Tutorial for browsing, searching, and visualizing the Human Microbial Metabolome Database MiMeDB

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Structure and design of the MimeDB

In simple terms, the Human Microbial Metabolome Database or MiMeDB (https://mimedb.org) contains data about human microbes, their associated metabolites, and the effects these metabolites have on humans.

The MiMeDB (https://mimedb.org) is a comprehensive, multi-omic, microbiome resource that connects:

1) microbes to microbial genomes
2) microbial genomes to microbial metabolites
3) microbial metabolites to the human exposome
4) all of these “omes” to human health.

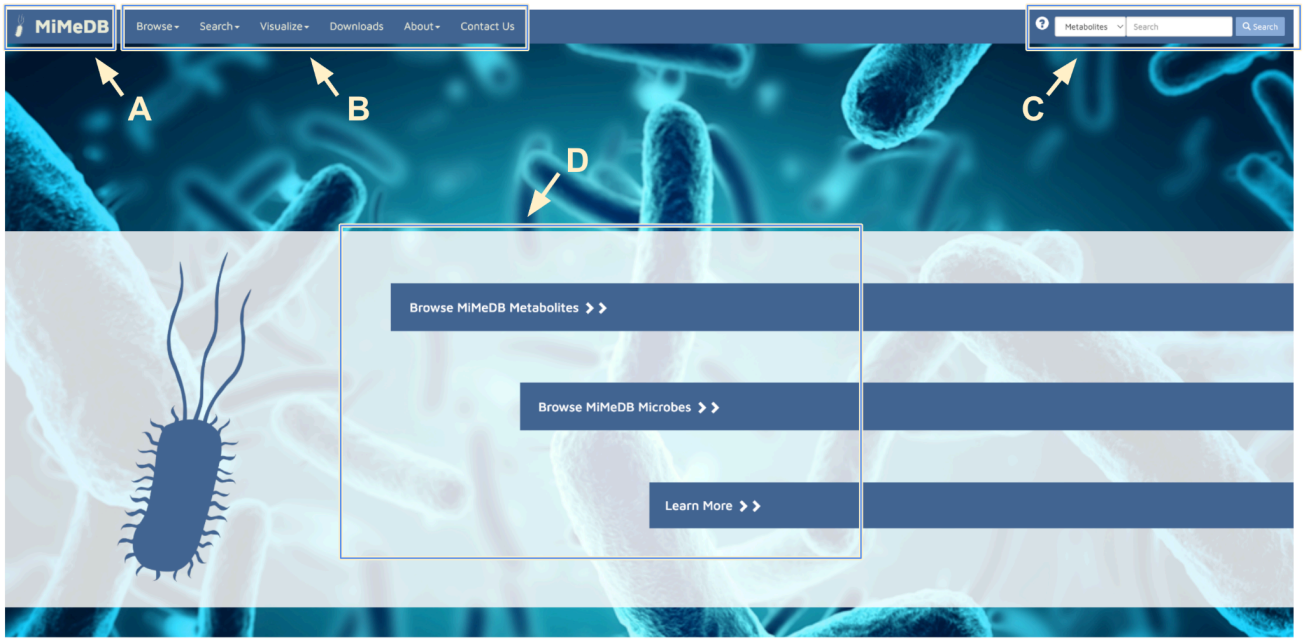
While the general content of MiMeDB can be grouped into three broad classes (microbes, metabolites, and effects), MiMeDB is actually divided into six smaller categories for more facile browsing, searching, and viewing. These six categories include:

1) Metabolites
2) Microbial Sources
3) Biospecimens & Location
4) Health Effects
5) Exposure Sources
6) Metabolic Reactions

The following sections provide details about how to “**Browse**” and “**Search**” the MiMeDB. The last section provides details on how to use the “**Visualize**” tabs, “**Genome Viewer**” and “**Network Viewer**”.

First, to access MiMeDB, open your preferred browser and type “https://mimedb.org” or simply “mimedb.org” into the search bar and press the “Enter” key. You will be first taken to the homepage.

Navigating the Homepage



A – Clicking the MiMeDB logo at the top left brings you back to the homepage

B – At the top of the page there are 6 menu headings, each with their own pulldown menu: **Browse**, **Search**, **Visualize**, **Downloads**, **About** and **Contact Us**.

C – At the top right corner there is a Search box that enables you to search the entire database. Here, you can either search for a microbe or a metabolite by name by selecting either **Metabolites** or **Microbes** from the pulldown menu. Clicking on the 

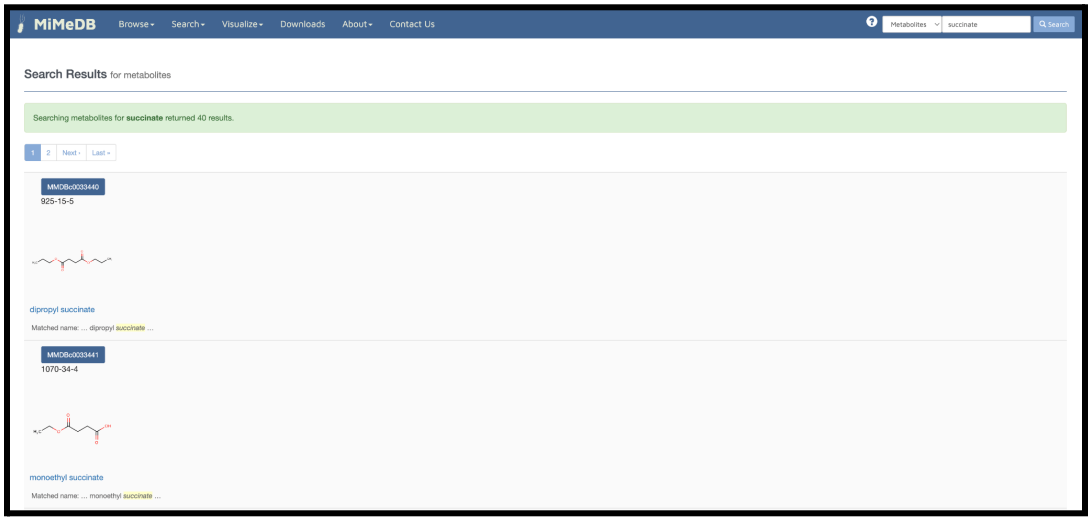
button returns a list of results that match your query.

D – There are hyperlinked bars at the center of the homepage that allow you to **Browse MiMeDB Metabolites**, **Browse MiMeDB Microbes**, or **Learn More** about MiMeDB.

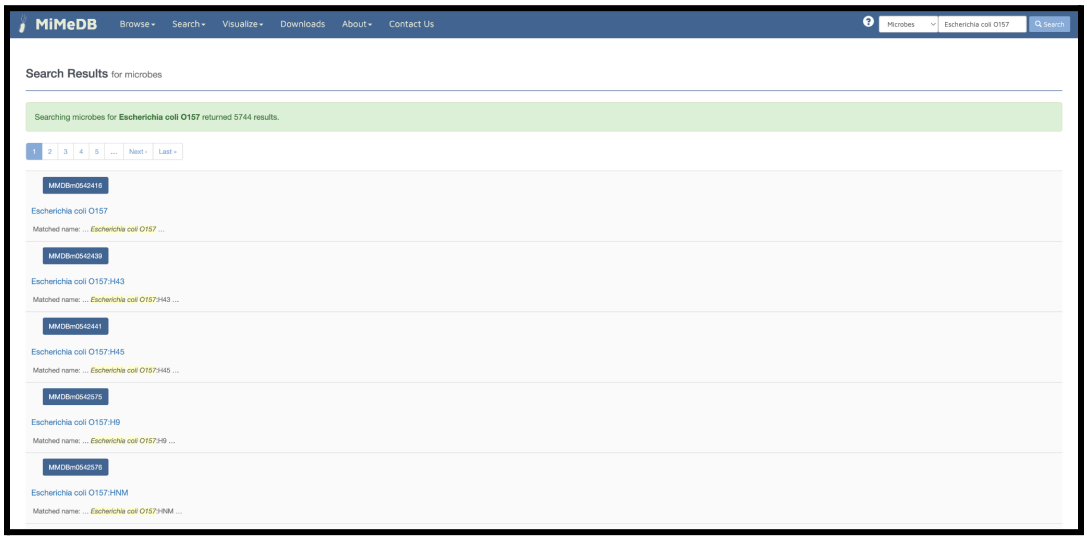
Search Box

Some general searches using the Search box

If you enter “succinate” in the search box and select **Metabolites** from the pulldown menu, 40 results are returned where “succinate” is found in the name or description.

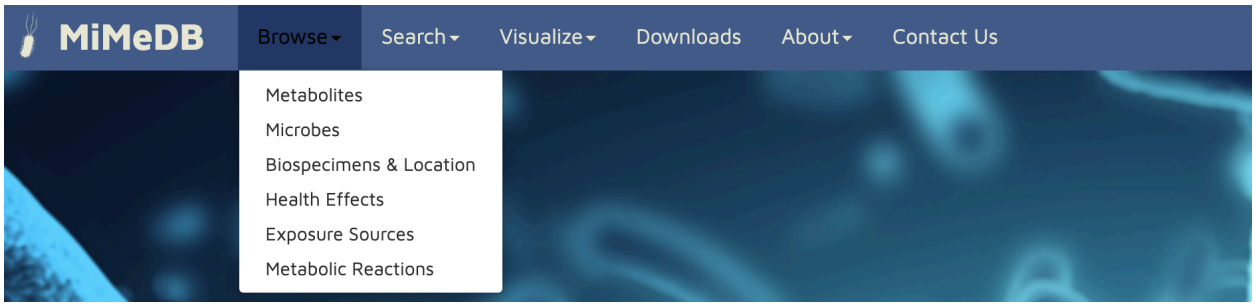


If you enter *Escherichia coli O157* in the Search box and select **Microbes** from the pulldown menu, 5744 results are returned containing “Escherichia”, “coli” or “O157” in the microbe name.



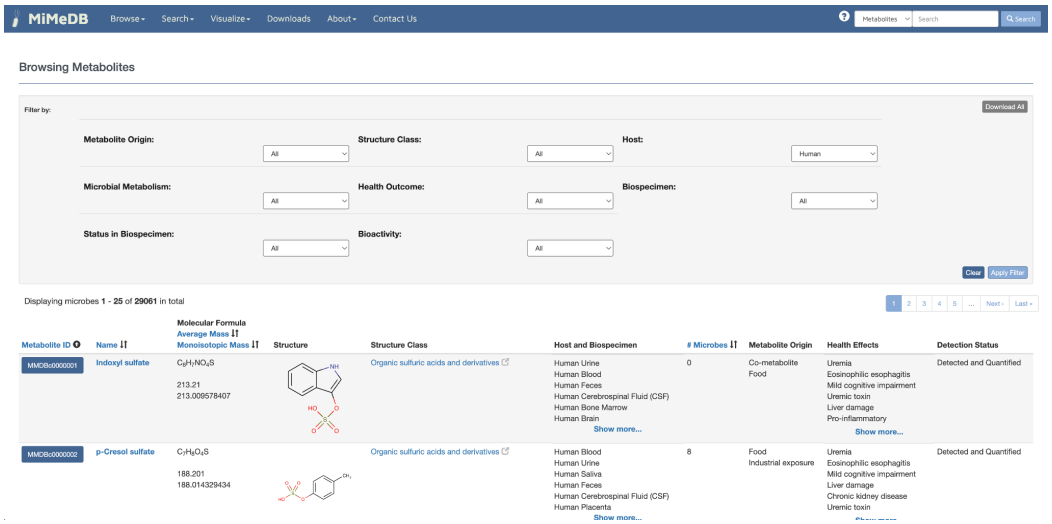
Browse

Browse at the top left of the homepage reveals a pulldown menu with 6 options.



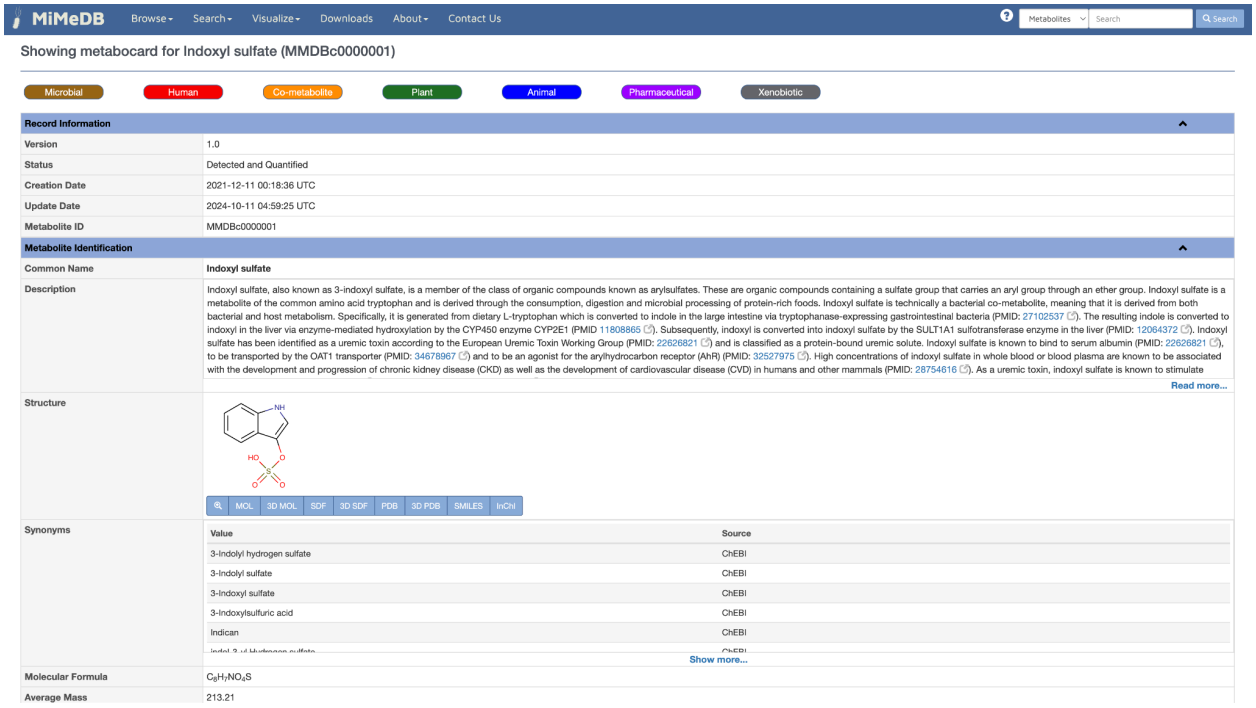
I. Metabolites

Metabolites in the pulldown menu will bring you to the Metabolites table.



Here there are various filters that can narrow your metabolite search such as **specific metabolite origin**, **structure class**, **host**, **microbial metabolism**, **health outcome**, **biospecimen**, **status in biospecimen**, and **bioactivity**. These each have their own corresponding pulldown menu, where you can then click **Apply Filter** to return a shorter table that matches your filter preferences.

Clicking on the MiMeDB compound button or the compound name will take you to the MiMeDB MetaboCard for that compound or metabolite. The MiMeDB MetaboCard for indoxyl sulfate (MMDBc0000001) is shown below.

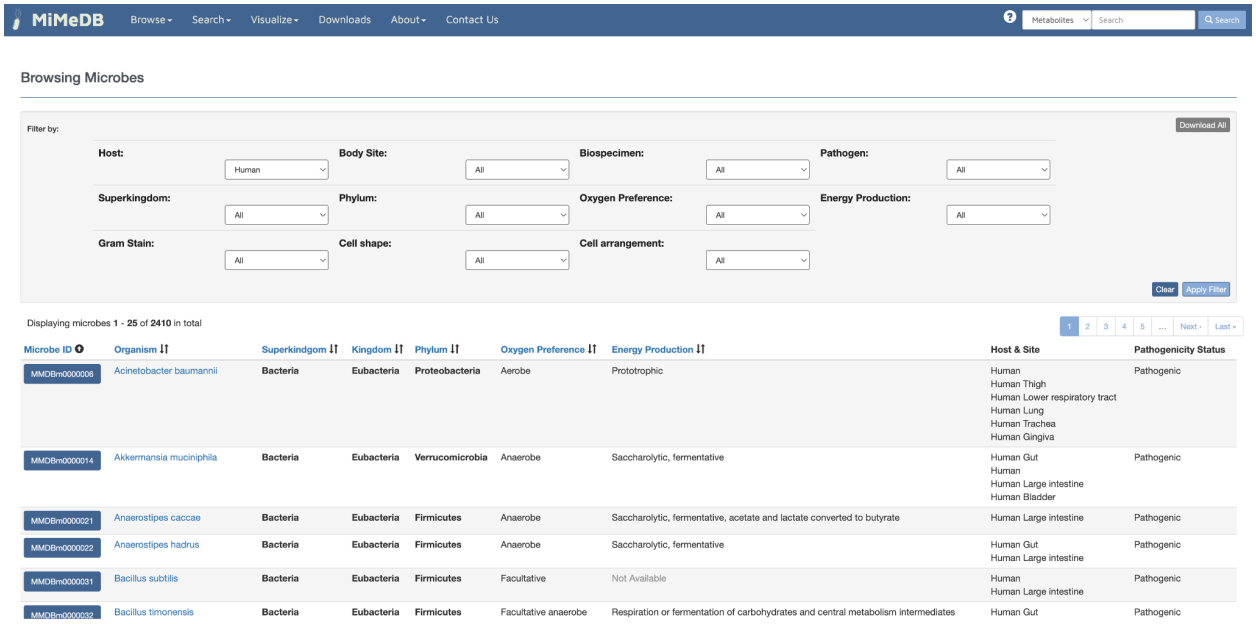


Each MiMeDB MetaboCard contains 16 data fields: **Record Information**; **Metabolite Identification**; **Chemical Taxonomy**; **Functional Ontology**; **Physical Properties**; **Spectra**; **Biological Properties**; **Human Proteins and Enzymes**; **Human Pathways**; **Metabolic Reactions**; **Health Effect and Bioactivity**; **Microbial Sources**; **Exposure Sources**; **Host Biospecimen and Location**; **External Links**; and **References**. The Record Information and Metabolite Information sections are expanded by default.

For any collapsed section, clicking on the down arrow on the righthand side expands it and reveals further information about that metabolite. Clicking on the up arrow for any expanded section collapses that section.

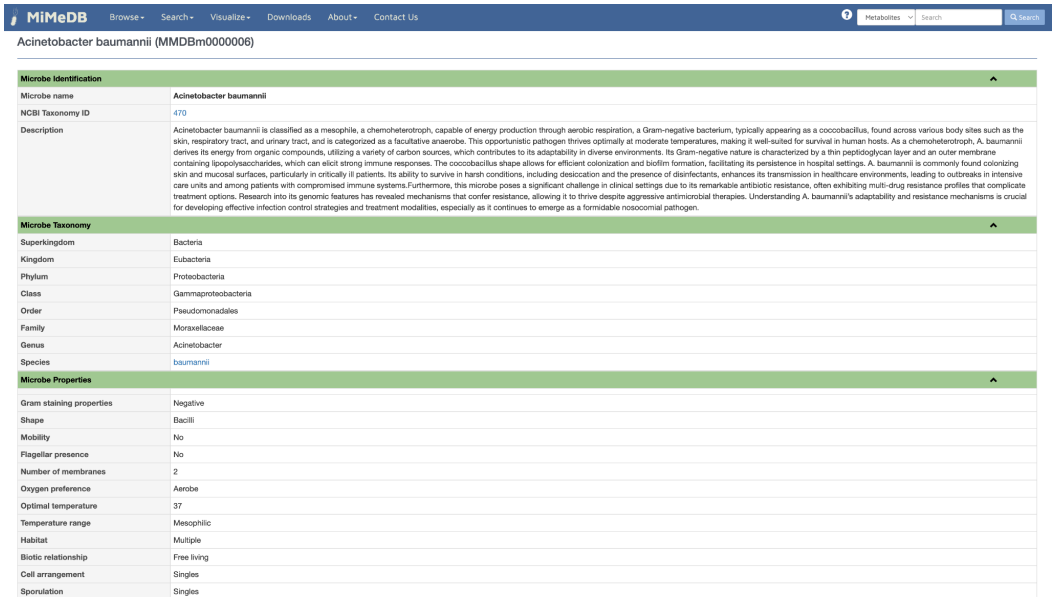
II. Microbes

From the top selection bar under **Browse**, **Microbes** in the pulldown menu will bring you to the Microbes table.

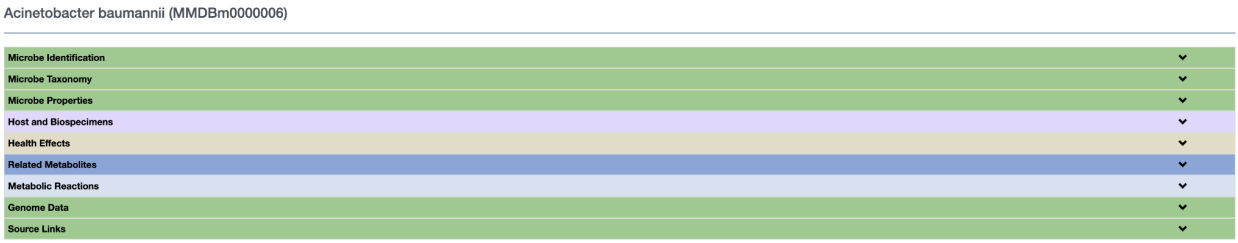


The Microbes table contains 11 filters that can specify your microbe search: **Host**, **Body site**, **Biospecimen**, **Pathogen**, **Superkingdom**, **Phylum**, **Oxygen Preference**, **Energy Preference**, **Energy Production**, **Gram Stain**, **Cell shape**, **Cell arrangement**. These each have their own corresponding pulldown menu, where you can then click **Apply Filter** to return a shorter table that matches your filter preferences.

Clicking on the MiMeDB microbe ID button or the Microbe name, will take you to the MiMeDB MicrobeCard for that organism. Acinetobacter baumannii (MMDBm0000006) is shown below.



Each MiMeDB MicrobeCard contains nine data fields: **Microbe Identification**; **Microbe Taxonomy**; **Microbe Properties**; **Hosts and Biospecimens**; **Health Effects**; **Related Metabolites**; **Metabolic Reactions**; **Genome Data**; and **Source Links**.
For any collapsed section, clicking on the down arrow on the righthand side expands it and reveals further information about that microbe. Clicking on the up arrow for any expanded section collapses that section.

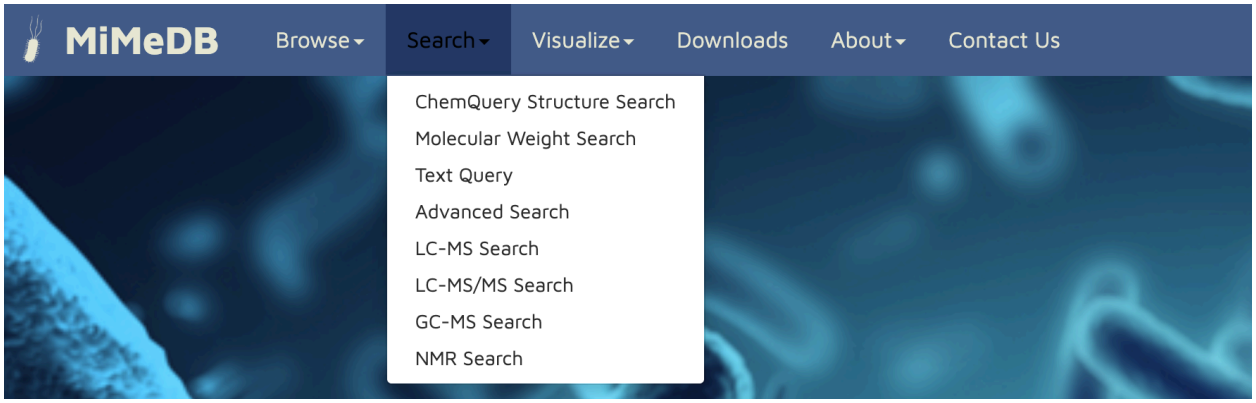


III. Other Browsing Options

Similar browsing options, similar layouts, and similar data tables are also available for each of the other Browse menu options including “Biospecimens & Locations”, “Health Effects”, “Exposure Sources” and “Metabolic Reactions”, each with their MiMeDB identifiers (named BiospeCard, HealthCard and ExposoCard, ReactCard respectively), filterable and sortable tables, and section-expandable viewing cards.

Search

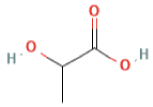
Clicking on the “Search” option at the top left of the homepage reveals a pulldown menu with 8 options.



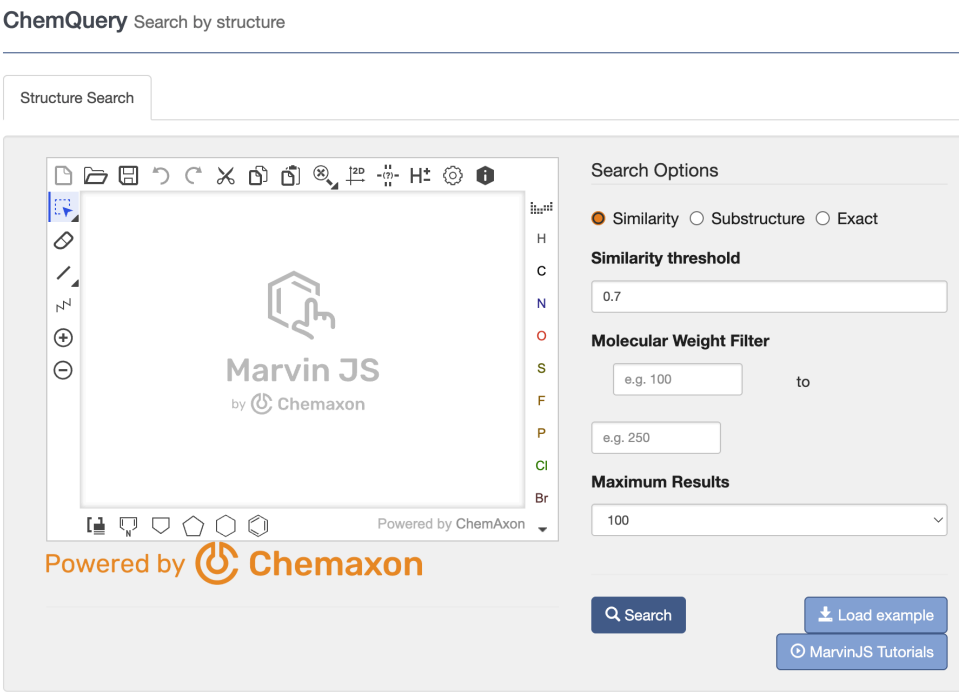
I. ChemQuery searches

The MarvinView applet from ChemAxon allows you to interactively draw structures or paste InChI or SMILES strings onto a palette (shown below).

If you were searching for the metabolite lactic acid, using the interactive palette, you could draw its chemical structure as below,



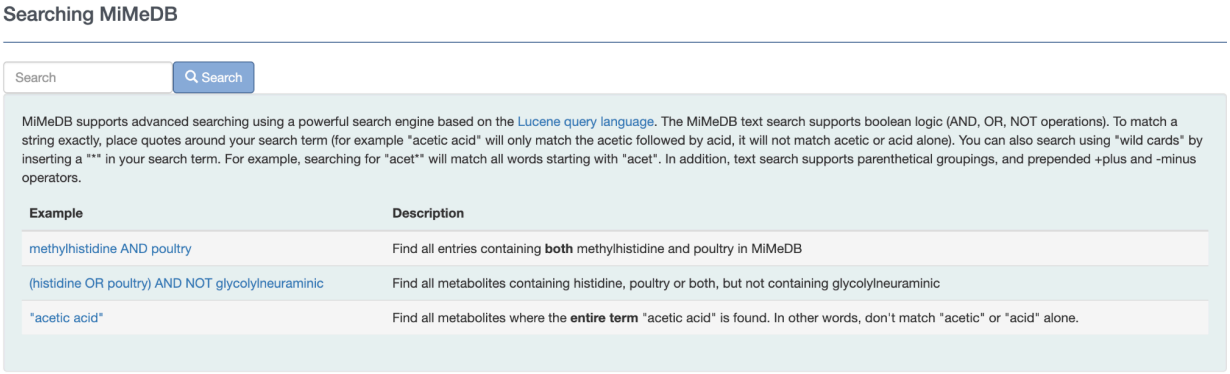
insert its InChI (InChI=1S/C3H6O3/c1-2(4)3(5)6/h2,4H,1H3,(H,5,6)); or insert one of its SMILES strings (e.g., CC(C(=O)O)O).



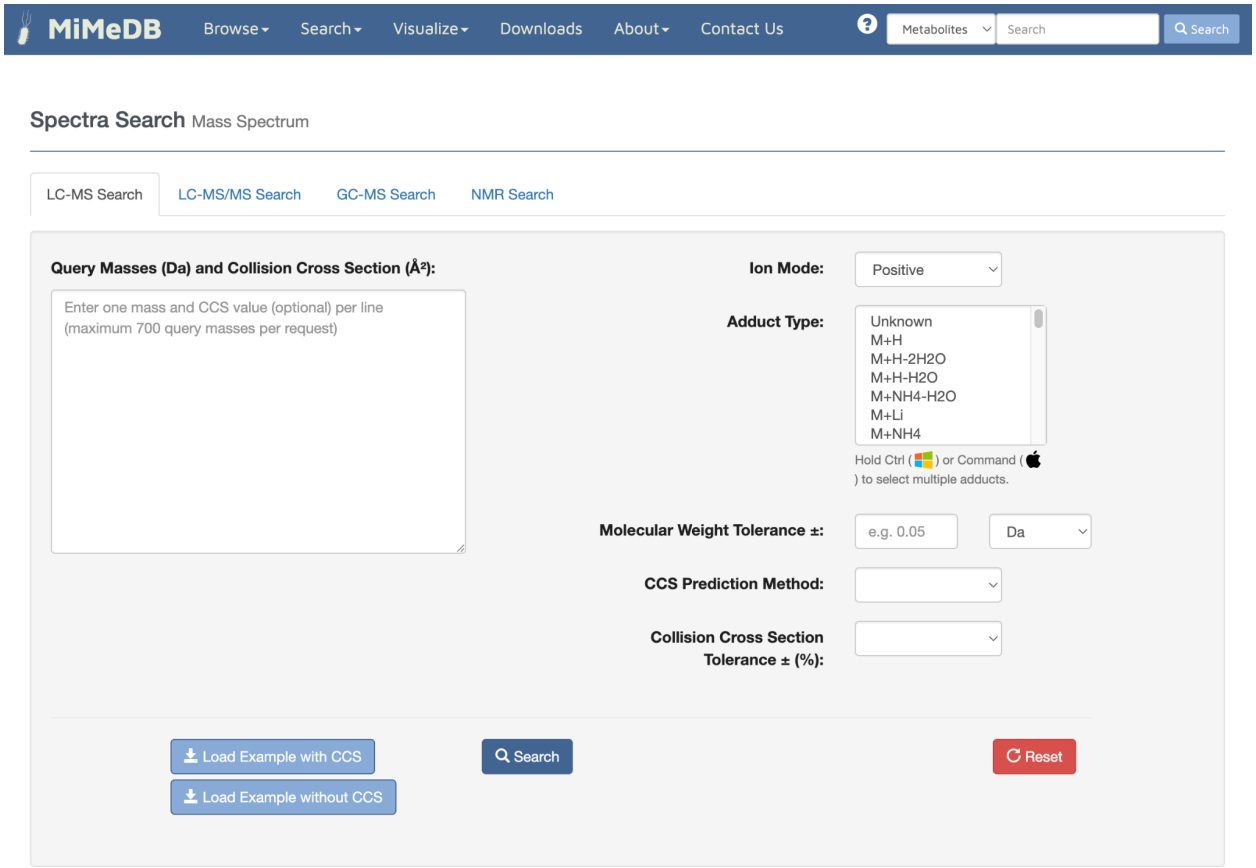
Selections for a narrowed search are also provided to specify the similarity threshold, add a range of molecular weight, and limit maximum results.

II. Text Query

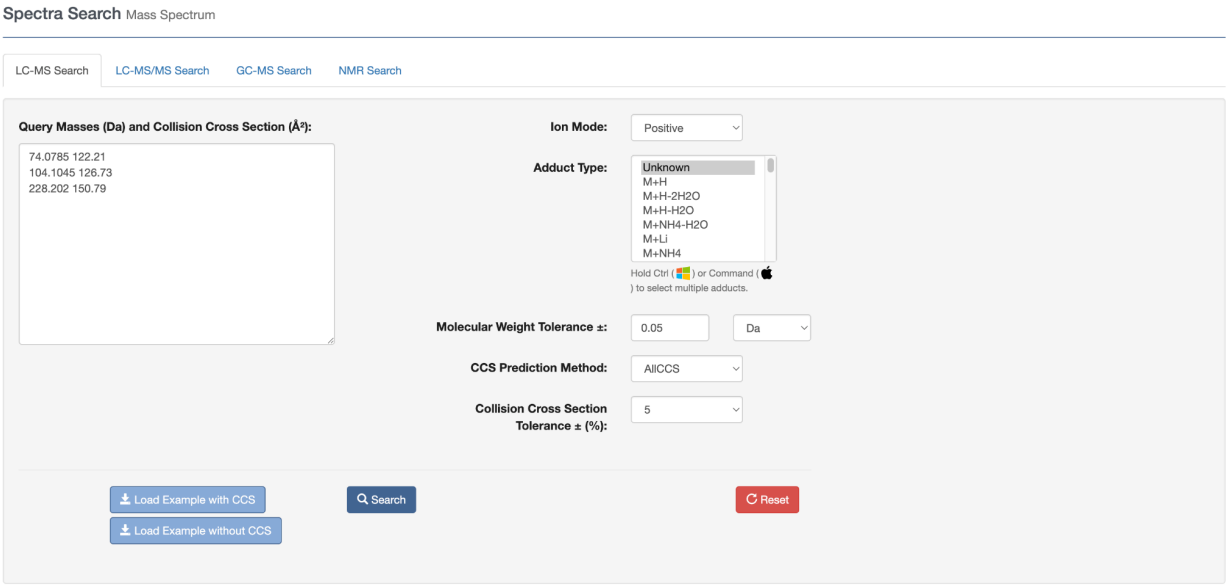
Using the provided instructions on the text query page, you can match strings you provide to data in MiMeDB.



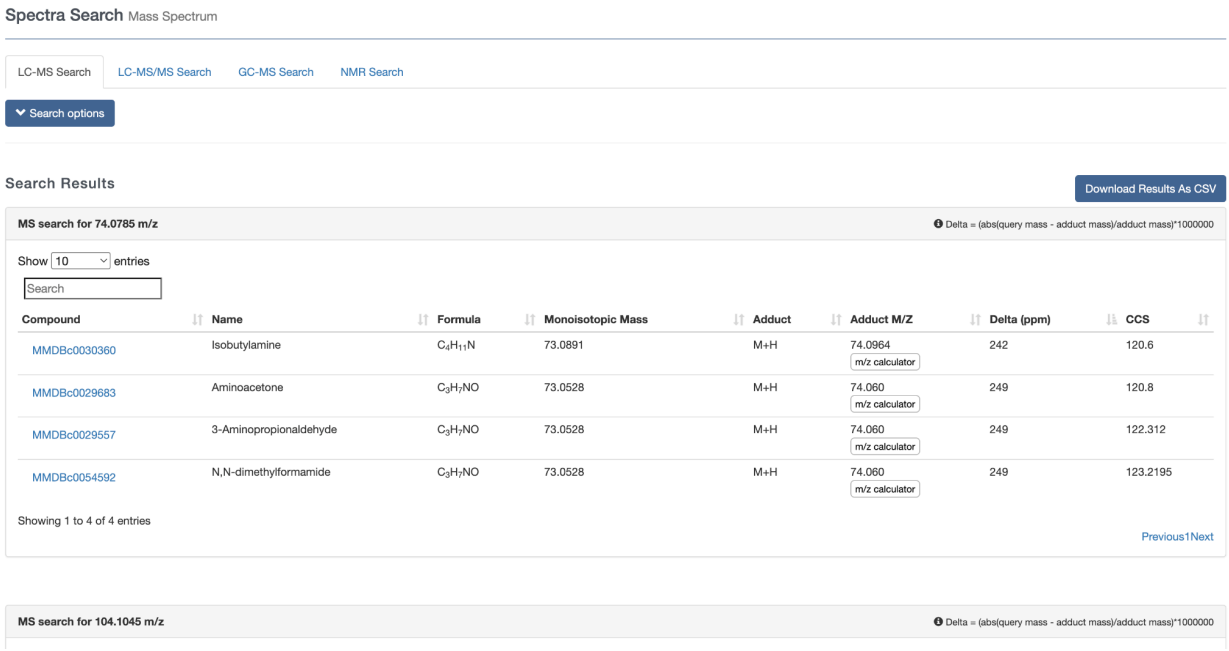
III. Spectra Search



There are four available spectral searches available on MiMeDB, Mass spectrum, Tandem mass spectrum, GC mass spectrum, and NMR spectrum. Each of these searches include a load example that can be clicked to fill in the required information with an example spectral search. By clicking search, you are brought to a table with your search results. For example, this is the propagated search box for the LC-MS search example:

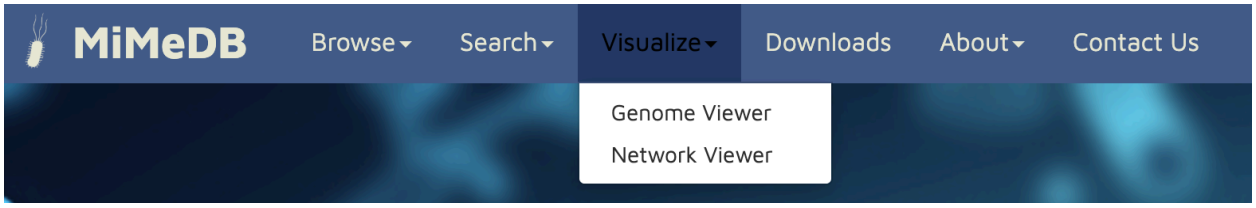


When clicking search, this is the result:



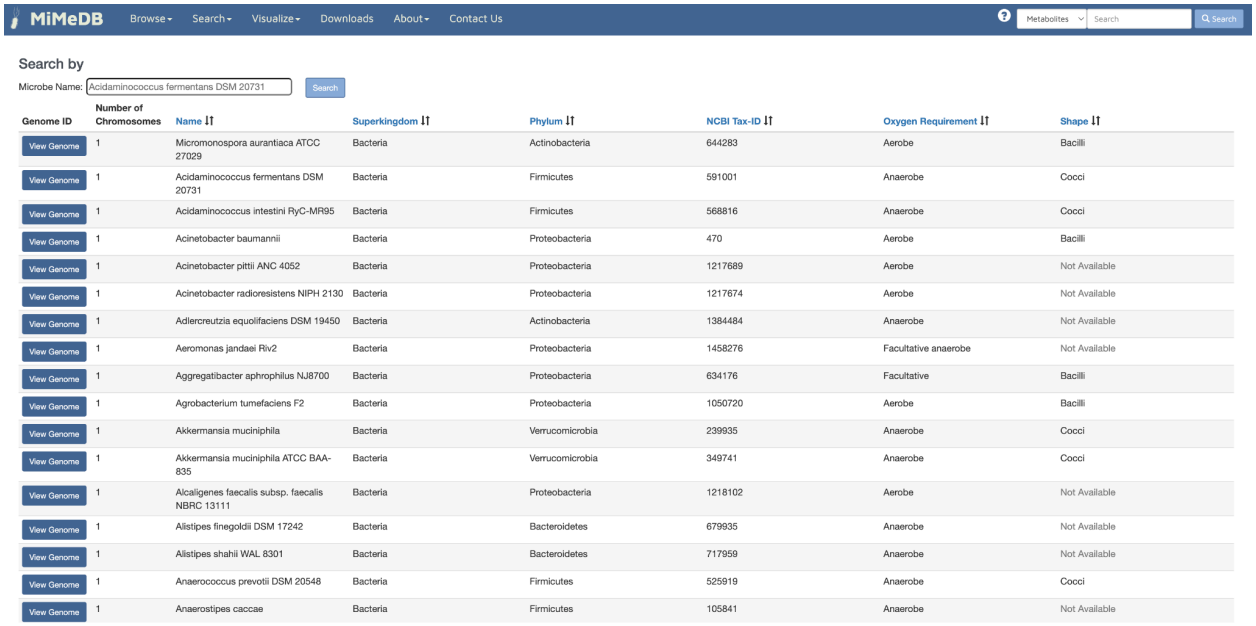
Visualize

Clicking on the “Visualize” at the top left of the homepage reveals a pulldown menu with 2 options: “Genome Viewer” and “Network Viewer”



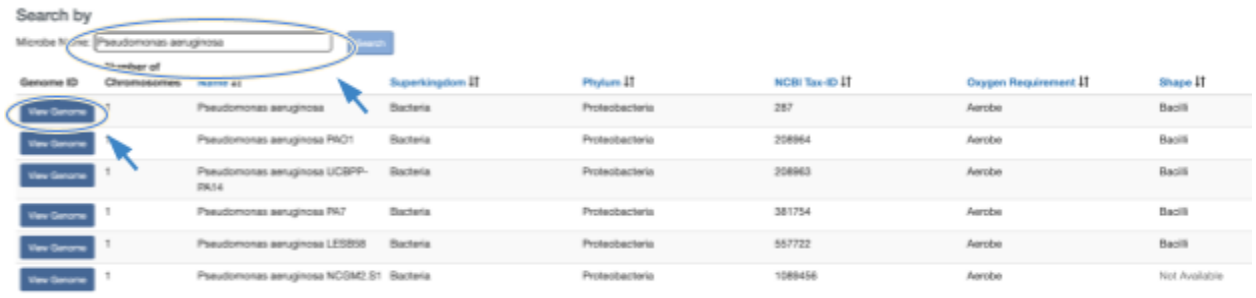
I. Genome Viewer

Selecting the “Chromosome Viewer” returns a default list of microbes with genomes that are available. One can scroll through the list to find a microorganism of interest.

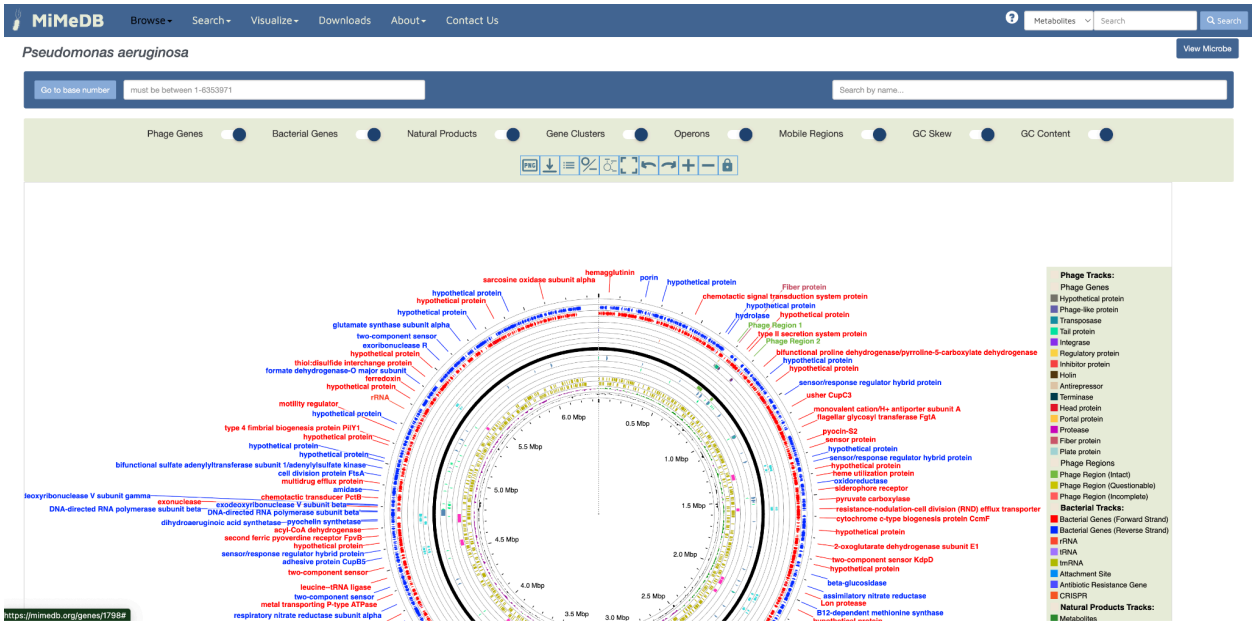


Genome ID	Number of Chromosomes	Name	Superkingdom	Phylum	NCBI Tax-ID	Oxygen Requirement	Shape
View Genome	1	Micromonospora aurantiaca ATCC 27029	Bacteria	Actinobacteria	644283	Aerobe	Bacilli
View Genome	1	Acidaminococcus fermentans DSM 20731	Bacteria	Firmicutes	591001	Anaerobe	Cocci
View Genome	1	Acidaminococcus intestini RyC-MR95	Bacteria	Firmicutes	568816	Anaerobe	Cocci
View Genome	1	Acinetobacter baumannii	Bacteria	Proteobacteria	470	Aerobe	Bacilli
View Genome	1	Acinetobacter pittii ANC 4052	Bacteria	Proteobacteria	1217689	Aerobe	Not Available
View Genome	1	Acinetobacter radioresistens NIPH 2130	Bacteria	Proteobacteria	1217674	Aerobe	Not Available
View Genome	1	Adlercreutzia equolifaciens DSM 19450	Bacteria	Actinobacteria	1384484	Anaerobe	Not Available
View Genome	1	Aeromonas jandaei Riv2	Bacteria	Proteobacteria	1458276	Facultative anaerobe	Not Available
View Genome	1	Aggregatibacter aphrophilus NJ8700	Bacteria	Proteobacteria	634176	Facultative	Bacilli
View Genome	1	Agrobacterium tumefaciens F2	Bacteria	Proteobacteria	1050720	Aerobe	Bacilli
View Genome	1	Akkermansia muciniphila	Bacteria	Verrucomicrobia	239935	Anaerobe	Cocci
View Genome	1	Akkermansia muciniphila ATCC BAA-835	Bacteria	Verrucomicrobia	349741	Anaerobe	Cocci
View Genome	1	Alcaligenes faecalis subsp. faecalis NBRC 13111	Bacteria	Proteobacteria	1218102	Aerobe	Not Available
View Genome	1	Alistipes finegoldii DSM 17242	Bacteria	Bacteroidetes	679935	Anaerobe	Not Available
View Genome	1	Alistipes shahii WAL 8301	Bacteria	Bacteroidetes	717959	Anaerobe	Not Available
View Genome	1	Anaerococcus prevotii DSM 20548	Bacteria	Firmicutes	525919	Anaerobe	Cocci
View Genome	1	Anaerostipes caccae	Bacteria	Firmicutes	105841	Anaerobe	Not Available

Alternatively, one can search for a specific microorganism by entering the name in the **Microbe Name** search box and clicking “Search”. Shown below are the 6 results returned when “Pseudomonas aeruginosa” is entered in the “Microbe Name” box.



By clicking **View Genome**, you are brought to the following page:



Widgets at the top of the genome viewer carry out the listed functions:

Download map snapshot as PNG

Download map snapshot as SVG

Toggle legends

Toggle Circular/Linear format

Toggle phage annotation labels

Reset view

Pan left

Pan right

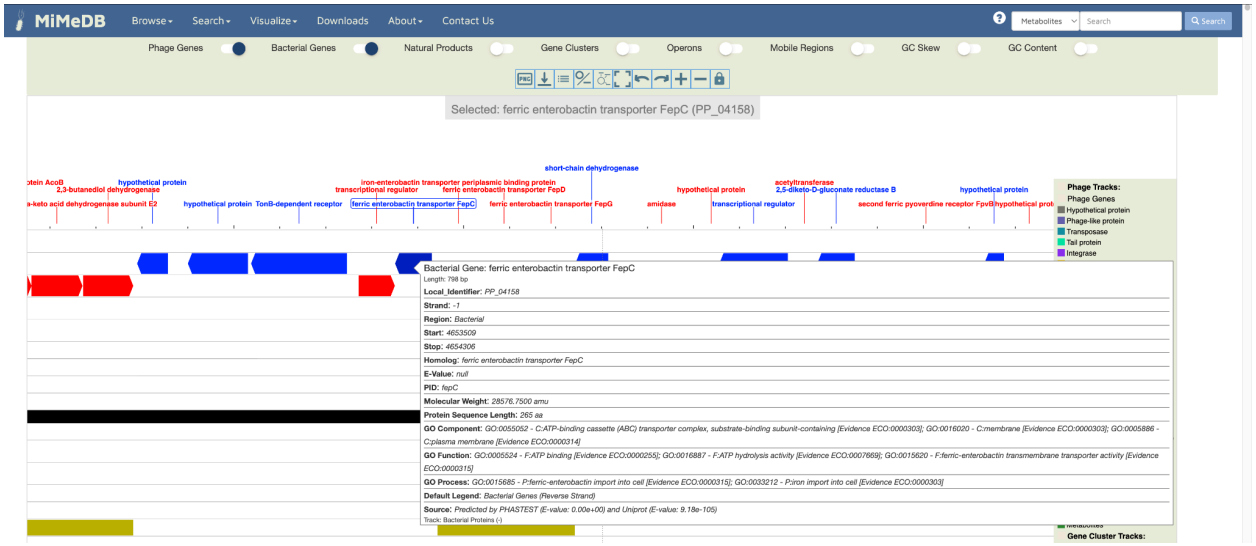
Zoom in

Zoom out

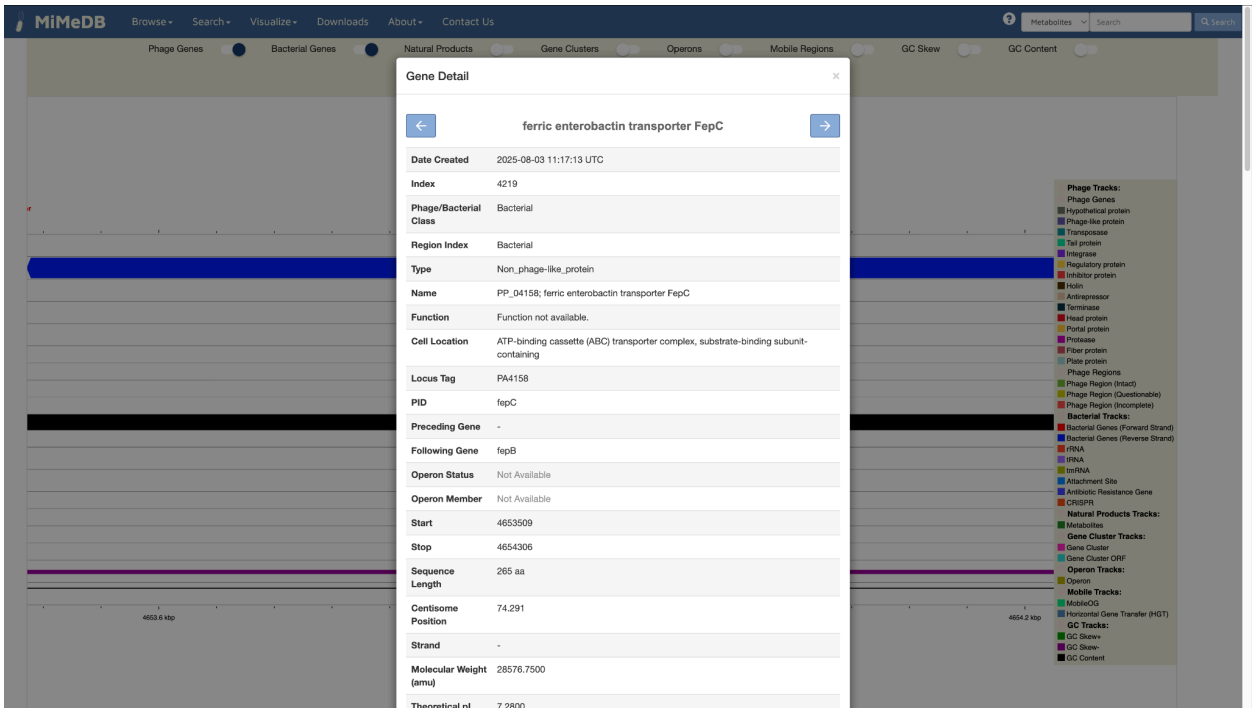
Lock zoom by scroll

Above these widgets are switches that toggle to alter the data shown on the tracks of the genome viewer.

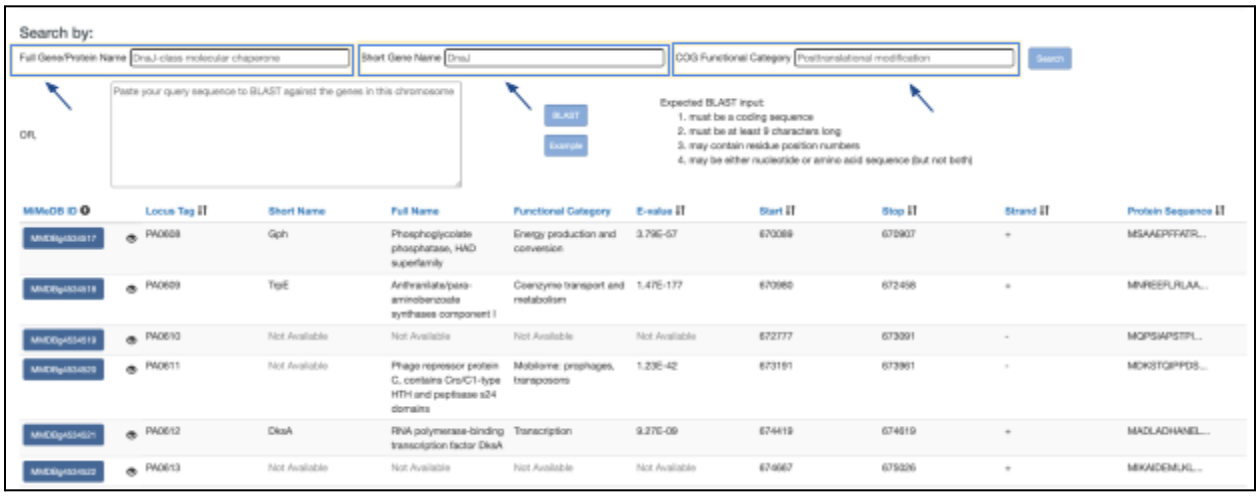
The Genome Viewer shows specific gene positions, names and orientations. Each chromosome is zoomable and each gene is clickable. By hovering over a gene you see the following popup:



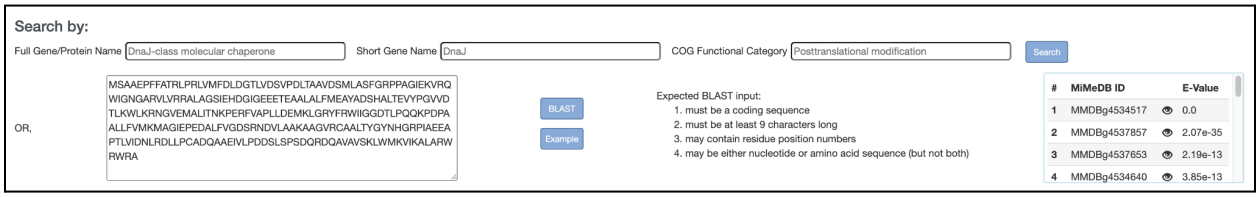
By clicking on this same gene you are provided a page with richer information on the gene, seen below:



Genes can also be searched for underneath the genome viewer:



Here you can search using the full gene name, short gene name, COG functional category or by sequence. Shown below is an example of a BLAST search by sequence, on the right side is a popup of the BLAST results.

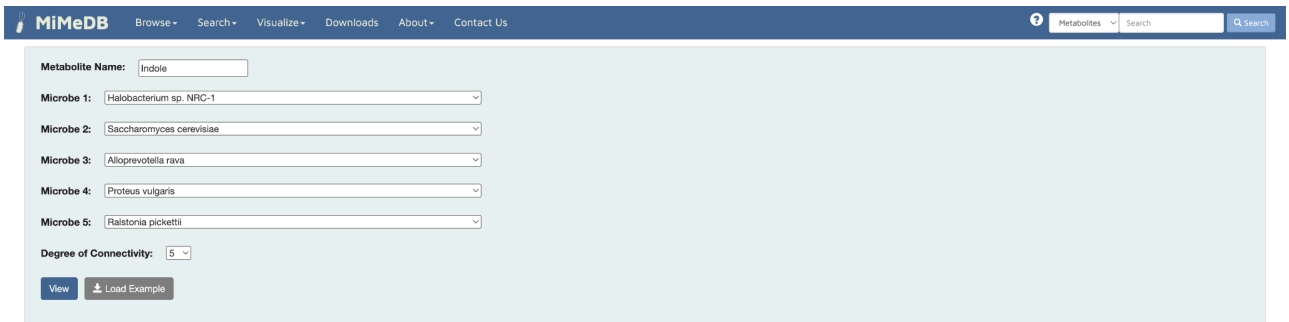


Clicking on any eye icon will bring you to the exact location of the gene on the chromosome map.

II. Network Viewer

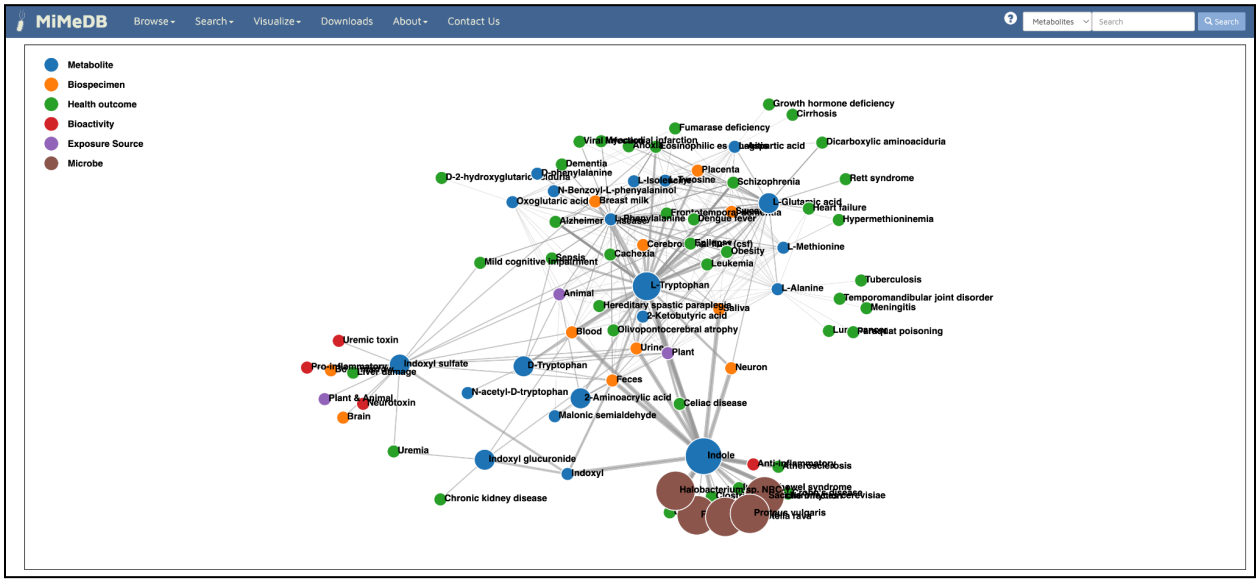
The network viewer allows you to see connections of metabolites to health effects to exposure to microbes to body sites. It is a tool to decipher/depict/visualize the relationship and interaction between metabolites and microbes. Clicking on Network viewer in the **Visualize** pulldown menu brings you to another page.
The following information is required for generating your network viewer:

A) Metabolite: Enter the metabolite of interest in the Metabolite Name box. Begin typing and a pulldown list of metabolites will appear below to select.
B) Microbe(s): Enter the names of up to 5 microbe(s) in the “Select Microbe” boxes. You must enter the scientific name or partial name and auto-select will reveal a list for you to choose your microbe of interest.
C) Degree of Connectivity: You must also select the degree of connectivity (default is “5”). The degree of connectivity affects the density of the network graph: the higher the connectivity, then more data (more interactivity) is loaded into the graph. From the pull-down menu, “1, 3, 5, 8 or 10” degrees of connectivity can be selected.
D) View: Once you have filled all desired boxes, click on view to be taken to the network viewer.
E) Load Example: To see an example of the network viewer, or how the boxes can be filled, click load example. All options will be filled by an example, the result is shown below:

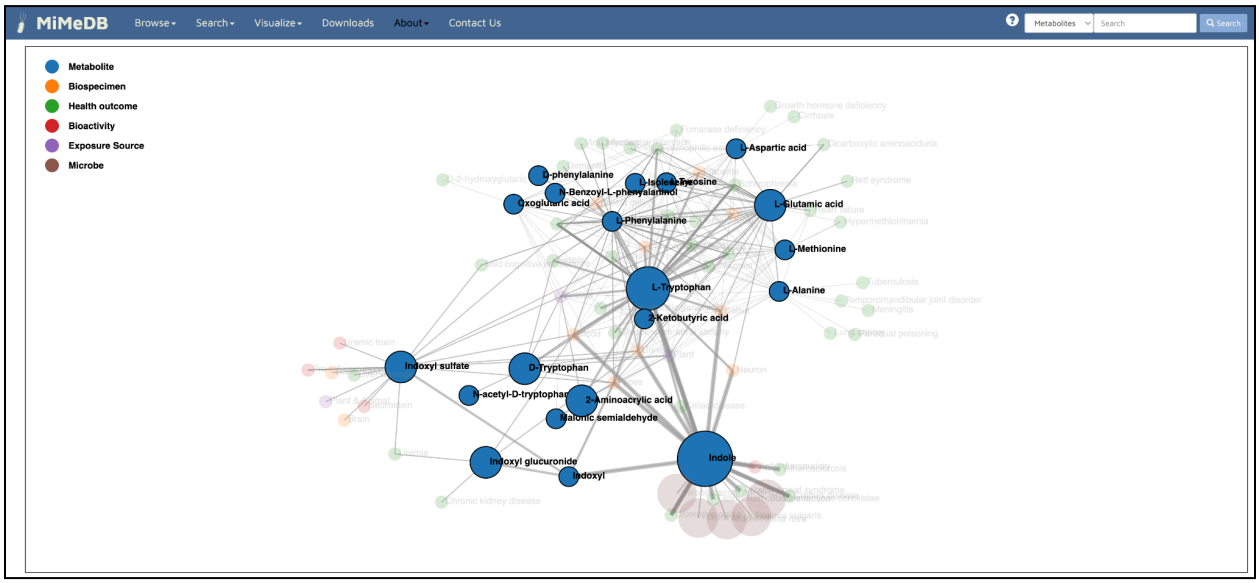


The generated network from the uploaded sample is shown below. All connections of metabolites, microbes, biospecimens and health effects within MiMeDB are shown. A color legend is provided on the top left to easily distinguish metabolites, biospecimens, health outcomes, bioactivity, exposure sources, and microbes within the network.

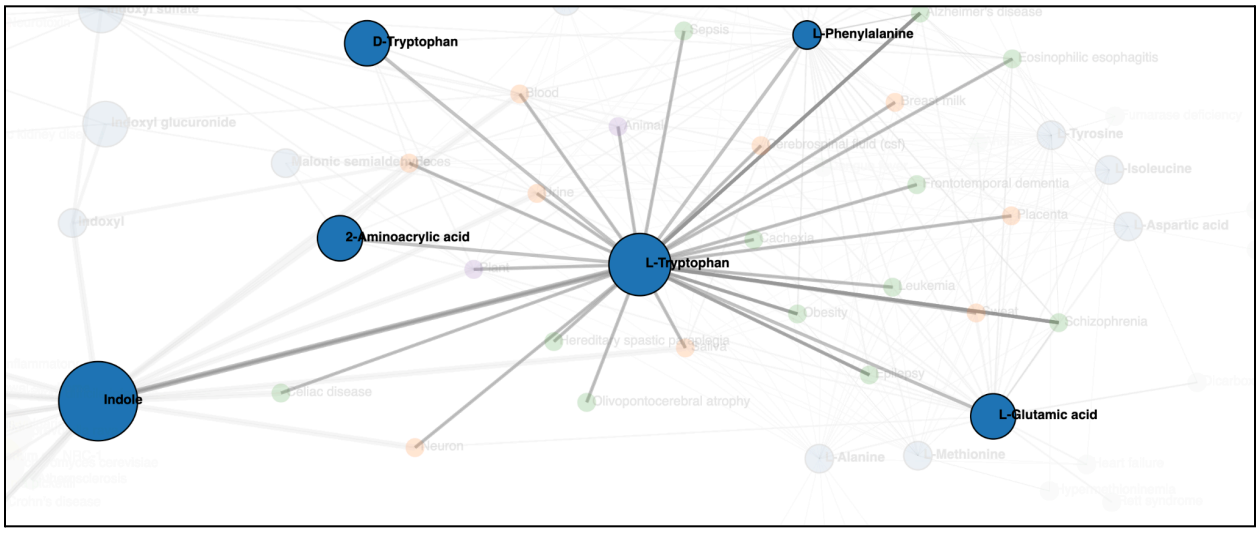
The viewer represents data in Nodes and Edges. **Nodes** are represented by metabolite, biospecimen, health outcome, exposure source and microbes. **Edges** depict the relationship among these different nodes. You can “Click” any of the nodes and edges. These nodes and edges can be adjusted or moved around to have a better view of the relationships among them.



Selecting on one of the labels in the legend isolates that specific data type. In the example below, Metabolite was clicked on in the legend to provide the following result



Hovering over the node, further isolates it for clearer viewing of the data point:



Clicking on nodes of metabolites or microbes, takes you to their metabocard or biocard. In this case, clocking on the L-Tryptophan node brings you to this page: