### Proposed URL ###

https://webapp.ufz.de/mgsmrdb/

### Title ###

MAG-based Genome-Scale Metabolic Reconstruction Database

### Subtitle ###

Explore bacterial and archaeal metagenome-assembled genome (MAG) based genome-scale metabolic reconstructions (GSMRs).

### About ###

We developed the MAG-based Genome-Scale Metabolic Reconstruction Database to facilitate the selection and download of the metagenome-assembled genome (MAG) based genome-scale metabolic reconstructions that were created from MAGs deposited in the CLUE-TERRA consortium [https://www.ufz.de/index.php?en=47300] and the Earth's microbiome genomic catalog (GEM) [https://doi.org/10.1038/s41587-020-0718-6]. The MAG-based Genome-Scale Metabolic Reconstruction Database (Release 1.0) contains the GTDB-tk [https://doi.org/10.1093/bioinformatics/btac672] determined taxonomic classifications, MAG quality and technical data from CheckM [https://doi.org/10.1101%2Fgr.186072.114] and the BioInfoTools BBMap genome statistics tool [https://github.com/BioInfoTools/BBMap/blob/master/sh/stats.sh], and metabolic reconstruction quality parameters from MEMOTE [https://www.nature.com/articles/s41587-020-0446-y] for 68,679 MAG-based metabolic reconstructions. The Quick Search and Advanced Search tabs allow users to select MAG-based metabolic reconstructions of interest. The download tool allows easy download of the source MAG sequence assemblies and the resulting genome-scale metabolic reconstructions.

### Attributes for quick search (min 6) ###

- Source database (database)

- Taxonomic domain (domain)

- Taxonomic phylum (phylum)

- Taxonomic class (class)

- Taxonomic order (order)

- Taxonomic family (family)

- Taxonomic genues (genus)

- Taxonomic species (species)

- MAG quality level (quality)

- Completeness

- Contamination

- Maximum growth rate on simulated minimal media ()

- Number of C-atom containing metabolites in simulated minimal media ()

- Growth yield on simulated minimal media ()

- r/K index

### contact page ###

The MAG-based Genome-Scale Metabolic Reconstruction Database was developed by Ulisses Nunes da Rocha, Avila Santos Anderson Paulo, Robson Parmezan Bonidia, Sanchita Kamath, Joao Pedro Saraiva, and Stefanía Magnúsdóttir at the Helmholz-Zentrum for Environmental Research (Leipzig, Germany) and the University of São Paulo (São Carlos, Brazil).

What is the reason of your contact?

- Feedback?

Feel free to use our Feedback Form to help us improve our database. You can also send an email to Dr. Ulisses Nunes da Rocha, ulisses.rocha@ufz.de

- Questions?

If our “Home” guide does not cover your questions, please post your question in the User Group for others to benefit.

- Other regards?

For other regards or questions please contact Dr. Ulisses Nunes da Rocha, ulisses.rocha@ufz.de.

### Help page ###

1. Home

The MAG-based Genome-Scale Metabolic Reconstruction Database user interface is divided into "Quick search" and "Advanced search" sections to help users choose a section that better fits their needs. The first section, “Quick search”, holds the full content of the databases’ current version, as well as the ability to filter the samples through their main characteristics. The “Advanced search” section dynamically generates filters for all the available features of the complete dataset, allowing the user to search for specific attributes.

2. How to use the Quick search?

The “Quick Search” is available for users to access the full content of MAG-based Genome-Scale Metabolic Reconstruction Database and filter the dataset according to the main available features.

Example usage:

All MAGs and metabolic reconstructions are are included in the “Quick Search” section, including the ones without valid features.

One can filter the entries by using the available main filters or typing in the search box at the top of the table.

You can further explore your selection by clicking the “Visualize” button. After filtering, you can download the data of your selected entries as a comma-separated values (.csv) file.

3. How to use the Advanced search?

The “Advanced Search” tab dynamically generates filters for all the available features of the complete dataset since not all the filters are present in the “Quick Search” tab. The checkbox allows the users to decide if they want to filter out samples with missing values for the selected attributes.

Example usage:

Click on “Search and add filters” and a window will open.

One can search for the available features either by name or by category. Click “Add filter” once you found the filters you would like to use.

Use the selected features to subset the MAGs and metabolic reconstructions.

Click the available checkbox if you would like to keep the samples with missing values.

You can further filter the entries by typing in the search box placed at the top right of the table or by using the filter boxes present at the top of each column.

You can further explore your selection by clicking the “Visualize” button.

After filtering your dataset, you can download the data of your selected entries as a comma-separated values (.csv) file.

4. How to download a metagenome-assembled genome?

We do not store the MAG sequence assemblies in our database. However, we created a graphical user interface (GUI) and script that makes it easy to download them directly from a data table downloaded from the database. You can find the GUI/script on the GitHub page of our research group [https://github.com/mdsufz].

You may use our Python scripts on all operating systems. For Windows (Win10), we recommend using the Windows executable provided for easy use without installing Python or any dependencies. To use it, when executing download\_gui.exe, you have to select the file with the mgsmrdb\_selected\_dataset.csv and execute it. You can download the graphical user interface for Windows by clicking on the “Download assemblies” button located on the other tabs of the database.

5. How to download a metabolic reconstruction?

We do not store the metabolic reconstructions in our database. However, we created a graphical user interface (GUI) and script that makes it easy to download them directly from a data table downloaded from the database. You can find the GUI/script on the GitHub page of our research group [https://github.com/mdsufz].

You may use our Python scripts on all operating systems. For Windows (Win10), we recommend using the Windows executable provided for easy use without installing Python or any dependencies. To use it, when executing download\_gui.exe, you have to select the file with the mgsmrdb\_selected\_dataset.csv and execute it. You can download the graphical user interface for Windows by clicking on the “Download reconstructions” button located on the other tabs of the database.

6. What does each attribute of the database mean?

[Table "resource.data.headers.csv"]