**from rdkit import** Chem

**from rdkit.Chem.Draw import** IPythonConsole

**from rdkit.Chem import** Draw

IPythonConsole.ipython\_useSVG=**True**

**def** mol\_with\_atom\_index(mol):

**for** atom **in** mol.GetAtoms():

atom.SetAtomMapNum(atom.GetIdx())

**return** mol

**from rdkit import** Chem

**from rdkit.Chem import** AllChem

m = Chem.MolFromSmiles('c1ncncc1C(=O)[O-]')

AllChem.ComputeGasteigerCharges(m)

m

m2 = Chem.Mol(m)

**for** at **in** m2.GetAtoms():

lbl = '*%s*:*%.2f*'%(at.GetSymbol(),at.GetDoubleProp("\_GasteigerCharge"))

at.SetProp('atomLabel',lbl)

m2

**from rdkit import** Chem

**from rdkit.Chem import** rdDepictor

**from rdkit.Chem.Draw import** rdMolDraw2D

**from IPython.display import** SVG

**def** mol\_with\_stereo(mol,molSize=(300,300), kekulize=**True**, fontSize = 0.8, LineWidth = 1):

*# check for defective molecule*

**if** mol **is None**:

**return None**

mol = rdMolDraw2D.PrepareMolForDrawing(mol, kekulize)

drawer = rdMolDraw2D.MolDraw2DSVG(molSize[0], molSize[1])

drawer.SetFontSize(fontSize) drawer.drawOptions().addStereoAnnotation = **True** *#drawer.drawOptions().addAtomIndices = True*

**try**:

drawer.SetLineWidth(LineWidth)

**except**:

**pass**

drawer.DrawMolecule(mol)

drawer.FinishDrawing()

svg = drawer.GetDrawingText()

**return** svg

m = Chem.MolFromSmiles('C[C@H](F)C\C=C/O')

SVG(mol\_with\_stereo(m))

**from rdkit import** Chem

**from rdkit.Chem.Draw import** IPythonConsole

**from rdkit.Chem import** Draw

ms = [Chem.MolFromSmiles(x) **for** x **in** ('Cc1onc(-c2ccccc2)c1C(=O)N[C@@H]1C(=O)N2[C@@H](C(=O)O)C(C)(C)S[C@H]12',

'Draw.MolsToGridImage(ms)

IPythonConsole.drawOptions.useBWAtomPalette()

Draw.MolsToGridImage(ms)

**from rdkit import** Chem

**from rdkit.Chem.Draw import** IPythonConsole

m = Chem.MolFromSmiles('c1cc(C(=O)O)c(OC(=O)C)cc1')

substructure = Chem.MolFromSmarts('C(=O)O')

print(m.GetSubstructMatches(substructure))

((3, 4, 5), (8, 9, 7))

m

m.\_\_sssAtoms = [0,1,2,6,11,12]

m