

Instructions for GC-MS

Printing Mass Spectral Data

- 1) On the computer, open **QualBrowser**.
- 2) **Open** your data file by either selecting **File..Open** from the menu bar or by clicking the **Open button** (first button from the right) from the toolbar. Your data file should be located in the **chm2211l** folder. Select this folder from the window that opens by double-clicking on the appropriate folder icon.
- 3) Then double-click on the appropriate data file (**Remember**: the file naming system used on the GC-MS). This will open the selected GC-MS data file giving you a double pane view of your data. The top pane is the actual GC trace for the sample you injected. The bottom pane is the Mass Spectrum for the area selected in the GC trace.
- 4) Using the cross-hairs, select the appropriate peak in the GC trace by clicking once on the peak. This will automatically change the Mass Spectrum in the bottom pane to that measured for the peak you selected. If a larger area is desired, you can click and drag on the area of interest in the GC trace which will give the total Mass Spectrum for the entire area.
- 5) When you have the desired Mass Spectrum displayed, click the **Print** button from the toolbar (fourth button from the right).
- 6) **Close** QualBrowser.

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Measuring Mass Spectrum

BEFORE STARTING THIS PROCESS YOU SHOULD HAVE YOUR UNKNOWN SOLUTION ALREADY PREPARED!! This is done by dissolving 1-2 drops of your liquid unknown or a small spatula tip of your solid unknown in 3-5 mL of acetone.

- 1) On the computer and in the Xcalibur software, ensure the **roadmap view** is selected. If the **roadmap view** is not showing, click the **roadmap view button** on the toolbar (first button from the left).
- 2) Select **sequence setup** from the right pane of the window by clicking the appropriate icon.
- 3) Under the file name column in the spreadsheet, select the first empty cell. Then, click the right mouse button and press the **browse** button on the menu that appears; you will get a new window that has the **C:\ drive** as the default. Change the drive to **D:\ drive** by selecting it from the dropdown menu at the **Lookin:** slot. Change folders to the **D:\Xcalibur\data\CHM3740I**. Enter your filename: YOU MUST ADD THE .raw file extension to your filename. The Click the **OPEN** button.
- 4) Select the row of the spreadsheet you just entered your filename by clicking on the number of your row on the right side of the spreadsheet pane, it should be highlighted in black.
- 5a) Depress the **run sample button** from the toolbar (seventh button from the right - looks like a test tube with a green arrow through it).
- 5b) A new window will appear where you should click the **OK button**. This will initiate the actual GC-MS. On the right panel, check that there are values in the filename and Inst. Method listings. **IF NOT, FIND YOU TA OR INSTRUCTOR IMMEDIATELY!!!!** There will be a short delay followed by the instrument display panel (front right of the GC-MS) indicating **Ready to Inject**.
- 6) During this delay time, carefully draw up 5 : L of your solution into the syringe. Depress the plunger until only 1 : L remains in the syringe.
- 7) **CAREFULLY**, inject 1: L of your sample into the injection port (**CAUTION: HOT!!!**) and immediately depress the **start button** on the instrument display panel. It will take ~15 minutes for your GC-MS run to be completed.
- 8) Clean the syringe with acetone by drawing up acetone into the syringe and injecting the acetone into the waste vial. Repeat several times.