

# Self-supervised contrastive learning on attribute and topology graphs for predicting relationships among lncRNAs, miRNAs and diseases

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**Supplementary Table 1 (ST1). Hyper-parameters on LDA, MDA and LMI prediction tasks under dataset 1 and dataset 2.**

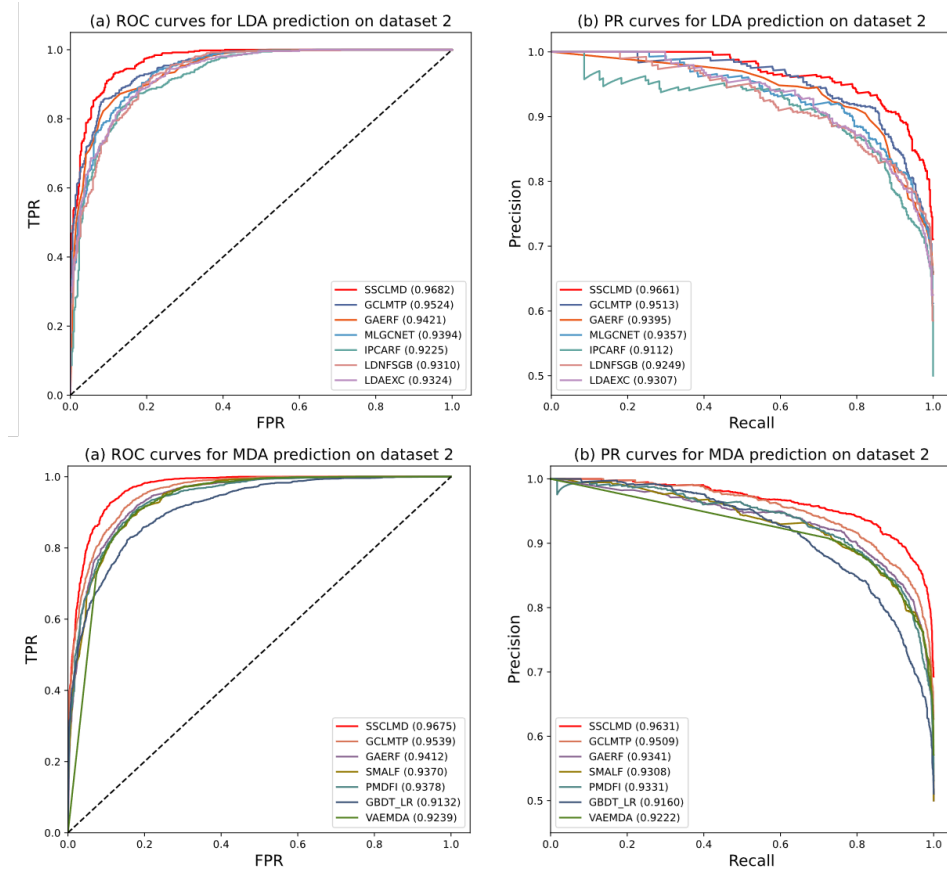
|           | Tasks | $k$ | $\alpha$ | $\theta$ | Nhid1 | Nhid2 | $\lambda$ | Epoch | $lr$   | Dropout |
|-----------|-------|-----|----------|----------|-------|-------|-----------|-------|--------|---------|
| Dataset 1 | LDA   | 22  | 0.9      | 0.6      | 256   | 128   | 1         | 80    | 0.0005 | 0.5     |
|           | MDA   | 26  | 0.9      | 0.5      | 512   | 256   | 0.1       | 80    | 0.0005 | 0.5     |
|           | LMI   | 30  | 0.5      | 0.5      | 512   | 256   | 0.1       | 80    | 0.0005 | 0.5     |
| Dataset 2 | LDA   | 18  | 0.9      | 0.5      | 256   | 128   | 1         | 80    | 0.0005 | 0.5     |
|           | MDA   | 26  | 0.9      | 0.7      | 512   | 256   | 0.1       | 80    | 0.0005 | 0.5     |
|           | LMI   | 34  | 0.5      | 0.5      | 512   | 256   | 1         | 80    | 0.0005 | 0.5     |

**Supplementary Table 2 (ST2).** The top 10 predicted BC-related lncRNA and miRNA candidates on dataset 2.

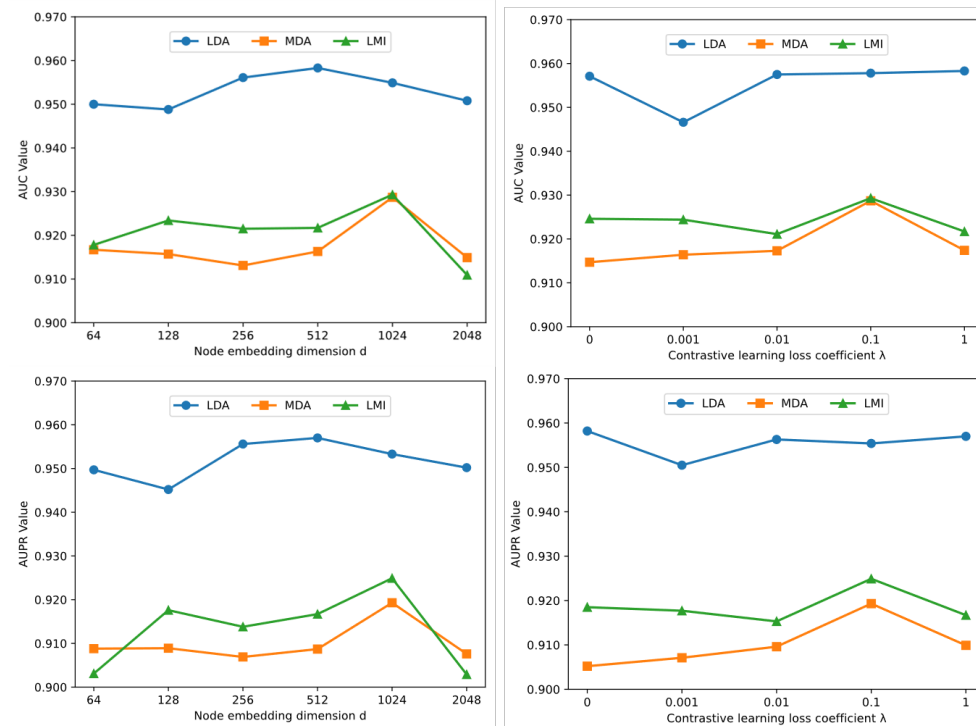
| Rank | LncRNA    | Evidence                               | Rank | MiRNA        | Evidence                  |
|------|-----------|--|------|--------------|---------------------------|
| 1    | MIR17HG   | PMID: 36943627                         | 1    | hsa-mir-150  | HMDD v4.0,<br>dbDEMC v3.0 |
| 2    | BANCR     | LncRNADisease v3.0,<br>Lnc2Cancer v3.0 | 2    | hsa-mir-15b  | HMDD v4.0,<br>dbDEMC v3.0 |
| 3    | HULC      | LncRNADisease v3.0,<br>Lnc2Cancer v3.0 | 3    | hsa-mir-142  | HMDD v4.0,<br>dbDEMC v3.0 |
| 4    | TUG1      | LncRNADisease v3.0,<br>Lnc2Cancer v3.0 | 4    | hsa-mir-192  | HMDD v4.0,<br>dbDEMC v3.0 |
| 5    | WT1-AS    | LncRNADisease v3.0                     | 5    | hsa-mir-181c | HMDD v4.0,<br>dbDEMC v3.0 |
| 6    | MIR155HG  | Unconfirmed                            | 6    | hsa-mir-144  | HMDD v4.0,<br>dbDEMC v3.0 |
| 7    | TUSC7     | LncRNADisease v3.0                     | 7    | hsa-mir-181d | HMDD v4.0,<br>dbDEMC v3.0 |
| 8    | DLEU2     | Unconfirmed                            | 8    | hsa-mir-106a | HMDD v4.0,<br>dbDEMC v3.0 |
| 9    | GHET1     | LncRNADisease v3.0,<br>Lnc2Cancer v3.0 | 9    | hsa-mir-378a | HMDD v4.0,<br>dbDEMC v3.0 |
| 10   | LINC01133 | LncRNADisease v3.0,<br>Lnc2Cancer v3.0 | 10   | hsa-mir-424  | HMDD v4.0,<br>dbDEMC v3.0 |

**Supplementary Table 3 (ST3).** The top 10 predicted BC-related lncRNAs and miRNA candidates on dataset 1.

| Rank | LncRNA      | Evidence       | Rank | MiRNA          | Evidence                 |
|------|-------------|----------------|------|----------------|--------------------------|
| 1    | FER1L4      | PMID: 31332783 | 1    | hsa-mir-211    | HMDD v4.0<br>dbDEMC v3.0 |
| 2    | MIR4435-2HG | PMID: 36105009 | 2    | hsa-mir-186    | HMDD v4.0<br>dbDEMC v3.0 |
| 3    | FTX         | Unconfirmed    | 3    | hsa-mir-28     | HMDD v4.0<br>dbDEMC v3.0 |
| 4    | MIR100HG    | PMID: 33088216 | 4    | hsa-mir-19b-2  | Unconfirmed              |
| 5    | LINC-PINT   | PMID: 32632453 | 5    | hsa-mir-181d   | HMDD v4.0<br>dbDEMC v3.0 |
| 6    | TUSC7       | PMID: 35296964 | 6    | hsa-mir-454    | HMDD v4.0<br>dbDEMC v3.0 |
| 7    | LINC00261   | PMID: 33274565 | 7    | hsa-mir-216a   | HMDD v4.0<br>dbDEMC v3.0 |
| 8    | HNF1A-AS1   | PMID: 32319789 | 8    | hsa-mir-136    | HMDD v4.0<br>dbDEMC v3.0 |
| 9    | MIR17HG     | PMID: 36943627 | 9    | hsa-mir-181a-1 | Unconfirmed              |
| 10   | DGCR5       | PMID: 32521856 | 10   | hsa-mir-138-2  | Unconfirmed              |



**Supplementary Figure 1 (SF1).** ROC and PR curves of SSCLMD and other baseline methods for LDA and MDA prediction on dataset 2.



**Supplementary Figure 2 (SF2).** Parameter sensitivity analysis of node embedding dimensions  $d$ , and contrastive learning loss coefficient  $\lambda$  on dataset 1.