PART 2: EXPLORATORY DATA ANALYSIS

```
# Tasks to be performed:
## Step 1: Import libraries
## Step 2: Import the database
## Step 3: Calculate the parameters of Lipink's rule of five
## Step 4: Normalize IC50 values
## Step 5: Carry out the exploratory analysis itself
## Step 6: Draw insights from the results of the exploratory analysis
```

Step 1: Import libraries

```
!pip install rdkit
import rdkit
import pandas as pd
```

```
Collecting rdkit
  Downloading rdkit-2024.3.6-cp310-cp310-manylinux_2_28_x86_64.whl.metadata (4.0 kB)
Requirement already satisfied: numpy in /usr/local/lib/python3.10/dist-packages (from rdkit) (1.26.4)
Requirement already satisfied: Pillow in /usr/local/lib/python3.10/dist-packages (from rdkit) (11.0.0)
Downloading rdkit-2024.3.6-cp310-cp310-manylinux_2_28_x86_64.whl (32.8 MB)
   ━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━ 32.8/32.8 MB 32.4 MB/s eta 0:00:00
Installing collected packages: rdkit
Successfully installed rdkit-2024.3.6
```

Step 2: Import the database

```
# Step 2: Import dataset

from google.colab import files
uploaded = files.upload()
```

Escolher arquivos Lepra Clofa…ART02 F.csv

- **Lepra Clofazimina_PART02 F.csv**(text/csv) - 169641 bytes, last modified: 21/12/2024 - 100% done

```
Saving Lepra Clofazimina_PART02 F.csv to Lepra Clofazimina_PART02 F.csv
```

```
df = pd.read_csv("Lepra Clofazimina_PART02 F.csv")
df
```

	molecule_chembl_id	canonical_smiles	bioactivity_class	standard_value
0	CHEMBL320553	Cc1oc(-c2ccccc2)nc1CCOc1ccc(C[C@](C)(Oc2ccccc2...	Active	14.0
1	CHEMBL149676	Cc1oc(-c2ccccc2)nc1CCOc1ccc(CC(C)(Oc2ccccc2)C(...	Intermediate	18.0
2	CHEMBL344282	Cc1oc(-c2ccccc2)nc1CCOc1ccc(CC(Oc2ccccc2)C(=O)...	Intermediate	128.0
3	CHEMBL278590	Cc1oc(C2CCCCC2)nc1CCOc1ccc(C[C@](C)(Oc2ccccc2)...	Active	15.0
4	CHEMBL424133	Cc1oc(-c2cccs2)nc1CCOc1ccc(C[C@](C)(Oc2ccccc2)...	Intermediate	10.0
...	...	...	...	...
1892	CHEMBL278501	COc1ccccc1CCC1(O)C(C)=C[C@@H](OC(C)=O)[C@@]2(C...	Inactive	142.0
1893	CHEMBL265334	CCOc1ccccc1CCC1(O)C(C)=C[C@@H](OC(C)=O)[C@@]2(...	Inactive	34.0
1894	CHEMBL16428	CCOc1ccccc1CCC1(O)C(C)=C[C@@H](OC(C)=O)[C@@]2(...	Inactive	80.0
1895	CHEMBL360583	COc1cccc(CCC2(O)C(C)=C[C@@H](OC(C)=O)[C@@]3(C)...	Intermediate	24.0
1896	CHEMBL516932	COc1cccc(CCC2(O)C(C)=C[C@@H](OC(C)=O)[C@@]3(C)...	Intermediate	1314.0

1897 rows × 4 columns

Next steps: Generate code with df | View recommended plots | New interactive sheet

Step 3: Calculate the parameters of Lipink's rule of five

```
## 3.1.  Importing libraries.

import numpy as np
```

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


## 3.2. Obtaining Lipinski descriptors.
# Inspired by : https://codeocean.com/explore/capsules?query=tag:data-curation

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"]
    descritores = pd.DataFrame(data=baseData,columns=columnNames)

    return descritores


df_lipinski = lipinski(df.canonical_smiles)
df_lipinski
```

	MW	LogP	NumHDonors	NumHAcceptors
0	457.526	5.73632	1.0	5.0
1	457.526	5.73632	1.0	5.0
2	443.499	5.34622	1.0	5.0
3	463.574	6.11702	1.0	5.0
4	463.555	5.79782	1.0	6.0
...	...	...	...	...
1892	710.861	5.30690	1.0	11.0
1893	724.888	5.69700	1.0	11.0
1894	724.888	5.69700	1.0	11.0
1895	710.861	5.30690	1.0	11.0
1896	710.861	5.30690	1.0	11.0

1897 rows × 4 columns

Next steps: Generate code with df_lipinski | View recommended plots | New interactive sheet

```
# Reading the initial dataframe
df
```

	molecule_chembl_id	canonical_smiles	bioactivity_class	standard_value
0	CHEMBL320553	Cc1oc(-c2ccccc2)nc1CCOc1ccc(C[C@](C)(Oc2ccccc2...	Active	14.0
1	CHEMBL149676	Cc1oc(-c2ccccc2)nc1CCOc1ccc(CC(C)(Oc2ccccc2)C(...	Intermediate	18.0
2	CHEMBL344282	Cc1oc(-c2ccccc2)nc1CCOc1ccc(CC(Oc2ccccc2)C(=O)...	Intermediate	128.0
3	CHEMBL278590	Cc1oc(C2CCCCC2)nc1CCOc1ccc(C[C@](C)(Oc2ccccc2)...	Active	15.0
4	CHEMBL424133	Cc1oc(-c2cccs2)nc1CCOc1ccc(C[C@](C)(Oc2ccccc2)...	Intermediate	10.0
...	...	...	...	...
1892	CHEMBL278501	COc1ccccc1CCC1(O)C(C)=C[C@@H](OC(C)=O)[C@@]2(C...	Inactive	142.0
1893	CHEMBL265334	CCOc1ccccc1CCC1(O)C(C)=C[C@@H](OC(C)=O)[C@@]2(...	Inactive	34.0
1894	CHEMBL16428	CCOc1ccccc1CCC1(O)C(C)=C[C@@H](OC(C)=O)[C@@]2(...	Inactive	80.0
1895	CHEMBL360583	COc1cccc(CCC2(O)C(C)=C[C@@H](OC(C)=O)[C@@]3(C)...	Intermediate	24.0
1896	CHEMBL516932	COc1cccc(CCC2(O)C(C)=C[C@@H](OC(C)=O)[C@@]3(C)...	Intermediate	1314.0

1897 rows × 4 columns

Next steps: Generate code with df | View recommended plots | New interactive sheet

```
## 3.2. Concatenating the two databases
df_combinado = pd.concat([df,df_lipinski], axis = 1)
```

```
display(df_combinado)
```

	molecule_chembl_id	canonical_smiles	bioactivity_class	standard_value	MW	LogP	NumHDonors
0	CHEMBL320553	Cc1oc(-c2ccccc2)nc1CCOc1ccc(C[C@](C)(Oc2ccccc2...	Active	14.0	457.526	5.73632	1.0
1	CHEMBL149676	Cc1oc(-c2ccccc2)nc1CCOc1ccc(CC(C)(Oc2ccccc2)C(...	Intermediate	18.0	457.526	5.73632	1.0
2	CHEMBL344282	Cc1oc(-c2ccccc2)nc1CCOc1ccc(CC(Oc2ccccc2)C(=O)...	Intermediate	128.0	443.499	5.34622	1.0
3	CHEMBL278590	Cc1oc(C2CCCCC2)nc1CCOc1ccc(C[C@](C)(Oc2ccccc2)...	Active	15.0	463.574	6.11702	1.0
4	CHEMBL424133	Cc1oc(-c2cccs2)nc1CCOc1ccc(C[C@](C)(Oc2ccccc2)...	Intermediate	10.0	463.555	5.79782	1.0
...	...	...	...	...	...	...	...
1892	CHEMBL278501	COc1ccccc1CCC1(O)C(C)=C[C@@H](OC(C)=O)[C@@]2(C...	Inactive	142.0	710.861	5.30690	1.0
1893	CHEMBL265334	CCOc1ccccc1CCC1(O)C(C)=C[C@@H](OC(C)=O)[C@@]2(...	Inactive	34.0	724.888	5.69700	1.0

Next steps: Generate code with df_combinado | View recommended plots | New interactive sheet

```
## 3.4. Descriptive analysis of non-standardized IC50 values
df_combinado.standard_value.describe()
```

	standard_value
count	1897.000000
mean	4654.286373
std	21746.199348
min	0.060000
25%	30.000000
50%	240.000000
75%	1676.000000
max	744000.000000

dtype: float64

Step 4: Normalize IC50 values

To ensure normal data distribution, we will convert the IC50 values to a negative logarithmic scale: -log10. To do this we will create the function "pIC50 ()" we will: a) First multiply all IC50 values by 10-9, converting nM into M. b) Second: From these results (M unit), we will calculate the "-log10". Finally, we will delete the variable that contains original IC50 values (non-standardized data) and create a new column with pIC50 values.

```
## 4.1. Creating the pIC50 function
# Inspired by: https://github.com/chaninlab/estrogen-receptor-alpha-qsar/blob/master/02_ER_alpha_RO5.ipynb

import numpy as np

def pIC50(input):
    pIC50 = []

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

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

    return x
```

```
## Important note:
# Values greater than 100,000,000 will be set to 100,000,000
# otherwise the negative logarithmic value will become negative.
```

```
-np.log10( (10**-9)* 100000000 )
```

```
1.0
```

```
-np.log10( (10**-9)* 10000000000 )
```

```
-1.0
```

```
## 4.2 Creating standardized normal values

def norm_value(input):
    norm = []

    for i in input['standard_value']:
        if i > 100000000:
          i = 100000000
        norm.append(i)

    input['standard_value_norm'] = norm
    x = input.drop('standard_value',axis = 1)

    return x
```

```
# We will first apply the normal_value() function, it is important to note that the "standar_value" variable is normalized
```

```
## 4.3. Viewing the data with normal values
df_normal = norm_value(df_combinado)
display(df_normal)
```

	molecule_chembl_id	canonical_smiles	bioactivity_class	MW	LogP	NumHDonors	NumHAcceptors	s
0	CHEMBL320553	Cc1oc(-c2ccccc2)nc1CCOc1ccc(C[C@](C)(Oc2ccccc2...	Active	457.526	5.73632	1.0	5.0	
1	CHEMBL149676	Cc1oc(-c2ccccc2)nc1CCOc1ccc(CC(C)(Oc2ccccc2)C(...	Intermediate	457.526	5.73632	1.0	5.0	
2	CHEMBL344282	Cc1oc(-c2ccccc2)nc1CCOc1ccc(CC(Oc2ccccc2)C(=O)...	Intermediate	443.499	5.34622	1.0	5.0	
3	CHEMBL278590	Cc1oc(C2CCCCC2)nc1CCOc1ccc(C[C@](C)(Oc2ccccc2)...	Active	463.574	6.11702	1.0	5.0	
4	CHEMBL424133	Cc1oc(-c2cccs2)nc1CCOc1ccc(C[C@](C)(Oc2ccccc2)...	Intermediate	463.555	5.79782	1.0	6.0	
...	...	...	...	...	...	...	...	
1892	CHEMBL278501	COc1ccccc1CCC1(O)C(C)=C[C@@H](OC(C)=O)[C@@]2(C...	Inactive	710.861	5.30690	1.0	11.0	
1893	CHEMBL265334	CCOc1ccccc1CCC1(O)C(C)=C[C@@H](OC(C)=O)[C@@]2(...	Inactive	724.888	5.69700	1.0	11.0	

Next steps: Generate code with `df_normal` View recommended plots New interactive sheet

```
## 4.4. Describing the new Dataframe
df_normal.describe()
```

	MW	LogP	NumHDonors	NumHAcceptors	standard_value_norm
count	1897.000000	1897.000000	1897.000000	1897.000000	1897.000000
mean	476.740182	5.799513	1.343173	4.733263	4654.286373
std	75.602010	1.492713	0.684208	1.738590	21746.199348
min	172.268000	-0.517500	0.000000	1.000000	0.060000
25%	433.504000	4.899020	1.000000	4.000000	30.000000
50%	480.576000	5.879620	1.000000	5.000000	240.000000
75%	526.054000	6.789400	2.000000	6.000000	1676.000000
max	788.840000	9.810640	7.000000	16.000000	744000.000000

```
## 4.5. Applying the pI50 function
df_final = pIC50(df_normal)
display(df_final)
```

	molecule_chembl_id	canonical_smiles	bioactivity_class	MW	LogP	NumHDonors	NumHAcceptors	
0	CHEMBL320553	Cc1oc(-c2ccccc2)nc1CCOc1ccc(C[C@](C)(Oc2ccccc2...	Active	457.526	5.73632	1.0	5.0	7.
1	CHEMBL149676	Cc1oc(-c2ccccc2)nc1CCOc1ccc(CC(C)(Oc2ccccc2)C(...	Intermediate	457.526	5.73632	1.0	5.0	7.
2	CHEMBL344282	Cc1oc(-c2ccccc2)nc1CCOc1ccc(CC(Oc2ccccc2)C(=O)...	Intermediate	443.499	5.34622	1.0	5.0	6.
3	CHEMBL278590	Cc1oc(C2CCCCC2)nc1CCOc1ccc(C[C@](C)(Oc2ccccc2)...	Active	463.574	6.11702	1.0	5.0	7.
4	CHEMBL424133	Cc1oc(-c2cccs2)nc1CCOc1ccc(C[C@](C)(Oc2ccccc2)...	Intermediate	463.555	5.79782	1.0	6.0	8.
...	...	...	...	...	...	...	...	
1892	CHEMBL278501	COc1ccccc1CCC1(O)C(C)=C[C@@H](OC(C)=O)[C@@]2(C...	Inactive	710.861	5.30690	1.0	11.0	6.
1893	CHEMBL265334	CCOc1ccccc1CCC1(O)C(C)=C[C@@H](OC(C)=O)[C@@]2(...	Inactive	724.888	5.69700	1.0	11.0	7.

Next steps: Generate code with `df_final` View recommended plots New interactive sheet

```
# Saving the dataset with three classes
df_final.to_csv("PART0 3 LEPRA_3classes.csv")
```

```
## 4.6. Describing the Final dataframe
df_final.pIC50.describe()
```

	pIC50
count	1897.000000
mean	6.628524
std	1.211388
min	3.128427
25%	5.775726
50%	6.619789
75%	7.522879
max	10.221849

dtype: float64

Step 5: Carry out the exploratory analysis itself: Pfizer Rule (lipinsk)

```
!pip install seaborn
```

```
Requirement already satisfied: seaborn in /usr/local/lib/python3.10/dist-packages (0.13.2)
Requirement already satisfied: numpy!=1.24.0,>=1.20 in /usr/local/lib/python3.10/dist-packages (from seaborn) (1.26.4)
Requirement already satisfied: pandas>=1.2 in /usr/local/lib/python3.10/dist-packages (from seaborn) (2.2.2)
Requirement already satisfied: matplotlib!=3.6.1,>=3.4 in /usr/local/lib/python3.10/dist-packages (from seaborn) (3.8.0)
Requirement already satisfied: contourpy>=1.0.1 in /usr/local/lib/python3.10/dist-packages (from matplotlib!=3.6.1,>=3.4->seaborn)
Requirement already satisfied: cycler>=0.10 in /usr/local/lib/python3.10/dist-packages (from matplotlib!=3.6.1,>=3.4->seaborn) (0.12
Requirement already satisfied: fonttools>=4.22.0 in /usr/local/lib/python3.10/dist-packages (from matplotlib!=3.6.1,>=3.4->seaborn)
Requirement already satisfied: kiwisolver>=1.0.1 in /usr/local/lib/python3.10/dist-packages (from matplotlib!=3.6.1,>=3.4->seaborn)
Requirement already satisfied: packaging>=20.0 in /usr/local/lib/python3.10/dist-packages (from matplotlib!=3.6.1,>=3.4->seaborn) (2
Requirement already satisfied: pillow>=6.2.0 in /usr/local/lib/python3.10/dist-packages (from matplotlib!=3.6.1,>=3.4->seaborn) (11
Requirement already satisfied: pyparsing>=2.3.1 in /usr/local/lib/python3.10/dist-packages (from matplotlib!=3.6.1,>=3.4->seaborn)
Requirement already satisfied: python-dateutil>=2.7 in /usr/local/lib/python3.10/dist-packages (from matplotlib!=3.6.1,>=3.4->seabor
Requirement already satisfied: pytz>=2020.1 in /usr/local/lib/python3.10/dist-packages (from pandas>=1.2->seaborn) (2024.2)
Requirement already satisfied: tzdata>=2022.7 in /usr/local/lib/python3.10/dist-packages (from pandas>=1.2->seaborn) (2024.2)
Requirement already satisfied: six>=1.5 in /usr/local/lib/python3.10/dist-packages (from python-dateutil>=2.7->matplotlib!=3.6.1,>=3
```

```
## 5.1. Importing libraries
import seaborn as sns
sns.set(style='ticks')
import matplotlib.pyplot as plt
```

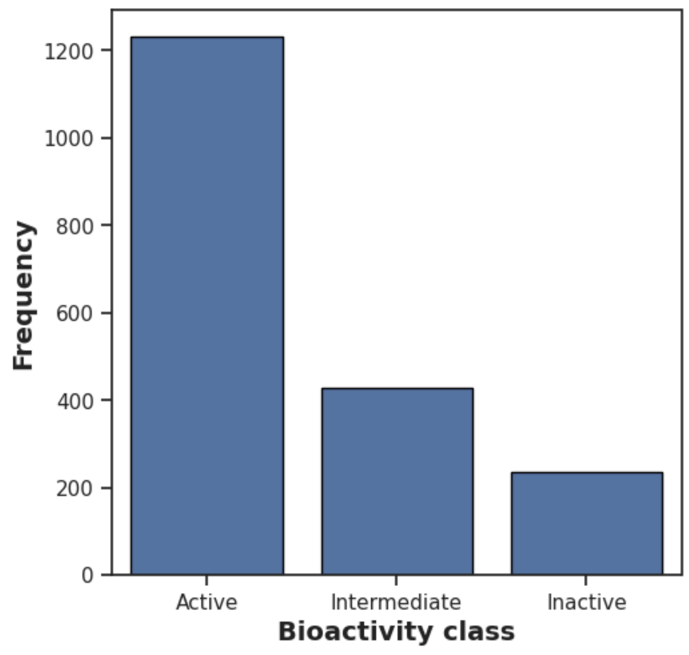
Creating the frequency graph of the three class of compounds

```
# Building the graph

plt.figure(figsize=(5.5, 5.5))
sns.countplot(x='bioactivity_class', data=df_final, edgecolor='black')
plt.xlabel('Bioactivity class', fontsize=14, fontweight='bold')
plt.ylabel('Frequency', fontsize=14, fontweight='bold')


## Saving the graph in PDF format.

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



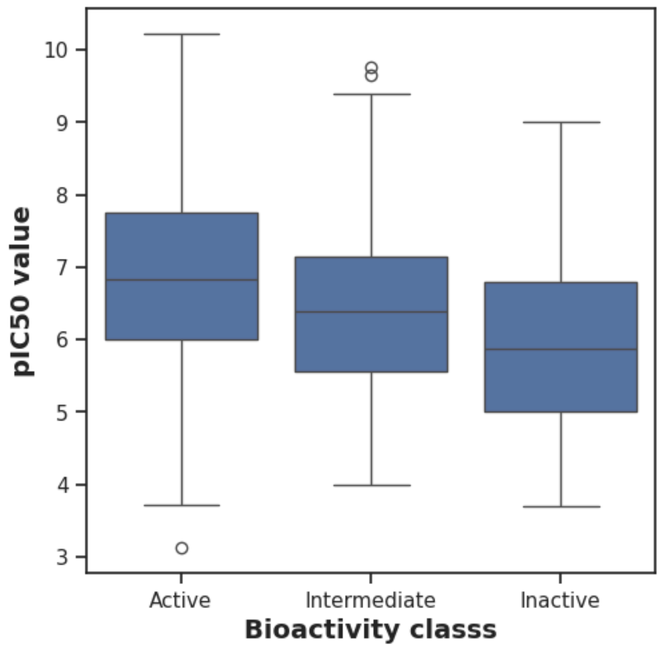
Creating the scatter plot of molecular weight versus LogP

Building the Box Plot graph of bioactivity versus pIC5 values: Kruskal-Wallis Test

```
## Building the graph

plt.figure(figsize=(5.5, 5.5))
sns.boxplot(x = 'bioactivity_class', y = 'pIC50', data = df_final)
plt.xlabel('Bioactivity classs', fontsize=14, fontweight='bold')
plt.ylabel('pIC50 value', fontsize=14, fontweight='bold')


## Saving the chart
plt.savefig('plot_ic50.pdf')
```



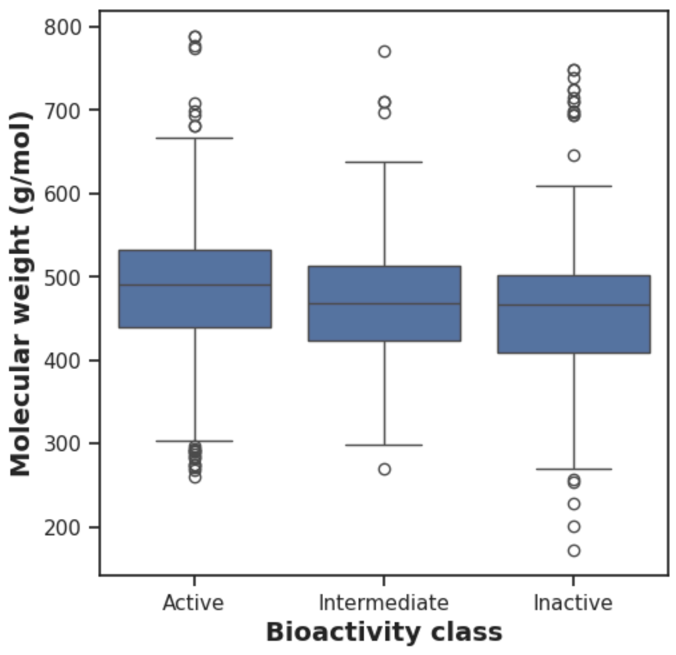
Comparing molecular weight values : Kruskal-Wallis Test

```
# Molecular weight
plt.figure(figsize=(5.5, 5.5))
```

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

plt.xlabel('Bioactivity class', fontsize=14, fontweight='bold')
plt.ylabel('Molecular weight (g/mol)', fontsize=14, fontweight='bold')

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



```
df_final
```

	molecule_chembl_id	canonical_smiles	bioactivity_class	MW	LogP	NumHDonors	NumHAcceptors	
0	CHEMBL320553	Cc1oc(-c2ccccc2)nc1CCOc1ccc(C[C@](C)(Oc2ccccc2...	Active	457.526	5.73632	1.0	5.0	7.
1	CHEMBL149676	Cc1oc(-c2ccccc2)nc1CCOc1ccc(CC(C)(Oc2ccccc2)C(...	Intermediate	457.526	5.73632	1.0	5.0	7.
2	CHEMBL344282	Cc1oc(-c2ccccc2)nc1CCOc1ccc(CC(Oc2ccccc2)C(=O)...	Intermediate	443.499	5.34622	1.0	5.0	6.
3	CHEMBL278590	Cc1oc(C2CCCCC2)nc1CCOc1ccc(C[C@](C)(Oc2ccccc2)...	Active	463.574	6.11702	1.0	5.0	7.
4	CHEMBL424133	Cc1oc(-c2cccs2)nc1CCOc1ccc(C[C@](C)(Oc2ccccc2)...	Intermediate	463.555	5.79782	1.0	6.0	8.
...	...	...	...	...	...	...	...	
1892	CHEMBL278501	COc1ccccc1CCC1(O)C(C)=C[C@@H](OC(C)=O)[C@@]2(C...	Inactive	710.861	5.30690	1.0	11.0	6.
1893	CHEMBL265334	CCOc1ccccc1CCC1(O)C(C)=C[C@@H](OC(C)=O)[C@@]2(...	Inactive	724.888	5.69700	1.0	11.0	7.

Next steps: Generate code with df_final | View recommended plots | New interactive sheet

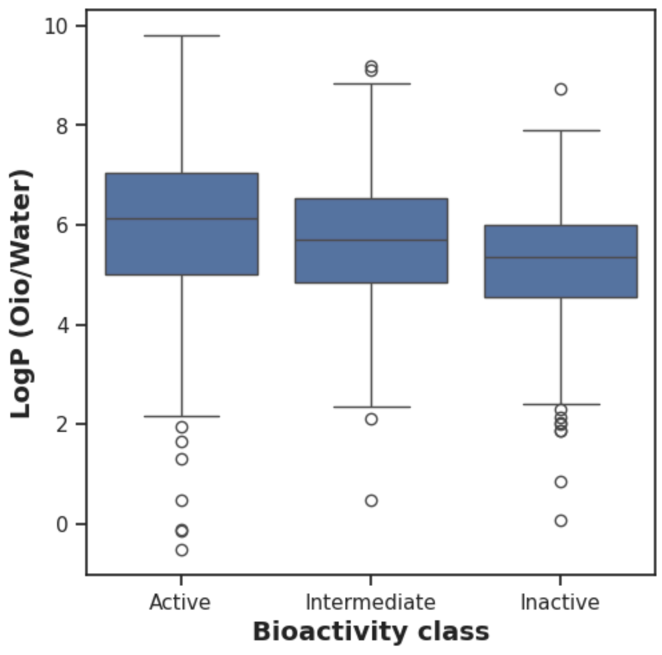
Comparing LogP values: Kruskal-Wallis Test

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

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

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

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



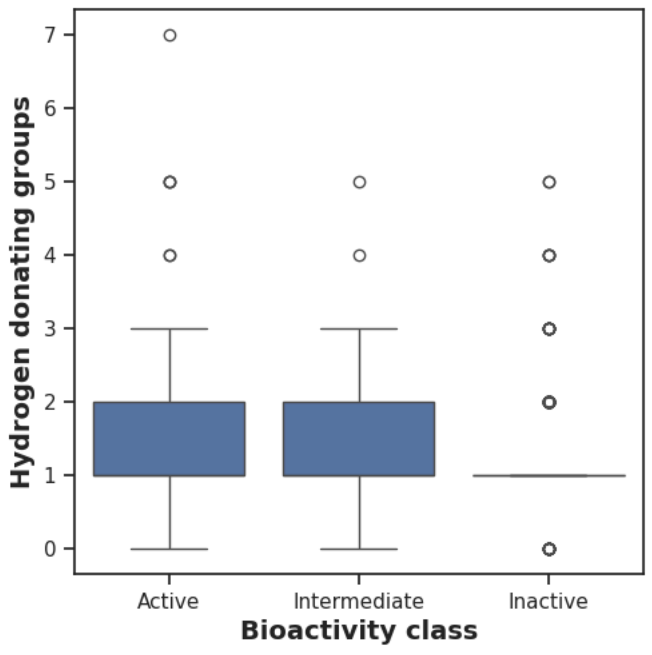
Comparing the number of hydrogen bond donor groups: Kruskal-Wallis Test

```
# Hydrogen bond donating groups
plt.figure(figsize=(5.5, 5.5))

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

plt.xlabel('Bioactivity class', fontsize=14, fontweight='bold')
plt.ylabel('Hydrogen donating groups', fontsize=14, fontweight='bold')

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

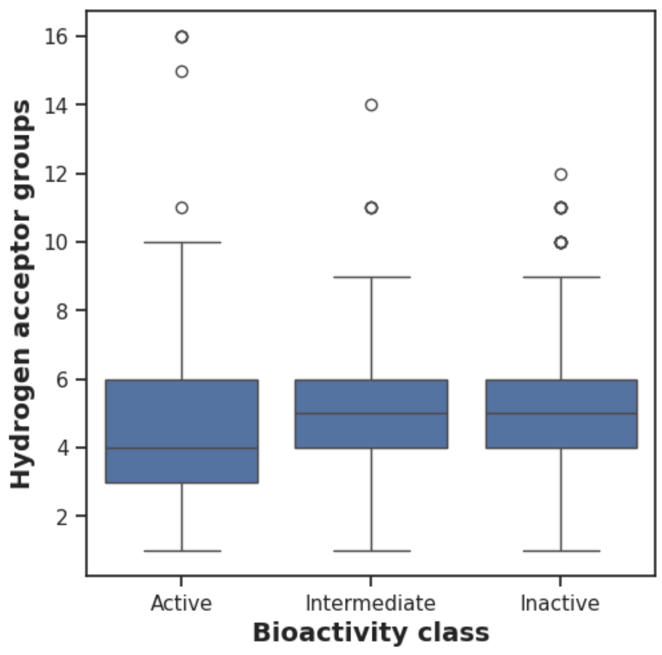


Comparing the number of hydrogen bond acceptor groups: Kruskal-Wallis Test

```
# Hydrogen bond acceptor groups
plt.figure(figsize=(5.5, 5.5))

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

plt.xlabel('Bioactivity class', fontsize=14, fontweight='bold')
plt.ylabel('Hydrogen acceptor groups', fontsize=14, fontweight='bold')
plt.savefig('plot_NumHAcceptors.pdf')
```



```
import seaborn as sns
import matplotlib.pyplot as plt
from random import seed
from scipy.stats import kruskal
import pandas as pd

# Seed the random number generator
seed(1)

# Define the list of quantitative descriptors
quantitative_vars = ['MW', 'LogP', 'NumHDonors', 'NumHAcceptors', 'pIC50']

# Initialize an empty list to collect results
all_results = []

# Loop through each quantitative variable to perform the Kruskal-Wallis test and plot
for descriptor in quantitative_vars:
    # Separate the dataset into groups based on the bioactivity class
    ativo = df_final[df_final.bioactivity_class == 'Active'][descriptor]
    inativo = df_final[df_final.bioactivity_class == 'Inactive'][descriptor]
    intermediario = df_final[df_final.bioactivity_class == 'Intermediate'][descriptor]

    # Perform the Kruskal-Wallis test
    stat, p = kruskal(ativo, inativo, intermediario)

    # Interpret the result
    alpha = 0.05
    if p > alpha:
        interpretation = 'Same distribution (fail to reject H0)'
    else:
        interpretation = 'Different distributions (reject H0)'

    # Store the results
    results = {
        'Descriptor': descriptor,
        'Statistics': stat,
        'p': p,
        'alpha': alpha,
        'Interpretation': interpretation
    }
    all_results.append(results)

    # Plot the box plot for the current descriptor
    plt.figure(figsize=(8, 6))
    sns.boxplot(x='bioactivity_class', y=descriptor, data=df_final, palette='Set2')
    plt.title(f'Box Plot of {descriptor} by Bioactivity Class')
    plt.xlabel('Bioactivity Class')
    plt.ylabel(descriptor)

    # Save the plot as a PNG file
    plot_filename = f'boxplot_{descriptor}.png'
    plt.savefig(plot_filename)
    plt.close()
```

```
        # Save each result to a separate CSV file
        filename = f'kruskal_{descriptor}.csv'
        pd.DataFrame([results]).to_csv(filename, index=False)

    # Convert all results to a DataFrame and return
    final_results_df = pd.DataFrame(all_results)
    final_results_df.to_csv('kruskal_all_results.csv', index=False)

    final_results_df
```

```
<ipython-input-32-aa17e4f31662>:45: FutureWarning:

Passing `palette` without assigning `hue` is deprecated and will be removed in v0.14.0. Assign the `x` variable to `hue` and set `le

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```

	Descriptor	Statistics	p	alpha	Interpretation
0	MW	40.127665	1.933696e-09	0.05	Different distributions (reject H0)
1	LogP	79.035183	6.882213e-18	0.05	Different distributions (reject H0)