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

(a) Title bar: This bar gives information about the query window and Lipid database in use.

(b) 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.

(c) 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)

(d) 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:

(a) Title Bar: It gives the summary of the database in use and chosen parameters queried-in.

(b) Queried Parameters: It gives the review of the selected parameters entered as input.

(c) Chosen Lipid categories: Population distribution of lipid(s) in different lipid categories is depicted here. These are clickable buttons that opens a new window

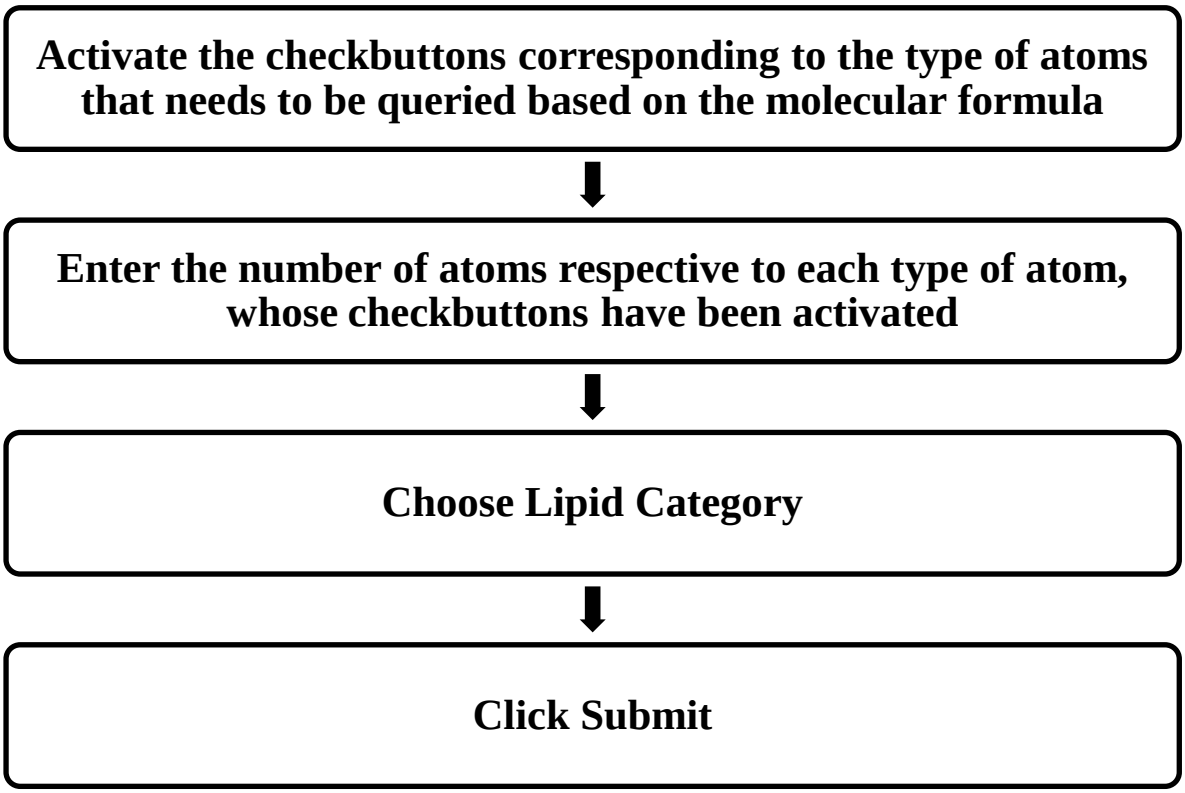
showing details (LM ID in case of General Lipidome MS-LAMP and Molecular Formulae in case of *Mycobacterium tuberculosis* (*M. tb*) Lipidome MS-LAMP) about the lipid(s) obtained as result of the query (see Figure 7.3).

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)

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

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

(e) 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).



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

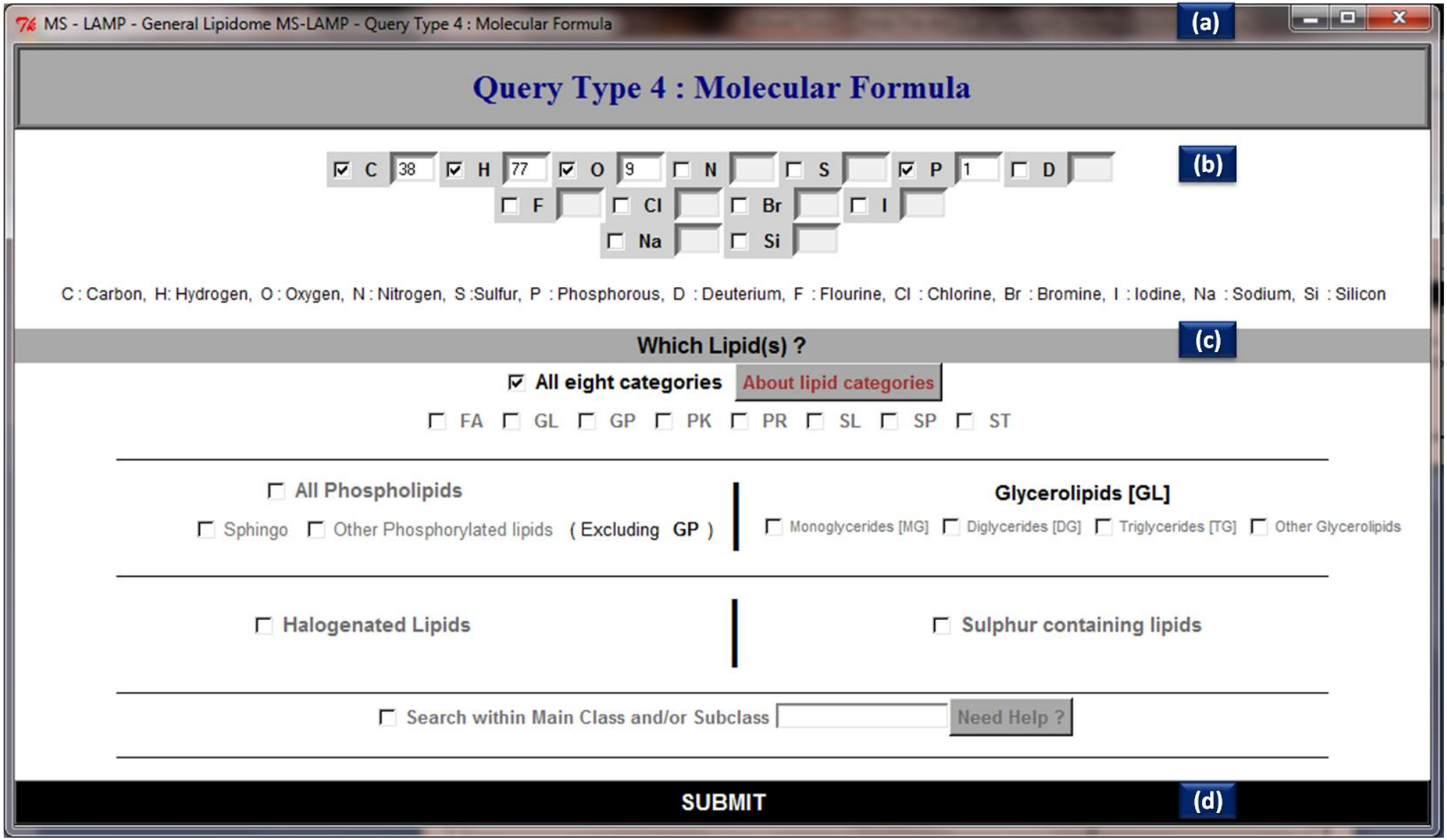


Figure 7.1: Snapshot of input window of "Query Type 4: Molecular Formula". Shown here is an example, wherein a molecular formula, C38 H77 O9 P is being searched in all eight lipid categories within General Lipidome MS-LAMP. (a) Title bar (b) To enter Molecular Formula (c) To select lipid category(ies)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

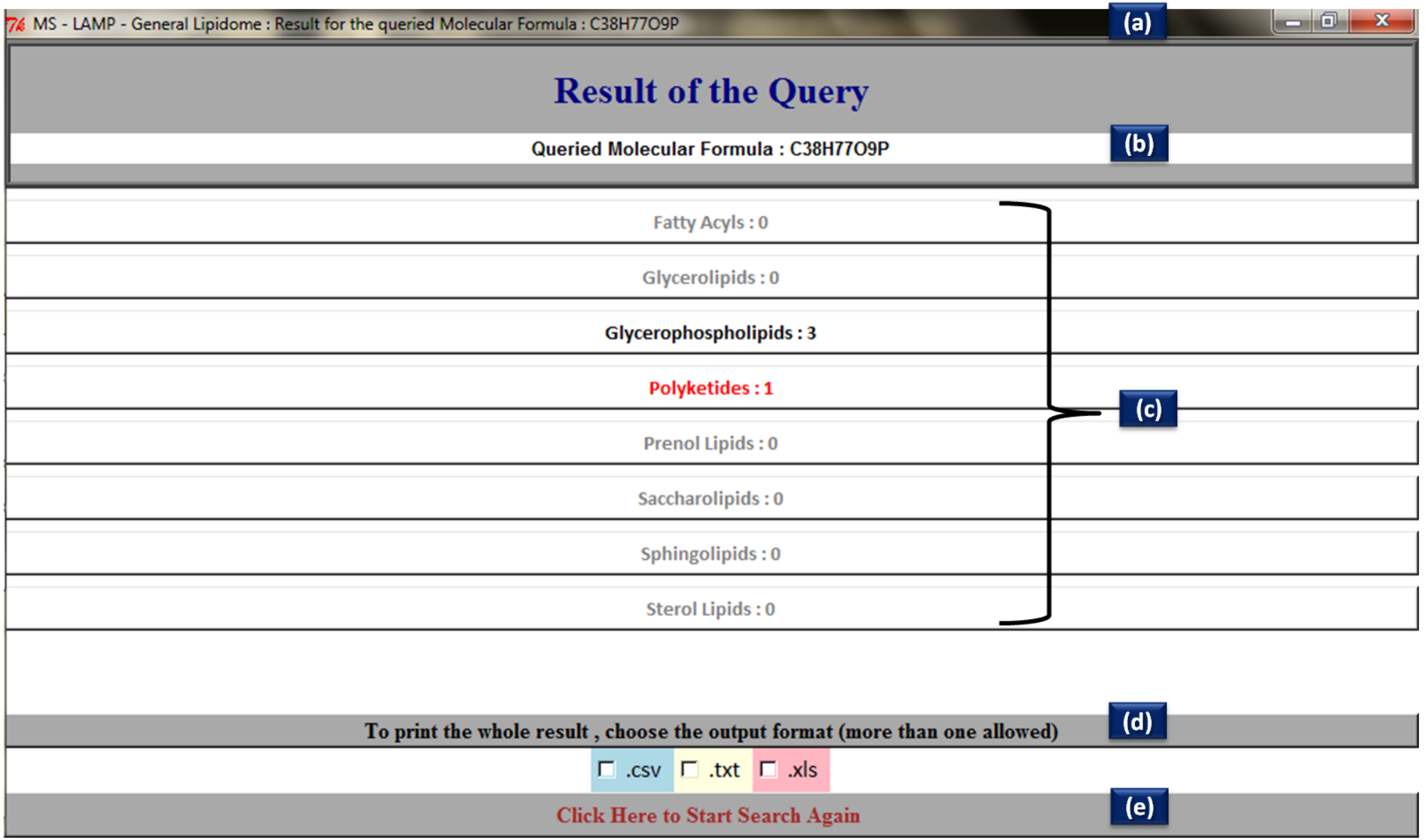


Figure 7.2: Snapshot of **Result of the Query** window showing a glimpse of different lipid categories : 3 glycerophospholipids and a polyketide, corresponding to queried molecular formula C38 H77 O9 P submitted to General lipidome MS-LAMP. (a) Title Bar (b) Queried Parameters (c) Chosen lipid category(ies)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

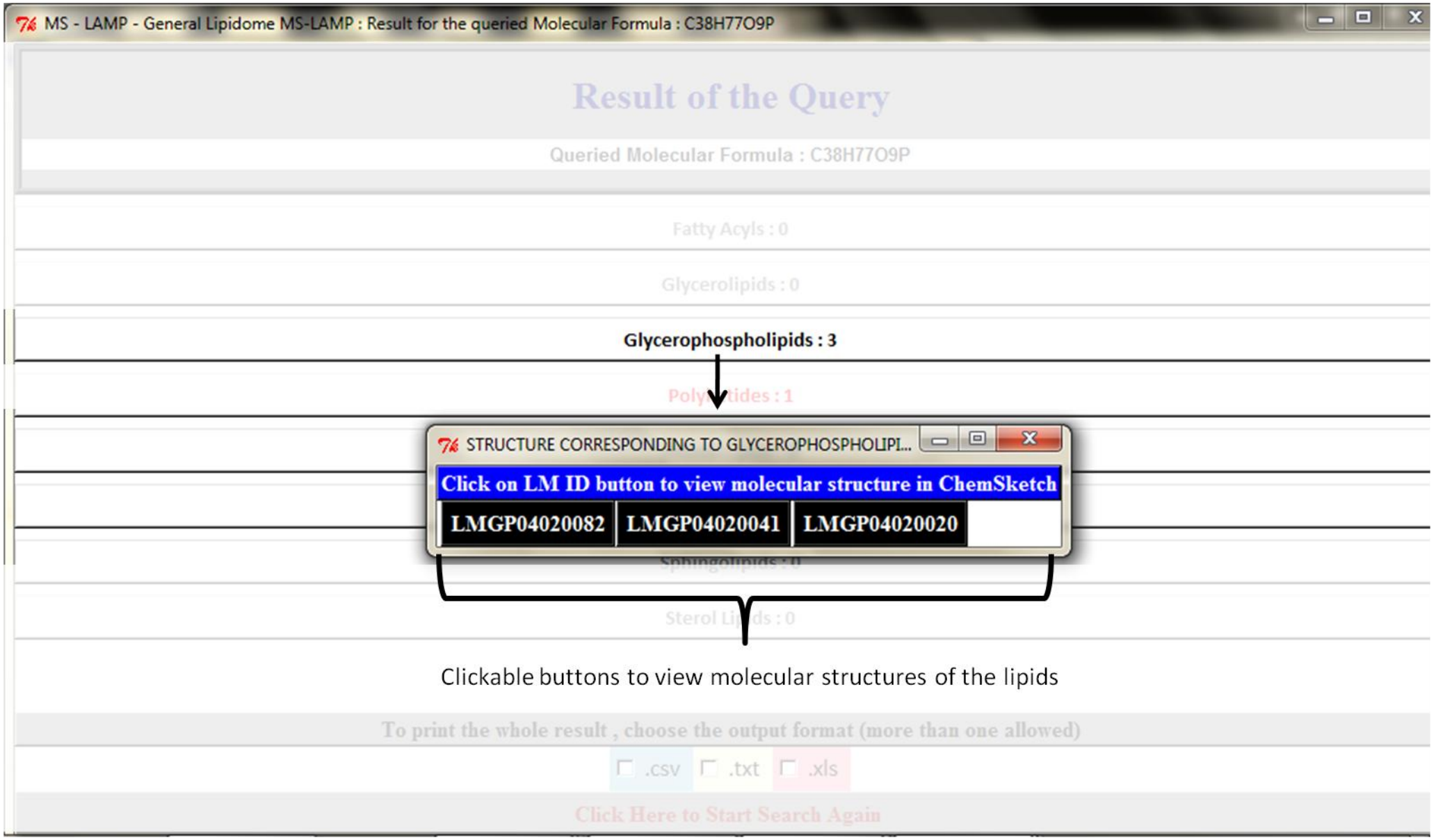


Figure 7.3: Figure showing snapshot of the window containing LM ID buttons, which can be clicked to view the molecular structure of lipids that are obtained as result of the query, shown in Figure 7.2 (**Refer section 4 for more details on this**).