Supplemental Materials

1 Loss Function Details

The contrastive learning component is optimized using this loss function:

$$L_{cont} = - \sum_{(d,c) \in D_{pos}} log \frac{e^{sim(\mathrm{h}_d, \mathrm{h}_c)/\tau}}{e^{sim(\mathrm{h}_d, \mathrm{h}_c)/\tau} + \sum_{c' \in N_d} e^{sim(\mathrm{h}_d, \mathrm{h}_{c'})/\tau}} , \qquad (1)$$

where D_{pos} denotes the set of drug-cell pairs (d,c), indicating that the interaction between drug d and cell line c is known to be true. The similarity function $sim(\mathrm{h}_d, \mathrm{h}_c)$ measures the similarity between the feature representations h_d for drugs and h_c for cell lines. The parameter τ controls the sharpness of the resulting similarity distribution. The link prediction task is optimized using:

$$L_{LinkPred} = \sum_{r \in R} \sum_{(i,j) \in E_r} \left[-log\ \sigma(s_{ij}^{(r)}) - \sum_{k=1}^{K} log\ \sigma(-s_{ik}^{(r)}) \right], \qquad (2)$$

where $s_{ij}^{(r)}$ denotes the score between node i and node j under relation r, and E_r represents the set of edges defined for relation r. The overall loss function used to train our model is therefore:

$$L = L_{LinkPred} + \lambda_1 L_{cont} + \lambda_2 \|\Theta\|_2^2 \qquad (3)$$

where Θ represents the model parameters.

2 Distribution of GT Numbers

Of the edges to be explained, 33.01% have a GT count of fewer than 1,009, which means that most of the edges to be explained have a corresponding GT count between 10 and 1,009. The specific distribution is shown in Extended Table 1.

Extended Table 1. Distribution of GT Numbers.

GT Num	Edge Count	Proportion	GT Num	Edge Count	Proportion
10-1009	1088	33.01	5010-6009	227	6.89
1010-2009	196	5.95	6010-7009	341	10.35
2010-3009	286	8.68	7010-8009	296	8.98
3010-4009	177	5.37	8010-9009	263	7.98
4010-5009	260	7.89	9010-10009	146	4.43

3 Prediction Performance Assessment

The AUC and PR curves of CETExplainer compared to the baselines are shown in Extended Fig. 1.
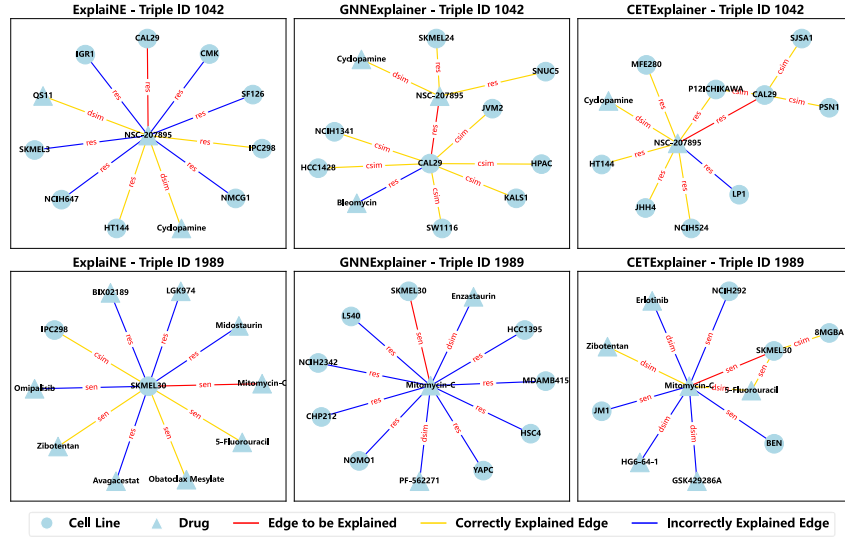
X. Li and J. Gui contributed equally to this work.
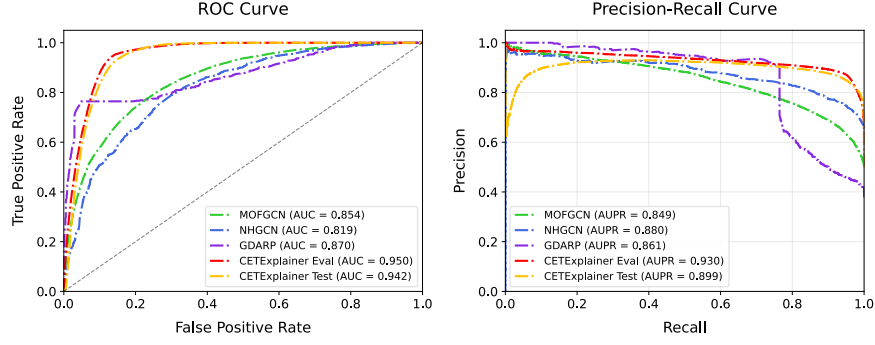
Extended Fig. 1. Performance Comparison of Models Using ROC and Precision-Recall

4   Qualitative Assessment

For the sen edge to be explained (Mitomycin-C, sen, SKMEL30) as shown in Extended Fig. 2, our model and ExplaiNE both correctly predict 4 edges, while GNNExplainer fails to predict any edges correctly.

Extended Fig. 2. Qualitative evaluation of the three explanation models on triplet instances 1266 and 1989.