

MASST Web Interface Tutorial

1) Paste M/Z value and spectrum peaks. Enter other information and click on “MASST Molecule”.

The screenshot shows the MASST web interface with the following sections:

- Search Parameters:** Includes fields for Minimum Cosine Score (0.7), Minimum Matched Peaks (6), Parent Mass Tolerance (2.0), Fragment Mass Tolerance (0.5), Analog Search (No), and Public Databases to Search (Non-redundant MS/MS).
- Spectrum Peaks:** A table with columns for Precursor M/Z (337.155) and Peaks. The peaks list includes: 30.033323, 207.030106, 41.037846, 1098.494019, 42.033474, 622.983582, 43.017254, 3939.47998, 43.053467, 804.571411, 53.037067, 142.545105, 55.017761, 1785.110962, 55.053783, 463.353699, 57.056606, 226.688507, 58.065262, 1169.906006, 67.017197, 4984.604004, 67.053978, 215.108902.
- Reporting Information:** Includes Analysis Description (Cyclopiiazonic acid), Email address (icarbon@ncsu.edu), and GNPS Login fields (Username and Password).

Red arrows point to the Precursor M/Z field, the Peaks list, the Email address field, and the MASST Molecule button.

2) Monitor progress of MASST run.

The screenshot shows the MASST job status page with the following details:

- Job Status:** SEARCH_SINGLE_SPECTRUM (version release_29)
- Status:** RUNNING
- User:** quickstart_GNPS (ccms.web@gmail.com)
- Title:** Cyclopiiazonic acid
- Date Created:** 2023-05-20 09:10:54.0
- Execution Time:** 2 minutes 58 seconds

The Progress section shows a workflow diagram with steps such as create_spectrum_file, library_search_single, find_single_dataset_matches_parallel_step_0 through 4, find_dataset_matches_parallel_merge, create_mast_network, build_tree, get_annotations, and write_description.

The Spectral Library section lists various libraries used in the search, including:

- speclibs/GNPS-SAM-SIK-KANG-LEGACY-LIBRARY/GNPS-SAM-SIK-KANG-LEGACY-LIBRARY.mgf
- speclibs/CASMI/CASMI.mgf
- speclibs/GNPS-SCIEX-LIBRARY/GNPS-SCIEX-LIBRARY.mgf
- speclibs/MONA/MONA.mgf
- speclibs/GNPS-NIH-CLINICALCOLLECTION2/GNPS-NIH-CLINICALCOLLECTION2.mgf
- speclibs/GNPS-SELLECKCHEM-FDA-PART1/GNPS-SELLECKCHEM-FDA-PART1.mgf
- speclibs/GNPS-COLLECTIONS-PESTICIDES-NEGATIVE/GNPS-COLLECTIONS-PESTICIDES-NEGATIVE.mgf
- speclibs/LDB_POSITIVE/LDB_POSITIVE.mgf
- speclibs/BIRMINGHAM-UHPLC-MS-NEG/BIRMINGHAM-UHPLC-MS-NEG.mgf
- speclibs/GNPS-NIH-NATURALPRODUCTSLIBRARY/GNPS-NIH-NATURALPRODUCTSLIBRARY.mgf
- speclibs/GNPS-NIH-CLINICALCOLLECTION1/GNPS-NIH-CLINICALCOLLECTION1.mgf
- speclibs/BERKELEY-LAB/BERKELEY-LAB.mgf
- speclibs/MMV_POSITIVE/MMV_POSITIVE.mgf
- speclibs/GNPS-NIH-NATURALPRODUCTSLIBRARY_ROUND2_NEGATIVE/GNPS-NIH-NATURALPRODUCTSLIBRARY_ROUND2_NEGATIVE.mgf
- speclibs/GNPS-SELLECKCHEM-FDA-PART2/GNPS-SELLECKCHEM-FDA-PART2.mgf
- speclibs/PNNL-LIPIDS/PNNL-LIPIDS-NEGATIVE.mgf
- speclibs/PNNL-LIPIDS/PNNL-LIPIDS-POSITIVE.mgf
- speclibs/GNPS-NIST14-MATCHES/GNPS-NIST14-MATCHES.mgf
- speclibs/DRUGS-OF-ABUSE-LIBRARY/DRUGS-OF-ABUSE-LIBRARY.mgf
- speclibs/INAMR/INAMR.mgf

3) Click on "Dataset Matches".

gnps.ucsd.edu/ProteoSAFe/status.jsp?task=1582659f1e5d49519f2c2aa93dc03f6d

GNPS: Global Natural Products Social Molecular Networking

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Job Status

Workflow
SEARCH_SINGLE_SPECTRUM (version release_29)
DONE
[Clone] [Clone to Latest Version]
[View All Library Hits]
Community Matches
[Dataset Matches]

Status
Reanalyze Files Found
[Analyze Files Found With Molecular Networking]
Foodomics Specific Analysis
[View Foodomics Specific Molecules | View Matched Files | View Interactive Tree | Download Tree (json) | Download Tree (HTML)]
Export/Download Network Files
[Download Cytoscape Data]
Advanced Views - External Visualization
[Direct Cytoscape Preview/Download]

User
quickstart_GNPS (ccms.web@gmail.com)

Title
Cycloplazonic acid

Re-Analyze Task Outputs
[Import to Re-analyze Task Data](#)

Date Created
2023-05-20 09:10:54.0

Execution Time
20 minutes 29 seconds

Progress

4) Click on "View File Matches".

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Cycloplazonic acid
Select columns

Hits 1 - 6 out of 6

Apply Filters	View Dataset	Title	Description	Organisms	Cosine Score	Matched Peaks	AZ Delta	NumFiles	View File Matches in GNPS
Filter By: USI Links 1	View MSV000086604	GNPS Chemodiversity in Aspergillus section Flavi	Show	Aspergillus sp. (NCBITaxon:5065)	0.92	14	0.00	14	View File Matches
View Mirror Match USI Links 2	View MSV000085858	GNPS Streptomycetes scabiei 87.22 MYMm/YM5m/OBA positive and negative ionization mode	Show	Streptomycetes scabiei 87.22	0.78	10	0.91	4	View File Matches
View Mirror Match USI Links 3	View MSV000085360	GNPS - 15_fungal isolates_bioconversion_ECGG	Show	Eurotium cristatum (NCBITaxon:41421); Cladosporium tenuissimum (NCBITaxon:70808); Penicillium sp. (NCBITaxon:5081); Penicillium oxalicum (NCBITaxon:69781); Aspergillus sp. (NCBITaxon:5065); Cladosporium sp. (NCBITaxon:1707700); Aspergillus ochraceus (NCBITaxon:40380); Candida metapsilosis (NCBITaxon:223772); Aspergillus niger (NCBITaxon:5061); Trametes hirsuta (NCBITaxon:5327); Bjerkandera adusta (NCBITaxon:5331); Penicillium stockii (NCBITaxon:303698)	0.75	6	0.00	7	View File Matches
View Mirror Match USI Links 4	View MSV000084595	GNPS - Comparative genomics metabolomics analysis of Streptomycetes species	Show	Streptomycetes	0.73	10	0.11	39	View File Matches
View Mirror Match USI Links 5	View MSV000079098	GNPS_Cichewicz_Fungi_Collection	Show	Fungi (NCBITaxon:4751)	0.72	8	0.00	3	View File Matches
View Mirror Match USI Links 6	View MSV000084855	GNPS_QINGLIN Fungi_20211126_Molecular networking parameters	Show	Fungi (NCBITaxon:4751)	0.70	10	0.00	1	View File Matches

5) Download tab-delimited MASST results file (.tsv).

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Download Option: Tab-Delimited Result Only
Include Entries: Filtered All [Download](#)

Cycloplazonic acid
Select columns

Hits 1 - 14 out of 14

Apply Filters	dataset_id	dataset_scan	filename	View Metadata	View Chromatogram (Beta)
Filter By: MSV000086604	MSV000086604	N/A	f.MSV000086604/ccms_peak/Group 1/sk1928.mzML	View Metadata	View LCMS
1	MSV000086604	N/A	f.MSV000086604/ccms_peak/Group 1/sk1927.mzML	View Metadata	View LCMS
2	MSV000086604	N/A	f.MSV000086604/ccms_peak/Group2/sk1926.mzML	View Metadata	View LCMS
3	MSV000086604	N/A	f.MSV000086604/ccms_peak/Group 1/sk1925.mzML	View Metadata	View LCMS
4	MSV000086604	N/A	f.MSV000086604/ccms_peak/Group2/sk1923.mzML	View Metadata	View LCMS
5	MSV000086604	N/A	f.MSV000086604/ccms_peak/Group2/sk1919.mzML	View Metadata	View LCMS
6	MSV000086604	N/A	f.MSV000086604/ccms_peak/Group 1/sk1915.mzML	View Metadata	View LCMS
7	MSV000086604	N/A	f.MSV000086604/ccms_peak/Group 5/sk1895.mzML	View Metadata	View LCMS
8	MSV000086604	N/A	f.MSV000086604/ccms_peak/Group 1/sk1891.mzML	View Metadata	View LCMS
9	MSV000086604	N/A	f.MSV000086604/ccms_peak/Group 1/sk1890.mzML	View Metadata	View LCMS
10	MSV000086604	N/A	f.MSV000086604/ccms_peak/Group 1/sk1889.mzML	View Metadata	View LCMS
11	MSV000086604	N/A	f.MSV000086604/ccms_peak/Group 6/sk1888.mzML	View Metadata	View LCMS
12	MSV000086604	N/A	f.MSV000086604/ccms_peak/Group 1/sk1885.mzML	View Metadata	View LCMS
13	MSV000086604	N/A	f.MSV000086604/ccms_peak/Group 4/sk1880.mzML	View Metadata	View LCMS
14	MSV000086604	N/A	f.MSV000086604/ccms_peak/Group 4/sk1880.mzML	View Metadata	View LCMS