



TUTORIAL

- 1. Work Flow.** There is a link entitled Work Flow on the left-hand side panel of the homepage. This work flow describes the steps required to do a metabolite search using MyCompoundID. The user is encouraged to take a look at this work flow to obtain an overall picture of how MyCompoundID works. For the user's convenience, a copy of it has been included in this tutorial. Please refer to Figure 1.

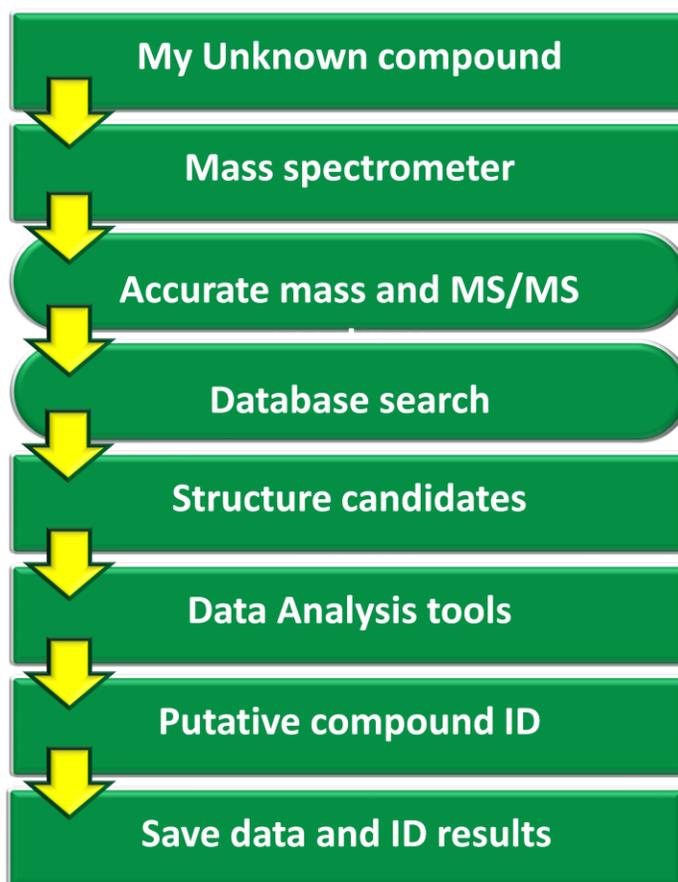


Figure 1. Workflow for the use of MyCompoundID.

- Human Metabolome Database.** MyCompoundID searches against a library of human endogenous metabolites found on the HMDB (Human Metabolome Database, URL: <http://www.hmdb.ca/>). This library consists of 8,021 entries, about 900 of which have MS/MS spectra acquired on a triple quadrupole instrument at three different collision energies. All this information is accessible by clicking on the HMDB links on the query results table.
- Mass list of unknown metabolites.** The user will require a mass list obtained from the sample of interest analyzed by MS or LC-MS. Mass accuracy plays an important role in narrowing down the number of possible candidates. It is therefore recommended that the mass list used has an error no greater than 5 ppm. Please refer to section 4-d.

The following describes how to use MyCompoundID using hydroxyoctanoylcarnitine as an example.

- Search parameters.** There are a number of parameters that need to be set by the user before submitting a query.

The screenshot shows the search interface for MyCompoundID. It includes several sections with radio button options and input fields:

- # Reactions:** Three radio buttons are present: "No reaction" (unselected), "1 reaction" (selected), and "2 reactions" (unselected).
- Neutral or Ion:** Seven radio buttons are present: "Neutral" (unselected), "[M+H]⁺" (selected), "[M+Na]⁺" (unselected), "[M+K]⁺" (unselected), "[M+NH₄]⁺" (unselected), "[M+H/Na/K/NH₄]⁺" (unselected), and "[M-H]" (unselected).
- Query Mass:** A text input field contains "304.210568" followed by "Da" and a link for "(Batch Mode)".
- Mass Tolerance:** Two radio buttons are present: "In Da (default: ± 0.005 Da):" (unselected) and "In ppm (default: ± 5 ppm):" (selected). The "In ppm" option has a text input field containing "5".
- A "Submit Query" button is located at the bottom center.

Figure 2. MyCompoundID's interface showing the default search parameters.

- Number of reactions.** MyCompoundID has a total of 76 possible metabolic reactions that are known to take place in metabolism. These include Phase I (e.g., hydroxylation) and Phase II (e.g., glucuronidation). A complete list of these reactions

can be found in the tab labelled "Possible Reactions" found at the top of the screen (Figure 3).

- i. If the user wants to search against endogenous metabolites found in the HMDB, "No reaction" can be selected.
- ii. "One reaction" can be selected to search for compounds that have undergone one metabolic reaction, whether it is a Phase I or Phase II reaction.
- iii. "Two reactions" can be selected to search for compounds that have undergone any two metabolic reactions, whether they are both Phase I or Phase II or one of each.

Figure 3. The link to the list of possible reactions as well as the area where the user selects the number of reactions are outlined in red.

- b. **Neutral species or type of ion.** The user has the option to search for neutral molecules, $[M+H]^+$ ions, $[M-H]^-$ ions and the most common adducts obtained by the ionization process, such as sodium and ammonium adducts. Alternatively, the user can do a search that includes all options. Please refer to Figure 4.

Neutral or Ion:

- Neutral
- [M+H]⁺
- [M+Na]⁺
- [M+K]⁺
- [M+NH₄]⁺
- [M+H/Na/K/NH₄]⁺
- [M-H]⁻

Figure 4. The area where the user selects the type of ion is outlined.

- c. **Mass.** The user can enter a single mass to search against the database or can choose to enter a list of masses (batch mode). Please refer to Figure 5.
- i. **Batch mode.** In batch mode the user can enter a list of masses, separated by one or more spaces or by a comma. Upon submitting a query, MyCompoundID will display a list that includes the masses entered, the ion type and the number of matched entries per compound. The user can then click on the number of hits to display all possible candidates for that particular mass.

Query Mass: Da ([Batch Mode](#))

Figure 5. A single mass or a list of masses (in batch mode) can be entered in the outlined area.

- d. **Mass tolerance.** The user can select a search mass error threshold in either parts Daltons (Da) or per million (ppm). The default is 0.005 Da or 5 ppm, which is the typical mass accuracy readily achievable by high resolution instruments, such as an FT (Fourier Transform) or a TOF (Time-of-Flight) mass spectrometer. The user can specify a mass tolerance threshold based on the mass accuracy obtainable from the user's instrument. Note that adjusting this search parameter will have a significant effect on the number of hits on the query. Please refer to Figure 6.

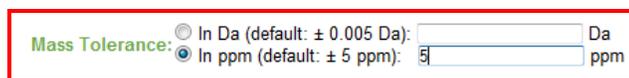
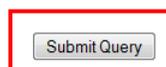


Figure 6. The desired mass tolerance threshold can be entered in either Da or ppm.

5. **Submitting a query.** Once all parameters have been set, the user can click on:



6. **Search results display.** The results page displays two tables, the parameter table and the results table. The parameter table is displayed at the top of the page in order to remind the user of the parameters selected for that particular search query. The results table is displayed immediately below. Note that the entries in the results table can be re-arranged by any column value, such as increasing or decrease mass, mass error, or reaction offset, by simply clicking on the heading of the desired column. The user also has the option of selecting and deleting particular matched entries as well as saving both tables as a .csv file that can be opened using Microsoft Excel.

The results table consists of the following columns:

- a. **Number of matched entries.** The first column on the left is simply used to number the hits observed by a particular search query.

Search Result										
Input Parameter Name	Parameter Value(s)									
# Reactions	1									
Ion Type	[M+H] ⁺									
Query Mass	304.210568 Da									
Neutral Mass	303.203292 Da									
Mass Tolerance	±5 ppm									

Parameter table

[Export as CSV](#) [Check All](#) [Uncheck All](#) [Delete Selected Entries](#) [Save Attachments](#)

#	HMDB ID	Common Name	Mass (Da)	Formula	Chemical Structure	Explore (for Firefox)	Possible Reactions	Reaction Offset (Da)	Mass Error (ppm)	To Del	Attachments
1	HMDB13324	2-Octenoylcarnitine	285.194	C ₁₅ H ₂₇ NO ₄	Structure	ChemDraw Pro ChemDraw Plugin	[+H ₂ O]	18.0105650	-4.199987	<input type="checkbox"/>	Add
2	HMDB00486	7-Hydroxyoctanoic acid	160.10994	C ₈ H ₁₆ O ₃		ChemDraw Pro ChemDraw Plugin	[+C ₇ H ₁₃ NO ₂]	143.094629	-4.213180	<input type="checkbox"/>	Add
3	HMDB00711	Hydroxyoctanoic acid	160.10994	C ₈ H ₁₆ O ₃		ChemDraw Pro ChemDraw Plugin	[+C ₇ H ₁₃ NO ₂]	143.094629	-4.213180	<input type="checkbox"/>	Add

Figure 7. The search result page displaying both the parameter table and the results table is shown. The first column in the results table where the matched entries are numbered is outlined in red.

- b. HMDB link.** The second column on the left (Figure 8) is a link to the HMDB. Clicking on it will open the compound's "MetaboCard". This "MetaboCard" contains a large amount of information on the metabolite of interest, including biological relevance, synonyms, chemical structure, physical properties and, in some cases, experimental ¹H and ¹³C NMR as well as MS/MS information.

[Export as CSV](#) [Check All](#) [Uncheck All](#) [Delete Selected Entries](#) [Save Attachments](#)

#	HMDB ID	Common Name	Mass (Da)	Formula	Chemical Structure	Explore (for Firefox)	Possible Reactions	Reaction Offset (Da)	Mass Error (ppm)	To Del	Attachments
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2	HMDB00486	7-Hydroxyoctanoic acid	160.10994	C ₈ H ₁₆ O ₃		ChemDraw Pro ChemDraw Plugin	[+C ₇ H ₁₃ NO ₂]	143.094629	-4.213180	<input type="checkbox"/>	Add
3	HMDB00711	Hydroxyoctanoic acid	160.10994	C ₈ H ₁₆ O ₃		ChemDraw Pro ChemDraw Plugin	[+C ₇ H ₁₃ NO ₂]	143.094629	-4.213180	<input type="checkbox"/>	Add

Figure 8. The link to the HMDB is located in the second column of the results table and is highlighted in red.

c. **Common name.** The metabolite's commonly used name is displayed in the third column (Figure 9).

Export as CSV Check All Uncheck All Delete Selected Entries Save Attachments

#	HMDB ID	Common Name	Mass (Da)	Formula	Chemical Structure	Explore (for Firefox)	Possible Reactions	Reaction Offset (Da)	Mass Error (ppm)	To Del	Attachments
1	HMDB13324	2-Octenoylcarnitine	285.194	C ₁₅ H ₂₇ NO ₄	Structure	ChemDraw Pro ChemDraw Plugin	[+H ₂ O]	18.0105650	-4.199987	<input type="checkbox"/>	Add
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3	HMDB00711	Hydroxyoctanoic acid	160.10994	C ₈ H ₁₆ O ₃		ChemDraw Pro ChemDraw Plugin	[+C ₇ H ₁₃ NO ₂]	143.094629	-4.213180	<input type="checkbox"/>	Add

Figure 9. The column displaying metabolite common names is outlined.

d. **Mass (Da).** The fourth column from the left shows the monoisotopic molecular mass of the compound (Figure 10).

Export as CSV Check All Uncheck All Delete Selected Entries Save Attachments

#	HMDB ID	Common Name	Mass (Da)	Formula	Chemical Structure	Explore (for Firefox)	Possible Reactions	Reaction Offset (Da)	Mass Error (ppm)	To Del	Attachments
1	HMDB13324	2-Octenoylcarnitine	285.194	C ₁₅ H ₂₇ NO ₄	Structure	ChemDraw Pro ChemDraw Plugin	[+H ₂ O]	18.0105650	-4.199987	<input type="checkbox"/>	Add
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3	HMDB00711	Hydroxyoctanoic acid	160.10994	C ₈ H ₁₆ O ₃		ChemDraw Pro ChemDraw Plugin	[+C ₇ H ₁₃ NO ₂]	143.094629	-4.213180	<input type="checkbox"/>	Add

Figure 10. The masses in Da of the matched entries are displayed in the fourth column.

e. **Chemical formula.** The chemical formula of the compound found from the HMDB is displayed in the fifth column (Figure 11).

Export as CSV Check All Uncheck All Delete Selected Entries Save Attachments

#	HMDB ID	Common Name	Mass (Da)	Formula	Chemical Structure	Explore (for Firefox)	Possible Reactions	Reaction Offset (Da)	Mass Error (ppm)	To Del	Attachments
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2	HMDB00486	7-Hydroxyoctanoic acid	160.10994	C ₈ H ₁₆ O ₃		ChemDraw Pro ChemDraw Plugin	[+C ₇ H ₁₃ NO ₂]	143.094629	-4.213180	<input type="checkbox"/>	Add
3	HMDB00711	Hydroxyoctanoic acid	160.10994	C ₈ H ₁₆ O ₃		ChemDraw Pro ChemDraw Plugin	[+C ₇ H ₁₃ NO ₂]	143.094629	-4.213180	<input type="checkbox"/>	Add

Figure 11. The chemical formula of each match entry is displayed in the outlined column.

f. Chemical structure. The chemical structure of the compound is displayed in the sixth column.

Export as CSV Check All Uncheck All Delete Selected Entries Save Attachments

#	HMDB ID	Common Name	Mass (Da)	Formula	Chemical Structure	Explore (for Firefox)	Possible Reactions	Reaction Offset (Da)	Mass Error (ppm)	To Del	Attachments
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3	HMDB00711	Hydroxyoctanoic acid	160.10994	C ₈ H ₁₆ O ₃		ChemDraw Pro ChemDraw Plugin	[+C ₇ H ₁₃ NO ₂]	143.094629	-4.213180	<input type="checkbox"/>	Add

Figure 12. The chemical structure of each match entry is displayed in the outlined column.

g. Link to ChemDraw Pro or Plug-in. The user who already owns a copy of ChemDraw software (<http://www.cambridgesoft.com/software/ChemDraw/>) can simply click on the link to open the structure of the metabolite of interest. For other users there is also the option of using the free-ware ChemDraw Plug-in (with Firefox only; it will not work with Internet Explorer). Users can manually compare their experimental MS/MS spectrum to the fragments formed using ChemDraw's fragmentation tool (see below).

Export as CSV Check All Uncheck All Delete Selected Entries Save Attachments

#	HMDB ID	Common Name	Mass (Da)	Formula	Chemical Structure	Explore (for Firefox)	Possible Reactions	Reaction Offset (Da)	Mass Error (ppm)	To Del	Attachments
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3	HMDB00711	Hydroxyoctanoic acid	160.10994	C ₈ H ₁₆ O ₃		ChemDraw Pro ChemDraw Plugin	[+C ₇ H ₁₃ NO ₂]	143.094629	-4.213180	<input type="checkbox"/>	Add

Figure 13. The link to either ChemDraw Pro or ChemDraw Plugin is displayed on the highlighted column.

- **Fragmentation tools.** A useful feature of this piece of software is its fragmentation tools which are within its main toolbar (see Figure 14) or can be found under other toolbars in the View menu. Note that the user is required to add or remove a proton (in the case of a positive or negative ion search, respectively) before breaking any bonds in the molecule. In the case of an adduct ion search, the user is also required to add the adduct counter ion to the displayed molecule.

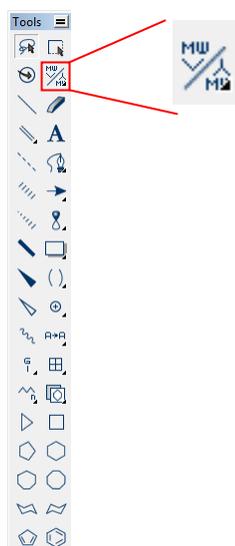


Figure 14. ChemDraw software contains a mass fragmentation tool within its main toolbar that can be used for the generation of fragments that can be compared to the experimental MS/MS spectra.

- Bond cleavage.** After clicking on the mass fragmentation tool icon, the user can draw a line across the bond to be broken. The software will automatically calculate the exact mass of each fragment which can be compared to the experimental MS/MS spectrum. Please refer to Figure 15. Note that the software can only do homolytic cleavage of bonds; as a result, radical species are formed. It is up to the user's discretion to assign charges to the produced fragments. Note that the exact mass of all structures can be displayed by selecting the molecule of interest with the lasso tool, right clicking on it and selecting exact mass under the Analysis option.

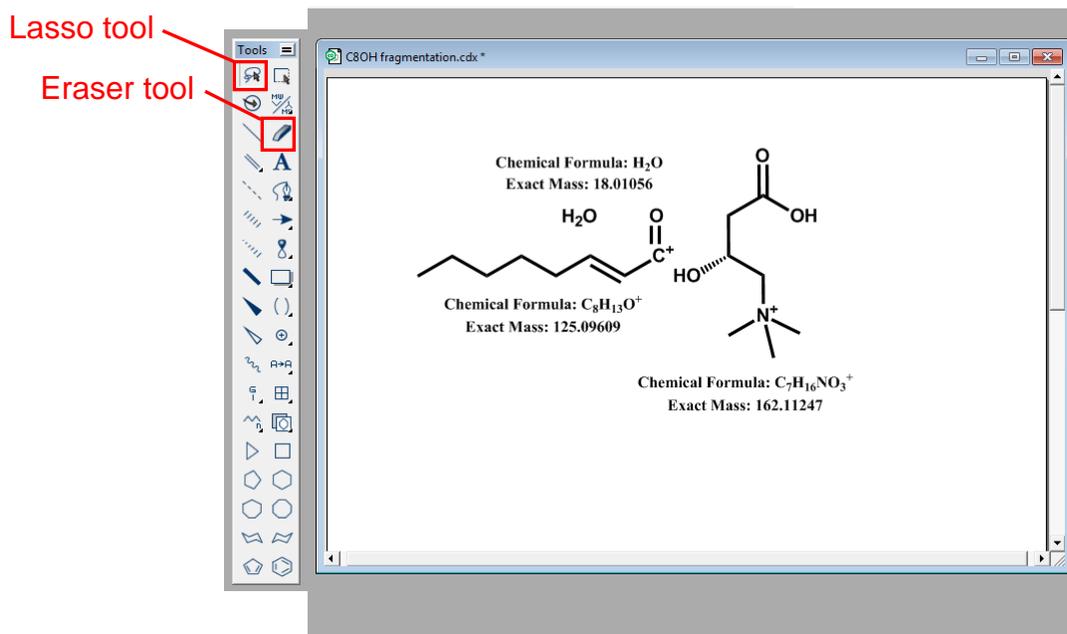


Figure 15. Metabolite fragments produced using the fragmentation tool. All radicals were removed with the eraser tool, positive charges were assigned and hydrogen atoms were added.

- Retrosynthesis tool.** Another useful component of the fragmentation capabilities of the ChemDraw software is the retrosynthesis tool. After clicking on it, the user can draw a line across the bond to be broken

and the software will automatically draw the products of the “retrosynthesis” reaction. As with the bond cleavage option, it is up to the user to account for charges and hydrogen atoms. Please refer to Figure 16 to see an example of how this tool works.

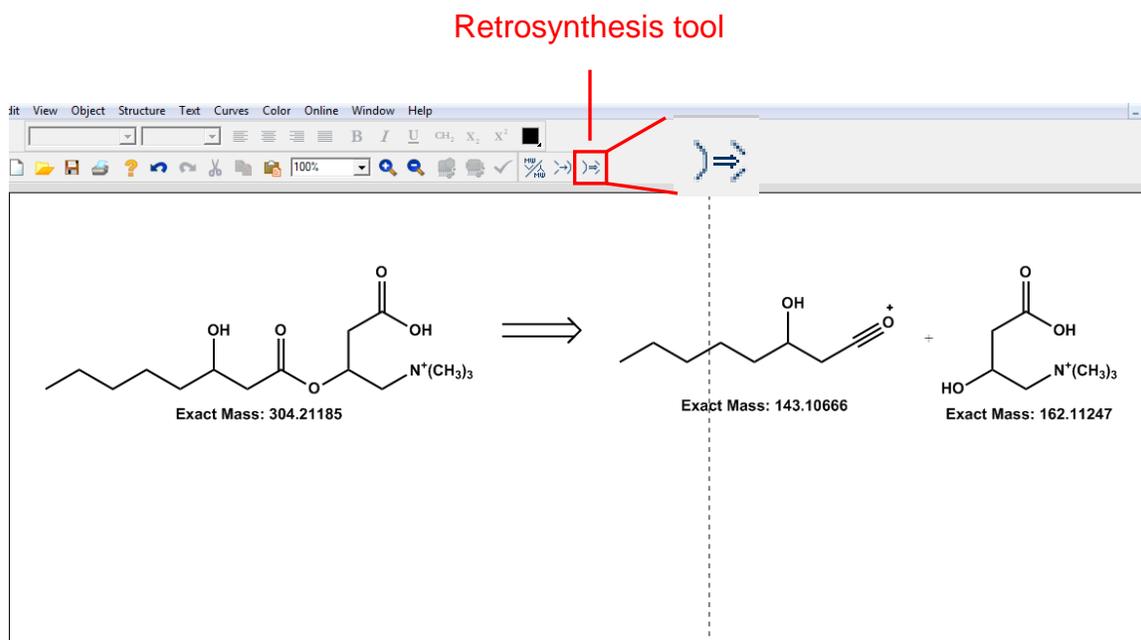


Figure 16. An example of how the retrosynthesis tool works.

- Rearrangements.** Although the fragmentation tool is not capable of carrying out rearrangements, such as McLafferty rearrangement, the user has the option of using the lasso tool to select a portion of the molecule that could correspond to a particular rearrangement and shift hydrogens as necessary. The lasso tool is found on the top left hand corner of the tool bar. Once a portion of the molecule has been selected, the user can then go to the view menu and select “Show Analysis Window”. A window will pop up containing the exact mass of the selected portion of the molecule. Please refer to Figure 17.

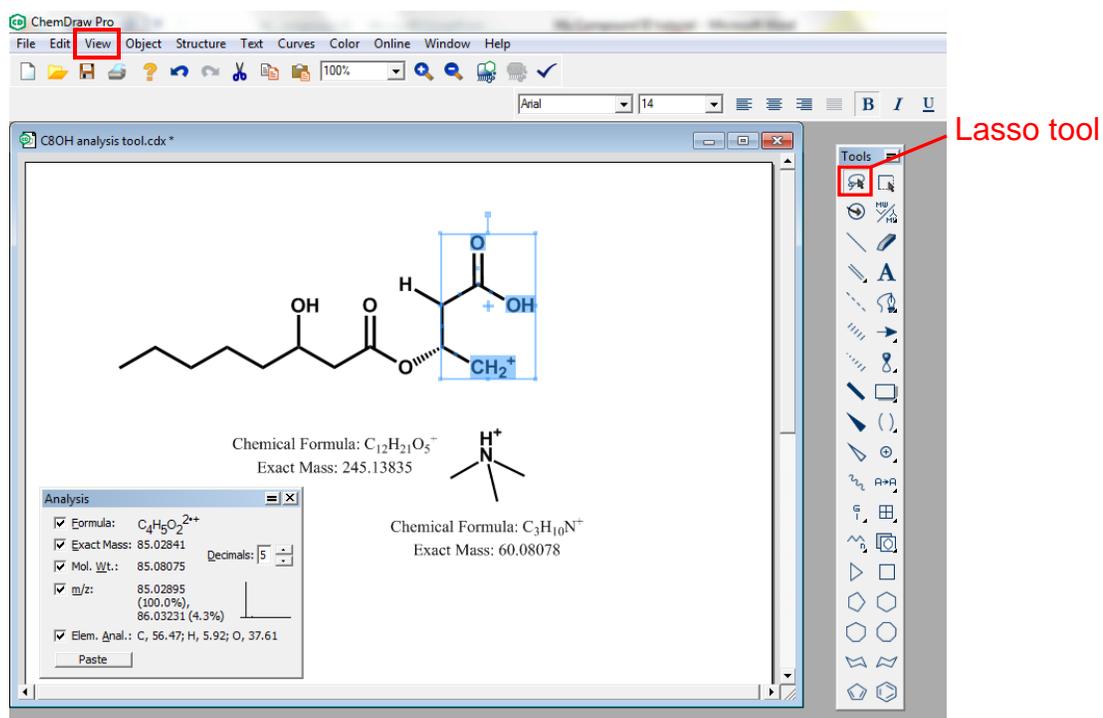


Figure 17. Using ChemDraw to calculate the mass of a fragment derived from a McLafferty rearrangement upon collision induced dissociation of a compound in a mass spectrometer.

- h. Possible reactions.** This column (Figure 18) shows the group that has been added or removed from the corresponding metabolite (as a result of a metabolic reaction) to obtain the mass that was searched for.

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2	HMDB00486	7-Hydroxyoctanoic acid	160.10994	C ₈ H ₁₆ O ₃		ChemDraw Pro ChemDraw Plugin	[+C ₇ H ₁₃ NO ₂]	143.094629	-4.213180	<input type="checkbox"/>	Add
3	HMDB00711	Hydroxyoctanoic acid	160.10994	C ₈ H ₁₆ O ₃		ChemDraw Pro ChemDraw Plugin	[+C ₇ H ₁₃ NO ₂]	143.094629	-4.213180	<input type="checkbox"/>	Add

Figure 18. The list of possible reactions is displayed in the 8th column of the results table.

- i. Reaction offset.** The mass of the group that was either added or removed as a result of a metabolic reaction is displayed in the ninth column (Figure 19).

Export as CSV Check All Uncheck All Delete Selected Entries Save Attachments

#	HMDB ID	Common Name	Mass (Da)	Formula	Chemical Structure	Explore (for Firefox)	Possible Reactions	Reaction Offset (Da)	Mass Error (ppm)	To Del	Attachments
1	HMDB13324	2-Octenoylcarnitine	285.194	C ₁₅ H ₂₇ NO ₄	Structure	ChemDraw Pro ChemDraw Plugin	[+H ₂ O]	18.0105650	-4.199987	<input type="checkbox"/>	Add
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3	HMDB00711	Hydroxyoctanoic acid	160.10994	C ₈ H ₁₆ O ₃		ChemDraw Pro ChemDraw Plugin	[+C ₇ H ₁₃ NO ₂]	143.094629	-4.213180	<input type="checkbox"/>	Add

Figure 19. The reaction offset for each matched entry is displayed on the 9th column of the results table.

- j. Mass error.** The difference in mass between the query mass and the mass of the matched entry is displayed (Figure 20). If the mass tolerance was set in Da the error will be displayed in Da. If it was set in ppm by the user the error will be displayed in ppm.

Export as CSV Check All Uncheck All Delete Selected Entries Save Attachments

#	HMDB ID	Common Name	Mass (Da)	Formula	Chemical Structure	Explore (for Firefox)	Possible Reactions	Reaction Offset (Da)	Mass Error (ppm)	To Del	Attachments
1	HMDB13324	2-Octenoylcarnitine	285.194	C ₁₅ H ₂₇ NO ₄	Structure	ChemDraw Pro ChemDraw Plugin	[+H ₂ O]	18.0105650	-4.199987	<input type="checkbox"/>	Add
2	HMDB00486	7-Hydroxyoctanoic acid	160.10994	C ₈ H ₁₆ O ₃		ChemDraw Pro ChemDraw Plugin	[+C ₇ H ₁₃ NO ₂]	143.094629	-4.213180	<input type="checkbox"/>	Add
3	HMDB00711	Hydroxyoctanoic acid	160.10994	C ₈ H ₁₆ O ₃		ChemDraw Pro ChemDraw Plugin	[+C ₇ H ₁₃ NO ₂]	143.094629	-4.213180	<input type="checkbox"/>	Add

Figure 20. The mass error (in ppm) for each matched entry is displayed on the 10th column of the results table.

- k. To del.** This column (Figure 21) is used to delete a particular row or hit. If the user finds a hit not likely to be a compound candidate, check the box and click the "Delete Selected Entries" button to delete this hit. There is also an option of selecting all the hits by click the "Check All" button and then de-selecting one or more hits from the "To Del"

column to keep the hit(s) of interest; clicking the "Delete Selected Entries" button will delete all hits except the de-selected ones. The "Unchecked All" button allows the user to de-select all the hits previously selected for deleting.

Export as CSV **Check All** **Uncheck All** **Delete Selected Entries** Save Attachments

#	HMDB ID	Common Name	Mass (Da)	Formula	Chemical Structure	Explore (for Firefox)	Possible Reactions	Reaction Offset (Da)	Mass Error (ppm)	To Del	Attachments
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2	HMDB00486	7-Hydroxyoctanoic acid	160.10994	C ₈ H ₁₆ O ₃		ChemDraw Pro ChemDraw Plugin	[+C ₇ H ₁₃ NO ₂]	143.094629	-4.213180	<input type="checkbox"/>	Add
3	HMDB00711	Hydroxyoctanoic acid	160.10994	C ₈ H ₁₆ O ₃		ChemDraw Pro ChemDraw Plugin	[+C ₇ H ₁₃ NO ₂]	143.094629	-4.213180	<input type="checkbox"/>	Add

Figure 21. The delete function buttons are highlighted.

I. Attachments. This feature allows the user to create a folder (in the user's destination of choice) where all metadata related to a metabolite of interest can be saved (Figure 22). This includes, but is not limited to, experimental MS and MS/MS information, fragmentation information from ChemDraw, all created .csv files, etc.

Export as CSV **Check All** **Uncheck All** **Delete Selected Entries** **Save Attachments**

#	HMDB ID	Common Name	Mass (Da)	Formula	Chemical Structure	Explore (for Firefox)	Possible Reactions	Reaction Offset (Da)	Mass Error (ppm)	To Del	Attachments
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3	HMDB00711	Hydroxyoctanoic acid	160.10994	C ₈ H ₁₆ O ₃		ChemDraw Pro ChemDraw Plugin	[+C ₇ H ₁₃ NO ₂]	143.094629	-4.213180	<input type="checkbox"/>	Add

Figure 22. An "Add" button is displayed on the last column on the right-hand side of the results table. Once a file has been selected, any file can be saved as an attachment by clicking on Save Attachments.

- 7. Arriving at a putative metabolite ID.** MyCompoundID will aid the user to obtain a putative metabolite identification by using all compiled data as evidence. However, in order to obtain a definitive chemical identification of the metabolite of interest, comparison to a chemical standard should be carried out.

- 8. Saving metadata in an “evidence folder”.** Experimental data, ChemDraw fragmentation results and .csv files corresponding to a particular compound can be saved in a folder created using MyCompoundID which can be used as supporting evidence when claiming the putative identification of a metabolite of interest.