How to get your MS-results

REVISED
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Log on to the computer:

- User name = chromuser and type in the password written on the side of the computer cabinet.
- Open VPN connection using the shortcut on the desk top or by a web browser

Transfer your files to the local hard drive:

- Open My Computer
    - Copy your datafiles from P:\filutveksling\MasseMAS to D:\"Supervisorname"\"Yourname.7pj"\DART/ESI.7fl (last folder may vary depending on experiment type Make the folder "Supervisorname" if it does not exist)

Analysing chromatograms – Mass Drift Compensation (once for every file)

- Open the Chromatogram Viewer
    - File > Open Chromatogram
        - Open your files from D:\"Supervisorname"\...
- Zoom to the peak of the standard by **left**clicking and dragging
- Open the MS of the first top on the IS by **right**clicking and dragging on the first small top
- Resize the two windows with the chromatorgram on the top half of the screen
- Open one of the last small peaks (rightclick and drag) [the molecular weight is increasing in the peaks from left to right]
    - Now you have two MS-spectra in the lower screen, if not doubleclick on the one you see
    - Zoom in to the MS-peak that is closest to your expected massrange
    - Click Spectrum > Calculate Mass Resolution
        - If Mass Resolution is >5000 then you can use that peak
        - If R<5000, make new spectrum by selecting a different time region in the chromatogram.
    - Rightclick on the spectra that you select, click Make Centroid Spectrum > Apply > Close
        - You should get one line with an exact mass
    - Click Tools > Change Mass Calibration
        - Click Change > Internal Mass Drift Compensation next to second box
            - Click next
            - Check that Mass Reference is PEG+H/PEG+Na etc
            - Click next and then finish
        - Rightclick on the top spectra and select Remove All Assignment
        - Zoom in to the peak you selected earlier
        - Mark it by leftclicking on it (it should turn red when selected)
        - The number the topmost box to the left should be very close to 1 (0,999)
        - Rightclick in the topmost spectra and select Remove All Assignments
        - Rightclick again and select Assign Peaks and choose the correct value from the list
        - Click File > Save as
            - Dataname should be pegxxx where xxx is the mass of the peak

        - File > Exit and Return
    - Change both Mass Drift Compensations to the file you just made (pegxxx)
    - Click OK

Analysing chromatograms – Exact mass of your sample

- Zoom in to the first sample in the chromatogram in the first windows
- Click Unzoom Y-Axis button in the top of the screen to maximize the peaks
- Rightclick and drag to open MS-spectrum of peak (should not use too broad)
- Zoom in the wanted peak in the MS-spectrum by leftclicking and dragging
- Check that the Mass Resolution is high enough by clicking Spectrum > Calculate Mass Resolution
    - If Mass Resolution is >5000 then you can use that peak
    - If R<5000, make new spectrum by selecting a different time region in the chromatogram.
- Rightclick in the spectrum and select Make Centroid Spectrum > Apply > Close
- This is your exact mass

Analysing chromatograms – Elemental composition of your sample

- Tools > Elemental Composition
    - Select you peak
    - Open the Elements tab and click Elements
        - Select the elements present in the molecule
    - Click Estimate to get a list over the possible elemental compositions

Printing results

- Go to print and select Office image writer as printer
- Click OK
- Write the desired filename and information
- Save the file in D:\"Supervisorname"\"Yourname.7pj
- Close the document if it opens automatically
- Open your file and print as normal or move the file to your home directory on server rasmus/rasurt/helix

Finishing

- Work done!
- Close everything using file / exit, and remember to log out

APPROVED

By Egil Nodland at 10:38 am, May 04, 2011