Standard Operation Procedure for Bruker Esquire LC Mass Spectrometer

Logging on the workstation and start up

1. Enter your user name and your password

2. Click on ESQUIRE-Control icon on the desktop to start the program

3. Wait until starting up finishes, it will open both the acquisition program called ESQUIRE control and Bruker DataAnalysis program.

Load MS method and change sample information

1. Find the "Method" menu on the top of ESQUIRE-Control window. Click and select "Load Method". Locate your method and load it into the program.

2. Click on "Tune" on the lower window, click on "Smart". Check the Nebulizer pressure (e.g. 20 psi), Dry Gas flow rate (e.g. 5 l/min) and Dry Temp (e.g. 300 C) are reasonable for your sample.

3. Click on "Mode", set positive or negative and Scan range. The actual scanning range is defined in the "Trap" box located in the lower right part of the window, and this can be modified. Typically the standard resolution is enough.

4. Find "Status" menu in the left of the lower window. Click to change from "Shutdown" to "Standby". The temperature should begin to rise.

5. Enter sample information. Click on "Acquisition" menu and click on "Sample info…". ***Find your subdirectory*** and enter your sample information. Select either manually or automatic Prefix/Counter for file name.

6. Click "Apply" then "Close".

Introducing your sample (direct infusion)

1. If the syringe pump is in shut off state, turn the switch on the back to turn it on.

2. Fill the syringe with about 50 ul of the solvent you use for your sample, infuse the sample at the rate of about 10ul/min (600ul/hour) to get a background.

3. Fill the syringe with your sample, infuse the sample at a rate <=600ul/hour, i.e. <=10ul/min. Typically a 300 ul/hour=5 ul/min gives very good signal.

Acquire MS data

1. When the temperature reaches the target, Click "Operate" in the "Status" menu.

2. Introducing your sample by directly pumping the sample solution in SYRINGE PUMP. Usually **1~10 ml/min** depending on your sample and source parameters (dry gas flow, nebulizer pressure and dry temperature) and sample concentration.

3. Click "Tune", click "Smart", then enter your Target Mass in the "Smart parameter Setting (SPS)". The software will automatically optimize the instrument for detecting the Target Mass.

Data Saving for single MS measurement

1. After getting a nice MS spectrum, you can A) click on the green icon (the 6^{th} from left) to save a profile spectrum. Or B) you can click on the green icon (the 4^{th} from left) to start saving a spectrum, then click the red icon next to it to stop the acquisition. For simple measurement, A is good enough and occupies much less disk space than B and is recommended.

2. If you need to run MS/MS, go to the next step. Otherwise skip the next step and go to the DataAnalysis for printing out.

Run MS/MS

1. Find and optimize the peak you want to run MS/MS

2. Click on "MS/MS", Under "Isolation" of the "Manual" menu, enter the m/z to be fragmented in "Stage 1" and check "on" for both "Isolation" and "Fragmentation"

3. After a while, you should see the MS/MS of the parent ion. Save a profile or a spectrum as you did in the previous step.

4. Continue to run the 2nd step if needed.

More samples

1. Stop the Syringe pump.

2. Click "Standby".

3. Change to another sample, enter new sample info, and collect MS spectra for the new sample. After finish all the measurement, stop the syringe pump and click "Standby".

Finishing up

1. Fill syringe full of solvent you used for your sample.

2. At a infusion rate of 40 ml/min (2400ml/h), wash the ion source until the solvent finishes. Click on "Operate", make sure your sample peaks are gone, only background and solvent signal present. Alternatively, you can manually inject the full syringe of solvent slowly. If you have a dilute sample and follow the above steps, one syringe of solvent is usually enough to clear any residue compound.

3. Click "Standby", click "Shutdown". Now you have finished measurement of your sample.

Data Analysis (For Profile Spectrum)

1. Click on "Bruker DataAnalysis Esquire" window
2. Open your file

3. Click "PeakList" on the top menu, and click "Find.."

4. Accept the criteria of peaks, and your peaks should be labeled. Print out your spectrum.

Leaving the instrument

1. "Exit" both of the program from the the "File" menu on the top.

2. Log out of the computer (DO NOT ShutDown the computer)

3. Clean up the instrument, put the syringe in its box, switch off the syringe pump.

4. ENTER YOUR USAGE AND REPORT ANY PROBLEM IN THE LOG BOOK.