

TReNDS 1.0

Manual

October 9, 2018

Abstract

The technique of time-resolved non-uniform sampling (TR-NUS) makes it possible to use standard multidimensional pulse sequences for process and reaction monitoring. It preserves the temporal resolution close to that achievable in 1D experiments.

TReNDS (Time-Resolved N-Dimensional NMR spectroscopy) is a free, user-friendly software kit for acquisition and processing of TR-NUS data. The program works on Bruker, Agilent and Magritek spectrometers, making it possible to carry out up to four experiments with an interleaved TR-NUS. It can be also used on data stations for spectral processing and data visualization.

The concept of TR-NUS has been described in several papers (see [1, 2, 3, 4, 5, 6] in the References below). In brief, the idea is to acquire NUS data in parallel to a certain process occurring in the sample and affecting the spectrum. The data is divided into subsets, each processed with NUS reconstruction algorithm (here iterative soft thresholding, IST or iteratively re-weighted least squares, IRLS). As a result, one obtains a stack of spectra constituting a “temporal pseudo-dimension”, that corresponds to the reaction progress. In other words, e.g. 2D HSQC is turned into 3D HSQC-movie.

1 Glossary

- NUS - non-uniform sampling [7]
- TR-NUS - time-resolved non-uniform sampling [1, 2, 3, 4, 5]
- “frame” - a subset of TR-NUS data used to reconstruct a single spectrum[1, 2, 3, 4, 5]
- “frame size” - a number of NUS points in a subset[1, 2, 3, 4, 5]
- “frame overlap” - a number of NUS points belonging to both consecutive “frames”
- IST - iterative soft thresholding algorithm[8]
- IRLS - iteratively re-weighted least squares algorithm[8]
- VE - virtual echo[9]

2 Programs in the TReNDS package

- trends-agilent-acq.py interleaved TR-NUS acquisition macro for Agilent
- makeFID - data management macro for Agilent
- trends-bruker-acq.py interleaved TR-NUS acquisition macro for Bruker
- trends-bruker-acq-temperature.py temperature-sweep TR-NUS acquisition macro for Bruker
- trends-magritek-acq , trends-magritek-acq_2exp interleaved TR-NUS acquisition macros (2 or 3 interleaved experiments) for Magritek
- trends-proc.py TR-NUS processing GUI

3 Installation

3.1 Linux

For Linux, we recommend installation via python-pip program. Additionally we recommend to download and install gtk-3 versiion of wxPython library from <https://wxpython.org/Phoenix/snapshot-builds/linux/gtk3/> using instructions provided in <https://wxpython.org/pages/downloads/index.html>

3.1.1 Using python-pip:

1. Install MddNMR package from <http://mddnmr.spektrino.com>
2. Install python-pip (e.g. `sudo apt-get install python-pip` or `yum install python-pip`)
3. Download Trends.whl from <http://trends.spektrino.com>
4. Install TReNDS : `pip install Trends.whl`
5. You can start TReNDS by typing in terminal: `trendsnmr`

3.1.2 Using source code:

1. Install MddNMR package from <http://mddnmr.spektrino.com>
2. Check if you have the following python packages:
 - wxpython (version 2.8 or newer. We recommend version 4)
 - matplotlib
 - scipy (version 0.14.0 or newer).
 - numpy
 - nmrglue (version 0.6 or newer)
 - python2.7
3. If your system does not have the above mentioned packages, you can install them via python-pip or use Anaconda python distribution (recommended for old systems)

4. Download the source code from <http://trends.spektrino.com> and unpack it
5. Run: `trends-proc.py` in the folder containing the source code

3.2 MacOS

3.2.1 Using dmg installer

1. Install MddNMR package from <http://mddnmr.spektrino.com>
2. Download TReNDS.dmg from <http://trends.spektrino.com>
3. Open TReNDS.dmg and drag TReNDS App to Application folder
4. Open TReNDS from Applications

3.2.2 Using python-pip

Follow the instructions for Linux

3.3 Windows

On Windows TReNDS works only under Windows 10 Creators Fall Update (or newer). The reason is that currently MddNMR package works only on UNIX systems and has to be installed in Windows for Linux Subsystem (WSL), the first stable version of which was released on Windows 10 Creators Fall Update.

1. Activate WSL: docs.microsoft.com/en-us/windows/wsl/install-win10
2. Install MDDNMR package in WSL: <http://mddnmr.spektrino.com>
3. Download TReNDSsetup.exe from <http://trends.spektrino.com>
4. Install TReNDS
5. Launch TReNDS from Start Menu

4 Using TReNDSacquisition macros

The acquisition system works for Agilent, Bruker and Magritek systems.

4.1 Agilent

Before the first use of TReNDS on Agilent system, copy file `makeFID` to `maclib` folder (e.g. `/userpath/vnmrsys/maclib/makeFID`). Ensure that `makeFID` file has read/write accessibility. `makeFID` can be downloaded from <http://trends.spektrino.com>.

1. Open Agilent's VnmrJ software
2. Type `listenon` in VnmrJ console

The return message shown in Figure 1 should appear:

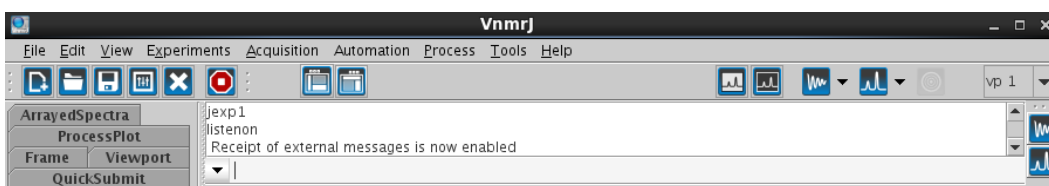


Figure 1: Typing `listenon` in VnmrJ console

3. Run `trends-agilent-acq.py` in the terminal
4. Choose the number of 2D spectra for interleaved acquisition

User can select up to three 2D spectra for interleaved acquisition. If more than one 2D spectrum is selected (one is default), a new panel or panels will appear. Every panel is separated by a horizontal line and corresponds to the acquisition and processing parameters of a single 2D spectrum (Figure 2).

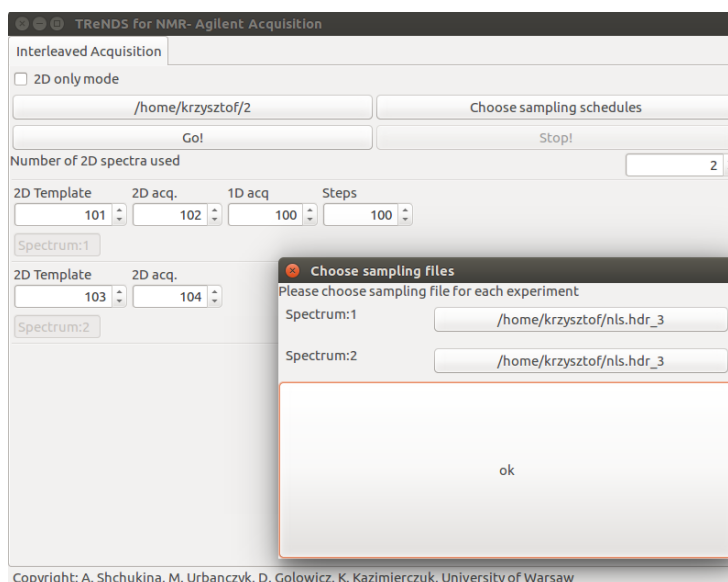


Figure 2: Acquisition setup interface for Agilent (`trends-agilent-acq.py`) with sampling schedule selection window open. Data will be saved in `/home/krzysztof/2`. NUS experiment templates are set in experiments number 101 and 103, acquisition will be run in 102 and 104. Additionally, 1D experiment set up in 100 will be run. Every step of acquisition will involve measurement of 1D spectrum in 100, 2 NUS points in 102, and 2 NUS points in 104. The 100 steps of acquisition will be performed (200 NUS points for every 2D experiment).

5. Prepare a 1D experiment in Agilent's VnmrJ software and put its number into TReNDS in the '`1Dacq`' field. The '`1Dacq`' field is located in the panel of the first 2D spectrum (shown in Figure 2). Acquiring a 1D spectrum in an interleaved manner can be disabled

by choosing *2D only* mode.

6. Prepare a 2D experiment in Agilent's VnmrJ software and put the experiment number into TReNDS in the '*2D Template*' field.

If user selects more than one 2D spectrum for interleaved acquisition, the following steps in this section must be repeated for every 2D spectrum in the corresponding panel: 6, 7, 9.

7. Click *Acquire* → *NUS tab* → *Enable non-uniform sampling* → *Use advanced schedule options* in VnmrJ workspace with a prepared 2D experiment and then click '*Build*' (See Figure 3).

IMPORTANT: in case of Biopack change 'Schedule mode' (Advanced options) from 'Auto' to 'Index'

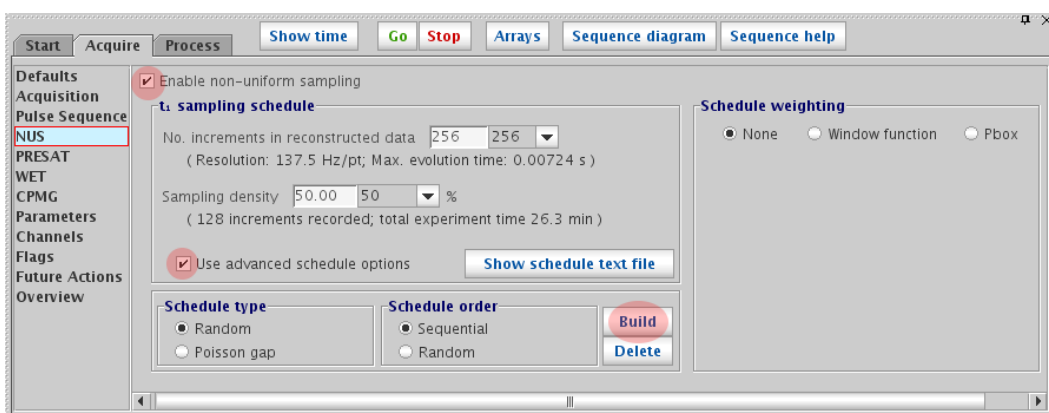


Figure 3: Enabling NUS and building schedule in VnmrJ

The parameters selected for building the NUS schedule in VnmrJ are not taken into account by an interleaved acquisition in TReNDS. However, it is important to enable NUS in VnmrJ experiment and create an appropriate file structure by clicking the **Build** button.

8. Set the number of *Steps*

TReNDS defines '*step*' as a measurement of 2 NUS points in the indirect dimension (2 increments) for every interleaved 2D experiment in a cycle. For example, for a set-up involving one 1D experiment and two 2D experiments, one step of an interleaved acquisition cycle means:

Acquire 1D spectrum → Acquire 2 indirect dimension points of the first 2D spectrum → Acquire 2 indirect dimension points of the second 2D spectrum.

The number of steps define the number of interleaved acquisition cycles.

9. Choose an empty experiment workspace in Agilent's VnmrJ software and put its number into TReNDS in '*2D acq*' field.

This will be the working directory for the acquisition of a 2D experiment. In practice, the experiment does not have to be empty. However, existing parameters and data stored in this experiment will be overwritten.

10. Choose *sampling schedule* file in TReNDS .

Non-uniform sampling schedule is a text file, which can be generated using `nussampler` program from MddNMR package (required for data processing - see installation section, Paragraph 3).

IMPORTANT NOTES:

- The number of points in a generated NUS schedule divided by 2 is the limiting maximum number of *Steps* (for example, 20,000 points in the NUS schedule file is the number limiting *Steps* to 10,000).
- The maximum increment value in a NUS schedule must be equal to the number of increments (`ni` parameter) in a prepared 2D experiment (see Point 6 in this section). For example, a 2D experiment prepared in Agilent's VnmrJ software has the `ni` parameter set to 256, and the generated NUS schedule includes *X* points from 0 to 255.
- TReNDS can exploit different NUS schedules for each of the interleaved 2D experiments.
- Acquisition macro sets a number of steady-state scans to zero.

11. Choose *Working Directory*.

Working directory is a place where TReNDS creates folders structure for a given interleaved measurement. Acquired and processed data will be saved there.

12. Click the '*Go!*' button to start acquisition.

13. User can stop the acquisition any time using the '*Stop!*' button. (Warning! The acquisition will stop after one cycle of interleaved experiments)

4.1.1 Agilent acquisition example

The example shows how to fill in TReNDS fields in compliance with prepared VnmrJ experiments to perform interleaved acquisition of one 1D spectrum (PROTON) and three 2D spectra (TOCSY, HSQC, and HMBC).

1. Actions in Agilent's VnmrJ software:

```
listenon
jexp100
PROTON
nt=1 d1=1 ...
jexp101
zTOCSY
ni=256 nt=2 ...
```

enabling NUS and clicking 'build' button (Figure 3)

jexp103

gHSQCAD

ni=256 nt=4 ...

enabling NUS and clicking 'build' button

2. TReNDS GUI filled according to prepared experiments

Figure 2 presents TReNDS ready for performing interleaved acquisition.

3. Click '*Go!*' to start acquisition

4.2 Bruker

Put file `trends-bruker-acq.py` into directory `/opt/topspin3.5p17/exp/stan/nmr/py/user/` (or appropriate, corresponding to your TopSpin distribution).

1. Open *Topspin*
2. Prepare experiments to acquire (standard 2D)
3. Type `edpy`
4. Execute `trends-bruker-acq.py` (see Figure 4)
5. Set the number of steps
6. Choose a sampling schedule file from `trends-bruker-acq.py`
7. Choose 2D and 1D experiments as templates. (**Do not use 'Find' button! - this will crash our script**)
8. Choose a folder to save the acquired data
9. Click *Start Acquisition!*
10. *Start Acquisition!* will show progress in the acquisition.

4.3 Magritek

To use TReNDS on Magritek Spinsolve spectrometers, you need to have SpinsolveExpert program installed. Four acquisition macros for Magritek are provided:

1. `trends-magritek-acq`
2. `trends-magritek-acq_2exp`
3. `trends-magritek-acq-calib`
4. `trends-magritek-acq_2exp-calib`

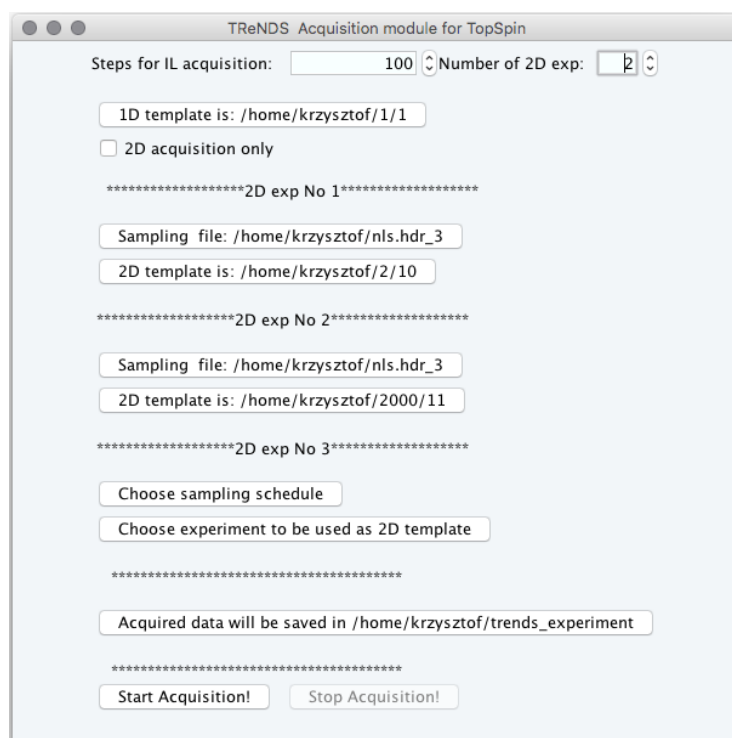


Figure 4: Acquisition setup interface for Bruker (`trends-bruker-acq.py`) with one 1D experiment and two 2D experiment templates set. Data will be saved in `/home/krzysztof/2`. NUS experiment templates are taken from `/home/krzysztof/2/10` and `/home/krzysztof/2000/11`. Every step of acquisition will involve measurement of 1D spectrum, 2 NUS points in experiment 1, and 2 NUS points in 2000. The 100 steps of acquisition will be performed (200 NUS points for every 2D experiment).

The first two allow to interleave 1D and 2D experiment (`trends-magritek-acq`) or 1D and two 2D experiments (`trends-magritek-acq_2exp`). The next two are their modifications ("`-calib`"), which include frequency calibration experiment, namely Findfo-H. The quick calibration experiment is placed before 1D experiment in the interleaved loop. The experiment finds proton resonant frequency for the highest peak and set transmitter offset to 4.72 ppm for ^1H and 110 ppm for ^{13}C (values can be set manually in a macro). Using "`-calib`" version may be useful when B_0 field remains unstable and peaks does not move in a course of monitored process.

Additionally, SpinsolveExpert's sequences do not have NUS support. Therefore, the pulse programs have to be modified before TReNDS interleaved acquisition can be run. The listed macros assign Sampling Schedule to a `NUSFile`. Variable `NUSFile` should be added to the pulse sequence "default parameters" and "user interface", and must be imported in "Experiment control" macro. The loop over mixing time in "Experiment control" needs to be modified for including `NUSFile`. If You need any help with pulse sequence modification, please contact us.

Follow these simple steps to acquire a data:

1. Place acquisition macros in "Scripts" catalogue in Spinsolve Expert directory

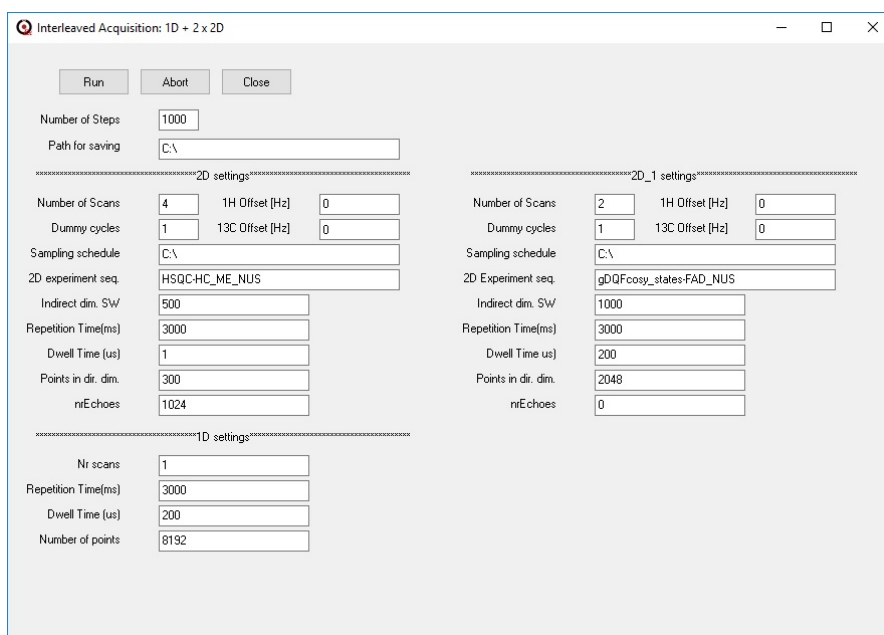


Figure 5: Acquisition macro GUI for Magritek

(/userpath/Applications/SpinsolveExpert/Scripts).

2. Open Spinsolve Expert software and select one of the earlier mentioned macros from Scripts list. The Interleaved Acquisition GUI should appear (Fig 5)
3. Define path for saving, 2D experiment pulse sequence name, sampling schedule and all required acquisition parameters.

Definition of *Steps* and informations regarding *Sampling Schedule* can be found in Agilent section (4.1). All fields must be filled. When correlation experiment other than H-C is performed, the *13C offset* field should be filled with anything (eg. "-" or "o"). The same rule concerns *nrEchoes* parameter, which is characteristic only for carbon correlation experiments.

4. Press **Run** button to start acquisition

The acquisition can be aborted anytime with **Abort** button

5. Acquired data can be processed in TReNDS running on Windows platform (See Paragraph 3.3) as well as on MacOS and Linux systems.

- **IMPORTANT NOTES:** Magritek's variables *nrPnts* (Points in dir. dimension) and *dwellTime* (Dwell Time) have different definitions when applied in H-C experiments. If you are not sure how to fill it, just copy values from standard Magritek parameters.
- Typically for Magritek, direct dimension is recorded with a very broad spectral width. When processing a data, remember to trim F2 dimension to reduce processing time.

4.4 Other platforms

TReNDS is developed on the platforms to which the authors have access. If we do not support your spectrometer please contact us. We can arrange a cooperation and develop TReNDS module (with your help) for the new platform.

5 Data processing and Analysis

5.1 Data storage system

All data are stored in a selected folder with the following subfolder structure:

- **Acquired**

- 1D

- 0,1,2... - number reflects TReNDS step

- 2D

- 0,1,2... - number reflects TReNDS step

- 2D_1 (if more than one 2D experiment is chosen)

- 0,1,2... - number reflects TReNDS step

- 2D_2 (if more than two 2D experiments are chosen)

- 0,1,2... - number reflects TReNDS step

- **Reconstructed**

- 2D

- 0,1,2... - the number of a reconstructed frame

- 2D_1 (if more than one 2D experiment is chosen)

- 0,1,2... - the number of a reconstructed frame

- 2D_2 (if more than two 2D experiments are chosen)

- 0,1,2... - the number of a reconstructed frame

- **Analysis**

- Peak tracking data, e.g., `Peak_at_3.398_77.678.txt`.

- **DynamicsCenter**

- Data saved in the DynamicsCenter format. To import the data to DynamicsCenter, use file `Filelist.txt` from this subfolder as the list of 2D spectra in the DynamicsCenter import menu.

5.2 Processing

5.2.1 MddNMR

Processing is performed using Compressed Sensing algorithms (IST and IRLS) from MddNMR package. Please refer to MddNMR manual for details (mddnmr.spektrino.com). IST, being usually faster, can be the method of choice for on-the-fly reaction monitoring. However, IRLS can give better results for low sampling levels[10].

By default, for Bruker and Agilent data the multi-threaded processing is used. A single-threaded standalone cssolver program is used for processing Magritek data on Windows.

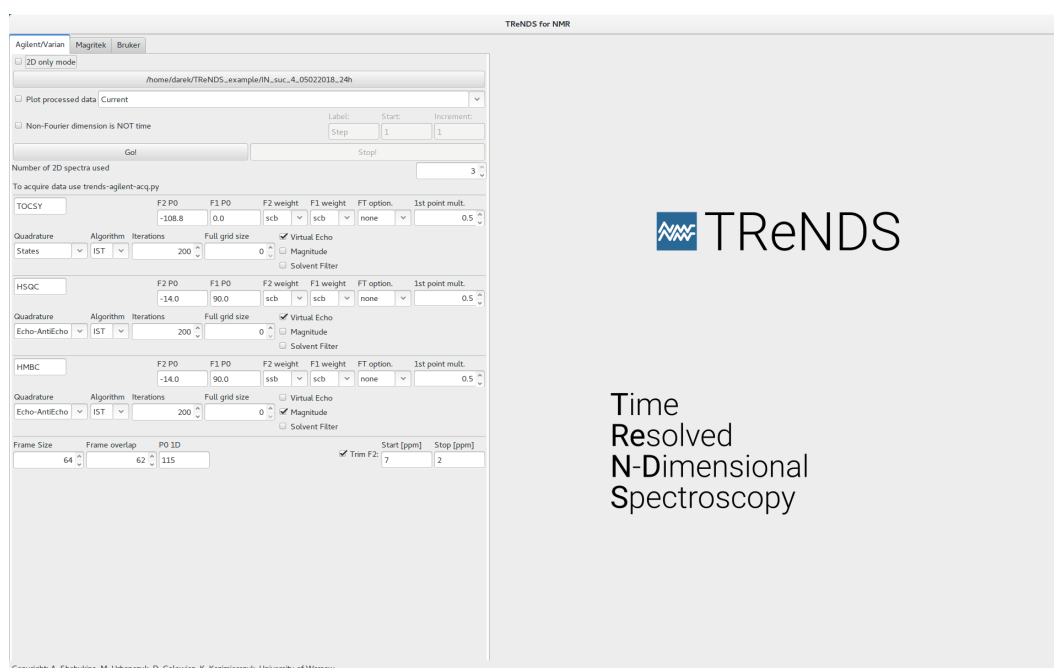


Figure 6: TReNDS processing GUI (before processing).

5.2.2 Using GUI

All the buttons and options in TReNDS have a tool-tip describing how to use it. Just hover the mouse pointer above the option to see it. Important points:

- Select a directory with the experimental data. If the folder contains previously measured data, they will be loaded together with the acquisition parameters.
- Set up all the processing parameters: frame size and frame “overlap”, quadrature mode, algorithm, number of iterations, weighting, Fourier transform option, Virtual Echo and solvent filter. It is possible to trim the direct dimension. If the size of the full sampling grid is not set, it will be set to the maximum t_1 index in the NUS schedule.
- Click ‘Go!’ to process all data acquired so far.

5.3 Data display

A simple tool for display of spectra is included in TReNDS. Once first frame is processed, the appropriate spectra are displayed and controls for setting contour levels and a region of interest become active. Peak analysis is also possible.

The number of processed and displayed spectra is controlled by *Number of 2D spectra used* and 2D only mode buttons in the GUI. Axes of all spectra are synchronized and the same frame is displayed in all plots. The time corresponding to a middle of a frame is displayed above every plot.

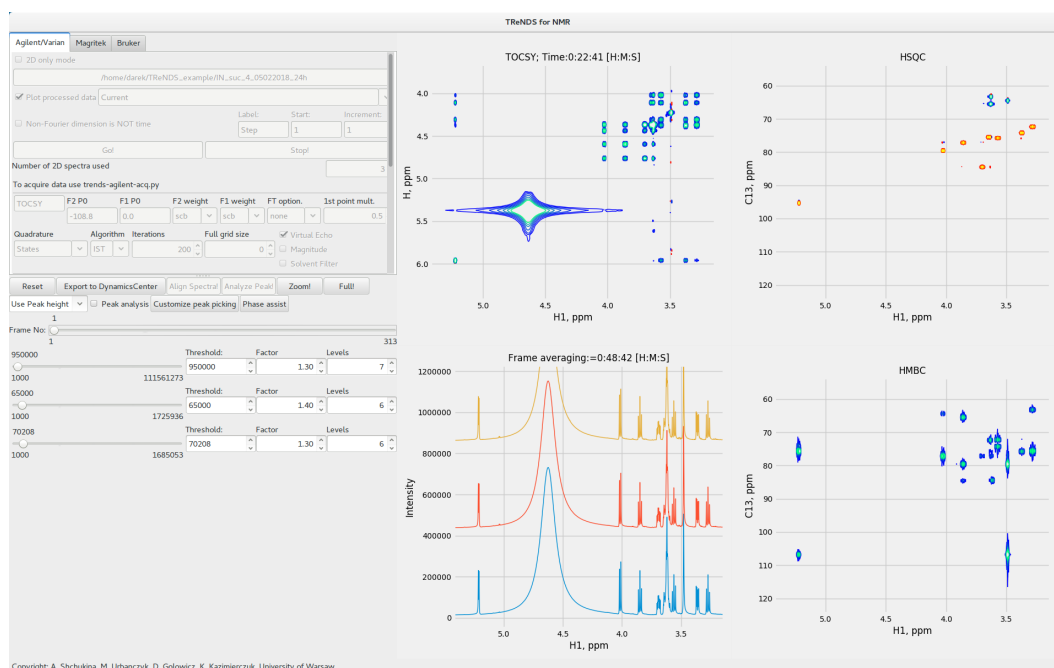


Figure 7: Data display in TRENDS - interleaved three 2D spectra and 1D

5.3.1 Display controls

The slider *Frame No* allows to set the frame that is currently displayed. The maximum frame available corresponds to most recently processed subset of TR-NUS data.

Below the *Frame No* slider one can find slider and controllers of contour levels for a 2D display. One can set the display threshold (will be the same for positive and negative contours), the number of contour lines and ratio between them.

5.3.2 Zoom

Set the bottom-left corner of the region to be zoomed in a 2D spectrum with the left mouse button click, and the top-right corner with the right button click. Then click button '*Zoom!*'. To restore the full view, click button '*Full!*'. Zoom is synchronized for all the spectra types, both 1D and 2D.

5.3.3 Phase assist

The zero-order phase correction can be adjusted using a *Phase assist* tool:

- Click *Phase assist*. The pop-up window will appear.
- Spectra for phasing are in separate tabs. Select appropriate spectrum.
- The contour level settings are passed from the main GUI and cannot be changed in *Phase assist*
- You can zoom spectrum in the same way as in the main GUI (*Zoom!* and *Full!* buttons)

- Select the peak for phasing by middle click. The vertical and horizontal 1D slices will appear.
- Adjust vertical scale by mouse scroll to see phase distortions
- Switch cursor mode from *Scroll zoom* to *Scroll phase*
- Adjust phase by scroll in both dimensions. You can adjust step to scroll more precisely
- When done, click *Exit & apply changes*. All frames will be recalculated with the new phase. This may take time.

5.3.4 Peak analysis

- Make sure that '*Peak Analysis*' box is checked.
- Choose peak intensity analysis mode from the dropdown menu: *Fit peak*, *Use peak height*, *Integrate peak*.
- Adjust the display threshold level for the spectrum of interest.
- Select a peak in a 2D spectrum with the middle mouse button. The peak closest to the clicked point will be selected.
- Click button '*Analyze Peak*'. The program will track the peak along all the frames and, depending on the intensity analysis mode:

Fit peak with a Lorentzian, determining its position, height and width (FWHM). For groups of close peaks, the parameters defined in *Customize peak picking* are used to check the number of peaks with a "neighbour test": if a point is higher than its N neighbors, it is considered a peak, otherwise not.

Use peak height as a peak intensity without integration.

Integrate peak using numerical integration according to the box defined in *Customize peak picking*.

If the peak is not present in some of the frames, the software will perform the analysis only on those frame where the peak is present.

- When the software has carried out the analysis, a peak analysis window pops up. It has three tabs: the intensity/integral of the peak and the positions of the peak in the two dimensions (ppm scale). All the three values are shown as functions of time. You can fit the intensity/integral changes of the peak with functions corresponding to zero, first or second order kinetics, as well as choose the time scale units.
- If peak analysis is performed on the given data for the first time, subfolder **Analysis** will be created. A text file, e.g., *Peak_at_3.398_77.678.txt*, with the intensity/integral function of time (written in the array form) will be generated in subfolder **Analysis**.

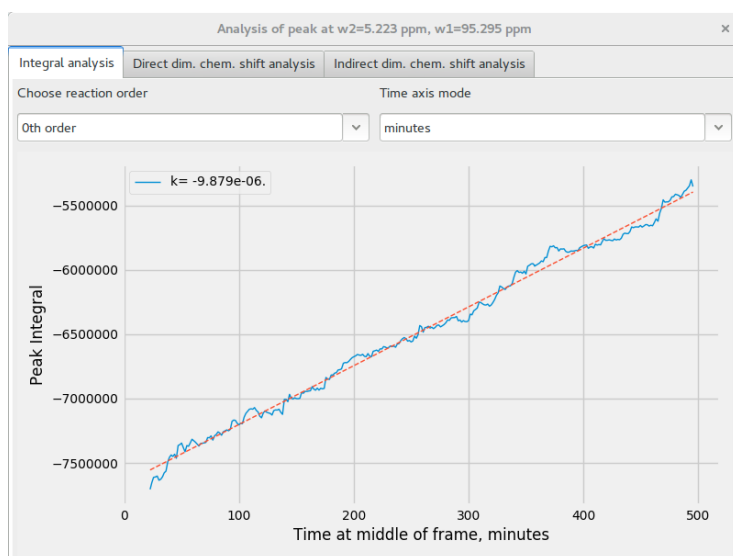


Figure 8: Peak intensity plot window

5.3.5 Aligning spectra

1. Disable 'Peak Analysis mode'
2. Select a peak using middle click
3. Click 'Align Spectra'

5.3.6 Export to other software

TReNDS allows to export spectra and peaklists to Bruker DynamicsCenter. To do so click '*Export to DynamicsCenter*'. Then, in the data folder, you will find DynamicsCentre subfolder with Filelist.txt which allows to import data directly to the DynamicsCenter.

All reconstructed frames are available in the nmrPipe format and can be found in subfolders of data directory: Reconstructed\2D\framenummer\MDD\Frame.proc. They can be opened by nmrDraw, ACD/Spectrus, MestReNova, Sparky and other software.

6 Using TReNDS library in your own scripts

Some of TReNDS functions can be used as a python functions.

6.1 VnmrJ acquisition control

package TReND.send2vnmr allows to create python based scripts to control acquisition and processing in VnmrJ similarly to TopSpin python programming

To allow VnmrJ control from python first type listenon in VnmrJ command line: in python:

```
from TReND.send2vnmr import *
```

Available commands are:

1. `change_exp(Number)` Function sends a request to VnmrJ to change active directory in to `jexpNumber`
2. `check_if_exp_exists(Number)`: Checks if the experiment "expNumber" exists. If not creates it;
3. `create_interleave_file_structure(Directory, num_of_exp)`: Creates the folder structure for saving the data in Directory in TReNDS fashion
4. `is_idle()`: Returns True if spectrometer is idle and False if is acquiring
5. `go_if_idle()`: activates the acquisition. Only when Idle;
6. `wait_for_idle_to_go()`: Runs go if idle if not idle checks the status every one second until idle and the runs go.
7. `Run_macro_on_idle(Macro)`: Runs any command when and only when Idle;
8. `wait_for_idle_to_Macro(Macro)`: Runs Macro if idle if not idle checks the status every one second until idle and then runs Macro
9. `Run_macro(Macro)`: Runs any (Macro) command immediately
10. `Save_experiment(Directory)`: Saves the experiment in given directory
11. `Interleaved_acquisition(ExpTemplate, ExpRunning, Exp1D, WorkingDirectory, Steps, SchedulePath, framesize, NumOfExp)`:
Runs interleaved acquisition.
ExpTemplate Number of Exp where the 2D NUS template is
ExpRunning is a directory where the interleaved 2D nus will be run
Exp1D directory for 1D acquisition
WorkingDirectory: Path to directory where the acquired data will be save and can be accessed by the processing program
Steps: Number of elements in the loop.
NumOfExp Number of 2D experiments to interleave

Example of acquisition script: This example shows how to acquire data for Sweep Coherence Transfer (SCoT) experiment.

```
from TReND.send2vnmr import *
import shutil
import time
import os
import numpy as np
##### PARAMETERS TO SET#####
SchedulePath = '/home/nmr700/timetab/IneptSweep.hdr_3' #Path for shedule of NUS for t1
GeneralPath = '/home/nmr700/IneptSweepNewSample_1/'
create_interleave_file_structure(GeneralPath)
SaveDir = GeneralPath + 'Acquired/2D/'
```

```

Steps = 512 #Number of Inept points to acquire (t1 point will be twice as big)
J_hc_start = 100 #Inept sweep start value
J_hc_stop = 200 #Inept sweep stop value
ExpTemplate = 2
ExpRunning = 3

#####ACTUAL MACRO#####
J_hc_array=np.linspace(J_hc_start, J_hc_stop, Steps)
with open(SchedulePath) as f:
    schedule = f.readlines()
shutil.copy2(SchedulePath, SaveDir + 'sampling.sch')
counter = 0;
# INEPT sweep loop
for N in xrange(0, 2 * Steps - 1, 2):
    schedule_one_step(ExpTemplate, ExpRunning, N, schedule)
    wait_until_idle()
    change_exp(ExpRunning)
    Macro = '"j1xh = ' + str(J_hc_array[counter]) + '"
    Run_macro_on_idle(Macro)
    go_if_idle()
    wait_until_idle()
    change_exp(ExpRunning)
    Save_experiment(SaveDir + str(counter) + '.fid')
    counter += 1

```

6.2 Magritek to nmrglue

Allows importin Magritek SpinsoleExpert data to nmrglue.

- `read_data(path)` Reads 2D spectrum from path and returns dictionary and data
- `read_data_1d(path)` Reads 1D spectrum from path and returns dictionary and data

References

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