In [3]:
```
%matplotlib inline

from IPython.display import Image

import io
import os

from Bio import SeqIO
from Bio.KEGG import REST
from Bio.KEGG.KGML import KGML_parser
from Bio.Graphics.KGML_vis import KGMLCanvas

import pandas as pd
```

In [5]:
```
def PDF(filename):
    return HTML('<iframe src=%s width=700 height=350></iframe>' % filename)

def to_df(result):
    return pd.read_table(io.StringIO(result), header=None)
```

In [6]:
```
result = REST.kegg_info("pathway").read()
print(result)
```

```
pathway          KEGG Pathway Database
path             Release 108.0+/10-08, Oct 23
                 Kanehisa Laboratories
                 1,094,015 entries

linked db        module
                 ko
                 <org>
                 genome
                 compound
                 glycan
                 reaction
                 rclass
                 enzyme
                 network
                 disease
                 drug
                 pubmed
```

In [10]:
```
result = REST.kegg_list("pathway").read()
to_df(result)
```

Out[10]:

	0	1
0	map01100	Metabolic pathways
1	map01110	Biosynthesis of secondary metabolites
2	map01120	Microbial metabolism in diverse environments
3	map01200	Carbon metabolism
4	map01210	2-Oxocarboxylic acid metabolism
...	...	...
561	map07035	Prostaglandins
562	map07110	Benzoic acid family
563	map07112	1,2-Diphenyl substitution family
564	map07114	Naphthalene family
565	map07117	Benzodiazepine family

566 rows × 2 columns

In [12]:
```
result = REST.kegg_info("pathway").read()
print(result)
```

```
pathway          KEGG Pathway Database
path             Release 108.0+/10-08, Oct 23
                 Kanehisa Laboratories
                 1,094,015 entries

linked db        module
                 ko
                 <org>
                 genome
                 compound
                 glycan
                 reaction
                 rclass
                 enzyme
                 network
                 disease
                 drug
                 pubmed
```

In [20]:
```
result = REST.kegg_find("drug","Ruxolitinib").read()
print(result)
```

```
dr:D09959        Ruxolitinib (USAN/INN)
dr:D09960        Ruxolitinib phosphate (JAN/USAN); Jakafi (TN); Jakavi (TN); Opzelura
(TN)
dr:D11866        Deuruxolitinib (USAN)
dr:D11867        Deuruxolitinib phosphate (USAN)
```

In [19]:
```
result = REST.kegg_get("dr:D09955").read()
print(result)
```

```
ENTRY       D09955                      Drug
NAME        Quizartinib (USAN/INN)
FORMULA     C29H32N6O4S
EXACT_MASS  560.2206
MOL_WEIGHT  560.6672
CLASS       Antineoplastic
             DG01918  Tyrosine kinase inhibitor
              DG01917  Receptor tyrosine kinase inhibitor
            Metabolizing enzyme substrate
             DG01633  CYP3A/CYP3A4 substrate
REMARK      ATC code: L01EX11
            Chemical structure group: DG01364
            Product (DG01364): D09956<JP/US>
EFFICACY    Antineoplastic, Receptor tyrosine kinase inhibitor
TARGET      FLT3 (CD135) [HSA:2322] [KO:K05092]
  PATHWAY   hsa04640(2322)  Hematopoietic cell lineage
            hsa05200(2322)  Pathways in cancer
METABOLISM  Enzyme: CYP3A [HSA:1576 1577 1551]
INTERACTION
STR_MAP     map07045  Antineoplastics - protein kinase inhibitors
BRITE       Anatomical Therapeutic Chemical (ATC) classification [BR:br08303]
             L ANTINEOPLASTIC AND IMMUNOMODULATING AGENTS
              L01 ANTINEOPLASTIC AGENTS
               L01E PROTEIN KINASE INHIBITORS
                L01EX Other protein kinase inhibitors
                 L01EX11 Quizartinib
                  D09955  Quizartinib (USAN/INN)
            Drug groups [BR:br08330]
             Antineoplastic
              DG01918  Tyrosine kinase inhibitor
               DG01917  Receptor tyrosine kinase inhibitor
                DG01364  Quizartinib
                 D09955  Quizartinib
             Metabolizing enzyme substrate
              DG01633  CYP3A/CYP3A4 substrate
               DG01364  Quizartinib
                D09955  Quizartinib
            Target-based classification of drugs [BR:br08310]
             Protein kinases
              Receptor tyrosine kinases (RTK)
               PDGFR family
                FLT3 (CD135)
                 D09955  Quizartinib (USAN/INN)
            Drug metabolizing enzymes and transporters [br08309.html]
             Drug metabolizing enzymes
              D09955
            Drug groups [BR:br08330]
             Antineoplastic
              DG01918  Tyrosine kinase inhibitor
               DG01917  Receptor tyrosine kinase inhibitor
                DG01364  Quizartinib
             Metabolizing enzyme substrate
              DG01633  CYP3A/CYP3A4 substrate
               DG01364  Quizartinib
DBLINKS     CAS: 950769-58-1
            PubChem: 135626680
            ChEBI: 90217
            PDB-CCD: P30
            LigandBox: D09955
ATOM        40
```

```
                1   C1x C    36.8374  -17.7901
                2   O2x O    36.8374  -19.1909
                3   C1x C    35.6467  -19.8912
                4   C1x C    34.3861  -19.1909
                5   N1y N    34.3861  -17.7901
                6   C1x C    35.6467  -17.0898
                7   C1b C    33.1954  -17.0898
                8   C1b C    32.0048  -17.7901
                9   O2a O    30.8142  -17.0898
                10  C8y C    29.6235  -17.7901
                11  C8x C    29.6235  -19.1909
                12  C8x C    28.3628  -19.8912
                13  C8y C    27.1722  -19.1909
                14  C8y C    27.1722  -17.7901
                15  C8x C    28.3628  -17.0898
                16  N4y N    25.8415  -19.6111
                17  C8y C    25.0011  -18.4905
                18  S2x S    25.8415  -17.3699
                19  C8x C    25.0011  -20.7317
                20  C8y C    23.6704  -20.3115
                21  N5x N    23.6704  -18.9107
                22  C8y C    22.4797  -21.0118
                23  C8x C    22.4797  -22.4126
                24  C8x C    21.2891  -23.1130
                25  C8y C    20.0284  -22.4126
                26  C8x C    20.0284  -21.0118
                27  C8x C    21.2891  -20.3115
                28  N1b N    18.8378  -23.1130
                29  C5a C    17.6472  -22.4126
                30  N1b N    16.4565  -23.1130
                31  O5a O    17.6472  -21.0118
                32  C8y C    15.2659  -22.4126
                33  N5x N    13.8651  -22.4126
                34  O2x O    13.3749  -21.0819
                35  C8y C    14.5655  -20.2414
                36  C8x C    15.6861  -21.0819
                37  C1d C    14.5655  -18.8407
                38  C1a C    14.5655  -17.4399
                39  C1a C    15.9655  -18.8407
                40  C1a C    13.1655  -18.8407
BOND            45
                1     1   2 1
                2     2   3 1
                3     3   4 1
                4     4   5 1
                5     5   6 1
                6     1   6 1
                7     5   7 1
                8     7   8 1
                9     8   9 1
                10    9  10 1
                11   10  11 1
                12   11  12 2
                13   12  13 1
                14   13  14 2
                15   14  15 1
                16   10  15 2
                17   13  16 1
                18   16  17 1
                19   17  18 1
```

```
            20   14  18 1
            21   16  19 1
            22   19  20 2
            23   20  21 1
            24   17  21 2
            25   20  22 1
            26   22  23 1
            27   23  24 2
            28   24  25 1
            29   25  26 2
            30   26  27 1
            31   22  27 2
            32   25  28 1
            33   28  29 1
            34   29  30 1
            35   29  31 2
            36   30  32 1
            37   32  33 2
            38   33  34 1
            39   34  35 1
            40   35  36 2
            41   32  36 1
            42   35  37 1
            43   37  38 1
            44   37  39 1
            45   37  40 1
///
```

In [23]:
```
lists =  pd.read_csv("Lists.csv")
arr = []
for k in lists['Drug Name'].tolist()[:15]:
    if ' ' in k:
        k= k.replace(" ", "+")
    result = REST.kegg_find("drug", k).read()
    if result != "\n":
        arr.append(result)
print(arr)
```

```
['dr:D09959\tRuxolitinib (USAN/INN)\ndr:D09960\tRuxolitinib phosphate (JAN/USAN); Jak
afi (TN); Jakavi (TN); Opzelura (TN)\ndr:D11866\tDeuruxolitinib (USAN)\ndr:D11867\tDe
uruxolitinib phosphate (USAN)\n', 'dr:D09864\tAmuvatinib (USAN/INN)\ndr:D09865\tAmuva
tinib hydrochloride (USAN)\n', 'dr:D03828\tPemetrexed disodium (USAN); Alimta (TN)\nd
r:D06503\tPemetrexed sodium hydrate (JAN); Pemetrexed disodium heptahydrate; Alimta
(TN)\ndr:D07472\tPemetrexed (INN); Alimta (TN); Pemetrexed (TN); Pemfexy (TN)\ndr:D10
596\tPemetrexed sodium hemipentahydrate (JAN); Pemetrexed disodium hemipentahydrate;
Pemetrexed accord (TN)\ndr:D11352\tPemetrexed tromethamine (USAN)\n']
```

In [24]:
```
lists =  pd.read_csv("Lists.csv")
arr = []
for k in lists['Drug Name'].tolist()[:150]:
    if ' ' in k:
        k= k.replace(" ", "+")
    result = REST.kegg_find("drug", k).read()
    if result != "\n":
        arr.append(result)
print(arr)
```

```
['dr:D09959\tRuxolitinib (USAN/INN)\ndr:D09960\tRuxolitinib phosphate (JAN/USAN); Jak
afi (TN); Jakavi (TN); Opzelura (TN)\ndr:D11866\tDeuruxolitinib (USAN)\ndr:D11867\tDe
uruxolitinib phosphate (USAN)\n', 'dr:D09864\tAmuvatinib (USAN/INN)\ndr:D09865\tAmuva
tinib hydrochloride (USAN)\n', 'dr:D03828\tPemetrexed disodium (USAN); Alimta (TN)\nd
r:D06503\tPemetrexed sodium hydrate (JAN); Pemetrexed disodium heptahydrate; Alimta
(TN)\ndr:D07472\tPemetrexed (INN); Alimta (TN); Pemetrexed (TN); Pemfexy (TN)\ndr:D10
596\tPemetrexed sodium hemipentahydrate (JAN); Pemetrexed disodium hemipentahydrate;
Pemetrexed accord (TN)\ndr:D11352\tPemetrexed tromethamine (USAN)\n', 'dr:D10630\tFed
ratinib (USAN/INN)\ndr:D11296\tFedratinib hydrochloride (USAN); Fedratinib hydrochlor
ide hydrate (JAN); Fedratinib dihydrochloride monohydrate; Inrebic (TN)\n', 'dr:D0539
9\tPelitinib (USAN/INN)\n', 'dr:D00142\tMethotrexate (JP18/USP/INN); Otrexup (TN); Xa
tmep (TN)\ndr:D02115\tMethotrexate sodium; Trexall (TN); Rasuvo (TN)\n', 'dr:D00753\t
Sirolimus (JAN/USAN/INN); Rapamune (TN); Rapamycin (TN)\n', 'dr:D05049\tMirincamycin
hydrochloride (USAN)\n', 'dr:D00961\tBicalutamide (JP18/USP/INN); Casodex (TN)\n', 'd
r:D06320\tVorinostat (JAN/USAN); Zolinza (TN)\n', 'dr:D01161\tFulvestrant (JAN/USP/IN
N); Faslodex (TN)\n', 'dr:D09338\tEntinostat (JAN/USAN/INN)\n', 'dr:D00961\tBicalutam
ide (JP18/USP/INN); Casodex (TN)\n', 'dr:D07741\tZibotentan (JAN/USAN/INN)\n', 'dr:D0
9666\tSelumetinib (USAN/INN)\ndr:D10024\tSelumetinib sulfate (JAN/USAN); Koselugo (T
N)\n', 'dr:D09869\tAvagacestat (USAN)\n', 'dr:D00966\tTamoxifen citrate (JP18/USP); N
olvadex (TN); Soltamox (TN)\ndr:D08559\tTamoxifen (INN); Tamoxifen (TN); Tamoplex (T
N)\n', 'dr:D08351\tPhenformin (BAN)\ndr:D08352\tPhenformin hydrochloride; Debei (TN)
\n', 'dr:D10560\tIdelalisib (JAN/USAN/INN); Zydelig (TN)\n', 'dr:D09692\tVeliparib (J
AN/USAN/INN)\n', 'dr:D06272\tSorafenib tosylate (USAN); Sorafenib tosilate (JAN); Nex
avar (TN)\ndr:D08524\tSorafenib (USAN/INN)\n', 'dr:D04696\tLestaurtinib (USAN/INN)
\n', 'dr:D10450\tAlectinib hydrochloride (JAN); Alecensa (TN)\ndr:D10542\tAlectinib
(USAN/INN)\n', 'dr:D03720\tTipifarnib (USAN/INN)\n', 'dr:D00125\tEtoposide (JP18/USP/
INN); Vepesid (TN)\ndr:D04107\tEtoposide phosphate (USAN); Etopophos (TN)\n', 'dr:D04
023\tErlotinib hydrochloride (JAN/USAN); Tarceva (TN)\ndr:D07907\tErlotinib (INN)\n',
'dr:D10019\tPanobinostat lactate (JAN); Farydak (TN)\ndr:D10319\tPanobinostat (USAN/I
NN); Farydak (TN)\n', 'dr:D04687\tLenalidomide (JAN/USAN/INN); Revlimid (TN)\ndr:D098
13\tLenalidomide hydrate (JAN); Revlimid (TN)\n', 'dr:D06402\tSunitinib malate (JAN/U
SAN); Sutent (TN)\ndr:D08552\tSunitinib (INN)\n', 'dr:D11727\tVoxtalisib (USAN/INN)
\n', 'dr:D10446\tMargetuximab (USAN/INN); Margetuximab-cmkb; Margenza (TN)\n', 'dr:D0
0275\tCisplatin (JP18/USP/INN); Platinol (TN)\n', 'dr:D00488\tPyrimethamine (JAN/USP/
INN); Daraprim (TN)\ndr:D02448\tPyrimethamine and sulfadoxine; Fansidar (TN)\n', 'dr:
D10257\tEzetimibe and simvastatin; Vytorin (TN)\n', 'dr:D09955\tQuizartinib (USAN/IN
N)\ndr:D09956\tQuizartinib dihydrochloride (USAN); Quizartinib hydrochloride (JAN); V
anflyta (TN)\n']
```

In [29]:

```python
csv_files = [
    'Lists (1).csv',
    'Lists (2).csv',
    'Lists (3).csv',
    'Lists (4).csv',
    'Lists (5).csv',
    'Lists (6).csv'
]

target_data = {}

for file in csv_files:
    df = pd.read_csv(file)
    print(f"Processing {file}, Columns in file: {df.columns.tolist()}")

    if 'Targets' in df.columns and 'Z Score' in df.columns:
        for index, row in df.iterrows():
            targets = row['Targets']

            if isinstance(targets, str):
                targets = targets.split(', ')
```

```
            else:
                targets = []

            z_score = row['Z Score']

            for target in targets:
                if target not in target_data:
                    target_data[target] = {'total_z_score': 0, 'drug_count': 0}

                target_data[target]['total_z_score'] += z_score
                target_data[target]['drug_count'] += 1
    else:
        print(f"Skipped {file} due to missing required columns.")

for target, data in target_data.items():
    data['average_z_score'] = data['total_z_score'] / data['drug_count']

sorted_targets = sorted(target_data.items(), key=lambda x: x[1]['average_z_score'], re

print("Sorted Targets by Average Z-Score:")
print(sorted_targets)
```

```
Processing Lists (1).csv, Columns in file: ['ID', 'Drug Name', 'Targets', 'Z Score',
'Count']
Processing Lists (2).csv, Columns in file: ['ID', 'Drug Name', 'Targets', 'Z Score',
'Count']
Processing Lists (3).csv, Columns in file: ['ID', 'Drug Name', 'Targets', 'Z Score',
'Count']
Processing Lists (4).csv, Columns in file: ['Drug Name']
Skipped Lists (4).csv due to missing required columns.
Processing Lists (5).csv, Columns in file: ['ID', 'Drug Name', 'Targets', 'Z Score',
'Count']
Processing Lists (6).csv, Columns in file: ['ID', 'Drug Name', 'Targets', 'Z Score',
'Count']
Sorted Targets by Average Z-Score:
[('DNA damage', {'total_z_score': 2.4593992292983433, 'drug_count': 2, 'average_z_sco
re': 1.2296996146491717}), ('DYRK1B', {'total_z_score': 1.7773576563095268, 'drug_cou
nt': 2, 'average_z_score': 0.8886788281547634}), ('FYN', {'total_z_score': 1.51025417
99169455, 'drug_count': 2, 'average_z_score': 0.7551270899584728}), ('PARP7', {'total
_z_score': 0.8910765187459387, 'drug_count': 2, 'average_z_score': 0.4455382593729693
7}), ('MCT1', {'total_z_score': 0.7714803095472053, 'drug_count': 2, 'average_z_scor
e': 0.38574015477360263}), ('Tankyrase 1/2 (PARP5a', {'total_z_score': 0.712810160667
7049, 'drug_count': 2, 'average_z_score': 0.3564050803338524 3}), ('PARP5b)', {'total_
z_score': 0.7128101606677049, 'drug_count': 2, 'average_z_score': 0.3564050803338524
3}), ('KS6B1 (p70S6K)', {'total_z_score': 0.6990975519028668, 'drug_count': 2, 'avera
ge_z_score': 0.3495487759514334}), ('LIMK1', {'total_z_score': 0.6156655835465211, 'd
rug_count': 2, 'average_z_score': 0.30783279177326056}), ('ALK5', {'total_z_score':
0.5957358825633687, 'drug_count': 2, 'average_z_score': 0.29786794128168437}), ('FGFR
4', {'total_z_score': 1.0735349567175085, 'drug_count': 4, 'average_z_score': 0.26838
373917937713}), ('IRAK1', {'total_z_score': 0.5029319080384665, 'drug_count': 2, 'ave
rage_z_score': 0.2514659540192333}), ('LCK', {'total_z_score': 2.0024528821504126, 'd
rug_count': 8, 'average_z_score': 0.2503066102688016}), (' BCL-W', {'total_z_score':
0.5880397657623906, 'drug_count': 3, 'average_z_score': 0.1960132552541302}), ('BCL-
B', {'total_z_score': 0.5880397657623906, 'drug_count': 3, 'average_z_score': 0.19601
32552541302}), ('BFL1', {'total_z_score': 0.5880397657623906, 'drug_count': 3, 'avera
ge_z_score': 0.1960132552541302}), ('Ephrins', {'total_z_score': 0.8689592264596184,
'drug_count': 5, 'average_z_score': 0.17379184529192368}), ('MAP4K2', {'total_z_scor
e': 0.34409510748251027, 'drug_count': 2, 'average_z_score': 0.17204755374125513}),
('IAP', {'total_z_score': 0.8361948434571232, 'drug_count': 9, 'average_z_score': 0.0
9291053816190259}), ('MCT4', {'total_z_score': 0.16767243758728545, 'drug_count': 2,
'average_z_score': 0.08383621879364273}), ('ERBB3', {'total_z_score': 0.4157056156569
172, 'drug_count': 5, 'average_z_score': 0.08314112313138344}), (' PDGFRA', {'total_z
_score': 0.12758807093754287, 'drug_count': 2, 'average_z_score': 0.0637940354687714
4}), ('SHP-1 (PTPN6)', {'total_z_score': 0.08775481514114958, 'drug_count': 2, 'avera
ge_z_score': 0.04387740757057479}), ('SHP-2 (PTPN11)', {'total_z_score': 0.0877548151
4114958, 'drug_count': 2, 'average_z_score': 0.04387740757057479}), ('PDGFRA', {'tota
l_z_score': 0.21935519562513095, 'drug_count': 5, 'average_z_score': 0.04387103912502
619}), ('EPHB4', {'total_z_score': 0.07688828931188812, 'drug_count': 4, 'average_z_s
core': 0.01922207232797203}), ('TRAIL receptor agonist', {'total_z_score': -0.0175356
37787329028, 'drug_count': 2, 'average_z_score': -0.008767818893664514}), ('TAK1',
{'total_z_score': -0.2416488148755438, 'drug_count': 6, 'average_z_score': -0.0402748
024792573}), ('IKK', {'total_z_score': -0.17829425474985633, 'drug_count': 4, 'averag
e_z_score': -0.04457356368746408}), ('PK3CG', {'total_z_score': -0.14931297565136853,
'drug_count': 2, 'average_z_score': -0.07465648782568426}), ('HDAC1-10', {'total_z_sc
ore': -0.1999115284744215, 'drug_count': 2, 'average_z_score': -0.0999557642372107
5}), ('PPARgamma', {'total_z_score': -0.236867747644269, 'drug_count': 2, 'average_z_
score': -0.1184338738221345}), ('PPARdelta', {'total_z_score': -0.236867747644269, 'd
rug_count': 2, 'average_z_score': -0.1184338738221345}), ('MNK1', {'total_z_score': -
0.2913846353346405, 'drug_count': 2, 'average_z_score': -0.14569231766732024}), ('MNK
2', {'total_z_score': -0.2913846353346405, 'drug_count': 2, 'average_z_score': -0.145
69231766732024}), ('dsDNA break induction', {'total_z_score': -1.7519493213381248, 'd
rug_count': 12, 'average_z_score': -0.1459957677817707}), ('PARP5a', {'total_z_scor
```

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('TGFB', {'total_z_score': -1.7309410559696143, 'drug_count': 1, 'average_z_score': -
1.7309410559696143}), ('ULK1', {'total_z_score': -5.2082605891348575, 'drug_count':
3, 'average_z_score': -1.7360868630449524}), ('Antimetabolite (DNA & RNA)', {'total_z
_score': -8.704862172812467, 'drug_count': 5, 'average_z_score': -1.740972434562493
3}), ('PPP1R15B', {'total_z_score': -5.243384438013174, 'drug_count': 3, 'average_z_s
core': -1.747794812671058}), ('PAK2', {'total_z_score': -5.34085333161303, 'drug_coun
t': 3, 'average_z_score': -1.7802844438710101}), ('BRD3', {'total_z_score': -30.32124
03376537, 'drug_count': 17, 'average_z_score': -1.7836023728031587}), ('NIK', {'total
_z_score': -5.388092295595326, 'drug_count': 3, 'average_z_score': -1.796030765198442
2}), ('BRD2', {'total_z_score': -36.70969246785452, 'drug_count': 20, 'average_z_scor
e': -1.8354846233927258}), ('S1P', {'total_z_score': -1.8492478791154008, 'drug_coun
t': 1, 'average_z_score': -1.8492478791154008}), ('Shh', {'total_z_score': -1.8575030
135205624, 'drug_count': 1, 'average_z_score': -1.8575030135205624}), ('DNA alkylatin
g agent', {'total_z_score': -20.683934443021624, 'drug_count': 11, 'average_z_score':
-1.8803576766383294}), ('NUAK1', {'total_z_score': -5.645235796578428, 'drug_count':
3, 'average_z_score': -1.8817452655261426}), ('NUAK2', {'total_z_score': -5.645235796
578428, 'drug_count': 3, 'average_z_score': -1.8817452655261426}), ('IDH2 R140Q mutan
t', {'total_z_score': -5.645933914975646, 'drug_count': 3, 'average_z_score': -1.8819
779716585485}), ('BRD4', {'total_z_score': -59.25666141382846, 'drug_count': 31, 'ave
rage_z_score': -1.9115052068976923}), ('KDM4A', {'total_z_score': -5.89881578869594,
'drug_count': 3, 'average_z_score': -1.9662719295653133}), ('KDM4C', {'total_z_scor
e': -5.89881578869594, 'drug_count': 3, 'average_z_score': -1.9662719295653133}), ('K
DM4E', {'total_z_score': -5.89881578869594, 'drug_count': 3, 'average_z_score': -1.96
62719295653133}), ('KDM3A', {'total_z_score': -5.89881578869594, 'drug_count': 3, 'av
erage_z_score': -1.9662719295653133}), ('BRD9', {'total_z_score': -11.80836508022428
3, 'drug_count': 6, 'average_z_score': -1.968060846704047}), ('CDK', {'total_z_scor
e': -1.9944746463128369, 'drug_count': 1, 'average_z_score': -1.9944746463128369}),
('CECR2', {'total_z_score': -6.388452130200821, 'drug_count': 3, 'average_z_score': -
2.1294840434002738}), ('VSP34', {'total_z_score': -6.628811130637253, 'drug_count':
3, 'average_z_score': -2.2096037102124177}), ('ACACA', {'total_z_score': -4.728463579
737365, 'drug_count': 2, 'average_z_score': -2.3642317898686827}), ('L3MBTL3', {'tota
l_z_score': -5.966245679795083, 'drug_count': 2, 'average_z_score': -2.98312283989754
16})]

In [34]:

```
target_df = pd.DataFrame(sorted_targets, columns=['Target', 'Metrics'])

target_df['Average_Z_Score'] = target_df['Metrics'].apply(lambda x: x['average_z_score
target_df['Drug_Count'] = target_df['Metrics'].apply(lambda x: x['drug_count'])

target_df.drop(['Metrics'], axis=1, inplace=True)

prefixes = set()
for target in target_df['Target']:
    for i in range(1, len(target)):
        prefix = target[:i]
        if any(other_target.startswith(prefix) for other_target in target_df['Target']
            prefixes.add(prefix)

def define_group(target):
    for prefix in sorted(prefixes, key=len, reverse=True):
        if target.startswith(prefix):
            return prefix
    return target

target_df['Group'] = target_df['Target'].apply(define_group)

aggregated_target_df = target_df.groupby('Group').agg({
    'Average_Z_Score': 'mean',
    'Drug_Count': 'sum'
```

```
}).reset_index()

aggregated_target_df.to_csv('Aggregated_Targets.csv', index=False)
print(aggregated_target_df)
```

```
           Group  Average_Z_Score  Drug_Count
0                        -0.749169           5
1              B         -1.676526           3
2           BCL-         -0.740256           6
3              A         -0.684700          30
4             AC         -2.364232           2
..           ...               ...         ...
157         mTOR         -1.062536           8
158        mTORC         -1.632148          10
159  not defined         -0.492752           4
160       others         -0.418350           8
161          p38         -1.162173          11

[162 rows x 3 columns]
```

In [35]:
```
print("Top 20 Targets by Average Z-Score:")
print(aggregated_target_df.sort_values(by='Average_Z_Score', ascending=False).head(20)
```

```
Top 20 Targets by Average Z-Score:
                     Group  Average_Z_Score  Drug_Count
78                      KS         0.349549           2
83                     MCT         0.234788           4
104                  PARP5         0.101944           4
130                   SHP-         0.043877           4
115                   PPAR        -0.118434           4
88                     MNK        -0.145692           4
154  dsDNA break induction        -0.145996          12
36                   DYRK1        -0.164770           5
18                      BC        -0.164923           2
20                    BCL-        -0.176218          34
14                    Anti        -0.226958           1
153                   cIAP        -0.232695           5
8                      ALK        -0.241644          13
105                  PDGFR        -0.258164          47
60                     IAP        -0.284543          15
103                   PARP        -0.298614          66
156        gamma-secretase        -0.309887           2
109                    PIK        -0.318043           4
112                    PKC        -0.344937           8
150                   XIAP        -0.348399           9
```

In [36]:
```
print("Top 20 Targets by Drug Count:")
print(aggregated_target_df.sort_values(by='Drug_Count', ascending=False).head(20))
```

```
Top 20 Targets by Drug Count:
     Group  Average_Z_Score  Drug_Count
7      AKT        -0.873587         101
23     BRD        -1.827917          81
29     CDK        -1.205253          70
103   PARP        -0.298614          66
86     MEK        -0.513478          60
107   PI3K        -0.976678          57
38      EG        -0.585990          54
49    FGFR        -0.621082          53
71     JAK        -1.375756          51
105  PDGFR        -0.258164          47
77      KI        -0.639288          43
55    HDAC        -0.874980          40
92   MTORC        -1.005075          39
147  VEGFR        -0.553514          38
99    NTRK        -0.935749          37
41    ERBB        -0.352906          36
11    AURK        -0.652512          36
50     FLT        -0.681538          36
127      S        -1.059467          35
20    BCL-        -0.176218          34
```

In [43]:

```python
data5 = pd.read_csv('receptors.csv')

mTOR_drugs = data5[data5['Targets'].str.contains('mTOR', case=False, na=False)]['Drug
AKT_drugs = data5[data5['Targets'].str.contains('AKT', case=False, na=False)]['Drug Na
PARP_drugs = data5[data5['Targets'].str.contains('PARP', case=False, na=False)]['Drug

mTOR_drugs_list = mTOR_drugs.tolist()
AKT_drugs_list = AKT_drugs.tolist()
PARP_drugs_list = PARP_drugs.tolist()

print('mTOR drugs:', mTOR_drugs_list)
print('AKT drugs:', AKT_drugs_list)
print('PARP drugs:', PARP_drugs_list)

max_length = max(len(mTOR_drugs_list), len(AKT_drugs_list), len(PARP_drugs_list))
mTOR_drugs_list.extend([None] * (max_length - len(mTOR_drugs_list)))
AKT_drugs_list.extend([None] * (max_length - len(AKT_drugs_list)))
PARP_drugs_list.extend([None] * (max_length - len(PARP_drugs_list)))

drug_data_1 = pd.DataFrame({
    'mTOR Drugs': mTOR_drugs_list,
    'AKT Drugs': AKT_drugs_list,
    'PARP Drugs': PARP_drugs_list
})

drug_data_1.to_csv('drug_lists.csv', index=False)
```

```
mTOR drugs: ['Voxtalisib', 'Dactolisib', 'Dactolisib', 'Dactolisib', 'Dactolisib', 'O
mipalisib', 'OSI-027', 'AZD8055', 'Dactolisib', 'OSI-027', 'AZD8055', 'Dactolisib',
'OSI-027', 'Dactolisib', 'AZD8055', 'Dactolisib', 'AZD8055', 'OSI-027', 'Omipalisib',
'AZD2014', 'AZD2014', 'AZD2014', 'AZD2014', 'Temsirolimus', 'Temsirolimus', 'JW-7-52-
1', 'Temsirolimus', 'Temsirolimus', 'Rapamycin', 'Rapamycin', 'Rapamycin', 'OSI-027',
'AZD8055', 'OSI-027', 'AZD8055', 'OSI-027', 'Rapamycin', 'AZD8055', 'AZD8055', 'OSI-0
27', 'Apitolisib', 'WYE-125132', 'Torin 2', 'CRT0105446', 'AZD2014', 'AZD2014', 'AZD2
014', 'AZD2014']
AKT drugs: ['Ipatasertib', 'Ipatasertib', 'Ipatasertib', 'MK-2206', 'GSK2110183B', 'B
AY AKT1', 'Uprosertib', 'Uprosertib', 'MK-2206', 'AKT inhibitor VIII', 'MK-2206', 'Af
uresertib', 'AZD5363', 'A-443654', 'AZD5363', 'GSK2110183B', 'Uprosertib', 'Uproserti
b', 'AKT inhibitor VIII', 'MK-2206', 'Uprosertib', 'Afuresertib', 'AZD5363', 'GSK2110
183B', 'GSK690693', 'Uprosertib', 'Afuresertib', 'GSK2110183B', 'BAY AKT1', 'Uprosert
ib', 'Uprosertib', 'AKT inhibitor VIII', 'Afuresertib', 'Ipatasertib', 'AZD5363', 'A-
443654', 'AZD5363', 'GSK2110183B', 'Ipatasertib', 'Uprosertib', 'Uprosertib', 'AKT in
hibitor VIII', 'Uprosertib', 'Afuresertib', 'AZD5363', 'GSK2110183B', 'GSK690693', 'I
patasertib', 'Uprosertib', 'Afuresertib', 'Capivasertib', 'AT7867', 'MK-2206', 'GSK21
10183B', 'BAY AKT1', 'Uprosertib', 'Uprosertib', 'MK-2206', 'AKT inhibitor VIII', 'MK
-2206', 'Afuresertib', 'Ipatasertib', 'AZD5363', 'A-443654', 'AZD5363', 'GSK2110183
B', 'AT13148', 'Ipatasertib', 'Uprosertib', 'Uprosertib', 'AKT inhibitor VIII', 'AT13
148', 'AT13148', 'MK-2206', 'Uprosertib', 'Afuresertib', 'AZD5363', 'GSK2110183B', 'G
SK690693', 'Ipatasertib', 'Uprosertib', 'Afuresertib']
PARP drugs: ['Rucaparib', 'Veliparib', 'Niraparib', 'Olaparib', 'Rucaparib', 'Nirapar
ib', 'Niraparib', 'Talazoparib', 'Veliparib', 'Veliparib', 'Talazoparib', 'Olaparib',
'Olaparib', 'PARP_0108', 'Veliparib', 'Olaparib', 'PARP_9482', 'Talazoparib', 'Rucapa
rib', 'Talazoparib', 'Rucaparib', 'Olaparib', 'PARP_9495', 'PARP_9482', 'TANK_1366',
'PARP_0108', 'PARP_9495', 'Rucaparib', 'Veliparib', 'Niraparib', 'Olaparib', 'Rucapar
ib', 'Niraparib', 'Niraparib', 'Talazoparib', 'Veliparib', 'Veliparib', 'Talazopari
b', 'Olaparib', 'Olaparib', 'PARP_0108', 'Veliparib', 'Olaparib', 'PARP_9482', 'Talaz
oparib', 'Rucaparib', 'Talazoparib', 'Rucaparib', 'Olaparib', 'PARP_9495', 'TANK_136
6']
```

In [53]:

```python
def process_pathway(pathway):

    pathway_data = data5[data5['Targets'].str.contains(pathway, case=False, na=False)]

    if pathway_data.empty:
        return pd.DataFrame(columns=['Drug Name', 'Z Score'])

    mean_z_scores = pathway_data.groupby('Drug Name')['Z Score'].mean().reset_index()

    return mean_z_scores

for pathway in ['mTOR', 'AKT', 'PARP']:
    mean_z_scores = process_pathway(pathway)

    mean_z_scores.to_csv(f'{pathway}_mean_z_scores.csv', index=False)

    print(f'Mean Z-Scores for {pathway} pathway:')
    print(mean_z_scores)
    print()
```

```
Mean Z-Scores for mTOR pathway:
       Drug Name   Z Score
0        AZD2014 -1.653557
1        AZD8055 -1.227507
2     Apitolisib -2.371608
3     CRT0105446  0.829741
4     Dactolisib -1.337519
5      JW-7-52-1 -1.300074
6        OSI-027 -1.084926
7     Omipalisib  1.098365
8      Rapamycin -2.297629
9   Temsirolimus -1.889939
10       Torin 2 -1.689402
11    Voxtalisib -2.940679
12    WYE-125132 -1.933757

Mean Z-Scores for AKT pathway:
             Drug Name   Z Score
0            A-443654 -1.198874
1   AKT inhibitor VIII -1.234553
2              AT13148 -0.803335
3               AT7867 -1.477580
4              AZD5363 -0.964885
5          Afuresertib -0.451088
6             BAY AKT1 -1.855045
7         Capivasertib -1.754816
8          GSK2110183B -1.026933
9            GSK690693  0.034443
10         Ipatasertib -0.746583
11             MK-2206 -1.442377
12          Uprosertib -0.954617

Mean Z-Scores for PARP pathway:
     Drug Name   Z Score
0    Niraparib -1.539296
1     Olaparib -0.328108
2    PARP_0108 -0.333051
3    PARP_9482 -0.132886
4    PARP_9495  1.481439
5    Rucaparib -0.756040
6    TANK_1366  0.941787
7  Talazoparib -0.466635
8    Veliparib -1.190144
```

In [60]:

```python
def process_pathway(pathway):
    pathway_data = data5[data5['Targets'].str.contains(pathway, case=False, na=False)]

    if pathway_data.empty:
        return pd.DataFrame(columns=['Drug Name', f'{pathway} Mean Z-Score'])

    mean_z_scores = pathway_data.groupby('Drug Name')['Z Score'].mean().reset_index()
    mean_z_scores.rename(columns={'Z Score': f'{pathway} Mean Z-Score'}, inplace=True)

    return mean_z_scores

combined_df = process_pathway('mTOR')

for pathway in ['AKT', 'PARP']:
    mean_z_scores = process_pathway(pathway)
```

```
    combined_df = pd.merge(combined_df, mean_z_scores, on='Drug Name', how='outer')

combined_df.to_csv('combined_mean_z_scores.csv', index=False)

print(combined_df)
```

	Drug Name	mTOR Mean Z-Score	AKT Mean Z-Score	PARP Mean Z-Score
0	AZD2014	-1.653557	NaN	NaN
1	AZD8055	-1.227507	NaN	NaN
2	Apitolisib	-2.371608	NaN	NaN
3	CRT0105446	0.829741	NaN	NaN
4	Dactolisib	-1.337519	NaN	NaN
5	JW-7-52-1	-1.300074	NaN	NaN
6	OSI-027	-1.084926	NaN	NaN
7	Omipalisib	1.098365	NaN	NaN
8	Rapamycin	-2.297629	NaN	NaN
9	Temsirolimus	-1.889939	NaN	NaN
10	Torin 2	-1.689402	NaN	NaN
11	Voxtalisib	-2.940679	NaN	NaN
12	WYE-125132	-1.933757	NaN	NaN
13	A-443654	NaN	-1.198874	NaN
14	AKT inhibitor VIII	NaN	-1.234553	NaN
15	AT13148	NaN	-0.803335	NaN
16	AT7867	NaN	-1.477580	NaN
17	AZD5363	NaN	-0.964885	NaN
18	Afuresertib	NaN	-0.451088	NaN
19	BAY AKT1	NaN	-1.855045	NaN
20	Capivasertib	NaN	-1.754816	NaN
21	GSK2110183B	NaN	-1.026933	NaN
22	GSK690693	NaN	0.034443	NaN
23	Ipatasertib	NaN	-0.746583	NaN
24	MK-2206	NaN	-1.442377	NaN
25	Uprosertib	NaN	-0.954617	NaN
26	Niraparib	NaN	NaN	-1.539296
27	Olaparib	NaN	NaN	-0.328108
28	PARP_0108	NaN	NaN	-0.333051
29	PARP_9482	NaN	NaN	-0.132886
30	PARP_9495	NaN	NaN	1.481439
31	Rucaparib	NaN	NaN	-0.756040
32	TANK_1366	NaN	NaN	0.941787
33	Talazoparib	NaN	NaN	-0.466635
34	Veliparib	NaN	NaN	-1.190144

In [64]:
```
from rdkit.Chem import AllChem
from rdkit import Chem
from rdkit.Chem import Descriptors
from rdkit.ML.Descriptors import MoleculeDescriptors

import numpy as np
from mordred import Calculator, descriptors
from chembl_webresource_client.new_client import new_client
```

In [65]:
```
compound_names = [
    "AZD2014", "AZD8055", "Apitolisib", "CRT0105446", "Dactolisib", "JW-7-52-1",
    "OSI-027", "Omipalisib", "Rapamycin", "Temsirolimus", "Torin 2", "Voxtalisib",
    "WYE-125132", "A-443654", "AKT inhibitor VIII", "AT-13148", "AT-7867", "AZD5363",
    "Afuresertib", "BAY AKT1", "Capivasertib", "GSK2110183B", "GSK690693",
    "Ipatasertib", "MK-2206", "Uprosertib", "Niraparib", "Olaparib", "PARP_0108",
    "PARP_9482", "PARP_9495", "Rucaparib", "TANK_1366", "Talazoparib", "Veliparib"
]
```

In [73]:

```
molecule = new_client.molecule

smiles_data = pd.DataFrame(columns=["Drug Name", "Canonical SMILES"])

for compound_name in compound_names:
    res = molecule.search(compound_name)

    if res:
        compound_info = res[0]

        if compound_info:
            molecule_structures = compound_info.get("molecule_structures")
            if molecule_structures:
                canonical_smiles = molecule_structures.get("canonical_smiles")

                smiles_data = smiles_data.append({
                    "Drug Name": compound_name,
                    "Canonical SMILES": canonical_smiles
                }, ignore_index=True)
            else:
                print(f"No molecule_structures found for {compound_name}")
        else:
            print(f"No data found for {compound_name}")
    else:
        print(f"No data found for {compound_name}")

smiles_data.to_csv("smiles_data.csv", index=False)


print(smiles_data)
```

```
No molecule_structures found for AZD8055
No molecule_structures found for Apitolisib
No data found for CRT0105446
No molecule_structures found for OSI-027
No molecule_structures found for Omipalisib
No molecule_structures found for Torin 2
No molecule_structures found for WYE-125132
No molecule_structures found for AT13148
No molecule_structures found for AT7867
No molecule_structures found for Afuresertib
No molecule_structures found for GSK690693
No molecule_structures found for Ipatasertib
No molecule_structures found for MK-2206
No molecule_structures found for Uprosertib
No data found for PARP_0108
No data found for PARP_9482
No data found for PARP_9495
No data found for TANK_1366
```

	Drug Name	Canonical SMILES
0	AZD2014	CNC(=O)c1cccc(-c2ccc3c(N4CCOC[C@@H]4C)nc(N4CCO...
1	Dactolisib	Cc1ccc(S(=O)(=O)O)cc1.Cn1c(=O)n(-c2ccc(C(C)(C)...
2	JW-7-52-1	O=C1Nc2ccccc2C12OCC1(CO2)COC2(OC1)C(=O)Nc1ccccc12
3	Rapamycin	CO[C@H]1C[C@@H]2CC[C@@H](C)[C@@](O)(O2)C(=O)C(...
4	Temsirolimus	CO[C@H]1C[C@@H]2CC[C@@H](C)[C@@](O)(O2)C(=O)C(...
5	Voxtalisib	CCn1c(=O)c(-c2cc[nH]n2)cc2c(C)nc(N)nc21
6	A-443654	Cc1n[nH]c2ccc(-c3cncc(OC[C@@H](N)Cc4c[nH]c5ccc...
7	AKT inhibitor VIII	O=c1[nH]c2ccccc2n1C1CCN(Cc2ccc(-c3[nH]c4cc5ncn...
8	AZD5363	NC1(C(=O)N[C@@H](CCO)c2ccc(Cl)cc2)CCN(c2nc[nH]...
9	BAY AKT1	Cc1cc(C)c(-n2ccn3nc(-c4cccnc4)cc23)cc1NC(=O)c1...
10	Capivasertib	NC1(C(=O)N[C@@H](CCO)c2ccc(Cl)cc2)CCN(c2nc[nH]...
11	GSK2110183B	Cl.Cn1ncc(Cl)c1-c1cc(C(=O)N[C@H](CN)Cc2cccc(F)...
12	Niraparib	NC(=O)c1cccc2cn(-c3ccc([C@@H]4CCCNC4)cc3)nc12
13	Olaparib	O=C(c1cc(Cc2n[nH]c(=O)c3ccccc23)ccc1F)N1CCN(C(...
14	Rucaparib	CNCc1ccc(-c2[nH]c3cc(F)cc4c3c2CCNC4=O)cc1
15	Talazoparib	Cn1ncnc1[C@H]1c2n[nH]c(=O)c3cc(F)cc(c23)N[C@@H...
16	Veliparib	C[C@]1(c2nc3c(C(N)=O)cccc3[nH]2)CCCN1

```
C:\Users\mkapt\AppData\Local\Temp\ipykernel_31676\1754174560.py:16: FutureWarning: Th
e frame.append method is deprecated and will be removed from pandas in a future versi
on. Use pandas.concat instead.
  smiles_data = smiles_data.append({
C:\Users\mkapt\AppData\Local\Temp\ipykernel_31676\1754174560.py:16: FutureWarning: Th
e frame.append method is deprecated and will be removed from pandas in a future versi
on. Use pandas.concat instead.
  smiles_data = smiles_data.append({
C:\Users\mkapt\AppData\Local\Temp\ipykernel_31676\1754174560.py:16: FutureWarning: Th
e frame.append method is deprecated and will be removed from pandas in a future versi
on. Use pandas.concat instead.
  smiles_data = smiles_data.append({
C:\Users\mkapt\AppData\Local\Temp\ipykernel_31676\1754174560.py:16: FutureWarning: Th
e frame.append method is deprecated and will be removed from pandas in a future versi
on. Use pandas.concat instead.
  smiles_data = smiles_data.append({
C:\Users\mkapt\AppData\Local\Temp\ipykernel_31676\1754174560.py:16: FutureWarning: Th
e frame.append method is deprecated and will be removed from pandas in a future versi
on. Use pandas.concat instead.
  smiles_data = smiles_data.append({
C:\Users\mkapt\AppData\Local\Temp\ipykernel_31676\1754174560.py:16: FutureWarning: Th
e frame.append method is deprecated and will be removed from pandas in a future versi
on. Use pandas.concat instead.
  smiles_data = smiles_data.append({
C:\Users\mkapt\AppData\Local\Temp\ipykernel_31676\1754174560.py:16: FutureWarning: Th
e frame.append method is deprecated and will be removed from pandas in a future versi
on. Use pandas.concat instead.
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C:\Users\mkapt\AppData\Local\Temp\ipykernel_31676\1754174560.py:16: FutureWarning: Th
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C:\Users\mkapt\AppData\Local\Temp\ipykernel_31676\1754174560.py:16: FutureWarning: Th
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  smiles_data = smiles_data.append({
C:\Users\mkapt\AppData\Local\Temp\ipykernel_31676\1754174560.py:16: FutureWarning: Th
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C:\Users\mkapt\AppData\Local\Temp\ipykernel_31676\1754174560.py:16: FutureWarning: Th
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C:\Users\mkapt\AppData\Local\Temp\ipykernel_31676\1754174560.py:16: FutureWarning: Th
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C:\Users\mkapt\AppData\Local\Temp\ipykernel_31676\1754174560.py:16: FutureWarning: Th
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on. Use pandas.concat instead.
  smiles_data = smiles_data.append({
```

```
C:\Users\mkapt\AppData\Local\Temp\ipykernel_31676\1754174560.py:16: FutureWarning: Th
e frame.append method is deprecated and will be removed from pandas in a future versi
on. Use pandas.concat instead.
  smiles_data = smiles_data.append({
C:\Users\mkapt\AppData\Local\Temp\ipykernel_31676\1754174560.py:16: FutureWarning: Th
e frame.append method is deprecated and will be removed from pandas in a future versi
on. Use pandas.concat instead.
  smiles_data = smiles_data.append({
```

In [74]:
```
data = pd.read_csv('smiles_data.csv')

akt_drugs_list = [
    "A-443654", "AKT inhibitor VIII", "AT13148", "AT7867", "AZD5363",
    "Afuresertib", "BAY AKT1", "Capivasertib", "GSK2110183B", "GSK690693",
    "Ipatasertib", "MK-2206", "Uprosertib"
]

akt_data = data[data['Drug Name'].isin(akt_drugs_list)]
akt_data.to_csv('akt_drugs.csv', index=False)
```

In [76]:
```
mtor_drugs = [
    "AZD2014",
    "AZD8055",
    "Apitolisib",
    "CRT0105446",
    "Dactolisib",
    "JW-7-52-1",
    "OSI-027",
    "Omipalisib",
    "Rapamycin",
    "Temsirolimus",
    "Torin 2",
    "Voxtalisib",
    "WYE-125132"
]
mtor_smiles_data = data[data['Drug Name'].isin(mtor_drugs)]
mtor_smiles_data.to_csv('mtor_drugs.csv', index=False)
```

In [77]:
```
parp_drugs = [
    "Niraparib",
    "Olaparib",
    "PARP_0108",
    "PARP_9482",
    "PARP_9495",
    "Rucaparib",
    "TANK_1366",
    "Talazoparib",
    "Veliparib"
]
parp_smiles_data = data[data['Drug Name'].isin(parp_drugs)]
parp_smiles_data.to_csv('parp_drugs.csv', index=False)
```

In [81]:
```
akt_data = pd.read_csv('akt_drugs.csv')

def RDkit_descriptors(smiles):
    mols = [Chem.MolFromSmiles(i) for i in smiles]
    calc = MoleculeDescriptors.MolecularDescriptorCalculator([x[0] for x in Descriptor
    desc_names = calc.GetDescriptorNames()
    Mol_descriptors = []
```

```
    for mol in mols:
        mol = Chem.AddHs(mol)
        descriptors = calc.CalcDescriptors(mol)
        Mol_descriptors.append(descriptors)
    return Mol_descriptors, desc_names

Mol_descriptors, desc_names = RDkit_descriptors(akt_data['Canonical SMILES'])

df_with_200_descriptors_akt = pd.DataFrame(Mol_descriptors, columns=desc_names)
df_with_200_descriptors_akt.to_csv('akt_descriptors.csv', index=False)
df_with_200_descriptors_akt
```

Out[81]:

	MaxEStateIndex	MinEStateIndex	MaxAbsEStateIndex	MinAbsEStateIndex	qed	MolWt	Heav
0	8.925933	-4.110077	8.925933	0.082105	0.396777	397.482	
1	13.792375	-4.510532	13.792375	0.184711	0.261050	551.654	
2	14.768705	-4.825164	14.768705	0.095096	0.476889	428.924	
3	14.145721	-11.220062	14.145721	0.218475	0.225291	558.536	
4	14.768705	-4.825164	14.768705	0.095096	0.476889	428.924	
5	14.621491	-4.218123	14.621491	0.161900	0.571782	463.793	
6	12.683225	-3.525434	12.683225	0.030695	0.468068	407.477	
7	8.589972	-3.674320	8.589972	0.198014	0.692988	313.788	

8 rows × 208 columns

In [83]:

```
data1 = pd.read_csv('akt_drugs.csv')

def morgan_fpts(smiles_data):
    Morgan_fpts = []
    for i in smiles_data:
        mol = Chem.MolFromSmiles(i)
        fpts =  AllChem.GetMorganFingerprintAsBitVect(mol,2,2048)
        mfpts = np.array(fpts)
        Morgan_fpts.append(mfpts)
    return np.array(Morgan_fpts)

Morgan_fpts = morgan_fpts(data1['Canonical SMILES'])
Morgan_fingerprints_akt = pd.DataFrame(Morgan_fpts,columns=['Col_{}'.format(i) for i i
Morgan_fingerprints_akt.to_csv('morgan_fingerprints_akt.csv', index=False)
Morgan_fingerprints_akt
```

Out[83]:

	Col_0	Col_1	Col_2	Col_3	Col_4	Col_5	Col_6	Col_7	Col_8	Col_9	...	Col_2038	Col_2039	Col_
0	0	1	0	0	0	0	0	0	0	0	...	0	0	
1	0	0	0	0	0	0	0	0	0	0	...	0	0	
2	0	1	0	0	0	0	0	0	0	0	...	0	0	
3	0	0	0	0	0	0	0	0	0	0	...	0	0	
4	0	1	0	0	0	0	0	0	0	0	...	0	0	
5	0	1	0	0	0	0	0	0	0	0	...	0	0	
6	0	0	0	0	0	0	0	0	0	1	...	0	0	
7	0	0	0	0	0	0	0	0	0	0	...	0	0	

8 rows × 2048 columns

In [85]:

```
data_mtor = pd.read_csv('mtor_drugs.csv')

def RDkit_descriptors(smiles):
    mols = [Chem.MolFromSmiles(i) for i in smiles]
    calc = MoleculeDescriptors.MolecularDescriptorCalculator([x[0] for x in Descriptor
    desc_names = calc.GetDescriptorNames()
    Mol_descriptors =[]
    for mol in mols:
        mol = Chem.AddHs(mol)
        descriptors = calc.CalcDescriptors(mol)
        Mol_descriptors.append(descriptors)
    return Mol_descriptors, desc_names

Mol_descriptors_mtor, desc_names_mtor = RDkit_descriptors(data_mtor['Canonical SMILES'

df_with_200_descriptors_mtor = pd.DataFrame(Mol_descriptors_mtor, columns=desc_names_m
df_with_200_descriptors_mtor.to_csv('mtor_descriptors.csv', index=False)
df_with_200_descriptors_mtor
```

Out[85]:

	MaxEStateIndex	MinEStateIndex	MaxAbsEStateIndex	MinAbsEStateIndex	qed	MolWt	Hea
0	13.215979	-4.344038	13.215979	0.624835	0.632373	462.554	
1	14.363054	-4.798796	14.363054	0.042962	0.202267	641.753	
2	13.458078	-4.250934	13.458078	0.186838	0.706043	394.383	
3	16.629391	-7.675282	16.629391	2.610034	0.155511	914.187	
4	16.883531	-7.949550	16.883531	2.716505	0.116173	1030.303	
5	13.401982	-3.576570	13.401982	0.070782	0.725310	270.296	

6 rows × 208 columns

In [87]:

```
def morgan_fpts(smiles):
    Morgan_fpts = []
    for i in smiles:
```

```
        mol = Chem.MolFromSmiles(i)
        fpts = AllChem.GetMorganFingerprintAsBitVect(mol, 2, 2048)
        mfpts = np.array(fpts)
        Morgan_fpts.append(mfpts)
    return np.array(Morgan_fpts)

Morgan_fpts_mtor = morgan_fpts(data_mtor['Canonical SMILES'])

Morgan_fingerprints_mtor = pd.DataFrame(Morgan_fpts_mtor, columns=['Col_{}'.format(i)
Morgan_fingerprints_mtor.to_csv('mtor_fingerprints.csv', index=False)
Morgan_fingerprints_mtor
```

Out[87]:

	Col_0	Col_1	Col_2	Col_3	Col_4	Col_5	Col_6	Col_7	Col_8	Col_9	...	Col_2038	Col_2039	Col_
0	0	0	0	0	0	0	0	0	0	0	...	0	0	
1	0	0	0	0	0	0	0	0	0	0	...	0	0	
2	0	0	0	0	0	0	0	0	0	0	...	0	0	
3	0	1	0	0	0	0	1	1	0	0	...	0	0	
4	0	1	0	0	0	1	1	1	0	0	...	0	0	
5	0	0	0	0	0	0	0	0	0	0	...	0	0	

6 rows × 2048 columns

In [88]:

```
data_parp = pd.read_csv('parp_drugs.csv')

def RDkit_descriptors(smiles):
    mols = [Chem.MolFromSmiles(i) for i in smiles]
    calc = MoleculeDescriptors.MolecularDescriptorCalculator([x[0] for x in Descriptor
    desc_names = calc.GetDescriptorNames()
    Mol_descriptors = []
    for mol in mols:
        mol = Chem.AddHs(mol)
        descriptors = calc.CalcDescriptors(mol)
        Mol_descriptors.append(descriptors)
    return Mol_descriptors, desc_names


Mol_descriptors_parp, desc_names_parp = RDkit_descriptors(data_parp['Canonical SMILES'

df_with_200_descriptors_parp = pd.DataFrame(Mol_descriptors_parp, columns=desc_names_p
df_with_200_descriptors_parp.to_csv('parp_descriptors.csv', index=False)
df_with_200_descriptors_parp
```

Out[88]:

	MaxEStateIndex	MinEStateIndex	MaxAbsEStateIndex	MinAbsEStateIndex	qed	MolWt	Heav
0	12.517046	-3.957997	12.517046	0.357732	0.778874	320.396	
1	15.918881	-4.443427	15.918881	0.339187	0.683092	434.471	
2	14.981622	-3.626891	14.981622	0.067114	0.693922	323.371	
3	15.150120	-3.612049	15.150120	0.009845	0.558167	380.358	
4	12.382471	-3.771370	12.382471	0.020458	0.743254	244.298	

5 rows × 208 columns

In [89]:

```
data_parp = pd.read_csv('parp_drugs.csv')

def morgan_fpts(smiles):
    Morgan_fpts = []
    for i in smiles:
        mol = Chem.MolFromSmiles(i)
        fpts =  AllChem.GetMorganFingerprintAsBitVect(mol,2,2048)
        mfpts = np.array(fpts)
        Morgan_fpts.append(mfpts)
    return np.array(Morgan_fpts)


Morgan_fpts_parp = morgan_fpts(data_parp['Canonical SMILES'])

Morgan_fingerprints_parp = pd.DataFrame(Morgan_fpts_parp, columns=['Col_{}'.format(i)
Morgan_fingerprints_parp.to_csv('parp_fingerprints.csv', index=False)
Morgan_fingerprints_parp
```

Out[89]:

	Col_0	Col_1	Col_2	Col_3	Col_4	Col_5	Col_6	Col_7	Col_8	Col_9	...	Col_2038	Col_2039	Col_
0	0	0	0	0	0	0	0	0	0	0	...	0	0	
1	0	0	0	0	0	0	0	0	0	0	...	0	0	
2	0	0	0	0	0	0	0	0	0	0	...	0	0	
3	0	0	0	0	0	0	0	0	0	0	...	0	0	
4	0	0	0	1	0	0	0	0	0	0	...	0	0	

5 rows × 2048 columns

In [93]:

```
akt_descriptors = pd.read_csv('akt_descriptors.csv')
akt_fingerprints = pd.read_csv('morgan_fingerprints_akt.csv')
akt_z_scores = pd.read_csv('AKT_mean_z_scores.csv')

selected_drugs = [
    'A-443654', 'AKT inhibitor VIII', 'AZD5363',
    'BAY AKT1', 'Capivasertib', 'GSK2110183B',
    'MK-2206', 'AT13148'
]
akt_z_scores = akt_z_scores[akt_z_scores['Drug Name'].isin(selected_drugs)]
```

```
akt_merged = pd.concat([akt_descriptors, akt_fingerprints, akt_z_scores], axis=1)
akt_merged.to_csv('akt_merged.csv', index=False)
```

In [94]:
```
mtor_descriptors = pd.read_csv('mtor_descriptors.csv')
mtor_fingerprints = pd.read_csv('mtor_fingerprints.csv')
mtor_z_scores = pd.read_csv('mTOR_mean_z_scores.csv')

selected_drugs_mtor = [
    'AZD2014', 'Dactolisib', 'JW-7-52-1',
    'Rapamycin', 'Temsirolimus', 'Voxtalisib'
]
mtor_z_scores = mtor_z_scores[mtor_z_scores['Drug Name'].isin(selected_drugs_mtor)]
mtor_merged = pd.concat([mtor_descriptors, mtor_fingerprints, mtor_z_scores], axis=1)
mtor_merged.to_csv('mtor_merged.csv', index=False)
```

In [95]:
```
parp_descriptors = pd.read_csv('parp_descriptors.csv')
parp_fingerprints = pd.read_csv('parp_fingerprints.csv')
parp_z_scores = pd.read_csv('PARP_mean_z_scores.csv')

selected_drugs_parp = [
    'Niraparib', 'Olaparib', 'Rucaparib',
    'Talazoparib', 'Veliparib'
]
parp_z_scores = parp_z_scores[parp_z_scores['Drug Name'].isin(selected_drugs_parp)]
parp_merged = pd.concat([parp_descriptors, parp_fingerprints, parp_z_scores], axis=1)
parp_merged.to_csv('parp_merged.csv', index=False)
```