



Knowledge that will change your world

Pathway software and databases

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Synopsis

- **Public and proprietary metabolite databases**
 - Instrument manufacturers provide software and search tools for their proprietary databases
 - Usually a single copy of the software is provided
 - Sciex and Waters provide additional copies at >\$35,000 for each
 - Metabolomics service companies have proprietary databases and do not allow investigators submitting samples to have access to them
 - This discourages deeper research to be performed on metabolomics data

Public databases

- North America
 - Metlin (<https://metlin.scripps.edu/index.php>)
 - Human metabolomics database <http://www.hmdb.ca/>
 - PubChem <http://pubchem.ncbi.nlm.nih.gov/>
 - Metabolomics Workbench
(<http://www.metabolomicsworkbench.org/data/index.php>)
- Europe
 - ChemSpider (<http://www.chemspider.com/>)
- Asia
 - Kyoto Encyclopedia of Genes and Genomes (KEGG)
(<http://www.genome.jp/kegg/>)

Choosing the ions to search

- Go to the Download file from Metaboanalyst and open the file "peak_normalized_rt_mz.csv"
- Use Excel to calculate the p-values for all the metabolites (they're ordered by m/z in the file)
- Now sort the entire file by the p-values
- Choose the ions with p-values <0.001 (there should be 233) and copy them into a Word file and save the file
 - We'll search these in multiple databases

Metlin

METLIN: Metabolite Search

Batch

[Simple \(Saved Searches\)](#) |
 [Advanced](#) |
 [Batch](#) |
 [Fragment](#) |
 [Neutral Loss](#) |
 [MS/MS Spectrum Match](#) |
 [Unknowns](#)

Masses:
 173.08163
 241.10831
 499.71989
 592.1392

Charge:
 Positive
 Negative

M-H
 M-H₂O-H
 M+Na-2H
 M+Cl
 M+K-2H
 M+FA-H
 M-2H
 M-3H
 M+CH₃COO
 M+F

*To select multiple Adducts:
 - Hit Ctrl + Adducts
 - Hit Command + Adducts
 Select: **all** | none

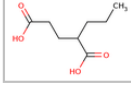
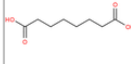
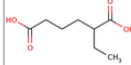
Accuracy (ppm):


Display Structure:

Remove peptides from search:

Metlin output-1

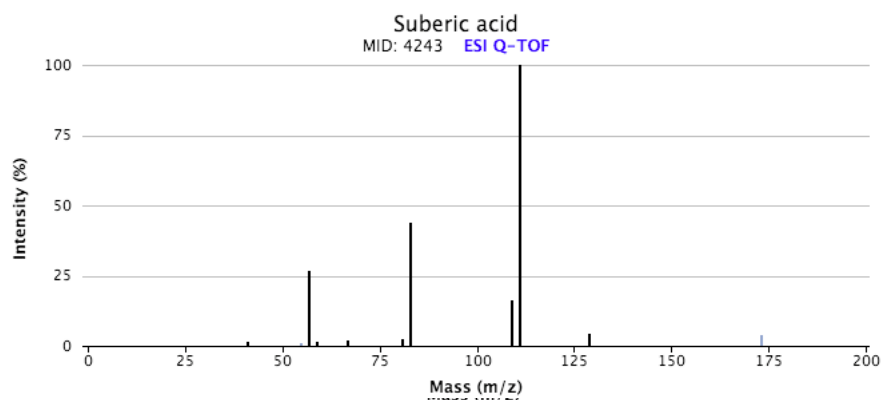
173.08163 m/z
 (174.0872 - 174.0906 daltons): 7 Metabolites [M-H]⁻

MetlinID	Mass	Δppm	Name	Formula	CAS	MS/MS	Structure
2998	174.0892	1	2-Propylglutaric acid	C ₈ H ₁₄ O ₄	32806-62-5	NO	
4243	174.0892	1	Suberic acid	C ₈ H ₁₄ O ₄	505-48-6	<input type="button" value="View"/>	
45928	174.0892	1	Ethyladipic acid	C ₈ H ₁₄ O ₄		NO	



Has MSMS data in this record

MSMS data of m/z 173.08163



Metlin output-2

197.11032 m/z

(198.1156 - 198.1196 daltons): 4 Metabolites [M-H]⁻

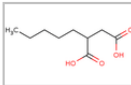
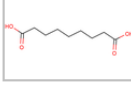
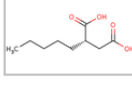
MetlinID	Mass	Δppm	Name	Formula	CAS	MS/MS	Structure
44521	198.1157	9	9-AMINO-1,2,3,4-TETRAHYDROACRIDINE	C13H14N2	NA	View	
2616	198.1157	9	Tacrine	C13H14N2	321-64-2	View	
69942	198.1157	9	4,4'-Methylenedianiline	C13H14N2	101-77-9	NO	
70631	198.1157	9	N-(Phenylmethyl)-N-methyl-2-pyridinamine	C13H14N2		NO	

Unlikely fits – high Δ ppm

Metlin output-3

187.09745 m/z

(188.1029 - 188.1066 daltons): 8 Metabolites [M-H]⁻

MetlinID	Mass	Δ ppm	Name	Formula	CAS	MS/MS	Structure
44183	188.1049	0	NONIC ACID	C ₉ H ₁₆ O ₄		View	
5750	188.1049	0	Nonanedioic acid	C ₉ H ₁₆ O ₄		View	
62450	188.1049	0	Nonate	C ₉ H ₁₆ O ₄		NO	

Spectra Search Mass Spectrum

MS Search **MS/MS Search** GC/MS Search 1D NMR Search 2D NMR Search **HMDB search**

Query Masses (Da)

165.0555
425.04502
658.45859
201.11197
501.1806
329.11214
177.05641
269.04555
426.03226
226.03738
199.09784
227.09225
193.05045
490.13636
608.13368

Enter one mass per line (maximum 150 query masses per request)

Ionization

Ion Mode
Negative

Adduct Type

M-H
M+Na-2H
M+Cl
M+K-2H
M+FA-H
M+Hac-H
M+Br

Hold Ctrl (⌘) or Command (⌘) to select multiple adducts

Molecular Weight Tolerance \pm
10 ppm

[Search](#) [Load Example](#)

HMDB search output-1

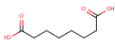
MS search for 173.08163 m/z Delta = abs(query mass - adduct mass)

Show entries

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB00893	Suberic acid	M-H	173.081933	174.089208936	0.000303
HMDB02023	Ethyladipic acid	M-H	173.081933	174.089208936	0.000303
HMDB33838	Diethyl succinate	M-H	173.081933	174.089208936	0.000303
HMDB59727	2,4-Dimethyladipic acid	M-H	173.081933	174.089208936	0.000303
HMDB59757	3-Methylpimelic acid	M-H	173.081933	174.089208936	0.000303
HMDB60684	2-Propylglutaric acid	M-H	173.081933	174.089208936	0.000303

Showing 1 to 6 of 6 entries Previous **1** Next

Click on HMDB record

Record Information	
Version	3.6
Creation Date	2005-11-16 15:48:42 UTC
Update Date	2015-12-02 05:10:07 UTC
HMDB ID	HMDB00893
Secondary Accession Numbers	<ul style="list-style-type: none"> • HMDB00837
Metabolite Identification	
Common Name	Suberic acid
Description	Suberic acid, also octanedioic acid, is a dicarboxylic acid, with formula C ₈ H ₁₂ (COOH) ₂ . It is present in the urine of patients with Fatty Acid Oxidation Disorders (PMID 10404733). A metabolic breakdown product derived from oleic acid. Elevated levels of this unsaturated dicarboxylic acid are found in individuals with dicarboxylic acid and medium-chain acyl-CoA dehydrogenase deficiency (MCAD).
Structure	 <div style="text-align: center;"> <input type="text" value="MOL"/> <input type="text" value="SDF"/> <input type="text" value="PDB"/> <input type="text" value="SMILES"/> <input type="text" value="InChI"/> </div>
Synonyms	<ol style="list-style-type: none"> 1,6-Dicarboxyhexane 1,6-Hexanedicarboxylate 1,6-Hexanedicarboxylic acid 1,8-Octanedioate 1,8-Octanedioic acid • Cork acid

ChemSpider
Search and share chemistry

Search ChemSpider

Simple Structure **Advanced** History

Advanced search

- Structure
- Identifier
- Elements
- Intrinsic Properties** ←
- Calculated Properties
- Data Source
- Lasso Similarity
- Supplementary Info
- Tags

FILTER ▾ Search Hits Limit: 100 CLEAR FORM SEARCH

Searching in ChemSpider

Monoisotopic Mass: ± min/max +/-

- Calculated Properties
- Data Source
- Lasso Similarity
- Supplementary Info
- Tags






FILTER ▾ Search Hits Limit: 100 CLEAR FORM SEARCH

ChemSpider output

Found 1374 results

Search term: $MM \geq 174.083906$ AND $MM \leq 174.093906$ AND $abs(Monoisotopic_Mass - 174.088906451991)$ as `mass_defect`

1 2 3 4 5

ID	Structure	Molecular Formula	Molecular Weight	# of Data Sources	# of References	# of PubMed	# of RSC	Mass defect ▲
10025 		C ₈ H ₁₄ O ₄	174.1944	109	264	73	275	0.0003
11364 		C ₈ H ₁₄ O ₄	174.1944	76	121	0	173	0.0003
11539		C ₈ H ₁₄ O ₄	174.1944	17	18	0	4	0.0003

MetaboSearch

- Find MetaboSearch using your browser
 - it's at <http://omics.georgetown.edu/metabosearch.html>
 - Note that this software may not work (for me, it won't allow me to output and save the data)

The screenshot shows the Resson Omics LAB website. The header features the logo and navigation links: Home, Projects, Publications, Members, Resources, and Software Tools. The main content area is titled "METABOSEARCH" and includes an "Introduction" section. A sidebar on the right lists the "CONTENT" menu items.

Resson Omics LAB

Home Projects Publications Members Resources Software Tools

METABOSEARCH

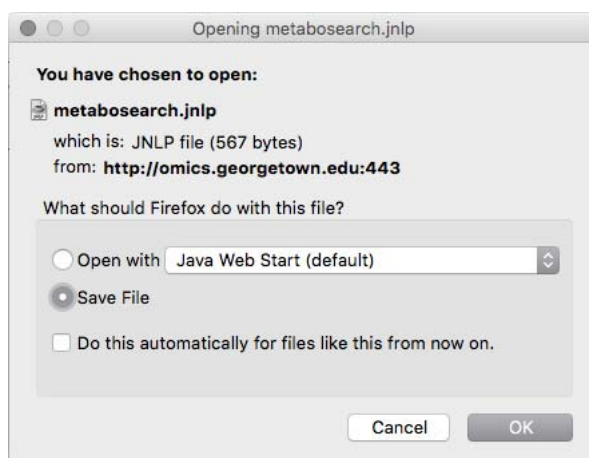
Introduction

- Mass-based search is an important step for metabolite identification in mass-spectrometry-based metabolomic analysis. The mass-to-charge ratio (m/z) value of a molecular ion of interest is searched against metabolite database(s). The metabolites having molecular weights within a specified tolerance to the query m/z value are retrieved from the databases as putative identifications. These putative identifications serve as a foundation for further metabolite verification. In addition to searching with m/z values only, the ion annotation information can be used to aid the mass-based search. Ion annotation groups the ions originating from the same metabolite together and annotates them as adducts/isotopes/in-source fragments. R package **CAMERA** (Collection of Algorithms for MEtabolite pRofile Annotation) was previously developed for ion annotation by Kuhl etc (Carsten Kuhl etc. CAMERA: Collection of annotation related methods for mass spectrometry data. R package version 1.10.0.). Using the ion annotation information, the appropriate mass values of ions can be calculated. Then the calculated mass values are searched against databases. This approach is expected to improve the accuracy for metabolite identification.

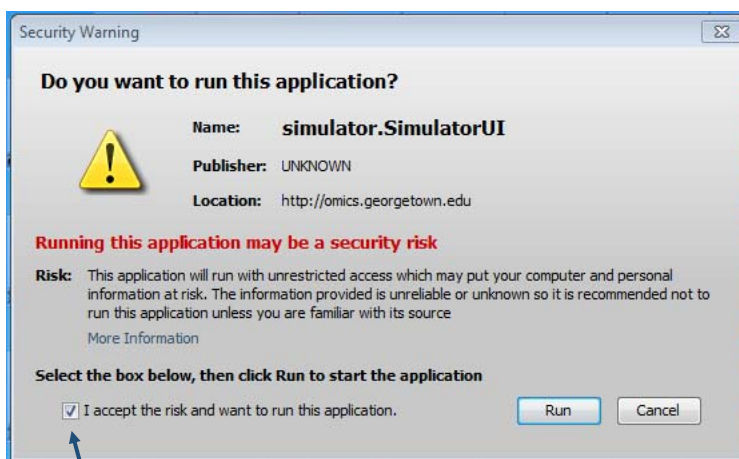
CONTENT

- Introduction
- Downloads
- User Guide
 - Input File Format
 - MetaboSearch Interface
 - Steps To Run MetaboSearch
 - Output File Format
- Questions & Answers

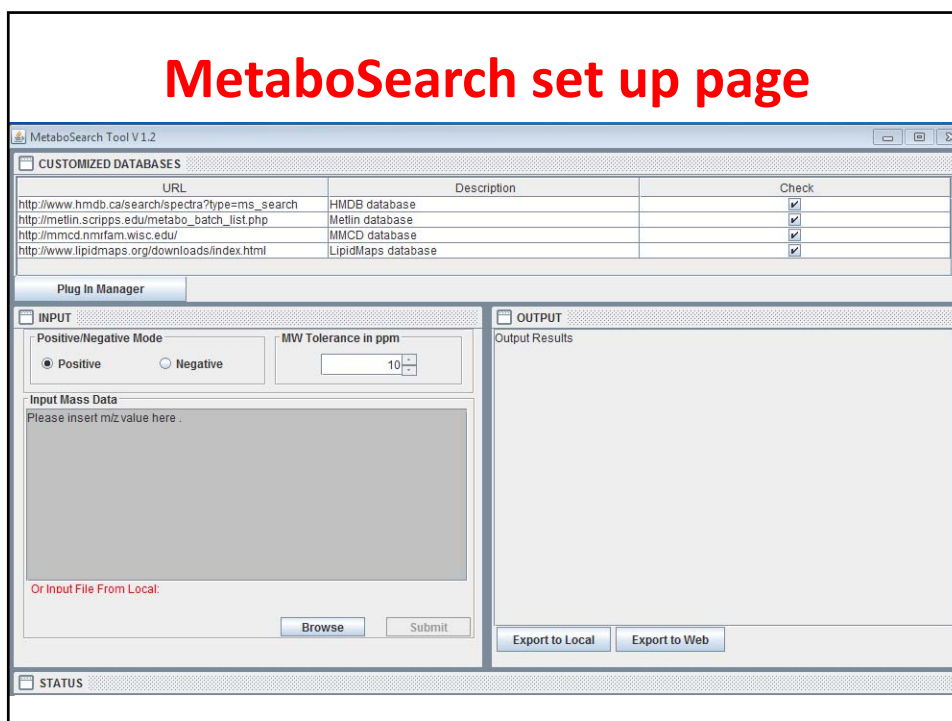
Download at Resson lab



Opening MetaboSearch gives you this



MetaboSearch set up page



Data loaded – note negative ions

MetaboSearch Tool V 1.2

CUSTOMIZED DATABASES

URL	Description	Check
http://www.hmdb.ca/search/spectra?type=ms_search	HMDB database	<input checked="" type="checkbox"/>
http://metlin.scripps.edu/metabo_batch_list.php	Metlin database	<input checked="" type="checkbox"/>
http://mmcd.nmrfam.wisc.edu/	MMCD database	<input checked="" type="checkbox"/>
http://www.lipidmaps.org/downloads/index.html	LipidMaps database	<input checked="" type="checkbox"/>

Plug In Manager

INPUT

Positive/Negative Mode
 Positive Negative

MW Tolerance in ppm: 10

Input Mass Data

- 329.11214
- 177.05641
- 269.04555
- 426.03226
- 226.03738
- 199.09784
- 227.09225
- 193.05045
- 490.13636
- 608.13368

Or Input File From Local:

Browse Submit

OUTPUT

Output Results

Export to Local Export to Web

STATUS

MetaboSearch completed

MetaboSearch Tool V 1.2

CUSTOMIZED DATABASES

URL	Description	Check
http://www.hmdb.ca/search/spectra?type=ms_search	HMDB database	<input checked="" type="checkbox"/>
http://metlin.scripps.edu/metabo_batch_list.php	Metlin database	<input checked="" type="checkbox"/>
http://mmcd.nmrfam.wisc.edu/	MMCD database	<input checked="" type="checkbox"/>
http://www.lipidmaps.org/downloads/index.html	LipidMaps database	<input checked="" type="checkbox"/>

Plug In Manager

INPUT

Positive/Negative Mode
 Positive Negative

MW Tolerance in ppm: 10

Input Mass Data

- 329.11214
- 177.05641
- 269.04555
- 426.03226
- 226.03738
- 199.09784
- 227.09225
- 193.05045
- 490.13636
- 608.13368

Or Input File From Local:

Browse Submit

OUTPUT

The directory of the result is: C:\Users\Stephen Barnes\Downloads\temp\search\

Searching databases, please wait...

Grasped Metlin is coming

Grasped MMCD is coming

Please save the result by clicking 'Export' button!

QueryID	Name	Chemical Structure
2	cq_0497	
2	cq_11996	
2	cq_13690	
2	cq_17537	
2	cq_16240	0.000302805800033 Ethyladipic acid C8H
2	cq_07883	0.000302805800033 Dimethyl adipate, Di
3	cq_09397	0.00180496030001 Diphenylcarbazide
5	cq_13056	0.00100951620004 Cefteram pivoxil; T.2
7	cq_05799	0.00258718569995 1,2-HYDRO-1-OXY-3
7	cq_10129	0.00258718569995 Athamantin C24
8	cq_00955	0.00189767219999 4,4'-Methylenedianil
8	cq_16789	0.00189767219999 Tacine C13
8	cq_16789	0.00189767219999 N-(Phenylmethyl)-N-

Export to Local Export to Web

Opening Metabosearch file

CUSTOMIZED DATABASES

URL	Description	Check
http://www.hmdb.ca/search/spectra?type=ms_search	HMDB database	<input checked="" type="checkbox"/>
http://metlin.scripps.edu/metabo_batch_list.php	Metlin database	<input checked="" type="checkbox"/>
http://mmcd.nmrfam.wisc.edu/	MMCD database	<input checked="" type="checkbox"/>
http://www.lipidmaps.org/downloads/index.html	LipidMaps database	<input checked="" type="checkbox"/>

INPUT

Positive/Negative Mode: Positive Negative

MW Tolerance in ppm: 10

Input Mass Data

329.11214
177.05641
269.04555
426.03226
226.03738
199.09784
227.09225
193.05045
490.13636
608.13368

Or Input File From Local:

Browse Submit

OUTPUT

The directory of the result is: C:\Users\Stephen Barnes\Downloads\tempforsearch//

Searching databases, please wait...

Grasped Metlin is coming...

Grasped MMCD is coming...

Would you like to open the output file?

Yes No


Export to Local Export to Web

MetaboSearch output

A	B	C	D	E	F	G	H	I	J	K	L	M
Query_ID	Query_m/	Input_RT	Name	Formula	Exact_Ma	KEGG ID	PubChem	PubChem	HMDB ID	Databases	dppm	Delta
1	417.1029	-	-	-	-	-	-	-	-	-	-	-
2	173.0816	-	[O4]-ACETOXY-2,3-DIDEOXYFI	C8H14O4	174.0892	-	-	-	-	MMCD	1.665336	2.90E-04
2	173.0816	-	2-(ALPHA-HYDROXYISOVALER	C8H14O4	174.0892	-	-	-	-	MMCD	1.665336	2.90E-04
2	173.0816	-	Ethyladipic acid	C8H14O4	174.0892	-	-	152459	HMDB020:	MMCD	1.665336	2.90E-04
2	173.0816	-	Dimethyl adipate;Dimethyl h	C8H14O4	174.0892	C14570	-	-	-	MMCD	1.665336	2.90E-04
2	173.0816	-	Suberic acid	C8H14O4	174.0892	C08278	10457;-	10457	HMDB008:	LIPIDMaps	1.665336	2.90E-04
2	173.0816	-	Ethyladipic acid	C8H14O4	174.0892	-	152459;-	152459	HMDB020:	LIPIDMaps	1.665336	2.90E-04
2	173.0816	-	Diethyl succinate	C8H14O4	174.0892	-	-	31249	HMDB338:	HMDB	1.665336	2.90E-04
2	173.0816	-	Suberic acid;Cork acid;1,8-Oct	C8H14O4	174.0892	C08278	153742	10457	HMDB008:	MMCD	1.665336	2.90E-04
3	241.1077	-	Diphenylcarbazine	C13H14N4	242.1168	C11232	151941	-	-	MMCD	7.436648	0.001801
4	499.7199	-	-	-	-	-	-	-	-	-	-	-
5	592.1392	-	Cefteram pivoxil;T 2588	C22H27N9	593.1475	C13147	192387	54885	-	MMCD	1.646408	9.77E-04
6	155.0716	-	-	C8H12O3	156.0786	-	5312943	-	-	LIPIDMaps	1.857506	2.90E-04
6	155.0716	-	8-Hydroxy-5,6-octadienoic ac	C8H12O3	156.0786	-	-	-	HMDB311:	HMDB	1.564215	2.44E-04
6	155.0716	-	2,5-Dimethyl-4-ethoxy-3(2H)-	C8H12O3	156.0786	-	-	3017596	HMDB322:	HMDB	1.564215	2.44E-04
7	429.1893	-	Mammea E/BA	C24H30O7	430.1992	-	-	11517592	HMDB308:	HMDB	6.029752	0.002594
7	429.1893	-	Armillarilin	C24H30O7	430.1992	-	-	21126389	HMDB316:	HMDB	6.029752	0.002594
7	429.1893	-	Athamantin	C24H30O7	430.1992	C09123	11315	442051	-	MMCD	6.029752	0.002594
7	429.1893	-	1,2-HYDRO-1-OXY-3,4-HYDRO	C24H30O7	430.1992	-	-	-	-	MMCD	6.029752	0.002594

Going to the KEGG Pathway website

- <http://www.genome.jp/kegg/pathway.html>
- We'll take the compounds detected in MetaboSearch that have KEGG identifiers
- These can be mapped to pathways
- If Metabosearch does not work, then we will use the Excel file on the class website for 2-10-17 class



KEGG PATHWAY Database
Wiring diagrams of molecular interactions, reactions, and relations

Menu **PATHWAY** BRITE MODULE KO GENOME GENES LIGAND DISEASE DRUG DBGET

Select prefix
map

Enter keywords [Help](#)

[[New pathway maps](#) | [Update history](#)]

Pathway Maps

KEGG PATHWAY is a collection of manually drawn [pathway maps](#) representing our knowledge on the molecular interaction and reaction networks for:

- 1. Metabolism**
Global/overview Carbohydrate Energy Lipid Nucleotide Amino acid Other amino Glycan Cofactor/vitamin Terpenoid/PK Other secondary metabolite Xenobiotics Chemical structure
- 2. Genetic Information Processing**
- 3. Environmental Information Processing**
- 4. Cellular Processes**
- 5. Organismal Systems**
- 6. Human Diseases**

and also on the structure relationships (KEGG drug structure maps) in:

- 7. Drug Development**

Pathway Mapping

KEGG PATHWAY mapping is the process to map molecular datasets, especially large-scale datasets in genomics, transcriptomics, proteomics, and metabolomics, to the KEGG pathway maps for biological interpretation of higher-level systemic functions.

- [Search Pathway](#) - basic pathway mapping tool
- [Search&Color Pathway](#) - advanced pathway mapping tool
- [Color Pathway](#) - selected pathway map coloring tool

Search against: Enter: map, ko, ec, rn, hsadd, or

Enter objects:

Copy in the values from the Excel table

Examples:

Alternatively, enter the file name containing the data:

No file chosen

[Filter1](#) [Filter2](#) (to extract K/C/G/D/R/RP/RC numbers)

- Include aliases
- Display objects not found in the search
- Search pathways containing all the objects (AND search)

Search against: Enter: map, ko, ec, rn, hsadd, or

Enter objects:

C00882
C01613
C02052
C03374
m2mn
C03170
C00016
C03374
C00016
C00016

Examples:

Alternatively, enter the file name containing the data:

No file chosen

Filter1 **Filter2** (to extract K/C/G/D/R/RC numbers)

Include aliases

Display objects not found in the search

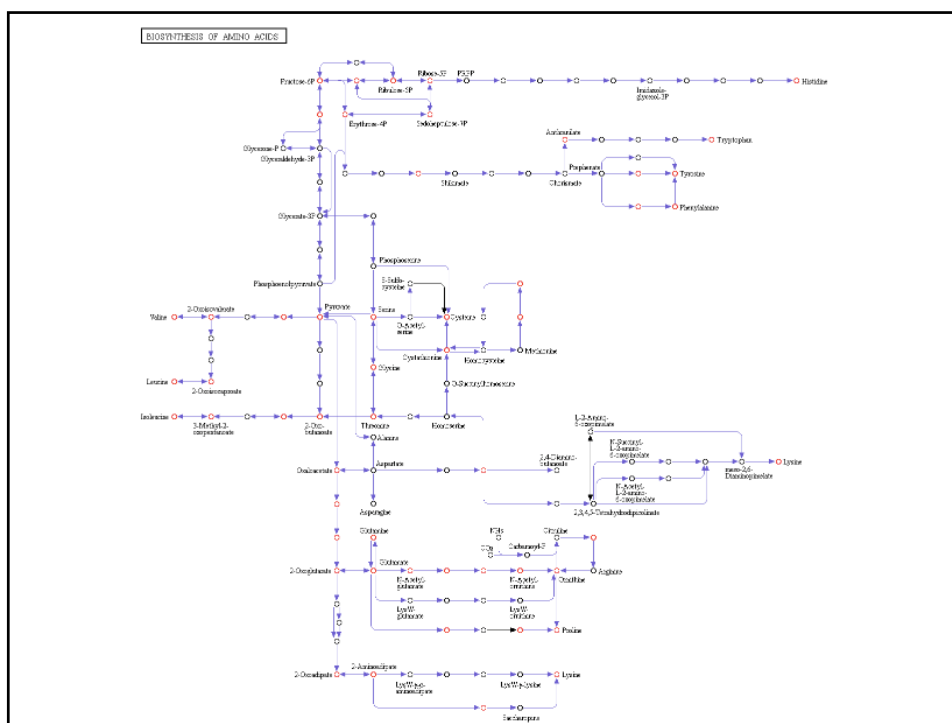
Search pathways containing all the objects (AND search)

Pathway Search Result

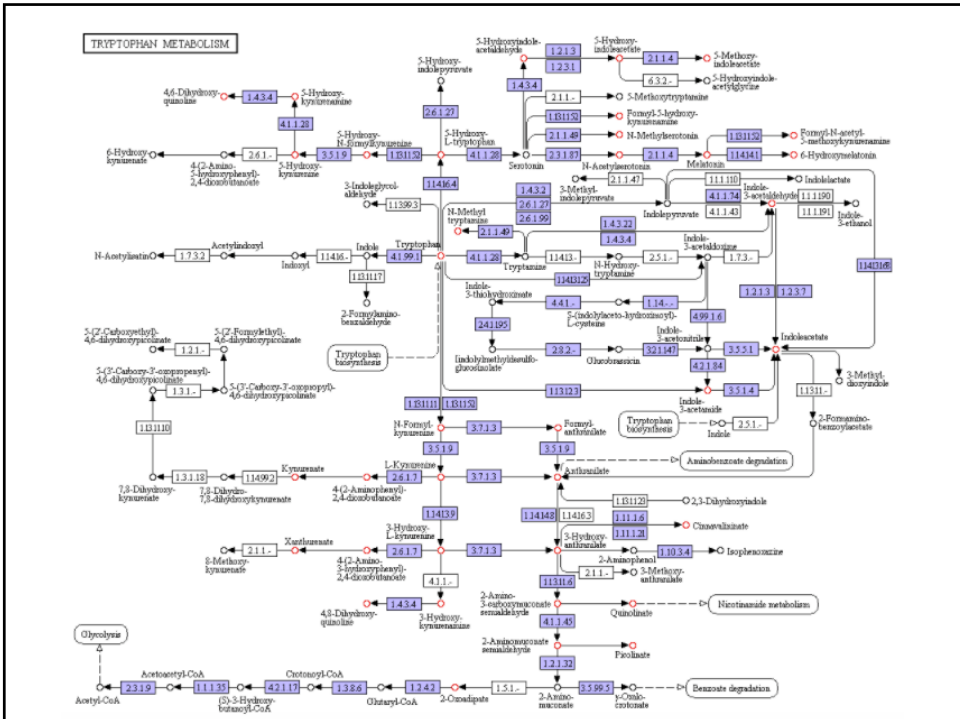
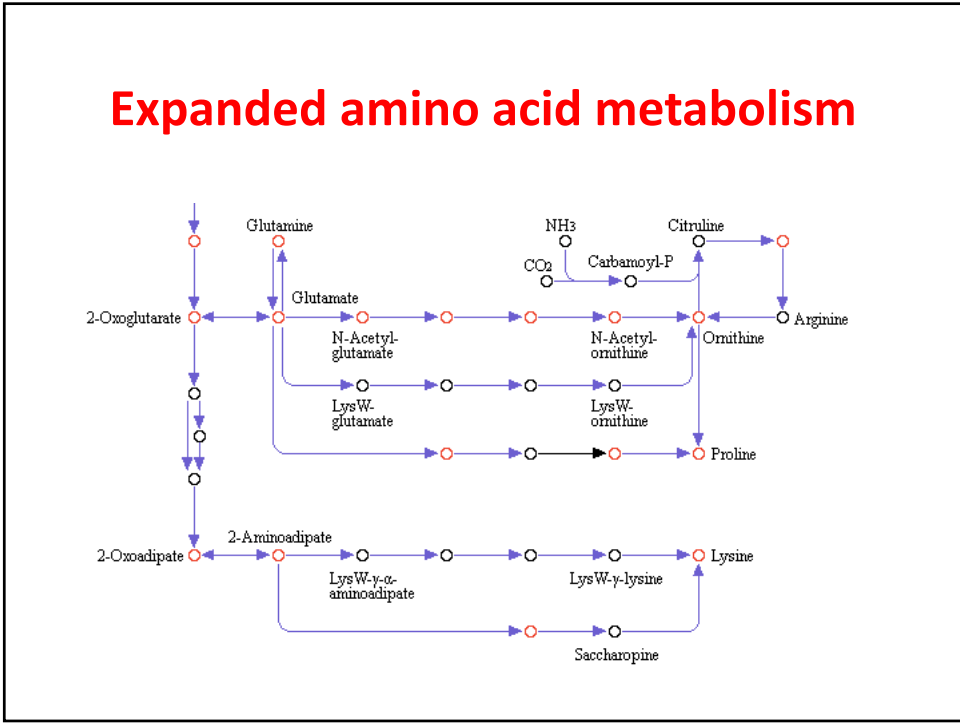
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- ko01100 Metabolic pathways (399)
- ko01110 Biosynthesis of secondary metabolites (142)
- ko01120 Microbial metabolism in diverse environments (115)
- ko01130 Biosynthesis of antibiotics (94)
- ko00140 Steroid hormone biosynthesis (63)
- ko01230 Biosynthesis of amino acids (52)
- ko00350 Tyrosine metabolism (43)
- ko02010 ABC transporters (43)
- ko00980 Metabolism of xenobiotics by cytochrome P450 (38)
- ko00380 Tryptophan metabolism (37)



Expanded amino acid metabolism



Expanded tryptophan metabolism

