```
import pandas as pd
import numpy as np
```

```
# Importing the chembl_database
! pip install chembl_webresource_client
```

```
Looking in indexes: https://pypi.org/simple, https://us-python.pkg.dev/colab-wheels/public/simple/
Requirement already satisfied: chembl_webresource_client in /usr/local/lib/python3.7/site-packages (0.10.8)
Requirement already satisfied: requests>=2.18.4 in /usr/local/lib/python3.7/site-packages (from chembl_webresource_client) (2.22.0)
Requirement already satisfied: easydict in /usr/local/lib/python3.7/site-packages (from chembl_webresource_client) (1.10)
Requirement already satisfied: urllib3 in /usr/local/lib/python3.7/site-packages (from chembl_webresource_client) (1.25.8)
Requirement already satisfied: requests-cache~=0.7.0 in /usr/local/lib/python3.7/site-packages (from chembl_webresource_client) (0.
Requirement already satisfied: certifi>=2017.4.17 in /usr/local/lib/python3.7/site-packages (from requests>=2.18.4->chembl_webresou
Requirement already satisfied: chardet<3.1.0,>=3.0.2 in /usr/local/lib/python3.7/site-packages (from requests>=2.18.4->chembl_webre
Requirement already satisfied: idna<2.9,>=2.5 in /usr/local/lib/python3.7/site-packages (from requests>=2.18.4->chembl_webresource_
Requirement already satisfied: itsdangerous>=2.0.1 in /usr/local/lib/python3.7/site-packages (from requests-cache~=0.7.0->chembl_we
Requirement already satisfied: attrs<22.0,>=21.2 in /usr/local/lib/python3.7/site-packages (from requests-cache~=0.7.0->chembl_webr
Requirement already satisfied: pyyaml>=5.4 in /usr/local/lib/python3.7/site-packages (from requests-cache~=0.7.0->chembl_webresourc
Requirement already satisfied: url-normalize<2.0,>=1.4 in /usr/local/lib/python3.7/site-packages (from requests-cache~=0.7.0->chemb
Requirement already satisfied: six in /usr/local/lib/python3.7/site-packages (from url-normalize<2.0,>=1.4->requests-cache~=0.7.0->
```

```
# Import necessary libraries
import pandas as pd
from chembl_webresource_client.new_client import new_client
```

```
# PART 1

# Target search for hcm using tnni3
target = new_client.target
target_query = target.search('tnni3')
targets = pd.DataFrame.from_dict(target_query)
targets
```

	cross_references	organism	pref_name	score	species_group_flag	target_chembl_id	target_compo
0	[]	Mus musculus	Serine/threonine-protein kinase TNNI3K	15.0	False	CHEMBL4879467	[{'accession': 'Q5 'component_desc
1	[]	Rattus norvegicus	Serine/threonine-protein kinase TNNI3K	14.0	False	CHEMBL4802010	[{'accession': 'Q7 'component_desc
2	[]	Homo sapiens	Serine/threonine-protein kinase TNNI3K	13.0	False	CHEMBL5260	[{'accession': 'Q5 'component_desc
3	[]	Homo sapiens	Troponin, cardiac muscle	11.0	False	CHEMBL2095202	[{'accession': 'P6 'component_desc

```
# Retrieve data for the single protein for humans
selected_target = targets.target_chembl_id[2]
selected_target
```

```
'CHEMBL5260'
```

```
activity = new_client.activity
res = activity.filter(target_chembl_id=selected_target).filter(standard_type="IC50")
```

```
df = pd.DataFrame.from_dict(res)
df.head()
```

	activity_comment	activity_id	activity_properties	assay_chembl_id	assay_description	assay_type	assa
0	None	15698897	[]	CHEMBL3615799	Displacement of 5-({[2-({[3-({4-[(5-hydroxy-2-...	B	
1	None	15698898	[]	CHEMBL3615799	Displacement of 5-({[2-({[3-({4-[(5-	B	

```
# Filtering the ones with unique value of IC50
df.standard_type.unique()
```

```
array(['IC50'], dtype=object)
```

```
df.to_csv('bioactivity_data.csv', index=False)
```

```
from google.colab import drive
drive.mount('/content/drive')
```

```
Drive already mounted at /content/drive; to attempt to forcibly remount, call drive.mount("/content/drive", force_remount=True).
```

```
# Dropping any values without the standard type
# Dropping rows with null values for standard type

df2 = df[df.standard_value.notna()]
df2
```

	activity_comment	activity_id	activity_properties	assay_chembl_id	assay_description	assay_type	as
0	None	15698897	[]	CHEMBL3615799	Displacement of 5-({[2-({[3-({4-[(5-hydroxy-2-...	B	
1	None	15698898	[]	CHEMBL3615799	Displacement of 5-({[2-({[3-({4-[(5-hydroxy-2-...	B	
2	None	15698899	[]	CHEMBL3615799	Displacement of 5-({[2-({[3-({4-[(5-hydroxy-2-...	B	
3	None	15698900	[]	CHEMBL3615799	Displacement of 5-({[2-({[3-({4-[(5-hydroxy-2-...	B	
4	None	15698901	[]	CHEMBL3615799	Displacement of 5-({[2-({[3-({4-[(5-hydroxy-2-...	B	
...	...	...	...	...	...	...	
294	None	23299501	[{'comments': None, 'relation': '=', 'result_f...	CHEMBL4841801	Inhibition of human myc-TNNI3K expressed in HE...	B	
295	None	23299502	[{'comments': None, 'relation': '=', 'result_f...	CHEMBL4841801	Inhibition of human myc-TNNI3K expressed in HE...	B	
296	None	23372920	[{'comments': None, 'relation': None, 'result_...	CHEMBL4884885	HH498(TNNILGY1) Takeda global kinase panel	B	
297	None	23373329	[{'comments': None, 'relation': None, 'result_...	CHEMBL4885176	HH498(TNNILGY1) Takeda global kinase panel	B	
298	None	23373683	[{'comments': None, 'relation': None, 'result_...	CHEMBL4885460	HH498(TNNILGY1) Takeda global kinase panel	B	

297 rows × 45 columns

```
# PART 2

# DATA PRE-PROCESSING

# Compounds are segregated based on a certain criteria of IC50 value

# Segregation is happening based on standard value

# Compounds having values of less than 1000 nM will be considered to be active
```

```
# those greater than 10,000 nM will be considered to be inactive.
# values in between 1,000 and 10,000 nM will be referred to as intermediate.

bioactivity_class = []
for i in df2.standard_value:
  if float(i) >= 10000:
    bioactivity_class.append("inactive")
  elif float(i) <= 1000:
    bioactivity_class.append("active")
  else:
    bioactivity_class.append("intermediate")
```

```
#Iterate the "molecule_chembl_id" to a list
mol_cid = []
for i in df2.molecule_chembl_id:
  mol_cid.append(i)
```

```
# Iterate "canonical_smiles" to a list
canonical_smiles = []
for i in df2.canonical_smiles:
  canonical_smiles.append(i)
```

```
# Iterate standard_value to a list
standard_value = []
for i in df2.standard_value:
  standard_value.append(i)
```

```
# Combine the 4 lists into a dataframe
data_tuples = list(zip(mol_cid, canonical_smiles, bioactivity_class, standard_value))
df3 = pd.DataFrame( data_tuples,  columns=['molecule_chembl_id', 'canonical_smiles', 'bioactivity_class', 'standard_value'])
df3
```

	molecule_chembl_id	canonical_smiles	bioactivity_class	standard_value
0	CHEMBL3612641	CNS(=O)(=O)c1cccc(Nc2ncnc3[nH]cnc23)c1	active	500.0
1	CHEMBL3612643	CNS(=O)(=O)c1cccc(Nc2ncnc3c2ncn3C)c1	inactive	25000.0
2	CHEMBL3612642	CNS(=O)(=O)c1cccc(Nc2nc(F)nc3[nH]cnc23)c1	intermediate	3200.0
3	CHEMBL3612644	CNS(=O)(=O)c1cccc(Nc2nc(N)nc3[nH]cnc23)c1	intermediate	8000.0
4	CHEMBL3612645	CNS(=O)(=O)c1cccc(Nc2nc(Cl)nc3[nH]cnc23)c1	inactive	16000.0
...	...	...	...	...
292	CHEMBL3815093	CNS(=O)(=O)c1ccc(N(C)C)c(Nc2ncnc3cc(OC)c(OC)cc...	active	100.0
293	CHEMBL4094739	CCS(=O)(=O)c1ccc(S(=O)(=O)NC)cc1Nc1cc(Nc2ccc(C...	active	8.0
294	CHEMBL4088216	CN1C(=O)[C@@H](N2CCc3cn(Cc4ccccc4)nc3C2=O)COc2...	active	1000.0
295	CHEMBL4549667	CN1C(=O)[C@@H](N2CCc3c(nn(Cc4ccccc4)c3Br)C2=O)...	active	1000.0

```
# storing df as a csv file
df3.to_csv('bioactivity_data_preprocessed.csv', index=False)
```

```
! ls -l
```

```
total 192832
-rw-r--r-- 1 root root   199379 Jan 10 15:22 bioactivity_data.csv
-rw-r--r-- 1 root root    23098 Jan 10 15:22 bioactivity_data_preprocessed.csv
-rw-r--r-- 1 root root   539408 Jan 10 15:11 descriptors_output.csv
-rw-r--r-- 1 root root    36852 Jan 10 15:08 df_combined.csv
drwx------ 5 root root     4096 Jan 10 14:47 drive
-rw-r--r-- 1 root root   538814 Jan 10 15:11 final_matrix_ic50_only.csv
drwxr-xr-x 3 root root     4096 Jan 10 15:10 __MACOSX
-rwxr-xr-x 1 root root 85055499 Mar 11  2020 Miniconda3-py37_4.8.2-Linux-x86_64.sh
-rw-r--r-- 1 root root 85055499 Mar 11  2020 Miniconda3-py37_4.8.2-Linux-x86_64.sh.1
-rw-r--r-- 1 root root    19122 Jan 10 15:10 molecule.smi
drwxrwxr-x 4 root root     4096 May 30  2020 PaDEL-Descriptor
-rw-r--r-- 1 root root      231 Jan 10 15:10 padel.sh
-rw-r--r-- 1 root root 25768637 Jan 10 15:10 padel.zip
-rw-r--r-- 1 root root    14170 Jan 10 15:08 plot_bioactivity_class.pdf
-rw-r--r-- 1 root root    15727 Jan 10 15:08 plot_ic50.pdf
-rw-r--r-- 1 root root    14577 Jan 10 15:08 plot_LogP.pdf
-rw-r--r-- 1 root root    13755 Jan 10 15:08 plot_MW.pdf
-rw-r--r-- 1 root root    16763 Jan 10 15:08 plot_NumHAcceptors.pdf
-rw-r--r-- 1 root root    15655 Jan 10 15:08 plot_NumHDonors.pdf
```

```
-rw-r--r-- 1 root root    81544 Jan 10 15:08 results.zip
drwxr-xr-x 1 root root     4096 Jan  5 14:34 sample_data
```

```
! wget https://repo.anaconda.com/miniconda/Miniconda3-py37_4.8.2-Linux-x86_64.sh
! chmod +x Miniconda3-py37_4.8.2-Linux-x86_64.sh
! bash ./Miniconda3-py37_4.8.2-Linux-x86_64.sh -b -f -p /usr/local
! conda install -c rdkit rdkit -y
import sys
sys.path.append('/usr/local/lib/python3.7/site-packages/')
```

```
--2023-01-10 15:22:32--  https://repo.anaconda.com/miniconda/Miniconda3-py37_4.8.2-Linux-x86_64.sh
Resolving repo.anaconda.com (repo.anaconda.com)... 104.16.131.3, 104.16.130.3, 2606:4700::6810:8303, ...
Connecting to repo.anaconda.com (repo.anaconda.com)|104.16.131.3|:443... connected.
HTTP request sent, awaiting response... 200 OK
Length: 85055499 (81M) [application/x-sh]
Saving to: ‘Miniconda3-py37_4.8.2-Linux-x86_64.sh.2’

Miniconda3-py37_4.8 100%[===================>]  81.12M   189MB/s    in 0.4s

2023-01-10 15:22:33 (189 MB/s) - ‘Miniconda3-py37_4.8.2-Linux-x86_64.sh.2’ saved [85055499/85055499]

PREFIX=/usr/local
Unpacking payload ...
Collecting package metadata (current_repodata.json): done
Solving environment: |
The environment is inconsistent, please check the package plan carefully
The following packages are causing the inconsistency:

  - defaults/linux-64::requests==2.22.0=py37_1
  - defaults/linux-64::pip==20.0.2=py37_1
  - defaults/linux-64::wheel==0.34.2=py37_0
  - defaults/linux-64::openssl==1.1.1s=h7f8727e_0
  - defaults/linux-64::pyopenssl==19.1.0=py37_0
  - defaults/linux-64::icu==58.2=he6710b0_3
  - rdkit/linux-64::rdkit==2020.09.1.0=py37hd50e099_1
  - defaults/linux-64::fontconfig==2.14.1=h52c9d5c_1
  - defaults/linux-64::jpeg==9e=h7f8727e_0
  - defaults/linux-64::readline==7.0=h7b6447c_5
  - defaults/linux-64::cffi==1.14.0=py37h2e261b9_0
  - defaults/linux-64::pysocks==1.7.1=py37_0
  - defaults/linux-64::libxcb==1.15=h7f8727e_0
  - defaults/linux-64::yaml==0.1.7=had09818_2
  - defaults/linux-64::xz==5.2.8=h5eee18b_0
  - defaults/linux-64::libffi==3.4.2=h6a678d5_6
  - defaults/noarch::python-dateutil==2.8.2=pyhd3eb1b0_0
  - defaults/linux-64::libstdcxx-ng==11.2.0=h1234567_1
  - defaults/linux-64::bzip2==1.0.8=h7b6447c_0
  - defaults/linux-64::libxml2==2.9.14=h74e7548_0
  - defaults/linux-64::zlib==1.2.13=h5eee18b_0
  - defaults/linux-64::packaging==22.0=py37h06a4308_0
  - defaults/linux-64::typing_extensions==4.4.0=py37h06a4308_0
  - defaults/linux-64::certifi==2022.12.7=py37h06a4308_0
  - defaults/linux-64::asn1crypto==1.3.0=py37_0
  - defaults/linux-64::toolz==0.12.0=py37h06a4308_0
  - defaults/linux-64::pixman==0.40.0=h7f8727e_1
  - defaults/linux-64::expat==2.4.9=h6a678d5_0
  - defaults/linux-64::pycosat==0.6.3=py37h7b6447c_0
  - defaults/linux-64::numexpr==2.8.4=py37he184ba9_0
  - defaults/linux-64::importlib-metadata==4.11.3=py37h06a4308_0
  - defaults/linux-64::mkl_fft==1.3.1=py37hd3c417c_0
  - defaults/linux-64::glib==2.69.1=he621ea3_2
  - defaults/linux-64::libgcc-ng==11.2.0=h1234567_1
  - defaults/linux-64::lerc==3.0=h295c915_0
  - defaults/linux-64::python==3.7.6=h0371630_2
  - defaults/linux-64::giflib==5.2.1=h7b6447c_0
  - defaults/linux-64::pcre==8.45=h295c915_0
  - defaults/linux-64::numpy==1.21.5=py37h6c91a56_3
  - defaults/linux-64::pandas==1.3.5=py37h8c16a72_0
```

```
df = pd.read_csv('bioactivity_data_preprocessed.csv')
```

```
# PART 3

# Calculating Lipinski descripters
# Describes the drug-likeness of a compound. Based on ADME (Absorptive, Distribution, Metabolism, and Excretion).
# The rule stays fixed where properties such as H-bond and molecular weight are to be lesser than a certain value only and such.

from rdkit import Chem
from rdkit.Chem import Descriptors, Lipinski
```

```
# To calculate the Lipinski descripters
def lipinski(smiles, verbose=False):

    moldata= []
    for elem in smiles:
```

```
        mol=Chem.MolFromSmiles(elem)
        moldata.append(mol)

    baseData= np.arange(1,1)
    i=0
    for mol in moldata:

        desc_MolWt = Descriptors.MolWt(mol)
        desc_MolLogP = Descriptors.MolLogP(mol)
        desc_NumHDonors = Lipinski.NumHDonors(mol)
        desc_NumHAcceptors = Lipinski.NumHAcceptors(mol)

        row = np.array([desc_MolWt,
                        desc_MolLogP,
                        desc_NumHDonors,
                        desc_NumHAcceptors])

        if(i==0):
            baseData=row
        else:
            baseData=np.vstack([baseData, row])
        i=i+1

    columnNames=["MW","LogP","NumHDonors","NumHAcceptors"]
    descriptors = pd.DataFrame(data=baseData,columns=columnNames)

    return descriptors
```

```
# Provides exact atomic details
df_lipinski = lipinski(df.canonical_smiles)

# Further details as per the Lipinski parameters
df_lipinski
```

	MW	LogP	NumHDonors	NumHAcceptors
0	304.335	1.0046	3.0	6.0
1	318.362	1.0150	2.0	7.0
2	322.325	1.1437	3.0	6.0
3	319.350	0.5868	4.0	7.0
4	338.780	1.6580	3.0	6.0
...	...	...	...	...
292	417.491	2.3647	2.0	8.0
293	482.975	2.7139	3.0	9.0
294	402.454	2.3537	0.0	5.0
295	481.350	3.1162	0.0	5.0
296	458.540	1.1302	0.0	7.0

297 rows × 4 columns

```
# The lipinski values and the original dataframe are combined to an all in one
df_combined = pd.concat([df,df_lipinski], axis=1)
df_combined.to_csv('df_combined.csv')
df_combined
```

molecule_chembl_id	canonical_smiles	bioactivity_class	standard_value	MW

```
# Convert ic50 to pic50
# pic50 is bsaically -log10 of ic50

def pIC50(input):
    pIC50 = []

    for i in input['standard_value']:
        molar = i*(10**-9) # Converts nM to M
        pIC50.append(-np.log10(molar))

    input['pIC50'] = pIC50
    x = input.drop('standard_value', 1)

    return x
```

```
# pic50 is performed on standard value in df_combined
df_final = pIC50(df_combined)
df_final
```

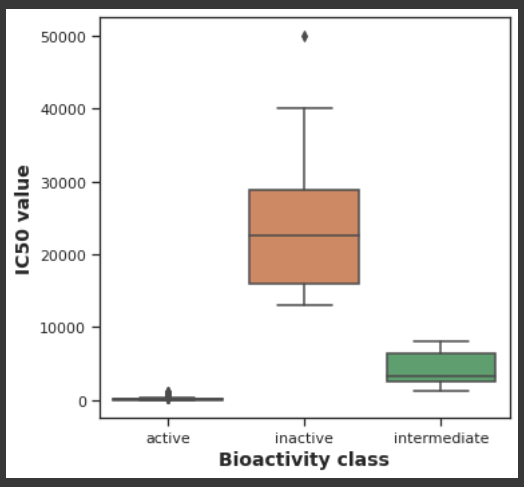
```
<ipython-input-126-9faa7b5de017>:12: FutureWarning: In a future version of pandas all arguments of DataFram
  x = input.drop('standard_value', 1)
```

	molecule_chembl_id	canonical_smiles	bioactivity_class	MW	LogP	NumHDo
0	CHEMBL3612641	CNS(=O)(=O)c1cccc(Nc2ncnc3[nH]cnc23)c1	active	304.335	1.0046	
1	CHEMBL3612643	CNS(=O)(=O)c1cccc(Nc2ncnc3c2ncn3C)c1	inactive	318.362	1.0150	
2	CHEMBL3612642	CNS(=O)(=O)c1cccc(Nc2nc(F)nc3[nH]cnc23)c1	intermediate	322.325	1.1437	
3	CHEMBL3612644	CNS(=O)(=O)c1cccc(Nc2nc(N)nc3[nH]cnc23)c1	intermediate	319.350	0.5868	
4	CHEMBL3612645	CNS(=O)(=O)c1cccc(Nc2nc(Cl)nc3[nH]cnc23)c1	inactive	338.780	1.6580	
...	...	...	...	...	...	
292	CHEMBL3815093	CNS(=O)(=O)c1ccc(N(C)C)c(Nc2ncnc3cc(OC)c(OC)cc...	active	417.491	2.3647	
293	CHEMBL4094739	CCS(=O)(=O)c1ccc(S(=O)(=O)NC)cc1Nc1cc(Nc2ccc(C...	active	482.975	2.7139	
294	CHEMBL4088216	CN1C(=O)[C@@H](N2CCc3cn(Cc4ccccc4)nc3C2=O)COc2...	active	402.454	2.3537	

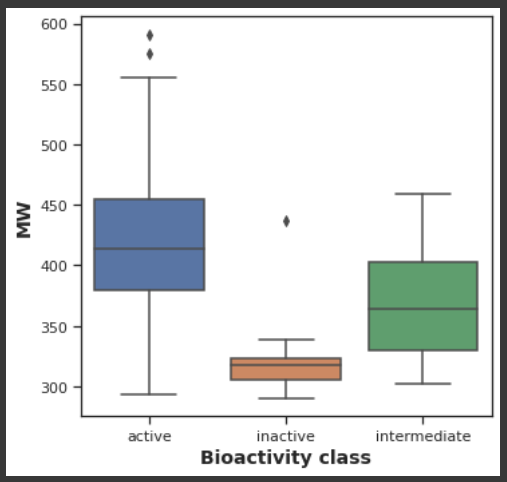
```
# PART 4

# Chemical space analysis w lipinski descriptors
import seaborn as sns
sns.set(style='ticks')
import matplotlib.pyplot as plt
```

```
# Frequency plot of the combined data
plt.figure(figsize=(5.5, 5.5))

sns.countplot(x='bioactivity_class', data=df_combined, edgecolor='black')

plt.xlabel('Bioactivity class', fontsize=14, fontweight='bold')
plt.ylabel('Frequency', fontsize=14, fontweight='bold')

plt.savefig('plot_bioactivity_class.pdf')
```

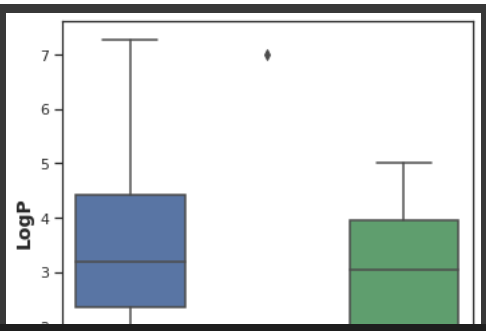
```
# Box plot for all the three variants wrt to their type and their respective standard values
plt.figure(figsize=(5.5, 5.5))

sns.boxplot(x = 'bioactivity_class', y = 'standard_value', data = df_combined)

plt.xlabel('Bioactivity class', fontsize=14, fontweight='bold')
plt.ylabel('IC50 value', fontsize=14, fontweight='bold')

plt.savefig('plot_ic50.pdf')
```



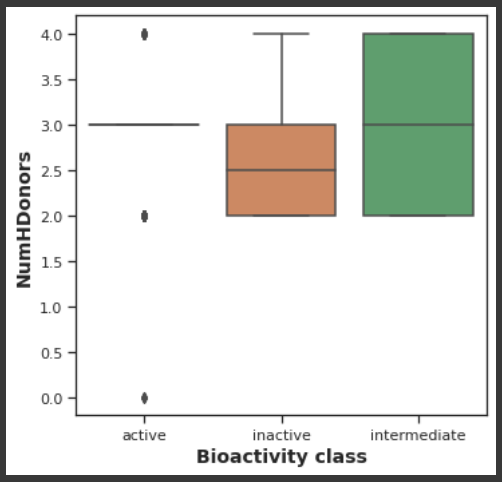

```
# Box plots for the other 4 Lipinski descripters

# M W

plt.figure(figsize=(5.5, 5.5))

sns.boxplot(x = 'bioactivity_class', y = 'MW', data = df_combined)

plt.xlabel('Bioactivity class', fontsize=14, fontweight='bold')
plt.ylabel('MW', fontsize=14, fontweight='bold')

plt.savefig('plot_MW.pdf')
```



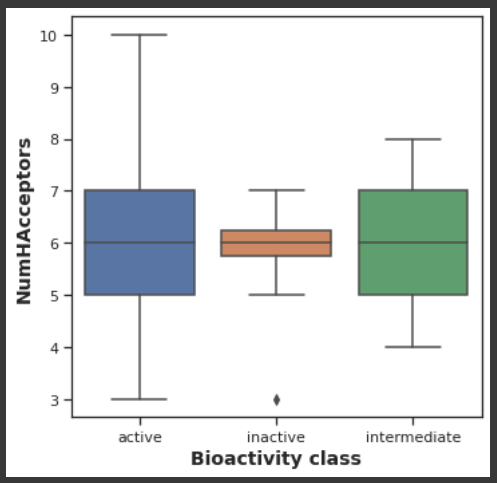

```
# Log P
plt.figure(figsize=(5.5, 5.5))

sns.boxplot(x = 'bioactivity_class', y = 'LogP', data = df_combined)

plt.xlabel('Bioactivity class', fontsize=14, fontweight='bold')
plt.ylabel('LogP', fontsize=14, fontweight='bold')

plt.savefig('plot_LogP.pdf')
```




```
# NumHDonors
plt.figure(figsize=(5.5, 5.5))

sns.boxplot(x = 'bioactivity_class', y = 'NumHDonors', data = df_combined)

plt.xlabel('Bioactivity class', fontsize=14, fontweight='bold')
plt.ylabel('NumHDonors', fontsize=14, fontweight='bold')

plt.savefig('plot_NumHDonors.pdf')
```




```
# NumHAcceptors
plt.figure(figsize=(5.5, 5.5))

sns.boxplot(x = 'bioactivity_class', y = 'NumHAcceptors', data = df_combined)

plt.xlabel('Bioactivity class', fontsize=14, fontweight='bold')
plt.ylabel('NumHAcceptors', fontsize=14, fontweight='bold')

plt.savefig('plot_NumHAcceptors.pdf')
```




```
! zip -r results.zip . -i *.csv *.pdf
```

```
  updating: plot_NumHAcceptors.pdf (deflated 35%)
  updating: plot_NumHDonors.pdf (deflated 37%)
  updating: plot_bioactivity_class.pdf (deflated 38%)
  updating: bioactivity_data.csv (deflated 94%)
  updating: bioactivity_data_preprocessed.csv (deflated 87%)
  updating: df_combined.csv (deflated 83%)
  updating: plot_MW.pdf (deflated 37%)
  updating: plot_ic50.pdf (deflated 36%)
```

```
  updating: plot_LogP.pdf (deflated 36%)
    adding: descriptors_output.csv (deflated 96%)
    adding: final_matrix_ic50_only.csv (deflated 96%)
```

```
# PART 5
# lipinski descriptors provide very simple molecular descriptor overview of the drug like properties
# padel will be used to calculate molecular descriptors
! wget /content/drive/MyDrive/padel.zip
```

```
/content/drive/MyDrive/padel.zip: Scheme missing.
```

```
! unzip padel.zip
```

```
Archive:  padel.zip
replace __MACOSX/._PaDEL-Descriptor? [y]es, [n]o, [A]ll, [N]one, [r]ename:
```

```
# The same file as that of df_combined
df4=pd.read_csv('df_combined.csv')
```

```
# canonical_smiles and molecule_chembl_id is filtered and placed into a new variable
selection = ['canonical_smiles','molecule_chembl_id']
df3_selection = df4[selection]
df3_selection.to_csv('molecule.smi', sep='\t', index=False, header=False)
```

```
# It contains the smiles notation and the particular molecule
# Smiles notation represents the chemical structure

! cat molecule.smi | head -5
```

```
CNS(=O)(=O)c1cccc(Nc2ncnc3[nH]cnc23)c1  CHEMBL3612641
CNS(=O)(=O)c1cccc(Nc2ncnc3c2ncn3C)c1    CHEMBL3612643
CNS(=O)(=O)c1cccc(Nc2nc(F)nc3[nH]cnc23)c1       CHEMBL3612642
CNS(=O)(=O)c1cccc(Nc2nc(N)nc3[nH]cnc23)c1       CHEMBL3612644
CNS(=O)(=O)c1cccc(Nc2nc(Cl)nc3[nH]cnc23)c1      CHEMBL3612645
```

```
# Cleans the data of any impurities like salts,acids and such.
# It then calculates the finger print values of the type pubchem finger prints

! cat padel.sh
```

```
java -Xms1G -Xmx1G -Djava.awt.headless=true -jar ./PaDEL-Descriptor/PaDEL-Descriptor.jar -removesalt -standardizenitro -fingerprint
```

```
! bash padel.sh
```

```
Processing CHEMBL4876578 in molecule.smi (246/297). Average speed: 0.22 s/mol.
Processing CHEMBL4864463 in molecule.smi (248/297). Average speed: 0.22 s/mol.
Processing CHEMBL4872243 in molecule.smi (247/297). Average speed: 0.22 s/mol.
Processing CHEMBL4877505 in molecule.smi (250/297). Average speed: 0.22 s/mol.
Processing CHEMBL4873406 in molecule.smi (249/297). Average speed: 0.22 s/mol.
Processing CHEMBL4871527 in molecule.smi (252/297). Average speed: 0.22 s/mol.
Processing CHEMBL4865829 in molecule.smi (251/297). Average speed: 0.22 s/mol.
Processing CHEMBL4859309 in molecule.smi (254/297). Average speed: 0.22 s/mol.
Processing CHEMBL4847826 in molecule.smi (253/297). Average speed: 0.22 s/mol.
Processing CHEMBL4854957 in molecule.smi (255/297). Average speed: 0.22 s/mol.
Processing CHEMBL4845883 in molecule.smi (256/297). Average speed: 0.22 s/mol.
Processing CHEMBL4867760 in molecule.smi (258/297). Average speed: 0.22 s/mol.
Processing CHEMBL4875220 in molecule.smi (257/297). Average speed: 0.22 s/mol.
Processing CHEMBL4856147 in molecule.smi (259/297). Average speed: 0.22 s/mol.
Processing CHEMBL4859818 in molecule.smi (261/297). Average speed: 0.22 s/mol.
Processing CHEMBL4855081 in molecule.smi (260/297). Average speed: 0.22 s/mol.
Processing CHEMBL4867053 in molecule.smi (262/297). Average speed: 0.22 s/mol.
Processing CHEMBL4870079 in molecule.smi (263/297). Average speed: 0.22 s/mol.
Processing CHEMBL4850964 in molecule.smi (264/297). Average speed: 0.22 s/mol.
Processing CHEMBL4868391 in molecule.smi (265/297). Average speed: 0.22 s/mol.
Processing CHEMBL4066096 in molecule.smi (267/297). Average speed: 0.22 s/mol.
```

```
# Preparing data matrices

# This matrix consists of the data descriptors (pubchem fingerprints) for every molecule
# Pubchem fingerprints are molecular features.

dataset3 = pd.read_csv('descriptors_output.csv')
dataset3
```

	Name	PubchemFP0	PubchemFP1	PubchemFP2	PubchemFP3	PubchemFP4	Pub
0	CHEMBL3612641	1	1	0	0	0	
1	CHEMBL3612643	1	1	0	0	0	
2	CHEMBL3612642	1	1	0	0	0	
3	CHEMBL3612644	1	1	0	0	0	
4	CHEMBL3612645	1	1	0	0	0	
...	...	...	...	...	...	...	
292	CHEMBL3815093	1	1	1	0	0	
293	CHEMBL4094739	1	1	1	0	0	
294	CHEMBL4088216	1	1	1	0	0	
295	CHEMBL4549667	1	1	1	0	0	
296	CHEMBL4097778	1	1	1	0	0	

297 rows × 882 columns

```
dataset3.to_csv('final_matrix_ic50_only.csv', index=False)
```

```
dataset3 = dataset3.drop(columns=['Name'])
```

```
# PART 6

# Model building
# X - pubchem finger prints
# Y - pic50 values

X = dataset3
Y = df_final.pIC50
X.shape
Y.shape
```

```
(297,)
```

```
# lipinski descriptors majorly talk about the global aspects of a molecule like solubility and h bond related stuff
# whereas pubchem fingerprints prev created talk more of the local aspects such as within the molecule prop stuff
```

```
# Remove low variance features
# Reduces the number of columns

from sklearn.feature_selection import VarianceThreshold
from sklearn.model_selection import train_test_split
```

```
from sklearn.ensemble import RandomForestRegressor
from sklearn.tree import DecisionTreeClassifier
from sklearn.preprocessing import StandardScaler
from sklearn.metrics import accuracy_score
import sklearn
import math

selection = VarianceThreshold(threshold=(.8 * (1 - .8)))
X = selection.fit_transform(X)
```

```
X.shape
```

```
(297, 110)
```

```
# Data split 8:2 ratio
X_train, X_test, Y_train, Y_test = train_test_split(X, Y, test_size=0.2, random_state = 1)
X_train.shape, Y_train.shape
```

```
((237, 110), (237,))
```

```
X_test.shape, Y_test.shape
```

```
((60, 110), (60,))
```

```
# Regression model using Random Forest
import numpy as np
model = RandomForestRegressor(n_estimators=100)
model.fit(X_train, Y_train)
Y_pred = model.predict(X_test)
Y_pred
```

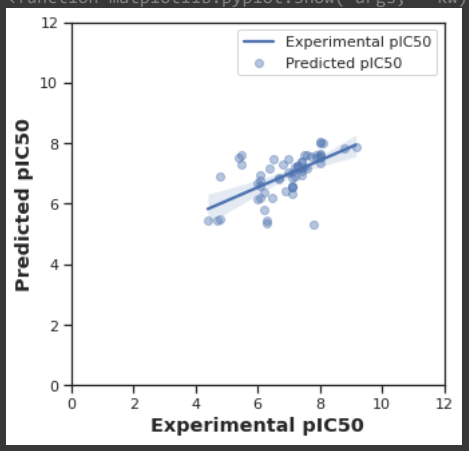
```
array([7.52354131, 7.21636048, 8.05524786, 7.48177767, 7.61269624,
       7.61269624, 7.58429707, 7.37016314, 7.15370809, 7.15151017,
       7.35744447, 6.7962181 , 5.44579219, 7.28731631, 7.46214788,
       6.3290617 , 6.13810772, 7.06832064, 6.61293386, 7.2286557 ,
       7.61856556, 5.44579219, 6.40193166, 6.89697034, 7.58429707,
       6.350455  , 6.6711189 , 6.17993531, 7.27861654, 7.98925896,
       5.32439161, 6.93192408, 6.88117518, 7.17742273, 5.44579219,
       7.04130832, 7.98925896, 7.26829504, 7.65154039, 6.86912189,
       5.46679562, 7.25016518, 6.75444138, 7.5224917 , 7.39108089,
       5.35697748, 6.93606089, 7.16456668, 7.84444579, 7.61856556,
       6.52662805, 7.59563688, 6.57935999, 7.88222955, 6.52662805,
       7.52503388, 5.80439251, 6.83784935, 7.03856112, 6.19454205])
```

```
mse = sklearn.metrics.mean_squared_error(Y_test,Y_pred)
rmse = math.sqrt(mse)
print('Accuracy for Random Forest',max(0,rmse))
```

```
Accuracy for Random Forest 0.7845668609056582
```

```
# Scatter plot of Experimental vs Predicted pic50 values

sns.set(color_codes=True)
sns.set_style("ticks")

ax = sns.regplot(Y_test, Y_pred, scatter_kws={'alpha':0.4})
ax.set_xlabel('Experimental pIC50', fontsize='large', fontweight='bold')
ax.set_ylabel('Predicted pIC50', fontsize='large', fontweight='bold')
ax.set_xlim(0, 12)
ax.set_ylim(0, 12)
ax.figure.set_size_inches(5, 5)
plt.legend(["Experimental pIC50","Predicted pIC50"])
plt.show
```

```
/usr/local/lib/python3.8/dist-packages/seaborn/_decorators.py:36: FutureWarning: Pass the following variabl
  warnings.warn(
<function matplotlib.pyplot.show(*args, **kw)>
```



✓ 0s completed at 8:55 PM