**Supplementary Table S1**: Robustness of SGCL-DPI to alternative graph-construction strategies (one validation fold, STITCH-hard split). Performance is reported after retraining the model with different similarity metrics or 𝑘 k-values for the drug and protein 𝑘 k-NN graphs. The default configuration (cosine similarity, 𝑘 = 5 k=5) is shown in bold. A “No-graph baseline” omits the GNN encoders entirely (retaining the deep-feature and RF components) for reference. Variations in F1 (≤ 0.3%) and AUC-ROC (≤ 0.1) indicate that SGCL-DPI is insensitive to reasonable changes in graph topology.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Variant (graph construction)** | **Accuracy** | **Precision** | **Recall** | **F1** | **AUC-ROC** | **AUC-PR** |
| **Cosine (k = 5)** – default | **0.749** | 0.588 | **0.814** | 0.683 | 0.807 | 0.659 |
| Cosine (k = 3) | 0.750 | 0.589 | 0.814 | **0.684** | 0.807 | 0.659 |
| Cosine (k = 7) | 0.750 | 0.589 | 0.814 | 0.684 | 0.807 | 0.659 |
| Euclidean (k = 5) | 0.750 | 0.589 | 0.814 | 0.684 | 0.807 | 0.657 |
| Correlation (k = 5) | 0.750 | 0.589 | 0.814 | 0.684 | 0.807 | 0.659 |
| **No-graph baseline**(Deep + RF, no GNN encoder) | 0.758 | **0.691** | 0.487 | 0.571 | **0.809** | **0.673** |