RDKIT TUTORIAL

Rdkit安装

In [1]:

```python
# conda install -c conda-forge rdkit
import rdkit
rdkit.__version__
```

Out[1]:

```
'2021.09.11'
```

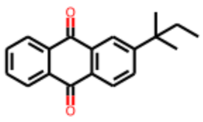
读写分子

In [18]:

```python
# mol -> smiles
from rdkit import Chem
from rdkit.Chem import Draw
mol_file = 'data/AAQ.mol'
mol = Chem.MolFromMolFile(mol_file)
smiles = Chem.MolToSmiles(mol)
#画分子图
# Draw.MolToFile(mol,'img/AAQ.png')
print(f'{mol}\n{smiles}')
Draw.MolToImage(mol, size=(150, 150),fitImage=True)
```

```
<rdkit.Chem.rdchem.Mol object at 0x7fa4b54e5fa0>
CCC(C)(C)c1ccc2c(c1)C(=O)c1ccccc1C2=O
```

Out[18]:



In [3]:

```python
# smiles -> mol
smile = 'COC1=C(C=C2C(=C1)CCN=C2C3=CC(=C(C=C3)Cl)Cl)Cl'
mol = Chem.MolFromSmiles(smile)
print(f'{mol}')
# 保存mol文件
Chem.MolToMolFile(mol,'data/CHEMBL1087421.mol')
#打印mol格式内容
print(Chem.MolToMolBlock(mol))
```

```
<rdkit.Chem.rdchem.Mol object at 0x7fa4b53e6220>

     RDKit          2D

 21 23  0  0  0  0  0  0  0  0999 V2000
    0.7500   -6.4952    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.5000   -5.1962    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
    0.7500   -3.8971    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.7500   -3.8971    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.5000   -2.5981    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.7500   -1.2990    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.7500   -1.2990    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.5000   -2.5981    0.0000 C   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
    0.7500    1.2990    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.7500    1.2990    0.0000 N   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
   -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 C   0  0  0  0  0  0  0  0  0  0  0  0
   -5.2500    1.2990    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -6.0000    0.0000    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -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 C   0  0  0  0  0  0  0  0  0  0  0  0
   -7.5000    0.0000    0.0000 Cl  0  0  0  0  0  0  0  0  0  0  0  0
   -6.0000    2.5981    0.0000 Cl  0  0  0  0  0  0  0  0  0  0  0  0
   -1.5000   -5.1962    0.0000 Cl  0  0  0  0  0  0  0  0  0  0  0  0
  1  2  1  0
  2  3  1  0
  3  4  2  0
  4  5  1  0
  5  6  2  0
  6  7  1  0
  7  8  2  0
  7  9  1  0
  9 10  1  0
 10 11  1  0
 11 12  2  0
 12 13  1  0
 13 14  2  0
 14 15  1  0
 15 16  2  0
 16 17  1  0
 17 18  2  0
 16 19  1  0
 15 20  1  0
  4 21  1  0
  8  3  1  0
 12  6  1  0
 18 13  1  0
M  END
```

In [4]:

```python
# sdf -> smiles
from rdkit.Chem import AllChem
sdf_file = 'data/Structure2D_CID_44138048.sdf'
mols = Chem.SDMolSupplier(sdf_file)
for mol in mols:
    smiles = Chem.MolToSmiles(mol)
    print(f'{smiles}')
```

```
COc1cc2c(cc1Cl)C(c1ccc(Cl)c(Cl)c1)=NCC2
```

分子指纹提取

In [5]:

```python
# MACCS指纹
from rdkit.Chem import MACCSkeys
from rdkit.DataStructs.cDataStructs import ConvertToNumpyArray
from rdkit import Chem
mol_file = 'data/AAQ.mol'
mol = Chem.MolFromMolFile(mol_file)
fps = MACCSkeys.GenMACCSKeys(mol)
fps.ToBitString()[1:]
```

Out[5]:

```
'00000000000000000000000000000000000000000000000000000000000000000100000001000000000000000000000000001000100000010110
00000000101000000001000010111000100101100011011110'
```

In [6]:

```python
# 摩根指纹
from rdkit.Chem import AllChem
import numpy as np
mol_file = 'data/AAQ.mol'
mol = Chem.MolFromMolFile(mol_file)
## GetMorganFingerprintAsBitVect((Mol)mol, (int)radius, (int)nBits=2048)
## @radius: scanning radius
## @nBits: Number of bits to store ECFP features
fp = AllChem.GetMorganFingerprintAsBitVect(mol,2,512)
#np.array(fp)
fp.ToBitString()

## 默认半径为2的摩根指纹就是ECFP4指纹
## 半径为2且考虑feature-based invariants得到的指纹为FCFP4指纹
## m1 = Chem.MolFromSmiles('c1ccccn1')
## ecfp4_mg = AllChem.GetMorganFingerprintAsBitVect(m1,2)
## fcfp4_mg = AllChem.GetMorganFingerprintAsBitVect(m1,2,useFeatures=True)
```

Out[6]:

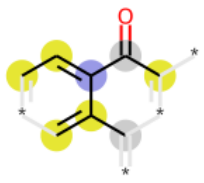
```
'011000000000000000000000000000000001001000000000000000000000001000001000000000000000100000000000000000000000000000000010
000000001000010000000010000000000000000000000000000001000000100000000000000000000000000000000000000010000000000000000000
000000000000000000000000000000000000000000100000000000000000001100000000000000000010000000000000000000000100000000000
001000100000010000000000000000000000000010011000000000000000000000000000000000000100000000000000000000010000000000000
000001000000000000000000000000000000000000000'
```

In [7]:

```python
#计算ECFP4指纹中有效的信息
from rdkit.Chem import AllChem
from rdkit import Chem
import numpy as np
mol_file = 'data/AAQ.mol'
mol = Chem.MolFromMolFile(mol_file)
bi = {}
fp = AllChem.GetMorganFingerprintAsBitVect(mol, radius=2, nBits=512,bitInfo=bi)
# print("num non zero bit in nBit=%d: %d"%(nbit,len(bi.keys())))

"""
里面的最小单元对应的是(atom index, radius)。
(19, 2)表示19号原子半径2的指纹。
((4, 2), (3, 2), (7, 2))表示4号原子、3号原子和7号原子 原子半径为1的指纹。

蓝色：表示中心原子
黄色：表示带有芳香性质的原子
灰色：表示在脂肪环中的原
"""
print(bi)
Draw.DrawMorganBit(mol, 1, bi)
#for v in info.values():
#    print(v)
```

```
{1: ((4, 2), (3, 2), (7, 2)), 2: ((19, 2),), 33: ((17, 0), (18, 0), (20, 0)), 36: ((12, 2),), 58: ((16, 1),), 64:
((1, 1), (0, 1)), 80: ((19, 0),), 114: ((16, 0),), 124: ((8, 2),), 129: ((11, 2),), 138: ((14, 0), (15, 0)), 168: ((1
0, 2),), 175: ((1, 2), (0, 2)), 214: ((2, 1), (5, 1), (10, 1), (11, 1)), 275: ((16, 2),), 294: ((20, 1),), 295: ((19,
1),), 314: ((14, 1), (15, 1)), 337: ((0, 0), (1, 0), (2, 0), (5, 0), (10, 0), (11, 0), (13, 0)), 352: ((3, 1), (4,
1), (7, 1), (8, 1)), 356: ((3, 0), (4, 0), (6, 0), (7, 0), (8, 0), (9, 0), (12, 0)), 363: ((13, 1),), 389: ((9, 2),
(6, 2)), 392: ((17, 1), (18, 1)), 393: ((12, 1),), 430: ((13, 2),), 452: ((9, 1), (6, 1)), 472: ((2, 2), (5, 2))}
```

Out[7]:



In [8]:

```
"""
以提取出2的结构为例，首先提取mol中，半径为2，第19个原子的结构
@submol1: 接收提取出的子结构
@amap: 用于接收原子索引的映射关系，键为原始分子中的原子索引，值为子结构中的原子索引
@env: 是被提取出的键的索引
"""
env = Chem.FindAtomEnvironmentOfRadiusN(mol,2,19)
amap={}
submol1 = Chem.PathToSubmol(mol,env,atomMap=amap)
print(amap)
# 用SMILES表示该子结构
print(Chem.MolToSmiles(submol1))
# env = Chem.FindAtomEnvironmentOfRadiusN(mol,1,1)
# amap={}
# submol11=Chem.PathToSubmol(mol,env,atomMap=amap)

# env = Chem.FindAtomEnvironmentOfRadiusN(mol,1,0)
# amap={}
# submol12=Chem.PathToSubmol(mol,env,atomMap=amap)

# mols=[submol25,submol11,submol12]
# Draw.MolsToGridImage(mols,molsPerRow=3,subImgSize=(300,200),legends=['' for x in mols])
```

```
{12: 0, 16: 1, 17: 2, 18: 3, 19: 4, 20: 5}
CCC(c)(C)C
```

In [9]:

```
# 设置不同的nBits 计算ECFP4指纹中有效信息的个数
from rdkit.Chem import AllChem
from rdkit import Chem
import numpy as np
from rdkit.Chem import Draw
nbitss=[64,128,256,512,1024,2048]
mol_file = 'data/AAQ.mol'
mol = Chem.MolFromMolFile(mol_file)
for nbit in nbitss:
    bi = {}
    fp = AllChem.GetMorganFingerprintAsBitVect(mol, radius=2, nBits=nbit,bitInfo=bi)
    print("num non zero bit in nBit=%d: %d"%(nbit,len(bi.keys())))
```

```
num non zero bit in nBit=64: 25
num non zero bit in nBit=128: 26
num non zero bit in nBit=256: 27
num non zero bit in nBit=512: 28
num non zero bit in nBit=1024: 28
num non zero bit in nBit=2048: 28
```

最大公共子结构

In [10]:

```
from rdkit.Chem import rdFMCS
from rdkit import Chem
mol1 = Chem.MolFromSmiles("O=C(NCc1cc(OC)c(O)cc1)CCCC/C=C/C(C)C")
mol2 = Chem.MolFromSmiles("CC(C)CCCCCC(=O)NCC1=CC(=C(C=C1)O)OC")
mol3 = Chem.MolFromSmiles("c1(C=O)cc(OC)c(O)cc1")
mols = [mol1,mol2,mol3]
res=rdFMCS.FindMCS(mols)
common=Chem.MolFromSmarts(res.smartsString)
#print(res.smartsString,Chem.MolToSmiles(common))

atom_indices = mol1.GetSubstructMatch(common)
print(atom_indices)
print("fragment smiles",Chem.MolFragmentToSmiles(mol1, atom_indices)) # returns the nitrile
```

```
(4, 3, 5, 6, 7, 8, 9, 11, 12, 10)
fragment smiles COc1cc(C)ccc1O
```

分子相似性计算

In [11]:

```
# 基于 MACCS 指纹和 Dice 相似性方法计算相似性
from rdkit import DataStructs
from rdkit.Chem import MACCSkeys
import rdkit
from rdkit import Chem
from rdkit.Chem import Draw
smis=[
    'CC(=O)CC(C1=CC=C(C=C1)[N+]([O-])=O)C1=C(O)C2=CC=CC=C2OC1=O',
    'CC(=O)CC(C1=CC=CC=C1)C1=C(O)C2=C(OC1=O)C=CC=C2',
    'CCC(C1=CC=CC=C1)C1=C(O)C2=C(OC1=O)C=CC=C2'
]
```

```
mols =[]
for smi in smis:
    m = Chem.MolFromSmiles(smi)
    mols.append(m)

fps = [MACCSkeys.GenMACCSKeys(x) for x in mols]
sm01=DataStructs.FingerprintSimilarity(fps[0],fps[1],metric=DataStructs.DiceSimilarity)
sm02=DataStructs.FingerprintSimilarity(fps[0],fps[2],metric=DataStructs.DiceSimilarity)
sm12=DataStructs.FingerprintSimilarity(fps[1],fps[2],metric=DataStructs.DiceSimilarity)

print("similarity between mol 1 and mol2: %.2f"%sm01)
print("similarity between mol 1 and mol3: %.2f"%sm02)
print("similarity between mol 2 and mol3: %.2f"%sm12)
```

```
similarity between mol 1 and mol2: 0.78
similarity between mol 1 and mol3: 0.70
similarity between mol 2 and mol3: 0.92
```

操作分子

原子操作	
对原子进行遍历	m.GetAtoms()
获取原子索引	GetIdx()
获取原子序号	GetAtomicNum()
获取原子符号	GetSymbol()
获取原子连接数（受H是否隐藏影响）	GetDegree()
获取原子总连接数（与H是否隐藏无关）	GetTotalDegree()
与该原子连接的氢原子个数	GetTotalNumHs()
获取原子形式电荷	GetFormalCharge()
获取原子杂化方式	GetHybridization()
获取原子显式化合价	GetExplicitValence()
获取原子隐式化合价	GetImplicitValence()
获取原子总的化合价	GetTotalValence()
该原子是否在芳香烃内	GetIsAromatic()
获取相连的原子	GetNeighbors()

In [12]:
```
from rdkit import Chem
mol_file = 'data/AAQ.mol'
mol = Chem.MolFromMolFile(mol_file)
print('\t'.join(['id', 'num', 'symbol', 'degree', 'HsNumber','explicit','implicit','aromatic','charge', 'hybrid']))
for atom in mol.GetAtoms():
    print(atom.GetIdx(), end='\t')
    print(atom.GetAtomicNum(), end='\t')
    print(atom.GetSymbol(), end='\t')
    print(atom.GetDegree(), end='\t')
    print(atom.GetTotalNumHs(), end='\t\t')
    print(atom.GetExplicitValence(), end='\t\t')
    print(atom.GetImplicitValence(), end='\t\t')
    print(atom.GetIsAromatic(), end='\t\t')
    print(atom.GetFormalCharge(), end='\t')
    print(atom.GetHybridization())
```

```
id      num     symbol  degree  HsNumber        explicit        implicit        aromatic        charge  hybrid
0       6       C       2       1               3               1               True            0       SP2
1       6       C       2       1               3               1               True            0       SP2
2       6       C       2       1               3               1               True            0       SP2
3       6       C       3       0               4               0               True            0       SP2
4       6       C       3       0               4               0               True            0       SP2
5       6       C       2       1               3               1               True            0       SP2
6       6       C       3       0               4               0               False           0       SP2
7       6       C       3       0               4               0               True            0       SP2
8       6       C       3       0               4               0               True            0       SP2
9       6       C       3       0               4               0               False           0       SP2
10      6       C       2       1               3               1               True            0       SP2
11      6       C       2       1               3               1               True            0       SP2
12      6       C       3       0               4               0               True            0       SP2
13      6       C       2       1               3               1               True            0       SP2
14      8       O       1       0               2               0               False           0       SP2
15      8       O       1       0               2               0               False           0       SP2
16      6       C       4       0               4               0               False           0       SP3
17      6       C       1       3               1               3               False           0       SP3
18      6       C       1       3               1               3               False           0       SP3
19      6       C       2       2               2               2               False           0       SP3
20      6       C       1       3               1               3               False           0       SP3
```

In [13]:
```
# 也可以通过索引获取原子：GetAtomWithIdx()
print(mol.GetAtomWithIdx(0).GetSymbol())
```

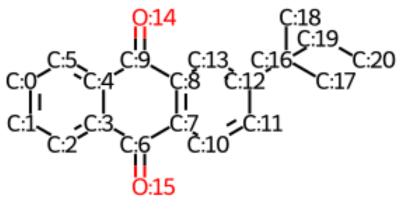
```
C
```

In [14]:
```
# 获取相连的原子：GetNeighbors()
from rdkit import Chem
```

```python
mol_file = 'data/AAQ.mol'
mol = Chem.MolFromMolFile(mol_file)
atom = mol.GetAtomWithIdx(9)
print([x.GetAtomicNum() for x in atom.GetNeighbors()])
# print([x.GetIdx() for x in atom.GetNeighbors()])

# 显示分子中原子的编号
from rdkit import Chem
from rdkit.Chem import  Draw

def mol_with_atom_index( mol ):
    atoms = mol.GetNumAtoms()
    for idx in range( atoms ):
        mol.GetAtomWithIdx( idx ).SetProp( 'molAtomMapNumber', str( mol.GetAtomWithIdx( idx ).GetIdx() ) )
    return mol

mol_with_atom_index(mol)
```

```
[6, 6, 8]
```

Out[14]:



键操作

对键进行遍历	m.GetBonds()
获取键的索引	GetIdx()
获取键的类型	GetGetBondType()
以数字形式显示键的类型	GetBondTypeAsDouble()
是否为芳香键	GetIsAromatic()
是否为共轭键	GetIsConjugated()
是否在环中	IsInRing()
是否在n元环中	IsInRingSize(n)
获取起始原子	GetBeginAtomIdx()
获取末尾原子	GetEndAtomIdx()

In [15]:

```python
from rdkit import Chem
mol_file = 'data/AAQ.mol'
mol = Chem.MolFromMolFile(mol_file)
print('\t'.join(['id', 'type', '\tdouble', 'aromic', 'conjug', 'ring', 'begin', 'end']))
for bond in mol.GetBonds():
    print(bond.GetIdx(), end='\t')
    print(bond.GetBondType(), end='\t')
    print(bond.GetBondTypeAsDouble(), end='\t')
    print(bond.GetIsAromatic(), end='\t')
    print(bond.GetIsConjugated(), end='\t')
    print(bond.IsInRing(), end='\t')
    print(bond.GetBeginAtomIdx(), end='\t')
    print(bond.GetEndAtomIdx())
```

```
id      type            double  aromic  conjug  ring    begin   end
0       AROMATIC        1.5     True    True    True    0       1
1       AROMATIC        1.5     True    True    True    1       2
2       AROMATIC        1.5     True    True    True    2       3
3       AROMATIC        1.5     True    True    True    3       4
4       AROMATIC        1.5     True    True    True    4       5
5       AROMATIC        1.5     True    True    True    5       0
6       SINGLE  1.0     False   True    True    3       6
7       SINGLE  1.0     False   True    True    6       7
8       AROMATIC        1.5     True    True    True    7       8
9       SINGLE  1.0     False   True    True    8       9
10      SINGLE  1.0     False   True    True    9       4
11      AROMATIC        1.5     True    True    True    7       10
12      AROMATIC        1.5     True    True    True    10      11
13      AROMATIC        1.5     True    True    True    11      12
14      AROMATIC        1.5     True    True    True    12      13
15      AROMATIC        1.5     True    True    True    13      8
16      DOUBLE  2.0     False   True    False   9       14
17      DOUBLE  2.0     False   True    False   6       15
18      SINGLE  1.0     False   False   False   12      16
19      SINGLE  1.0     False   False   False   16      17
20      SINGLE  1.0     False   False   False   16      18
21      SINGLE  1.0     False   False   False   16      19
22      SINGLE  1.0     False   False   False   19      20
```

In [16]:

```python
# 也可以通过索引获取键：GetBondWithIdx()
print(mol.GetBondWithIdx(0).GetBondType())
```

```
AROMATIC
```

```
In [17]: # 获得两个atom(atom_index1, atom_index2)之间的键的信息
         mol.GetBondBetweenAtoms(0, 1).GetIdx()

Out[17]: 0
```