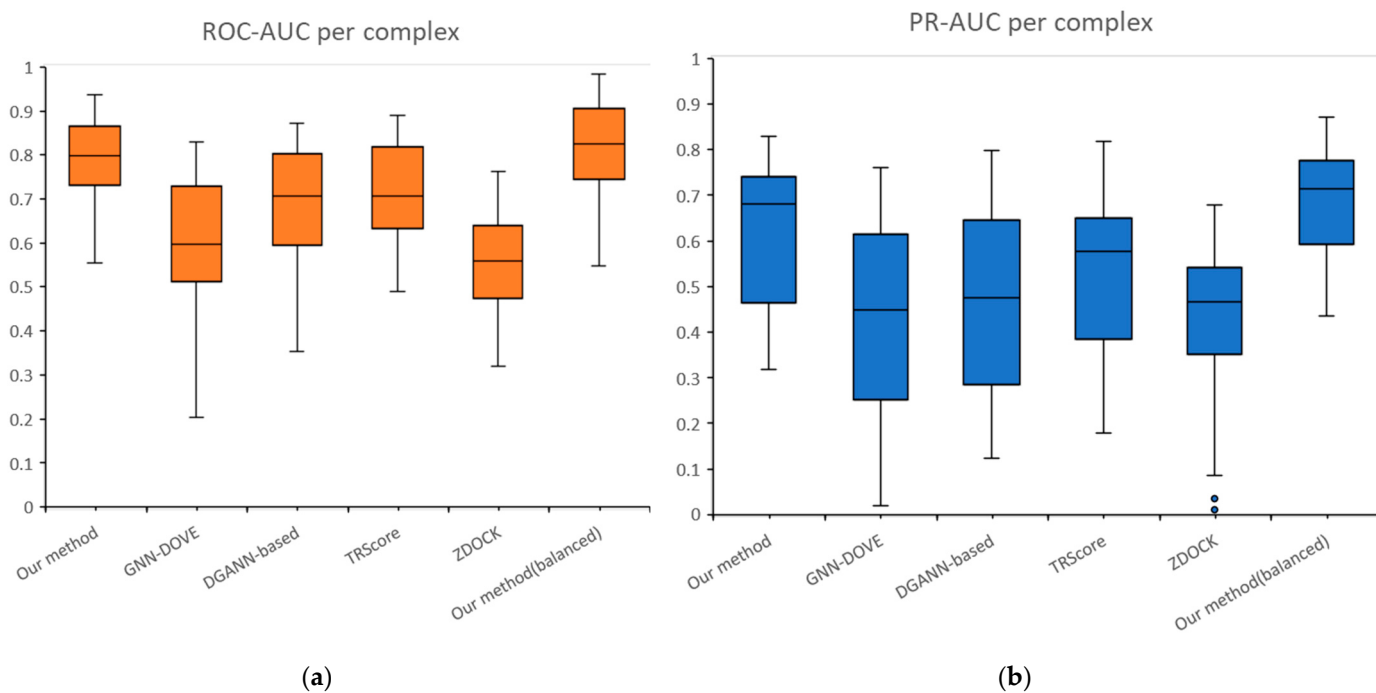


**Table S1.** the Precision and Recall of different scoring functions on Benchmark 4.0

| Scoring functions    | Precision | Recall |
|----------------------|-----------|--------|
| Our method           | 0.66      | 0.23   |
| Our-method(balanced) | 0.83      | 0.23   |
| DGANN-based          | 0.41      | 0.17   |
| ZDOCK                | 0.41      | 0.18   |
| GNN-DOVE             | 0.38      | 0.16   |
| TRScore              | 0.61      | 0.20   |



**Figure S1.** Comparison of our scoring function with DGANN-based method, ZDOCK, GNN-DOVE and TRScore for the cross-validation ZDOCK benchmark 4.0. (a) ROC-AUC per complex of different methods. (b) PR-AUC per complex of different methods