SmallMoleculesEDA_Preprocessing_Submission

May 13, 2025

1 Small Molecules EDA and processing

[1]:
```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
```

[2]:
```
from rdkit import Chem
from rdkit.Chem import Draw
from rdkit.Chem import AllChem
from rdkit.Chem import DataStructs
from rdkit.Chem import rdMolDescriptors
from IPython.display import display, HTML
```

[3]:
```
from rdkit.Chem import Descriptors
from rdkit.Chem import MolFromSmiles
from rdkit import Chem
from rdkit.Chem import PandasTools
PandasTools.RenderImagesInAllDataFrames(True)
from rdkit import Chem
from rdkit.Chem import Draw
```

[4]:
```
from rdkit.Chem import Lipinski
from rdkit.DataStructs import TanimotoSimilarity
```

[5]:
```
import plotly.express as px
```

[6]:
```
SmallMolecules = pd.read_csv("data/HarvardSmallMolecules.csv")
```

[7]:
```
columns = ['Name', 'Molecular Mass', 'SMILES']
drugs_EDA = SmallMolecules[columns]
```

[8]:
```
PandasTools.AddMoleculeColumnToFrame(drugs_EDA, smilesCol='SMILES',␣
  ↪molCol='structure')
```

```
/opt/anaconda3/lib/python3.12/site-packages/rdkit/Chem/PandasTools.py:376:
SettingWithCopyWarning:
```

```
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-
docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  frame[molCol] = frame[smilesCol].map(Chem.MolFromSmiles)
```

[9]:
```
def compute_descriptors(smiles):
    mol = Chem.MolFromSmiles(smiles)
    if mol is None:
        return {"LogP": None,
            "NumHDonors": None,
            "NumHAcceptors": None,
            "TPSA": None,
            "Fingerprint": None}
    return {"LogP": Descriptors.MolLogP(mol),
        "NumHDonors": Lipinski.NumHDonors(mol),
        "NumHAcceptors": Lipinski.NumHAcceptors(mol),
        "TPSA": Descriptors.TPSA(mol),
        "Fingerprint": AllChem.GetMorganFingerprintAsBitVect(mol, radius=3,␣
 ↪nBits=2048)}
```

[10]:
```
descriptor_df = drugs_EDA["SMILES"].apply(compute_descriptors).apply(pd.Series)
drugs_EDA = pd.concat([drugs_EDA, descriptor_df], axis=1)
```

```
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[03:24:37] DEPRECATION WARNING: please use MorganGenerator
```

[11]:
```
drugs_EDA
```

[11]:
```
            Name  Molecular Mass  \
0        AZD7762          362.12
1      Neratinib          556.20
2      Dasatinib          487.16
3    Saracatinib          541.21
4     Pictilisib          513.16
5    Palbociclib          447.24
6         Torin2          432.12
7          Taxol          853.33
8     Tivantinib          369.15
9     Trametinib          615.08
10      Olaparib          434.18
11    Buparlisib          410.17
12    Luminespib          465.23
13        TGX221          364.19
14       ABT-737          812.26
15  Cabozantinib          501.17
16       INK-128          309.13
17     Alpelisib          441.14
18    Everolimus          957.58
19     Cisplatin          298.96
20   Doxorubicin          543.17
21     Etoposide          588.18
22     Topotecan          421.16
23    Vorinostat          264.15
24    Dinaciclib          396.23
25   Ipatasertib          457.22
26    Volasertib          618.40
27   Abemaciclib          506.27
28     Ceritinib          557.22
29    PF-4708671          390.18
30     Cediranib          450.21
31     Taselisib          460.23
```

```
32    A-1210477          849.39
33    Bleomycin         1414.52

                                                   SMILES  \
0   C1C[C@H](CNC1)NC(=O)C2=C(C=C(S2)C3=CC(=CC=C3)F...
1   CCOC1=C(C=C2C(=C1)N=CC(=C2NC3=CC(=C(C=C3)OCC4=...
2   CC1=C(C(=CC=C1)Cl)NC(=O)C2=CN=C(S2)NC3=NC(=NC(...
3   CN1CCN(CC1)CCOC2=CC(=C3C(=C2)N=CN=C3NC4=C(C=CC...
4   CS(=O)(=O)N1CCN(CC1)CC2=CC3=C(S2)C(=NC(=N3)C4=...
5   CC1=C(C(=O)N(C2=NC(=NC=C12)NC3=NC=C(C=C3)N4CCN...
6   C1=CC(=CC(=C1)N2C(=O)C=CC3=CN=C4C=CC(=CC4=C32)...
7   CC1=C2[C@H](C(=O)[C@@]3([C@H](C[C@@H]4[C@](C3[...
8   C1CC2=CC=CC3=C2N(C1)C=C3[C@H]4[C@@H](C(=O)NC4=...
9   CC1=C2C(=C(N(C1=O)C)NC3=C(C=C(C=C3)I)F)C(=O)N(...
10  C1CC1C(=O)N2CCN(CC2)C(=O)C3=C(C=CC(=C3)CC4=NNC...
11  C1COCCN1C2=NC(=NC(=C2)C3=CN=C(C=C3C(F)(F)F)N)N...
12  CCNC(=O)C1=C(C(=C2C=C(C(=CC2=O)O)C(C)C)ON1)C3=...
13  CC1=CN2C(=O)C=C(N=C2C(=C1)C(C)NC3=CC=CC=C3)N4C...
14  CN(C)CC[C@H](CSC1=CC=CC=C1)NC2=C(C=C(C=C2)S(=O...
15  COC1=CC2=C(C=CN=C2C=C1OC)OC3=CC=C(C=C3)NC(=O)C...
16  CC(C)N1C2=C(C(=N1)C3=CC4=C(C=C3)OC(=N4)N)C(=NC...
17  CC1=C(SC(=N1)NC(=O)N2CCC[C@H]2C(=O)N)C3=CC(=NC...
18  CC1CCC2CC(C(=CC=CC=CC(CC(C(=O)C(C(C(=CC(C(=O)C...
19                                N.N.[Cl-].[Cl-].[Pt+2]
20  C[C@H]1[C@H]([C@H](C[C@@H](O1)O[C@H]2C[C@@](CC...
21  C[C@@H]1OC[C@@H]2[C@@H](O1)[C@@H]([C@H]([C@@H]...
22  CC[C@@]1(C2=C(COC1=O)C(=O)N3CC4=C(C3=C2)N=C5C=...
23                    C1=CC=C(C=C1)NC(=O)CCCCCCC(=O)NO
24  CCC1=C2N=C(C=C(N2N=C1)NCC3=C[N+](=CC=C3)[O-])N...
25  C[C@@H]1C[C@H](C2=C1C(=NC=N2)N3CCN(CC3)C(=O)[C...
26  O=C(N[C@H]1CC[C@H](N2CCN(CC3CC3)CC2)CC1)C4=CC=...
27  CCN1CCN(CC1)CC2=CN=C(C=C2)NC3=NC=C(C(=N3)C4=CC...
28  CC1=CC(=C(C=C1C2CCNCC2)OC(C)C)NC3=NC=C(C(=N3)N...
29  CCC1=CN=CN=C1N2CCN(CC2)CC3=NC4=C(N3)C=C(C=C4)C...
30  CC1=CC2=C(N1)C=CC(=C2F)OC3=NC=NC4=CC(=C(C=C43)...
31  CC1=NN(C(=N1)C2=CN3CCOC4=C(C3=N2)C=CC(=C4)C5=C...
32  CN(C)S(=O)(=O)N1CCN(CC1)C1=CC=C(OCC2=C(C(C)=NN...
33  CC1=C(N=C(N=C1N)[C@H](CC(=O)N)NC[C@@H](C(=O)N)...

                                         structure     LogP  NumHDonors  \
0   <rdkit.Chem.rdchem.Mol object at 0x36b922030>  2.52660           4
1   <rdkit.Chem.rdchem.Mol object at 0x36b922880>  5.93248           2
2   <rdkit.Chem.rdchem.Mol object at 0x36b922730>  3.31354           3
3   <rdkit.Chem.rdchem.Mol object at 0x36b9229d0>  3.93950           1
4   <rdkit.Chem.rdchem.Mol object at 0x36b922a40>  2.14840           1
5   <rdkit.Chem.rdchem.Mol object at 0x36b922ab0>  2.96582           2
6   <rdkit.Chem.rdchem.Mol object at 0x36b922b20>  5.20190           1
```

```
7   <rdkit.Chem.rdchem.Mol object at 0x36b922b90>  3.73570           4
8   <rdkit.Chem.rdchem.Mol object at 0x36b922c00>  3.59260           2
9   <rdkit.Chem.rdchem.Mol object at 0x36b922c70>  3.94012           2
10  <rdkit.Chem.rdchem.Mol object at 0x36b922ce0>  2.34740           1
11  <rdkit.Chem.rdchem.Mol object at 0x36b922d50>  1.81280           1
12  <rdkit.Chem.rdchem.Mol object at 0x36b922dc0>  2.76190           3
13  <rdkit.Chem.rdchem.Mol object at 0x36b922e30>  3.01262           1
14  <rdkit.Chem.rdchem.Mol object at 0x36b922ea0>  7.88060           2
15  <rdkit.Chem.rdchem.Mol object at 0x36b922f10>  5.54080           2
16  <rdkit.Chem.rdchem.Mol object at 0x36b922f80>  2.37980           2
17  <rdkit.Chem.rdchem.Mol object at 0x36b922ff0>  3.83502           2
18  <rdkit.Chem.rdchem.Mol object at 0x36b923060>  6.19720           3
19  <rdkit.Chem.rdchem.Mol object at 0x36b9230d0> -5.67050           2
20  <rdkit.Chem.rdchem.Mol object at 0x36b923140>  0.00130           6
21  <rdkit.Chem.rdchem.Mol object at 0x36b9231b0>  1.33860           3
22  <rdkit.Chem.rdchem.Mol object at 0x36b923220>  1.84680           2
23  <rdkit.Chem.rdchem.Mol object at 0x36b923290>  2.47110           3
24  <rdkit.Chem.rdchem.Mol object at 0x36b923300>  2.27850           2
25  <rdkit.Chem.rdchem.Mol object at 0x36b923370>  3.10100           2
26  <rdkit.Chem.rdchem.Mol object at 0x36b9233e0>  4.26720           2
27  <rdkit.Chem.rdchem.Mol object at 0x36b923450>  4.93692           1
28  <rdkit.Chem.rdchem.Mol object at 0x36b9234c0>  6.36192           3
29  <rdkit.Chem.rdchem.Mol object at 0x36b923530>  3.25630           1
30  <rdkit.Chem.rdchem.Mol object at 0x36b9235a0>  5.22422           1
31  <rdkit.Chem.rdchem.Mol object at 0x36b923610>  3.17422           1
32  <rdkit.Chem.rdchem.Mol object at 0x36b923680>  6.05282           1
33  <rdkit.Chem.rdchem.Mol object at 0x36b9236f0> -7.70358          20

    NumHAcceptors    TPSA                                        Fingerprint
0               4   96.25  [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, …
1               8  112.40  [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, …
2               9  106.51  [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, …
3              10   90.44  [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 1, 1, …
4               9  107.55  [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, …
5               9  105.04  [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, …
6               5   73.80  [0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, …
7              14  221.29  [0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, …
8               3   66.89  [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, …
9               8  107.13  [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, …
10              4   86.37  [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, …
11              8   89.63  [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, …
12              7  100.13  [0, 1, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, …
13              6   58.87  [0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, …
14             10  128.13  [0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 1, 0, …
15              6   98.78  [0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, …
16              8  121.67  [0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, …
17              5  101.21  [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, …
```

```
18              14  204.66  [0, 1, 0, 0, 0, 0, 1, 1, 0, 0, 0, 0, 0, 1, 0, …
19               2   70.00  [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, …
20              12  206.07  [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, …
21              13  160.83  [0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, …
22               8  104.89  [0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, …
23               3   78.43  [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, …
24               7   92.63  [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, …
25               6   81.59  [0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, …
26               9  106.17  [0, 1, 0, 0, 0, 1, 0, 0, 0, 1, 0, 0, 0, 0, 0, …
27               8   75.00  [0, 1, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, …
28               8  105.24  [0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, …
29               5   60.94  [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, …
30               6   72.50  [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, …
31               9  118.67  [0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, …
32              11  134.84  [0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 1, 0, …
33              31  627.07  [0, 1, 0, 0, 0, 0, 0, 0, 1, 0, 0, 1, 0, 0, 0, …
```

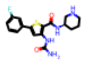
```
[13]: drugs_EDA[["Name","Molecular Mass", "LogP", "NumHDonors", "NumHAcceptors",␣
      ↪"TPSA"]]
```

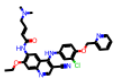
```
[13]:          Name  Molecular Mass     LogP  NumHDonors  NumHAcceptors    TPSA
      0     AZD7762          362.12  2.52660           4              4   96.25
      1   Neratinib          556.20  5.93248           2              8  112.40
      2   Dasatinib          487.16  3.31354           3              9  106.51
      3  Saracatinib         541.21  3.93950           1             10   90.44
      4  Pictilisib          513.16  2.14840           1              9  107.55
      5  Palbociclib         447.24  2.96582           2              9  105.04
      6      Torin2          432.12  5.20190           1              5   73.80
      7       Taxol          853.33  3.73570           4             14  221.29
      8  Tivantinib          369.15  3.59260           2              3   66.89
      9  Trametinib          615.08  3.94012           2              8  107.13
      10   Olaparib          434.18  2.34740           1              4   86.37
      11 Buparlisib          410.17  1.81280           1              8   89.63
      12 Luminespib          465.23  2.76190           3              7  100.13
      13     TGX221          364.19  3.01262           1              6   58.87
      14    ABT-737          812.26  7.88060           2             10  128.13
      15 Cabozantinib        501.17  5.54080           2              6   98.78
      16    INK-128          309.13  2.37980           2              8  121.67
      17  Alpelisib          441.14  3.83502           2              5  101.21
      18 Everolimus          957.58  6.19720           3             14  204.66
      19  Cisplatin          298.96 -5.67050           2              2   70.00
      20 Doxorubicin         543.17  0.00130           6             12  206.07
      21  Etoposide          588.18  1.33860           3             13  160.83
      22  Topotecan          421.16  1.84680           2              8  104.89
      23 Vorinostat          264.15  2.47110           3              3   78.43
      24 Dinaciclib          396.23  2.27850           2              7   92.63
      25 Ipatasertib         457.22  3.10100           2              6   81.59
```

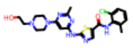
```
26    Volasertib          618.40  4.26720           2               9  106.17
27   Abemaciclib          506.27  4.93692           1               8   75.00
28     Ceritinib          557.22  6.36192           3               8  105.24
29    PF-4708671          390.18  3.25630           1               5   60.94
30     Cediranib          450.21  5.22422           1               6   72.50
31     Taselisib          460.23  3.17422           1               9  118.67
32     A-1210477          849.39  6.05282           1              11  134.84
33     Bleomycin         1414.52 -7.70358          20              31  627.07
```

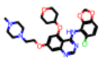
[14]:

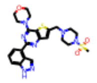
```
mols = [Chem.MolFromSmiles(smiles) for smiles in SmallMolecules["SMILES"]]
names = SmallMolecules["Name"].tolist()

img = Draw.MolsToGridImage(
    mols,
    legends=names,
    molsPerRow=5,
    subImgSize=(200,200)

from IPython.display import display
display(img)
```

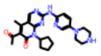

AZD7762

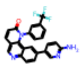

Neratinib

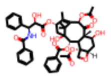

Dasatinib

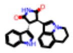

Saracatinib

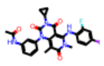

Pictilisib

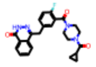

Palbociclib

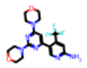

Torin2

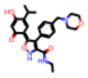

Taxol

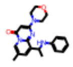

Tivantinib

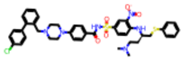

Trametinib

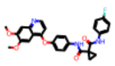

Olaparib

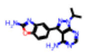

Buparlisib

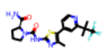

Luminespib

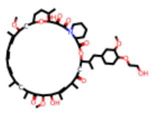

TGX221


ABT-737

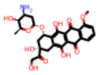

Cabozantinib

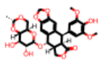

INK-128

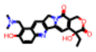

Alpelisib

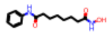

Everolimus

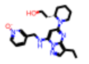
Cisplatin

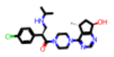

Doxorubicin

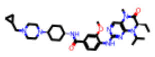

Etoposide

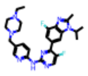

Topotecan

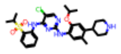

Vorinostat

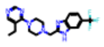

Dinaciclib

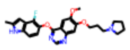

Ipatasertib

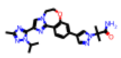

Volasertib

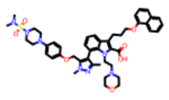

Abemaciclib

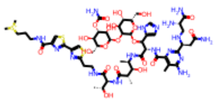

Ceritinib


PF-4708671


Cediranib

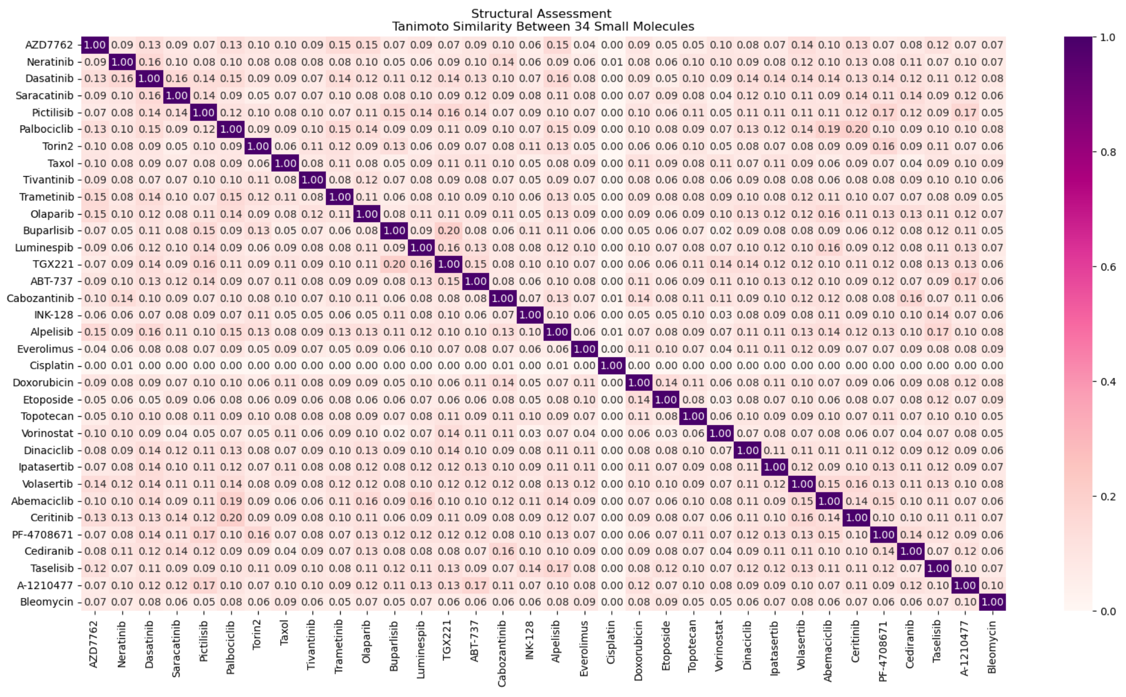

Taselisib


A-1210477

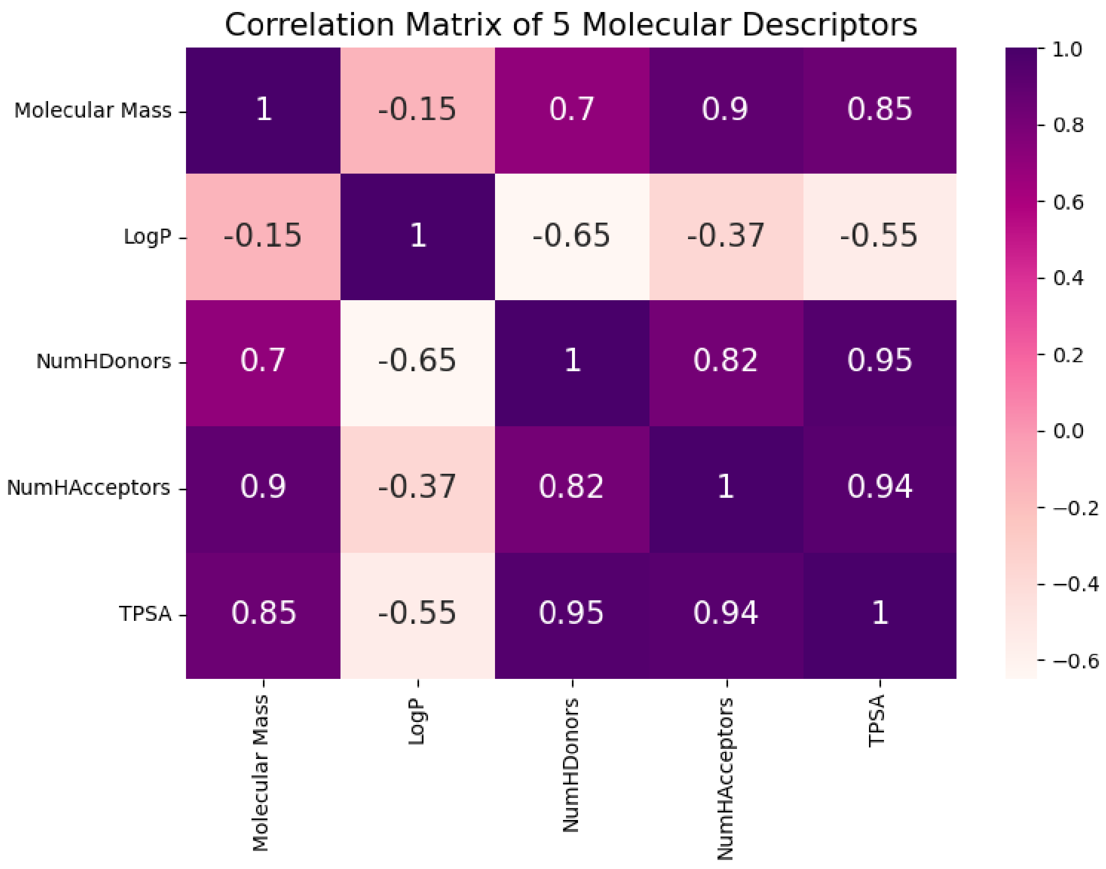

Bleomycin

[15]:
```python
fps = drugs_EDA["Fingerprint"].tolist()
names = drugs_EDA["Name"].tolist()
n = len(fps)

# similarity matrix
sim_matrix = np.zeros((n, n))
for i in range(n):
    for j in range(n):
        sim_matrix[i, j] = TanimotoSimilarity(fps[i], fps[j])

sim_df = pd.DataFrame(sim_matrix, index=names, columns=names)
```

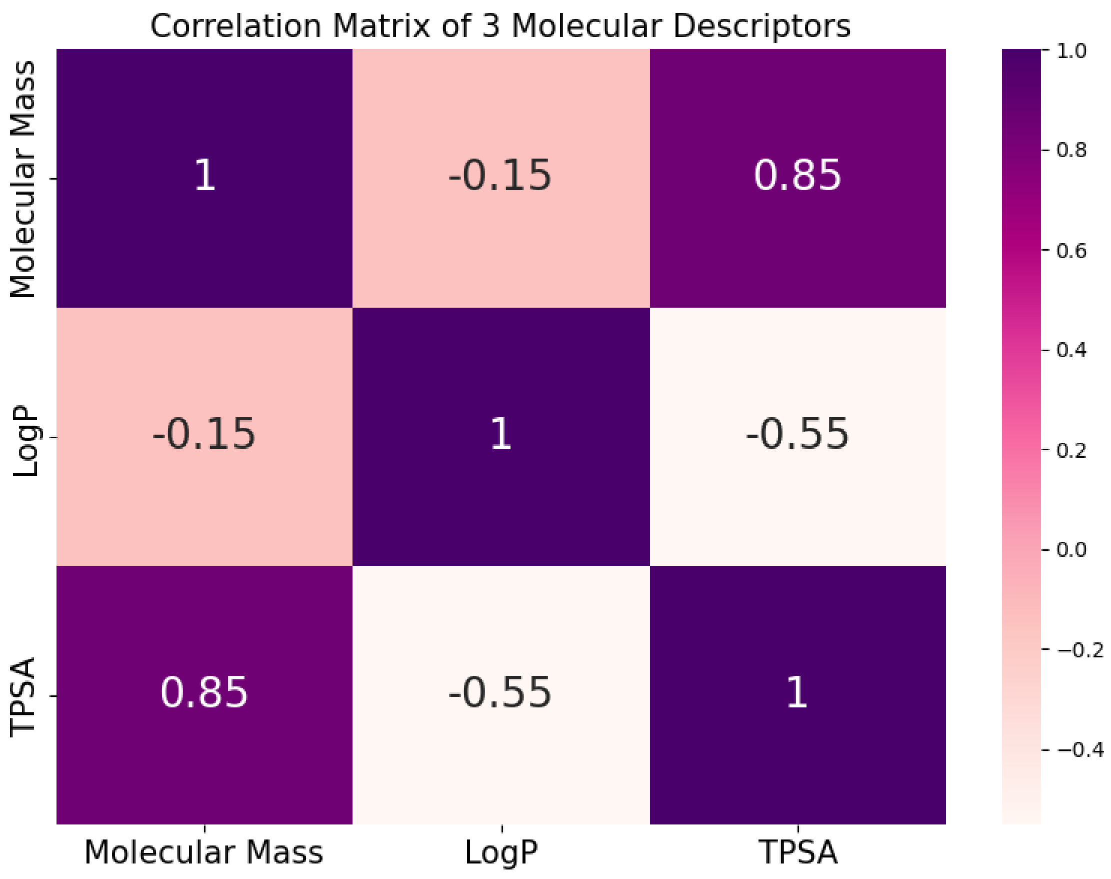
[72]:
```python
plt.figure(figsize=(20,10))
sns.heatmap(sim_df, annot=True, fmt=".2f", cmap="RdPu")
plt.title("Structural Assessment \nTanimoto Similarity Between 34 Small␣
 ↪Molecules")
plt.show()
```



[18]:
```python
# correlation matrix
descriptor_cols = ['Molecular Mass', 'LogP', 'NumHDonors', 'NumHAcceptors',␣
 ↪'TPSA']
corr_matrix = drugs_EDA[descriptor_cols].corr()
plt.figure(figsize=(8, 6))
sns.heatmap(corr_matrix, annot=True, cmap="RdPu", annot_kws={"size": 15})
plt.xticks(fontsize=10)
plt.yticks(fontsize=10)
plt.title("Correlation Matrix of 5 Molecular Descriptors", fontsize=15)
plt.tight_layout()
plt.show()
```

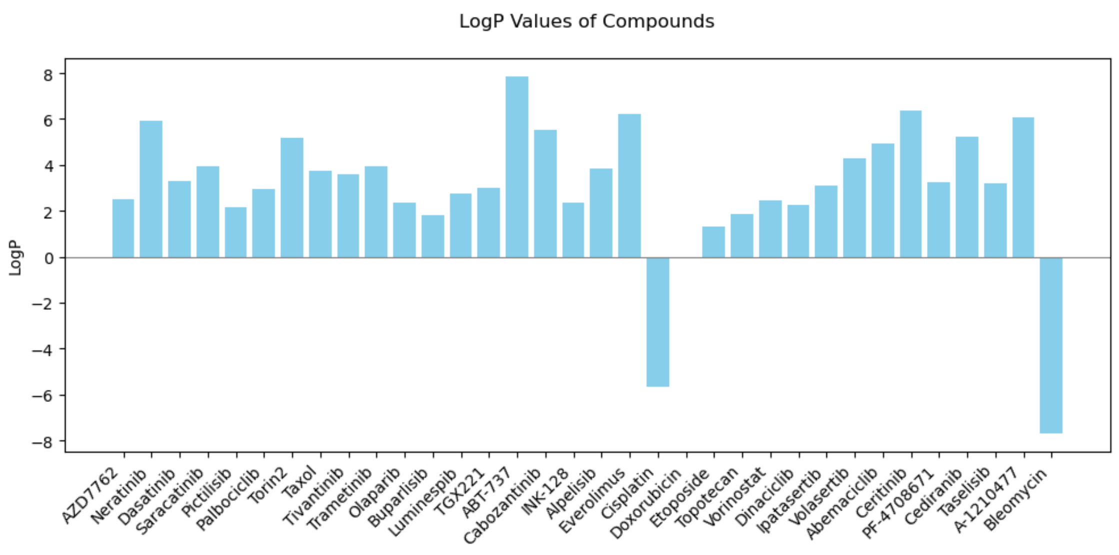


[28]:
```
descriptor_cols = ["Molecular Mass", "LogP", "TPSA"] # TPSA abd Hacceptors/
  ↪donors tend to be correlated with one another.
corr_matrix = drugs_EDA[descriptor_cols].corr()
plt.figure(figsize=(8, 6))
sns.heatmap(corr_matrix, annot=True, cmap="RdPu", annot_kws={"size": 20} )
plt.xticks(fontsize=15)
plt.yticks(fontsize=15)
plt.title("Correlation Matrix of 3 Molecular Descriptors", fontsize=15)
plt.tight_layout()
plt.show()
```

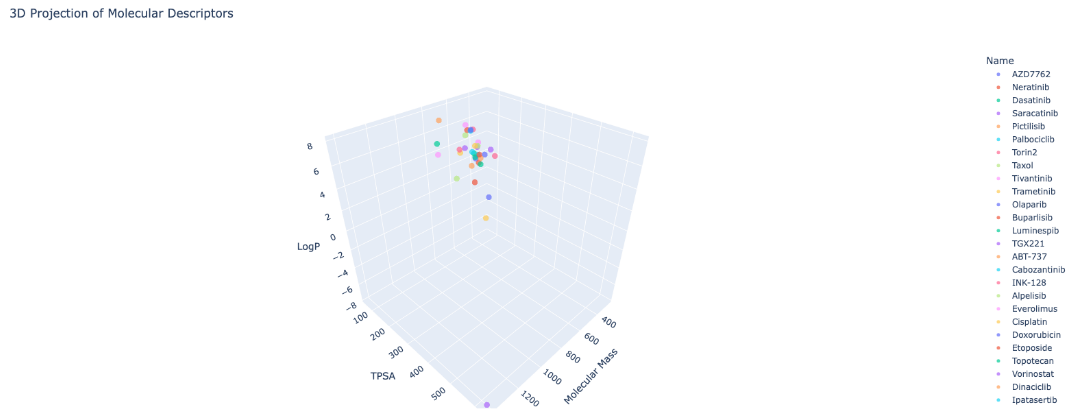


[33]:

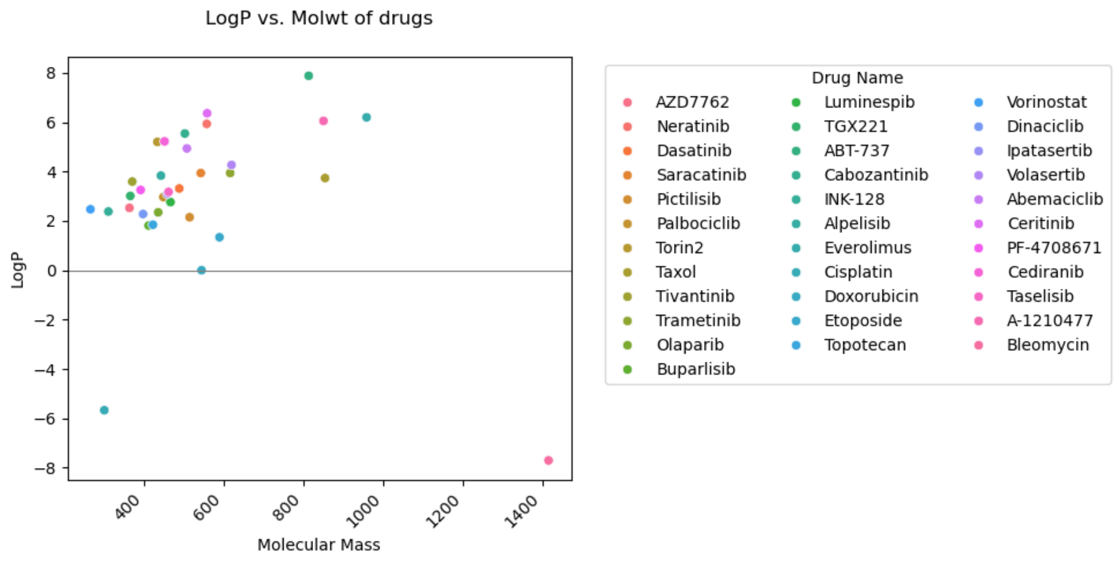
```
plt.figure(figsize=(10, 5))
bars = plt.bar(drugs_EDA["Name"], drugs_EDA["LogP"], color='skyblue')
plt.axhline(0, color='gray', linewidth=0.8)
plt.ylabel("LogP")
plt.title("LogP Values of Compounds", pad=20)
plt.xticks(rotation=45, ha='right')
plt.tight_layout()
plt.show()
```



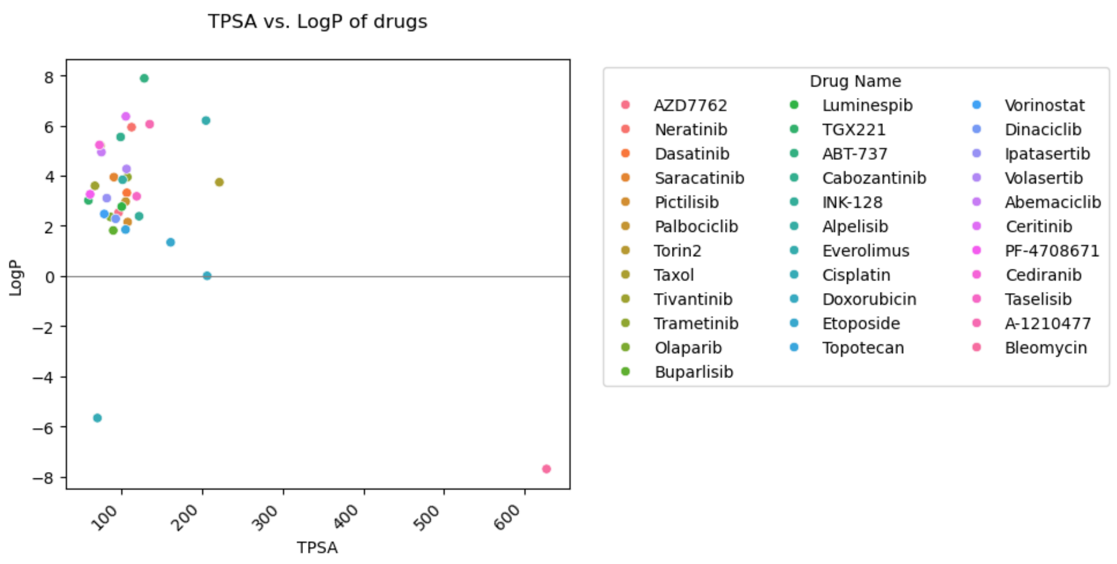
```
[38]: fig = px.scatter_3d(
          drugs_EDA,
          width=900,
          height=700,
          x="Molecular Mass",
          y="TPSA",
          z="LogP",
          color="Name",
          title="3D Projection of Molecular Descriptors",
          labels={"MolWt": "Molecular Weight", "TPSA": "TPSA", "LogP": "LogP"},
          opacity=0.7,)
      fig.update_traces(marker=dict(size=5))
      fig.show()
```



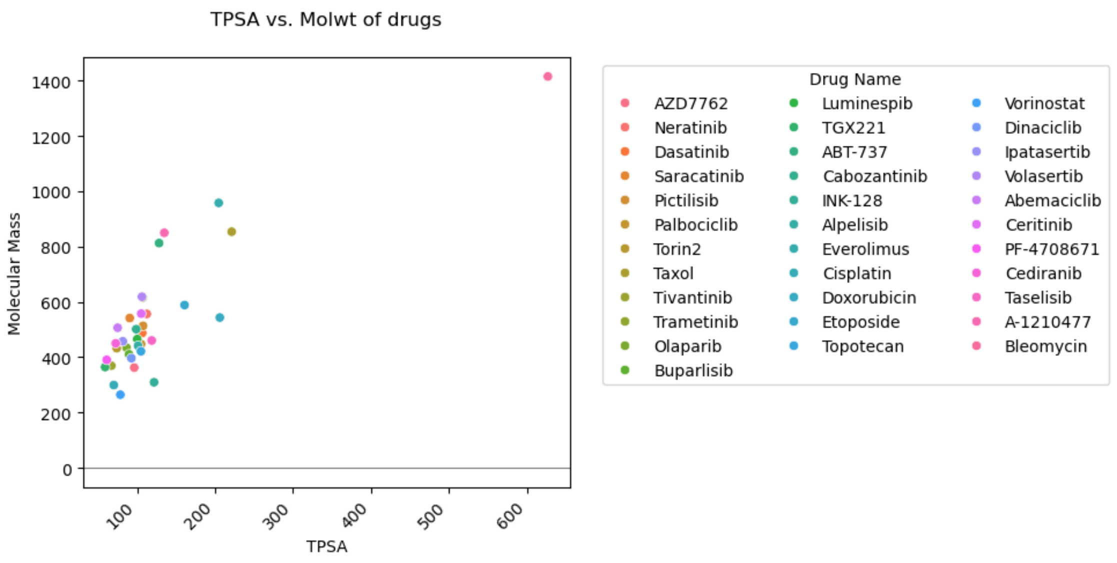
[40]:
```python
plt.figure(figsize=(10,5))
bars = sns.scatterplot(drugs_EDA, x = drugs_EDA["Molecular Mass"], y =␣
↪drugs_EDA["LogP"], hue = "Name")
plt.axhline(0, color='gray', linewidth=0.8)
plt.title("LogP vs. Molwt of drugs", pad=20)
plt.xticks(rotation=45, ha='right')
plt.legend(title="Drug Name", bbox_to_anchor=(1.05, 1), loc='upper left',␣
↪ncol=3)
plt.tight_layout()
plt.show()
```



[42]:
```python
plt.figure(figsize=(10,5))
bars = sns.scatterplot(drugs_EDA, x = drugs_EDA["TPSA"], y = drugs_EDA["LogP"],␣
↪hue = "Name")
plt.axhline(0, color='gray', linewidth=0.8)
plt.title("TPSA vs. LogP of drugs", pad=20)
plt.xticks(rotation=45, ha='right')
plt.legend(title="Drug Name", bbox_to_anchor=(1.05, 1), loc='upper left',␣
↪ncol=3)
plt.tight_layout()
plt.show()
```



[45]:
```
plt.figure(figsize=(10,5))
bars = sns.scatterplot(drugs_EDA, x = drugs_EDA["TPSA"], y =␣
  ↪drugs_EDA["Molecular Mass"], hue = "Name")
plt.axhline(0, color='gray', linewidth=0.8)
plt.title("TPSA vs. Molwt of drugs", pad=20)
plt.xticks(rotation=45, ha='right')
plt.legend(title="Drug Name", bbox_to_anchor=(1.05, 1), loc='upper left',␣
  ↪ncol=3)
plt.tight_layout()
plt.show()
```



```
[46]: drugs_EDA = drugs_EDA[['Name', 'Molecular Mass', 'LogP', 'NumHDonors',␣
       ↪'NumHAcceptors', 'TPSA', 'structure','SMILES', 'Fingerprint']]
```

Importance of TPSA:

https://pressbooks.openeducationalberta.ca/abcofpkpd/chapter/tpsa/

Topological polar surface area (TPSA), sometimes referred to simply as "polar surface area" (PSA) is a value that can be calculated for a drug that provides an indication of the drug's polarity, and thus an indication of its lipid solubility.

Drugs with higher TPSA values are less lipid-soluble and will, in general, be absorbed less extensively and more slowly, and will distribute less extensively, than drugs with lower TPSA values.

Once TPSA is known for a drug, the value can be used, for example, to predict the extent to which an oral dose of the drug will be absorbed from the GI tract into the portal circulation, or the extent to which the drug will partition into the brain from the plasma, by consulting published graphs that relate TPSA values to these drug behaviours.

TPSA is used as a translation for PK/PD.

```
[50]: drugs_EDA.to_csv("Descriptors_Small_Molecules.csv")
```

```
[ ]:
```

```
[ ]:
```

```
[ ]:
```