Supplementary information

for

DCABM-TCM: A Database of Constituents Absorbed into the Blood and Metabolites of Traditional Chinese Medicine

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Tutorials

for

the analysis functions of

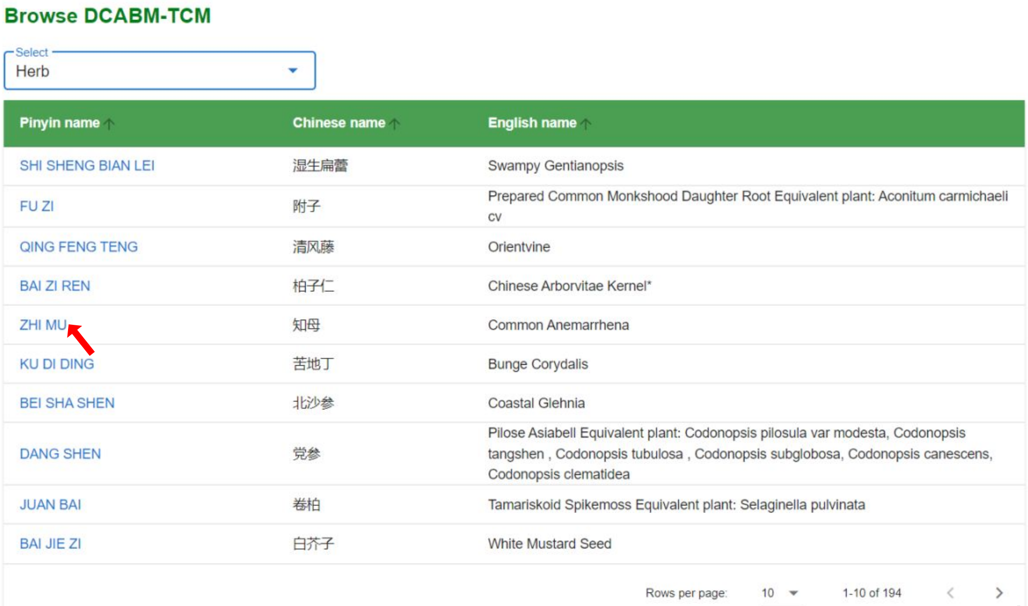
DCABM-TCM

Updated on 2023-06-16
By Zhongyang Liu and Jinying Liu

Tutorial for the network pharmacology analysis function

Taking the herb “ZHI MU” as an example, we show the tutorial for the network pharmacology analysis function.

Step 1: By database browse (A) or search page (B), users can enter the detailed annotation page of "ZHI MU", on which the results of the network pharmacology analysis of "ZHI MU" will be given in the bottom column (shown in the next step).



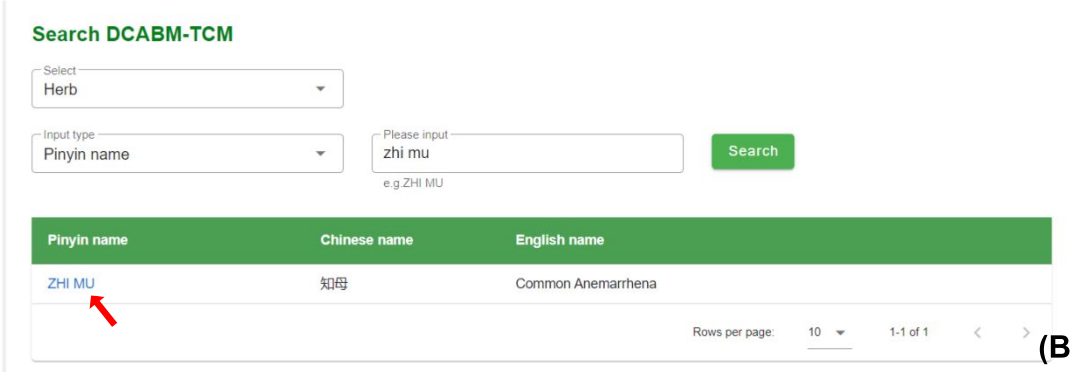
Browse DCABM-TCM

Select: Herb

Pinyin name	Chinese name	English name
SHI SHENG BIAN LEI	湿生扁蕾	Swampy Gentianopsis
FU ZI	附子	Prepared Common Monkshood Daughter Root Equivalent plant: Aconitum carmichaeli cv
QING FENG TENG	清风藤	Orientvine
BAI ZI REN	柏子仁	Chinese Arborvitae Kernel*
ZHI MU	知母	Common Anemarrhena
KU DI DING	苦地丁	Bunge Corydalis
BEI SHA SHEN	北沙参	Coastal Glehnia
DANG SHEN	党参	Pilose Asiabell Equivalent plant: Codonopsis pilosula var modesta, Codonopsis tangshen , Codonopsis tubulosa , Codonopsis subglobosa, Codonopsis canescens, Codonopsis clematidea
JUAN BAI	卷柏	Tamariskoid Spikemoss Equivalent plant: Selaginella pulvinata
BAI JIE ZI	白芥子	White Mustard Seed

Rows per page: 10 1-10 of 194

(A)



Search DCABM-TCM

Select: Herb

Input type: Pinyin name

Please input: zhi mu

e.g.ZHI MU

Pinyin name	Chinese name	English name
ZHI MU	知母	Common Anemarrhena

Rows per page: 10 1-1 of 1

(B)

Step2: The network pharmacology analysis results are given here. The results include three sections: Result1, target prediction result; Result2, bioinformatics analyses of potential targets (including KEGG pathway, GO functional term, CTR/OMIM disease enrichment analyses); Result3: blood constituent-target-pathway-disease association network visualization.

Step3: Parameter adjustment

Score_cutoff: For each blood constituent, DCABM-TCM ranks its predicted candidate targets according to the order of decreasing scores given by the target prediction algorithm previously constructed by us [Sci Rep. 2016, 6:21146] for the drug-target interaction prediction. The predicted candidate targets with scores>="Score_cutoff" (including known direct targets backed by DrugBank, KEGG and TTD) will be hypothesized as the potential targets of the blood constituent. The following network pharmacology analyses are based on these potential targets. The default value is 20.

Adjusted P-value cutoff: The significantly enriched GO functional terms, KEGG biological pathways and TTD/OMIM diseases among the potential targets are analyzed. The cutoff of the P-value after Benjamini-Hochberg multiple testing correction (i.e. adjusted P-value cutoff) for the significant level can be set. The default value is 0.05.

Users can change the two parameters here. If the parameters are changed, all results will be updated.

Network pharmacology analysis based on BATMAN-TCM

The following are the target prediction and analysis results of the blood constituents of the interested prescription/herb. This function is implemented by BATMAN-TCM previously developed by our group. This aims to reveal potential molecular mechanism of the prescription/herb.

Parameter setting

Target Prediction: For the blood constituent, proteins whose target prediction scores exceed a given cutoff **"Score cutoff"** (including known targets) will be considered as the potential targets, and will be presented and further analyzed.

Please input **Score cutoff** : 20

Target Analyses: The significantly enriched Gene Ontology functional terms, KEGG biological pathways and OMIM/CTD diseases among the potential targets of the blood constituents of the prescription/herb are analyzed

Please set the cutoff of **P-value after Benjamini-Hochberg multiple testing correction (Adjusted P-value)** for the enrichment analysis: 0.05

You can change the two parameters and re-analyze all results below.

Result 1: Target Prediction Result | Result 2: Bioinformatics analyses of potential targets | Result 3: Network visualization

As you set, only the predicted candidate target proteins with scores >= **20** are presented.

herb_ZHI_MU

Summary

There are 10 blood constituent(s) (with chemical structure(s)) whose targets can be predicted.

Target Prediction Result

Show 10 **compounds each page**

Search your interested protein (Gene Symbol):

Compound	Predicted targets [Gene Symbol] ranked according to the decreasing (score)
46173862	CXCR4(48.000)
167691	DPP4(48.000)GANC(48.000)MGAM(48.000)GANAB(48.000)UGCG(48.000) GAA(48.000)
44575944	ATP1A1(48.000)
131900	CPT2(48.000)MGAM(48.000)GANC(48.000)GAA(48.000)GANAB(48.000) CPT1A(48.000)UGCG(48.000)
44575945	CXCR4(48.000)
101389834	ATP1A1(48.000)
6918448	This compound doesn't have any potential target with score larger than 20.
15953793	CXCR4(48.000)
5281647	This compound doesn't have any potential target with score larger than 20.
5281656	This compound doesn't have any potential target with score larger than 20.

Showing 1 to 10 of 10 entries

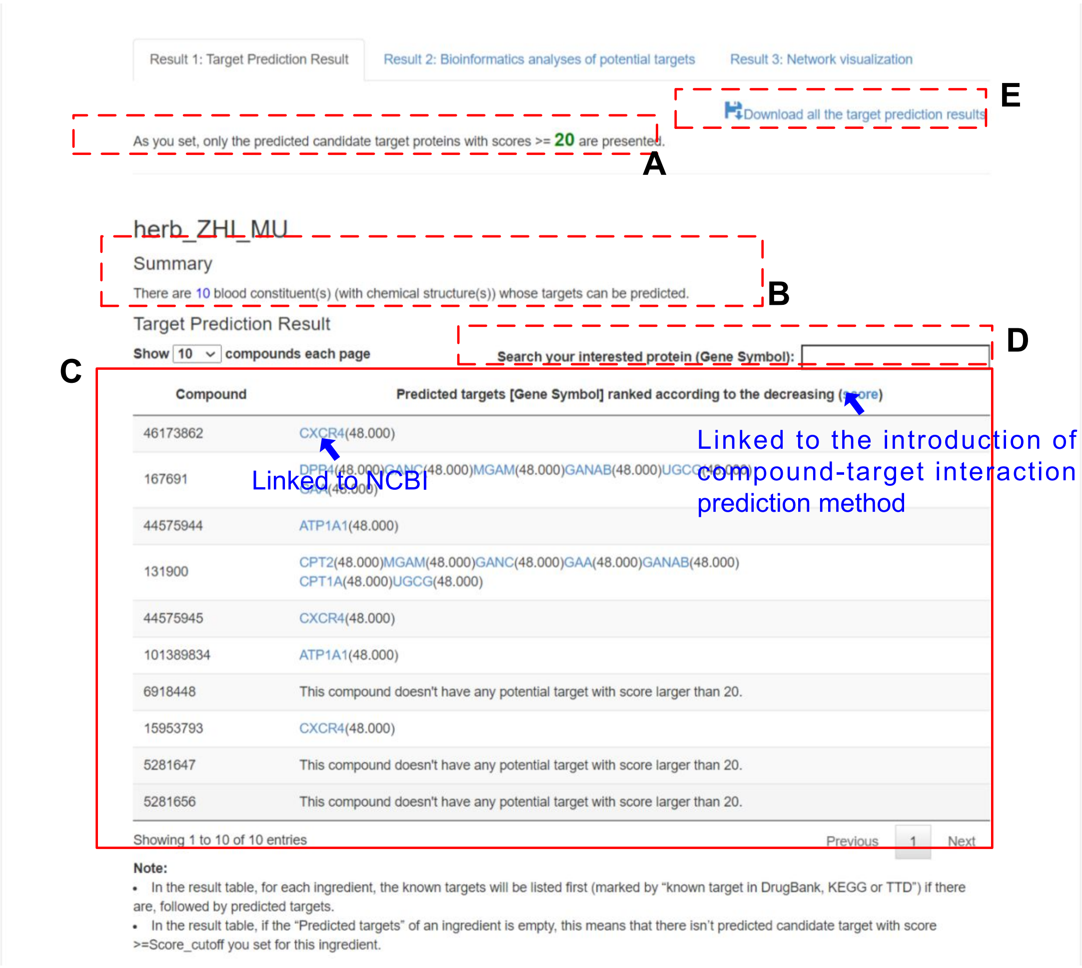
Previous 1 Next

Note:

- In the result table, for each ingredient, the known targets will be listed first (marked by "known target in DrugBank, KEGG or TTD") if there are, followed by predicted targets.
- In the result table, if the "Predicted targets" of an ingredient is empty, this means that there isn't predicted candidate target with score >=Score_cutoff you set for this ingredient.

Result1: Target prediction result

For each blood constituent of "ZHI MU", the predicted candidate targets (denoted by Gene Symbol) with scores>=Score_cutoff ranked according to the order of decreasing scores given by the target prediction method are listed in the result table (including known targets).



As you set, only the predicted candidate target proteins with scores >= 20 are presented.

herb_ZHI_MU

Summary

There are 10 blood constituent(s) (with chemical structure(s)) whose targets can be predicted.

Target Prediction Result

Compound	Predicted targets [Gene Symbol] ranked according to the decreasing (score)
46173862	CXCR4(48.000)
167691	DPP4(48.000)GANC(48.000)MGAM(48.000)GANAB(48.000)UGCG(48.000) GAA(48.000)
44575944	ATP1A1(48.000)
131900	CPT2(48.000)MGAM(48.000)GANC(48.000)GAA(48.000)GANAB(48.000) CPT1A(48.000)UGCG(48.000)
44575945	CXCR4(48.000)
101389834	ATP1A1(48.000)
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15953793	CXCR4(48.000)
5281647	This compound doesn't have any potential target with score larger than 20.
5281656	This compound doesn't have any potential target with score larger than 20.

Showing 1 to 10 of 10 entries

Note:

- In the result table, for each ingredient, the known targets will be listed first (marked by “known target in DrugBank, KEGG or TTD”) if there are, followed by predicted targets.
- In the result table, if the “Predicted targets” of an ingredient is empty, this means that there isn’t predicted candidate target with score >=Score_cutoff you set for this ingredient.

A: According to user-defined parameter, only the predicted candidate targets with scores>=Score_cutoff (also including known targets) will be presented in the result table and be considered as potential targets.

B: Only for blood constituents with chemical structures, targets can be predicted.

C: The target prediction result table. For each blood constituent, known targets reported by DrugBank (version: 20150726), KEGG (version: July 31, 2014) and TTD (version: 4.3.02) database (marked by “known target in DrugBank, KEGG or TTD”) will be given first if there are, followed by predicted targets.

D: Users can search the interested gene among these targets.

E: The complete target prediction result can be downloaded.

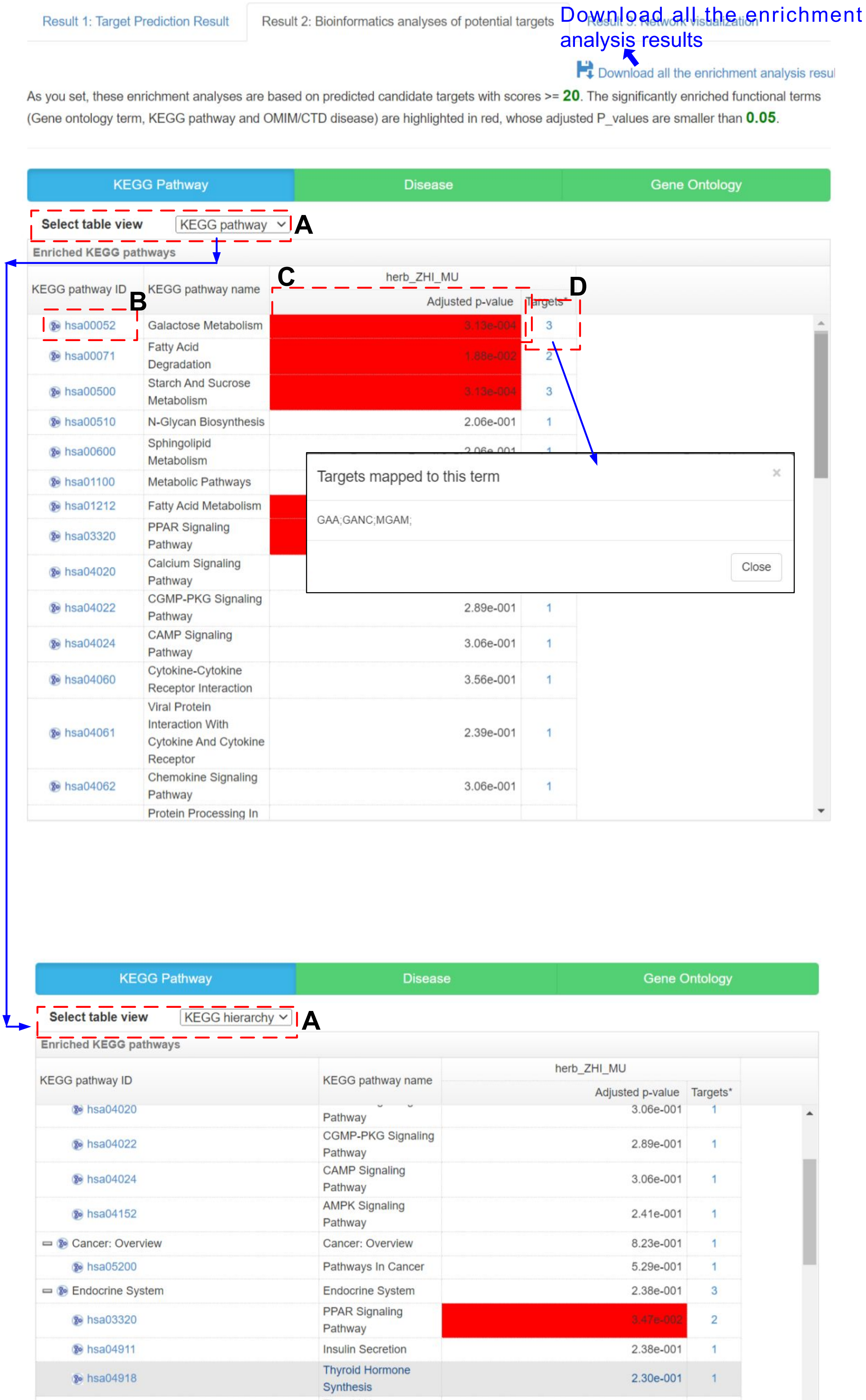
Result 2: Bioinformatics analyses of potential targets

Further for the potential targets of blood constituents, DCABM-TCM provides three enrichment analyses, including KEGG biological pathway, GO functional term and OMIM/TTD disease enrichment analyses.

The significantly enriched KEGG biological pathways, GO functional terms and OMIM disease phenotypes/TTD diseases among the potential targets of blood constituents together with corresponding adjusted P-value and targets mapped to this term will be presented in the result table.

Attention: The enrichment analyses are based on the predicted candidate targets with scores>=Score_cutoff (also including known targets).

KEGG pathway enrichment analysis result



As you set, these enrichment analyses are based on predicted candidate targets with scores >= **20**. The significantly enriched functional terms (Gene ontology term, KEGG pathway and OMIM/CTD disease) are highlighted in red, whose adjusted P_values are smaller than **0.05**.

Enriched KEGG pathways

KEGG pathway ID	KEGG pathway name	herb_ZHI_MU	
		Adjusted p-value	Targets*
hsa00052	Galactose Metabolism	3.13e-004	3
hsa00071	Fatty Acid Degradation	1.88e-002	2
hsa00500	Starch And Sucrose Metabolism	3.13e-004	3
hsa00510	N-Glycan Biosynthesis	2.06e-001	1
hsa00600	Sphingolipid Metabolism	2.06e-001	1
hsa01100	Metabolic Pathways		
hsa01212	Fatty Acid Metabolism		
hsa03320	PPAR Signaling Pathway		
hsa04020	Calcium Signaling Pathway		
hsa04022	CGMP-PKG Signaling Pathway	2.89e-001	1
hsa04024	CAMP Signaling Pathway	3.06e-001	1
hsa04060	Cytokine-Cytokine Receptor Interaction	3.56e-001	1
hsa04061	Viral Protein Interaction With Cytokine And Cytokine Receptor	2.39e-001	1
hsa04062	Chemokine Signaling Pathway	3.06e-001	1
	Protein Processing In		

Targets mapped to this term

GAA;GANC;MGAM;

Enriched KEGG pathways

KEGG pathway ID	KEGG pathway name	herb_ZHI_MU	
		Adjusted p-value	Targets*
hsa04020	Pathway	3.06e-001	1
hsa04022	CGMP-PKG Signaling Pathway	2.89e-001	1
hsa04024	CAMP Signaling Pathway	3.06e-001	1
hsa04152	AMPK Signaling Pathway	2.41e-001	1
▭ Cancer: Overview	Cancer: Overview	8.23e-001	1
hsa05200	Pathways In Cancer	5.29e-001	1
▭ Endocrine System	Endocrine System	2.38e-001	3
hsa03320	PPAR Signaling Pathway	3.47e-002	2
hsa04911	Insulin Secretion	2.38e-001	1
hsa04918	Thyroid Hormone Synthesis	2.30e-001	1

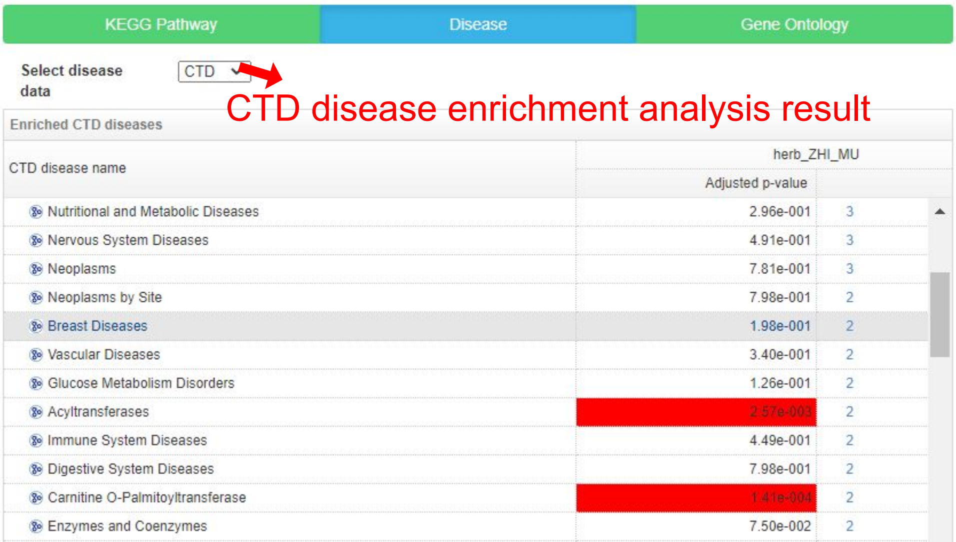
A: Here we provide two kinds of views to present the KEGG pathway enrichment analysis results. Tree view (“KEGG hierarchy”) shows the hierarchy of pathways.

B: The “KEGG pathway IDs” are crosslinked to the KEGG database.

C: The significantly enriched pathways with adjusted P-value smaller than the cutoff set by users are highlighted in red.

D: “Targets” are referred to as the targets mapped to the pathway and clicking on the number will present the detailed target list.

Disease enrichment analysis result

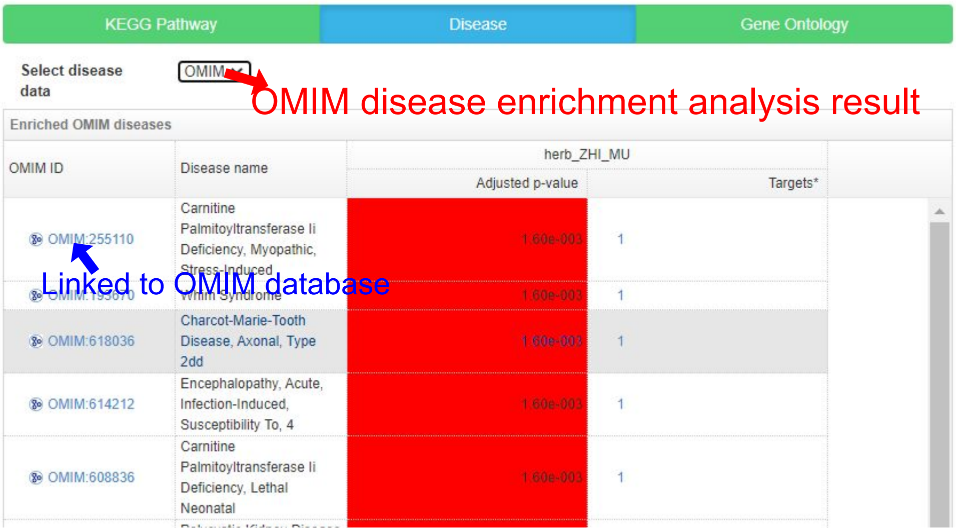


Select disease data: CTD

CTD disease enrichment analysis result

Enriched CTD diseases

CTD disease name	herb_ZHI_MU	
	Adjusted p-value	
Nutritional and Metabolic Diseases	2.96e-001	3
Nervous System Diseases	4.91e-001	3
Neoplasms	7.81e-001	3
Neoplasms by Site	7.98e-001	2
Breast Diseases	1.98e-001	2
Vascular Diseases	3.40e-001	2
Glucose Metabolism Disorders	1.26e-001	2
Acyltransferases	2.57e-003	2
Immune System Diseases	4.49e-001	2
Digestive System Diseases	7.98e-001	2
Carnitine O-Palmitoyltransferase	1.41e-004	2
Enzymes and Coenzymes	7.50e-002	2



Select disease data: OMIM

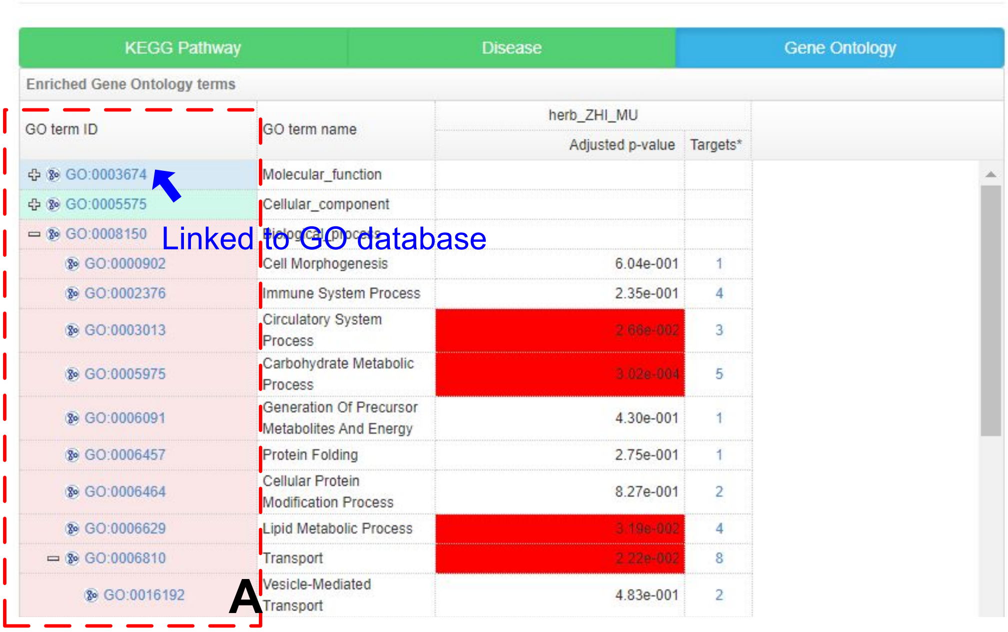
OMIM disease enrichment analysis result

Linked to OMIM database

Enriched OMIM diseases

OMIM ID	Disease name	herb_ZHI_MU	
		Adjusted p-value	Targets*
OMIM:255110	Carnitine Palmitoyltransferase Ii Deficiency, Myopathic, Stress-Induced	1.60e-003	1
OMIM:193670	Whim Syndrome	1.60e-003	1
OMIM:618036	Charcot-Marie-Tooth Disease, Axonal, Type 2dd	1.60e-003	1
OMIM:614212	Encephalopathy, Acute, Infection-Induced, Susceptibility To, 4	1.60e-003	1
OMIM:608836	Carnitine Palmitoyltransferase Ii Deficiency, Lethal Neonatal	1.60e-003	1

GO term enrichment analysis result



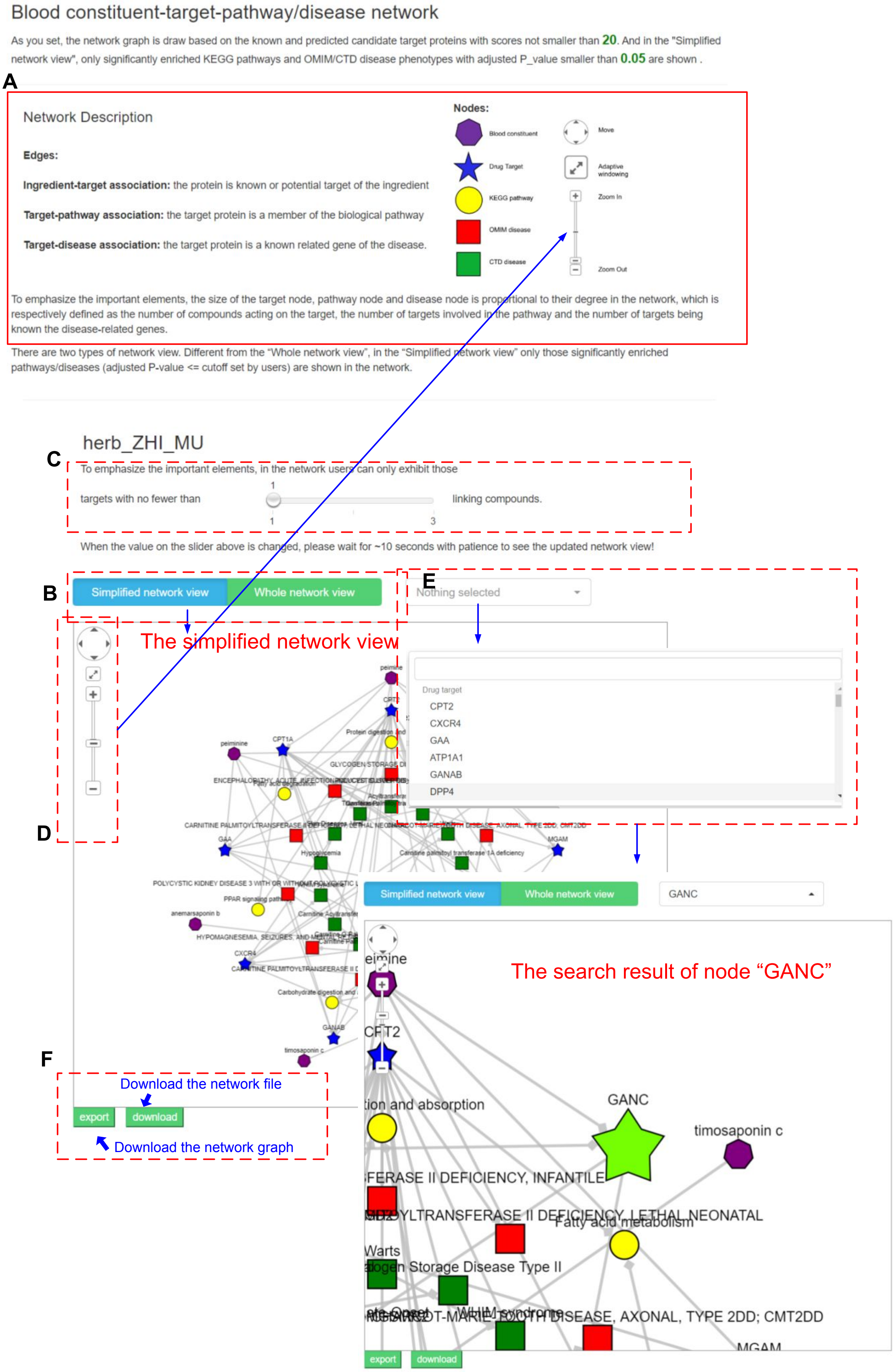
Enriched Gene Ontology terms

GO term ID	GO term name	herb_ZHI_MU	
		Adjusted p-value	Targets*
GO:0003674	Molecular_function		
GO:0005575	Cellular_component		
GO:0008150	Biological_process		
GO:0000902	Cell Morphogenesis	6.04e-001	1
GO:0002376	Immune System Process	2.35e-001	4
GO:0003013	Circulatory System Process	2.66e-002	3
GO:0005975	Carbohydrate Metabolic Process	3.02e-004	5
GO:0006091	Generation Of Precursor Metabolites And Energy	4.30e-001	1
GO:0006457	Protein Folding	2.75e-001	1
GO:0006464	Cellular Protein Modification Process	8.27e-001	2
GO:0006629	Lipid Metabolic Process	3.19e-002	4
GO:0006810	Transport	2.22e-002	8
GO:0016192	Vesicle-Mediated Transport	4.83e-001	2

A: The GO enrichment analysis result is presented as a tree structure which shows the hierarchical relationship between GO terms. GO terms of three categories are painted by different colors.

Result 3: Blood constituent-target-pathway/disease association network visualization

The network graph is drew based on the predicted candidate target proteins with scores>=Score_cutoff (user defined) of the constituents.



Blood constituent-target-pathway/disease network

As you set, the network graph is draw based on the known and predicted candidate target proteins with scores not smaller than **20**. And in the "Simplified network view", only significantly enriched KEGG pathways and OMIM/CTD disease phenotypes with adjusted P_value smaller than **0.05** are shown .

Network Description

Edges:

Ingredient-target association: the protein is known or potential target of the ingredient

Target-pathway association: the target protein is a member of the biological pathway

Target-disease association: the target protein is a known related gene of the disease.

Nodes:

To emphasize the important elements, the size of the target node, pathway node and disease node is proportional to their degree in the network, which is respectively defined as the number of compounds acting on the target, the number of targets involved in the pathway and the number of targets being known the disease-related genes.

There are two types of network view. Different from the "Whole network view", in the "Simplified network view" only those significantly enriched pathways/diseases (adjusted P-value <= cutoff set by users) are shown in the network.

herb_ZHI_MU

To emphasize the important elements, in the network users can only exhibit those targets with no fewer than 1 linking compounds.

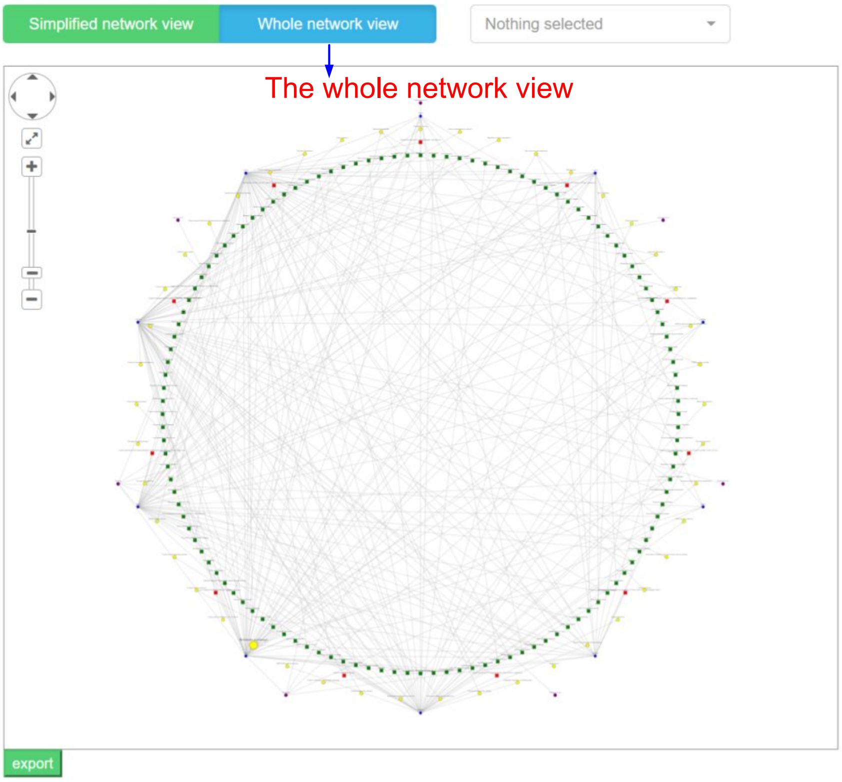
When the value on the slider above is changed, please wait for ~10 seconds with patience to see the updated network view!

The simplified network view

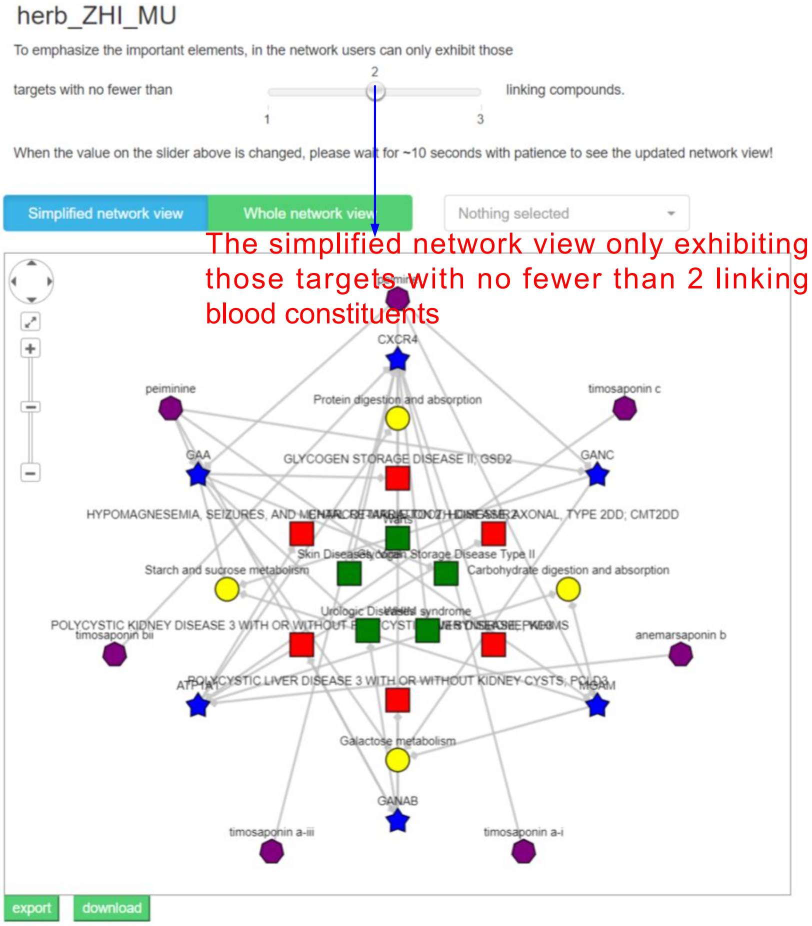
The search result of node "GANC"

Download the network file

Download the network graph



The whole network view


herb_ZHI_MU

To emphasize the important elements, in the network users can only exhibit those targets with no fewer than 2 linking compounds.

When the value on the slider above is changed, please wait for ~10 seconds with patience to see the updated network view!

The simplified network view only exhibiting those targets with no fewer than 2 linking blood constituents

A: In the association network, there are four kinds of nodes distinguished by different shapes and colors including blood constituents, targets, biological pathways and OMIM/TTD diseases and three types of edges including constituents-target association (if the protein is a known or potential target of the constituents), target-pathway association (if the target protein is a member of the biological pathway) and target-disease association (if the target protein is a known related gene of the disease). In addition, to emphasize the important elements, the size of the target node, pathway node and disease node is proportional to their degree in the network, which is respectively defined as the number of compounds acting on the target, the number of targets involved in the pathway and the number of targets being known the disease-related genes.

B: There are two types of network view. Different from the “Whole network view”, in the “Simplified network view” only those significantly enriched pathways /diseases (adjusted P-value <= cutoff set by users) are shown in the network.

C: Users can only exhibit those targets with no fewer than M linking blood constituents (which can be adjusted by the slider) in the network.

D: The network graph navigation buttons. In addition, to further facilitate navigation, besides using these navigation buttons, users can also pan the network view by directly holding down the left mouse button in a blank area and moving the mouse. Users can also move the nodes on the graph by holding down the left mouse button on the node and moving it.

E: Node search function using the node name. Once the interested node is found in the network, the node will be highlighted in size and color on the network graph, and the area around it will be zoomed in.

F: The network graph and corresponding network file can also be downloaded.

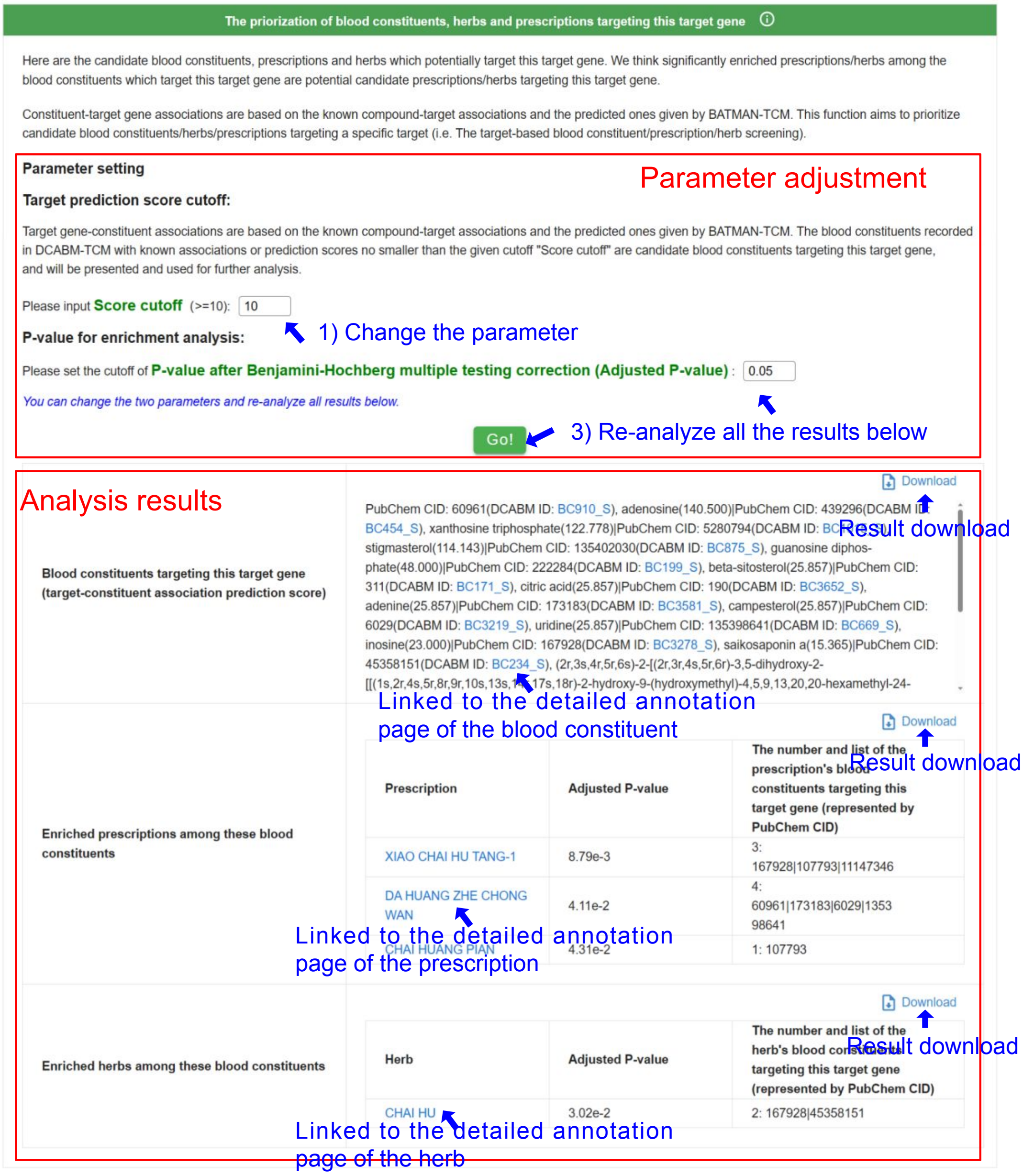
Tutorial for the analysis function of the “the priorization of blood constituents, herbs and prescriptions targeting the target gene”

For an interested target, this analysis function prioritizes the candidate blood constituents, prescriptions and herbs which potentially target this target gene (i.e. The target-based blood constituent/prescription/herb screening).
Blood constituent-target gene associations are predicted by a prediction method (BATMAN-TCM) previously constructed by us [Sci Rep. 2016, 6:21146]. Further, we think significantly enriched prescriptions/herbs among the blood constituents which target this target gene are potential candidate prescriptions/herbs targeting this target gene.

Parameter adjustment

Target prediction score cutoff: Target gene-blood constituent associations are based on the known compound-target associations and the predicted ones given by BATMAN-TCM. The blood constituents recorded in DCABM-TCM with known associations or prediction scores no smaller than the given cutoff "Score cutoff" are candidate blood constituents targeting this target gene, and will be presented and used for further analyses. The default cutoff value is set to 10.
P-Value cutoff: We think significantly enriched prescriptions/herbs among the blood constituents which target this target gene are potential candidate prescriptions/herbs targeting this target gene. The enrichment analysis is performed by the hypergeometric cumulative distribution test. This parameter is the cutoff of P-value after Benjamini-Hochberg multiple testing correction for the enrichment analysis (Adjusted P-value). The default value is set to 0.05.

You can change the two parameters and re-analyze all results.



The priorization of blood constituents, herbs and prescriptions targeting this target gene ⓘ

Here are the candidate blood constituents, prescriptions and herbs which potentially target this target gene. We think significantly enriched prescriptions/herbs among the blood constituents which target this target gene are potential candidate prescriptions/herbs targeting this target gene.

Constituent-target gene associations are based on the known compound-target associations and the predicted ones given by BATMAN-TCM. This function aims to prioritize candidate blood constituents/herbs/prescriptions targeting a specific target (i.e. The target-based blood constituent/prescription/herb screening).

Parameter setting

Target prediction score cutoff:

Target gene-constituent associations are based on the known compound-target associations and the predicted ones given by BATMAN-TCM. The blood constituents recorded in DCABM-TCM with known associations or prediction scores no smaller than the given cutoff "Score cutoff" are candidate blood constituents targeting this target gene, and will be presented and used for further analysis.

Please input **Score cutoff** (>=10): 10

P-value for enrichment analysis:

Please set the cutoff of **P-value after Benjamini-Hochberg multiple testing correction (Adjusted P-value)** : 0.05

You can change the two parameters and re-analyze all results below.

Blood constituents targeting this target gene (target-constituent association prediction score)

PubChem CID: 60961(DCABM ID: BC910_S), adenosine(140.500)|PubChem CID: 439296(DCABM ID: BC454_S), xanthosine triphosphate(122.778)|PubChem CID: 5280794(DCABM ID: BC[illegible]), stigmasterol(114.143)|PubChem CID: 135402030(DCABM ID: BC875_S), guanosine diphosphate(48.000)|PubChem CID: 222284(DCABM ID: BC199_S), beta-sitosterol(25.857)|PubChem CID: 311(DCABM ID: BC171_S), citric acid(25.857)|PubChem CID: 190(DCABM ID: BC3652_S), adenine(25.857)|PubChem CID: 173183(DCABM ID: BC3581_S), campesterol(25.857)|PubChem CID: 6029(DCABM ID: BC3219_S), uridine(25.857)|PubChem CID: 135398641(DCABM ID: BC669_S), inosine(23.000)|PubChem CID: 167928(DCABM ID: BC3278_S), saikosaponin a(15.365)|PubChem CID: 45358151(DCABM ID: BC234_S), (2r,3s,4r,5r,6s)-2-[(2r,3r,4s,5r,6r)-3,5-dihydroxy-2-[[(1s,2r,4s,5r,8r,9r,10s,13s,1[illegible],17s,18r)-2-hydroxy-9-(hydroxymethyl)-4,5,9,13,20,20-hexamethyl-24-

Enriched prescriptions among these blood constituents

Prescription	Adjusted P-value	The number and list of the prescription's blood constituents targeting this target gene (represented by PubChem CID)
XIAO CHAI HU TANG-1	8.79e-3	3: 167928|107793|11147346
DA HUANG ZHE CHONG WAN	4.11e-2	4: 60961|173183|6029|135398641
CHAI HUANG PIAN	4.31e-2	1: 107793

Enriched herbs among these blood constituents

Herb	Adjusted P-value	The number and list of the herb's blood constituents targeting this target gene (represented by PubChem CID)
CHAI HU	3.02e-2	2: 167928|45358151

Tutorial for the analysis function of the “the priorization of blood constituents, herbs and prescriptions targeting the pathway”

Here are the candidate blood constituents, prescriptions and herbs which potentially target this pathway. This function aims to prioritize candidate blood constituents/herbs/prescriptions targeting a specific pathway (i.e. The pathway-based blood constituent/prescription/herb screening).

We think that significantly enriched blood constituents among the pathway’s member genes are potential candidate blood constituents targeting this pathway. Further significantly enriched herbs/prescriptions among these potential candidate blood constituents are thought to be potential candidate herbs/prescriptions targeting this pathway. Constituent-gene associations are based on the known compound-target associations and the predicted ones given by BATMAN-TCM.

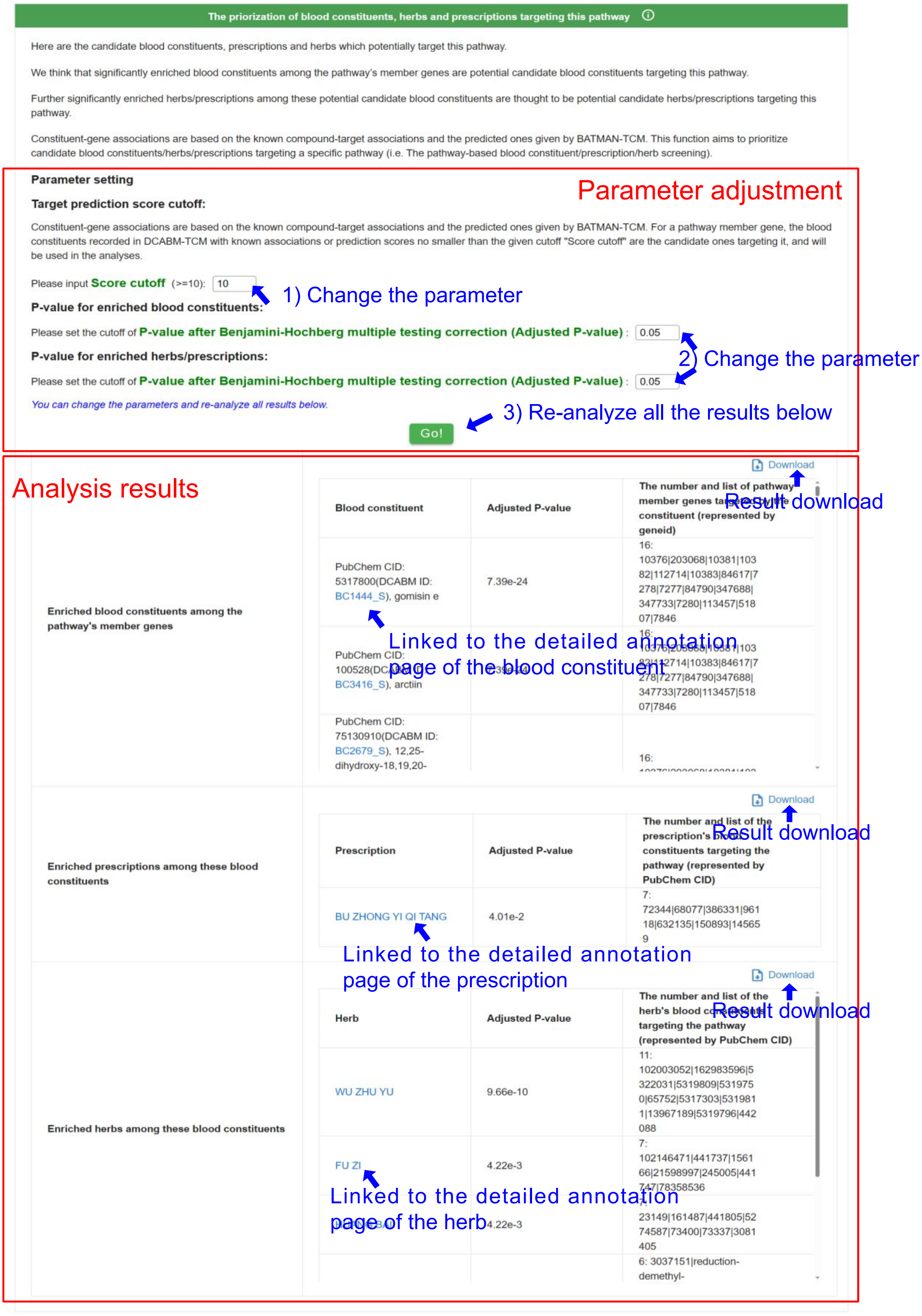
Parameter adjustment

Target prediction score cutoff: Constituent-gene associations are based on the known compound-target associations and the predicted ones given by BATMAN-TCM. For a pathway member gene, the blood constituents recorded in DCABM-TCM with known associations or prediction scores no smaller than the given cutoff "Score cutoff" are the candidate ones targeting it, and will be used in the analyses. The default value is 10.

P-value for enriched blood constituents: The enrichment analysis is performed by the hypergeometric cumulative distribution test. This parameter is the cutoff of P-value after Benjamini-Hochberg multiple testing correction for the enrichment analysis (Adjusted P-value). The default value is set to 0.05.

P-value for enriched herbs/prescriptions: The enrichment analysis is performed by the hypergeometric cumulative distribution test. This parameter is the cutoff of P-value after Benjamini-Hochberg multiple testing correction (Adjusted P-value). The default value is set to 0.05.

Users can change the three parameters and re-analyze all results.



The priorization of blood constituents, herbs and prescriptions targeting this pathway

Here are the candidate blood constituents, prescriptions and herbs which potentially target this pathway.

We think that significantly enriched blood constituents among the pathway's member genes are potential candidate blood constituents targeting this pathway.

Further significantly enriched herbs/prescriptions among these potential candidate blood constituents are thought to be potential candidate herbs/prescriptions targeting this pathway.

Constituent-gene associations are based on the known compound-target associations and the predicted ones given by BATMAN-TCM. This function aims to prioritize candidate blood constituents/herbs/prescriptions targeting a specific pathway (i.e. The pathway-based blood constituent/prescription/herb screening).

Parameter setting

Target prediction score cutoff:

Constituent-gene associations are based on the known compound-target associations and the predicted ones given by BATMAN-TCM. For a pathway member gene, the blood constituents recorded in DCABM-TCM with known associations or prediction scores no smaller than the given cutoff "Score cutoff" are the candidate ones targeting it, and will be used in the analyses.

Please input **Score cutoff** (>=10): 10

P-value for enriched blood constituents:

Please set the cutoff of **P-value after Benjamini-Hochberg multiple testing correction (Adjusted P-value)** : 0.05

P-value for enriched herbs/prescriptions:

Please set the cutoff of **P-value after Benjamini-Hochberg multiple testing correction (Adjusted P-value)** : 0.05

You can change the parameters and re-analyze all results below.

Enriched blood constituents among the pathway's member genes

Blood constituent	Adjusted P-value	The number and list of pathway member genes targeted by the constituent (represented by geneid)
PubChem CID: 5317800(DCABM ID: BC1444_S), gomisin e	7.39e-24	16: 10376|203068|10381|10382|112714|10383|84617|7278|7277|84790|347688|347733|7280|113457|51807|7846
PubChem CID: 100528(DCABM ID: BC3416_S), arctiin	7.39e-24	16: 10376|203068|10381|10382|112714|10383|84617|7278|7277|84790|347688|347733|7280|113457|51807|7846
PubChem CID: 75130910(DCABM ID: BC2679_S), 12,25-dihydroxy-18,19,20-		16:

Enriched prescriptions among these blood constituents

Prescription	Adjusted P-value	The number and list of the prescription's blood constituents targeting the pathway (represented by PubChem CID)
BU ZHONG YI QI TANG	4.01e-2	7: 72344|68077|386331|96118|632135|150893|145659

Enriched herbs among these blood constituents

Herb	Adjusted P-value	The number and list of the herb's blood constituents targeting the pathway (represented by PubChem CID)
WU ZHU YU	9.66e-10	11: 102003052|162983596|5322031|5319809|5319750|65752|5317303|5319811|13967189|5319796|442088
FU ZI	4.22e-3	7: 102146471|441737|156166|21598997|245005|441747|78358536
[illegible]	4.22e-3	7: 23149|161487|441805|5274587|73400|73337|3081405
		6: 3037151|reduction-demethyl-

Tutorial for the analysis function of the “the priorization of blood constituents, herbs and prescriptions targeting the disease”

Here are the candidate blood constituents, prescriptions and herbs which potentially target this disease. This function aims to prioritize candidate blood constituents/herbs/prescriptions targeting a specific disease (i.e. The disease-based blood constituent/prescription/herb screening).

We think that significantly enriched blood constituents among the disease-related genes are potential candidate blood constituents targeting this disease. Further significantly enriched herbs/prescriptions among these potential candidate blood constituents are thought to be potential candidate herbs/prescriptions targeting this disease. Constituent-gene associations are based on the known compound-target associations and the predicted ones given by BATMAN-TCM.

Parameter adjustment

Target prediction score cutoff: For a disease-related gene, the blood constituents recorded in DCABM-TCM with known associations or prediction scores given by BATMAN-TCM no smaller than the given cutoff "Score cutoff" are the candidate ones targeting it, and will be used in the analyses. The default value is 10.

P-value for enriched blood constituents: The enrichment analysis is performed by the hypergeometric cumulative distribution test. This parameter is the cutoff of P-value after Benjamini-Hochberg multiple testing correction (Adjusted P-value). The default value is set to 0.05.

P-value for enriched herbs/prescriptions: The enrichment analysis is performed by the hypergeometric cumulative distribution test. This parameter is the cutoff of P-value after Benjamini-Hochberg multiple testing correction (Adjusted P-value) .The default value is set to 0.05.

Users can change the parameters and re-analyze all results.

The priorization of blood constituents, herbs and prescriptions targeting this disease ⓘ

Here are the candidate blood constituents, prescriptions and herbs which potentially target this disease.

We think that significantly enriched blood constituents among the disease-related genes are potential candidate blood constituents targeting this disease.

Further significantly enriched herbs/prescriptions among these potential candidate blood constituents are thought to be potential candidate herbs/prescriptions targeting this disease.

Constituent-gene associations are based on the known compound-target associations and the predicted ones given by BATMAN-TCM. This function aims to prioritize candidate blood constituents/herbs/prescriptions targeting a specific disease (i.e. The disease-based blood constituent/prescription/herb screening).

Parameter setting

Target prediction score cutoff:

For a disease-related gene, the blood constituents recorded in DCABM-TCM with known associations or prediction scores given by BATMAN-TCM no smaller than the given cutoff "Score cutoff" are the candidate ones targeting it, and will be used in the analyses.

Please input **Score cutoff** (>=10): 10

P-value for enriched blood constituents:

Please set the cutoff of **P-value after Benjamini-Hochberg multiple testing correction (Adjusted P-value)** : 0.05

P-value for enriched herbs/prescriptions:

Please set the cutoff of **P-value after Benjamini-Hochberg multiple testing correction (Adjusted P-value)** : 0.05

You can change the parameters and re-analyze all results below.

Enriched blood constituents among the disease-related genes

Blood constituent	Adjusted P-value	The number and list of the disease-related genes targeted by the constituent (represented by geneid)
PubChem CID: 637540(DCABM ID: BC1892_S), 2-hydroxycinnamic acid	3.54e-2	1: 100506658
PubChem CID: 637541(DCABM ID: BC2789_S), 3-hydroxycinnamic acid	3.54e-2	1: 100506658
PubChem CID: 1549106(DCABM ID: BC154_S), cis-p-coumaric acid	3.54e-2	1: 100506658
PubChem CID: 54708747(DCABM ID: BC3327_S), 2,4-dihydroxycinnamate	3.54e-2	1: 100506658

Enriched prescriptions among these blood constituents

Prescription	Adjusted P-value	The number and list of the prescription's blood constituents targeting the disease (represented by PubChem CID)
GUA LOU GUI ZHI TANG	5.71e-4	3: 637540|637541|637542
NAN SHI JIAO NANG	2.99e-3	2: 54708747|637542
DANG GUI HONG HUA TANG	3.56e-2	1: 637542

Enriched herbs among these blood constituents

Herb	Adjusted P-value	The number and list of the herb's blood constituents targeting the disease (represented by PubChem CID)
QING PI ZHU	1.47e-4	2: 1549106|637542
GUI ZHI	1.47e-4	3: 637540|637541|637542
GOU QI	2.21e-2	1: 637542

Parameter adjustment

1) Change the parameter

3) Re-analyze all the results below

Analysis results

Result download

Linked to the detailed annotation page of the blood constituent

Result download

Linked to the detailed annotation page of the prescription

Result download

Linked to the detailed annotation page of the herb