manual

目录

1. Overview

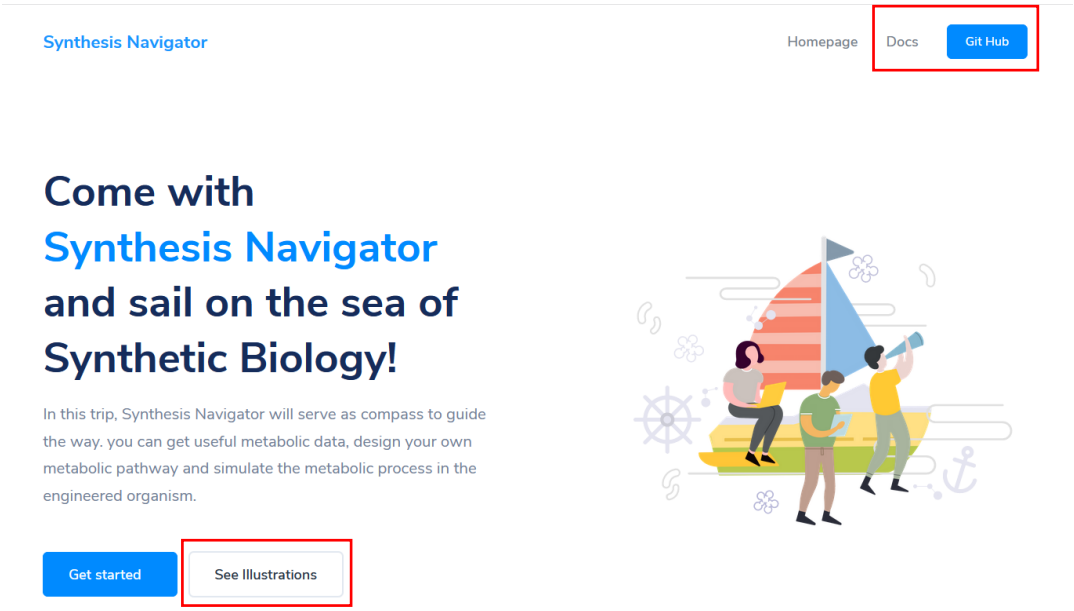
Our project aims to design a metabolic platform that simulates changes in the metabolic network to provide comprehensive results for the researcher. You can take the data from our platform, search the pathways between molecules, and perform the metabolic simulations mentioned above.

These functions, which are hosted on the web, are divided into three main modules: Synthetic Bay (DB), Pathway Finder (PF), and Deep Metabolic Simulation (DMS). Through '/Home', we can enter the Home page of the project. On this page, users can get our project's leading content and this manual (Handbook) of the software. At the same time, they can enter the three functional pages by clicking the navigation card.

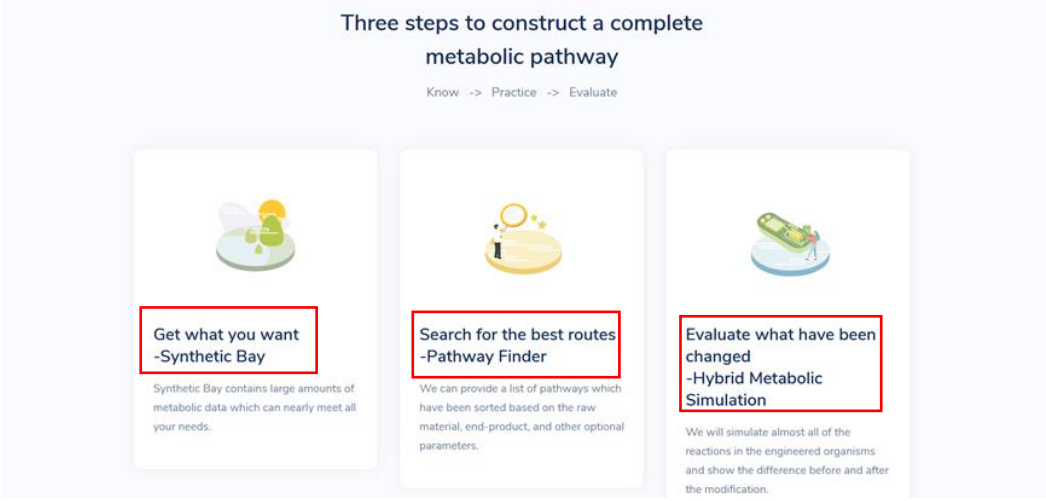
2. Getting start

>>You can input this url '/Home' to visit our web page.

>>'Docs' bar to get this handbook, 'Git Hub' bar to visit our Git Hub page to get more code details and Click the white bottom 'See Illustrations' you can watch our demonstration video



>>The main part of Home page is these three access interfaces to three function modules. Click on any of the cards, you can visit our function page.



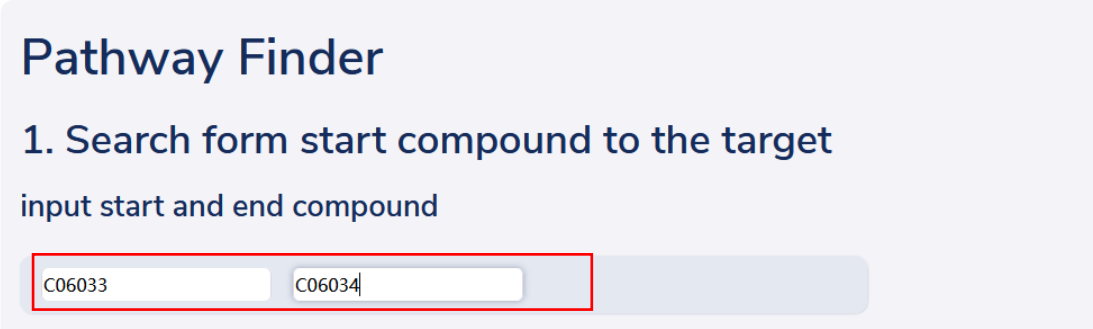
>>Click the first navigation card from the home page or input '/database' to enter the database module.

>>On the database page, click the blue botton 'Download Data' to download the data.

>>click each link you want to download, you can download this data. Then you can click the text 'Back to The Home Page' to redirect to Home page.

>> Click the second navigation card from the home page or input '/PF' to enter the Pathway Finder module.

>> In the forward pathway finder, you can input a start compound and a end compound, we will search the pathway from start to end and rank them by scores.

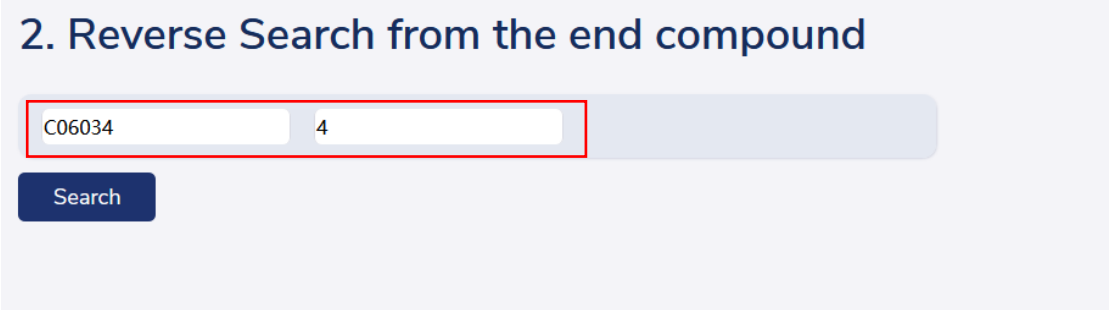


>> There are five parameters: KM, KKM, Toxicity, PH, Temperature. You can assign value to the five parameters according to their importance in the experimental environment or your priori knowledge.

>>Click the search button, you will get a PDF results, and you can download this PDF.

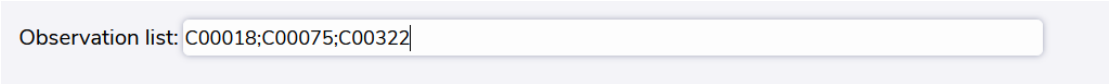
pathway_res_2020_10_24_65507017.pdf
Back to The Home Page

>> You should input the target compound a and the search depth——steps b to get the pathway target to a wth Steps no more than b. And click the search button you will get a similar PDF file.

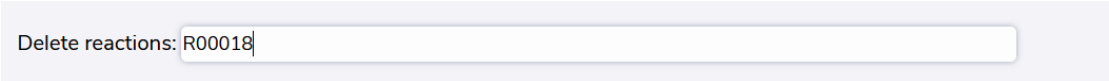


>> Click the third navigation card on the home page or '/HMS' to enter the Deep Metabolic Simulation module.

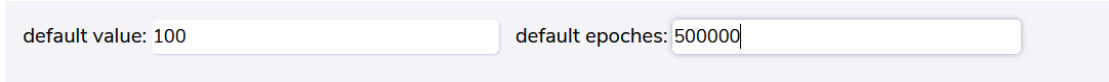
>>you should input observation_list first, which is the compound you want to observe and we will show them in the top of results with red color.



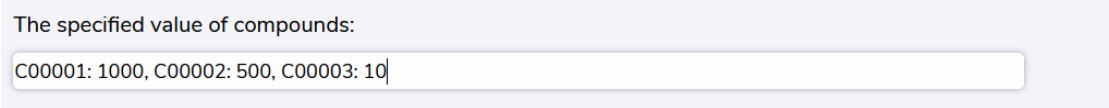
>>second, in delete_reaction_list, You can delete some reactions to block the paths between molecules.



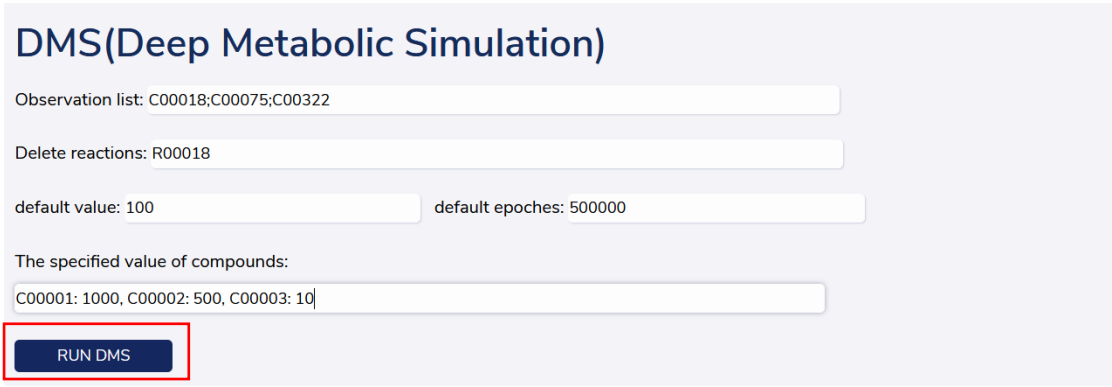
>>you should enter two default value, the first is a default initial value of all the compounds, we will define the compounds' amount with this number, and the second is the iteration times our algorithm will go through.



>>At the last, the most important parameter is specified_values. you can define every specified compound with a initial value, and we will replace this compound's default value with it.



>>When you input all the parameters, you can click the RUN DMS button to run the algorithm. You may be need wait some minutes and then you can get two results.



>>One is PDF file in which we show the compounds in observation_list and whose

value's change is in rank TOP50, other one is csv file, we output all the change information of all compounds.

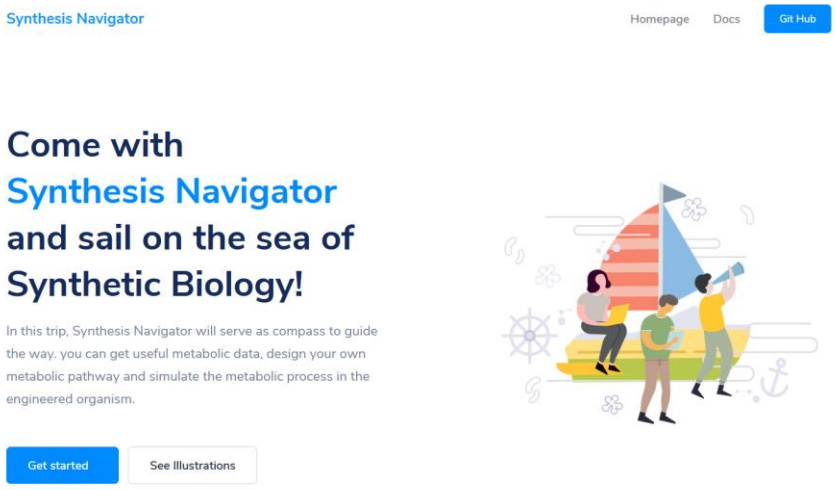
randomwalk_res_2020_10_24_98104347.pdf
randomwalk_res_2020_10_24_98104347.csv
Back to The Home Page

3. Details about our software

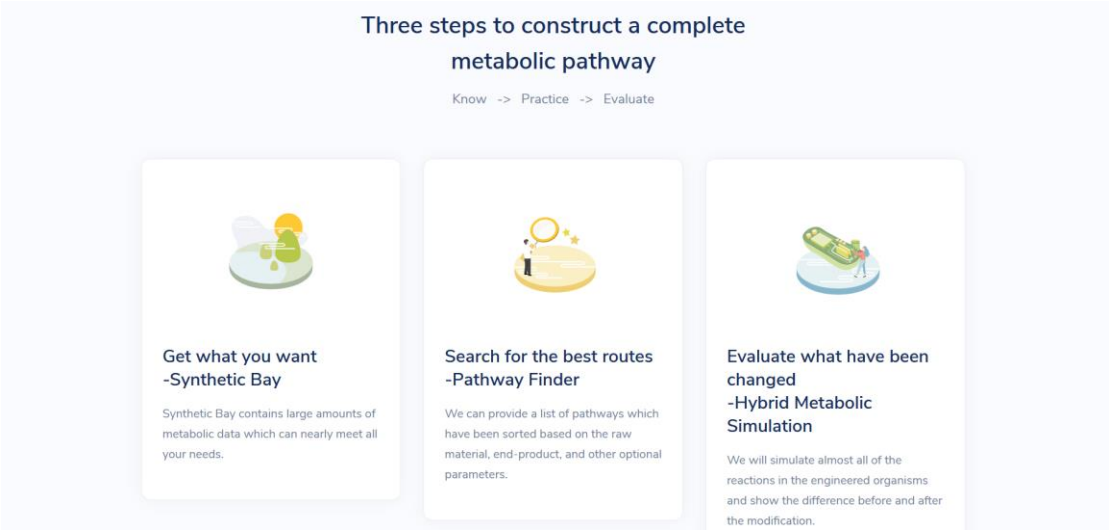
Home and handbook

On this page, you can see a brief introduction of our project. And on the top of this page, there are three navigator bar you can click to visit. *'Homepage'* bar to redirect to Home page, *'Docs'* bar to get this handbook and *'Git Hub'* bar to visit our Git Hub page to get more code details.

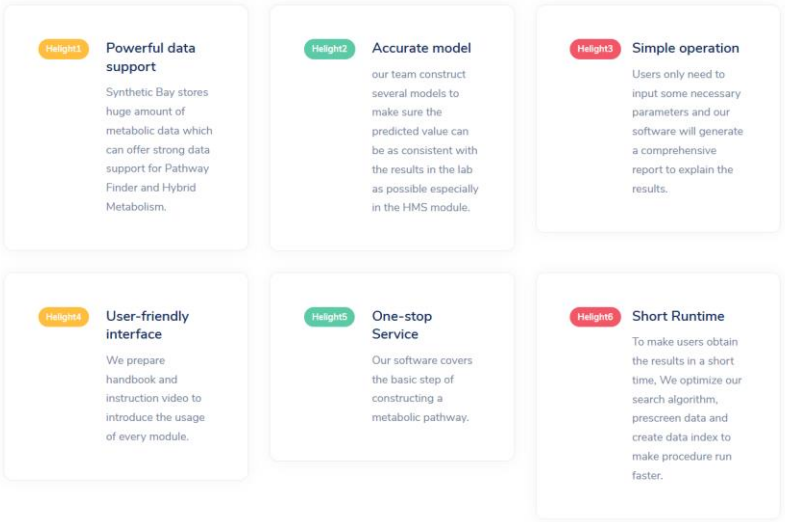
Under the overview text, you can see two bottoms colored with blue and white, respectively. Click the white bottom you can watch our demonstration video, in which we show how to use our function modules.



The main part of Home page is these three access interfaces to three function modules. Click on any of the cards, you can visit our function page.



Meanwhile, we have summarized six advantages in the bottom: Powerful database, Accurate models, Simple operation, User-friendly interface, One-stop service and Short Runtime. You can read more conclusions about our software on the Home page.



Synthetic Bay

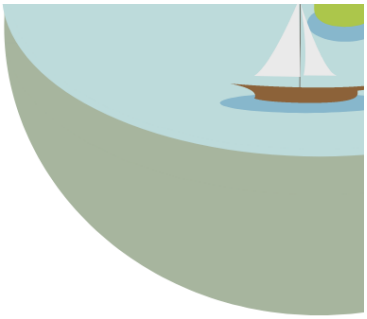
- About pages

Click the navigation card from the home page or input '/database' to enter the database module.

Here, you will know the basic framework of our data and download the data. Our data provides four downloadable files, named "reaction.csv", "compound.csv", "enzyme.csv" and "SyntheticBay.db", respectively.

In the Synthetic Bay, you can have a good knowledge of all the compounds, enzymes and reactions which might be significant components of your pathway.

Download Data



- About database

To provide data support for the Synthesis Navigator software's pathway search function and metabolic simulation function, we integrated several databases, including MetaCyc, ChEBI, BRENDA, eQuilibrator, and KEGG. Finally, we have constructed a database in *sqlite* and *sql* form, in which we create three tables: compounds, reactions and enzymes.

Compounds data is integrated from KEGG and ChEBI. We have selected 1.8k compound entries, include the information about KEGG id, compound name, formula, smile, toxicity, molecule mass, and sdf string.

Smile: a 2D pattern of molecules which can show you the structure of these molecules.

Toxicity: The value is associated with high or low toxicity of this compound. When have high toxicity, it will be harmful to biological chassis.

Sdf string: a 3D pattern involves spatial position of every atom.

```
cid,name,formula,smile,toxicity,weight,sdf
C00001,water,H2O,O,,18.0153,'  Marvin  01211112152D           3  2  0  0  0  0
C00002,ATP,C10H16N5O13P3,Nc1ncnc2c1ncn2[C@@H]1O[C@H](COP(=O)(O)OP(=O)(O)OP(=O)(O)O)[C@
C00003,NAD(+),C21H28N7O14P2,NC(=O)c1ccc[n+]([C@@H]2O[C@H](COP(=O)(O)OP(=O)(O)OC[C@H]3C
C00004,NADH,C21H29N7O14P2,NC(=O)C1=CN([C@@H]2O[C@H](COP(=O)(O)OP(=O)(O)OC[C@H]3O[C@@H]
C00005,NADPH,C21H30N7O17P3,NC(=O)C1=CN([C@@H]2O[C@H](COP(=O)(O)OP(=O)(O)OC[C@H]3O[C@@H
C00006,NADP(+),C21H29N7O17P3,NC(=O)c1ccc[n+]([C@@H]2O[C@H](COP(=O)(O)OP(=O)(O)OC[C@H]3
C00007,dioxygen,O2,O=O,,31.9988,'  Marvin  02030822342D            2  1  0  0  0  0
C00008,ADP,C10H15N5O10P2,Nc1ncnc2c1ncn2[C@@H]1O[C@H](COP(=O)(O)OP(=O)(O)O)[C@@H](O)[C@
C00009,phosphate(3-),O4P,O=P([O-])([O-])[O-],,94.97136,'  Marvin  10300609012D
C00010,coenzyme A,C21H36N7O16P3S,CC(C)(COP(=O)(O)OP(=O)(O)OC[C@H]1O[C@@H](n2cnc3c(N)nc
C00011,carbon dioxide,CO2,O=C=O,,44.01,'  Marvin  10290522252D            3  2  0  0
C00012,peptide,(C2H2NOR)nC2H3NOR,*C(N)C(=O)NC(*)C(=O)O,,,'  Marvin  07051116182D
C00013,diphosphate(4-),O7P2,O=P([O-])([O-])OP(=O)([O-])[O-],,173.94332,'  Marvin  1205
C00014,ammonia,H3N,N,,17.03056,'  Marvin  09260512442D           4  3  0  0  0  0
C00015,UDP,C9H14N2O12P2,O=c1ccn([C@@H]2O[C@H](COP(=O)(O)OP(=O)(O)O)[C@@H](O)[C@H]2O)c(
C00016,FAD,C27H33N9O15P2,Cc1cc2nc3c(=O)[nH]c(=O)nc-3n(C[C@H](O)[C@H](O)[C@H](O)COP(=O)
C00017,protein polypeptide chain,,,,,
C00018,pyridoxal 5'-phosphate,C8H10NO6P,Cc1ncc(COP(=O)(O)O)c(C=O)c1O,,247.1419,'  Marv
C00019,S-adenosyl-L-methionine,C15H23N6O5S,C[S+](CC[C@H](N)C(=O)O)C[C@H]1O[C@@H](n2cnc
C00020,adenosine 5'-monophosphate,C10H14N5O7P,Nc1ncnc2c1ncn2[C@@H]1O[C@H](COP(=O)(O)O)
C00021,S-adenosyl-L-homocysteine,C14H20N6O5S,Nc1ncnc2c1ncn2[C@@H]1O[C@H](CSCC[C@H](N)C
C00022,pyruvate,C3H3O3,CC(=O)C(=O)[O-],,87.05412,'  Marvin  11220615062D            6
```

Reaction data is integrated from KEGG, including above 10k rows. This data table have record six feature of reactions: KEGG id, EC number of enzymes participate in reaction, equation of reaction, reaction class, Gibbs energy from experiment, frequency about the reaction.

```
rid,ecnum,equation,reactionclass,energy,frequency
R00002,1.18.6.1,16 C00002 + 16 C00001 + 8 C00138 <=> 8 C05359 + 16 C00009 + 16 C0000
R00004,3.6.1.1,C00013 + C00001 <=> 2 C00009,,-15.8  0.4,
R00005,3.5.1.54,C01010 + C00001 <=> 2 C00011 + 2 C00014,C00011_C01010,-78.5 15.1,
R00006,2.2.1.6,C00900 + C00011 <=> 2 C00022,C00022_C00900,32.3  7.4,
R00008,4.1.3.17,C06033 <=> 2 C00022,C00022_C06033,16.3  4.6,
R00009,1.11.1.6 1.11.1.21,2 C00027 <=> C00007 + 2 C00001,C00007_C00027,-193.1   13.3
R00010,3.2.1.28,C01083 + C00001 <=> 2 C00031,C00031_C01083,-11.7    2.1,
R00011,1.11.1.13    1.11.1.16,2 C19610 + C00027 + 2 C00080 <=> 2 C19611 + 2 C00001,,
R00012,2.7.7.45,2 C00044 <=> C00013 + C01261,C00044_C01261,nan  nan,
R00013,4.1.1.47,2 C00048 <=> C01146 + C00011,C00048_C01146,-19.6    8.8,
R00014,1.2.4.1  2.2.1.6 4.1.1.1,C00022 + C00068 <=> C05125 + C00011,C00068_C05125
R00015,2.4.1.99,2 C00089 <=> C00031 + C03661,C00031_C00089  C00089_C03661,-6.1  10.7
R00017,1.11.1.5,C00027 + 2 C00126 <=> 2 C00125 + 2 C00001,C00125_C00126,nan nan,
R00018,2.5.1.44,2 C00134 <=> C06366 + C00014,C00134_C06366,-0.9 8.0,
R00019,1.12.7.2 1.12.99.-,2 C00138 + 2 C00080 <=> C00282 + 2 C00139,,18.0   13.0,
R00021,1.4.7.1,2 C00025 + 2 C00139 <=> C00064 + C00026 + 2 C00138 + 2 C00080,C00025_
R00022,3.2.1.52,C01674 + C00001 <=> 2 C00140,C00140_C01674,-13.8    10.8,
R00023,1.7.1.5,2 C00192 + 2 C00003 <=> C01818 + 2 C00004 + 2 C00080,C00003_C00004,na
R00024,4.1.1.39,C01182 + C00011 + C00001 <=> 2 C00197,C00197_C01182,-28.4   7.5,
R00025,1.13.12.16,C18091 + C00007 + C01847 <=> C00084 + C00088 + C00061 + C00001,C00
R00026,3.2.1.21,C00185 + C00001 <=> 2 C00221,C00185_C00221,-12.9    3.7,
R00027,4.1.2.38,C01408 <=> 2 C00261,C00261_C01408,7.8   10.2,
```

Enzyme data is integrated from KEGG, BRENDA and eQuilibrator. This data is too big to load because of its 28k items and also 14 columns. We try to include more comprehensive enzyme information, and use them for pathway finding. We will show you the meaning of these features below:

pid: protein id corresponds to the sequence.

name: enzyme name.

ecnum: EC number.

organism: chassis.

localization: where the enzyme located in enzyme.

ph & phr: *Pondus Hydrogenii*, PH and PH range for normal enzyme function.

t & tr: temperature and temperature range for normal enzyme function.

KM: Michaelis constant.

KKM: Kcat/Km.

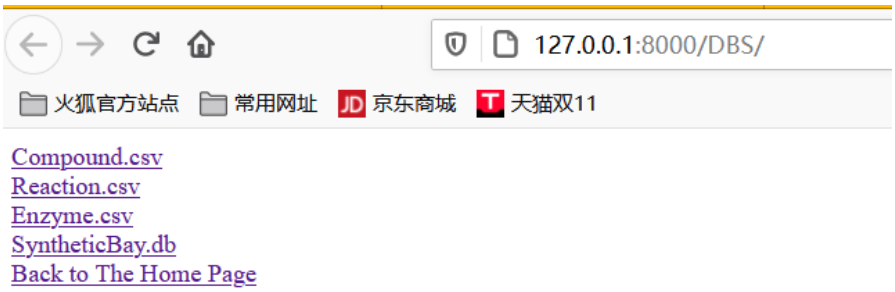
sequence: the protein sequence of enzyme.

```
pid,name,ecnum,organism,localization,ph,phr,t,tr,km,kkm,sequence
P43309,catechol oxidase,1.10.3.1,Malus domestica,membrane,6.5#6.8,2.5-9,20#30,20-80,,,
O81103,catechol oxidase,1.10.3.1,Prunus armeniaca,,,,,,,MATAPSPTTMGTYSSLISTNSFSTFLPNK
P43311,catechol oxidase,1.10.3.1,Vitis vinifera,,5,,25,,,,MASLPWSLTTSTAIANTTNISAFPPSPL
Q9MB14,catechol oxidase,1.10.3.1,Ipomoea batatas,,,,,,-999 {more}#9 {catechol}#3.9 {4-
Q08303,catechol oxidase,1.10.3.1,Solanum lycopersicum,,4.8,4.1-4.4,40,30-50,,,MASLCSNS
Q08304,catechol oxidase,1.10.3.1,Solanum lycopersicum,,4.8,4.1-4.4,40,30-50,,,MASVVCNS
Q06355,catechol oxidase,1.10.3.1,Solanum tuberosum,,6.5,,25,,21.1 {catechol},,SSSSTTTI
Q9ZP19,catechol oxidase,1.10.3.1,Ipomoea batatas,,,,,,-999 {more}#9 {catechol}#3.9 {4-
Q08305,catechol oxidase,1.10.3.1,Solanum lycopersicum,,4.8,4.1-4.4,40,30-50,,,MASLCSNS
Q08306,catechol oxidase,1.10.3.1,Solanum lycopersicum,,4.8,4.1-4.4,40,30-50,,,MASLCSNS
Q08307,catechol oxidase,1.10.3.1,Solanum lycopersicum,,4.8,4.1-4.4,40,30-50,,,MSSSSSIT
Q08296,catechol oxidase,1.10.3.1,Solanum lycopersicum,,4.8,4.1-4.4,40,30-50,,,MSSSTPNT
B3VQ03,catechol oxidase,1.10.3.1,Camellia sinensis,,5.3-5.7,,,,,MASILPPTTTKTTTTSSTLYS
B5M677,catechol oxidase,1.10.3.1,Ipomoea batatas,,,,,,-999 {more}#9 {catechol}#3.9 {4-
A6N8J4,catechol oxidase,1.10.3.1,Camellia sinensis,,5.3-5.7,,,,,MASILPPTTTKTTTTSSTLYS
O24057,catechol oxidase,1.10.3.1,Malus domestica,membrane,6.5#6.8,2.5-9,20#30,20-80,,,
Q5ENY2,catechol oxidase,1.10.3.1,Ipomoea batatas,,,,,,-999 {more}#9 {catechol}#3.9 {4-
D6QY28,catechol oxidase,1.10.3.1,Solanum melongena,,,,,,,MASVCNTSTATLKSSFIPSPNSLGSTPK
Q6ZXV3,catechol oxidase,1.10.3.1,Solanum lycopersicum,,4.8,4.1-4.4,40,30-50,,,YGVANAIP
B5M678,catechol oxidase,1.10.3.1,Ipomoea batatas,,,,,,-999 {more}#9 {catechol}#3.9 {4-
B5M680,catechol oxidase,1.10.3.1,Ipomoea batatas,,,,,,-999 {more}#9 {catechol}#3.9 {4-
Q6ZXV2,catechol oxidase,1.10.3.1,Solanum lycopersicum,,4.8,4.1-4.4,40,30-50,,,DIQNKDWL
```

- About results

You can download three tables data in the form of '.csv' file, and one database in the form of '.db' file.

Three tables data is split with ',' and you can read the information with Excel or Text Reader (Notepat++). This form is convenient for data analysis, manage with commands and other pipelines. The database can be use with sql commands or sql softwares (MySQL, SQLsever).

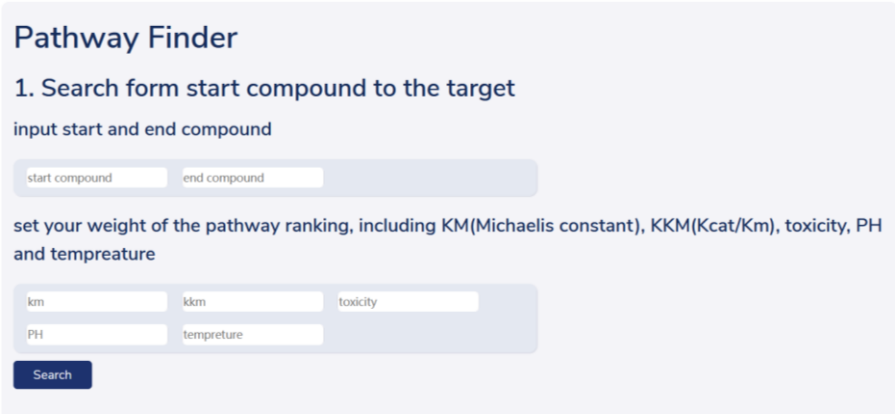


Pathway Finder

- About page

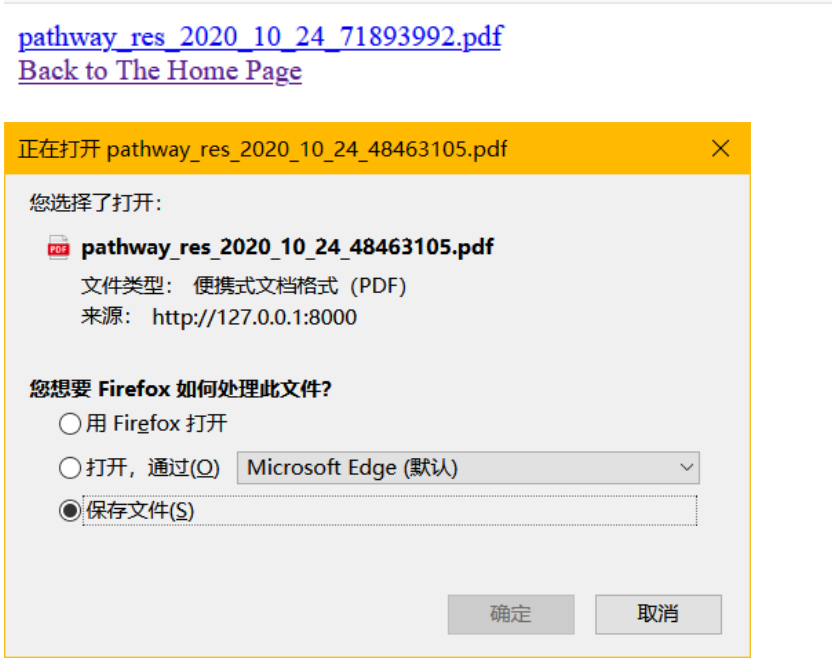
Click the navigation card on the home page or '/PF' to enter the Pathway Finder module.

In the middle of this page, you can find one gray windows consist of many entry bar. This is main part of pathway finder, which includes two functions: forward pathway search and reverse pathway search.



In the first function, you can input a start compound and a end compound, we will search the pathway from start to end and rank them by scores. There are five parameters: KM, KKM, Toxicity, PH, Temperature. You can assign value to the five parameters according to their importance in the experimental environment or

your priori knowledge. Click the search button, you will get a PDF results, and you can download this PDF.



The reverse pathway search is very much like the forward. You should input the target compound a and the search depth——steps b to get the pathway target to a wth Steps no more than b. And click the search button you will get a similar PDF file.

- About functions

The core of our Pathway Finder is traditional graph algorithms. A*, Dijkstra, and Yen's k shortest way algorithm are used.

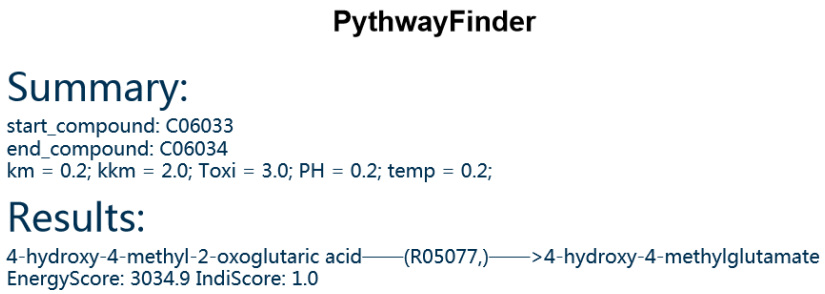
Forward pathway search function, According to the length of the path (energy score of reactions) and weighted score, will calculate scores and sort all the pathways between the start and end compound to output the better pathways (TOP10) and their scores.

Weighted score is computed by the five features (KM, KKM, Toxicity, PH, temperature) and user's weight ratio, which is entered by you through the five parameters input bar. This five ratio parameters means the weight ratio of the feature's influence. A weight matrix will be created based on the value you input and the content of data, and then a score will be given to these pathways.

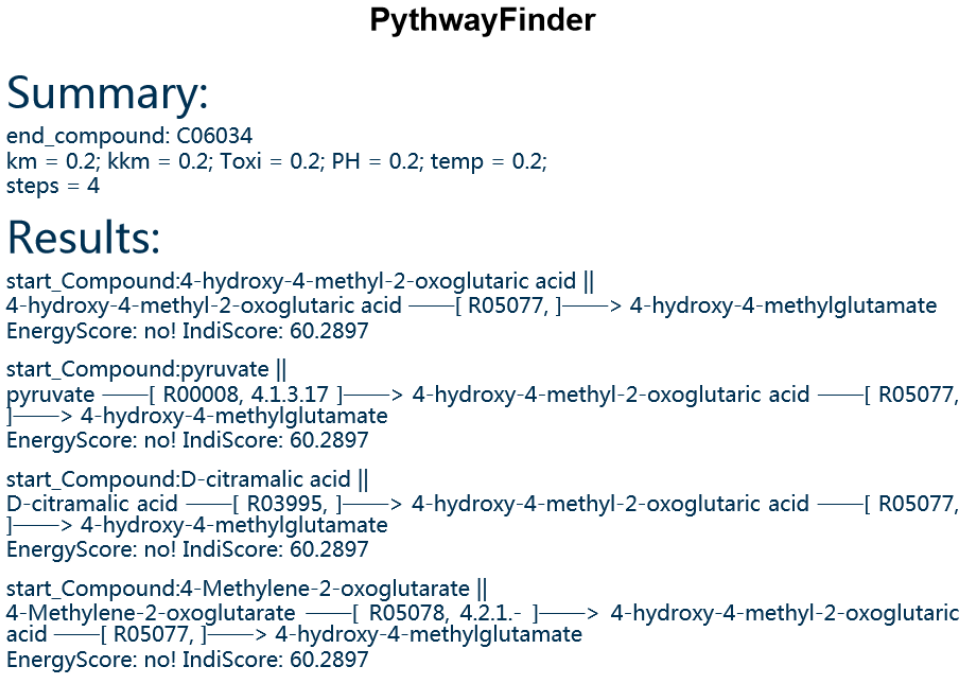
In the reverse pathway search, you will get some pathways that can produce the target molecule no more than steps. The scores of these pathways will be presented to you, too.

- About results

We will show you a download link for our results. The results is output in PDF format and divided into two parts: Summary and Results.



Summary part conclude all the parameters you input or default, through it you can know what you have input and what you want to get. In forward pathway finder you see the start_compound and end_compound but in reverse pathway finder you can just see the target (end_compound).

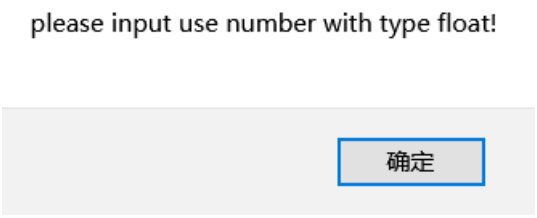


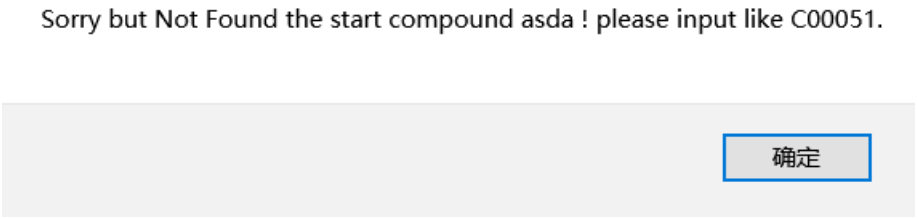
Results part displays all the Top pathways it found. Each pathway will be show by the form of “compound 1-----[reaction 1, enzyme 1]---->compound 2”, and followed by EnergyScore (score calculated by Gibbs energy) and IndiScore (score calculated by the five features). In additions, reverse pathway finder will output the start compound, which is end with ‘||’, at the beginning of each result.

However, you may not know which one to choose. The EnergyScore is the first choice criteria, the lower which is, the better this pathway may be. Then, you should consider the higher IndiScore. If you input a big ratio to any feature(KM, KKM, Toxicity, PH, Temperature), which means you value a particular condition, you should consider IndiScore first or take both into consideration.

- About debug

Our software is the 1.0 version, so there will be many bugs in it although we have fixed some bugs. For more normal functions, this version may not really fit the user. If you input a illogical compound or number, we popup a windows to warning you and then return to the page and fill in the default values. Meanwhile, we will show you an example about the compound id. If you input a compound our database not found, we will also warning but you may need to try other compound.



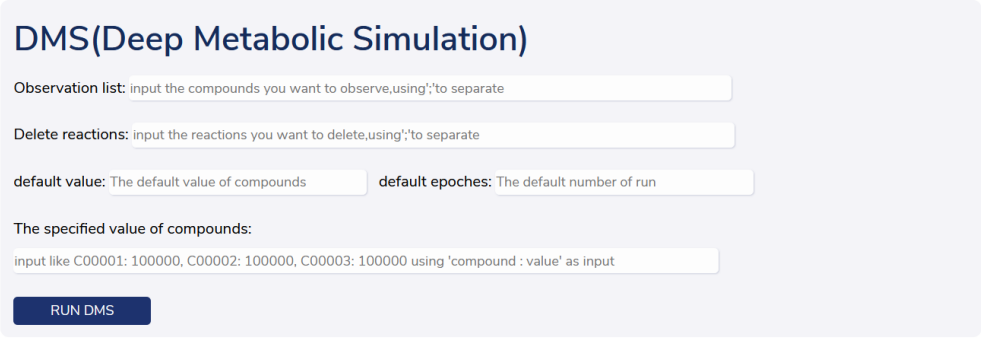


Deep Metabolic Simulation

- About page

Click the navigation card on the home page or '/HMS' to enter the Deep Metabolic Simulation module.

Similar as pathway finder page, DMS search is put in the center of this page.



In the search windows, there are some input parameters. First one is observation_list, which is the compound you want to observe and we will show them in the top of results with red color. Second one is delete_reaction_list. You can delete some reactions to block the paths between molecules. Default value is a default initial value of all the compounds, we will define the compounds' amount with this number. Default_epochs is the iteration times our algorithm will go through. At the last, the most important parameter is specified_values. you can define every specified compound with a initial value, and we will replace this compound's default value with it. When you input all the parameters, you can click the RUN DMS button to run the algorithm. You may be need wait some minutes and then you can get two results. One is PDF file in which we show the compounds in observation_list and whose value's change is in rank TOP50, other one is csv file, we output all the change information of all compounds.

randomwalk_res_2020_10_24_2543771.pdf
randomwalk_res_2020_10_24_2543771.csv
Back to The Home Page

- About functions

DMS aims to provide simulations of metabolism in a computational environment. Our Metabolism Simulation tool's core is random walking, which is like the Monte-Carlo method, and the difference is that random walking is applied to a graph.

Users input the default value of common compounds and the specified values of particular compounds, which are hypothetical parameters that refer to the number of molecules or the molecular level. Then, we construct an environment (or graph) that contains all reactions and all molecules (compounds), giving these reactants initial states with the user-defined values; You can also eliminate some reaction (the reaction_deficient_list) according to the demand; these reactions may be which you want to block or have inhibited in gene level. Eliminated reactions will no longer provide the molecules' transformation on both sides of the reaction. Then we simulate the process of metabolic reactions, let these molecules randomly transform to others until it reaches an equilibrium state. Users can adjust the times of metabolic simulations through epochs. The larger the epochs, the more times DMS functions iterate, and the more stable DMS results are. For users' convenience,

we've provided an observation list for the compounds that you want to observe (get the change of these compounds), and we're going to put them first on the top in PDF with red color.

- About results

We will show you two download link for our results. One is PDF divided into three parts: Summary, Results and Annotation, and other one is csv data file.

RandomWalking

Summary:

observation compound(the compound you want to observe, which is label with color red!):
C00797,C00008
reaction deficient:
default_value: 100, epoches: 5000, thread: 8
specified_value(the compound you altered, which is label with color red!):
C00002: 500, C00008: 595, C00020: 955, C00003: 10, C00004: 100, C00006: 195, C00005: 62, C00010: 123, C00009: 100, C00011: 1350, C00014: 10000, C00031: 220000, C00095: 230000, C00092: 3480, C00085: 600, C00354: 272, C00118: 218, C00111: 167, C03339: 8, C00197: 2500, C00074: 2670, C00022: 2670, C04442: 808, C00199: 111, C01101: 111, C00117: 398, C00231: 138, C03291: 138, C00279: 980, C05382: 276, C00024: 300, C00036: 680, C00158: 150, C00311: 170, C00026: 180, C00042: 190, C00149: 60, C00497: 60, C00049: 1340, C00402: 1340, C00575: 8, C00001: 1000,

You can find the initial state value in summary part, which is shown in default_value and specified_value. The specified values include some values of compound in experiment we get from article and the values you input in. In this condition, most of compounds will begin with default value and the specified compounds will begin with specified values (of course, the specified values you input have highest priority).

The observation compounds are the compounds you want to observe, which is label with color red and we put them on the TOP of results!

For better experience, we show the TOP50 (now TOP100) of the compounds' normalize delta. Every result is output in "compound id: compounds name, final state, change *delta*, normalized *delta*". Change *delta* is equal to final value minus initial value: $delta = final\ value - initial\ value$, and normalized *delta* is equal to change *delta* divided by initial value: $normalized\ delta = \frac{\Delta value(delta)}{initial\ value}$.

Results(TOP50):

C00797: ethylamine, 97.875, delta:-2.125, normalize_delta:-0.02125
C00008: ADP, 405.375, delta:-189.625, normalize_delta:-0.3187
C00003: NAD(+), 110.75, delta:100.75, normalize_delta:10.075
C00007: dioxygen, 945.0, delta:845.0, normalize_delta:8.45
C00019: S-adenosyl-L-methionine, 238.5, delta:138.5, normalize_delta:1.385
C00009: phosphate(3-), 0.0, delta:-100.0, normalize_delta:1.0
C00013: diphosphate(4-), 0.0, delta:-100.0, normalize_delta:1.0
C00015: UDP, 0.0, delta:-100.0, normalize_delta:1.0
C03024: Reduced flavoprotein, 200.0, delta:100.0, normalize_delta:1.0
C03161: Oxidized flavoprotein, 0.0, delta:-100.0, normalize_delta:1.0
C00021: S-adenosyl-L-homocysteine, 0.125, delta:-99.875, normalize_delta:0.99875
C00010: coenzyme A, 0.25, delta:-122.75, normalize_delta:0.99797
C00004: NADH, 1.5, delta:-98.5, normalize_delta:0.985
C00027: hydrogen peroxide, 9.25, delta:-90.75, normalize_delta:0.9075
C00138: reduced ferredoxin, 189.625, delta:89.625, normalize_delta:0.89625
C00139: oxidized ferredoxin, 10.375, delta:-89.625, normalize_delta:0.89625

C00229: holo-[acyl-carrier protein], 80.5, delta:-19.5, normalize_delta:0.195
C00060: monocarboxylic acid anion, 81.75, delta:-18.25, normalize_delta:0.1825
C00043: UDP-N-acetyl-alpha-D-glucosamine, 117.0, delta:17.0, normalize_delta:0.17
C00048: glyoxylic acid, 83.125, delta:-16.875, normalize_delta:0.16875
C05359: electron, 116.125, delta:16.125, normalize_delta:0.16125
C00028: acceptor, 115.875, delta:15.875, normalize_delta:0.15875

Annotation:

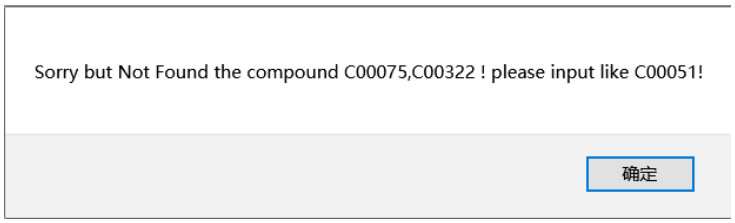
we output the compound you want to observe, and the top50 compound which altered and ordered by alter number(delta). the output features are compound id, compound name, the Final state value, altered value and normalized altered value from left to right. if you want to get all results, please download the .csv file!

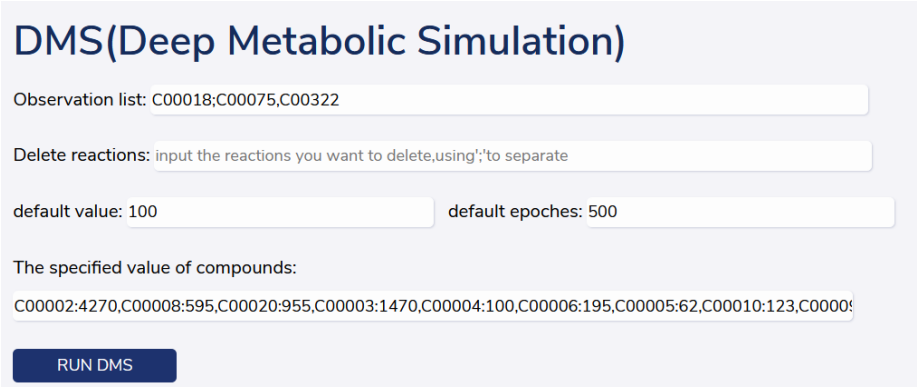
At the end of this PDF, we give you Annotation for find this handbook to know more details, and also you can download the csv file for more analysis, in which we output all the compounds and their values.

```
compound,start_value,end_value,delta,normalize_delta
C00001,1000,873.25,-126.75,0.12675
C00002,500,730.75,230.75,0.4615
C00003,10,110.75,100.75,10.075
C00004,100,1.5,-98.5,0.985
C00005,62,85.625,23.625,0.38105
C00006,195,171.0,-24.0,0.12308
C00007,100,945.0,845.0,8.45
C00008,595,405.375,-189.625,0.3187
C00009,100,0.0,-100.0,1.0
C00010,123,0.25,-122.75,0.99797
C00011,1350,1017.625,-332.375,0.2462
C00012,100,98.75,-1.25,0.0125
C00013,100,0.0,-100.0,1.0
C00014,10000,9860.375,-139.625,0.01396
C00015,100,0.0,-100.0,1.0
C00016,100,108.0,8.0,0.08
C00017,100,104.375,4.375,0.04375
C00018,100,97.75,-2.25,0.0225
C00019,100,238.5,138.5,1.385
C00020,955,904.875,-50.125,0.05249
C00021,100,0.125,-99.875,0.99875
C00022,2670,2638.875,-31.125,0.01166
C00023,100,100.0,0.0,0.0
```

- About debug

Our software is the 1.0 version, so there will be many bugs in it although we have fixed some bugs. For more normal functions, this version may not really fit the user. If you input a illogical compound, reaction or number, we will popup a windows to warning you and then return to the page and fill in the default values. Meanwhile, we will show you an example about the compound id or the reaction id. If you input a compound or reaction our database not found, we will also warning but you may need to try other one. Last but not least, if you input a text in a invalid format, for instance, you input a false separator but not the example we show you in the page, you will get a warning and must modify the error until the function is running.





4. Other pipelines

Our three modules are inter-related. Users can not only analyze the metabolic system with these modules but also cooperate with other software to form a more standard pipeline. First, you can see the correlation between the reactants from DMS. In DMS, that changes of one molecule will result in other compounds' changes dramatically. Then you can go to Pathway Finder and search for the pathways between these two reactants. Second, users can search pathways between two compounds, and the reactions in these pathways can be deleted in DMS. as a result, you will find some unexpected results when you use DMS. Third, when you use other IGEM modules for project operation, such as eliminating a particular gene of one reaction or making part of the molecular level changes, you can input the changed level as the initial value into our DMS module, obtain a more comprehensive molecules change within the metabolic system.

Meanwhile, you will find some alternative parameters to get more different results in our DMS code. You can choose better value or functions according to your demand. And we will give how to deploy:

Our software can be deployed on your own Linux server for a better performance. We have tested the deployment steps on CentOS 7.7.

STEP I
Update your system and install docker.
>>curl -fsSL https://get.docker.com | bash -s docker --mirror Aliyun

STEP II
Clone our repo and download extra data.
Put the downloaded files into the following directories.

>>mv ~/Download/db.sqlite3 Synthesis_Navigator-master/
>>mv ~/Download/Compound.csv Synthesis_Navigator-master/statics/data_download/
>>mv ~/Download/Enzyme.csv Synthesis_Navigator-master/statics/data_download/
>>mv ~/Download/Reaction.csv Synthesis_Navigator-master/statics/data_download/
>>mv ~/Download/SyntheticBay.db Synthesis_Navigator-master/statics/data_download/

STEP III
Build docker image.
>>cd Synthesis_Navigator-master/
>>docker build -t TongjiSoftware/Synthesis_Navigator:1.0 .

STEP IV
Run the container.
>>docker run -it --rm -p 8000:8000 TongjiSoftware/Synthesis_Navigator:1.0

STEP V
Open 127.0.0.1:8000/Home in your browser (Chrome is recommended).Enjoy:)
You can modify settings.py to suit your environment.