metID: A R package for Automatable Compound Annotation for LC–MS-based Data

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OUTLINE

</> metID: Compound Annotation for LC-MS Data

- In-house Database Construction
- Databases Provided in metID
- Database Sharing
- Case Study

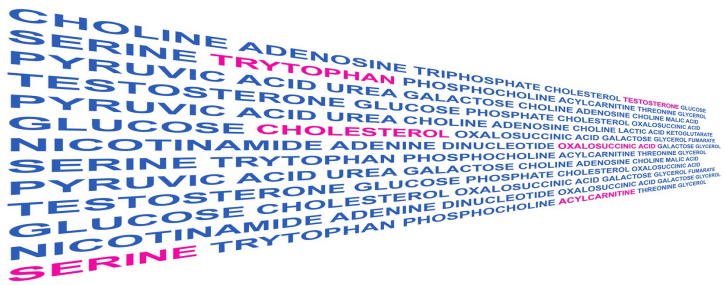
</> TidyMass: A Computational Framework for LC-MS Data Processing and Analysis

metID: Compound Annotation for LC-MS Data

Background

LipidIMMS Analyzer

Metabolite identification and
Dysregulated **N**etwork **A**nalysis

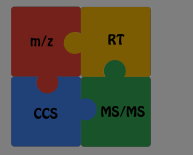


 More tools are not listed here.

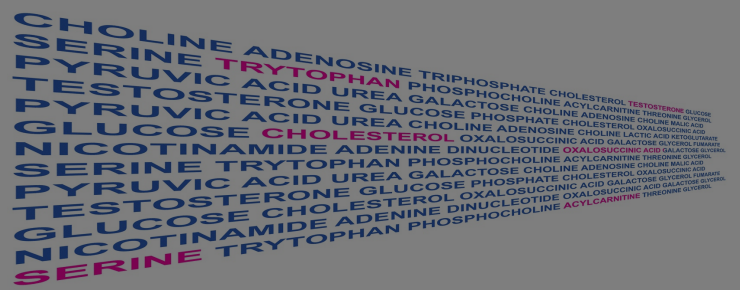
Background

1. User-friendly,
2. Simple.

1. For GUI software, most of them only support Windows,
2. Not flexible.



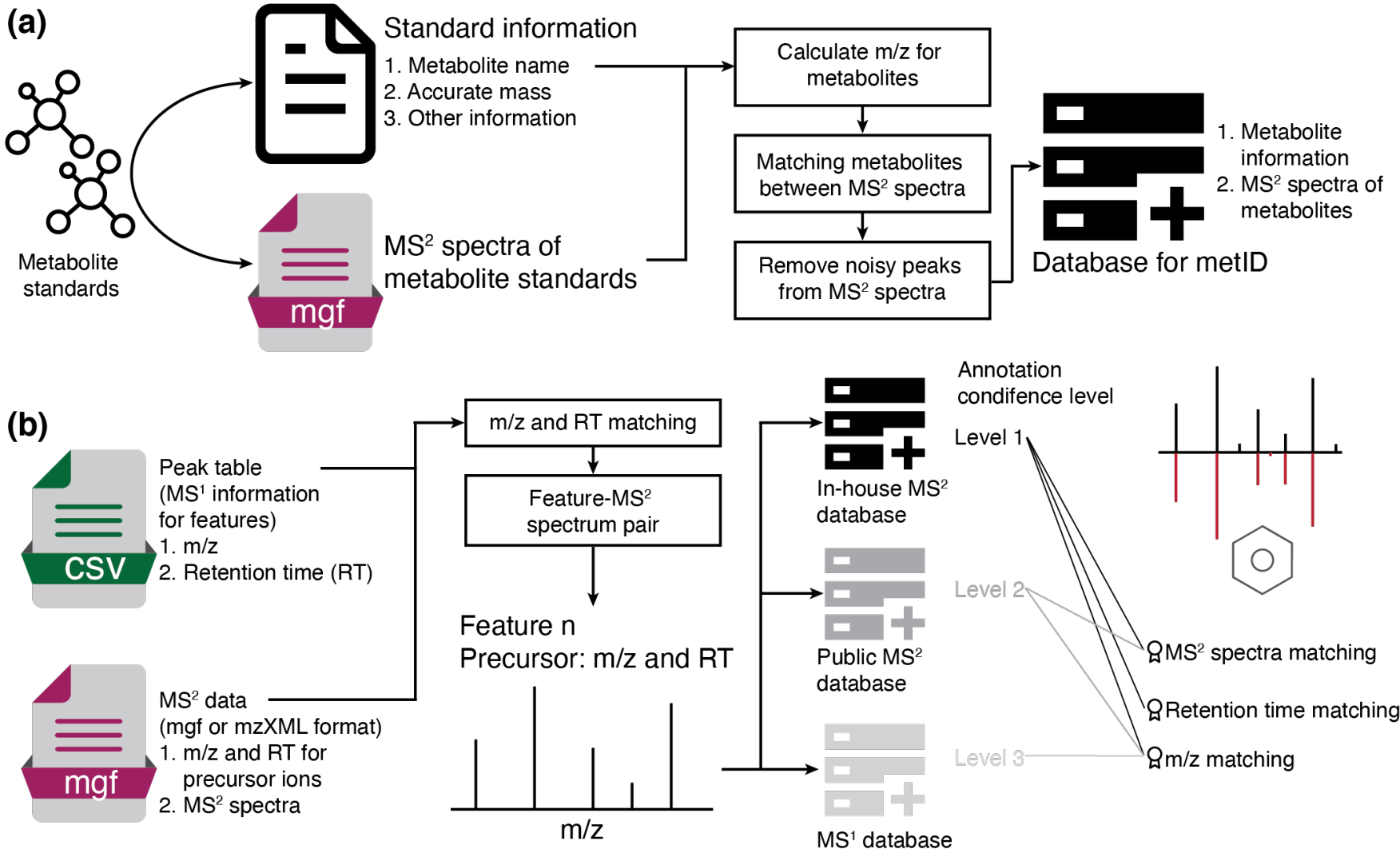
LipidIMMS Analyzer



More tools are not listed here.

metID: Design and Overview

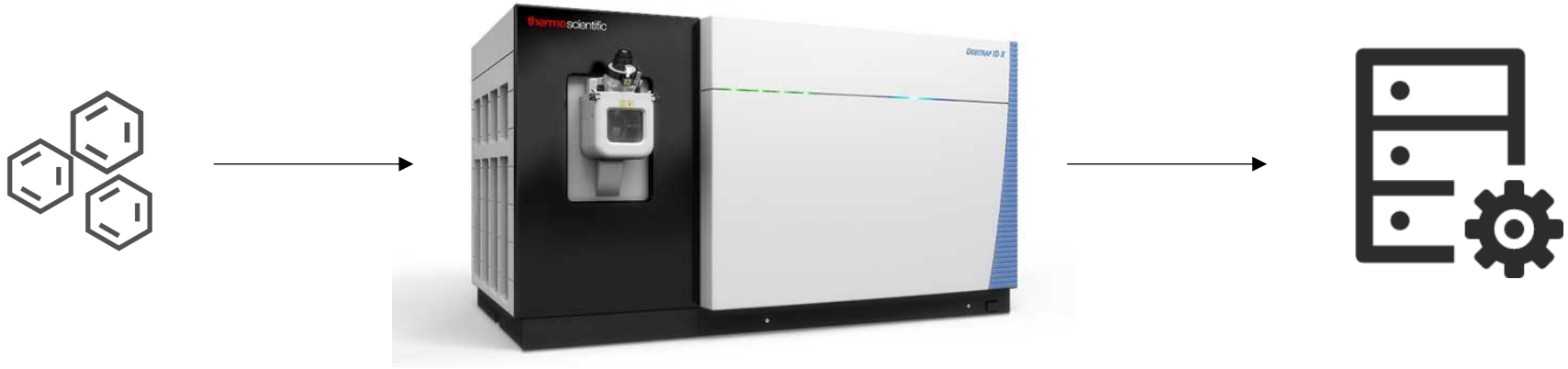
1. R-based: can be installed any platform (Windows, Mac and Linux).
2. Universal format database.
3. Support multiple database format from other common tools (GNPS, MoNA and so on).
4. Automatable metabolite annotation functions.



Xiaotao Shen et al. Bioinformatics, 2021.

In-house Database Construction

A lot of labs have compound standard information (retention time and MS/MS spectra).

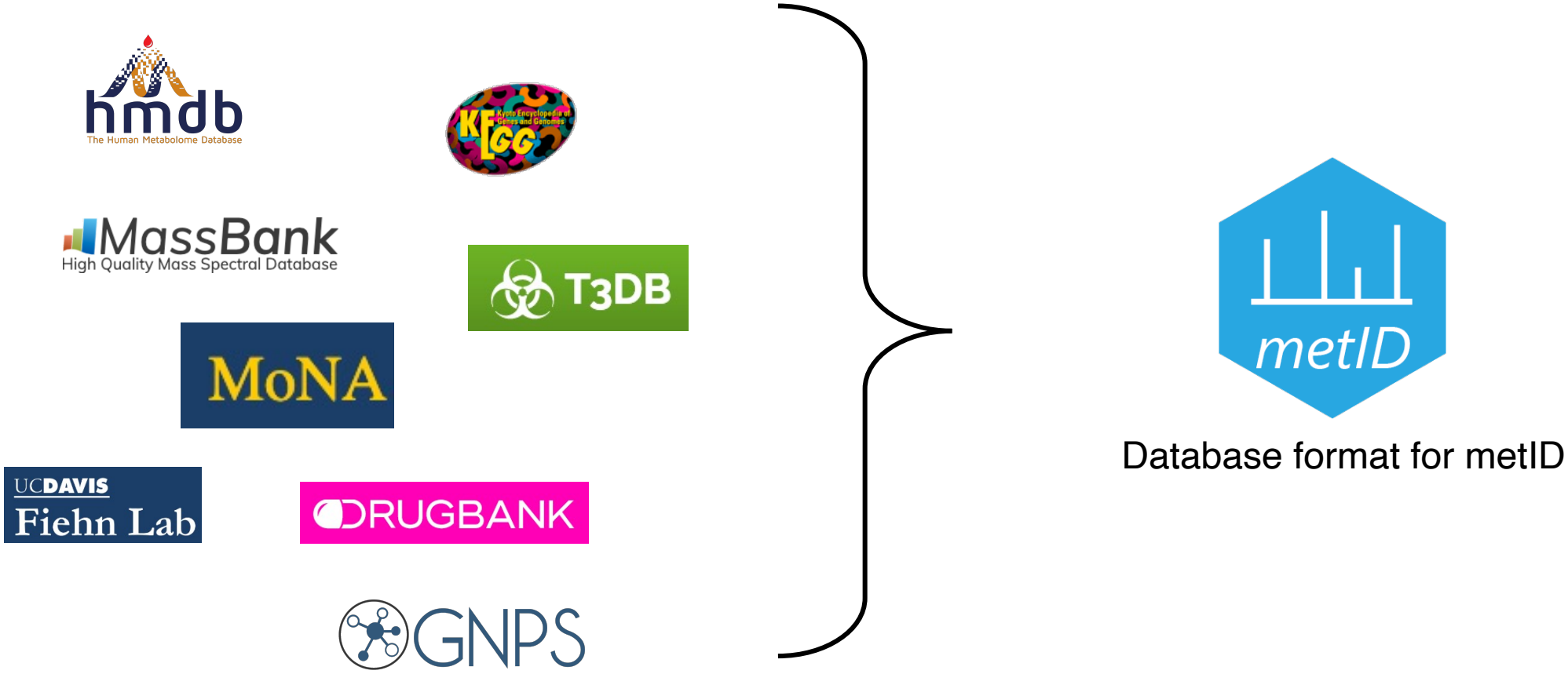


Metabolite information

Spectrum information

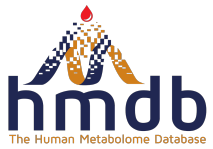
Database format for metID

Public Databases



Database format for metID

Public Databases



Example Code

Read databases from other tools

```
> massbank_database <-
> construct_mona_database(file = “MassBank.msp”,
  source = ”MassBank")

> mona_database <-
  construct_mona_database(file = “MoNA.msp”,
  source = "MoNA")

> gnps_database <-
  construct_gnps_database(file = “GNPS.msp”,
  source = ”GNPS")
```

Output databases for other tools

```
> write_msp_mona(database = database, path = ".")
> write_msp_massbank(database = database, path = ".")
> write_msp_gnps(database = database, path = ".")

> write_mgf_mona(database = database, path = ".")
> write_mgf_massbank(database = database, path = ".")
> write_mgf_gnps(database = database, path = ".")
```

Databases Provided in metID

Database	Compound number	Spectrum number	Information	Level	Source
msDatabase_rplc0.0.2	**917**	**2,047**	**mz/RT/MS^2**	**1**	**Snyder lab**
msDatabase_hilic0.0.2	**846**	**2,570**	**mz/RT/MS^2**	**1**	**Snyder lab**
hmdbDatabase0.0.2	5,646	22,331	mz/MS^2	2	https://hmdb.ca/downloads
massbankDatabase0.0.2	18,311	91,148	mz/MS^2	2	https://massbank.eu/MassBank
monaDatabase0.0.2	19,537	40,315	mz/MS^2	2	https://mona.fiehnlab.ucdavis.edu
orbitrapDatabase0.0.1[3]	8,360	23,227	mz/MS^2	2	https://mona.fiehnlab.ucdavis.edu
fiehn_hilic_database0.0.1	3,042	3,042	mz/MS^2	2	https://fiehnlab.ucdavis.edu/staff/kind/publications

Databases Provided in metID

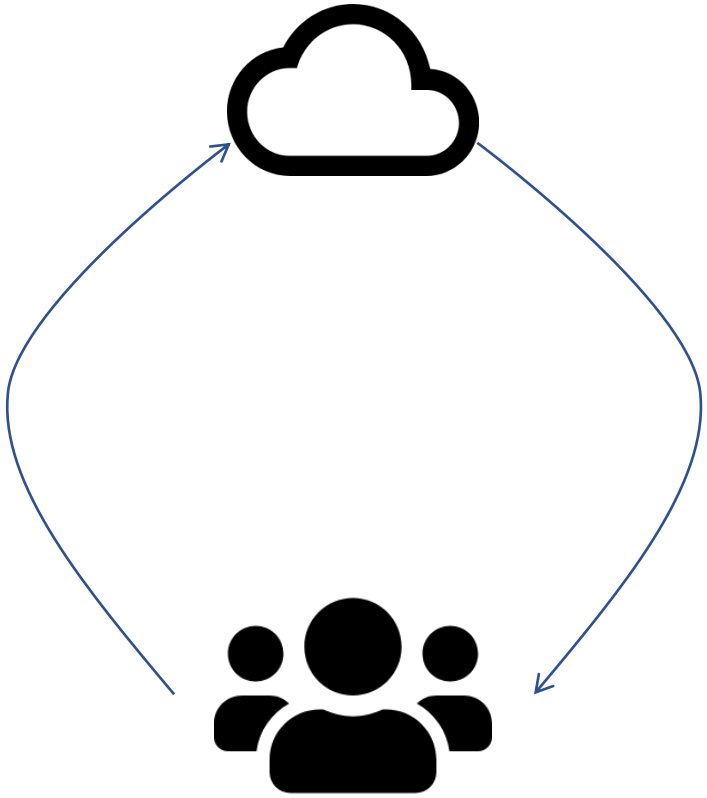
Database	Compound number	Spectrum number	Information	Level	Source
hmdbMS1Database0.0.1	114,004	0	mz	3	https://hmdb.ca/downloads
keggMS1Database_1.0	16,409	0	mz	3	https://www.genome.jp/kegg/compound/
drugbankMS1Database5.1.8	11,174	0	mz	3	https://go.drugbank.com/releases/latest
T3DBMS1Database_1.0	3,533	0	mz	3	http://www.t3db.ca/downloads
bloodExposomeMS1Database_1.0	65,957	0	mz	3	https://bloodexposome.org/#/download

Databases Provided in metID

Database	Compound number	Spectrum number	Information	Level	Source
hmdbMS1Database0.0.1	114,004	0	mz	3	https://hmdb.ca/downloads
keggMS1Database_1.0	16,409	0	mz	3	https://www.genome.jp/kegg/compound/
drugbankMS1Database5.1.8	11,174	0	mz	3	https://go.drugbank.com/releases/latest
T3DBMS1Database_1.0	3,533	0	mz	3	http://www.t3db.ca/downloads
bloodExposomeMS1Database_1.0	65,957	0	mz	3	https://bloodexposome.org/#/download

54,896 compound and 180,063 spectra in total
(Only the databases with MS/MS spectra)

Database Sharing



metID 1.0.0 | Help documents | News | Public databases | Reference | Get started | Search...

Database provided for `metID`

Xiaotao Shen PhD (https://www.shenxt.info/)

Si Wu PhD

School of Medicine, Stanford University

Created on 2020-03-28 and updated on 2021-05-10

Source: `vignettes/public_databases.Rmd`

Contents

- In-house MS2MS^2 databases from Michael Snyder lab
- Public MS2MS^2 databases
- Public MS1MS^1 databases

In-house MS^2 databases from Michael Snyder lab

1. Michael Snyder HILIC databases

- Professor Michael Snyder's lab. More than 1,000 metabolites.
- Download here

> If you need this database, please contact shenxt@stanford.edu

2. Michael Snyder HILIC databases

- Professor Michael Snyder's lab. More than 1,000 metabolites.
- Download here

Automatable Metabolite annotation

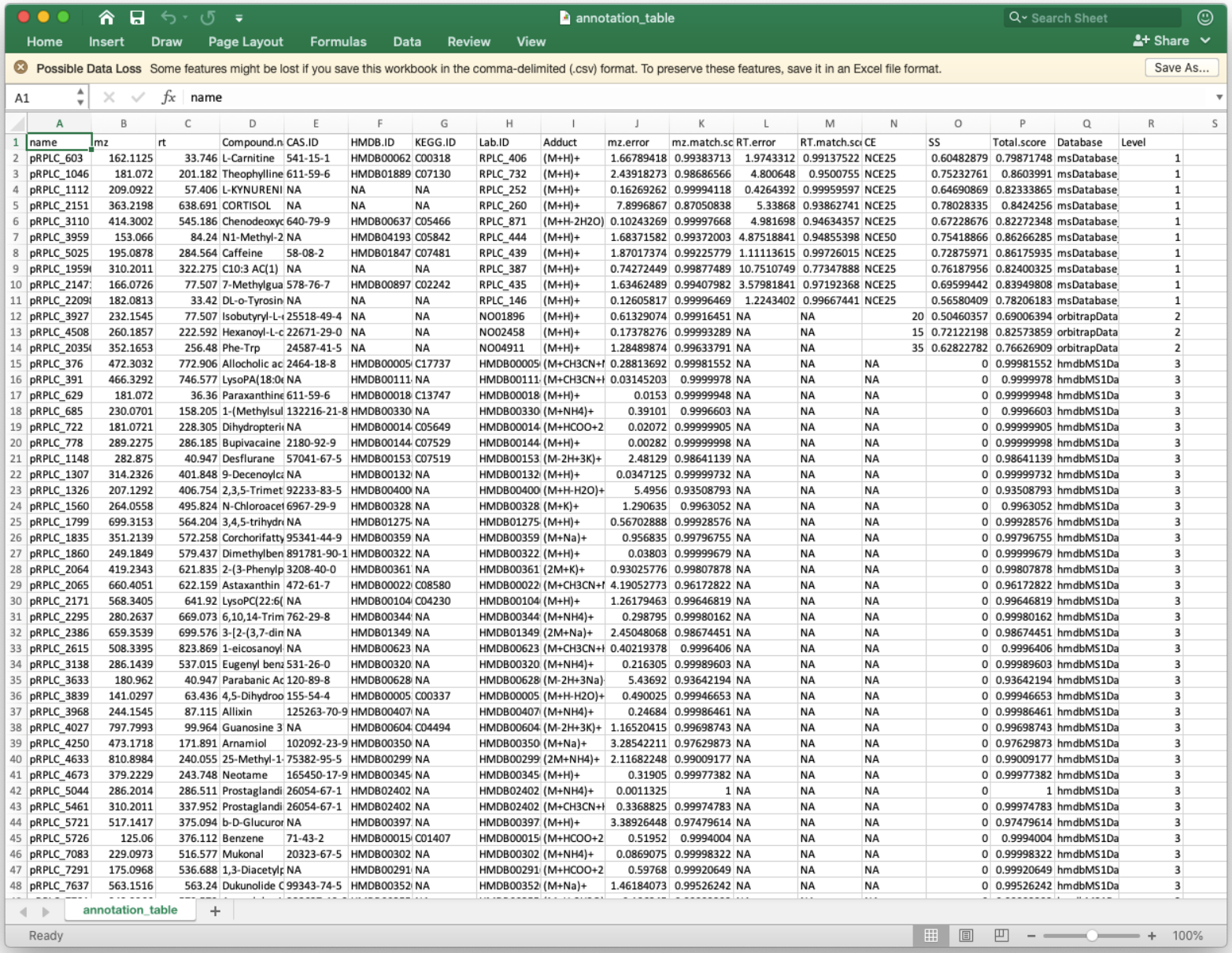
Example Code

```
> param1 <-
  identify_metabolites_params(ms1.match.ppm = 15, rt.match.tol = 15, polarity = "positive", ce = "all", column = "rp",
  total.score.tol = 0.5, candidate.num = 3, threads = 3, database = "msDatabase_rplc0.0.2" )
> param2 <-
  identify_metabolites_params(ms1.match.ppm = 15, rt.match.tol = 15, polarity = “positive”, ce = “all”, column = “rp”,
  total.score.tol = 0.5, candidate.num = 3, threads = 3, database = ”MoNA")

> result <-
  identify_metabolite_all(ms1.data = “ms1.peak.table.csv”,
                          ms2.data = “QC1_MSMS_NCE25.mgf”,
                          parameter.list = c(param1, param2))
```

```
result[[1]]
#> --------------metID version-----------
#> 0.4.1
#> -----------Identifications------------
#> (Use get_identification_table() to get identification table)
#> There are 100 peaks
#> 23 peaks have MS2 spectra
#> There are 14 metabolites are identified
#> There are 10 peaks with identification
#> -----------Parameters------------
#> (Use get_parameters() to get all the parameters of this processing)
#> Polarity: positive
#> Collision energy: all
#> database: msDatabase_rplc0.0.2
#> Total score cutoff: 0.5 #> Column: rp
#> Adduct table: #> (M+H)+;(M+H-H2O)+;(M+H-2H2O)+
```

Automatable Metabolite annotation



annotation_table

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Possible Data Loss Some features might be lost if you save this workbook in the comma-delimited (.csv) format. To preserve these features, save it in an Excel file format. Save As...

A1 name

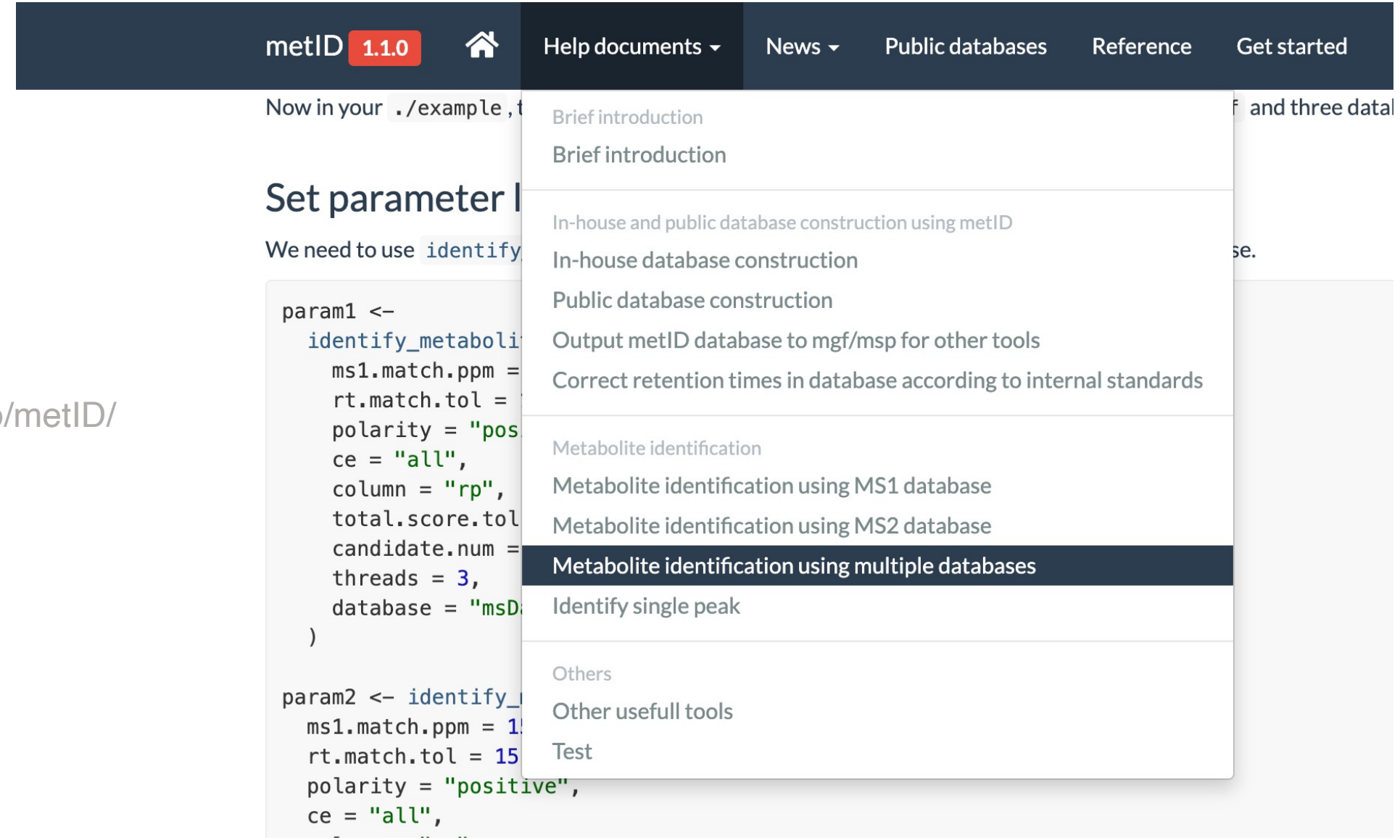
	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S
1	name	mz	rt	Compound.n	CAS.ID	HMDB.ID	KEGG.ID	Lab.ID	Adduct	mz.error	mz.match.sc	RT.error	RT.match.sc	CE	SS	Total.score	Database	Level	
2	pRPLC_603	162.1125	33.746	L-Carnitine	541-15-1	HMDB00062	C00318	RPLC_406	(M+H)+	1.66789418	0.99383713	1.9743312	0.99137522	NCE25	0.60482879	0.79871748	msDatabase	1	
3	pRPLC_1046	181.072	201.182	Theophylline	611-59-6	HMDB01889	C07130	RPLC_732	(M+H)+	2.43918273	0.98686566	4.800648	0.9500755	NCE25	0.75232761	0.8603991	msDatabase	1	
4	pRPLC_1112	209.0922	57.406	L-KYNURENI	NA	NA	NA	RPLC_252	(M+H)+	0.16269262	0.99994118	0.4264392	0.99959597	NCE25	0.64690869	0.82333865	msDatabase	1	
5	pRPLC_2151	363.2198	638.691	CORTISOL	NA	NA	NA	RPLC_260	(M+H)+	7.8996867	0.87050838	5.33868	0.93862741	NCE25	0.78028335	0.8424256	msDatabase	1	
6	pRPLC_3110	414.3002	545.186	Chenodeoxyc	640-79-9	HMDB00637	C05466	RPLC_871	(M+H-2H2O)	0.10243269	0.99997668	4.981698	0.94634357	NCE25	0.67228676	0.82272348	msDatabase	1	
7	pRPLC_3959	153.066	84.24	N1-Methyl-2	NA	HMDB04193	C05842	RPLC_444	(M+H)+	1.68371582	0.99372003	4.87518841	0.94855398	NCE50	0.75418866	0.86266285	msDatabase	1	
8	pRPLC_5025	195.0878	284.564	Caffeine	58-08-2	HMDB01847	C07481	RPLC_439	(M+H)+	1.87017374	0.99225779	1.11113615	0.99726015	NCE25	0.72875971	0.86175935	msDatabase	1	
9	pRPLC_1959	310.2011	322.275	C10:3 AC(1)	NA	NA	NA	RPLC_387	(M+H)+	0.74272449	0.99877489	10.7510749	0.77347888	NCE25	0.76187956	0.82400325	msDatabase	1	
10	pRPLC_2147	166.0726	77.507	7-Methylgua	578-76-7	HMDB00897	C02242	RPLC_435	(M+H)+	1.63462489	0.99407982	3.57981841	0.97192368	NCE25	0.69599442	0.83949808	msDatabase	1	
11	pRPLC_2209	182.0813	33.42	DL-o-Tyrosin	NA	NA	NA	RPLC_146	(M+H)+	0.12605817	0.99996469	1.2243402	0.99667441	NCE25	0.56580409	0.78206183	msDatabase	1	
12	pRPLC_3927	232.1545	77.507	Isobutyryl-L-(	25518-49-4	NA	NA	NO01896	(M+H)+	0.61329074	0.99916451	NA	NA	20	0.50460357	0.69006394	orbitrapData	2	
13	pRPLC_4508	260.1857	222.592	Hexanoyl-L-c	22671-29-0	NA	NA	NO02458	(M+H)+	0.17378276	0.99993289	NA	NA	15	0.72122198	0.82573859	orbitrapData	2	
14	pRPLC_2035	352.1653	256.48	Phe-Trp	24587-41-5	NA	NA	NO04911	(M+H)+	1.28489874	0.99633791	NA	NA	35	0.62822782	0.76626909	orbitrapData	2	
15	pRPLC_376	472.3032	772.906	Allocholic ac	2464-18-8	HMDB00005	C17737	HMDB00005	(M+CH3CN+H	0.28813692	0.99981552	NA	NA	NA	0	0.99981552	hmdbMS1Da	3	
16	pRPLC_391	466.3292	746.577	LysoPA(18:0(	NA	HMDB00111	NA	HMDB00111	(M+CH3CN+H	0.03145203	0.9999978	NA	NA	NA	0	0.9999978	hmdbMS1Da	3	
17	pRPLC_629	181.072	36.36	Paraxanthine	611-59-6	HMDB00018	C13747	HMDB00018	(M+H)+	0.0153	0.99999948	NA	NA	NA	0	0.99999948	hmdbMS1Da	3	
18	pRPLC_685	230.0701	158.205	1-(Methylsul	132216-21-8	HMDB00330	NA	HMDB00330	(M+NH4)+	0.39101	0.9996603	NA	NA	NA	0	0.9996603	hmdbMS1Da	3	
19	pRPLC_722	181.0721	228.305	Dihydropteri	NA	HMDB00014	C05649	HMDB00014	(M+HCOO+2	0.02072	0.99999905	NA	NA	NA	0	0.99999905	hmdbMS1Da	3	
20	pRPLC_778	289.2275	286.185	Bupivacaine	2180-92-9	HMDB00144	C07529	HMDB00144	(M+H)+	0.00282	0.99999998	NA	NA	NA	0	0.99999998	hmdbMS1Da	3	
21	pRPLC_1148	282.875	40.947	Desflurane	57041-67-5	HMDB00153	C07519	HMDB00153	(M-2H+3K)+	2.48129	0.98641139	NA	NA	NA	0	0.98641139	hmdbMS1Da	3	
22	pRPLC_1307	314.2326	401.848	9-Decenoylca	NA	HMDB00132	NA	HMDB00132	(M+H)+	0.0347125	0.99999732	NA	NA	NA	0	0.99999732	hmdbMS1Da	3	
23	pRPLC_1326	207.1292	406.754	2,3,5-Trimet	92233-83-5	HMDB00400	NA	HMDB00400	(M+H-H2O)+	5.4956	0.93508793	NA	NA	NA	0	0.93508793	hmdbMS1Da	3	
24	pRPLC_1560	264.0558	495.824	N-Chloroacet	6967-29-9	HMDB00328	NA	HMDB00328	(M+K)+	1.290635	0.9963052	NA	NA	NA	0	0.9963052	hmdbMS1Da	3	
25	pRPLC_1799	699.3153	564.204	3,4,5-trihydr	NA	HMDB01275	NA	HMDB01275	(M+H)+	0.56702888	0.99928576	NA	NA	NA	0	0.99928576	hmdbMS1Da	3	
26	pRPLC_1835	351.2139	572.258	Corchorifatty	95341-44-9	HMDB00359	NA	HMDB00359	(M+Na)+	0.956835	0.99796755	NA	NA	NA	0	0.99796755	hmdbMS1Da	3	
27	pRPLC_1860	249.1849	579.437	Dimethylben	891781-90-1	HMDB00322	NA	HMDB00322	(M+H)+	0.03803	0.99999679	NA	NA	NA	0	0.99999679	hmdbMS1Da	3	
28	pRPLC_2064	419.2343	621.835	2-(3-Phenylp	3208-40-0	HMDB00361	NA	HMDB00361	(2M+K)+	0.93025776	0.99807878	NA	NA	NA	0	0.99807878	hmdbMS1Da	3	
29	pRPLC_2065	660.4051	622.159	Astaxanthin	472-61-7	HMDB00022	C08580	HMDB00022	(M+CH3CN+H	4.19052773	0.96172822	NA	NA	NA	0	0.96172822	hmdbMS1Da	3	
30	pRPLC_2171	568.3405	641.92	LysoPC(22:6(	NA	HMDB00104	C04230	HMDB00104	(M+H)+	1.26179463	0.99646819	NA	NA	NA	0	0.99646819	hmdbMS1Da	3	
31	pRPLC_2295	280.2637	669.073	6,10,14-Trim	762-29-8	HMDB00344	NA	HMDB00344	(M+NH4)+	0.298795	0.99980162	NA	NA	NA	0	0.99980162	hmdbMS1Da	3	
32	pRPLC_2386	659.3539	699.576	3-[2-(3,7-dim	NA	HMDB01349	NA	HMDB01349	(2M+Na)+	2.45048068	0.98674451	NA	NA	NA	0	0.98674451	hmdbMS1Da	3	
33	pRPLC_2615	508.3395	823.869	1-eicosanoyl	NA	HMDB00623	NA	HMDB00623	(M+CH3CN+H	0.40219378	0.9996406	NA	NA	NA	0	0.9996406	hmdbMS1Da	3	
34	pRPLC_3138	286.1439	537.015	Eugenyl benz	531-26-0	HMDB00320	NA	HMDB00320	(M+NH4)+	0.216305	0.99989603	NA	NA	NA	0	0.99989603	hmdbMS1Da	3	
35	pRPLC_3633	180.962	40.947	Parabanic Ac	120-89-8	HMDB00628	NA	HMDB00628	(M-2H+3Na)	5.43692	0.93642194	NA	NA	NA	0	0.93642194	hmdbMS1Da	3	
36	pRPLC_3839	141.0297	63.436	4,5-Dihydroo	155-54-4	HMDB00005	C00337	HMDB00005	(M+H-H2O)+	0.490025	0.99946653	NA	NA	NA	0	0.99946653	hmdbMS1Da	3	
37	pRPLC_3968	244.1545	87.115	Allixin	125263-70-9	HMDB00407	NA	HMDB00407	(M+NH4)+	0.24684	0.99986461	NA	NA	NA	0	0.99986461	hmdbMS1Da	3	
38	pRPLC_4027	797.7993	99.964	Guanosine 3	NA	HMDB00604	C04494	HMDB00604	(M-2H+3K)+	1.16520415	0.99698743	NA	NA	NA	0	0.99698743	hmdbMS1Da	3	
39	pRPLC_4250	473.1718	171.891	Arnamiol	102092-23-9	HMDB00350	NA	HMDB00350	(M+Na)+	3.28542211	0.97629873	NA	NA	NA	0	0.97629873	hmdbMS1Da	3	
40	pRPLC_4633	810.8984	240.055	25-Methyl-1-	75382-95-5	HMDB00299	NA	HMDB00299	(2M+NH4)+	2.11682248	0.99009177	NA	NA	NA	0	0.99009177	hmdbMS1Da	3	
41	pRPLC_4673	379.2229	243.748	Neotame	165450-17-9	HMDB00345	NA	HMDB00345	(M+H)+	0.31905	0.99977382	NA	NA	NA	0	0.99977382	hmdbMS1Da	3	
42	pRPLC_5044	286.2014	286.511	Prostaglandi	26054-67-1	HMDB02402	NA	HMDB02402	(M+NH4)+	0.0011325	1	NA	NA	NA	0	1	hmdbMS1Da	3	
43	pRPLC_5461	310.2011	337.952	Prostaglandi	26054-67-1	HMDB02402	NA	HMDB02402	(M+CH3CN+H	0.3368825	0.99974783	NA	NA	NA	0	0.99974783	hmdbMS1Da	3	
44	pRPLC_5721	517.1417	375.094	b-D-Glucuror	NA	HMDB00397	NA	HMDB00397	(M+H)+	3.38926448	0.97479614	NA	NA	NA	0	0.97479614	hmdbMS1Da	3	
45	pRPLC_5726	125.06	376.112	Benzene	71-43-2	HMDB00015	C01407	HMDB00015	(M+HCOO+2	0.51952	0.9994004	NA	NA	NA	0	0.9994004	hmdbMS1Da	3	
46	pRPLC_7083	229.0973	516.577	Mukonal	20323-67-5	HMDB00302	NA	HMDB00302	(M+NH4)+	0.0869075	0.99998322	NA	NA	NA	0	0.99998322	hmdbMS1Da	3	
47	pRPLC_7291	175.0968	536.688	1,3-Diacetyl	NA	HMDB00291	NA	HMDB00291	(M+HCOO+2	0.59768	0.99920649	NA	NA	NA	0	0.99920649	hmdbMS1Da	3	
48	pRPLC_7637	563.1516	563.24	Dukunolide C	99343-74-5	HMDB00352	NA	HMDB00352	(M+Na)+	1.46184073	0.99526242	NA	NA	NA	0	0.99526242	hmdbMS1Da	3	

annotation_table

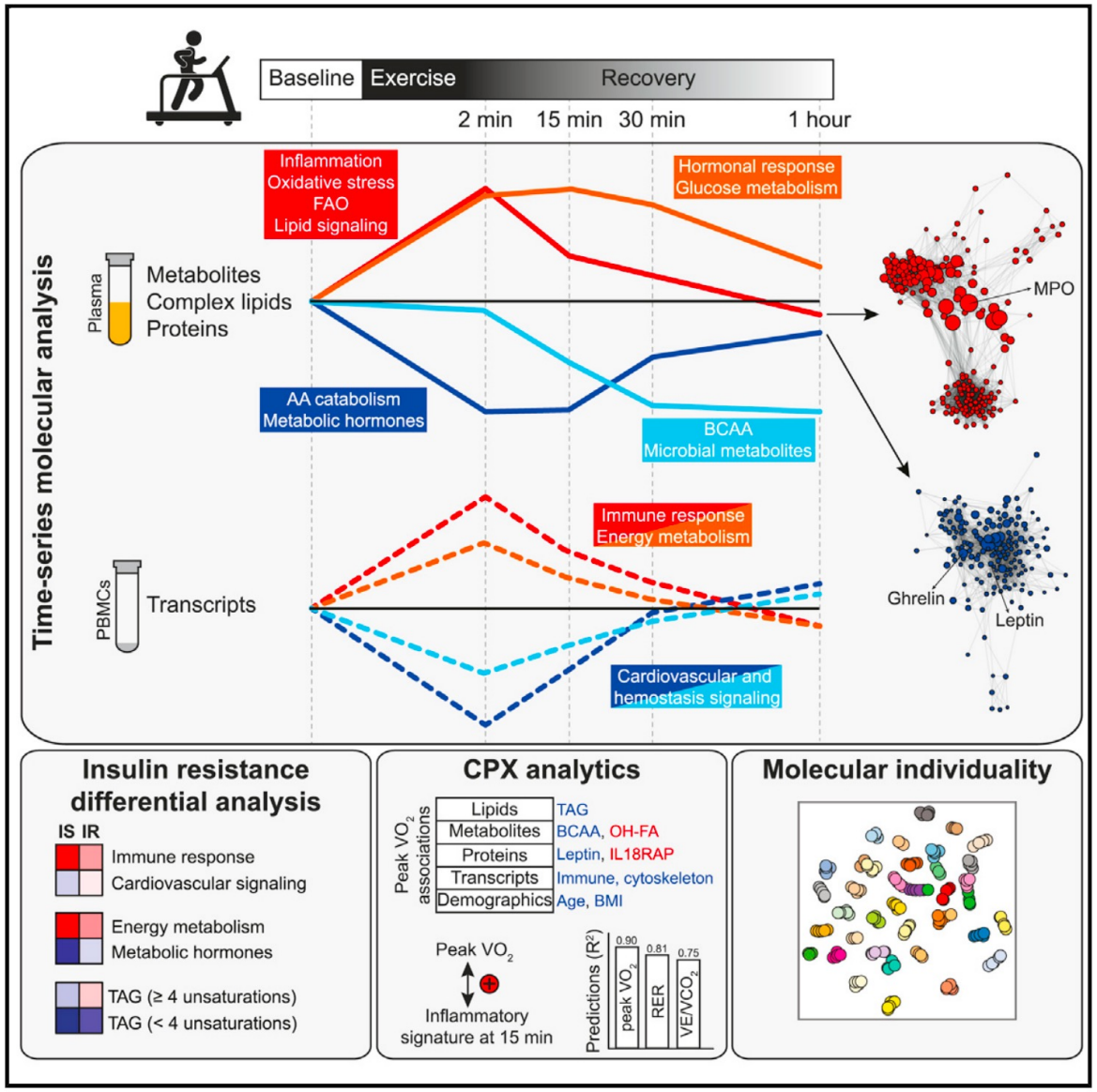
Ready 100%

Other functions from metID and website of metID

https://jaspershen.github.io/metID/



Case Study



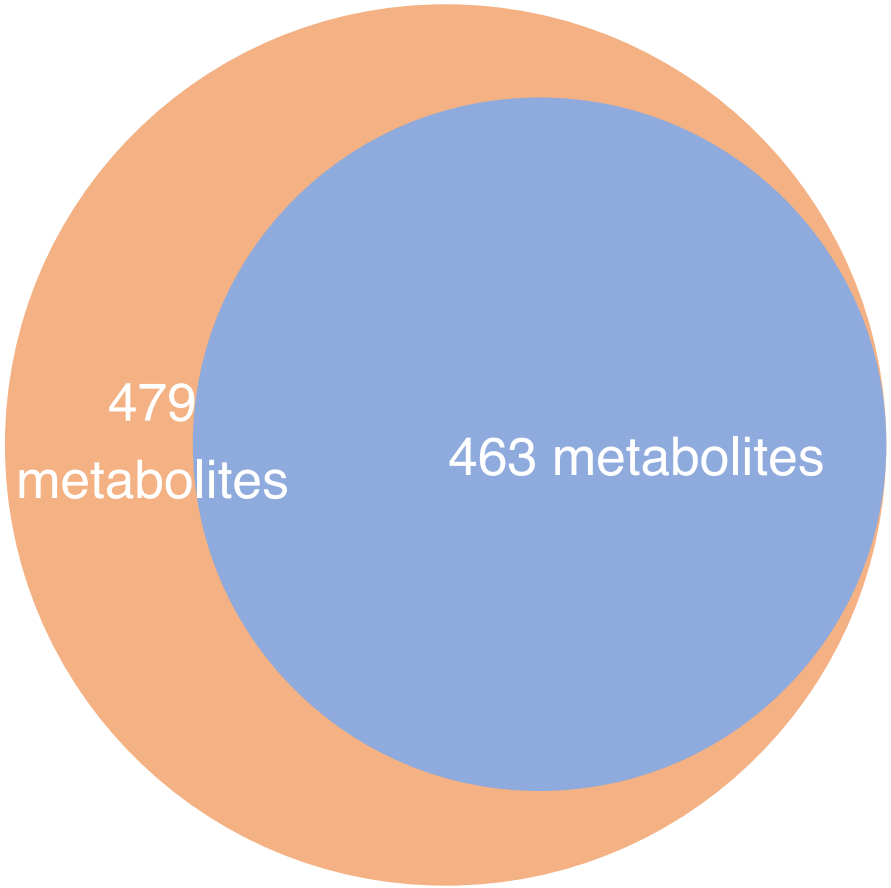
Variable	Information
Sample type	Plasma
Subject sample number	310
QC sample number	36
Data acquisition	Untargeted metabolomics
Instrument platform	LC-MS
Chromatographic condition	RPLC + HILIC
Polarity mode	Positive + negative

463 manually annotate metabolites. (Golden standard)

Contrepois et al. Cell, 2020.

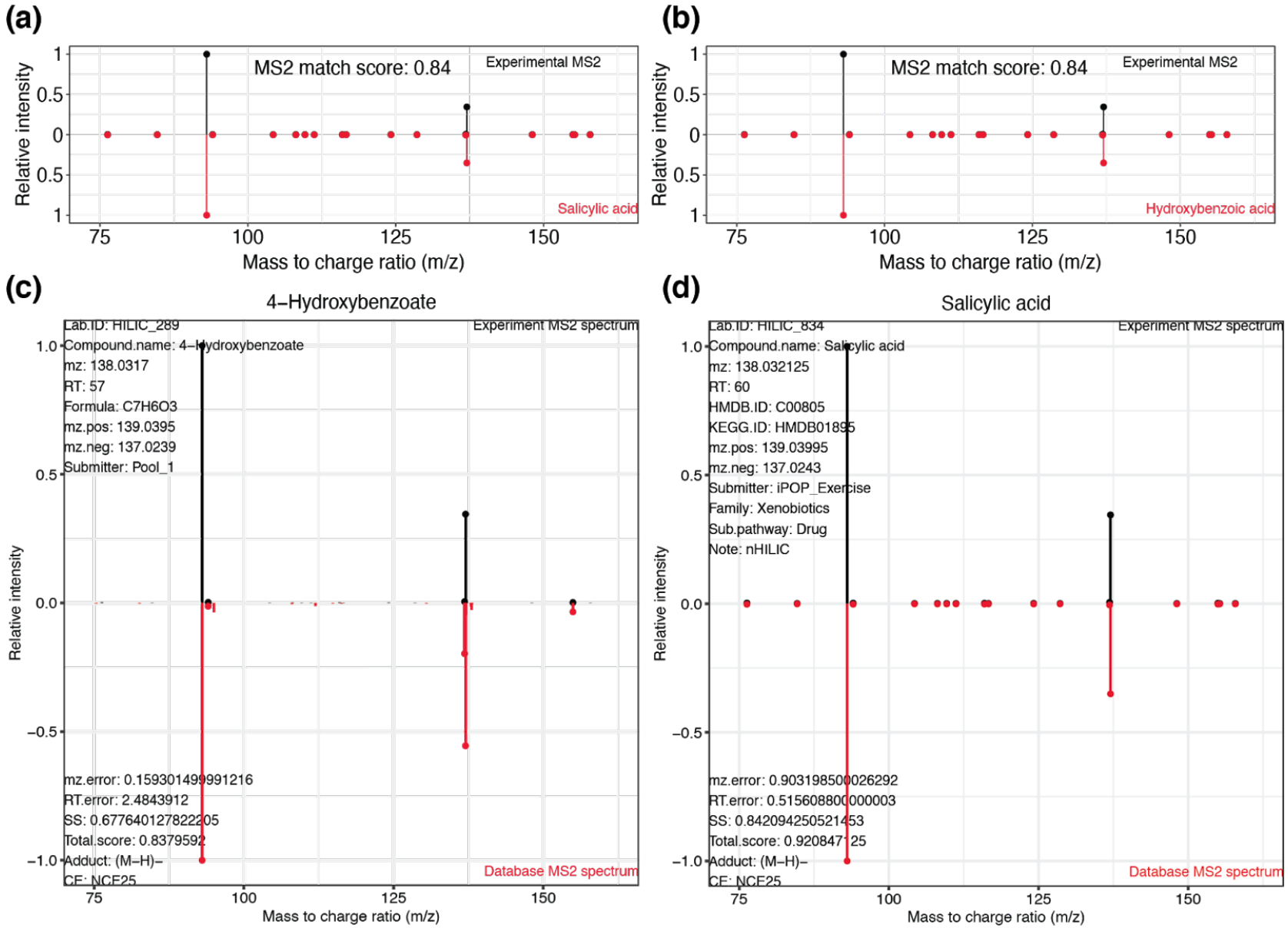
Case Study

Same dataset processed by metID



1. We retrieved all the 463 metabolites annotated in the original paper.
2. 457 out of 463 annotation are consistent with exercise paper.
3. We additionally annotate 479 more metabolites.

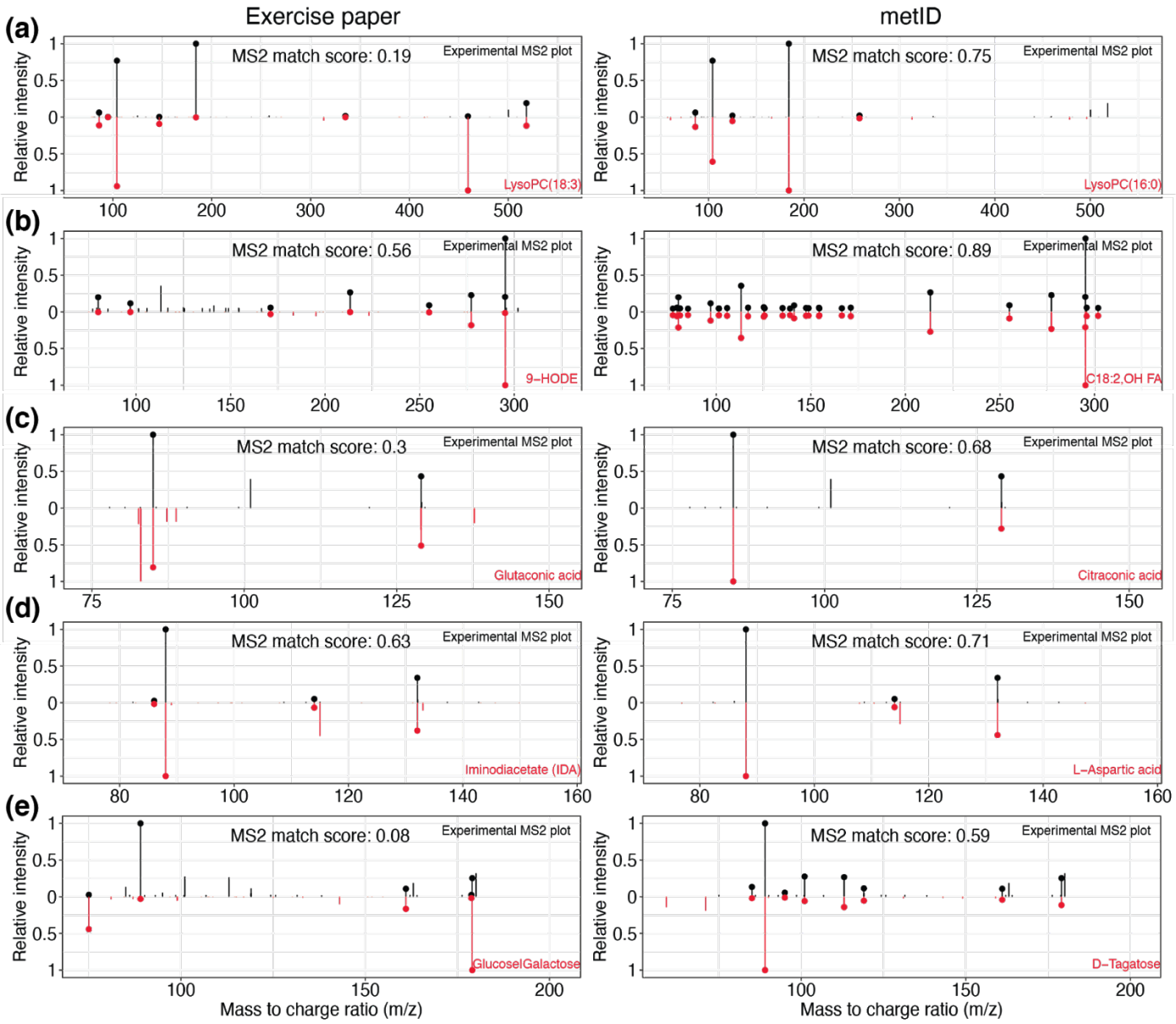
Non-consistent Annotations



peak 1.00_137.0243m/z

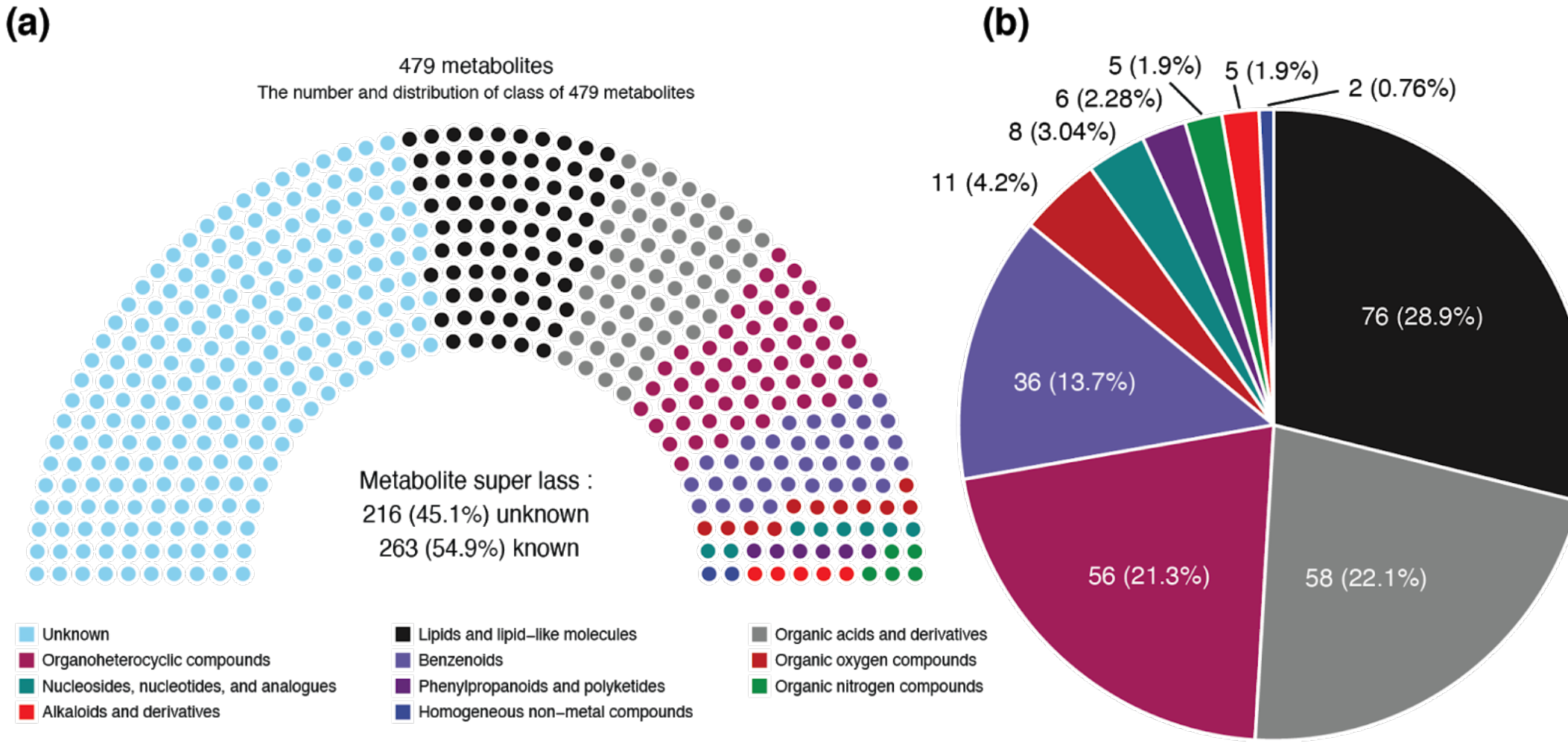
For metID, rank 2 annotation is consistent with the original paper annotation.

Non-consistent Annotations



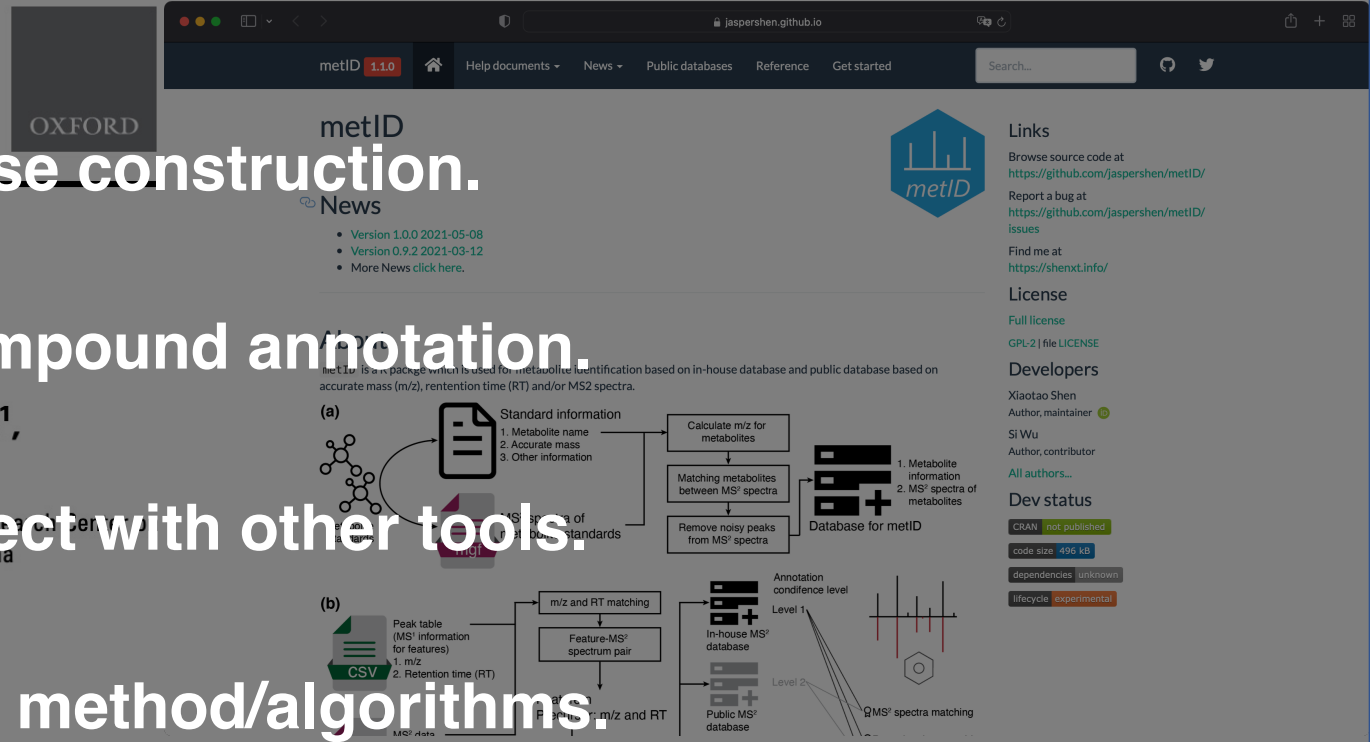
For the other five metabolites with the inconsistency of annotation, we found that the annotation by metID has higher MS/MS scores than the annotation in the original paper, indicating metID has high annotation accuracy.

479 More Metabolites



Summary

- In-house database construction.
- Automatable compound annotation.
- Flexible to connect with other tools.
- Easy to add new method/algorithms.



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Applications Note

OXFORD

Systems biology

metID: an R package for automatable compound annotation for LC–MS-based data

Xiaotao Shen [1,†], Si Wu[1,†], Liang Liang[1], Songjie Chen[1], Kévin Contrepois[1], Zheng-Jiang Zhu[2,*] and Michael Snyder[1,*]

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†The authors wish it to be known that, in their opinion, the first two authors should be regarded as Joint First Authors.
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jaspershen.github.io

metID 1.1.0 | Help documents | News | Public databases | Reference | Get started | Search...

metID

News

- Version 1.0.0 2021-05-08
- Version 0.9.2 2021-03-12
- More News click here.

accurate mass (m/z), rentention time (RT) and/or MS2 spectra.

(a) Standard information 1. Metabolite name 2. Accurate mass 3. Other information; Calculate m/z for metabolites; Matching metabolites between MS² spectra; Remove noisy peaks from MS² spectra; Database for metID: 1. Metabolite information 2. MS² spectra of metabolites

(b) Peak table (MS¹ information for features) 1. m/z 2. Retention time (RT); CSV; m/z and RT matching; Feature-MS² spectrum pair; In-house MS² database; Public MS² database; Annotation confidence level; Level 1; Level 2; MS² spectra matching

Links

Browse source code at https://github.com/jaspershen/metID/

Report a bug at https://github.com/jaspershen/metID/issues

Find me at https://shenxt.info/

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Developers

Xiaotao Shen
Author, maintainer

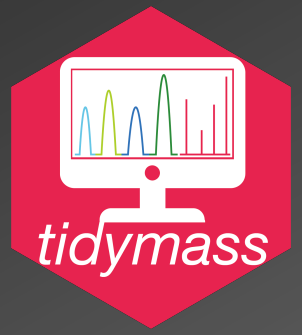
Si Wu
Author, contributor

All authors...

Dev status

CRAN not published | code size 496 kB | dependencies unknown | lifecycle experimental

https://jaspershen.github.io/tidymass/



TidyMass: A Computational Framework for LC-MS Data processing and analysis

R is the most important language for bioinformatics analysis

Bioconductor

2,083 packages
(10/31/2021)

Comprehensive R Archive Network (CRAN)

18,357 packages
(10/31/2021)

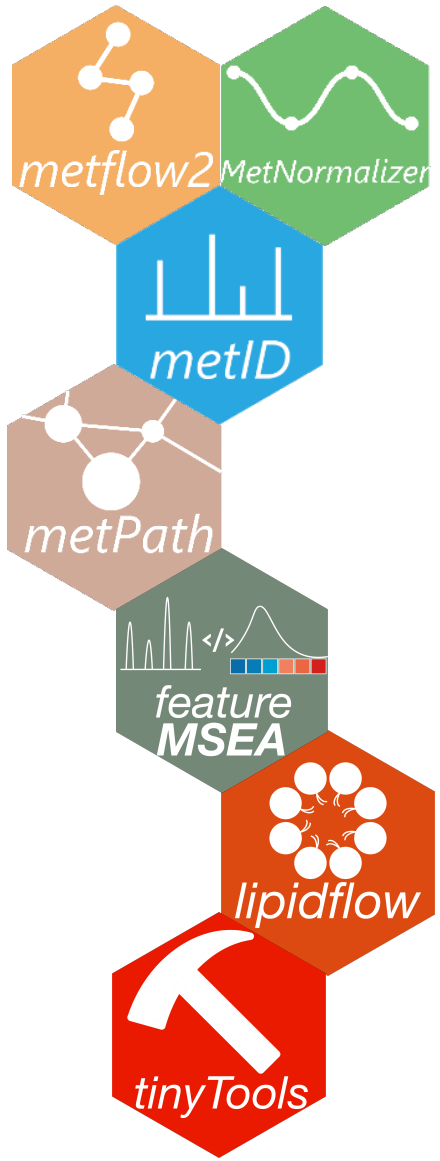
GitHub

34,268 active repos
(10/31/2021)

R-Forge

2,148 packages
(10/31/2021)

TidyMass: Collection of R Packages for Mass Spectrometry Data Analysis



lifecycle maturing **metflow2**: Raw MS data processing and data cleaning

https://jaspershen.github.io/metflow2/

lifecycle maturing **metNormalizer**: Data normalization and integration

https://jaspershen.github.io/MetNormalizer/

lifecycle maturing **metID**: Compound identification

https://jaspershen.github.io/metID/

lifecycle experimental **metPath:** Biological information mining

https://jaspershen.github.io/metPath/

lifecycle experimental **lipidflow:** Lipidomics data analysis. (Chuchu Wang)

https://jaspershen.github.io/lipidflow/

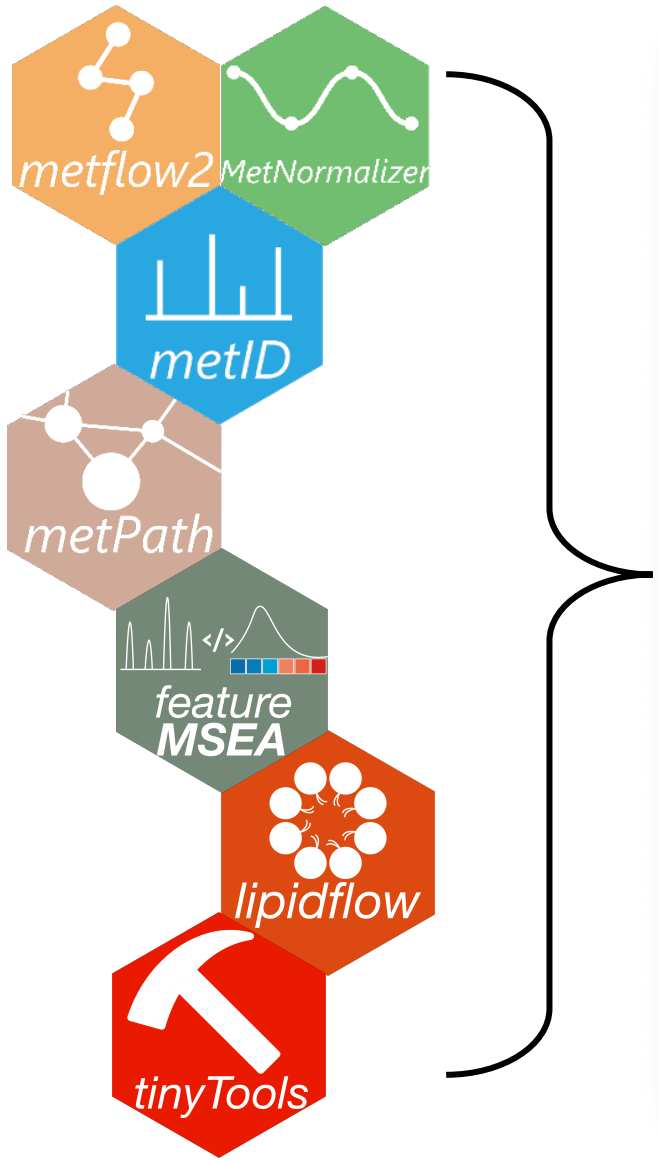
lifecycle experimental **fMSEA:** feature based metabolite set enrichment analysis

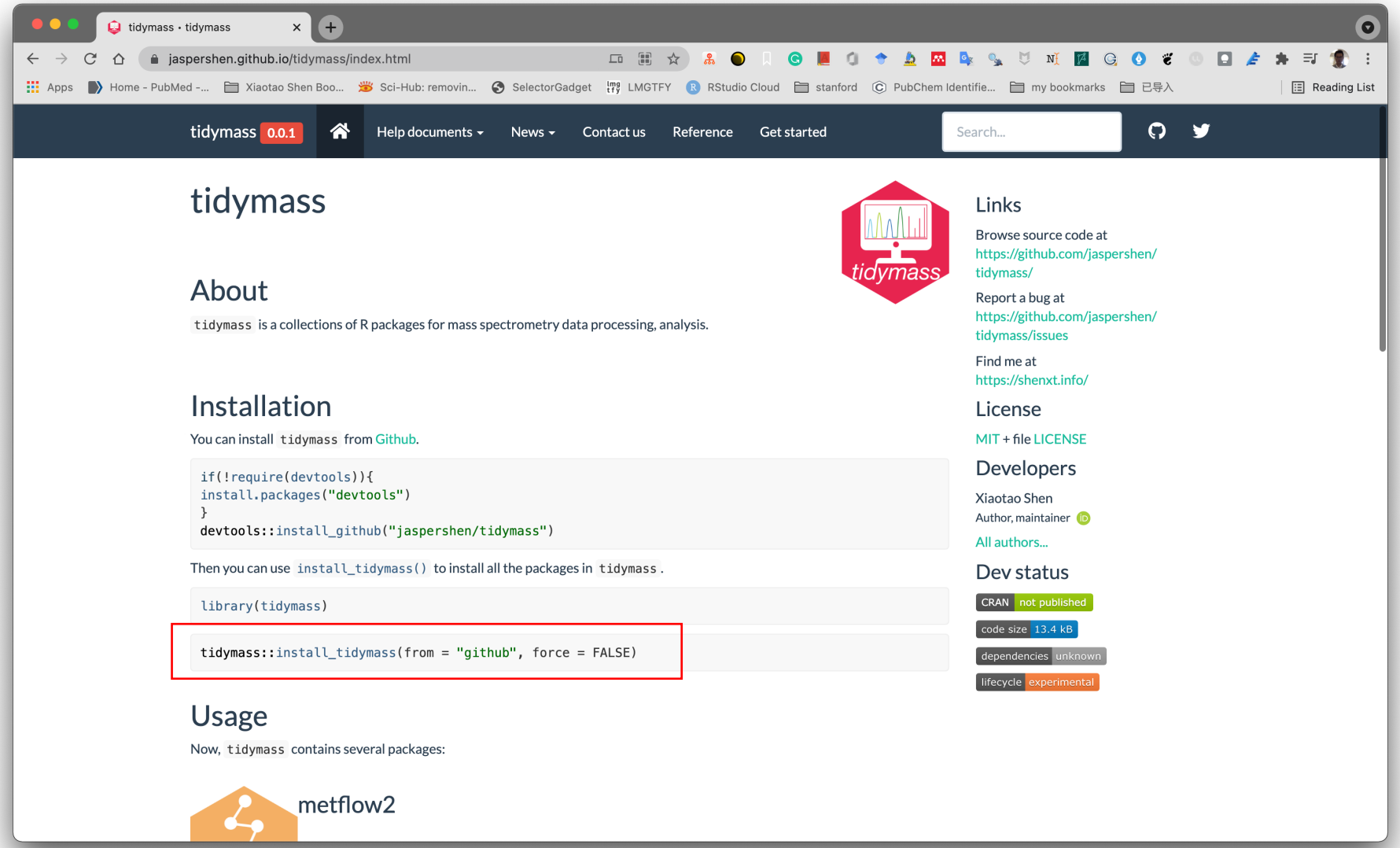
https://jaspershen.github.io/fMSEA/

lifecycle maturing **tinyTools:** Toolkit for MS data processing.

https://jaspershen.github.io/tinyTools/

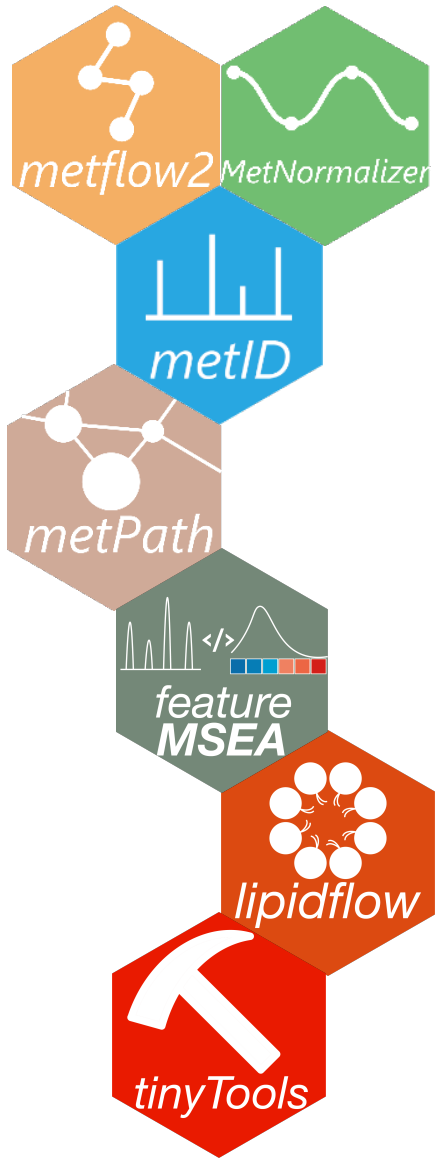
TidyMass: Collection of R Packages for Mass Spectrometry Data Analysis

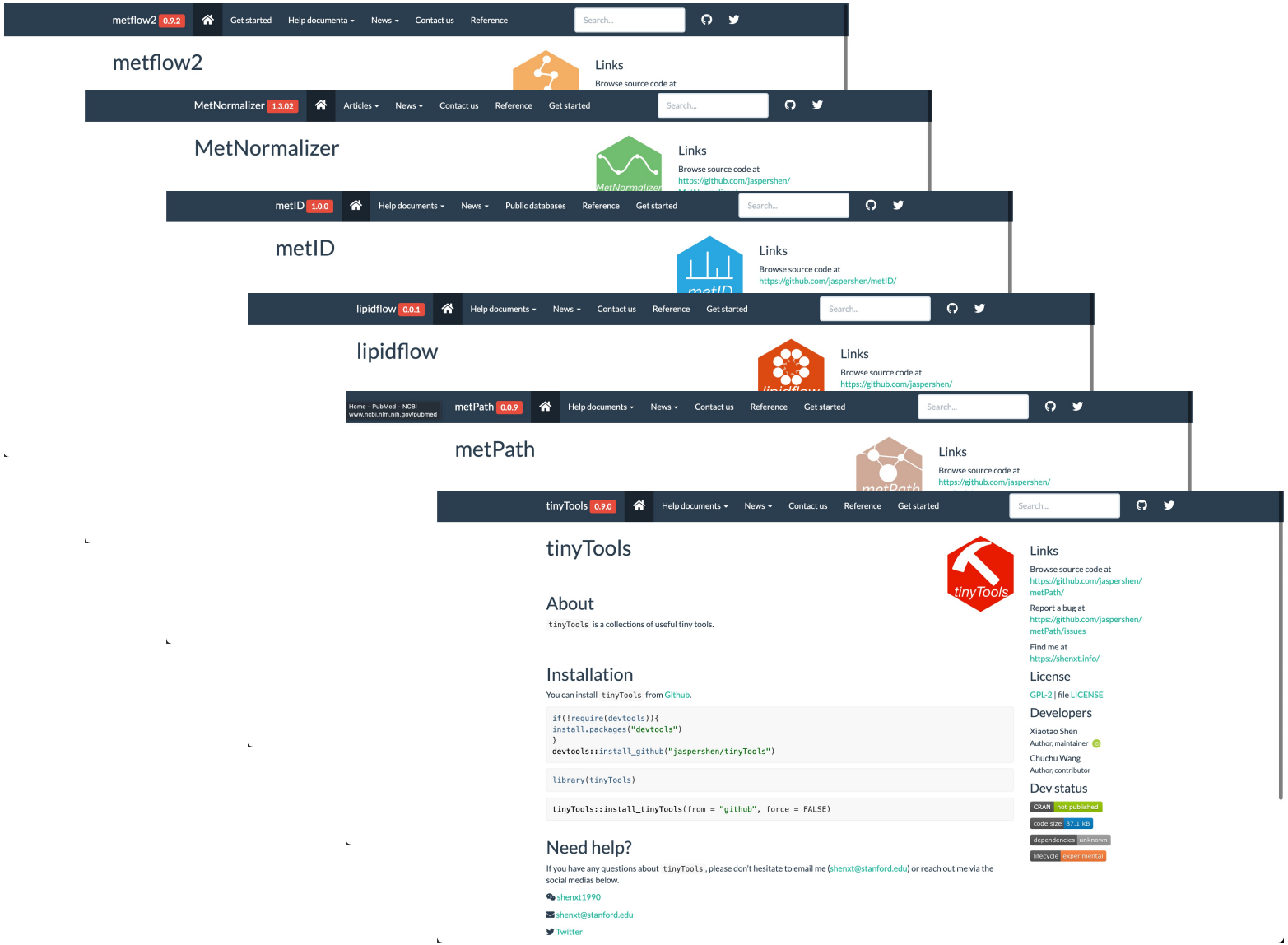




https://jaspershen.github.io/tidymass/

TidyMass: Collection of R Packages for Mass Spectrometry Data Analysis

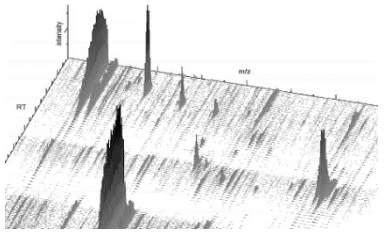




https://jaspershen.github.io/tidymass/

Workflow of LC-MS Data Processing and Analysis

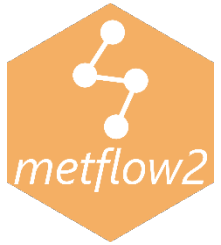
MS raw data



Data processing

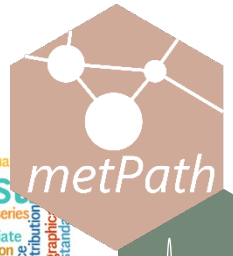
Peak table

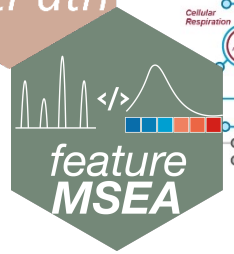
Data Cleaning



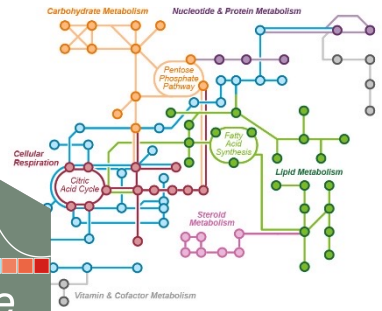
Compound identification

Statistical analysis





Biological interpretation



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Prof. Zheng-Jiang Zhu
(CAS)

Prof. Michael Snyder
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30