IC50 Prediction with cells Submission

May 13, 2025

1 Simple feed forward NN to predict IC50 based on patient demographic and molecular drug information (INCLUDES CELL LINE FEATURE FOR TRAINING)

[2]: from CHEM277B functions import *

```
[3]: |valid_IC50s = pd.read_csv("data/valid_IC50s_within_range.csv")
    merged_df = pd.read_csv("data/final_merged_imputed_race_CSV.csv")
    lucas_df = pd.read_csv("data/Raw_Mapping_Imputed_Race.csv")
    cell_lines_df = pd.read_csv("data/HarvardCellLines.csv")
    /var/folders/s8/ghqk114n7n9_w17t7hx21g2m0000gn/T/ipykernel_12486/1684730604.py:2
    : DtypeWarning: Columns (3,4,5,6,7,9,12,15,16,17,18,22,24,26,28,29,30,67) have
    mixed types. Specify dtype option on import or set low_memory=False.
      merged df = pd.read csv("final merged imputed race CSV.csv")
[4]: valid_IC50s.drop(columns = ['Unnamed: 0', 'N Points'], inplace = True)
[5]: columns = ["HMS LINCS Batch ID", "Name", "T Stage"]
     cell_lines_df = cell_lines_df[columns]
    2 USE LUCAS' DATASET STARTING HERE
[7]: merged_df['T_stage_by_size'] = merged_df.apply(lambda row: row['T Stage'] if pd.
      anotnull(row['T Stage']) else T_stage_by_size(row['Tumor Size']), axis=1)
[8]: columns = ['Age', 'Race', 'T_stage_by_size']
    patients_df = merged_df[columns]
[9]: patients_df["cell_lines"] = lucas_df["Matched Cell Line ID"]
    /var/folders/s8/ghqk114n7n9_w17t7hx21g2m0000gn/T/ipykernel_12486/3231217547.py:1
    : SettingWithCopyWarning:
    A value is trying to be set on a copy of a slice from a DataFrame.
    Try using .loc[row_indexer,col_indexer] = value instead
```

```
docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
       patients_df["cell_lines"] = lucas_df["Matched Cell Line ID"]
[11]: cell_lines_df_dict = cell_lines_df.set_index("HMS LINCS Batch ID").

sto_dict()["Name"]

[13]: def mapping(row, dictionary):
          return dictionary[row]
[14]: patients_df["Cell Name"] = patients_df["cell_lines"].apply(mapping, dictionary_
       ⇔= cell_lines_df_dict)
     /var/folders/s8/ghqk114n7n9_w17t7hx21g2m0000gn/T/ipykernel_12486/1850949227.py:1
     : SettingWithCopyWarning:
     A value is trying to be set on a copy of a slice from a DataFrame.
     Try using .loc[row_indexer,col_indexer] = value instead
     See the caveats in the documentation: https://pandas.pydata.org/pandas-
     docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
       patients_df["Cell Name"] = patients_df["cell_lines"].apply(mapping, dictionary
     = cell_lines_df_dict)
[15]: patients_df.dropna(inplace=True)
      patients_df.isna().sum()
     /var/folders/s8/ghqk114n7n9_w17t7hx21g2m0000gn/T/ipykernel_12486/2483854490.py:1
     : SettingWithCopyWarning:
     A value is trying to be set on a copy of a slice from a DataFrame
     See the caveats in the documentation: https://pandas.pydata.org/pandas-
     docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
       patients df.dropna(inplace=True)
[15]: Age
                         0
                         0
     Race
      T_stage_by_size
                         0
      cell_lines
                         0
      Cell Name
      dtype: int64
```

See the caveats in the documentation: https://pandas.pydata.org/pandas-

3 Add Small Molecule descriptors for each row.

- 3.0.1 Cell lines are proxy for patients, so drop the cell lines column.
- 3.0.2 Need to one-hot-encode categorical features

```
[42]: categorical_cols = ['Race', 'T_stage_by_size', 'Small Molecule Name', 'Cell

→Name']

patient_drug_df[categorical_cols] = patient_drug_df[categorical_cols].

→astype('category')
```

```
[44]: patient_drug_df_encoded = pd.get_dummies(patient_drug_df,_u columns=categorical_cols, drop_first=True)
```

```
[46]: bool_cols = patient_drug_df_encoded.select_dtypes(include='bool').columns patient_drug_df_encoded[bool_cols] = patient_drug_df_encoded[bool_cols].

astype(int)
```

3.0.3 PRE-PROCESSING DONE. ONTO MODEL TRAINING.

```
[49]: # Separate features (X) and target (y)

X = patient_drug_df_encoded.drop(columns=['EC50 (uM)']) # Drop EC50 and

→non-features

y = patient_drug_df_encoded['EC50 (uM)'] # EC50 is the target

# Standardize numerical features
scaler = StandardScaler()
```

```
X[['Age', 'Molecular Mass', 'LogP', 'NumHDonors', 'NumHAcceptors', 'TPSA']] =
      ⇒scaler.fit_transform(X[['Age', 'Molecular Mass', 'LogP', 'NumHDonors', ⊔
       →'NumHAcceptors', 'TPSA']])
[51]: # Train/Test Split
     →random state=42)
[53]: # FEED FORWARD NEURAL NETWORK
     class DrugEncoder(nn.Module):
         def __init__(self, input_dim=5): # 5 molecular descriptors
             super().__init__()
             self.encoder = nn.Sequential(
                 nn.Linear(input_dim, 32),
                nn.ReLU(),
                 nn.Linear(32, 32)
             )
         def forward(self, x):
             return self.encoder(x.float())
     # SIMGPLE FEED FORWARD NEURAL NETWORK
     class PatientEncoder(nn.Module):
         def __init__(self, input_dim):
             super().__init__()
             self.encoder = nn.Sequential(
                 nn.Linear(input_dim, 32),
                nn.ReLU(),
                 nn.Linear(32, 32)
             )
         def forward(self, x):
             return self.encoder(x.float())
     # REGRESSION PREDICTION WITH SIMPLE FEED FORWARD NEURAL NETWORK
     class DrugResponsePredictor(nn.Module):
         def __init__(self, drug_input_dim, patient_input_dim):
             super().__init__()
             self.drug_encoder = DrugEncoder(drug_input_dim)
             self.patient_encoder = PatientEncoder(patient_input_dim)
             self.fc = nn.Sequential(
                 nn.Linear(32 + 32, 32),
                nn.ReLU(),
                nn.Linear(32, 1) # IC50 prediction
             )
```

```
def forward(self, drug_feat, patient_feat):
    drug_vec = self.drug_encoder(drug_feat)
    patient_vec = self.patient_encoder(patient_feat)
    combined = torch.cat([drug_vec, patient_vec], dim=1)
    return self.fc(combined).squeeze(-1)
```

```
[55]: # Data
      # Select drug descriptor columns
      drug_feature_cols = ['Molecular Mass', 'LogP', 'NumHDonors', 'NumHAcceptors', |
      drug_features = X_train[drug_feature_cols].to_numpy() # (n_samples, 5)
      # Drop drug features to get patient features
      patient_features = X_train.drop(columns=drug_feature_cols).to_numpy()
      # Convert to tensors
      drug_tensor = torch.tensor(drug_features).float()
      patient_tensor = torch.tensor(patient_features).float()
      ic50_tensor = torch.tensor(y_train.to_numpy()).float()
      model = DrugResponsePredictor(drug_input_dim=5,__
       spatient_input_dim=patient_tensor.shape[1])
      optimizer = torch.optim.Adam(model.parameters(), lr=1e-3)
      loss_fn = nn.MSELoss()
      # Training loop
      model.train()
      start_time = time.time()
      my_epochs = []
      my_losses = []
      for epoch in range (500):
          optimizer.zero_grad()
          preds = model(drug_tensor, patient_tensor)
          loss = loss_fn(preds, ic50_tensor)
          loss.backward()
          optimizer.step()
          end_time = time.time()
          elapsed = end_time - start_time
          print(f"Epoch {epoch} | Loss: {loss.item():.4f}")
          print(f"Time elapsed: {elapsed:.2f} seconds")
          my_epochs.append(epoch)
          my_losses.append(loss.item())
```

Epoch 0 | Loss: 3.2312

Time elapsed: 0.06 seconds Epoch 1 | Loss: 3.1874 Time elapsed: 0.10 seconds Epoch 2 | Loss: 3.1462 Time elapsed: 0.13 seconds Epoch 3 | Loss: 3.1065 Time elapsed: 0.16 seconds Epoch 4 | Loss: 3.0681 Time elapsed: 0.20 seconds Epoch 5 | Loss: 3.0308 Time elapsed: 0.23 seconds Epoch 6 | Loss: 2.9941 Time elapsed: 0.26 seconds Epoch 7 | Loss: 2.9579 Time elapsed: 0.30 seconds Epoch 8 | Loss: 2.9220 Time elapsed: 0.33 seconds Epoch 9 | Loss: 2.8867 Time elapsed: 0.36 seconds Epoch 10 | Loss: 2.8524 Time elapsed: 0.40 seconds Epoch 11 | Loss: 2.8190 Time elapsed: 0.43 seconds Epoch 12 | Loss: 2.7866 Time elapsed: 0.46 seconds Epoch 13 | Loss: 2.7546 Time elapsed: 0.50 seconds Epoch 14 | Loss: 2.7230 Time elapsed: 0.53 seconds Epoch 15 | Loss: 2.6914 Time elapsed: 0.56 seconds Epoch 16 | Loss: 2.6596 Time elapsed: 0.59 seconds Epoch 17 | Loss: 2.6275 Time elapsed: 0.63 seconds Epoch 18 | Loss: 2.5950 Time elapsed: 0.66 seconds Epoch 19 | Loss: 2.5623 Time elapsed: 0.69 seconds Epoch 20 | Loss: 2.5291 Time elapsed: 0.73 seconds Epoch 21 | Loss: 2.4955 Time elapsed: 0.76 seconds Epoch 22 | Loss: 2.4616 Time elapsed: 0.79 seconds Epoch 23 | Loss: 2.4276 Time elapsed: 0.82 seconds Epoch 24 | Loss: 2.3936

Time elapsed: 0.85 seconds Epoch 25 | Loss: 2.3598 Time elapsed: 0.88 seconds Epoch 26 | Loss: 2.3263 Time elapsed: 0.92 seconds Epoch 27 | Loss: 2.2932 Time elapsed: 0.95 seconds Epoch 28 | Loss: 2.2607 Time elapsed: 0.98 seconds Epoch 29 | Loss: 2.2290 Time elapsed: 1.01 seconds Epoch 30 | Loss: 2.1983 Time elapsed: 1.05 seconds Epoch 31 | Loss: 2.1688 Time elapsed: 1.08 seconds Epoch 32 | Loss: 2.1408 Time elapsed: 1.11 seconds Epoch 33 | Loss: 2.1145 Time elapsed: 1.14 seconds Epoch 34 | Loss: 2.0903 Time elapsed: 1.17 seconds Epoch 35 | Loss: 2.0683 Time elapsed: 1.21 seconds Epoch 36 | Loss: 2.0486 Time elapsed: 1.24 seconds Epoch 37 | Loss: 2.0316 Time elapsed: 1.27 seconds Epoch 38 | Loss: 2.0171 Time elapsed: 1.30 seconds Epoch 39 | Loss: 2.0051 Time elapsed: 1.33 seconds Epoch 40 | Loss: 1.9954 Time elapsed: 1.37 seconds Epoch 41 | Loss: 1.9876 Time elapsed: 1.40 seconds Epoch 42 | Loss: 1.9811 Time elapsed: 1.43 seconds Epoch 43 | Loss: 1.9755 Time elapsed: 1.46 seconds Epoch 44 | Loss: 1.9700 Time elapsed: 1.49 seconds Epoch 45 | Loss: 1.9643 Time elapsed: 1.53 seconds Epoch 46 | Loss: 1.9581 Time elapsed: 1.56 seconds Epoch 47 | Loss: 1.9510 Time elapsed: 1.59 seconds Epoch 48 | Loss: 1.9431

Time elapsed: 1.62 seconds Epoch 49 | Loss: 1.9345 Time elapsed: 1.65 seconds Epoch 50 | Loss: 1.9254 Time elapsed: 1.69 seconds Epoch 51 | Loss: 1.9157 Time elapsed: 1.72 seconds Epoch 52 | Loss: 1.9058 Time elapsed: 1.75 seconds Epoch 53 | Loss: 1.8957 Time elapsed: 1.78 seconds Epoch 54 | Loss: 1.8857 Time elapsed: 1.82 seconds Epoch 55 | Loss: 1.8758 Time elapsed: 1.85 seconds Epoch 56 | Loss: 1.8660 Time elapsed: 1.88 seconds Epoch 57 | Loss: 1.8563 Time elapsed: 1.91 seconds Epoch 58 | Loss: 1.8467 Time elapsed: 1.94 seconds Epoch 59 | Loss: 1.8370 Time elapsed: 1.98 seconds Epoch 60 | Loss: 1.8271 Time elapsed: 2.01 seconds Epoch 61 | Loss: 1.8170 Time elapsed: 2.04 seconds Epoch 62 | Loss: 1.8066 Time elapsed: 2.07 seconds Epoch 63 | Loss: 1.7957 Time elapsed: 2.11 seconds Epoch 64 | Loss: 1.7844 Time elapsed: 2.14 seconds Epoch 65 | Loss: 1.7726 Time elapsed: 2.17 seconds Epoch 66 | Loss: 1.7603 Time elapsed: 2.20 seconds Epoch 67 | Loss: 1.7475 Time elapsed: 2.24 seconds Epoch 68 | Loss: 1.7342 Time elapsed: 2.27 seconds Epoch 69 | Loss: 1.7206 Time elapsed: 2.30 seconds Epoch 70 | Loss: 1.7067 Time elapsed: 2.33 seconds Epoch 71 | Loss: 1.6923 Time elapsed: 2.37 seconds Epoch 72 | Loss: 1.6776

Time elapsed: 2.40 seconds Epoch 73 | Loss: 1.6626 Time elapsed: 2.43 seconds Epoch 74 | Loss: 1.6471 Time elapsed: 2.46 seconds Epoch 75 | Loss: 1.6312 Time elapsed: 2.49 seconds Epoch 76 | Loss: 1.6146 Time elapsed: 2.52 seconds Epoch 77 | Loss: 1.5974 Time elapsed: 2.56 seconds Epoch 78 | Loss: 1.5796 Time elapsed: 2.59 seconds Epoch 79 | Loss: 1.5610 Time elapsed: 2.62 seconds Epoch 80 | Loss: 1.5416 Time elapsed: 2.65 seconds Epoch 81 | Loss: 1.5213 Time elapsed: 2.69 seconds Epoch 82 | Loss: 1.5004 Time elapsed: 2.72 seconds Epoch 83 | Loss: 1.4792 Time elapsed: 2.75 seconds Epoch 84 | Loss: 1.4575 Time elapsed: 2.78 seconds Epoch 85 | Loss: 1.4352 Time elapsed: 2.82 seconds Epoch 86 | Loss: 1.4121 Time elapsed: 2.85 seconds Epoch 87 | Loss: 1.3883 Time elapsed: 2.88 seconds Epoch 88 | Loss: 1.3637 Time elapsed: 2.91 seconds Epoch 89 | Loss: 1.3387 Time elapsed: 2.94 seconds Epoch 90 | Loss: 1.3135 Time elapsed: 2.98 seconds Epoch 91 | Loss: 1.2879 Time elapsed: 3.01 seconds Epoch 92 | Loss: 1.2620 Time elapsed: 3.04 seconds Epoch 93 | Loss: 1.2357 Time elapsed: 3.07 seconds Epoch 94 | Loss: 1.2092 Time elapsed: 3.10 seconds Epoch 95 | Loss: 1.1826 Time elapsed: 3.14 seconds Epoch 96 | Loss: 1.1559

Time elapsed: 3.17 seconds Epoch 97 | Loss: 1.1294 Time elapsed: 3.20 seconds Epoch 98 | Loss: 1.1032 Time elapsed: 3.23 seconds Epoch 99 | Loss: 1.0775 Time elapsed: 3.26 seconds Epoch 100 | Loss: 1.0526 Time elapsed: 3.30 seconds Epoch 101 | Loss: 1.0285 Time elapsed: 3.33 seconds Epoch 102 | Loss: 1.0054 Time elapsed: 3.36 seconds Epoch 103 | Loss: 0.9833 Time elapsed: 3.39 seconds Epoch 104 | Loss: 0.9624 Time elapsed: 3.42 seconds Epoch 105 | Loss: 0.9428 Time elapsed: 3.45 seconds Epoch 106 | Loss: 0.9246 Time elapsed: 3.49 seconds Epoch 107 | Loss: 0.9079 Time elapsed: 3.52 seconds Epoch 108 | Loss: 0.8925 Time elapsed: 3.55 seconds Epoch 109 | Loss: 0.8785 Time elapsed: 3.58 seconds Epoch 110 | Loss: 0.8659 Time elapsed: 3.61 seconds Epoch 111 | Loss: 0.8545 Time elapsed: 3.64 seconds Epoch 112 | Loss: 0.8442 Time elapsed: 3.68 seconds Epoch 113 | Loss: 0.8348 Time elapsed: 3.71 seconds Epoch 114 | Loss: 0.8261 Time elapsed: 3.74 seconds Epoch 115 | Loss: 0.8182 Time elapsed: 3.77 seconds Epoch 116 | Loss: 0.8107 Time elapsed: 3.80 seconds Epoch 117 | Loss: 0.8035 Time elapsed: 3.83 seconds Epoch 118 | Loss: 0.7964 Time elapsed: 3.87 seconds Epoch 119 | Loss: 0.7897 Time elapsed: 3.90 seconds Epoch 120 | Loss: 0.7826

Time elapsed: 3.93 seconds Epoch 121 | Loss: 0.7758 Time elapsed: 3.96 seconds Epoch 122 | Loss: 0.7688 Time elapsed: 3.99 seconds Epoch 123 | Loss: 0.7617 Time elapsed: 4.02 seconds Epoch 124 | Loss: 0.7545 Time elapsed: 4.06 seconds Epoch 125 | Loss: 0.7473 Time elapsed: 4.09 seconds Epoch 126 | Loss: 0.7401 Time elapsed: 4.12 seconds Epoch 127 | Loss: 0.7329 Time elapsed: 4.15 seconds Epoch 128 | Loss: 0.7259 Time elapsed: 4.18 seconds Epoch 129 | Loss: 0.7189 Time elapsed: 4.21 seconds Epoch 130 | Loss: 0.7120 Time elapsed: 4.25 seconds Epoch 131 | Loss: 0.7053 Time elapsed: 4.28 seconds Epoch 132 | Loss: 0.6988 Time elapsed: 4.31 seconds Epoch 133 | Loss: 0.6924 Time elapsed: 4.34 seconds Epoch 134 | Loss: 0.6861 Time elapsed: 4.37 seconds Epoch 135 | Loss: 0.6799 Time elapsed: 4.41 seconds Epoch 136 | Loss: 0.6737 Time elapsed: 4.44 seconds Epoch 137 | Loss: 0.6675 Time elapsed: 4.47 seconds Epoch 138 | Loss: 0.6614 Time elapsed: 4.50 seconds Epoch 139 | Loss: 0.6551 Time elapsed: 4.53 seconds Epoch 140 | Loss: 0.6490 Time elapsed: 4.56 seconds Epoch 141 | Loss: 0.6429 Time elapsed: 4.59 seconds Epoch 142 | Loss: 0.6369 Time elapsed: 4.63 seconds Epoch 143 | Loss: 0.6307 Time elapsed: 4.66 seconds Epoch 144 | Loss: 0.6245

Time elapsed: 4.69 seconds Epoch 145 | Loss: 0.6183 Time elapsed: 4.72 seconds Epoch 146 | Loss: 0.6120 Time elapsed: 4.75 seconds Epoch 147 | Loss: 0.6057 Time elapsed: 4.78 seconds Epoch 148 | Loss: 0.5994 Time elapsed: 4.82 seconds Epoch 149 | Loss: 0.5930 Time elapsed: 4.85 seconds Epoch 150 | Loss: 0.5867 Time elapsed: 4.88 seconds Epoch 151 | Loss: 0.5803 Time elapsed: 4.91 seconds Epoch 152 | Loss: 0.5740 Time elapsed: 4.95 seconds Epoch 153 | Loss: 0.5676 Time elapsed: 4.98 seconds Epoch 154 | Loss: 0.5612 Time elapsed: 5.01 seconds Epoch 155 | Loss: 0.5548 Time elapsed: 5.04 seconds Epoch 156 | Loss: 0.5483 Time elapsed: 5.07 seconds Epoch 157 | Loss: 0.5419 Time elapsed: 5.10 seconds Epoch 158 | Loss: 0.5356 Time elapsed: 5.14 seconds Epoch 159 | Loss: 0.5292 Time elapsed: 5.17 seconds Epoch 160 | Loss: 0.5229 Time elapsed: 5.20 seconds Epoch 161 | Loss: 0.5167 Time elapsed: 5.23 seconds Epoch 162 | Loss: 0.5104 Time elapsed: 5.26 seconds Epoch 163 | Loss: 0.5042 Time elapsed: 5.29 seconds Epoch 164 | Loss: 0.4980 Time elapsed: 5.32 seconds Epoch 165 | Loss: 0.4918 Time elapsed: 5.36 seconds Epoch 166 | Loss: 0.4856 Time elapsed: 5.39 seconds Epoch 167 | Loss: 0.4794 Time elapsed: 5.42 seconds Epoch 168 | Loss: 0.4732

Time elapsed: 5.45 seconds Epoch 169 | Loss: 0.4670 Time elapsed: 5.49 seconds Epoch 170 | Loss: 0.4608 Time elapsed: 5.52 seconds Epoch 171 | Loss: 0.4547 Time elapsed: 5.55 seconds Epoch 172 | Loss: 0.4486 Time elapsed: 5.58 seconds Epoch 173 | Loss: 0.4425 Time elapsed: 5.61 seconds Epoch 174 | Loss: 0.4364 Time elapsed: 5.64 seconds Epoch 175 | Loss: 0.4303 Time elapsed: 5.68 seconds Epoch 176 | Loss: 0.4243 Time elapsed: 5.71 seconds Epoch 177 | Loss: 0.4184 Time elapsed: 5.74 seconds Epoch 178 | Loss: 0.4124 Time elapsed: 5.77 seconds Epoch 179 | Loss: 0.4066 Time elapsed: 5.80 seconds Epoch 180 | Loss: 0.4008 Time elapsed: 5.84 seconds Epoch 181 | Loss: 0.3950 Time elapsed: 5.87 seconds Epoch 182 | Loss: 0.3893 Time elapsed: 5.90 seconds Epoch 183 | Loss: 0.3837 Time elapsed: 5.93 seconds Epoch 184 | Loss: 0.3781 Time elapsed: 5.96 seconds Epoch 185 | Loss: 0.3727 Time elapsed: 6.00 seconds Epoch 186 | Loss: 0.3673 Time elapsed: 6.03 seconds Epoch 187 | Loss: 0.3619 Time elapsed: 6.06 seconds Epoch 188 | Loss: 0.3567 Time elapsed: 6.09 seconds Epoch 189 | Loss: 0.3516 Time elapsed: 6.13 seconds Epoch 190 | Loss: 0.3465 Time elapsed: 6.16 seconds Epoch 191 | Loss: 0.3415 Time elapsed: 6.19 seconds Epoch 192 | Loss: 0.3366

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Time elapsed: 7.77 seconds Epoch 241 | Loss: 0.1763 Time elapsed: 7.80 seconds Epoch 242 | Loss: 0.1740 Time elapsed: 7.83 seconds Epoch 243 | Loss: 0.1716 Time elapsed: 7.86 seconds Epoch 244 | Loss: 0.1694 Time elapsed: 7.90 seconds Epoch 245 | Loss: 0.1671 Time elapsed: 7.93 seconds Epoch 246 | Loss: 0.1649 Time elapsed: 7.96 seconds Epoch 247 | Loss: 0.1628 Time elapsed: 7.99 seconds Epoch 248 | Loss: 0.1607 Time elapsed: 8.03 seconds Epoch 249 | Loss: 0.1586 Time elapsed: 8.06 seconds Epoch 250 | Loss: 0.1566 Time elapsed: 8.09 seconds Epoch 251 | Loss: 0.1546 Time elapsed: 8.12 seconds Epoch 252 | Loss: 0.1526 Time elapsed: 8.15 seconds Epoch 253 | Loss: 0.1507 Time elapsed: 8.19 seconds Epoch 254 | Loss: 0.1488 Time elapsed: 8.22 seconds Epoch 255 | Loss: 0.1470 Time elapsed: 8.25 seconds Epoch 256 | Loss: 0.1451 Time elapsed: 8.28 seconds Epoch 257 | Loss: 0.1433 Time elapsed: 8.31 seconds Epoch 258 | Loss: 0.1416 Time elapsed: 8.34 seconds Epoch 259 | Loss: 0.1398 Time elapsed: 8.38 seconds Epoch 260 | Loss: 0.1381 Time elapsed: 8.41 seconds Epoch 261 | Loss: 0.1364 Time elapsed: 8.44 seconds Epoch 262 | Loss: 0.1347 Time elapsed: 8.47 seconds Epoch 263 | Loss: 0.1331 Time elapsed: 8.50 seconds Epoch 264 | Loss: 0.1315

Time elapsed: 8.53 seconds Epoch 265 | Loss: 0.1299 Time elapsed: 8.57 seconds Epoch 266 | Loss: 0.1283 Time elapsed: 8.60 seconds Epoch 267 | Loss: 0.1267 Time elapsed: 8.63 seconds Epoch 268 | Loss: 0.1252 Time elapsed: 8.66 seconds Epoch 269 | Loss: 0.1237 Time elapsed: 8.69 seconds Epoch 270 | Loss: 0.1222 Time elapsed: 8.73 seconds Epoch 271 | Loss: 0.1208 Time elapsed: 8.76 seconds Epoch 272 | Loss: 0.1194 Time elapsed: 8.79 seconds Epoch 273 | Loss: 0.1180 Time elapsed: 8.82 seconds Epoch 274 | Loss: 0.1166 Time elapsed: 8.86 seconds Epoch 275 | Loss: 0.1152 Time elapsed: 8.89 seconds Epoch 276 | Loss: 0.1139 Time elapsed: 8.92 seconds Epoch 277 | Loss: 0.1126 Time elapsed: 8.95 seconds Epoch 278 | Loss: 0.1113 Time elapsed: 8.98 seconds Epoch 279 | Loss: 0.1100 Time elapsed: 9.02 seconds Epoch 280 | Loss: 0.1087 Time elapsed: 9.05 seconds Epoch 281 | Loss: 0.1075 Time elapsed: 9.08 seconds Epoch 282 | Loss: 0.1062 Time elapsed: 9.11 seconds Epoch 283 | Loss: 0.1050 Time elapsed: 9.15 seconds Epoch 284 | Loss: 0.1037 Time elapsed: 9.21 seconds Epoch 285 | Loss: 0.1025 Time elapsed: 9.24 seconds Epoch 286 | Loss: 0.1013 Time elapsed: 9.28 seconds Epoch 287 | Loss: 0.1001 Time elapsed: 9.31 seconds Epoch 288 | Loss: 0.0989

Time elapsed: 9.35 seconds Epoch 289 | Loss: 0.0978 Time elapsed: 9.38 seconds Epoch 290 | Loss: 0.0966 Time elapsed: 9.42 seconds Epoch 291 | Loss: 0.0955 Time elapsed: 9.45 seconds Epoch 292 | Loss: 0.0944 Time elapsed: 9.48 seconds Epoch 293 | Loss: 0.0933 Time elapsed: 9.52 seconds Epoch 294 | Loss: 0.0922 Time elapsed: 9.55 seconds Epoch 295 | Loss: 0.0911 Time elapsed: 9.58 seconds Epoch 296 | Loss: 0.0901 Time elapsed: 9.61 seconds Epoch 297 | Loss: 0.0890 Time elapsed: 9.65 seconds Epoch 298 | Loss: 0.0880 Time elapsed: 9.68 seconds Epoch 299 | Loss: 0.0869 Time elapsed: 9.71 seconds Epoch 300 | Loss: 0.0859 Time elapsed: 9.74 seconds Epoch 301 | Loss: 0.0849 Time elapsed: 9.78 seconds Epoch 302 | Loss: 0.0839 Time elapsed: 9.81 seconds Epoch 303 | Loss: 0.0829 Time elapsed: 9.84 seconds Epoch 304 | Loss: 0.0819 Time elapsed: 9.89 seconds Epoch 305 | Loss: 0.0810 Time elapsed: 9.93 seconds Epoch 306 | Loss: 0.0800 Time elapsed: 9.96 seconds Epoch 307 | Loss: 0.0791 Time elapsed: 10.00 seconds Epoch 308 | Loss: 0.0781 Time elapsed: 10.03 seconds Epoch 309 | Loss: 0.0772 Time elapsed: 10.06 seconds Epoch 310 | Loss: 0.0763 Time elapsed: 10.10 seconds Epoch 311 | Loss: 0.0754 Time elapsed: 10.13 seconds Epoch 312 | Loss: 0.0745

Time elapsed: 10.16 seconds Epoch 313 | Loss: 0.0736 Time elapsed: 10.20 seconds Epoch 314 | Loss: 0.0728 Time elapsed: 10.23 seconds Epoch 315 | Loss: 0.0719 Time elapsed: 10.26 seconds Epoch 316 | Loss: 0.0711 Time elapsed: 10.30 seconds Epoch 317 | Loss: 0.0702 Time elapsed: 10.33 seconds Epoch 318 | Loss: 0.0694 Time elapsed: 10.37 seconds Epoch 319 | Loss: 0.0686 Time elapsed: 10.40 seconds Epoch 320 | Loss: 0.0678 Time elapsed: 10.44 seconds Epoch 321 | Loss: 0.0671 Time elapsed: 10.47 seconds Epoch 322 | Loss: 0.0663 Time elapsed: 10.53 seconds Epoch 323 | Loss: 0.0656 Time elapsed: 10.56 seconds Epoch 324 | Loss: 0.0648 Time elapsed: 10.60 seconds Epoch 325 | Loss: 0.0641 Time elapsed: 10.63 seconds Epoch 326 | Loss: 0.0633 Time elapsed: 10.67 seconds Epoch 327 | Loss: 0.0626 Time elapsed: 10.70 seconds Epoch 328 | Loss: 0.0619 Time elapsed: 10.74 seconds Epoch 329 | Loss: 0.0612 Time elapsed: 10.77 seconds Epoch 330 | Loss: 0.0605 Time elapsed: 10.80 seconds Epoch 331 | Loss: 0.0598 Time elapsed: 10.83 seconds Epoch 332 | Loss: 0.0592 Time elapsed: 10.87 seconds Epoch 333 | Loss: 0.0585 Time elapsed: 10.90 seconds Epoch 334 | Loss: 0.0578 Time elapsed: 10.93 seconds Epoch 335 | Loss: 0.0572 Time elapsed: 10.97 seconds Epoch 336 | Loss: 0.0565

Time elapsed: 11.00 seconds Epoch 337 | Loss: 0.0559 Time elapsed: 11.03 seconds Epoch 338 | Loss: 0.0553 Time elapsed: 11.06 seconds Epoch 339 | Loss: 0.0546 Time elapsed: 11.10 seconds Epoch 340 | Loss: 0.0540 Time elapsed: 11.13 seconds Epoch 341 | Loss: 0.0534 Time elapsed: 11.16 seconds Epoch 342 | Loss: 0.0528 Time elapsed: 11.19 seconds Epoch 343 | Loss: 0.0522 Time elapsed: 11.23 seconds Epoch 344 | Loss: 0.0516 Time elapsed: 11.26 seconds Epoch 345 | Loss: 0.0510 Time elapsed: 11.29 seconds Epoch 346 | Loss: 0.0505 Time elapsed: 11.33 seconds Epoch 347 | Loss: 0.0499 Time elapsed: 11.36 seconds Epoch 348 | Loss: 0.0494 Time elapsed: 11.39 seconds Epoch 349 | Loss: 0.0488 Time elapsed: 11.43 seconds Epoch 350 | Loss: 0.0483 Time elapsed: 11.46 seconds Epoch 351 | Loss: 0.0477 Time elapsed: 11.49 seconds Epoch 352 | Loss: 0.0472 Time elapsed: 11.53 seconds Epoch 353 | Loss: 0.0467 Time elapsed: 11.56 seconds Epoch 354 | Loss: 0.0462 Time elapsed: 11.59 seconds Epoch 355 | Loss: 0.0456 Time elapsed: 11.62 seconds Epoch 356 | Loss: 0.0451 Time elapsed: 11.66 seconds Epoch 357 | Loss: 0.0446 Time elapsed: 11.69 seconds Epoch 358 | Loss: 0.0442 Time elapsed: 11.72 seconds Epoch 359 | Loss: 0.0437 Time elapsed: 11.75 seconds Epoch 360 | Loss: 0.0432

Time elapsed: 11.79 seconds Epoch 361 | Loss: 0.0427 Time elapsed: 11.82 seconds Epoch 362 | Loss: 0.0423 Time elapsed: 11.85 seconds Epoch 363 | Loss: 0.0418 Time elapsed: 11.89 seconds Epoch 364 | Loss: 0.0414 Time elapsed: 11.92 seconds Epoch 365 | Loss: 0.0409 Time elapsed: 11.95 seconds Epoch 366 | Loss: 0.0405 Time elapsed: 11.98 seconds Epoch 367 | Loss: 0.0400 Time elapsed: 12.01 seconds Epoch 368 | Loss: 0.0396 Time elapsed: 12.05 seconds Epoch 369 | Loss: 0.0392 Time elapsed: 12.08 seconds Epoch 370 | Loss: 0.0388 Time elapsed: 12.11 seconds Epoch 371 | Loss: 0.0384 Time elapsed: 12.14 seconds Epoch 372 | Loss: 0.0380 Time elapsed: 12.18 seconds Epoch 373 | Loss: 0.0376 Time elapsed: 12.21 seconds Epoch 374 | Loss: 0.0372 Time elapsed: 12.24 seconds Epoch 375 | Loss: 0.0368 Time elapsed: 12.27 seconds Epoch 376 | Loss: 0.0364 Time elapsed: 12.31 seconds Epoch 377 | Loss: 0.0360 Time elapsed: 12.34 seconds Epoch 378 | Loss: 0.0356 Time elapsed: 12.37 seconds Epoch 379 | Loss: 0.0352 Time elapsed: 12.40 seconds Epoch 380 | Loss: 0.0348 Time elapsed: 12.43 seconds Epoch 381 | Loss: 0.0344 Time elapsed: 12.47 seconds Epoch 382 | Loss: 0.0341 Time elapsed: 12.50 seconds Epoch 383 | Loss: 0.0337 Time elapsed: 12.53 seconds Epoch 384 | Loss: 0.0333

Time elapsed: 12.57 seconds Epoch 385 | Loss: 0.0330 Time elapsed: 12.60 seconds Epoch 386 | Loss: 0.0326 Time elapsed: 12.63 seconds Epoch 387 | Loss: 0.0322 Time elapsed: 12.67 seconds Epoch 388 | Loss: 0.0319 Time elapsed: 12.70 seconds Epoch 389 | Loss: 0.0315 Time elapsed: 12.73 seconds Epoch 390 | Loss: 0.0312 Time elapsed: 12.76 seconds Epoch 391 | Loss: 0.0308 Time elapsed: 12.79 seconds Epoch 392 | Loss: 0.0305 Time elapsed: 12.83 seconds Epoch 393 | Loss: 0.0302 Time elapsed: 12.86 seconds Epoch 394 | Loss: 0.0299 Time elapsed: 12.89 seconds Epoch 395 | Loss: 0.0295 Time elapsed: 12.92 seconds Epoch 396 | Loss: 0.0292 Time elapsed: 12.96 seconds Epoch 397 | Loss: 0.0289 Time elapsed: 12.99 seconds Epoch 398 | Loss: 0.0286 Time elapsed: 13.02 seconds Epoch 399 | Loss: 0.0283 Time elapsed: 13.05 seconds Epoch 400 | Loss: 0.0280 Time elapsed: 13.09 seconds Epoch 401 | Loss: 0.0277 Time elapsed: 13.12 seconds Epoch 402 | Loss: 0.0274 Time elapsed: 13.15 seconds Epoch 403 | Loss: 0.0271 Time elapsed: 13.18 seconds Epoch 404 | Loss: 0.0268 Time elapsed: 13.21 seconds Epoch 405 | Loss: 0.0266 Time elapsed: 13.24 seconds Epoch 406 | Loss: 0.0263 Time elapsed: 13.28 seconds Epoch 407 | Loss: 0.0260 Time elapsed: 13.31 seconds Epoch 408 | Loss: 0.0257

Time elapsed: 13.34 seconds Epoch 409 | Loss: 0.0254 Time elapsed: 13.37 seconds Epoch 410 | Loss: 0.0251 Time elapsed: 13.41 seconds Epoch 411 | Loss: 0.0248 Time elapsed: 13.44 seconds Epoch 412 | Loss: 0.0246 Time elapsed: 13.47 seconds Epoch 413 | Loss: 0.0243 Time elapsed: 13.50 seconds Epoch 414 | Loss: 0.0240 Time elapsed: 13.53 seconds Epoch 415 | Loss: 0.0238 Time elapsed: 13.56 seconds Epoch 416 | Loss: 0.0235 Time elapsed: 13.60 seconds Epoch 417 | Loss: 0.0232 Time elapsed: 13.63 seconds Epoch 418 | Loss: 0.0230 Time elapsed: 13.66 seconds Epoch 419 | Loss: 0.0227 Time elapsed: 13.69 seconds Epoch 420 | Loss: 0.0224 Time elapsed: 13.72 seconds Epoch 421 | Loss: 0.0222 Time elapsed: 13.76 seconds Epoch 422 | Loss: 0.0219 Time elapsed: 13.79 seconds Epoch 423 | Loss: 0.0217 Time elapsed: 13.82 seconds Epoch 424 | Loss: 0.0214 Time elapsed: 13.85 seconds Epoch 425 | Loss: 0.0212 Time elapsed: 13.88 seconds Epoch 426 | Loss: 0.0209 Time elapsed: 13.92 seconds Epoch 427 | Loss: 0.0207 Time elapsed: 13.95 seconds Epoch 428 | Loss: 0.0205 Time elapsed: 13.98 seconds Epoch 429 | Loss: 0.0203 Time elapsed: 14.01 seconds Epoch 430 | Loss: 0.0201 Time elapsed: 14.04 seconds Epoch 431 | Loss: 0.0198 Time elapsed: 14.07 seconds Epoch 432 | Loss: 0.0195

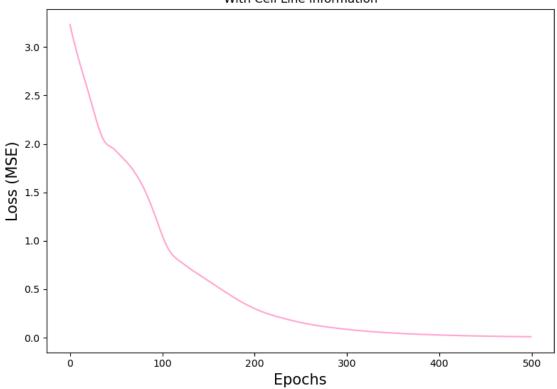
Time elapsed: 14.11 seconds Epoch 433 | Loss: 0.0193 Time elapsed: 14.15 seconds Epoch 434 | Loss: 0.0191 Time elapsed: 14.19 seconds Epoch 435 | Loss: 0.0189 Time elapsed: 14.22 seconds Epoch 436 | Loss: 0.0187 Time elapsed: 14.25 seconds Epoch 437 | Loss: 0.0185 Time elapsed: 14.29 seconds Epoch 438 | Loss: 0.0183 Time elapsed: 14.32 seconds Epoch 439 | Loss: 0.0181 Time elapsed: 14.35 seconds Epoch 440 | Loss: 0.0179 Time elapsed: 14.39 seconds Epoch 441 | Loss: 0.0177 Time elapsed: 14.42 seconds Epoch 442 | Loss: 0.0175 Time elapsed: 14.45 seconds Epoch 443 | Loss: 0.0173 Time elapsed: 14.48 seconds Epoch 444 | Loss: 0.0171 Time elapsed: 14.51 seconds Epoch 445 | Loss: 0.0169 Time elapsed: 14.55 seconds Epoch 446 | Loss: 0.0168 Time elapsed: 14.58 seconds Epoch 447 | Loss: 0.0166 Time elapsed: 14.61 seconds Epoch 448 | Loss: 0.0164 Time elapsed: 14.64 seconds Epoch 449 | Loss: 0.0162 Time elapsed: 14.68 seconds Epoch 450 | Loss: 0.0161 Time elapsed: 14.71 seconds Epoch 451 | Loss: 0.0159 Time elapsed: 14.74 seconds Epoch 452 | Loss: 0.0157 Time elapsed: 14.77 seconds Epoch 453 | Loss: 0.0156 Time elapsed: 14.80 seconds Epoch 454 | Loss: 0.0154 Time elapsed: 14.84 seconds Epoch 455 | Loss: 0.0153 Time elapsed: 14.87 seconds Epoch 456 | Loss: 0.0151

Time elapsed: 14.90 seconds Epoch 457 | Loss: 0.0149 Time elapsed: 14.93 seconds Epoch 458 | Loss: 0.0148 Time elapsed: 14.96 seconds Epoch 459 | Loss: 0.0147 Time elapsed: 14.99 seconds Epoch 460 | Loss: 0.0145 Time elapsed: 15.03 seconds Epoch 461 | Loss: 0.0144 Time elapsed: 15.06 seconds Epoch 462 | Loss: 0.0142 Time elapsed: 15.09 seconds Epoch 463 | Loss: 0.0141 Time elapsed: 15.12 seconds Epoch 464 | Loss: 0.0139 Time elapsed: 15.16 seconds Epoch 465 | Loss: 0.0138 Time elapsed: 15.19 seconds Epoch 466 | Loss: 0.0137 Time elapsed: 15.22 seconds Epoch 467 | Loss: 0.0135 Time elapsed: 15.25 seconds Epoch 468 | Loss: 0.0134 Time elapsed: 15.29 seconds Epoch 469 | Loss: 0.0133 Time elapsed: 15.32 seconds Epoch 470 | Loss: 0.0131 Time elapsed: 15.35 seconds Epoch 471 | Loss: 0.0130 Time elapsed: 15.38 seconds Epoch 472 | Loss: 0.0129 Time elapsed: 15.41 seconds Epoch 473 | Loss: 0.0128 Time elapsed: 15.45 seconds Epoch 474 | Loss: 0.0127 Time elapsed: 15.48 seconds Epoch 475 | Loss: 0.0125 Time elapsed: 15.51 seconds Epoch 476 | Loss: 0.0125 Time elapsed: 15.54 seconds Epoch 477 | Loss: 0.0124 Time elapsed: 15.57 seconds Epoch 478 | Loss: 0.0123 Time elapsed: 15.61 seconds Epoch 479 | Loss: 0.0121 Time elapsed: 15.64 seconds Epoch 480 | Loss: 0.0120

Time elapsed: 15.67 seconds Epoch 481 | Loss: 0.0119 Time elapsed: 15.70 seconds Epoch 482 | Loss: 0.0117 Time elapsed: 15.74 seconds Epoch 483 | Loss: 0.0116 Time elapsed: 15.77 seconds Epoch 484 | Loss: 0.0115 Time elapsed: 15.80 seconds Epoch 485 | Loss: 0.0114 Time elapsed: 15.83 seconds Epoch 486 | Loss: 0.0113 Time elapsed: 15.86 seconds Epoch 487 | Loss: 0.0112 Time elapsed: 15.90 seconds Epoch 488 | Loss: 0.0111 Time elapsed: 15.93 seconds Epoch 489 | Loss: 0.0110 Time elapsed: 15.96 seconds Epoch 490 | Loss: 0.0109 Time elapsed: 16.00 seconds Epoch 491 | Loss: 0.0108 Time elapsed: 16.03 seconds Epoch 492 | Loss: 0.0107 Time elapsed: 16.06 seconds Epoch 493 | Loss: 0.0106 Time elapsed: 16.09 seconds Epoch 494 | Loss: 0.0105 Time elapsed: 16.13 seconds Epoch 495 | Loss: 0.0104 Time elapsed: 16.16 seconds Epoch 496 | Loss: 0.0104 Time elapsed: 16.19 seconds Epoch 497 | Loss: 0.0103 Time elapsed: 16.22 seconds Epoch 498 | Loss: 0.0102 Time elapsed: 16.26 seconds Epoch 499 | Loss: 0.0101 Time elapsed: 16.29 seconds

[57]: epochs_vs_loss_with_cells(my_epochs,my_losses)

Epochs vs. Loss during training With Cell Line information



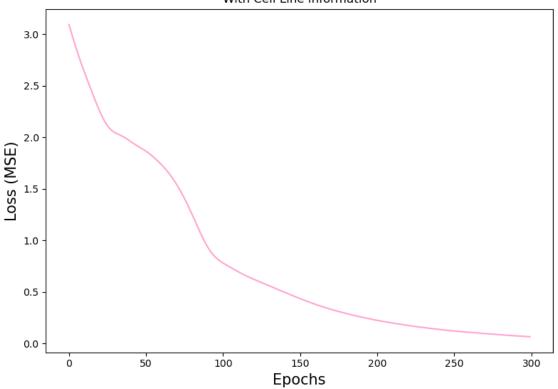
```
[59]: model = DrugResponsePredictor(drug_input_dim=5,__
       patient_input_dim=patient_tensor.shape[1])
      optimizer = torch.optim.Adam(model.parameters(), lr=1e-3)
      loss_fn = nn.MSELoss()
      # Training loop
      model.train()
      start_time = time.time()
      my_epochs = []
      my_losses = []
      for epoch in range(300):
          optimizer.zero_grad()
          preds = model(drug_tensor, patient_tensor)
          loss = loss_fn(preds, ic50_tensor)
          loss.backward()
          optimizer.step()
          end_time = time.time()
          elapsed = end_time - start_time
```

```
print(f"Epoch {epoch} | Loss: {loss.item():.4f}")
print(f"Time elapsed: {elapsed:.2f} seconds")
my_epochs.append(epoch)
my_losses.append(loss.item())
```

Epoch 0 | Loss: 3.0935 Time elapsed: 0.06 seconds Epoch 1 | Loss: 3.0416 Time elapsed: 0.10 seconds Epoch 2 | Loss: 2.9909 Time elapsed: 0.14 seconds Epoch 3 | Loss: 2.9418 Time elapsed: 0.17 seconds Epoch 4 | Loss: 2.8942 Time elapsed: 0.21 seconds Epoch 5 | Loss: 2.8478 Time elapsed: 0.24 seconds Epoch 6 | Loss: 2.8023 Time elapsed: 0.27 seconds Epoch 7 | Loss: 2.7578 Time elapsed: 0.31 seconds Epoch 8 | Loss: 2.7144 Time elapsed: 0.34 seconds Epoch 9 | Loss: 2.6727 Time elapsed: 0.37 seconds Epoch 10 | Loss: 2.6321 Time elapsed: 0.41 seconds Epoch 11 | Loss: 2.5922 Time elapsed: 0.44 seconds Epoch 12 | Loss: 2.5527 Time elapsed: 0.47 seconds Epoch 13 | Loss: 2.5135 Time elapsed: 0.50 seconds Epoch 14 | Loss: 2.4743 Time elapsed: 0.54 seconds Epoch 15 | Loss: 2.4354 Time elapsed: 0.57 seconds Epoch 16 | Loss: 2.3968 Time elapsed: 0.60 seconds Epoch 17 | Loss: 2.3586 Time elapsed: 0.63 seconds Epoch 18 | Loss: 2.3212 Time elapsed: 0.66 seconds Epoch 19 | Loss: 2.2852 Time elapsed: 0.70 seconds Epoch 20 | Loss: 2.2507 Time elapsed: 0.73 seconds Epoch 21 | Loss: 2.2181 Time elapsed: 0.76 seconds Epoch 22 | Loss: 2.1877 Time elapsed: 0.79 seconds Epoch 23 | Loss: 2.1599 Time elapsed: 0.83 seconds Epoch 24 | Loss: 2.1347 Time elapsed: 0.86 seconds Epoch 25 | Loss: 2.1125 Time elapsed: 0.89 seconds Epoch 26 | Loss: 2.0933 Time elapsed: 0.92 seconds Epoch 27 | Loss: 2.0772 Time elapsed: 0.95 seconds Epoch 28 | Loss: 2.0638 Time elapsed: 0.99 seconds Epoch 29 | Loss: 2.0530 Time elapsed: 1.02 seconds Epoch 30 | Loss: 2.0441 Time elapsed: 1.05 seconds Epoch 31 | Loss: 2.0365 Time elapsed: 1.08 seconds Epoch 32 | Loss: 2.0296 Time elapsed: 1.11 seconds Epoch 33 | Loss: 2.0230 Time elapsed: 1.15 seconds Epoch 34 | Loss: 2.0158 Time elapsed: 1.18 seconds Epoch 35 | Loss: 2.0081 Time elapsed: 1.21 seconds Epoch 36 | Loss: 1.9995 Time elapsed: 1.24 seconds Epoch 37 | Loss: 1.9901 Time elapsed: 1.27 seconds Epoch 38 | Loss: 1.9801 Time elapsed: 1.31 seconds Epoch 39 | Loss: 1.9697 Time elapsed: 1.34 seconds Epoch 40 | Loss: 1.9593 Time elapsed: 1.37 seconds Epoch 41 | Loss: 1.9490 Time elapsed: 1.40 seconds Epoch 42 | Loss: 1.9391 Time elapsed: 1.43 seconds Epoch 43 | Loss: 1.9296 Time elapsed: 1.47 seconds Epoch 44 | Loss: 1.9204 Time elapsed: 1.50 seconds Epoch 45 | Loss: 1.9115 Time elapsed: 1.53 seconds Epoch 46 | Loss: 1.9026 Time elapsed: 1.56 seconds Epoch 47 | Loss: 1.8937 Time elapsed: 1.59 seconds Epoch 48 | Loss: 1.8845 Time elapsed: 1.63 seconds Epoch 49 | Loss: 1.8750 Time elapsed: 1.66 seconds Epoch 50 | Loss: 1.8650 Time elapsed: 1.69 seconds Epoch 51 | Loss: 1.8544 Time elapsed: 1.72 seconds Epoch 52 | Loss: 1.8433 Time elapsed: 1.75 seconds Epoch 53 | Loss: 1.8315 Time elapsed: 1.79 seconds Epoch 54 | Loss: 1.8192 Time elapsed: 1.82 seconds Epoch 55 | Loss: 1.8063 Time elapsed: 1.85 seconds Epoch 56 | Loss: 1.7930 Time elapsed: 1.88 seconds Epoch 57 | Loss: 1.7791 Time elapsed: 1.91 seconds Epoch 58 | Loss: 1.7648 Time elapsed: 1.94 seconds Epoch 59 | Loss: 1.7500 Time elapsed: 1.98 seconds Epoch 60 | Loss: 1.7348 Time elapsed: 2.01 seconds Epoch 61 | Loss: 1.7190 Time elapsed: 2.04 seconds Epoch 62 | Loss: 1.7026 Time elapsed: 2.07 seconds Epoch 63 | Loss: 1.6854 Time elapsed: 2.10 seconds Epoch 64 | Loss: 1.6674 Time elapsed: 2.13 seconds Epoch 65 | Loss: 1.6486 Time elapsed: 2.17 seconds Epoch 66 | Loss: 1.6288 Time elapsed: 2.20 seconds Epoch 67 | Loss: 1.6081 Time elapsed: 2.23 seconds Epoch 68 | Loss: 1.5863 Time elapsed: 2.26 seconds Epoch 69 | Loss: 1.5635 Time elapsed: 2.29 seconds Epoch 70 | Loss: 1.5396 Time elapsed: 2.33 seconds Epoch 71 | Loss: 1.5146 Time elapsed: 2.36 seconds Epoch 72 | Loss: 1.4887 Time elapsed: 2.39 seconds Epoch 73 | Loss: 1.4618 Time elapsed: 2.42 seconds Epoch 74 | Loss: 1.4339 Time elapsed: 2.45 seconds Epoch 75 | Loss: 1.4051 Time elapsed: 2.49 seconds Epoch 76 | Loss: 1.3754 Time elapsed: 2.52 seconds Epoch 77 | Loss: 1.3448 Time elapsed: 2.55 seconds Epoch 78 | Loss: 1.3135 Time elapsed: 2.58 seconds Epoch 79 | Loss: 1.2815 Time elapsed: 2.61 seconds Epoch 80 | Loss: 1.2488 Time elapsed: 2.65 seconds Epoch 81 | Loss: 1.2157 Time elapsed: 2.68 seconds Epoch 82 | Loss: 1.1822 Time elapsed: 2.71 seconds Epoch 83 | Loss: 1.1487 Time elapsed: 2.74 seconds Epoch 84 | Loss: 1.1153 Time elapsed: 2.77 seconds Epoch 85 | Loss: 1.0824 Time elapsed: 2.80 seconds Epoch 86 | Loss: 1.0502 Time elapsed: 2.84 seconds Epoch 87 | Loss: 1.0192 Time elapsed: 2.87 seconds Epoch 88 | Loss: 0.9898 Time elapsed: 2.90 seconds Epoch 89 | Loss: 0.9621 Time elapsed: 2.93 seconds Epoch 90 | Loss: 0.9363 Time elapsed: 2.96 seconds Epoch 91 | Loss: 0.9126 Time elapsed: 3.00 seconds Epoch 92 | Loss: 0.8911 Time elapsed: 3.03 seconds Epoch 93 | Loss: 0.8717 Time elapsed: 3.06 seconds Epoch 94 | Loss: 0.8542 Time elapsed: 3.09 seconds Epoch 95 | Loss: 0.8386 Time elapsed: 3.12 seconds Epoch 96 | Loss: 0.8246 Time elapsed: 3.16 seconds Epoch 97 | Loss: 0.8120 Time elapsed: 3.19 seconds Epoch 98 | Loss: 0.8008 Time elapsed: 3.22 seconds Epoch 99 | Loss: 0.7905 Time elapsed: 3.25 seconds Epoch 100 | Loss: 0.7810 Time elapsed: 3.28 seconds Epoch 101 | Loss: 0.7720 Time elapsed: 3.32 seconds Epoch 102 | Loss: 0.7633 Time elapsed: 3.35 seconds Epoch 103 | Loss: 0.7547 Time elapsed: 3.38 seconds Epoch 104 | Loss: 0.7462 Time elapsed: 3.41 seconds Epoch 105 | Loss: 0.7376 Time elapsed: 3.44 seconds Epoch 106 | Loss: 0.7290 Time elapsed: 3.47 seconds Epoch 107 | Loss: 0.7204 Time elapsed: 3.51 seconds Epoch 108 | Loss: 0.7118 Time elapsed: 3.54 seconds Epoch 109 | Loss: 0.7035 Time elapsed: 3.57 seconds Epoch 110 | Loss: 0.6952 Time elapsed: 3.60 seconds Epoch 111 | Loss: 0.6871 Time elapsed: 3.63 seconds Epoch 112 | Loss: 0.6792 Time elapsed: 3.67 seconds Epoch 113 | Loss: 0.6715 Time elapsed: 3.70 seconds Epoch 114 | Loss: 0.6640 Time elapsed: 3.73 seconds Epoch 115 | Loss: 0.6568 Time elapsed: 3.76 seconds Epoch 116 | Loss: 0.6498 Time elapsed: 3.80 seconds Epoch 117 | Loss: 0.6431 Time elapsed: 3.83 seconds Epoch 118 | Loss: 0.6365 Time elapsed: 3.86 seconds Epoch 119 | Loss: 0.6300 Time elapsed: 3.89 seconds Epoch 120 | Loss: 0.6236 Time elapsed: 3.92 seconds Epoch 121 | Loss: 0.6172 Time elapsed: 3.96 seconds Epoch 122 | Loss: 0.6108 Time elapsed: 3.99 seconds Epoch 123 | Loss: 0.6044 Time elapsed: 4.02 seconds Epoch 124 | Loss: 0.5981 Time elapsed: 4.05 seconds Epoch 125 | Loss: 0.5917 Time elapsed: 4.08 seconds Epoch 126 | Loss: 0.5852 Time elapsed: 4.12 seconds Epoch 127 | Loss: 0.5788 Time elapsed: 4.15 seconds Epoch 128 | Loss: 0.5724 Time elapsed: 4.18 seconds Epoch 129 | Loss: 0.5659 Time elapsed: 4.21 seconds Epoch 130 | Loss: 0.5595 Time elapsed: 4.24 seconds Epoch 131 | Loss: 0.5532 Time elapsed: 4.28 seconds Epoch 132 | Loss: 0.5468 Time elapsed: 4.31 seconds Epoch 133 | Loss: 0.5405 Time elapsed: 4.34 seconds Epoch 134 | Loss: 0.5343 Time elapsed: 4.37 seconds Epoch 135 | Loss: 0.5280 Time elapsed: 4.41 seconds Epoch 136 | Loss: 0.5218 Time elapsed: 4.44 seconds Epoch 137 | Loss: 0.5155 Time elapsed: 4.47 seconds Epoch 138 | Loss: 0.5094 Time elapsed: 4.50 seconds Epoch 139 | Loss: 0.5032 Time elapsed: 4.53 seconds Epoch 140 | Loss: 0.4970 Time elapsed: 4.57 seconds Epoch 141 | Loss: 0.4909 Time elapsed: 4.60 seconds Epoch 142 | Loss: 0.4847 Time elapsed: 4.63 seconds Epoch 143 | Loss: 0.4785 Time elapsed: 4.66 seconds Epoch 144 | Loss: 0.4724 Time elapsed: 4.69 seconds Epoch 145 | Loss: 0.4662 Time elapsed: 4.73 seconds Epoch 146 | Loss: 0.4601 Time elapsed: 4.76 seconds Epoch 147 | Loss: 0.4540 Time elapsed: 4.79 seconds Epoch 148 | Loss: 0.4480 Time elapsed: 4.82 seconds Epoch 149 | Loss: 0.4420 Time elapsed: 4.86 seconds Epoch 150 | Loss: 0.4360 Time elapsed: 4.89 seconds Epoch 151 | Loss: 0.4301 Time elapsed: 4.92 seconds Epoch 152 | Loss: 0.4244 Time elapsed: 4.95 seconds Epoch 153 | Loss: 0.4186 Time elapsed: 4.98 seconds Epoch 154 | Loss: 0.4130 Time elapsed: 5.02 seconds Epoch 155 | Loss: 0.4074 Time elapsed: 5.05 seconds Epoch 156 | Loss: 0.4019 Time elapsed: 5.08 seconds Epoch 157 | Loss: 0.3964 Time elapsed: 5.11 seconds Epoch 158 | Loss: 0.3910 Time elapsed: 5.15 seconds Epoch 159 | Loss: 0.3857 Time elapsed: 5.18 seconds Epoch 160 | Loss: 0.3805 Time elapsed: 5.21 seconds Epoch 161 | Loss: 0.3753 Time elapsed: 5.24 seconds Epoch 162 | Loss: 0.3703 Time elapsed: 5.27 seconds Epoch 163 | Loss: 0.3653 Time elapsed: 5.31 seconds Epoch 164 | Loss: 0.3603 Time elapsed: 5.34 seconds Epoch 165 | Loss: 0.3555 Time elapsed: 5.37 seconds Epoch 166 | Loss: 0.3507 Time elapsed: 5.40 seconds Epoch 167 | Loss: 0.3461 Time elapsed: 5.44 seconds Epoch 168 | Loss: 0.3415 Time elapsed: 5.47 seconds Epoch 169 | Loss: 0.3369 Time elapsed: 5.50 seconds Epoch 170 | Loss: 0.3325 Time elapsed: 5.53 seconds Epoch 171 | Loss: 0.3282 Time elapsed: 5.56 seconds Epoch 172 | Loss: 0.3240 Time elapsed: 5.60 seconds Epoch 173 | Loss: 0.3198 Time elapsed: 5.63 seconds Epoch 174 | Loss: 0.3157 Time elapsed: 5.66 seconds Epoch 175 | Loss: 0.3116 Time elapsed: 5.69 seconds Epoch 176 | Loss: 0.3075 Time elapsed: 5.72 seconds Epoch 177 | Loss: 0.3035 Time elapsed: 5.76 seconds Epoch 178 | Loss: 0.2996 Time elapsed: 5.79 seconds Epoch 179 | Loss: 0.2958 Time elapsed: 5.82 seconds Epoch 180 | Loss: 0.2920 Time elapsed: 5.85 seconds Epoch 181 | Loss: 0.2882 Time elapsed: 5.89 seconds Epoch 182 | Loss: 0.2845 Time elapsed: 5.92 seconds Epoch 183 | Loss: 0.2809 Time elapsed: 5.95 seconds Epoch 184 | Loss: 0.2773 Time elapsed: 5.98 seconds Epoch 185 | Loss: 0.2738 Time elapsed: 6.01 seconds Epoch 186 | Loss: 0.2703 Time elapsed: 6.05 seconds Epoch 187 | Loss: 0.2668 Time elapsed: 6.08 seconds Epoch 188 | Loss: 0.2634 Time elapsed: 6.11 seconds Epoch 189 | Loss: 0.2601 Time elapsed: 6.14 seconds Epoch 190 | Loss: 0.2568 Time elapsed: 6.18 seconds Epoch 191 | Loss: 0.2535 Time elapsed: 6.21 seconds Epoch 192 | Loss: 0.2503 Time elapsed: 6.24 seconds Epoch 193 | Loss: 0.2471 Time elapsed: 6.27 seconds Epoch 194 | Loss: 0.2439 Time elapsed: 6.30 seconds Epoch 195 | Loss: 0.2408 Time elapsed: 6.34 seconds Epoch 196 | Loss: 0.2377 Time elapsed: 6.37 seconds Epoch 197 | Loss: 0.2346 Time elapsed: 6.40 seconds Epoch 198 | Loss: 0.2317 Time elapsed: 6.43 seconds Epoch 199 | Loss: 0.2287 Time elapsed: 6.46 seconds Epoch 200 | Loss: 0.2259 Time elapsed: 6.50 seconds Epoch 201 | Loss: 0.2231 Time elapsed: 6.53 seconds Epoch 202 | Loss: 0.2203 Time elapsed: 6.56 seconds Epoch 203 | Loss: 0.2176 Time elapsed: 6.59 seconds Epoch 204 | Loss: 0.2149 Time elapsed: 6.63 seconds Epoch 205 | Loss: 0.2122 Time elapsed: 6.66 seconds Epoch 206 | Loss: 0.2096 Time elapsed: 6.69 seconds Epoch 207 | Loss: 0.2071 Time elapsed: 6.72 seconds Epoch 208 | Loss: 0.2045 Time elapsed: 6.75 seconds Epoch 209 | Loss: 0.2020 Time elapsed: 6.78 seconds Epoch 210 | Loss: 0.1995 Time elapsed: 6.82 seconds Epoch 211 | Loss: 0.1971 Time elapsed: 6.85 seconds Epoch 212 | Loss: 0.1947 Time elapsed: 6.88 seconds Epoch 213 | Loss: 0.1924 Time elapsed: 6.91 seconds Epoch 214 | Loss: 0.1900 Time elapsed: 6.95 seconds Epoch 215 | Loss: 0.1877 Time elapsed: 6.98 seconds Epoch 216 | Loss: 0.1854 Time elapsed: 7.01 seconds Epoch 217 | Loss: 0.1831 Time elapsed: 7.04 seconds Epoch 218 | Loss: 0.1809 Time elapsed: 7.07 seconds Epoch 219 | Loss: 0.1787 Time elapsed: 7.11 seconds Epoch 220 | Loss: 0.1765 Time elapsed: 7.14 seconds Epoch 221 | Loss: 0.1743 Time elapsed: 7.17 seconds Epoch 222 | Loss: 0.1722 Time elapsed: 7.20 seconds Epoch 223 | Loss: 0.1700 Time elapsed: 7.23 seconds Epoch 224 | Loss: 0.1680 Time elapsed: 7.27 seconds Epoch 225 | Loss: 0.1659 Time elapsed: 7.30 seconds Epoch 226 | Loss: 0.1639 Time elapsed: 7.33 seconds Epoch 227 | Loss: 0.1619 Time elapsed: 7.36 seconds Epoch 228 | Loss: 0.1599 Time elapsed: 7.39 seconds Epoch 229 | Loss: 0.1579 Time elapsed: 7.43 seconds Epoch 230 | Loss: 0.1560 Time elapsed: 7.46 seconds Epoch 231 | Loss: 0.1541 Time elapsed: 7.49 seconds Epoch 232 | Loss: 0.1522 Time elapsed: 7.52 seconds Epoch 233 | Loss: 0.1503 Time elapsed: 7.55 seconds Epoch 234 | Loss: 0.1485 Time elapsed: 7.59 seconds Epoch 235 | Loss: 0.1467 Time elapsed: 7.62 seconds Epoch 236 | Loss: 0.1449 Time elapsed: 7.65 seconds Epoch 237 | Loss: 0.1431 Time elapsed: 7.68 seconds Epoch 238 | Loss: 0.1414 Time elapsed: 7.71 seconds Epoch 239 | Loss: 0.1397 Time elapsed: 7.75 seconds Epoch 240 | Loss: 0.1380 Time elapsed: 7.78 seconds Epoch 241 | Loss: 0.1364 Time elapsed: 7.81 seconds Epoch 242 | Loss: 0.1347 Time elapsed: 7.84 seconds Epoch 243 | Loss: 0.1331 Time elapsed: 7.87 seconds Epoch 244 | Loss: 0.1315 Time elapsed: 7.91 seconds Epoch 245 | Loss: 0.1300 Time elapsed: 7.94 seconds Epoch 246 | Loss: 0.1284 Time elapsed: 7.97 seconds Epoch 247 | Loss: 0.1269 Time elapsed: 8.00 seconds Epoch 248 | Loss: 0.1255 Time elapsed: 8.03 seconds Epoch 249 | Loss: 0.1240 Time elapsed: 8.06 seconds Epoch 250 | Loss: 0.1226 Time elapsed: 8.10 seconds Epoch 251 | Loss: 0.1211 Time elapsed: 8.13 seconds Epoch 252 | Loss: 0.1198 Time elapsed: 8.16 seconds Epoch 253 | Loss: 0.1184 Time elapsed: 8.19 seconds Epoch 254 | Loss: 0.1170 Time elapsed: 8.23 seconds Epoch 255 | Loss: 0.1156 Time elapsed: 8.26 seconds Epoch 256 | Loss: 0.1143 Time elapsed: 8.29 seconds Epoch 257 | Loss: 0.1130 Time elapsed: 8.32 seconds Epoch 258 | Loss: 0.1118 Time elapsed: 8.35 seconds Epoch 259 | Loss: 0.1105 Time elapsed: 8.39 seconds Epoch 260 | Loss: 0.1093 Time elapsed: 8.42 seconds Epoch 261 | Loss: 0.1081 Time elapsed: 8.45 seconds Epoch 262 | Loss: 0.1069 Time elapsed: 8.48 seconds Epoch 263 | Loss: 0.1057 Time elapsed: 8.51 seconds Epoch 264 | Loss: 0.1046 Time elapsed: 8.55 seconds Epoch 265 | Loss: 0.1034 Time elapsed: 8.58 seconds Epoch 266 | Loss: 0.1023 Time elapsed: 8.61 seconds Epoch 267 | Loss: 0.1012 Time elapsed: 8.64 seconds Epoch 268 | Loss: 0.1000 Time elapsed: 8.68 seconds Epoch 269 | Loss: 0.0989 Time elapsed: 8.71 seconds Epoch 270 | Loss: 0.0978 Time elapsed: 8.74 seconds Epoch 271 | Loss: 0.0967 Time elapsed: 8.77 seconds Epoch 272 | Loss: 0.0956 Time elapsed: 8.80 seconds Epoch 273 | Loss: 0.0944 Time elapsed: 8.84 seconds Epoch 274 | Loss: 0.0932 Time elapsed: 8.87 seconds Epoch 275 | Loss: 0.0920 Time elapsed: 8.90 seconds Epoch 276 | Loss: 0.0908 Time elapsed: 8.93 seconds Epoch 277 | Loss: 0.0896 Time elapsed: 8.97 seconds Epoch 278 | Loss: 0.0885 Time elapsed: 9.00 seconds Epoch 279 | Loss: 0.0873 Time elapsed: 9.03 seconds Epoch 280 | Loss: 0.0862 Time elapsed: 9.06 seconds Epoch 281 | Loss: 0.0850 Time elapsed: 9.09 seconds Epoch 282 | Loss: 0.0839 Time elapsed: 9.12 seconds Epoch 283 | Loss: 0.0827 Time elapsed: 9.16 seconds Epoch 284 | Loss: 0.0816 Time elapsed: 9.19 seconds Epoch 285 | Loss: 0.0805 Time elapsed: 9.22 seconds Epoch 286 | Loss: 0.0795 Time elapsed: 9.25 seconds Epoch 287 | Loss: 0.0784 Time elapsed: 9.28 seconds Epoch 288 | Loss: 0.0773 Time elapsed: 9.31 seconds Epoch 289 | Loss: 0.0763 Time elapsed: 9.35 seconds Epoch 290 | Loss: 0.0752 Time elapsed: 9.38 seconds Epoch 291 | Loss: 0.0743 Time elapsed: 9.41 seconds Epoch 292 | Loss: 0.0733 Time elapsed: 9.44 seconds Epoch 293 | Loss: 0.0723 Time elapsed: 9.47 seconds Epoch 294 | Loss: 0.0714 Time elapsed: 9.51 seconds Epoch 295 | Loss: 0.0705 Time elapsed: 9.54 seconds Epoch 296 | Loss: 0.0696 Time elapsed: 9.57 seconds Epoch 297 | Loss: 0.0687 Time elapsed: 9.60 seconds Epoch 298 | Loss: 0.0678 Time elapsed: 9.63 seconds Epoch 299 | Loss: 0.0669 Time elapsed: 9.67 seconds

[61]: epochs_vs_loss_with_cells(my_epochs,my_losses)

Epochs vs. Loss during training With Cell Line information

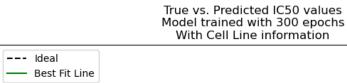


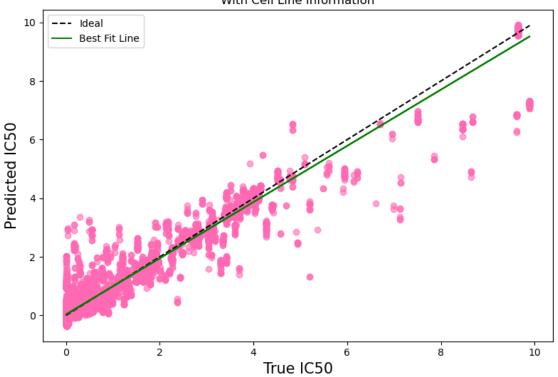
```
[63]: drug_features_test = X_test[['Molecular Mass', 'LogP', 'NumHDonors', __
       ⇔'NumHAcceptors', 'TPSA']]
      patient_features_test = X_test.drop(columns=drug_features_test.columns)
      metrics = evaluate_model(model, drug_features_test, patient_features_test,__

y_test)

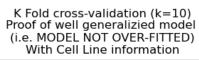
      print(f"MSE: {metrics[0]:.4f}")
      print(f"MAE: {metrics[1]:.4f}")
      print(f"R2: {metrics[2]:.4f}")
     MSE: 0.0650
     MAE: 0.1026
     R2: 0.9706
[65]: with torch.no_grad():
          preds = model(torch.tensor(drug_features_test.values).float(),
                        torch.tensor(patient_features_test.values).float()).cpu().
       →numpy()
      plot_pred_vs_true_with_cells(y_test.to_numpy(), preds)
```

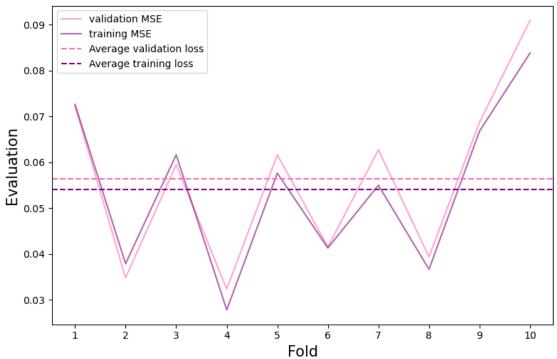
/Users/joyceyu/Documents/CHEM277B - ML Algorithms/Final project/Data_277_-Cancer/CHEM277B_functions.py:108: UserWarning: color is redundantly defined by the 'color' keyword argument and the fmt string "r--" (-> color='r'). The keyword argument will take precedence. plt.plot([true.min(), true.max()], [true.min(), true.max()], 'r--', label='Ideal', color = "Black")





```
[69]: k_fold_cv = compute_CV_error(X_train, y_train)
[71]: Kfold_CV_plot_with_cells(k_fold_cv)
```





[]: