

M-IOLITE tutorial

- Edit your file based on the M.E.S.B.L data template (can be found attached)
- Unzip M-IOLITE folder
- Run the .exe file
- Insert user name, password and login
- M-IOLITE can read and process excel files. Sheet name='Sheet1'
- The results can be found in M-IOLITE folder

Metabolomic Data Analysis using

M-IOLITE

**Upload data to
mesbl standardized
repository**

1

M.E.S.B.L
Data Bank

Data
Normalization

3

**Specialized data
normalization
methods**

**Peak library,
unknown peak
identification
method**

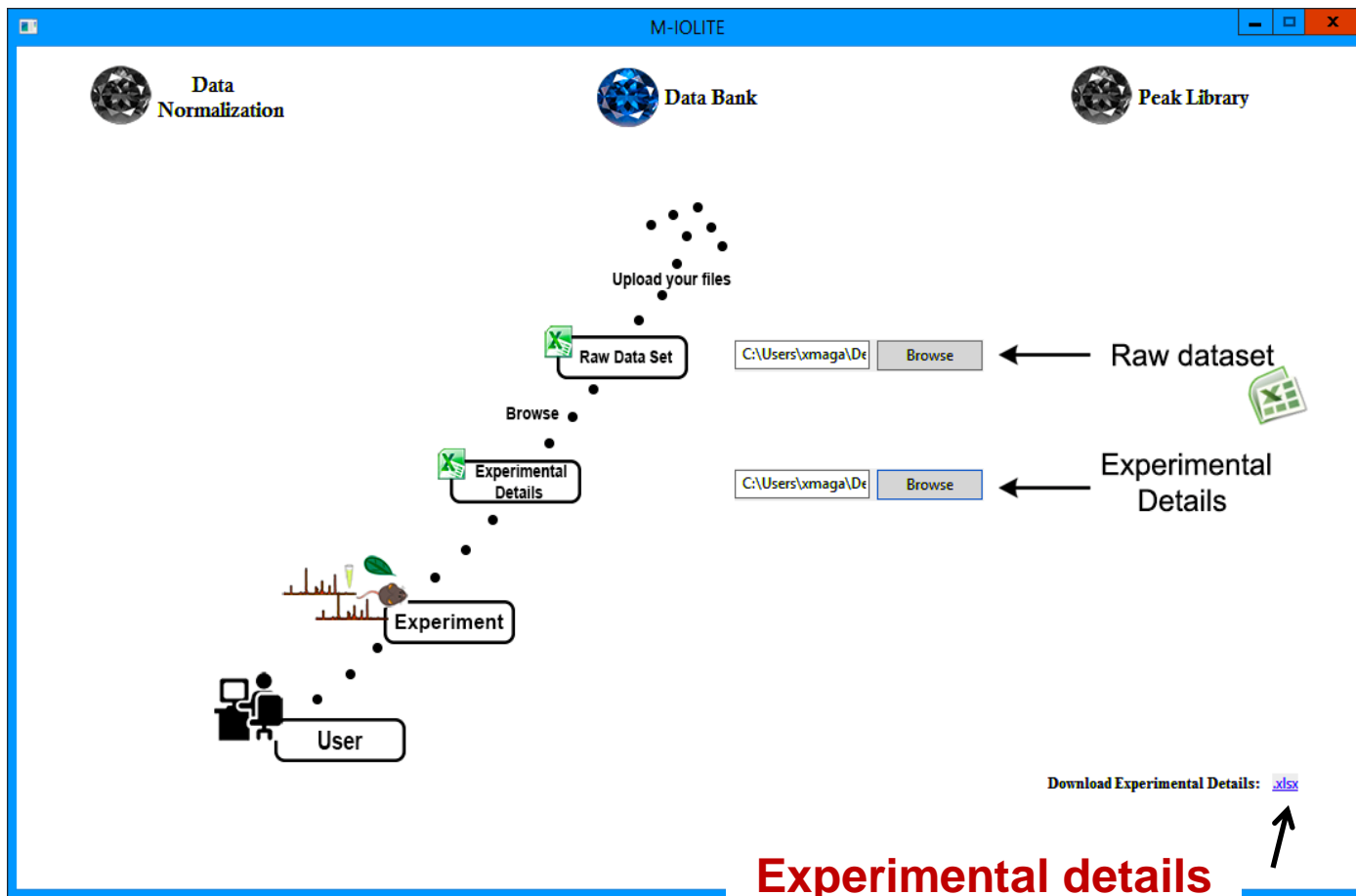
M.E.S.B.L
Peak Library

2

user_id password
Login:
[Create account](#)

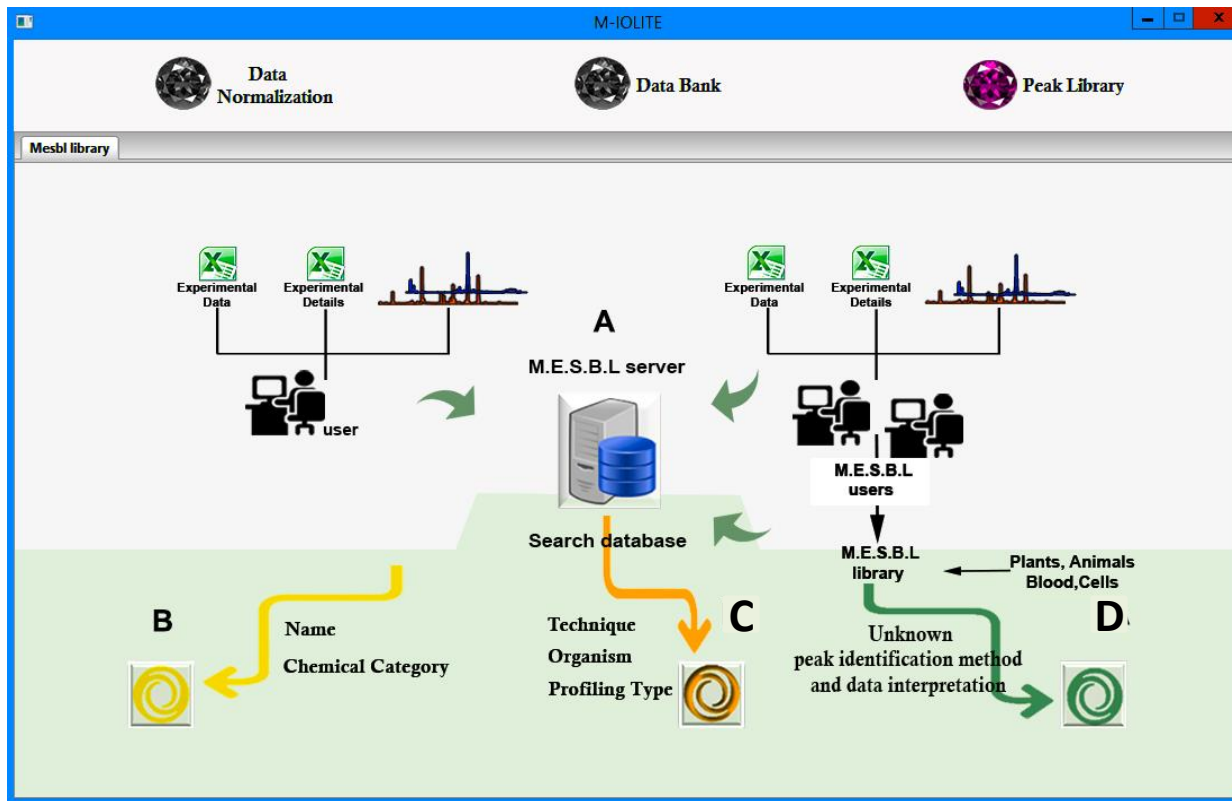
Insert user_id and password

1.

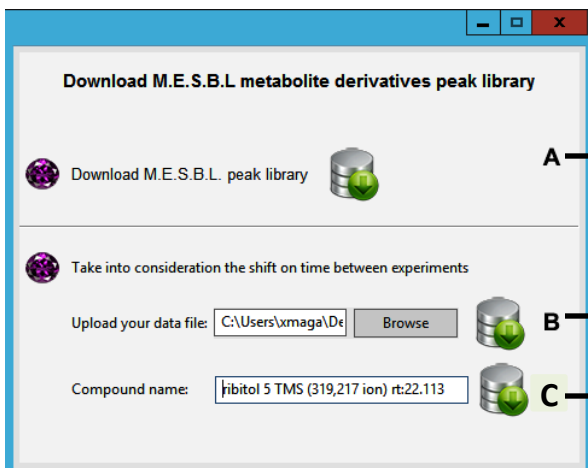


**Experimental details
can be downloaded
as a file here**

2.



A. Download standardized peak library

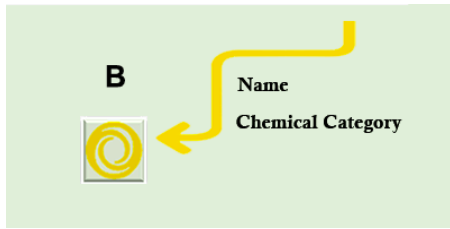


Download standardized peak library locally to your computer

Retention time shift between experiments. Upload excel file with 2 columns (1st peak name, 2nd retention time).

Provide peak name (i.e ribitol)

2.



M.E.S.B.L peak library

Search by compound name or chemical category

Filtering by model organism

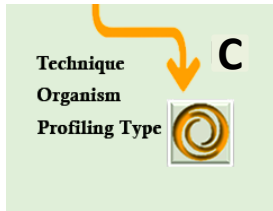
The screenshot shows the M-IOLITE_SEARCH application window. On the left, there is a search panel with the following options:

- Search metabolite by:**
 - Compound name
 - Chemical category
- Search** button
- Filtering by model organism:**
 - Mus musculus
 - Solanum lycopersicum(tomato)
 - Arabidopsis thaliana
- Filtering by line/tissue:**
 - Baby hamster kidney cell
 - Brain(mouse)
 - Heart(mouse)

The main window displays the **Mesbl library** search results. A large red watermark 'Results' is overlaid on the results list. The results are as follows:

Peak ID	Retention Time (min)	Marker Ion (m/z)	Fragm. pattern	TMS category	Species
Un_0199	4.4	190	'190,117,221,226,'	None	'BhK,Mouse(BALB/cJ),Serum,'
Un_0203	4.723	110	'110'	None	'
m_3(xri)/C_008 (Lena)	4.87	184	'184,228,117,77'	3	'Mouse(BALB/cJ),HeLa'
Un_0226	5.148	128	'128,103,100,162,206'	1	'
ethanolamine 2TMS	5.152	102	'206,128,102,218,162'	3	'BhK,Mouse(BALB/cJ),Arabidopsis,'

2.



M.E.S.B.L repository

Search
experiments

M-IOLITE_EXPERIMENTS

Mesbl library

Search Results

Next >>

Sex-comparative study of mouse cerebellum physiology under adult-onset hypothyroidism:937

Species: mouse | Strain: balb/cj | Tissue: cerebellum | Culture_type: primary culture

Profiling_type: METABOLOMICS | Released date: 2017/1/27

GC-MS Metabolomic Analysis Cerebellar Metabolic Physiology in...

Species: mouse | Strain: balb/cj | Tissue: cerebellum | Culture_type: primary culture

Profiling_type: METABOLOMICS | Released date: 2017/1/27

Technology

GC-MS

Organism

Mus musculus

Lycopersicon(tomato)

Arabidopsis thaliana

Cell/Tissue

Blood(serum)

Kidney(BalB/cJ mouse)

Brain(Balb/cJ mouse)

Search

experiments

Study Name: GC-MS Metabolomic Analysis

User Contact Info:


Experimental Data:

Experimental Info:


Download
experimental
data

3. Options from M-IOLITE workflow


M-IOLITE
[-] [] [X]



Data Normalization

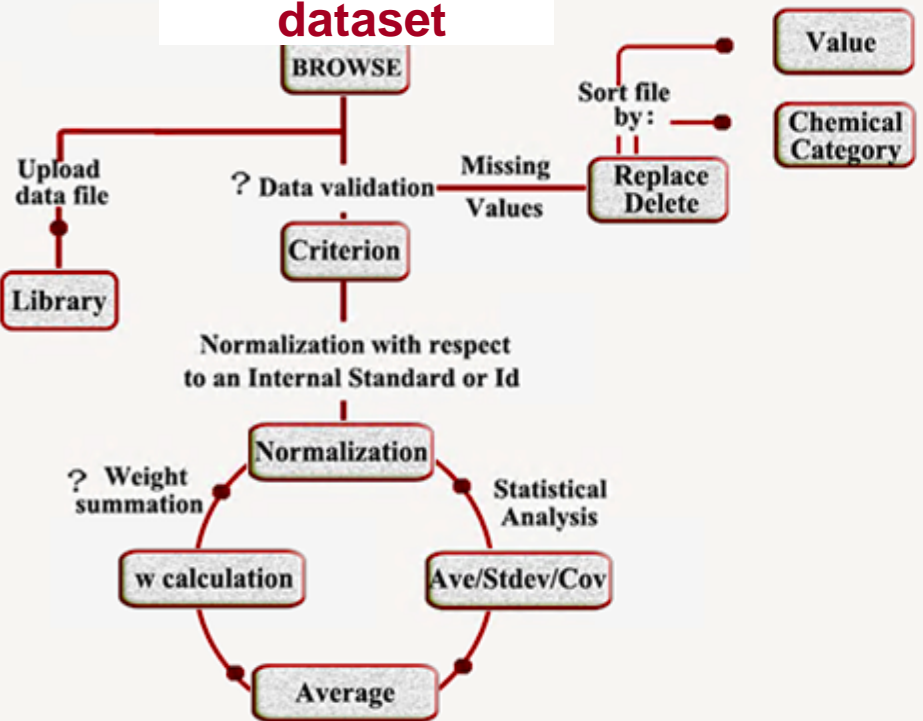


Data Bank



Peak Library

Raw metabolic dataset



Select samples for further analysis and then select a node from the network

Sample1

Sample2

Sample3

Sample4

Sample5

Sample6

Sample7

Sample8

Sample9

Sample10

Sample11

Sample12

Sample13

Sample14

Sample15

Sample16

Sample17

Sample18

Sample19

Sample20

M_1E_Cb_Inj1

M_1E_Cb_Inj2

M_2E_Cb_Inj1

M_2E_Cb_Inj3

M_2E_Cb_Inj4

M_3E_Cb_Inj1

M_3E_Cb_Inj2

M_3E_Cb_Inj3

M_3E_Cb_Inj4

M_3E_Cb_Inj5

M_3E_Cb_Inj6

M_3E_Cb_Inj7

M_3E_Cb_Inj8

M_3E_Cb_Inj9

M_3E_Cb_Inj10

M_3E_Cb_Inj11

M_3E_Cb_Inj12

M_3E_Cb_Inj13

M_3E_Cb_Inj14

M_3E_Cb_Inj15

M_3E_Cb_Inj16

M_3E_Cb_Inj17

M_3E_Cb_Inj18

M_3E_Cb_Inj19

M_3E_Cb_Inj20

Biological Samples
Technical Replicates

P1016

2-Hydroxybutanoic-acid

P1091

Valine_2TMS(2/2)

P1099/f_12/d_13

Oxalic-Acid_2TMS

Valine_3TMS(3/3)

isoLeucine_2TMS(2/3)

isoLeucine_1TMS(1/3)

P1229

Ribitol(319)

D-13C-Leucine

3. Options from M-IOLITE workflow

BROWSE

Upload data file

Normalization

Normalization with respect to an IS

Criterion

Data validation criterion (Constant operating conditions)

Ave/Stdev/Cov

Statistical methods

Value

Sort by value

Average

Statistical methods

Chemical Category

Sort by chemical category based on 1,2

w calculation

Normalization with respect to the derivatization artifacts

Replace Delete

Filtering unreliable data

- Zero concentration
- Internal Standards
- Unknown cat.3
- Artifacts (*i.e.* bleeding)
- Metabolites of cat.2

Library

Upload normalized data to the library

1.Kanani H, Chrysanthopoulos PK, Klapa MI. 2008,J . Chromatogr. B. Analyt. Technol. Biomed Life Sci. 871:91- 201
2.Kanani and Klapa. 2007, *Metab Eng.* 1:39-51