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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**)

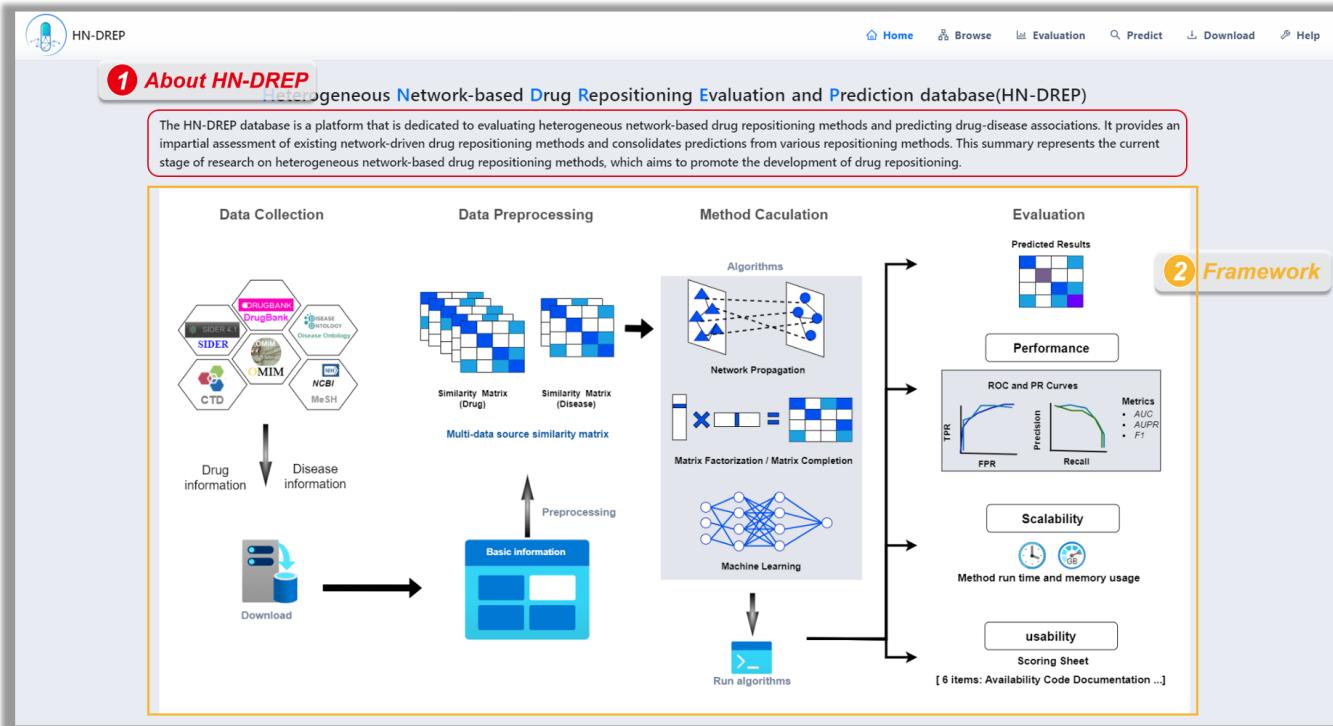


Fig 1. The HN-DREP homepage

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**)

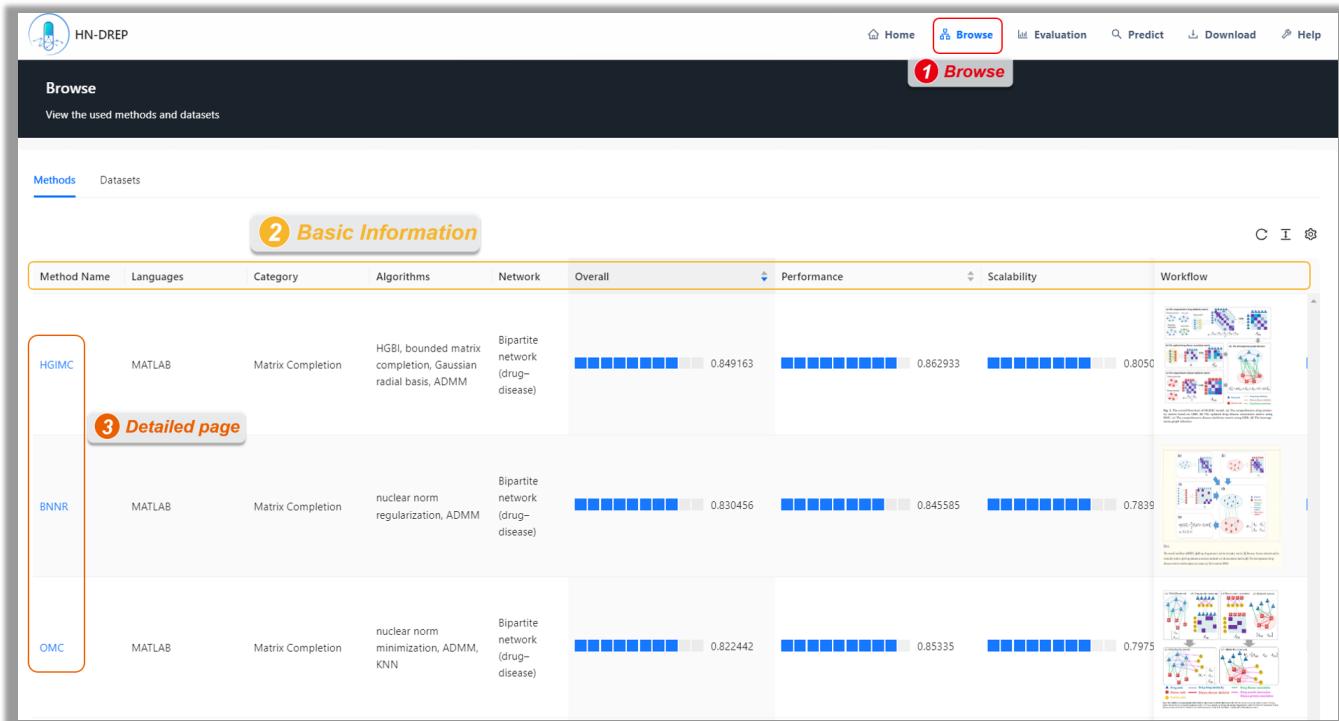


Fig 3. The Browse methods page of the HN-DREP

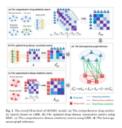
HN-DREP

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Evaluation / Method

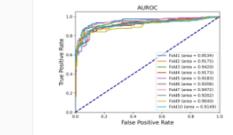
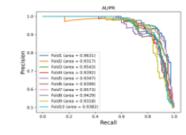
Method Details

2 Basic Information

Method Name	HGIMC	Languages	MATLAB	Category	Matrix Completion
Algorithms	HGBI, bounded matrix completion, Gaussian radial basis, ADMM	Network	Bipartite network (drug-disease)	Overall	 0.849163
Performance	 0.862933	Scalability	 0.80509	Usability	 0.896
Code Address	https://github.com/BioinformaticsCSU/HGIMC	Description	HGIMC is a heterogeneous graph inference with matrix completion method to predict potential indications for approved and novel drugs.		
Dois	10.1093/bioinformatics/btaa1024	Workflow			

HGIMC Performance On All Datasets

3 Evaluation Results

Fdataset		Numbers of drug		593	Numbers of disease		313
Numbers of drug-disease associations		1933	Dois	10.1093/msb.2011.26			
AUC	0.9255	AUPR	0.9433	F1			
AUC Curve		AUPR Curve		F1	0.6768		
Time	14s	Memory	0.76GB				

Method Predicted Results

4 Predicted Results

DrugName	DrugBankID	Disease Name	OMIM ID	MeSH ID	DO ID	MedGen ID	Score
Fenofibrate	DB01039	HYPOALPHALIPOPROTEINEMIA, PRIMARY, 1	-	-	-	-	0.9
Selegiline	DB01037	DEMENTIA/PARKINSONISM WITH NON-ALZHEIMER AMYLOID PLAQUES	-	-	-	-	0.9
Fluocinolone acetonide	DB00591	DERMATITIS, ATOPIC, 3; ATOD3	-	-	-	-	0.9
Fluocinolone acetonide	DB00591	DERMATITIS, ATOPIC, 5; ATOD5	-	-	-	-	0.9
Fluocinolone acetonide	DB00591	DERMATTIS, ATOPIC, 4; ATOD4	-	-	-	-	0.9
Primidone	DB00794	DENTATORUBRAL-PALLIDOLYSIAN ATROPHY; DRPLA	-	-	-	-	0.9
Rotigotine	DB05271	PARALYSIS AGITANS, JUVENILE, OF HUNT	168100	-	-	-	0.9
Teniposide	DB00444	LEUKEMIA, CHRONIC LYMPHOCYTIC; CLL	151400	D015451	D015451	-	0.9
Ibandronate	DB00710	BONE MINERAL DENSITY QUANTITATIVE TRAIT LOCUS 1; BMND1	-	-	-	-	0.9
Triamterene	DB00384	NEPHROTIC SYNDROME, TYPE 4; NPHS4	256370	-	D015451	-	0.9
Lisuride	DB00589	PARALYSIS AGITANS, JUVENILE, OF HUNT	168100	-	-	-	0.8
Profenamine	DB00392	PARALYSIS AGITANS, JUVENILE, OF HUNT	168100	-	-	-	0.8
Bendroflumethiazide	DB00436	ASCITES, CHYLOUS	208300	-	-	-	0.8

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**)

Dataset Name	Numbers of drug	Numbers of disease	Numbers of drug-disease associations	Dois
Cdataset	663	409	2352	10.1093/bioinformatics/btw228
deepDR	1519	1229	6677	10.1093/bioinformatics/btz418
Ddataset	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

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

HN-DREP

Evaluation / Dataset

← Dataset Details

2 Basic Information

Dataset Name	Fdataset	Numbers of drug	593	Numbers of disease	313
Numbers of drug-disease associations	1933	Dois	10.1038/msb.2011.26		

Method Performance On Fdataset

3 Evaluation Results

MBIRW					
Method Name	MBIRW	Languages	MATLAB	Category	Network Propagation
Algorithms	bi-random walk	Network	Bipartite network (drug-disease)	Code Address	https://github.com/bioinformaticsCSU/MBIRW
Description	a novel computational method, which utilizes some comprehensive similarity measures and Bi-Random walk algorithm to identify potential novel indications for a given drug.	Dataset Used In Paper	Fdataset;Cdataset	Dois	10.1093/bioinformatics/btw228
Workflow					
AUC	AUC	0.9120	AUPR	0.9294	F1
AUC Curve					
Time	Time	17s	Memory	Memory	0.76GB

4 Predicted Results

DrugName	DrugBankID	Disease Name	OMIM ID	MeSH ID	DO ID	MedGen ID	Score
Enalapril	DB00584	RENAL FAILURE, PROGRESSIVE, WITH HYPERTENSION: RFH1	161900	C562889	-	-	1
Triamcinolone	DB00620	DERMATOSIS PAPULOSA NIGRA	125600	-	-	-	1
Prochlorperazine	DB00433	SCHIZOPHRENIA: SCZD	181500	D012559	D0ID:5419	-	1
Pamidronic acid	DB00282	PAGET DISEASE OF BONE 2, EARLY-ONSET; PD82	602080	D010001	D0ID:5408	-	0.9999
Propranolol	DB00571	ATRIAL FIBRILLATION, FAMILIAL 3; AFB3	607554	C563817	-	-	0.9998
Bleomycin	DB00290	MISMATCH REPAIR CANCER SYNDROME 1; MMRC51	276300	C536928	-	-	0.9997
Dihydrocodeine	DB01551	INSENSITIVITY TO PAIN WITH HYPERPLASTIC MYELINOPATHY	147530	-	-	-	0.9996
Triamcinolone	DB00620	GROWTH RETARDATION, SMALL AND PUFFY HANDS AND FEET, AND ECZEMA	233810	-	-	-	0.9995
Dextromethorphan	DB00514	INSENSITIVITY TO PAIN WITH HYPERPLASTIC MYELINOPATHY	147530	-	-	-	0.9992
Prednisone	DB00635	SPASTIC PARAPLEGIA AND EVANS SYNDROME	601608	-	-	-	0.9992
Ethinylestradiol	DB00977	BREAST CANCER	114480	D001943	D0ID:3459_D0ID:1612	-	0.9992
Teniposide	DB00444	MISMATCH REPAIR CANCER SYNDROME 1; MMRC51	276300	C536928	-	-	0.999

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**)

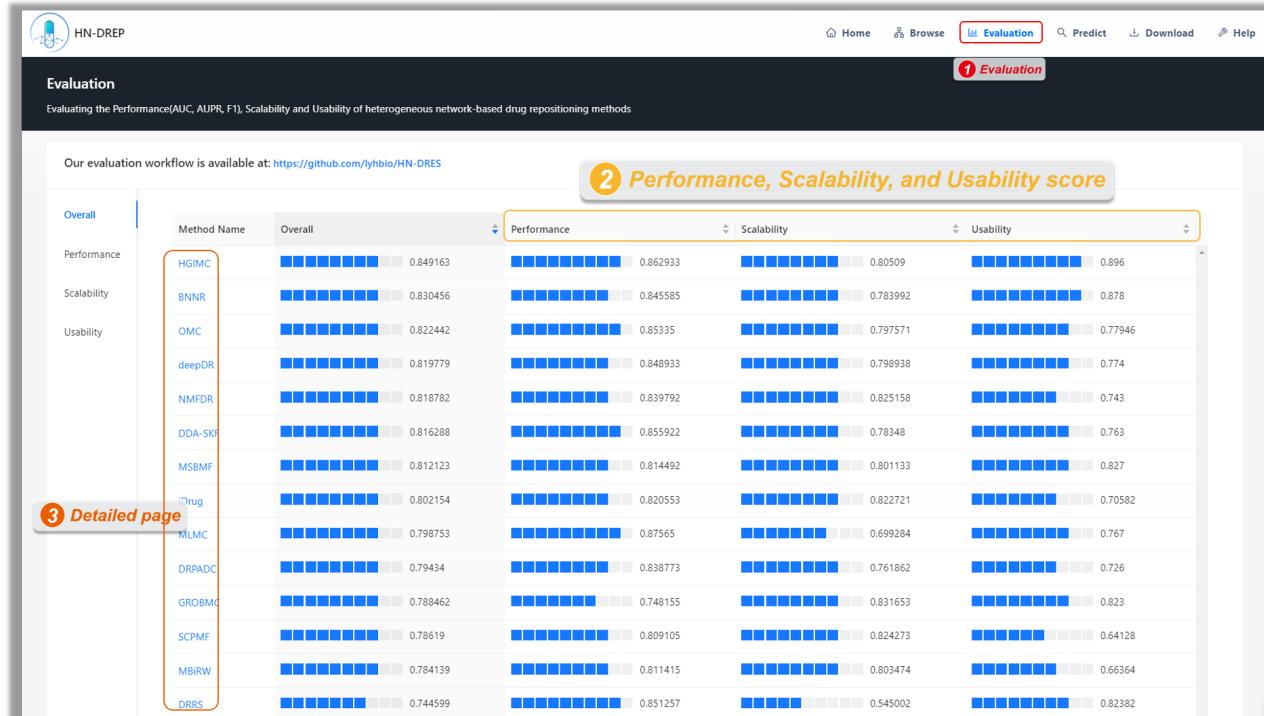


Fig 7. The overall evalutaion results: Performance, Scalability and Usability

- **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)

Overall	Performance	Scalability	Usability	Switch Display Mode Button											
				Cdataset			deepDR			DNdataset			Fdataset		
Method Name	AUC	AUPR	F1	AUC	AUPR	F1	AUC	AUPR	F1	AUC	AUPR	F1	AUC	AUPR	F1
ANMF	0.8981	0.2119	0.3103	0.8676	0.0320	0.0870	NA	NA	NA	0.9362	0.2795	0.3357	NA	NA	NA
	0.9497	0.9627	0.6889	0.9085	0.9414	0.6711	0.9257	0.9516	0.6780	0.9312	0.9490	0.6799	NA	NA	NA
	0.9450	0.9450	0.9450	NA	NA	NA	NA	NA	NA	0.9332	0.9475	0.6799	NA	NA	NA
	0.9428	0.6394	0.6218	NA	NA	NA	NA	NA	NA	0.9313	0.5639	0.5627	NA	NA	NA
	NA	NA	NA	0.9269	0.9413	0.6786	NA	NA	NA	NA	NA	NA	NA	NA	NA
	0.9627	0.6641	0.6461	0.9403	0.5357	0.5544	0.9237	0.2034	0.1582	0.9450	0.5772	0.5762	NA	NA	NA
	0.9678	0.3770	0.0101	NA	NA	NA	NA	NA	NA	0.9571	0.3003	0.0105	NA	NA	NA
	0.9348	0.9494	0.6810	0.9134	0.9403	0.6729	0.9666	0.9737	0.6895	0.9296	0.9475	0.6788	NA	NA	NA
	0.9500	0.9615	0.6881	0.8901	0.9242	0.6630	0.9440	0.9642	0.6870	0.9343	0.9497	0.6809	NA	NA	NA
	0.9807	0.7537	0.6132	0.9192	0.4042	0.6137	0.9573	0.5076	0.6146	0.9773	0.7247	0.6131	NA	NA	NA
HGIMC	0.9440	0.9577	0.6859	NA	NA	NA	NA	NA	NA	0.9255	0.9433	0.6768	NA	NA	NA

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)

Overall	Performance	Scalability	Usability	Time or Memory Usage											
				Cdataset	deepDR	DNdataset	Fdataset	HDVD	iDrug	LAGCN	LRSSL	SCMFDD_L	TLHGBI	Ydataset	
ANMF	1m14s	16m14s	NA	47s	7s	NA	3m52s	2m38s	3h10m	NA	8m4s	NA	NA	NA	NA
	38s	1m49s	27m46s	28s	10s	11m23s	51s	48s	20m13s	28m12s	1m49s	NA	NA	NA	NA
	29s	NA	NA	NA	NA	NA	NA	51s	NA	NA	NA	NA	NA	NA	NA
	56s	NA	NA	41s	NA	NA	NA	NA	1m34s	NA	NA	NA	NA	NA	NA
	NA	6m36s	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
	2m44s	17m54s	1h14m	2m9s	43s	58m41s	2m6s	4m53s	39m32s	1h20m	9m3s	NA	NA	NA	NA
	31s	NA	NA	24s	NA	NA	NA	56s	NA	NA	NA	NA	NA	NA	NA
	45s	11m26s	38m0s	35s	10s	19m37s	25s	1m24s	11m45s	37m0s	2m29s	NA	NA	NA	NA
	4m26s	14m39s	41m51s	3m7s	NA	1h22m	5m14s	4m39s	45m55s	1h7m	11m12s	NA	NA	NA	NA
	16s	1m2s	4m41s	13s	8s	3m29s	13s	22s	1m49s	6m29s	42s	NA	NA	NA	NA
HGIMC	17s	NA	NA	14s	NA	7m44s	NA	NA	NA	NA	50s	NA	NA	NA	NA
	NA	NA	NA	18s	NA	NA	3m58s	NA	NA	NA	NA	NA	NA	NA	NA

Fig 9. The method scalability evalutaion results

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

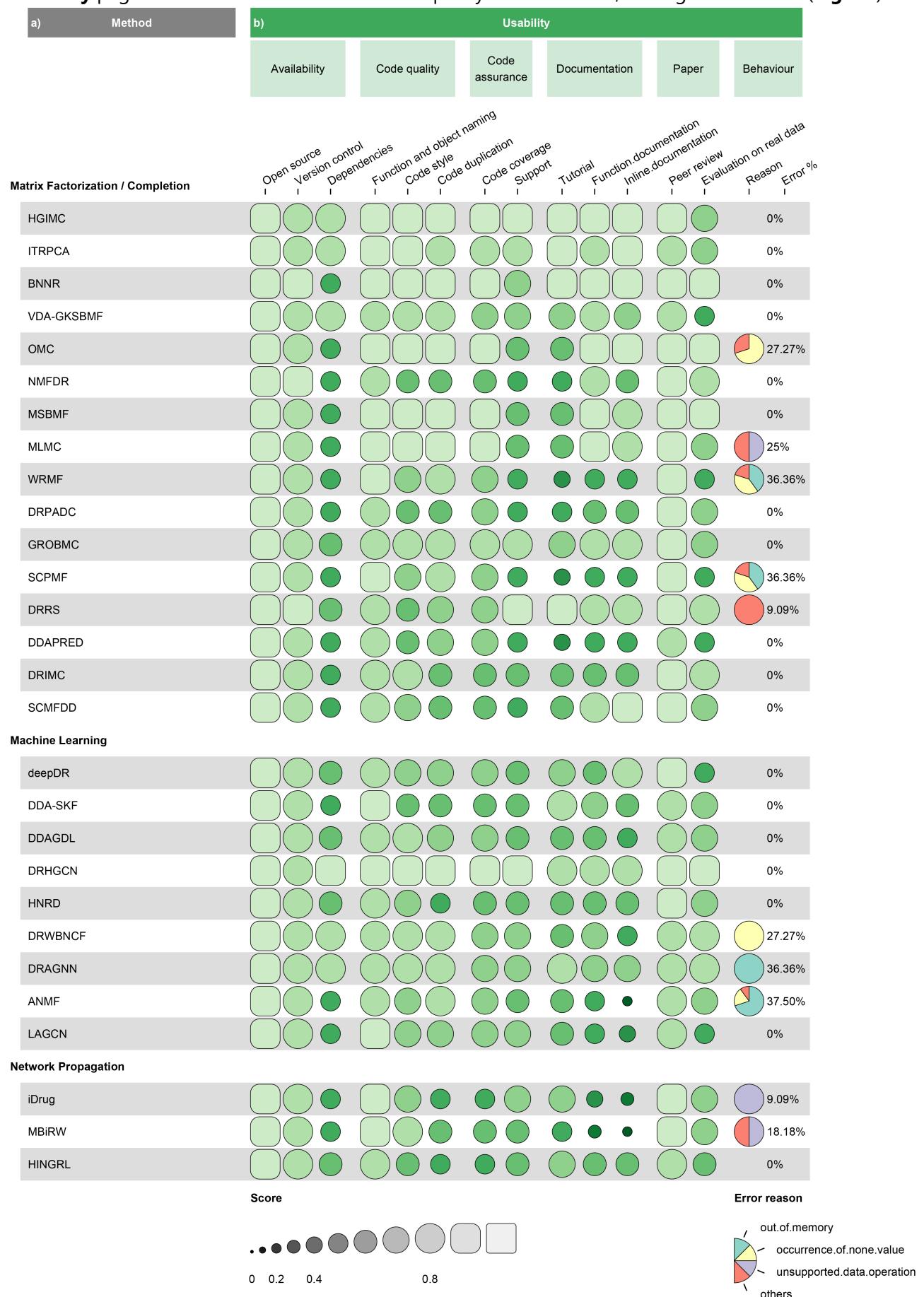


Fig 10. The method usability evalutaion results

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**)

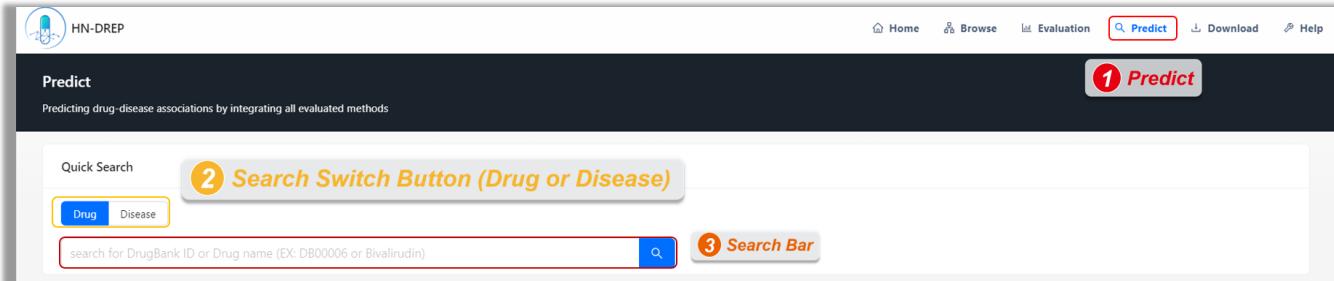


Fig 11. The HN-DREP search page

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

IDs.(Fig. 12)

HN-DREP

Predict / Predicting Results

← Drug Details

2 Basic Information

DrugName	Bivalirudin	DrugBankID	DB00006	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@H](C)[C@H](C)C(=O)C(=O)CCC(O)=ONC(=O)C@H</chem> <chem>CC(C)O=ONC(=O)C@H</chem> <chem>(CC1=CC=CC=C1)NC(=O)C@H</chem> <chem>(CC(O)=O)NCl=O)CNC(=O)C@H</chem> <chem>(CC(N)=O)NCl=O)CNC(=O)CNC(=O)C</chem> <chem>NC(=O)CNC(=O)</chem> <chem>[C@H]1CCCCNC(=O)C@H</chem> <chem>(CCCN(N)=N)NC(=O)</chem> <chem>[C@H]1CCCCNC(=O)C@H</chem> <chem>(N)CC1=CC=C1C(=O)N1CC[C@H]1C(=O)N[C@@H]</chem> <chem>(CC(O)=O)C(=O)N[C@@H]</chem> <chem>(CCC(O)=O)C(=O)N[C@@H]</chem> <chem>(CC1=CC=C(O)C=C1)C(=O)N[C@@H]</chem> <chem>(CC(C)C)C(=O)O</chem>	2D Structure		3D Structure	

3 Overview

Disease Name	Count	Methods
HYPERTENSION, ESSENTIAL	5	DRRS LAGCN DRHGCN SCPMF iDrug
ASTHMA, SUSCEPTIBILITY TO	4	DRRS LAGCN DRHGCN SCPMF
MIGRAINE WITH OR WITHOUT AURA, SUSCEPTIBILITY TO, 1	4	DRRS LAGCN DRHGCN SCPMF
MALARIA, SUSCEPTIBILITY TO	4	DRRS LAGCN DRHGCN SCPMF
CHOLESTASIS, PROGRESSIVE FAMILIAL INTRAHEPATIC, 2; PFIC2	3	DRRS SCPMF iDrug
INFLAMMATORY BOWEL DISEASE (CROHN DISEASE) 1; IBD1	3	DRRS LAGCN DRHGCN
CYSTIC FIBROSIS; CF	3	DRRS DRHGCN iDrug
ARTERIOVENOUS MALFORMATIONS OF THE BRAIN	3	DRRS DRHGCN SCPMF
MYCOBACTERIUM TUBERCULOSIS, SUSCEPTIBILITY TO	3	DRRS LAGCN DRHGCN
BREAST CANCER	3	DRRS DRHGCN ANMF

4 Predicted Results

DRRS	LAGCN	SCMFDD	DRHGCN	SCPMF	HNRD	iDrug	ANMF	MSBMF
Order	Disease Name	OMIM ID		MeSH	Score			
1	ASTHMA, SUSCEPTIBILITY TO	600807		D0012+	1			
2	INTERMEDIATE CORONARY SYNDROME	-		-	1			
3	LONG QT SYNDROME 2; LQT2	613688		C56361	0.9449			
4	HYPERTENSION, ESSENTIAL	145500		D0000+	0.9325			
5	SHORT QT SYNDROME 1; SQT1	609620		C5665C	0.9307			
6	MIGRAINE WITH OR WITHOUT AURA, SUSCEPTIBILITY TO, 1	157300		-	0.9133			
7	DRUG METABOLISM, POOR, CYP2D6-RELATED	608902		C5638+	0.9049			
8	MALARIA, SUSCEPTIBILITY TO	611162		D0082+	0.9027			
9	CORONARY THROMBOSIS	-		D0033+	0.8925			
10	Venous Thrombosis	-		D0202+	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**)

Basic Information

Disease Name	PRUNE BELLY SYNDROME; PBS	OMIM ID	100100	MeSH ID	D011535
DO ID	DOID-0006089	Synonyms	ABDOMINAL MUSCLES, ABSENCE OF, WITH URINARY TRACT ABNORMALITY AND CRYPTORCHIDISM EAGLE-BARRETT SYNDROME; EGBRS		

Predicted Results

Overview

Drug Name	Count	Methods
Acetaminophen	8	DRRS LAGCN SCPMF iDrug DRHGCN MSBMF SCMF1
Cyclosporine	7	DRRS LAGCN SCPMF iDrug DRHGCN MSBMF SCMF1
Cocaine	7	DRRS LAGCN SCPMF iDrug DRHGCN MSBMF DRPAI
Cisplatin	7	DRRS LAGCN SCPMF iDrug DRHGCN MSBMF SCMF1
Doxorubicin	6	DRRS LAGCN SCPMF iDrug DRHGCN MSBMF
Dexamethasone	6	DRRS LAGCN SCPMF DRHGCN MSBMF SCMFDD
Tamoxifen	6	DRRS LAGCN SCPMF iDrug DRHGCN MSBMF

4 Predicted Results

Order	Drug Name	Drug ID	Score
1	Cyclosporine	DB00091	1
2	Gentamicin	DB00798	0.923
3	Beta-D-Glucose	DB02379	0.9174
4	Methionine	DB00134	0.9027
5	Decitabine	DB01262	0.8956
6	Cocaine	DB00007	0.8709

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.

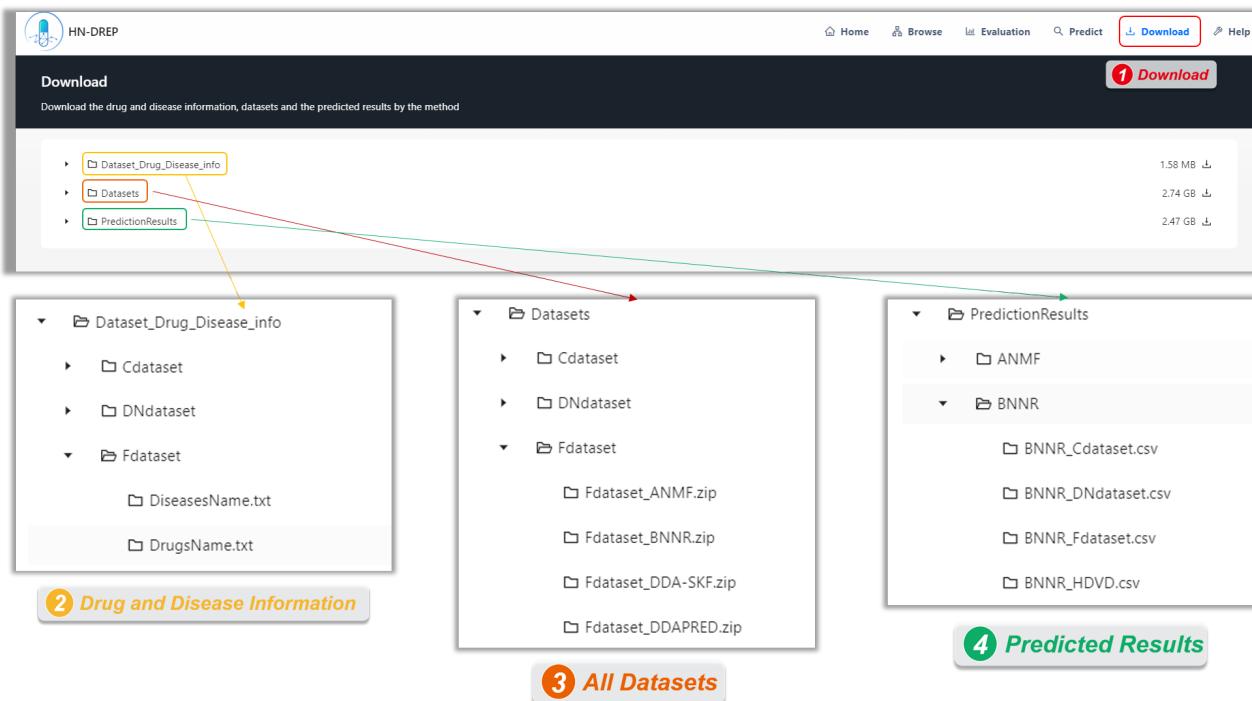


Fig 14. The download page of HN-DREP