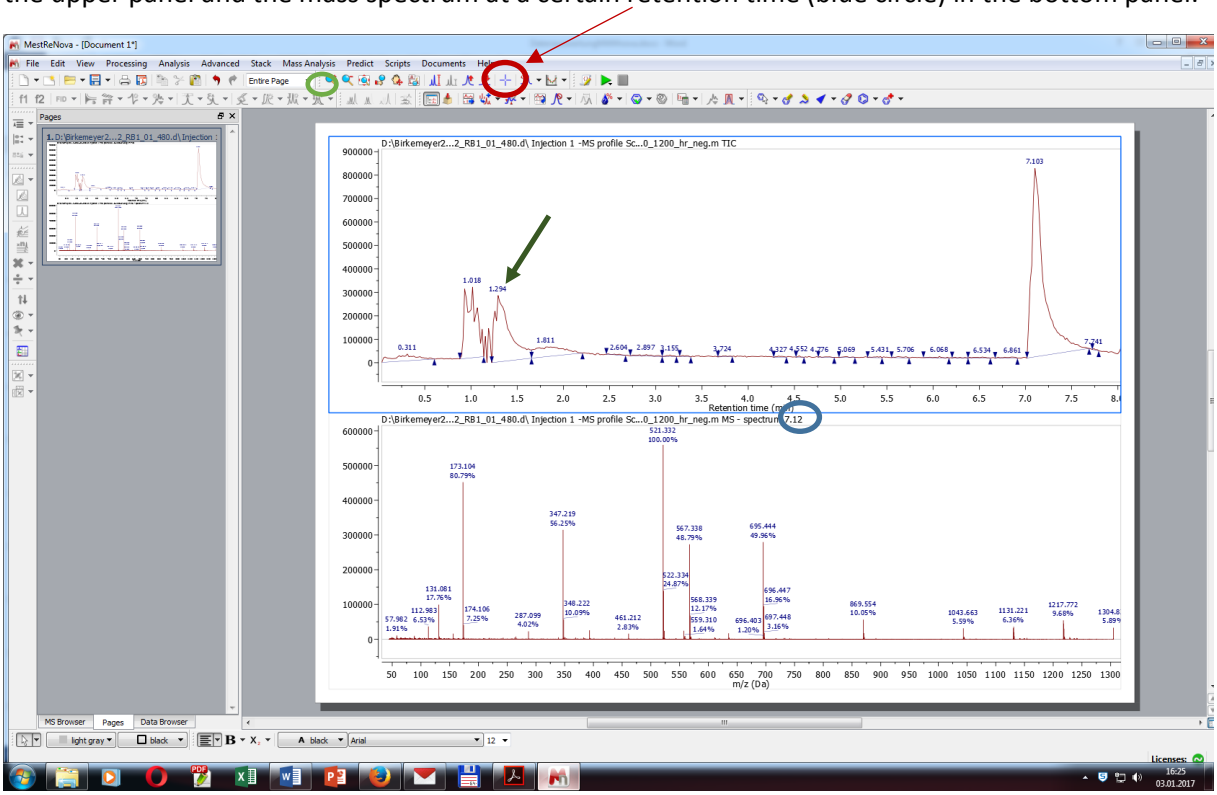
Data Evaluation with Mnova

1. Open Data file and view spectra

After opening the software, you can upload your calibrated data file by File/Open/[select analysis.baf or analysis.yep from the data file]. The software will show the file with the TIC (total ion current) in the upper panel and the mass spectrum at a certain retention time (blue circle) in the bottom panel:



Select the “cross hair” button from the tool bar (red arrow) and view the mass spec at each selected time by clicking on the desired region in the upper panel (left mouse click) which will bring out the corresponding MS to that particular time point in the bottom panel. Select either the mass spectrum at the peak apex from injection of your sample (highest signal intensity, green arrow) or average the signal over the apex region between 0.7-2.0 min by holding down the left mouse button and pulling over the desired region before releasing the button. The late peak at 7.1 min is our control and calibration signal and may be neglected during your evaluation.

2. Format and export the mass spectrum as a graphic

You can change the spectrum appearance by activating the bottom panel by clicking, selecting “properties/mass spectrum” from the “Edit” menu of the tool bar, e.g.:

- “Line” will change the color of the peaks
- “Peaks”: you can select the color of the labels and decimals (4 for accurate measurements and 0 for low resolution. However, please keep in mind that the used digits should comply with the precision of the instrument, which is at least 5 ppm for high resolution analysis but 1 amu for low resolution.
- Accept changes with “OK” or “Apply”

Please consider that the identity of your substance is NOT confirmed if the deviation in an accurate measurement is >5ppm; in low resolution the deviation should be <0.5 m/z.

Select the “zoom” button from the toolbar to zoom in the desired mass region drawing a rectangle by holding down the left mouse button. Now you can export the picture by selecting “copy” from the menu appearing when clicking the right mouse button in the lower panel and paste it to the desired destination or using the “Save as…” and “Export pdf” from the File menu.

3. Data interpretation:

ESI MS analysis will produce ions that correspond to adducts of the target compound with protons $[M+1]^+$, sodium $[M+23]^+$ or potassium ions $[M+39]^+$. If more than one of these ions or mixtures of them are attached to the target compound, it will have a morefold charge and you will be observing the resulting *m/*z, e.g. *m/z* = $([M+23+23]/2)^{2+}$ for attachment of two sodium ions. The distance between the isotopic peaks is 1/charge number. Acid H may be also replaced by alkali ions in solution: $[M+2\ Na\text{-}H]^+$. In this case, no change in charge is observed.

In the negative mode, deprotonation or adducts with negative ions in solution such as chloride can be observed.

In addition to that, you may have your target molecule associated with neutral solvent molecules or any other additives present in the sample solution.

The isotopic pattern of your signal can give valuable hints on the identity of the adducts. You can simulate the expected isotopic pattern under “Mass analysis/Spectrum prediction/predict” for comparison with the analysis.

In addition, you can calculate the possible elemental composition of your unknown substance using “Mass analysis/Elemental composition/Calculate from m/z”; however, we recommend editing “Mass analysis/Elemental composition/Constraints” before.

Should you need any further support in interpretation of your spectra, please feel free to contact us: Frau Oehme (36095), Frau Billig (36077), Frau Birkemeyer (senior executive, 36092).

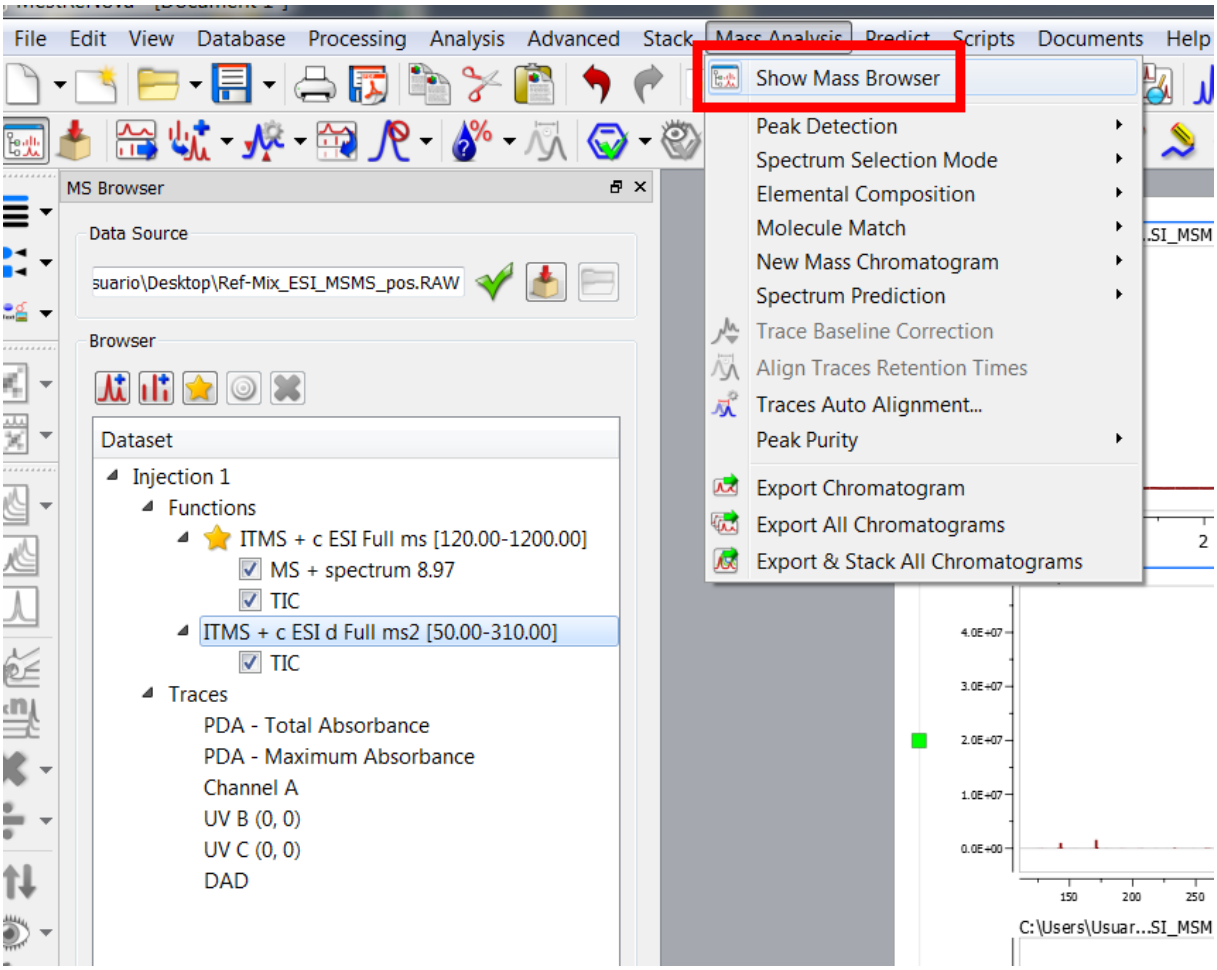
GC-MS, LC-MS and MSMS data

Please open the file and check your spectra as described before at the apices of the peaks of interest.

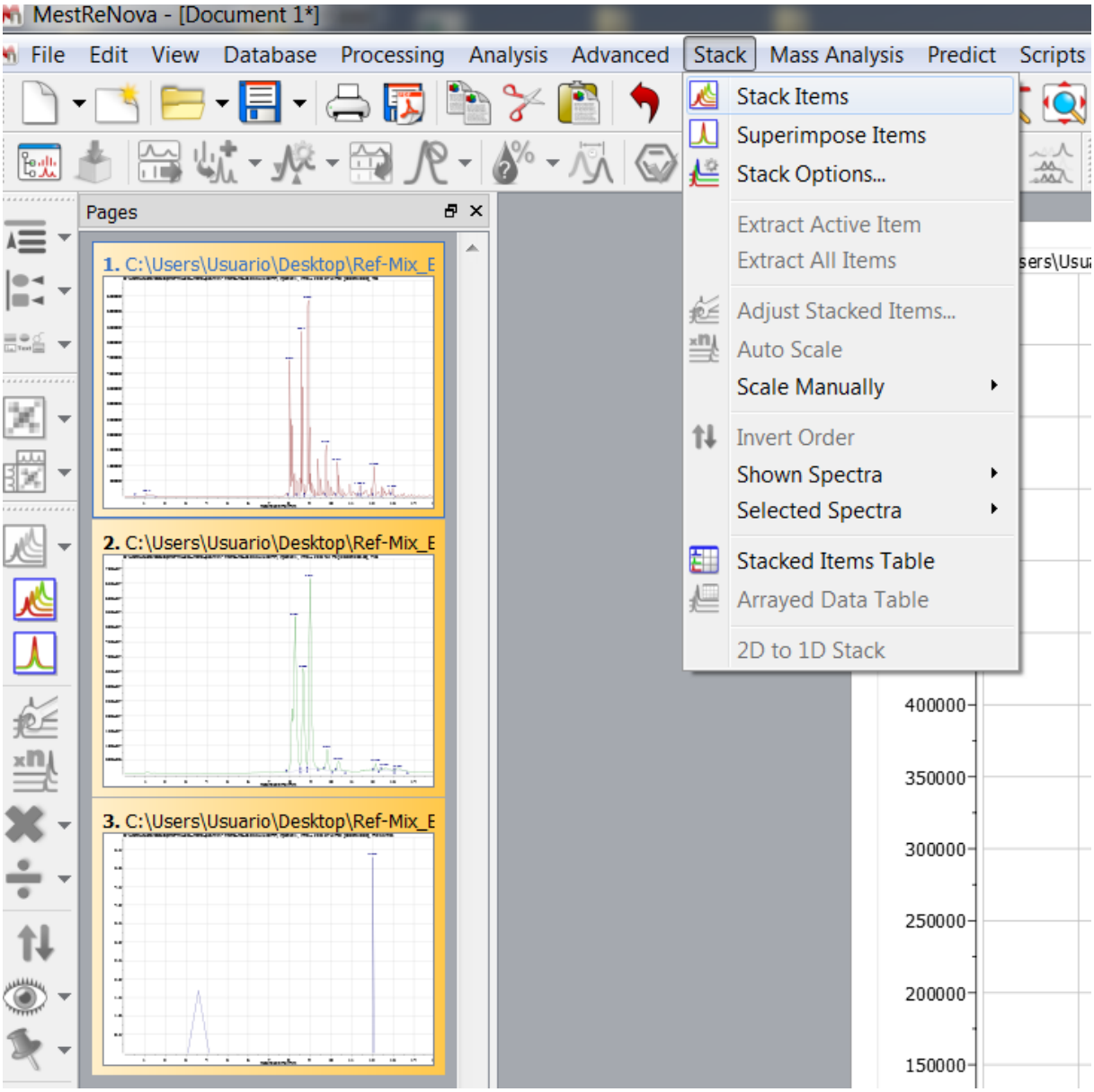
You can extract particular ions you search for using the drop down menu from the 'Mass Analysis/New Mass Chromatogram" manually typing the desired m/z.

The software features an automated peak detection for each chromatogram trace (defined as signal intensity over time, total ion current or extracted ion current) accessible from the drop down menu after clicking the right mouse button in the upper right panel and select "detect peaks".

Also, you can work with MSMS with Mnova. Following the menu 'Mass Analysis/Show Mass Browser' will display the MS Browser; from there, just double click on the MSMS function to open the applicable TIC (or the Base Peak or MS chromatogram):



You can stack/superimpose chromatograms from the same dataset by following the menu 'Mass Analysis/Export&Stack Chromatograms'. If you have different chromatograms, you will need to copy them to the same MestReNova document; next highlight all the pages from the page navigator and follow the menu 'Stack/Stack Items':



You can produce figures according to your personal needs as described in the first section.

Should you feel lost evaluating the data yourself, please don't hesitate to seek our cooperation. In particular, please get back to us for EI spectra library searches.

More detailed instructions you can find in the Mnova Manual (http://research.uni-leipzig.de/nmr/MNOVA/).