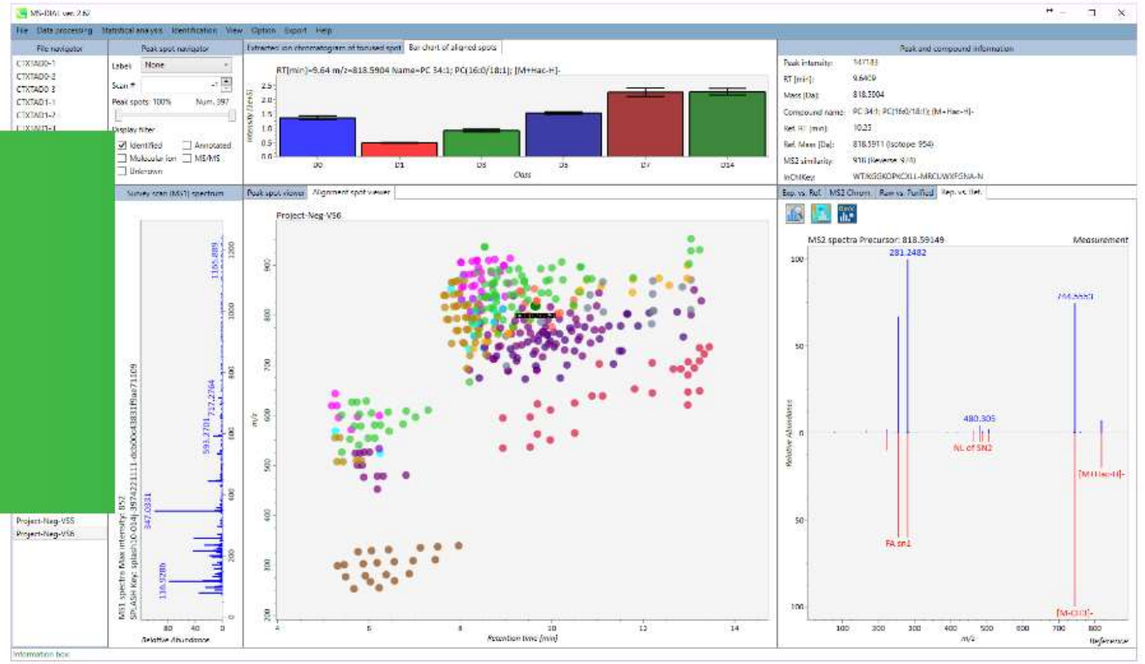
Untargeted Metabolomics Analysis
MS-DIAL

Shadab Ahmad, Ph.D. [C-CAMP]

CompMS | MS-DIAL (systemsomicslab.github.io)



MS-DIAL

Objective

MS-DIAL was launched as a universal program for untargeted metabolomics that supports multiple instruments (GC/MS, GC/MS/MS, LC/MS, and LC/MS/MS) and MS vendors (Agilent, Bruker, LECO, Sciex, Shimadzu, Thermo, and Waters). Common data formats such as netCDF (AIA) and mzML, can also be managed in our project. In addition, we released several MSP files including both EI- and MS/MS spectra as a 'start-up kit'. Moreover, MS-DIAL internally has a version of Fiehn lab's GC/MS database (oriented by FAME RI index), and in silico retention time- and MS/MS database for LC/MS/MS based lipidomics. The isotope labeled tracking can also be executed in LC/MS project.

It features
(1) spectral deconvolution for both GC/MS and data-independent MS/MS,
(2) streamlined criteria for peak identification,
(3) support of all data processing steps from raw data import to statistical analysis,
and (4) user-friendly graphic user interface.

Citation

✔ General, and lipidomics: A lipidome atlas in MS-DIAL 4. *Nature Biotechnology*, 38, 1159–1163, 2020 [NPG link]
Springer Nature 'SharedIt': full-text access to a view-only version of this paper

✔ Plant metabolomics and stable isotope labeling technology: A cheminformatics approach to characterize metabolomes in stable-isotope-labeled organisms. *Nature Methods*, 16, 295–298, 2019 [NPG link]
Springer Nature 'SharedIt': full-text access to a view-only version of this paper

MS-DIAL


Open recent projects
New project
Load project
MS-DIAL
5.3.240328-alpha.5
YouTube
Twitter
GitHub

Setting project parameters

Project parameters

Start up new project

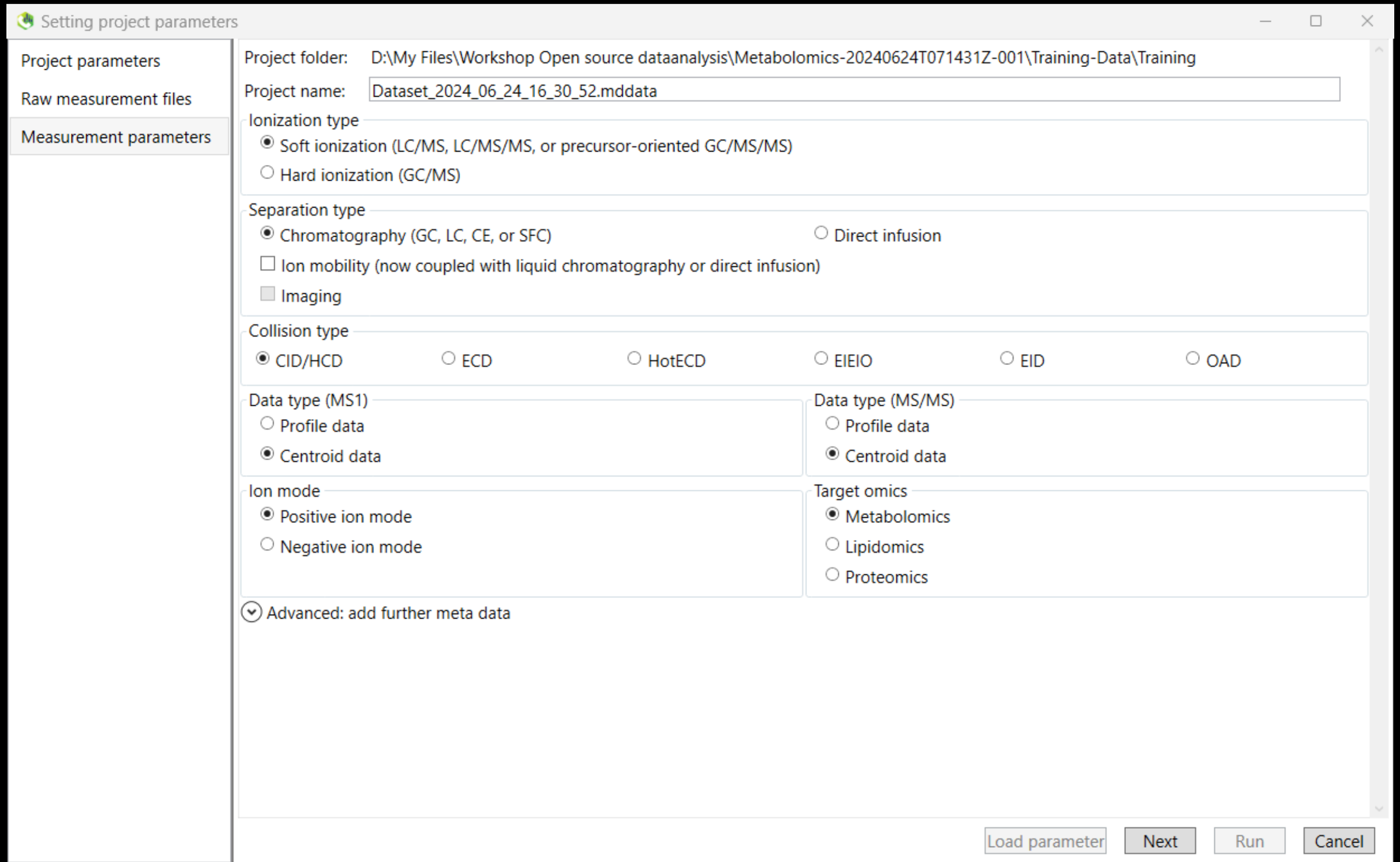
Project title: 2024_06_24_17_53_24.mdproject

Project file pa

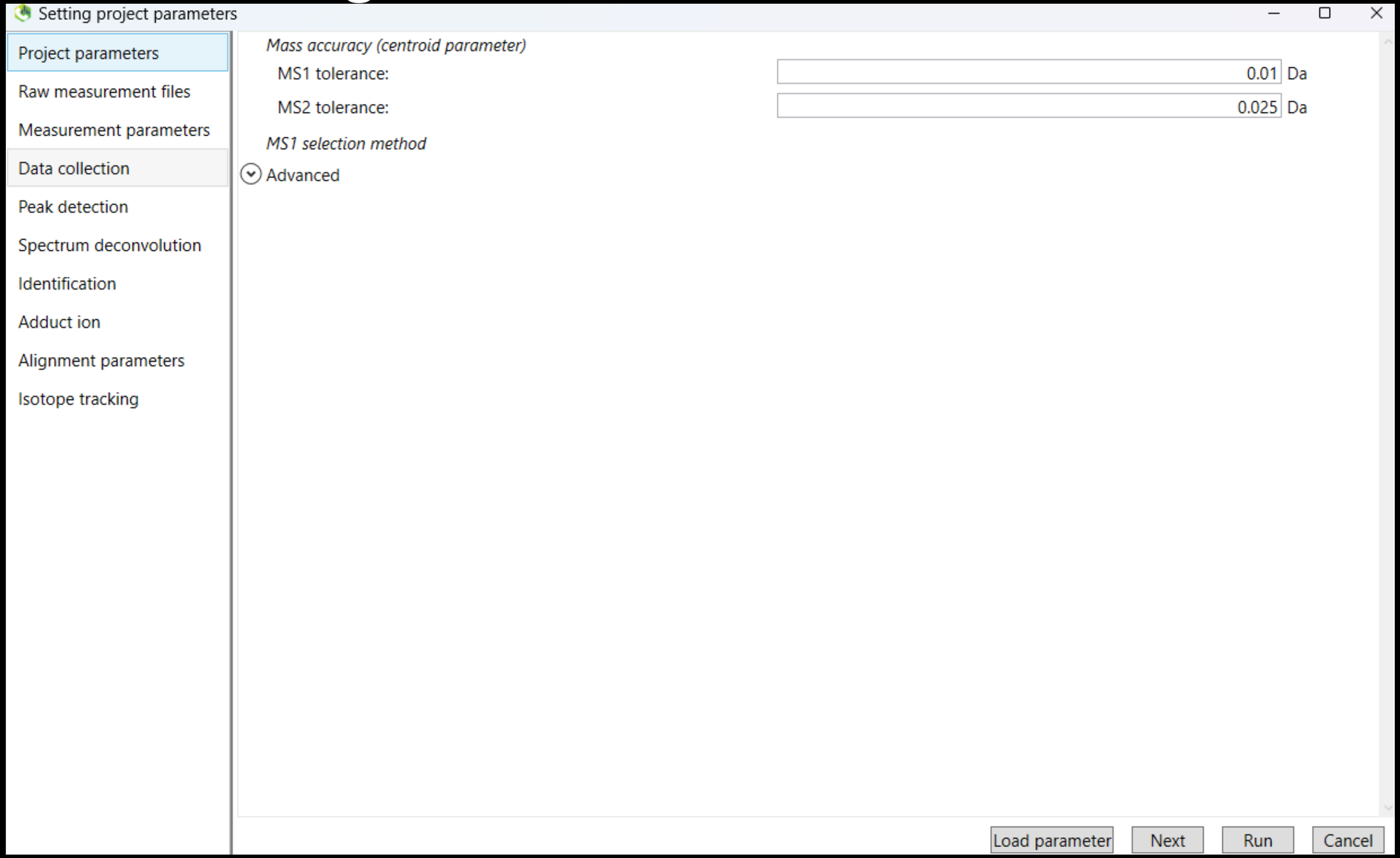
Browse

Load parameter | Next | Run | Cancel

Parameter setting



Parameter setting



Setting project parameters

- Project parameters
- Raw measurement files
- Measurement parameters
- Data collection
- Peak detection
- Spectrum deconvolution
- Identification
- Adduct ion
- Alignment parameters
- Isotope tracking

Peak detection parameters

Minimum peak height: 1000 amplitude

Mass slice width: 0.1 Da

Advanced

Load parameter | Next | Run | Cancel

Setting project parameters

- Project parameters
- Raw measurement files
- Measurement parameters
- Data collection
- Peak detection
- Spectrum deconvolution
- Identification
- Adduct ion
- Alignment parameters
- Isotope tracking

Deconvolution parameters

Sigma window value: 0.5

MS/MS abundance cut off: 0 amplitude

Advanced

Load parameter | Next | Run | Cancel

Setting project parameters

- Project parameters
- Raw measurement files
- Measurement parameters
- Data collection
- Peak detection
- Spectrum deconvolution
- Identification
- Adduct ion
- Alignment parameters
- Isotope tracking

Database setting

MSMS_Public_EXP_Pos_VS17 (1)

Annotation method setting

MSMS_Public_EXP_Pos_VS17 (1)_1

DataBase

Database type: Msp

Database path: D:\MS Dial Library\MSMS_Public_EXP_Pos_VS17 (1).msp Browse

Database name: MSMS_Public_EXP_Pos_VS17 (1)

Annotation method

Annotation method name: MSMS_Public_EXP_Pos_VS17 (1)_1

MS/MS identification setting

Accurate mass tolerance (MS1): 0.01 Da

Accurate mass tolerance (MS2): 0.025 Da

Retention time tolerance: 100 min

MS2 spectrum cut off

Annotation cut off

Retention time setting

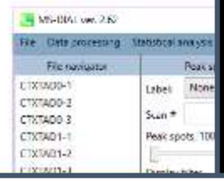
Load parameter | Next | Run | Cancel

CompMS | MS-DIAL –Spectral Database

Software Database Contact License

MSP spectral database

MRM database



MS-DIAL

Objective

Software Database Contact License

MS-DIAL metabolomics MSP spectral kit containing EI-MS, MS/MS, and CCS values

Last edited in Aug. 8th, 2024

ESI(+)-MS/MS from authentic standards (16,232 unique compounds)	MS/MS Positive	324,191 records	
ESI(-)-MS/MS from authentic standards (8,887 unique compounds)	MS/MS Negative	44,669 records	
ESI(+)-MS/MS from standards+bio+in silico (16,746 unique compounds)	MS/MS Positive	326,575 records	
ESI(-)-MS/MS from standards+bio+in silico (15,100 unique compounds)	MS/MS Negative	53,337 records	
MassBank	MS/MS Positive	8,068 records	
MassBank	MS/MS Negative	4,782 records	
MassBank-EU	MS/MS Positive	701 records	
MassBank-EU	MS/MS Negative	100 records	
ReSpect	MS/MS Positive	2,737 records	

Setting project parameters

- Project parameters
- Raw measurement files
- Measurement parameters
- Data collection
- Peak detection
- Spectrum deconvolution
- Identification
- Adduct ion
- Alignment parameters
- Isotope tracking

Adduct ion setting

Adduct: Mass: 0 AdductIonXmer: 0 ChargeNumber: 0 IonMode: Positive

Add user-defined adduc | Remove selected adduc

Molecular species	Charge	Accurate mass [Da]	Included
[M+H]+	1	1.00782503207	☑
[M+NH4]+	1	18.03437413	☑
[M+Na]+	1	22.9897692809	☑
[M+CH3OH+H]+	1	33.03403978207	☑
[M+K]+	1	38.96370668	☐
[M+Li]+	1	7.01600455	☐
[M+ACN+H]+	1	42.03437413207	☐
[M+H-H2O]+	1	-17.00273964793	☐
[M+H-2H2O]+	1	-35.01330432793	☐
[M+2Na-H]+	1	44.97171352973	☐
[M+IsoProp+H]+	1	61.06533991207	☐
[M+ACN+Na]+	1	64.0163183809	☐
[M+2K-H]+	1	76.91958832793	☐
[M+DMSO+H]+	1	79.02176103207	☐
[M+2ACN+H]+	1	83.06092323207	☐
[M+IsoProp+Na+H]+	1	84.05510919297	☐
[M-C6H10O4+H]+	1	-145.05008376687	☐
[M-C6H10O5+H]+	1	-161.04499838643	☐
[M-C6H8O6+H]+	1	-175.02426294185	☐
[2M+H]+	1	1.00782503207	☐
[2M+NH4]+	1	18.03437413	☐
[2M+Na]+	1	22.9897692809	☐
[2M+3H2O+2H]+	1	56.04734410414	☐
[2M+K]+	1	38.96370668	☐

Load parameter | Next | Run | Cancel

Processing | Data visualization | Search | View | Option | Export | Help | Filter

All processing (from peak detection) | Identification | Alignment | Correlation-based deconvolution (LC-MS only) | Amalgamation of different polarity peak list | Quant mass manager

Data | Post processing

File navigator

Con_1

Alignment navigator

Peak spot navigator

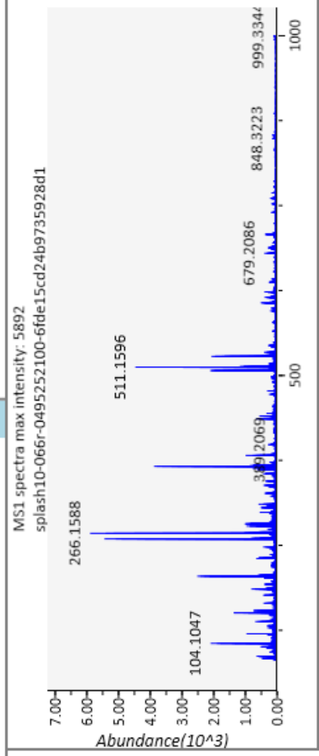
Label: None

Peak spots: 100% Num: 30

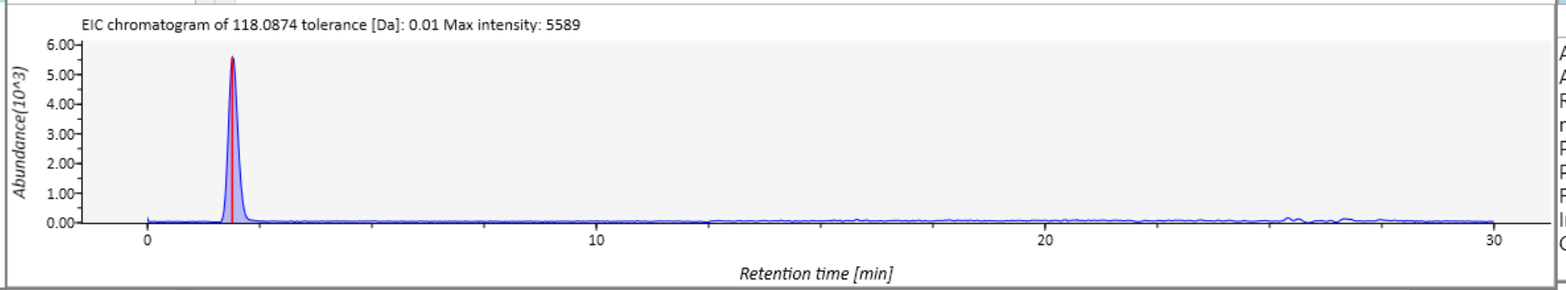
Display filter

Ref. matched | Suggested | CCS matched | Unknown | Molecular ion | MS2 acquired | Blank filter | Unique ions

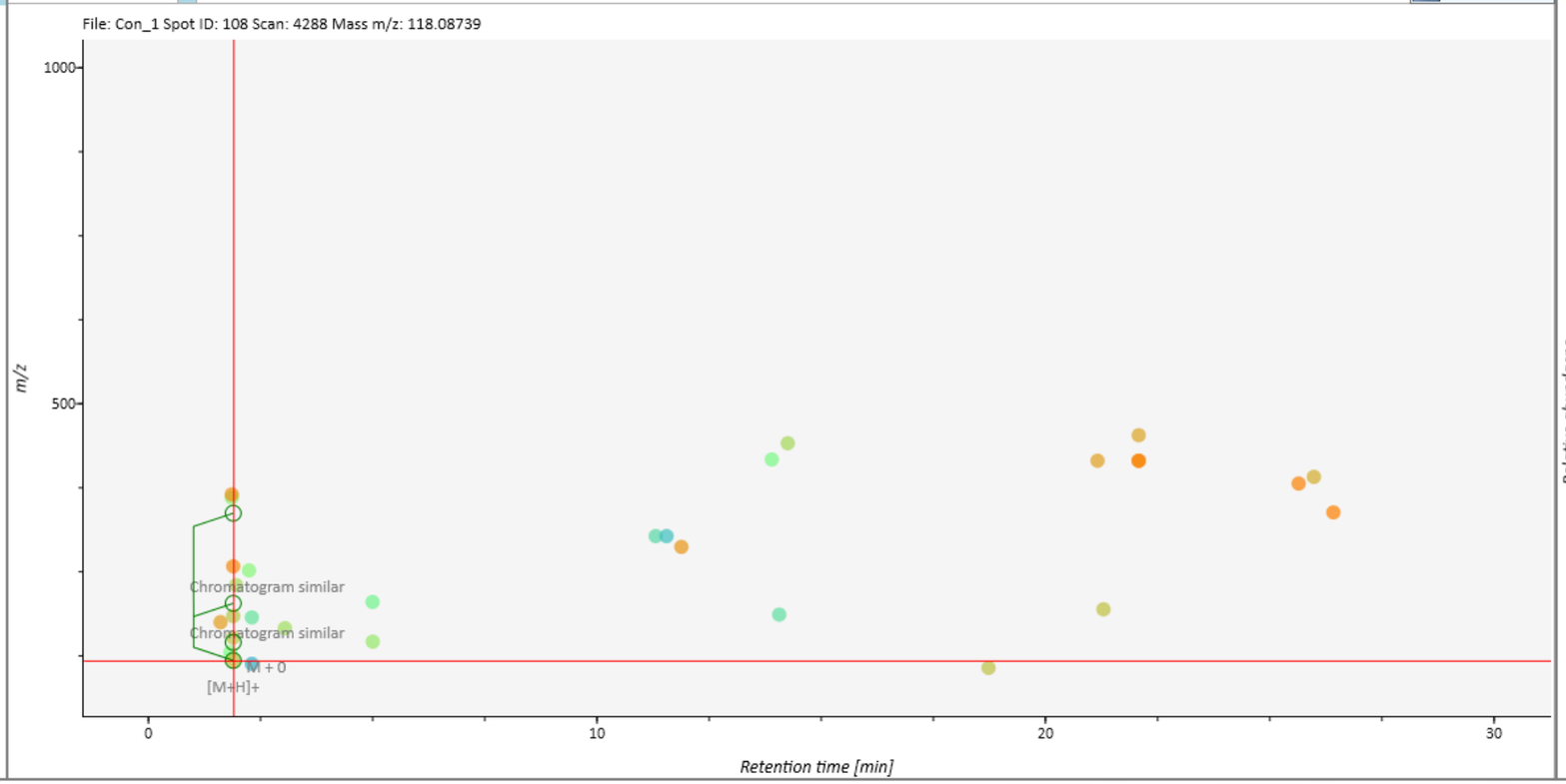
Survey scan (MS1) spectrum



Eic of focused spot



Peak spot viewer | Show ion tab

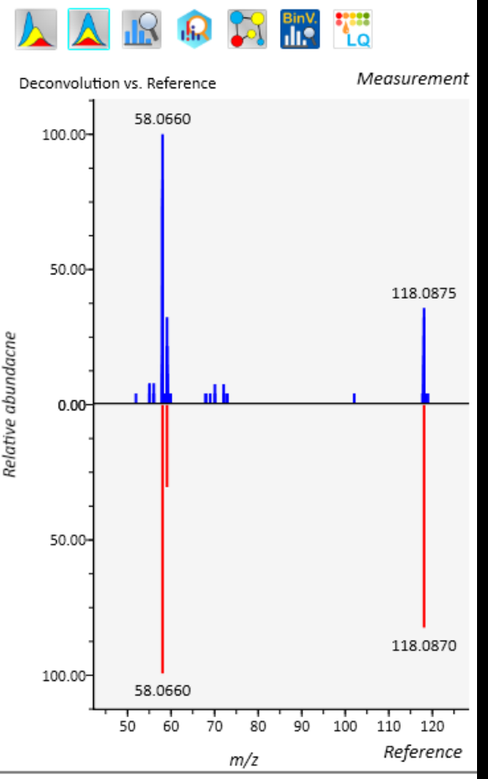


Structure | Candidates

Basic peak property | Compund detail

Annotation:	Betaine
Adduct type:	[M+H]+
RT [min]:	1.889|ref=-1.000|diff=2.89
m/z:	118.08739|ref=118.08677|diff(mDa)=
Peak height:	5589
Peak area:	84807
Formula|Ontolog	C5H11NO2|Alpha amino acids
InChIKey:	KWIUHFFTVRNATP-UHFFFAOYSA-N
Comment:	NA

Exp. vs.Rep. | MS2 Chrom. | Raw vs. Purified



Region focus by ID: 108 > RT(min): 1.89 > m/z: 118.087 >

Information box: Ctr+D, metabolite name to 'Unknown'

Untargeted Metabolomics Comparative Analysis

Graph tools Dataset: D:\My Files\Workshop Open source dataanalysis\Metabolomics-202...

Processing | Data visualization | Search | View | Option | Export | Help | Filter

All processing (from peak detection) | Identification | Alignment | Correlation-based deconvolution (LC-MS only) | Amalgamation of different polarity peak list | Quant mass manager

Data | Post processing

File navigator

Con_1
Con_2
Con_3
Treat_1
Treat_2
Treat_3

Alignment navigator

AlignmentResult_2024

Peak spot navigator

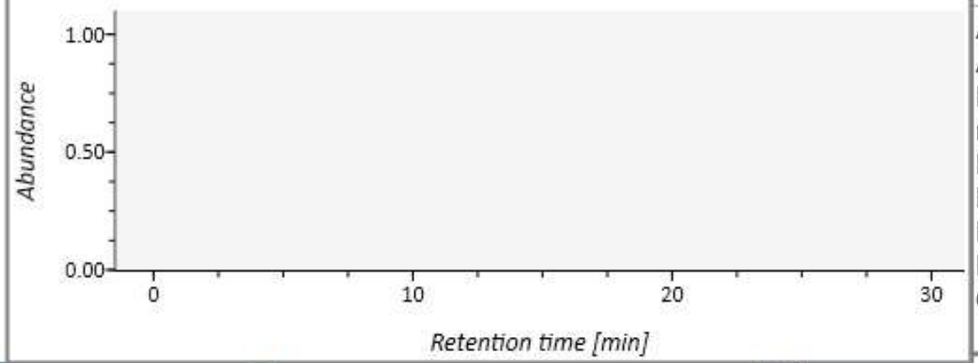
Label: None

Peak spots: 100% Num: 1310

Display filter

Ref. matched | Suggested
CCS matched | Unknown
Molecular ion | MS2 acquired
Blank filter | Unique ions

Eic of focused spot

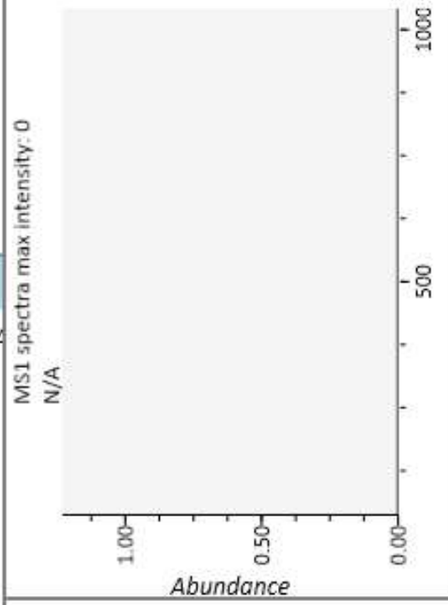


Structure | Candidates

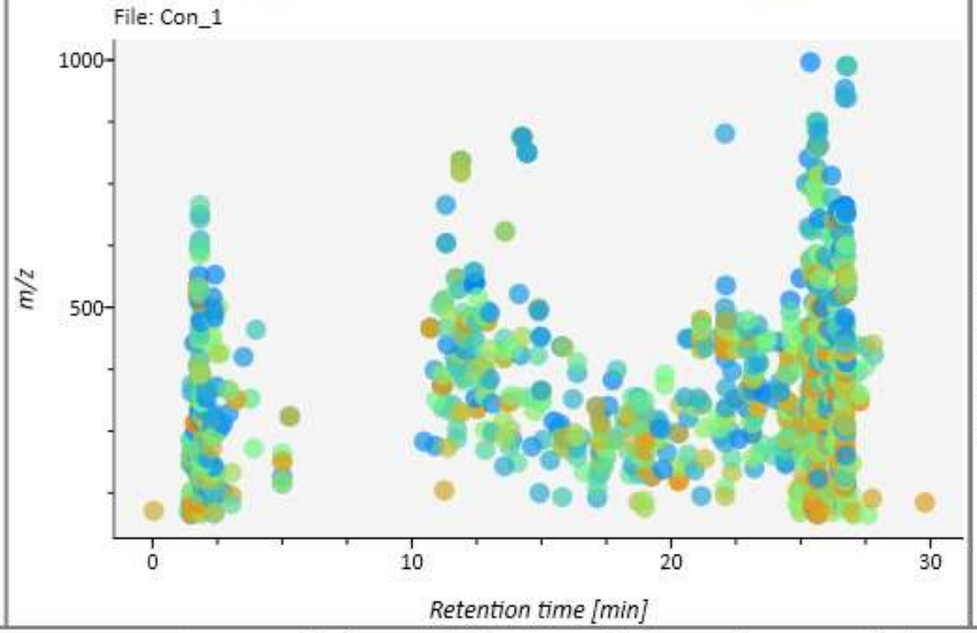
Basic peak property | Compund detail

Annotation:	Unknown
Adduct type:	NA
RT [min]:	0.000
m/z:	0.00000
Peak height:	0
Peak area:	0
Formula|Ontolog	NA|NA
InChIKey:	NA
Comment:	NA

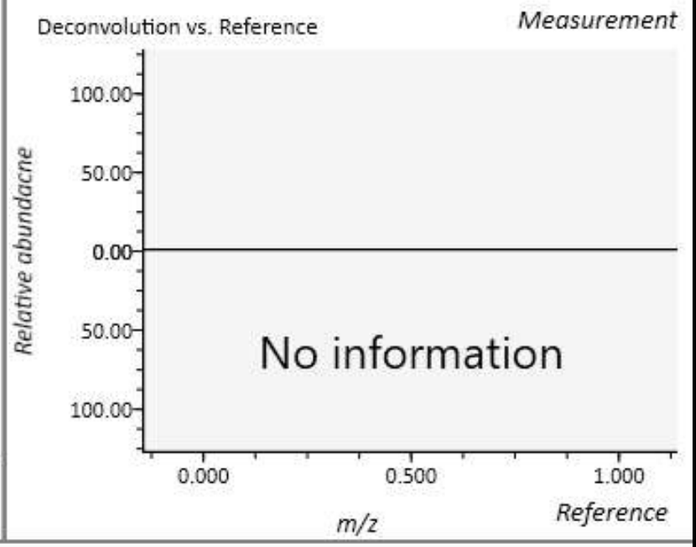
Survey scan (MS1) spectrum



Peak spot viewer | Show ion tal

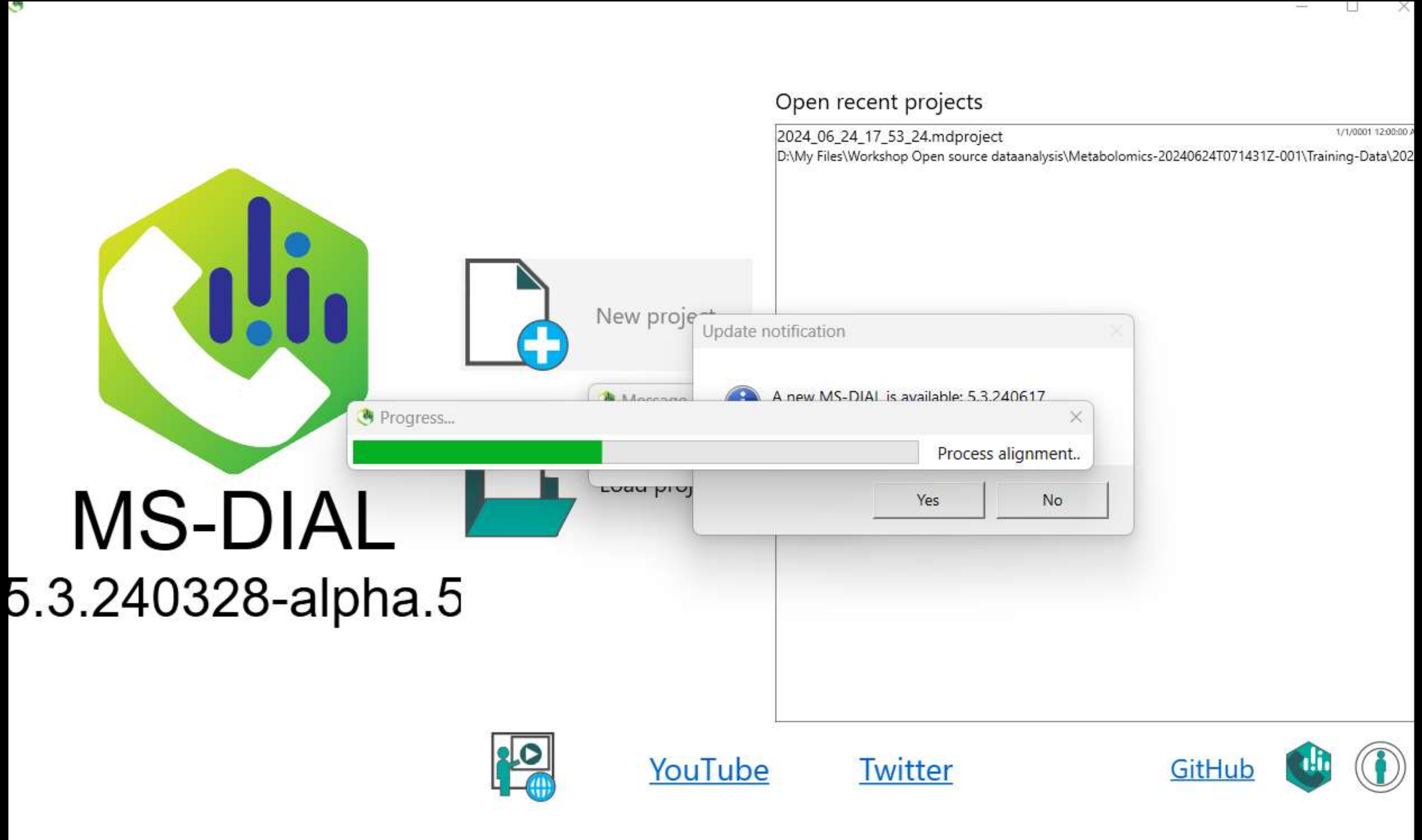


Exp. vs.Rep. | MS2 Chrom. | Raw vs. Purified



Region focus by ID: 0 > RT(min): 0.00 > m/z: 0.000 >

Information box: Ctr+D, metabolite name to 'Unknown'


Open recent projects
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1/1/0001 12:00:00 A
D:\My Files\Workshop Open source dataanalysis\Metabolomics-20240624T071431Z-001\Training-Data\202
New project
Update notification
A new MS-DIAL is available: 5.3.240617
Progress...
Process alignment..
Yes
No
MS-DIAL
5.3.240328-alpha.5
YouTube
Twitter
GitHub

ID	m/z	RT(min)	Type	Fill %	Metabolite name	Ontology	Comment	Tag	Annotation meth	Match sco	S/N	ANOVA P-value	Fold chanc (Max/Min)	BarChart
234	182.0801	2.1185	[M+H]+	1.00	Tyrosine	Tyrosine and derivatives		L M C O	MSMS_Public_EX	1.8351	104.9	2.63E-01	1.06	
312	205.0930	4.9892	[M+H]+	0.50	Tryptophan	Indolyl carboxylic acids and deriv		L M C O	MSMS_Public_EX	1.8249	21.4	1.19E-03	1.55	
771	327.0779	24.2157	[M+H]+	1.00	Triphenylphosphate	Aryl phosphotriesters		L M C O	MSMS_Public_EX	1.6993	193.7	1.71E-01	1.34	
1035	399.2467	25.2771	[M+H]+	1.00	Tri(butoxyethyl) phosphate	Trialkyl phosphates		L M C O	MSMS_Public_EX	1.7902	633.0	2.72E-01	1.19	
117	133.0625	17.1477	[M+H]+	1.00	trans-Cinnamaldehyde	Cinnamaldehydes		L M C O	MSMS_Public_EX	1.5807	110.2	4.65E-02	1.38	
905	365.1014	1.9163	[M+Na]+	1.00	SUCROSE	O-glycosyl compounds		L M C O	MSMS_Public_EX	1.9050	2025.6	2.44E-05	2.18	
889	360.1508	1.8840	[M+NH4]+	1.00	SUCROSE	O-glycosyl compounds		L M C O	MSMS_Public_EX	1.7133	284.6	2.31E-02	1.16	
512	258.1071	1.8786	[M]+	1.00	sn-Glycero-3-phosphocholine	Glycerophosphocholines		L M C O	MSMS_Public_EX	1.7521	2947.7	1.85E-03	1.43	
1377	527.1531	1.9420	[M+Na]+	0.50	RAFFINOSE	Oligosaccharides		L M C O	MSMS_Public_EX	1.7085	3434.3	2.56E-05	2.41	
699	303.0461	11.5518	[M+H]+	1.00	Quercetin	Flavonols		L M C O	MSMS_Public_EX	1.6932	90.1	2.05E-02	1.49	
242	184.0740	1.8733	[M+H]+	1.00	Phosphocholine	Phosphocholines		L M C O	MSMS_Public_EX	1.6832	247.8	1.46E-03	1.38	
191	166.0844	3.0270	[M+H]+	1.00	Phenylalanine	Phenylalanine and derivatives		L M C O	MSMS_Public_EX	1.7829	102.8	1.60E-04	2.70	
1197	441.2412	14.2777	[M+Na]+	1.00	Ophiopogonoside A	Terpene glycosides		L M C O	MSMS_Public_EX	1.6418	135.5	1.84E-01	1.18	
460	244.2259	23.1277	[M+H]+	1.00	N-lauroylethanolamine	Carboximidic acids		L M C O	MSMS_Public_EX	1.8091	541.3	3.71E-01	1.10	
92	124.0395	25.4290	[M+H]+	0.50	NICOTINATE	Pyridinecarboxylic acids		L **M** C O	MSMS_Public_EX	1.7861	47.9	2.29E-04	21.40	
1085	415.2091	22.9477	[M-H2O+H]+	0.67	NCGC00385811-01!6-[3-[(3,4-dimethoxyphe	Dibenzylbutane lignans		L M C O	MSMS_Public_EX	1.6547	317.2	1.11E-03	2.60	
1086	415.2093	22.0841	[M-H2O+H]+	0.83	NCGC00385811-01!6-[3-[(3,4-dimethoxyphe	Dibenzylbutane lignans		L M C O	MSMS_Public_EX	1.7143	9944.9	7.73E-04	3.63	
868	355.1698	12.5107	[M+Na]+	0.50	NCGC00385387-01_C16H28O7_4-(Hydroxym	Terpene glycosides		L M C O	MSMS_Public_EX	1.4904	17.5	1.02E-01	1.63	
1182	437.3373	15.4525	[M-H2O+H]+	0.50	NCGC00380944-01_C30H46O3_(3beta,5xi,9x	Triterpenoids		L M C O	MSMS_Public_EX	1.6914	15217.9	2.66E-04	215.77	
741	315.1905	24.0121	[M+H]+	1.00	NCGC00347651-02_C20H26O3_1-Phenanthr	Diterpenoids		L M C O	MSMS_Public_EX	1.6979	43.1	8.02E-01	1.03	
1215	449.1044	11.8922	[M+H]+	1.00	NCGC00169187-02!5,7-dihydroxy-2-(4-hydr	Flavonoid-3-O-glycosides		L M C O	MSMS_Public_EX	1.6834	424.7	7.56E-04	1.80	
1348	511.2263	21.1421	[M+H]+	0.50	methyl 3-(6-((4-formylpiperazin-1-yl)methyl)	Imidazolyl carboxylic acids and d		L M C O	MSMS_Public_EX	1.5576	121.1	1.93E-04	3.97	
272	194.1167	21.2943	[M+H]+	1.00	m-Cumenyl methylcarbamate	Phenyl methylcarbamates		L M C O	MSMS_Public_EX	1.7961	243.4	4.70E-02	1.10	
1368	522.3499	25.7143	[M+H]+	0.50	LPC 18:1	1-acyl-sn-glycero-3-phosphocho		L M C O	MSMS_Public_EX	1.7104	3794.7	7.54E-04	211.04	
1323	496.3354	25.3133	[M+H]+	0.50	LPC 16:0	1-acyl-sn-glycero-3-phosphocho		L M C O	MSMS_Public_EX	1.6520	1897.8	3.47E-03	100.48	
609	281.2467	25.1765	[M+H]+	0.50	Linoleic acid	Lineolic acids and derivatives		L M C O	MSMS_Public_EX	1.6747	417.0	3.73E-04	14.29	
146	148.0579	1.8256	[M+H]+	1.00	L-Glutamic acid	Glutamic acid and derivatives		L M C **O**	MSMS_Public_EX	1.7456	158.9	1.29E-04	2.15	
577	274.2735	18.3776	[M+H]+	1.00	Lauryldiethanolamine	1,2-aminoalcohols		L M C O	MSMS_Public_EX	1.8688	4515.1	3.59E-03	2.14	
837	343.2932	19.7692	[M]+	1.00	Lauramidopropyl betaine	Alpha amino acids		L M C O	MSMS_Public_EX	1.7672	381.1	7.61E-01	1.04	
413	230.0951	1.9266	[M+H]+	1.00	L-(+)-Ergothioneine	Histidine and derivatives		L M C O	MSMS_Public_EX	1.7151	277.5	5.70E-03	1.48	
634	287.0533	11.8922	[M+H]+	1.00	Kaempferol	Flavonols		L M C O	MSMS_Public_EX	1.8543	1268.7	1.89E-03	1.58	
633	287.0532	11.5833	[M+H]+	1.00	Kaempferol	Flavonols		L M C O	MSMS_Public_EX	1.8456	115.9	1.01E-02	1.37	
141	146.0579	4.9805	[M+H]+	0.50	Indole-3-carboxyaldehyde	Indoles		L **M** C O	MSMS_Public_EX	1.8294	80.9	1.12E-03	1.96	
625	285.2394	26.8987	[M-H2O+H]+	0.50	GLYCEROL-MYRISTATE	1-monoacylglycerols		L M C O	MSMS_Public_EX	1.7294	463.9	2.31E-04	15.41	
196	167.0689	22.3529	[M+H]+	1.00	Ethylparaben	p-Hydroxybenzoic acid alkyl este		L M C O	MSMS_Public_EX	1.5802	112.2	3.09E-01	1.04	
810	338.3380	24.6175	[M+H]+	0.67	Erucamide	Fatty amides		L M C O	MSMS_Public_EX	1.7918	1524.5	3.90E-01	1.63	
811	338.3383	26.5121	[M+H]+	1.00	Erucamide	Fatty amides		L M C O	MSMS_Public_EX	1.8173	106789.	6.94E-04	9.02	

CompMS | MS-DIAL –Tutorial

Software Database Contact License

It features
(1) spectral deconvolution for both GC/MS and data-independent MS/MS,
(2) streamlined criteria for peak identification,
(3) support of all data processing steps from raw data import to statistical analysis,
and (4) user-friendly graphic user interface.

Direct links

GitHub repository
that contains MS-DIAL source code
Link

Releases
All recent MS-DIAL5 releases
Link

Tutorial
for MS-DIAL5
Link

https://systemsomicslab.github.io/msdial5tutorial/

MS-DIAL 5 tutorial | Home | Lipidomics | Metabolomics | Proteomics | Mass spectrometry imaging | Other utilities | About

MS-DIAL5 tutorial

ABSTRACT
MS-DIAL was launched as a universal program for untargeted metabolomics that supports multiple instruments (GC/MS, GC/MS/MS, LC/MS, and LC/MS/MS) and MS vendors (Agilent, Bruker, LECO, Sciex, Shimadzu, Thermo, and Waters). Common data formats such as netCDF (AIA) and mzML, can also be managed in our project. In addition, we released several MSP files including both EI- and MS/MS spectra as a 'start-up kit'. Moreover, MS-DIAL internally has a version of Fiehn lab's GC/MS database (oriented by FAME RI index), and in silico retention time- and MS/MS database for LC/MS/MS based lipidomics. The isotope labeled tracking can also be executed in LC/MS project.

Keep in touch with us and follow the latest developments

YouTube @msdialproject channel

General introduction of MS-DIAL5

The current MS-DIAL program provides a stream pipeline for untargeted metabolomics, lipidomics and proteomics. In this latest version, the user experience has been greatly improved with a new graphical interface and also due to the fact it is no longer necessary to convert raw MS data from different vendor formats into a common ABF format (which is still supported), but the data can now be imported directly (supported file formats and analytical techniques are summarized in Figure 1).