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:

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

(b) Queried Parameters: It gives the review of the chosen parameters queried-in.

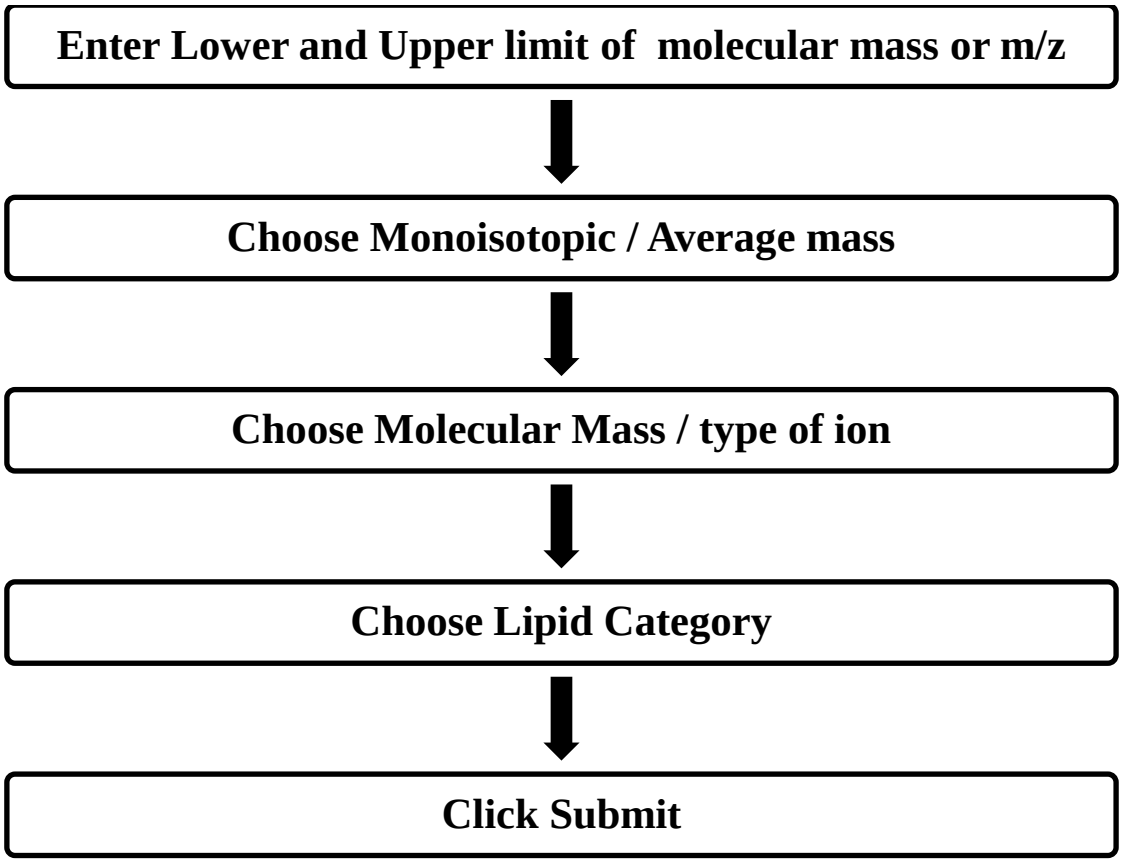
(c) Chosen Lipid categories: Shown here is the population distribution of lipid(s) in different lipid categories chosen while making a query. These are clickable buttons that yield a new window showing details (LM ID in case of General Lipidome MS-LAMP and Molecular formulae for *M. tb* Lipidome MS-LAMP) 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.

(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 start the search again, this button can be clicked that would redirect to the input window of Query Type 3 (Figure 6.1).



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

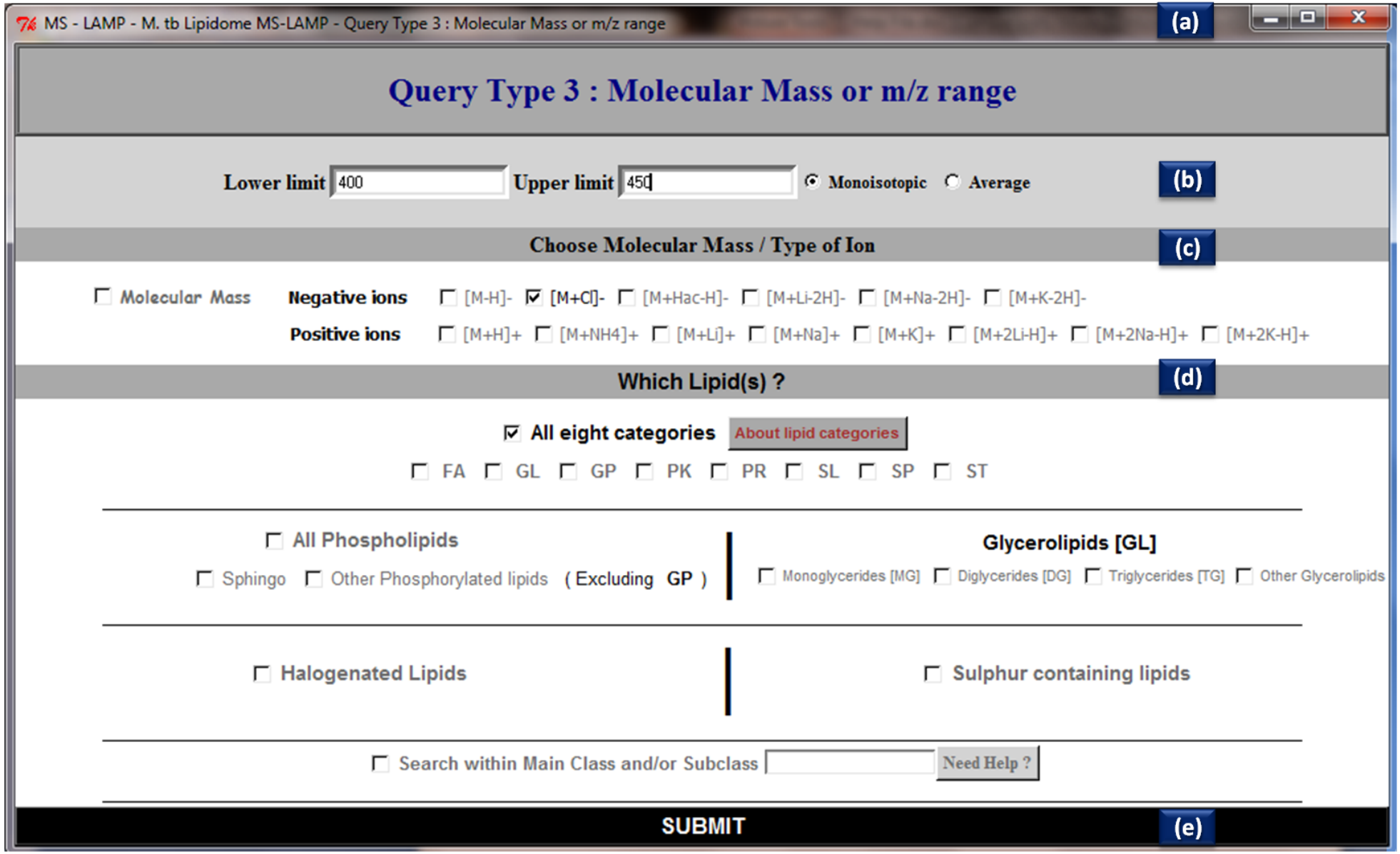


Figure 6.1: Snapshot of input window for "**Query Type 3**: Molecular Mass or m/z range". **(a)** Title Bar **(b)** To enter lower and upper limits of Molecular Mass or m/z value and for choosing monoisotopic or average mass **(c)** To Choose Molecular Mass/ Type of Ion **(d)** For selecting lipid category(ies)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

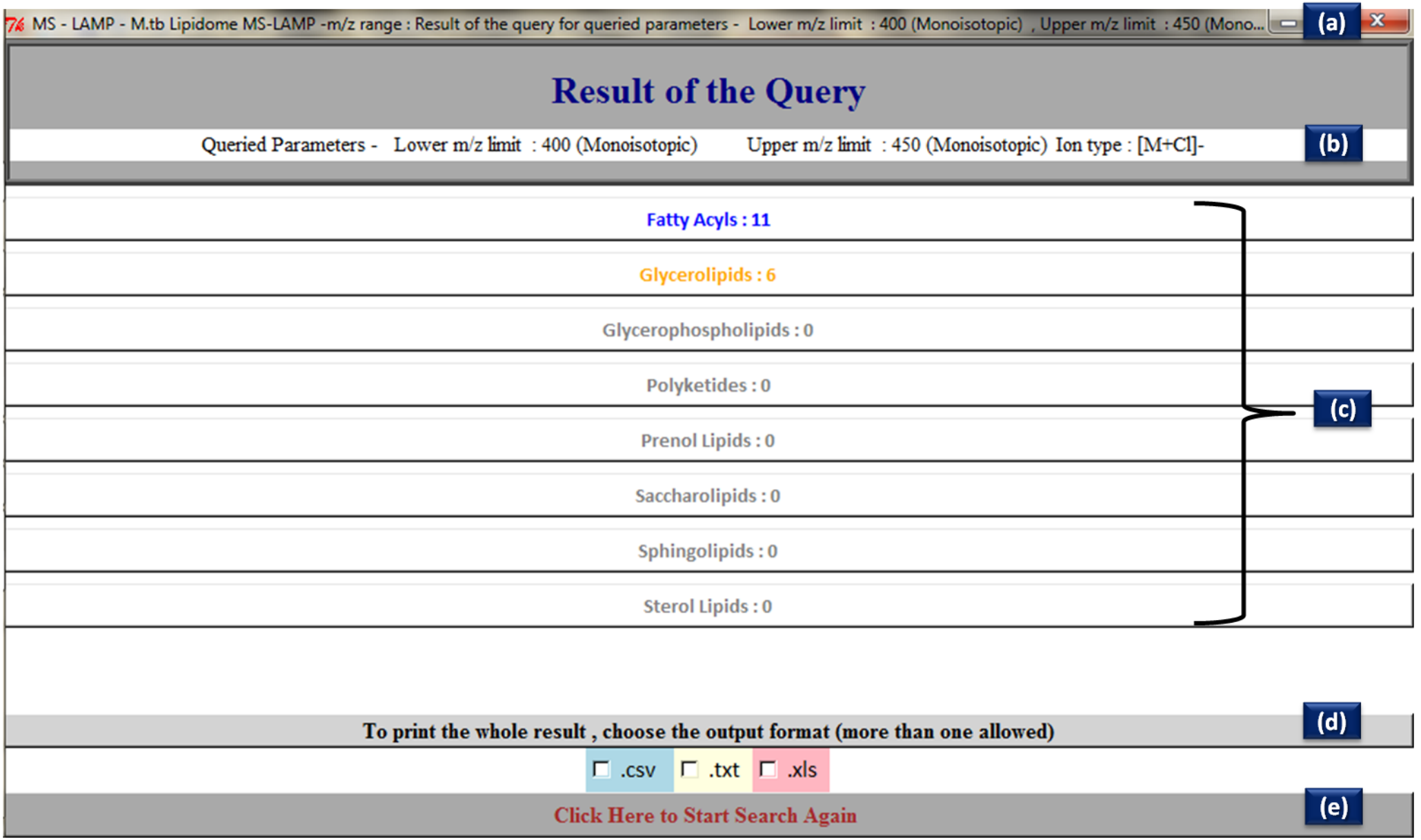


Figure 6.2: Snapshot of **Result of the query** window providing a glance of different lipid categories and number of lipids in each category matching to the queried criteria submitted to *M. tb* Lipidome MS-LAMP, as shown in Figure 6.1 **(a)** Title Bar **(b)** Queried Parameters **(c)** Chosen lipid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

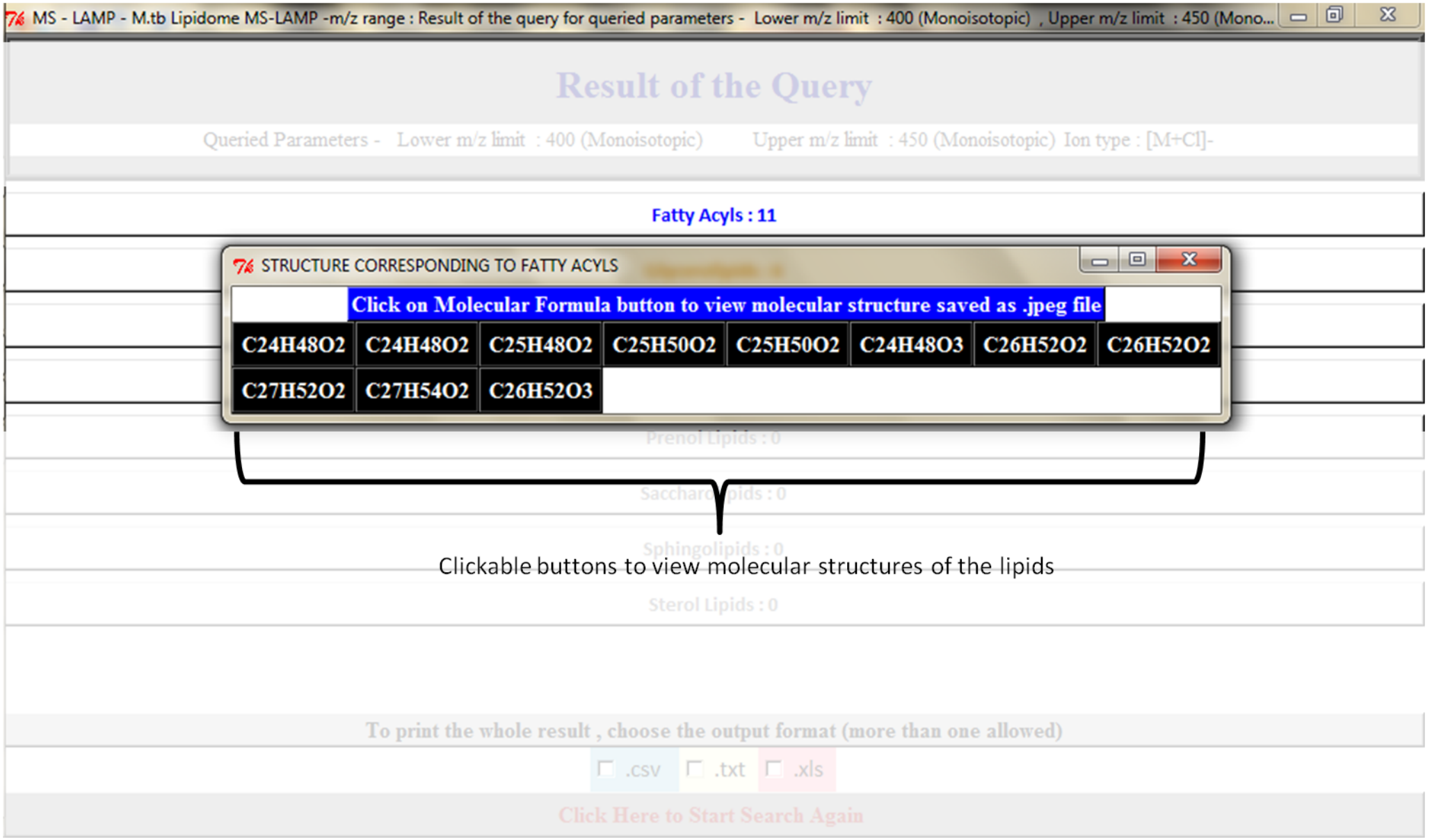


Figure 6.3: Figure showing snapshot of the window containing molecular formulae buttons, which are to be clicked to view the molecular structure of lipids corresponding to those obtained as result of the query, shown in Figure 6.2 (**Refer section 4 for more details on this**).