

メタボロームデータベースを用いて代謝を理解する

津川裕司 (Tokyo University of Agriculture and Technology)

メタボロームデータを出す側と使う側

出す側

- 分析化学
- 質量分析
- イオン
- マススペクトル
- 質量分析インフォマティクス
- アノテーション
- データ標準化

使う側

- データの特徴理解
- 化合物IDの取得
- データの正規化
- 統計・多変量解析
- データベース検索
- 代謝マップ投影
- 適切な数理モデルの選択
- オミクスモジュールへ統合

メタボロームデータを出す側と使う側



メタボロミクスのデータ解析プロトコール

メタボロームデータを「出す側」
(4-2~4-5)

メタボロームデータを「使う側」
(4-6~4-8)

質量分析インフォマティクス

ケムインフォマティクス

バイオインフォマティクス

データ処理(ノンターゲット解析)

XCMS

MS-DIAL

OpenMS

MZmine 2

未知代謝物アノテーション

MS-FINDER

GNPS

SIRIUS

代謝データベース

KEGG

HMDB

ID変換ツール(CTSなど)

パスウェイ解析

VANTED

MSEA

多変量解析及び統合解析

MetaboAnalyst

transomics2cytoscape

Garudaプラットホーム

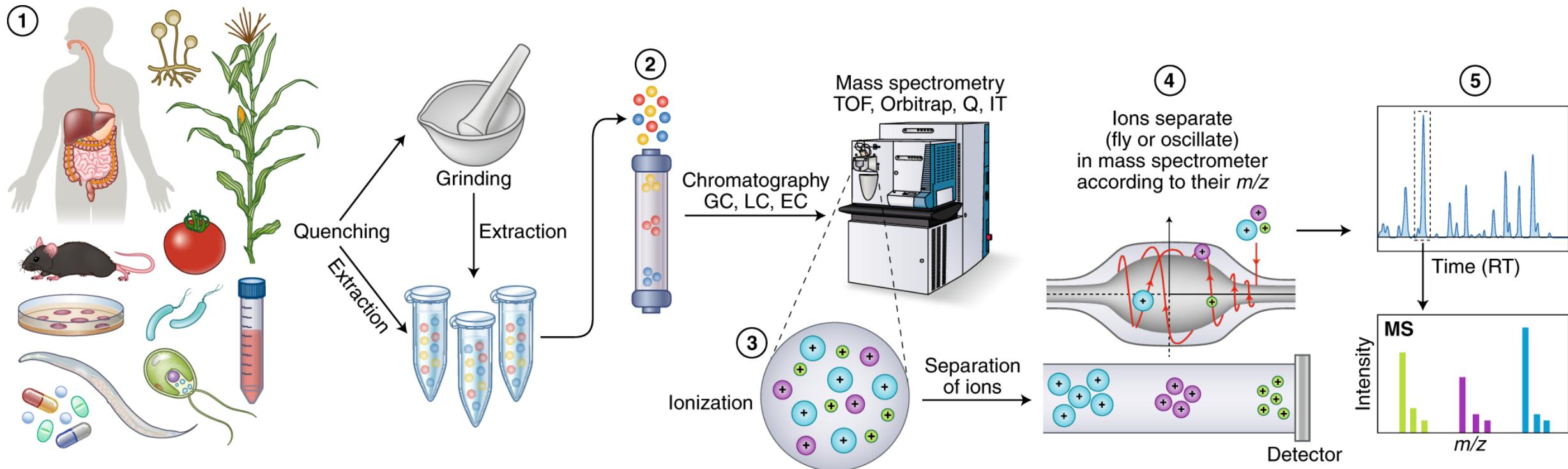
データ処理(ターゲット解析)

MRM PROBS

Skyline

その他
データ標準化・レポジトリ
(4-9, 4-10)

Metabolomics workflow



Sample preparation and extraction

- Avoid environmental perturbation during harvesting
- Control environment: harvesting at the same time and under the same conditions
- Snap-freezing in liquid nitrogen
- Enzyme quenching: completely terminate all enzyme activities
- Standards spiked into the quenching solvent
- Grinding, isolation of cells, fast-filtration or aspiration

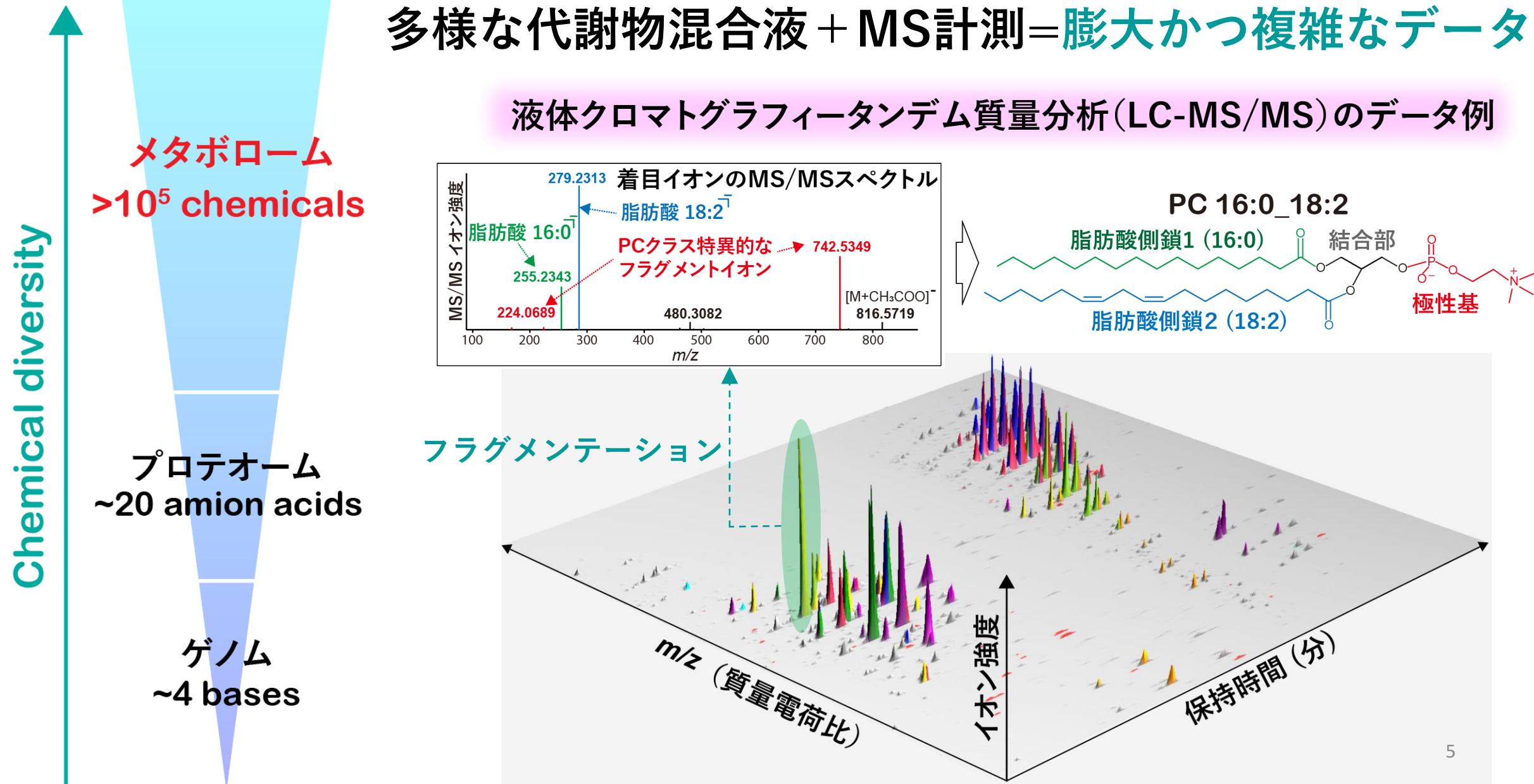
Sample replication and randomization

- At least four biological replicates, preferably more
- Technical and analytic replicates are worthy of consideration
- Randomization of samples throughout workflows is essential
- In large-scale studies, quality-control samples and batch correction are essential

Chromatography–mass spectrometry

- Separation methods, composition of the mobile phase, column properties and injection volume
- Metabolites are within their range of detection
- Avoid ion suppression: dilution of extracts, sonication, filtration or centrifugation, recovery test
- Choosing ionization source and type of detection mode, MS method, scan number and speed, MS/MS and energy for fragmentation

メタボロームの多様性とデータ解析の複雑さ



データ形式：生データ（一次データ）

Vendor formats

Agilent
.D

Bruker
.D

LECO
.PEG

SCIEX
.WIFF .WIFF2

Shimadzu
QGD .LCD

Thermo .RAW

Waters .RAW

Data conversion

netCDF (by vendors software), [mzML](#) (by ProteoWizard), ABF (by Reifycs), IBF (by MS-DIAL package)

mzML data structure by ProteoWizard

m/z values binary: [44] 112.9876 174.9537 182.9914 212.0731

Intensities binary: [44] 4.67 1.94 14.88 10.68...

MS-DIAL環境による質量分析データの解析

MS formats

Agilent	Bruker	SCIEX	Shimadzu	Thermo	Waters	Common data formats
.D	.D	.WIFF .WIFF2	.QGD .LCD	.RAW	.RAW	.CDF .mzML .ABF .IBF

Peak picking, Annotation, and Integration



Hard ionization

Soft ionization

GC-MS

Conventional

With ion mobility (IM)

LC-MS

SWATH DIA

AIF-MS

LC-IM-MS

LC-IM-AIF-MS

LC-MS/MS (DDA)

LC-IM-MS/MS (PASEF)

Data output

Metabolome table (.TXT, .mztabM) & Spectral information (.MSP, .MGF, .MassBank)

メタボロームのアノテーション

1. 計測方法によって方法が異なる

- GC-MS
- LC-MS/MS
- IM-MS/MS (LC-IM-MS/MS)

2. アノテーションのレベル分けをする必要がある

- Metabolomics Standards Initiativeの定義 *Metabolomics* 2007, **3**, 211–221
- Schymanski E.L. et al. の5段階レベル *Environ. Sci. Technol.* 2014, **48**, 2097–2098
- Lipidomics Standards Initiativeの定義 *Nature Metabolism* 2022, **4**, 1086–1088

アノテーション用のライブラリーファイルとフォーマット

<http://prime.psc.riken.jp/compms/msdial/main.html#MSP>

Last edited in Aug. 21th, 2022

ESI(+) - MS/MS from authentic standards (16,481 unique compounds)	MS/MS Positive	324,191 records		
ESI(-) - MS/MS from authentic standards (9,033 unique compounds)	MS/MS Negative	44,669 records		
ESI(+) - MS/MS from standards+bio+in silico (16,995 unique compounds)	MS/MS Positive	326,575 records		
ESI(-) - MS/MS from authentic standards (15,245 unique compounds)	MS/MS Negative	53,337 records		
All records with Kovats RI (9062 unique compounds)	EI-MS	28,220 records		
Fiehn BinBase DB (Rtx5-Sil MS, predicted Kovats RI)	EI-MS	1,021 records		
RIKEN DB (Rtx5-Sil MS, Kovats RI)	EI-MS	241 records		
Kazusa DB (Rtx5-Sil MS, Kovats RI)	EI-MS	273 records		

整理しておくべきライブラリーフォーマット (MSP形式)

GC-MS用

```
1 NAME: 1-NITROPYRENE; EI-B; MS
2 EXACTMASS: 247.0633285
3 FORMULA: C16H9NO2
4 SMILES: [O-1] [N+1] (=O) c(c4)c(c1)c(c3c4)
5 ONTOLOGY: Pyrenes
6 INCHIKEY: ALRLPDGCPYIVHP-UHFFFAOYSA-N
7 RETENTIONTIME: -1
8 RETENTIONINDEX: 1872.217
9 QUANTMASS: 201
10 IONMODE: Positive
11 COLLISIONENERGY: 70eV
12 LICENSE: CC BY-SA
13 Comment:
14 Num Peaks: 75
15 51 27
16 55 80
17 57 73
18 58 13
19 59 13
20 60 140
21 61 13
22 62 33
23 63 33
24 66 13
25 68 87
```

MS/MS用 (LC-MS、IM-MS、LC-IM-MSに対応)

```
1 NAME: Corosolic acid; PlaSMA ID-1295
2 PRECURSORMZ: 471.34798
3 PRECURSORTYPE: [M-H]-
4 FORMULA: C30H48O4
5 Ontology: Triterpenoids
6 INCHIKEY: HFGSQOYIOKBQOW-UHFFFAOYNA-N
7 SMILES: CC1CCC2(CCC3(C)C(=CCC4C5(C)CC
8 RETENTIONTIME: 9.88
9 CCS: 222.7776231
10 IONMODE: Negative
11 Comment: Annotation level-1; PlaSMA I
12 Num Peaks: 5
13 196.13573 18
14 407.32126 20
15 471.30518 21
16 471.34604 3406
17 471.40079 20
18
19 NAME: Ginsenoside compound K; PlaSMA
20 PRECURSORMZ: 621.43719
21 PRECURSORTYPE: [M-H]-
22 FORMULA: C36H62O8
```

整理しておくべきライブラリーフォーマット (TXT形式)

LC-MS、IM-MS、LC-IM-MSデータに便利

	A	B	C	D	E	F	G	H	I
1	Name	MZ	RT	Adduct	InChIKey	Formula	SMILES	Ontology	CCS
2	PC 15:0_18:1(d7)	811.6199	9.5	[M+CH3COO]-	ZEWLMKXMNQOCOO-GCHPQBSENA-N	C41H73D7NO8P	[C@](COP(=O)([O-])OCC[N+](C)PC	284.786	
3	PE 15:0_18:1(d7)	709.55191	9.64	[M-H]-	ADCNXGARWPJRBV-RGLIIYCRNA-N	C38H67D7NO8P	[C@](COP(=O)(O)OCCN)([H])(O)PE	258.184	
4	PS 15:0_18:1(d7)	753.54179	8.38	[M-H]-	KVBAVKWITJZQEG-UDKXCJCZNA-N	C39H67D7NO10P	C(O)(=O)[C@@]([H])(N)COP(OCPS	268.427	
5	PG 15:0_18:1(d7)	740.54655	8.42	[M-H]-	CAKDJPLOYWLK-AHOXJELVNA-N	C39H68D7O10P	[H][C@](O)(CO)COP(OC[C@]([H]PG	264.974	
6	PI 15:0_18:1(d7)	828.56261	8.35	[M-H]-	XCKYASHMOHAUQB-OAFUKSMZNA-N	C42H72D7O13P	[C@]([H])(OC(CCCCCC/C=C\CCPI	279.073	
7	PA 15:0_18:1(d7)	666.50975	8	[M-H]-	NKHIVFXDPYZIBK-ZYYJESQNA-N	C36H62D7O8P	[C@](COP(=O)(O)O)([H])(OC(CCPA	250	
8	LPC 18:1(d7)	587.40594	6.33	[M+CH3COO]-	YAMUFBLWGFFICM-HNNXNMBSNA-N	C26H45D7NO7P	C(COP(=O)([O-])OCC[N+](C)(C)CLPC	239.829	
9	LPE 18:1(d7)	485.33783	6.4	[M-H]-	PYVRVRFVLRNJLY-CCLUNVSZNA-N	C23H39D7NO7P	[C@](COP(=O)(O)OCCN)([H])(OLPE	209.347	
10	SM 18:1;2O/18:1(d9)	796.65303	9.11	[M+CH3COO]-	NBEADXWAAWCCDG-KYPZZJCONA-N	C41H72D9N206P	[C@](COP(=O)([O-])OCC[N+](C)SM	287.235	
11	Cer 18:1;2O/15:0(d7)	589.554235	9.34	[M+CH3COO]-	HBULQAPKKLNTLT-BXLQGFJZSA-N	C33H58D7NO3	[H][C@@](O)(\C=C\CCCCCCCCCer-NS	249.173	
12	FA 18:0(d3)	286.283084	6.96	[M-H]-	QIQXTHQIDYTFRH-FIBGUPNXSA-N	C18H33D3O2	[2H]C([2H])([2H])CCCCCCCCCCCCFA	177.728	
13	FA 16:0(d3)	258.251784	6.3	[M-H]-	IPCSVZSSVZVIGE-FIBGUPNXSA-N	C16H29D3O2	[2H]C([2H])([2H])CCCCCCCCCCCCFA	169.563	

*必ずTab区切りテキストで保存すること

メタボロームのアノテーション

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2. アノテーションのレベル分けをする必要がある

- Metabolomics Standards Initiativeの定義

Metabolomics 2007, **3**, 211–221

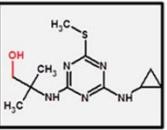
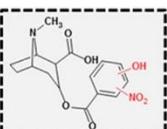
- Schymanski E.L. et al. の5段階レベル

Environ. Sci. Technol. 2014, **48**, 2097–2098

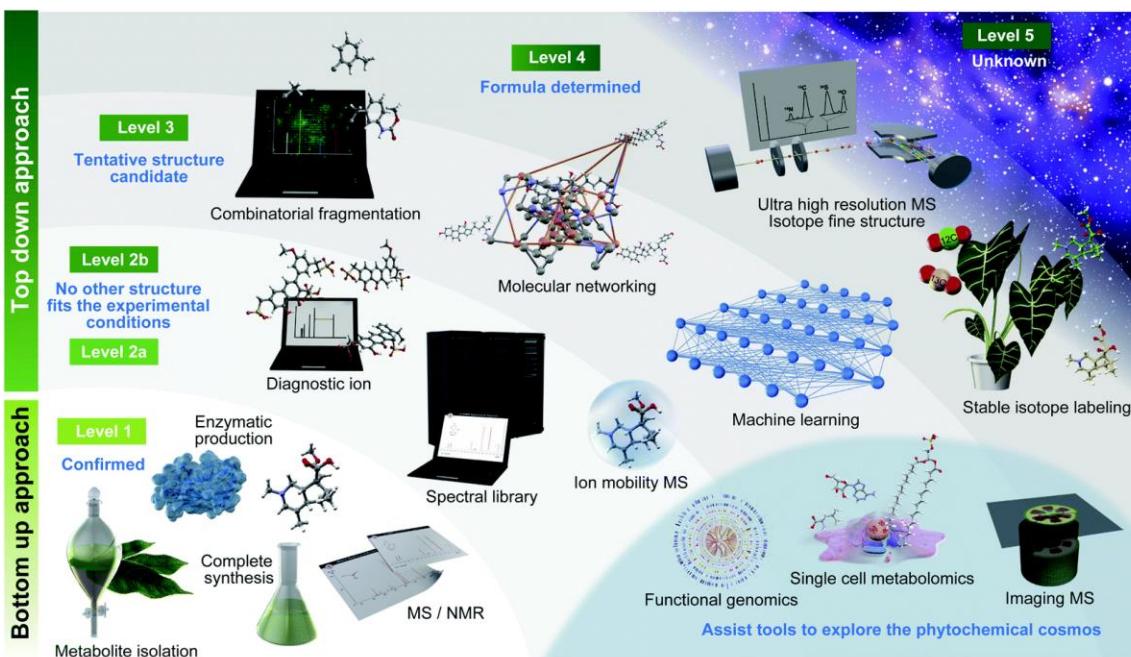
- Lipidomics Standards Initiativeの定義

Nature Metabolism 2022, **4**, 1086–1088

Schymanski E.L. et al. の5段階レベル (脂質は別に定義)

Example	Identification confidence	Minimum data requirements
	Level 1: Confirmed structure by reference standard	MS, MS ² , RT, Reference Std.
	Level 2: Probable structure a) by library spectrum match b) by diagnostic evidence	MS, MS ² , Library MS ² MS, MS ² , Exp. data
	Level 3: Tentative candidate(s) structure, substituent, class	MS, MS ² , Exp. data
C ₆ H ₅ N ₃ O ₄	Level 4: Unequivocal molecular formula	MS isotope/adduct
192.0757	Level 5: Exact mass of interest	MS

Environ. Sci. Technol. 2014, **48**, 2097–2098



Nat. Prod. Rep. 2021 **38**, 1729-1759

Level 1: Confirmed structure represents the ideal situation, where the proposed structure has been confirmed via appropriate measurement of a reference standard with MS, MS/MS and retention time matching. If possible, an orthogonal method should also be used.

Level 2a: Library this involves matching literature or library spectrum data where the spectrum-structure match is unambiguous.

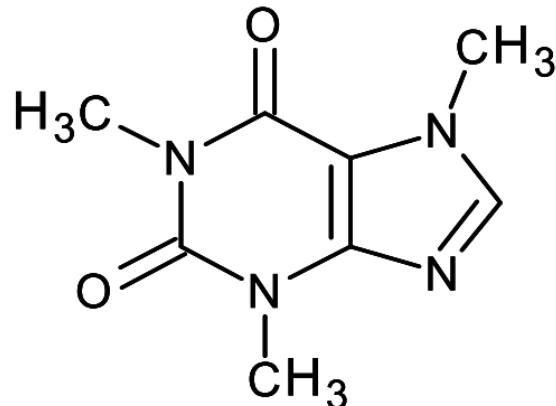
Level 2b: Diagnostic represents the case where no other structure fits the experimental information, but no standard or literature information is available for confirmation. Evidence can include diagnostic MS/MS fragments and/or ionization behavior, parent compound information and the experimental context.

Level 3: Tentative candidate(s) describes a “grey zone”, where evidence exists for possible structure(s), but insufficient information for one exact structure only (e.g., positional isomers).

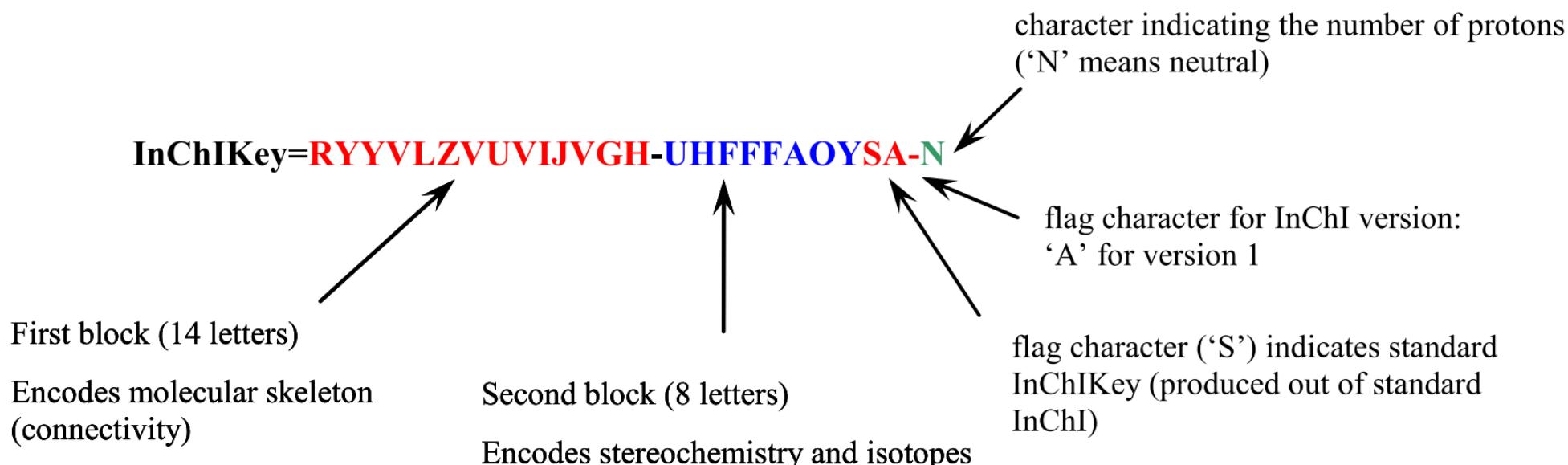
Level 4: Unequivocal molecular formula is possible when a formula can be unambiguously assigned using the spectral information (e.g., adduct, isotope, and/or fragment information), but insufficient evidence exists to propose possible structures.

Level 5: Exact mass (m/z) can be measured in a sample and be of specific interest for the investigation, but lack information to assign even a formula.

Let's use InChIKey as a unique identifier of metabolite



InChI=1S/C8H10N4O2/c1-10-4-9-6-5(10)7(13)12(3)8(14)11(6)2/h4H,1-3H3 (caffeine)



InChIKeyがあれば様々なIDに変換可能

Alanine

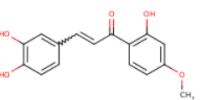
InChIKey: QNAYBMKLOCPYGJ-REOHCLBHSA-N

The screenshot shows the 'Batch Conversion' page of the CTS (Chemical Translation Service) web application. The URL in the address bar is `cts.fiehnlab.ucdavis.edu/batch`. The main title is 'Batch Conversion'. Below it, instructions state: 'To convert multiple identifiers, enter them in the box below or upload them as a text file. IDs should be separated by line breaks. Select your source and target types, and click the Convert button. You may select multiple target types.' A text input field contains the InChIKey: `QNAYBMKLOCPYGJ-REOHCLBHSA-N`. To its right are dropdown menus for 'Source' (set to 'InChIKey') and 'Target' (set to 'KEGG'). A 'Convert' button is located between these dropdowns. Below the input field is a 'Choose File' button with the message 'No file chosen'. Under the conversion results, there are two rows: one for 'InChIKey' showing the input value and one for 'KEGG' showing the output value 'C00041'. At the bottom, there are sections for 'Download Style' (set to 'Table'), 'File Type' (set to 'CSV'), and a checked checkbox for 'Top Hit Only'. A final 'Download' button is at the bottom right.

ClassyFire categorizing metabolite into a chemical class

ClassyFire Browse▼ Classify About ClassyFire Contact Downloads Help▼

Structure Information



Compound Identification

SMILES
COC1=CC(O)=C(C=C1)C(=O)C=CC1=CC(O)=C(O)C=C1

InChIKey
InChIKey=IULVGTQZKYHCS-UHFFFAOYSA-N

Formula
C₁₆H₁₄O₅

Mass
286.283

Export to:

JSON SDF CSV

Taxonomic Classification

Taxonomy Tree

- Kingdom [Organic compounds](#)
- Superclass [Phenylpropanoids and polyketides](#)
- Class [Linear, 1,3-diarylpropanoids](#)
- Subclass [Chalcones and dihydrochalcones](#)
- Level 5 [2'-Hydroxychalcones](#)

J Cheminform 8, 61 (2016)

ClassyFire Batch by Fiehn Lab

Batch Compound Classification

ClassyFire¹ is a web-based application developed by the [Wishart Research Group](#) for automated structural classification. It is an independent tool that retrieves and formats ClassyFire results for a list of InChIKey identifiers.

If you encounter any bugs or problems, please let us know using our [issue tracker](#).

August 2019: We are migrating to an updated server with a local database cache. Speeds are still slower than they used to be, but should be minimal.

InChIKeys (one per line):

FZWWJIXYNHHJI-QBZLNYABNA-N
HHARWONQTCORMN-UHFFFAOYNA-N
UYALDZZEAZIEME-YWGUMEFLNA-N
YIEPZDPKKNJALX-CKPZSVDJNA-N
ZAZHPBXBNGWCDV-UHFFFAOYNA-N
NFBYZSYLZUMCFV-JJRRTKJUSA-N
RPMNUQRUHXIGHK-PYXJVEIZSA-N
JRNZEGAFLBTZDT-JTVHLFNZNA-N
WKEMJKQOLOHJLZ-UHFFFAOYSA-N
RAMPQQLLROWEJQ-JJASCTQYNA-N

Please enter one InChIKey per line

ClassyFy

ClassyFire categorizing metabolite into a chemical class

InChIKey	Status	Kingdom	Superclass	Class	Subclass	Parent Level 1	Parent Level 2	Parent Level 3
PFRVZQKEOAYKSC-UHFFAOYNA-N	Completed	Organic compounds	Alkaloids and derivatives	Amaryllidaceae alkaloids	Galanthamine-type amaryllidaceae alkaloids	Galanthamine-type amaryllidaceae alkaloids		
GJHTVUOIDXUACV-UHFFAOYNA-N	Completed	Organic compounds	Phenylpropanoids and polyketides	Flavonoids	Flavonoid glycosides	Flavonoid C-glycosides	Flavonoid 8-C-glycosides	
MMJPRTHFLGOVBZ-UHFFAOYSA-N	Completed	Organic compounds	Bzenoids	Benzene and substituted derivatives	Benzenesulfonic acids and derivatives	Benzenesulfonic acids and derivatives		
UJSYMVCGDZCLO-DILIWBYS-A-N	Completed	Organic compounds	Lipids and lipid-like molecules	Prenol lipids	Monoterpenoids	Aromatic monoterpenoids		
ZWDZSGCQFGIYBE-UHFFAOYSA-N	Completed	Organic compounds	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	Amino acids and derivatives	Beta amino acids and derivatives	
SEOZHEFAHJQWFY-USNXYBSJSA-N	Completed	Organic compounds	Phenylpropanoids and polyketides	Stilbenes	Stilbene glycosides	Stilbene glycosides		

Failed classifications occur when ClassyFire does not contain the given InChIKey in its database. If all results fail, this could be due to network issues - in this case, please try again later.

[Export as CSV](#)[Reset](#)

曖昧な脂質表記からでも、明確な定義構造のリストを出力する

	Cholic acid (3 α ,7 α ,12 α -Trihydroxy-5 β -cholan-24-oic acid) (Sterol lipids)	Diacylglycerol (Glycerolipids)	Sulfatide (Sphingolipids)
Species level	ST 24:1;O5	DG 34:1	SHexCer 36:1;3O
Molecular species level		DG 16:0_18:1	SHexCer 18:1;O2/18:0;O
sn-Position level		DG 16:0/18:1	
Structure defined level			SHexCer 18:1;(1OH,3OH)/18:0;(2OH)
Full structure level	ST 24:0;(5bH);(3aOH,7aOH,12aOH)(24COOH)	DG 16:0/18:1(9Z)/0:0	3'-sulfo Gal β Cer 18:1(4E);(1OH,3OH)/18:0;(2OH)

<http://prime.psc.riken.jp/compms/msdial/lipidnomenclature.html>

LipidLynxXによるIDコンバート



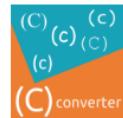
LipidLynxX

PLPC

Check resources

LipidLynxX Tools

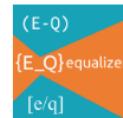
Nomenclature & Levels



Lipid ID Converter

Convert different abbreviations
to unified LipidLynxX identifier.

Run Converter



Lipid ID Equalizer

Bring lipid identifiers to the
same level of annotation and
perform cross-level matching
between different datasets.

Run Equalizer



Lipid Resource Linker

Collect available resources
across databases.

Run Linker

LipidLynxXによるIDコンバート

LipidLynxX Converter

Convert list

Convert file

Input lipid abbreviations

lipid_names

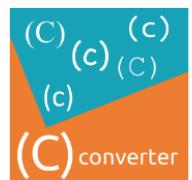
palmitic acid
DHA
HETE
PLPE
PC O-16:0_18:2
FaCoA 18:2;O
C18 Sphingomyelin

Choose the export style:

Choose the export Level:

- COMP_DB and BioPAN export in Bulk level only.
- LipidCreator export supports Molecular species and sn specific species.
- LPPtiger export in sn specific species level only.

Choose the export format:



Lipid ID Converter

Convert different abbreviations to unified
LipidLynxX identifier.

他 Shorthand notation...

他 Molecular species level

Shorthand, Bulkを選択

TextInput

▲ TextInputConverted

C18 Sphingomyelin

SM 36:1;2

DHA

FA 22:6

FaCoA 18:2;O

CoA 18:2;O

HETE

FA 20:4+16

palmitic acid

FA 16:0

PC O-16:0_18:2

PC O-34:2

PLPE

PE 34:2

Shorthand, Maxを選択

TextInput

▲ TextInputConverted

C18 Sphingomyelin

SM 18:1;2/18:0

DHA

FA 22:6(4Z,7Z)

FaCoA 18:2;O

CoA 18:2;O

HETE

FA 20:4(OH)

palmitic acid

FA 16:0

PC O-16:0_18:2

PC O-16:0_18:2

PLPE

PE 16:0/18:2(9Z,12Z)

LipidLynxXによるresourceリンク

LipidLynxX Linker

Link list

Link file

Input lipid abbreviations:

lipid names (max 100 rows)

PLPC
PLPE
PC O-16:0_18:2
C18 Sphingomyelin



Lipid Resource Linker

Collect available resources across databases.

Choose the export format:



Save output: LipidLynxX-Linker-20221119-102101-25c6.xlsx

Input Lipid	Converted Notation (LipidLynxX)	Resources
PLPC	PC(16:0/18:2<{9Z,12Z}>)	<input type="button" value="View resource details"/>
PLPE	PE(16:0/18:2<{9Z,12Z}>)	<input type="button" value="View resource details"/>
PC O-16:0_18:2	PC(O-16:0_18:2)	<input type="button" value="View resource details"/>
C18 Sphingomyelin	SM(18:1;02/18:0)	<input type="button" value="View resource details"/>

Input Lipid: PLPC

Shorthand Notation: PC 16:0/18:2(9Z,12Z)

LipidLynxX Notation: PC(16:0/18:2<{9Z,12Z}>)

BioPAN Notation: PC 34:2

§ Lipid database

⇄ lipidmaps

LMGP01010594 : <https://www.lipidmaps.org/data/LMSDRecord.php?LMID=LMGP01010594>

⇄ swisslipids

SLM:000000792 : <https://www.swisslipids.org/#/entity/SLM:000000792/>

§ Metabolites database

⇄ hmdb

HMDB0007973 : <https://hmdb.ca/metabolites/HMDB0007973>

§ Lipid ontology

⇄ lion

0003021 : http://bioportal.bioontology.org/ontologies/LION/?p=classes&conceptid=http%3A%2F%2Fpurl.obolibrary.org%2Fobo%2FLION_0003021

§ General database

⇄ chebi

73002 : <https://www.ebi.ac.uk/chebi/searchId.do?chebiId=CHEBI:73002>

⇄ pubchem

5287971 : <https://pubchem.ncbi.nlm.nih.gov/compound/5287971>

§ Pathways

⇄ kegg

C00157 : https://www.kegg.jp/dbget-bin/www_bget?cpd:C00157

メタボロームデータを出す側と使う側



メタボロミクスのデータ解析プロトコール

メタボロームデータを「出す側」
(4-2~4-5)

メタボロームデータを「使う側」
(4-6~4-8)

質量分析インフォマティクス

ケムインフォマティクス

バイオインフォマティクス

データ処理(ノンターゲット解析)

XCMS

MS-DIAL

OpenMS

MZmine 2

未知代謝物アノテーション

MS-FINDER

GNPS

SIRIUS

代謝データベース

KEGG

HMDB

ID変換ツール(CTSなど)

パスウェイ解析

VANTED

MSEA

多変量解析及び統合解析

MetaboAnalyst

transomics2cytoscape

Garudaプラットホーム

データ処理(ターゲット解析)

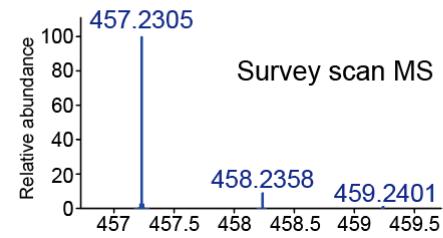
MRM PROBS

Skyline

その他
データ標準化・レポジトリ
(4-9, 4-10)

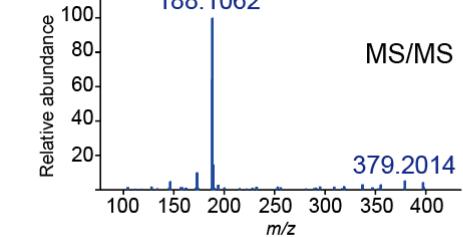
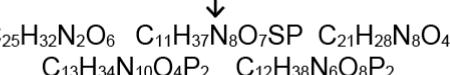
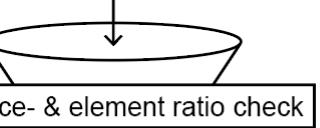
未知マススペクトルのアノテーション

a. Get MS & MS/MS spectrum

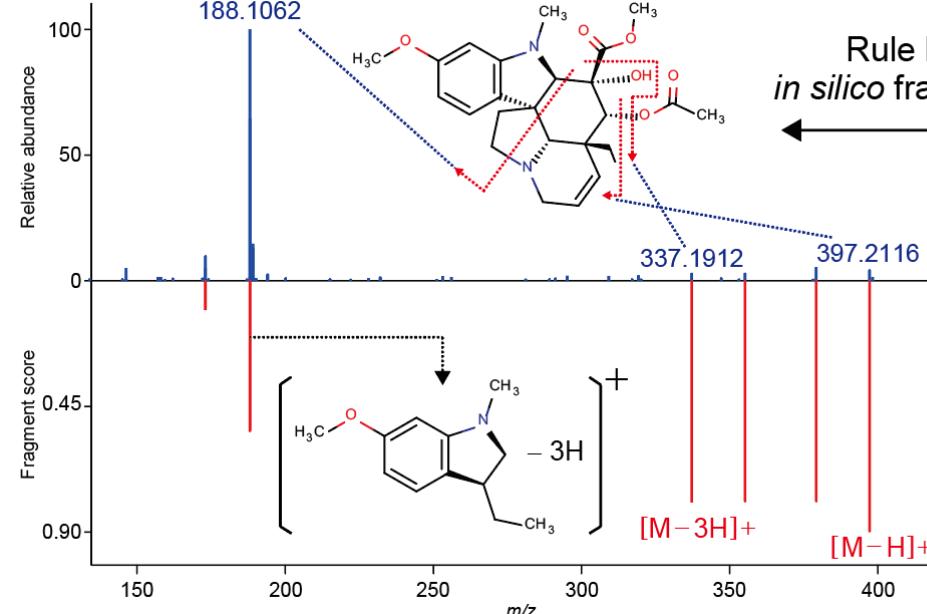


b. Formula generation

Input
 m/z : 457.23053
 Adduct: $[M+H]^+$
 Tolerance: 0.003 Da



e. Structure ranking



c. Formula ranking

Candidates

Scoring
 Mass error
 Isotopic ratio
 Product ion annotation
 Neutral loss annotation
 Inclusion in metabolome DBs

Top: $C_{25}H_{32}N_2O_6$

Metabolome databases

HMDB
 YMDB
 SMPDB
 UNPD
 ChEBI
 PlantCyc
 PubChem (Biopathway)
 DrugBank
 BMDB
 KNApSAcK
 FooDB
 ECMDB
 T3DB

d. Structure searching

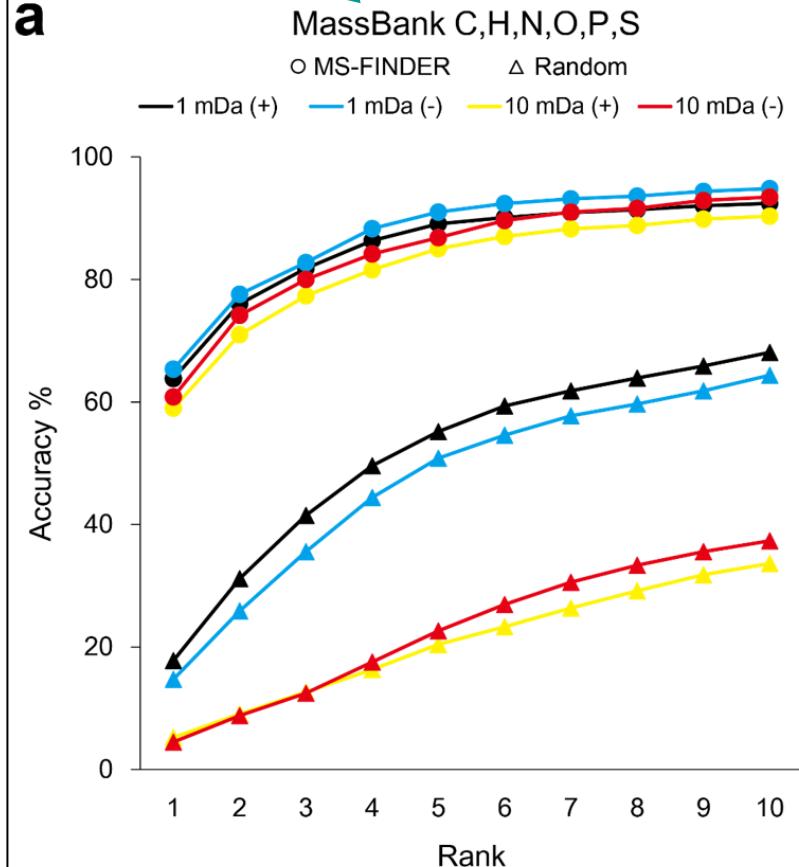
PubChem database

Structure candidates

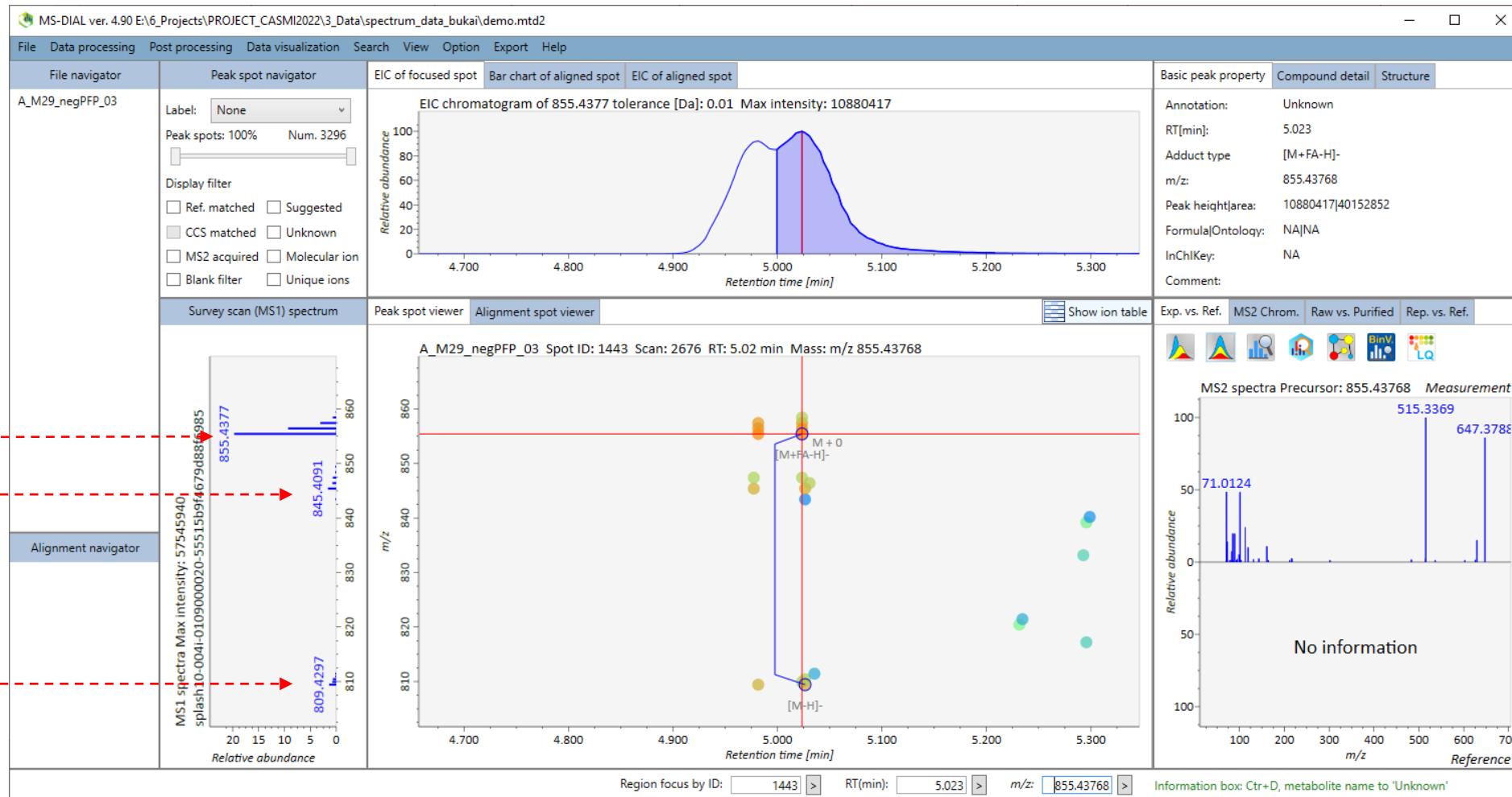
XBGOBGJHGGWIE-*****-*
 ITHNZGQTXZZCTI-*****-*
 HYEXIINDBCFMOM-*****-*
 NVRFOCOGUIYAQQL-*****-*
 NQKHZSNXAUQSHC-*****-*

Validation using 3,000 MS/MS data

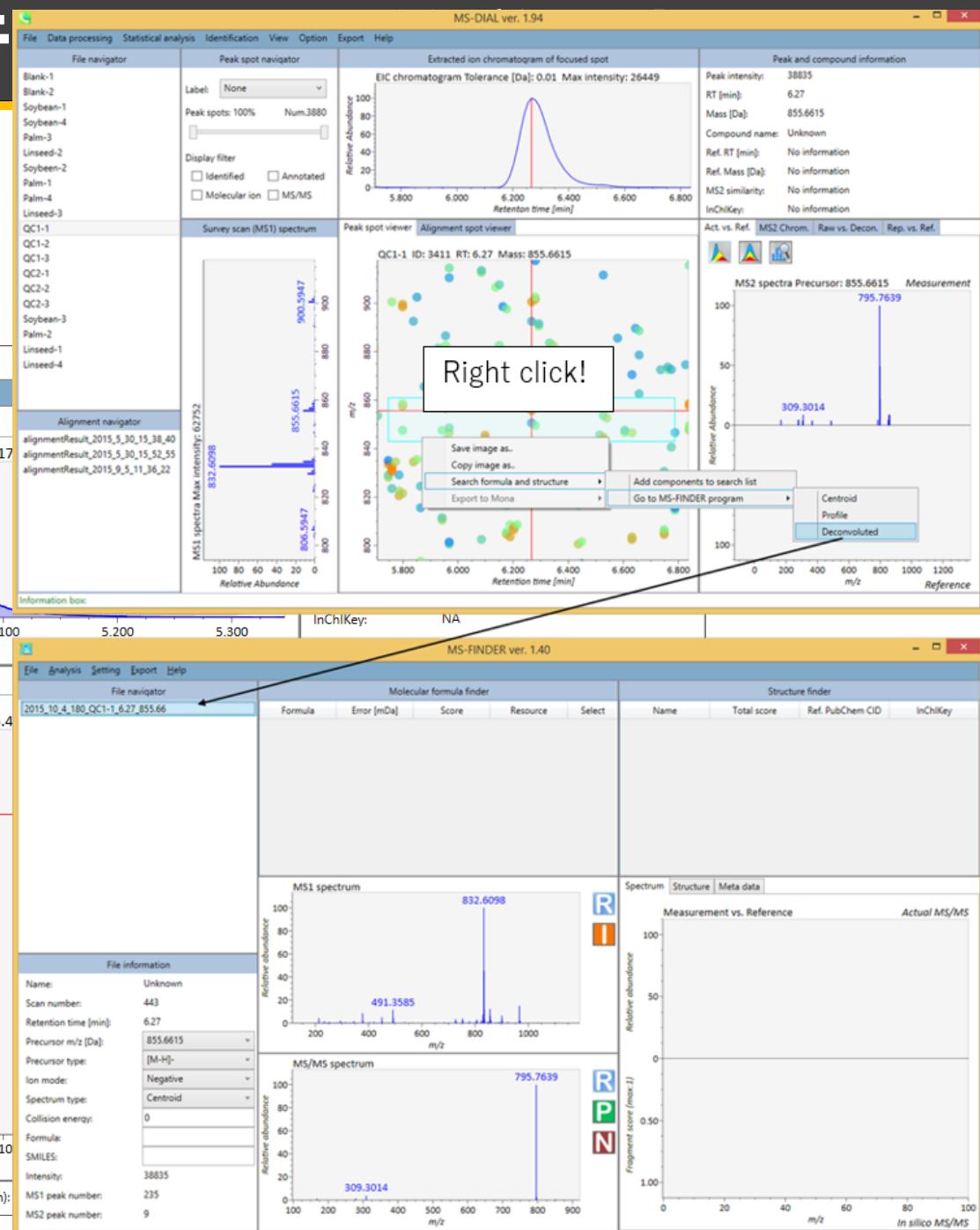
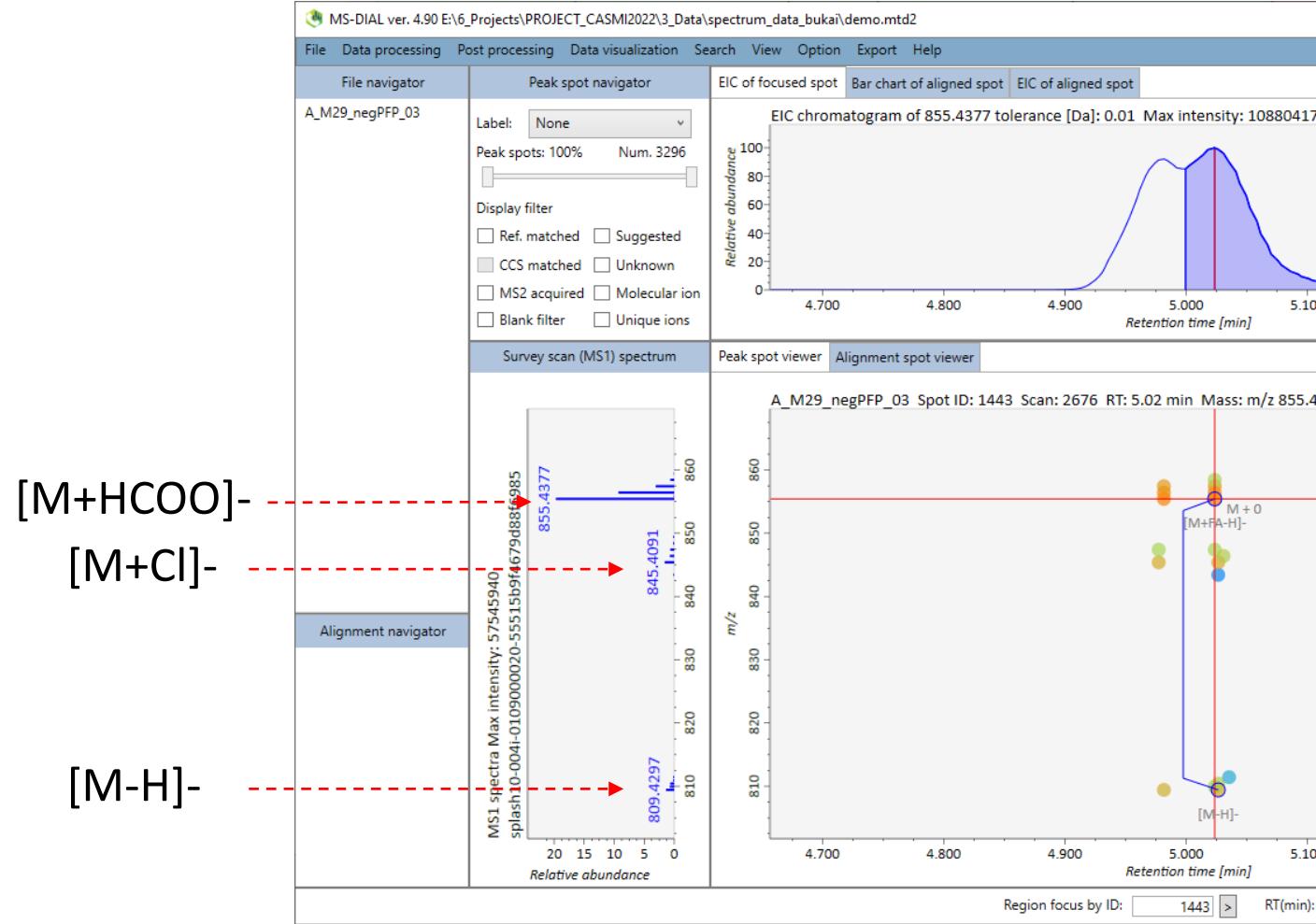
a



未知マススペクトルのアノテーションの簡単な流れ



未知マススペクトルのアノテ



未知マススペクトルのアノテーションの簡単な流れ

Analysis parameter setting

- Method**: Basic
- Formula finder**: Structure finder
- Data source**: Retention time
- Retention time**: CCS

Formula calculation setting

- LEWIS and SENIOR check:
- Isotopic ratio tolerance: 20 %
- Element ratio check: Common range (99.7%) covering
- Element probability check:

Element selection

- O
- N
- P
- S
- F
- Cl
- Br
- I
- Si

TMS-MEOX derivative compound

Minimum TMS count: 1

Minimum MEOX count: 0

Options

Maximum report number: 100 up to 100

Time out (-1 means infinite): -1 min

Advanced settings for AIF: Setting

Finish **Cancel**

Analysis parameter setting

- Method**: Basic
- Formula finder**: Structure finder
- Data source**: Retention time
- Retention time**: CCS

Local Databases

- HMDB (Human)
- Urine (Human)
- Saliva (Human)
- Feces (Human)
- Serum (Human)
- CSF (Human)
- SMPDB (Human)
- LipidMAPS (Lipids)
- YMDB (Yeast)
- ECMDB (E.coli)
- BMDB (Bovine)
- DrugBank (Drug)
- FooDB (Food)
- PlantCyc (Plant)
- ChEBI (Biomolecules)
- T3DB (Toxin)
- STOFF (Environment)
- BLEXP (blood exposome)
- NPA (Natural Products Atlas)
- NANPDB (Natural product)
- COCONUT (Natural product)
- KNApSack (Natural product)
- PubChem (Biomolecules)
- UNPD (Natural product)
- User-defined DB Browse

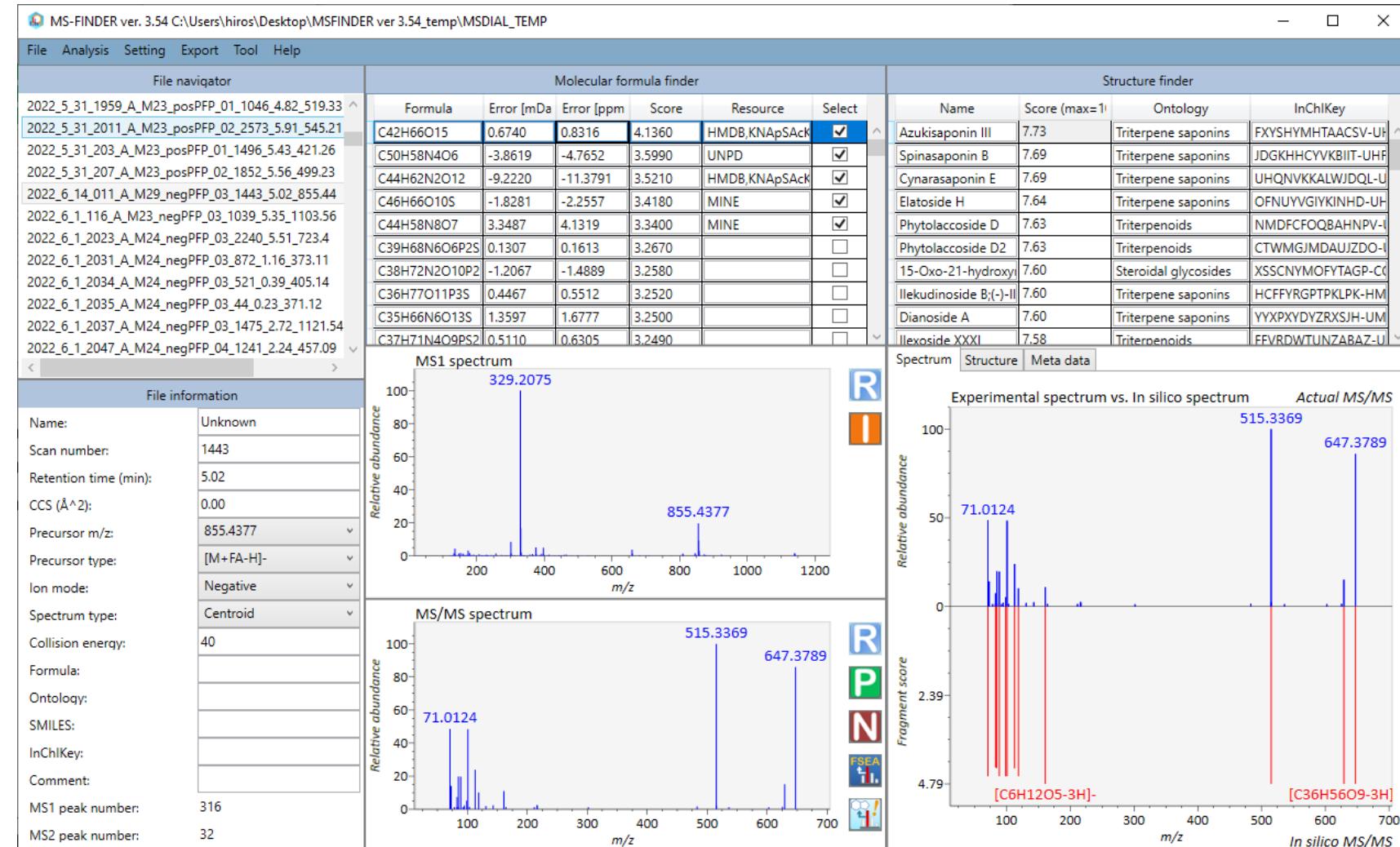
MINEs (Metabolic In silico Network Expansions) setting

- Never use it.
- Only use when there is no query in local DBs.
- Always use it.

PubChem Online setting

- Never use it.
- Only use when there is no query in local DBs.
- Always use it.

Finish **Cancel**



MS-FINDERデータベースは化合物構造情報が豊富

MSFINDER ver 3.56 > Resources	
Name	Date modified
AdductNegatives.anf	4/7/2021 9:46 AM
AdductPositives.apf	4/7/2021 9:46 AM
Biotransformation-VS1.fbt	4/7/2021 9:46 AM
ChemOntologyDB_vs2.cho	4/7/2021 9:46 AM
EiFragmentDB_vs1.eif	4/7/2021 9:46 AM
EIMS-DBs-vs1.egm	4/7/2021 9:46 AM
InchikeyClassyfireDB-VS5.icd	4/7/2021 9:46 AM
LipidQueryMaster.txt	4/19/2022 11:18 PM
MINEs-StructureDB-vs1.msd	4/7/2021 9:46 AM
MINEs-StructureDB-vs1_bin.msd	3/10/2022 6:38 PM
MsfinderFormulaDB-VS13.esd	4/7/2021 9:46 AM
MsfinderFormulaDB-VS13_bin.esd	3/10/2022 6:38 PM
MsfinderStructureDB-VS15.esd	4/7/2021 9:46 AM
MsfinderStructureDB-VS15_bin.esd	3/10/2022 6:38 PM
MSMS-DBs-vs1.etm	4/7/2021 9:46 AM
Msp20201228141756_converted.lbm2	4/7/2021 9:46 AM
NeutralLossDB_vs2.ndb	4/7/2021 9:46 AM
ProductionLib_vs1.pid	4/7/2021 9:46 AM
UniqueFragmentLib_vs1.ufd	4/7/2021 9:46 AM

A	B	C	E	F	G	H	I	J	K	L	M	N	O	P	Q
1 Title	InChikey	Short InChI	Exact mass	Formula	SMILES	HMDB	KNAPSAc	ChEBI	DrugBank	SMPDB	YMDB	T3DB	FooDB	NANPDB	STOFF
2 buta-1,3-diyne	LLCSWKVOHI	LLCSWKVC	50.01565	C4H2	C#CC#C	N/A	N/A	CHEBI:378	N/A	N/A	N/A	N/A	N/A	N/A	N/A
3 fluoromethanol	RLWXXXHAQ	RLWXXXH	50.01679	CH3FO	C(O)F	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
4 oxalonitrile	JMANVNJQN	JMANVNJ	52.00615	C2N2	N#CC#N	N/A	N/A	CHEBI:293	N/A	N/A	N/A	N/A	T3D0754	N/A	N/A
5 oxalonitrile.(1-)	SELGXVYREW	SELGXVYR	52.00615	C2N2	[N-]=[C]C#N	N/A	N/A	CHEBI:298	N/A	N/A	N/A	N/A	N/A	N/A	N/A
6 difluoromethane	RWRIBAII	RWRIBA	52.01246	CH2F2	FCF	N/A	N/A	CHEBI:478	N/A	N/A	N/A	N/A	N/A	N/A	STOFF_52
7 tetrahedrane	FJGIHZCEAZ	FJGIHZCEZ	52.0313	C4H4	C12C3C1C	N/A	N/A	CHEBI:365	N/A	N/A	N/A	N/A	N/A	N/A	N/A
8 cyclobuta-1,3-diene	HWEQKSVYKI	HWEQKSV	52.0313	C4H4	C1=CC=C1	N/A	N/A	CHEBI:336	N/A	N/A	N/A	N/A	N/A	N/A	N/A
9 butenyne	WFYPICNXBK	WFYPICNX	52.0313	C4H4	C=CC#C	N/A	N/A	CHEBI:480	N/A	N/A	N/A	N/A	N/A	N/A	N/A
10 butatriene	WHVXVDDUY	WHVXVDC	52.0313	C4H4	C=C=C=C	N/A	N/A	CHEBI:376	N/A	N/A	N/A	N/A	N/A	N/A	N/A
11 prop-2-yn-1-one	NONQAKWU	NONQAKV	53.00274	C3HO	C#[C]=O	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
12 acrylonitrile	NLHHRLWOU	NLHHRLW	53.02655	C3H3N	C=CC#N	N/A	N/A	CHEBI:282	N/A	N/A	N/A	N/A	T3D1688	N/A	N/A
13 2-Propyn-1-al	IJNJLGFTSIAH	IJNJLGFTS	54.01056	C3H2O	O=CC#C	HMDB000	N/A	CHEBI:279	N/A	N/A	N/A	N/A	FDB02408	N/A	N/A
14 prop-1,2-dien-1-one	TURAMGVWIT	TURAMGV	54.01056	C3H2O	C=C=C=O	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
15 propanenitrile	VQGISNOMG	VQGISNOI	54.03437	C3H4N	C#[CH]C#N	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
16 1,3-Butadiene	KAKZBPTYRL	KAKZBPTY	54.04695	C4H6	C=CC=C	HMDB004	N/A	CHEBI:394	N/A	N/A	N/A	N/A	T3D0156	N/A	N/A
17 cyclobutene	CFBGXYDUOD	CFBGXYDU	54.04695	C4H6	C1CC=C1	N/A	N/A	CHEBI:512	N/A	N/A	N/A	N/A	N/A	N/A	N/A
18 but-1-yne	KDKYADYSIPS	KDKYADYS	54.04695	C4H6	CCC#C	N/A	N/A	CHEBI:480	N/A	N/A	N/A	N/A	N/A	N/A	N/A
19 buta-1,2-diene	QNRMTGGDF	QNRMTGC	54.04695	C4H6	CC=C=C	N/A	N/A	CHEBI:394	N/A	N/A	N/A	N/A	FDB00364	N/A	STOFF_56
20 1-methylcyclopropene	SHDPRTQPPV	SHDPRTQI	54.04695	C4H6	CC1=CC1	N/A	N/A	CHEBI:132	N/A	N/A	N/A	N/A	N/A	N/A	STOFF_43
21 UNPD155200	XNMQEEKYCX	XNMQEEK	54.04695	C4H6	CC#CC	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
22 Cyanoformaldehyde	TUHMQDODLTUHMQDC		55.00581	C2HNO	O=CC#N	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	STOFF_42
23 N-Methylene-ethenamine	TUVFMMNNATUVFMMN		55.0422	C3H5N	C=CN=C	HMDB006	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
24 propionitrile	FVSKHRXBFI	FVSKHRXE	55.0422	C3H5N	CCC#N	N/A	N/A	CHEBI:263	N/A	N/A	N/A	N/A	T3D1708	N/A	NANPDB
25 prop-2-yn-1-amine	JKANAVGODJKANAVG		55.0422	C3H5N	C#CCN	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
26 prop-1-en-2-ylazanide	LUWREKROQ	LUWREKR	55.0422	C3H5N	C=C([CH2]N)A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
27 cyclopropanimine	QAVALNTZAV	QAVALNTZ	55.0422	C3H5N	C1CC1=N	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
28 Acrolein	HGINCPLSRV	HGINCPLS	56.02621	C3H4O	C=CC=O	HMDB004	N/A	CHEBI:153	N/A	PW_C022tYMDB0081T3D0037	FDB00830	N/A	N/A	STOFF_24	
29 oxetene	CRYATLIDHPFCRYATLDI		56.02621	C3H4O	C1OC=C1	N/A	N/A	CHEBI:511	N/A	N/A	N/A	N/A	N/A	N/A	N/A
30 prop-2-yn-1-ol	TVDSBUOJIPE	TVDSBUO	56.02621	C3H4O	OCC#C	N/A	N/A	CHEBI:289	N/A	N/A	YMDB013	N/A	N/A	N/A	STOFF_53
31 prop-1-en-1-one	UYLUJGRCKKUYLUJGR		56.02621	C3H4O	CC=C=O	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
32 cyclopropanone	VBBRYJMZLY	VBBRYJMZ	56.02621	C3H4O	C1CC1=O	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
33 diazoethane	WLXALCKAKCWLXALCK		56.03745	C2H4N2	CC=[N+]=[N]	N/A	N/A	CHEBI:874	N/A	N/A	N/A	N/A	N/A	N/A	N/A
34 2-aminoacetonitrile	DFNYGALUNI	DFNYGALL	56.03745	C2H4N2	C(C#N)N	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
35 methylcyanamide	MCLITRXWHZ	MCLITRXV	56.03745	C2H4N2	CNC#N	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
36 N-(methylideneamino)me	NBHLEUNJGN	NBHLEUN	56.03745	C2H4N2	C=NN=C	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
37 Ethyl Isocyanide	JEGVKBYNUP	JEGVKBYN	56.05002	C3H6N	CC[N+]=C	N/A	N/A	N/A	DB03399	N/A	N/A	N/A	N/A	N/A	N/A

作成すべきメタボロームテーブルの目標

代謝物アノテーションのメタデータ・定量値が整理されてるテーブル

メタボロームデータを出す側と使う側



メタボロミクスのデータ解析プロトコール

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(4-2~4-5)

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MRM PROBS

Skyline

その他
データ標準化・レポジトリ
(4-9, 4-10)

パスウェイ解析に使えるリソース

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nature > npj systems biology and applications > technology features > article

Technology Feature | Open Access | Published: 13 December 2018

ComPath: an ecosystem for exploring, analyzing, and curating mappings across pathway databases

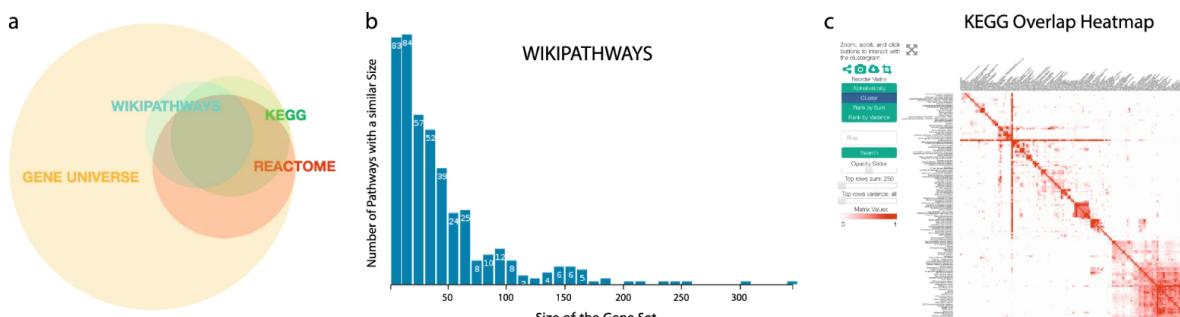
Daniel Domingo-Fernández , Charles Tapley Hoyt, Carlos Bobis-Álvarez, Josep Marín-Llao & Martin Hofmann-Apitius

[npj Systems Biology and Applications](#) 4, Article number: 43 (2018) | [Cite this article](#)

4625 Accesses | 11 Citations | 18 Altmetric | [Metrics](#)

Fig. 2

From: ComPath: an ecosystem for exploring, analyzing, and curating mappings across pathway databases



a An Euler diagram summarizing the human gene-centric coverage of KEGG, Reactome, and WikiPathways compared to the universe of all genes from HGNC (more details in Supplementary Table 1). **b** Histogram views present gene promiscuity or pathway size distributions. **c** The pathway similarity landscape of KEGG visualized as a heatmap.

Cytoscape is an open source software platform for visualizing complex networks and integrating these with any type of attribute data. A lot of Apps are available for various kinds of problem domains, including bioinformatics, social network analysis, and semantic web.

[Learn more...](#)

[Cytoscape Tutorials](#) [App Developers Docs](#)

MetaboAnalyst is a great (really top) tool for analyses.

The screenshot shows the MetaboAnalyst 4.0 homepage. On the left is a sidebar with links: Home, User Stats, Overview, Data Formats, FAQs, Tutorials, MetaboAnalystR, Contact, Resources, APIs, Update History, and About. Logos for GenomeCanada and GenomeQuébec are also present. The main content area features a large circular diagram with various analysis modules. A legend on the right maps colors to analysis types:

- Display R command history
- Targeted or untargeted metabolomics
- Targeted or annotated metabolomics
- Untargeted metabolomics
- Multiple metabolomics data
- Integrating other omics

The modules shown in the diagram include:

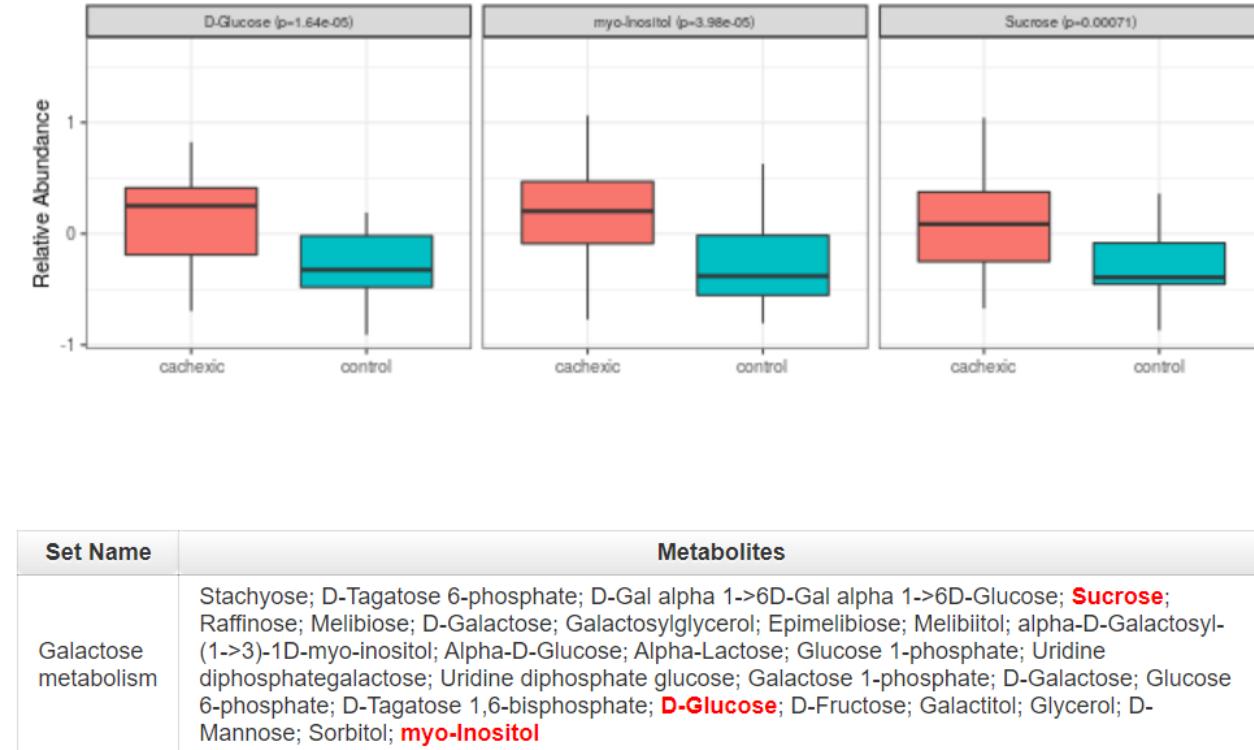
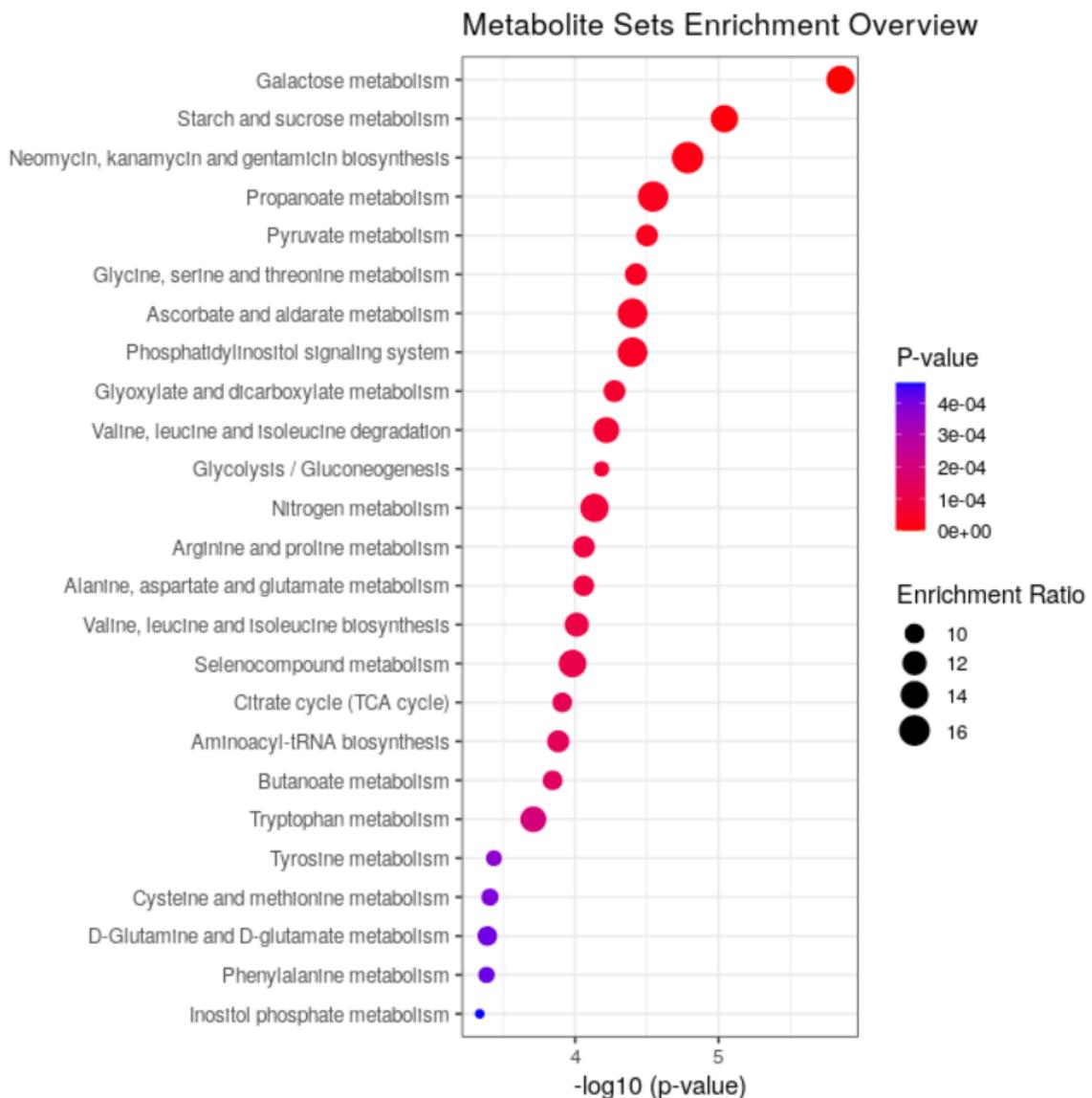
- Statistical Analysis
- Enrichment Analysis
- Pathway Analysis
- MS Peaks to Pathways
- MS Spectral Processing
- Joint Pathway Analysis
- Network Explorer
- Other Utilities
- Biomarker Meta-analysis
- Power Analysis
- Time-series / Two-factor
- Biomarker Analysis

A call-to-action text "Click a module to proceed, or scroll down for more details:" is located above the circular diagram.

MetaboAnalyst is a great (really top) tool for analyses.

A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X	Y	Z	AA	AB	AC	AD	AE	AF	AG	AH	AI	
Patient ID	Muscle loss	1,6-Anhydri	1-Methyl	2-Aminob	2-Hydroxy	2-Oxoglut	3-Amino	3-Hydroxy	3-Hydroxy	3-Indoxyl	4-Hydroxy	Acetate	Acetone	Adipate	Alanine	Asparagin	Betaine	Carnitine	Citrate	Creatine	Creatinin	Dimethyl	Ethanol	Formate	Fucose	Fumarate	Glucose	Glutamine	Glycine	Glycolate	Guano	Hippuric	Histidine	Hyp	
2	PIF_178	cachexic	40.85	65.37	18.73	26.05	71.52	1480.3	56.83	10.07	566.8	120.3	126.47	9.49	38.09	314.19	159.17	109.95	265.07	3714.5	196.37	16481.6	632.7	645.48	441.42	336.97	7.69	395.44	871.31	2038.56	685.4	154.47	4582.5	925.19	1
3	PIF_087	cachexic	62.18	340.36	24.29	41.68	67.36	116.75	43.82	79.84	368.71	432.68	212.72	11.82	327.01	871.31	157.59	244.69	120.3	2617.57	212.72	15835.35	607.89	487.85	252.14	198.34	18.92	8690.62	601.85	1107.65	651.97	109.95	1737.15	845.56	1
4	PIF_090	cachexic	270.43	64.72	12.18	65.37	23.81	14.3	5.64	23.34	665.14	292.95	314.19	4.44	131.63	464.05	89.12	116.75	25.03	862.64	221.41	24587.66	735.1	407.48	249.64	186.79	7.1	1352.89	301.87	620.17	141.17	183.09	4315.64	284.29	1
5	NETL_005_V1	cachexic	154.47	52.98	172.43	74.44	1199.91	555.57	175.91	25.03	411.58	214.86	37.34	206.44	144.03	589.93	273.14	278.66	200.34	13629.61	85.63	20952.22	1064.22	820.57	468.72	407.48	96.54	862.64	1685.81	5064.45	70.81	102.51	757.48	1043.15	2
6	PIF_115	cachexic	22.2	73.7	15.64	83.93	33.12	29.67	76.71	69.41	165.67	97.51	407.48	44.26	15.03	1118.79	42.52	391.51	84.77	854.06	105.64	6768.26	242.26	365.04	114.43	26.05	19.69	6836.29	432.68	395.44	26.58	52.98	1152.86	327.01	1
7	PIF_110	cachexic	212.72	31.82	18.36	80.64	47.94	17.46	31.82	35.16	183.09	132.95	81.45	14.44	25.28	237.46	157.59	66.69	40.04	1958.63	200.34	15677.78	614	459.44	314.19	123.97	5.05	512.86	298.87	482.99	428.38	57.97	3568.85	459.44	1
8	NETL_019_V1	cachexic	151.41	36.6	8.67	42.52	223.63	56.26	11.59	25.79	223.63	59.15	51.42	3.25	8.41	336.97	71.52	149.9	127.74	3944.19	383.75	8022.46	333.62	217.02	67.36	55.7	4.71	237.46	561.16	3428.92	290.03	101.49	2368.47	327.01	1
9	NETCR_014_V1	cachexic	31.5	6.82	4.18	12.94	25.03	8.67	1.73	8.76	111.05	33.78	7.46	2.8	3.53	69.41	13.87	15.33	9.87	788.4	5.81	2208.35	73.7	55.7	49.9	18.17	1.86	80.64	71.52	196.37	70.11	42.52	254.68	130.32	1
10	NETCR_014_V2	cachexic	51.42	30.27	7.54	34.81	80.64	17.99	9.03	3.25	391.51	145.47	9.97	8.67	8.25	102.51	32.79	31.19	7.32	1669.03	35.16	6634.24	214.86	183.09	68.03	72.97	3.56	177.68	145.47	292.95	33.12	56.26	365.04	183.09	1
11	PIF_154	cachexic	117.92	52.46	19.49	72.24	73.7	57.97	26.84	28.5	116.75	50.4	100.48	9.12	14.59	962.95	221.41	149.9	487.85	4675.07	126.47	8690.62	350.72	437.03	320.54	57.4	12.06	972.63	1022.49	3294.47	589.93	188.67	632.7	706.27	1
12	NETL_022_V1	cachexic	20.7	221.41	15.18	28.79	357.81	93.69	13.07	4.26	361.41	59.74	27.94	6.49	18.54	164.02	32.14	219.2	230.44	3533.34	1450.99	8433.78	361.41	184.93	83.93	138.38	10.91	170.72	179.47	497.25	132.95	137	2697.28	247.15	1
13	NETL_022_V2	cachexic	127.74	177.68	12.68	15.03	68.03	105.64	29.08	53.52	376.15	160.77	30.88	7.92	259.82	502.7	64.72	137	35.87	854.06	1863.11	694.09	273.14	175.91	165.67	94.63	11.47	473.43	445.86	607.89	149.9	154.47	1934.31	497.7	1
14	NETL_008_V1	cachexic	59.74	50.91	6.82	46.06	111.05	8.08	17.12	16.78	379.93	174.16	55.15	9.21	11.02	217.02	32.14	167.34	14.88	1772.24	125.21	15677.78	678.58	354.25	46.06	210.61	6.05	419.89	237.46	880.07	288.15	83.93	427.69	154.47	1
15	PIF_146	cachexic	89.12	32.79	10.38	32.14	32.46	43.38	8.08	20.49	317.35	86.49	95.58	8.67	9.03	167.34	47.94	56.83	16.95	323.76	102.51	12209.87	437.03	144.03	91.84	101.49	3.49	183.09	121.51	330.3	249.64	99.48	2643.87	190.57	1
16	PIF_119	cachexic	23.57	6.89	2.12	7.85	8.33	2.97	1.7	5.58	82.27	17.64	69.41	6.23	3.16	34.47	13.33	41.68	24.53	265.07	11.7	1480.3	46.99	37.34	79.84	24.05	1.48	43.82	36.6	104.58	12.06	18.17	113.3	24.05	1
17	PIF_099	cachexic	41.26	8.67	2.56	7.85	6.89	6.36	3.42	6.23	90.02	25.03	79.84	3.16	4.81	26.84	14.3	4.06	18.36	80.64	18.54	1635.98	56.26	29.96	57.4	31.19	2.23	57.97	26.84	36.23	25.28	92.76	22.87	1	
18	PIF_162	cachexic	589.93	21.98	15.18	46.06	32.79	31.82	25.03	7.69	109.95	148.41	91.84	17.64	22.87	441.42	79.04	157.59	62.8	897.85	419.98	970.15	395.44	200.34	53.52	64.07	10.49	105.64	512.86	160.77	181.27	112.17	934.49	160.77	1
19	PIF_160	cachexic	112.17	25.28	15.49	47.94	28.79	16.12	30.27	21.33	347.23	73.7	70.81	4.22	15.8	188.67	54.05	78.26	24.05	2489.91	170.72	10198.54	1422.26	244.69	89.12	26.84	3.39	387.61	214.86	1141.39	190.57	51.42	4023.87	190.57	1
20	PIF_113	cachexic	167.34	19.89	13.46	31.19	47.94	79.04	11.7	12.55	184.93	74.44	42.52	9.39	12.43	237.46	35.87	60.34	12.06	4447.07	97.51	6974.39	275.89	290.03	160.77	61.56	5.21	221.41	225.88	2298.47	141.17	18.54	2807.36	343.78	1
21	PIF_143	cachexic	183.09	90.92	8.94	64.07	20.49	18.73	26.05	51.42	204.38	115.58	28.22	3.82	20.49	333.62	61.56	68.72	15.18	2643.87	55.7	11158.98	379.93	407.48	314.19	117.92	3.1	473.43	399.41	1096.63	595.86	123.95	420.18	419.89	1
22	NETCR_007_V1	cachexic	208.51	53.52	5.26	47.94	212.72	50.4	30.27	6.82	200.34	46.53	25.03	5.05	18.54	254.68	96.54	131.63	29.37	2835.57	44.26	978.95	361.41	450.34	130.32	82.27	4.85	267.74	487.85	99.27	437.03	57.4	4675.07	347.23	1
23	NETCR_007_V2	cachexic	34.81	95.58	23.57	68.03	287.15	104.58	60.34	42.95	333.62	117.92	82.27	5.26	28.79	555.57	94.63	170.72	19.3	5377.61	48.91	14328.42	665.14	713.37	198.34	156.02	7.85	528.48	888.91	1261.43	478.19	98.49	6438.17	437.03	1
24	PIF_137	cachexic	333.62	35.87	7.92	54.6	20.49	63.43	29.96	47.47	247.15	237.46	50.4	4.35	23.1	399.41	102.51	66.02	20.91	1958.63	71.52	13357.93	539.15	350.72	154.47	93.69	19.11	845.56	445.86	1958.63	23.81	49.4	6568.23	720.54	1
25	PIF_100	cachexic	32.46	9.68	3.9	11.02	170.72	2.97	6.36	2.46	34.81	70.11	77.48	2.29	3.6	78.26	16.61	50.91	4.44	223.63	9.58	1261.43	102.51	16.12	58.56	13.6	17.46	5943.18	38.09	52.46	10.91	19.69	217.02	14.15	1
26	NETL_004_V1	cachexic	4.71	11.13	43.38	30.88	104.58	54.05	7.61	7.92	20.61	31.19	13.07	7.61	6.11	27.66	94.63	28.79	1422.26	38.86	4865.87	214.86	86.49	36.23	24.29	8.17	109.95	116.75	518.01	107.77	108.85	645.48	146.94	1	
27	PIF_094	cachexic	68.72	13.87	12.18	25.03	28.22	72.97	11.47	25.03	119.1	134.29	103.54	12.06	32.14	454.86	98.49	88.23	42.52	3677.54	43.82	8349.86	350.72	252.14	202.35	86.49	7.17	403.43	415.72	1422.26	204.38	95.58	1919.85	383.75	1
28	PIF_132	cachexic	214.86	127.74	31.5	33.78	88.23	64.07	54.05	164.02	692.29	278.66	411.58	14.73	68.72	1312.91	132.95	156.02	33.78	9045.29	105.64	33860.35	1556.2	1436.55	1480.3	181.27	7.54	1							

Enrichment Analysis in MetaboAnalyst



Integrated analysis in MetaboAnalyst



MetaboAnalyst - statistical, functional and integrative analysis of metabolomics data



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Please upload a gene list and a metabolite list below.

Gene List Metabolite List

Gene list with optional fold changes

```
#Official logFC
AASS -0.139042168
ACAA2 1.401267672
ACADL -2.608712824
ACADM -0.876538515
ACADS 0.150535255
ACADSB -1.637743607
ACHE 2.567118372
ACSM1 -2.348501729
ACTA2 -0.282176735
ACTB 1.559623747
ACTC1 -1.690352151
ADCY1 2.916857724
ADH1A -0.87610472
AGL -0.399133917
AGTR1 -1.078340189
AKR1A1 2.178398898
AKR1B1 -1.077265882
AKT1 0.221500016
```

ID Type: Official Gene Symbol

Compound list with optional fold changes

```
#KEGG logFC
C0006 0.512160717
C0024 0.351757155
C0026 -2.669056963
C0029 0.379186578
C0031 1.669222153
C0047 -2.492289379
C0049 2.963835134
C0062 -2.558919927
C0064 1.77810046
C0072 0.632536475
C0077 -2.09045808
C0084 0.347392968
C0089 -1.460843412
C0097 3.046798674
C00101 -1.495004303
C00109 0.476718643
C00111 -2.672997377
C00115 -0.572141500
```

ID Type: KEGG ID

Specify organism: Homo sapiens (human)

Try our example data

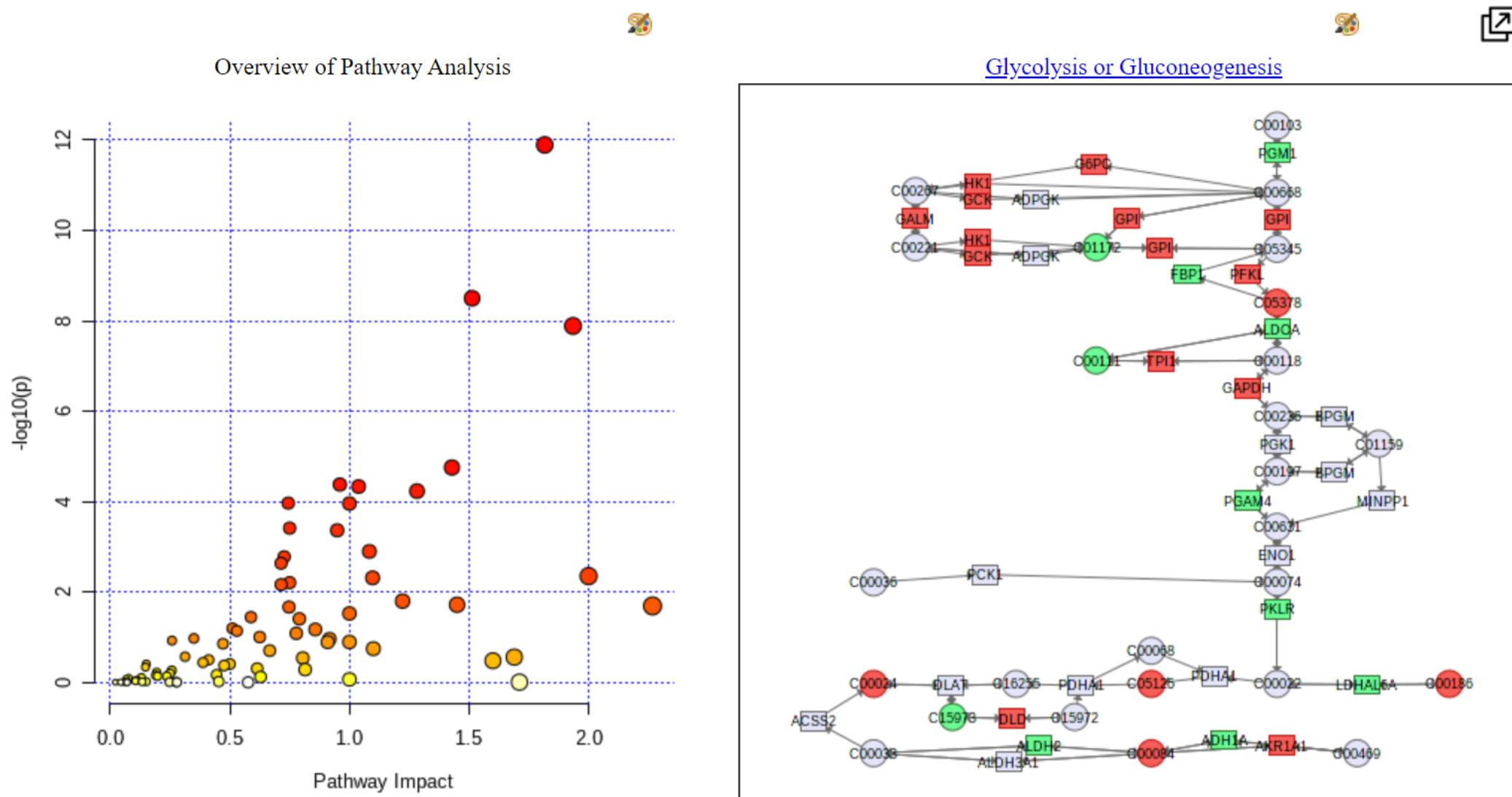
Submit

R Command History

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```
1. mSet<-InitDataObjects("conc", "msetqea", FALSE)
2. mSet<-Read.TextData(mSet, "Replacing_with_your_file_path", "rowu", "disc");
3. mSet<-CrossReferencing(mSet, "name");
4. mSet<-CreateMappingResultTable(mSet)
5. mSet<-SanityCheckData(mSet)
6. mSet<-ReplaceMin(mSet);
7. mSet<-PreparePrenormData(mSet)
8. mSet<-Normalization(mSet, "NULL", "LogNorm", "MeanCenter", ratio=FALSE, ratioNum=2 0)
9. mSet<-PlotNormSummary(mSet, "norm_0_", "png", 72, width=NA)
10. mSet<-PlotSampleNormSummary(mSet, "snorm_0_", "png", 72, width=NA)
11. mSet<-SetMetabolomeFilter(mSet, F);
12. mSet<-SetCurrentMsetLib(mSet, "kegg_pathway", 2);
13. mSet<-CalculateGlobalTestScore(mSet)
14. mSet<-PlotQEA.Overview(mSet, "qea_0_", "net", "png", 72, width=NA)
15. mSet<-PlotEnrichDotPlot(mSet, "qea", "qea_dot_0_", "png", 72, width=NA)
16. mSet<-PlotQEA.MetSet(mSet, "Galactose metabolism", "png", 72, width=NA)
17. mSet<-PlotQEA.MetSet(mSet, "Galactose metabolism", "png", 72, width=NA)
18. mSet<-PlotQEA.MetSet(mSet, "Galactose metabolism", "png", 72, width=NA)
19. mSet<-PreparePrenormData(mSet)
20. mSet<-SanityCheckData(mSet)
21. mSet<-CreateMappingResultTable(mSet)
```

Integrated analysis in MetaboAnalyst



Integrated analysis in MetaboAnalyst

Click the corresponding **Pathway Name** to view its graphical presentation; click **Match Status** to view the pathway members (with matched ones highlighted).

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Pathway Name	Match Status	p	-log(p)	Holm p	FDR	Impact	Link
Glycolysis or Gluconeogenesis	28/61	1.2805E-12	11.893	1.0756E-10	1.0756E-10	1.8167	KEGG
Fructose and mannose metabolism	19/40	3.1764E-9	8.4981	2.6364E-7	1.3341E-7	1.5128	KEGG
Pentose phosphate pathway	20/47	1.2988E-8	7.8865	1.065E-6	3.6367E-7	1.9348	KEGG
Starch and sucrose metabolism	15/43	1.7621E-5	4.754	0.0014273	3.7004E-4	1.4286	KEGG
Galactose metabolism	16/51	4.1966E-5	4.3771	0.0033573	6.5122E-4	0.96	KEGG
Arginine biosynthesis	11/27	4.6516E-5	4.3324	0.0036748	6.5122E-4	1.0385	KEGG
Retinol metabolism	15/47	5.8685E-5	4.2315	0.0045774	7.0422E-4	1.2826	KEGG
beta-Alanine metabolism	14/44	1.082E-4	3.9658	0.0083311	0.0010314	0.74419	KEGG
Pantothenate and CoA biosynthesis	12/34	1.1051E-4	3.9566	0.0083989	0.0010314	1.0	KEGG
Lysine degradation	14/49	3.8705E-4	3.4122	0.029029	0.0032513	0.75	KEGG
Amino sugar and nucleotide sugar metabolism	19/79	4.3262E-4	3.3639	0.032014	0.0033036	0.94872	KEGG
Ascorbate and aldarate metabolism	6/13	0.001268	2.8969	0.092562	0.0088758	1.0833	KEGG
Glutathione metabolism	14/56	0.0016645	2.7787	0.11984	0.010755	0.72727	KEGG
Butanoate metabolism	9/29	0.0023213	2.6343	0.16481	0.013928	0.71429	KEGG
Neomycin, kanamycin and gentamicin biosynthesis	3/4	0.0044608	2.3506	0.31225	0.02498	2.0	KEGG
Pentose and glucuronate interconversions	9/32	0.0048735	2.3122	0.33627	0.025586	1.0968	KEGG
Pyruvate metabolism	11/45	0.0062287	2.2056	0.42355	0.030777	0.75	KEGG
Arginine and proline metabolism	16/78	0.0068754	2.1627	0.46065	0.032085	0.71429	KEGG
D-Glutamine and D-glutamate metabolism	4/10	0.015946	1.7973	1.0	0.0705	1.2222	KEGG
Biotin metabolism	6/21	0.019191	1.7169	1.0	0.080601	1.45	KEGG

1 2 3 4

Integrated analysis in MetaboAnalyst

Click the corresponding **Pathway Name** to view its graphical presentation; click **Match Status** to view t

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Pathway Name	Match Status	
Glycolysis or Gluconeogenesis	28/61	1.2805
Fructose and mannose metabolism	19/40	3.1764
Pentose phosphate pathway	20/47	1.2988
Starch and sucrose metabolism	15/43	1.7621
Galactose metabolism	16/51	4.1966
Arginine biosynthesis	11/27	4.6516
Retinol metabolism	15/47	5.8685
beta-Alanine metabolism	14/44	1.082E-1
Pantothenate and CoA biosynthesis	12/34	1.1051
Lysine degradation	14/49	3.8705
Amino sugar and nucleotide sugar metabolism	19/79	4.3262
Ascorbate and aldarate metabolism	6/13	0.0012
Glutathione metabolism	14/56	0.0016
Butanoate metabolism	9/29	0.0023
Neomycin, kanamycin and gentamicin biosynthesis	3/4	0.0044
Pentose and glucuronate interconversions	9/32	0.0048
Pyruvate metabolism	11/45	0.0062
Arginine and proline metabolism	16/78	0.0068
D-Glutamine and D-glutamate metabolism	4/10	0.0159
Biotin metabolism	6/21	0.0191

Matched Features	
Pathway	Members
Glycolysis or Gluconeogenesis	Acetaldehyde; Ethanol; Thiamin diphosphate; Pyruvate; 2-(alpha-Hydroxyethyl)thiamine diphosphate; Enzyme N6-(lipoyl)lysine; Acetyl-CoA; Enzyme N6-(dihydrolipoyl)lysine; (S)-Lactate; Phosphoenolpyruvate; 2-Phospho-D-glycerate; D-Glyceraldehyde 3-phosphate; beta-D-Fructose 1,6-bisphosphate; beta-D-Fructose 6-phosphate; alpha-D-Glucose 6-phosphate; D-Glucose 1-phosphate; beta-D-Glucose 6-phosphate; beta-D-Glucose; alpha-D-Glucose; 3-Phospho-D-glycerate; Oxaloacetate; 2,3-Bisphospho-D-glycerate; 3-Phospho-D-glyceroyl phosphate; Acetate; [Dihydrolipoyllysine-residue acetyltransferase] S-acetyl dihydrolipoyllysine; Glycerone phosphate; ALDH2, ALDH-E2, ALDHI, ALDM...; ALDH3A1, ALDH3, ALDHIII...; AKR1A1, ALDR1, ALR, ARM, DD3, HEL-S-6; ADH1A, ADH1...; PDHA1, PDHA, PDHAD, PDHCE1A, PHE1A...; DLAT, DLTA, E2, PDC-E2, PDCE2; LDHAL6A, LDH6A...; PKLR, PK1, PKL, PKRL, RPK...; ENO1, ENO1L1, HEL-S-17, MPB1, NNE, PPH...; PGAM4, PGAM-B, PGAM1, PGAM3, dJ1000K24.1...; GAPDH, G3PD, GAPD, HEL-S-162eP...; TPI1, HEL-S-49, TIM, TPI, TPID; ALDOA, ALDA, GSD12, HEL-S-87p...; PFKL, ATP-PFK, PFK-B, PFK-L...; FBP1, FBP...; GPI, AMF, GNPI, NLK, PGI, PHI, SA-36, SA36; PGM1, CDG1T, GSD14...; HK1, HK, HK1-ta, HK1-tb, HK1-tc, HKD, HKI, HMSN, HXK1, RP79, hexokinase...; GCK, FGQTL3, GK, GLK, HHF3, HK4, HKIV, HXKP, LGLK, MODY2; GALM, BLOCK25, GLAT, HEL-S-63p, IBD1; G6PC, G6PC1, G6PT, G6Pase, GSD1, GSD1a...; DLD, DLDD, DLDH, E3, GCSL, LAD, PHE3; PGK1, HEL-S-68p, MIG10, PGKA...; PCK1, PCKDC, PEPCK-C, PEPCK1, PEPCKC...; BPGM, DPGM, ECYT8; ACSS2, ACAS2, ACECS, ACS, ACSA, dJ1161H23.1...; ADPGK, 2610017G09Rik, ADP-GK; MINPP1, HIPER1, MINPP2, MIPP

質量分析データの性質を理解し、データ再解析により新たな知見を創出

 MetaboBank integrated metabolome data repository



Instrument

- LC-MS 46
- GC-MS 45
- LC-PDA 1

Data Format

- .abf 59
- .txt 47
- .cdf 44
- .csv 39
- .RAW 28
- .zip 10
- .CDF 4
- .xls 4
- .xlsx 3

Organism

- filter
- Arabidopsis thaliana 28
- Solanum lycopersicum 13
- Oryza sativa 10
- Brassica oleracea 4
- Glycine max 4
- Spinacia oleracea 4
- Homo sapiens 3
- Allium cepa 2
- Glycyrrhiza glabra 2
- Glycyrrhiza 2

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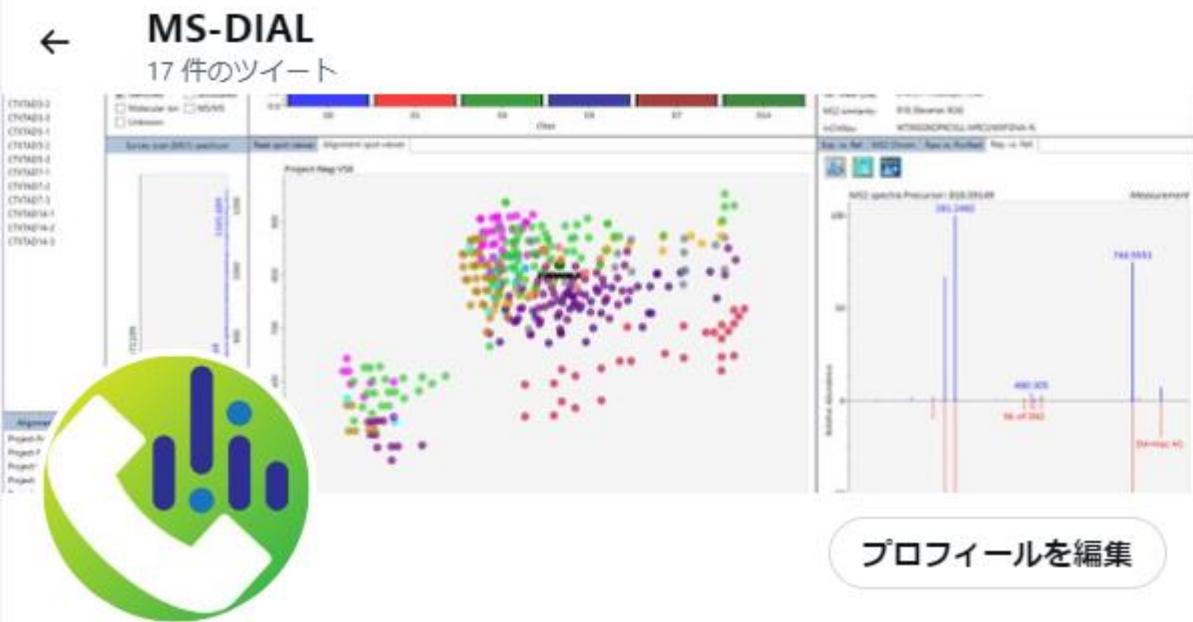
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PR001483	Dietary inclusion of nitrite-containing frankfurter exacerbates colorectal cancer pathology, increases oxidative stress, alters metabolism and causes gut dysbiosis in APCmin mice	Institute for Global Food Security	Institute for Global Food Security	1
PR001457	Machine Learning Reveals Lipidome Dynamics in a Mouse Model of Ovarian Cancer	Georgia Institute of Technology	Georgia Institute of Technology	1
PR001455	1-deoxysphingolipid synthesis compromises anchorage-independent growth and plasma membrane endocytosis in cancer cells	TU Braunschweig	Salk Institute for Biological Studies	1
PR001425	Application of Artificial Intelligence to Plasma Metabolomics Profiles to Predict Response to Neoadjuvant Chemotherapy in Triple-Negative Breast Cancer	University of Texas MD Anderson Cancer Center	University of Texas MD Anderson Cancer Center	1
PR001418	Dynamic partitioning of branched-chain amino acids-derived nitrogen supports renal cancer progression	CECAD Research Center, University Hospital Cologne	CECAD Research Center	8
PR001416	The microbiome-derived metabolite TMAO drives immune activation and boosts response to immune checkpoint blockade in pancreatic cancer	The Wistar Institute	The Wistar Institute	2

メタボロームデータを出す側と使う側

本日取り扱った内容

出す側	使う側
・ 分析化学	・ データの特徴理解
・ 質量分析	・ 化合物IDの取得
・ イオン	・ データの正規化
・ マススペクトル	・ 統計・多変量解析
・ 質量分析インフォマティクス	・ データベース検索
・ アノテーション	・ 代謝マップ投影
・ データ標準化	・ 適切な数理モデルの選択
	・ オミクスモジュールへ統合

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MS-DIAL
@msdial_project

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

自己紹介を翻訳

[prime.psc.riken.jp/compmis/msdial/...](https://prime.psc.riken.jp/compmis/msdial/)

2022年8月からTwitterを利用しています

16 フォロー中 324 フォロワー

The figure shows the YouTube channel page for the MS-DIAL project. The channel has 8 subscribers. The main content area displays a grid of video thumbnails for various topics related to MS-DIAL, such as PCA function, Retention time correction function, and different mass spectrometry techniques for lipidomics. Each thumbnail includes a title, duration, and a brief description.

質量分析の情報計測で新しいバイオロジーを探求したい方→ htsugawa@go.tuat.ac.jp