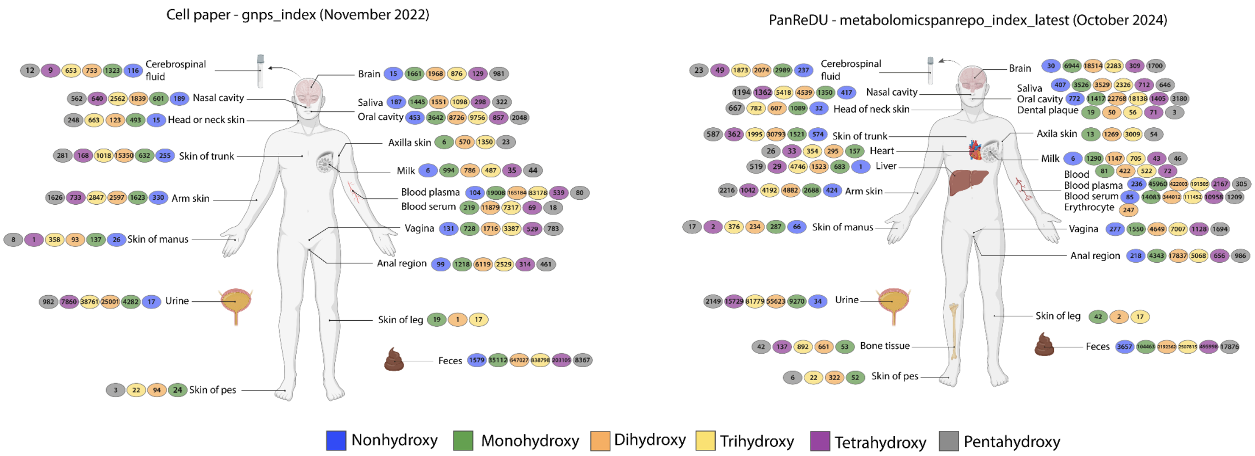
Supplementary Information

Supplementary Figure 1



Supplementary Figure 1. Bile acid matches the number of hydroxy groups on the bile acid core. Updated numbers of a human organ distribution search of bile acids from a recently published Candidate Bile Acid Library utilizing Pan-ReDU. The left panel shows the numbers before the update, and the right panel shows the numbers after the Pan-ReDU update[7]. On average, the increase was 246% per tissue/biofluid type. The numbers are given separately by the number of hydroxyl groups on the bile acid core. This figure was made using BioRender.com. Source data are provided as a Source Data file.

Supplementary Table 1

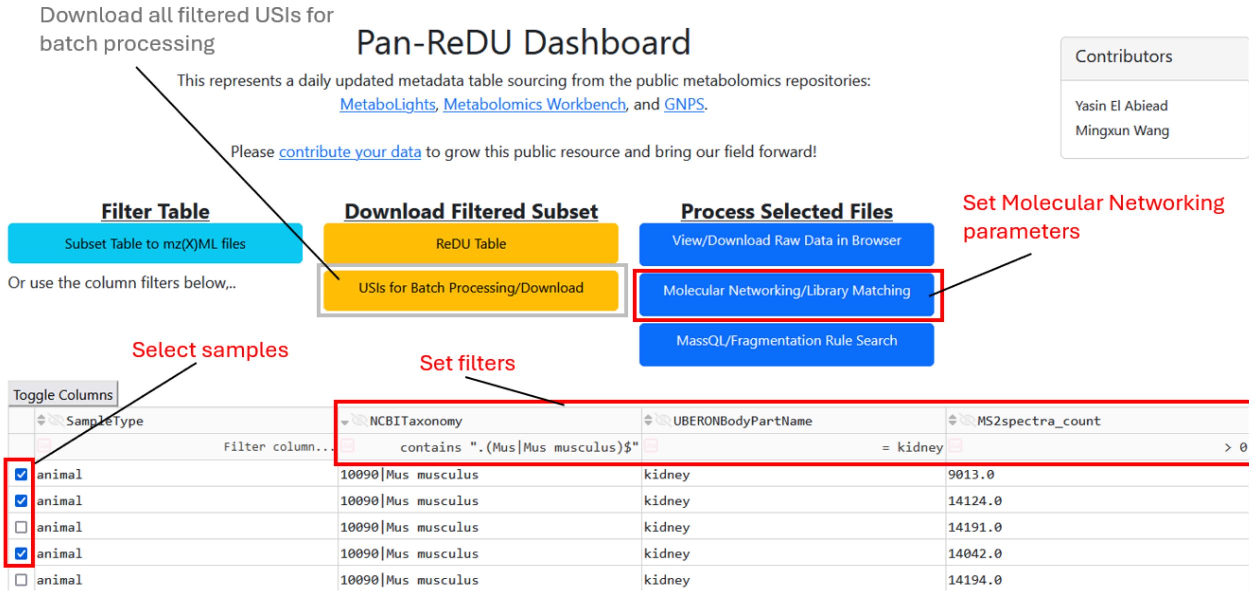
Supplementary Table 1 | Linkouts demonstrating the accessibility of different file formats across different repositories within the browser

MS Run Identifier (MRI)
mzspec:MSV000094405:MSV000094405/raw/SCCe0064.mzML
mzspec:MTBLS300:FILES/Method 4 stool/QXA07POSLAT20190401_MSST010118ML_HUMAN_FECAL4_08.mzML
mzspec:MSV000094460:raw/FIR094/20221108_C1_094_R2A_ext_POS_2-B,7_01_35551.d.mzXML
mzspec:MTBLS1039:FILES/DERIVED_FILES/13-124_12hpi_Chitin_1_150306.mzXML
mzspec:MSV000094118:raw/Raw/20210552_QC5.raw
mzspec:MTBLS1024:FILES/KN210_1019_ppl_neg_400k.raw
mzspec:ST002244:Positive_QC_16.raw

Supplementary Note 1

Here we demonstrate how we can select and process *Mus* and *Mus musculus* mzML and mzXML with files with MS/MS scans to retrieve GNPS library annotations and molecular networking results.

1. Go to the ReDU data selection dashboard at https://redu.gnps2.org/selection/
2. Set the NCBITaxonomy column filter to ‘contains ".(Mus|Mus musculus)$"’ which retrieves all NCBI Taxonomy values ending on ‘Mus’ or ‘Mus musculus’.
3. Set the UBERONBodyPartName filter to ‘= kidney’ which retains all kidney samples.
4. Subset to files that contain MS/MS spectra by setting the MS2spectra_count to ‘> 0’.
5. Select a few rows via the checkboxes on the left side of the table and click the ‘Molecular Networking/Library Matching’ button (or download all filtered MRIs to submit more than can be selected on a single page).



Download all filtered USIs for batch processing

Pan-ReDU Dashboard

This represents a daily updated metadata table sourcing from the public metabolomics repositories: MetaboLights, Metabolomics Workbench, and GNPS.

Please contribute your data to grow this public resource and bring our field forward!

Contributors

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Set Molecular Networking parameters

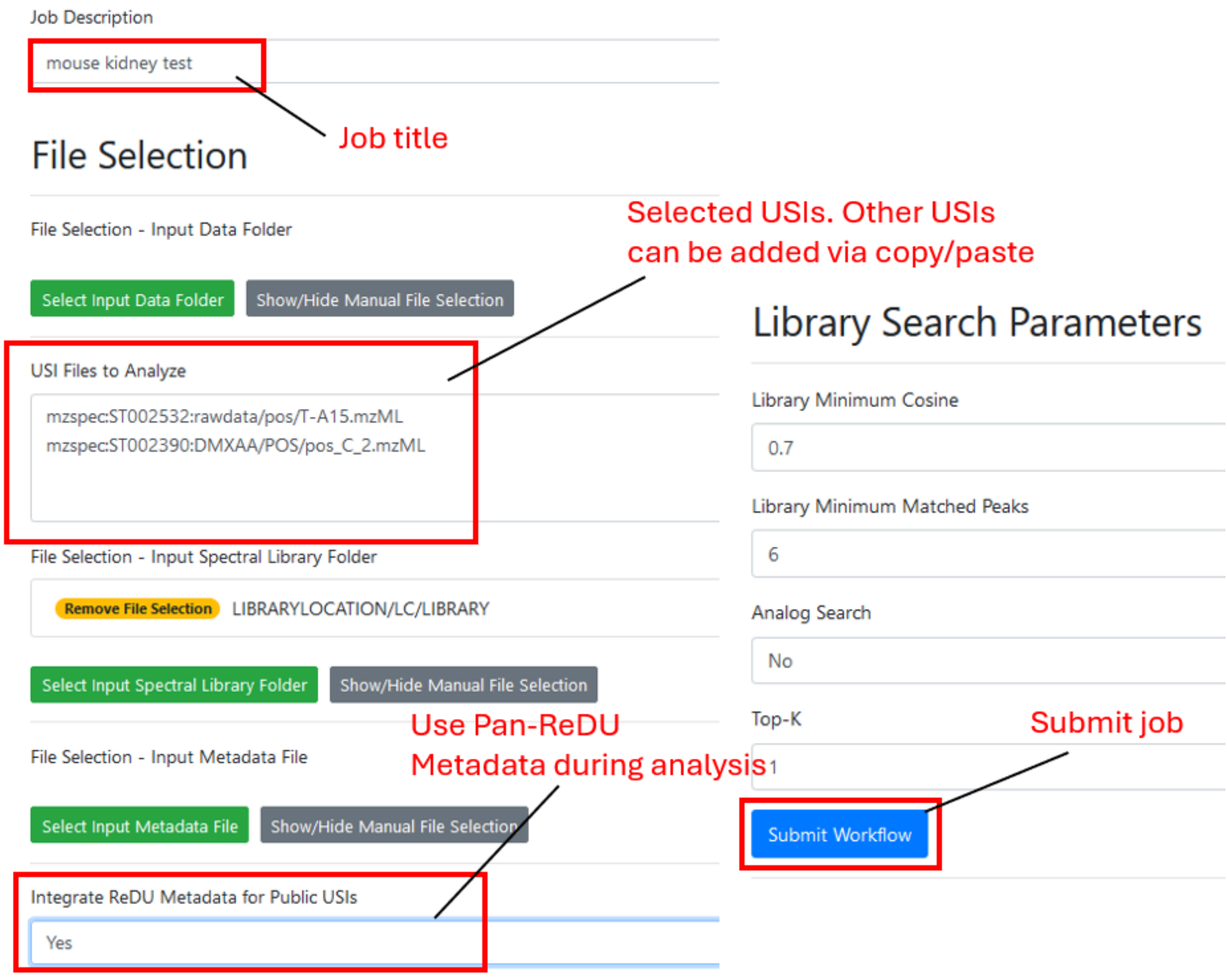
Or use the column filters below,..

Select samples

Set filters

	SampleType	NCBITaxonomy	UBERONBodyPartName	MS2spectra_count
	Filter column...	contains ".(Mus|Mus musculus)$"	= kidney	> 0
☑	animal	10090|Mus musculus	kidney	9013.0
☑	animal	10090|Mus musculus	kidney	14124.0
☐	animal	10090|Mus musculus	kidney	14191.0
☑	animal	10090|Mus musculus	kidney	14042.0
☐	animal	10090|Mus musculus	kidney	14194.0

6. This will bring you to the Molecular Networking submission page with the MRIs of the selected files already populated.
7. Give a title to your job, set ‘Integrate ReDU Metadata for Public USIs’ to ‘Yes’, and the other parameters to your satisfaction.
8. Submit workflow through the ‘Submit Workflow’ button.



Job Description: mouse kidney test

File Selection

File Selection - Input Data Folder

USI Files to Analyze:
mzspec:ST002532:rawdata/pos/T-A15.mzML
mzspec:ST002390:DMXAA/POS/pos_C_2.mzML

File Selection - Input Spectral Library Folder: LIBRARYLOCATION/LC/LIBRARY

File Selection - Input Metadata File

Integrate ReDU Metadata for Public USIs: Yes

Library Search Parameters

Library Minimum Cosine: 0.7

Library Minimum Matched Peaks: 6

Analog Search: No

Top-K: 1

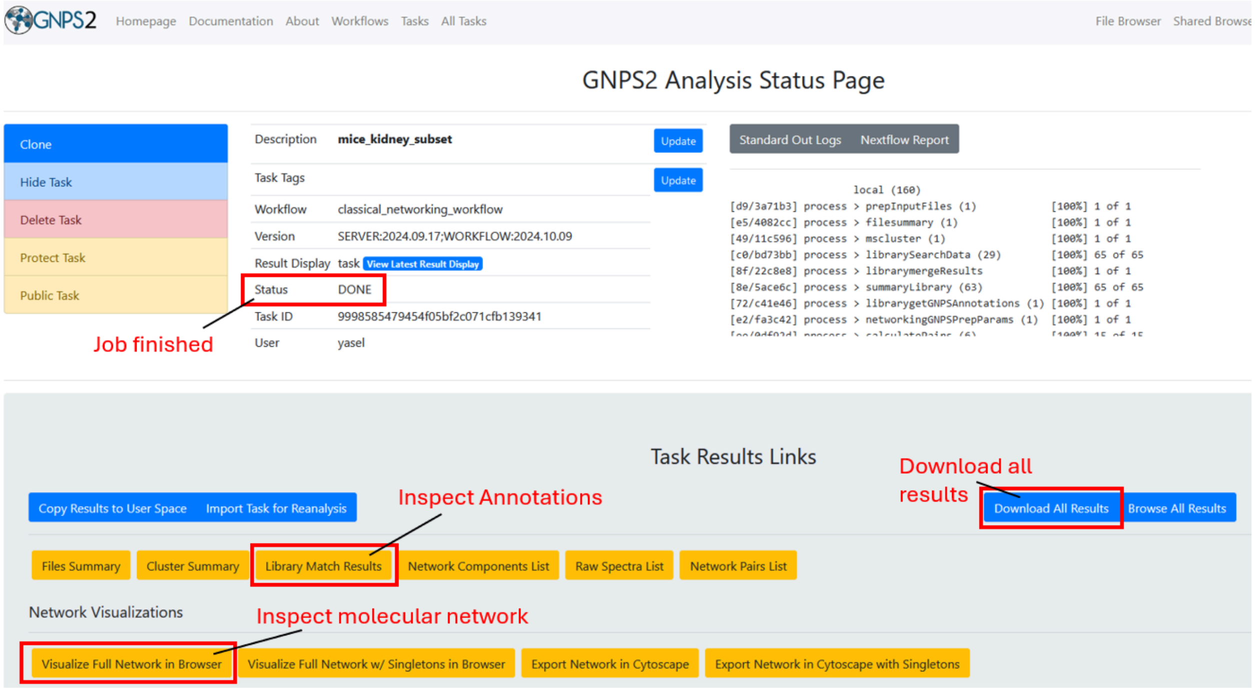
Job title

Selected USIs. Other USIs can be added via copy/paste

Use Pan-ReDU Metadata during analysis

Submit job

9. Once the status page switches from Status ‘Running’ to ‘Done’ you can download all results via the ‘Download All Results’ button.



GNPS2 Analysis Status Page

Description	**mice_kidney_subset**
Task Tags	
Workflow	classical_networking_workflow
Version	SERVER:2024.09.17;WORKFLOW:2024.10.09
Result Display	task
Status	DONE
Task ID	9998585479454f05bf2c071cfb139341
User	yasel

```
                    local (160)
[d9/3a71b3] process > prepInputFiles (1)           [100%] 1 of 1
[e5/4082cc] process > filesummary (1)              [100%] 1 of 1
[49/11c596] process > mscluster (1)                [100%] 1 of 1
[c0/bd73bb] process > librarySearchData (29)       [100%] 65 of 65
[8f/22c8e8] process > librarymergeResults          [100%] 1 of 1
[8e/5ace6c] process > summaryLibrary (63)          [100%] 65 of 65
[72/c41e46] process > librarygetGNPSAnnotations (1) [100%] 1 of 1
[e2/fa3c42] process > networkingGNPSPrepParams (1)  [100%] 1 of 1
```

Job finished

Task Results Links

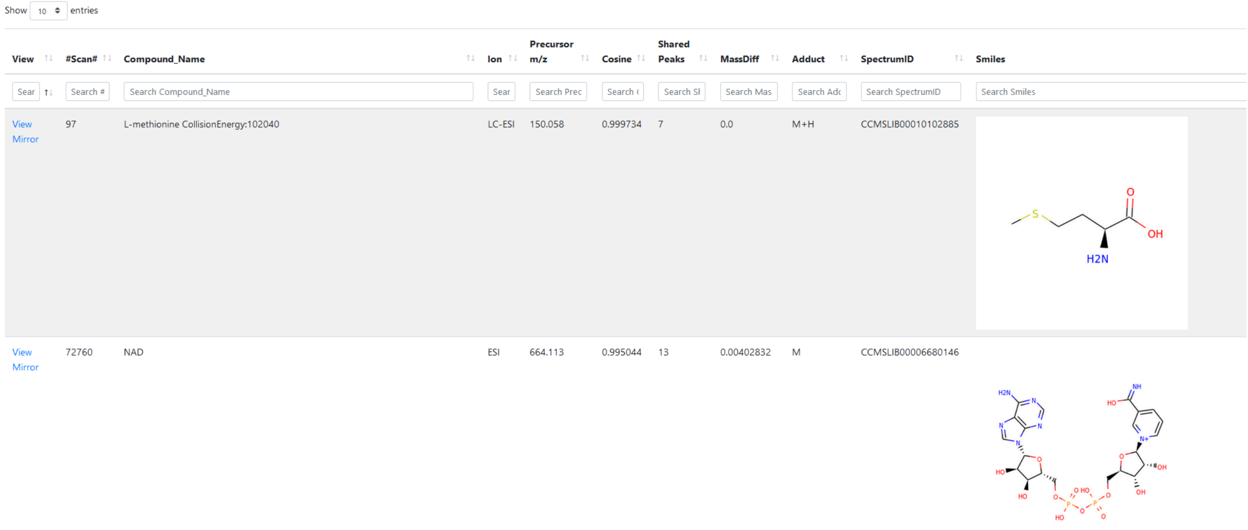
Download all results

Inspect Annotations

Network Visualizations

Inspect molecular network

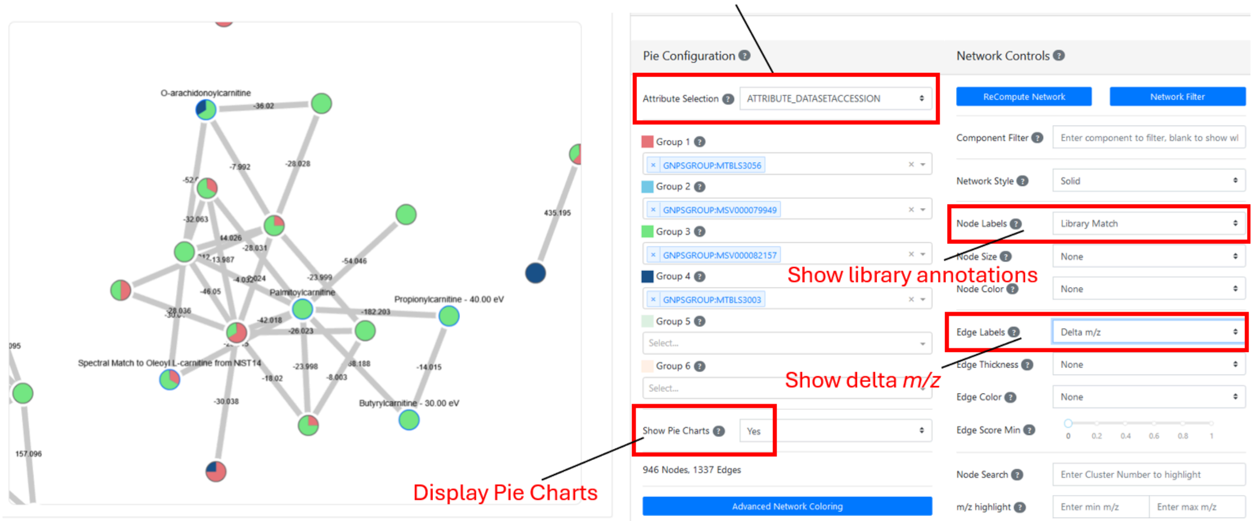
10. Click the ‘Library Match Results’ button to inspect all molecular annotations.



View	#Scan#	Compound_Name	Ion	Precursor m/z	Cosine	Shared Peaks	MassDiff	Adduct	SpectrumID	Smiles
View Mirror	97	L-methionine CollisionEnergy:102040	LC-ESI	150.058	0.999734	7	0.0	M+H	CCMSLIB00010102885	
View Mirror	72760	NAD	ESI	664.113	0.995044	13	0.00402832	M	CCMSLIB00006680146	

11. You can click the ‘Visualize Full Network in Browser’ button for an interactive Molecular Network.

Select Pan-ReDU variable



Attribute Selection: ATTRIBUTE_DATASETACCESSION

🟥 Group 1: GNPSGROUP:MTBLS3056

Group 2: GNPSGROUP:MSV000079949

🟩 Group 3: GNPSGROUP:MSV000082157

Group 4: GNPSGROUP:MTBLS3003

Group 5: Select...

Group 6: Select...

Show Pie Charts: Yes

946 Nodes, 1337 Edges

Component Filter: Enter component to filter, blank to show wl

Network Style: Solid

Node Labels: Library Match

Node Size: None

Node Color: None

Edge Labels: Delta m/z

Edge Thickness: None

Edge Color: None

Edge Score Min: 0 0.2 0.4 0.6 0.8 1

Node Search: Enter Cluster Number to highlight

m/z highlight: Enter min m/z Enter max m/z

Show library annotations

Show delta *m/z*

Display Pie Charts

12. The ‘Visualize Full Network in Browser’ button will bring you to an interactive network. It might require some time to load depending on the size.
13. To integrate with metadata set ‘Show Pie Charts’ to ‘Yes’, and select any ReDU column from the ‘Attribute Selection’ dropdown menu. This will show the relative number of observed spectra for every node as a pie chart per selected grouping.
14. To display annotations set ‘Node Labels’ to ‘Library match’. Clicking on individual nodes allows to show structures of molecules if available for the respective annotation, as well as MS2 spectral matches.