In [1]:
```
import glob
import csv
import pandas as pd
import flexynesis
from collections import defaultdict
from itertools import islice
from tabulate import tabulate
```

```
[rank: 0] Seed set to 42
```

- Input files were generated using a Slurm array job and `flex_conf.tsv`, so very easy to iterate over many combinations (98 in total)
- Files are on github
  - KH_day3_test_models_gpu_array.job was used to generate the data
    - Used flex_conf.tsv for list of variables to test
  - flexynesis_runs_gpu contains the outputs
- Command used to run `flexynesis` was:

```
flexynesis --data_path ./ccle_vs_gdsc/ --target_variables Erlotinib
\
    --hpo_iter 100 --features_top_percentile 10 --outdir ./
flexynesis_runs \
    --model_class ${class} \
    --data_types ${data_type} \
    --fusion_type ${fusion_type} \
    --prefix ${prefix}
```

- Where `class`, `data_type`, `fusion_type` and `prefix` (to name the output files) were taken from the config file
- Was based on the other parameters. e.g:
  - class = `DirectPred`
  - data_type = `cnv,rna`
  - fusion_type = `early`
  - prefix = `DP_cnv_rna_early`

In [2]:
```
#First get list of files, check we have correct number
stats_files = glob.glob("flexynesis_runs_gpu/*.stats.csv")
if len(stats_files)==0:
    raise Exception("WARNING - No stats files found!")
else:
    print(len(stats_files))
```

```
70
```

In [3]:
```
#Get pearson corr values for each file and store in default dict
pearson_values=defaultdict(float)
for file in stats_files:
    with open(file,"rt") as f_in:
        data_in=csv.DictReader(f_in)
        for row in data_in:
            if row["metric"]=="pearson_corr":
                pearson_values[file.removesuffix(".stats.csv")]=float(row["value"])
```

In [4]:
```
# Sort by value to get highest first
# NOTE - use abs since Pearson correlation goes from -1 to +1
print(tabulate([[k.split("/")[1], v] for k, v in sorted(pearson_values.items(), key
File                                     Rank
----------------------------------  ----------
DP_cnv_rna_intermediate             0.442977
DP_rna_early                        0.432765
DP_mutation_rna_intermediate        0.431637
DP_mutation_rna_early               0.407984
RF_rna_intermediate                 0.395603
SVAE_cnv_rna_intermediate           0.393623
RF_mutation_rna_early               0.393196
SVAE_mutation_rna_early             0.391337
RF_cnv_rna_intermediate             0.390664
XGB_mutation_rna_early              0.386213
SVAE_cnv_mutation_rna_intermediate  0.383251
RF_mutation_rna_intermediate        0.382885
XGB_rna_early                       0.381653
RF_cnv_rna_early                    0.381051
RF_rna_early                        0.380996
XGB_mutation_rna_intermediate       0.380361
RF_cnv_mutation_rna_intermediate    0.37719
SVAE_mutation_rna_intermediate      0.374065
RF_cnv_mutation_rna_early           0.373031
DP_rna_intermediate                 0.36828
SVAE_rna_intermediate               0.367124
XGB_rna_intermediate                0.358608
DP_cnv_rna_early                    0.349215
XGB_cnv_rna_early                   0.343795
XGB_cnv_rna_intermediate            0.342156
XGB_cnv_mutation_rna_early          0.339035
XGB_cnv_mutation_rna_intermediate   0.339035
SVAE_rna_early                      0.33199
SVM_mutation_rna_intermediate       0.324508
SVM_mutation_rna_early              0.323144
SVM_rna_early                       0.321807
SVM_rna_intermediate                0.321807
DP_cnv_mutation_rna_early           0.320266
SVAE_cnv_mutation_rna_early         0.319364
DP_cnv_mutation_rna_intermediate    0.25389
SVM_cnv_mutation_early              0.248631
SVM_cnv_mutation_intermediate       0.248579
SVAE_cnv_mutation_early             0.242968
DP_cnv_mutation_intermediate        0.224292
SVAE_cnv_rna_early                  0.220405
SVM_cnv_mutation_rna_early          0.220324
SVM_cnv_mutation_rna_intermediate   0.219508
DP_cnv_intermediate                 0.212797
SVAE_cnv_mutation_intermediate      0.212756
SVM_cnv_early                       0.204805
SVM_cnv_intermediate                0.204805
SVM_cnv_rna_early                   0.188696
SVM_cnv_rna_intermediate            0.188696
SVAE_cnv_early                      0.171016
DP_cnv_early                        0.149677
RF_cnv_mutation_early               0.145631
RF_cnv_mutation_intermediate        0.14257
XGB_cnv_mutation_early              0.115657
XGB_cnv_mutation_intermediate       0.115657
```

```
RF_cnv_intermediate                  0.108834
RF_cnv_early                         0.103964
SVAE_cnv_intermediate                0.103218
DP_cnv_mutation_early                0.101767
XGB_mutation_early                   0.0969347
XGB_mutation_intermediate            0.0969347
SVAE_mutation_intermediate           0.0852483
XGB_cnv_early                        0.0736077
XGB_cnv_intermediate                 0.0736077
SVM_mutation_intermediate            0.0537542
RF_mutation_early                    0.0444553
RF_mutation_intermediate             0.0417318
SVM_mutation_early                   0.0301753
DP_mutation_intermediate             0.0195059
DP_mutation_early                    0.0171416
SVAE_mutation_early                  0.00551811
```

In [5]:
```
# Above gives complete ranking, but we just want to take the best. Could just copy
best_score=float('-inf')
best_file=None
for file, score in pearson_values.items():
    if abs(score)>best_score:
        best_score=abs(score)
        best_file=file
#Note - Taking Pearson value from the dictionary here, rather than "best_score". Si
print(f"The best model was {best_file.split('/')[1]} with a pearson correlation of
```

```
The best model was DP_cnv_rna_intermediate with a pearson correlation of 0.443
```

In [6]:
```
best_test_E = pd.read_csv(f"{best_file}.embeddings_test.csv",index_col=0)
best_test_E.head()
```

Out[6]:

	E0	E1	E2	E3	E4	E5	E6	
HT-29	-3.171900	18.702538	16.695679	-18.600662	-0.033051	-22.472208	-15.506233	9.3
TE-10	-5.035516	9.025412	2.040252	-9.834312	4.803314	-3.681761	-6.823434	8.0
HN	-0.640362	11.684107	11.424771	-10.792943	-1.444747	-14.353040	-9.421462	4.3
SW872	-0.449053	22.439035	25.262285	-20.846043	-3.861798	-28.585697	-16.333190	8.7
HuP-T3	11.866579	-10.889995	-6.932766	5.245561	-2.116546	7.728584	-4.267910	2.0

5 rows × 256 columns

In [7]:
```
best_train_E = pd.read_csv(f"{best_file}.embeddings_train.csv",index_col=0)
best_train_E.head()
```

Out[7]:

	E0	E1	E2	E3	E4	E5	E6
HT-29	-1.091322	15.224613	16.648972	-14.422094	-2.383394	-19.867304	-11.618456
EFE-184	-1.686388	2.033938	-1.647987	-5.170491	3.086606	-3.286962	-7.165794
SNU-738	18.399225	-16.493600	-5.161220	10.380494	-6.891843	8.851066	-2.662938
UM-RC-6	4.603933	24.928680	48.100100	-20.128560	-19.839441	-42.647026	-13.696178
JHH-2	-5.058876	10.372157	3.365797	-16.254572	6.690586	-13.717236	-16.479500

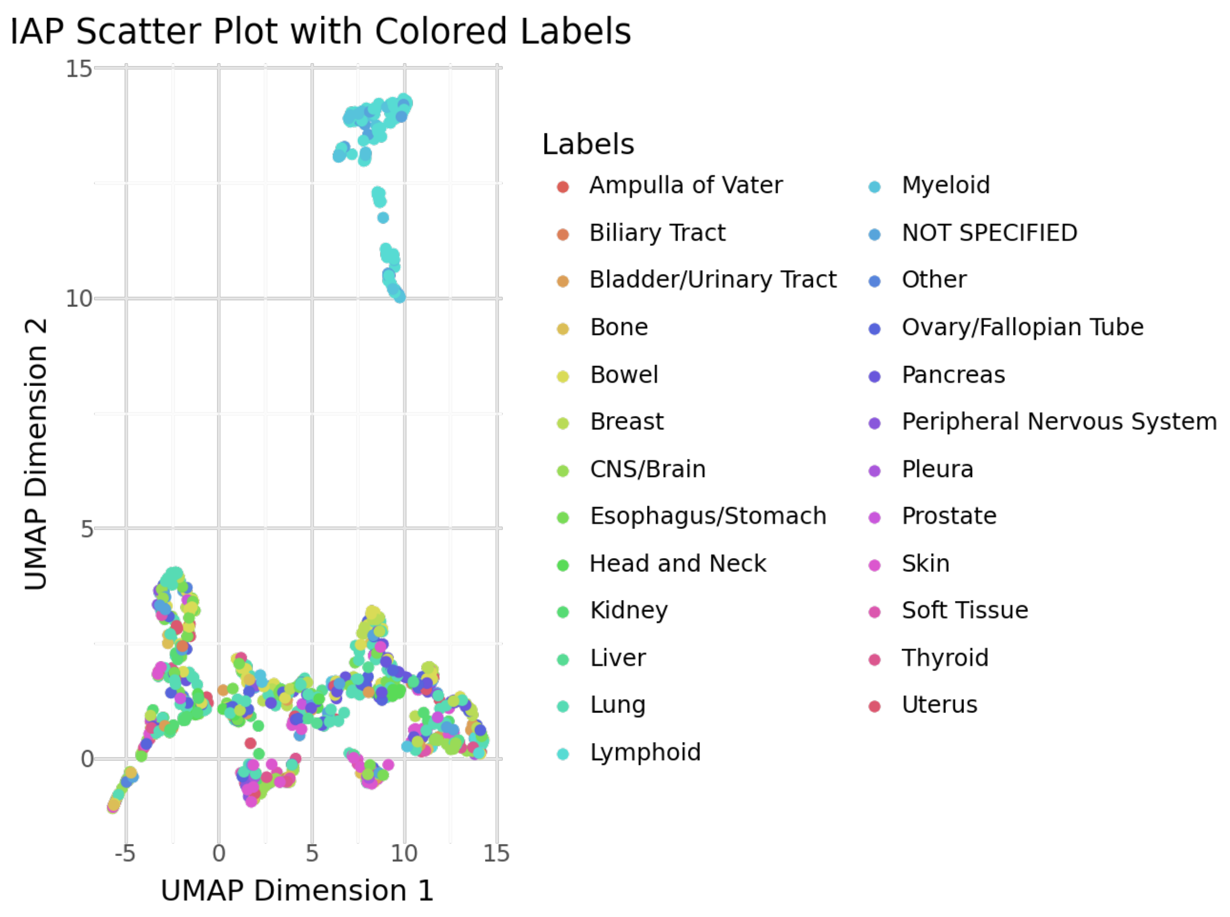
5 rows × 256 columns

In [8]:
```
clin_data=pd.read_csv("./ccle_vs_gdsc/train/clin.csv",index_col=0)
```

In [9]:
```
#Get sample types for PCA
sample_tissues=defaultdict(str)
for i,row in clin_data.iterrows():
    if row["Erlotinib"]:
        sample_tissues[row.name]=row["tissueid"]
train_labels = [sample_tissues[x] if x in sample_tissues.keys() else "NOT SPECIFIED
```

In [10]:
```
flexynesis.plot_dim_reduced(best_train_E, labels=train_labels, color_type = 'catego
```

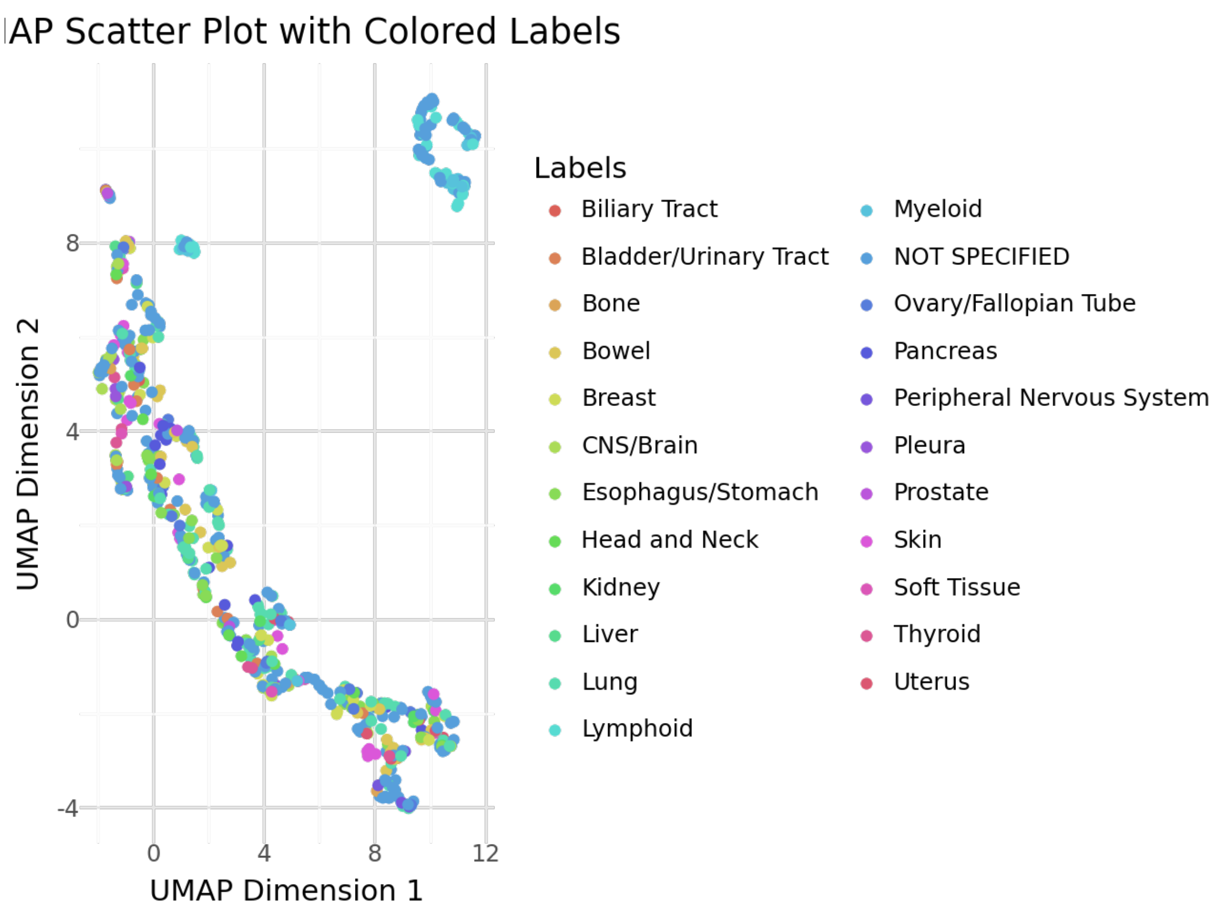
```
/usr/local/lib/python3.11/site-packages/sklearn/utils/deprecation.py:151: FutureWarn
ing: 'force_all_finite' was renamed to 'ensure_all_finite' in 1.6 and will be remove
d in 1.8.
```



```
In [11]: #Get sample types for PCA
         sample_tissues=defaultdict(str)
         for i,row in clin_data.iterrows():
             if row["Erlotinib"]:
                 sample_tissues[row.name]=row["tissueid"]
         test_labels = [sample_tissues[x] if x in sample_tissues.keys() else "NOT SPECIFIED"
```

```
In [12]: flexynesis.plot_dim_reduced(best_test_E, labels=test_labels, color_type = 'categori
```

```
/usr/local/lib/python3.11/site-packages/sklearn/utils/deprecation.py:151: FutureWarn
ing: 'force_all_finite' was renamed to 'ensure_all_finite' in 1.6 and will be remove
d in 1.8.
```



In [13]:
```
feature_scores_rna={}
feature_scores_cnv={}
feature_scores_mut={}
with open(f"{best_file}.feature_importance.IntegratedGradients.csv","rt") as f:
    data_in=csv.DictReader(f)
    for row in data_in:
        if row["layer"]=="cnv":
            feature_scores_cnv[row["name"]]=float(row["importance"])
        elif row["layer"]=="rna":
            feature_scores_rna[row["name"]]=float(row["importance"])
        elif row["layer"]=="mutation":
            feature_scores_mut[row["name"]]=float(row["importance"])
```

In [14]:
```
print(tabulate([[k, v] for k, v in sorted(feature_scores_rna.items(), key=lambda it
Gene       Importance
-------  ------------
EVPL       0.00245805
SACS       0.00241299
VILL       0.00230411
PCYOX1     0.00226497
ICA1       0.00214187
HKDC1      0.00206526
SLC44A4    0.00201588
NUAK2      0.00196789
LRRC8E     0.00194765
CELF2      0.00191327
LPAR1      0.00185839
XDH        0.00184949
EGFR       0.0018306
DPYSL3     0.00177932
DKK1       0.00176761
LYPD3      0.00175193
FAM216A    0.00174877
CLDN4      0.00174467
POU2AF1    0.00174066
EAF2       0.0017343
```

Top 10 features from RNA data:

- EVPL
- SACS
- VILL
- PCYOX1
- ICA1
- HKDC1
- SLC44A4
- NUAK2
- LRRC8E
- CELF2

None of these seem to have any known association with Erlotinib, however NUAK2 and HKDC1 has been implicated in progression of some cances and are kinases, so may have some possible interactions with Erlotinib

```
In [15]: print(tabulate([[k, v] for k, v in sorted(feature_scores_cnv.items(), key=lambda it
Gene         Importance
--------  ------------
SLC15A3    1.13261e-05
NOL4L      1.12278e-05
CD6        1.12201e-05
DUSP15     1.11505e-05
BPIFA4P    1.10506e-05
NOL4L-DT   1.09723e-05
DNMT3B     1.09312e-05
SUN5       1.09196e-05
REM1       1.08833e-05
BPIFB6     1.08729e-05
MAPRE1     1.08286e-05
BPIFB2     1.08128e-05
APLNR      1.0798e-05
BPIFA1     1.07818e-05
MIR3193    1.0776e-05
ZP1        1.0686e-05
TTLL9      1.06706e-05
COMMD7     1.06662e-05
BPIFA3     1.06413e-05
DHFRP3     1.064e-05
```

Importance of cnv data so low, not done lit search due to time constraints

```
In [16]: print(tabulate([[k, v] for k, v in sorted(feature_scores_mut.items(), key=lambda it
```

```
Gene    Importance
------  ------------
```

Mutation data was not used for the best model