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About HN-DREP

The HN-DREP database is a platform that is dedicated to evaluating heterogeneous network-based drug repositioning methods and predicting drug-disease associations. It provides an impartial assessment of existing network-driven drug repositioning methods and consolidates predictions from various repositioning methods. This summary represents the current stage of research on heterogeneous network-based drug repositioning methods, which aims to promote the development of drug repositioning.

1. Homepage

The HN-DREP homepage briefly describes the database and research framework. It contains three main sections: About HN-DREP, Research Framework, and Statistics.

- About HN-DREP: This section provides an introduction to HN-DREP, clarifying what it does, what functions it provides, and what it means. **(Fig. 1 ①)**
- Research Framework: This section is a framework for our evaluation of heterogeneous network-based drug repositioning methods. **(Fig. 1 ②)**
- Statistics: This section is the statistics of the data, including the methods evaluated, the datasets used, the drugs included, the diseases, and the number of drug-disease associations predicted. **(Fig. 2)**

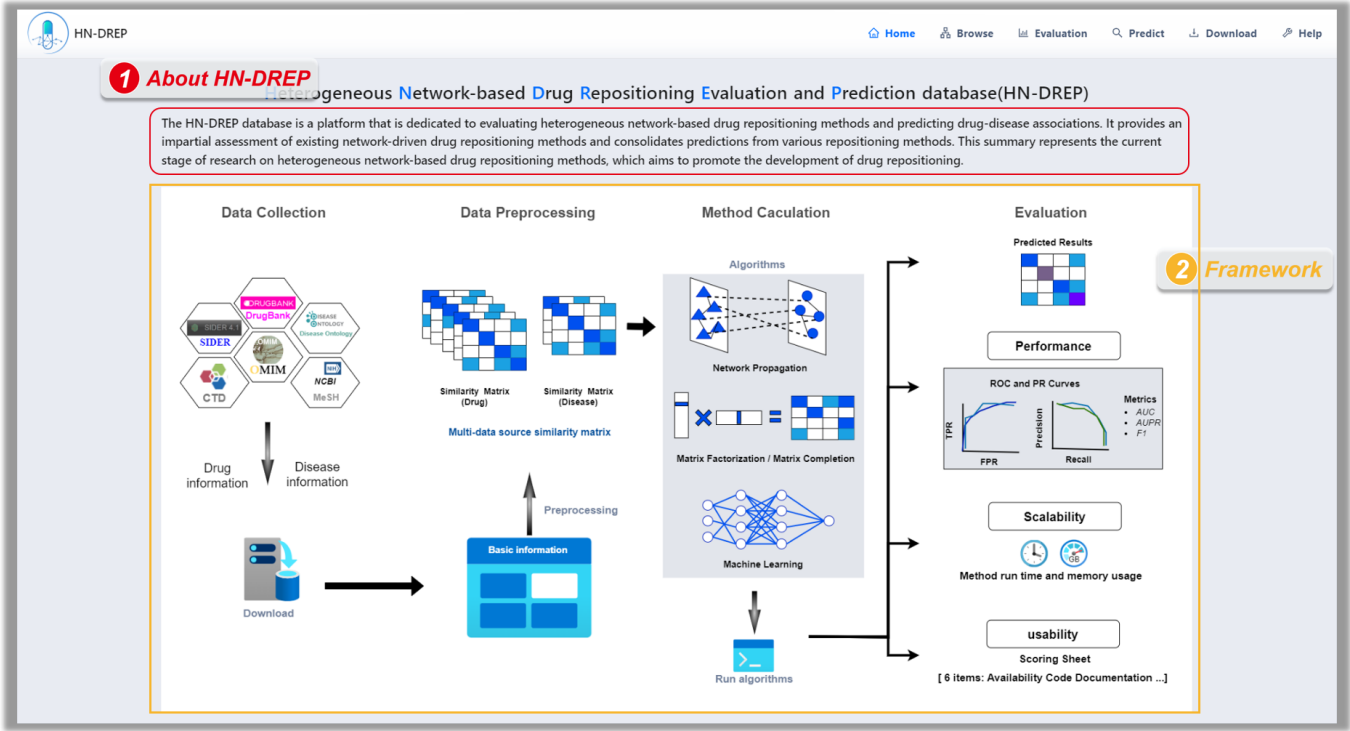


Fig 1. The HN-DREP homepage

Statistics

Overview of Database

Methods	Disease ID Type	Datasets	Drugs	Diseases	Drug-Disease associations
28	OMIM	5	2794	4220	1805270
	MeSH	3		2892	984676
	MedGen	1		1229	874245
	Disease Name	2		4552	3499069

Fig 2. The statistics section of the HN-DREP homepage

2. Browse

Clicking the **Browse** button in the navigation bar will take you to the **Browse page**. The Browse page lists the used drug repositioning **methods** and **datasets** in our evaluation. Click on the hyperlinks to access more detailed information and the evaluation results.

2.1. Methods

- Users can directly browse all heterogeneous network-based drug repositioning methods used in our evaluation in this page. This page gives the basic information for each method: languages, category, algorithms, network, overall score, performance score, scalability score, workflow, and swipe the table to the right to see more information, such as code address, doi number and method description etc. You can also click on settings to show only what you choose and sort the methods the way you want. (Fig. 3 ②)

- For more detailed method information, click on the corresponding method line to navigate to the **method detail page**. (Fig. 3 ③)
 - The method info block displays the basic method information shown in the Browse page.(Fig. 4 ②)
 - The method performance on all datasets block displays the basic dataset information and the evaluation performance results of the method on this dataset, including AUC, AUPR, F1, AUC Curve, AUPR Curve, Time usage and Memory Usage.(Fig. 4 ③)
 - The Method Predicted Results block shows the prediction results of the methods for all datasets, categorized according to the dataset. The page block shows only the first 100 prediction results of the methods for each dataset with a prediction score greater than 0.5. If you want to get the full results, you can get them on the download page.(Fig. 4 ④)

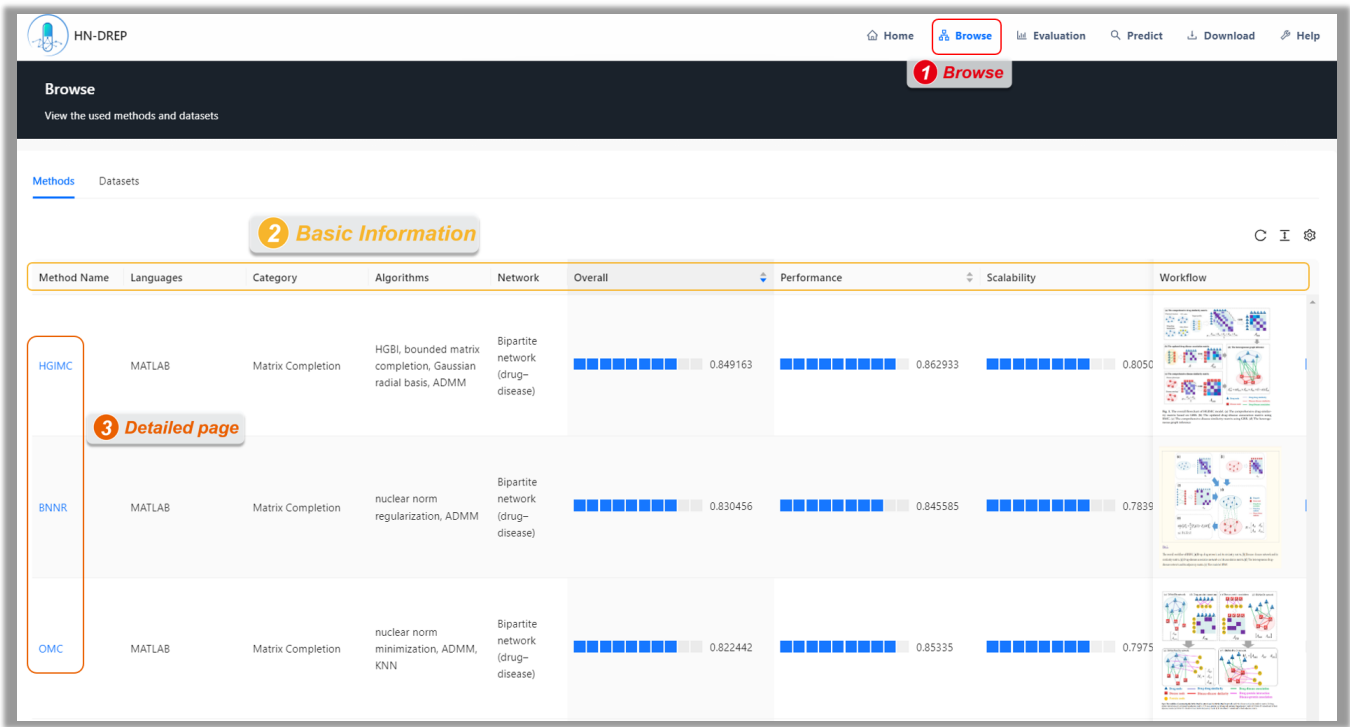


Fig 3. The Browse methods page of the HN-DREP

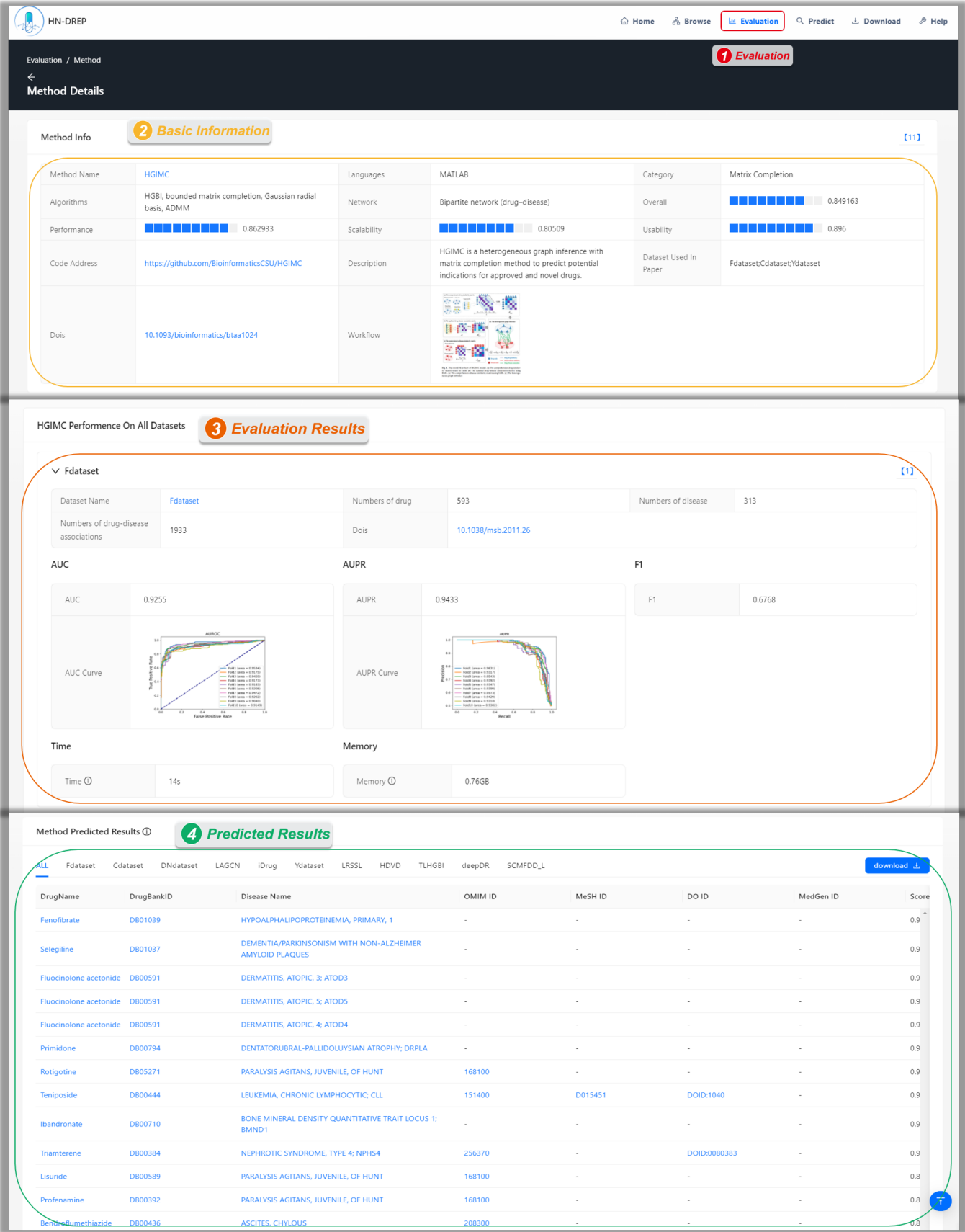


Fig 4. The method detailed page of the HN-DREP

2.2. Datasets

- Users can directly browse all datasets we used by clicking on the Datasets button in Browse page. This page gives the basic information for each dataset, including the dataset name, numbers of drug,

numbers of disease, numbers of drug-disease associations and doi number.(Fig. 5 ②)

- For more detailed dataset information, click on the corresponding dataset line to navigate to the **dataset detail page**. (Fig. 5 ③)
 - The dataset info block displays the basic dataset information.(Fig. 6 ②)
 - The method performance on dataset block displays the basic method information and the evaluation performance results of the method on this dataset, including AUC, AUPR, F1, AUC Curve, AUPR Curve, Time usage and Memory Usage.(Fig. 6 ③)
 - The Method Predicted Results block shows the prediction results of the methods on datasets, categorized by the methods. The page block only shows the first 100 prediction results of the method on each dataset with a prediction score greater than 0.5. If you wish to access the complete results, you can find them on the **download page**.(Fig. 6 ④)

HN-DREP

Home Browse Evaluation Predict Download Help

Browse

View the used methods and datasets

Methods Datasets

2 Basic Information

Dataset Name	Numbers of drug	Numbers of disease	Numbers of drug-disease associations	Dois
Cdataset	667	409	2352	10.1093/bioinformatics/btw228
deepDR	1219	1229	6677	10.1093/bioinformatics/btz418
DNdataset	1490	4516	1008	10.1016/j.artmed.2014.11.003
Fdataset	593	313	1933	10.1038/msb.2011.26
HDVD	219	34	455	10.1016/j.asoc.2021.107135
IDrug	1321	3966	111481	10.1371/journal.pcbi.1008040
LAGCN	269	598	18416	10.1186/s12859-018-2220-4
LRSSL	763	681	3051	10.1093/bioinformatics/btw770
SCMFDD_L	1323	2834	49217	10.1186/s12859-018-2220-4
TLHGBI	1409	5080	1461	10.1093/bioinformatics/btu403
Ydataset	1478	655	8448	10.1093/bib/bbaa267

1-11 of 11 items 1

Fig 5. The Browse datasets page of the HN-DREP

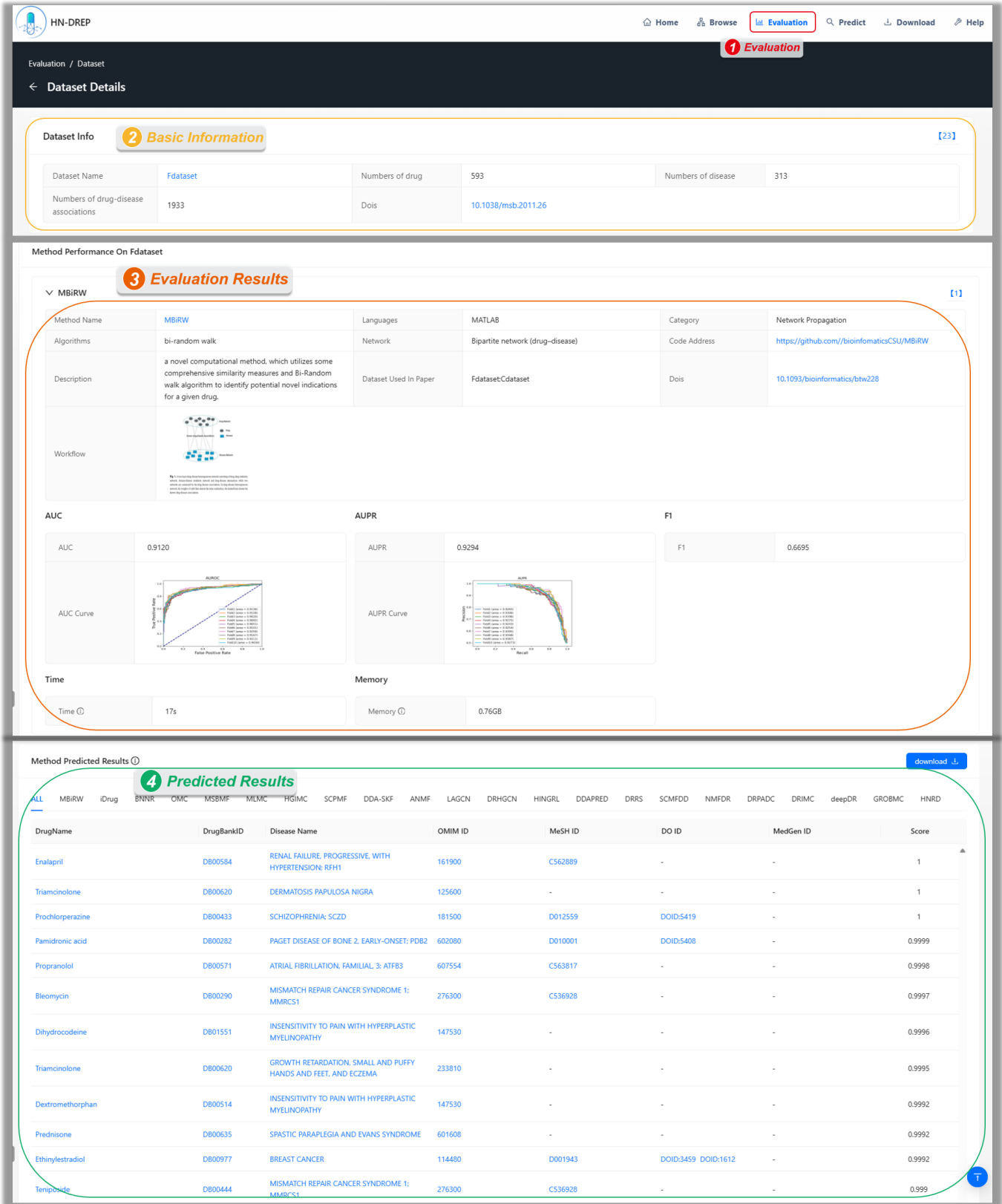


Fig 6. The dataset detailed page of the HN-DREP

3. Evaluation

Click the **Evaluation** button in the navigation bar to enter the **evaluation results page**. The Evaluation page presents the comprehensive evaluation results for the various methods we have employed, focusing on three

critical aspects: Performance, Scalability and Usability. Click on the hyperlinks to access more detailed information within the evaluation results. The detail pages contain essential information about the method and dataset, as well as specific evaluation results. Our evaluation workflow is available at: <https://github.com/lyhbio/HN-DRES> .

- **Overall** page provides a concise summary of three aspects: Performance, Scalability and Usability. You can click the corresponding button to sort the methods the way you want. For more detailed method evaluation results, click on the corresponding method line to navigate to the method detail page.(Fig. 7)

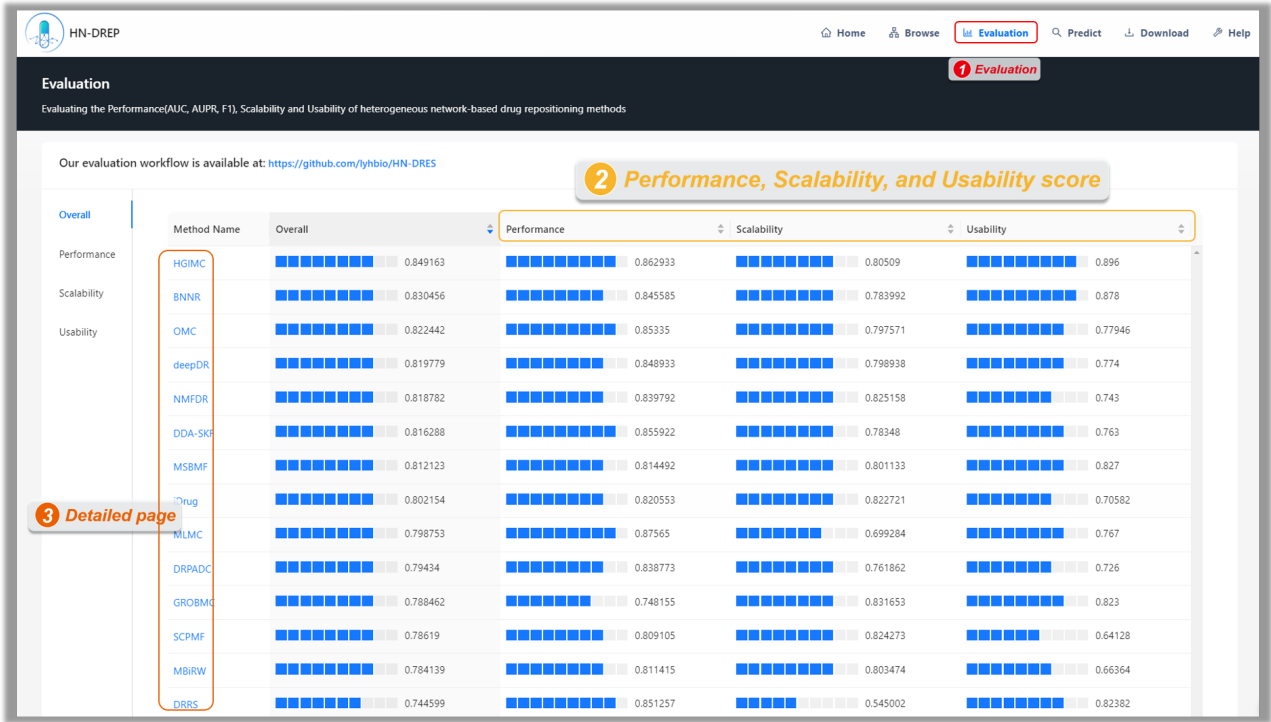


Fig 7. The overall evalutaion results: Performance, Scalability and Usability

- **Performance** page displays the performance of the evaluated method, as measured by metrics such as AUC, AUPR, and F1 value. You can click on the corresponding buttons to display the results in Table show, Shape show, 3D show. You can also click on a method, dataset, or table element to access the

evaluation details.(Fig. 8)

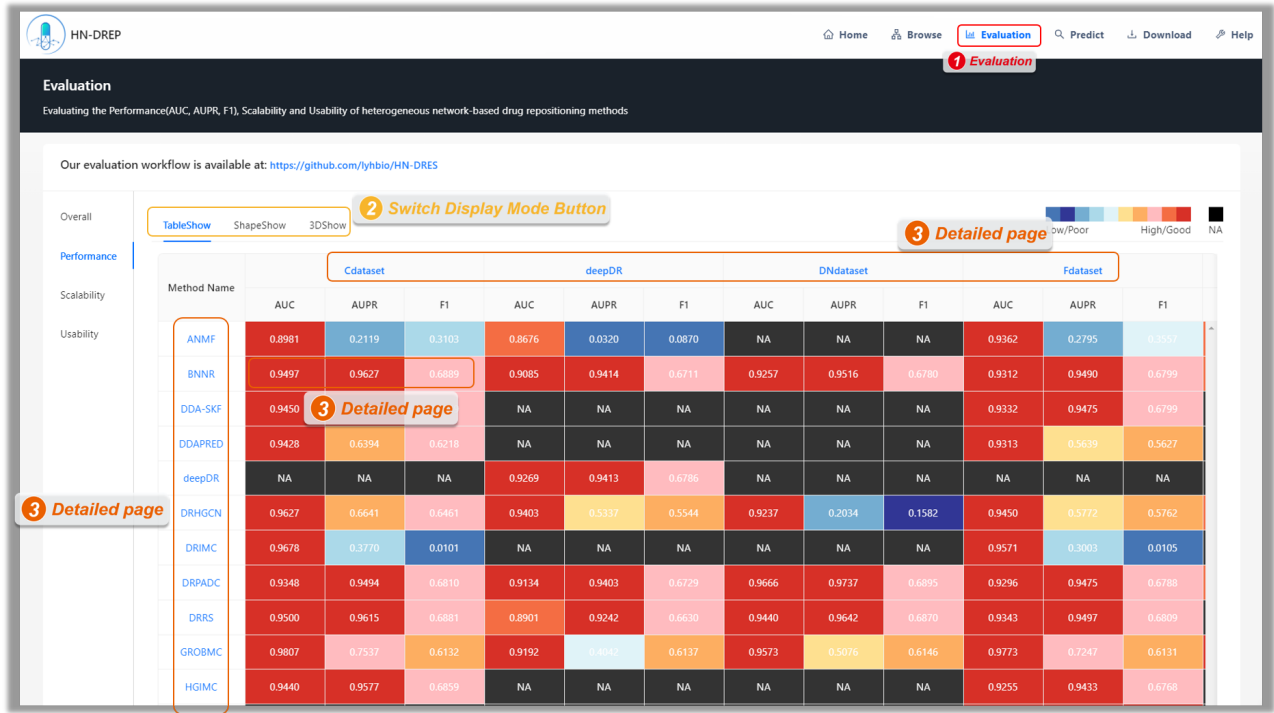


Fig 8. The method performance evalutaion results

- **Scalability** page offers insights into the computational demands in terms of time and memory required for method execution. Similarly, you can access the assessment details by clicking on the corresponding hyperlinks.(Fig. 9)

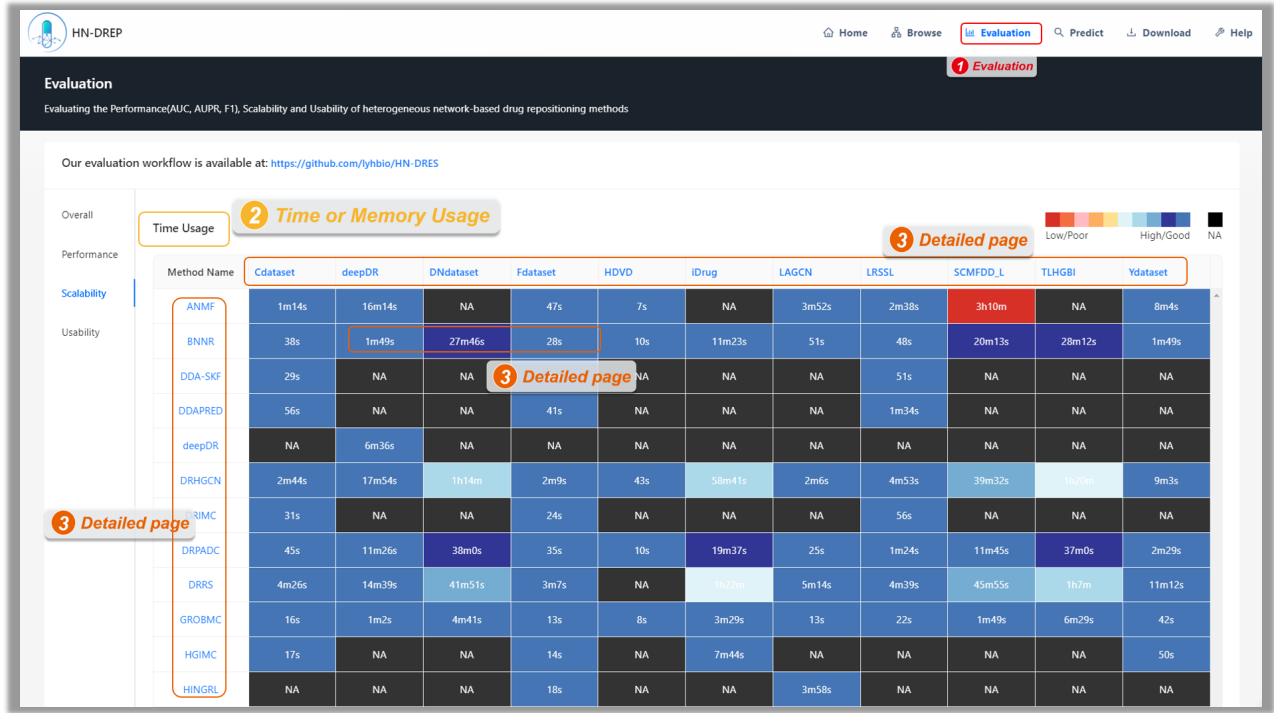


Fig 9. The method scalability evalutaion results

- **Usability** page shows the user-friendliness and quality of the method, among other factors. (Fig. 10)

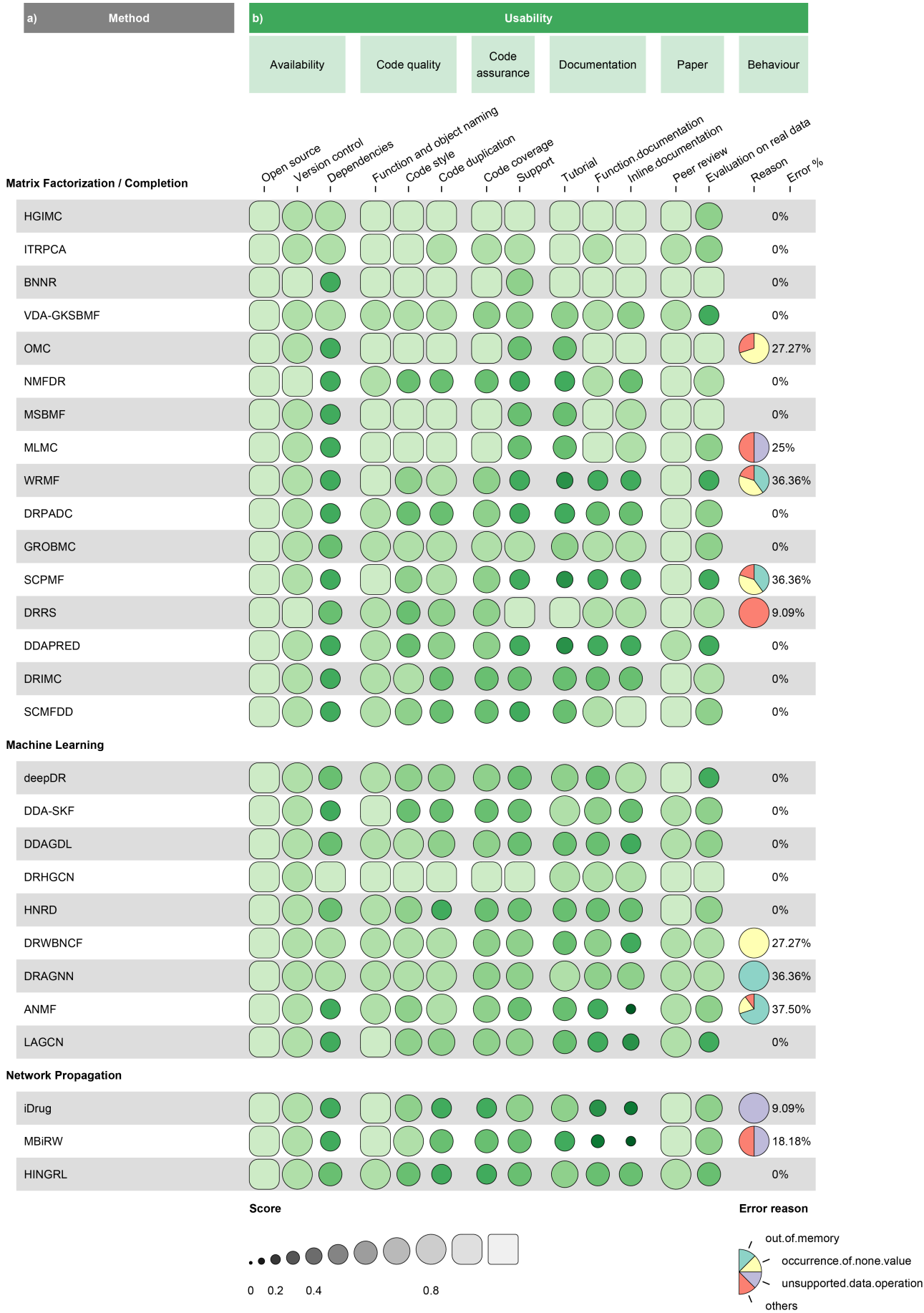


Fig 10. The method usability evalutaion results

4. Predict

Click the **Predict** button in the navigation bar to enter the **predict page**. The prediction menu integrates multiple drug repositioning methods to provide drug-disease association prediction functions. You can query the entries related to the drug or disease based on its ID and name and download them. **(Fig. 11)**

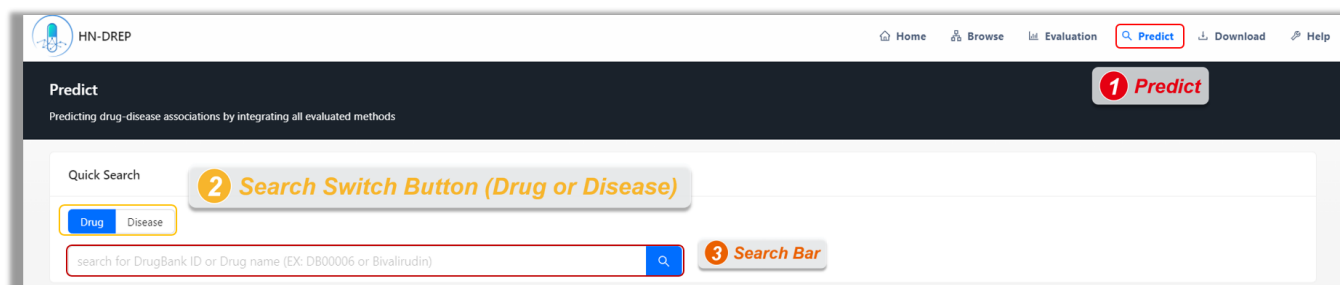


Fig 11. The HN-DREP search page

4.1. Drug

- You can search by drug id or name to get to the drug details, a page that includes basic information about the drug (DrugBank ID, targets, Type, Chemical Formula, ATC codes, Smiles, 2D structure, 3D structure etc.), as well as entries on associated diseases that are predicted by integrating all the methods.
- The detailed page has the basic information of the searched drug, and the prediction results associated with it. The left form is an aggregation of all the results on the right, including the name of the predicted diseases, the number of times it occurs, and which methods predicted the entry, and the right side is the prediction disease results of a single method for this drug, including disease name and its

 HN-DREP

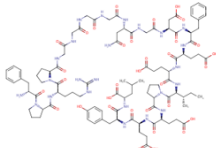
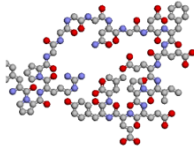
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Predict / Predicting Results

1 Predict

[<](#) Drug Details

Drug Info 2 Basic Information

DrugName	Bivalirudin	DrugBankID	D800006	Target	P00734
Type	small molecule	Synonyms	Bivalirudin, Bivalirudina, Bivalirudinum	Brand Name	Angiomax
Weight	Average: 2180.2853, Monoisotopic: 2178.985813062	Chemical Formula	C98H138N24O33	ATC Codes	B01AE06
Smiles	<chem>CC(C)[C@H](C)(C)[C@@H](NC(=O)C[C@H](CCC(O)=O)NC(=O)C[C@H](CCC(O)=O)NC(=O)C[C@H](CC1=CC=C(C=C1)NC(=O)C[C@H](CC(O)=O)NC(=O)CNC(=O)C[C@H](CC(N)=O)NC(=O)CNC(=O)CNC(=O)CNC(=O)CNC(=O)C)[C@@H](CCCC(N)=N)NC(=O)C[C@H](CCCC(N)=N)NC(=O)C[C@H](N)CC1=CC=C(C=C1)C(=O)N1CCCC[C@H]1C(=O)N[C@@H](CCCC(O)=O)C(=O)N[C@@H](CCCC(O)=O)C(=O)N[C@@H](CC1=CC=C(C=C1)C(=O)N[C@@H](CCCC(C)C)C(=O)O)</chem>	2D Structure		3D Structure	 download ↓

Predicted Results 3 Overview

Overview
[download ↓](#)

Disease Name	Count	Methods
HYPERTENSION, ESSENTIAL	5	DRRS LAGCN DRHGNC SCPMF iDrug
ASTHMA, SUSCEPTIBILITY TO	4	DRRS LAGCN DRHGNC SCPMF
MIGRAINE WITH OR WITHOUT AURA, SUSCEPTIBILITY TO, 1	4	DRRS LAGCN DRHGNC SCPMF
MALARIA, SUSCEPTIBILITY TO	4	DRRS LAGCN DRHGNC SCPMF
CHOLESTASIS, PROGRESSIVE FAMILIAL INTRAHEPATIC, 2; PFIC2	3	DRRS SCPMF iDrug
INFLAMMATORY BOWEL DISEASE (CROHN DISEASE) 1; IBID1	3	DRRS LAGCN DRHGNC
CYSTIC FIBROSIS; CF	3	DRRS DRHGNC iDrug
ARTERIOVENOUS MALFORMATIONS OF THE BRAIN	3	DRRS DRHGNC SCPMF
MYCOBACTERIUM TUBERCULOSIS, SUSCEPTIBILITY TO	3	DRRS LAGCN DRHGNC
BREAST CANCER	3	DRRS DRHGNC ANMF

Predicted Results 4

DRRS LAGCN SCMPFD DRHGNC SCPMF HNRD iDrug ANMF MS8MF
[download ↓](#)

Order	Disease Name	OMIM ID	MeSH	Score
1	ASTHMA, SUSCEPTIBILITY TO	600807	D0012x	1
2	INTERMEDIATE CORONARY SYNDROME	-	-	1
3	LONG QT SYNDROME 2; LQT2	613688	C56361	0.9449
4	HYPERTENSION, ESSENTIAL	145500	D0000x	0.9325
5	SHORT QT SYNDROME 1; SQT1	609620	C5665x	0.9307
6	MIGRAINE WITH OR WITHOUT AURA, SUSCEPTIBILITY TO, 1	157300	-	0.9133
7	DRUG METABOLISM, POOR, CYP2D6-RELATED	608902	C5668x	0.9049
8	MALARIA, SUSCEPTIBILITY TO	611162	D0082x	0.9027
9	CORONARY THROMBOSIS	-	D0033x	0.8925
10	Venous Thrombosis	-	D0202x	0.867

Fig 12. The drug detailed page of HN-DREP

4.2 Disease

- You can search by disease id (Mesh ID, OMIM ID, DO ID, MedGen ID) or disease name to get to the disease details, a page that includes basic information about the disease (OMIM ID, MeSH ID, DO ID, MedGen ID, etc.), as well as entries on associated drugs that are predicted by integrating all the methods.
- The detailed page has the basic information of the searched disease, and the prediction results associated with it. The left form is an aggregation of all the results on the right, including the name of the predicted drugs, the number of times it occurs, and which methods predicted the entry, and the right side is the prediction disease results of a single method for this diseases, including drug name and

its DrugBank ID.(Fig. 13)

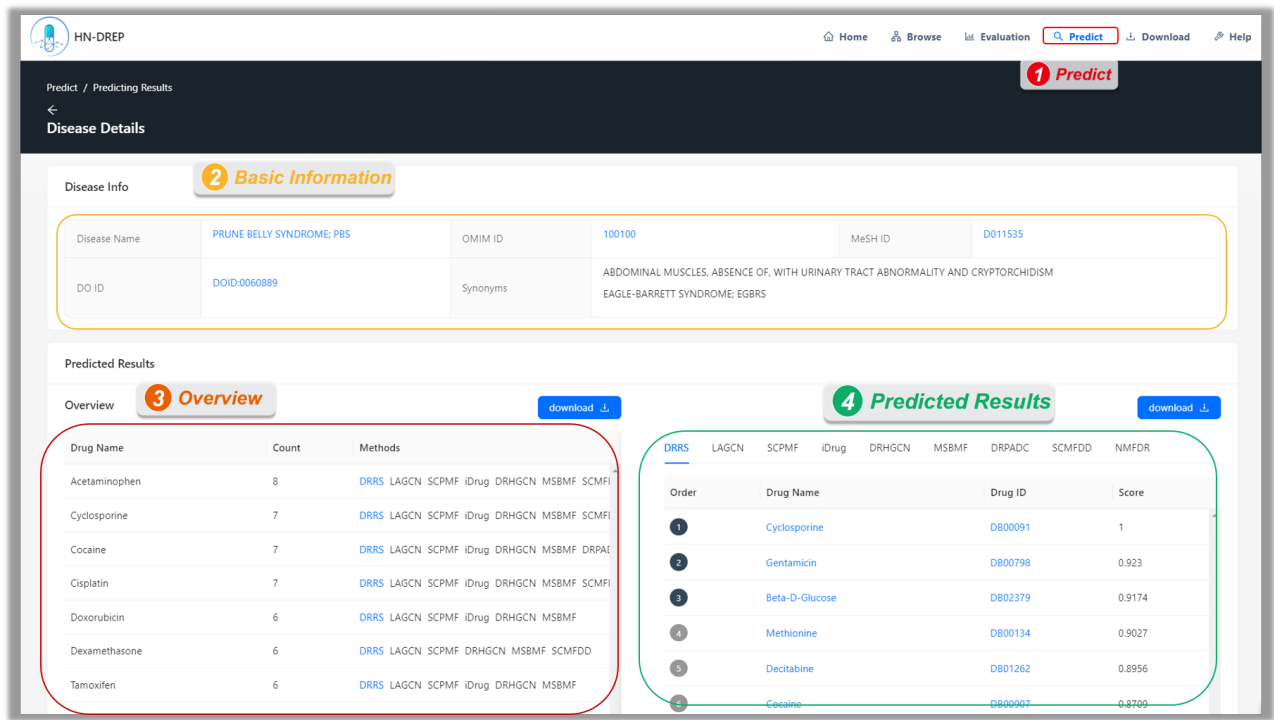


Fig 13. The disease detailed page of HN-DREP

5. Download

Click the **Download** button in the navigation bar to enter the download page. On the download page, you can download the all data we used.(Fig. 14)

- The drug and disease information contained in the dataset. It includes drug name and drug id, disease name and disease id.
- All datasets we used. It contains the dataset required by the method.

- The prediction results of all methods on the datasets.

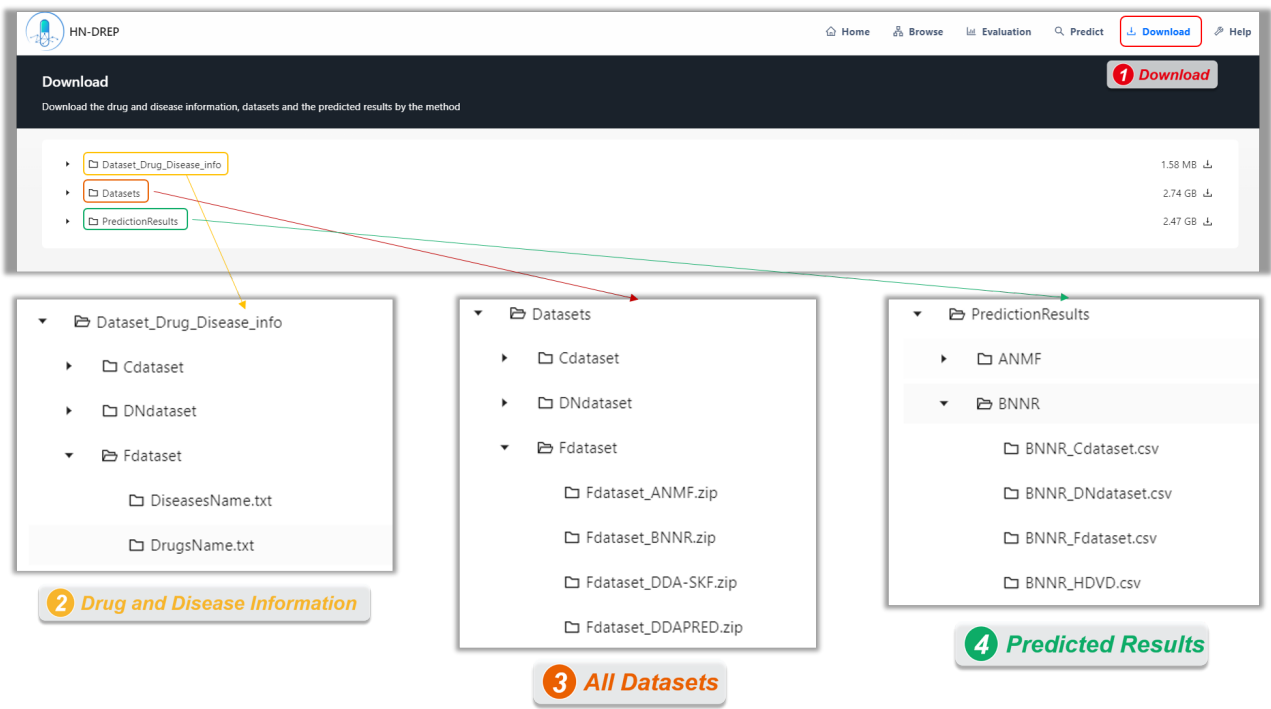


Fig 14. The download page of HN-DREP