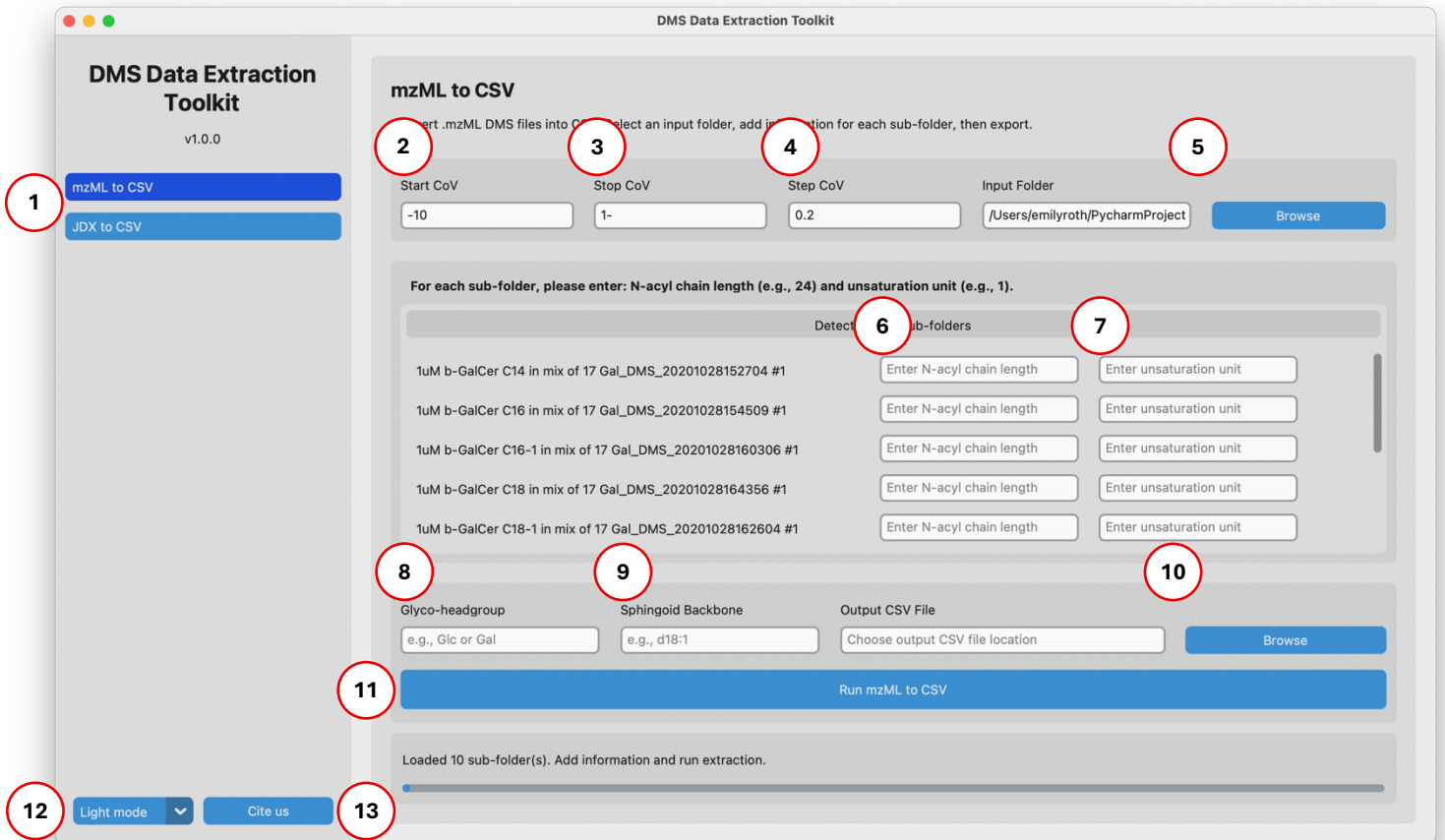


Understanding the DMS Data Extraction Toolkit Application Interface:

Specify the CoV parameters, lipid properties, input, and output directories to extract data from a collection of .mzml or .jdx files, saved to a single .csv file.



The screenshot shows the DMS Data Extraction Toolkit v1.0.0 interface. It features a sidebar on the left with two buttons: 'mzML to CSV' (1) and 'JDX to CSV'. The main area is titled 'mzML to CSV' and contains several input fields and buttons. At the top, there's a description: 'Import .mzML DMS files into CSV. Select an input folder, add information for each sub-folder, then export.' Below this are three input fields for 'Start CoV' (2, value -10), 'Stop CoV' (3, value 1), and 'Step CoV' (4, value 0.2). To the right is an 'Input Folder' field (5) with the value '/Users/emilyroth/PycharmProject' and a 'Browse' button. Below these is a section for sub-folders with a 'Detect' button (6) and a table of sub-folders (7). Each sub-folder entry has two input fields: 'Enter N-acyl chain length' (8) and 'Enter unsaturation unit' (9). At the bottom, there are three input fields: 'Glyco-headgroup' (10, value 'e.g., Glc or Gal'), 'Sphingoid Backbone' (11, value 'e.g., d18:1'), and 'Output CSV File' (12, value 'Choose output CSV file location') with a 'Browse' button. A large blue button labeled 'Run mzML to CSV' (13) is at the bottom. A status bar at the very bottom shows 'Loaded 10 sub-folder(s). Add information and run extraction.'

- 1. Select tool:** Select the option to extract from either .mzml or .jdx files.
- 2. Start CoV:** Input the start value of the CoV range.
- 3. Stop CoV:** Input the stop value of the CoV range.
- 4. Step CoV:** Input the step by which the CoV increases.
- 5. Input folder & browse button:** Select the directory where the input sub-directories are located.
- 6. Input N-acyl chain length:** For each sub-directory, specify the given N-acyl chain length as a single number (i.e., 14)
- 7. Input unsaturation unit:** For each sub-directory, specify the given unsaturation unit as a number (i.e., 0)
- 8. Glyco-headgroup:** Specify which sugar headgroup is relevant to the set of input experimental runs uploaded

9. **Sphingoid backbone:** Specify the sphingoid backbone relevant to the set of input experimental runs. Use the following nomenclature (e.g., d18:0, d18:1, d18:2)
10. **Output browse:** Select the directory where DMS Extract will save the extracted data (.csv).
11. **Run:** Start the extraction pipeline.
12. **Theme selector:** Change the application appearance between light (default) and dark mode.
13. **Cite us:** Open the citation information for DMS Extract in a browser.

Understanding the DMS Extract Application Output:

DMS Extract outputs a single .csv file formatted for use as sample data input for [iDMS](#).