Generate conformers
mol = dm.conformers.generate(mol, n_confs=None, rms_cutoff=None, minimize_energy=False)
mol.GetNumConformers()
```

```
50
```

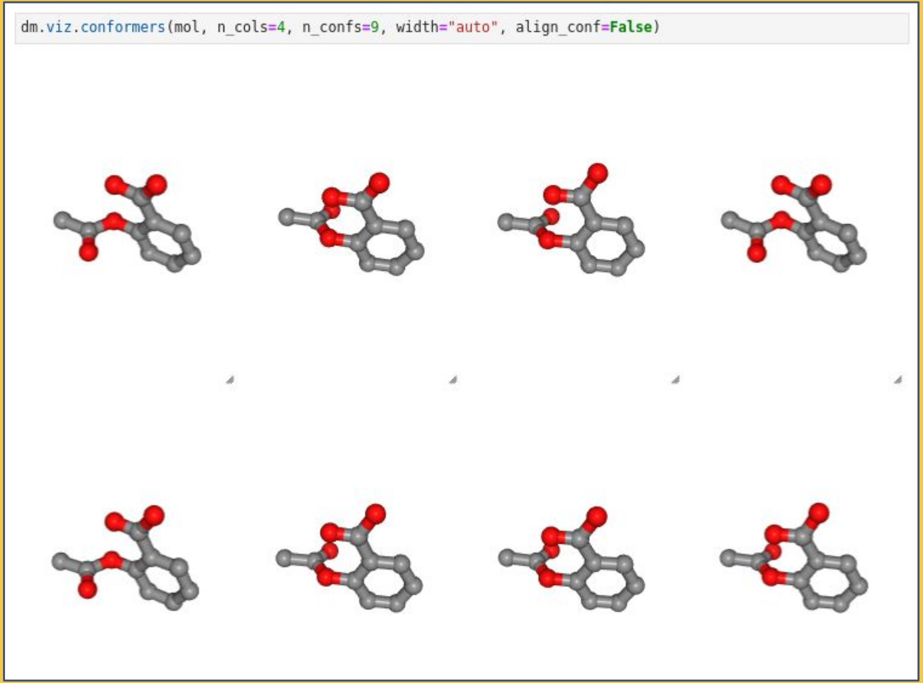
```
# Compute SASA from conformers (not on windows)
sasa = dm.conformers.sasa(mol)
sasa[:10]
```

```
array([331.15806948, 333.12688155, 331.84964809, 332.48508474,
       332.58994178, 327.96942053, 332.29747657, 333.99595928,
       333.02506343, 330.72611764])
```

```
# Compute RMSD between conformers
rmsd = dm.conformers.rmsd(mol)
rmsd[:4, :4]
```

```
array([[4.67577303e-08, 7.04409149e-02, 1.01514928e+00, 1.01300938e+00],
       [7.04409149e-02, 4.67577303e-08, 1.00597281e+00, 1.00270357e+00],
       [1.01514928e+00, 1.00597281e+00, 0.00000000e+00, 3.38150622e-02],
       [1.01300938e+00, 1.00270357e+00, 3.38150631e-02, 0.00000000e+00]])
```

3D viz of conformers

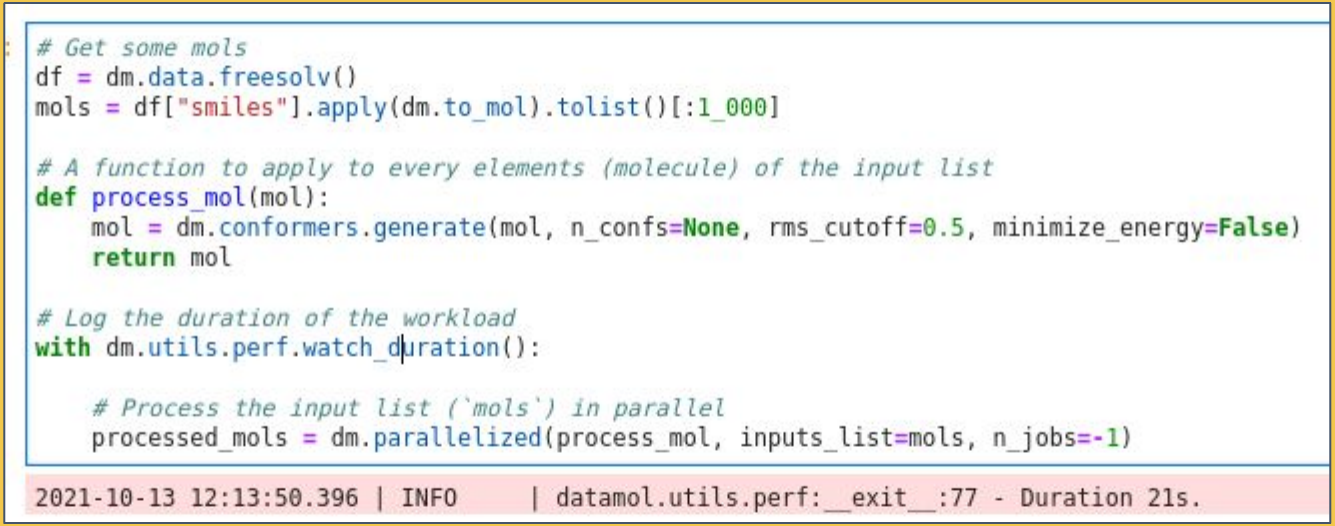


```
dm.viz.conformers(mol, n_cols=4, n_confs=9, width="auto", align_conf=False)
```

Based on the `nglview` Python library.

API Tour - Distributed computing

Easy workload parallelization

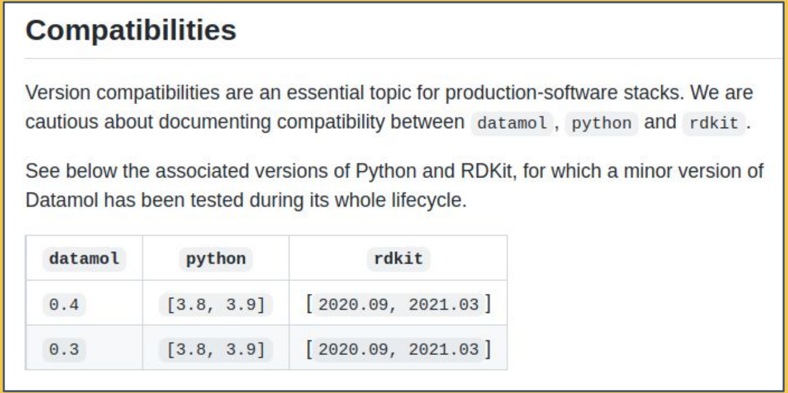


```python
# Get some mols
df = dm.data.freesolv()
mols = df["smiles"].apply(dm.to_mol).tolist()[:1_000]

# A function to apply to every elements (molecule) of the input list
def process_mol(mol):
    mol = dm.conformers.generate(mol, n_confs=None, rms_cutoff=0.5, minimize_energy=False)
    return mol

# Log the duration of the workload
with dm.utils.perf.watch_duration():

    # Process the input list (`mols`) in parallel
    processed_mols = dm.parallelized(process_mol, inputs_list=mols, n_jobs=-1)
```

```
2021-10-13 12:13:50.396 | INFO     | datamol.utils.perf:__exit__:77 - Duration 21s.
```

Built on top of `joblib` and its `loky` backend.

Datamol is production ready

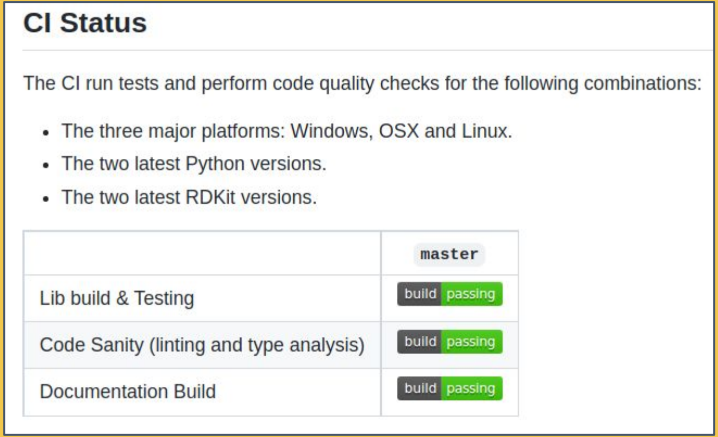


Compatibilities

Version compatibilities are an essential topic for production-software stacks. We are cautious about documenting compatibility between `datamol`, `python` and `rdkit`.

See below the associated versions of Python and RDKit, for which a minor version of Datamol has been tested during its whole lifecycle.

`datamol`	`python`	`rdkit`
`0.4`	`[3.8, 3.9]`	[`2020.09, 2021.03`]
`0.3`	`[3.8, 3.9]`	[`2020.09, 2021.03`]



CI Status

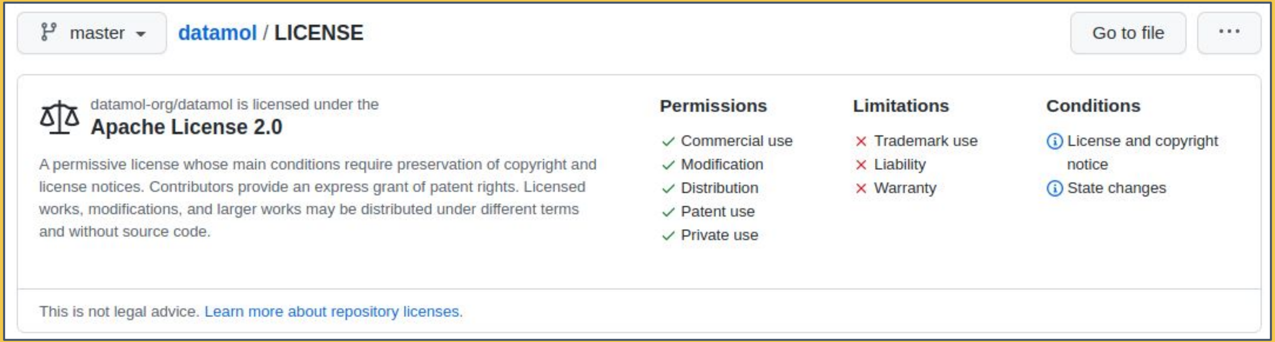
The CI run tests and perform code quality checks for the following combinations:

- The three major platforms: Windows, OSX and Linux.
- The two latest Python versions.
- The two latest RDKit versions.

	`master`
Lib build & Testing	build passing
Code Sanity (linting and type analysis)	build passing
Documentation Build	build passing

"Release fast and often."

Datamol is business friendly



master

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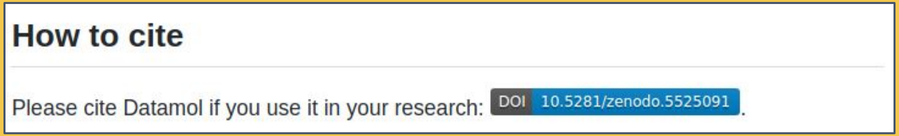
Cite Datamol



How to cite

Please cite Datamol if you use it in your research: DOI 10.5281/zenodo.5525091.

Datamol

Get started at https://github.com/datamol-org/datamol

RDKit

Valence
The Drug Design Company