

Manipulating Molecular Structures of Drugs in Python

July 11, 2020

Manipulating Molecular Structures of Drugs in Python

Contact: [Rongui Zhou](#)

Python code can be found [here](#).

RDKit package is used for processing chemical structure. [Tutorial](#)

Installation: follow this [link](#).

```
conda install -c rdkit rdkit
```

```
[1]: # import libraries
import os
import pandas as pd
from rdkit import Chem

# read in the csv file and display the head
file = 'Drugs.csv'
drugs = pd.read_csv(file)
drugs.head()
```

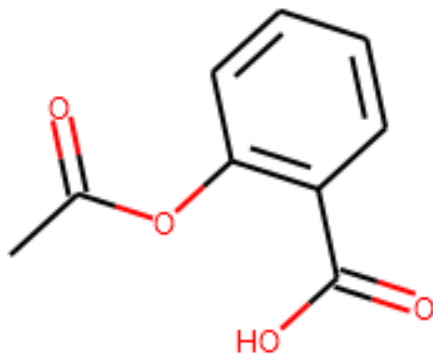
```
[1]:
```

	Drug Name	SMILES
0	Aspirin	<chem>O=C(C1=C(OC(C)=O)C=CC=C1)O</chem>
1	Morphine	<chem>OC1=C2O[C@H]3[C@]45C2=C(C=C1)C[C@H](N(CC5)C)...</chem>
2	Apixaban	<chem>COC1=CC=C(N2N=C(C3=C2C(N(C4=CC=C(N5CCCCC5=O)C=...</chem>
3	Lenalidomide	<chem>NC1=CC=CC2=C1CN(C2=O)C3CCC(NC3=O)=O</chem>
4	Rivaroxaban	<chem>C1C1=CC=C(C(NC[C@H]2CN(C3=CC=C(N4CCOCC4=O)C=C3...</chem>

```
[2]: # Use Chem module from rdkit to read the SMILES string and display the structure
aspirin = Chem.MolFromSmiles('O=C(C1=C(OC(C)=O)C=CC=C1)O')
print('Aspirin structure:')
aspirin
```

Aspirin structure:

```
[2]:
```



```
[3]: # set up directories for image, SMILES and mol files
smi_dir = './smi'
mol_dir = './mol'
sdf_dir = './sdf'
img_dir = './img'

# make the directories if not exist
for d in [smi_dir, mol_dir, sdf_dir, img_dir]:
    if not os.path.exists(d):
        os.makedirs(d)
```

```
[4]: # initiate an empty list to accept all drug structure
structure_lst = []

# iterate through the whole csv file
for i in range(drugs.shape[0]):

    #####
    # get the drug name
    drug = drugs.loc[i, 'Drug Name']
    print(f'\n\033[1m{drug}\033[0m:')

    # get the SMILES string
    smiles = drugs.loc[i, 'SMILES']

    # convert SMILES string to structure
    structure = Chem.MolFromSmiles(smiles)

    # append the structure to the list
    structure_lst.append(structure)

    #####
    # configure the filename and path for .smi files
    smi_file = drug + '.smi'
```

```

smi_path = os.path.join(smi_dir, smi_file)

#####
# configure the filename and path for .mol files
mol_file = drug + '.mol'
mol_path = os.path.join(mol_dir, mol_file)

#####
# configure the filename and path for .sdf files
sdf_file = drug + '.sdf'
sdf_path = os.path.join(sdf_dir, sdf_file)

#####
# configure the filename and path for .png files
img_file = drug + '.png'
img_path = os.path.join(img_dir, img_file)

#####
# iterate through .smi, .mol and .sdf files
for item in [smi_path, mol_path, sdf_path]:
    try:
        w = Chem.SDWriter(item)
        w.write(structure)
        w.close()
        print(f"\t.{item.rsplit('.',1)[1]} file saved")
    except:
        print(f"\t{item.rsplit('.',1)[1]} file failed")
        pass

# export individual png file
try:
    Chem.Draw.MolToFile(structure, img_path, size = (200,200), legend =
↳drug)
    print('\t.png file saved')
except:
    print('\tImage failed')
    pass

#####
# configure the filename and path for drug_all.sdf file
sdf_all_file = 'Drugs.sdf'
sdf_all_path = os.path.join(sdf_dir, sdf_all_file)

try:
    w = Chem.SDWriter(sdf_all_path)

```

```

for structure in structure_lst:
    w.write(structure)
w.close()
print('\nA big sdf file saved for all drugs as "drug_all.sdf".')

except:
    print('\tBig sdf for all drugs failed')

#####
↪
img_all_path = os.path.join(img_dir, 'drug_all.png')
# export a big png file for all drugs
try:
    img_all = Chem.Draw.MolsToGridImage(structure_lst, molsPerRow=4,
    ↪subImgSize=(200,200),legends = drugs['Drug Name'].tolist())
    img_all.save(img_all_path)
    print('\nA big image saved for all drugs as "drug_all.png".')
except:
    print('\tBig image for all drugs failed')
    pass

print('\n\x1b[6;30;42m' + 'All DONE!' + '\x1b[0m')

```

Aspirin:

```

.smi file saved
.mol file saved
.sdf file saved
.png file saved

```

Morphine:

```

.smi file saved
.mol file saved
.sdf file saved
.png file saved

```

Apixaban:

```

.smi file saved
.mol file saved
.sdf file saved
.png file saved

```

Lenalidomide:

```

.smi file saved
.mol file saved

```

.sdf file saved
.png file saved

Rivaroxaban:

.smi file saved
.mol file saved
.sdf file saved
.png file saved

Ibuprofen:

.smi file saved
.mol file saved
.sdf file saved
.png file saved

Propranolol:

.smi file saved
.mol file saved
.sdf file saved
.png file saved

Nicotine:

.smi file saved
.mol file saved
.sdf file saved
.png file saved

A big sdf file saved for all drugs as "drug_all.sdf".

A big image saved for all drugs as "drug_all.png".

ALL DONE!