**Python Scripts**

Need to know how to write Error handlers in python.

How to look up for variables in a python scripts.

\n = Start a new line.

\\* or \# = This means python will write the special character(\* or #) in the script.

Name = ‘Adele’ => means it is assigning the value Adele to Name.

Concatenation = Pending a string to another one like Name + ‘Like Cake’.

Functions = Block of code that can do specific operation ( modification or get info).

Example Functions: abs(); pow(,); max(,); min(,); round(,); floor(); ceil();

Print(Name.upper()) => so the function upper turn the value ‘Adele’ into Upper Case.

Print(Name.upper().isupper()) => so turn The value into Upper Case and check if the value in Name is upper Case.

Print(len(name)) = > give us the number of characters in Name = 5.

Print(Name[0]) => Here we specify that we want the character of index = 0 in the string Name which is = A, so A= 0, D=1, E=2, L=3, E=4. Or we can do “ print(name.index(‘L’)) ” which will give us = 3.

Everytime you wanna print a number next to a string, you have to convert the number into a string.

Num= 5; print( str (Num) + “oranges sont sur la table”).

How to import function libraries: “ from math import \* ”.

Data Type: Int(all numbers);

How to train a model in python.

import rdkit  
from rdkit import Chem  
m = Chem.MolFromSmiles('CC(=0)NCCC1=CNc2c1cc(0C)cc2')  
print(m)

from rdkit import Chem  
from rdkit.Chem import Draw  
from rdkit.Chem.Draw import IPythonConsole  
from rdkit.Chem import Descriptors  
from rdkit.Chem import AllChem  
from rdkit import DataStructs  
import numpy as np  
  
  
  
m = Chem.MolFromSmiles('COc1cc(C=O)ccc1O')  
print(m)

import pandas as pd  
from rdkit import Chem  
from rdkit.Chem import Draw  
  
from rdkit.Chem import Descriptors  
from rdkit.Chem import AllChem  
from rdkit import DataStructs  
import numpy as np  
  
  
  
m = Chem.MolFromSmiles('COc1cc(C=O)ccc1O')  
print(m)  
  
  
  
# How to read a csv smile file  
# data = pd.read\_csv('./location of the file', index\_col=0) data.head()  
  
#we define a variable to take individual smile string 1 by 1; data defined at the top; Smiles\_std is the column in our table when smiles are stored; and index 0  
# my\_one\_smile\_string = data['SMILE\_STD'][0]  
  
#Transform a smile to a mol; our one smile that we save, we redifining it and transform it into a mol from a smile  
#my\_one\_smile\_string = chem.MolFromSmiles(my\_one\_smile\_string, sanitizer=True)  
  
#so we will see what the mol object looks like  
#print(my\_one\_mol\_object)  
  
#Transform mols to smiles; so we can tranform what we saved into our variable into smiles  
#chem.MolToSmiles(my\_one\_mol\_object)  
  
  
  
#With Panda DataFrame, you can just write it like this: so we copy the first 40 entries of the data table  
#data\_small = data.head(40).copy()  
#print('data\_small.head()')  
  
  
#Here we are creating a new table with the first column having smiles code and 2nd col with mol object  
#from rdkit.chem import PandasTools  
#pandasTools.AddMoleculeCOlumnToFrame(data\_small, smilesCol = 'Smile\_STD', molCol='RoMol')  
  
  
#so we can draw mol files to grid image to see them; here we will use the data from our mol object col RoMol  
#from rdkit.chem import Draw  
#Draw.MolsToGridImage(list(data\_small.RoMol), useSVG=True)

**N2S icon code**

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Benzene Icon:

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Monomers Icon:

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31.927693 31.88481 32.8125 31 A 1.0001 1.0001 0 0 0 33.09375 30.8125 L 37.21875 26.71875 C 38.074094 25.863406 38.354518 24.629218 38.25 23.375 C 38.145482 22.120782 37.662564 20.778852 36.84375 19.46875 C 36.84375 19.46875 35.859943 17.868123 35.34375 17.03125 L 39.3125 19.8125 A 1.0001 1.0001 0 0 0 40.6875 19.625 L 45.5625 13.625 A 1.0001 1.0001 0 0 0 45.375 12.1875 C 45.375 12.1875 38.935404 7.7199367 37.90625 7 C 37.89418 6.99072 37.88708 6.977971 37.875 6.96875 C 36.47265 5.8979906 35.021431 5.2571621 33.625 5.09375 C 33.276711 5.0529927 32.934171 5.0357098 32.59375 5.0625 z M 32.71875 7.0625 C 32.917493 7.0503808 33.139614 7.0662048 33.375 7.09375 C 34.316544 7.2039307 35.500942 7.6810134 36.6875 8.59375 A 1.0001 1.0001 0 0 0 36.71875 8.625 C 37.619 9.2551752 42.156122 12.396476 43.34375 13.21875 L 39.71875 17.65625 L 32.6875 12.75 C 32.491679 12.433169 32.305431 12.115985 32.15625 11.875 C 31.430145 10.664824 31.039219 9.0086711 30.875 8.125 L 31.3125 7.71875 A 1.0001 1.0001 0 0 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21.34375 A 1.0001 1.0001 0 0 0 23.625 21.5 C 23.70221 21.5383 23.786821 21.59422 23.90625 21.65625 C 24.217804 21.818077 24.643756 22.047199 25.125 22.3125 C 26.087489 22.843103 27.252089 23.506867 28.0625 24.03125 A 1.0001 1.0001 0 0 0 28.25 24.15625 C 28.705001 24.873462 29.273532 25.784681 29.5625 26.21875 C 29.5693 26.22953 29.5557 26.23916 29.5625 26.25 C 30.399038 27.585625 30.928511 29.019912 31.1875 29.75 C 30.847475 29.960152 30.336511 30.06803 29.625 29.96875 C 28.748256 29.846414 27.661161 29.38869 26.5625 28.65625 A 1.0001 1.0001 0 0 0 26.46875 28.625 C 26.46875 28.625 23.242525 26.88986 21.71875 25.9375 A 1.0001 1.0001 0 0 0 21.59375 25.875 C 21.004579 24.920711 20.624149 24.291895 20.25 23.6875 C 19.442756 22.342093 18.892805 21.155442 18.5625 20.40625 L 18.875 20.125 A 1.0001 1.0001 0 0 0 18.90625 20.09375 C 19.031258 19.968742 19.191121 19.874322 19.40625 19.84375 z M 17.09375 21.8125 C 17.420395 22.56799 17.701005 23.335008 18.53125 24.71875 A 1.0001 1.0001 0 0 0 18.5625 24.71875 C 19.861925 26.817821 23.25 32.3125 23.25 32.3125 A 1.0001 1.0001 0 0 0 23.25 32.34375 C 23.931186 33.433648 24.304518 34.497968 24.375 35.34375 C 24.44548 36.189532 24.250906 36.749094 23.90625 37.09375 L 20.65625 40.3125 C 20.417409 39.265825 20.042527 37.985665 19.34375 36.9375 C 18.186419 35.201504 14.65625 29.46875 14.65625 29.46875 C 13.975064 28.378852 13.601732 27.314532 13.53125 26.46875 C 13.46077 25.622968 13.655344 25.063406 14 24.71875 L 16.65625 22.0625 A 1.0001 1.0001 0 0 0 17.09375 21.8125 z M 10.46875 32.25 L 16.8125 36.8125 A 1.0001 1.0001 0 0 0 16.90625 36.875 A 1.0001 1.0001 0 0 0 16.96875 36.9375 C 17.182388 37.270317 17.501118 37.829801 17.65625 38.0625 C 18.428002 39.220127 18.844375 41.340544 18.96875 42.125 C 18.46452 42.607774 17.761045 42.797331 16.8125 42.6875 C 15.843237 42.57527 14.664058 42.108771 13.46875 41.28125 C 12.573114 40.654305 8.0969755 37.53356 6.875 36.6875 L 10.46875 32.25 z"></path></svg></span>  
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**Mol File Representation**:

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