**Figure S1:** The figure is showed the ratio of the drug and target in the negative samples to drug and target in all samples. The proportion of negative samples is more than 82%, which basically covers the kinds of drugs and targets in the experimental data.

radio_negative_sample_f1

**Figure S2：**PPDTS is set the optimal weight value α for the linear combination drug-target similarity network model and target-drug similarity network model. Abscissa represents the combination probability α (0<α<1). The red line represents the AUC value with the change ofα values, and the blue line represents the AUPR value with the change of α values.



**Figure S3:** This figure shows the AUC curve of PPDTS compared with baseline methods in dataset1 after 5- fold cross validation.

data1_auc

**Table S1:** The Dataset 2 contains 575 drugs, 981 targets and 8008 known drug target interactions. After 5-fold cross validation, the comparison of PPDTS and baseline methods in each evaluation parameter results is shown in the table.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Metrics**  **Methods** | **AUPR** | **AUC** | **F1\_SCORE** | **RECALL** | **PRECISION** |
| **ProCF** | 0.574596 | 0.970665 | 0.592547 | 0.578014 | 0.609193 |
| **NP** | 0.574659 | 0.970665 | 0.592496 | 0.577888 | 0.609199 |
| **RWR(0.1)** | 0.548859 | 0.955862 | 0.578524 | 0.478951 | 0.741943 |
| **LP (0.1)** | 0.582472 | 0.961169 | 0.577862 | 0.563273 | 0.596959 |
| **PPDTS** | **0.780761** | **0.974878** | **0.758846** | **0.725547** | **0.795864** |