

GNPS Hands-on – Exploring Chemical Diversity with Molecular Networks

Pieter C. Dorrestein and Mingxun Wang
Download URL: <https://tinyurl.com/2z8n5k93>

1

Samples Background

MassIVE MSV000088828 Partial Public

GNPS - Nicotinamide Adenine Dinucleotide Biosynthetic Impairment and Urinary Metabolomic Alterations Observed in Hospitalized Adults With COVID-19

[Subscribe](#) [Comment](#) [Convert Spectra](#) [Reanalyze Spectra](#) [Add Reanalysis](#)

Description

Nicotinamide Adenine Dinucleotide Biosynthetic Impairment and Urinary Metabolomic Alterations Observed in Hospitalized Adults With COVID-19 Nicotinamide Adenine Dinucleotide Biosynthetic Impairment and Urinary Metabolomic Alterations Observed in Hospitalized Adults With COVID-19 Nicotinamide Adenine Dinucleotide Biosynthetic Impairment and Urinary Metabolomic Alterations Observed in Hospitalized Adults With COVID-19 [doi:10.25345/C53P23] [dataset license: [CC0 1.0 Universal \(CC0 1.0\)](#)]

Keywords: Metabolomics

Contact

Principal Investigators: Stephen Barnes, University of Alabama, USA
(in alphabetical order)
Submitting User: [mwang87](#)

Number of Files: 60
Total Size: 15.40 GB
Subscribers: 1

Owner Reanalyses

Identification Results

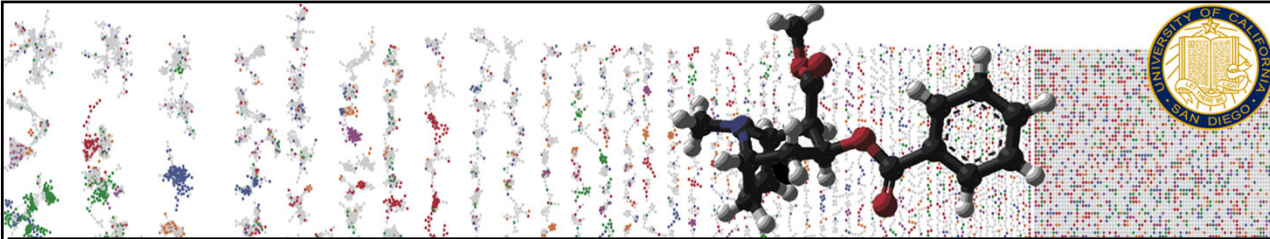
Proteins (Reported):	1	N/A	N/A
Peptides:	1	N/A	N/A
Variant Peptides:	1	N/A	N/A
PSMs:	1	N/A	N/A

[Browse Dataset Files](#)

[Browse Metadata](#)


Raines et al. 2021


2



**GNPS Classic Molecular Networking Job Submission
HANDS ON**

**Ming Wang, Pieter Dorrestein, University of California San
Diego**



 @Pdorrestein1
<https://dorresteinlab.ucsd.edu/>

3

Outline for today

- Submit a molecular networking job (Hands-on, Pieter).
- Explanation of what was just submitted (Pieter).
- Exploring the molecular network (Ming).
- GNPS dashboard for inspecting the data (Ming).
- MASST (If we have time, Pieter)

4

Outline for today

- **Submit a molecular networking job (Hands-on, Pieter).**
- Explanation of what was just submitted (Pieter).
- Exploring the molecular network (Ming).
- GNPS dashboard for inspecting the data (Ming).
- MASST (If we have time, Pieter)

5

Go to GNPS (gnps.ucsd.edu)

GNPS: Global Natural Products Social Molecular Network

MassIVE Datasets | Documentation | Forum | Contact

Please Login to Analyze Data at GNPS

Login to Existing Account Register New Account

GNPS

GNPS is a web-based mass spectrometry ecosystem that aims to be an open-access knowledge base for community-wide organization and sharing of raw, processed, or annotated fragmentation mass spectrometry data (MS/MS). GNPS aids in identification and discovery throughout the entire life cycle of data, from initial data acquisition/analysis to post publication.

Tweets by @GNPS_UCSD

GNPS - UC San Diego Retweeted
@NatureBiotech

High-confidence structural annotation of metabolites absent from spectral libraries
go.nature.com/9aD5jy

6

Create an Account (If you don't have one already)

Please Login to Analyze Data at GNPS

Login to Existing Account

Register New Account

Username	<input type="text"/>
Name	<input type="text"/>
Organization	<input type="text"/>
Email	<input type="text"/>
Password	<input type="password"/>
	<input type="password"/> (confirmation)
	<input type="submit" value="submit"/>

7

Select Molecular Networking

Data Analysis

Molecular Networking Organize Spectra by Family Visualize Large Datasets Discover New Molecules <input type="button" value="Create Molecular Network"/> <input type="button" value="Help"/>	Library Search High-Throughput Dereplication Comprehensive MS/MS Libraries Find Analogs of Knowns <input type="button" value="Match Libraries"/> <input type="button" value="Help"/>	Molecular BLAST Put Spectrum in Context Query Across Public Spectra Infer Metadata of Spectrum <input type="button" value="Query Spectrum"/> <input type="button" value="Help"/>
---	--	--

8

Select Molecular Networking

Molecular Networking

Organize Spectra by Family
Visualize Large Datasets
Discover New Molecules

Create Molecular Network

Help

GNPS: Global Natural Products Social Molecular Networking
Logout | My User | Update Profile | Jobs | MassIVE Datasets | Documentation | Forum | Contact

Workflow Selection
Search Protocol: [Reset Form](#) [Save as Protocol](#)
Title:

Networking Parameter Presets
[Small Data Preset](#) [Medium Data Preset](#) [Big Data Preset](#)

Basic Options
Spectrum files must be centroided and be in an open spectrum format (mzXML, mzML, or mgf)
[See here for further documentation about molecular networking.](#)
[Click Here here to run a demo molecular network.](#)

Spectrum Files (Required): [Select Input Files](#)
Spectrum Files G2: [Select Input Files](#)
Spectrum Files G3: [Select Input Files](#)
Spectrum Files G4: [Select Input Files](#)
Spectrum Files G5: [Select Input Files](#)
Spectrum Files G6: [Select Input Files](#)
[For custom group/attribute documentation click here](#)

Precursor Ion Mass Tolerance: Da Fragment Ion Mass Tolerance: Da

9

Select Molecular Networking

Molecular Networking

Organize Spectra by Family
Visualize Large Datasets
Discover New Molecules

Create Molecular Network

Help

GNPS: Global Natural Products Social Molecular Networking
Logout | My User | Update Profile | Jobs | MassIVE Datasets | Documentation | Forum | Contact

Workflow Selection
Search Protocol: [Reset Form](#) [Save as Protocol](#)
Title:

Networking Parameter Presets
[Small Data Preset](#) [Medium Data Preset](#) [Big Data Preset](#)

Basic Options
Spectrum files must be centroided and be in an open spectrum format (mzXML, mzML, or mgf)
[See here for further documentation about molecular networking.](#)
[Click Here here to run a demo molecular network.](#)

Spectrum Files (Required): [Select Input Files](#)
Spectrum Files G2: [Select Input Files](#)
Spectrum Files G3: [Select Input Files](#)
Spectrum Files G4: [Select Input Files](#)
Spectrum Files G5: [Select Input Files](#)
Spectrum Files G6: [Select Input Files](#)
[For custom group/attribute documentation click here](#)

Precursor Ion Mass Tolerance: Da Fragment Ion Mass Tolerance: Da

10

CCMS ProteoSAFe File/Resource Manager

gnps.ucsd.edu/ProteoSAFe/upload.jsp

Select Input Files | Upload Files | Share Files

Select Input File

Spectrum Files G1
Spectrum Files G2
Spectrum Files G3
Spectrum Files G4
Spectrum Files G5
Spectrum Files G6
Metadata File
Group Mapping (Legacy)
Attribute Mapping (Legacy)
Library Files
STL Model for iti

Selected Files

Selected Spectrum Files G1
Selected Spectrum Files G2
Selected Spectrum Files G3
Selected Spectrum Files G4
Selected Spectrum Files G5
Selected Spectrum Files G6
Selected Metadata File
Selected Group Mapping (Legacy)
Selected Attribute Mapping (Legacy)
Selected Library Files
speclibs
Selected STL Model for iti

Clear Selection | Finish Selection

[Task 383f...] - "Drug metabolism ASM Microbe Demo 3 ions 0.6"
[Task 86be...] - "Hodskins"
CCMS_ProteomeDatabases
CCMS_School_2019
CCMS_SpectralLibraries
[Dataset MSV000081098] - "GNPS Drug Metabolism Demo Data"
[Dataset MSV000081344] - "GNPS - SEED - Palmer"
[Dataset MSV000081486] - "GNPS - Malawi Legume Study"
[Dataset MSV000082374] - "GNPS_Nobel_twin_study"
[Dataset MSV000082406] - "GNPS Pediatric CF samples"
[Dataset MSV000082802] - "GNPS Bile Acid Bioreactor Samples"
[Dataset MSV000083357] - "GNPS - Pitt Hopkins"
[Dataset MSV000083666] - "GNPS - SEED - Perez-Lopez Mouse Fecal Samples"
[Dataset MSV000084322] - "GNPS - Postmortem interval prediction using metabolomics - Skin samples during decomposition "

Folders in your space

11

Select Input Files | Upload Files | Share Files

Share Files With User

Share

Import Data Share

Import

Shared Users

Imported Data Shares

[Dataset MSV000081098] - "GNPS Drug Metabolism Demo Data"
[Dataset MSV000081344] - "GNPS - SEED - Palmer"
[Dataset MSV000081486] - "GNPS - Malawi Legume Study"
[Dataset MSV000082374] - "GNPS_Nobel_twin_study"
[Dataset MSV000082406] - "GNPS Pediatric CF samples"
[Dataset MSV000082802] - "GNPS Bile Acid Bioreactor Samples"
[Dataset MSV000083357] - "GNPS - Pitt Hopkins"
[Dataset MSV000083666] - "GNPS - SEED - Perez-Lopez Mouse Fecal Samples"
[Dataset MSV000084322] - "GNPS - Postmortem interval prediction using metabolomics - Skin samples during decomposition "
[Dataset MSV000084475] - "GNPS-Human-associated bacteria cultured with bile acids"
[Dataset MSV000084847] - "Circadian_IHC_ApoE_KO_mice_acute_study"
[Dataset MSV000086109] - "GNPS - Moorena bouillonii extracts"
[Dataset MSV000086415] - "GNPS ROSMAP - U19-600 LCMS Metabolomics Sample Cohort"
[Dataset MSV000086889] - "GNPS Fecal Cultures with Microbially Conjugated Bile Acids"
[Dataset MSV000086989] - "GNPS_NIST_Human_Fecal_Material_Standards_Positive_Polarity"
[Dataset MSV000087087] - "GNPS_U19_BEAM-Wake_Forest_Metabolomic_Samples"
[Dataset MSV000087562] - "GNPS_Pooled fecal samples from iHMP2 dataset"
[Dataset MSV000087790] - "GNPS Undernourished Mouse Metabolomics Protein Restriction"

Datasets you have imported into your space

12

Select Input Files Upload Files **Share Files**


Share Files With User Share

Import Data Share Import

Shared Users

Imported Data Shares

[Dataset MSV000081098] - "GNPS Drug Metabolism Demo Data"
 [Dataset MSV000081344] - "GNPS - SEED - Palmer"
 [Dataset MSV000081486] - "GNPS - Malawi Legume Study"
 [Dataset MSV000082374] - "GNPS_Nobel_twin_study"
 [Dataset MSV000082406] - "GNPS Pediatric CF samples"
 [Dataset MSV000082802] - "GNPS Bile Acid Bioreactor Samples"
 [Dataset MSV000083357] - "GNPS - Pitt Hopkins"
 [Dataset MSV000083666] - "GNPS - SEED - Perez-Lopez Mouse Fecal Samples"
 [Dataset MSV000084322] - "GNPS - Postmortem interval prediction using metabolomics - Skin samples during decomposition"
 [Dataset MSV000084475] - "GNPS-Human-associated bacteria cultured with bile acids"
 [Dataset MSV000084847] - "Circadian_IHC_ApoE_KO_mice_acute_study"
 [Dataset MSV000086109] - "GNPS - Moorena bouillonii extracts"
 [Dataset MSV000086415] - "GNPS ROSMAP - U19-600 LCMS Metabolomics Sample Cohort"
 [Dataset MSV000086889] - "GNPS Fecal Cultures with Microbially Conjugated Bile Acids"
 [Dataset MSV000086989] - "GNPS_NIST_Human_Fecal_Material_Standards_Positive_Polarity"
 [Dataset MSV000087087] - "GNPS_U19_BEAM-Wake_Forest_Metabolomic_Samples"
 [Dataset MSV000087562] - "GNPS_Pooled fecal samples from iHMP2 dataset"
 [Dataset MSV000087790] - "GNPS Undernourished Mouse Metabolomics Protein Restriction"

Datasets you have imported into your space 

13

Select Input Files Upload Files **Share Files**


Share Files With User Share

Import Data Share Import

Shared Users

Imported Data Shares

[Dataset MSV000081098] - "GNPS Drug Metabolism Demo Data"
 [Dataset MSV000081344] - "GNPS - SEED - Palmer"
 [Dataset MSV000081486] - "GNPS - Malawi Legume Study"
 [Dataset MSV000082374] - "GNPS_Nobel_twin_study"
 [Dataset MSV000082406] - "GNPS Pediatric CF samples"
 [Dataset MSV000082802] - "GNPS Bile Acid Bioreactor Samples"
 [Dataset MSV000083357] - "GNPS - Pitt Hopkins"
 [Dataset MSV000083666] - "GNPS - SEED - Perez-Lopez Mouse Fecal Samples"
 [Dataset MSV000084322] - "GNPS - Postmortem interval prediction using metabolomics - Skin samples during decomposition"
 [Dataset MSV000084475] - "GNPS-Human-associated bacteria cultured with bile acids"
 [Dataset MSV000084847] - "Circadian_IHC_ApoE_KO_mice_acute_study"
 [Dataset MSV000086109] - "GNPS - Moorena bouillonii extracts"
 [Dataset MSV000086415] - "GNPS ROSMAP - U19-600 LCMS Metabolomics Sample Cohort"
 [Dataset MSV000086889] - "GNPS Fecal Cultures with Microbially Conjugated Bile Acids"
 [Dataset MSV000086989] - "GNPS_NIST_Human_Fecal_Material_Standards_Positive_Polarity"
 [Dataset MSV000087087] - "GNPS_U19_BEAM-Wake_Forest_Metabolomic_Samples"
 [Dataset MSV000087562] - "GNPS_Pooled fecal samples from iHMP2 dataset"
 [Dataset MSV000087790] - "GNPS Undernourished Mouse Metabolomics Protein Restriction"

MSV000088828 

14

The screenshot shows a file selection interface with two main panels: "Select Input Files" and "Selected Files".

Select Input Files:

- Spectrum Files G1
- Spectrum Files G2
- Spectrum Files G3
- Spectrum Files G4
- Spectrum Files G5
- Spectrum Files G6
- Metadata File
- Group Mapping (Legacy)
- Attribute Mapping (Legacy)
- Library Files
- STL Model for ili

Selected Files:

- Selected Spectrum Files G1
- Selected Spectrum Files G2
- Selected Spectrum Files G3
- Selected Spectrum Files G4
- Selected Spectrum Files G5
- Selected Spectrum Files G6
- Selected Metadata File
- Selected Group Mapping (Legacy)
- Selected Attribute Mapping (Legacy)
- Selected Library Files
- Selected STL Model for ili

Dataset List (Yellow Box):

- [Task 383f...] - "Drug metabolism ASM Microbe Demo 3 ions 0.6"
- [Task 86be...] - "Hodskins"
- CCMS_ProteomeDatabases
- CCMS_School_2019
- CCMS_SpectralLibraries
- [Dataset MSV000081098] - "GNPS Drug Metabolism Demo Data"
- [Dataset MSV000088137] - "GNPS U19_Wisconsin_Stool_Samples"
- [Dataset MSV000088335] - "GNPS - Foodomics - Workshop Dataset"
- [Dataset MSV000088570] - "GNPS In vitro cultured bacteria with or with bile salts"
- [Dataset MSV000088828] - "GNPS - Nicotinamide Adenine Dinucleotide Biosynthetic Impairment and Urinary Metabolomic Alterations Observed in Hospitalized Adults With COVID-19"
- ccms_metadata
- ccms_parameters
- peak
 - Neg_PooledSample_NEW MSMS repeat.mzML
 - Pos_PooledSample MSMS_1.mzML
- neg
- pos
- updates

Buttons: Clear Selection, Finish Selection

15

This screenshot is identical to the one above, but includes two orange arrows:

- An arrow pointing to "Spectrum Files G1" in the "Select Input Files" list.
- An arrow pointing to "Pos_PooledSample MSMS_1.mzML" in the "peak" sub-directory of the dataset list.

16

Select Input Files | Upload Files | Share Files

Select Input Files

Spectrum Files G1
Spectrum Files G2
Spectrum Files G3
Spectrum Files G4
Spectrum Files G5
Spectrum Files G6
Metadata File
Group Mapping (Legacy)
Attribute Mapping (Legacy)
Library Files
STL Model for ili

Selected Files

Selected Spectrum Files G1
MSV000088828/peak/Pos_PooledSample MSMS_1.mzML
Selected Spectrum Files G2
Selected Spectrum Files G3
Selected Spectrum Files G4
Selected Spectrum Files G5
Selected Spectrum Files G6
Selected Metadata File
Selected Group Mapping (Legacy)
Selected Attribute Mapping (Legacy)
Selected Library Files
speclibs
Selected STL Model for ili

Clear Selection | Finish Selection

[Task 383f...] - "Drug metabolism ASM Microbe Demo 3 ions 0.6"
[Task 86be...] - "Hodskins"
CCMS_ProteomeDatabases
CCMS_School_2019
CCMS_SpectralLibraries
[Dataset MSV000081098] - "GNPS Drug Metabolism Demo Data"
[Dataset MSV000088137] - "GNPS U19_Wisconsin_Stool_Samples"
[Dataset MSV000088335] - "GNPS - Foodomics - Workshop Dataset"
[Dataset MSV000088570] - "GNPS In vitro cultured bacteria with or with bile salts"
[Dataset MSV000088828] - "GNPS - Nicotinamide Adenine Dinucleotide Biosynthetic Impairment and Urinary Metabolomic Alterations Observed in Hospitalized Adults With COVID-19"
ccms_metadata
ccms_parameters
peak
Neg_PooledSample_NEW MSMS repeat.mzML
Pos_PooledSample MSMS_1.mzML
neg
pos
updates

17

Networking Parameter Presets

Small Data Preset | Medium Data Preset | Big Data Preset

Basic Options

Spectrum files must be centroided and be in an open spectrum format (mzXML, mzML, or mgf)

Spectrum Files (Required): Select Input Files | 1 file and 0 folders are selected | See here for further documentation about molecular networking.
Click Here here to run a demo molecular network.

Spectrum Files G2: Select Input Files
Spectrum Files G3: Select Input Files
Spectrum Files G4: Select Input Files
Spectrum Files G5: Select Input Files
Spectrum Files G6: Select Input Files | For custom group/attribute documentation click here

Precursor Ion Mass Tolerance: 0.1 Da | Fragment Ion Mass Tolerance: 0.1 Da

Advanced Network Options | Show Fields

Advanced Library Search Options | Show Fields

18

Basic Options

Spectrum files must be centroided and be in an open spectrum format (mzXML, mzML, or mgf)

Spectrum Files (Required): 1 file and 0 folders are selected [See here for further documentation about molecular networking.](#)

Spectrum Files G2: [Click Here here to run a demo molecular network.](#)

Spectrum Files G3:

Spectrum Files G4:

Spectrum Files G5:

Spectrum Files G6: [For custom group/attribute documentation click here](#)

Precursor Ion Mass Tolerance: Da Fragment Ion Mass Tolerance: Da

Advanced Network Options

Min Pairs Cos: Minimum Matched Fragment Ions: Maximum shift: Da

Network TopK: **Minimum Cluster Size:** Run MSCluster:

Maximum Connected Component Size:

Google Sheets Metadata URL (Experimental):

Metadata File:

Group Mapping (Legacy):

Attribute Mapping (Legacy):

Advanced Library Search Options

Spectral Library: 0 files and 1 folder are selected [To import libraries for search click here](#)

Library Search Min Matched Score Threshold:

Peaks:

Search Analogs: Maximum Analog Search Mass Difference:

19

Basic Options

Spectrum files must be centroided and be in an open spectrum format (mzXML, mzML, or mgf)

Spectrum Files (Required): 1 file and 0 folders are selected [See here for further documentation about molecular networking.](#)

Spectrum Files G2: [Click Here here to run a demo molecular network.](#)

Spectrum Files G3:

Spectrum Files G4:

Spectrum Files G5:

Spectrum Files G6: [For custom group/attribute documentation click here](#)

Precursor Ion Mass Tolerance: Da Fragment Ion Mass Tolerance: Da

Advanced Network Options

Min Pairs Cos: Minimum Matched Fragment Ions: Maximum shift: Da

Network TopK: **Minimum Cluster Size:** Run MSCluster:

Maximum Connected Component Size:

Google Sheets Metadata URL (Experimental):

Metadata File:

Group Mapping (Legacy):

Attribute Mapping (Legacy):

Advanced Library Search Options

Spectral Library: 0 files and 1 folder are selected [To import libraries for search click here](#)

Library Search Min Matched Score Threshold:

Peaks:

Search Analogs: Maximum Analog Search Mass Difference:

Workflow Submission

Email me at

20

Outline for today

- **Submit a molecular networking job (Hands-on, Pieter).**
- **Explanation of what was just submitted (Pieter).**
- Exploring the molecular network (Ming).
- GNPS dashboard for inspecting the data (Ming).
- MASST (If we have time, Pieter)

21

Mass spectral molecular networking of living microbial colonies

Jeramie Watrous^{a,b,c}, Patrick Roach^{d,1}, Theodore Alexandrov^{c,e}, Brandi S. Heath^d, Jane Y. Yang^{a,b,c}, Roland D. Kersten^{a,b,1}, Menno van der Voort^g, Kit Pogliano^h, Harald Grossⁱ, Jos M. Raaijmakers^g, Bradley S. Moore^{c,f}, Julia Laskin^{d,2}, Nuno Bandeira^{c,i,k,2}, and Pieter C. Dorrestein^{a,b,c,f,2}

Departments of ^aPharmacology and ^bChemistry and Biochemistry, University of California at San Diego, La Jolla, CA 92093; ^cPharmaceutical Sciences, University of California at San Diego, La Jolla, CA 92093; ^dDepartment of Microbiology and Immunobiology, Harvard Medical School, Boston, MA 02115; ^eDepartment of Chemistry, University of California at San Diego, La Jolla, CA 92093; ^fDepartment of Chemistry, University of California at San Diego, La Jolla, CA 92093; ^gDepartment of Microbiology, University of California at San Diego, La Jolla, CA 92093; ^hDepartment of Chemistry, University of California at San Diego, La Jolla, CA 92093; ⁱDepartment of Chemistry, University of California at San Diego, La Jolla, CA 92093; ^jDepartment of Chemistry, University of California at San Diego, La Jolla, CA 92093; ^kDepartment of Chemistry, University of California at San Diego, La Jolla, CA 92093

A massively spectacular view of the chemical lives of microbes

Matthew F. Traxler and Roberto Kolter¹

Sharing and community curation of mass spectrometry data with Global Natural Products Social Molecular Networking

Mingxun Wang, Jeremy J Carver, Vanessa V Phelan, Laura M Sanchez, Neha Garg, Yao Peng, Don Duy Nguyen, Jeramie Watrous, Clifford A Kapon, Tal Luzzatto-Knaan, Carla Porto, Amin...

Electrospray → MS Inlet → Tandem MS Spectra

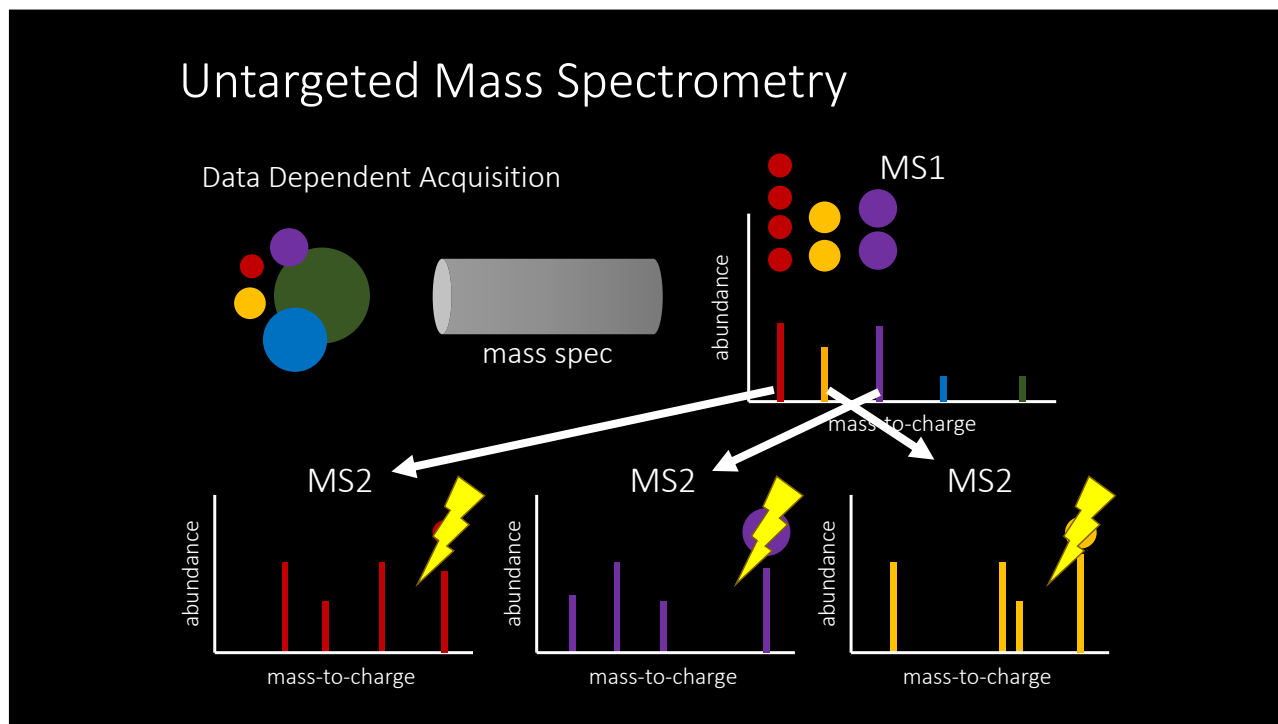
2' Capillary

MS Inlet

Tandem MS Spectra

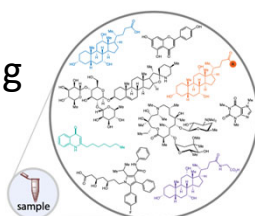
22

Untargeted Mass Spectrometry



23

Molecular Networking



24

Molecular Networking



Robert Quinn

nature

Explore content ▾ About the journal ▾ Publish with us ▾ Subscribe

nature > articles > article

Article | Published: 26 February 2020

Global chemical effects of the microbiome include new bile-acid conjugations

Robert A. Quinn, Alexey V. Melnik, ... Pieter C. Dorrestein ✉ + Show authors

Nature 579, 123–129 (2020) | Cite this article

How much does the microbiome impact the chemistry of the host?

25

Molecular Networking

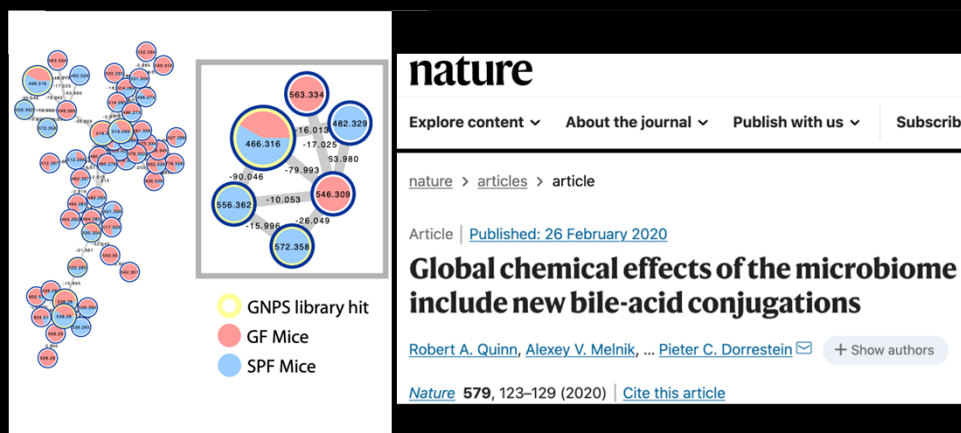
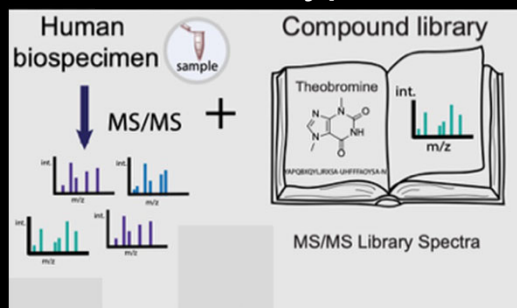


Figure from Aron, Gentry Nature Protocols 2020

26

Growing public reference libraries
(>620,000 public ref spectra) can be
used to hypothesize the structure.



5%
Annotated
(10% human)



Julia Gauglitz and Kiana West Wang et al Nature Biotech. 2016, Bauemeister et al, Microbiome Metabolomics Nature Micro. Reviews, 2021

27

Molecular Networking

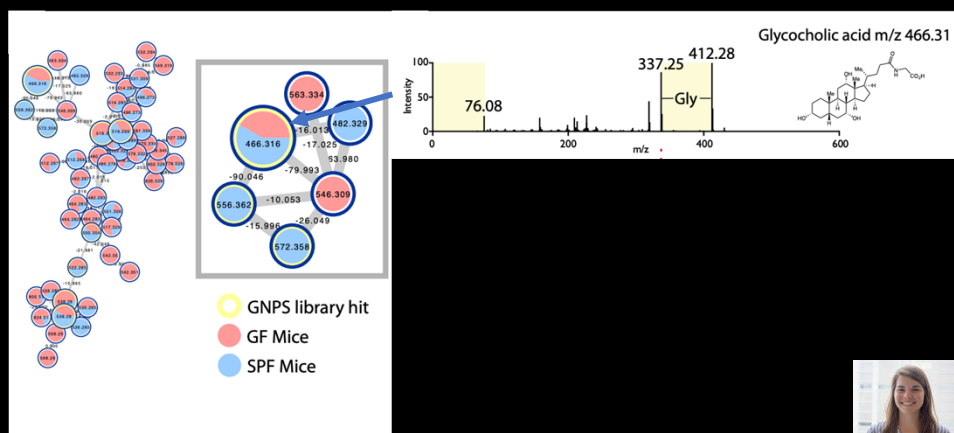


Figure by
Emily
Gentry

Figure from Aron, Gentry Nature Protocols 2020

28

Molecular Networking

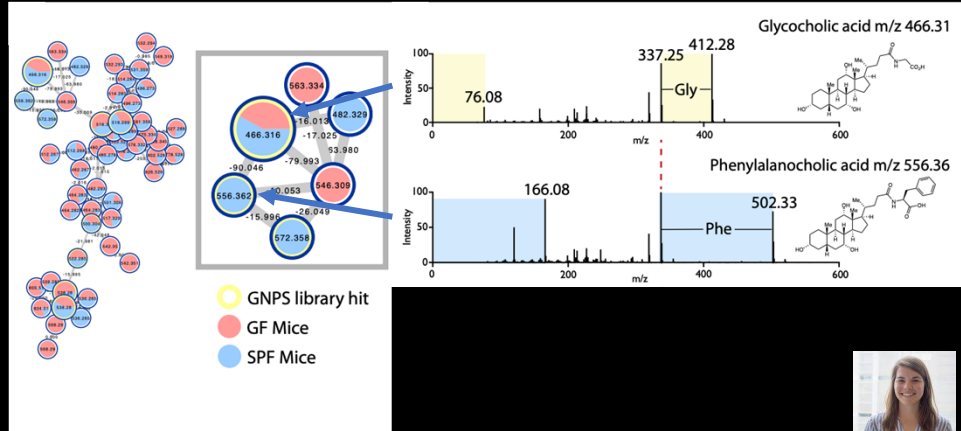


Figure by
Emily
Gentry

Figure from Aron, Gentry Nature Protocols 2020

29

Molecular Networking



UniMod-

https://www.unimod.org/modifications_list.php?a=search&value=1&SearchFor=15.99&SearchOption=Contains&SearchField=

Curated list of delta masses (we don't vouch for accuracy so use your thinking caps).

https://docs.google.com/spreadsheets/d/1RbhwM8KPUUBTrppcYrKp5hs8B_ZPJkxO-WcyHDoU074/edit#gid=566878567

Figure from Aron, Gentry Nature Protocols 2020

30

Molecular Networking

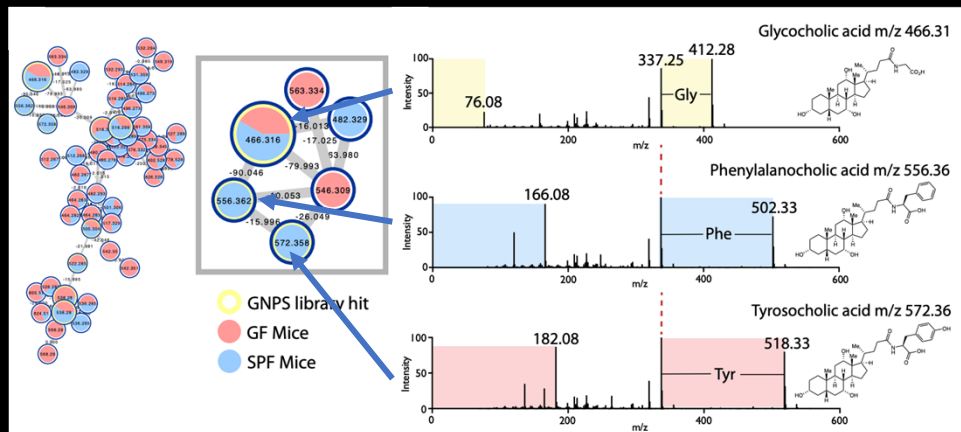


Figure from Aron, Gentry Nature Protocols 2020

31

From untargeted data to chemicals

1,894,519 MS² spectra



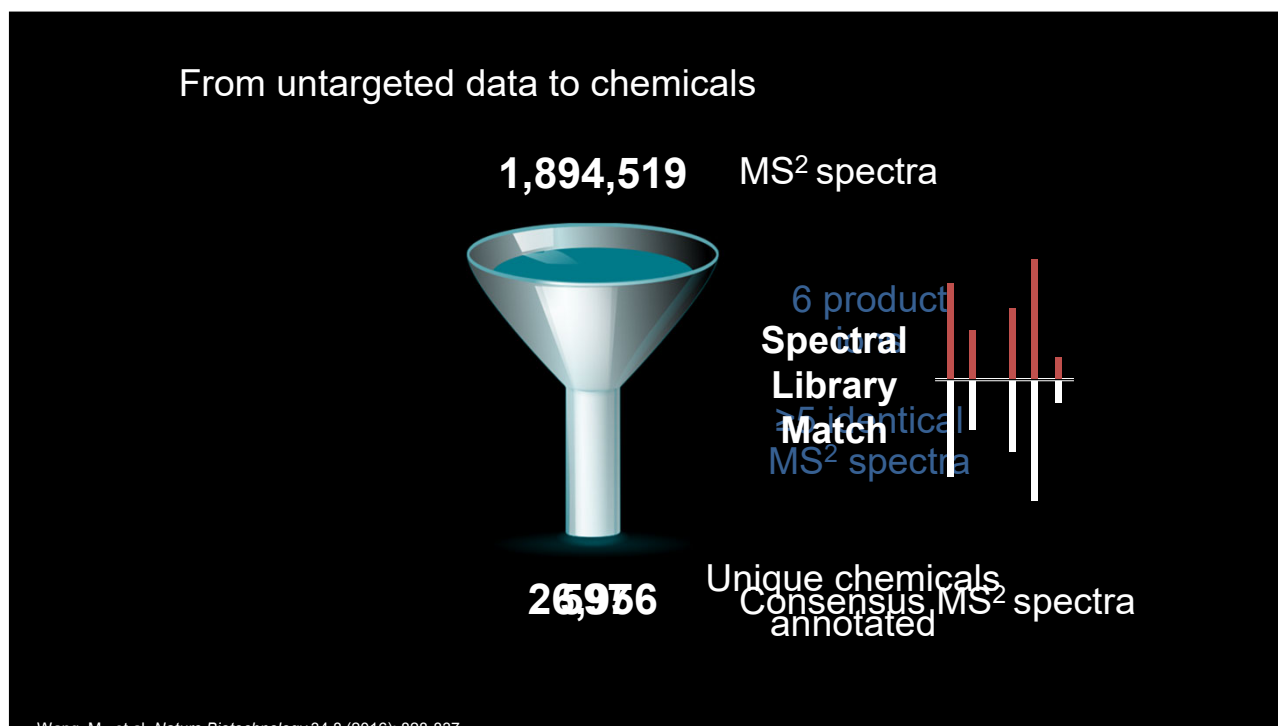
6 product ions

≥5 identical MS² spectra

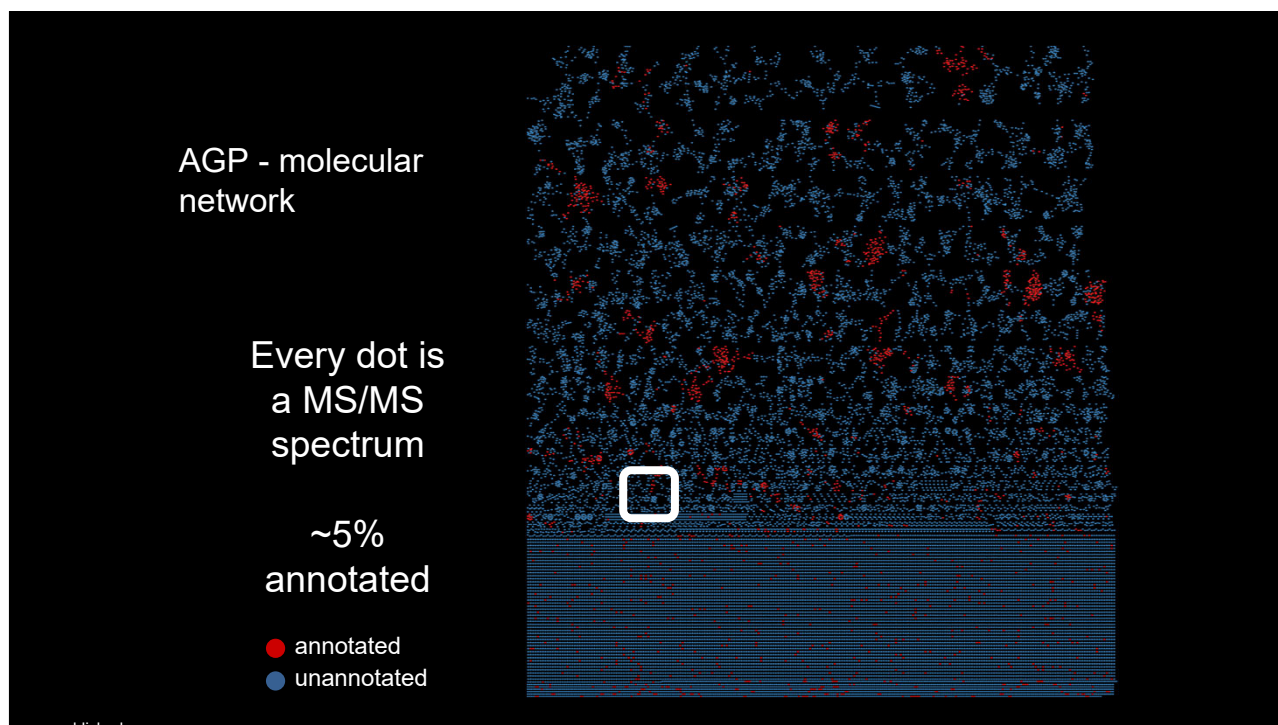
26,956 Consensus MS² spectra

Wang, M. et al. Nature Biotechnology 34, 8 (2016): 828-837

32

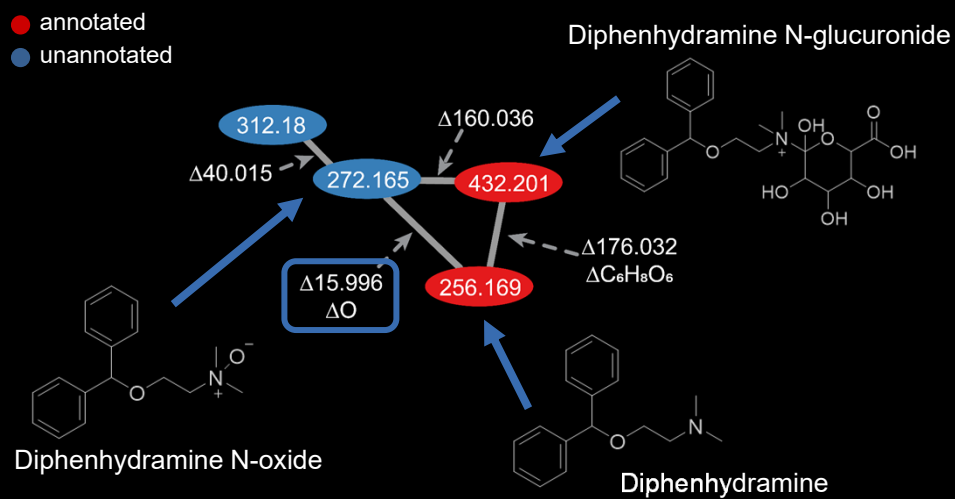


33



34

Identifying unknowns using molecular networking



35

5 min break

Before we analyze the submitted job!

36

Outline for today

- Submit a molecular networking job (Hands-on, Pieter).
- Explanation of what was just submitted (Pieter).
- Exploring the molecular network (Ming).
- GNPS dashboard for inspecting the data (Ming).
- MASST (If we have time, Pieter)

[Catch up Link](#) - In case the MN failed for anyone.

37

Ming will carry you through the analysis.



[Back to main page](#)

Total: 331 jobs, occupying 41.91 GB of storage space (0 bytes in 0 protected jobs)

ProteoSAFe Workflow Tasks

Hits 1 - 30 out of 331

Go to

Go

[Select columns](#)

Apply Filters	Description	User	Workflow	Workflow Version	Status	Protected	Create Time	Total
<input type="checkbox"/>	Select All	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="text"/>	<input type="checkbox"/>
<input type="checkbox"/>	Steve Barnes Class Pooled Test - min cluster 1 - Positive Only [5] ID=f9d55f2e4c4a4d63bdd9f1270fc98bcc	workshop	METABOLOMICS-SNETS-V2	release_30	DONE	<input type="checkbox"/> 0	Feb. 15, 2022, 3:04 PM	0
<input type="checkbox"/>	foodMASST Analysis Cumarin cosine 0.8 ID=3d5bbaef692e4a32b844edbb36718f86	workshop	SEARCH_SINGLE_SPECTRUM	release_29	DONE	<input type="checkbox"/> 0	Feb. 14, 2022, 4:09 PM	5
<input type="checkbox"/>	CURCUMIN second version ID=15c69657eb83452c9ecc134bec2c6122	workshop	SEARCH_SINGLE_SPECTRUM	release_29	DONE	<input type="checkbox"/> 0	Feb. 14, 2022, 3:54 PM	5
<input type="checkbox"/>	foodMASST Analysis Cumarin second version ID=ec671ce0c17742a19d0b17000c4eeaae	workshop	SEARCH_SINGLE_SPECTRUM	release_29	DONE	<input type="checkbox"/> 0	Feb. 14, 2022, 3:54 PM	5
<input type="checkbox"/>	foodMASST Analysis Cumarin ID=70edaf08c9b84fc6b90bff595f1fa904	workshop	SEARCH_SINGLE_SPECTRUM	release_29	DONE	<input type="checkbox"/> 0	Feb. 14, 2022, 3:51 PM	6
<input type="checkbox"/>	CURCUMIN	workshop	SEARCH_SINGLE_SPECTRUM	release_29	DONE	<input type="checkbox"/> 0	Feb. 14, 2022,	6

[Catch up Link](#) - In case the MN failed for anyone.

38

Job Status	
Workflow	METABOLOMICS-SNETS-V2 (version release_30)
	<p>DONE [Clone] [Clone to Latest Version] [Restart][Delete]</p> <p>Default Molecular Networking Results Views [View All Library Hits] [View Unique Library Compounds] [View All Clusters With IDs] [File Summaries]</p> <p>Network Visualizations [View Spectral Families (In Browser Network Visualizer)] [Network Summarizing Graphs]</p> <p>Methods and Citation for Manuscripts [Workflow Written Description]</p> <p>Export/Download Network Files [Download Clustered Spectra as MGF] [Download GraphML for Cytoscape] [Download Bucket Table] [Download BioM For Qiime/Qiita] [Download Metadata For Qiime] [Download Ili Data]</p> <p>Advanced Views - Metadata Views [View Metadata]</p> <p>Status</p> <p>Advanced Views - Global Public Dataset Matches [View Matches to All Public Datasets]</p> <p>Advanced Views - External Visualization [View Ili in GNPS] [Direct Cytoscape Preview/Download] [Visualize with Upset Plots (Beta)]</p> <p>Advanced Views - Networking Graphs/Histograms [Nodes, MZ Histogram] [Edges, MZ Delta Histogram] [Edges, Score vs MZ Delta Plot] [Library Search, PPM Error Histogram]</p> <p>Advanced Views - Misc Views [View Network, Node Centric] [View Network Pairs] [Networking Statistics] [View Raw/Unclustered Spectra] [View Compounds and File Occurrence]</p> <p>Advanced Views - Make Dataset Public [Make Public Dataset Documentation] [Make Dataset Public Direct Link]</p> <p>Advanced Views - Experimental Views [Analyze with MS2LDA] [Enhance with MolNetEnhancer] [Global Comparison with ReDU PCA] [Annotate with DEREPLICATOR] [Annotate with DEREPLICATOR+] [Network with Spec2vec]</p> <p>Advanced Views - qiime2 Views [View qiime2 Emperor Plots] [Download qiime2 Emperor qzv] [Download qiime2 features biom qza]</p>

39

Let's Explore What Molecules are in these Urine Sample

Job Status	
Workflow	METABOLOMICS-SNETS-V2 (version release_30)
	<p>DONE [Clone] [Clone to Latest Version] [Restart][Delete]</p> <p>Default Molecular Networking Results Views [View All Library Hits] [View Unique Library Compounds] [View All Clusters With IDs] [File Summaries]</p> <p>Network Visualizations [View Spectral Families (In Browser Network Visualizer)] [Network Summarizing Graphs]</p> <p>Methods and Citation for Manuscripts [Workflow Written Description]</p> <p>Export/Download Network Files [Download Clustered Spectra as MGF] [Download GraphML for Cytoscape] [Download Bucket Table] [Download BioM For Qiime/Qiita] [Download Metadata For Qiime] [Download Ili Data]</p> <p>Advanced Views - Metadata Views [View Metadata]</p> <p>Status</p> <p>Advanced Views - Global Public Dataset Matches [View Matches to All Public Datasets]</p> <p>Advanced Views - External Visualization [View Ili in GNPS] [Direct Cytoscape Preview/Download] [Visualize with Upset Plots (Beta)]</p> <p>Advanced Views - Networking Graphs/Histograms [Nodes, MZ Histogram] [Edges, MZ Delta Histogram] [Edges, Score vs MZ Delta Plot] [Library Search, PPM Error Histogram]</p> <p>Advanced Views - Misc Views</p>

40

Let's see if any drugs are being detected

Steve Barnes Class Pooled Test - min cluster 1 - Positive Only [5] Hits 1 ~ 1 out of 1 Go to Go

Select columns

Apply Filters	ViewLib	Explore	Compound Name	ClusterIdx	View All Spectra	Library Class
Filter By:	<input type="text"/>	<input type="text"/>	<input type="text" value="desv"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>
View Mirror Match USI Links 1	ViewLib	Explore Molecule in 0 Files and 0 Datasets	<p>desv</p> <p>Massbank:EA105309 O-desmethylvenlafaxine Desvenlafaxine 4-[2-(dimethylamino)-1-(1-hydroxycyclohexyl)ethyl]phenol</p>	483	View Raw Spectra	Bronze



Desmethylvenlafaxine is an antidepressant

41

Let's compare this to GNPS MS/MS Reference Spectrum

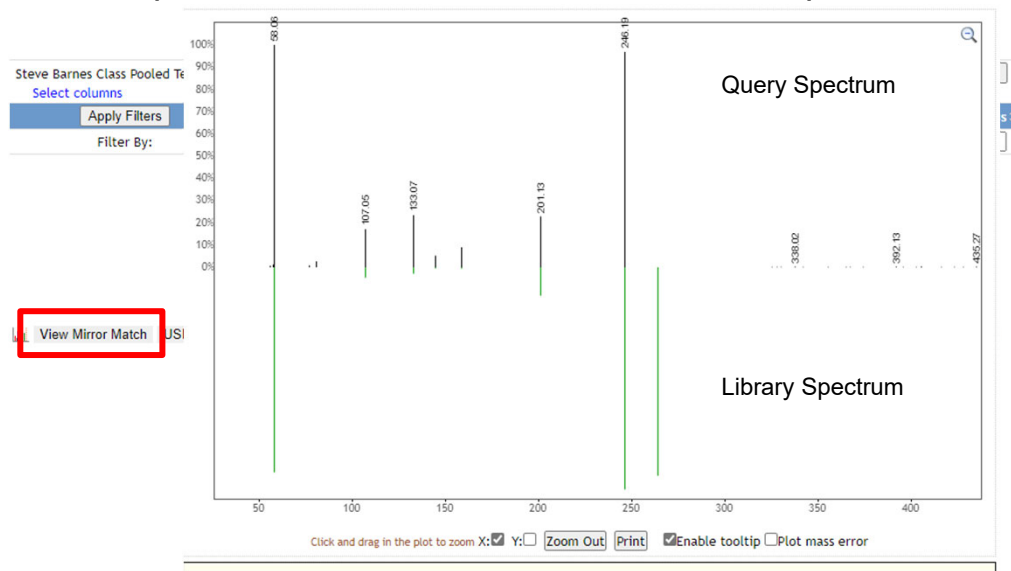
Steve Barnes Class Pooled Test - min cluster 1 - Positive Only [5] Hits 1 ~ 1 out of 1 Go to Go

Select columns

Apply Filters	ViewLib	Explore	Compound Name	ClusterIdx	View All Spectra	Library Class
Filter By:	<input type="text"/>	<input type="text"/>	<input type="text" value="desv"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>
View Mirror Match USI Links 1	ViewLib	Explore Molecule in 0 Files and 0 Datasets	<p>Massbank:EA105309 O-desmethylvenlafaxine Desvenlafaxine 4-[2-(dimethylamino)-1-(1-hydroxycyclohexyl)ethyl]phenol</p>	483	View Raw Spectra	Bronze

42

Let's compare this to GNPS MS/MS Reference Spectrum



43

Let's explore potential analogs of Desmethylvenlafaxine

Back to main page [Back to status page](#)

Steve Barnes Class Pooled Test - min cluster 1 - Positive Only [5] Hits 1 ~ 1 out of 1 Go to

Select columns

Apply Filters	ViewLib	Explore	Compound_Name	ClusterIdx
Filter By:			desv	
View Mirror Match	USI Links 1	ViewLib	Massbank:EA105309 O-desmethylvenlafaxine Desvenlafaxine 4-[2-(dimethylamino)-1-(1-hydroxycyclohexyl)ethyl]phenol	483

44

Let's explore potential analogs of Desmethylvenlafaxine

Job Status

Workflow: METABOLOMICS-SNETS-V2 (version [release_30](#))

DONE
[\[Clone\]](#) [\[Clone to Latest Version\]](#) [\[Restart\]](#) [\[Delete\]](#)

Default Molecular Networking Results Views
[\[View All Library Hits \]](#) [\[View Unique Library Compounds \]](#) [\[View All Clusters With IDs \]](#) [\[File Summaries \]](#)

Network Visualizations
[\[View Spectral Families \(In Browser Network Visualizer\) \]](#) [\[Network Summarizing Graphs \]](#)

Methods and Citation for Manuscripts
[\[Workflow Written Description \]](#)

Export/Download Network Files
[\[Download Clustered Spectra as MGF \]](#) [\[Download GraphML for Cytoscape \]](#) [\[Download Bucket Table \]](#) [\[Download BioM For Otime/Qiita \]](#)
[\[Download Metadata For Otime \]](#) [\[Download Ili Data \]](#)

Advanced Views - Metadata Views
[\[View Metadata \]](#)

<https://gnps.ucsd.edu/ProteoSAFe/status.jsp?task=f9d55f2e4c4a4d63bbd9f1270fc98bcc>

45

Let's explore potential analogs of Desmethylvenlafaxine

Steve Barnes Class Pooled Test - min cluster 1 - Positive Only [5] Hits 1 - 1 out of 1 Go to Go

Select columns

Apply Filters	Visualize Network	View Network Nodes	NodeCount	%ID	#Spectra	desv
Filter By: <input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text" value="desv"/>
1	Visualize Network	Network Nodes	4	0.250	6	Show

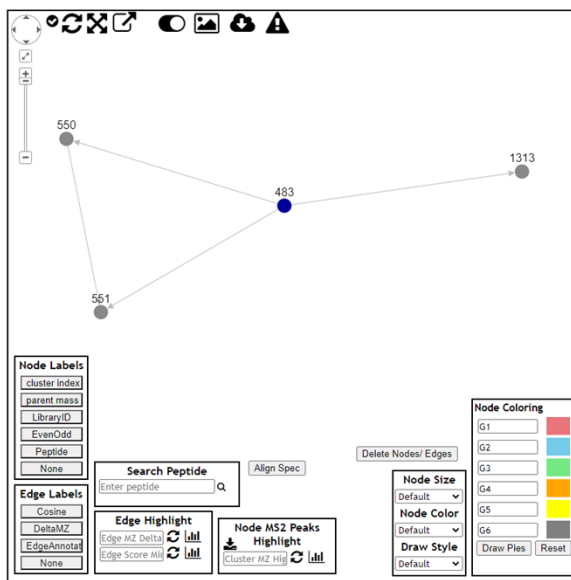
desv

[Catch up Link](#)

46

Let's explore potential analogs of Desmethylvenlafaxine

- Each Circle (node) is a molecule in data
- Blue nodes are identified to known compounds
- Connected nodes mean similar MS/MS fragmentation



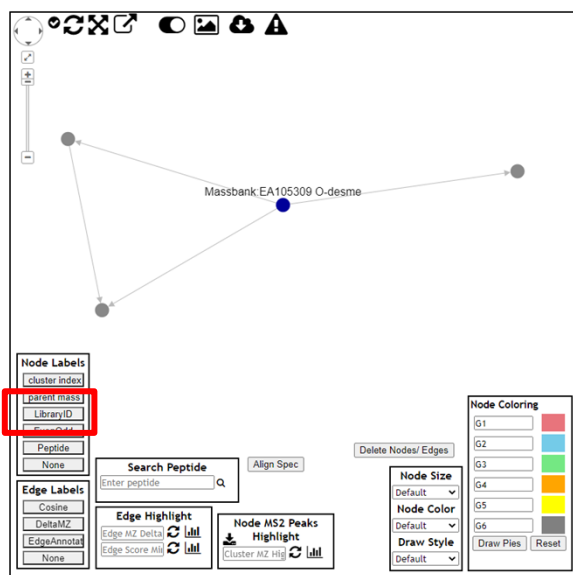
[Catch up Link](#)

47

Let's explore potential analogs of Desmethylvenlafaxine

Show the Library ID for the network

We can see it is Desvenlafaxine



[Catch up Link](#)

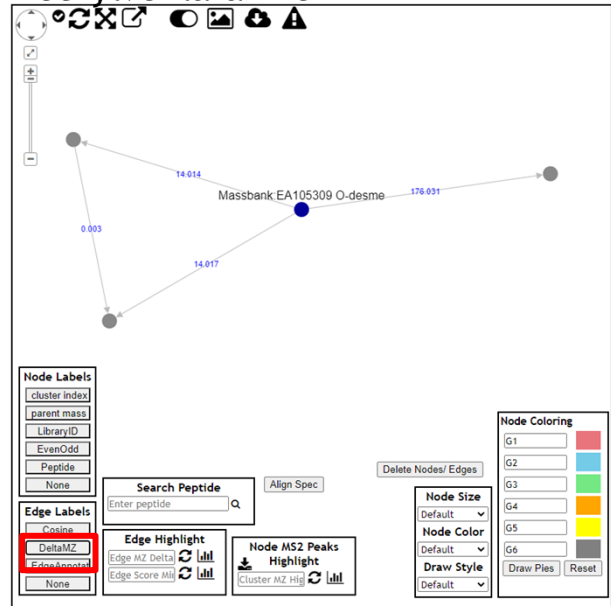
48

Let's explore potential analogs of Desmethylvenlafaxine

Show the mass deltas to putative analogs

Can you explain what these mass deltas could mean?

[Catch up Link](#)



49

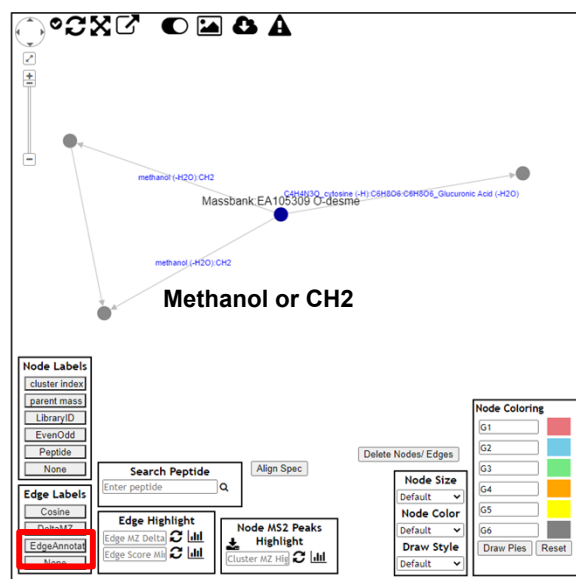
Let's explore potential analogs of Desmethylvenlafaxine

Show the mass deltas to putative analogs

Can you explain what these mass deltas could mean?

We try to help with that by curating a common but not exhaustive list of potential modifications. Could also be multiple options for you to decide what makes sense biologically and chemically.

[Catch up Link](#)

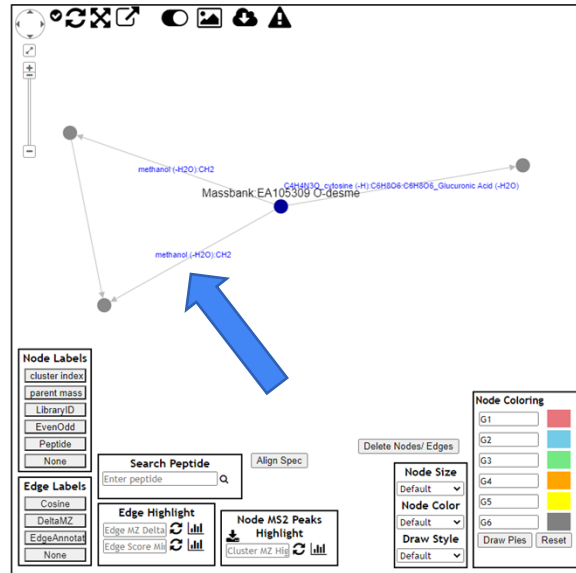


50

Let's explore potential analogs of Desmethylvenlafaxine

Let's inspect the MS/MS spectra!

[Catch up Link](#)

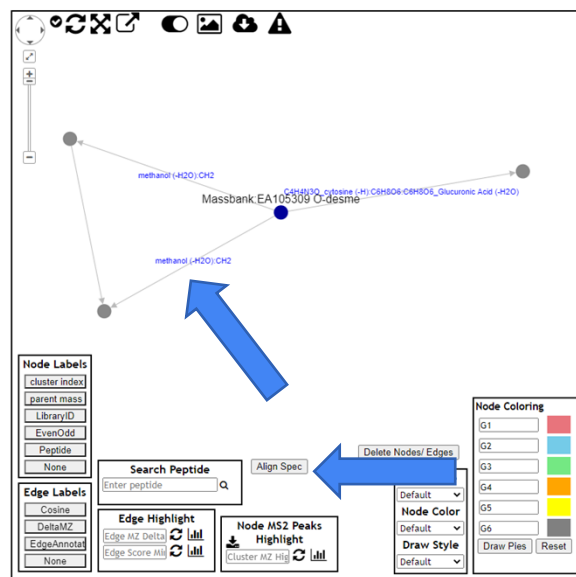


51

Let's explore potential analogs of Desmethylvenlafaxine

Let's inspect the MS/MS spectra!

[Catch up Link](#)



52

Let's explore p

Blue peaks shifted
Red peaks same

Click and drag in the plot to zoom X: Y: Zoom Out Enable tooltip
 Plot mass error

cluster index 483
parent mass 264.197
LibraryID Massbank:EA105309 O-d
number of spectra 2
DefaultGroups G1
precursor charge 0
Peptide
RT Info 186.78, $\sigma = 0.35$
ClusterSpectra [Cluster Spectra](#)

cluster index 551
parent mass 278.214
LibraryID N/A
number of spectra 1
DefaultGroups G1
precursor charge 0
Peptide
RT Info 235.51, $\sigma = 0.00$
ClusterSpectra [Cluster Spectra](#)

Node Coloring
G1
G2
G3
G4
G5
G6
Default
Draw Style

53

Explore endogenous molecule - Carnitines

Job Status

Workflow METABOLOMICS-SNETS-V2 (version [release_30](#))

DONE
[Clone] [Clone to Latest Version] [Restart][Delete]

Default Molecular Networking Results Views
[View All Library Hits] [View Unique Library Compounds] [View All Clusters With IDs] [File Summaries]

Network Visualizations
[View Spectral Families (In Browser Network Visualizer)] [Network Summarizing Graphs]

Methods and Citation for Manuscripts
[Workflow Written Description]

Export/Download Network Files
[Download Clustered Spectra as MGF] [Download GraphML for Cytoscape] [Download Bucket Table] [Download BioM For Qiime/Qiita]
[Download Metadata For Qiime] [Download Iii Data]

Advanced Views - Metadata Views
[View Metadata]

[Catch up Link](#)

54

Explore endogenous molecule - Carnitines

Steve Barnes Class Pooled Test - min cluster 1 - Positive Only [5] Hits 1 - 1 out of 1 Go to Go

Select columns

Apply Filters	Visualize Network	View Network Nodes	NodeCount	%ID	#Spectra	Carnitine
Filter By:	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>
1	Visualize Network	Network Nodes	38	0.158	129	Carnitine (Show)

[Catch up Link](#)

55

Explore endogenous molecule - Carnitines

Steve Barnes Class Pooled Test - min cluster 1 - Positive Only [5] Hits 1 - 1 out of 1 Go to Go

Select columns

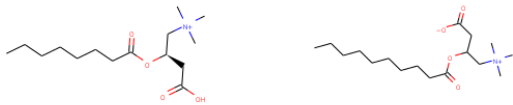
Apply Filters	Visualize Network	View Network Nodes	NodeCount	%ID	#Spectra	Carnitine
Filter By:	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>
1	Visualize Network	Network Nodes	38	0.158	129	Carnitine (Show)

[Catch up Link](#)

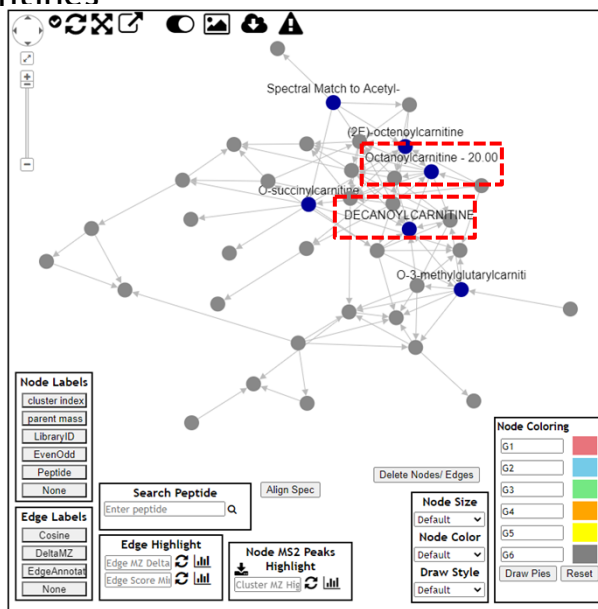
56

Let's explore potential analogs of Carnitines

- Octanoylcarnitine related to Decanoylcarnitine



[Catch up Link](#)

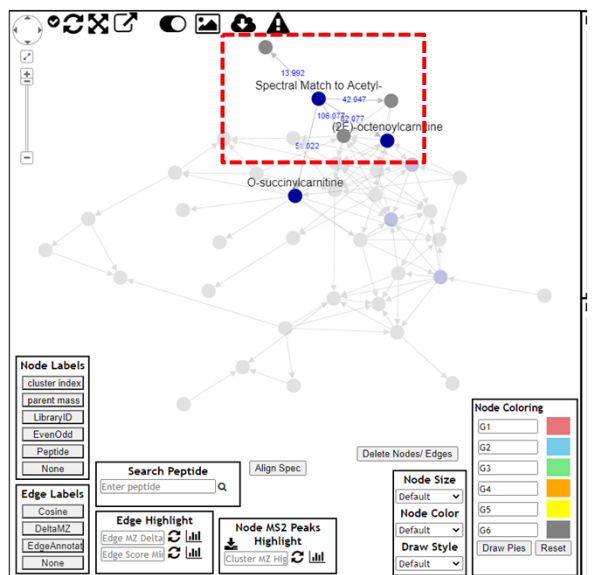


57

Let's explore potential analogs of Carnitines

- Activity: Can you find new putative analog of Acetyl-DL-carnitine?

[Catch up Link](#)



58

Outline for today

- Submit a molecular networking job (Hands-on, Pieter).
- Explanation of what was just submitted (Pieter).
- Exploring the molecular network (Ming).
- GNPS dashboard for inspecting the data (Ming).
- MASST (If we have time, Pieter)

59

Connecting Networks Back to Raw Data - Visualizing Data GNPS Dashboard

- Let's use GNPS Explorer to Select Data to Visualize
<https://gnps-explorer.ucsd.edu/>
- COVID-19 Urine Samples

GNPS Dataset Dashboard - Version - 0.4

MSV00008828

GNPS/Metabolights/PX Dataset Accession MSV00008828

Dataset Password (if private MSV) - Beta Feature Enter Dataset Password

[Link](#)

60

Visualizing Data GNPS Dashboard

- Select Metadata to Use

Metadata Source: MASSIVE

Metadata Options: DEFAULT, REDU, **MASSIVE**

Metadata Source: MASSIVE

Page Size: 10

Metadata Options: f.MSV000088828/updates/2022-02-13_mwang87_0874e95a/metadata/metadata_..., f.MSV000088828/updates/2022-02-12_mwang87_887552af/metadata/metadata.txt, **f.MSV000088828/updates/2022-02-13_mwang87_0874e95a/metadata/metadata_with_AKI.txt**

MSV000088828

61

Visualizing Data GNPS Dashboard

- Select Positive AKI (Acute Kidney Injury Samples)

Export

	filename	collection	update_name	size_mb	ms2	Vendor	Model	ATTRIBUTE_polarity	ATTRIBUTE_type	ATTRIBUTE_AKI	Unnamed: 4
	filter data...							Positive		AKI	
<input checked="" type="checkbox"/>	peak/pos/Pos_NRSP_04.mzXML.mzML	peak		316	0			Positive	Sample	AKI	
<input checked="" type="checkbox"/>	peak/pos/Pos_NRSP_05.mzXML.mzML	peak		321	0			Positive	Sample	AKI	
<input type="checkbox"/>	peak/pos/Pos_NRSP_06.mzXML.mzML	peak		300	0			Positive	Sample	no_AKI	
<input checked="" type="checkbox"/>	peak/pos/Pos_NRSP_07.mzXML.mzML	peak		301	0			Positive	Sample	AKI	
<input checked="" type="checkbox"/>	peak/pos/Pos_NRSP_08.mzXML.mzML	peak		318	0			Positive	Sample	AKI	
<input type="checkbox"/>	peak/pos/Pos_NRSP_10.mzXML.mzML	peak		360	0			Positive	Sample	no_AKI	
<input type="checkbox"/>	peak/pos/Pos_NRSP_11.mzXML.mzML	peak		339	0			Positive	Sample	no_AKI	
<input checked="" type="checkbox"/>	peak/pos/Pos_NRSP_12.mzXML.mzML	peak		299	0			Positive	Sample	AKI	
<input checked="" type="checkbox"/>	peak/pos/Pos_NRSP_13.mzXML.mzML	peak		344	0			Positive	Sample	AKI	
<input type="checkbox"/>	peak/pos/Pos_NRSP_24.mzXML.mzML	peak		325	0			Positive	Sample	no_AKI	

« < 1 / 2 > »

62

Visualizing Data GNPS Dashboard

- Select Positive no_AKI (Acute Kidney Injury Samples) in Comparison Selector Below

Comparison File Selection List (Optional)

Export

	filename	collection	update_name	size_mb	ms2	Vendor	Model	ATTRIBUTE_polarity	ATTRIBUTE_type	ATTRIBUTE_AKI	Unnamed: 4
	filter data...							Positive		no_AKI	
<input checked="" type="checkbox"/>	beak/pos/Pos_NRSP_06.mzXML.mzML	peak		300	0			Positive	Sample	no_AKI	
<input checked="" type="checkbox"/>	beak/pos/Pos_NRSP_10.mzXML.mzML	peak		360	0			Positive	Sample	no_AKI	
<input checked="" type="checkbox"/>	beak/pos/Pos_NRSP_11.mzXML.mzML	peak		339	0			Positive	Sample	no_AKI	
<input checked="" type="checkbox"/>	beak/pos/Pos_NRSP_24.mzXML.mzML	peak		325	0			Positive	Sample	no_AKI	
<input checked="" type="checkbox"/>	beak/pos/Pos_NRSP_26.mzXML.mzML	peak		315	0			Positive	Sample	no_AKI	

63

Visualizing Data GNPS Dashboard

Selected 6 Default Files and 5 Comparison Files for LCMS Analysis

Visualize 11 Files

Visualize All Filtered 18 Files (24 max each)

Molecular Network 11 Files at GNPS

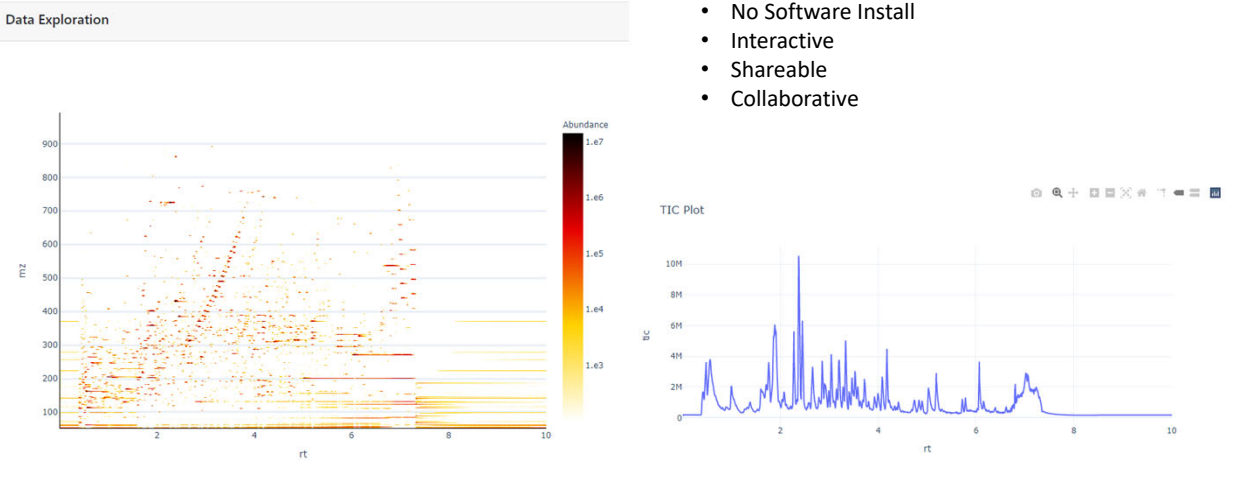
Molecular Network All 18 Files at GNPS

Download First Selected File

64

The GNPS Dashboard – Visualizing Raw MS Data in the Browser

Data Exploration



- No Software Install
- Interactive
- Shareable
- Collaborative

[Catch up Link](#)

Petras et al. Nature Methods 2021

65

Connecting to Raw Data – which samples have drugs?

- Extracted Ion Chromatogram
Desmethylvenlafaxine
- **264.20 m/z**
- **3 min Retention Time**

XIC Options

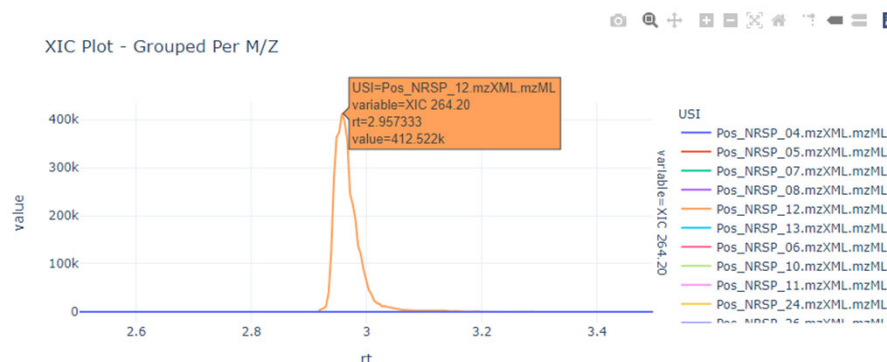
Advanced XIC Options

XIC m/z	264.20	XIC Formula	Enter Molecular Formula to XIC
XIC Tolerance (Da)	0.5	XIC Tolerance (ppm)	10
XIC Retention Time View/Integration Limits	3	XIC Tolerance Unit	p...

66

Connecting to Raw Data – which samples have drugs?

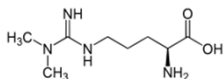
- Extracted Ion Chromatogram – Desmethylvenlafaxine
- A single AKI Sample – what might this mean?



67

Validating Differentially Expressed Metabolites in Publication

Metabolites	Metabolic pathways involved	Boston	
		FC	Raw <i>P</i>
Decreased			
Xanthine (+)	Purine, caffeine	0.26	4.00e-6
N,N-dimethylarginine (+)	Arginine, urea	0.36	5.45e-6
Cyclic AMP (-)	Purine, cellular signaling	0.42	5.80e-6



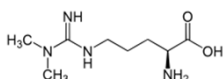
Observed in Positive Mode
203.150 m/z @ 0.6 min retention time

Raines et al. 2021

68

Validating Differentially Expressed Metabolites in Publication

Metabolites	Metabolic pathways involved	Boston	
		FC	Raw <i>P</i>
Decreased			
Xanthine (+)	Purine, caffeine	0.26	4.00e-6
N,N-dimethylarginine (+)	Arginine, urea	0.36	5.45e-6
Cyclic AMP (-)	Purine, cellular signaling	0.42	5.80e-6

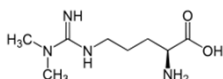


Observed in Positive Mode
203.150 m/z @ 0.6 min retention time

69

Validating Differentially Expressed Metabolites in Publication

Metabolites	Metabolic pathways involved	Boston	
		FC	Raw <i>P</i>
Decreased			
Xanthine (+)	Purine, caffeine	0.26	4.00e-6
N,N-dimethylarginine (+)	Arginine, urea	0.36	5.45e-6
Cyclic AMP (-)	Purine, cellular signaling	0.42	5.80e-6



Observed in Positive Mode
203.150 m/z @ 0.6 min retention time

XIC Options

XIC m/z XIC Formula

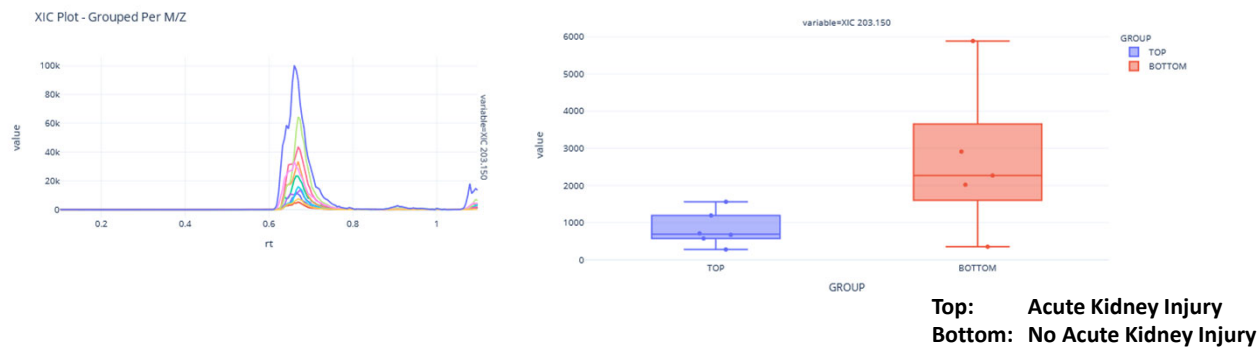
XIC Tolerance (Da) XIC Tolerance (ppm) XI

XIC Retention Time View/Integration Limits

XIC Integration XIC Normalization

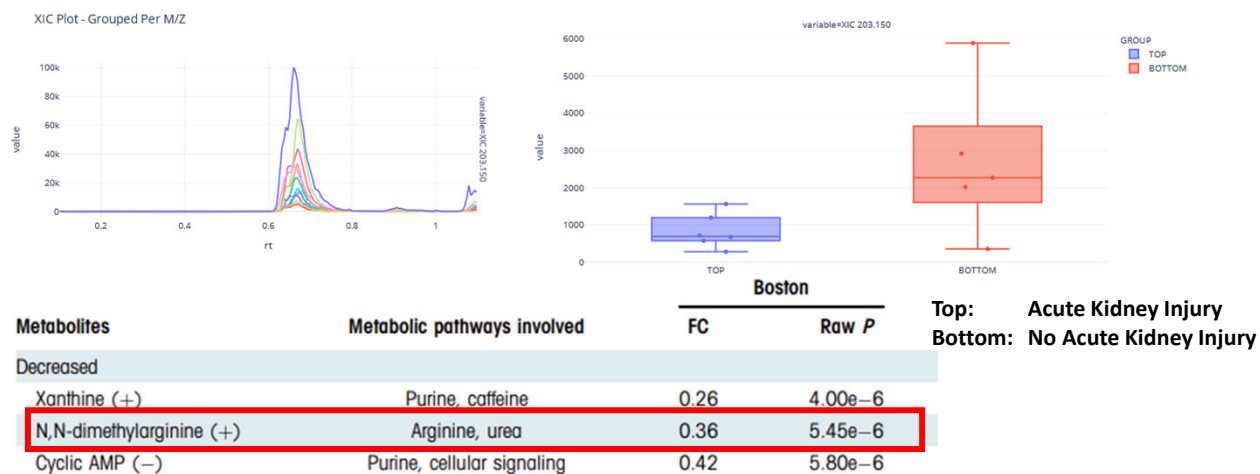
70

Validating Differentially Expressed Metabolites in Publication



71

Validating Differentially Expressed Metabolites in Publication



72

Sharing Visualization – Share exactly what you see with others

The screenshot shows the 'Data Selection' interface. It includes a 'File Selection' section with an 'Upload Files' button. Below this are two 'GNPS USI' input fields. The first field contains two file paths: 'mzspec:MSV000088828:peak/pos/Pos_NRSP_04.mzXML.mzML' and 'mzspec:MSV000088828:peak/pos/Pos_NRSP_05.mzXML.mzML'. The 'USI View Selection' dropdown is set to 'mzspec:MSV000088828:peak/pos/Pos_NRSP_04.mzXML.mzML'. The second 'GNPS USI' field contains two file paths: 'mzspec:MSV000088828:peak/pos/Pos_NRSP_06.mzXML.mzML' and 'mzspec:MSV000088828:peak/pos/Pos_NRSP_10.mzXML.mzML'. Two buttons are visible: 'Copy URL Link to this Visualization' (highlighted with a red box) and 'Copy Short Temporary URL'. A status bar at the bottom indicates 'Molecular Network 11 Files at GNPS'. A 'Comment' field is at the bottom.

73

Outline for today

- **Submit a molecular networking job (Hands-on, Pieter).**
- **Explanation of what was just submitted (Pieter).**
- **Exploring the molecular network (Ming).**
- **GNPS dashboard for inspecting the data (Ming).**
- **MASST (If we have time, Pieter)**

74

Growing repositories

Leveraging repository scale information to
annotate unknowns



= BLAST for molecules



Ming Wang

Wang Et al Nature Biotechnology 2020

75

m/z

① Dataset 1 Dataset 2 Dataset 3

② Annotated Suspects

③

Global Molecular Network

NCBI taxonomic ontology

Age

Uberon Ontology

Sex

Altitude/Depth

Disease Ontology

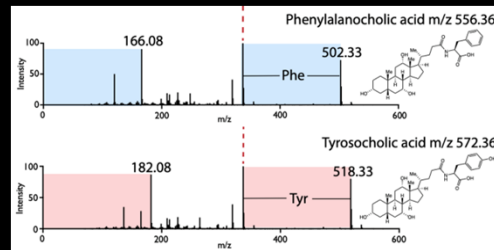
Longitude/Latitude

Mass Spectrometry Ontology

Wang Et al Nature Biotechnology 2020

76

Question:
Is the work in an animal model
translational to humans?

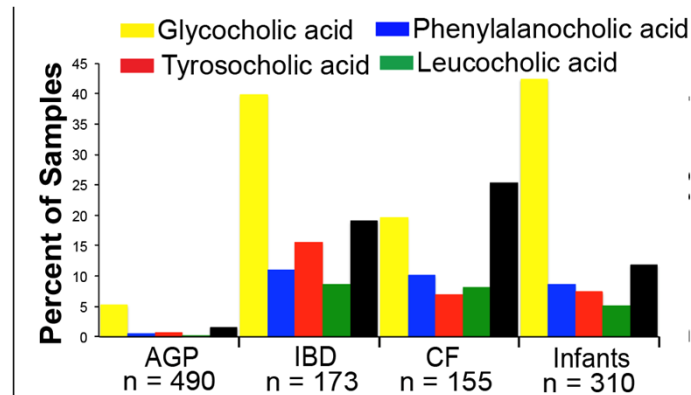


Wang Et al Nature Biotechnology 2020

Quinn et al Nature 2020

77

Now we know these bile acids are found in humans
and that the work is translational.



+27 other public projects
from human samples.

78

Topic/domain specific MASST's



Kiana West



Robin Schmid

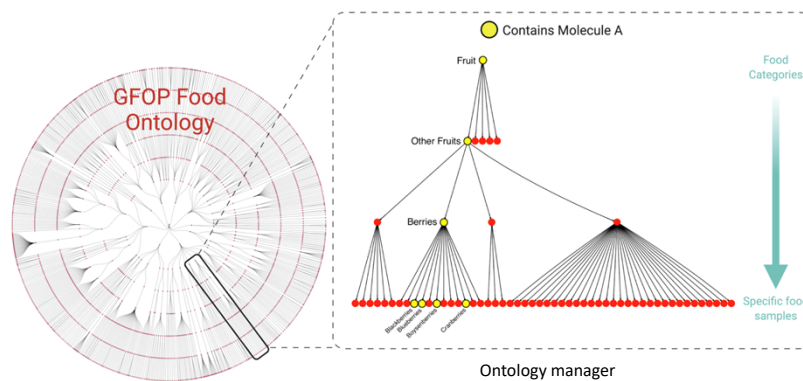


Ming Wang

PhyloMASST, DiseaseMASST, MicrobeMASST,
ExposureMASST etc will be available in the future

79

Connect molecules to food ontologies.



Kiana West

80

80

Is this drug often observed?
 What sample types is this drug found in?
 Is there evidence it is found in the environment?

Google search results for **desfenlafaxine**. The search bar shows "desfenlafaxine" and the results indicate "Showing results for **desvenlafaxine**". The text states: "Desvenlafaxine is used to treat depression. Desvenlafaxine is in a class of medications called selective serotonin and norepinephrine reuptake inhibitors (SNRIs). It works by increasing the amounts of serotonin and norepinephrine, natural substances in the brain that help maintain mental balance." Below the text are two images: a row of five small white pill bottles and two pink, oval-shaped tablets, one with "W 50" and the other with a logo.

Showing results for **desvenlafaxine**
 Search instead for **desvenlafaxine**

Desvenlafaxine is used to treat depression. Desvenlafaxine is in a class of medications called selective serotonin and norepinephrine reuptake inhibitors (SNRIs). It works by increasing the amounts of serotonin and norepinephrine, natural substances in the brain that help maintain mental balance.

<https://medlineplus.gov/druginfo/meds/>
Desvenlafaxine: MedlinePlus Drug Information

81

Job Status	
Workflow	METABOLOMICS-SNETS-V2 (version release_30) DONE [Clone] [Clone to Latest Version] [Restart] [Delete] Default Molecular Networking Results Views [View All Library Hits] [View Unique Library Compounds] [View All Clusters With IDs] [File Summaries] Network Visualizations [View Spectral Families (In Browser Network Visualizer)] [Network Summarizing Graphs] Methods and Citation for Manuscripts [Workflow Written Description] Export/Download Network Files [Download Clustered Spectra as MGF] [Download GraphML for Cytoscape] [Download Bucket Table] [Download BioM For Qiime/Qiita] [Download Metadata For Qiime] [Download ILL Data] Advanced Views - Metadata Views [View Metadata]
Status	Advanced Views - Global Public Dataset Matches [View Matches to All Public Datasets] Advanced Views - External Visualization [View ILL in GNP5] [Direct Cytoscape Preview/Download] [Visualize with Upset Plots (Beta)] Advanced Views - Networking Graphs/Histograms [Nodes_MZ Histogram] [Edges_MZ Delta Histogram] [Edges_Score vs MZ Delta Plot] [Library Search_PPM Error Histogram] Advanced Views - Misc Views [View Network_Node Centric] [View Network Pairs] [Networking Statistics] [View Raw/Unclustered Spectra] [View Compounds and File Occurrence] Advanced Views - Make Dataset Public [Make Public Dataset Documentation] [Make Dataset Public Direct Link] Advanced Views - Experimental Views [Analyze with MS2LDA] [Enhance with MolNetEnhancer] [Global Comparison with ReDU PCA] [Annotate with DEREPLICATOR] [Annotate with DEREPLICATOR+] [Network with Spec2vec] Advanced Views - qiime2 Views [View qiime2 Emperor Plots] [Download qiime2 Emperor qzv] [Download qiime2 features biom gza]

Or
 masst.ucsd.edu

82

Pooled Test - min cluster 1 - Positive Only [5] Hits 1 - 1 out of 1 Go to Go

Apply Filters	ClusterIdx	Spec Family	AddToLibrary	NumSpectra	NumFiles	PrecursorMZ	PrecursorInt	RTMean	AllGroups	DefaultGroups	EvenOdd	LibraryID	
Filter By:	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	Desvenlafaxine	
MASST Spectrum	USI Links 1	Cluster - 483	View Network	AddToLibrary	2	1	264.19700	-2.00000	186.778		G1	1	Massbank:EA105309 O-desmethylvenlafaxine [Desvenlafaxine (Z-(dimethylamino)-1-(1-hydroxycyclohexyl)ethyl)ph

83

Search Protocol: [Reset Form](#) [Save as Protocol](#)

Title:

Workflow Description

SEARCH_SINGLE_SPECTRUM

Use MASST to query a single MS/MS spectrum across all public GNPS datasets. The mass spectrometry equivalent of NCBI BLAST helps to put the query spectrum in context of where else it occurs (including sample information) as well as search a single MS/MS spectrum against all public spectral libraries.

Workflow version release_29

Spectrum Input

Precursor M/Z:

Spectrum Input:

56.049	3.762
57.892	7.49
58.064	700.333
77.039	4.626

Search Options

Find Related Datasets: Select Databases to Search:

Parent Mass Tolerance: Da Ion Tolerance: Da

Min Matched Peaks: Score Threshold:

Advanced Search Options [Show Fields](#)

Advanced Filtering Options [Show Fields](#)

Workflow Submission


Email me at

[Submit](#)

84

Job Status	
Workflow	SEARCH_SINGLE_SPECTRUM (version release_29)
Status	RUNNING [Clone] [Clone to Latest Version] [Delete]
User	workshop (pdorresteinstein@hotmail.com), UCSD
Title	Desvenlafaxine
Date Created	2022-02-15 15:45:13.0
Execution Time	0 seconds
Progress	
Spectral Library	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/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/IQAMDB/IQAMDB.mgf speclibs/GNPS-IOBA-NHC/GNPS-IOBA-NHC.mgf speclibs/GNPS-NIH-SMALLMOLECULEPHARMACOLOGICALLYACTIVE/GNPS-NIH-SMALLMOLECULEPHARMACOLOGICALLYACTIVE.mgf speclibs/BILELIB19/BILELIB19.mgf

85



GNPS: Global Natural Products Social Molecular Networking

[Logout](#) | [My User](#) | [Update Profile](#) | [Jobs](#) | [MassIVE Datasets](#) | [Documentation](#) | [Forum](#) | [Contact](#)

[Back to main page](#)


Total: 333 jobs, occupying 41.91 GB of storage space (0 bytes in 0 protected jobs)

ProteoSAFE Workflow Tasks Hits 1 - 30 out of 333 Go to Go [Export Filtered Results](#) [Delete Selected](#)

Select columns

Apply Filters	Description	User	Workflow	Workflow Version	Status	Protected	Create Time	Total Size (MIB)	Site	Delete Task
<input type="checkbox"/> Select All						<input type="checkbox"/>				
<input type="checkbox"/> 1	Desvenlafaxine ID=79cab77fa1de46cf89913a26c9b4a5e5	workshop	SEARCH_SINGLE_SPECTRUM	release_29	RUNNING	<input type="checkbox"/> 0	Feb. 15, 2022, 3:45 PM	0	GNPS	Delete
<input type="checkbox"/> 2	Desvenlafaxine ID=cf11835cb14c494586cf91684a22e401	workshop	SEARCH_SINGLE_SPECTRUM	release_29	RUNNING	<input type="checkbox"/> 0	Feb. 15, 2022, 3:39 PM	0	GNPS	Delete
<input type="checkbox"/> 3	Steve Barnes Class Pooled Test - min cluster 1 - Positive Only [5] ID=f905572e4c4e4463bb0911270c98b8cc	workshop	METABOLOMICS-SNETS-V2	release_30	DONE	<input type="checkbox"/> 0	Feb. 15, 2022, 3:04 PM	0	GNPS	Delete
<input type="checkbox"/> 4	foodMASST Analysis Cumarin cosine 0.8 ID=3d5bbaef692e4a32b844db36718f86	workshop	SEARCH_SINGLE_SPECTRUM	release_29	DONE	<input type="checkbox"/> 0	Feb. 14, 2022, 4:09 PM	5	GNPS	Delete
<input type="checkbox"/> 5	CURCUMIN second version ID=15c69657eb83452c9ecc134bec2c6122	workshop	SEARCH_SINGLE_SPECTRUM	release_29	DONE	<input type="checkbox"/> 0	Feb. 14, 2022, 3:54 PM	5	GNPS	Delete
<input type="checkbox"/> 6	foodMASST Analysis Cumarin second version ID=ec671ce0c17742a19d0b17000c4eeaae	workshop	SEARCH_SINGLE_SPECTRUM	release_29	DONE	<input type="checkbox"/> 0	Feb. 14, 2022, 3:54 PM	5	GNPS	Delete
<input type="checkbox"/> 7	foodMASST Analysis Cumarin ID=70eda08c9b84fc6b90bf959f1fa904	workshop	SEARCH_SINGLE_SPECTRUM	release_29	DONE	<input type="checkbox"/> 0	Feb. 14, 2022, 3:51 PM	6	GNPS	Delete
<input type="checkbox"/> 8	CURCUMIN ID=c9a6e4d6544e4384b85de2350e7c1b0c	workshop	SEARCH_SINGLE_SPECTRUM	release_29	DONE	<input type="checkbox"/> 0	Feb. 14, 2022, 3:49 PM	6	GNPS	Delete
<input type="checkbox"/> 9	DIE in environmental samples Jan 31 2022 ID=093a4a912405428891ca1dfc43add84f	workshop	SEARCH_SINGLE_SPECTRUM	release_29	DONE	<input type="checkbox"/> 0	Jan. 31, 2022, 9:35 AM	3	GNPS	Delete
<input type="checkbox"/> 10	rats ceacum and cognition 4 ion 0.6 cos ID=c3c8a8e2079411f8a21770f8ca45c88	workshop	METABOLOMICS-SNETS-V2	release_30	DONE	<input type="checkbox"/> 0	Jan. 28, 2022, 12:17 PM	66	GNPS	Delete
<input type="checkbox"/> 11	rats ceacum and cognition with suspect ID=f4438769a43440208a74c5a276dce5	workshop	METABOLOMICS-SNETS-V2	release_30	DONE	<input type="checkbox"/> 0	Jan. 28, 2022, 12:15 PM	67	GNPS	Delete
<input type="checkbox"/> 12	rats ceacum and cognition ID=9959e654e99747b2b89b95cabfc274d6	workshop	METABOLOMICS-SNETS-V2	release_30	DONE	<input type="checkbox"/> 0	Jan. 28, 2022, 11:10 AM	66	GNP	Delete
<input type="checkbox"/> 13	229 TMAP based on https://pubs.acs.org/doi/abs/10.1021/acs.analchem.1c04378 ID=f680bcb8e164624a379b3b178b37f45	workshop	ADD-SINGLE-ANNOTATED-BRONZE	1.2.5	DONE	<input type="checkbox"/> 0	Jan. 19, 2022, 2:32 PM	5	GNP	Delete

86



GNPS: Global Natural Products Social Molecular Networking

Logout | My User | Update Profile | Jobs | Massive Datasets | Documentation | Forum | Contact

[Back to main page](#)

Total: 333 jobs, occupying 41.91 GB of storage space (0 bytes in 0 protected jobs)

ProteoSAFE Workflow Tasks Hits 1 - 30 out of 333 Go to Go Export Filtered Results Delete Selected

[Select columns](#)

Apply Filters	Description	User	Workflow	Workflow Version	Status	Protected	Create Time	Total Size (MiB)	Site	Delete Task
<input type="checkbox"/>	Select All									
<input type="checkbox"/>	1 Desvenlafaxine ID=79cab777fa1de46cf89913a26c9b4a5e5	workshop	SEARCH_SINGLE_SPECTRUM	release_29	RUNNING	<input type="checkbox"/>	Feb. 15, 2022, 3:45 PM	0	GNPS	Delete
<input type="checkbox"/>	2 Desvenlafaxine ID=cf1f835cb14c494586cf91684a22e401	workshop	SEARCH_SINGLE_SPECTRUM	release_29	RUNNING	<input type="checkbox"/>	Feb. 15, 2022, 3:39 PM	0	GNPS	Delete
<input type="checkbox"/>	3 Steve Barnes Class Pooled Test - min cluster 1 - Positive Only [5] ID=f9d55f2e4c4a4d63bb9f1270fc98bccc	workshop	METABOLOMICS-SNETS-V2	release_30	DONE	<input type="checkbox"/>	Feb. 15, 2022, 3:04 PM	0	GNPS	Delete
<input type="checkbox"/>	4 foodMASST Analysis Cumarin cosine 0.8 ID=3d5bbaef692e4a32b84aedbb36718f86	workshop	SEARCH_SINGLE_SPECTRUM	release_29	DONE	<input type="checkbox"/>	Feb. 14, 2022, 4:09 PM	5	GNPS	Delete
<input type="checkbox"/>	5 CURCUMIN second version ID=15c69657eb83452c9ecc134bec2c6122	workshop	SEARCH_SINGLE_SPECTRUM	release_29	DONE	<input type="checkbox"/>	Feb. 14, 2022, 3:54 PM	5	GNPS	Delete
<input type="checkbox"/>	6 foodMASST Analysis Cumarin second version ID=ec671ce0c17742a1900b17000c4eeaae						Feb. 14, 2022, 3:44 PM	5	GNPS	Delete
<input type="checkbox"/>	7 foodMASST Analysis Cumarin ID=70edaf08c9b84f6cb90bfrf595f1fa904						Feb. 14, 2022, 3:11 PM	6	GNPS	Delete
<input type="checkbox"/>	8 CURCUMIN ID=c9a6e4d6544e4384b85de2350e7c1b0c						Feb. 14, 2022, 3:09 PM	6	GNPS	Delete
<input type="checkbox"/>	9 DIE in environmental samples Jan 31 2022 ID=095a4a912405428891ca1dfc43ddd84f	workshop	SEARCH_SINGLE_SPECTRUM	release_29	DONE	<input type="checkbox"/>	Jan. 31, 2022, 9:35 AM	3	GNPS	Delete
<input type="checkbox"/>	10 rats caecum and cognition 4 ion 0.6 cos ID=c3c8a8ea207b41fc8a2d770f8ca45c88	workshop	METABOLOMICS-SNETS-V2	release_30	DONE	<input type="checkbox"/>	Jan. 28, 2022, 12:17 PM	66	GNPS	Delete
<input type="checkbox"/>	11 rats caecum and cognition with suspect ID=f4438769a43440208a67a4c5a276dce5	workshop	METABOLOMICS-SNETS-V2	release_30	DONE	<input type="checkbox"/>	Jan. 28, 2022, 12:15 PM	67	GNPS	Delete
<input type="checkbox"/>	12 rats caecum and cognition ID=9959e654e99747b2b89b95cabfc274d6	workshop	METABOLOMICS-SNETS-V2	release_30	DONE	<input type="checkbox"/>	Jan. 28, 2022, 11:10 AM	66	GNP	Delete
<input type="checkbox"/>	13 229 TMAPA based on https://pubs.acs.org/doi/abs/10.1021/acs.analchem.1c04378 ID=f6680b0c8e164624a379b3b178b37f45	workshop	ADD-SINGLE-ANNOTATED-BRONZE	1.2.5	DONE	<input type="checkbox"/>	Jan. 19, 2022, 2:32 PM	5	GNP	Delete

https://gnps.ucsd.edu/ProteoSAFE/result.jsp?task=cf1f835cb14c494586cf91684a22e401&view=view_all_datasets_matched

87