

MS - LAMP

Mass Spectrometry based Lipid(ome) Analyzer & Molecular Platform

Help File

Contents

S. No.	Section	Page No.
1	Introduction to MS-LAMP	3 - 4
2	Mycobacterium tuberculosis Lipidome MS-LAMP search window	5 - 6
3	General Lipidome MS-LAMP search window	7 - 8
4	Query Type 1: Single molecular mass or m/z value	9 - 17
5	Query Type 2: List of Molecular Masses or m/z values	18 - 26
6	Query Type 3: Range of Molecular Mass or m/z value	27 - 32
7	Query Type 4: Molecular Formula	33 - 37
8	Query Type 5: LIPID MAPS ID (LM ID) or List of LM IDs	38 - 43
9	Permissible combination of checkboxes to choose a lipid category	44 - 45
10	Search within Main Class and/or Subclass	46 - 63
11	Monoisotopic mass & Atomic weight values considered by MS-LAMP	64

MS-LAMP

Mass Spectrometry based Lipid(ome) Analyzer & Molecular Platform (MS-LAMP) has been developed to facilitate analysis and interpretation of data obtained from mass spectrometry, in particular of electrospray ionization (ESI) and matrix assisted laser desorption and ionization (MALDI), towards identification of lipids. The main window of the software, whose snapshot is shown in [Figure 1.1](#), consists of buttons to independently search two databases:

- ***Mycobacterium tuberculosis* Lipidome MS-LAMP**
- **General Lipidome MS-LAMP**

There is also an audio based introduction to MS-LAMP, which is included utilizing Microsoft SAPI module. Refer to [Figure 1.1](#)

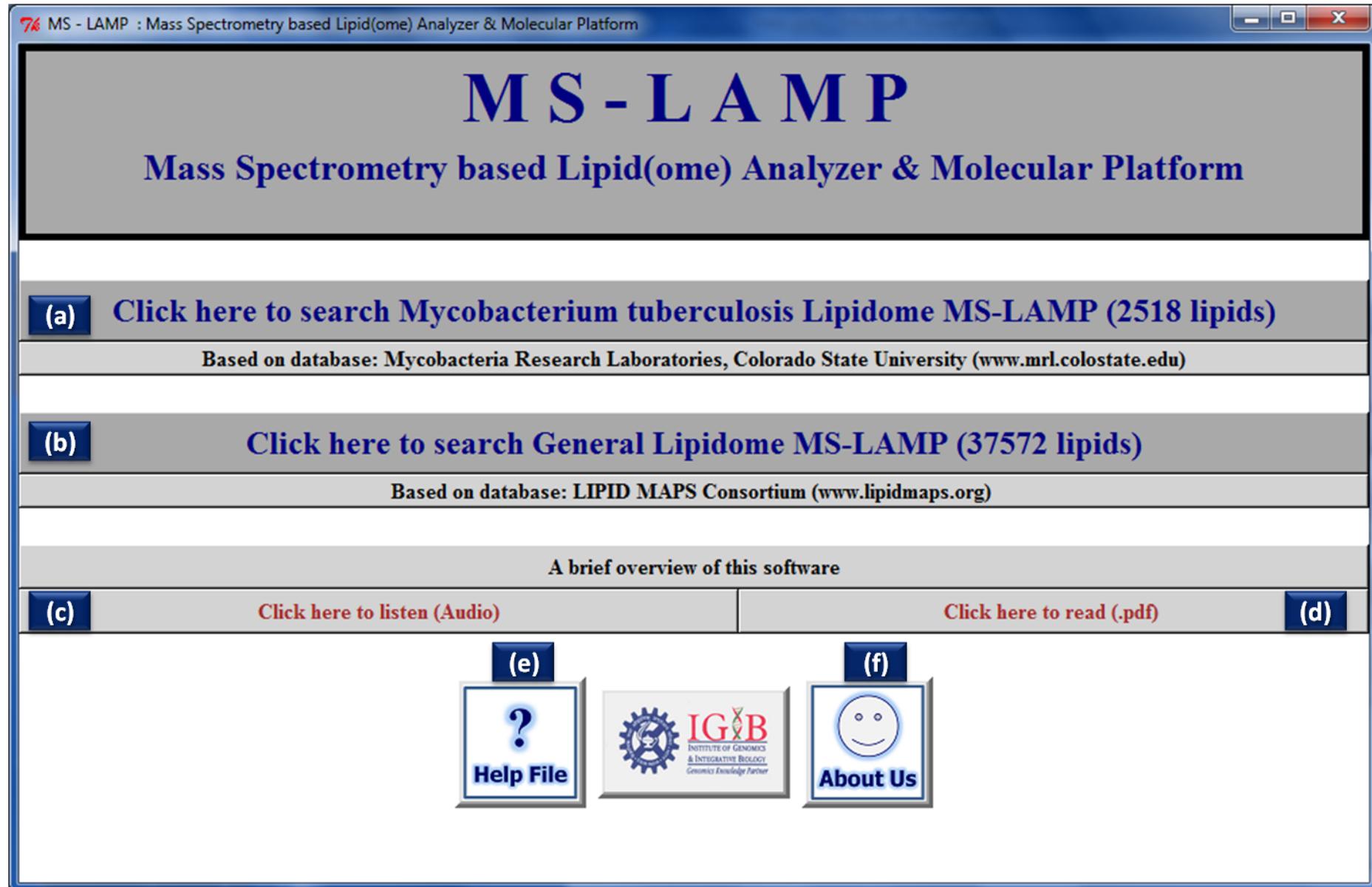


Figure 1.1: Snapshot of main window of Mass Spectrometry based Lipid(ome) Analyzer & Molecular Platform (MS-LAMP): There are buttons to choose and obtain search window of (a) General Lipidome MS-LAMP or (b) Mycobacterium tuberculosis Lipidome MS-LAMP. Clickable buttons: (c) to listen to an audio or (d) to read (a .pdf file) for getting a brief overview of this software; (e) to open Help File (.pdf file) containing entire details of MS-LAMP; (f) to know about the people who have contributed and responsible for the making of MS-LAMP.

2. Mycobacterium tuberculosis Lipidome MS-LAMP search window

Lipid database from The Mycobacterium Research Laboratories, Colorado State University (www.mrl.colostate.edu) was used to construct *Mycobacterium tuberculosis* Lipidome MS-LAMP that consists of 2518 lipids. There are 4 different query types available in this search window (see [Figure 2.1](#)), viz.

- [**Query Type 1**](#) - Single Molecular Mass or m/z value
- [**Query Type 2**](#) - List of Molecular Masses or m/z values
- [**Query Type 3**](#) - Molecular Mass or m/z range
- [**Query Type 4**](#) - Molecular Formula

MS - L A M P

Mass Spectrometry based Lipid(ome) Analyzer & Molecular Platform

Mycobacterium tuberculosis Lipidome MS-LAMP (2518 Lipids)

(a)

[Click to listen about search options \(Audio\)](#)

Choose a Query Type

(b) Query Type 1

Single Molecular Mass or m/z value

For example :
m/z : 369.37268 : [M+H]⁺
 corresponds to
Mycocerosic acid (C24)
 a Fatty Acyls (FA)

(f) Need Help?

(c) Query Type 2

List of Molecular Masses or m/z values

For example :

m/z	Intensity	Relative	Charge
377.09	287946.8	69.30	1.00
485.14	314223.8	77.76	1.00
521.12	931672.5	22.99	1.00

(g) Need Help?

(d) Query Type 3

Molecular Mass Or m/z range

For example :
 search in the range of
m/z : 200 – 300

(h) Need Help?

(e) Query Type 4

Molecular Formula

For example :
C31 H62 O2
 corresponds to
Phthioceranic acid (C31)
 a Fatty Acyls (FA)

(i) Need Help?

Figure 2.1: *Mycobacterium tuberculosis* Lipidome MS-LAMP search window showing four options (Query Type 1-4) to search within 2518 lipids belonging to *Mycobacterium tuberculosis* Lipidome MS-LAMP database. Clickable buttons are denoted as (a) - (i):

- (a) To listen to audio that provides introduction to available search options
- (b) To open “Query Type 1 - Single Molecular Mass or m/z value” window
- (c) To open “Query Type 2 - List of Molecular Masses or m/z values ” window
- (d) To open “Query Type 3 - Molecular Mass or m/z range ” window
- (e) To open “Query Type 4 - Molecular Formula” window
- (f) Help File for “Query Type 1 - Single Molecular Mass or m/z value” window
- (g) Help File for “Query Type 2 - List of Molecular Masses or m/z values ” window
- (h) Help File for “Query Type 3 - Molecular Mass or m/z range ” window
- (i) Help File for “Query Type 4 - Molecular Formula” window

3. General Lipidome MS-LAMP search window

General Lipidome MS-LAMP is a database, which has been constructed based on the database of LIPID MAPS Consortium (www.lipidmaps.org) that consists of 30,476 lipids. Using General Lipidome MS-LAMP search window the user can make 5 different types of query viz. (see [Figure 3.1](#))

- [**Query Type 1**](#) - Single Molecular Mass or m/z value
- [**Query Type 2**](#) - List of Molecular Masses or m/z values
- [**Query Type 3**](#) - Molecular Mass or m/z range
- [**Query Type 4**](#) - Molecular Formula
- [**Query Type 5**](#) - LM ID (LIPID MAPS ID)

MS - LAMP

Mass Spectrometry based Lipid(ome) Analyzer & Molecular Platform

General Lipidome MS - LAMP (37572 Lipids)

(a)

[Click to listen about search options \(Audio\)](#)

Choose a Query Type

(b) Query Type 1

Single Molecular Mass or m/z value

For example :
m/z : 309.336 : [M-H]
corresponds to
Flavonoid
a Polyketide [PK]

(c) Query Type 2

List of Molecular Masses or m/z values

For example :

m/z	Intensity	Relative	Charge
377.09	287946.8	69.30	1.00
485.14	314223.8	77.76	1.00
521.12	931672.5	22.99	1.00

(d) Query Type 3

Molecular Mass Or m/z range

For example :
search in the range of
m/z : 200 – 300

(e) Query Type 4

Molecular Formula

For example :
C₂₉ H₅₀ O₂
corresponds to
α - Tocopherol (Vitamin - E)
a Prenol lipid [PR]

(f) Query Type 5

LM ID (LIPID MAPS)

For example :
LMSP01020001
corresponds to
"Sphinganine"
a Sphingolipid [SP]

(g) Need Help?

(h) Need Help?

(i) Need Help?

(j) Need Help?

(k) Need Help?

Figure 3.1: General Lipidome MS-LAMP search window showing five options (Query Type 1-5) to search within 30,476 lipids belonging to General Lipidome MS-LAMP database. Clickable buttons are denoted as (a) - (k):

- (a) To listen to audio that provides introduction to available search options
- (b) To open “Query Type 1 - Single Molecular Mass or m/z value” window
- (c) To open “Query Type 2 - List of Molecular Masses or m/z values ” window
- (d) To open “Query Type 3 - Molecular Mass or m/z range ” window
- (e) To open “Query Type 4 - Molecular Formula” window
- (f) To open “Query Type 5 - LM ID (LIPID MAPS ID) ” window
- (g) Help File for “Query Type 1 - Single Molecular Mass or m/z value” window
- (h) Help File for “Query Type 2 - List of Molecular Masses or m/z values ” window
- (i) Help File for “Query Type 3 - Molecular Mass or m/z range ” window
- (j) Help File for “Query Type 4 - Molecular Formula” window
- (k) Help File for “Query Type 5 - LM ID (LIPID MAPS ID) ” window

4. Query Type 1: Single molecular mass or m/z value

[Scheme 4.1](#) delineates the syntax for making a query of single molecular mass or m/z value.

[Figure 4.1](#) shows the snapshot of the query window, which is explained below:

- (a) Title bar:** This bar gives information about the query window and the chosen lipid database.
- (b) Enter Molecular Mass or m/z value:** Molecular Mass or m/z value to be queried should be entered in the text box provided. Upon entering the value, choice between Monoisotopic or Average mass needs to be made. However, by default monoisotopic mass will be automatically selected.
- (c) Choose Molecular Mass / Type of Ion:** A choice between six negative and eight positive ions have been provided, in addition to ‘Molecular Mass’ for making a query.
- (d) Window range:** Depending on the resolution of the instrument used and the level of accuracy required by the user, it is possible to define the search within a mass range of -1.00000 to +1.00000 about the queried m/z or mass value. However, the default value is set at 0.5.
- (e) Lipid categories:** MS-LAMP has multiple search ability. More than one lipid category can be chosen by activating the check-buttons corresponding to lipid category(ies). (Note: Refer [Section 9](#) to know about permissible combinations of check-buttons)
- (f) Submit:** By clicking the ‘Submit’ button, the above selected parameters are entered as input to the programme.

Upon submitting the input, ‘Result of the Query’ window appears (see [Figure 4.2](#)), which shows population distribution of lipids belonging to different lipid categories present in the database of General or *Mycobacterium tuberculosis* (*M. tb*) Lipidome MS-LAMP, corresponding to the queried parameters. The ‘Result of the Query’ window has the following features:

- (a) Title Bar:** It gives the summary of the database in use and the input parameters.
- (b) Queried Parameters:** It gives review of the selected parameters.

(c) Population distribution of lipids in different lipid categories chosen are shown here.

These are clickable buttons that gives rise to a new window showing details (LM ID in case of General Lipidome MS-LAMP and Molecular Formulae in case of *M. tb* Lipidome MS-LAMP) about the lipid(s) obtained as result of the query (see [Figure 4.3](#)).

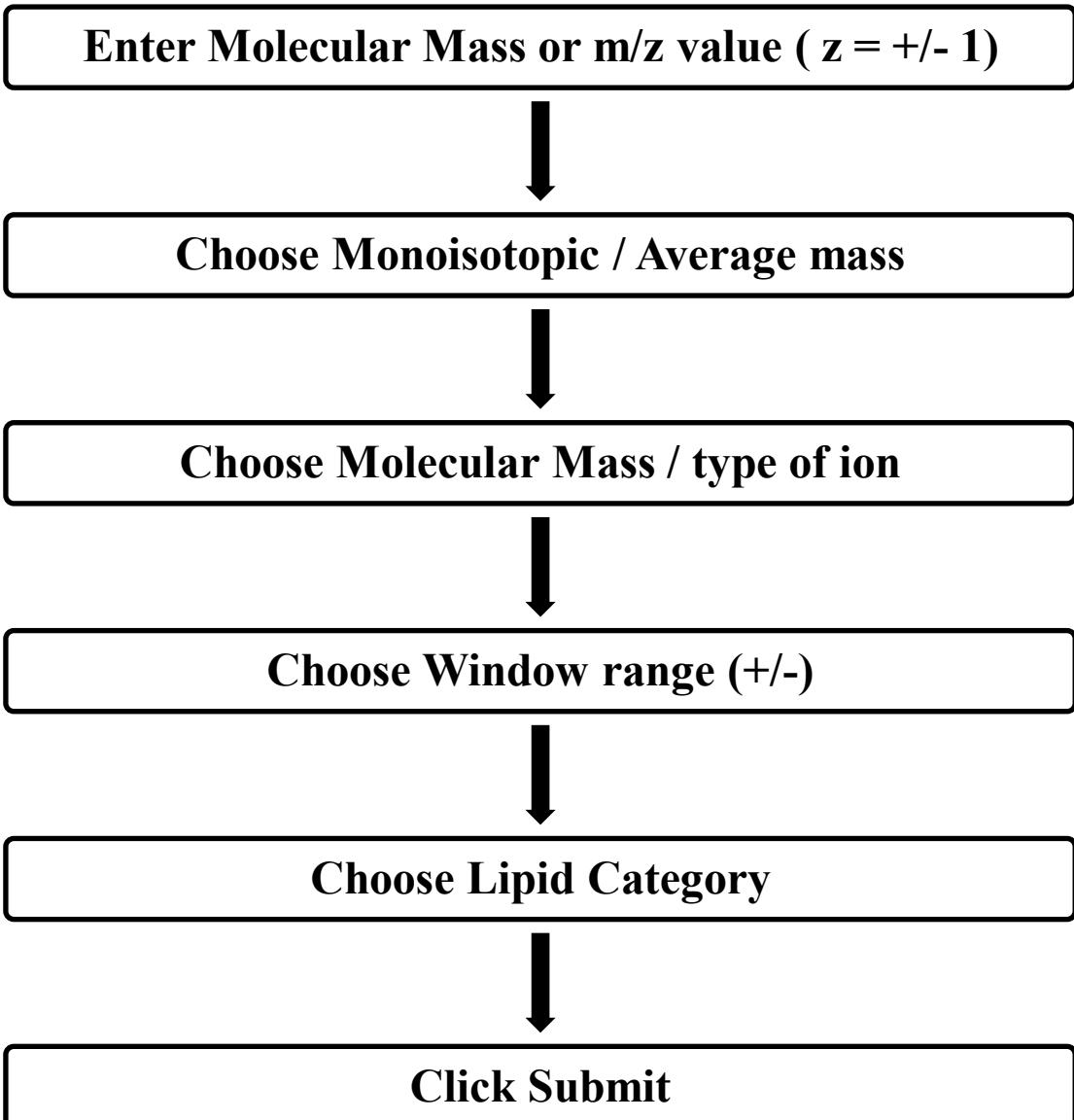
Upon clicking a button in this new window, the molecular structure corresponding to that lipid is shown. In case of General Lipidome MS-LAMP, the structures are available as MD mol file, which can be opened using ChemSketch (See [Figure 4.4](#)); while for *M. tb* Lipidome MS-LAMP, structures are available as .jpeg files (See [Figure 4.6](#)).

(d) Output file types: Result of the query can be saved in 3 different file formats.viz,

1. Comma separated Value (.csv)
2. Text file (.txt)
3. Excel File (.xls)

(e) Search again: To begin a new search, this button can be clicked, which will redirect to input window of Query Type 1.

[Figure 4.2](#) shows snapshot of the ‘Result of the query’ window from General Lipidome MS-LAMP database for the query of monoisotopic m/z 425; $[M+H]^+$ is the chosen Type of Ion; window range selected is ± 1 , which is about m/z 425, i.e. 425 ± 1 and the search is directed to all eight categories of lipids.



Scheme 4.1: Flowchart describing steps to enter **Query Type 1**: querying single molecular mass or m/z value.

(a)

Query Type 1 : Single Molecular Mass or m/z value

Enter Molecular Mass or m/z value (z = +/- 1) Monoisotopic Average (b)

Choose Molecular Mass / Type of Ion (c)

<input type="checkbox"/> Molecular Mass	Negative ions	<input type="checkbox"/> [M-H] ⁻	<input type="checkbox"/> [M+Cl] ⁻	<input type="checkbox"/> [M+HOAc-H] ⁻	<input type="checkbox"/> [M+Li-2H] ⁻	<input type="checkbox"/> [M+Na-2H] ⁻	<input type="checkbox"/> [M+K-2H] ⁻		
Positive ions		<input checked="" type="checkbox"/> [M+H] ⁺	<input type="checkbox"/> [M+NH ₄] ⁺	<input type="checkbox"/> [M+Li] ⁺	<input type="checkbox"/> [M+Na] ⁺	<input type="checkbox"/> [M+K] ⁺	<input type="checkbox"/> [M+2Li-H] ⁺	<input type="checkbox"/> [M+2Na-H] ⁺	<input type="checkbox"/> [M+2K-H] ⁺

Window Range (+/-) (d)

Molecular Mass or m/z : 0.005 0.01 0.05 0.1 0.25 0.5 0.75 1

Which Lipid(s) ? (e)

All eight categories [About lipid categories](#)

FA GL GP PK PR SL SP ST

All Phospholipids

Sphingo Other Phosphorylated lipids (Excluding GP)

Monoglycerides [MG] Diglycerides [DG] Triglycerides [TG] Other Glycerolipids **Glycerolipids [GL]**

Halogenated Lipids

Sulphur containing lipids

Search within Main Class and/or Subclass [Need Help ?](#)

SUBMIT (f)

Figure 4.1: Snapshot of “Query Type 1: Single Molecular Mass or m/z value” query window: (a) Title bar (b) To enter Molecular Mass or m/z value and select monoisotopic or average mass (c) To choose Molecular Mass / Type of Ion (d) For selecting Window range (e) To choose lipid categor(y/ies) (f) To submit the query.

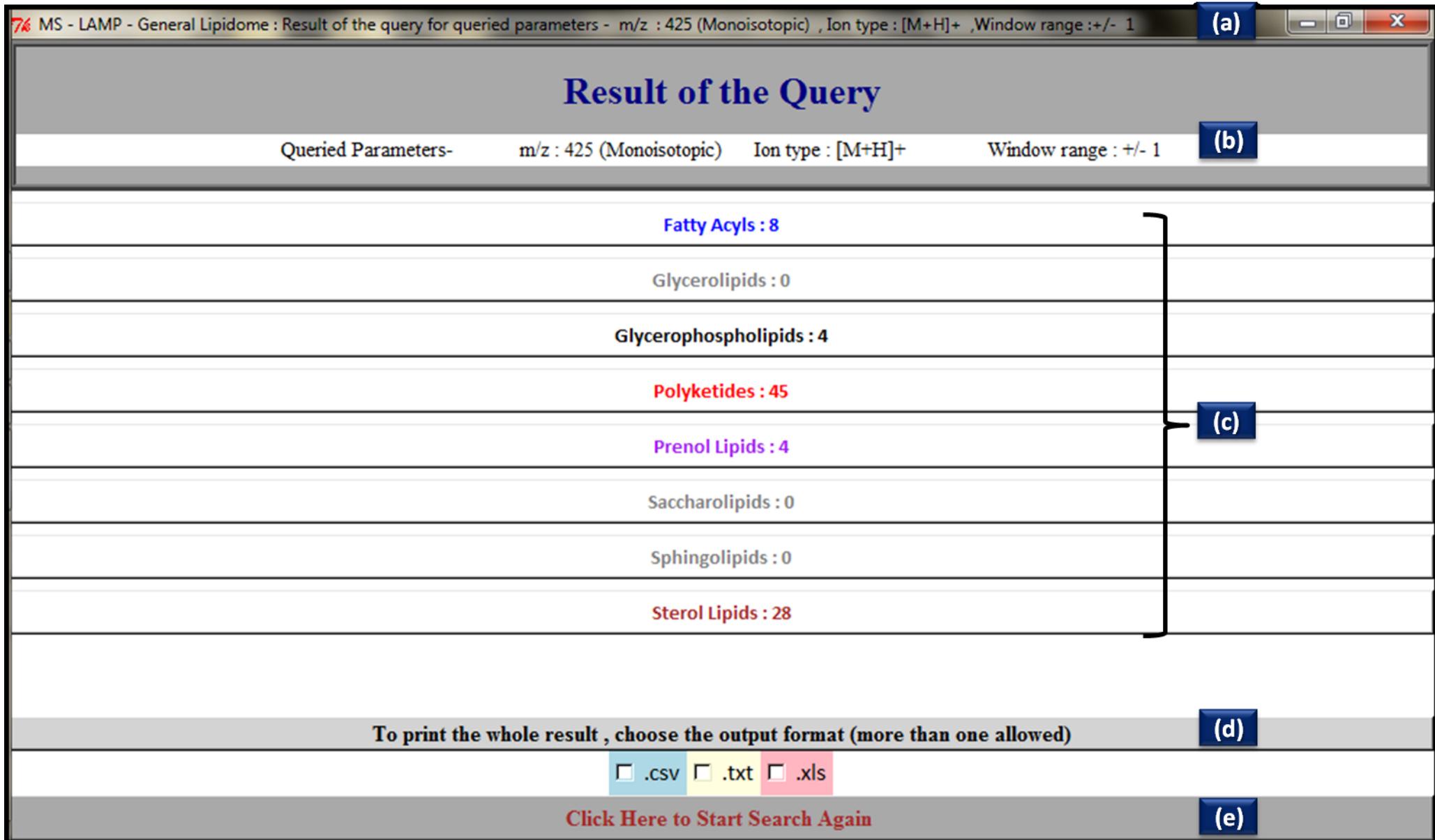


Figure 4.2: Snapshot of ‘Result of the Query’ window displaying a glimpse of different lipid categories and number of lipids in each category that match to the queried criteria shown in [Figure 4.1](#). **(a)** Title Bar **(b)** Queried Parameters **(c)** Chosen Lipid categories **(d)** To choose different file types for saving the output **(e)** For beginning the search again, this button has to be clicked. Shown here is the result yielded from General Lipidome MS-LAMP.

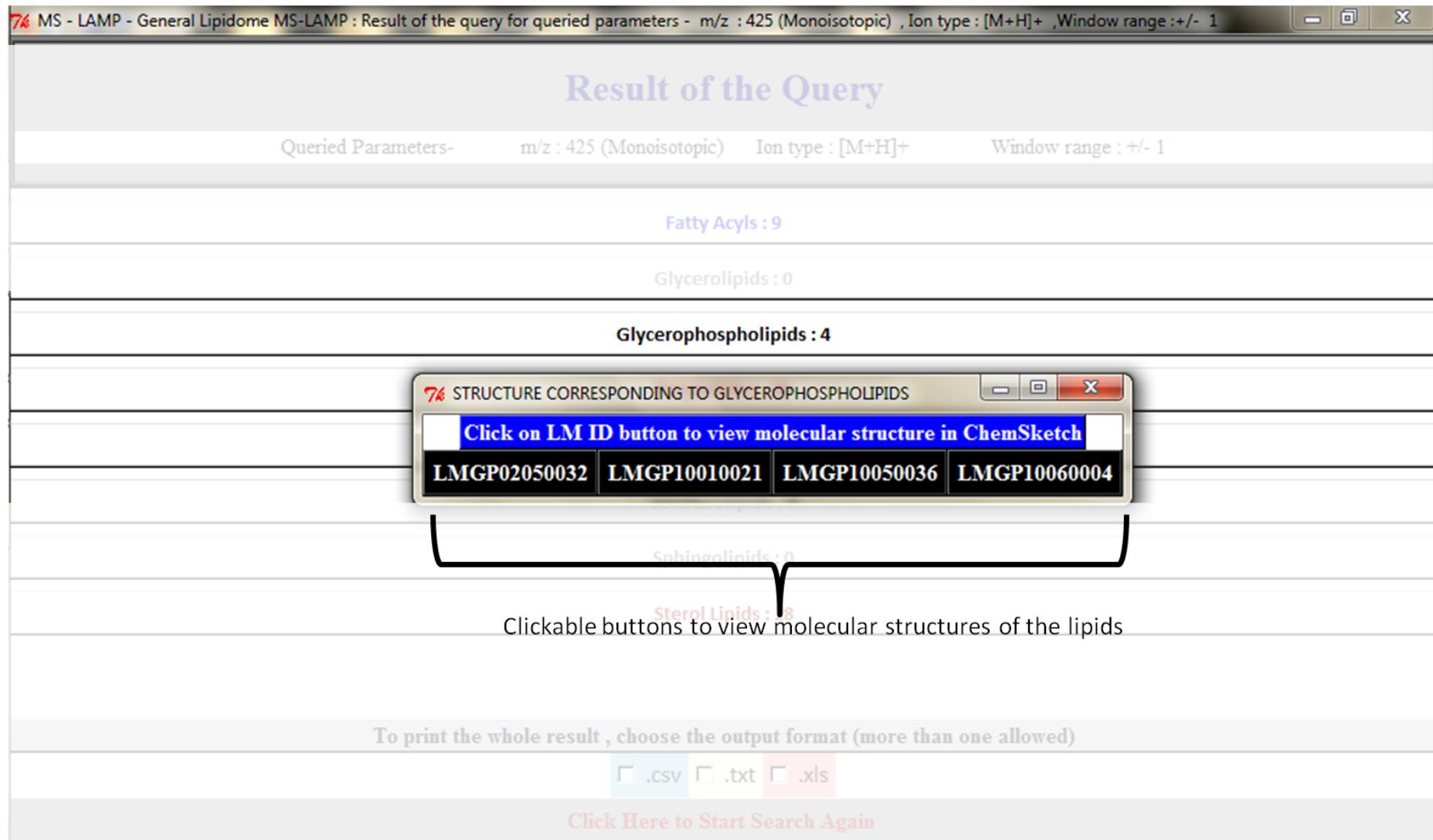


Figure 4.3: To view molecular structures of the lipids obtained as result of the query, button corresponding to a lipid category (in Results of the query window see [Figure 4.2](#)) can be clicked that will give rise to a new window containing clickable buttons showing LM ID(s). On clicking a LM ID button in the new pop-up window, molecular structure of the respective lipid opens in ChemSketch (See [Figure 4.4](#)). Shown here is an example from General Lipidome MS-LAMP. Only one structure can be viewed, at a given instance. In order to view another, previously opened structure needs to be closed. However, the already opened molecular structure can be saved and then closed. Subsequently, another LM ID button can be clicked to view another molecular structure. With respect to this aspect of *M. tb* Lipidome MS-LAMP, see [Figures 4.5](#) and [4.6](#).

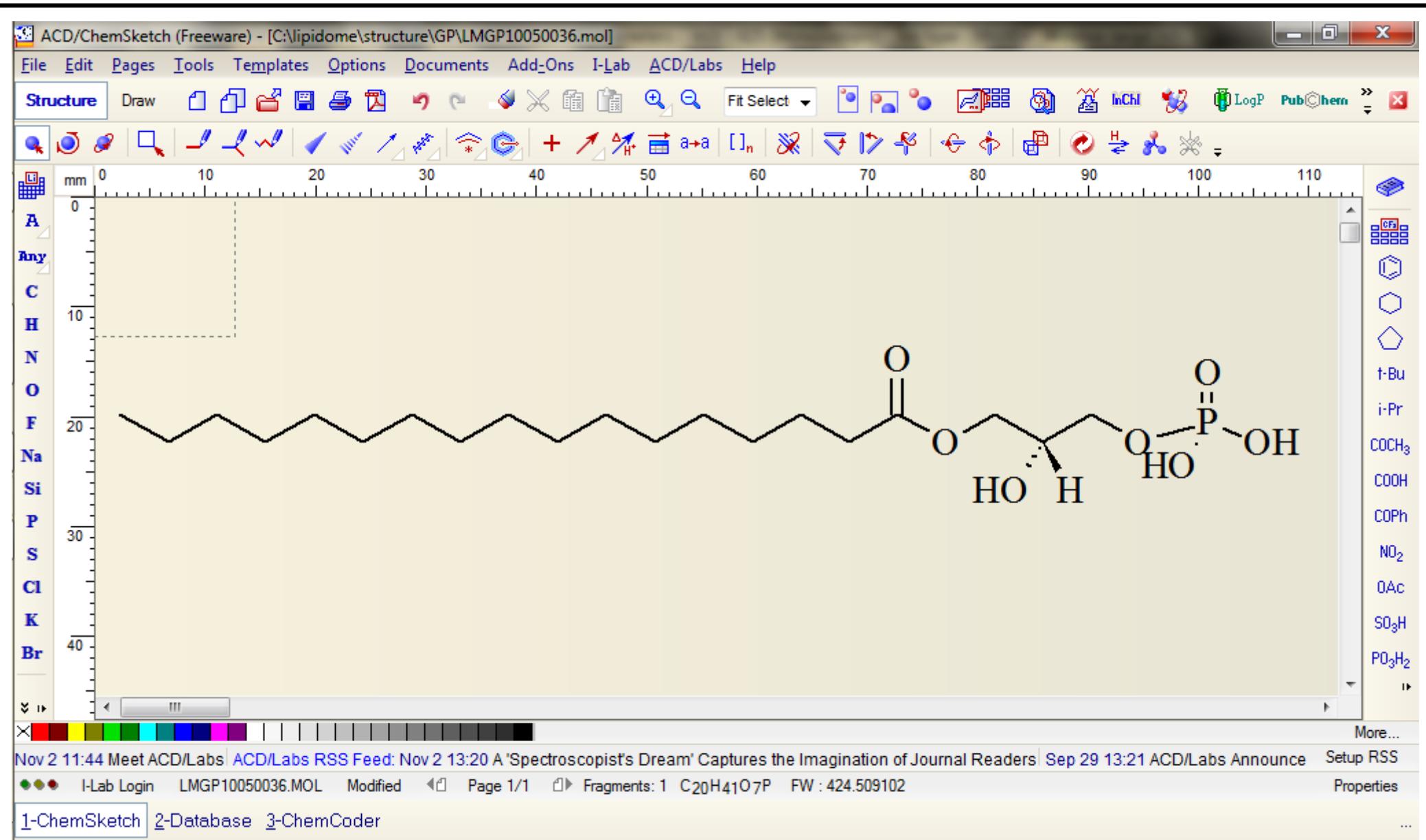


Figure 4.4: Molecular structure of a lipid shown in ChemSketch, which opens on clicking a LM ID button (see [Figure 4.3](#)). This is the molecular structure of the lipid corresponding to LM ID: LMGP10050036.

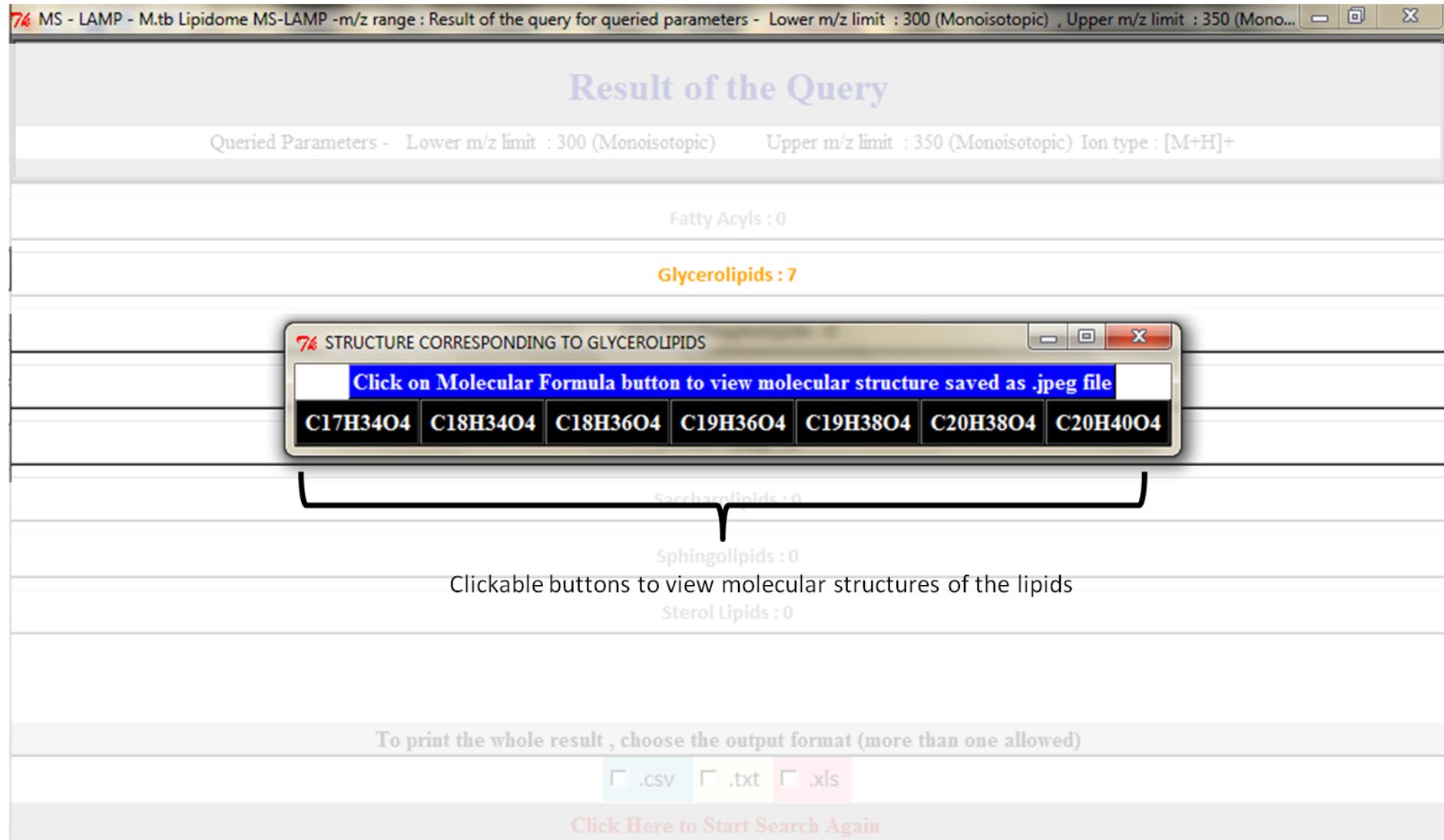


Figure 4.5: Shown here is an example from *M. tb* Lipidome MS-LAMP. To view molecular structures of the lipids obtained as results of the query, button corresponding to a lipid category (in Results of the query window) can be clicked that will give rise to a new window containing clickable buttons showing Molecular Formula(e). On clicking a button of molecular formula in the new pop-up window, molecular structure of the respective lipid, which is saved as .jpeg file, opens (See [Figure 4.6](#)). Only one structure can be viewed, at a given instance. In order to view another, previously opened structure needs to be closed. However, the already opened molecular structure can be saved and then closed. Thereafter, another molecular formula button can be clicked to view another structure.

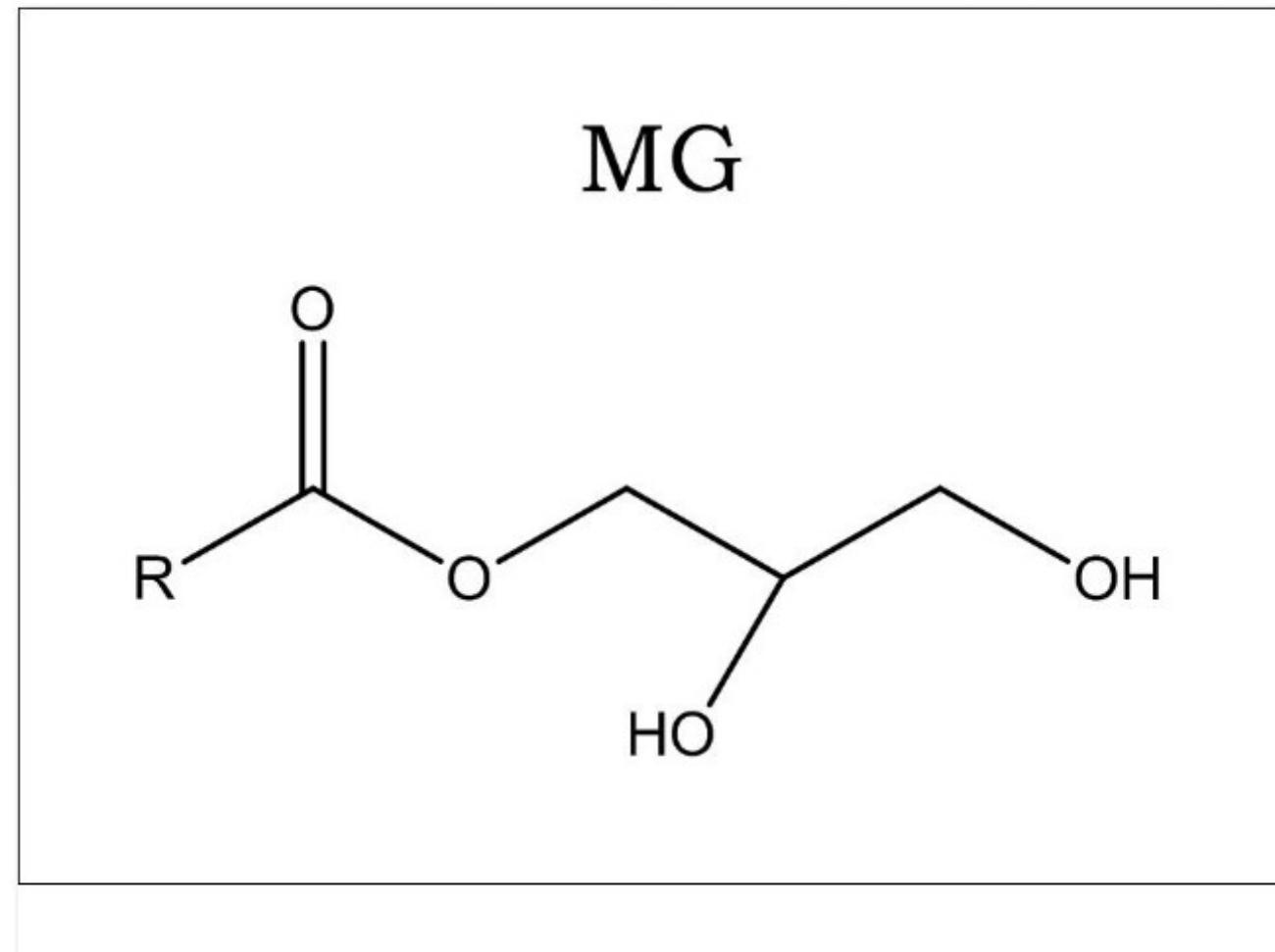


Figure 4.6: Molecular structure of a lipid available as .jpeg file in the *M. tb* lipid database (<http://mrl.colostate.edu>). The structure opens on clicking the respective Molecular Formula button shown in Figure 4.5. This is the molecular structure of a monoglyceride (MG) as present in the *M. tb* lipid database.

5. Query Type 2: List of Molecular Masses or m/z values

There are two ways to input this Query Type (see [Figure 5.1](#))

Option 1: By uploading a .txt file of molecular mass or m/z and no intensity values
(See [Figure 5.2](#))

Option 2: By uploading a .txt file of m/z and relative intensity values (see [Figure 5.2](#))

[Scheme 5.1](#) depicts flowchart describing the syntax to input query as list of molecular masses or m/z values.

[Figure 5.2](#) shows the snapshot of the window to input Query Type 2. Different parts of the window are explained below:

- (a) Title bar:** This bar gives information about the query window and the selected lipid database in use.
- (b) File Upload:** As the list of mass values can be queried using two different options ([Figure 5.1](#)), the input window rearranges itself accordingly. [Figure 5.2](#) shows the change in input window for both the options.

For Option 1:

1. **Back:** This button rearranges the main window of Query Type 2 ([Figure 5.1](#))
2. **Upload .txt file:** On clicking this button a file window opens, by which a .txt file containing Molecular Mass or m/z & no intensity values can be selected and uploaded.
3. **Mass Type:** After uploading the text file, Monoisotopic or Average Mass can be chosen. However, monoisotopic mass is set as default.

For Option 2:

1. **Back:** This button rearranges the main window of Query Type 2 ([Figure 5.1](#))
2. **Relative Intensity Threshold (%):** A scrollbar has been provided to select an intensity threshold value for the uploaded text file containing m/z and relative intensity values (see [Figure 5.2](#)).

3. **Upload .txt file:** Clicking this button opens a file window to select and upload a .txt file consisting of Molecular Mass or m/z & intensity values.

4. **Mass Type:** After uploading a text file Monoisotopic or Average Mass can be selected. Monoisotopic mass is however set as default.

(c) **Choose Molecular Mass / Type of Ion:** A choice between six negative and eight positive ions have been provided in addition to ‘Molecular Mass’, for making a query using MS-LAMP.

(d) **Window range:** Depending on the resolution of the instrument used and the level of accuracy required by the user, it is possible to define the search within a mass range of -1.00000 to +1.00000 about the queried *m/z* or mass value. However, the default value is set at 0.5.

(e) **Lipid category(ies):** MS-LAMP has multiple search ability. More than one lipid category can be chosen by activating the check-buttons corresponding to lipid category (ies). (Note: refer section 9 to know about permissible combinations of check-buttons)

(f) **Submit:** By clicking the ‘Submit’ button, the above selected parameters are entered as input to the programme.

The result of the input query can be seen in [Figure 5.3](#) consisting of different parts as explained below:

(e) **Title Bar:** Summary of the database in use and the input parameters are shown here.

(f) **Queried Parameters:** It gives review of the queried parameters.

(g) Population distribution of lipids in different lipid categories chosen are shown here.

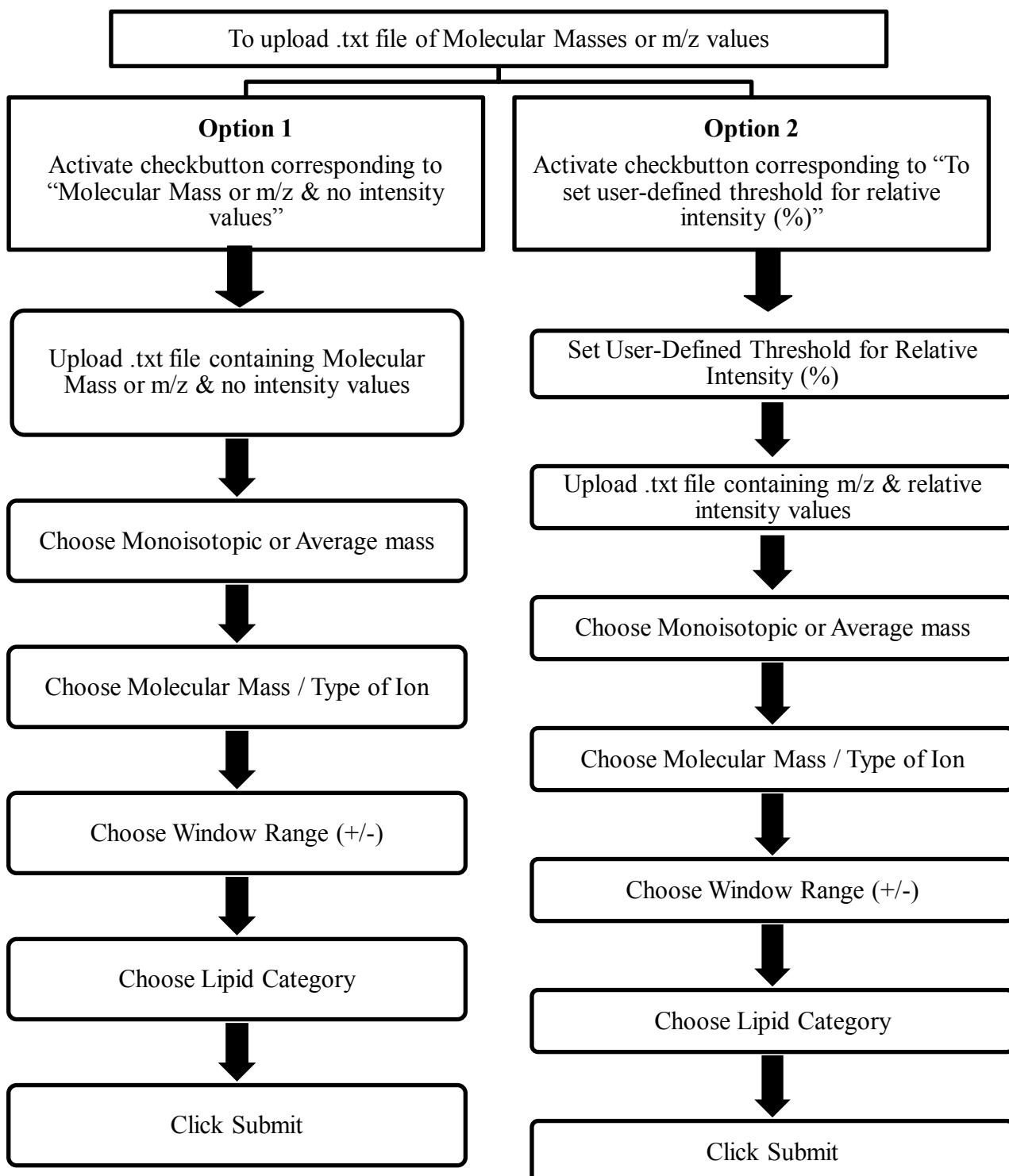
These are clickable buttons that gives rise to a new window showing details (LM ID in case of General Lipidome MS-LAMP and Molecular Formulae in case of *Mycobacterium tuberculosis* (*M. tb*) Lipidome MS-LAMP) about lipid(s) obtained as result of the query (see [Figure 5.4](#)).

Upon clicking a button in this new window, molecular structure corresponding to that lipid can be viewed. In case of General Lipidome MS-LAMP, the structures are available as MD mol file, which can be opened using ChemSketch; while for *M. tb* Lipidome MS-LAMP, structures are available as jpeg files.

(h) **Output file types:** Result of the query can be saved in 3 different formats:

4. Comma separated Value (.csv)
5. Text file (.txt)
6. Excel File (.xls)

(f) Search again: To start another search, this button can be clicked that would redirect to input window of Query Type 2 ([Figure 5.1](#)).



Scheme 5.1: Syntax to be followed to input **Query Type 2**: List of molecular masses or m/z values.

Query Type 2 : List of Molecular Masses or m/z values

(a)**(b)**

To upload .txt file of Molecular Masses or m/z values Molecular Mass or m/z & no intensity values To set user-defined threshold for relative intensity (%)
 (Not for Molecular Masses, only for m/z values)

Choose Molecular Mass / Type of Ion

Molecular Mass Negative ions [M-H]⁻ [M+Cl]⁻ [M+HOAc-H]⁻ [M+Li-2H]⁻ [M+Na-2H]⁻ [M+K-2H]⁻

Positive ions [M+H]⁺ [M+NH4]⁺ [M+Li]⁺ [M+Na]⁺ [M+K]⁺ [M+2Li-H]⁺ [M+2Na-H]⁺ [M+2K-H]⁺

Window Range (+/-)

Molecular Mass or m/z : 0.005 0.01 0.05 0.1 0.25 0.5 0.75 1

Which Lipid(s) ?

All eight categories [About lipid categories](#)

FA GL GP PK PR SL SP ST

All Phospholipids

Sphingo Other Phosphorylated lipids (Excluding GP)

Glycerolipids [GL]

Monoglycerides [MG] Diglycerides [DG] Triglycerides [TG] Other Glycerolipids

Halogenated Lipids

Sulphur containing lipids

Search within Main Class and/or Subclass

[Need Help ?](#)

SUBMIT

Figure 5.1: Snapshot of the main window of “Query Type 2: List of Molecular Masses or m/z values”. There are two options to input: **(a) Option 1:** For uploading a text file of Molecular Masses or m/z & no intensity values, this check-button should be activated. Following this the window rearranges and buttons for uploading text file appear as shown in [Figure 5.2](#). **(b) Option 2:** Activating this check-button allows a user to set a threshold for relative intensity values and then a text file containing m/z values can be uploaded (see [Figure 5.2](#)). Refer to [Figure 5.5](#) for more details on the type of .txt files to be uploaded using these two options.

74 MS - LAMP - General Lipidome - Query type 2 : List of Molecular Masses or m/z values

(a) **Query Type 2 : List of Molecular Masses or m/z values**

Back

To upload .txt file containing Molecular Mass or m/z & no intensity values

[Click here to upload .txt file](#)

Monoisotopic Average

(b) Option 1

Back

User-Defined Threshold for Relative Intensity (%)

5

5 10 15 20 25 30 35 40 45 50 55 60 65 70

Monoisotopic Average

[Click here to upload .txt file containing m/z & relative intensity values](#)

(b) Option 2

(c) Choose Molecular Mass / Type of Ion

Molecular Mass **Negative ions** [M-H]⁻ [M+C]⁻ [M+HOAc-H]⁻ [M+Li-2H]⁻ [M+Na-2H]⁻ [M+K-2H]⁻
Positive ions [M+H]⁺ [M+NH₄]⁺ [M+Li]⁺ [M+Na]⁺ [M+K]⁺ [M+2Li-H]⁺ [M+2Na-H]⁺ [M+2K-H]⁺

(d) Window Range (+/-)

Molecular Mass or m/z : 0.005 0.01 0.05 0.1 0.25 0.5 0.75 1

(e) Which Lipid(s) ?

All eight categories [About lipid categories](#)

FA GL GP PK PR SL SP ST

All Phospholipids

Sphingo Other Phosphorylated lipids (Excluding GP)

Glycerolipids [GL]

Monoglycerides [MG] Diglycerides [DG] Triglycerides [TG] Other Glycerolipids

Halogenated Lipids

Sulphur containing lipids

Search within Main Class and/or Subclass [Need Help ?](#)

SUBMIT **(f)**

Figure 5.2: Snapshot of **Query Type 2** input window: **(a)** Title Bar **(b)** Two different features that would appear in this window depending on the choice of two different options, Option 1 & Option 2. In both the options, there is provision to choose monoisotopic or average mass. **(c)** To choose Molecular Mass/Type of Ion **(d)** For selecting Window Range (+/-) **(e)** To choose lipid category(ies) **(f)** For submitting the chosen input parameters.

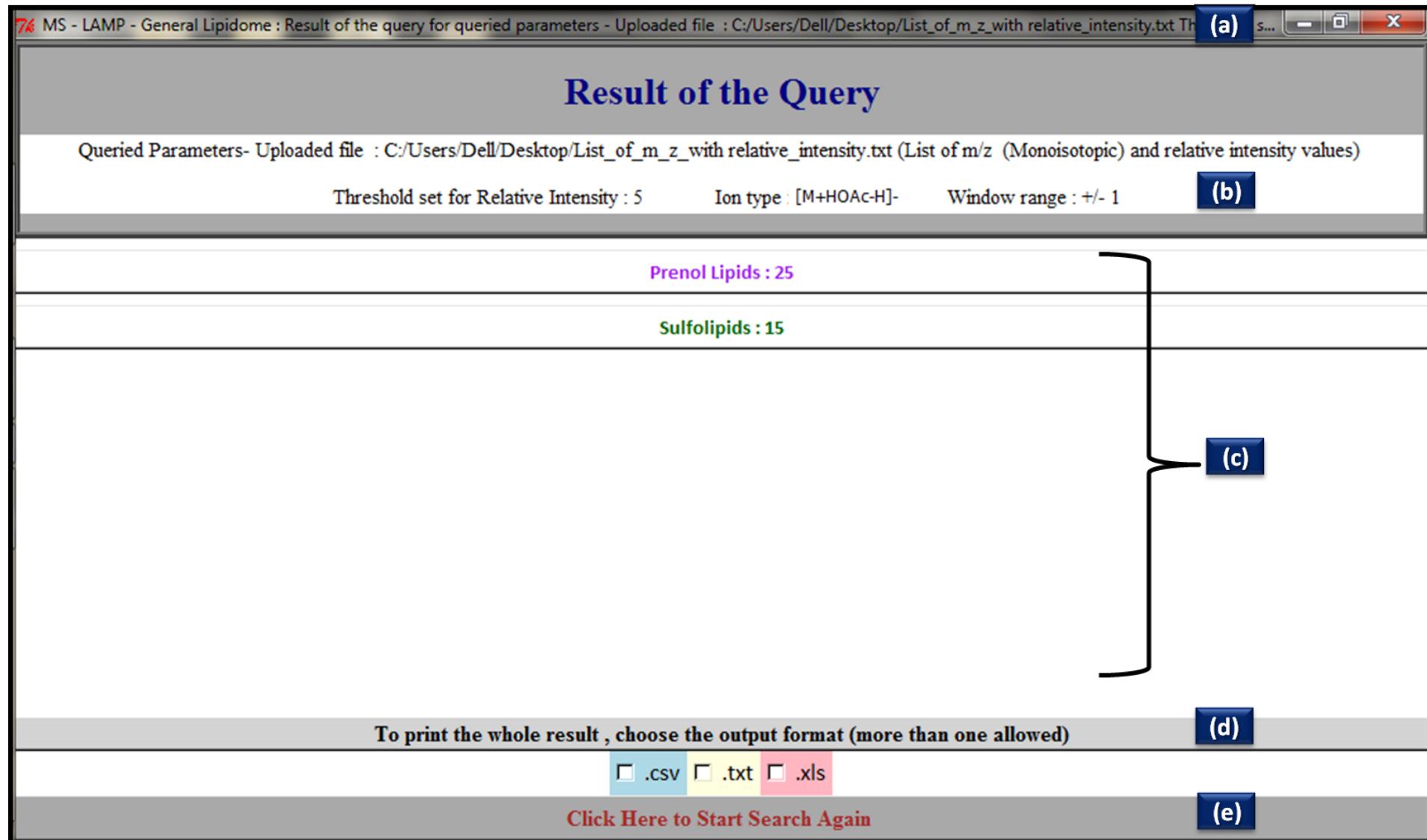


Figure 5.3: Snapshot of **Result of the Query** window displaying a glimpse of different lipid categories and number of lipids in each category that match to the queried criteria: A file containing list of m/z values and relative intensities was uploaded. As depicted in [Figure 5.2](#), monoisotopic mass was selected; the threshold for relative intensity was set to 5; window range of 1 and type of ion, $[M+Hac-H]^-$ were chosen; and the search was directed to prenol and sulfur-containing lipids. It can be noted that corresponding to the input parameters, there are 25 prenol lipids and 15 sulfolipids. **(a)** Title Bar **(b)** Queried Parameters **(c)** Chosen lipid category(ies) **(d)** To choose different file types for saving the result **(e)** For beginning a new search, this button is to be clicked. The result obtained on querying General Lipidome MS-LAMP is shown here.

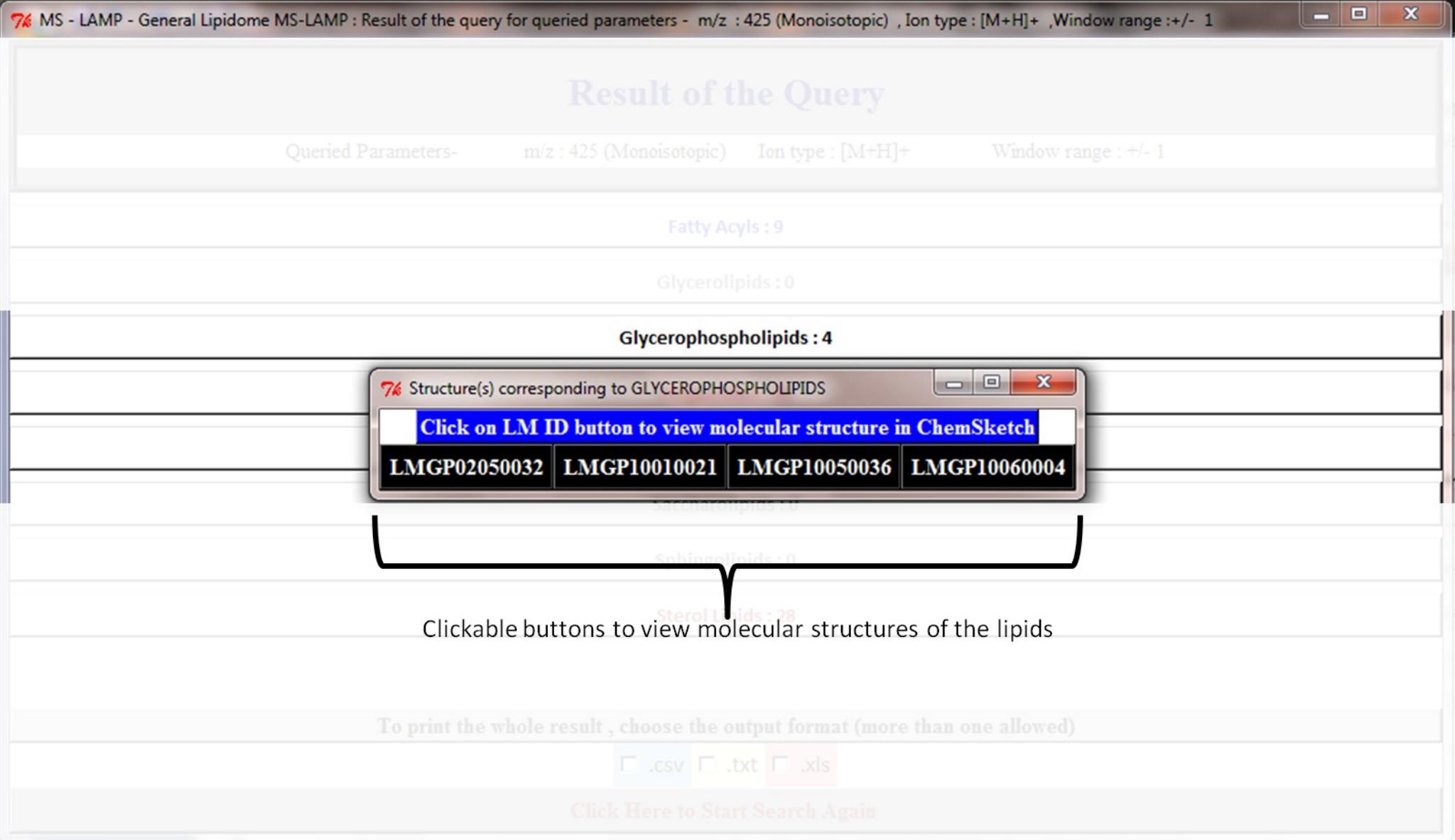


Figure 5.4: Figure showing snapshot of the window containing LM ID buttons, which can be clicked to view molecular structure of lipids that are obtained as result of the query , shown in [Figure 5.3](#) ([Refer section 4](#) for more details on this).

(a)

(b)

m/z	Intensity	Relative	Charge
377.09	287946.8	69.30	1.00
485.14	314223.8	77.76	1.00
521.12	931672.5	22.99	1.00

Figure 5.5: Files suitable to input **Query Type 2**: (a) **Option 1**: Example of a text file containing Molecular Mass or m/z and no intensity values. This file contains a single column and can be used for making a query corresponding to only “Molecular Mass or m/z & no intensity values” (Refer [Figures 5.1 & 5.2](#)) (b) **Option 2**: Example of a text file containing m/z and relative intensity values (To set user-defined threshold for relative intensity (%)) (Refer [Figures 5.1 & 5.2](#)). In this case, the .txt file to be submitted must have four columns comprising m/z , absolute intensity, relative intensity and charge, respectively in column numbers 1, 2, 3 and 4, where each column is separated by a tab (as shown here). This file is suitable for the entering query using **Option 1** as well, i.e. for making a query using “Molecular Mass or m/z & no intensity values”. In that case, the software will consider column 1 only and ignore other three columns.

Note: Regarding submitting query by **Option 2**; where the user sets a threshold for relative intensity (%) (See [Figure 5.2](#)): When this option is chosen, the programme considers values in columns 1 (m/z values) and 3 (Relative Intensity values) only, while the entries in columns 2 and 4 are disregarded.

6. Query Type 3: Range of Molecular Mass or m/z value

Range of Molecular Mass or *m/z* value can also be used to search lipids. [Scheme 6.1](#) summarizes the steps to enter this query type.

[Figure 6.1](#) shows the input parameters to look for lipids within monoisotopic molecular mass in the range of 400 - 450. $[M+Cl]^-$ is chosen as ion type and the search is directed to entire *Mycobacterium tuberculosis* (*M. tb*) lipidome. Various parts of this window are explained, which are as follows:

(a) Title bar: This bar gives information about the query window and the selected lipid database in use. An example of a case from *M. tb* Lipidome MS-LAMP is shown here.

(b) Molecular Mass or m/z value and mass type:

1. **Lower Limit:** A mass value entered in this box will be considered as lower limit of the range being queried.

2. **Upper Limit:** Upper limit of the mass range should be entered in this text box.

(Note: Mass value entered as “Lower limit” should be less than the value entered as “Upper Limit”.)

3. **Mass type:** Monoisotopic or Average Mass can be chosen, however, monoisotopic mass is the default type.

(c) Choose Molecular Mass / Type of Ion: A choice between six negative and eight positive ions have been provided, in addition to ‘Molecular Mass’ for making a query using MS-LAMP.

(d) Lipid category (ies): MS-LAMP has multiple search ability; thereby multiple lipid categories can be chosen by activating the check-buttons corresponding to lipid category(ies). (Note: refer section 9 to know about permissible combinations of check-buttons)

(e) Submit: This button can be clicked to input the above chosen parameters to the programme.

On submitting the above mentioned parameters as input (as depicted [Figure 6.1](#)), a total of 17 lipids (11 fatty acyls and 6 glycerolipids) were found satisfying to the queried-in

parameters in the *M. tb* Lipidome MS-LAMP database. This can be seen from the “Result of the query” window shown in [Figure 6.2](#) and various parts of the same are explained as follows:

- (i) **Title Bar:** It gives the summary of the database in use and the queried parameters.
- (j) **Queried Parameters:** It gives the review of the chosen parameters queried-in.
- (k) **Chosen Lipid categories:** Shown here is the population distribution of lipid(s) in different lipid categories chosen while making a query. These are clickable buttons that yield a new window showing details (LM ID in case of General Lipidome MS-LAMP and Molecular formulae for *M. tb* Lipidome MS-LAMP) about the lipid(s) obtained as result of the query (see [Figure 6.3](#)).

Upon clicking a button in the new pop-up window, molecular structure corresponding to that lipid can be viewed. In case of General Lipidome MS-LAMP, the structure is available as MD mol file, which could be seen using ChemSketch; whereas for *M. tb* Lipidome MS-LAMP, structures are available as .jpeg files.

- (l) **Output file types:** Result of the query can be saved in 3 different formats.viz,

7. Comma separated Value (.csv)
8. Text file (.txt)
9. Excel File (.xls)

- (g) **Search again:** To start the search again, this button can be clicked that would redirect to the input window of Query Type 3 ([Figure 6.1](#)).

Enter Lower and Upper limit of molecular mass or m/z



Choose Monoisotopic / Average mass



Choose Molecular Mass / type of ion



Choose Lipid Category



Click Submit

Scheme 6.1: Flowchart delineating the procedure to search lipids by **Query Type 3**: querying range of molecular mass or m/z values.

(a)



Query Type 3 : Molecular Mass or m/z range

Lower limit Upper limit
 Monoisotopic Average

(b)

Choose Molecular Mass / Type of Ion

(c)

 Molecular Mass**Negative ions** [M-H]⁻ [M+Cl]⁻ [M+HOAc-H]⁻ [M+Li-2H]⁻ [M+Na-2H]⁻ [M+K-2H]⁻**Positive ions** [M+H]⁺ [M+NH₄]⁺ [M+Li]⁺ [M+Na]⁺ [M+K]⁺ [M+2Li-H]⁺ [M+2Na-H]⁺ [M+2K-H]⁺

Which Lipid(s) ?

(d)

 All eight categories [About lipid categories](#)
 FA GL GP PK PR SL SP ST
 All Phospholipids

Glycerolipids [GL]

 Sphingo Other Phosphorylated lipids (Excluding GP) Monoglycerides [MG] Diglycerides [DG] Triglycerides [TG] Other Glycerolipids Halogenated Lipids Sulphur containing lipids Search within Main Class and/or Subclass[Need Help ?](#)

SUBMIT

(e)

Figure 6.1: Snapshot of input window for “Query Type 3: Molecular Mass or m/z range”. (a) Title Bar (b) To enter lower and upper limits of Molecular Mass or m/z value and for choosing monoisotopic or average mass (c) To Choose Molecular Mass/ Type of Ion (d) For selecting lipid category(ies) (e) To Submit the selected parameters.

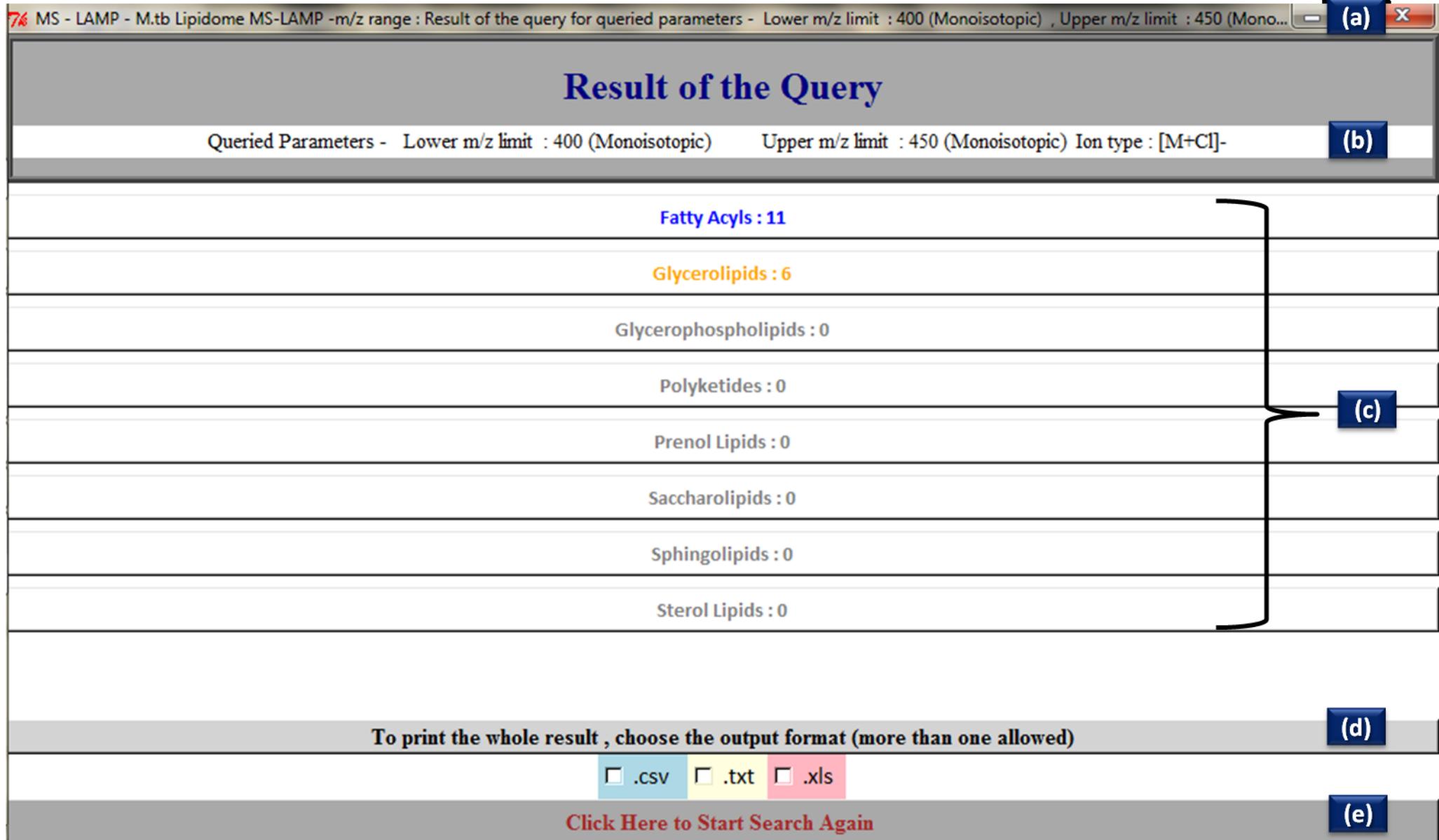


Figure 6.2: Snapshot of **Result of the query** window providing a glance of different lipid categories and number of lipids in each category matching to the queried criteria submitted to *M. tb* Lipidome MS-LAMP, as shown in [Figure 6.1](#) (a) Title Bar (b) Queried Parameters (c) Chosen lipid category(ies) (d) For selecting different file types to save the output (e) To begin another search, this button needs to be clicked.

Result of the Query

Queried Parameters - Lower m/z limit : 400 (Monoisotopic) Upper m/z limit : 450 (Monoisotopic) Ion type : [M+Cl]-

Fatty Acyls : 11

STRUCTURE CORRESPONDING TO FATTY ACYLS							
Click on Molecular Formula button to view molecular structure saved as .jpeg file							
C24H48O2	C24H48O2	C25H48O2	C25H50O2	C25H50O2	C24H48O3	C26H52O2	C26H52O2
C27H52O2	C27H54O2	C26H52O3					

Prenol Lipids : 0

Saccharolipids : 0

Sphingolipids : 0

Clickable buttons to view molecular structures of the lipids

Sterol Lipids : 0

To print the whole result , choose the output format (more than one allowed)

.csv .txt .xls

[Click Here to Start Search Again](#)

Figure 6.3: Figure showing snapshot of the window containing molecular formulae buttons, which are to be clicked to view the molecular structure of lipids corresponding to those obtained as result of the query, shown in [Figure 6.2 \(Refer section 4 for more details on this\)](#).

7. Query Type 4: Molecular Formula

To enter the query as molecular formula, the user first has to activate check-buttons corresponding to the type of atoms and the number of atoms respective to the each type needs to be typed-in, depending on the molecular formula to be searched. Upon entering these values, user can choose to search within specific lipid category (ies). [Scheme 7.1](#) shows a flowchart summarizing the steps to input Query Type 4.

As shown in [Figure 7.1](#), a molecular formula C38 H77 O9 P was queried within all eight lipid categories. Highlighted parts of the window are being explained as follows

- (f) **Title bar:** This bar gives information about the query window and Lipid database in use.
- (g) **Molecular formula input:** to make an input check-buttons corresponding to the atoms contained in molecular formula being queried needs to be activated and the number of atoms respective to the each type needs to be typed-in the text box provided for each atom.
- (h) **Lipid category (ies):** MS-LAMP has multiple search ability. Thereby multiple lipid categories can be chosen by activating the check-buttons corresponding to lipid category (ies). (Note: refer section 9 to know about permissible combinations of check-buttons)
- (i) **Submit Input:** Upon choosing the query parameters, this button can be clicked to submit the input.

[Figure 7.2](#) shows the result of the queried parameters (see [Figure 7.1](#)): 3 Glycerophospholipids and 1 Polyketide correspond to queried molecular formula in General Lipidome MS-LAMP database. Various elements of the output window are explained in the following:

- (m) **Title Bar:** It gives the summary of the database in use and chosen parameters queried-in.
- (n) **Queried Parameters:** It gives the review of the selected parameters entered as input.
- (o) **Chosen Lipid categories:** Population distribution of lipid(s) in different lipid categories is depicted here. These are clickable buttons that opens a new window

showing details (LM ID in case of General Lipidome MS-LAMP and Molecular Formulae in case of *Mycobacterium tuberculosis* (*M. tb*) Lipidome MS-LAMP) about the lipid(s) obtained as result of the query (see [Figure 7.3](#)).

Upon clicking a button in this new window, structure corresponding to that lipid is shown (In case of General Lipidome MS-LAMP, the structure is available as MD mol file and structure is shown in Chemsketch; whereas for *M. tb* Lipidome MS-LAMP, structures are available as .jpeg files)

(p) Output file types: Result of the query can be saved in 3 different formats.viz,

10. Comma separated Value (.csv)
11. Text file (.txt)
12. Excel File (.xls)

(h) Search again: To begin another search, this button can be clicked, which would redirect to input window for Query Type 4 (See [Figure 7.1](#)).

Activate the checkboxes corresponding to the type of atoms that needs to be queried based on the molecular formula



Enter the number of atoms respective to each type of atom, whose checkboxes have been activated



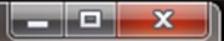
Choose Lipid Category



Click Submit

Scheme 7.1: Steps to enter **Query Type 4:** Molecular formula

(a)



Query Type 4 : Molecular Formula

<input checked="" type="checkbox"/> C	38	<input checked="" type="checkbox"/> H	77	<input checked="" type="checkbox"/> O	9	<input type="checkbox"/> N	<input type="checkbox"/> S	<input checked="" type="checkbox"/> P	1	<input type="checkbox"/> D	<input type="checkbox"/>
<input type="checkbox"/> F		<input type="checkbox"/> Cl		<input type="checkbox"/> Br		<input type="checkbox"/> I					
		<input type="checkbox"/> Na		<input type="checkbox"/> Si							

(b)

C : Carbon, H: Hydrogen, O : Oxygen, N : Nitrogen, S :Sulfur, P : Phosphorous, D :Deuterium, F :Flourine, Cl :Chlorine, Br :Bromine, I :Iodine, Na :Sodium, Si :Silicon

Which Lipid(s) ?

(c)

All eight categories [About lipid categories](#)

FA GL GP PK PR SL SP ST

All Phospholipids

Sphingo Other Phosphorylated lipids (Excluding GP)

Glycerolipids [GL]

Monoglycerides [MG] Diglycerides [DG] Triglycerides [TG] Other Glycerolipids

Halogenated Lipids

Sulphur containing lipids

Search within Main Class and/or Subclass

Need Help ?

SUBMIT

(d)

Figure 7.1: Snapshot of input window of “Query Type 4: Molecular Formula”. Shown here is an example, wherein a molecular formula, C₃₈ H₇₇ O₉ P is being searched in all eight lipid categories within General Lipidome MS-LAMP. (a) Title bar (b) To enter Molecular Formula (c) To select lipid category(ies) (d) To submit queried parameters as input.

76 MS - LAMP - General Lipidome : Result for the queried Molecular Formula : C38H77O9P

(a)

Result of the Query

Queried Molecular Formula : C38H77O9P

(b)

Fatty Acyls : 0

Glycerolipids : 0

Glycerophospholipids : 3

Polyketides : 1

Prenol Lipids : 0

Saccharolipids : 0

Sphingolipids : 0

Sterol Lipids : 0

(c)

To print the whole result , choose the output format (more than one allowed)

.csv .txt .xls

(d)

[Click Here to Start Search Again](#)

(e)

Figure 7.2: Snapshot of **Result of the Query** window showing a glimpse of different lipid categories : 3 glycerophospholipids and a polyketide, corresponding to queried molecular formula C38 H77 O9 P submitted to General lipidome MS-LAMP. (a) Title Bar (b) Queried Parameters (c) Chosen lipid category(ies) (d) To choose different file types for saving the output (e) To begin another search.

76 MS - LAMP - General Lipidome MS-LAMP : Result for the queried Molecular Formula : C38H77O9P

Result of the Query

Quered Molecular Formula : C38H77O9P

Fatty Acyls : 0

Glycerolipids : 0

Glycerophospholipids : 3

Polytides : 1

STRUCTURE CORRESPONDING TO GLYCEROPHOSPHOLIPI...

Click on LM ID button to view molecular structure in ChemSketch

LMGP04020082 | LMGP04020041 | LMGP04020020

Sphingolipids : 0

Sterol Lipids : 0

Clickable buttons to view molecular structures of the lipids

To print the whole result , choose the output format (more than one allowed)

.csv .txt .xls

[Click Here to Start Search Again](#)

Figure 7.3: Figure showing snapshot of the window containing LM ID buttons, which can be clicked to view the molecular structure of lipids that are obtained as result of the query, shown in Figure 7.2 (Refer section 4 for more details on this).

8. Query Type 5: LIPID MAPS ID (LM ID) or List of LM IDs

This option is available only in General Lipidome MS-LAMP search window. LIPID MAPS ID (LM ID) is a unique identifier designated by LIPID MAPS Consortium (www.lipidmaps.org) to every lipid and this has been adopted in General Lipidome MS-LAMP database. Currently as on Feb 2012 only 57 lipids (47 FA, 5 PK, and 5 PR) in *Mycobacterium tuberculosis* database (<http://mrl.colostate.edu>) have been designated with LM IDs. Therefore, this Query Type is meant for General Lipidome MS-LAMP only.

There are two different ways to submit a query:

1. Option 1: Single LM ID
2. Option 2: List of LM IDs

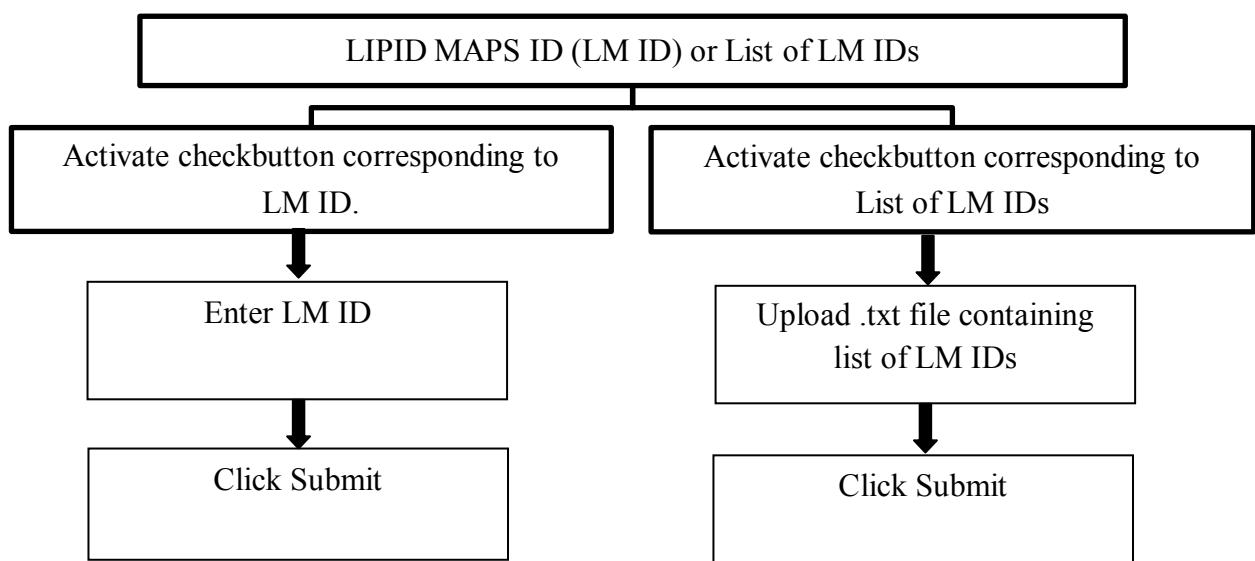
A flowchart describing the steps to use this option is shown in [Scheme 8.1](#).

Single LM ID can be entered by first activating the check-button respective to LM ID and then the LM ID of a lipid needs to be entered in the space provided, as depicted in [Figure 8.1b option 1](#). A text file containing list of LM IDs also can be uploaded as shown in [Figure 8.1b option 2](#). Different parts of the input window are explained in the following:

- (a) **Title bar:** This bar gives information about the query window and the selected lipid database in use.
- (b) **LM ID Query options:** As shown in [Figure 8.1](#), for making query of LM ID(s) two different options have been provided. To enter a single LM ID query, option 1 can be used, whereby the ID can be entered in the provided text box after clicking the “**LM ID**” check-button. In order to input list of LM IDs, a text file containing list of the same, each separated by a new line, can be uploaded. In an attempt, only one option can be used to submit the query.
- (c) **Submit:** By clicking this button the above selected parameters are entered as input to the programme.

[Figure 8.2](#) shows snapshot of ‘Result of the Query’ window obtained on using option 1, i.e., Single LM ID query; while [Figure 8.3](#) shows output details when lipids are queried utilizing option 2, i.e., list of LM IDs.

To view molecular structure of lipid(s) obtained as result of the query through option 1, the output window contains a button (as shown in [Figure 8.2](#)) that can be clicked to view the corresponding structure. On following option 2 to input query, [Figure 8.4](#) shows the way to view molecular structure of lipids.



Scheme 8.1: Flowchart explaining to input **Query Type 5**: LIPID MAPS ID (LM ID) or List of LM IDs

Query type 5 : LIPID MAPS ID (LM ID) / List of LM IDs

For example, LMSP01020001 corresponds to Sphinganine, a Sphingolipid [SP]

 LM ID List of LM IDs

Enter LM ID

LMFA01010040

(b) Option 1

 LM ID List of LM IDs

Upload a text file containing list of LM ID

Click here to upload file

(b) Option 2

SUBMIT

(c)

Figure 8.1: Snapshot of input window of “Query Type 5: LIPID MAPS ID (LM ID) / List of LM IDs”. **(a)** Title Bar **(b)** Two different options available for making this query: Option 1, Single LM ID and Option 2, List of LM IDs **(c)** To submit the query. In an attempt, only one option can be used to input query.

Details of Queried LM ID : LMSP01020001

LM ID :	LMSP01020001
M-Monoisotopic (db)* :	301.298079
M-Average (db)* :	301.50928
Common name :	Sphinganine
Scientific name :	Sphinganine
Category :	Sphingolipids [SP]
Main class :	Sphingoid bases [SP01]
Sub class :	Sphinganines [SP0102]
Structure	Click to view the structure of LMSP01020001

To print the whole result , choose the output format (more than one allowed)

.csv .txt .xls

[Click Here to Start Search Again](#)

Figure 8.2: Snapshot of ‘Result of the query’ window on submitting query through Option 1: Details corresponding to the queried LM ID are enlisted.

Result of the Query

Uploaded Filename : C:/Users/Dell/Desktop/List_of_LM_IDs.txt

Fatty Acyls : 9

Glycerolipids : 0

Glycerophospholipids : 0

Polyketides : 0

Prenol Lipids : 4

Saccharolipids : 0

Sphingolipids : 3

Sterol Lipids : 0

To print the whole result , choose the output format (more than one allowed)

.csv .txt .xls

[Click Here to Start Search Again](#)

Figure 8.3: Snapshot of ‘Result of the query’ window while entering the input through Option 2: A glimpse of different lipid categories and number of lipids in each category that match to the list of LM IDs submitted in a .txt file as query, are displayed.

Result of the Query

Uploaded Filename : C:/Users/Dell/Desktop/List_of_LM IDs.txt

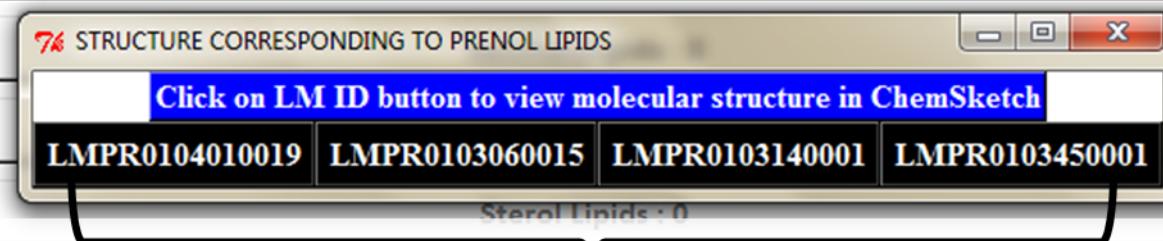
Fatty Acyls : 9

Glycerolipids : 0

Glycerophospholipids : 0

Polyketides : 0

Prenol Lipids : 4



Clickable buttons to view molecular structures of the lipids
To print the whole result, choose the output format (more than one allowed)

.csv .txt .xls

Click Here to Start Search Again

Figure 8.4: Figure showing snapshot of the window containing LM ID buttons obtained from ‘Result of the Query’ window (shown in [Figure 8.3](#)). These LM ID buttons can be clicked to view molecular structure of lipids. ([Refer section 4 for more details on this](#)).

9. Permissible combination of checkbuttons to choose a lipid category

MS-LAMP has multiple search ability and permits to guide search to multiple lipid categories in an attempt and hence it is possible to obtain a glimpse of population distribution of different lipid categories, corresponding to the queried parameters.

[Table 9.1](#) delineates the permissible combination of checkbuttons to select lipid category (ies).

Table 9.1: Permissible combination of checkboxes to choose lipid category(ies) (N.A. refers to not applicable; ✓ tells that this combination is allowed whereas ✗ indicates that this combination is not allowed.)

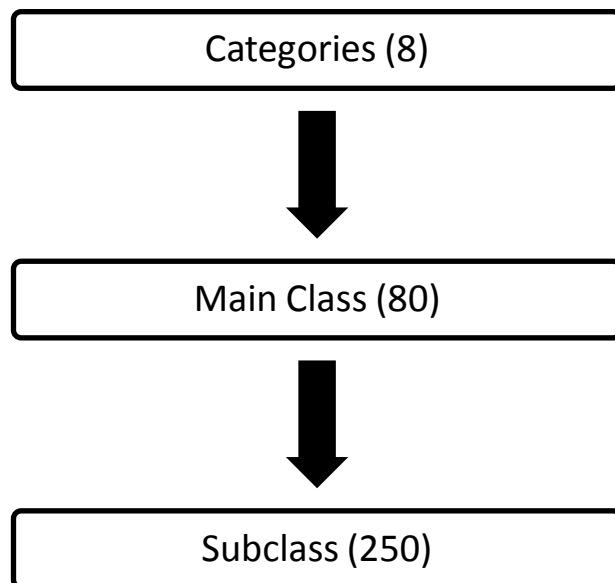
LAMP - LAMP

Spectrometry based Lipid(ome) Analyzer & Molecular Platform

ossible combination of checkboxes for searching within Lipidome

10. Search within Main Class and/or Subclass

This option in MS-LAMP can be used to focus the search to a specific lipid class. The lipids in General and *Mycobacterium tuberculosis* (*M. tb*) Lipidome MS-LAMP databases are categorised as shown in [Scheme 10.1](#), which follows the convention of LIPID MAPS Consortium (www.lipidmaps.org).



Scheme 10.1: Hierarchy of lipid classification

In order to focus the search to a particular Main Class and/or Subclass of lipids, it is essential to understand the codes defined by LIPID MAPS to address categories, main classes and subclasses; these are summarized in [Tables 10.1](#), [10.2](#) and [10.3](#).

[Tables 10.1](#) and [10.2](#) show eight-category classification of lipids, abbreviations for the categories and the number of Main Classes and Subclasses in every category for General and *M. tb* Lipidome MS-LAMP, respectively.

[Table 10.3](#) describes the format for denoting the LIPID MAPS identifier (LM ID)

Table 10.1: Eight-category classification of Lipids (General Lipidome MS-LAMP)

S.No.	Category	Abbreviation	Number of Main Classes	Number of Subclasses
1	Fatty Acids	FA	15	51
2	Glycerolipids	GL	6	14
3	Glycerophospholipid	GP	21	67
4	Polyketide	PK	15	28
5	Prenol Lipids	PR	4	19
6	Saccharolipids	SL	4	5
7	Sphingolipids	SP	9	30
8	Sterol Lipids	ST	5	39

Source: LIPID MAPS Consortium (www.lipidmaps.org)**Table 10.2:** Eight-category classification of Lipids (*M. tb* Lipidome MS-LAMP)

S.No.	Category	Abbreviation	Number of Main Classes	Number of Subclasses
1	Fatty Acyls	FA	2	11
2	Glycerolipids	GL	3	3
3	Glycerophospholipids	GP	5	30
4	Polyketides	PK	1	2
5	Prenol Lipids	PR	2	4
6	Saccharolipids	SL	2	7
7	Sphingolipids	SP	0	0
8	Sterol Lipids	ST	0	0

Source: The Mycobacterium Research Laboratories, Colorado State University (www.mrl.colostate.edu)

Table 10.3: Format for unique twelve-character LIPID MAPS identifier (LM ID).

LIPID ID : LMFA02012012		
Characters	Description	Example
1 - 2	Database designation	LM
3 - 4	Category code	FA
5 - 6	Main Class code	02
7 - 8	Subclass code	01
9 - 12	unique four character identifier within subclass	2012

To search within a

1. **Main Class:** To target search specifically to a Main class, code specific to that class is to be entered in the text box. For example, the **Main Class** code for ‘Fatty Esters’ in the **Category, Fatty Acyls** (FA) is 07 (Refer Tables [10.3](#) and [10.4](#)). Therefore, to search within Fatty Esters, **FA07** may be entered. MS-LAMP will then interrogate specifically with lipids belonging to this class.
2. **Subclass:** To aim the search within a subclass, appropriate code meant for a subclass is to be entered in the text box. For instance, information on Ceramide phosphocholines (sphingomyelins) can be obtained by entering SP0301, which corresponds to **Category:** SP, **Main Class code:** 03 and **Subclass code:** 01 (Refer Tables [10.3](#), [10.10](#) and Figure [10.1](#)).

This search option is available in Query Types 1, 2, 3 and 4.

[Figure 10.1](#) shows a snapshot of window that illustrates about searching within Main Class and/or Subclass. In this example, the query is directed specifically to “**Ceramide phosphocholines (sphingomyelins)**”; SP0301 is entered in the text box provided. [Figure 10.2](#) shows result of the query window for this input.

To know the details regarding codes meant for Main Classes and Subclasses in every category for General Lipidome MS-LAMP, refer Tables [10.4](#) - [10.11](#).

For details regarding codes meant for Main Classes ad Subclasses in every category for *M. tb* Lipidome MS-LAMP, refer Tables [10.12](#) - [10.17](#).

Query Type 3 : Molecular Mass or m/z range

Lower limit Upper limit
 Monoisotopic Average

Choose Molecular Mass / Type of Ion

 Molecular Mass**Negative ions** [M-H]⁻ [M+Cl]⁻ [M+HOAc-H]⁻ [M+Li-2H]⁻ [M+Na-2H]⁻ [M+K-2H]⁻**Positive ions**
 [M+H]⁺ [M+NH₄]⁺ [M+Li]⁺ [M+Na]⁺ [M+K]⁺ [M+2Li-H]⁺ [M+2Na-H]⁺ [M+2K-H]⁺

Which Lipid(s) ?

 All eight categories [About lipid categories](#)
 FA GL GP PK PR SL SP ST

All Phospholipids

 Sphingo Other Phosphorylated lipids (Excluding GP)

Glycerolipids [GL]

 Monoglycerides [MG] Diglycerides [DG] Triglycerides [TG] Other Glycerolipids

Halogenated Lipids

Sulphur containing lipids

Search within Main Class and/or Subclass

[Need Help ?](#)

SUBMIT

Figure 10.1: Snapshot of the window of Query Type 3 of General Lipidome MS-LAMP, illustrating to search within Main Class and/or Subclass. As an example, here the search is aimed at ‘Ceramide phosphocholine’, which corresponds to the code SP0301 that is entered in the text box provided (shaded in pink colour). In an attempt, only a Main Class and/or a Subclass can be entered. This option is available in Query Types 1, 2, 3 and 4.

Result of the Query

Queried Parameters - Lower m/z limit : 600 (Monoisotopic) Upper m/z limit : 800 (Monoisotopic) Ion type : [M+H]⁺

SP0301 : 60

To print the whole result , choose the output format (more than one allowed)

.csv .txt .xls

[Click Here to Start Search Again](#)

Figure 10.2: Result of the Query window showing number of lipids in subclass SP0301, corresponding to the input parameters queried, as depicted in [Figure 10.1.](#)

Table 10.4: List of classes within **Fatty Acyls** belonging to **General Lipidome MS-LAMP**. Code shown in the bracket ([]) may be entered in the text box to search specifically within that class.

Category	Main Class	Sub Class
Fatty Acyls [FA]	Acyltrehaloses [SL03]	-
Fatty Acyls [FA]	Docosanoids [FA04]	-
Fatty Acyls [FA]	Eicosanoids [FA03]	Hydroxy/hydroperoxyeicosatrienoic acids [FA0305]
Fatty Acyls [FA]	Eicosanoids [FA03]	Clavulones and derivatives [FA0312]
Fatty Acyls [FA]	Eicosanoids [FA03]	Prostaglandins [FA0301]
Fatty Acyls [FA]	Eicosanoids [FA03]	Isoprostanes [FA0311]
Fatty Acyls [FA]	Eicosanoids [FA03]	Other Eicosanoids [FA0300]
Fatty Acyls [FA]	Eicosanoids [FA03]	Leukotrienes [FA0302]
Fatty Acyls [FA]	Eicosanoids [FA03]	Hydroxy/hydroperoxyeicosatetraenoic acids [FA0306]
Fatty Acyls [FA]	Eicosanoids [FA03]	Hydroxy/hydroperoxyeicosapentaenoic acids [FA0307]
Fatty Acyls [FA]	Eicosanoids [FA03]	Epoxyeicosatrienoic acids [FA0308]
Fatty Acyls [FA]	Eicosanoids [FA03]	Hepoxilins [FA0309]
Fatty Acyls [FA]	Eicosanoids [FA03]	Thromboxanes [FA0303]
Fatty Acyls [FA]	Eicosanoids [FA03]	Lipoxins [FA0304]
Fatty Acyls [FA]	Eicosanoids [FA03]	Levuglandins [FA0310]
Fatty Acyls [FA]	Fatty Acids and Conjugates [FA01]	Straight chain fatty acids [FA0101]
Fatty Acyls [FA]	Fatty Acids and Conjugates [FA01]	Unsaturated fatty acids [FA0103]
Fatty Acyls [FA]	Fatty Acids and Conjugates [FA01]	Oxo fatty acids [FA0106]
Fatty Acyls [FA]	Fatty Acids and Conjugates [FA01]	Branched fatty acids [FA0102]
Fatty Acyls [FA]	Fatty Acids and Conjugates [FA01]	Halogenated fatty acids [FA0109]
Fatty Acyls [FA]	Fatty Acids and Conjugates [FA01]	Hydroxy fatty acids [FA0105]
Fatty Acyls [FA]	Fatty Acids and Conjugates [FA01]	Amino fatty acids [FA0110]
Fatty Acyls [FA]	Fatty Acids and Conjugates [FA01]	Dicarboxylic acids [FA0117]
Fatty Acyls [FA]	Fatty Acids and Conjugates [FA01]	Carbocyclic fatty acids [FA0114]
Fatty Acyls [FA]	Fatty Acids and Conjugates [FA01]	Thia fatty acids [FA0113]
Fatty Acyls [FA]	Fatty Acids and Conjugates [FA01]	Heterocyclic fatty acids [FA0115]
Fatty Acyls [FA]	Fatty Acids and Conjugates [FA01]	Epoxy fatty acids [FA0107]
Fatty Acyls [FA]	Fatty Acids and Conjugates [FA01]	Methoxy fatty acids [FA0108]
Fatty Acyls [FA]	Fatty Acids and Conjugates [FA01]	Hydroperoxy fatty acids [FA0104]
Fatty Acyls [FA]	Fatty Acids and Conjugates [FA01]	Nitro fatty acids [FA0112]
Fatty Acyls [FA]	Fatty Acids and Conjugates [FA01]	Cyano fatty acids [FA0111]
Fatty Acyls [FA]	Fatty Acids and Conjugates [FA01]	Mycolic acids [FA0116]
Fatty Acyls [FA]	Fatty acyl glycosides [FA13]	Fatty acyl glycosides of mono- and disaccharides [FA1301]
Fatty Acyls [FA]	Fatty acyl glycosides [FA13]	Rhamnolipids [FA1303]

Fatty Acyls [FA]	Fatty acyl glycosides [FA13]	Sophorolipids [FA1302]
Fatty Acyls [FA]	Fatty alcohols [FA05]	-
Fatty Acyls [FA]	Fatty aldehydes [FA06]	-
Fatty Acyls [FA]	Fatty amides [FA08]	Primary amides [FA0801]
Fatty Acyls [FA]	Fatty amides [FA08]	N-acyl amines [FA0802]
Fatty Acyls [FA]	Fatty amides [FA08]	Fatty acyl homoserine lactones [FA0803]
Fatty Acyls [FA]	Fatty amides [FA08]	N-acyl ethanolamines (endocannabinoids) [FA0804]
Fatty Acyls [FA]	Fatty esters [FA07]	Lactones [FA0704]
Fatty Acyls [FA]	Fatty esters [FA07]	Wax monoesters [FA0701]
Fatty Acyls [FA]	Fatty esters [FA07]	Fatty acyl ACPs [FA0706]
Fatty Acyls [FA]	Fatty esters [FA07]	Fatty acyl carnitines [FA0707]
Fatty Acyls [FA]	Fatty esters [FA07]	Fatty acyl adenylates [FA0708]
Fatty Acyls [FA]	Fatty esters [FA07]	Cyano esters [FA0703]
Fatty Acyls [FA]	Fatty esters [FA07]	Wax diesters [FA0702]
Fatty Acyls [FA]	Fatty esters [FA07]	Fatty acyl CoAs [FA0705]
Fatty Acyls [FA]	Fatty ethers [FA10]	-
Fatty Acyls [FA]	Fatty nitriles [FA09]	-
Fatty Acyls [FA]	Hydrocarbons [FA11]	-
Fatty Acyls [FA]	Octadecanoids [FA02]	Jasmonic acids [FA0202]
Fatty Acyls [FA]	Octadecanoids [FA02]	12-oxophytodienoic acid metabolites [FA0201]
Fatty Acyls [FA]	Octadecanoids [FA02]	Other Octadecanoids [FA0200]
Fatty Acyls [FA]	Other Fatty Acyls [FA00]	-
Fatty Acyls [FA]	Oxygenated hydrocarbons [FA12]	-

Table 10.5: List of classes within **Glycerolipids** belonging to **General Lipidome MS-LAMP**. Code shown in the bracket ([]) may be entered in the text box to search specifically within that class.

Category	Main Class	Sub Class
Glycerolipids [GL]	Diradylglycerols [GL02]	Diacylglycerols [GL0201]
Glycerolipids [GL]	Diradylglycerols [GL02]	1Z-alkenylacylglycerols [GL0204]
Glycerolipids [GL]	Diradylglycerols [GL02]	Dialkylglycerols [GL0203]
Glycerolipids [GL]	Diradylglycerols [GL02]	1-alkyl,2-acylglycerols [GL0202]
Glycerolipids [GL]	Diradylglycerols [GL02]	1-acyl,2-alkylglycerols [GL0207]
Glycerolipids [GL]	Diradylglycerols [GL02]	Di-glycerol tetraethers [GL0205]
Glycerolipids [GL]	Diradylglycerols [GL02]	Di-glycerol tetraether glycans [GL0206]
Glycerolipids [GL]	Glycosyldiradylglycerols [GL05]	Glycosyldiacylglycerols [GL0501]

Glycerolipids [GL]	Glycosyldiradylglycerols [GL05]	Glycosyldialkylglycerols [GL0503]
Glycerolipids [GL]	Glycosylmonoradylglycerols [GL04]	Glycosylmonoacylglycerols [GL0401]
Glycerolipids [GL]	Monoradylglycerols [GL01]	Monoalkylglycerols [GL0102]
Glycerolipids [GL]	Monoradylglycerols [GL01]	Monoacylglycerols [GL0101]
Glycerolipids [GL]	Other Glycerolipids [GL00]	-
Glycerolipids [GL]	Triradylglycerols [GL03]	Triacylglycerols [GL0301]
Glycerolipids [GL]	Triradylglycerols [GL03]	Estolides [GL0305]

Table 10.6: List of classes within **Glycerophospholipids** belonging to **General Lipidome MS-LAMP**. Code shown in the bracket ([]) may be entered in the text box to search specifically within that class.

Category	Main Class	Sub Class
Glycerophospholipids [GP]	CDP-Glycerols [GP13]	CDP-diacylglycerols [GP1301]
Glycerophospholipids [GP]	CDP-Glycerols [GP13]	CDP-Monoacylglycerols [GP1305]
Glycerophospholipids [GP]	Di-glycerol tetraether phospholipids (caldarchaeols) [GP18]	-
Glycerophospholipids [GP]	Glycerol-nonitol tetraether phospholipids [GP19]	-
Glycerophospholipids [GP]	Glycerophosphates [GP10]	1-(1Z-alkenyl),2-acylglycerophosphates [GP1003]
Glycerophospholipids [GP]	Glycerophosphates [GP10]	1-alkyl,2-acylglycerophosphates [GP1002]
Glycerophospholipids [GP]	Glycerophosphates [GP10]	1Z-alkenylglycerophosphates [GP1007]
Glycerophospholipids [GP]	Glycerophosphates [GP10]	Diacylglycerophosphates [GP1001]
Glycerophospholipids [GP]	Glycerophosphates [GP10]	Dialkylglycerophosphates [GP1004]
Glycerophospholipids [GP]	Glycerophosphates [GP10]	Monoacylglycerophosphates [GP1005]
Glycerophospholipids [GP]	Glycerophosphates [GP10]	Monoalkylglycerophosphates [GP1006]
Glycerophospholipids [GP]	Glycerophosphocholines [GP01]	1-(1Z-alkenyl),2-acylglycerophosphocholines [GP0103]
Glycerophospholipids [GP]	Glycerophosphocholines [GP01]	1-acyl,2-(1Z-alkenyl)-glycerophosphocholines [GP0109]
Glycerophospholipids [GP]	Glycerophosphocholines [GP01]	1-acyl,2-alkylglycerophosphocholines [GP0108]
Glycerophospholipids [GP]	Glycerophosphocholines [GP01]	1-alkyl,2-acylglycerophosphocholines [GP0102]
Glycerophospholipids [GP]	Glycerophosphocholines [GP01]	1Z-alkenylglycerophosphocholines [GP0107]
Glycerophospholipids [GP]	Glycerophosphocholines [GP01]	Diacylglycerophosphocholines [GP0101]
Glycerophospholipids [GP]	Glycerophosphocholines [GP01]	Dialkylglycerophosphocholines [GP0104]
Glycerophospholipids [GP]	Glycerophosphocholines [GP01]	Monoacylglycerophosphocholines [GP0105]
Glycerophospholipids [GP]	Glycerophosphocholines [GP01]	Monoalkylglycerophosphocholines [GP0106]
Glycerophospholipids [GP]	Glycerophosphoethanolamines [GP02]	1-(1Z-alkenyl),2-acylglycerophosphoethanolamines [GP0203]
Glycerophospholipids [GP]	Glycerophosphoethanolamines [GP02]	1-acyl,2-alkylglycerophosphoethanolamines [GP0208]

Glycerophospholipids [GP]	Glycerophosphoethanolamines [GP02]	1-alkyl,2-acylglycerophosphoethanolamines [GP0202]
Glycerophospholipids [GP]	Glycerophosphoethanolamines [GP02]	1Z-alkenylglycerophosphoethanolamines [GP0207]
Glycerophospholipids [GP]	Glycerophosphoethanolamines [GP02]	Diacylglycerophosphoethanolamines [GP0201]
Glycerophospholipids [GP]	Glycerophosphoethanolamines [GP02]	Dialkylglycerophosphoethanolamines [GP0204]
Glycerophospholipids [GP]	Glycerophosphoethanolamines [GP02]	Monoacylglycerophosphoethanolamines [GP0205]
Glycerophospholipids [GP]	Glycerophosphoethanolamines [GP02]	Monoalkylglycerophosphoethanolamines [GP0206]
Glycerophospholipids [GP]	Glycerophosphoglycerols [GP04]	1-(1Z-alkenyl),2-acylglycerophosphoglycerols [GP0403]
Glycerophospholipids [GP]	Glycerophosphoglycerols [GP04]	1-acyl,2-alkylglycerophosphoglycerols [GP0411]
Glycerophospholipids [GP]	Glycerophosphoglycerols [GP04]	1-alkyl,2-acylglycerophosphoglycerols [GP0402]
Glycerophospholipids [GP]	Glycerophosphoglycerols [GP04]	1Z-alkenylglycerophosphoglycerols [GP0407]
Glycerophospholipids [GP]	Glycerophosphoglycerols [GP04]	Diacylglycerophosphoglycerols [GP0401]
Glycerophospholipids [GP]	Glycerophosphoglycerols [GP04]	Diacylglycerophosphomonoradylglycerols [GP0409]
Glycerophospholipids [GP]	Glycerophosphoglycerols [GP04]	Dialkylglycerophosphoglycerols [GP0404]
Glycerophospholipids [GP]	Glycerophosphoglycerols [GP04]	Monoacylglycerophosphoglycerols [GP0405]
Glycerophospholipids [GP]	Glycerophosphoglycerols [GP04]	Monoacylglycerophosphomonoradylglycerols [GP0410]
Glycerophospholipids [GP]	Glycerophosphoglycerols [GP04]	Monoalkylglycerophosphoglycerols [GP0406]
Glycerophospholipids [GP]	Glycerophosphoglycerophosphates [GP05]	Diacylglycerophosphoglycerophosphates [GP0501]
Glycerophospholipids [GP]	Glycerophosphoglycerophosphates [GP05]	Dialkylglycerophosphoglycerophosphates [GP0504]
Glycerophospholipids [GP]	Glycerophosphoglycerophosphoglycerols [GP12]	Diacylglycerophosphoglycerophosphodiradylglycerols [GP1201]
Glycerophospholipids [GP]	Glycerophosphoglycerophosphoglycerols [GP12]	Diacylglycerophosphoglycerophosphomonoradylglycerols [GP1202]
Glycerophospholipids [GP]	Glycerophosphoglycerophosphoglycerols [GP12]	Dialkylglycerophosphoglycerophosphodiradylglycerols [GP1212]
Glycerophospholipids [GP]	Glycerophosphoglycerophosphoglycerols [GP12]	Monoacylglycerophosphoglycerophosphomonoradylglycerols [GP1207]
Glycerophospholipids [GP]	Glycerophosphoinositol bisphosphates [GP08]	Diacylglycerophosphoinositol bisphosphates [GP0801]
Glycerophospholipids [GP]	Glycerophosphoinositol monophosphates [GP07]	Diacylglycerophosphoinositol monophosphates [GP0701]
Glycerophospholipids [GP]	Glycerophosphoinositol trisphosphates [GP09]	Diacylglycerophosphoinositol trisphosphates [GP0901]
Glycerophospholipids [GP]	Glycerophosphoinositolglycans [GP15]	Diacylglycerophosphoinositolglycans [GP1501]
Glycerophospholipids [GP]	Glycerophosphoinositols [GP06]	1-(1Z-alkenyl),2-acylglycerophosphoinositols [GP0603]
Glycerophospholipids [GP]	Glycerophosphoinositols [GP06]	1-alkyl,2-acylglycerophosphoinositols [GP0602]
Glycerophospholipids [GP]	Glycerophosphoinositols [GP06]	1Z-alkenylglycerophosphoinositols [GP0607]
Glycerophospholipids [GP]	Glycerophosphoinositols [GP06]	Diacylglycerophosphoinositols [GP0601]
Glycerophospholipids [GP]	Glycerophosphoinositols [GP06]	Dialkylglycerophosphoinositols [GP0604]
Glycerophospholipids [GP]	Glycerophosphoinositols [GP06]	Monoacylglycerophosphoinositols [GP0605]
Glycerophospholipids [GP]	Glycerophosphoinositols [GP06]	Monoalkylglycerophosphoinositols [GP0606]
Glycerophospholipids [GP]	Glycerophosphonocholines [GP16]	Diacylglycerophosphonocholines [GP1601]

Glycerophospholipids [GP]	Glycerophosphonoethanolamines [GP17]	Diacylglycerophosphonoethanolamines [GP1701]
Glycerophospholipids [GP]	Glycerophosphoserines [GP03]	1-(1Z-alkenyl),2-acylglycerophosphoserines [GP0303]
Glycerophospholipids [GP]	Glycerophosphoserines [GP03]	1-alkyl,2-acylglycerophosphoserines [GP0302]
Glycerophospholipids [GP]	Glycerophosphoserines [GP03]	1Z-alkenylglycerophosphoserines [GP0307]
Glycerophospholipids [GP]	Glycerophosphoserines [GP03]	Diacylglycerophosphoserines [GP0301]
Glycerophospholipids [GP]	Glycerophosphoserines [GP03]	Monoacylglycerophosphoserines [GP0305]
Glycerophospholipids [GP]	Glycerophosphoserines [GP03]	Monoalkylglycerophosphoserines [GP0306]
Glycerophospholipids [GP]	Glyceropyrophosphates [GP11]	Diacylglyceropyrophosphates [GP1101]
Glycerophospholipids [GP]	Glycosylglycerophospholipids [GP14]	Diacylglycosylglycerophospholipids [GP1401]
Glycerophospholipids [GP]	Glycosylglycerophospholipids [GP14]	Dialkylglycosylglycerophospholipids [GP1407]
Glycerophospholipids [GP]	Other Glycerophospholipids [GP00]	-
Glycerophospholipids [GP]	Oxidized glycerophospholipids [GP20]	Oxidized Cardiolipins [GP2003]
Glycerophospholipids [GP]	Oxidized glycerophospholipids [GP20]	Oxidized glycerophosphocholines [GP2001]
Glycerophospholipids [GP]	Oxidized glycerophospholipids [GP20]	Oxidized glycerophosphoethanolamines [GP2002]

Table 10.7: List of classes within **Polyketides** belonging to **General Lipidome MS-LAMP**. Code shown in the bracket ([]) may be entered in the text box to search specifically within that class.

Category	Main Class	Sub Class
Polyketides [PK]	Aflatoxins and related substances [PK10]	-
Polyketides [PK]	Angucyclines [PK08]	-
Polyketides [PK]	Annonaceae acetogenins [PK03]	-
Polyketides [PK]	Ansamycins and related polyketides [PK05]	-
Polyketides [PK]	Aromatic polyketides [PK13]	Monocyclic aromatic polyketides [PK1301]
Polyketides [PK]	Aromatic polyketides [PK13]	Diphenyl ethers, biphenyls, dibenzyls and stilbenes [PK1309]
Polyketides [PK]	Aromatic polyketides [PK13]	Benzopyranoids [PK1311]
Polyketides [PK]	Aromatic polyketides [PK13]	Anthracenes and phenanthrenes [PK1304]
Polyketides [PK]	Aromatic polyketides [PK13]	Benzoisochromanquinones [PK1303]
Polyketides [PK]	Aromatic polyketides [PK13]	Other aromatic polyketides [PK1312]
Polyketides [PK]	Aromatic polyketides [PK13]	Depsides and depsidones [PK1308]
Polyketides [PK]	Aromatic polyketides [PK13]	Dibenzofurans, griseofulvins, dibenzopyrans and xanthones [PK1306]
Polyketides [PK]	Aromatic polyketides [PK13]	Benzofuranoids [PK1310]
Polyketides [PK]	Aromatic polyketides [PK13]	Diphenylmethanes, acylphloroglucinols and benzophenones [PK1307]

Polyketides [PK]	Aromatic polyketides [PK13]	Naphthalenes and naphthoquinones [PK1302]
Polyketides [PK]	Aromatic polyketides [PK13]	Anthracyclinones [PK1305]
Polyketides [PK]	Cytochalasins [PK11]	-
Polyketides [PK]	Flavonoids [PK12]	Chalcones and dihydrochalcones [PK1212]
Polyketides [PK]	Flavonoids [PK12]	Flavones and Flavanols [PK1211]
Polyketides [PK]	Flavonoids [PK12]	Flavans, Flavanols and Leucoanthocyanidins [PK1202]
Polyketides [PK]	Flavonoids [PK12]	Flavanones [PK1214]
Polyketides [PK]	Flavonoids [PK12]	Other Flavonoids [PK1216]
Polyketides [PK]	Flavonoids [PK12]	Isoflavans [PK1208]
Polyketides [PK]	Flavonoids [PK12]	Isoflavonoids [PK1205]
Polyketides [PK]	Flavonoids [PK12]	Pterocarpans [PK1207]
Polyketides [PK]	Flavonoids [PK12]	Neoflavanoids [PK1210]
Polyketides [PK]	Flavonoids [PK12]	Aurone flavonoids [PK1213]
Polyketides [PK]	Flavonoids [PK12]	Coumestan flavonoids [PK1209]
Polyketides [PK]	Flavonoids [PK12]	Anthocyanidins [PK1201]
Polyketides [PK]	Flavonoids [PK12]	Rotenoid flavonoids [PK1206]
Polyketides [PK]	Flavonoids [PK12]	Dihydroflavonols [PK1215]
Polyketides [PK]	Flavonoids [PK12]	Proanthocyanidins [PK1203]
Polyketides [PK]	Flavonoids [PK12]	Biflavonoids and polyflavonoids [PK1204]
Polyketides [PK]	Halogenated acetogenins [PK02]	-
Polyketides [PK]	Linear polyketides [PK01]	-
Polyketides [PK]	Linear tetracyclines [PK07]	-
Polyketides [PK]	Macrolides and lactone polyketides [PK04]	-
Polyketides [PK]	Non-ribosomal peptide/polyketide hybrids [PK14]	-
Polyketides [PK]	Other Polyketides [PK00]	-
Polyketides [PK]	Polyenes [PK06]	-
Polyketides [PK]	Polyether polyketides [PK09]	-

Table 10.8: List of classes within **Prenol Lipids** belonging to **General Lipidome MS-LAMP**. Code shown in the bracket ([]) may be entered in the text box to search specifically within that class.

Category	Main Class	Sub Class
Prenol Lipids [PR]	Hopanoids [PR04]	-

Prenol Lipids [PR]	Isoprenoids [PR01]	C10 isoprenoids (monoterpenes) [PR0102]
Prenol Lipids [PR]	Isoprenoids [PR01]	C15 isoprenoids (sesquiterpenes) [PR0103]
Prenol Lipids [PR]	Isoprenoids [PR01]	C40 isoprenoids (tetraterpenes) [PR0107]
Prenol Lipids [PR]	Isoprenoids [PR01]	C5 isoprenoids (hemiterpenes) [PR0101]
Prenol Lipids [PR]	Isoprenoids [PR01]	C20 isoprenoids (diterpenes) [PR0104]
Prenol Lipids [PR]	Isoprenoids [PR01]	Retinoids [PR0109]
Prenol Lipids [PR]	Isoprenoids [PR01]	C25 isoprenoids (sesterterpenes) [PR0105]
Prenol Lipids [PR]	Isoprenoids [PR01]	C30 isoprenoids (triterpenes) [PR0106]
Prenol Lipids [PR]	Isoprenoids [PR01]	Polyterpenes [PR0108]
Prenol Lipids [PR]	Polyprenols [PR03]	Dolichols [PR0307]
Prenol Lipids [PR]	Polyprenols [PR03]	Dolichol monophosphates [PR0308]
Prenol Lipids [PR]	Polyprenols [PR03]	Dolichol diphosphates [PR0309]
Prenol Lipids [PR]	Polyprenols [PR03]	Bactoprenol diphosphates [PR0303]
Prenol Lipids [PR]	Polyprenols [PR03]	Phytoprenols [PR0304]
Prenol Lipids [PR]	Polyprenols [PR03]	Bactoprenols [PR0301]
Prenol Lipids [PR]	Polyprenols [PR03]	Bactoprenol monophosphates [PR0302]
Prenol Lipids [PR]	Quinones and hydroquinones [PR02]	Vitamin E [PR0202]
Prenol Lipids [PR]	Quinones and hydroquinones [PR02]	Ubiquinones [PR0201]
Prenol Lipids [PR]	Quinones and hydroquinones [PR02]	Vitamin K [PR0203]

Table 10.9: List of classes within **Saccharolipids** belonging to **General Lipidome MS-LAMP**. Code shown in the bracket ([]) may be entered in the text box to search specifically within that class.

Category	Main Class	Sub Class
Saccharolipids [SL]	Acylaminosugar glycans [SL02]	-
Saccharolipids [SL]	Acylaminosugars [SL01]	Monoacylaminosugars [SL0101]
Saccharolipids [SL]	Acylaminosugars [SL01]	Diacylaminosugars [SL0102]
Saccharolipids [SL]	Acylaminosugars [SL01]	Tetraacylaminosugars [SL0104]
Saccharolipids [SL]	Acylaminosugars [SL01]	Pentaacylaminosugars [SL0105]
Saccharolipids [SL]	Acylaminosugars [SL01]	Hexaacylaminosugars [SL0106]
Saccharolipids [SL]	Acyltrehaloses [SL03]	-
Saccharolipids [SL]	Other acyl sugars [SL05]	-

Table 10.10: List of classes within **Sphingolipids** belonging to **General Lipidome MS-LAMP**. Code shown in the bracket ([]) may be entered in the text box to search specifically within that class.

Category	Main Class	Sub Class
Sphingolipids [SP]	Acidic glycosphingolipids [SP06]	Glucuronosphingolipids [SP0603]
Sphingolipids [SP]	Acidic glycosphingolipids [SP06]	Sulfoglycosphingolipids (sulfatides) [SP0602]
Sphingolipids [SP]	Acidic glycosphingolipids [SP06]	Gangliosides [SP0601]
Sphingolipids [SP]	Acidic glycosphingolipids [SP06]	Phosphoglycosphingolipids [SP0604]
Sphingolipids [SP]	Amphoteric glycosphingolipids [SP08]	-
Sphingolipids [SP]	Basic glycosphingolipids [SP07]	-
Sphingolipids [SP]	Ceramides [SP02]	N-acylsphingosines (ceramides) [SP0201]
Sphingolipids [SP]	Ceramides [SP02]	Ceramide 1-phosphates [SP0205]
Sphingolipids [SP]	Ceramides [SP02]	N-acylsphinganines (dihydroceramides) [SP0202]
Sphingolipids [SP]	Ceramides [SP02]	N-acyl-4-hydroxysphinganines (phytoceramides) [SP0203]
Sphingolipids [SP]	Ceramides [SP02]	Acylceramides [SP0204]
Sphingolipids [SP]	Neutral glycosphingolipids [SP05]	Simple Glc series [SP0501]
Sphingolipids [SP]	Neutral glycosphingolipids [SP05]	Gal- (Gala series) [SP0509]
Sphingolipids [SP]	Neutral glycosphingolipids [SP05]	GalNAcbeta1-3Galalpha1-4Galbeta1-4Glc- (Globo series) [SP0502]
Sphingolipids [SP]	Neutral glycosphingolipids [SP05]	Galbeta1-4GlcNAcbeta1-3Galbeta1-4Glc- (Neolacto series) [SP0505]
Sphingolipids [SP]	Neutral glycosphingolipids [SP05]	GlcNAcbeta1-2Manalpha1-3Manbeta1-4Glc- (Mollu series) [SP0507]
Sphingolipids [SP]	Neutral glycosphingolipids [SP05]	Other Neutral glycosphingolipids [SP0500]
Sphingolipids [SP]	Neutral glycosphingolipids [SP05]	GalNAcbeta1-4Galbeta1-4Glc- (Ganglio series) [SP0503]
Sphingolipids [SP]	Neutral glycosphingolipids [SP05]	Galbeta1-3GlcNAcbeta1-3Galbeta1-4Glc- (Lacto series) [SP0504]
Sphingolipids [SP]	Neutral glycosphingolipids [SP05]	GalNAcbeta1-4GlcNAcbeta1-3Manbeta1-4Glc- (Arthro series) [SP0508]
Sphingolipids [SP]	Neutral glycosphingolipids [SP05]	GalNAcbeta1-3Galalpha1-3Galbeta1-4Glc- (Isoglobo series) [SP0506]
Sphingolipids [SP]	Other Sphingolipids [SP00]	-
Sphingolipids [SP]	Phosphonosphingolipids [SP04]	-
Sphingolipids [SP]	Phosphosphingolipids [SP03]	Ceramide phosphocholines (sphingomyelins) [SP0301]
Sphingolipids [SP]	Phosphosphingolipids [SP03]	Ceramide phosphoethanolamines [SP0302]
Sphingolipids [SP]	Phosphosphingolipids [SP03]	Ceramide phosphoinositols [SP0303]
Sphingolipids [SP]	Sphingoid bases [SP01]	Sphingoid base analogs [SP0108]
Sphingolipids [SP]	Sphingoid bases [SP01]	Sphingoid base homologs and variants [SP0104]
Sphingolipids [SP]	Sphingoid bases [SP01]	Sphing-4-enines (Sphingosines) [SP0101]
Sphingolipids [SP]	Sphingoid bases [SP01]	Sphinganines [SP0102]

Sphingolipids [SP]	Sphingoid bases [SP01]	4-Hydroxysphinganines (Phytosphingosines) [SP0103]
Sphingolipids [SP]	Sphingoid bases [SP01]	N-methylated sphingoid bases [SP0107]
Sphingolipids [SP]	Sphingoid bases [SP01]	Sphingoid base 1-phosphates [SP0105]
Sphingolipids [SP]	Sphingoid bases [SP01]	Lysosphingomyelins and lysoglycosphingolipids [SP0106]

Table 10.11: List of classes within **Sterol Lipids** belonging to **General Lipidome MS-LAMP**. Code shown in the bracket ([]) may be entered in the text box to search specifically within that class.

CATEGORY	MAIN_CLASS	SUB_CLASS
Sterol Lipids [ST]	Bile acids and derivatives [ST04]	C22 bile acids, alcohols, and derivatives [ST0405]
Sterol Lipids [ST]	Bile acids and derivatives [ST04]	C23 bile acids, alcohols, and derivatives [ST0406]
Sterol Lipids [ST]	Bile acids and derivatives [ST04]	C24 bile acids, alcohols, and derivatives [ST0401]
Sterol Lipids [ST]	Bile acids and derivatives [ST04]	C25 bile acids, alcohols, and derivatives [ST0407]
Sterol Lipids [ST]	Bile acids and derivatives [ST04]	C26 bile acids, alcohols, and derivatives [ST0402]
Sterol Lipids [ST]	Bile acids and derivatives [ST04]	C27 bile acids, alcohols, and derivatives [ST0403]
Sterol Lipids [ST]	Bile acids and derivatives [ST04]	C27 bile acids, alcohols, and derivatives [ST0403]
Sterol Lipids [ST]	Bile acids and derivatives [ST04]	C28 bile acids, alcohols, and derivatives [ST0404]
Sterol Lipids [ST]	Bile acids and derivatives [ST04]	C29 bile acids, alcohols, and derivatives [ST0408]
Sterol Lipids [ST]	Secosteroids [ST03]	Vitamin D2 and derivatives [ST0301]
Sterol Lipids [ST]	Secosteroids [ST03]	Vitamin D3 and derivatives [ST0302]
Sterol Lipids [ST]	Secosteroids [ST03]	Vitamin D4 and derivatives [ST0303]
Sterol Lipids [ST]	Secosteroids [ST03]	Vitamin D5 and derivatives [ST0304]
Sterol Lipids [ST]	Secosteroids [ST03]	Vitamin D6 and derivatives [ST0305]
Sterol Lipids [ST]	Secosteroids [ST03]	Vitamin D7 and derivatives [ST0306]
Sterol Lipids [ST]	Steroid conjugates [ST05]	Glucuronides [ST0501]
Sterol Lipids [ST]	Steroid conjugates [ST05]	Glycine conjugates [ST0503]
Sterol Lipids [ST]	Steroid conjugates [ST05]	Other Steroid conjugates [ST0505]
Sterol Lipids [ST]	Steroid conjugates [ST05]	Sulfates [ST0502]
Sterol Lipids [ST]	Steroid conjugates [ST05]	Sulfates [ST0502]
Sterol Lipids [ST]	Steroid conjugates [ST05]	Taurine conjugates [ST0504]
Sterol Lipids [ST]	Steroids [ST02]	C18 steroids (estrogens) and derivatives [ST0201]
Sterol Lipids [ST]	Steroids [ST02]	C19 steroids (androgens) and derivatives [ST0202]
Sterol Lipids [ST]	Steroids [ST02]	C21 steroids (gluco/mineralocorticoids, progestogens) and derivatives [ST0203]
Sterol Lipids [ST]	Sterols [ST01]	Brassinolides and derivatives [ST0114]

Sterol Lipids [ST]	Sterols [ST01]	Bufanolides and derivatives [ST0113]
Sterol Lipids [ST]	Sterols [ST01]	C24-propyl sterols and derivatives [ST0105]
Sterol Lipids [ST]	Sterols [ST01]	Calysterols and cyclopropyl sidechain derivatives [ST0111]
Sterol Lipids [ST]	Sterols [ST01]	Cardanolides and derivatives [ST0112]
Sterol Lipids [ST]	Sterols [ST01]	Cholesterol and derivatives [ST0101]
Sterol Lipids [ST]	Sterols [ST01]	Cholesteryl esters [ST0102]
Sterol Lipids [ST]	Sterols [ST01]	Cholesteryl esters [ST0102]
Sterol Lipids [ST]	Sterols [ST01]	Cycloartanols and derivatives [ST0110]
Sterol Lipids [ST]	Sterols [ST01]	Ergosterols and C24-methyl derivatives [ST0103]
Sterol Lipids [ST]	Sterols [ST01]	Ergosterols and C24-methyl derivatives [ST0103]
Sterol Lipids [ST]	Sterols [ST01]	Furospirostanols and derivatives [ST0109]
Sterol Lipids [ST]	Sterols [ST01]	Furostanols and derivatives [ST0107]
Sterol Lipids [ST]	Sterols [ST01]	Gorgosterols and derivatives [ST0106]
Sterol Lipids [ST]	Sterols [ST01]	Solanidines and alkaloid derivatives [ST0115]
Sterol Lipids [ST]	Sterols [ST01]	Spirostanols and derivatives [ST0108]
Sterol Lipids [ST]	Sterols [ST01]	Stigmasterols and C24-ethyl derivatives [ST0104]
Sterol Lipids [ST]	Sterols [ST01]	Stigmasterols and C24-ethyl derivatives [ST0104]
Sterol Lipids [ST]	Sterols [ST01]	Withanolides and derivatives [ST0116]

Table 10.12: List of classes within **Fatty Acyls** belonging to ***M. tb* Lipidome MS-LAMP**. Code shown in the bracket ([]) may be entered in the text box to search specifically within that class.

CLASS	MAIN CLASS	SUBCLASS
Fatty Acyls [FA]	Fatty Acids and Conjugates [FA01]	Branched Fatty Acids [FA0102]
Fatty Acyls [FA]	Fatty Acids and Conjugates [FA01]	Alpha Mycolic Acids (Alpha-MA) [FA0116z]
Fatty Acyls [FA]	Fatty Acids and Conjugates [FA01]	Keto Mycolic Acids (Keto-MA) [FA0116z]
Fatty Acyls [FA]	Fatty Acids and Conjugates [FA01]	Methoxy Mycolic Acids (Methoxy-MA) [FA0116z]
Fatty Acyls [FA]	Fatty Acids and Conjugates [FA01]	Glucose Monomycolates (GMM) [FA0116z]
Fatty Acyls [FA]	Fatty Acids and Conjugates [FA01]	Trehalose Monomycolates (TMM) [FA0116z]
Fatty Acyls [FA]	Fatty Acids and Conjugates [FA01]	Trehalose Dimycolates (TDM) [FA0116z]
Fatty Acyls [FA]	Fatty Esters [FA07]	Phthiodiolone Dimycocerosates (DIMB) [FA0707z]
Fatty Acyls [FA]	Fatty Esters [FA07]	Phthiocerol Dimycocerosates (DIMA) [FA0707z]
Fatty Acyls [FA]	Fatty Esters [FA07]	Glycosylated Phthiodiolone Dimycocerosates [FA07yz]
Fatty Acyls [FA]	Fatty Esters [FA07]	Glycosylated Phthiocerol Dimycocerosates (PGL-tb) [FA07yz]

Table 10.13: List of classes within **Glycerolipids** belonging to ***M. tb* Lipidome MS-LAMP**. Code shown in the bracket ([]) may be entered in the text box to search specifically within that class.

Category	Main Class	SUBCLASS
Glycerolipids [GL]	Monoradylglycerols [GL01]	Monoacylglycerols (MG) [GL0101]
Glycerolipids [GL]	Diradylglycerols [GL02]	Diacylglycerols (DG) [GL0201]
Glycerolipids [GL]	Triradylglycerols [GL03]	Triacylglycerols (TG) [GL0301]

Table 10.14: List of classes within **Glycerophospholipids** belonging to ***M. tb* Lipidome MS-LAMP**. Code shown in the bracket ([]) may be entered in the text box to search specifically within that class.

Category	Main Class	SUBCLASS
Glycerophospholipids [GP]	Glycerophosphoethanolamines [GP02]	Monoacylglycerolphosphoethanolamines (Lyso-PE) [GP0205]
Glycerophospholipids [GP]	Glycerophosphoethanolamines [GP02]	Diacylglycerolphosphoethanolamines (PE) [GP0201]
Glycerophospholipids [GP]	Glycerophosphoglycerols [GP04]	Monoacylglycerophosphoglycerols (Lyso-GP) [GP0405]
Glycerophospholipids [GP]	Glycerophosphoglycerols [GP04]	Diacylglycerophosphoglycerols (PG) [GP0401]
Glycerophospholipids [GP]	Glycerophosphoinositols [GP06]	Monoacylglycerophosphoinositols (Lyso-PI) [GP0605]
Glycerophospholipids [GP]	Glycerophosphoinositols [GP06]	Diacylglycerophosphoinositols (PI) [GP0601]
Glycerophospholipids [GP]	Glycerophosphoglycerophosphoglycerols [GP12]	Diacylglycerophosphoglycerophosphodiradylglycerols (CL) [GP1201]
Glycerophospholipids [GP]	Glycerophosphoinositolglycans [GP15]	Monoacylglycerophosphoinositolmonomannosides (Lyso-PIM1) [GP15y]
Glycerophospholipids [GP]	Glycerophosphoinositolglycans [GP15]	Monoacylglycerophosphoinositoldimannosides (Lyso-PIM2) [GP15y]
Glycerophospholipids [GP]	Glycerophosphoinositolglycans [GP15]	Diacylglycerophosphoinositolmonomannosides (PIM1) [GP15y]
Glycerophospholipids [GP]	Glycerophosphoinositolglycans [GP15]	Monoacylglycerophosphoinositoltrimannosides (Lyso-PIM3) [GP15y]
Glycerophospholipids [GP]	Glycerophosphoinositolglycans [GP15]	Diacylglycerophosphoinositoldimannosides (PIM2) [GP15y]
Glycerophospholipids [GP]	Glycerophosphoinositolglycans [GP15]	Monoacylated diacylglycerophosphoinositolmonomannosides (Ac1PIM1) [GP15y]
Glycerophospholipids [GP]	Glycerophosphoinositolglycans [GP15]	Monoacylglycerophosphoinositoltetramannosides (Lyso-PIM4) [GP15y]
Glycerophospholipids [GP]	Glycerophosphoinositolglycans [GP15]	Diacylglycerophosphoinositoltrimannosides (PIM3) [GP15y]
Glycerophospholipids [GP]	Glycerophosphoinositolglycans [GP15]	Monoacylated diacylglycerophosphoinositoldimannosides (Ac1PIM2) [GP15y]
Glycerophospholipids [GP]	Glycerophosphoinositolglycans [GP15]	Monoacylglycerophosphoinositolpentamannosides (Lyso-PIM5) [GP15y]
Glycerophospholipids [GP]	Glycerophosphoinositolglycans [GP15]	Diacylglycerophosphoinositoltetramannosides (PIM4) [GP15y]
Glycerophospholipids [GP]	Glycerophosphoinositolglycans [GP15]	Monoacylated diacylglycerophosphoinositoltrimannosides (Ac1PIM3) [GP15y]
Glycerophospholipids [GP]	Glycerophosphoinositolglycans [GP15]	Monoacylglycerophosphoinositolhexamannosides (Lyso-PIM6) [GP15y]
Glycerophospholipids [GP]	Glycerophosphoinositolglycans [GP15]	Diacylated diacylglycerophosphoinositoldimannosides (Ac2PIM2) [GP15y]

Glycerophospholipids [GP]	Glycerophosphoinositolglycans [GP15]	Diacylglycerophosphoinositolpentamannosides (PIM5) [GP15y]
Glycerophospholipids [GP]	Glycerophosphoinositolglycans [GP15]	Monoacylated diacylglycerophosphoinositoltetramannosides (Ac1PIM4) [GP15y]
Glycerophospholipids [GP]	Glycerophosphoinositolglycans [GP15]	Diacylated diacylglycerophosphoinositoltrimannosides (Ac2PIM3) [GP15y]
Glycerophospholipids [GP]	Glycerophosphoinositolglycans [GP15]	Diacylglycerophosphoinositolhexamannosides (PIM6) [GP15y]
Glycerophospholipids [GP]	Glycerophosphoinositolglycans [GP15]	Monoacylated diacylglycerophosphoinositolpentamannosides (Ac1PIM5) [GP15y]
Glycerophospholipids [GP]	Glycerophosphoinositolglycans [GP15]	Diacylated diacylglycerophosphoinositoltetramannosides (Ac2PIM4) [GP15y]
Glycerophospholipids [GP]	Glycerophosphoinositolglycans [GP15]	Monoacylated diacylglycerophosphoinositolhexamannosides (Ac1PIM6) [GP15y]
Glycerophospholipids [GP]	Glycerophosphoinositolglycans [GP15]	Diacylated diacylglycerophosphoinositolpentamannosides (Ac2PIM5) [GP15y]
Glycerophospholipids [GP]	Glycerophosphoinositolglycans [GP15]	Diacylated diacylglycerophosphoinositolhexamannosides (Ac2PIM6) [GP15y]

Table 10.15: List of classes within **Polyketides** belonging to ***M. tb* Lipidome MS-LAMP**. Code shown in the bracket ([]) may be entered in the text box to search specifically within that class.

Category	Main Class	SUBCLASS
Polyketides [PK]	Linear polyketides [PK01]	Mannosyl-b1-phosphomycoketides (MPM) [PK01y]
Polyketides [PK]	Linear polyketides [PK01]	Non-ribosomal peptides/polyketide hybrids [PK14]

Table 10.16: List of classes within **Prenol Lipids** belonging to ***M. tb* Lipidome MS-LAMP**. Code shown in the bracket ([]) may be entered in the text box to search specifically within that class.

Category	Main Class	SUBCLASS
Prenol Lipids [PR]	Quinones and Hydroquinones [PR02]	Ubiquinones [PR0201]
Prenol Lipids [PR]	Polyprenols [PR03]	Bactoprenols [PR0301]
Prenol Lipids [PR]	Polyprenols [PR03]	Bactoprenol monophosphates [PR0302]
Prenol Lipids [PR]	Polyprenols [PR03]	Bactoprenol diphosphates (DP-PP) [PR0303]

Table 10.17: List of classes within **Saccharolipids** belonging to ***M. tb* Lipidome MS-LAMP**. Code shown in the bracket ([]) may be entered in the text box to search specifically within that class.

Category	Main Class	SUBCLASS
Saccharolipids [SL]	Acyltrehaloses [SL03]	2,3-di-O-acyltrehaloses (DAT1) [SL03yz]
Saccharolipids [SL]	Acyltrehaloses [SL03]	2,3-di-O-acyltrehaloses (DAT2) [SL03yz]

Saccharolipids [SL]	Acyltrehaloses [SL03]	Polyacyltrehaloses (PAT) [SL03y]
Saccharolipids [SL]	Sulfolipids [SL03y]	Diacylated Sulfolipid (Ac2SGL) [SL03yz]
Saccharolipids [SL]	Sulfolipids [SL03y]	Sulfolipid III (SL-III) [SL03yz]
Saccharolipids [SL]	Sulfolipids [SL03y]	Sulfolipid I (SL-I) [SL03yz]
Saccharolipids [SL]	Sulfolipids [SL03y]	Sulfolipid II or II' (SL-II or SL-II') [SL03yz]

11. Monoisotopic mass & Atomic weight values considered by MS-LAMP

S. No.	Element	Monoisotopic Mass (Atomic Mass)	Atomic Weight (Relative Atomic Mass)
1	Hydrogen	1.007825	1.00794
2	Carbon	12.000000	12.01078
3	Nitrogen	14.003074	14.00672
4	Oxygen	15.994915	15.99943
5	Phosphorus	30.973761	30.973761
6	Sulphur	31.972070	32.06550
7	Lithium (7)	7.016004	6.94120
8	Sodium	22.989769	22.989770
9	Potassium (39)	38.963707	39.09831
10	Fluorine (19)	18.998403	18.998403
11	Chlorine (35)	34.968852	35.45320
12	Bromine (79)	78.918338	79.90410
13	Iodine	126.904468	126.90447
14	Silicon	27.976926	28.08553
15	Deuterium	2.014102	2.014102

Note : Monoisotopic Mass is the atomic mass of the most abundant isotope of an element.

Atomic weight is the weighted average of atomic masses of all the isotopes of an element.

The values given in the table are from International Union of Pure and Applied Chemistry (IUPAC);

Reference: De Laeter J.R., Bohlke J.K., De Bievre P., Hidaka H., Peiser H.S., Rosman K.J.R., Taylor P.D.P. Atomic Weights of the Elements: Review 2000 (IUPAC Technical Report). Pur. Appl. Chem. 2003, 75, 683 - 800.