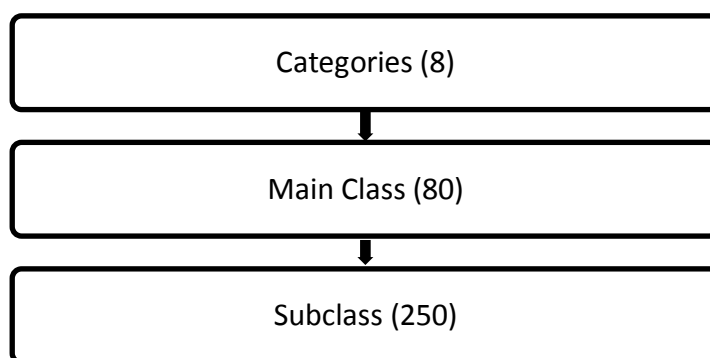


10. Search within Main Class and/or Subclass

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 Diacylglycerophosphoglycerophosphodiradylglycerols (CL) can be obtained by entering GP1201, which corresponds to **Category:** GP, **Main Class code:** 12 and **Subclass code:** 01 (Refer Tables [10.3](#), [10.6](#) 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 “**Diacylglycerophosphoglycerophosphodiradylglycerols (CL)**”; GP1201 is entered in the text box provided. [Figure 10.2](#) shows result of the query window for this input.

For details regarding codes meant for Main Classes and Subclasses in every category for *M. tb* Lipidome MS-LAMP, refer Tables [10.4](#) - [10.9](#).

MS - LAMP - M. tb Lipidome MS-LAMP - Query Type 3 : Molecular Mass or m/z range

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 *M. tb* Lipidome MS-LAMP, illustrating to search within Main Class and/or Subclass. As an example, here the search is aimed at ‘Diacylglycerophosphoglycerophosphodiradylglycerols (CL)’, which corresponds to the code GP1201 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 : 1600 (Average) Upper m/z limit : 1800 (Average) Ion type : [M+H]⁺

GP1201 : 31

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 GP1201, corresponding to the input parameters queried, as depicted in [Figure 10.1](#).

Table 10.4: 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 10.5: 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 10.6: 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 10.7: 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 10.8: 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 10.9: 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]