MestReNova – A quick Guide (8. April 2021)

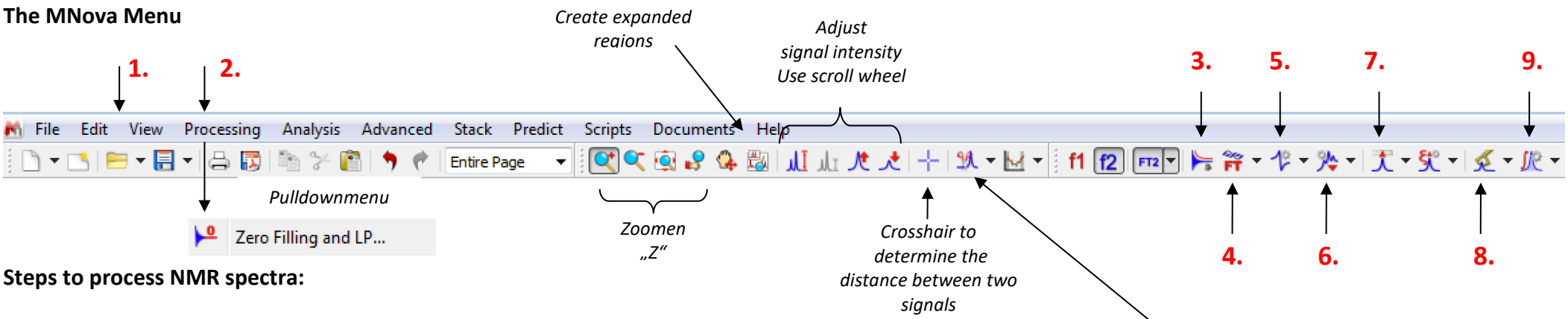
MNova is a program to analyze 1D- and 2D NMR data.

Start of MNova

Start → Chemie → MNova

Hint: This Quick-Guide refers to the classical view. If you see a red menu bar on the top, change the THEME to classic (File --> Preferences) and restart MNOVA

The MNova Menu



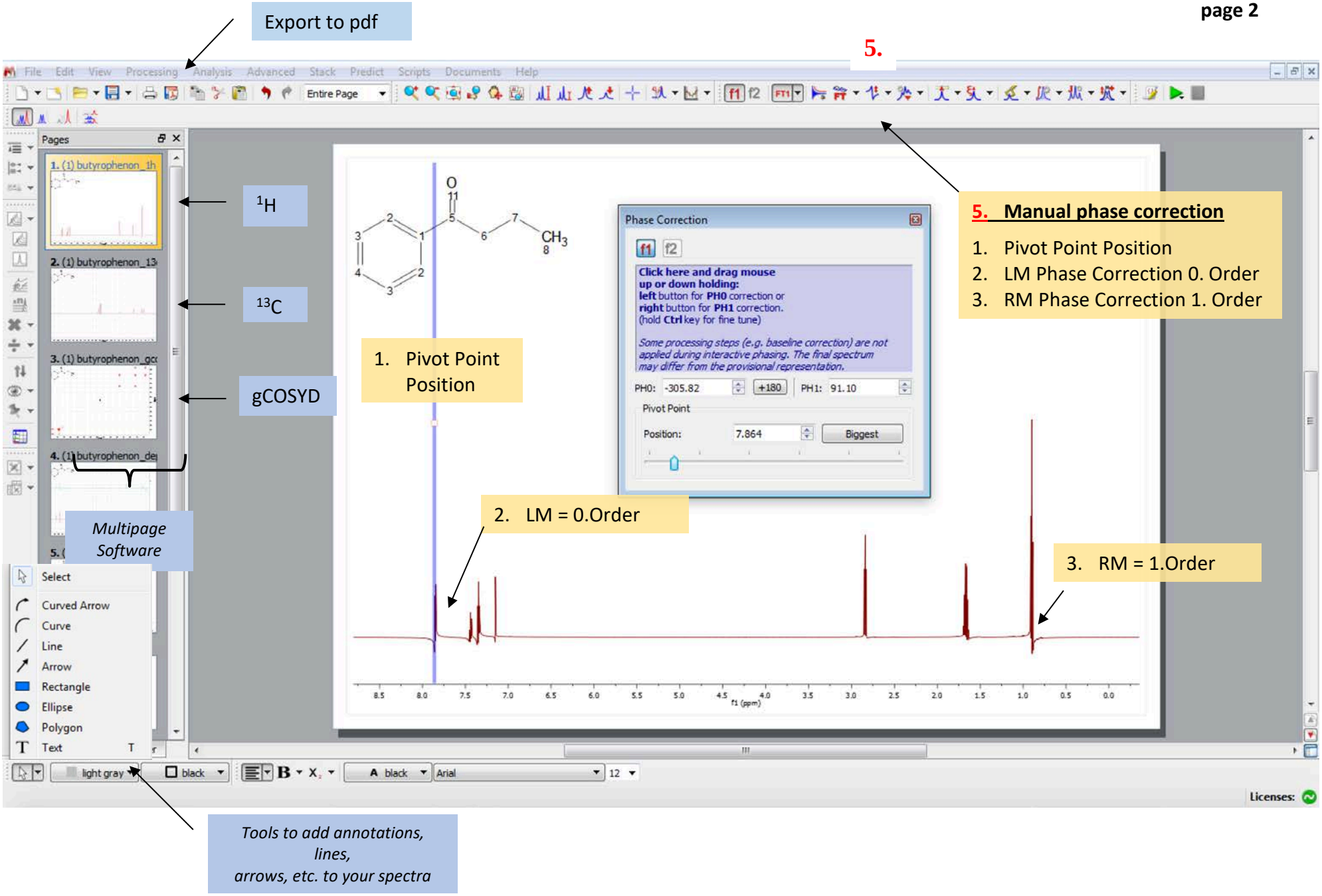
Steps to process NMR spectra:

1. Load NMR Data N:\Group\Fachbereiche\Chemie und Pharmazie\q0ocstud\MNova\MNova-Einführung
2. Zerofilling and Linear Prediction = Increase the number of digital points, resolution enhancement
3. Apodization = Apply these functions to improve S/N **or** the resolution
4. FT = Fourier transformation
   After loading the fid, MNova applies the Fourier Transformation automatically (this procedure includes also phase correction).
5. Phase Correction
6. Baseline Correction
7. Referencing to the TMS or the solvent signal
8. Peak picking
9. Integration

Manuals on the internet:

http://www.uni-muenster.de/Chemie.oc/nmr/software.html

http://mestrelab.com/software/mnova/manuals/


Export to pdf
5.
^{1}H
^{13}C
gCOSYD
Multipage Software
1. Pivot Point Position
2. LM = 0.Order
3. RM = 1.Order
5. Manual phase correction
1. Pivot Point Position
2. LM Phase Correction 0. Order
3. RM Phase Correction 1. Order
Phase Correction
Click here and drag mouse up or down holding:
left button for PH0 correction or
right button for PH1 correction.
(hold Ctrl key for fine tune)
Some processing steps (e.g. baseline correction) are not applied during interactive phasing. The final spectrum may differ from the provisional representation.
PH0: -305.82
+180
PH1: 91.10
Pivot Point
Position: 7.864
Biggest
Select
Curved Arrow
Curve
Line
Arrow
Rectangle
Ellipse
Polygon
Text
Tools to add annotations, lines, arrows, etc. to your spectra

NMR data processing with MNova

The structure of the MNova program is comparable to Powerpoint. So, you can create for each spectrum a separate page: ^{1}H-, ^{13}C-, gCOSY- and gHSQC. After loading the raw data (FID file), the data will be processed (FT, phase correction) automatically. Unfortunately, the automatic phase correction doesn't work properly all the time, thus sometimes it's necessary to redo the phase correction manually. After you've finished the processing, save these data as MNova file. In this way, you will be able to reload these data later, without the necessity to redo the processing.

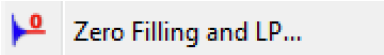
Start the Program

- PC of NWZ: Start → Chemie → MNova Private PC: Start → MNova

1. Load data

- Strg O
- For the practical course OCF browse to N:\Group\Fachbereiche\Chemie und Pharmazie\q0ocstud\OC-Praktika\ocf
- Choose the right fid or ser-file
- Fourier Transformation and Phase Correction are executed automatically, so that the transformed spectrum will appear after loading the fid.

2. Zero Filling and Linear Prediction

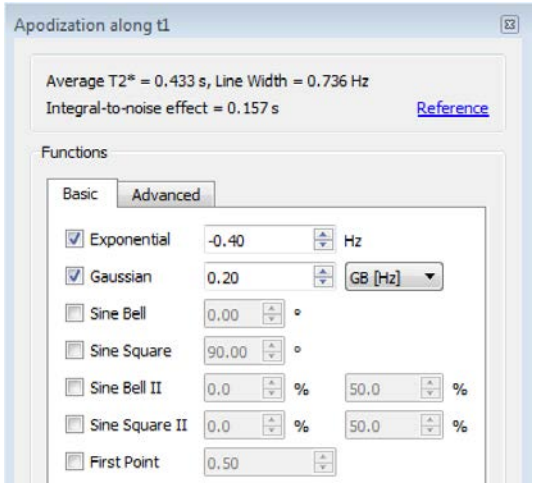
Processing → 

- Generally, the data points of the raw data (*Spectrum Size*) are doubled by zero filling → After zerofilling the signal shape will be smoothed.
- Linear Prediction is an algorithm to calculate the expected data points at the zero filled end of the FID (*forward prediction*).
  The alternative *backward prediction* is primarily used for nuclei with extreme short T1-values to calculate the beginning of the FID. In this way the problem of baseline distortions (due to probe ringing) is solved.

3. Apodization

a) **Improvement of Signal to Noise (S/N), e.g. in case of ^{13}C NMR spectra**
The exponential multiplication emphasizes the beginning of the FID (signal), whereas the end of the FID (noise) is weighted less. In this way the S/N ratio is improved, but at the cost of getting broader lines (*linebroadening*). The bigger the lb value is, the broader appears the resulting line. Typical lb values for ^{13}C: *Exponential* lb = + 1 Hz.

b) **Improvement of Resolution, e.g. in case of ^{1}H spectra to resolve small line splitting**
The Gaussian multiplication emphasizes the end of the FID's (coupling and noise), whereas the beginning of the FID (signal) is weighted less. The resolution of the signal will be improved on the cost of a worse signal to noise ratio. Typical values for ^{1}H: *Gaussian* = **0.1 to 0.5**, *Exponential*: lb= **-0.1 to – 1.0**



4. FT = Fourier transformation

- The Fourier transformation is executed automatically after opening the fid file.

5. Phase correction

- Chose the option *Manual Correction* within the pull-down menu **Phase Correction**. The procedure of phase correction is described in detail on the screenshot on the next page.
- Bear in mind that the automatic phase correction results quite often in poor results.

6. Baseline correction

- Select the option *Baseline Correction* within the pull-down menu **Baseline Correction**. Then select the *Whittaker Smoother* as method.
- From now on the method *Whittaker Smoother* is used during the *Full Auto* baseline correction.

7. Reference the TMS or the solvent signal

- Click on the **TMS** button.
- Place the appearing red cursor line to the signal which should be referenced and click the LM.
- Either you enter the corresponding ppm value manually, or you select the corresponding solvent after clicking the **Solvents** button.

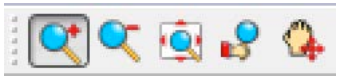
8. Peak-Picking

- Select the option manual threshold within the pull-down menu **Peak Picking**.
- Press the LM left to the signal, hold the LM and drag the cursor over the signal.
- The appearing horizontal line defines the lowest intensity of all signals which should be labeled with peak picking.

9. Integration

- Select the option *Manual* within the pull-down menu **Integration**.
- Press the LM left to the signal, hold the LM and drag the cursor over the signal.
- To normalize an integral value, place the cursor to the integral and click the LM two times. Enter the right integral value in the appearing window (e.g. 3 for a single CH_3 group).

10. Zoomen



Expand

Zoom out

Full

Enter the limits manually

11. Vertical Scale

- The easiest way to adjust the vertical scale is done with the scroll wheel.

Scale the most intense signal to the height of

Decrease signal intensity

Increase signal intensity

12. Crosshair to determine line splitting

- It appears an info-box and a blue cursor line.
- Move the blue cursor line to the left signal of the multiplet.
- Press the LM, hold the LM and move the additional appearing line to the next signal.
- The info box will display the line splitting in Hz.

13. Stack two or more spectra on one page (e.g. ^{13}C and DEPT)

- 1st page: Load ^{13}C spectrum (fid)
- 2nd page: Load DEPT
- Mark both pages on the left by using the Strg-key + the LM (→ blue border)
- Menu bar on the top: **Stack** → *Stack Spectra*

14. Selective processing of *„stacked“* spectra

- left menu bar

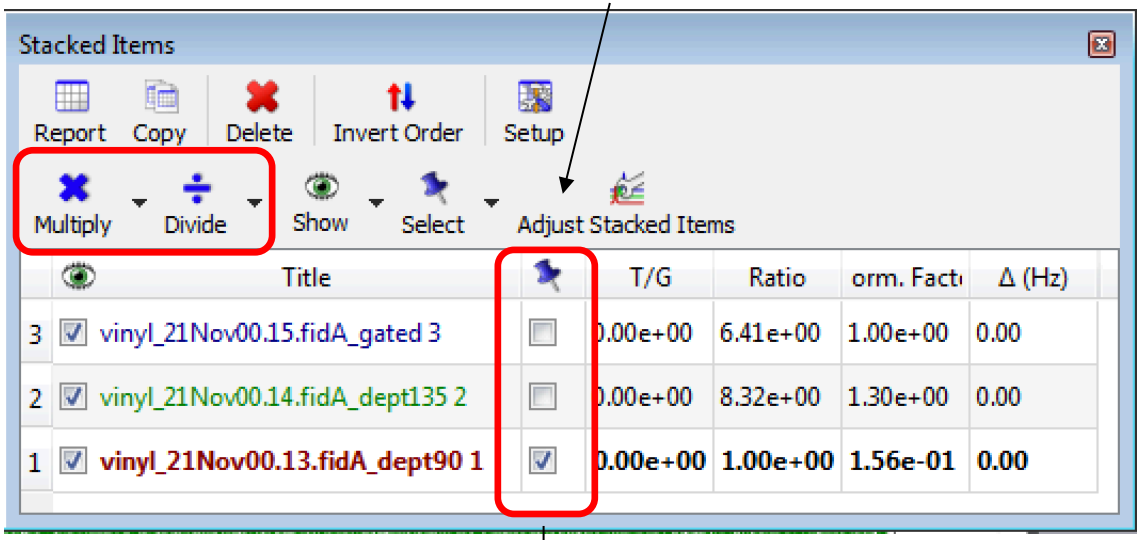
Adjust vertical scale selectively (e.g. carbon only)

Autoscale spectra

Increase vertical scale of selected spectra

Decrease vertical scale of selected spectra

Select spectra for processing



*^{13}C is activated for processing, so during phase correction only the phase of the carbon spectrum is changed, **but not** the phase of the dept spectra.*

*Three methods, to process one spectrum **or** several spectra simultaneously*

- If you use the scroll wheel, the vertical scale of all spectra will be changed simultaneously.
- If you want to change only the active spectrum (blue bar, right to the spectrum), you've to deselect all spectra. To change the active spectrum, point the cursor to the selected spectrum and press the left mouse button. Then click or .
- If you want to process several spectra simultaneously, you've to select them by clicking the corresponding checkboxes.

15. Cut function

- With the aid of this function you can suppress the display of certain spectral regions (e.g. regions, which show no signal).
- Select the button which shows a **signal & scissors** on the top menu bar.
- Move the appearing cursor left to the region which you like to suppress, press and hold the LM and drag the mouse over the region to suppress.

16. Copy/Paste into other Windows programs (Word, Powerpoint)

- Click with the LM inside the spectrum, so that a green border will appear around the specified spectrum.
- Now you can copy the specified spectrum from MNova to e.g. Word by using **Ctrl C** and **Ctrl V**.

17. Create spectral expansions on the top of the page

- Click on the button **spectrum & glasses**, so that the cursor appears as magnifier and a plus sign.
- Press the LM left to the signal, hold the LM and drag the cursor over the region, which should be expanded.
- If you like, you can process the expanded region after activating this expanded region by clicking the LM inside the expanded region.

18. IUPAC Chemical Shift referencing

If you measure a set of NMR data, firstly, the proton NMR spectrum has to be referenced to the TMS signal (0 ppm). According to the IUPAC recommendation from 2001, the referencing of all other spectra will then be calculated by the UNIFIED SCALE. Thus, using a suitable secondary reference compound is no longer recommended!

In case of inaccurate referencing of the proton NMR spectrum by the spectrometer, you have to redo referencing for the whole NMR data set:

1st step: Reference the TMS signal of proton NMR:

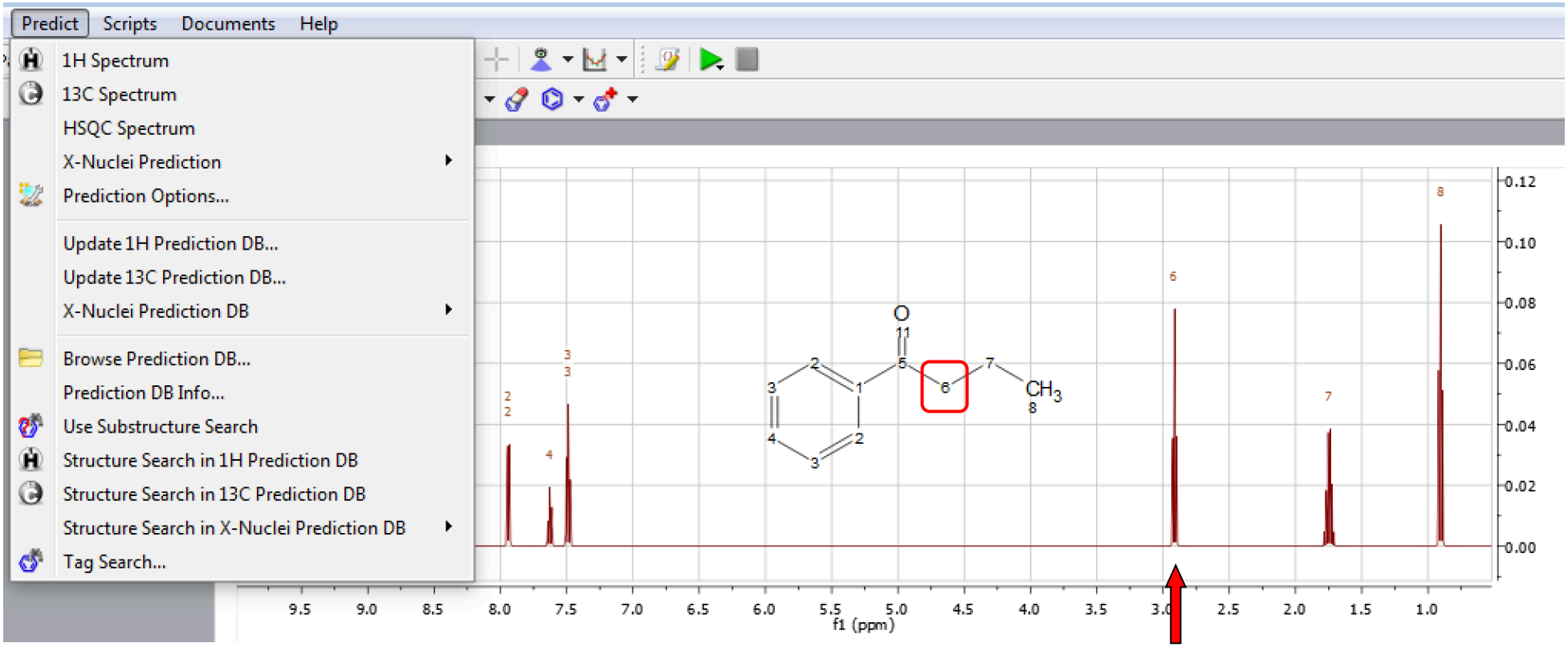
- Load the proton NMR spectrum
- Upper menu bar: *Analysis* ⇒ *Reference* ⇒ *Reference* ⇒ Point the cursor to the TMS signal and enter 0
  (If no TMS was added to the sample, you can reference the residual protonated solvent signal instead)

2nd step: All other spectra of your sample, which were recorded on the same day and with the same spectrometer (same lockfrequency!), have to be referenced by using the *UNIFIED SCALE* relative to the before referenced proton NMR spectrum (see 1st step):

- Load all other spectra of your sample, which have been measured on the same day and spectrometer as the proton NMR spectrum
- Upper menu bar: *Analysis* ⇒ *Reference* ⇒ *Absolute Reference* ⇒
  At the top of the appearing dialog box you'll find the proton NMR of your dataset predefined as reference
  All other spectra are preselected for absolute referencing
- Click OK

19. Predict NMR Spectra

- Draw your structure with ChemDraw and copy and paste this structure on a new page in MNova.
- Menu bar on the top: **Predict** → *^{13}C Spectrum.*
- If you move the cursor to a carbon of the structure the corresponding carbon signal will be highlighted by a blue line.



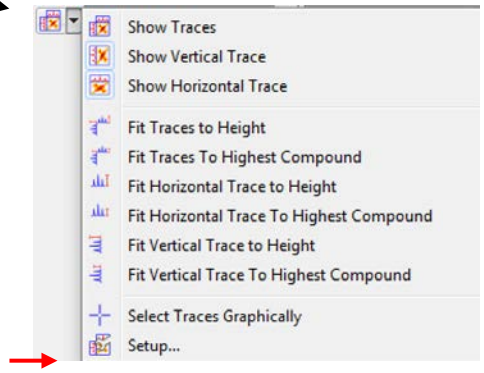
If you move the cursor on a specific signal the corresponding carbon of the structure will be highlighted by a red box.

20. Shortcuts

- Ctrl C / Ctrl V : Copy/Paste e.g. to copy a structure from ChemDraw to a page of MNova or to copy a spectrum from MNova to Word.
- Ctrl O : Open NMR data
- Ctrl M : New page
- Ctrl Z : Undo the last action
- Z : Select the **Zoom** mode
- C : Select the **Crosshair** mode
- E : Select the **Expand** mode
- Hold Space bar : While you're holding the space bar, the panning mode is selected temporarily. So, you can move the displayed spectral region.
- Esc : Leave the last chosen mode

21. 2D spectra with external projections (see screenshot on the next page)

- 1st page : Load ^{1}H spectrum (fid)
- 2nd page : Load ^{13}C spectrum (fid)
- 3rd page : Load gHSQC spectrum (fid oder ser)
- **Left menu bar**: Select the pull-down menu *Show Traces* (Icon with 2D-Plot + projections) and select *Setup*.
- Select the right ^{1}H and ^{13}C projections and define them as vertical and horizontal projection (cp. screenshot).

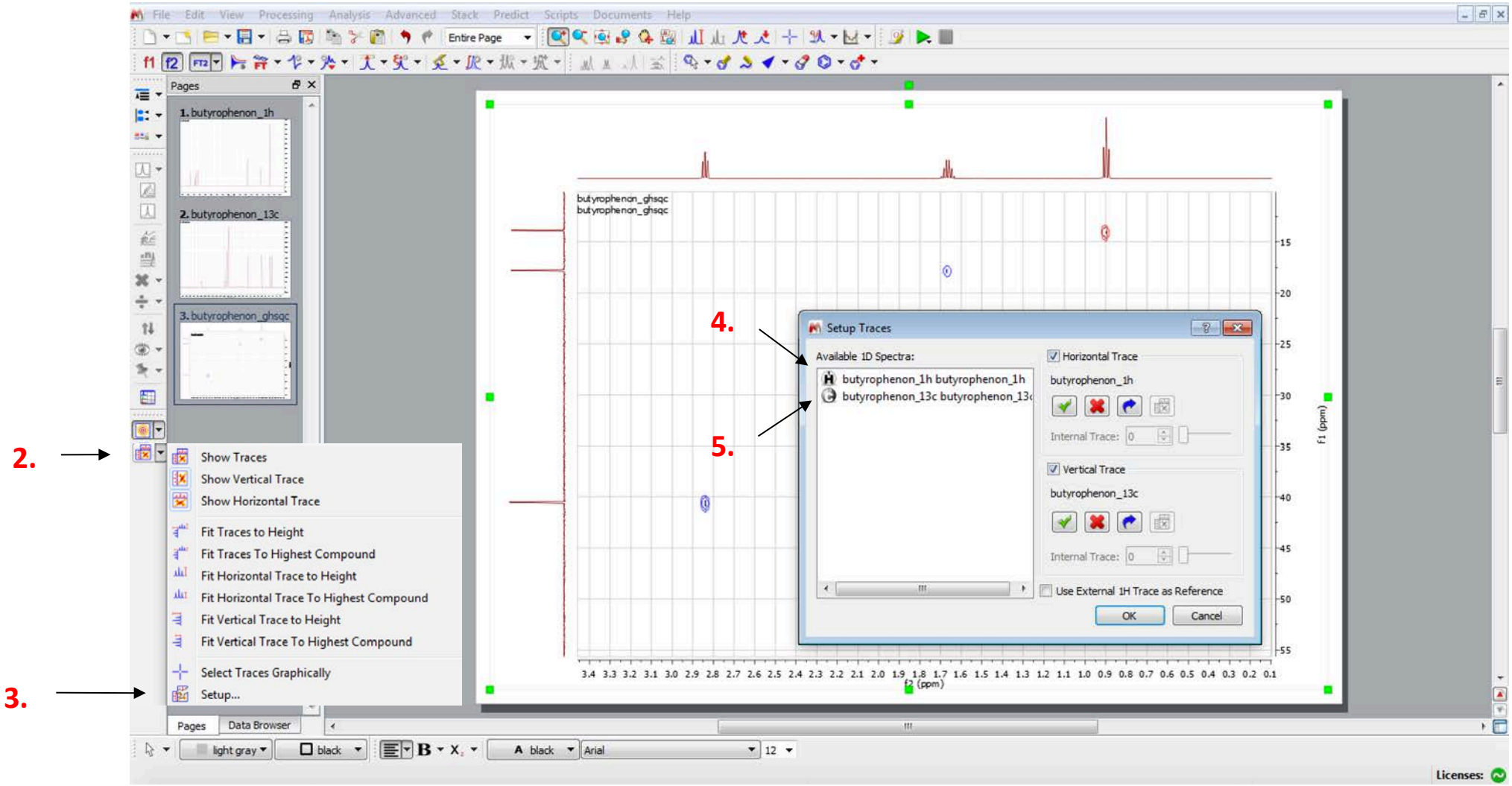


22. Phase correction of phase sensitive 2D NMR Spectra (^{1}J(C,H) correlation = gHSQC)

- Phase sensitive 2D NMR spectra need a phase correction along the F2 (^{1}H) and the F1 (^{13}C) axis. The main principle of 2D phase correction is comparable to that one for 1D phase correction. The only difference is that you have to choose the direction which should be adjusted (F1 or F2) by clicking on the corresponding F1 or F2 button.

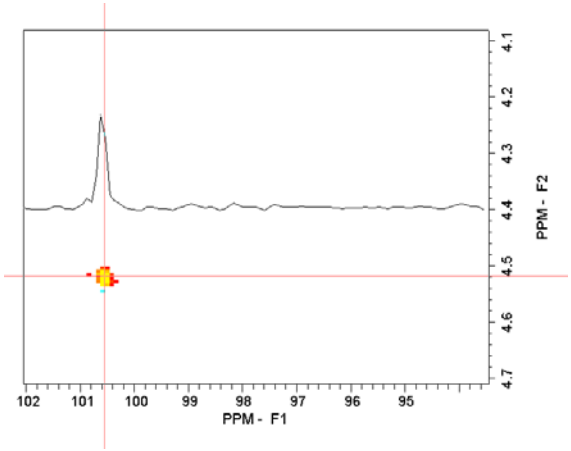
2D NMR: $^{1}J(C,H)$-Korrelation

1. Load ghsqc/fid
2. Select Show Traces
3. Setup
4. Select H for the horizontal trace
5. Select C for the vertical trace

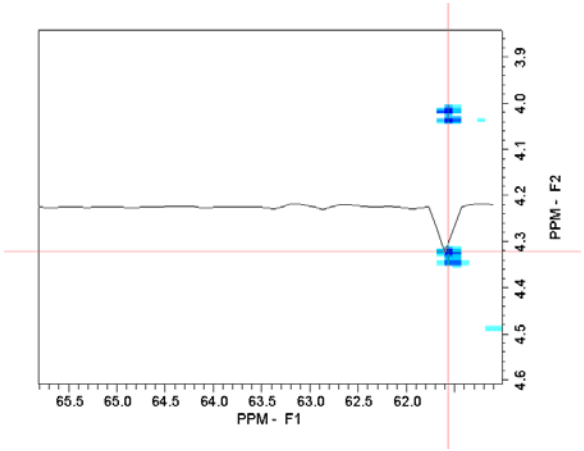


Right phase along F1 und F2:

Positive absorption signal in F1 and F2
e.g. CH_3 or CH in gHSQC

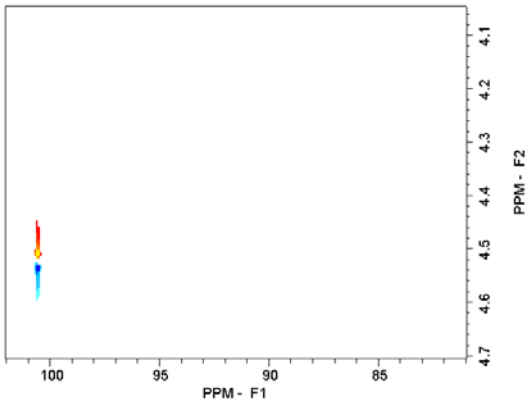


Negative absorption signal in F1 and F2
e.g. diastereotopic CH_2 in gHSQC



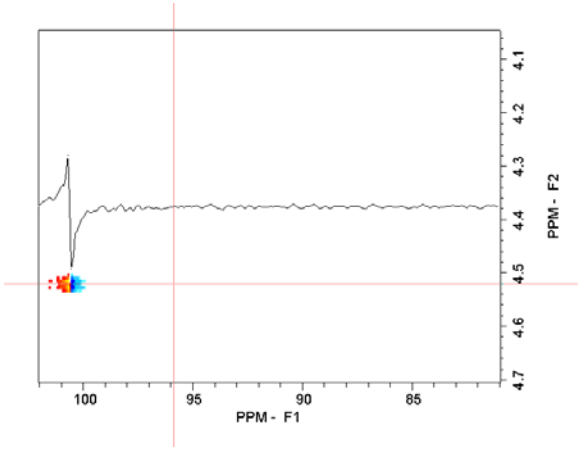
Phase error along F2:

Dispersion signal
Positive and negative parts along F2



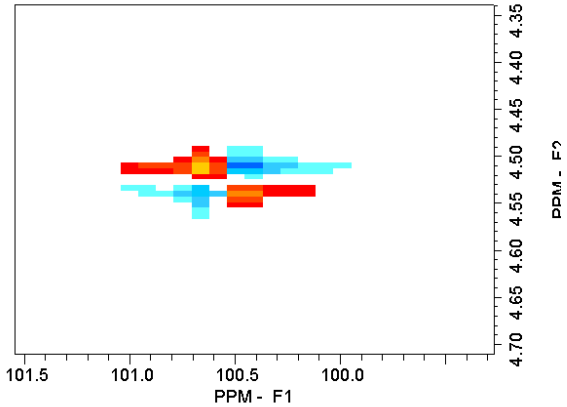
Phase error along F1:

Dispersion signal along F1
Positive and negative parts along F1



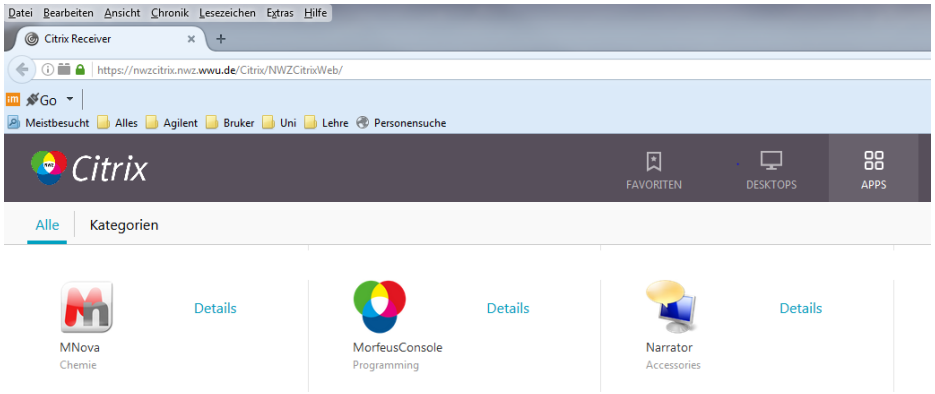
Phase error along F1 and F2:

Dispersion signal along F1and F2
Positive and negative parts along F1 and F2



23. MNova by Citrix Receiver

Start Citrix-Receiver: https://nwzcitrix.nwz.wwu.de/Citrix/NWZCitrixWeb/



24. Local installation of MNova

see: http://www.uni-muenster.de/Chemie.oc/en/nmr/software.html