

## Appendix A FPSC-DTI supplement

### A.1 Mean percentile ranking *MPR*

The mean percentile ranking (*MPR*) [1–3], a recall-based statistical metric, is adopted to evaluate the method’s performance. This is a good evaluation criterion for one-class datasets [4, 5]. Specifically, for each drug  $d_i$  in the test set, we generate a ranked list of the targets sorted in descending order by the predicted scores between the current drug with all targets in the dataset. Let  $rank_{ji}$  denote the percentile ranking (PR) of target  $t_j$  with drug  $d_i$ . The smaller the *rank* value is, the better the prediction performance of the algorithm. For example,  $rank_{ji} = 0\%$  indicates that drug  $d_i$  is predicted to interact with target  $t_j$  with the highest probability. Similarly,  $rank_{ji} = 100\%$  signifies that drug  $d_i$  is predicted to interact with target  $t_j$  with the lowest probability. Herein, the definition of *MPR* is as follows:

$$MPR = \frac{\sum_{i=1}^{N_D^t} R_i}{N_D^t} \quad (1)$$

where  $N_D^t$  denotes the number of drugs in the test set, and  $R_i$  can be computed as follows:

$$R_i = \frac{\sum_{j=1}^{N_T^t} rank_{ji}}{N_T^t} \quad (2)$$

where  $N_T^t$  denotes the number of targets in the test set for the current drug  $d_i$ .

### A.2 Cluster analysis of the four benchmark datasets

Since there is no class label information in the drug and target data of the four benchmark datasets, we firstly determine them the number of clusters. In this paper, we use the decision graph of DPCSA [6] to determine the number of clusters, which requires none predefined parameter. Then, we use INCK [7], an improved K-medoids algorithm, to cluster drug and target data, respectively. All the clustering results are given in Table A1.

**Table A1:** Clustering results of four benchmark datasets

Dataset	Number of objects in each cluster	
	Drug	Target
Enzyme	59,19,17,101,15,7,46,4,13,3	123,40,19,2,2,43,20,25,6,9
	10,10,19,19,33,12,12,20,11,15	9,15,21,3,10,6,289,6,10,6
GPCR	48,27,11,19,16,6,14,11,6,22	30,23,10,4,5,16,7
	9,10,10,14	
IC	72,10,12,14,12,10	39,17,6,41,9,4,7,20
	15,22,11,14,18	6,5,14,5,11,8,12
NR	18,15,7,9,5	12,5,5,4

## References

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