

Untitled

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2 ChEMBL Database

ChEMBL is a manually curated database of bioactive molecules with drug-like properties. It brings together chemical, bioactivity and genomic data to aid the translation of genomic information into effective new drugs. The ChEMBL Database contains curated bioactivity data of more than 2.2 million compounds.

3 Installing ChEMBL web service package

```
[1]: ! pip install chembl_webresource_client
```

```
Requirement already satisfied: chembl_webresource_client in  
/home/pandey/anaconda3/lib/python3.8/site-packages (0.10.8)
```

Requirement already satisfied: urllib3 in
 /home/pandey/anaconda3/lib/python3.8/site-packages (from
 chembl_webresource_client) (1.25.11)

Requirement already satisfied: requests>=2.18.4 in
 /home/pandey/anaconda3/lib/python3.8/site-packages (from
 chembl_webresource_client) (2.24.0)

Requirement already satisfied: requests-cache~=0.7.0 in
 /home/pandey/anaconda3/lib/python3.8/site-packages (from
 chembl_webresource_client) (0.7.5)

Requirement already satisfied: easydict in
 /home/pandey/anaconda3/lib/python3.8/site-packages (from
 chembl_webresource_client) (1.9)

Requirement already satisfied: idna<3,>=2.5 in
 /home/pandey/anaconda3/lib/python3.8/site-packages (from
 requests>=2.18.4->chembl_webresource_client) (2.10)

Requirement already satisfied: certifi>=2017.4.17 in
 /home/pandey/anaconda3/lib/python3.8/site-packages (from
 requests>=2.18.4->chembl_webresource_client) (2020.6.20)

Requirement already satisfied: chardet<4,>=3.0.2 in
 /home/pandey/anaconda3/lib/python3.8/site-packages (from
 requests>=2.18.4->chembl_webresource_client) (3.0.4)

Requirement already satisfied: attrs<22.0,>=21.2 in
 /home/pandey/anaconda3/lib/python3.8/site-packages (from requests-
 cache~=0.7.0->chembl_webresource_client) (21.2.0)

Requirement already satisfied: pyyaml>=5.4 in
 /home/pandey/anaconda3/lib/python3.8/site-packages (from requests-
 cache~=0.7.0->chembl_webresource_client) (6.0)

Requirement already satisfied: itsdangerous>=2.0.1 in
 /home/pandey/anaconda3/lib/python3.8/site-packages (from requests-
 cache~=0.7.0->chembl_webresource_client) (2.1.2)

Requirement already satisfied: url-normalize<2.0,>=1.4 in
 /home/pandey/anaconda3/lib/python3.8/site-packages (from requests-
 cache~=0.7.0->chembl_webresource_client) (1.4.3)

Requirement already satisfied: six in /home/pandey/anaconda3/lib/python3.8/site-
 packages (from url-normalize<2.0,>=1.4->requests-
 cache~=0.7.0->chembl_webresource_client) (1.15.0)

4 Importing libraries

```
[2]: import pandas as pd
import numpy as np
from rdkit import Chem
from rdkit.Chem import Descriptors, Lipinski
from rdkit.Chem.MolStandardize import rdMolStandardize
from chembl_webresource_client.new_client import new_client
from numpy.random import seed
```

```

from numpy.random import randn
from scipy.stats import mannwhitneyu
import seaborn as sns
from IPython.display import display
import matplotlib.pyplot as plt

```

5 Search for target tubulin protein

```

[3]: target = new_client.target
target_query = target.search('tubulin')
targets = pd.DataFrame.from_dict(target_query)
targets

```

```

[3]:
                                cross_references \
0                                           []
1                                           []
2                                           []
3                                           []
4                                           []
5  [{'xref_id': 'P68366', 'xref_name': None, 'xre...
6  [{'xref_id': 'Q13509', 'xref_name': None, 'xre...
7  [{'xref_id': 'Q71U36', 'xref_name': None, 'xre...
8  [{'xref_id': 'P68370', 'xref_name': None, 'xre...
9  [{'xref_id': 'P02550', 'xref_name': None, 'xre...
10 [{'xref_id': 'P02554', 'xref_name': None, 'xre...
11 [{'xref_id': 'Q25270', 'xref_name': None, 'xre...
12                                           []
13                                           []
14                                           []
15                                           []
16                                           []
17                                           []
18  [{'xref_id': 'P68371', 'xref_name': None, 'xre...
19  [{'xref_id': 'P07437', 'xref_name': None, 'xre...
20  [{'xref_id': 'P04350', 'xref_name': None, 'xre...
21                                           []
22                                           []
23                                           []
24                                           []
25                                           []
26                                           []
27                                           []
28                                           []
29                                           []
30                                           []

```

```

31 [{ 'xref_id': 'Q6B856', 'xref_name': None, 'xre...
32 [{ 'xref_id': 'Q9H4B7', 'xref_name': None, 'xre...
33 [{ 'xref_id': 'Q8NG68', 'xref_name': None, 'xre...
34 []
35 []
36 []
37 [{ 'xref_id': 'Q9UBN7', 'xref_name': None, 'xre...
38 []
39 []
40 []
41 []
42 [{ 'xref_id': 'POA9A6', 'xref_name': None, 'xre...
43 [{ 'xref_id': 'P64170', 'xref_name': None, 'xre...
44 [{ 'xref_id': 'POA031', 'xref_name': None, 'xre...
45 [{ 'xref_id': 'P17865', 'xref_name': None, 'xre...
46 [{ 'xref_id': 'P47204', 'xref_name': None, 'xre...
47 []
48 []
49 []
50 []
51 []
52 []
53 []
54 []

```

```

                                organism \
0                                Homo sapiens
1                                Nematoda
2                                Homo sapiens
3                                Homo sapiens
4                                Candida albicans
5                                Homo sapiens
6                                Homo sapiens
7                                Homo sapiens
8                                Rattus norvegicus
9                                Sus scrofa
10                               Sus scrofa
11                               Leishmania donovani
12                               Sus scrofa
13                               Trichophyton
14                               Taeniidae
15                               Homo sapiens
16                               Homo sapiens
17                               Homo sapiens
18                               Homo sapiens
19                               Homo sapiens
20                               Homo sapiens

```

21	Bos taurus
22	Bos taurus
23	Arabidopsis thaliana
24	Homo sapiens
25	Homo sapiens
26	Gallus gallus
27	Homo sapiens
28	Ovis aries
29	Mus musculus
30	Trypanosoma cruzi
31	Bos taurus
32	Homo sapiens
33	Homo sapiens
34	Homo sapiens
35	Mus musculus
36	Mus musculus
37	Homo sapiens
38	Homo sapiens
39	Bos taurus
40	Bacillus subtilis
41	Homo sapiens
42	Escherichia coli K-12
43	Mycobacterium tuberculosis
44	Staphylococcus aureus
45	Bacillus subtilis (strain 168)
46	Pseudomonas aeruginosa (strain ATCC 15692 / PA...
47	Homo sapiens
48	Homo sapiens
49	Mus musculus
50	Homo sapiens
51	Mus musculus
52	Homo sapiens
53	Homo sapiens
54	Mus musculus

	pref_name	score	species_group_flag \
0	Tubulin	16.0	False
1	Tubulin	16.0	True
2	Tubulin alpha	16.0	False
3	Tubulin beta	16.0	False
4	Tubulin	16.0	False
5	Tubulin alpha-1 chain	15.0	False
6	Tubulin beta-3 chain	15.0	False
7	Tubulin alpha-3 chain	15.0	False
8	Tubulin alpha-1 chain	15.0	False
9	Tubulin alpha chain	15.0	False
10	Tubulin beta chain	15.0	False

11	Beta tubulin	15.0	False
12	Tubulin	15.0	False
13	Tubulin	15.0	True
14	Tubulin	15.0	True
15	Tubulin alpha-1B chain	15.0	False
16	Tubulin alpha-1C chain	15.0	False
17	Tubulin alpha-1A /beta chains	15.0	False
18	Tubulin beta-2 chain	14.0	False
19	Tubulin beta-5 chain	14.0	False
20	Tubulin beta-4 chain	14.0	False
21	Tubulin	14.0	False
22	Tubulin	14.0	False
23	Tubulin beta-6 chain	14.0	False
24	Tubulin alpha-8 chain	14.0	False
25	Tubulin beta-2A chain	14.0	False
26	Tubulin beta-4 chain	14.0	False
27	Putative tubulin-like protein alpha-4B	14.0	False
28	Tubulin alpha 4a	13.0	False
29	Tubulin polyglutamylase TTL7	13.0	False
30	Tubulin alpha chain	13.0	False
31	Tubulin beta chain	12.0	False
32	Tubulin beta-1 chain	12.0	False
33	Tubulin--tyrosine ligase	12.0	False
34	Tau-tubulin kinase 2	12.0	False
35	Tubulin beta-5 chain	12.0	False
36	Histone deacetylase 6	10.0	False
37	Histone deacetylase 6	10.0	False
38	Tau-tubulin kinase 1	10.0	False
39	Tubulin polymerization-promoting protein	10.0	False
40	Cell division protein FtsZ	10.0	False
41	Cereblon/Histone deacetylase 6	10.0	False
42	Cell division protein ftsZ	9.0	False
43	Cell division protein FtsZ	9.0	False
44	Cell division protein ftsZ	9.0	False
45	Cell division protein ftsZ	9.0	False
46	Cell division protein ftsZ	9.0	False
47	Histone deacetylase 1/6	9.0	False
48	Histone deacetylase 6/3	9.0	False
49	Cereblon/Histone deacetylase 6	9.0	False
50	VHL/Histone deacetylase 6	9.0	False
51	VHL/Histone deacetylase 6	9.0	False
52	Histone deacetylase 1/2/3/6	7.0	False
53	Histone deacetylase	3.0	False
54	Histone deacetylase	3.0	False

	target_chembl_id		target_components \
0	CHEMBL2095182	[{'accession': 'P68371', 'component_descriptio...	

1	CHEMBL2364705	[{'accession': 'F1L5G6', 'component_descriptio...
2	CHEMBL3832941	[{'accession': 'PODPH7', 'component_descriptio...
3	CHEMBL3832942	[{'accession': 'P68371', 'component_descriptio...
4	CHEMBL3988634	[{'accession': 'P87066', 'component_descriptio...
5	CHEMBL2070	[{'accession': 'P68366', 'component_descriptio...
6	CHEMBL2597	[{'accession': 'Q13509', 'component_descriptio...
7	CHEMBL3661	[{'accession': 'Q71U36', 'component_descriptio...
8	CHEMBL4139	[{'accession': 'P68370', 'component_descriptio...
9	CHEMBL3658	[{'accession': 'P02550', 'component_descriptio...
10	CHEMBL2788	[{'accession': 'P02554', 'component_descriptio...
11	CHEMBL3186	[{'accession': 'Q25270', 'component_descriptio...
12	CHEMBL2111354	[{'accession': 'P02554', 'component_descriptio...
13	CHEMBL2364703	[{'accession': 'F2SZD3', 'component_descriptio...
14	CHEMBL2364704	[{'accession': 'C4PKY4', 'component_descriptio...
15	CHEMBL3797010	[{'accession': 'P68363', 'component_descriptio...
16	CHEMBL3797011	[{'accession': 'Q9BQE3', 'component_descriptio...
17	CHEMBL3885647	[{'accession': 'Q71U36', 'component_descriptio...
18	CHEMBL1848	[{'accession': 'P68371', 'component_descriptio...
19	CHEMBL5444	[{'accession': 'P07437', 'component_descriptio...
20	CHEMBL3838	[{'accession': 'P04350', 'component_descriptio...
21	CHEMBL2094134	[{'accession': 'Q6B856', 'component_descriptio...
22	CHEMBL2111464	[{'accession': 'Q6B856', 'component_descriptio...
23	CHEMBL2424501	[{'accession': 'P29514', 'component_descriptio...
24	CHEMBL3714503	[{'accession': 'Q9NY65', 'component_descriptio...
25	CHEMBL3797012	[{'accession': 'Q13885', 'component_descriptio...
26	CHEMBL4295707	[{'accession': 'P09652', 'component_descriptio...
27	CHEMBL4295944	[{'accession': 'Q9H853', 'component_descriptio...
28	CHEMBL2366421	[{'accession': 'C5ISA2', 'component_descriptio...
29	CHEMBL2401604	[{'accession': 'A4Q9F0', 'component_descriptio...
30	CHEMBL3988589	[{'accession': 'Q27352', 'component_descriptio...
31	CHEMBL3394	[{'accession': 'Q6B856', 'component_descriptio...
32	CHEMBL1915	[{'accession': 'Q9H4B7', 'component_descriptio...
33	CHEMBL5549	[{'accession': 'Q8NG68', 'component_descriptio...
34	CHEMBL3337327	[{'accession': 'Q6IQ55', 'component_descriptio...
35	CHEMBL4739682	[{'accession': 'P99024', 'component_descriptio...
36	CHEMBL2878	[{'accession': 'Q9Z2V5', 'component_descriptio...
37	CHEMBL1865	[{'accession': 'Q9UBN7', 'component_descriptio...
38	CHEMBL1926492	[{'accession': 'Q5TCY1', 'component_descriptio...
39	CHEMBL2366491	[{'accession': 'Q27957', 'component_descriptio...
40	CHEMBL2417349	[{'accession': 'A5Z1V5', 'component_descriptio...
41	CHEMBL4296129	[{'accession': 'Q9UBN7', 'component_descriptio...
42	CHEMBL3999	[{'accession': 'POA9A6', 'component_descriptio...
43	CHEMBL4213	[{'accession': 'P9WN95', 'component_descriptio...
44	CHEMBL5096	[{'accession': 'POA031', 'component_descriptio...
45	CHEMBL5690	[{'accession': 'P17865', 'component_descriptio...
46	CHEMBL1075206	[{'accession': 'P47204', 'component_descriptio...
47	CHEMBL4106187	[{'accession': 'Q13547', 'component_descriptio...

48	CHEMBL4296072	[{'accession': 'O15379', 'component_descriptio...
49	CHEMBL4630735	[{'accession': 'Q9Z2V5', 'component_descriptio...
50	CHEMBL4630736	[{'accession': 'Q9UBN7', 'component_descriptio...
51	CHEMBL4630747	[{'accession': 'Q9Z2V5', 'component_descriptio...
52	CHEMBL3430896	[{'accession': 'Q13547', 'component_descriptio...
53	CHEMBL2093865	[{'accession': 'Q13547', 'component_descriptio...
54	CHEMBL3832944	[{'accession': 'Q8VH37', 'component_descriptio...

	target_type	tax_id
0	PROTEIN COMPLEX GROUP	9606
1	PROTEIN COMPLEX GROUP	6231
2	PROTEIN FAMILY	9606
3	PROTEIN FAMILY	9606
4	PROTEIN COMPLEX GROUP	5476
5	SINGLE PROTEIN	9606
6	SINGLE PROTEIN	9606
7	SINGLE PROTEIN	9606
8	SINGLE PROTEIN	10116
9	SINGLE PROTEIN	9823
10	SINGLE PROTEIN	9823
11	SINGLE PROTEIN	5661
12	PROTEIN FAMILY	9823
13	PROTEIN COMPLEX GROUP	5550
14	PROTEIN COMPLEX GROUP	6208
15	SINGLE PROTEIN	9606
16	SINGLE PROTEIN	9606
17	PROTEIN COMPLEX GROUP	9606
18	SINGLE PROTEIN	9606
19	SINGLE PROTEIN	9606
20	SINGLE PROTEIN	9606
21	PROTEIN FAMILY	9913
22	PROTEIN COMPLEX	9913
23	SINGLE PROTEIN	3702
24	SINGLE PROTEIN	9606
25	SINGLE PROTEIN	9606
26	SINGLE PROTEIN	9031
27	SINGLE PROTEIN	9606
28	SINGLE PROTEIN	9940
29	SINGLE PROTEIN	10090
30	SINGLE PROTEIN	5693
31	SINGLE PROTEIN	9913
32	SINGLE PROTEIN	9606
33	SINGLE PROTEIN	9606
34	SINGLE PROTEIN	9606
35	SINGLE PROTEIN	10090
36	SINGLE PROTEIN	10090
37	SINGLE PROTEIN	9606

38	SINGLE PROTEIN	9606
39	SINGLE PROTEIN	9913
40	SINGLE PROTEIN	1423
41	PROTEIN-PROTEIN INTERACTION	9606
42	SINGLE PROTEIN	83333
43	SINGLE PROTEIN	1773
44	SINGLE PROTEIN	1280
45	SINGLE PROTEIN	224308
46	SINGLE PROTEIN	208964
47	PROTEIN FAMILY	9606
48	PROTEIN FAMILY	9606
49	PROTEIN-PROTEIN INTERACTION	10090
50	PROTEIN-PROTEIN INTERACTION	9606
51	PROTEIN-PROTEIN INTERACTION	10090
52	PROTEIN FAMILY	9606
53	PROTEIN FAMILY	9606
54	PROTEIN FAMILY	10090

5.0.1 Select and retrieve bioactivity data for tubulin (homo sapiens organism)

```
[4]: selected_target = targets.target_chembl_id[0]
      selected_target
```

```
[4]: 'CHEMBL2095182'
```

5.0.2 Extracting IC50 data

- We will retrieve only bioactivity data for ABL kinase (CHEMBL2095182) that are reported as IC₅₀ values in nM (nanomolar) unit.

```
[5]: activity = new_client.activity
      res = activity.filter(target_chembl_id=selected_target).
      ↪filter(standard_type="IC50")
```

5.0.3 Converting data to dataframe

```
[6]: df = pd.DataFrame.from_dict(res)
      df.head(3)
```

```
[6]:  activity_comment  activity_id  activity_properties  assay_chembl_id  \
0             None          97337                []    CHEMBL815107
1             None          265761                []    CHEMBL622599
2             None          268214                []    CHEMBL622599
```

	assay_description	assay_type		
0	Inhibition of tubulin polymerization in S180 (...)	F		
1	Inhibition of tubulin polymerization in human ...	F		
2	Inhibition of tubulin polymerization in human ...	F		

	assay_variant_accession	assay_variant_mutation	bao_endpoint	bao_format	
0	None	None	BAO_0000190	BAO_0000219	
1	None	None	BAO_0000190	BAO_0000219	
2	None	None	BAO_0000190	BAO_0000219	

	target_organism	target_pref_name	target_tax_id	text_value	toid	type	
0	...	Homo sapiens	Tubulin	9606	None	None	IC50
1	...	Homo sapiens	Tubulin	9606	None	None	IC50
2	...	Homo sapiens	Tubulin	9606	None	None	IC50

	units	uo_units	upper_value	value
0	uM	UO_0000065	None	2.0
1	uM	UO_0000065	None	0.67
2	uM	UO_0000065	None	0.72

[3 rows x 45 columns]

```
[7]: df.standard_type.unique()
```

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

6 Handling missing data

- If any compounds has missing value for the standard_value column then drop it

```
[8]: df = df[df.standard_value.notna()]
```

7 Data pre-processing

7.0.1 Labeling compounds as either being active, inactive or intermediate

- The bioactivity data is in the IC₅₀ unit. Compounds having values of less than 1000 nM will be considered to be active while those greater than 10,000 nM will be considered to be inactive. As for those values in between 1,000 and 10,000 nM will be referred to as intermediate.

```
[9]: df['standard_value'] = df['standard_value'].astype(float)
df['bioactivity_class'] = df['standard_value'].map(lambda x : 'active' if x <= 1000
↪ else ('inactive' if x >= 10000 else 'intermediate'))
```

```
[10]: selection = ['molecule_chembl_id', 'canonical_smiles',
    ↪ 'standard_value', 'bioactivity_class']
df = df[selection]
df.head(10)
```

```
[10]: molecule_chembl_id canonical_smiles \
0 CHEMBL89905 COc1cc([C@@H]2c3cc4c(cc3C[C@H]3COC(=O)[C@@H]32...
1 CHEMBL2369028 C=CC[C@H](CC/C(C)=C/C=C/CC/C=C\[C@@H]1CSC([C@@...
2 CHEMBL89138 C=CC[C@@H](CC/C(C)=C/C=C/CC/C=C\[C@@H]1CSC([C@...
3 CHEMBL299279 C=CC[C@@H](CC/C(C)=C/C=C/CC/C=C\[C@@H]2C...
4 CHEMBL2115069 C=CC[C@@H](CC/C(C)=C/C=C/CC/C=C\[C@H]1CSC([C@@...
5 CHEMBL2369027 C=CC[C@@H](CC/C(C)=C/C=C/CC/C=C\[C@@H]1CSC([C@...
6 CHEMBL2369023 C=CC[C@@H](CC/C(C)=C/C=C/CC/C=C\[C@@H]1CSC([C@...
7 CHEMBL264716 C=CC[C@H](O)CC/C(C)=C/C=C/CC/C=C\C1CSC([C@@H]2...
8 CHEMBL91937 C=CC[C@@H](CC/C(C)=C/C=C/CC/C=C\[C@@H]1CSC([C@...
9 CHEMBL89124 CCCCCCc1cccc(CC/C=C\[C@@H]2CSC([C@@H]3C[C@@H]...

standard_value bioactivity_class
0 2000.0 intermediate
1 670.0 active
2 720.0 active
3 740.0 active
4 5500.0 intermediate
5 640.0 active
6 5400.0 intermediate
7 870.0 active
8 2100.0 intermediate
9 50000.0 inactive
```

```
[11]: df.canonical_smiles.replace('nan',np.nan, inplace=True)
df.dropna(inplace=True)
df.reset_index(inplace=True)
```

```
[12]: '''
function to estimate molecule Lipinski descriptors
'''

def lipinski(smiles, verbose=False):
    moldata= []
    problematic_smiles=[]
    for i,elem in enumerate(smiles):
        try:
            mol=Chem.MolFromSmiles(elem)
            mol = rdMolStandardize.Cleanup(mol)
            moldata.append(mol)
        except:
```

```

        problematic_smiles.append(i)
    pass
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, problematic_smiles

```

```
[13]: df_lipinski, problematic_smiles = lipinski(df.canonical_smiles)
```

```

[15:06:19] Initializing MetalDisconnector
[15:06:19] Running MetalDisconnector
[15:06:19] Initializing Normalizer
[15:06:19] Running Normalizer
[15:06:19] Initializing MetalDisconnector
[15:06:19] Running MetalDisconnector
[15:06:19] Initializing Normalizer
[15:06:19] Running Normalizer
[15:06:19] Initializing MetalDisconnector
[15:06:19] Running MetalDisconnector
[15:06:19] Initializing Normalizer
[15:06:19] Running Normalizer
[15:06:19] Initializing MetalDisconnector
[15:06:19] Running MetalDisconnector
[15:06:19] Initializing Normalizer
[15:06:19] Running Normalizer
[15:06:19] Initializing MetalDisconnector
[15:06:19] Running MetalDisconnector
[15:06:19] Initializing Normalizer

```

[15:06:19] Running Normalizer
[15:06:19] Initializing MetalDisconnector
[15:06:19] Running MetalDisconnector
[15:06:19] Initializing Normalizer
[15:06:19] Running Normalizer
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```
[14]: df_lipinski.head(10).style.background_gradient()
```

```
[14]: <pandas.io.formats.style.Styler at 0x7f7127434550>
```

```
[15]: df = pd.concat([df,df_lipinski], axis=1)
```

8 Convert IC50 to pIC50

- To allow IC50 data to be more uniformly distributed, we will convert IC50 to the negative logarithmic scale which is essentially $-\log_{10}(\text{IC50})$.

```
[16]: def pIC50(i):
        molar = i*(10**-9) # Converts nM to M
        pIC50 = -np.log10(molar)
        return pIC50
```

```
[17]: df.standard_value.describe()
```

```
[17]: count      1.087000e+03
      mean      3.254848e+05
      std      3.436745e+06
      min      5.000000e-01
      25%      1.226130e+03
      50%      2.600000e+03
      75%      1.450000e+04
      max      4.000000e+07
      Name: standard_value, dtype: float64
```

```
[18]: df['norm_value'] = df['standard_value'].map(lambda x: 100000000 if x> 100000000
        ↪ else x)
      df['pIC50'] = df['norm_value'].map(pIC50)
```

8.0.1 Removing the ‘intermediate’ bioactivity class

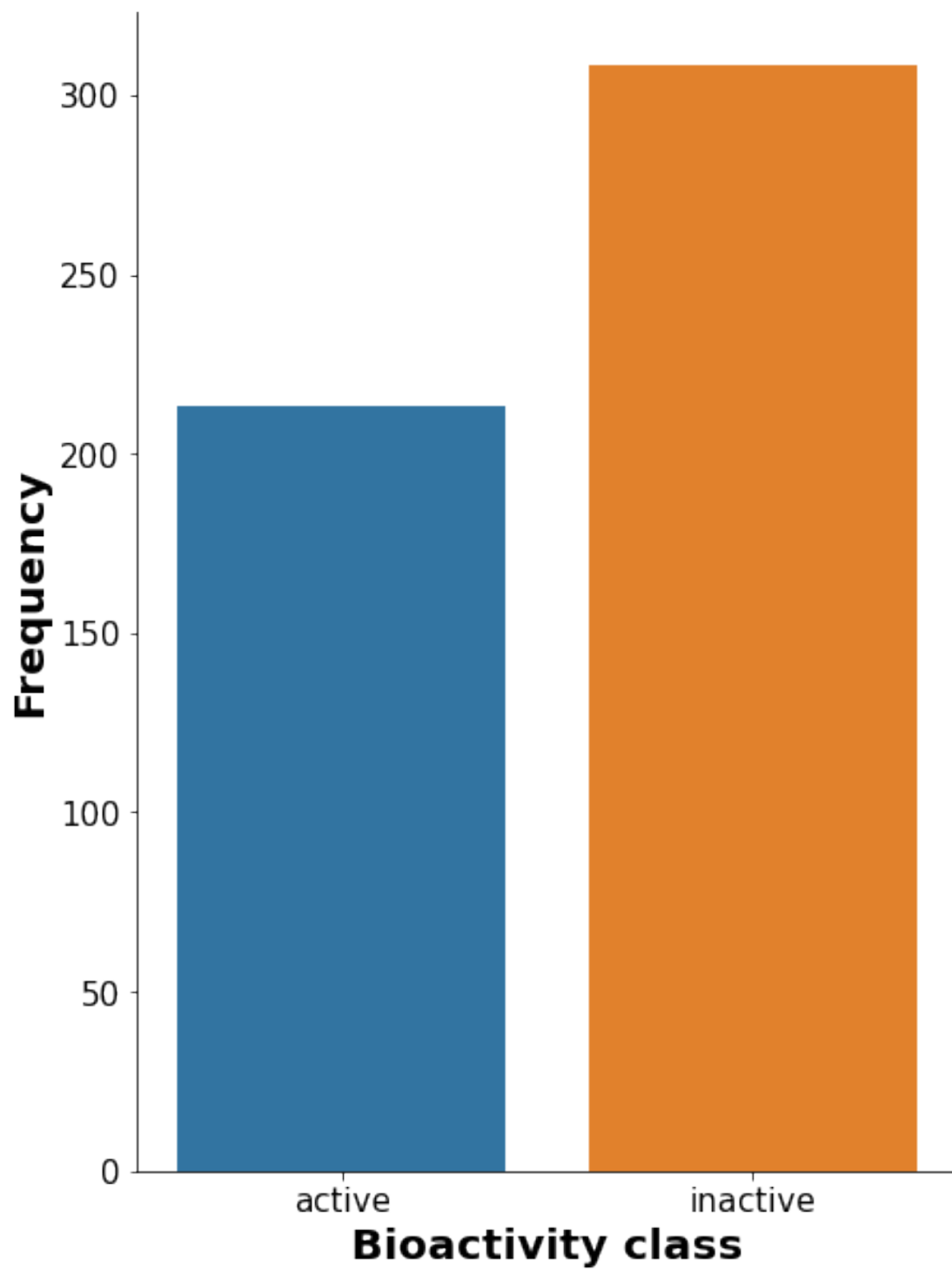
```
[19]: df = df[df['bioactivity_class'] != 'intermediate']
```

```
[20]: df['bioactivity_class'].value_counts()
```

```
[20]: inactive    308  
      active      213  
      Name: bioactivity_class, dtype: int64
```

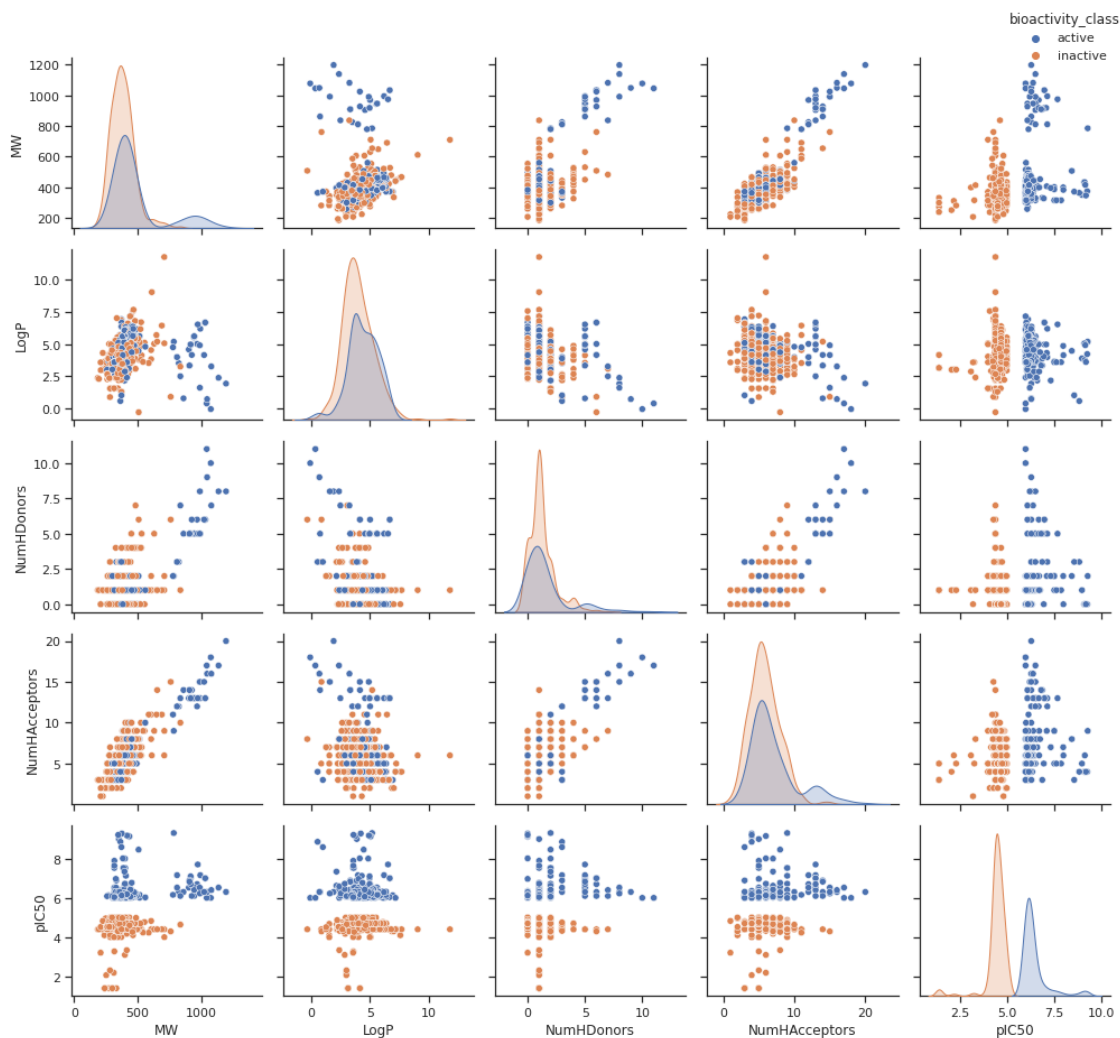
9 Exploratory Data Analysis

```
[21]: plt.figure(figsize=(6.5, 8.5))  
  
      sns.countplot(x='bioactivity_class', data=df)  
      plt.xlabel('Bioactivity class', size=20, fontweight='bold')  
      plt.ylabel('Frequency', fontsize=20, fontweight='bold')  
      plt.xticks(size=15)  
      plt.yticks(size=15)  
      sns.set(style='ticks')  
      sns.despine(top=True)  
      plt.tight_layout()  
      plt.savefig('plot_bioactivity_class.png')
```

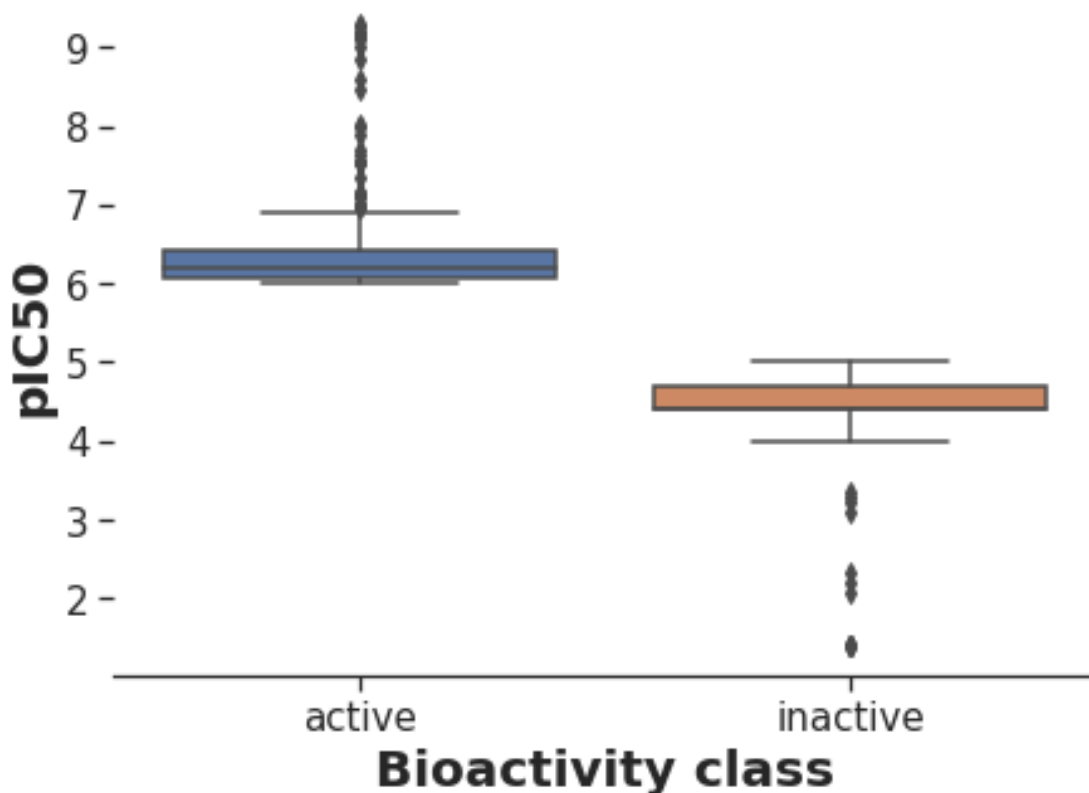
9.0.1 Pairplot of the features

```
[33]: selection = □  
      ↪ ['bioactivity_class', 'MW', 'LogP', 'NumHDonors', 'NumHAcceptors', 'pIC50']  
      sns.pairplot(df[selection], hue='bioactivity_class')._legend.  
      ↪ set_bbox_to_anchor((1, 1))  
      plt.tight_layout()  
      plt.savefig('Pairplot.png', dpi=300)
```



9.0.2 Boxplot of pIC50

```
[34]: fig = plt.figure(figsize=(7,5))
sns.boxplot(x='bioactivity_class', y='pIC50', data = df)
plt.xlabel('Bioactivity class', size=20, fontweight='bold')
plt.ylabel('pIC50', size=20, fontweight='bold')
plt.xticks(size=15)
plt.yticks(size=15)
sns.despine(top=True, left=True)
plt.savefig('boxplot_pIC50.png',dpi=300);
```



9.0.3 Boxplot of Lipinski descriptors

```
[35]: fig = plt.figure(figsize=(12,10))
fig.subplots_adjust(hspace=0.5,wspace=0.5)
fig.add_subplot(2,2,1)
sns.boxplot(x='bioactivity_class', y='NumHAcceptors', data = df)
plt.xlabel('Bioactivity class', size=20, fontweight='bold')
plt.ylabel('NumHAcceptors', size=20, fontweight='bold')
```

```

plt.xticks(size=15)
plt.yticks(size=15)

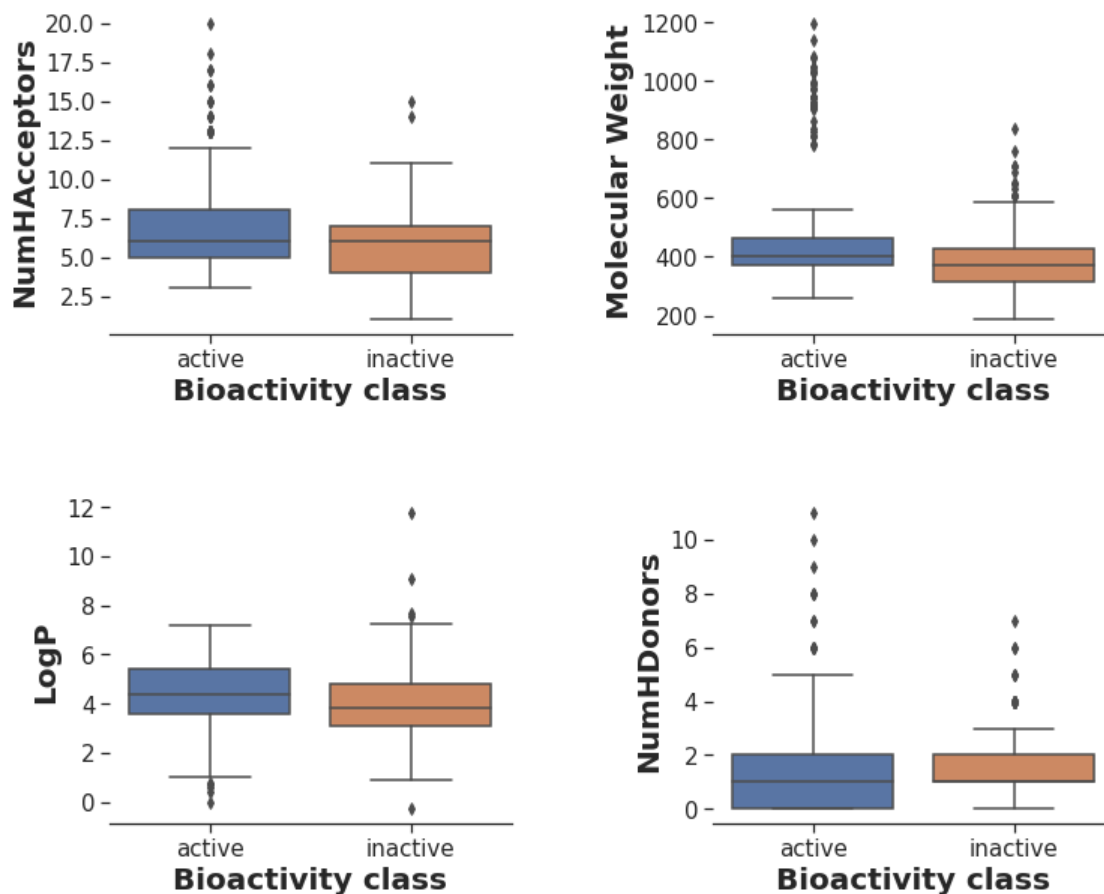
fig.add_subplot(2,2,2)
sns.boxplot(x='bioactivity_class', y='MW', data = df)
plt.xlabel('Bioactivity class', size=20, fontweight='bold')
plt.ylabel('Molecular Weight', size=20, fontweight='bold')
plt.xticks(size=15)
plt.yticks(size=15)

fig.add_subplot(2,2,3)
sns.boxplot(x='bioactivity_class', y='LogP', data = df)
plt.xlabel('Bioactivity class', size=20, fontweight='bold')
plt.ylabel('LogP', size=20, fontweight='bold')
plt.xticks(size=15)
plt.yticks(size=15)

fig.add_subplot(2,2,4)
sns.boxplot(x='bioactivity_class', y='NumHDonors', data = df)
plt.xlabel('Bioactivity class', size=20, fontweight='bold')
plt.ylabel('NumHDonors', size=20, fontweight='bold')
plt.xticks(size=15)
plt.yticks(size=15)

sns.despine(top=True, left=True)
plt.savefig('boxplot_lipinski_descriptors.png',dpi=300);

```



10 Statistical analysis | Mann-Whitney U Test

```
[36]: def mannwhitney_(active, inactive, descriptor):
    stat, p = mannwhitneyu(active, inactive)
    alpha = 0.05
    if p > alpha:
        interpretation = 'Same distribution (fail to reject H0)'
    else:
        interpretation = 'Different distribution (reject H0)'

    results = pd.DataFrame({'Descriptor': descriptor,
                           'Statistics': stat,
                           'p': p,
                           'alpha': alpha,
                           'Interpretation': interpretation}, index=[0])

    filename = 'mannwhitneyu_' + descriptor + '.csv'
    results.to_csv(filename)
```

```
return results
```

```
[37]: for feature in selection[1:]:
      results=mannwhitney_(df[df['bioactivity_class'] != 'inactive'][feature],
                           df[df['bioactivity_class'] == 'inactive'][feature],
                           feature)
      display(results)
```

	Descriptor	Statistics	p	alpha	\
0	MW	22581.5	7.244730e-10	0.05	

Interpretation

0 Different distribution (reject H0)

	Descriptor	Statistics	p	alpha	Interpretation
0	LogP	25280.5	0.000004	0.05	Different distribution (reject H0)

	Descriptor	Statistics	p	alpha	\
0	NumHDonors	32711.5	0.477251	0.05	

Interpretation

0 Same distribution (fail to reject H0)

	Descriptor	Statistics	p	alpha	\
0	NumHAcceptors	27272.0	0.000456	0.05	

Interpretation

0 Different distribution (reject H0)

	Descriptor	Statistics	p	alpha	\
0	pIC50	0.0	3.325100e-85	0.05	

Interpretation

0 Different distribution (reject H0)

```
[38]: df.to_csv('tubulin-data.csv')
```

11 Conclusion

Taking a look at pIC₅₀ values, the actives and inactives displayed statistically significant difference, which is to be expected since threshold values (IC₅₀ < 1,000 nM = Actives while IC₅₀ > 10,000 nM = Inactives, corresponding to pIC₅₀ > 6 = Actives and pIC₅₀ < 5 = Inactives) were used to define actives and inactives.