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).

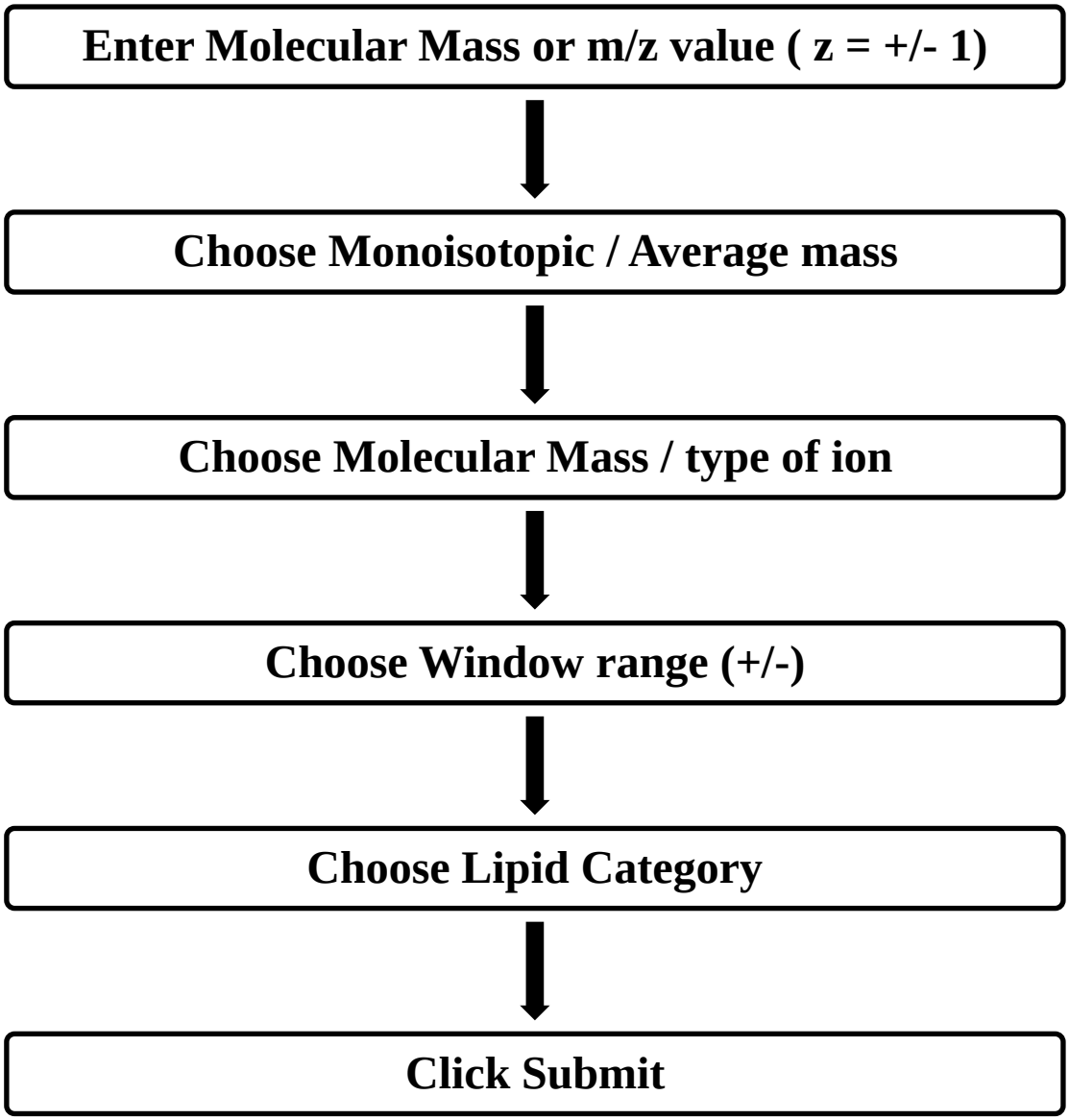
Upon clicking a button in this new window, the molecular structure corresponding to that lipid is shown. In case of General Lipidome MS-LAMP, the structures are available as MD mol file, which can be opened using ChemSketch (See Figure 4.4); while for *M. tb* Lipidome MS-LAMP, structures are available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

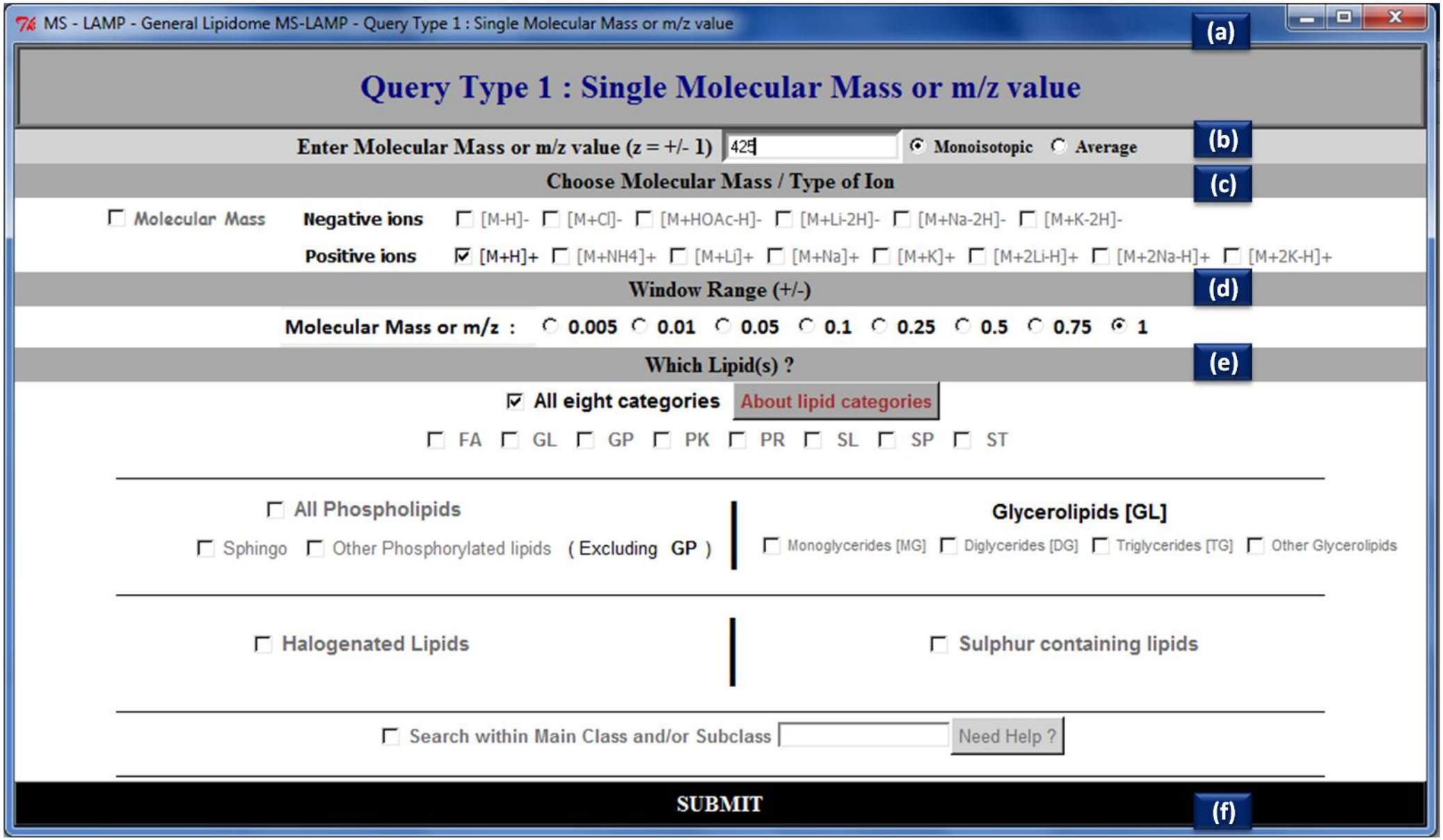


Figure 4.1: Snapshot of "**Query Type 1**: Single Molecular Mass or *m/z* value" query window: **(a)** Title bar **(b)** To enter Molecular Mass or *m/z* value and select monoisotopic or average mass **(c)** To choose Molecular Mass / Type of Ion **(d)** For selecting Window range **(e)** To choose lipid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

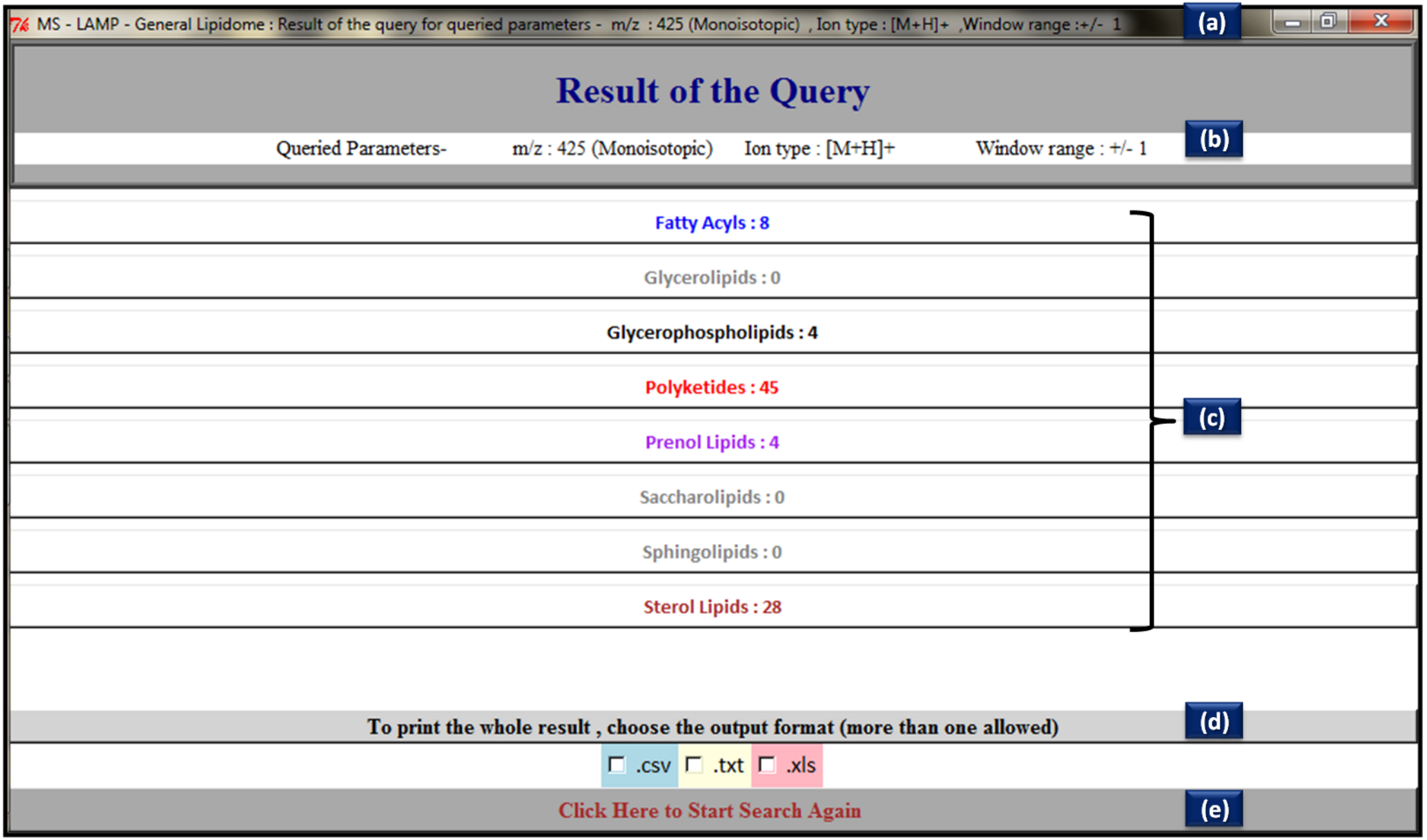


Figure 4.2: Snapshot of '**Result of the Query**' window displaying a glimpse of different lipid categories and number of lipids in each category that match to the queried criteria shown in Figure 4.1. **(a)** Title Bar **(b)** Queried Parameters **(c)** Chosen Lipid categories **(d)** To choose different 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.

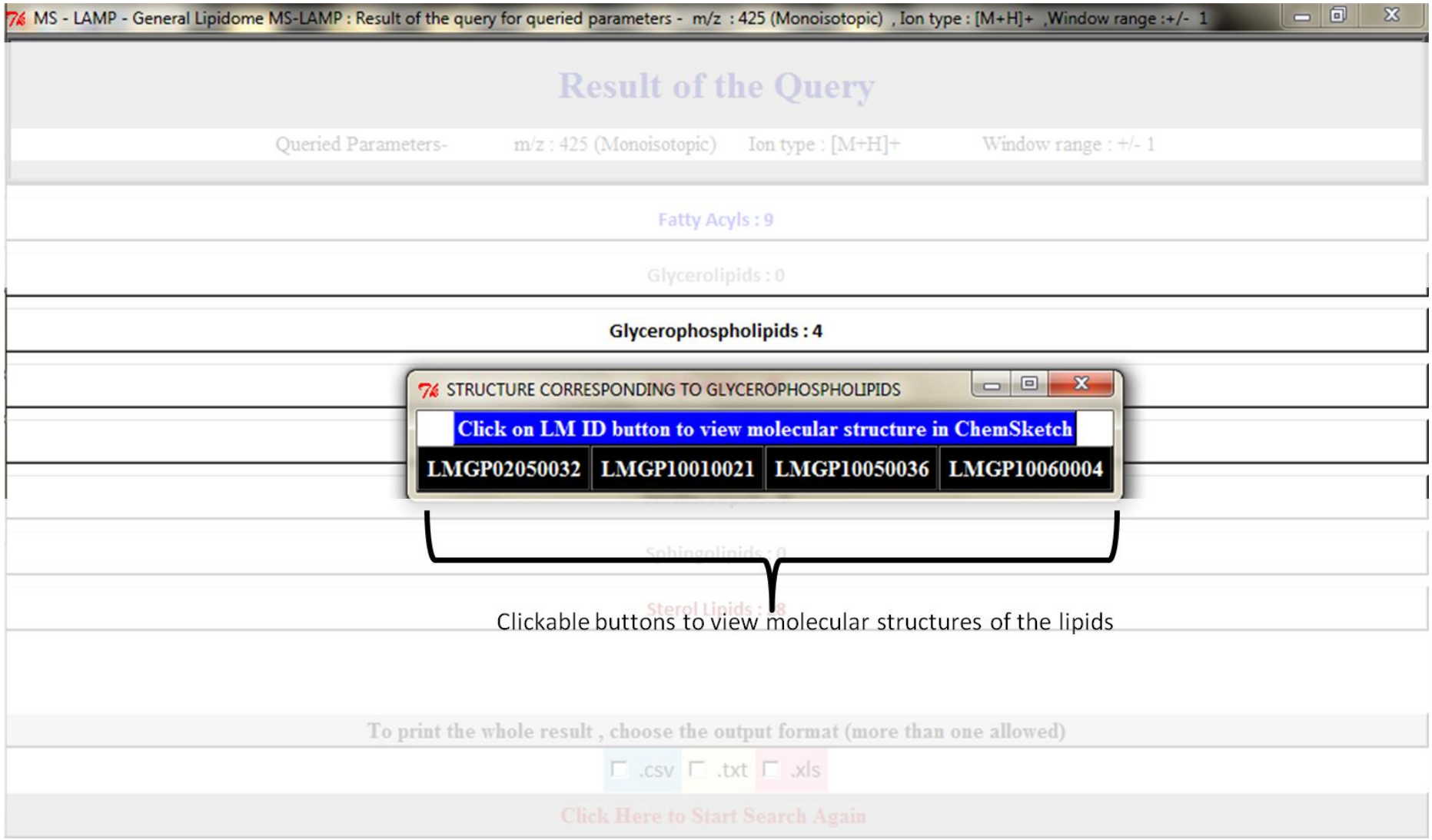


Figure 4.3: To view molecular structures of the lipids obtained as result of the query, button corresponding to a lipid category (in Results of the query window see Figure 4.2) can be clicked that will give rise to a new window containing clickable buttons showing LM ID(s). On clicking a LM ID button 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.

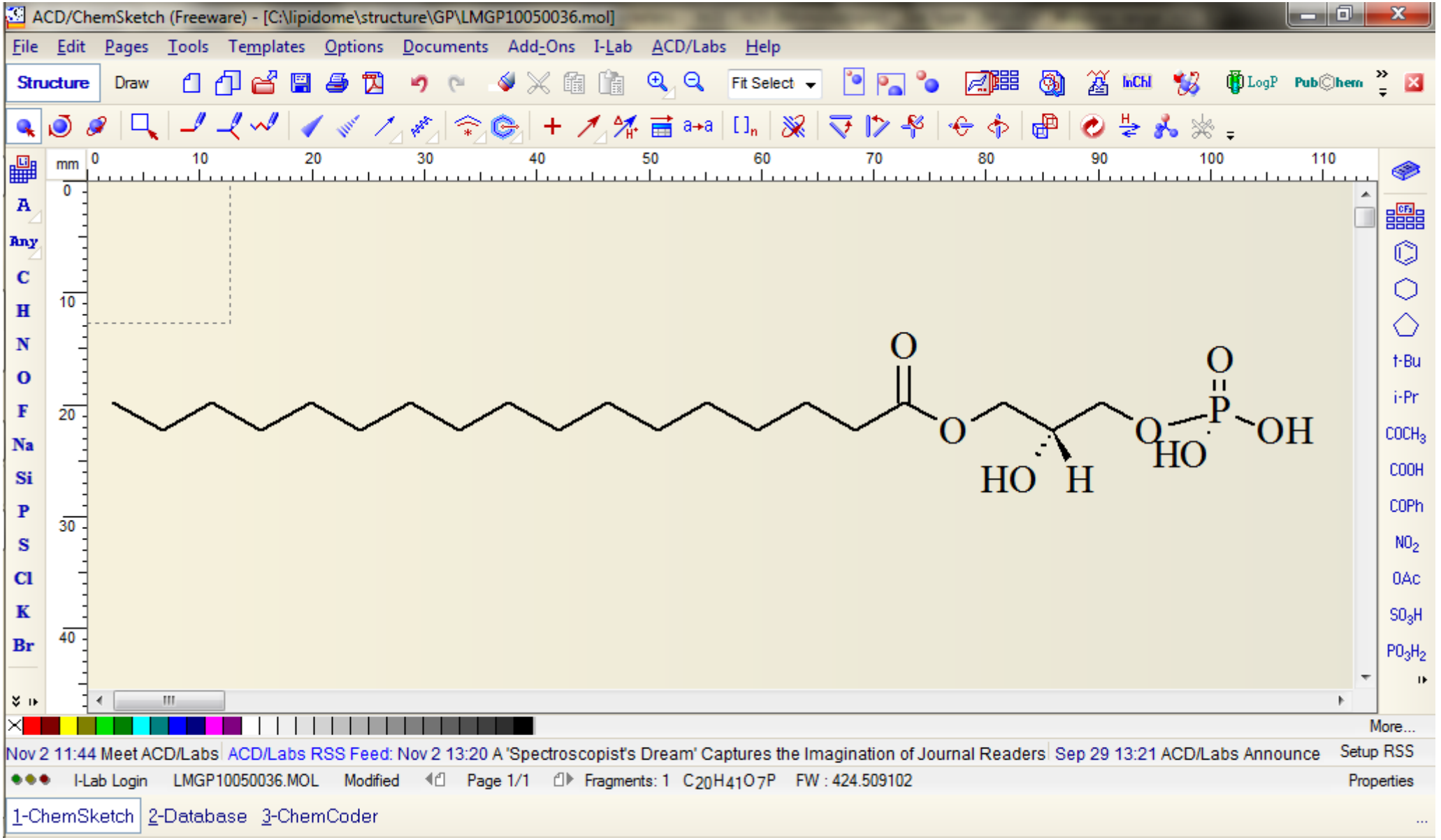


Figure 4.4: Molecular structure of a lipid shown in ChemSketch, which opens on clicking a LM ID button (see Figure 4.3). This is the molecular structure of the lipid corresponding to LM ID: LMGP10050036.

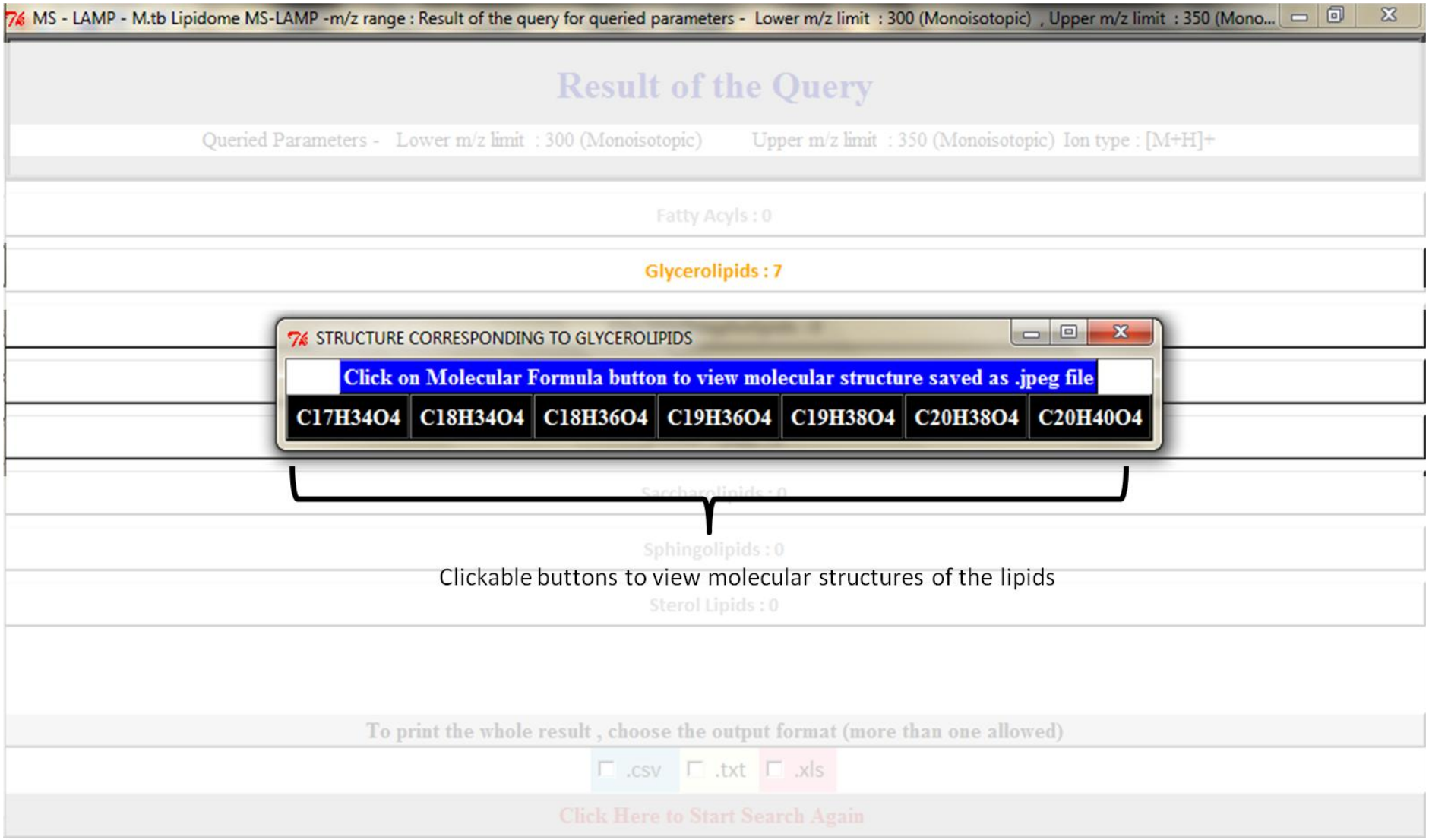


Figure 4.5: Shown here is an example from *M. tb* Lipidome MS-LAMP. To view molecular structures of the lipids obtained as results of the query, button corresponding to a lipid category (in Results of the query window) can be clicked that will give rise to a new window containing clickable buttons showing 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.

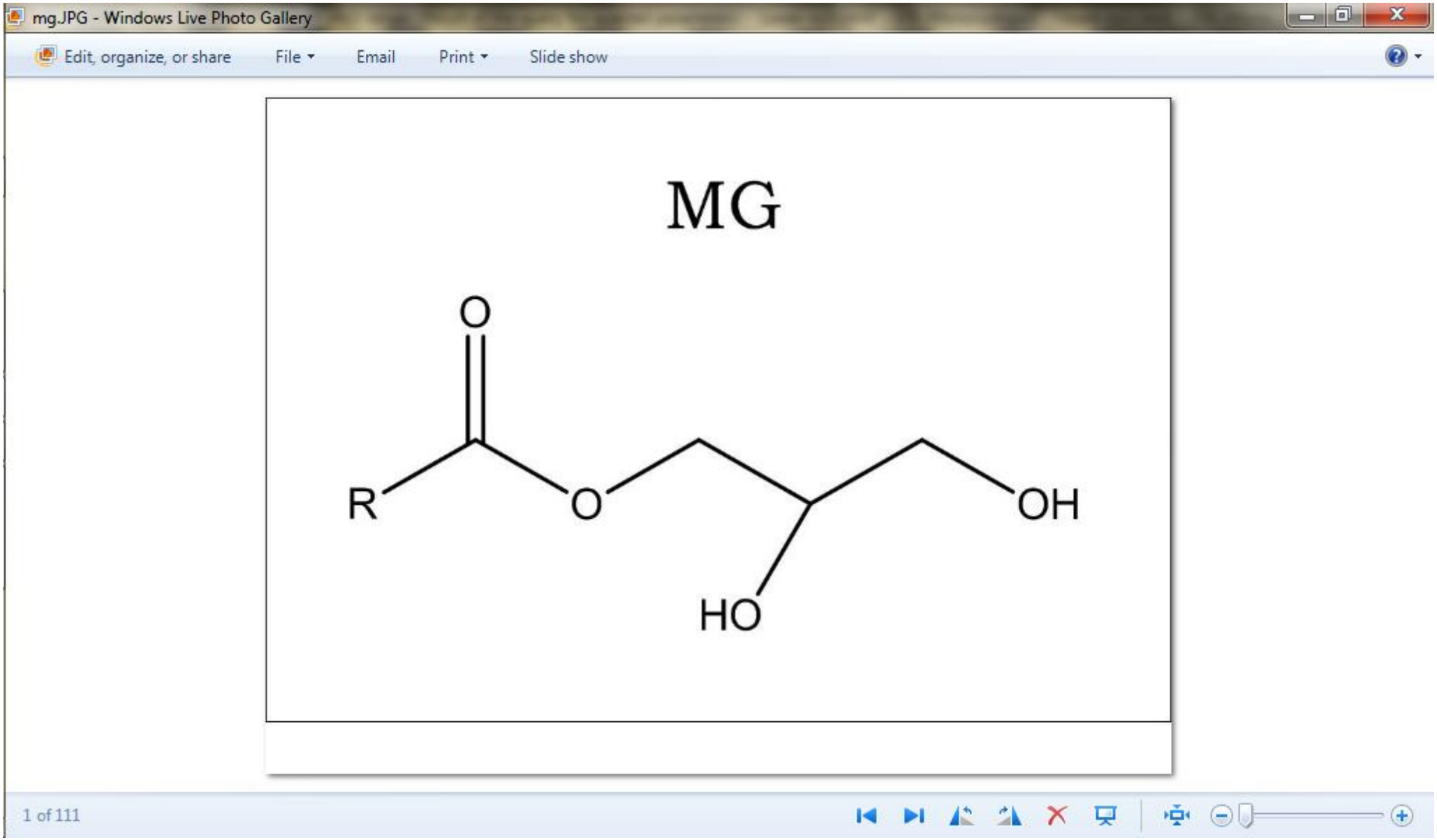


Figure 4.6: Molecular structure of a lipid available as .jpeg file in the *M. tb* lipid database (http://mrl.colostate.edu). The structure opens on clicking the respective Molecular Formula button shown in Figure 4.5. This is the molecular structure of a monoglyceride (MG) as present in the *M. tb* lipid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