**Supplemental Table S1: The list of data used in this study and their sources**

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| --- | --- | --- |
| Groups of data | Data sets | Data sources |
| Drug-target interaction data | Drug-target interactions | DrugBank |
| Drug-related data | Chemical structures | DrugBank |
| Drug-drug interactions | DrugBank |
| Drug-disease associations | CTD |
| Drug side effects | SIDER |
| Target-related data | Protein sequences | DrugBank |
| Protein-protein interactions | STRING |
| GO annotations | GOA |
| Protein pathways | KEGG |