With this homework, I practiced building multiple models on the command-line

- (1) Use multi-omics data from human cancer cell lines from the CCLE and GDSC databases.

- (2) Build the models on the CCLE dataset and evaluate the models on the GDSC dataset.

- (3) Benchmarking of different deep learning architectures and different combinations of omic data modalities used as input.

- (4) This jupyter notebook explores the best performing models.

In [1]:
```
import os
import glob
import flexynesis
import torch
import numpy as np
import seaborn as sns
import pandas as pd
import math
import random
import lightning as pl
from flexynesis import plot_dim_reduced
import matplotlib.pyplot as plt
from sklearn.decomposition import PCA
from IPython.display import display
```

```
Seed set to 42
```

Download and unpack the data: https://bimsbstatic.mdc-berlin.de/akalin/buyar/flexynesis-benchmark-datasets/ccle_vs_gdsc.tgz

In [2]:
```
if not os.path.exists("ccle_vs_gdsc"):
    !wget -O ccle_vs_gdsc.tgz "https://bimsbstatic.mdc-berlin.de/akalin/b
```

Use flexynesis on the command-line to predict drug responses for “Erlotinib”. Write a bash script to run the following experiments: Try a combination of:

a) different architectures: e.g. DirectPred, Supervised VAE, GNN (Test at least 2 of these).

b) data type combinations (e.g. mutation, mutation + rna, mutation + cnv) (Test at least 2 of these)

c) fusion methods: early, intermediate (applies only to tools other than GNN)

So, in total, you will run maximally 3 x 3 x 2 = 18 different flexynesis runs (and minimally 2 x 2 x 2 = 8 different runs).

Note: GNNs actually only support "early" fusion, so you can skip "intermediate" fusion for GNNs, but you can try different graph convolution options for GNNs. For GNNs, try "GC" and "SAGE" as different options in your experiment (See --gnn_conv_type argument).

Hint 1: Restrict your analysis to 5-10% of the features (use a combination of variance and laplacian score filtering).

Hint 2: It is okay to use few HPO iterations for this exercise (e.g. 15 iterations or so) (considering the resourse/time limits etc). The point of this exercise is not to find the perfect model, but to get an insight on the idea of benchmarking different setups.

In [3]:
```
data_importer = flexynesis.DataImporter(path ='ccle_vs_gdsc',
                                        data_types = ['mutation', 'rna',
                                        concatenate=False, top_percentile
                                       variance_threshold=0.5)
train_dataset, test_dataset = data_importer.import_data()
```

```
[INFO] ================= Importing Data =================
[INFO] Validating data folders...

[INFO] ----------------- Reading Data -----------------
[INFO] Importing ccle_vs_gdsc/train/mutation.csv...
[INFO] Importing ccle_vs_gdsc/train/clin.csv...
[INFO] Importing ccle_vs_gdsc/train/cnv.csv...
[INFO] Importing ccle_vs_gdsc/train/rna.csv...

[INFO] ----------------- Reading Data -----------------
[INFO] Importing ccle_vs_gdsc/test/mutation.csv...
[INFO] Importing ccle_vs_gdsc/test/clin.csv...
[INFO] Importing ccle_vs_gdsc/test/cnv.csv...
[INFO] Importing ccle_vs_gdsc/test/rna.csv...

[INFO] ----------------- Checking for problems with the input data
-----------------

[WARNING] Warnings:

[WARNING] 1. Warning: Some sample labels in train/clin.csv are missing in
train/cnv.csv: {'KP-1NL', 'IOMM-Lee', 'MKN45', 'DOV13', 'EW-8', 'UACC-62',
'HCC2108', 'TE 617.T', 'HCC2814', 'YD-8', 'HT115', 'OV56', 'NCI-H211', 'NC
I-H684', 'ESS-1', 'SaOS-2', 'LN-443', 'LK-2', 'LN-428', 'TE-1', 'HCC1833',
'LN-308', 'SLR24', 'Hs 255.T', 'ChaGo-K-1', 'CL-14', 'COLO 818', '253J-B
V', 'RS-5', 'BFTC-905', 'LN-340', '253J', 'SF8657', 'BICR 16', 'SNU-1066',
'T3M-10', 'HCC364', 'HCC1588', 'KMS-27', 'UM-UC-1', 'CH-157MN', 'MV4-11',
'MKN7', 'KP-1N', 'HCC2935', 'UOK101', 'LN-215', 'SNU-1033', 'SNU-245', '64
7V', 'SF767', 'CMK', 'LN-319', 'NU-DUL-1', 'THP-1', 'Hs 888.T', 'Hs 895.T'
, 'COLO 201', 'RMG-I', 'Evsa-T', 'MHH-CALL-3', 'KP-N-YN', 'IST-Mes2', 'HCC
827 GR5', 'MUTZ-3', 'TF-1', 'SNU-1041', 'HCC1438', 'COLO 677', 'LN-464',
'A-1207', 'LN-382', 'Rh18', 'NCI-H69', 'OCI-Ly10', 'VMRC-RCW', 'SK-RC-31',
'Caki-2', 'JeKo-1', 'M059J', 'SK-RC-20', 'JH-EsoAd1', 'HCT 8', 'SNU-5', 'B
GC-823', 'JJN-3', 'SNU-869', 'HCC827', 'HCC1806', 'ACCS', 'SNU-475', 'G
B-1', 'GLC-82', 'U-BLC1', 'SNU-626', 'MOLM-6', 'Hs 834.T', 'SNU-C2B', 'GaM
G', 'HCC1359', 'HEC-6', 'DFCI024', 'LN-235', 'T1-73', 'COLO 699', 'U-343MG
a', 'OC 315'}
[WARNING] 2. Warning: Some sample labels in train/clin.csv are missing in
train/rna.csv: {'KP-1NL', 'HN', 'SF8657', 'GLC-82', 'OE21', 'M059J', 'KP-1
N', 'JHUEM-7', 'DOV13', 'HRT-18', 'NCI-H2073', 'ACCS', 'SNU-C2B', 'COLO 69
9', 'BGC-823', 'MUTZ-3'}
[WARNING] 3. Warning: Some sample labels in test/clin.csv are missing in t
est/mutation.csv: {'RKN', 'WIL2 NS', 'OVMIU', 'NCI-N417', 'KYM-1', 'NCI-H3
255', 'NCI-ADR-RES', 'WERI-Rb-1', 'Ishikawa (Heraklio) 02 ER-', 'HARA [Hum
an squamous cell lung carcinoma]', 'JM-1', 'SUP-B15', 'NCI-H2731', 'SNU-6
1', 'NCC-IT-A3', 'Rh41', 'SNB-19', '201T', 'HeLaSF', 'JIMT-1', 'VAL', 'NC
I-H1435', 'COR-L51', 'Namalwa', 'TC-71', 'ESO-51', 'NCI-H660', 'SCCH-26',
'Kelly', 'KMS-11', 'AML-193', 'PC-3 [Human lung carcinoma]', 'NB4', 'KCL-2
2', 'KP-2', 'D556 Med', 'Hs 940.T', 'KYSE-30', 'ML-1 [Human thyroid carcin
oma]', 'STS-0421', 'KP-1N', 'NCI-H2085', 'KMH-2', 'NCC010', 'JHU-029', 'U
D-SCC-2', 'TE-4', 'TE 161.T', 'NCC021', 'PD1503a', 'BT-483', 'SNU-283', 'N
CI-H2373', 'TT2609-C02', 'NCI-H2110', 'SBC-3', 'GOTO.P3', 'CL-40', 'Karpa
s-231', 'OSC-20', 'VL51', 'IHH-4', 'Malme-3M', 'NCI-H2591', 'RC-K8', 'OACP
4 C', 'VMRC-RCW', 'LIM1215', 'CCK-81', 'KATO III', 'JJN-3', 'UPCI-SCC-09
0', 'SUP-HD1', 'HCC827', 'CL-11', 'LC-1/sq', 'HCC15', 'NCI-H1876', 'NB(T
U)1', 'ITO-II', 'PWR-1E', 'MS751', 'KOPN-8', 'JURL-MK1', 'K2 [Human melano
ma]', 'KTCTL-13', 'SUP-B8', 'WM35', 'DOV13', 'MOLM-16', 'SNU-81', 'COR-L9
5', 'NCC-IT', 'Jurkat E6.1', 'NCI-H889', 'SU-DHL-6', 'NCI-H211', 'QGP-1',
'Panc 04.03', 'OV-90', 'CAL-78', 'NCI-H2172', 'LS174T', 'SiSo', 'ESO-26',
'HuH-1', 'C8166', 'KTCTL-21', 'NCI-H2795', 'T.T', 'PL-21', 'RCH-ACV', 'NC
```

```
I-H2722', 'G-mel', 'MY-M12', 'COR-L32', 'CHSA0011', 'OACM5.1 C', 'KON', 'B
2-17', 'OVISE', '42-MG-BA', 'SUP-M2', 'OCUM-1', 'HCC366', 'WSU-DLCL2', 'NC
I-H2444', 'NCI-H196', 'OVK18', 'GA-10 clone 20', 'KTCTL-140', 'RF-48', 'C
S-1 [Human chondrosarcoma]', 'UWB1.289', 'NU-DUL-1', 'MOLM-13', 'EMC-BA
C-1', 'MUTZ-1', 'JHU-022', 'RERF-LC-Sq1', 'SNU-182', 'SNU-C5', 'P32/ISH',
'IGR-37', 'NCI-H2023', 'OCI-AML-3', 'NCI-H820', 'COR-L96-CAR', 'NH-6', 'JH
H-7', 'PCI-04B', 'GA-10 clone 4', 'OVTOKO', 'KTCTL-195', 'SU.86.86', 'SK-E
S-1', 'MOG-G-UVW', 'MOG-G-CCM', 'Panc 02.03', 'COR-L311', 'HCE-T', 'Fu97',
'MJ', 'Hs 939.T', 'TASK1', 'BICR 78', 'DiFi', 'MFE-319', 'TMK-1', 'NCI-H19
15', 'PaTu 8988t', 'BONNA-12', 'COLO 783', 'D-245MG', 'SKN-3', 'MCC13', 'H
CC44', 'COR-L321', 'TCO-1 [Human cervical carcinoma]', 'OV17R', 'GEO', 'KY
SE-50', 'OV56', 'TOV-21G', 'NCI-H2135', 'MHH-CALL-4', 'D-397MG', 'VMRC-MEL
G', 'JHOS-4', 'SUIT-2', 'HeLa', 'KMRC-1', 'Karpas-620', 'Hs 683', 'D384 Me
d', 'OSC-19', 'NCI-H1944', 'DAN-G', 'OCI-Ly19', 'G-292 clone A141B1', 'Hs
445', 'MM1.S', 'FLO-1', 'LOU-NH91', 'Granta-519', 'SNU-398', 'NCI-H290',
'CL-34', 'NCI-H1781', 'ROS-50', 'L-1236', 'HPAC', 'NALM-1', 'C-4-I', 'HC
C-56', 'MDST8', 'NB16', 'OCI-Ly7', 'SET-2', 'SU-DHL-4', 'Farage', 'HDQ-P
1', 'HuH-28', 'SU-DHL-16', 'SNU-407', 'NCI-H740', '380', 'NCI-H2803', 'CHS
A0108', 'PL18 [Human pancreatic adenocarcinoma]', 'NCI-H2869', 'KP-N-SI9
s', 'MDA-MB-435', 'SK-N-SH', 'D458 Med', 'SNU-175', 'NCI-H1836', 'CRO-AP
3', 'SK-N-BE(2)-M17', 'LS180', 'NCI-H841', 'GP2d', 'HCC202', 'MDA-MB-436',
'NCI-H647', 'RERF-GC-1B', 'PCI-30', 'HEY', 'OVKATE', 'RTSG', 'NCI-H2595',
'TOV-112D', 'KMS-12-PE', '451Lu', 'EN', 'SW1271', 'YMB-1-E', 'LN-229', 'AS
H-3', 'FU-OV-1', 'JHOS-3', 'MC-1010', 'OCI-M1', 'NCI-H2818', 'JHU-011', 'P
CI-38', 'SK-GT-4', 'ALL-SIL', 'Karpas-1106P', 'LNZTA3WT4', 'EJM', 'U-CH2',
'NCI-H3122', 'HuNS1', 'WM793', 'OUMS-23', 'OVCA433', 'HT115', 'TK [Human
B-cell lymphoma]', 'NCI-H2330', 'NCI-H2066', 'HSC-39', 'AMO1', 'PCI-06A',
'NCI-H2804', 'KTCTL-1M', 'PaTu 8902', 'JHH-1', 'Sarc9371', 'ES-2', 'Hs 746
.T', 'MCAS', 'LA-N-1', 'HuH-6 Clone 5', 'D-538MG', 'KTCTL-26A', 'CML-T1',
'SK-MEL-31', 'NCI-H1568', 'OV7', 'SU-DHL-10', 'NCI-H1341', 'SAT [Human HNS
CC]', 'OCI-AML-5', 'SNU-1040', 'NCI-H2810', 'NCI-H295', 'VMRC-LCD', 'OVCA4
20', 'Hep 3B2.1-7', 'NCI-H146', 'NCI-H157', 'COLO 720E', 'KMS-12-BM', 'HA
7-RCC', 'NCI-H508', 'HCC78', 'LA-N-5', 'C-4-II', 'NCI-H1105', 'NCI-H3118',
'NCI-H847', 'RERF-LC-FM', 'GA-10', 'MOLP-8', 'CAL-29', 'NCI-H2369', 'BICR
31', 'CHSA8926', 'NUGC-4', 'KP-3', 'HCC1428', 'NCI-H1869', 'WM1552C', 'L
N-18', 'NCI-H1688', 'NCI-H1930', 'JeKo-1', 'EFM-192A', 'NCI-H513', 'NCI-H9
29', 'PCI-15A', 'SCaBER', 'HCC1500', 'CRO-AP5', 'WM278', 'SW403', 'PE/CA-P
J15', 'JHH-6', 'CADO-ES1', 'NK-92MI', 'PL4', 'SU-DHL-8', 'MCC26', 'SK-G
T-2', 'HO-1-u-1', 'ME-1 [Human leukemia]', 'OE21', 'JSC-1', 'EMC-BAC-2', '
Hs 766T', 'COR-L303', 'IM95', 'RERF-LC-KJ', 'PEO1', 'KYSE-220', 'JHOS-2'}
[WARNING] 4. Warning: Some sample labels in test/clin.csv are missing in t
est/cnv.csv: {'DMS 153', 'PLC/PRF/5', 'HuNS1', 'M14', 'TCO-1 [Human cervic
al carcinoma]', 'NCI-N417', 'NCI-H889', 'NCI-H1648', 'Calu-1', 'SR', 'NCI-
ADR-RES', 'WERI-Rb-1', 'SCC-15', 'NCI-H2330', 'FTC-133', 'ES6', 'CPC-N',
'D-397MG', 'DV-90', 'ECC12', 'SBC-5', 'SNU-387', 'LS174T', 'BOKU', 'MC/CA
R', 'EC-GI-10', 'NCC-IT-A3', 'SNB-19', 'EoL-1', 'D384 Med', 'C8166', 'LA-
N-1', 'MDA-MB-175-VII', 'HeLaSF', 'NCI-H1522', 'D-538MG', 'RPMI-7951', 'CO
R-L51', 'SCCH-26', 'B2-17', 'NT2-D1', 'AML-193', 'NCI-H250', 'EFE-184', 'M
DA-MB-134-VI', 'J.RT3-T3.5', 'D556 Med', 'NCI-H295', 'NALM-1', 'KYSE-140',
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', 'LA-N-5', 'CP50-MEL-B', 'CAL-39', 'KYSE-150', 'HuH-28', 'OVCAR-4',
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'380', 'IPC-298', 'S-117', 'NCI-H719', 'COR-L96-CAR', 'LC-1F', 'GOTO.P3',
'NH-6', 'SJNB-13', 'KP-N-SI9s', 'MDA-MB-435', 'D458 Med', 'GA-10 clone 4',
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T', 'MDA-MB-231', 'CP66-MEL', 'ECC10', 'MC116', 'CRO-AP5', 'MJ', 'ECC4',
'DBTRG-05MG', 'NCI-H1618', 'GB-1', 'ITO-II', 'NCI-H2107', 'MCF-7', 'LS411N
', 'UACC-893', 'SCLC-21H', 'T1-73'}
[WARNING] 5. Warning: Some sample labels in test/clin.csv are missing in t
est/rna.csv: {'SW756', 'RKN', 'WIL2 NS', 'OVMIU', 'KYM-1', 'NCI-H3255', 'I
```

```
shikawa (Heraklio) 02 ER-', 'HARA [Human squamous cell lung carcinoma]',
'JM-1', 'SUP-B15', 'NCI-H2731', 'SNU-61', 'MC/CAR', 'Rh41', '201T', 'JIM
T-1', 'VAL', 'SNB-75', 'NCI-H1435', 'KLE', 'NCI-H322M', 'Namalwa', 'TC-7
1', 'ESO-51', 'NCI-H660', 'KMS-11', 'NCI-H1581', 'PC-3 [Human lung carcino
ma]', 'KCL-22', 'KP-2', 'Hs 940.T', 'KYSE-30', 'ML-1 [Human thyroid carcin
oma]', 'STS-0421', 'KP-1N', 'NCI-H2085', 'KMH-2', 'NCC010', 'JHU-029', 'U
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'CHP-126', 'NCI-H2373', 'NCI-H2110', 'TT2609-C02', 'SBC-3', 'NCI-H187', 'C
L-40', 'Karpas-231', 'OSC-20', 'VL51', 'IHH-4', 'RC-K8', 'NCI-H2591', 'OAC
P4 C', 'VMRC-RCW', '8305C', 'LIM1215', 'MLMA', 'CCK-81', 'JJN-3', 'UPCI-SC
C-090', 'SUP-HD1', 'HCC827', 'CL-11', 'LC-1/sq', 'HCC15', 'NCI-H1876', 'NB
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[Human melanoma]', 'KTCTL-13', 'TE 441.T', 'WM35', 'DOV13', 'MOLM-16', 'SN
U-81', 'COR-L95', 'NCC-IT', 'Jurkat E6.1', 'SU-DHL-6', 'NCI-H211', 'QG
P-1', 'Panc 04.03', 'OV-90', 'CAL-78', 'NCI-H2172', 'SiSo', 'ESO-26', 'Hu
H-1', 'KTCTL-21', 'NCI-H2795', 'T.T', 'PL-21', 'RCH-ACV', 'NCI-H2722', 'G-
mel', 'MY-M12', 'COR-L32', 'CHSA0011', 'KG-1', 'KON', 'OACM5.1 C', 'OVISE'
, '42-MG-BA', 'SUP-M2', 'OCUM-1', 'HCC366', 'WSU-DLCL2', 'NCI-H2444', 'NC
I-H196', 'OVK18', 'KTCTL-140', 'SK-PN-DW', 'CS-1 [Human chondrosarcoma]',
'UWB1.289', 'SH-4', 'NU-DUL-1', 'MOLM-13', 'EMC-BAC-1', 'JHU-022', 'RT-4',
'RERF-LC-Sq1', 'SNU-182', 'SNU-C5', 'P32/ISH', 'IGR-37', 'NCI-H2023', 'OC
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'NCI-H1915', 'PaTu 8988t', 'NCI-H128', 'NCI-H1734', 'G-402', 'COLO 783',
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V56', 'TOV-21G', 'AU565', 'NCI-H2135', 'LC-2/ad', 'JHOS-4', 'SUIT-2', 'HeL
a', 'KMRC-1', 'Karpas-620', 'Hs 683', 'OSC-19', 'ES4', 'NCI-H1944', 'DAN-
G', 'OCI-Ly19', 'G-292 clone A141B1', 'Hs 445', 'MM1.S', 'FLO-1', 'LOU-NH9
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y7', 'SET-2', 'SU-DHL-4', 'CP50-MEL-B', 'Farage', 'HDQ-P1', 'SU-DHL-16',
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a]', 'CHSA0108', 'NCI-H719', 'NCI-H2869', 'SK-N-SH', 'SNU-175', 'NCI-H183
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6', 'NCI-H647', 'RERF-GC-1B', 'PCI-30', 'HEY', 'OVKATE', 'TOV-112D', 'NCI-
H2595', '451Lu', 'EN', 'SW1271', 'ECC10', 'MC116', 'Ku812', 'YMB-1-E', 'L
N-229', 'ASH-3', 'HCC1569', 'GB-1', 'FU-OV-1', 'JHOS-3', 'OCI-M1', 'NCI-H2
818', 'JHU-011', 'PCI-38', 'SK-GT-4', 'MZ-PC-1', 'ALL-SIL', 'Karpas-1106
P', 'LNZTA3WT4', 'EJM', 'U-CH2', 'NCI-H3122', 'K-562', 'WM793', 'OUMS-23',
'OVCA433', 'HT115', 'NCI-H748', 'NCI-H1648', 'TK [Human B-cell lymphoma]',
'NCI-H2066', 'HSC-39', 'NCI-H1963', 'AMO1', 'PCI-06A', 'NCI-H2804', 'BT-47
4', 'KTCTL-1M', 'PaTu 8902', 'JHH-1', 'Sarc9371', 'ES-2', 'Hs 746.T', 'MCA
S', 'KTCTL-26A', 'SK-MEL-31', 'NCI-H1568', 'Lu-165', 'OV7', 'SU-DHL-10',
'NCI-H1341', 'SAT [Human HNSCC]', 'OCI-AML-5', 'SNU-1040', 'NCI-H2810', 'M
V4-11', 'VMRC-LCD', 'OVCA420', 'Hep 3B2.1-7', 'NCI-H2122', 'HCC78', 'NCI-H
3118', 'NCI-H847', 'GA-10', 'MOLP-8', 'A-388', 'CAL-29', 'SIG-M5', 'NCI-H2
369', 'BICR 31', 'CHSA8926', 'NUGC-4', 'KP-3', 'HCC1428', 'NCI-H1869', 'WM
1552C', 'LN-18', 'NCI-H1688', 'JeKo-1', 'EFM-192A', 'NCI-H513', 'NCI-H92
9', 'PCI-15A', 'SCaBER', 'HCC1500', 'WM278', 'YT', 'PE/CA-PJ15', 'JHH-6',
'CADO-ES1', 'NK-92MI', 'PL4', 'SU-DHL-8', 'MCC26', 'SK-GT-2', 'HO-1-u-1',
'ME-1 [Human leukemia]', 'UACC-893', 'OE21', 'JSC-1', 'EMC-BAC-2', 'Hs 766
T', 'COR-L303', 'IM95', 'RERF-LC-KJ', 'PEO1', 'KYSE-220', 'JHOS-2'}

[INFO] ----------------- Processing Data (train) -----------------

[INFO] ----------------- Cleaning Up Data -----------------

[INFO] working on layer:  mutation
[INFO] Imputing NA values to median of features, affected # of cells in th
```

```
e matrix 76760  # of rows: 808
[INFO] Number of NA values:  0
[INFO] DataFrame mutation - Removed 859 features.

[INFO] working on layer:  rna
[INFO] Number of NA values:  0
[INFO] DataFrame rna - Removed 9098 features.

[INFO] working on layer:  cnv
[INFO] Imputing NA values to median of features, affected # of cells in th
e matrix 19914  # of rows: 373
[INFO] Number of NA values:  0
[INFO] DataFrame cnv - Removed 11603 features.
[INFO] DataFrame mutation - Removed 3 samples (0.29%).
[INFO] DataFrame rna - Removed 3 samples (0.29%).
[INFO] DataFrame cnv - Removed 3 samples (0.32%).
[INFO] Implementing feature selection using laplacian score for layer: mut
ation with  808 features  and  935  samples
[INFO] No feature selection applied. Returning original matrix. Demanded #
of features is  larger than existing number of features
[INFO] Implementing feature selection using laplacian score for layer: rna
with  9098 features  and  935  samples
Calculating Laplacian scores: 100%|
| 9098/9098 [00:00<00:00, 12672.74it/s]
Filtering redundant features: 100%|
| 1000/1000 [00:00<00:00, 3395.59it/s]
[INFO] Implementing feature selection using laplacian score for layer: cnv
with  11304 features  and  935  samples
Calculating Laplacian scores: 100%|
| 11304/11304 [00:12<00:00, 921.57it/s]
Filtering redundant features: 100%|
| 1130/1130 [00:00<00:00, 45548.20it/s]
```

```
[INFO] ----------------- Processing Data (test) -----------------

[INFO] ----------------- Cleaning Up Data -----------------

[INFO] working on layer:  mutation
[INFO] Imputing NA values to median of features, affected # of cells in th
e matrix 1  # of rows: 1
[INFO] Number of NA values:  0
[INFO] DataFrame mutation - Removed 41 features.

[INFO] working on layer:  rna
[INFO] Number of NA values:  0
[INFO] DataFrame rna - Removed 5824 features.

[INFO] working on layer:  cnv
[INFO] Imputing NA values to median of features, affected # of cells in th
e matrix 19540  # of rows: 329
[INFO] Number of NA values:  0
[INFO] DataFrame cnv - Removed 11634 features.
[INFO] DataFrame mutation - Removed 61 samples (8.63%).
[INFO] DataFrame rna - Removed 53 samples (7.29%).
[INFO] DataFrame cnv - Removed 56 samples (5.79%).

[INFO] ----------------- Harmonizing Data Sets -----------------

[INFO] ----------------- Finished Harmonizing -----------------

[INFO] ----------------- Normalizing Data -----------------

[INFO] ----------------- Normalizing Data -----------------
[INFO] Training Data Stats:  {'feature_count in: rna': 689, 'feature_count
in: cnv': 989, 'feature_count in: mutation': 24, 'sample_count': 935}
[INFO] Test Data Stats:  {'feature_count in: rna': 689, 'feature_count in:
cnv': 989, 'feature_count in: mutation': 24, 'sample_count': 560}
[INFO] Merging Feature Logs...
[INFO] Data import successful.
```

Exploratory Data Analysis

In [4]:
```
train_dataset.dat, test_dataset.dat
```

Out[4]:
```
({'rna': tensor([[-0.0208, -0.3414, -0.4249,  ..., -0.2060, -0.3766,
0.6584],
          [-0.3612, -0.2744, -0.4973,  ..., -0.1911, -0.1769, -0.6552],
          [-0.3049, -0.2824, -0.3996,  ..., -0.3177, -0.2875, -0.6266],
          ...,
          [-0.1632, -0.3509, -0.4916,  ..., -0.2083, -0.0203, -0.6274],
          [-0.1413, -0.3829, -0.4328,  ..., -0.5116, -0.2376, -0.4091],
          [-0.3027, -0.2340, -0.4338,  ..., -0.2162,  0.1707, -0.478
9]]),
  'cnv': tensor([[ 0.7062,  0.3192,  0.7958,  ..., -0.7854,  0.0438,
-0.7831],
          [-0.8651, -0.8125, -0.8801,  ..., -0.5187, -0.8108, -0.5191],
          [ 0.1955,  0.0308,  0.3297,  ..., -1.7013,  0.1330, -1.6903],
          ...,
          [-0.4542, -0.5713, -0.4280,  ..., -0.1911, -0.3265, -0.1945],
          [ 0.0040,  0.9154,  0.0940,  ...,  0.6679,  0.9288,  0.6562],
          [ 0.7815, -0.4772, -1.1490,  ..., -0.4251, -2.4611, -0.426
3]]),
  'mutation': tensor([[-0.4054, -0.3480, -0.2249,  ..., -0.3142, -0.162
3,  0.7577],
          [-0.4054, -0.3480, -0.2249,  ...,  3.1829, -0.1623, -1.3198],
          [-0.4054, -0.3480, -0.2249,  ..., -0.3142, -0.1623, -1.3198],
          ...,
          [ 2.4664, -0.3480, -0.2249,  ..., -0.3142, -0.1623,  0.7577],
          [-0.4054, -0.3480,  4.4472,  ..., -0.3142, -0.1623,  0.7577],
          [-0.4054, -0.3480, -0.2249,  ..., -0.3142, -0.1623,  0.757
7]])},
 {'rna': tensor([[-0.0402,  0.1191, -0.5291,  ...,  0.5134,  0.4189,
-0.0526],
          [-0.2169,  0.0027, -0.6846,  ...,  0.6502,  0.7320, -0.3932],
          [-0.3680, -0.0615, -0.8491,  ...,  0.3458,  0.4300, -0.4533],
          ...,
          [-0.2175, -0.0195, -0.7529,  ...,  0.4056,  0.6370,  0.0419],
          [-0.1532, -0.0346, -0.7010,  ...,  0.8062,  0.5223, -0.2598],
          [-0.2513, -0.0108, -0.7570,  ...,  0.3753,  0.6749, -0.388
6]]),
  'cnv': tensor([[ 2.5704,  2.3923,  2.7841,  ..., -0.4740,  2.2923,
-0.4747],
          [ 1.9550, -0.8479,  2.1277,  ...,  0.7004, -0.8450,  0.6884],
          [ 0.6783,  1.1174,  0.7661,  ..., -1.1334,  0.9459, -1.1278],
          ...,
          [ 0.7536,  0.8703,  0.8464,  ...,  1.5410,  0.3306,  1.5210],
          [-0.9043, -0.7635, -0.9220,  ..., -0.4455, -0.7633, -0.4465],
          [ 0.8682,  0.7232,  0.8848,  ...,  1.0973,  0.9933,  1.081
5]]),
  'mutation': tensor([[-0.4054, -0.3480, -0.2249,  ..., -0.3142, -0.162
3,  0.7577],
          [-0.4054,  2.8736, -0.2249,  ..., -0.3142, -0.1623,  0.7577],
          [-0.4054, -0.3480, -0.2249,  ..., -0.3142, -0.1623, -1.3198],
          ...,
          [-0.4054, -0.3480, -0.2249,  ..., -0.3142, -0.1623,  0.7577],
          [-0.4054, -0.3480, -0.2249,  ...,  3.1829, -0.1623,  0.7577],
          [-0.4054, -0.3480, -0.2249,  ..., -0.3142, -0.1623,  0.757
7]])})
```

In [5]:
```
train_dataset.dat['mutation'].shape, train_dataset.dat['cnv'].shape, trai
```

Out[5]:
```
(torch.Size([935, 24]), torch.Size([935, 989]), torch.Size([935, 689]))
```

In [6]:
```
test_dataset.dat['mutation'].shape, test_dataset.dat['cnv'].shape, test_d
```

Out[6]:
```
(torch.Size([560, 24]), torch.Size([560, 989]), torch.Size([560, 689]))
```

In [7]:
```
train_dataset.samples[1:20], train_dataset.features
```

Out[7]:
```
(['COLO 704',
  'Hs 274.T',
  'B-CPAP',
  'NCI-H2452',
  'NCO2',
  'Hs 821.T',
  'RKN',
  'TEN',
  'DMS 153',
  'NCI-H596',
  'SW620',
  'EFM-19',
  'NCI-H1666',
  'KYM-1',
  'MKN74',
  'NCI-H3255',
  'HCC1395',
  'Ishikawa (Heraklio) 02 ER-',
  'JHUEM-3'],
 {'rna': Index(['SOX10', 'TNFRSF17', 'CD53', 'TCL1A', 'CD19', 'VPREB3',
'MLANA',
         'LGALS4', 'YAP1', 'BTK',
         ...
         'S100B', 'IKZF1', 'TYR', 'RAB25', 'PMEL', 'SLC45A2', 'SCG3', 'A
ZU1',
         'RAG1', 'HLA-DRA'],
        dtype='object', length=689),
  'cnv': Index(['GNAS-AS1', 'SNORA22', 'LINC01260', 'LUZP6', 'POLR2J2',
'HCK', 'NUPL2',
         'KIAA0586', 'RNASEH2C', 'ANKRD9',
         ...
         'PRSS58', 'GCH1', 'MIR4308', 'PLD4', 'AHNAK2', 'SUGCT', 'GPR6
8',
         'ITPK1', 'ZNHIT1', 'CCDC88C'],
        dtype='object', length=989),
  'mutation': Index(['APC', 'BRAF', 'CDH1', 'CDKN2A', 'CTNNB1', 'EGFR',
'FBXW7', 'KDM6A',
         'KRAS', 'MAP2K4', 'MLH1', 'MSH2', 'NF1', 'NF2', 'NOTCH1', 'NRA
S',
         'PIK3CA', 'PIK3R1', 'PTEN', 'RB1', 'SMAD4', 'SMARCA4', 'STK11',
'TP53'],
        dtype='object')})
```

In [8]:
```
test_dataset.samples[1:20], test_dataset.features
```

Out[8]:
```
(['B-CPAP',
  'NCI-H2452',
  'NCI-H596',
  'SW620',
  'EFM-19',
  'NCI-H1666',
  'OMC-1 [Human cervical carcinoma]',
  'HCC1395',
  'Lu-134-A',
  'ESS-1',
  'RCM-1 [Human rectum adenocarcinoma]',
  'NCI-H2052',
  'BB49-HNC',
  'UACC-257',
  'D-263MG',
  'NALM-6',
  'MZ-MEL-2',
  'AM-38',
  'OVCAR-8'],
 {'rna': Index(['SOX10', 'TNFRSF17', 'CD53', 'TCL1A', 'CD19', 'VPREB3',
'MLANA',
         'LGALS4', 'YAP1', 'BTK',
         ...
         'S100B', 'IKZF1', 'TYR', 'RAB25', 'PMEL', 'SLC45A2', 'SCG3', 'A
ZU1',
         'RAG1', 'HLA-DRA'],
        dtype='object', length=689),
  'cnv': Index(['GNAS-AS1', 'SNORA22', 'LINC01260', 'LUZP6', 'POLR2J2',
'HCK', 'NUPL2',
         'KIAA0586', 'RNASEH2C', 'ANKRD9',
         ...
         'PRSS58', 'GCH1', 'MIR4308', 'PLD4', 'AHNAK2', 'SUGCT', 'GPR6
8',
         'ITPK1', 'ZNHIT1', 'CCDC88C'],
        dtype='object', length=989),
  'mutation': Index(['APC', 'BRAF', 'CDH1', 'CDKN2A', 'CTNNB1', 'EGFR',
'FBXW7', 'KDM6A',
         'KRAS', 'MAP2K4', 'MLH1', 'MSH2', 'NF1', 'NF2', 'NOTCH1', 'NRA
S',
         'PIK3CA', 'PIK3R1', 'PTEN', 'RB1', 'SMAD4', 'SMARCA4', 'STK11',
'TP53'],
        dtype='object')})
```

In [9]:
```
train_dataset.ann
```

Out[9]:
```
{'Crizotinib': tensor([       nan,        nan,        nan, 2.4927e-02,
1.5810e-02, 3.1539e-01,
                nan, 1.5027e-02, 0.0000e+00,        nan,        nan, 1.0
264e-01,
         4.3664e-02, 2.0824e-02, 4.1460e-02, 0.0000e+00, 1.1192e-01, 0.0
000e+00,
         1.5148e-02,        nan,        nan, 5.8767e-02,        nan, 7.2
986e-03,
                nan,        nan, 0.0000e+00,        nan, 0.0000e+00,
nan,
         4.6343e-03,        nan,        nan, 5.2503e-02,        nan,
nan,
         2.6602e-02,        nan,        nan,        nan,        nan,
nan,
                nan,        nan, 3.4074e-02, 6.6740e-02, 2.6957e-01,
nan,
         1.2539e-01, 9.5140e-02,        nan, 1.4447e-02,        nan,
nan,
                nan,        nan, 1.3735e-02,        nan,        nan,
nan,
         1.0407e-01, 0.0000e+00, 2.0031e-02,        nan,        nan, 0.0
000e+00,
                nan, 0.0000e+00, 1.9905e-02,        nan, 3.5230e-02,
nan,
         3.8792e-02,        nan, 5.3306e-02, 4.0237e-02, 7.3804e-02, 2.6
462e-01,
         6.9279e-02, 1.5212e-02, 6.6552e-02,        nan,        nan, 0.0
000e+00,
         3.1578e-02,        nan,        nan, 2.3900e-01, 4.2099e-02, 2.6
464e-02,
                nan, 1.0601e-02,        nan, 4.3016e-02,        nan,
nan,
                nan, 8.8745e-02, 1.0592e-02, 2.5919e-03, 1.0572e-02, 6.6
150e-02,
                nan,        nan, 4.4803e-02,        nan,        nan,
nan,
         2.4201e-02,        nan,        nan,        nan,        nan, 1.9
586e-02,
                nan, 1.7947e-02,        nan, 1.7956e-02, 1.0154e-02, 1.6
169e-02,
                nan,        nan,        nan, 5.2924e-02, 5.4500e-03,
nan,
                nan,        nan,        nan,        nan, 4.8394e-02, 1.4
038e-01,
                nan,        nan,        nan, 2.2537e-02,        nan, 1.0
550e-02,
                nan, 0.0000e+00,        nan, 2.9930e-02, 3.6015e-02, 7.2
477e-02,
         8.0449e-03,        nan,        nan,        nan,        nan, 3.4
882e-02,
         4.0681e-02, 8.6601e-02, 0.0000e+00, 4.2998e-02,        nan,
nan,
                nan,        nan,        nan,        nan, 3.9493e-02, 4.3
364e-02,
         1.0232e-01,        nan,        nan,        nan, 1.1148e-01,
nan,
                nan, 5.4665e-02, 2.1003e-02,        nan,        nan,
nan,
         6.0332e-03,        nan,        nan, 3.7980e-02,        nan,
nan,
```

```
        6.5476e-02,        nan, 5.3854e-03,        nan,        nan, 1.6
194e-02,
               nan,        nan,        nan, 3.6860e-02,        nan, 6.6
986e-02,
        7.3939e-02,        nan, 1.3543e-01,        nan, 7.9504e-02,
nan,
               nan, 2.9640e-02,        nan, 9.1054e-03,        nan,
nan,
               nan, 1.2137e-01,        nan, 9.0245e-02, 6.8550e-02,
nan,
               nan, 8.9969e-02, 0.0000e+00,        nan, 9.3349e-02, 1.0
157e-02,
               nan,        nan, 8.7442e-02, 2.0691e-02,        nan, 1.9
136e-02,
        1.1262e-01, 3.0324e-02,        nan, 2.1585e-02, 1.8824e-02, 1.6
765e-02,
               nan,        nan,        nan,        nan, 7.5827e-02,
nan,
               nan,        nan,        nan, 2.8895e-02, 7.9667e-02,
nan,
        1.7940e-01,        nan, 2.0184e-02, 2.8050e-02,        nan, 0.0
000e+00,
        1.1849e-02,        nan, 0.0000e+00,        nan, 7.4971e-02,
nan,
        7.0804e-02, 5.1676e-02,        nan, 5.0374e-02, 1.4604e-02,
nan,
        3.6295e-02,        nan,        nan, 3.3994e-02,        nan, 1.9
549e-02,
               nan, 6.5340e-02,        nan,        nan,        nan,
nan,
        4.2129e-02,        nan, 4.2845e-02,        nan,        nan,
nan,
        4.3716e-02,        nan, 6.5293e-02,        nan, 7.3845e-02,
nan,
        2.9628e-02,        nan,        nan,        nan,        nan,
nan,
        2.6741e-02,        nan,        nan, 7.1612e-02,        nan, 1.4
609e-02,
               nan, 1.3157e-02, 2.9713e-02, 3.9443e-03, 1.3916e-01, 5.0
588e-02,
               nan, 1.8443e-01, 4.8498e-02, 7.4733e-02,        nan, 2.1
345e-03,
               nan,        nan, 7.3643e-02, 2.2609e-02,        nan,
nan,
        7.0189e-02, 0.0000e+00,        nan,        nan,        nan,
nan,
               nan,        nan,        nan, 5.1251e-02, 1.0335e-01,
nan,
        4.6535e-02,        nan,        nan,        nan, 4.2579e-02,
nan,
        1.4558e-02, 0.0000e+00,        nan,        nan,        nan, 3.7
887e-02,
               nan,        nan, 1.9563e-02,        nan, 2.8222e-02,
nan,
        2.1843e-02,        nan,        nan,        nan, 2.7937e-01,
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               nan, 5.5484e-02,        nan, 4.0625e-02, 5.8670e-02, 9.7
346e-03,
        1.6250e-02, 6.7953e-02,        nan, 2.8483e-02,        nan, 5.2
095e-02,
```

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                nan,        nan, 5.3985e-02,        nan, 0.0000e+00,
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                nan, 2.9732e-02,        nan, 4.6414e-02,        nan,
nan,
                nan, 9.3542e-02,        nan, 3.6225e-02, 1.1066e-01,
nan,
        5.8962e-02, 1.4255e-02, 1.2100e-02, 4.6026e-03,        nan, 3.1
363e-02,
        7.7346e-02,        nan, 2.9748e-02, 6.9612e-02,        nan, 1.4
803e-02,
                nan,        nan, 9.2848e-03,        nan,        nan, 8.1
892e-02,
        1.0044e-02, 1.6254e-02, 2.3456e-02, 1.4511e-02, 2.5283e-02, 3.9
785e-02,
                nan, 7.8923e-02, 5.6249e-02, 9.5728e-03,        nan, 1.2
751e-02,
                nan,        nan, 1.1135e-01,        nan,        nan, 2.6
292e-02,
                nan, 7.1696e-03, 2.8946e-02, 1.1484e-02, 2.8771e-02,
nan,
                nan, 3.5706e-01, 1.4547e-01,        nan, 5.5703e-02, 7.4
591e-02,
        0.0000e+00, 5.6117e-02,        nan,        nan,        nan, 1.0
288e-01,
                nan, 1.0568e-02, 3.4002e-02, 7.7410e-02, 2.6865e-02, 1.6
962e-02,
                nan, 7.9777e-02,        nan,        nan, 1.9542e-03, 7.3
080e-02,
        2.0987e-02, 5.3565e-02,        nan,        nan, 1.0518e-02, 1.1
418e-01,
        5.4500e-03,        nan,        nan,        nan,        nan,
nan,
                nan, 1.2795e-02, 0.0000e+00, 4.0183e-02,        nan, 0.0
000e+00,
                nan,        nan,        nan,        nan,        nan,
nan,
                nan, 1.9082e-02, 1.0438e-01,        nan,        nan,
nan,
        7.7776e-14,        nan, 1.2828e-02, 5.9465e-02, 7.1477e-02, 8.0
474e-03,
        0.0000e+00,        nan, 8.5628e-02, 8.7868e-02, 2.2866e-02,
nan,
                nan, 1.5911e-01,        nan, 1.4679e-02, 1.6844e-02,
nan,
                nan,        nan, 1.1950e-01, 2.6518e-02,        nan,
nan,
        3.8888e-02,        nan,        nan, 6.8732e-02, 5.9177e-02, 2.0
907e-02,
        4.6181e-02,        nan,        nan,        nan, 8.4947e-03,
nan,
                nan, 1.0835e-02,        nan, 3.2341e-02,        nan, 2.5
387e-02,
                nan,        nan, 1.1171e-01, 1.4451e-01,        nan,
nan,
```

```
               nan, 5.7785e-02, 2.1813e-02,        nan,        nan,
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nan,
               nan,        nan, 3.4646e-02,        nan,        nan, 1.0
639e-01,
               nan, 1.1211e-01,        nan, 3.3875e-02, 2.5890e-02,
nan,
               nan,        nan, 2.8134e-02, 0.0000e+00,        nan,
nan,
        2.0388e-02,        nan,        nan, 7.9382e-02,        nan,
nan,
        1.1031e-02, 2.2438e-02,        nan,        nan,        nan,
nan,
        1.5007e-01, 6.8697e-03, 2.3249e-02,        nan, 4.4105e-01,
nan,
        0.0000e+00,        nan,        nan, 3.8256e-02, 7.8115e-02, 0.0
000e+00,
        6.7685e-02,        nan,        nan,        nan, 1.7093e-01,
nan,
        4.1013e-02, 1.8887e-01,        nan,        nan, 5.5392e-02, 7.1
735e-02,
        4.3298e-02,        nan, 1.6214e-02,        nan,        nan, 1.1
390e-01,
               nan,        nan, 2.8212e-02, 2.8383e-02,        nan,
nan,
        1.5738e-02,        nan, 0.0000e+00,        nan,        nan, 2.2
417e-02,
               nan,        nan, 1.6770e-11, 2.3736e-02,        nan, 6.4
336e-03,
               nan,        nan,        nan,        nan, 6.3532e-02,
nan,
        5.5213e-02, 3.4295e-02, 2.0210e-02,        nan,        nan,
nan,
        3.3204e-02, 2.3526e-02, 7.6318e-02, 9.1580e-02,        nan, 0.0
000e+00,
        1.1473e-02, 1.8715e-01, 3.8909e-02, 1.5792e-02, 3.3004e-02, 1.4
309e-02,
               nan,        nan,        nan, 4.6166e-03,        nan,
nan,
        8.1937e-02, 2.1047e-02,        nan, 8.0364e-02,        nan, 5.8
808e-02,
        2.4615e-02,        nan,        nan,        nan, 3.7503e-02,
nan,
        5.5094e-02, 4.5938e-02,        nan, 5.2248e-02,        nan,
nan,
        0.0000e+00, 1.2746e-02, 2.7480e-01, 0.0000e+00,        nan,
nan,
               nan, 1.6000e-02,        nan, 0.0000e+00, 4.5768e-02, 1.7
889e-02,
        2.1169e-02, 1.2429e-01, 9.7134e-03,        nan,        nan, 3.6
069e-03,
        6.1220e-02, 4.2340e-02,        nan, 4.1552e-02,        nan,
nan,
               nan,        nan, 2.8747e-01, 5.7746e-02,        nan, 3.2
154e-02,
               nan,        nan, 6.0789e-03,        nan,        nan, 1.5
608e-02,
```

```
               nan, 3.1143e-02,        nan,        nan,        nan,
nan,
               nan, 4.0493e-02,        nan, 9.4153e-02, 5.8741e-02,
nan,
               nan, 8.3219e-02,        nan, 3.6584e-03,        nan, 7.7
494e-02,
        7.8838e-02, 5.8099e-02, 2.3817e-01,        nan, 5.0708e-02, 1.1
794e-02,
        6.5048e-03, 2.3098e-02,        nan, 2.3679e-02,        nan, 3.6
863e-02,
        1.5603e-02,        nan, 1.7811e-02, 4.4544e-01, 0.0000e+00, 4.2
602e-02,
               nan,        nan, 0.0000e+00, 6.6314e-02, 2.2592e-01, 1.5
085e-02,
               nan, 6.1436e-03, 2.5789e-02,        nan,        nan,
nan,
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nan,
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0.3215,
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0.1161,
           nan,    nan,    nan, 0.4512,    nan, 0.4791, 0.1648, 0.6755,
nan,
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0.2814,
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0.0495,
        0.0847,    nan,    nan,    nan,    nan,    nan,    nan, 0.1265,
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0.0624,
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0.1137,
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,  7.,
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In [10]:
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flexynesis.print_summary_stats(train_dataset)
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Summary for variable: Crizotinib
Numerical Variable Summary: Median = 0.0348820359866738, Mean = 0.05367918
925271896
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Summary for variable: Dovitinib
Numerical Variable Summary: Median = 0.0747548468378515, Mean = 0.08868079
986988005
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Summary for variable: Erlotinib
Numerical Variable Summary: Median = 0.0401425137728223, Mean = 0.06560994
516154504
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Summary for variable: Irinotecan
Numerical Variable Summary: Median = 0.3920620379485415, Mean = 0.38968231
036548984
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Summary for variable: L-685458
Numerical Variable Summary: Median = 0.0144951759575499, Mean = 0.03070823
3328112813
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Summary for variable: Lapatinib
Numerical Variable Summary: Median = 0.0390705370047462, Mean = 0.06683012
778667083
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Summary for variable: LBW242
Numerical Variable Summary: Median = 0.0547794573417837, Mean = 0.07822785
863411183
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Summary for variable: Nilotinib
Numerical Variable Summary: Median = 0.0296334712782784, Mean = 0.05127125
47926707
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Summary for variable: Nutlin-3
Numerical Variable Summary: Median = 0.02887548099037655, Mean = 0.0382131
4938196926
------
Summary for variable: Nvp-aew541
Numerical Variable Summary: Median = 0.08536779367827185, Mean = 0.1054708
2695911461
------
Summary for variable: Nvp-tae 684
Numerical Variable Summary: Median = 0.113250919137906, Mean = 0.133551583
34062392
------
Summary for variable: Paclitaxel
Numerical Variable Summary: Median = 0.7024549570648385, Mean = 0.68550655
25644032
------
Summary for variable: Palbociclib
Numerical Variable Summary: Median = 0.0514853892367603, Mean = 0.06758314
475498992
------
Summary for variable: Panobinostat
Numerical Variable Summary: Median = 0.579730990993632, Mean = 0.587535053
3648767
------
Summary for variable: PD-0325901
Numerical Variable Summary: Median = 0.210611029735158, Mean = 0.258129052
7645829
------
```

```
Summary for variable: Pha-665752
Numerical Variable Summary: Median = 0.0285848706863142, Mean = 0.04603632
441340321
------
Summary for variable: PLX4720
Numerical Variable Summary: Median = 0.0175275051401726, Mean = 0.04373662
688995133
------
Summary for variable: Raf265(chir-265)
Numerical Variable Summary: Median = 0.171325890850019, Mean = 0.177927035
56795297
------
Summary for variable: Saracatinib
Numerical Variable Summary: Median = 0.081563188355603, Mean = 0.098159203
51291245
------
Summary for variable: Selumetinib
Numerical Variable Summary: Median = 0.12481214197078, Mean = 0.1646180651
4609872
------
Summary for variable: Sorafenib
Numerical Variable Summary: Median = 0.0150700837472094, Mean = 0.02800836
756646312
------
Summary for variable: Tanespimycin
Numerical Variable Summary: Median = 0.418851454650132, Mean = 0.420476989
8479707
------
Summary for variable: Topotecan
Numerical Variable Summary: Median = 0.353837474649707, Mean = 0.354359686
28481546
------
Summary for variable: Vandetanib
Numerical Variable Summary: Median = 0.0995465385663049, Mean = 0.11613698
597641095
------
Summary for variable: tissueid
Categorical Variable Summary:
  Label: Ampulla of Vater, Count: 1
  Label: Biliary Tract, Count: 5
  Label: Bladder/Urinary Tract, Count: 22
  Label: Bone, Count: 23
  Label: Bowel, Count: 55
  Label: Breast, Count: 57
  Label: CNS/Brain, Count: 53
  Label: Esophagus/Stomach, Count: 60
  Label: Head and Neck, Count: 30
  Label: Kidney, Count: 29
  Label: Liver, Count: 25
  Label: Lung, Count: 166
  Label: Lymphoid, Count: 119
  Label: Myeloid, Count: 47
  Label: Other, Count: 5
  Label: Ovary/Fallopian Tube, Count: 49
  Label: Pancreas, Count: 45
  Label: Peripheral Nervous System, Count: 16
  Label: Pleura, Count: 9
  Label: Prostate, Count: 8
  Label: Skin, Count: 57
  Label: Soft Tissue, Count: 14
```

```
  Label: Thyroid, Count: 13
  Label: Uterus, Count: 27
------
```

In [11]:
```
flexynesis.print_summary_stats(test_dataset)
```

```
Summary for variable: (2R,6aS,12aS)-2-Isopropyl-8,9-dimethoxy-1,2,12,12a-t
etrahydrochromeno[3,4-b]furo[2,3-h]chromen-6(6aH)-one
Numerical Variable Summary: Median = 0.137673879066792, Mean = 0.159211630
01570104
------
Summary for variable: (5R,5aR,8aR)-9-Bromo-5-(3,4,5-trimethoxypheny
l)-5,8,8a,9-tetrahydrofuro[3',4':6,7]naphtho[2,3-d][1,3]dioxol-6(5aH)-one
Numerical Variable Summary: Median = 0.192777551603734, Mean = 0.194352971
25740514
------
Summary for variable: 1,3-Bis(2-chloroethyl)-1-nitrosourea
Numerical Variable Summary: Median = 0.0082343323580145, Mean = 0.02037577
440306922
------
Summary for variable: 2-fluoroAraA (fludarabine)
Numerical Variable Summary: Median = 0.0321679832898623, Mean = 0.07052042
918700793
------
Summary for variable: 2-Pyridinecarboxylic acid
Numerical Variable Summary: Median = 0.03230051266080725, Mean = 0.0371784
7227732785
------
Summary for variable: 2H-Indol-2-one, 3,3-bis[4-(acetyloxy)phenyl]-1,3-dih
ydro-
Numerical Variable Summary: Median = 0.035339022156573655, Mean = 0.119453
17799052205
------
Summary for variable: 5-Fluorouracil
Numerical Variable Summary: Median = 0.07126794671261805, Mean = 0.0886336
3743432202
------
Summary for variable: 681640
Numerical Variable Summary: Median = 0.12662899337835798, Mean = 0.1466487
1591791448
------
Summary for variable: Abt-737
Numerical Variable Summary: Median = 0.165004506242306, Mean = 0.217655012
18058061
------
Summary for variable: Adavosertib
Numerical Variable Summary: Median = 0.285982692816003, Mean = 0.302392278
99901705
------
Summary for variable: Afatinib
Numerical Variable Summary: Median = 0.13876149157029, Mean = 0.1781418142
7262513
------
Summary for variable: Afuresertib
Numerical Variable Summary: Median = 0.1679609546952085, Mean = 0.18833065
12221515
------
Summary for variable: AGI-5198
Numerical Variable Summary: Median = 0.0679615486856224, Mean = 0.06723030
897393395
------
Summary for variable: AGI-6780
Numerical Variable Summary: Median = 0.0592344239954875, Mean = 0.06223544
685338492
------
Summary for variable: Alisertib
```

```
Numerical Variable Summary: Median = 0.130837634051094, Mean = 0.167224602
8388208
------
Summary for variable: Alpelisib
Numerical Variable Summary: Median = 0.04815732992382665, Mean = 0.0600300
5774342829
------
Summary for variable: AMG-319
Numerical Variable Summary: Median = 0.0294939330030171, Mean = 0.04198020
510782494
------
Summary for variable: Aminofurazanyl-azabenzimidazole 6n
Numerical Variable Summary: Median = 0.109202954629959, Mean = 0.126984643
98976225
------
Summary for variable: AT13148
Numerical Variable Summary: Median = 0.07008470391144955, Mean = 0.0846575
3237420244
------
Summary for variable: Axitinib
Numerical Variable Summary: Median = 0.0874749017302966, Mean = 0.09429443
221114304
------
Summary for variable: AZ6102
Numerical Variable Summary: Median = 0.0909220727240594, Mean = 0.10144304
516019803
------
Summary for variable: AZ960
Numerical Variable Summary: Median = 0.186811086432691, Mean = 0.201079804
29000508
------
Summary for variable: AZD1208
Numerical Variable Summary: Median = 0.0088841617903957, Mean = 0.02232247
197281744
------
Summary for variable: AZD1332
Numerical Variable Summary: Median = 0.0520963604259877, Mean = 0.07121663
719313022
------
Summary for variable: AZD2014
Numerical Variable Summary: Median = 0.185847255081387, Mean = 0.189098606
5841021
------
Summary for variable: AZD3759
Numerical Variable Summary: Median = 0.0493469648615842, Mean = 0.05602630
953863077
------
Summary for variable: Azd4547
Numerical Variable Summary: Median = 0.0441379749843096, Mean = 0.05876369
4594327204
------
Summary for variable: AZD5153
Numerical Variable Summary: Median = 0.259018297480865, Mean = 0.286237931
20394353
------
Summary for variable: AZD5363
Numerical Variable Summary: Median = 0.128220138219499, Mean = 0.143724895
2593584
------
Summary for variable: AZD5438
```

```
Numerical Variable Summary: Median = 0.1242695279942605, Mean = 0.13130596
111785248
------
Summary for variable: AZD5582
Numerical Variable Summary: Median = 0.107782509250554, Mean = 0.179522820
46314924
------
Summary for variable: AZD5991
Numerical Variable Summary: Median = 0.0110089501588448, Mean = 0.11358533
499419965
------
Summary for variable: AZD6482
Numerical Variable Summary: Median = 0.0932121757683784, Mean = 0.14377360
907686
------
Summary for variable: AZD6738
Numerical Variable Summary: Median = 0.16924468806743348, Mean = 0.1754659
158433335
------
Summary for variable: AZD7762
Numerical Variable Summary: Median = 0.3369458930845335, Mean = 0.35518420
032657916
------
Summary for variable: AZD8055
Numerical Variable Summary: Median = 0.212114814805803, Mean = 0.206938647
19834698
------
Summary for variable: AZD8186
Numerical Variable Summary: Median = 0.113197037821832, Mean = 0.132874616
11341733
------
Summary for variable: BDP-00009066
Numerical Variable Summary: Median = 0.09952290445278705, Mean = 0.1108817
6547678175
------
Summary for variable: BI-2536
Numerical Variable Summary: Median = 0.41979450728111145, Mean = 0.4387851
1328692527
------
Summary for variable: BIBR-1532
Numerical Variable Summary: Median = 0.036634433496126204, Mean = 0.048060
18816692138
------
Summary for variable: BMS-345541 free base
Numerical Variable Summary: Median = 0.0634836207410898, Mean = 0.07174193
751035776
------
Summary for variable: Bms-754807
Numerical Variable Summary: Median = 0.3179233165153445, Mean = 0.38319744
4258751
------
Summary for variable: Bortezomib
Numerical Variable Summary: Median = 0.1737528386571065, Mean = 0.17365221
68877125
------
Summary for variable: BPD-00008900
Numerical Variable Summary: Median = 0.0639612712968786, Mean = 0.06854094
040768992
------
Summary for variable: Buparlisib
```

```
Numerical Variable Summary: Median = 0.24561796331874802, Mean = 0.2464717
1539538093
------
Summary for variable: Camptothecin
Numerical Variable Summary: Median = 0.139344783080692, Mean = 0.162343597
92617148
------
Summary for variable: Carbamic acid, N,N'-(1,2,3,4-tetrahydro-6,7,8-trimet
hoxy-4-oxo-2-quinazolinylidene)bis-, dimethyl ester
Numerical Variable Summary: Median = 0.03061011953821045, Mean = 0.0429463
1767765323
------
Summary for variable: CDK9_5038
Numerical Variable Summary: Median = 0.49361815746772697, Mean = 0.4894003
7117712426
------
Summary for variable: CDK9_5576
Numerical Variable Summary: Median = 0.402751480576129, Mean = 0.399207366
65438394
------
Summary for variable: Cediranib
Numerical Variable Summary: Median = 0.113045711493415, Mean = 0.126747289
5487129
------
Summary for variable: Cisplatin
Numerical Variable Summary: Median = 0.0452709817981214, Mean = 0.06258708
619389618
------
Summary for variable: Crizotinib
Numerical Variable Summary: Median = 0.022591880530659, Mean = 0.036520107
6905007
------
Summary for variable: Cyclophosphamide
Numerical Variable Summary: Median = 0.0165513286418755, Mean = 0.02784069
1555297285
------
Summary for variable: Cytarabine
Numerical Variable Summary: Median = 0.0985125647297326, Mean = 0.14482692
884051887
------
Summary for variable: CZC24832
Numerical Variable Summary: Median = 0.02262950891832785, Mean = 0.0327198
1612293745
------
Summary for variable: Dabrafenib
Numerical Variable Summary: Median = 0.0378018636648292, Mean = 0.07371340
44213426
------
Summary for variable: Dactinomycin
Numerical Variable Summary: Median = 0.623115021413368, Mean = 0.610720043
3010896
------
Summary for variable: Dactolisib
Numerical Variable Summary: Median = 0.1701141530495485, Mean = 0.17404734
378627107
------
Summary for variable: Daporinad
Numerical Variable Summary: Median = 0.3166049171189555, Mean = 0.34493796
326143406
------
```

```
Summary for variable: Dasatinib
Numerical Variable Summary: Median = 0.106995282501268, Mean = 0.142382653
55681484
------
Summary for variable: Dinaciclib
Numerical Variable Summary: Median = 0.409717665060277, Mean = 0.403186280
3843454
------
Summary for variable: Docetaxel
Numerical Variable Summary: Median = 0.153945128163699, Mean = 0.164325046
63100264
------
Summary for variable: Doramapimod
Numerical Variable Summary: Median = 0.024591269921731, Mean = 0.032172645
41870581
------
Summary for variable: Eg5_9814
Numerical Variable Summary: Median = 0.222056116016654, Mean = 0.232174106
19978163
------
Summary for variable: Elephantin
Numerical Variable Summary: Median = 0.09758446028264339, Mean = 0.1082963
5080240023
------
Summary for variable: Entinostat
Numerical Variable Summary: Median = 0.108252874141887, Mean = 0.133900859
86473585
------
Summary for variable: Entospletinib
Numerical Variable Summary: Median = 0.0867402327328646, Mean = 0.08997669
123422676
------
Summary for variable: Epirubicin
Numerical Variable Summary: Median = 0.2042371543372995, Mean = 0.23042549
89938525
------
Summary for variable: EPZ004777
Numerical Variable Summary: Median = 0.0301993749890132, Mean = 0.03644847
494731088
------
Summary for variable: EPZ5676
Numerical Variable Summary: Median = 0.014078723749542651, Mean = 0.019729
37353458294
------
Summary for variable: ERK_2440
Numerical Variable Summary: Median = 0.149743683350577, Mean = 0.165164738
03550902
------
Summary for variable: ERK_6604
Numerical Variable Summary: Median = 0.115181432888578, Mean = 0.130366943
0344123
------
Summary for variable: Erlotinib
Numerical Variable Summary: Median = 0.063671450526157, Mean = 0.075696420
7850125
------
Summary for variable: Foretinib
Numerical Variable Summary: Median = 0.229865396134536, Mean = 0.248703069
4720553
------
```

```
Summary for variable: Fulvestrant
Numerical Variable Summary: Median = 0.03192612588573675, Mean = 0.0352385
61386565094
------
Summary for variable: GDC0810
Numerical Variable Summary: Median = 0.02966284702109085, Mean = 0.0401036
04221934264
------
Summary for variable: Gefitinib
Numerical Variable Summary: Median = 0.0358360006728427, Mean = 0.05029654
1081314344
------
Summary for variable: Gemcitabine
Numerical Variable Summary: Median = 0.418912494419359, Mean = 0.457717193
88297644
------
Summary for variable: GNE-317
Numerical Variable Summary: Median = 0.3174731988021, Mean = 0.32194241945
548985
------
Summary for variable: GSK-1904529A
Numerical Variable Summary: Median = 0.0641124717038122, Mean = 0.06879057
655592222
------
Summary for variable: GSK2578215A
Numerical Variable Summary: Median = 0.0275913409389102, Mean = 0.03659125
073284348
------
Summary for variable: GSK2606414
Numerical Variable Summary: Median = 0.056563101634848054, Mean = 0.067472
04297796466
------
Summary for variable: GSK343
Numerical Variable Summary: Median = 0.0337663448757752, Mean = 0.03934935
99747645
------
Summary for variable: GSK591
Numerical Variable Summary: Median = 0.0738143516803852, Mean = 0.08201231
571109546
------
Summary for variable: I-BRD9
Numerical Variable Summary: Median = 0.0299123709285814, Mean = 0.04351894
5617176785
------
Summary for variable: IAP_5620
Numerical Variable Summary: Median = 0.01601398106051065, Mean = 0.0495325
7680043384
------
Summary for variable: Ibrutinib
Numerical Variable Summary: Median = 0.02382782148163955, Mean = 0.0660468
2444602498
------
Summary for variable: IGF1R_3801
Numerical Variable Summary: Median = 0.222721844174502, Mean = 0.237037403
26931827
------
Summary for variable: Ipatasertib
Numerical Variable Summary: Median = 0.101024232941507, Mean = 0.114624406
46859097
------
```

```
Summary for variable: IRAK4_4710
Numerical Variable Summary: Median = 0.04362765075681025, Mean = 0.0499152
07457087385
------
Summary for variable: Irinotecan
Numerical Variable Summary: Median = 0.102981599098958, Mean = 0.129358678
15155355
------
Summary for variable: IWP-2
Numerical Variable Summary: Median = 0.038680501283413, Mean = 0.048307060
42254878
------
Summary for variable: JAK_8517
Numerical Variable Summary: Median = 0.09456570091840524, Mean = 0.1112015
2837758916
------
Summary for variable: JAK1_8709
Numerical Variable Summary: Median = 0.063345944135781, Mean = 0.071861626
4931288
------
Summary for variable: JQ1 compound
Numerical Variable Summary: Median = 0.155017241995235, Mean = 0.187088780
56808392
------
Summary for variable: KRAS (G12C) Inhibitor-12
Numerical Variable Summary: Median = 0.0638592658833109, Mean = 0.07653996
375180178
------
Summary for variable: KU-55933
Numerical Variable Summary: Median = 0.0500234175550616, Mean = 0.04613808
907799042
------
Summary for variable: Lapatinib
Numerical Variable Summary: Median = 0.0750681746357749, Mean = 0.09492503
825283853
------
Summary for variable: LCL161
Numerical Variable Summary: Median = 0.032473800409850304, Mean = 0.043790
85395715869
------
Summary for variable: Leflunomide
Numerical Variable Summary: Median = 0.113580305539292, Mean = 0.122090874
68322662
------
Summary for variable: LGK974
Numerical Variable Summary: Median = 0.0638007357343557, Mean = 0.06874459
375718858
------
Summary for variable: Linsitinib
Numerical Variable Summary: Median = 0.08459862042075075, Mean = 0.0975715
5094682766
------
Summary for variable: LJI308
Numerical Variable Summary: Median = 0.0186879419360599, Mean = 0.03142082
091782486
------
Summary for variable: Luminespib
Numerical Variable Summary: Median = 0.2851973502944765, Mean = 0.28653761
48342891
------
```

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Summary for variable: LY2109761
Numerical Variable Summary: Median = 0.009852845218781499, Mean = 0.027292
041179400744
------
Summary for variable: MIM1
Numerical Variable Summary: Median = 0.0781213862627144, Mean = 0.07817671
520990044
------
Summary for variable: Mirin
Numerical Variable Summary: Median = 0.0780818847645854, Mean = 0.09048230
027401072
------
Summary for variable: Mitoxantrone
Numerical Variable Summary: Median = 0.187032241378891, Mean = 0.233926197
66799094
------
Summary for variable: MK-2206
Numerical Variable Summary: Median = 0.114088633406747, Mean = 0.139769944
77214996
------
Summary for variable: MK-8776
Numerical Variable Summary: Median = 0.05333009582154315, Mean = 0.0721434
5060357318
------
Summary for variable: ML323
Numerical Variable Summary: Median = 0.0562029431961973, Mean = 0.06446454
352327623
------
Summary for variable: MN-64
Numerical Variable Summary: Median = 0.0297173022052086, Mean = 0.03839425
356423396
------
Summary for variable: Molibresib
Numerical Variable Summary: Median = 0.113553489562935, Mean = 0.124680618
11258553
------
Summary for variable: Navitoclax
Numerical Variable Summary: Median = 0.118443351153085, Mean = 0.186842963
23462915
------
Summary for variable: Nelarabine
Numerical Variable Summary: Median = 0.000952944979808, Mean = 0.022852463
943272235
------
Summary for variable: Nilotinib
Numerical Variable Summary: Median = 0.023313717219065798, Mean = 0.044060
354286870475
------
Summary for variable: Niraparib
Numerical Variable Summary: Median = 0.0617493048787766, Mean = 0.07587064
586904897
------
Summary for variable: NSC19630
Numerical Variable Summary: Median = 0.0, Mean = 0.012695791729793923
------
Summary for variable: NU-7441
Numerical Variable Summary: Median = 0.0787671964305607, Mean = 0.10243041
366027293
------
Summary for variable: Nutlin-3a (-)
```

```
Numerical Variable Summary: Median = 0.0166945512527916, Mean = 0.04597038
466781325
------
Summary for variable: NVP-ADW742
Numerical Variable Summary: Median = 0.07734291760101786, Mean = 0.0915289
6600527094
------
Summary for variable: Obatoclax
Numerical Variable Summary: Median = 0.195220657472774, Mean = 0.208316302
0713849
------
Summary for variable: OF-1
Numerical Variable Summary: Median = 0.0608276516976701, Mean = 0.06996444
5722596
------
Summary for variable: Olaparib
Numerical Variable Summary: Median = 0.04971908561671745, Mean = 0.0615415
6922181187
------
Summary for variable: Osi-027
Numerical Variable Summary: Median = 0.0693300142366928, Mean = 0.07748478
210092667
------
Summary for variable: Osimertinib
Numerical Variable Summary: Median = 0.056290242187945, Mean = 0.071807212
40955075
------
Summary for variable: OTX015
Numerical Variable Summary: Median = 0.177487524613953, Mean = 0.200215937
0328717
------
Summary for variable: Oxaliplatin
Numerical Variable Summary: Median = 0.0510100496413189, Mean = 0.06731489
885335461
------
Summary for variable: P22077
Numerical Variable Summary: Median = 0.018167113023867497, Mean = 0.034104
13225249717
------
Summary for variable: Paclitaxel
Numerical Variable Summary: Median = 0.024706069276433, Mean = 0.043623458
950266446
------
Summary for variable: PAK_5339
Numerical Variable Summary: Median = 0.1696781990815815, Mean = 0.19480824
274269223
------
Summary for variable: Palbociclib
Numerical Variable Summary: Median = 0.0862517725279007, Mean = 0.10324969
724617794
------
Summary for variable: PCI-34051
Numerical Variable Summary: Median = 0.03602146056459585, Mean = 0.0448447
0722922453
------
Summary for variable: PD 173074
Numerical Variable Summary: Median = 1.3380492214447915e-15, Mean = 0.0227
13745490322367
------
Summary for variable: PD-0325901
```

```
Numerical Variable Summary: Median = 0.071244194806611, Mean = 0.097264488
74543198
------
Summary for variable: Pevonedistat
Numerical Variable Summary: Median = 0.301269271510871, Mean = 0.314783101
43603017
------
Summary for variable: PF-4708671
Numerical Variable Summary: Median = 0.0743254862289325, Mean = 0.07671013
512291913
------
Summary for variable: PFI-3
Numerical Variable Summary: Median = 0.01197123360442715, Mean = 0.0241976
1913940294
------
Summary for variable: Pictilisib
Numerical Variable Summary: Median = 0.192462117414503, Mean = 0.204548203
16915223
------
Summary for variable: PLX4720
Numerical Variable Summary: Median = 0.03405423010569175, Mean = 0.0516741
9258365804
------
Summary for variable: PRIMA-1-Met
Numerical Variable Summary: Median = 0.06634643857066494, Mean = 0.0749189
7802959324
------
Summary for variable: PRT062607
Numerical Variable Summary: Median = 0.0893740082771621, Mean = 0.09377116
165243293
------
Summary for variable: Pyridostatin
Numerical Variable Summary: Median = 0.05103481606942205, Mean = 0.0584911
7780826185
------
Summary for variable: Ribociclib
Numerical Variable Summary: Median = 0.0654982829655131, Mean = 0.06162310
951456875
------
Summary for variable: RO-3306
Numerical Variable Summary: Median = 0.0766385053424526, Mean = 0.09813865
736783388
------
Summary for variable: Ruxolitinib
Numerical Variable Summary: Median = 0.0624223704041464, Mean = 0.06817581
593436206
------
Summary for variable: RVX-208
Numerical Variable Summary: Median = 0.0363369801910583, Mean = 0.04486293
999850898
------
Summary for variable: Sabutoclax
Numerical Variable Summary: Median = 0.4135586166065325, Mean = 0.42055621
04715481
------
Summary for variable: Sapatinib
Numerical Variable Summary: Median = 0.050913187010466, Mean = 0.086670261
36128127
------
Summary for variable: Savolitinib
```

```
Numerical Variable Summary: Median = 0.0262184697811065, Mean = 0.05076320
288108072
------
Summary for variable: SB 216763
Numerical Variable Summary: Median = 0.0071112205311183, Mean = 0.01982831
4469208318
------
Summary for variable: SB 505124
Numerical Variable Summary: Median = 0.1115767653742705, Mean = 0.12720165
951042736
------
Summary for variable: SCH772984
Numerical Variable Summary: Median = 0.101705090495233, Mean = 0.135879965
99036178
------
Summary for variable: Selumetinib
Numerical Variable Summary: Median = 0.057674748728164846, Mean = 0.102047
28410274645
------
Summary for variable: Sepantronium bromide
Numerical Variable Summary: Median = 0.86358556430109, Mean = 0.8146561003
420442
------
Summary for variable: Sinularin
Numerical Variable Summary: Median = 0.036695848112981, Mean = 0.043945856
00659171
------
Summary for variable: Sirolimus
Numerical Variable Summary: Median = 0.102054739724453, Mean = 0.121380330
20402579
------
Summary for variable: Sorafenib
Numerical Variable Summary: Median = 0.07279843427807381, Mean = 0.0837650
1490878531
------
Summary for variable: TAF1_5496
Numerical Variable Summary: Median = 0.0724297762718277, Mean = 0.09107869
025188899
------
Summary for variable: Talazoparib
Numerical Variable Summary: Median = 0.129447458303138, Mean = 0.169067611
1784775
------
Summary for variable: Tamoxifen
Numerical Variable Summary: Median = 0.09156109723534385, Mean = 0.0962574
3786826572
------
Summary for variable: Taselisib
Numerical Variable Summary: Median = 0.155866901425658, Mean = 0.178964906
9532792
------
Summary for variable: Telomerase Inhibitor IX
Numerical Variable Summary: Median = 0.3013347020447395, Mean = 0.29914830
47874932
------
Summary for variable: Temozolomide
Numerical Variable Summary: Median = 0.0484297955503224, Mean = 0.05733120
641970658
------
Summary for variable: Teniposide
```

```
Numerical Variable Summary: Median = 0.201313052718005, Mean = 0.231449544
25565506
------
Summary for variable: Topotecan
Numerical Variable Summary: Median = 0.226478520496089, Mean = 0.250047956
0907472
------
Summary for variable: Tozasertib
Numerical Variable Summary: Median = 0.0903720782415113, Mean = 0.11142140
442666044
------
Summary for variable: Trametinib
Numerical Variable Summary: Median = 0.181029253437023, Mean = 0.215839778
72749557
------
Summary for variable: Ulixertinib
Numerical Variable Summary: Median = 0.0977135092685724, Mean = 0.11335231
72506973
------
Summary for variable: ULK1_4989
Numerical Variable Summary: Median = 0.208059475767644, Mean = 0.224293594
32293025
------
Summary for variable: UMI-77
Numerical Variable Summary: Median = 0.08311125555203461, Mean = 0.0862919
5840672524
------
Summary for variable: Unii-40E3azg1MX
Numerical Variable Summary: Median = 0.14438782935975147, Mean = 0.1681975
4639904133
------
Summary for variable: Uprosertib
Numerical Variable Summary: Median = 0.1357560650313545, Mean = 0.16052127
351701445
------
Summary for variable: VE-822
Numerical Variable Summary: Median = 0.0407958176718728, Mean = 0.06102469
155101414
------
Summary for variable: VE821
Numerical Variable Summary: Median = 0.0555030567479457, Mean = 0.06919394
401341336
------
Summary for variable: Venetoclax
Numerical Variable Summary: Median = 0.0764372069338673, Mean = 0.10017555
965546272
------
Summary for variable: Vincaleukoblastine
Numerical Variable Summary: Median = 0.292758603683214, Mean = 0.291835613
3688447
------
Summary for variable: Vincristine
Numerical Variable Summary: Median = 0.457711312042171, Mean = 0.466557971
90351866
------
Summary for variable: Vinorelbine
Numerical Variable Summary: Median = 0.2206900611017935, Mean = 0.23645457
570214554
------
Summary for variable: Vorinostat
```

```
Numerical Variable Summary: Median = 0.165587667682214, Mean = 0.181345846
47459515
------
Summary for variable: VSP34_8731
Numerical Variable Summary: Median = 0.1910789128548845, Mean = 0.19751443
643291872
------
Summary for variable: VX-11e
Numerical Variable Summary: Median = 0.0868024916118665, Mean = 0.11664547
972912143
------
Summary for variable: WEHI-539
Numerical Variable Summary: Median = 0.117360471517225, Mean = 0.148244843
06945596
------
Summary for variable: WIKI4
Numerical Variable Summary: Median = 0.107234452011319, Mean = 0.109199574
20053418
------
Summary for variable: Wnt-C59
Numerical Variable Summary: Median = 0.0438928825420606, Mean = 0.05374682
933812989
------
Summary for variable: WZ4003
Numerical Variable Summary: Median = 0.0458950115806167, Mean = 0.05250517
950267002
------
Summary for variable: XAV-939
Numerical Variable Summary: Median = 0.0731079865882327, Mean = 0.07665802
398719392
------
Summary for variable: YK 4-279
Numerical Variable Summary: Median = 0.2049389871738635, Mean = 0.22190902
152642297
------
Summary for variable: ZM-447439
Numerical Variable Summary: Median = 0.0704123332258365, Mean = 0.10256456
086307027
------
Summary for variable: Zolendronic Acid
Numerical Variable Summary: Median = 0.0, Mean = 0.013884325043733207
------
Summary for variable: tissueid
Categorical Variable Summary:
  Label: -1.0, Count: 13
  Label: Biliary Tract, Count: 5
  Label: Bladder/Urinary Tract, Count: 17
  Label: Bone, Count: 25
  Label: Bowel, Count: 33
  Label: Breast, Count: 33
  Label: CNS/Brain, Count: 44
  Label: Esophagus/Stomach, Count: 34
  Label: Head and Neck, Count: 21
  Label: Kidney, Count: 17
  Label: Liver, Count: 6
  Label: Lung, Count: 106
  Label: Lymphoid, Count: 64
  Label: Myeloid, Count: 20
  Label: Other, Count: 2
  Label: Ovary/Fallopian Tube, Count: 18
```

```
  Label: Pancreas, Count: 16
  Label: Peripheral Nervous System, Count: 16
  Label: Pleura, Count: 7
  Label: Prostate, Count: 4
  Label: Skin, Count: 32
  Label: Soft Tissue, Count: 9
  Label: Thyroid, Count: 9
  Label: Uterus, Count: 9
------
```

In [12]:
```
train_dataset.label_mappings, test_dataset.label_mappings
```

Out[12]:
```
({'tissueid': {0: 'Ampulla of Vater',
   1: 'Biliary Tract',
   2: 'Bladder/Urinary Tract',
   3: 'Bone',
   4: 'Bowel',
   5: 'Breast',
   6: 'CNS/Brain',
   7: 'Esophagus/Stomach',
   8: 'Head and Neck',
   9: 'Kidney',
   10: 'Liver',
   11: 'Lung',
   12: 'Lymphoid',
   13: 'Myeloid',
   14: 'Other',
   15: 'Ovary/Fallopian Tube',
   16: 'Pancreas',
   17: 'Peripheral Nervous System',
   18: 'Pleura',
   19: 'Prostate',
   20: 'Skin',
   21: 'Soft Tissue',
   22: 'Thyroid',
   23: 'Uterus'}},
 {'tissueid': {0: 'Ampulla of Vater',
   1: 'Biliary Tract',
   2: 'Bladder/Urinary Tract',
   3: 'Bone',
   4: 'Bowel',
   5: 'Breast',
   6: 'CNS/Brain',
   7: 'Esophagus/Stomach',
   8: 'Head and Neck',
   9: 'Kidney',
   10: 'Liver',
   11: 'Lung',
   12: 'Lymphoid',
   13: 'Myeloid',
   14: 'Other',
   15: 'Ovary/Fallopian Tube',
   16: 'Pancreas',
   17: 'Peripheral Nervous System',
   18: 'Pleura',
   19: 'Prostate',
   20: 'Skin',
   21: 'Soft Tissue',
   22: 'Thyroid',
   23: 'Uterus'}})
```

In [13]:
```
Erlotinib_vals = train_dataset.ann["Erlotinib"][:10]
mapping = train_dataset.label_mappings["tissueid"]
df = pd.DataFrame({
    "STUDY": Erlotinib_vals.tolist(),
    "Mapped Label": [
        mapping[int(x.item())] if not math.isnan(x.item()) else "NaN"
        for x in Erlotinib_vals
    ]
})
display(df)
```

	STUDY	Mapped Label
0	NaN	NaN
1	NaN	NaN
2	NaN	NaN
3	0.026610	Ampulla of Vater
4	0.078255	Ampulla of Vater
5	0.105692	Ampulla of Vater
6	NaN	NaN
7	0.021037	Ampulla of Vater
8	0.000000	Ampulla of Vater
9	NaN	NaN

In [14]:
```
df = pd.DataFrame(train_dataset.dat['mutation'], index = train_dataset.sa
```

In [15]:
```
df.head()
```

Out[15]:

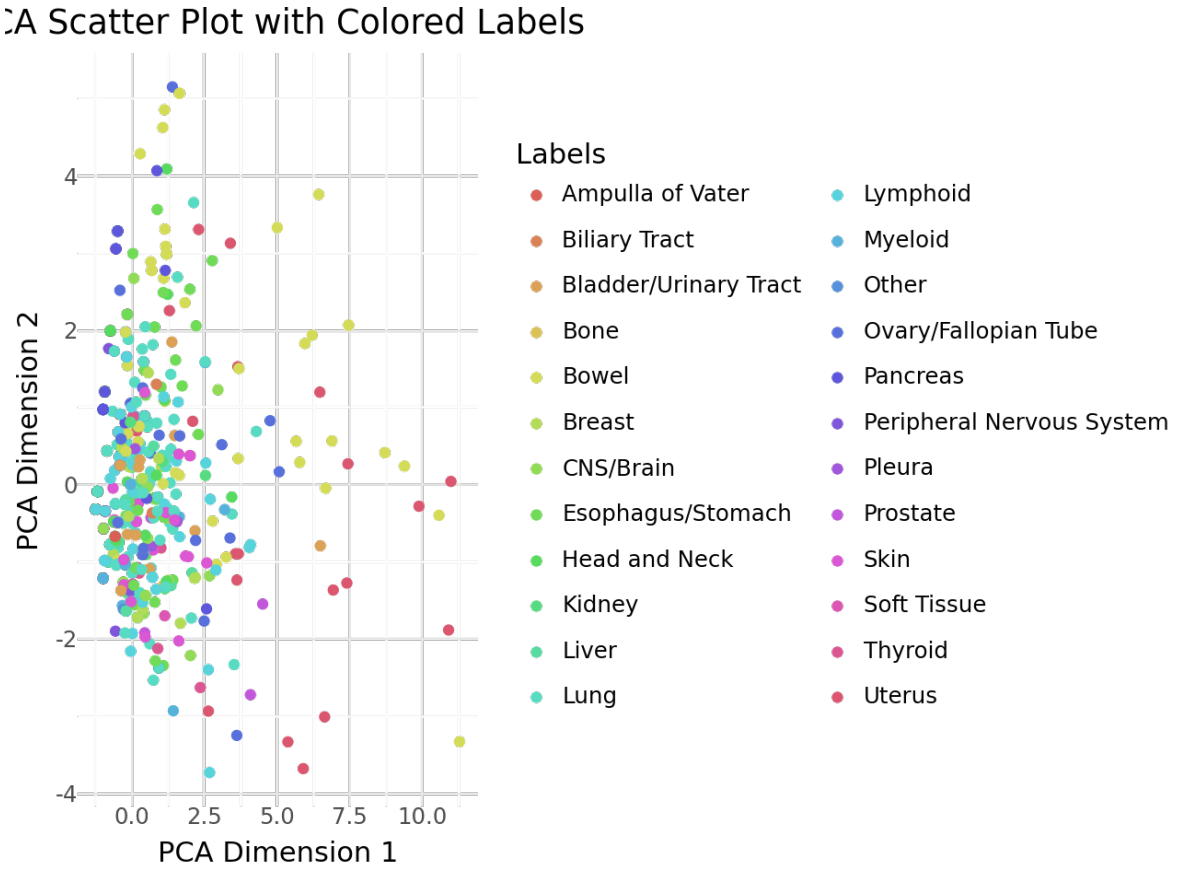
	APC	BRAF	CDH1	CDKN2A	CTNNB1	EGFR	FBXW7	KDM
Caov-4	-0.405442	-0.347999	-0.22486	-0.205824	-0.23517	-0.23517	-0.247576	-0.230(
COLO 704	-0.405442	-0.347999	-0.22486	-0.205824	-0.23517	-0.23517	-0.247576	-0.230(
Hs 274.T	-0.405442	-0.347999	-0.22486	-0.205824	-0.23517	-0.23517	-0.247576	-0.230(
B-CPAP	2.466441	2.873574	-0.22486	-0.205824	-0.23517	-0.23517	-0.247576	-0.230(
NCI-H2452	-0.405442	-0.347999	-0.22486	-0.205824	-0.23517	-0.23517	-0.247576	-0.230(

5 rows × 24 columns

In [16]:
```
ds = train_dataset
```

In [17]:
```
f = 'tissueid'
labels = [ds.label_mappings[f][x] for x in ds.ann[f].numpy()]
```

In [18]:
```
flexynesis.plot_dim_reduced(df, labels, color_type = 'categorical', metho
```



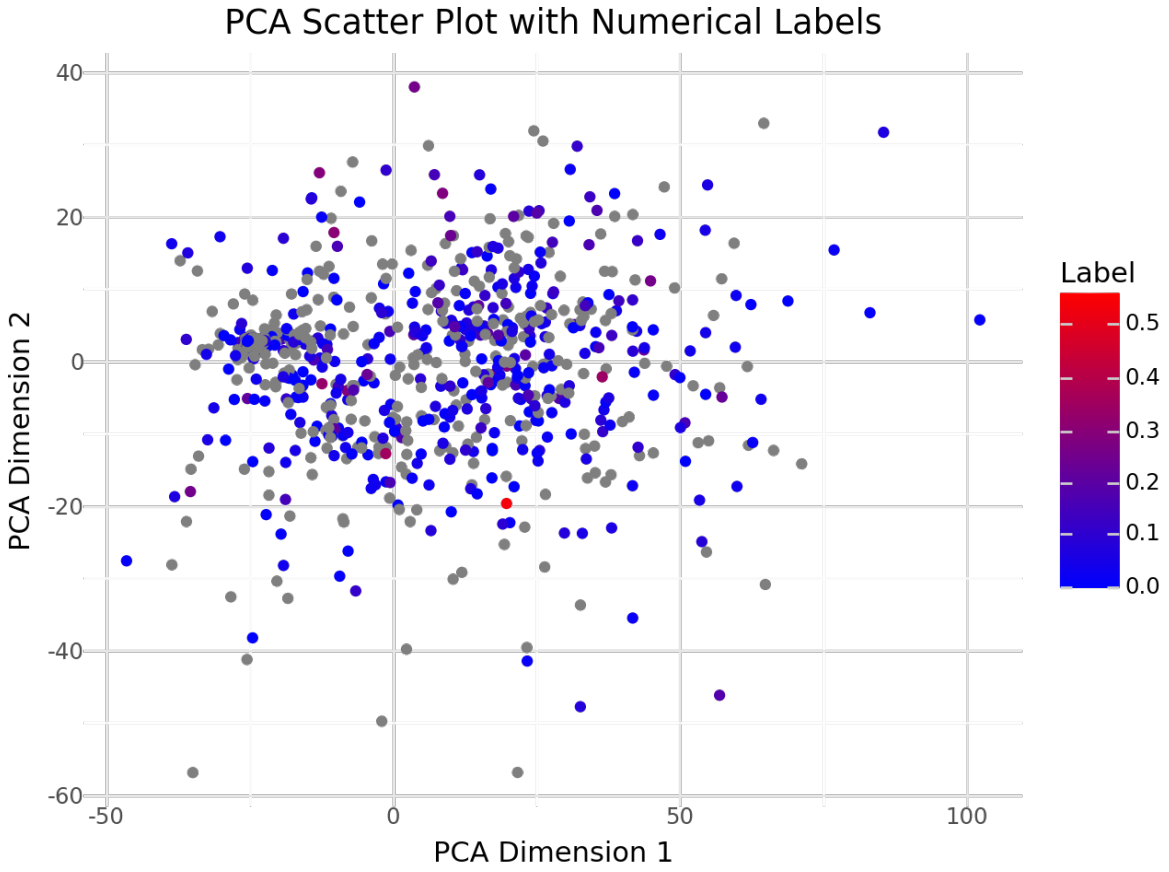
In [19]:
```
train_dataset.ann.keys()
```

Out[19]:
```
dict_keys(['Crizotinib', 'Dovitinib', 'Erlotinib', 'Irinotecan', 'L-6854
58', 'Lapatinib', 'LBW242', 'Nilotinib', 'Nutlin-3', 'Nvp-aew541', 'Nvp-
tae 684', 'Paclitaxel', 'Palbociclib', 'Panobinostat', 'PD-0325901', 'Ph
a-665752', 'PLX4720', 'Raf265(chir-265)', 'Saracatinib', 'Selumetinib',
'Sorafenib', 'Tanespimycin', 'Topotecan', 'Vandetanib', 'tissueid'])
```

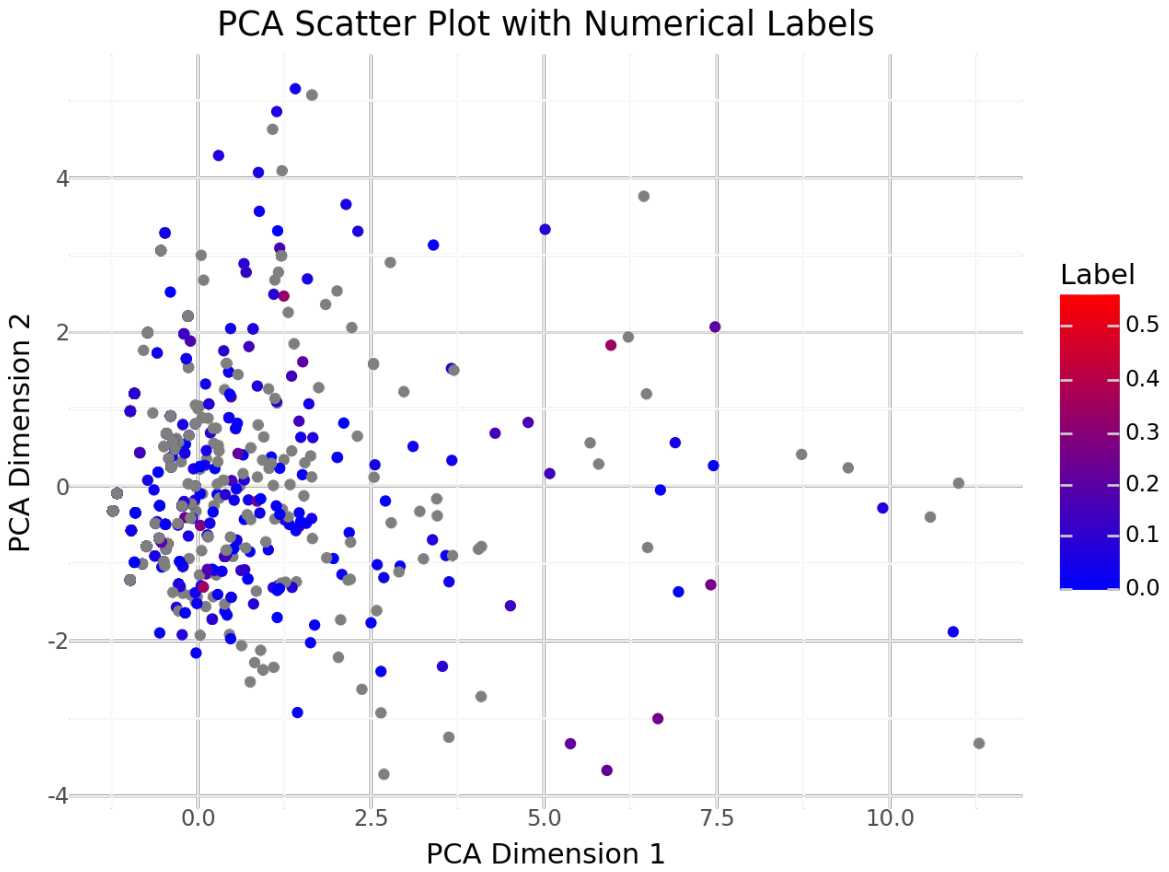
In [20]:
```
# List available clinical variables in the training dataset (from .ann)
clinical_vars = ['Erlotinib', 'Crizotinib', 'Paclitaxel', 'Tanespimycin']

# Prepare the data matrices for CNV, RNA, and MUT
ds = train_dataset
df_cnv = pd.DataFrame(ds.dat["cnv"], index=ds.samples, columns=ds.feature
df_mut = pd.DataFrame(ds.dat["mutation"], index=ds.samples, columns=ds.fe
df_rna = pd.DataFrame(ds.dat["rna"], index=ds.samples, columns=ds.feature

def get_labels(variable):
    """
    For a given clinical variable, returns a tuple:
      (labels, color_type)
    If a mapping exists, labels are mapped (categorical);
    otherwise, raw values are returned (numerical).
    """
    vals = ds.ann[variable].numpy()
    if variable in ds.label_mappings:
        labels = [ds.label_mappings[variable][int(x.item())] if not math.
                  for x in ds.ann[variable]]
        color_type = "categorical"
    else:
        labels = vals  # Use raw numeric values
        color_type = "numerical"
    return labels, color_type
```

In [21]:
```
# Loop over each clinical variable and generate PCA plots for both CNA an
for var in clinical_vars:
    labels, color_type = get_labels(var)

    # Plot PCA for CNV data
    print(f"PCA plot for CNV data colored by: {var}")
    fig1 = plot_dim_reduced(df_cnv, labels=labels, color_type=color_type,
    # If fig is returned, display it:
    if fig1 is not None:
        fig1.show()
    else:
        plt1.show()

    # Plot PCA for MUT data
    print(f"PCA plot for MUT data colored by: {var}")
    fig2 = plot_dim_reduced(df_mut, labels=labels, color_type=color_type,
    # If fig is returned, display it:
    if fig2 is not None:
        fig2.show()
    else:
        plt2.show()

    # Plot PCA for RNA data
    print(f"PCA plot for RNA data colored by: {var}")
    fig3 = plot_dim_reduced(df_rna, labels=labels, color_type=color_type,
    # If fig is returned, display it:
    if fig3 is not None:
        fig3.show()
    else:
        plt3.show()
```

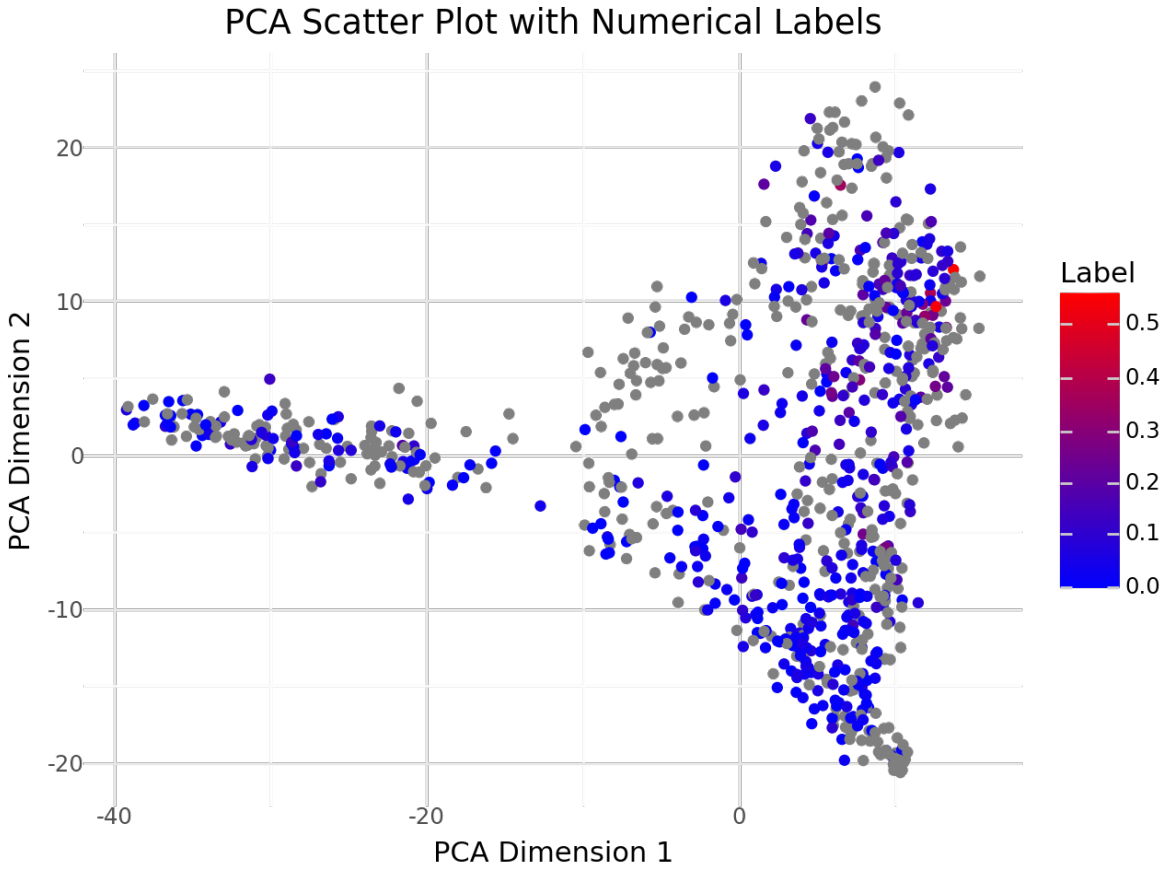
```
PCA plot for CNV data colored by: Erlotinib
```



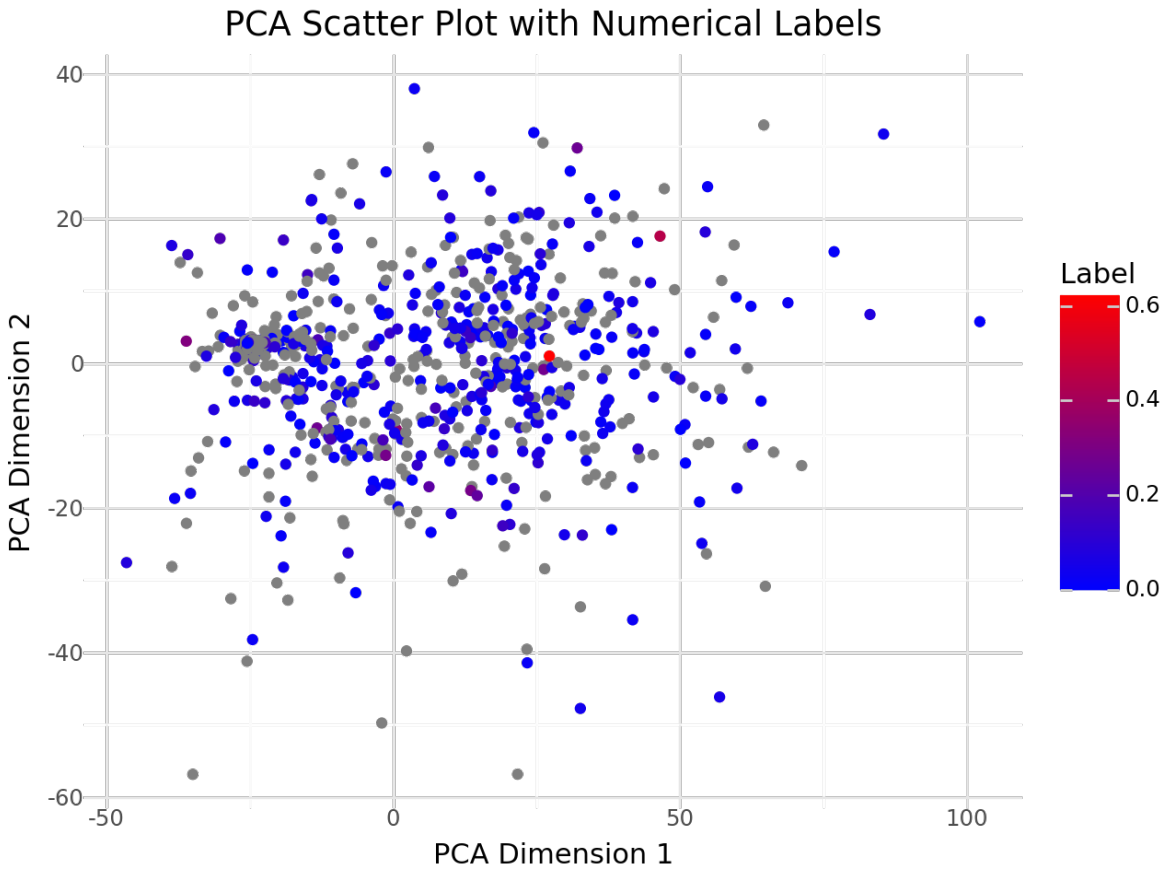
PCA plot for MUT data colored by: Erlotinib



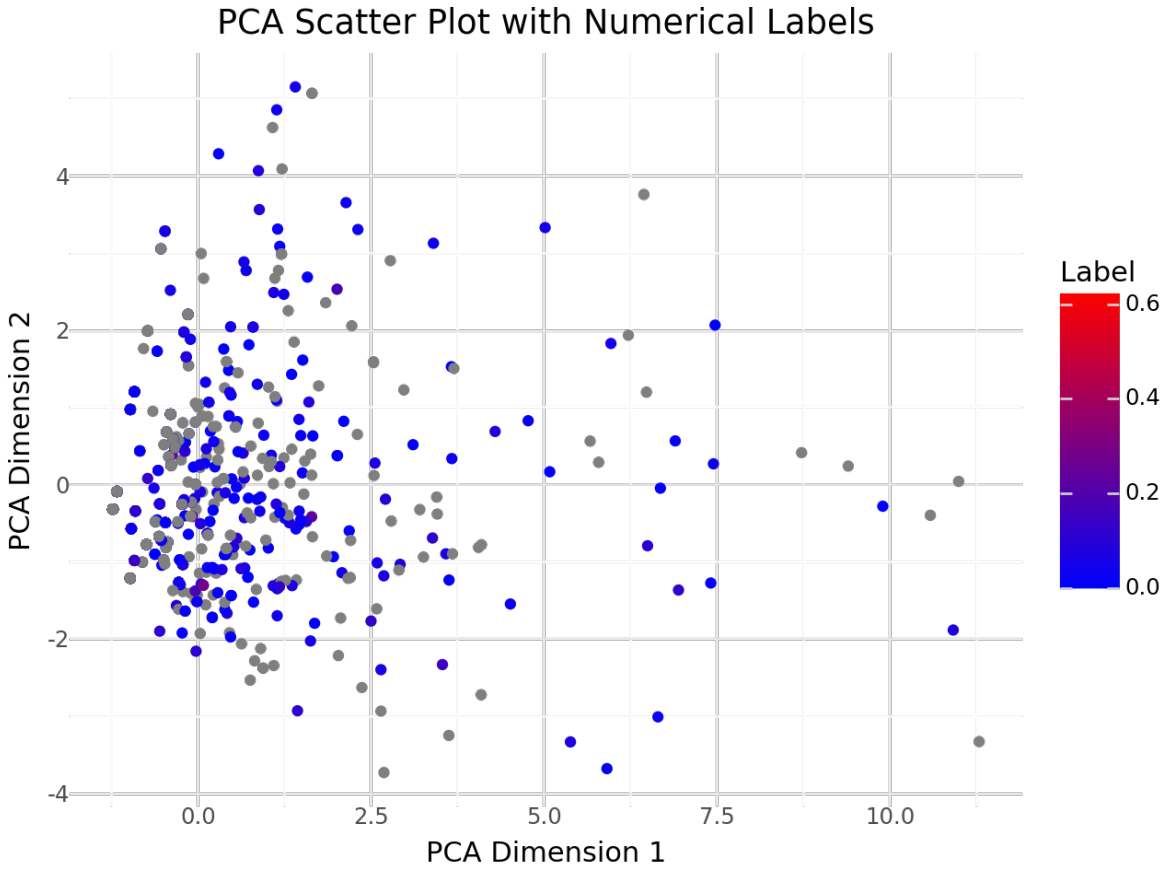
PCA plot for RNA data colored by: Erlotinib



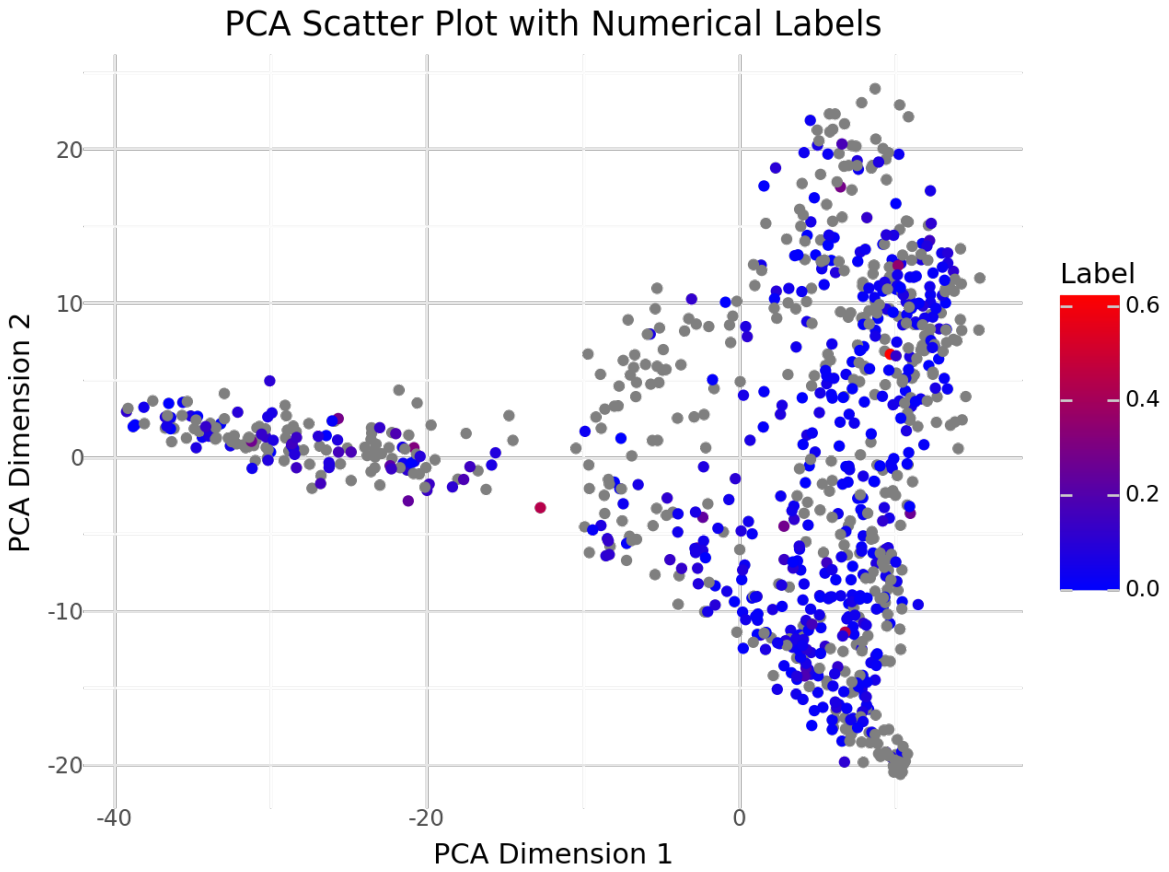
PCA plot for CNV data colored by: Crizotinib



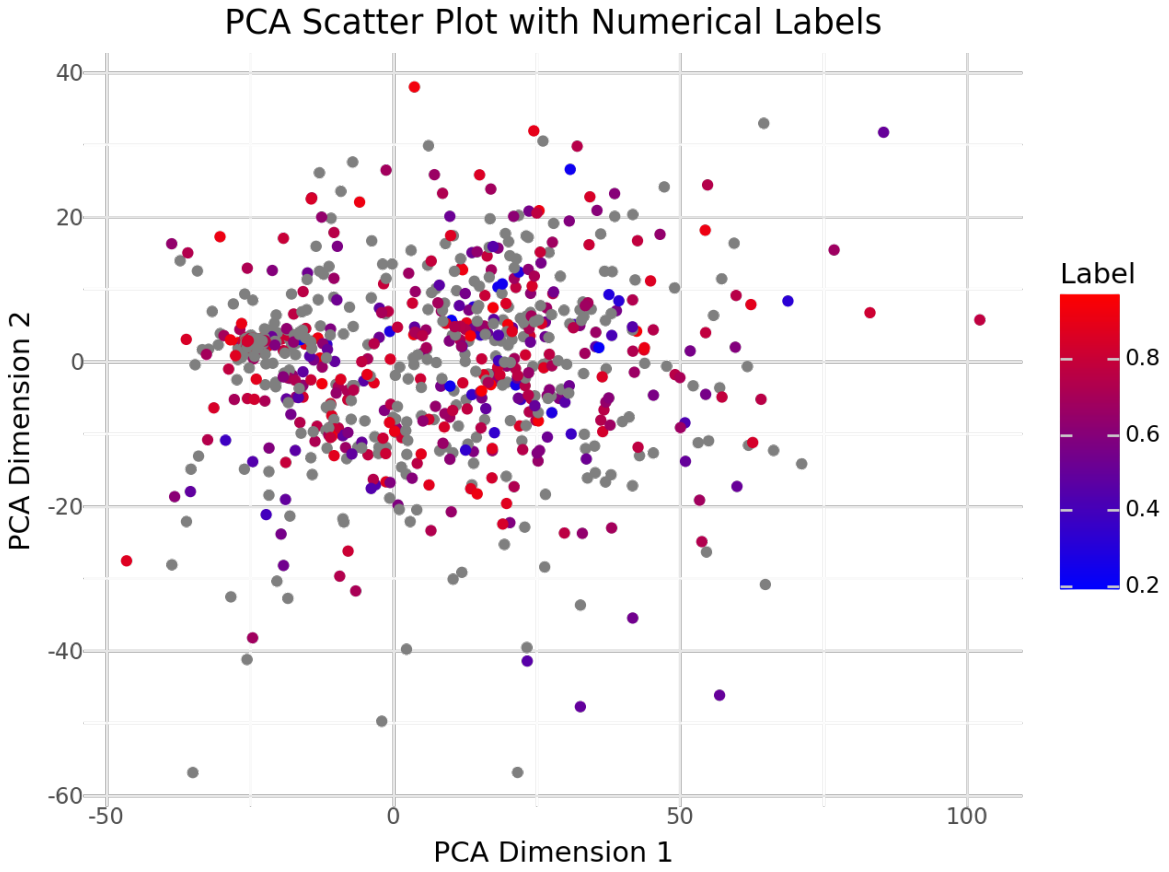
PCA plot for MUT data colored by: Crizotinib



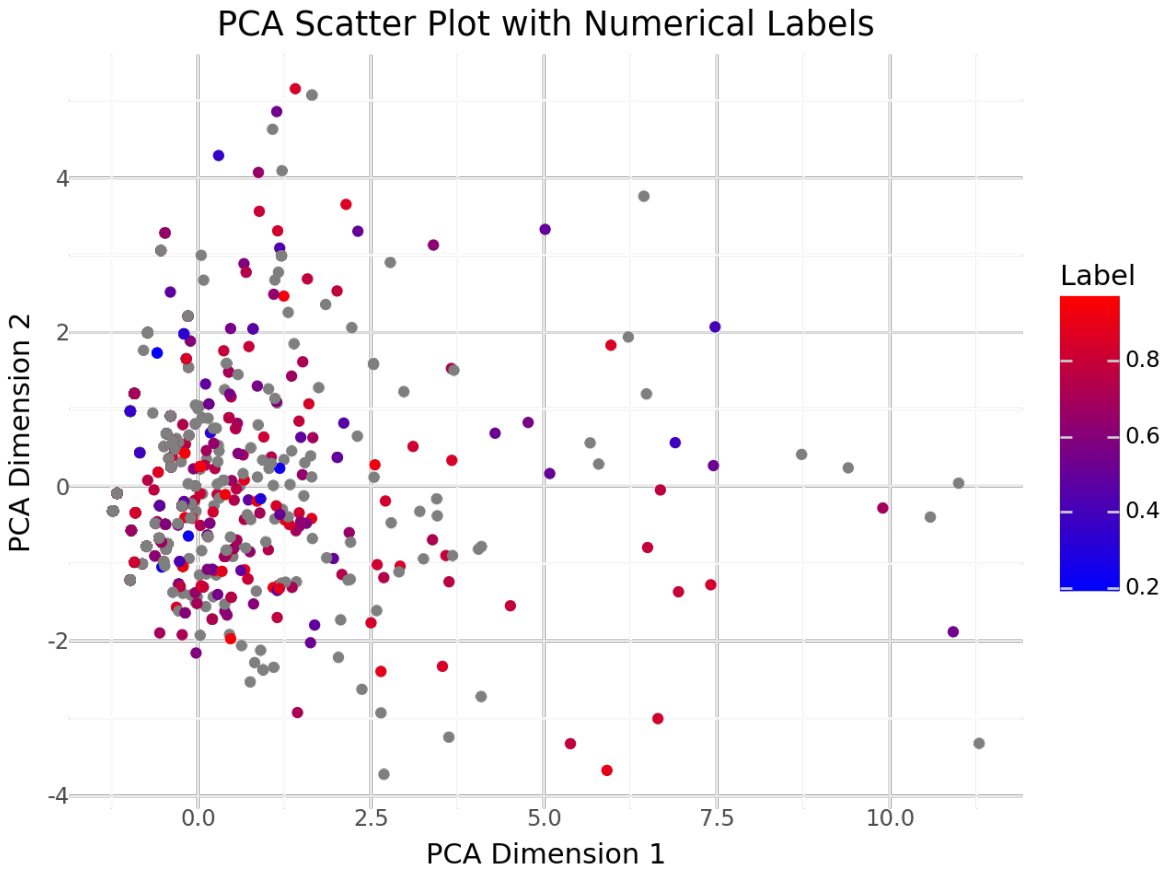
PCA plot for RNA data colored by: Crizotinib



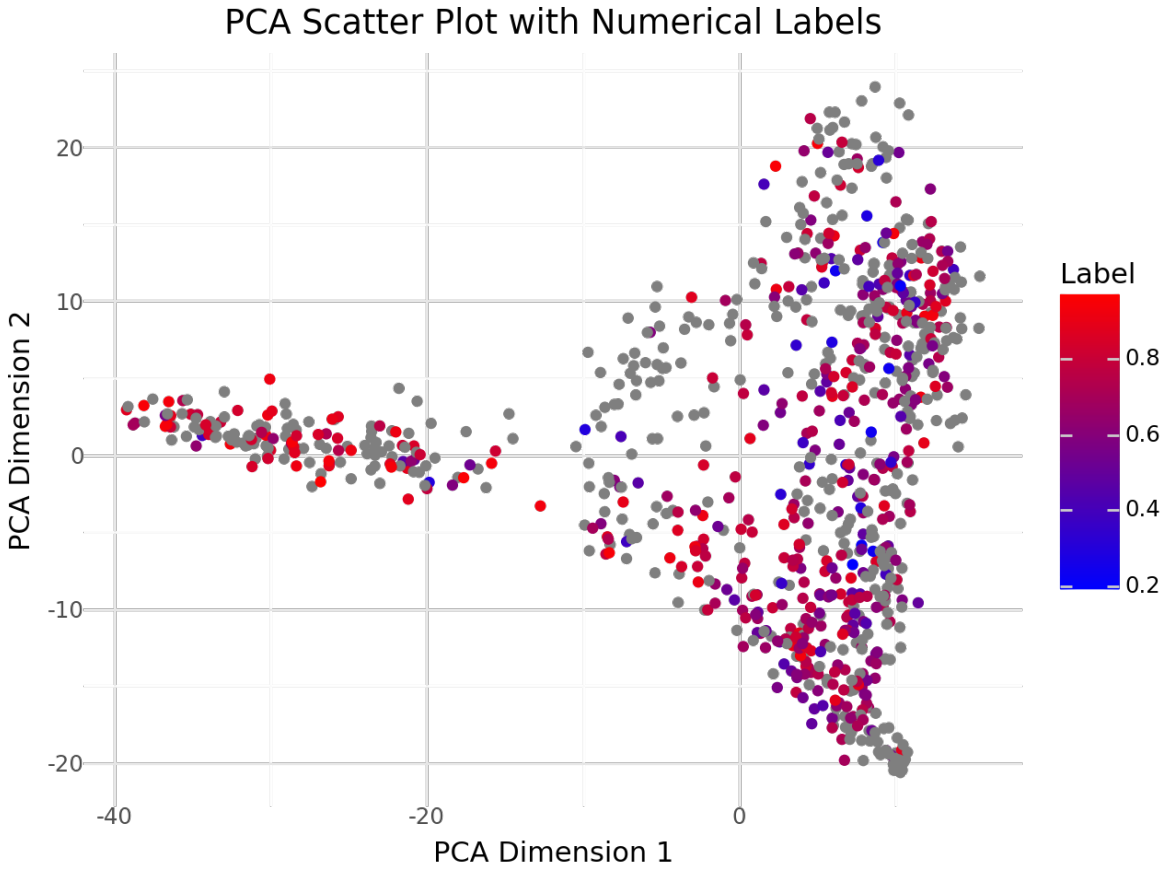
PCA plot for CNV data colored by: Paclitaxel



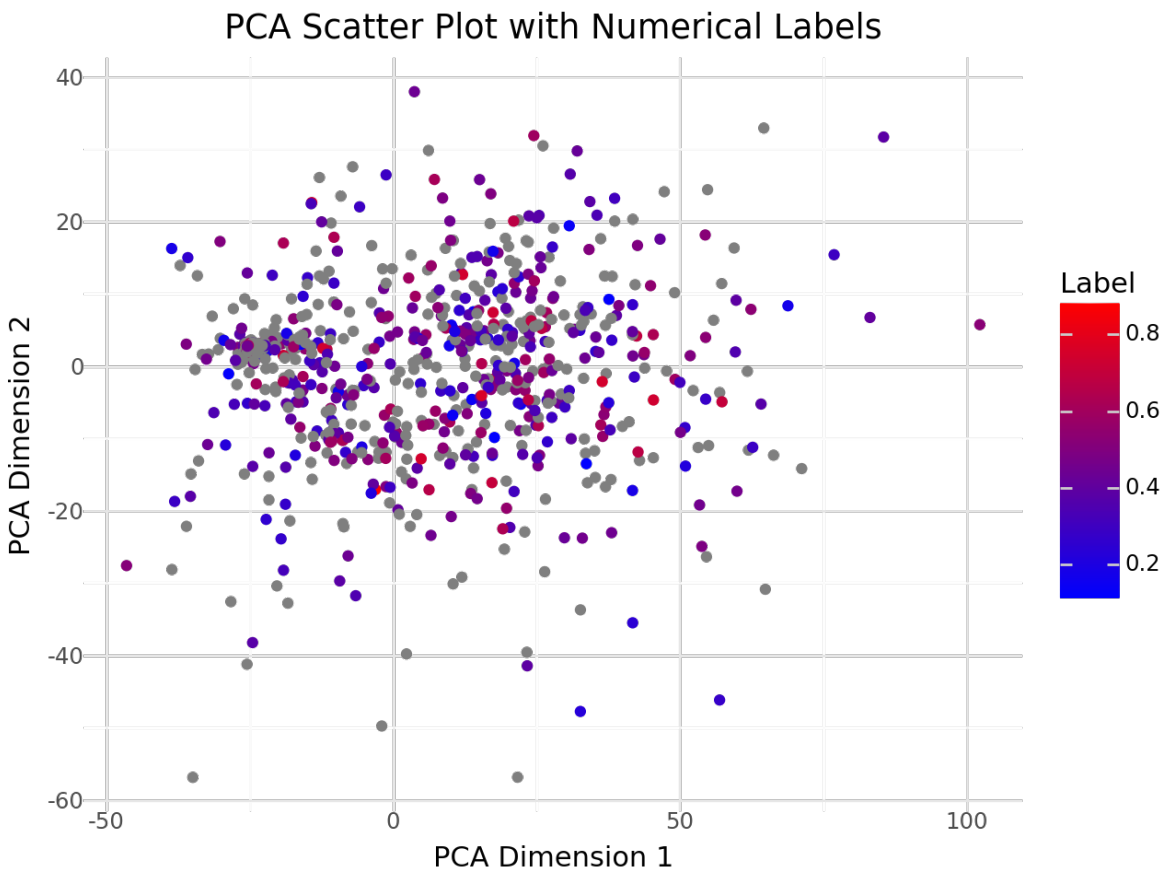
PCA plot for MUT data colored by: Paclitaxel



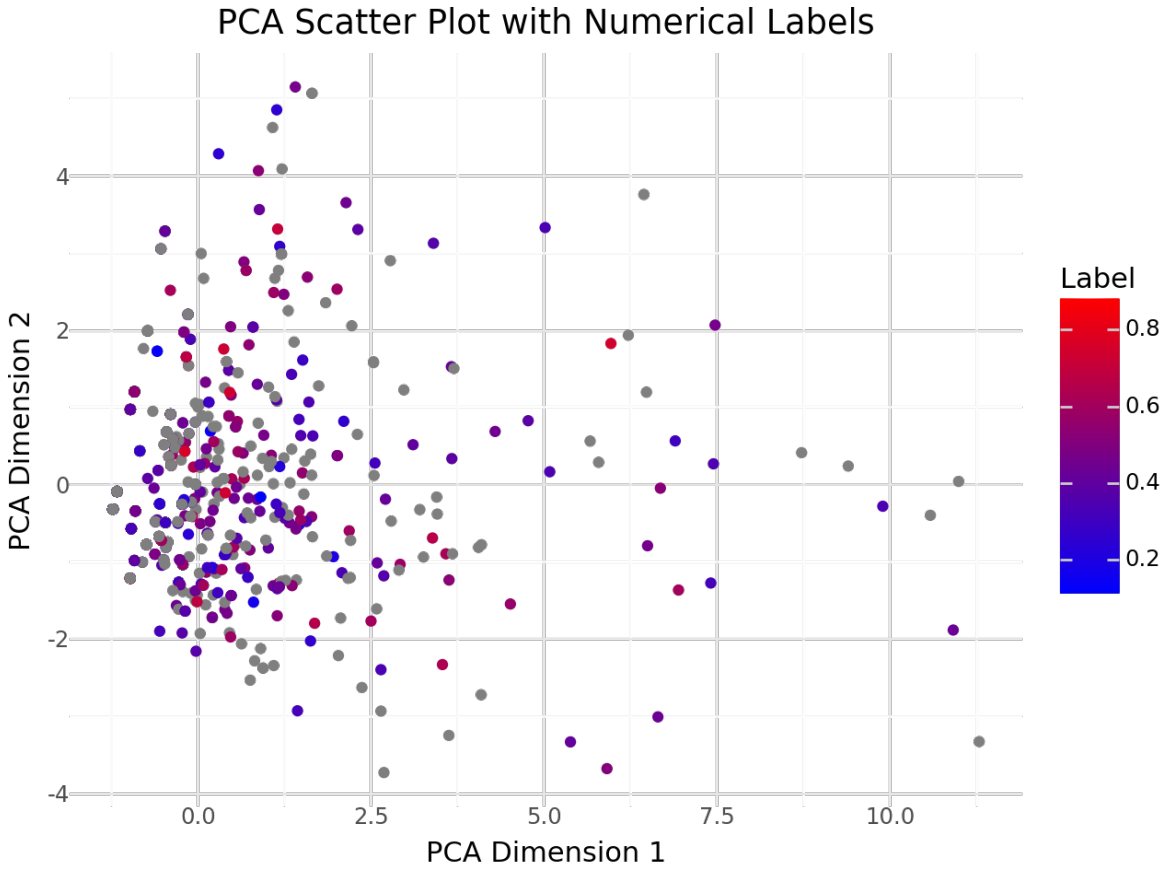
PCA plot for RNA data colored by: Paclitaxel



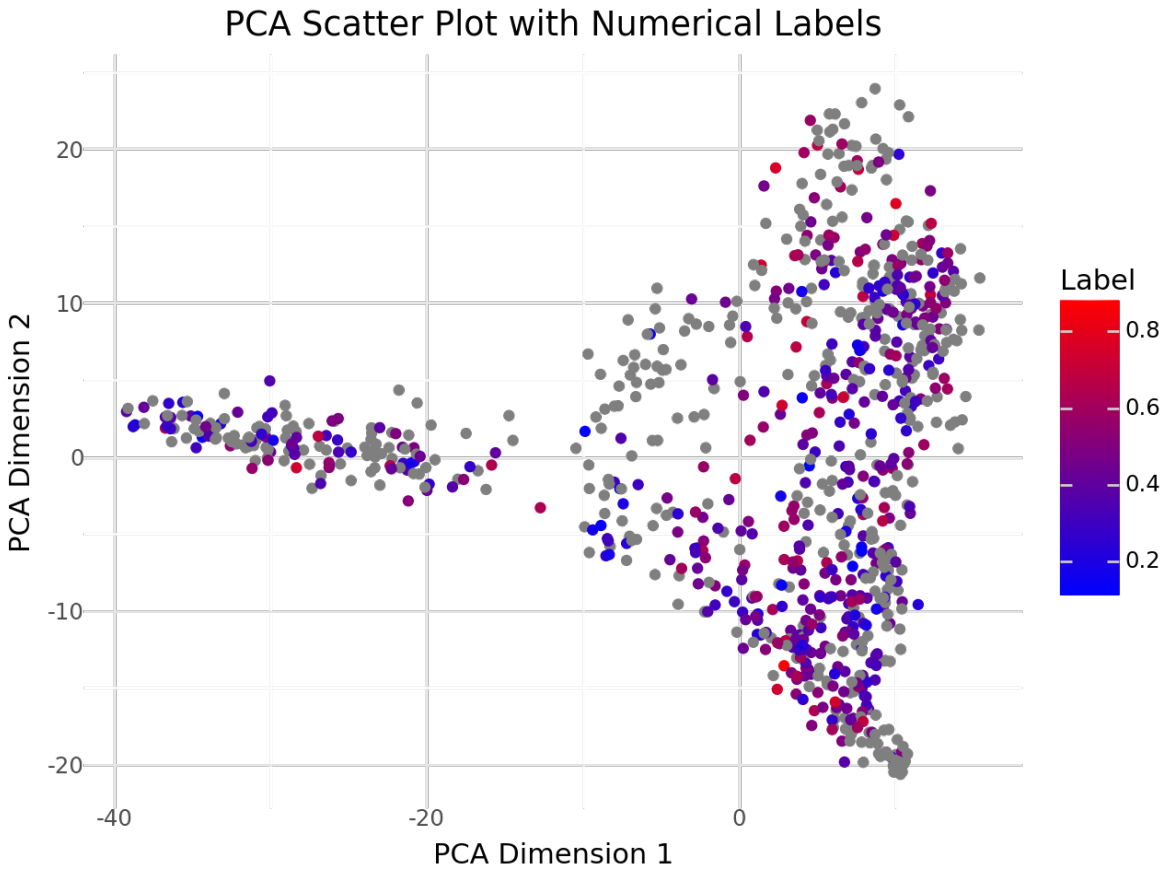
PCA plot for CNV data colored by: Tanespimycin



PCA plot for MUT data colored by: Tanespimycin



PCA plot for RNA data colored by: Tanespimycin



Generate all models

Total: 24 (non-GNN) + 12 (GNN) = 36

Different data modality combinations

DATA_TYPE_LIST=("mutation" "rna" "cnv" "mutation,cnv" "mutation,rna" "rna,cnv")

Two fusion types for non-GNN models

FUSION_MODES=("early" "intermediate")

Non-GNN model classes

NON_GNN_CLASSES=("DirectPred" "supervised_vae")

GNN model class and convolution types

GNN_CLASS="GNN"; GNN_CONV_TYPES=("GC" "SAGE")

In [22]:
```
!bash check_multiomics_ccle_vs_gdsc_eval.sh
```

```
================================================================
Running Flexynesis for Erlotinib (CCLE vs GDSC) with skipping if present
Data path:         /home/thesamurai/sciebo/Project_Allocation/module3_tria
l_multiomics/compgen_course_2025_module3_my_session/submissions/day3/ccle_
vs_gdsc/
Target variable:   Erlotinib
HPO iterations:    15
Threads:           12
Num workers:       6
================================================================
----------------------------------------------------------
Model: DirectPred | Data: mutation | Fusion: early
Prefix: run_DirectPred_mutation_early
----------------------------------------------------------
Checking if all required files exist for run_DirectPred_mutation_early ...
All output files found for run_DirectPred_mutation_early. Skipping.
----------------------------------------------------------
----------------------------------------------------------
Model: DirectPred | Data: mutation | Fusion: intermediate
Prefix: run_DirectPred_mutation_intermediate
----------------------------------------------------------
Checking if all required files exist for run_DirectPred_mutation_intermedi
ate ...
All output files found for run_DirectPred_mutation_intermediate. Skipping.
----------------------------------------------------------
----------------------------------------------------------
Model: DirectPred | Data: rna | Fusion: early
Prefix: run_DirectPred_rna_early
----------------------------------------------------------
Checking if all required files exist for run_DirectPred_rna_early ...
All output files found for run_DirectPred_rna_early. Skipping.
----------------------------------------------------------
----------------------------------------------------------
Model: DirectPred | Data: rna | Fusion: intermediate
Prefix: run_DirectPred_rna_intermediate
----------------------------------------------------------
Checking if all required files exist for run_DirectPred_rna_intermediate
...
All output files found for run_DirectPred_rna_intermediate. Skipping.
----------------------------------------------------------
----------------------------------------------------------
Model: DirectPred | Data: cnv | Fusion: early
Prefix: run_DirectPred_cnv_early
----------------------------------------------------------
Checking if all required files exist for run_DirectPred_cnv_early ...
All output files found for run_DirectPred_cnv_early. Skipping.
----------------------------------------------------------
----------------------------------------------------------
Model: DirectPred | Data: cnv | Fusion: intermediate
Prefix: run_DirectPred_cnv_intermediate
----------------------------------------------------------
Checking if all required files exist for run_DirectPred_cnv_intermediate
...
All output files found for run_DirectPred_cnv_intermediate. Skipping.
----------------------------------------------------------
----------------------------------------------------------
Model: DirectPred | Data: mutation,cnv | Fusion: early
Prefix: run_DirectPred_mutation,cnv_early
----------------------------------------------------------
Checking if all required files exist for run_DirectPred_mutation,cnv_early
```

```
...
All output files found for run_DirectPred_mutation,cnv_early. Skipping.
------------------------------------------------------------
------------------------------------------------------------
Model: DirectPred | Data: mutation,cnv | Fusion: intermediate
Prefix: run_DirectPred_mutation,cnv_intermediate
------------------------------------------------------------
Checking if all required files exist for run_DirectPred_mutation,cnv_inter
mediate ...
All output files found for run_DirectPred_mutation,cnv_intermediate. Skipp
ing.
------------------------------------------------------------
------------------------------------------------------------
Model: DirectPred | Data: mutation,rna | Fusion: early
Prefix: run_DirectPred_mutation,rna_early
------------------------------------------------------------
Checking if all required files exist for run_DirectPred_mutation,rna_early
...
All output files found for run_DirectPred_mutation,rna_early. Skipping.
------------------------------------------------------------
------------------------------------------------------------
Model: DirectPred | Data: mutation,rna | Fusion: intermediate
Prefix: run_DirectPred_mutation,rna_intermediate
------------------------------------------------------------
Checking if all required files exist for run_DirectPred_mutation,rna_inter
mediate ...
All output files found for run_DirectPred_mutation,rna_intermediate. Skipp
ing.
------------------------------------------------------------
------------------------------------------------------------
Model: DirectPred | Data: rna,cnv | Fusion: early
Prefix: run_DirectPred_rna,cnv_early
------------------------------------------------------------
Checking if all required files exist for run_DirectPred_rna,cnv_early ...
All output files found for run_DirectPred_rna,cnv_early. Skipping.
------------------------------------------------------------
------------------------------------------------------------
Model: DirectPred | Data: rna,cnv | Fusion: intermediate
Prefix: run_DirectPred_rna,cnv_intermediate
------------------------------------------------------------
Checking if all required files exist for run_DirectPred_rna,cnv_intermedia
te ...
All output files found for run_DirectPred_rna,cnv_intermediate. Skipping.
------------------------------------------------------------
------------------------------------------------------------
Model: supervised_vae | Data: mutation | Fusion: early
Prefix: run_supervised_vae_mutation_early
------------------------------------------------------------
Checking if all required files exist for run_supervised_vae_mutation_early
...
All output files found for run_supervised_vae_mutation_early. Skipping.
------------------------------------------------------------
------------------------------------------------------------
Model: supervised_vae | Data: mutation | Fusion: intermediate
Prefix: run_supervised_vae_mutation_intermediate
------------------------------------------------------------
Checking if all required files exist for run_supervised_vae_mutation_inter
mediate ...
All output files found for run_supervised_vae_mutation_intermediate. Skipp
ing.
```

```
------------------------------------------------------------
------------------------------------------------------------
Model: supervised_vae | Data: rna | Fusion: early
Prefix: run_supervised_vae_rna_early
------------------------------------------------------------
Checking if all required files exist for run_supervised_vae_rna_early ...
All output files found for run_supervised_vae_rna_early. Skipping.
------------------------------------------------------------
------------------------------------------------------------
Model: supervised_vae | Data: rna | Fusion: intermediate
Prefix: run_supervised_vae_rna_intermediate
------------------------------------------------------------
Checking if all required files exist for run_supervised_vae_rna_intermedia
te ...
All output files found for run_supervised_vae_rna_intermediate. Skipping.
------------------------------------------------------------
------------------------------------------------------------
Model: supervised_vae | Data: cnv | Fusion: early
Prefix: run_supervised_vae_cnv_early
------------------------------------------------------------
Checking if all required files exist for run_supervised_vae_cnv_early ...
All output files found for run_supervised_vae_cnv_early. Skipping.
------------------------------------------------------------
------------------------------------------------------------
Model: supervised_vae | Data: cnv | Fusion: intermediate
Prefix: run_supervised_vae_cnv_intermediate
------------------------------------------------------------
Checking if all required files exist for run_supervised_vae_cnv_intermedia
te ...
All output files found for run_supervised_vae_cnv_intermediate. Skipping.
------------------------------------------------------------
------------------------------------------------------------
Model: supervised_vae | Data: mutation,cnv | Fusion: early
Prefix: run_supervised_vae_mutation,cnv_early
------------------------------------------------------------
Checking if all required files exist for run_supervised_vae_mutation,cnv_e
arly ...
All output files found for run_supervised_vae_mutation,cnv_early. Skippin
g.
------------------------------------------------------------
------------------------------------------------------------
Model: supervised_vae | Data: mutation,cnv | Fusion: intermediate
Prefix: run_supervised_vae_mutation,cnv_intermediate
------------------------------------------------------------
Checking if all required files exist for run_supervised_vae_mutation,cnv_i
ntermediate ...
All output files found for run_supervised_vae_mutation,cnv_intermediate. S
kipping.
------------------------------------------------------------
------------------------------------------------------------
Model: supervised_vae | Data: mutation,rna | Fusion: early
Prefix: run_supervised_vae_mutation,rna_early
------------------------------------------------------------
Checking if all required files exist for run_supervised_vae_mutation,rna_e
arly ...
All output files found for run_supervised_vae_mutation,rna_early. Skippin
g.
------------------------------------------------------------
------------------------------------------------------------
Model: supervised_vae | Data: mutation,rna | Fusion: intermediate
```

```
Prefix: run_supervised_vae_mutation,rna_intermediate
------------------------------------------------------------
Checking if all required files exist for run_supervised_vae_mutation,rna_i
ntermediate ...
All output files found for run_supervised_vae_mutation,rna_intermediate. S
kipping.
------------------------------------------------------------
------------------------------------------------------------
Model: supervised_vae | Data: rna,cnv | Fusion: early
Prefix: run_supervised_vae_rna,cnv_early
------------------------------------------------------------
Checking if all required files exist for run_supervised_vae_rna,cnv_early
...
All output files found for run_supervised_vae_rna,cnv_early. Skipping.
------------------------------------------------------------
------------------------------------------------------------
Model: supervised_vae | Data: rna,cnv | Fusion: intermediate
Prefix: run_supervised_vae_rna,cnv_intermediate
------------------------------------------------------------
Checking if all required files exist for run_supervised_vae_rna,cnv_interm
ediate ...
All output files found for run_supervised_vae_rna,cnv_intermediate. Skippi
ng.
------------------------------------------------------------
------------------------------------------------------------
Model: GNN | Data: mutation | gnn_conv_type=GC
Prefix: run_GNN_mutation_GC
------------------------------------------------------------
Checking if all required files exist for run_GNN_mutation_GC ...
All output files found for run_GNN_mutation_GC. Skipping.
------------------------------------------------------------
------------------------------------------------------------
Model: GNN | Data: mutation | gnn_conv_type=SAGE
Prefix: run_GNN_mutation_SAGE
------------------------------------------------------------
Checking if all required files exist for run_GNN_mutation_SAGE ...
All output files found for run_GNN_mutation_SAGE. Skipping.
------------------------------------------------------------
------------------------------------------------------------
Model: GNN | Data: rna | gnn_conv_type=GC
Prefix: run_GNN_rna_GC
------------------------------------------------------------
Checking if all required files exist for run_GNN_rna_GC ...
All output files found for run_GNN_rna_GC. Skipping.
------------------------------------------------------------
------------------------------------------------------------
Model: GNN | Data: rna | gnn_conv_type=SAGE
Prefix: run_GNN_rna_SAGE
------------------------------------------------------------
Checking if all required files exist for run_GNN_rna_SAGE ...
All output files found for run_GNN_rna_SAGE. Skipping.
------------------------------------------------------------
------------------------------------------------------------
Model: GNN | Data: cnv | gnn_conv_type=GC
Prefix: run_GNN_cnv_GC
------------------------------------------------------------
Checking if all required files exist for run_GNN_cnv_GC ...
All output files found for run_GNN_cnv_GC. Skipping.
------------------------------------------------------------
------------------------------------------------------------
```

```
Model: GNN | Data: cnv | gnn_conv_type=SAGE
Prefix: run_GNN_cnv_SAGE
------------------------------------------------------------
Checking if all required files exist for run_GNN_cnv_SAGE ...
All output files found for run_GNN_cnv_SAGE. Skipping.
------------------------------------------------------------
------------------------------------------------------------
Model: GNN | Data: mutation,cnv | gnn_conv_type=GC
Prefix: run_GNN_mutation,cnv_GC
------------------------------------------------------------
Checking if all required files exist for run_GNN_mutation,cnv_GC ...
All output files found for run_GNN_mutation,cnv_GC. Skipping.
------------------------------------------------------------
------------------------------------------------------------
Model: GNN | Data: mutation,cnv | gnn_conv_type=SAGE
Prefix: run_GNN_mutation,cnv_SAGE
------------------------------------------------------------
Checking if all required files exist for run_GNN_mutation,cnv_SAGE ...
All output files found for run_GNN_mutation,cnv_SAGE. Skipping.
------------------------------------------------------------
------------------------------------------------------------
Model: GNN | Data: mutation,rna | gnn_conv_type=GC
Prefix: run_GNN_mutation,rna_GC
------------------------------------------------------------
Checking if all required files exist for run_GNN_mutation,rna_GC ...
All output files found for run_GNN_mutation,rna_GC. Skipping.
------------------------------------------------------------
------------------------------------------------------------
Model: GNN | Data: mutation,rna | gnn_conv_type=SAGE
Prefix: run_GNN_mutation,rna_SAGE
------------------------------------------------------------
Checking if all required files exist for run_GNN_mutation,rna_SAGE ...
All output files found for run_GNN_mutation,rna_SAGE. Skipping.
------------------------------------------------------------
------------------------------------------------------------
Model: GNN | Data: rna,cnv | gnn_conv_type=GC
Prefix: run_GNN_rna,cnv_GC
------------------------------------------------------------
Checking if all required files exist for run_GNN_rna,cnv_GC ...
All output files found for run_GNN_rna,cnv_GC. Skipping.
------------------------------------------------------------
------------------------------------------------------------
Model: GNN | Data: rna,cnv | gnn_conv_type=SAGE
Prefix: run_GNN_rna,cnv_SAGE
------------------------------------------------------------
Checking if all required files exist for run_GNN_rna,cnv_SAGE ...
All output files found for run_GNN_rna,cnv_SAGE. Skipping.
------------------------------------------------------------
============================================================
All 36 Flexynesis runs completed or skipped if previously found.
Total: 24 (non-GNN) + 12 (GNN) = 36
Logs and best models are saved under 'logs_flexynesis'.
This script is designed by Dr. Karan Kumar, Postdoc at Institute of
Applied Microbiology, RWTH Aachen University, Germany.
Dr. Kumar Acknowledges compgen2025 module organized by Dr. Bora.
============================================================
```

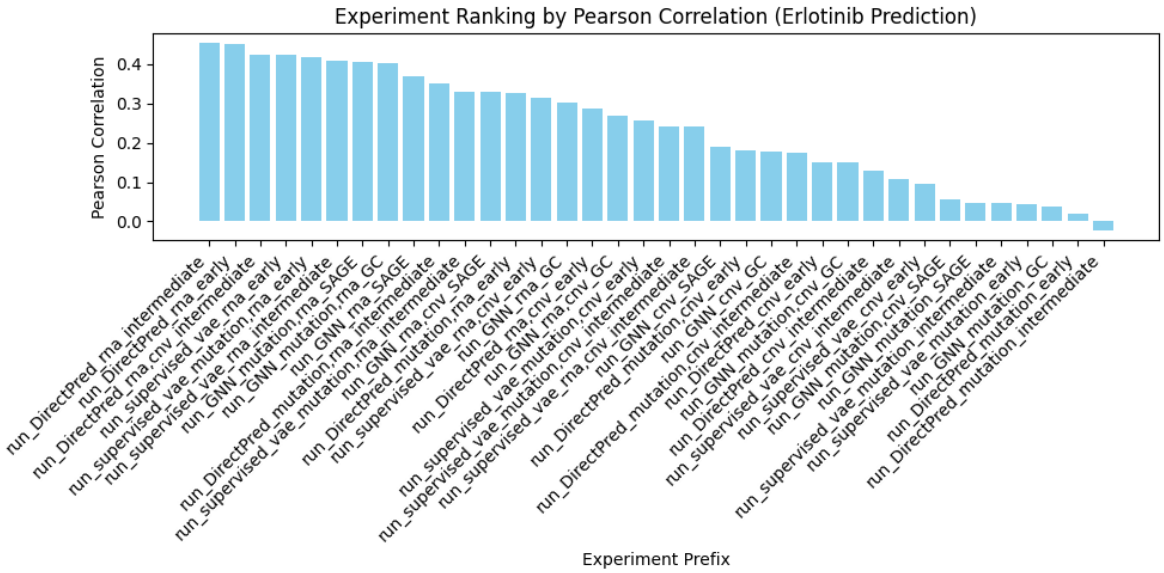
a) Import the results of the experiments from step 3, and rank the experiments based on performance (pearson_corr) Which combination yields the best results?

In [23]:
```
# Directory where logs and results are stored
LOGS_DIR = "logs_flexynesis"

# 1. Gather all .stats.csv files in LOGS_DIR
stats_files = glob.glob(os.path.join(LOGS_DIR, "**", "*.stats.csv"), recu

results = []
for file_path in stats_files:
    # Derive prefix from the filename (assuming e.g. "run_DirectPred_mut_
    prefix = os.path.basename(file_path).replace(".stats.csv", "")

    df_stats = pd.read_csv(file_path)

    # 2. Locate the row with metric == "pearson_corr"
    df_pearson = df_stats[df_stats["metric"] == "pearson_corr"]

    if not df_pearson.empty:
        pearson_val = df_pearson["value"].iloc[0]
    else:
        pearson_val = None  # if it doesn't exist

    results.append({
        "Prefix": prefix,
        "FilePath": file_path,
        "PearsonCorr": pearson_val
    })

# Convert to a DataFrame
results_df = pd.DataFrame(results)

# Drop rows with no pearson_corr available (if any)
results_df.dropna(subset=["PearsonCorr"], inplace=True)

# Sort experiments by pearson_corr descending (best at top)
results_df.sort_values(by="PearsonCorr", ascending=False, inplace=True)
results_df.reset_index(drop=True, inplace=True)

print("Ranking of experiments by Pearson correlation (descending):")
display(results_df)

# Visualize the Pearson correlation across experiments in a simple bar ch
plt.figure(figsize=(10, 5))
plt.bar(results_df["Prefix"], results_df["PearsonCorr"], color="skyblue")
plt.xticks(rotation=45, ha="right")
plt.xlabel("Experiment Prefix")
plt.ylabel("Pearson Correlation")
plt.title("Experiment Ranking by Pearson Correlation (Erlotinib Predictio
plt.tight_layout()
plt.show()

# Identify the best model (highest PearsonCorr)
best_model_prefix = results_df.iloc[0]["Prefix"]
print(f"The best model prefix is: {best_model_prefix}")
```

```
Ranking of experiments by Pearson correlation (descending):
```

	Prefix	FilePath	Pearso
0	run_DirectPred_rna_intermediate	logs_flexynesis/ run_DirectPred_rna_intermediat...	0.4
1	run_DirectPred_rna_early	logs_flexynesis/ run_DirectPred_rna_early/run_D...	0.4
2	run_DirectPred_rna,cnv_intermediate	logs_flexynesis/ run_DirectPred_rna,cnv_interme...	0.4
3	run_supervised_vae_rna_early	logs_flexynesis/ run_supervised_vae_rna_early/r...	0.4
4	run_supervised_vae_mutation,rna_early	logs_flexynesis/ run_supervised_vae_mutation,rn...	0.4
5	run_supervised_vae_rna_intermediate	logs_flexynesis/ run_supervised_vae_rna_interme...	0.4
6	run_GNN_mutation,rna_SAGE	logs_flexynesis/ run_GNN_mutation,rna_SAGE/ run_...	0.4
7	run_GNN_mutation,rna_GC	logs_flexynesis/ run_GNN_mutation,rna_GC/ run_GN...	0.4
8	run_GNN_rna_SAGE	logs_flexynesis/ run_GNN_rna_SAGE/ run_GNN_rna_S...	0.3
9	run_DirectPred_mutation,rna_intermediate	logs_flexynesis/ run_DirectPred_mutation,rna_in...	0.3
10	run_supervised_vae_mutation,rna_intermediate	logs_flexynesis/ run_supervised_vae_mutation,rn...	0.3
11	run_GNN_rna,cnv_SAGE	logs_flexynesis/ run_GNN_rna,cnv_SAGE/ run_GNN_r...	0.3
12	run_DirectPred_mutation,rna_early	logs_flexynesis/ run_DirectPred_mutation,rna_ea...	0.3
13	run_supervised_vae_rna,cnv_early	logs_flexynesis/ run_supervised_vae_rna,cnv_ear...	0.3
14	run_GNN_rna_GC	logs_flexynesis/run_GNN_rna_GC/ run_GNN_rna_GC....	0.3
15	run_DirectPred_rna,cnv_early	logs_flexynesis/ run_DirectPred_rna,cnv_early/r...	0.2
16	run_GNN_rna,cnv_GC	logs_flexynesis/ run_GNN_rna,cnv_GC/ run_GNN_rna...	0.2
17	run_supervised_vae_mutation,cnv_early	logs_flexynesis/ run_supervised_vae_mutation,cn...	0.2
18	run_supervised_vae_mutation,cnv_intermediate	logs_flexynesis/ run_supervised_vae_mutation,cn...	0.2
19	run_supervised_vae_rna,cnv_intermediate	logs_flexynesis/ run_supervised_vae_rna,cnv_int...	0.2

	Prefix	FilePath	Pearso
20	run_GNN_cnv_SAGE	logs_flexynesis/ run_GNN_cnv_SAGE/ run_GNN_cnv_S...	0.1
21	run_DirectPred_mutation,cnv_early	logs_flexynesis/ run_DirectPred_mutation,cnv_ea...	0.1
22	run_GNN_cnv_GC	logs_flexynesis/run_GNN_cnv_GC/ run_GNN_cnv_GC....	0.1
23	run_DirectPred_mutation,cnv_intermediate	logs_flexynesis/ run_DirectPred_mutation,cnv_in...	0.1
24	run_DirectPred_cnv_early	logs_flexynesis/ run_DirectPred_cnv_early/run_D...	0.1
25	run_GNN_mutation,cnv_GC	logs_flexynesis/ run_GNN_mutation,cnv_GC/ run_GN...	0.1
26	run_DirectPred_cnv_intermediate	logs_flexynesis/ run_DirectPred_cnv_intermediat...	0.1
27	run_supervised_vae_cnv_intermediate	logs_flexynesis/ run_supervised_vae_cnv_interme...	0.1
28	run_supervised_vae_cnv_early	logs_flexynesis/ run_supervised_vae_cnv_early/r...	0.0
29	run_GNN_mutation,cnv_SAGE	logs_flexynesis/ run_GNN_mutation,cnv_SAGE/ run_...	0.0
30	run_GNN_mutation_SAGE	logs_flexynesis/ run_GNN_mutation_SAGE/ run_GNN_...	0.0
31	run_supervised_vae_mutation_intermediate	logs_flexynesis/ run_supervised_vae_mutation_in...	0.0
32	run_supervised_vae_mutation_early	logs_flexynesis/ run_supervised_vae_mutation_ea...	0.0
33	run_GNN_mutation_GC	logs_flexynesis/ run_GNN_mutation_GC/ run_GNN_mu...	0.0
34	run_DirectPred_mutation_early	logs_flexynesis/ run_DirectPred_mutation_early/...	0.0
35	run_DirectPred_mutation_intermediate	logs_flexynesis/ run_DirectPred_mutation_interm...	-0.0



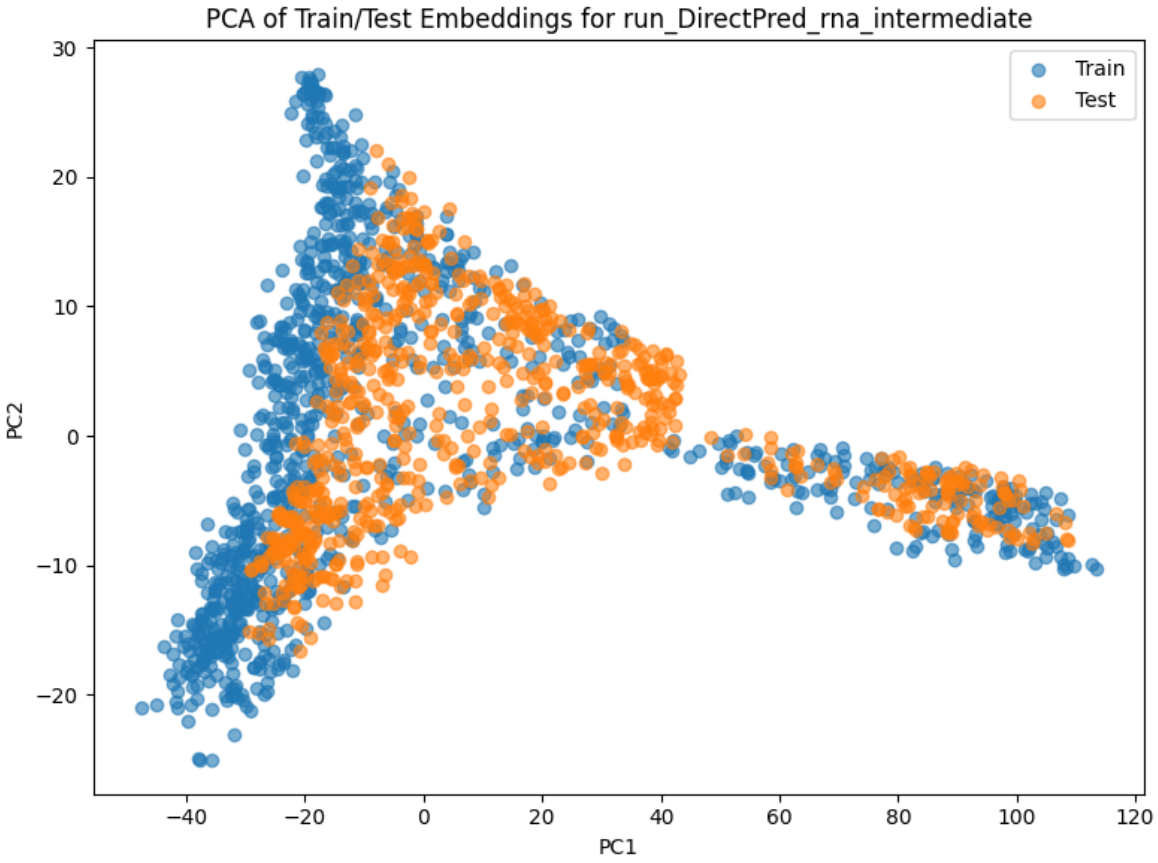

```
The best model prefix is: run_DirectPred_rna_intermediate
```

b) Explore the train/test embeddings from the best model (from 4a).

In [24]:
```
BEST_MODEL_DIR = os.path.join(LOGS_DIR, best_model_prefix)

# Embedding files look like: "<prefix>.embeddings_train.csv" and "<prefix
train_embeddings_path = os.path.join(BEST_MODEL_DIR, f"{best_model_prefix
test_embeddings_path  = os.path.join(BEST_MODEL_DIR, f"{best_model_prefix

# 1) Read and rename columns so the first column = "sample_id"
df_train_embed = pd.read_csv(train_embeddings_path)
df_test_embed = pd.read_csv(test_embeddings_path)

# Rename the first column in each to "sample_id" (since it's originally t
df_train_embed.rename(columns={df_train_embed.columns[0]: "sample_id"}, i
df_test_embed.rename(columns={df_test_embed.columns[0]: "sample_id"}, inp

print("Train Embeddings Shape:", df_train_embed.shape)
print("Test Embeddings Shape:", df_test_embed.shape)

# 2) Identify the embedding columns ("E0", "E1", ..., "E17").
#    We assume all columns except the first one are the embedding feature
embedding_cols = df_train_embed.columns[1:]  # E0..E17 for train

# 3) Run PCA on the numeric embedding columns only
pca = PCA(n_components=2)

# Fit on train, transform train and test
train_pca = pca.fit_transform(df_train_embed[embedding_cols])
test_pca  = pca.transform(df_test_embed[embedding_cols])

# 4) Plot the train/test embeddings in PCA space
plt.figure(figsize=(8, 6))
plt.scatter(train_pca[:,0], train_pca[:,1], alpha=0.6, label="Train")
plt.scatter(test_pca[:,0], test_pca[:,1], alpha=0.6, label="Test")
plt.title(f"PCA of Train/Test Embeddings for {best_model_prefix}")
plt.xlabel("PC1")
plt.ylabel("PC2")
plt.legend()
plt.tight_layout()
plt.show()
```

```
# 5) Display a small sample of each embedding DataFrame
print("Sample Train Embeddings:")
display(df_train_embed.head())

print("Sample Test Embeddings:")
display(df_test_embed.head())
```

```
Train Embeddings Shape: (1034, 17)
Test Embeddings Shape: (727, 17)
```



Sample Train Embeddings:

	sample_id	E0	E1	E2	E3	E4	E5	
0	CAS-1	-9.521608	3.208619	-6.779980	8.682497	0.630838	-5.129259	6.183
1	AU565	-3.748832	-3.107173	2.502489	-7.949045	0.658635	3.967231	3.281
2	HARA [Human squamous cell lung carcinoma]	-3.183113	-2.197794	-0.365624	-2.435834	1.628433	0.856045	1.761
3	MJ	24.992676	12.755637	-0.364261	-10.412441	1.358003	30.916039	-15.354
4	SU-DHL-4	37.493378	17.792190	4.345458	-14.346065	0.566390	46.487186	-23.227

Sample Test Embeddings:

	sample_id	E0	E1	E2	E3	E4	E5	
0	CAS-1	-2.699492	4.467287	-4.155583	4.622183	-0.218824	-1.142177	0.671
1	DJM-1	-4.247461	-3.437389	-0.124484	-3.895321	2.442992	1.929470	2.074
2	MN-60	35.054073	17.645554	3.266762	-13.409164	0.220840	42.818493	-22.172
3	Rh1	12.148687	8.613775	0.155137	-5.376956	-0.524279	12.207080	-8.110
4	MJ	25.870636	13.899988	-0.703533	-10.501465	1.698678	31.867535	-16.658

c) Import the feature importance scores from the best model (from 4a). Get top 10 markers.

In [25]:
```
feature_importance_path = os.path.join(BEST_MODEL_DIR, f"{best_model_pref

# 1. Read the feature importance CSV
df_importance = pd.read_csv(feature_importance_path)

# Columns: target_variable, target_class, target_class_label, layer, name
# 2. Sort by highest 'importance'
df_importance.sort_values(by="importance", ascending=False, inplace=True)

# 3. Extract the top 10 markers
top10 = df_importance.head(10)

print(f"Top 10 markers from {best_model_prefix}:")
display(top10)

# 4. Provide placeholders for further analysis
print("Next step: check if these markers (in 'name' column) are known to
```

```
Top 10 markers from run_DirectPred_rna_intermediate:
```

	target_variable	target_class	target_class_label	layer	name	importance	
847	Erlotinib	0	NaN	rna	HKDC1	0.001761	Integ
118	Erlotinib	0	NaN	rna	EGFR	0.001344	Integ
1116	Erlotinib	0	NaN	rna	XDH	0.001312	Integ
612	Erlotinib	0	NaN	rna	CTSV	0.001202	Integ
1008	Erlotinib	0	NaN	rna	GLS2	0.001201	Integ
528	Erlotinib	0	NaN	rna	ACSL5	0.001139	Integ
1224	Erlotinib	0	NaN	rna	VILL	0.001129	Integ
435	Erlotinib	0	NaN	rna	ICA1	0.001120	Integ
572	Erlotinib	0	NaN	rna	SH3YL1	0.001118	Integ
707	Erlotinib	0	NaN	rna	TBC1D30	0.001102	Integ

```
Next step: check if these markers (in 'name' column) are known to be relat
ed to Erlotinib response.
```

Do literature search. Are any of the top markers associated to “Erlotinib”?

Here is a summary of the associations between each gene from the provided table and Erlotinib treatment in the context of cancer therapies, supported by relevant research references:

1. HKDC1: Research indicates that HKDC1 (Hexokinase Domain Containing 1) plays a significant role in the metabolic processes of cancer cells, particularly in gastric cancer. The silencing of HKDC1 has been shown to inhibit the proliferation and glycolysis of gastric cancer cells, potentially enhancing the effectiveness of Erlotinib as a treatment. This suggests that targeting HKDC1 may complement the therapeutic impacts of Erlotinib in metabolic regulation Chen et al. (2023).

2. EGFR: The epidermal growth factor receptor (EGFR) is the primary target of Erlotinib. Erlotinib's efficacy is heavily reliant on its ability to inhibit EGFR signaling pathways, which are crucial in promoting cell growth and survival in non-small cell lung cancer (NSCLC). Studies have demonstrated that the presence of specific EGFR mutations can predict response to Erlotinib treatment, reinforcing its standing as a foundational therapy for cancers harboring these mutations (Abourbeh et al., 2015; Sette et al., 2015).

3. XDH: Xanthine dehydrogenase (XDH) has been implicated in various metabolic processes, yet its association with Erlotinib treatment is not well-established. Some studies suggest metabolic alterations in cancer cells can impact drug resistance, but the evidence directly linking XDH expression or activity to Erlotinib effectiveness is minimal. Further research is needed to clarify this relationship (Shen et al., 2019).

4. CTSV: Cathepsin V (CTSV) has not been directly associated with Erlotinib treatment in the current cancer literature. However, cathepsins are involved in cancer progression and may influence tumor microenvironments, which could be relevant in targeted therapies like Erlotinib. Without specific studies connecting CTSV to Erlotinib, its role remains speculative (Shen et al., 2019).

5. GLS2: Glutaminase 2 (GLS2) is involved in glutamine metabolism, which cancer cells often exploit. While a study demonstrated that GLS1 inhibitors can enhance the sensitivity of NSCLC cells to Erlotinib, direct studies on GLS2 specifically in the context of Erlotinib are limited (Wu et al., 2017).

6. ACSL5: Acyl-CoA synthetase long-chain family member 5 (ACSL5) has been reported to play a role in fatty acid metabolism and has implications in cancer biology. However, the influence of ACSL5 on Erlotinib resistance has not been extensively explored in the literature, indicating a need for further investigation into its potential interactions with Erlotinib therapy (Shen et al., 2019).

7. VILL: Villin (VILL) is a protein linked to cytoskeletal dynamics in epithelial cells. While its exact role in Erlotinib sensitivity is not well-documented, proteins that modulate cell architecture may influence drug responses indirectly. However, specific evidence linking VILL to Erlotinib treatment is lacking (Shen et al., 2019).

8. ICA1: ICA1 (Inducible cAMP early repressor) has not been studied directly in

connection with Erlotinib. Its involvement in intracellular signaling could hypothetically affect how cancer cells respond to various treatments, including Erlotinib, but further research is required to establish any direct correlations (Shen et al., 2019).

9. SH3YL1: The relationship of SH3YL1 to Erlotinib or cancer treatment in general has not been well-characterized in existing literature. As such, it does not appear to be a primary focus in Erlotinib research, indicating a need for more targeted studies to reveal its potential role (Shen et al., 2019).

10. TBC1D30: The gene TBC1D30 does not have established connections with Erlotinib treatment in the available cancer research literature. Its involvement in intracellular processes suggests a possible role in cancer cell communication, but it does not provide direct insights into Erlotinib efficacy (Shen et al., 2019).

References:

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