The xpy3-tools tutorial

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Version 1.7

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1 Introduction

`xpy3-tools` is a collection of Python scripts for NMR data processing, intended to be suitable for use with Bruker's Topspin. As such, they rely on Bruker's Python API available since Topspin version 4.1.3 [1]. Later versions conveniently allow one to run the scripts from the command line by typing `xpy3 <script name>`, in a similar manner to regular Jython scripts. The scripts are meant to solve the tasks from the author's own practice but hopefully can be of interest to all NMR practitioners using Topspin. The current version of `xpy3-tools` comprises 17 scripts (see the table below), which number is meant to grow according to a to-do list.

Using Topspin environment means, among other things, a direct access to its GUI. Yet some of `xpy3-tools` have their own GUI – a pop-up window for interactive parameter optimization and visual control. The GUI functionality is implemented by using `matplotlib` / `Tkinter`. The I/O functionality is provided by a module `BrukerIO` from a `JTutils` package (https://github.com/jtrebosc/JTutils).

`xpy3-tools` will not modify in place `fid`, `ser`, `acqu(123)` or other files containing raw data, in which respect they are safe to play with. When those files are to be overwritten by design, as *e.g.* in de-noising or linear prediction scripts, it will be done after first copying and pasting the entire dataset under a new `EXPNO` thus keeping original data intact. Otherwise data are processed in-place, the result being saved in a `pdata` folder under the same `EXPNO` from whence the script has been called.

2 List of scripts

Script name	*Function*	*Comments*
`baseline`	Baseline correction of a 1D spectrum.	Uses a rolling standard deviation distribution method to identify baseline points [4] and a Whittaker method for interpolation [5].
`baseline2`	`baseline` applied to individual 1D spectra from a pseudo-2D data set.	Allows navigation throughout individual spectra for manual baseline adjustment.
`baseplane`	Baseline correction of a 2D spectrum along both axes.	Works in automatic mode (there is no pop-up GUI, nor does it take external arguments).
`cpmg_fp`	Whole-echo processing for CPMG multi-echo trains.	Relies on zero points in a CPMG signal to split it into individual echoes. To have such zeros, consider using the `op_qcpmg` pulse program included in the package.
`cpmg_recursive`	T_2 relaxation analysis of a CPMG echo train using a mono-exponential recursive formula.	Quantifies individual echoes, plots their cumulative sum vs time, and fits it with a mono-exponential recursive model [6].
`cpmg_relaxation`	T_2 relaxation analysis of a CPMG echo train using mono- or stretched-exponential model.	Plots individual echo intensity vs echo time and fits the curve with mono- or stretched exponential.
`denoise`	Low-rank SVD approximation of a 1D signal in time domain (a Cadzow's de-noising scheme).	Uses a Toepitz matrix format to represent the FID in 2D. An optimum SVD threshold value is computed according to [7].
`denoise2`	Approximation of a 2D signal in time domain using noise-adaptive principal components.	Uses NUS type data randomization to perturb signal's principal components (PCs) and thus to average their noise-related content prior to using them for data approximation [8].
`icoshift`	Peak alignment over a series of spectra – either stacked in a pseudo-2D data set or linked via Topspin's multi display.	A number of peak regions can be selected for individual alignment; or you can choose one particular region to align the entire spectrum.
`lp`	Forward linear prediction on 1D data	Employs an original method of LP based on repetitive projection of PCs on an extended data set (see below).
`phase_fid`	Zero-order phasing of 1D time-domain signals, including CPMG type signals.	Handy for maximizing the Re-part of the signal; has the option to nullify the Im-part.
`rotsync`	Construction of a rotor-synchronized MAS spectrum from an arbitrary sampled FID.	Enables quantitation of distinct chemical shift components through direct integration; comes in handy for line shape analysis.
`rotsync_plus`	Same as `rotsync` but more involved rotary-echo quantitation.	In theory should provide better SNR than `rotsync`.
`sino_fid`	Signal-to-noise ratio (SNR) calculator for time-domain signals in 1D.	SNR is defined as the ratio of FID amplitude to 2 * std of noise per channel.

`symmetrize`	MAS sideband symmetrization for quadrupolar spectra of half-integer spins	Comes in handy for fitting the 1st-order quadrupolar model to MAS spinning sidebands; gives good-looking spectra for presentations.
`t1denoise`	Removal of t1 noise in 2D spectra	Uses standard deviation distribution method [4] to identify noise regions along the F1 axis (the same as in `baseline` / `baseplane`).
`t1t2`	Basic relaxation analysis module	Allows interactive integration over pseudo-2D spectra with optional correction for baseline shifts; currently restricted to mono-, two- and stretched exponential fit.
`utils`	Contains common utility functions and classes.	Ever growing collection of `def`s.

3 Installation

3.1 Python environment setup

Topspin 4.1.4+ comes with a preinstalled Python 3 environment in `<topspin>/python/lib/python3.x/` that includes Bruker Python API and few packages necessary for running demo scripts. To use another Python environment, you need to specify a path to its prefix. In Topspin 4.2+, you can do that via Topspin's Preferences going `Preferences` → `Python 3+` → `Select Python 3+ Environment`. In Topspin 4.1.x, you are bound to use the prefix `<topspin>/python/...` unless you backport a Jython script `xpy3.py` from Topspin 4.2+ where you can hard-code the path to Python of your choice. Backporting `xpy3.py` will also render `xpy3-tools` callable from Topspin 4.1.x command line, otherwise you can run them as regular console applications (using CLI or Windows' CMD) or from within a dedicated IDE such as Spyder or VSCode.

For instance, imagine that you have chosen to use a Python 3.x interpreter from `/usr/local/bin` on your Linux machine. Imagine also that your package installer is `pip`, namely `pip3.x`. To proceed to installation, open the terminal (CLI), change the current directory to `/usr/local/bin` and run the command

```
python3.x pip3.x install -r path/to/requirements.txt
```

with the configuration file `requirements.txt` shipped with `xpy3-tools`. This will install the required dependencies. Next, provide a search path for the Bruker Python API modules stored a `site-package` (or `dist-package`) folder in a Topspin's installation prefix. It can be done using a `.pth` file with a text line containing the path to the prefix, *e.g.*

```
/opt/topspin4.2.0/python/lib/python3.10/site-package/
```

The `.pth` file needs to be placed in a `site-package` directory of the chosen Python 3.x environment. Alternatively, you may re-install the Bruker Python API modules directly to the place using `.whl` files shipped with `<topspin>/python/examples`, as follows:

```
python3.x pip3.x install -r path/to/ts_remote_api*.whl
python3.x pip3.x install -r path/to/bruker_nmr_api*.whl
```

A special care is required for the module `BrukerIO`. The package `JTutils` where this module comes from cannot be installed via `pip`. Hence copy the `brukerIO.py` file directly from the `JTutils` repository at `https://github.com/jtrebosc/JTutils/blob/master/CpyLib/` and put it in the folder where `xpy3-tools` scripts are kept (see the next paragraph).

Installation on a Windows machine is supposed to be similar (not tested though).

3.2 Placement of scripts

Running `xpy3-tools` scripts directly from Topspin's command line requires a proper script location. The search path for Python 3 scripts is hard-coded in a `xpy3.py` file as `<topspin>/python/examples`. A simple workaround will be, therefore, to move the `xpy3-tools` files, including `brukerIO.py`, into `<topspin>/python/examples`. Should you prefer another location, add a path as follows. In a text editor,

open the file `<topspin>/exp/stan/nmr/py/xpy3.py` (you might need administrator's privileges for that), then find and comment out the line

```
return getParfileDirs(PYTHON_3_INDEX)
```

and put instead the lines (mind indents):

```
    defaultDir = getParfileDirs(PYTHON_3_INDEX)
    extras = ['/my/path/to/scripts']
    for x in extras: defaultDir.append(x)
return defaultDir
```

Here `'/my/path/to/scripts'` is where you want to keep your Python scripts for Topspin. You may add as many paths in `extras` as you wish, separated with commas. As mentioned in paragraph 3.1, `xpy3-tools` can be run as regular console applications, *i.e.* `python3.x <script name>`, or be launched from within a dedicated IDE. All you need in this case is open a target NMR dataset in Topspin and make sure that the network service is running – either through `Preferences` → `Python 3+` → `Manage TopSpin Network Interface` in Topspin 4.2+ or by executing command `start_rest_interface` when using Topspin 4.1.3. The examples below presume that Topspin 4.2+ is used.

4 Usage examples

4.1 baseline

This script allows interactive baseline correction of 1D spectra. For a baseline classification part, the script employs a function `std_distribution()` from the package `pybaselines` [2], which identifies baseline points by analyzing a rolling standard deviation distribution across a spectrum. This part is controlled by two parameters – `half_window` and `num_std` – adjusting, respectively, the number of points involved in the rolling standard deviation calculation and a number of standard deviations to be used as a baseline threshold. For a baseline interpolation part, it uses a Whittaker smoother `ws2d()` from the package `vam.whittaker` [3]. It gives the third adjustable parameter – `lambda` – to control the interpolation smoothness. Running `xpy3 baseline` in Topspin's command line (Fig. 1) brings about a two-graph window (Fig. 2). The upper graph shows the classified baseline points and baseline interpolation overlapping the original spectrum. The lower graph shows the spectrum after subtracting the estimated baseline.

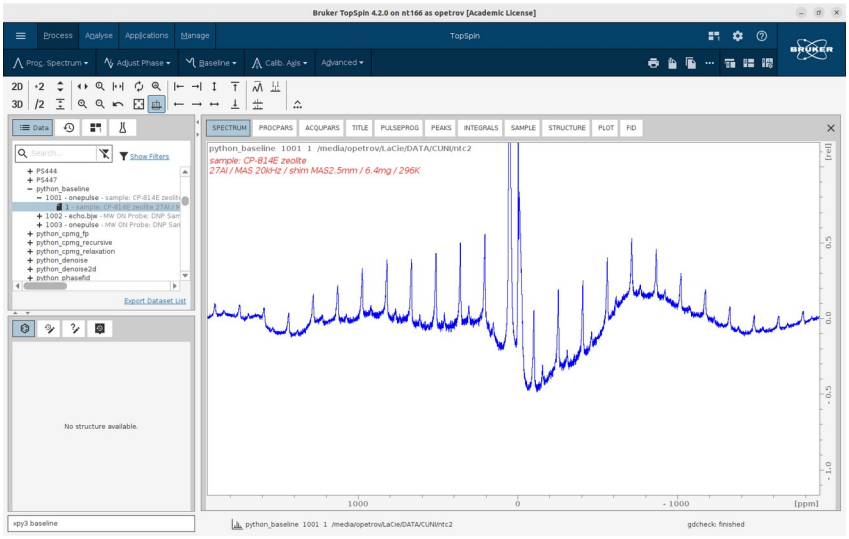


Fig. 1

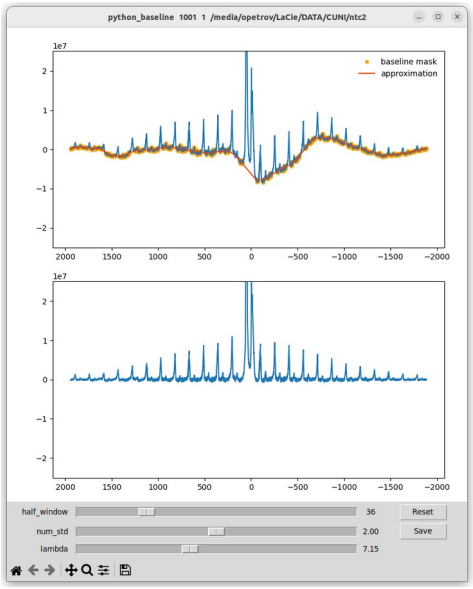


Fig. 2

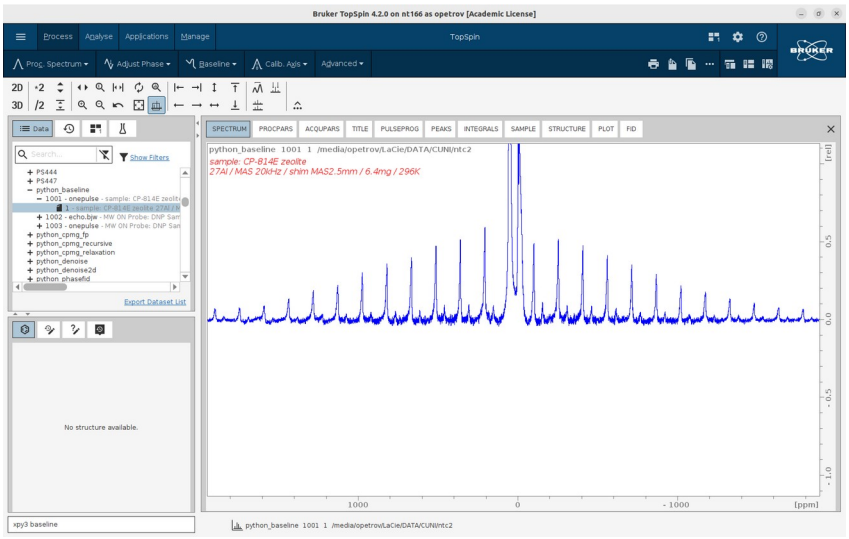


Fig. 3

The baseline estimate can be improved manually using sliders. Clicking `Reset` restores the automatically estimated baseline. Clicking `Save` writes the spectrum shown on the bottom graph to the `pdata` folder and updates Topspin's window accordingly (Fig. 3). You may run the script few times for additive corrections.

The script checks modification times of `1r` and `1i` files, and when they coincide (meaning that in-built baseline corrections have never been applied, hence Re and Im parts of processed data are still coherent), the estimated baseline is subtracted from both Re- and Im-part of the spectrum. This is handy if you plan to process the spectrum any further, and the processing involves both of the parts (*e.g.* phasing, conversion to magnitude mode, inverse FT). The script is applicable to datasets with `1i` files missing, *i.e.* to magnitude spectra.

4.2 baseline2

This script is used to correct baselines of individual 1D spectra from pseudo-2D data sets (those having `2rr` and `2ii` files but not `2ir` or `2ri` files). As an example, Fig. 4 shows a series of 24 spectra from a T_1 inversion-recovery experiment on methane confined in a MOF.

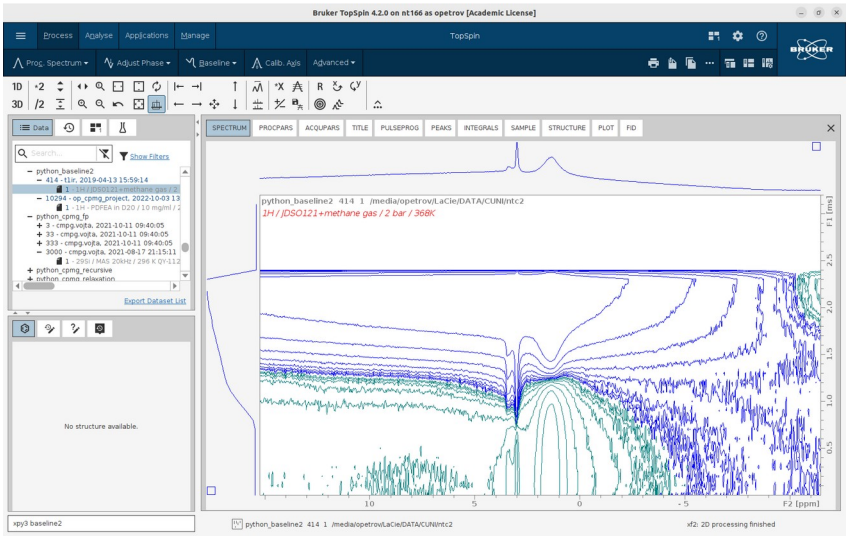


Fig. 4

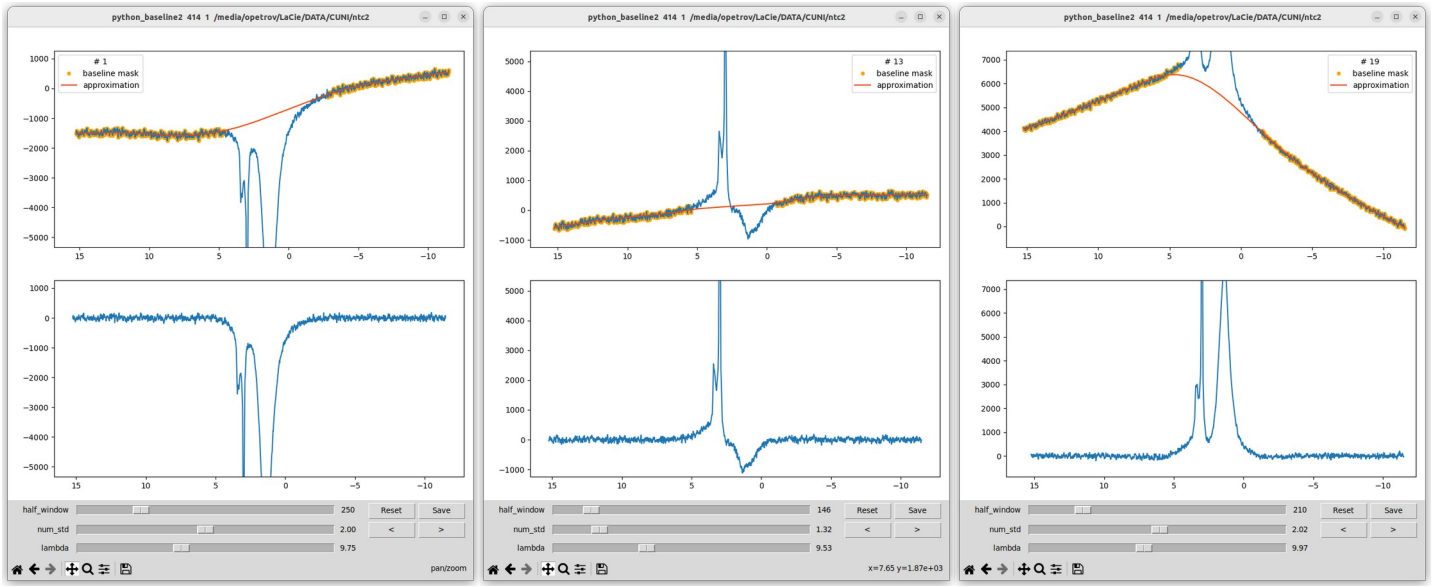


Fig. 5

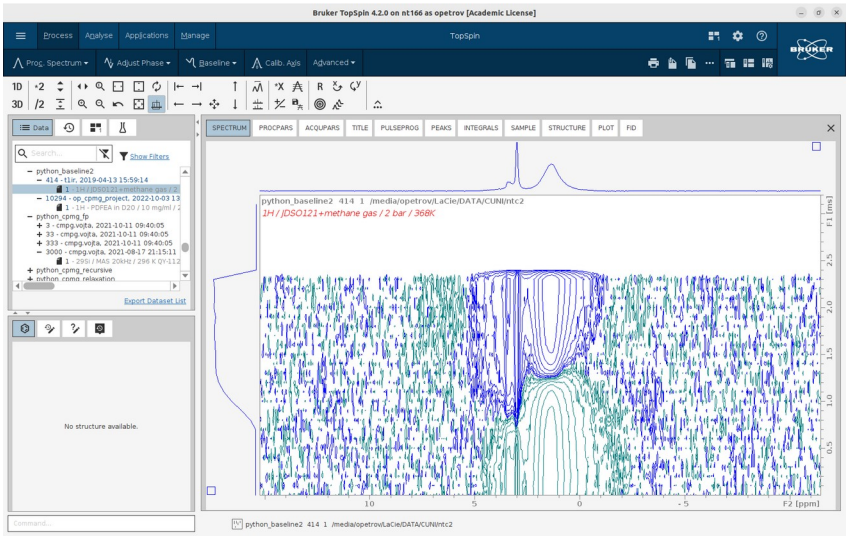


Fig. 6

Running the `xpy3 baseline2` command brings about a pop-up window which is identical to Fig. 2 except for the buttons ">" and "<" enabling navigation through the spectra. By default, the first spectrum in a series is displayed. Once you inspect and optimize a baseline estimate for this spectrum, you switch to another, and so on (Fig. 5). Eventually you click `Save` to write the entire baseline-corrected series to the disk (Fig. 6).

Tip: If you find matplotlib too slow at interactive re-drawing (zooming and such), you can try and improve it by increasing a line segment simplification parameter `path.simplify_threshold` in a matplotlib's configuration file `[PYTHON]/.../matplotlib/mpl-data/matplotlibrc`.

4.3 baseplane

This script runs a `baseline` correction procedure first on a series of rows and then on a series of columns of a 2D NMR spectrum. Unlike `baseline`, this one does not have a GUI for interactive parameter adjustment thus relying on automatically optimized `half-window` and `lambda` values and a default `num_std = 3`. The parameter optimization is done once for rows and once for columns, using the data arrays that have the greatest norm in corresponding dimensions.

Fig. 7, left, shows a 2D EASY-ROESY spectrum of cyclosporine taken from Bruker's example dataset `/examdata/Cyclosporine/`. Fig. 7, right, shows the same spectrum after running `xpy3 baseplane` at Topspin's command line. For dealing with t1-noise that manifests as vertical stripes in the spectrum, see `t1denoise`.

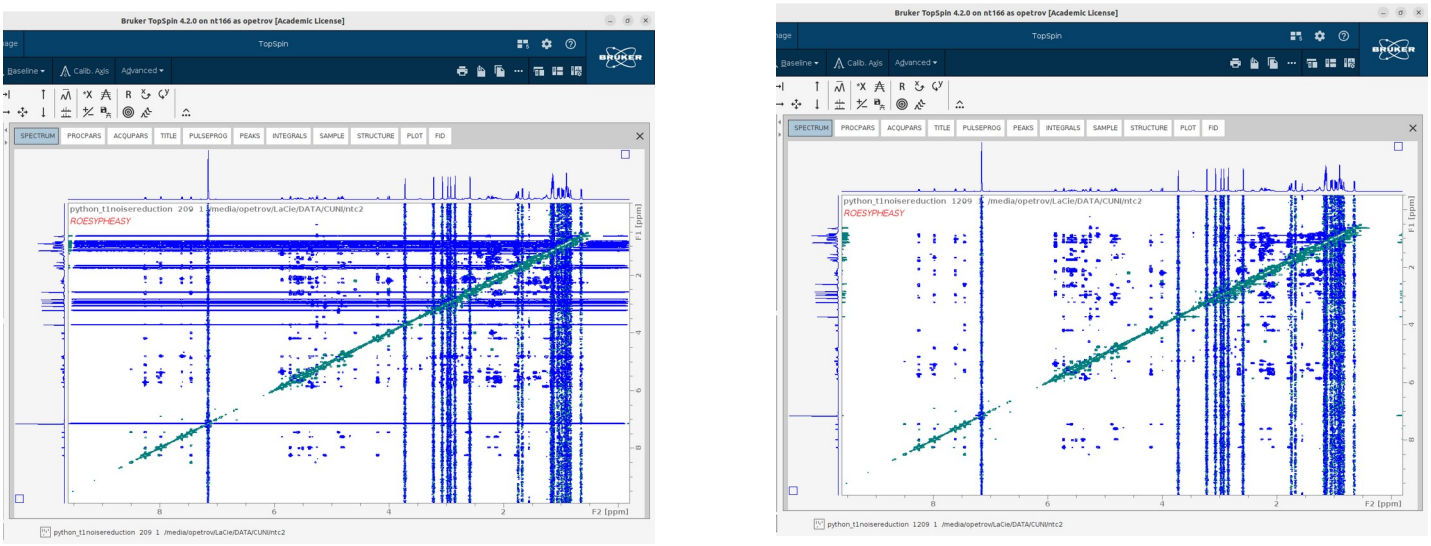


Fig. 7

4.4 cpmg_fp

This script is intended for `qcpmg` type pulse programs that generate continuously sampled echo decays (a.k.a. echo trains). Processing the echo train as a regular FID – *e.g.* with the command `fp` – results in a discrete 'spikelet' spectrum. To get a conventional continuous spectrum, you need to collapse the train into a single echo (a sum of echoes) and follow whole-echo processing steps, which are splitting the echo in the middle, swapping the halves and only then `fp`. The `cpmg_fp` script automates these very steps plus it does the first-order phase correction to maximize the Re part of the spectrum.

Fig. 8 shows a train of 256 spin echoes from a zeolite sample (^{29}Si MAS NMR). Typing `xpy3 cpmg_fp` brings about a two-graph window (Fig. 9). Top graph shows the echo train (same as in Topspin's FID window). The bottom graph the average echo (a sum of echoes) after splitting the train into individual echo segments. By default, the average echo is calculated with all segments included, which can be changed with the slider `# echoes` to include only a number of leading echoes. Playing with `# echoes` affects both SNR and a spectral line shape provided the spectrum comprises differently T_2-relaxing components. Once you are certain about `# echoes`, click `OK` to get to the spectrum (Fig. 10).

For the script to work, individual echo segments in the echo train must be separated by at least one zero point. A pulse program `op_qcpmg` is shipped with `xpy3-tools` which is the variant of a standard `qcpmg` that inserts such zeros in the CPMG train.

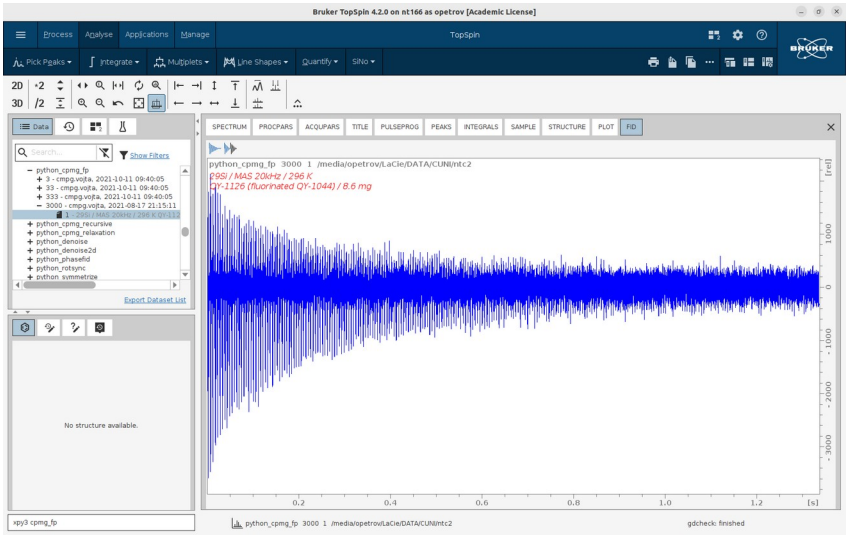


Fig. 8

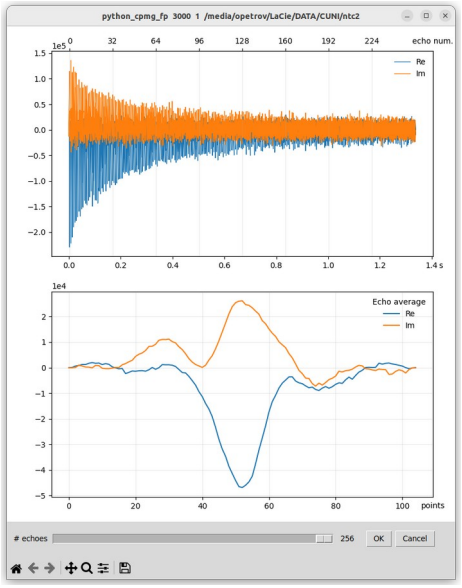


Fig. 9

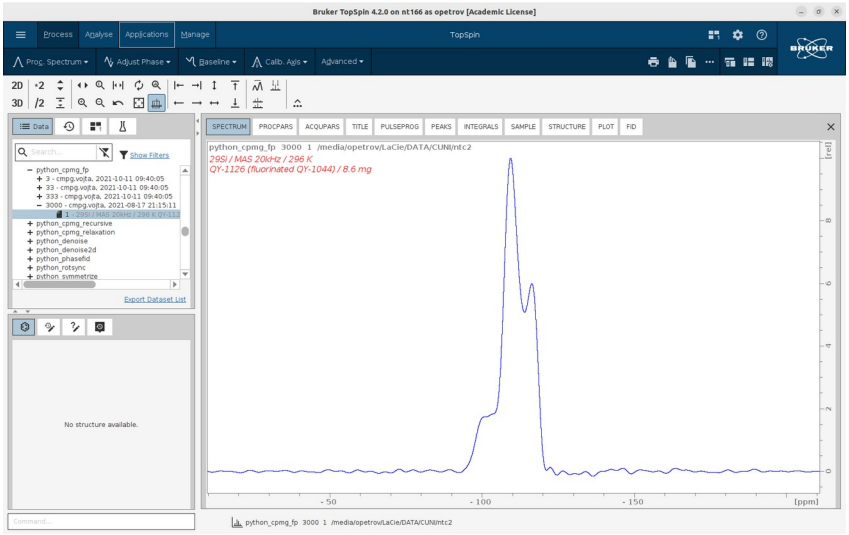


Fig. 10

4.5 cpmg_relaxation

This script is again relevant to the `qcpmg` type pulse programs generating continuous trains of zero-separated echoes. Individual echoes are quantifies using either midpoints (by default) or integral intensities. The resultant echo-decay curve – the echo signal *vs.* echo time – is fitted with either mono or stretched exponential model.

Fig. 11 shows an echo decay for a fluorine-containing zeolite (^{19}F NMR) acquired with the pulse program `op_qcpmg` (included to the package). Running `xpy3 cpmg_relaxation` brings about a two-graph window (Fig. 12). The top graph shows the experimental signal, with detected echo positions marked with asterisks, and the bottom graph the echo decay curve, on a semi-log scale, measured from echo midpoints (with the option to switch to integrals). Clicking `Fit Me!` fits a mono-exponential model to the curve, with the best-fit parameters reported in as annotation box (Fig. 13). There is an option for a stretched exponential fit, in which case a mean

relaxation time is reported (Fig. 14). Clicking `Save&Quit` saves the decay curve in a two-column text file in `<EXPNO>/pdata/1/ct1t2.txt`, for further processing (*e.g.* for Inverse Laplace transformation). Note that the annotation text with best-fit model parameters is not saved – so mind that you write them down before clicking `Save&Quit`.

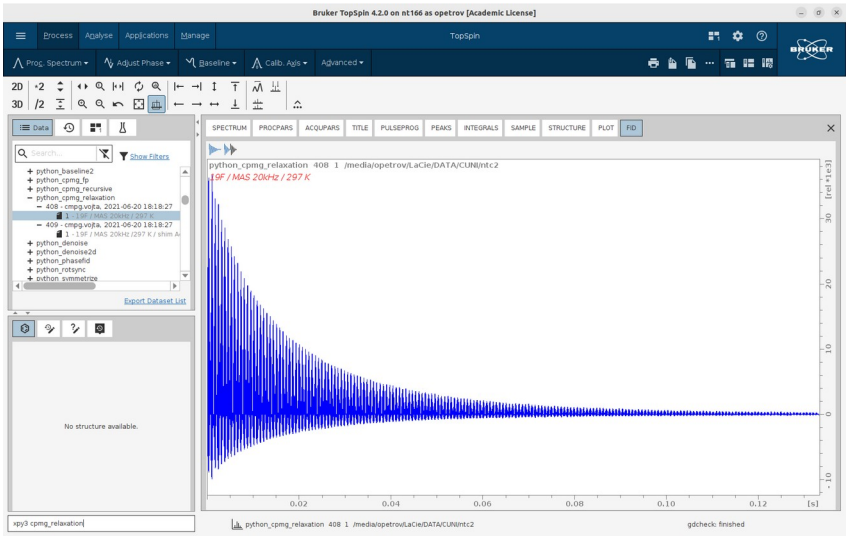


Fig. 11

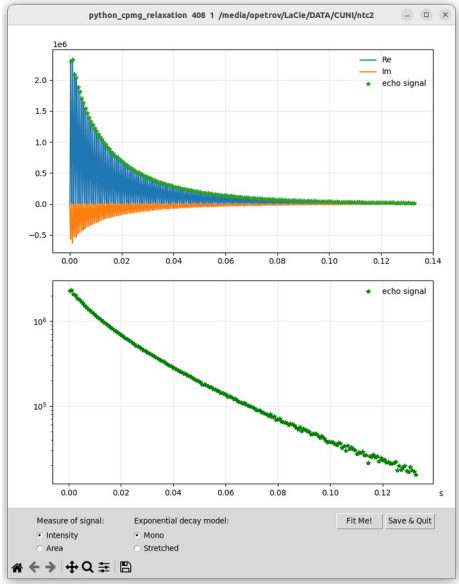


Fig. 12

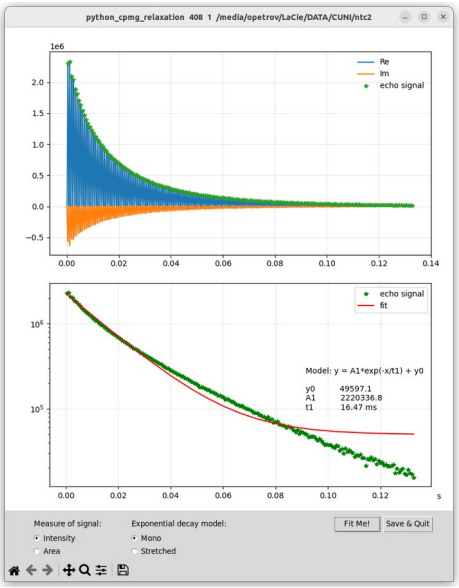


Fig. 13

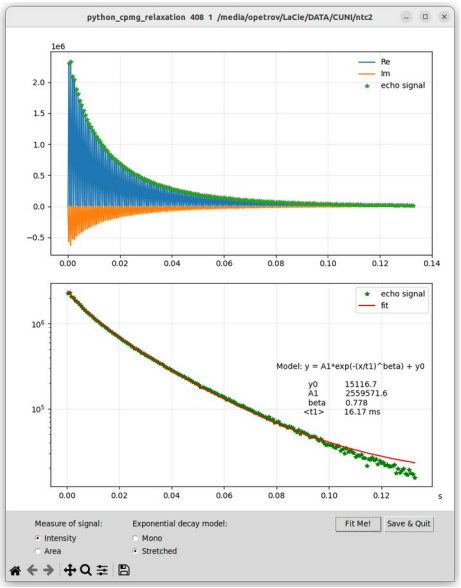


Fig. 14

4.6 cpmg_recursive

The function of `cpmg_recursive` is identical to `cpmg_relaxation` except for its using a cumulative sum of consecutive echoes intensity instead of individual echo intensity as a measure of relaxation. The cumulative sum is fitted with a recursive mono-exponential relaxation model given in [6]. The summation decreases a scatter in points on longer relaxation times and it renders the best-fit parameters less sensitive to fast relaxation

of few initial points, thereby better capturing an overall relaxation behavior. Fig. 15 shows the performance of `cpmg_recursive` on the same data as in Fig. 11. The GUI's controls are analogous to `cpmg_relaxation`.

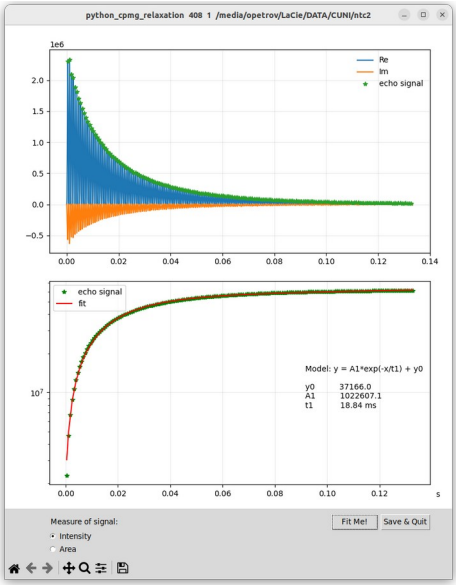


Fig. 15

4.7 denoise

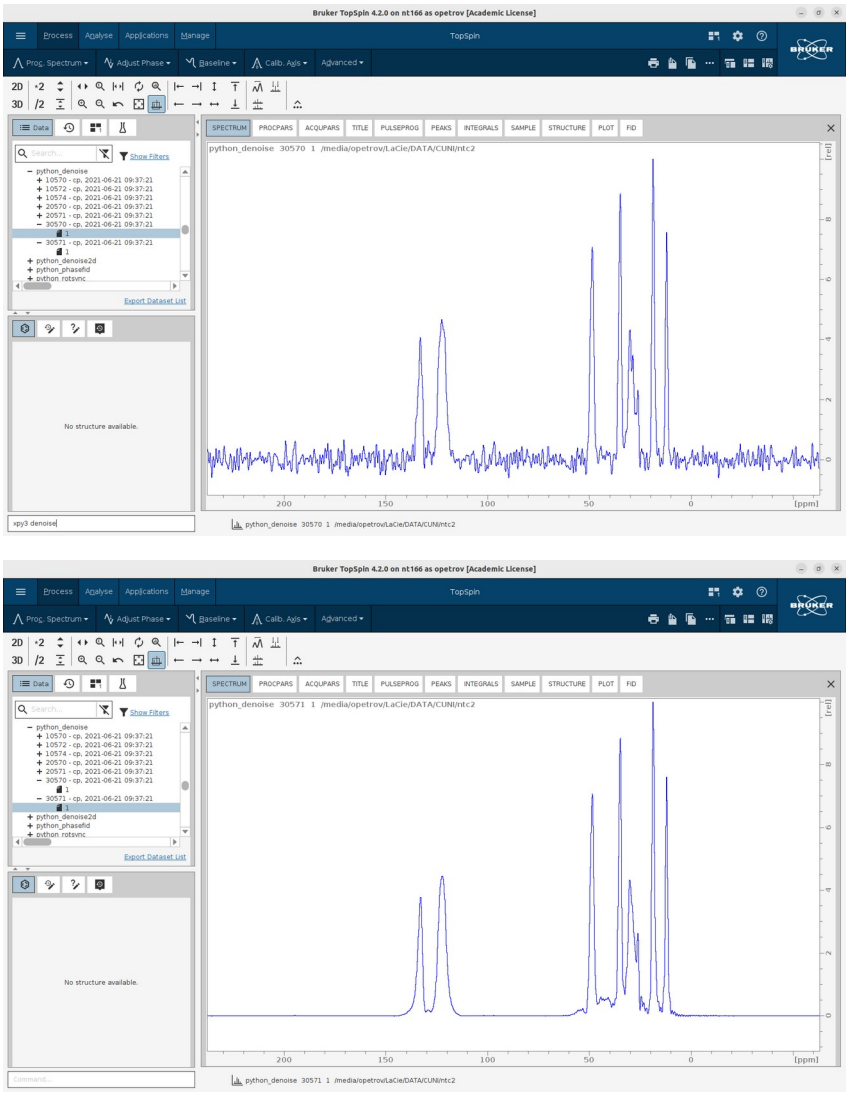
This script implements a Cadzow type denoising of 1D time-domain signals [9]. The Cadzow method consists of a low-rank decomposition of a data matrix constructed from the FID – of either a Hankel or Toeplitz format – where each row is a lagged (one-point shifted) sample of FID. The data matrix is subjected to a singular value decomposition (SVD), where only a few most significant singular eigenvectors are retained. The retained terms are then employed to reconstruct (approximate) the data matrix, which is finally re-arranged back into a 1D signal. To avoid problems with group delay's points, the FID signal is automatically converted to an AMX ('analog filter') type by Topspin's `convdta`.

The script does not have a dedicated GUI. There are a couple of things that may help you optimize it in terms of performance. Firstly, you may try and truncate the FID signal by setting the Topspin's processing parameter `TDeff` somewhere between the actual `TD` and the value at which truncation artifacts ('sinc wiggles') become visible. Secondly, you may change the number of eigenvectors used in data approximation. By default, this number is set automatically according to a Gavish-Donoho's (G.-D.) formula of thresholding [7] and can be adjusted by running the script with an external argument `offset` as

```
xpy3 denoise --offset n
```

Here `n` is an integer (either positive or negative) which will be added to the G.-D.'s threshold value.

Fig. 16 shows a ^{13}C spectrum of an organic precursor inside a zeolite sample (on the top) and the same spectrum after applying `denoise` (on the bottom), demonstrating a flawless performance. Another example is a ^{13}C spectrum of alginate (Fig. 17), in which case `denoise` is not that perfect leaving two noisy spikes at 47 and 170 ppm. As a rule, such spikes appear 'off-phase' w.r.t. real peaks and therefore are readily recognizable as noise-related artifacts.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Bruker TopSpin 4.2.0 on nt166 as opetrov [Academic License]
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Fig. 16

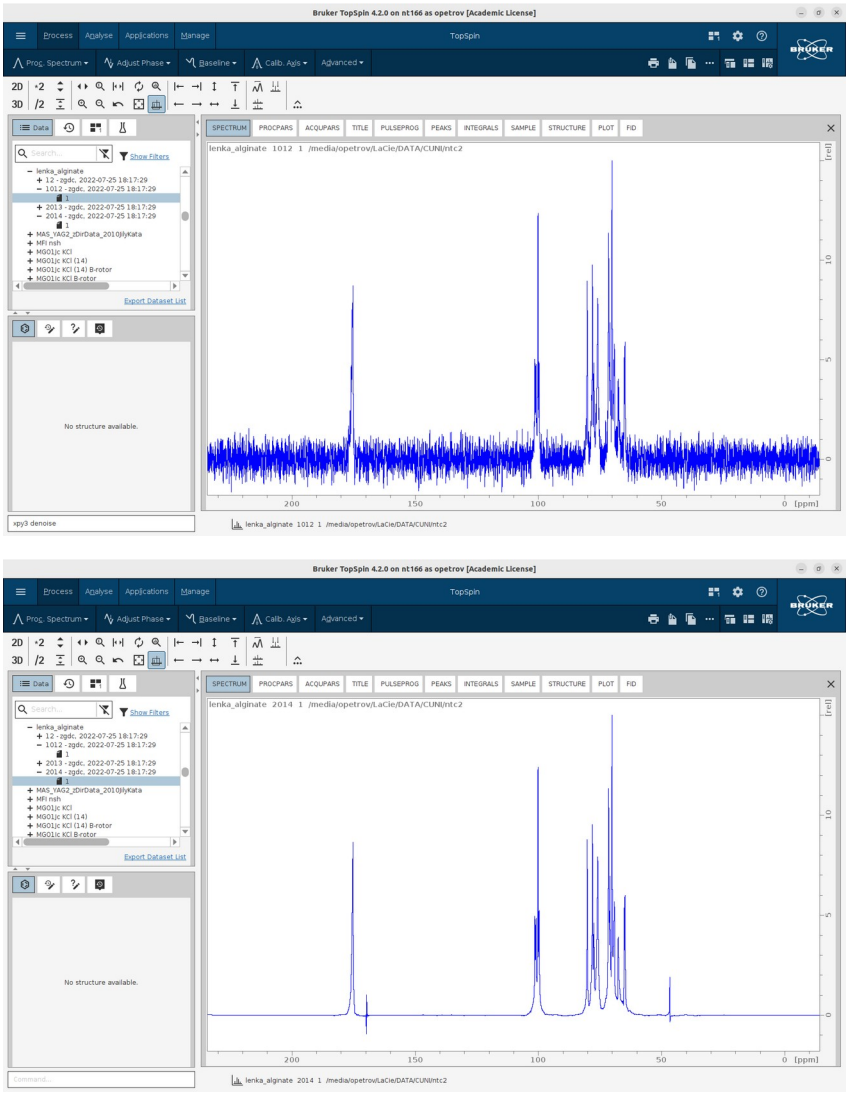


Fig. 17

4.8 denoise2

This script reduces noise in 2D data sets using an original de-noising method [8]. In brief, it is a PCA-based method where the principal components (PCs) used as a basis for data approximation are attenuated in norm proportionally to their noise-related content. You may think of it as a regularized SVD approximation in contrast to the hard-threshold SVD approximation employed in `denoise`. The PC attenuation is achieved through 'averaging' PCs of same ranks in a repetitive SVD applied to randomly chosen data rows. The number of rows is controlled by a parameter `nus` ranging from 0.25 to 1.0 and the number of repetitions by the parameter `samples`. Both parameters are set through external arguments provided at the command line (the square brackets indicate that these arguments are indeed optional):

```
xpy3 denoise2 [--nus nus] [--samples samples]
```

Given no arguments, the script will estimate `nus` by itself and use the default `samples` = `20`.

Fig. 18, left shows a phase-sensitive 2D INADEQUATE spectrum of strychnine in $CDCl_3$ (taken from Bruker's example dataset `/examdata/exam_CMCse_3/`). Fig. 18, right shows the same spectrum after applying `denoise2`, demonstrating a factor of 2.3 improvement in SNR.

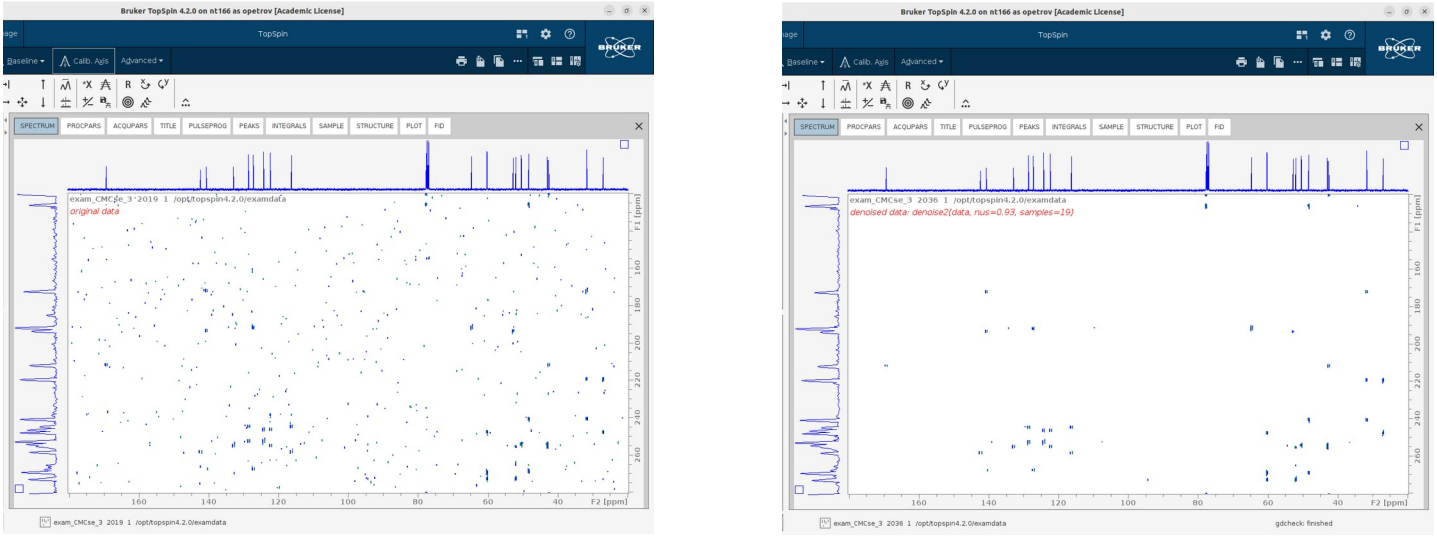


Fig. 18

Running `denoise2` on large datasets and with the number of `samples` greater than the default `20` may take annoyingly long (more than a minute). Shouldn't you want to wait that long, interrupt the script by closing the progress bar widget and restart it with less number of `samples`. Like its 1D counterpart `denoise`, `denoise2` copies the entire data set to a nearest available `EXPNO` beforehand.

4.9 icoshift

This is a front-end to the functions from `pyicoshift` [11] – a Python implementation of the *icoshift*, which stands for '*interval correlation optimized shifting'* algorithm for peak alignment. It is applicable to spectra of the same pattern with the peaks at certain positions sensible to fluctuations in pH, ion content, temperature *etc.*, or where the entire spectrum is shifted *e.g.* due to instrumental factors. The `icoshift` script can be run either on a pseudo-2D dataset or the 1D spectra that are linked to each other in the multi-display (`md`) mode, provided they are of the same size.

Fig. 19 shows spectra of a polyacrylamide hydrogel in D_2O from a variable-temperature experiment, opened in a Topspin's multi-display window (`.md`). Typing `xpy3 icoshift` brings about a two-graph GUI (Fig. 20). The top graph replicates the content of the Topspin's window, thus enabling peak intervals selection. Omitting the selection means treating the whole spectrum as one interval. Note that once selected, the intervals cannot be edited, you can only clear them altogether with a `Clear` button and start over. In Figs. 21 and 22, one interval is chosen that encloses a single peak from a reference compound (TMMS). With `Align mode` options, you can choose whether to align only this selected peak, keeping the rest intact (the option `n_intervals`), or to apply the shifts which will be found for this peak to the whole spectra (the option `whole`). When `n_intervals` is chosen, the gaps in the shifted spectra are filled with adjacent values, whereas for the `whole` option, the spectra are completed with `nan`'s on either of their sides. With the radio-buttons `Target`, you choose a reference

signal to which the spectra are shifted to match its position. The default target is `maxcorr` (“*the signal with the highest correlation with all input signals*” [10]), the others are `average` (arithmetic mean of spectra), `median` (median of spectra), `max` (spectrum of maximum intensity), and `average2` (uses the average target spectrum twice). For more information about the targets and which one it is better to use, see a tutorial to the Matlab version of `icoshift` [11]. In practice, you just go through all those targets and watch the difference it makes.

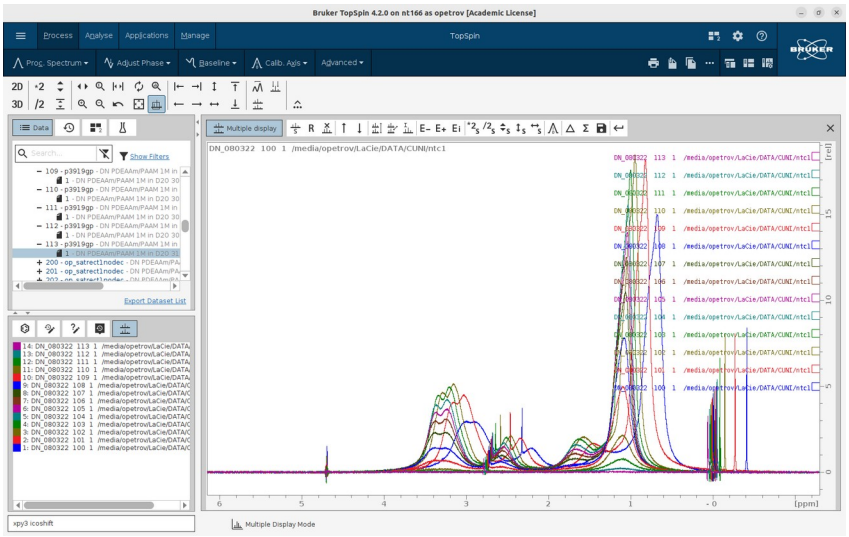


Fig. 19

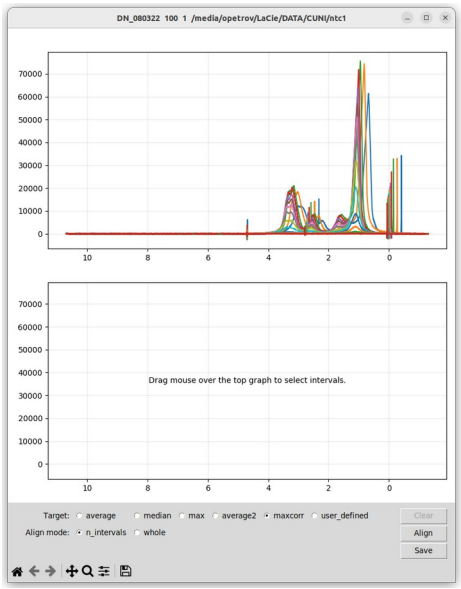


Fig. 20

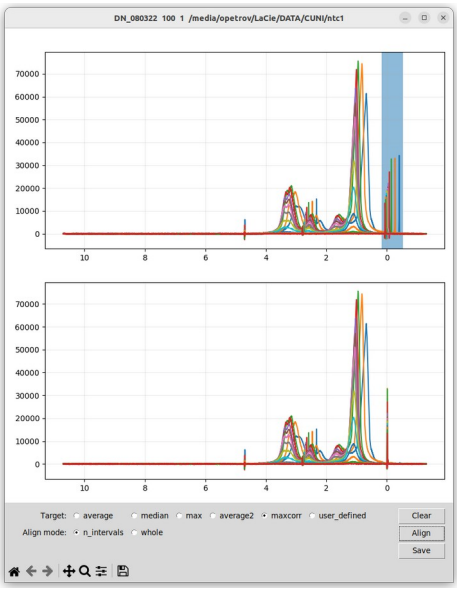


Fig. 21

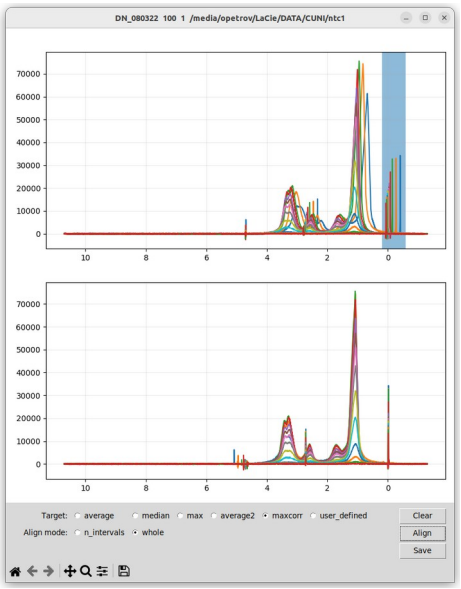


Fig. 22

4.10 lp

This plugin aims to provide an alternative method of *forward* linear prediction (LP) in 1D in case the built-in LP method will not work. What it does is finds principal components of a Toeplitz matrix of available data and projects them on an upper triangle matrix representing the extended part of FID with trailing zeros. The result of such projection is blended in with the available data (the diagonal averaging), then the projection/ averaging

steps are repeated, until convergence. Because of the repetition, it takes longer than the built-in LP method, but in return it is free of problems inherent in recursive prediction based on LP coefficient calculation (which is presumably what the built-in LP method is about).

The script requires three parameters be specified. First is `ME_mod` – to define whether to use a plain FID (`ME_mod` = `LPfc`) or mirror-image FID (`ME_mod` = `LPmifc`) as input data. Second is `LPBIN` – to define the size of an extended FID (including original data). Both `ME_mod` and `LPBIN` are taken from Topspin's PROCPARS. The third parameter `lpblk` gives the number of simultaneously predicted points expressed as a fraction of the FID size and can be varied from 0.5 to 0.9. By default, it is set to 0.7 meaning that the FID is simultaneously extended by 70%, then by another 70% and so on until all `LPBIN` points are delivered. To adjust `lpblk`, say to 0.8, run the script with an external argument `--lpblk` followed by the value, *i.e.*

```
xpy3 lp --lpblk 0.8
```

Tips: (i) Low `lpblk` (< 0.7) readily lead to unstable results, meaning that the calculated FID values skyrocket to several orders of magnitude instead of approaching zero. When this happens, increase `lpblk`. (ii) Apparently, `lp` with `ME_mod` = `LPmifc` is more stable than with `LPfc`. However, the former requires a specific FID structure to work (hard to tell what structure exactly), whereas `LPfc` suits them all.

Topspin doesn't have a dedicated command for LP. To see the result of extrapolation in time domain, one has to disable FT via `FT_mod` = `no` and run a `trf` command which would know whether LP was required from a `ME_mod` value. The extrapolated FID is saved in this case in `~/pdata/.../1r` and `1i` files. In contrast, `lp` saves the extrapolated FID to a `fid` file and modifies relevant parameters – `TD`, `AQ` and `FIDRES` – according to its new size. Like all scripts aiming at modification of time-domain data, `lp` writes in `fid` after first copying the entire data set under a new EXPNO. Should another run of `lp` be necessary, don't forget switching back to a the initial data set. Once you find the extended FID adequate, proceed to FT normally.

Fig. 23a shows a ^{31}P FID of H_6NO_4P from a CP MAS experiment with proton decoupling which allowed max. 50 ms acquisition time to avoid problems with applying high-power decoupling pulses. Consequently, FT has severe truncation artifacts. Figs. 23b shows this FID extrapolated up to 400 ms employing `lp` with `ME_mod=LPfc`, `LPBIN=4096`, and `lpblk=0.9`, as well as a new spectrum. For another example, Fig. 24a shows a truncated ^{1}H FID from a gelatin derivative in H_2O and the FID extrapolation with `ME_mod=LPmifc`, `LPBIN=11776`, and `lpblk=0.6` (only a part of the spectrum is shown).

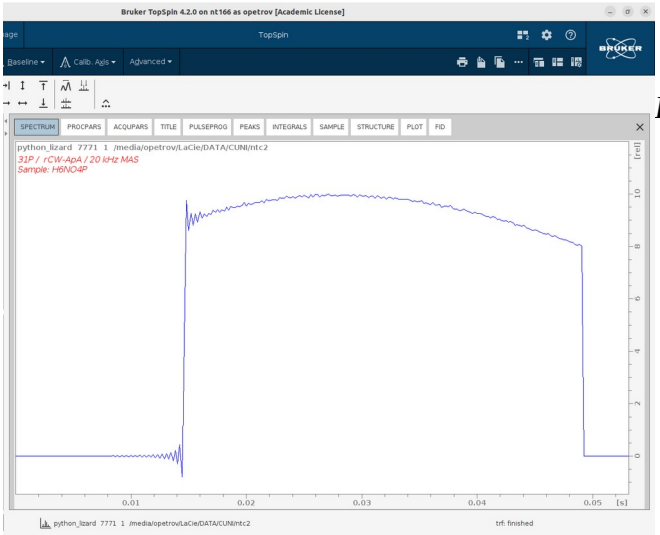
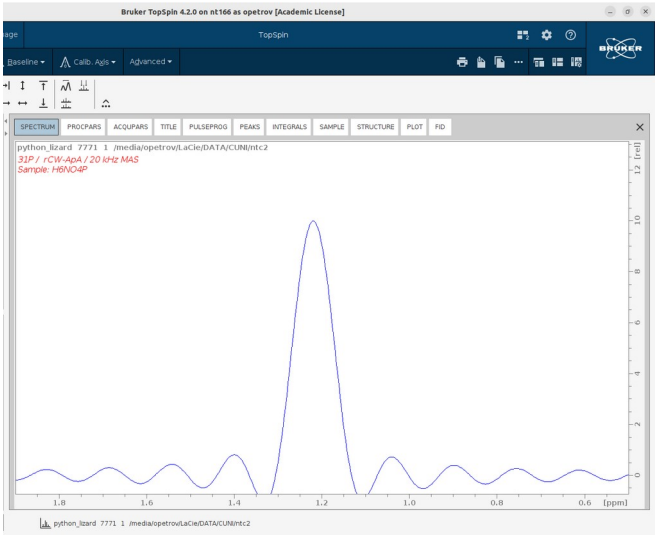
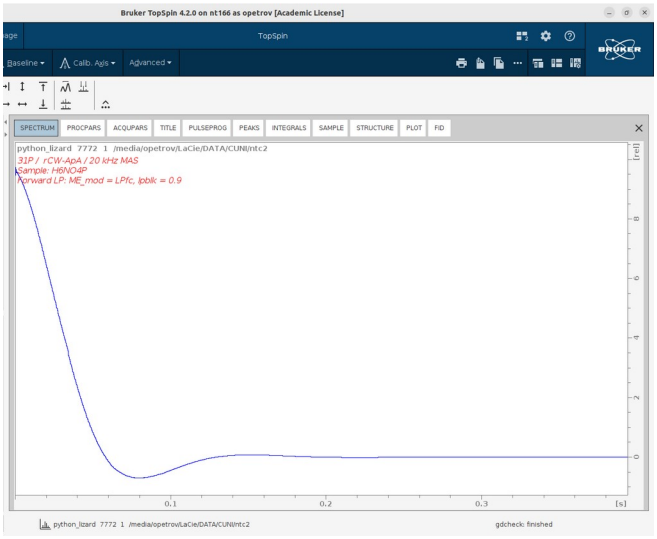


Fig. 23a





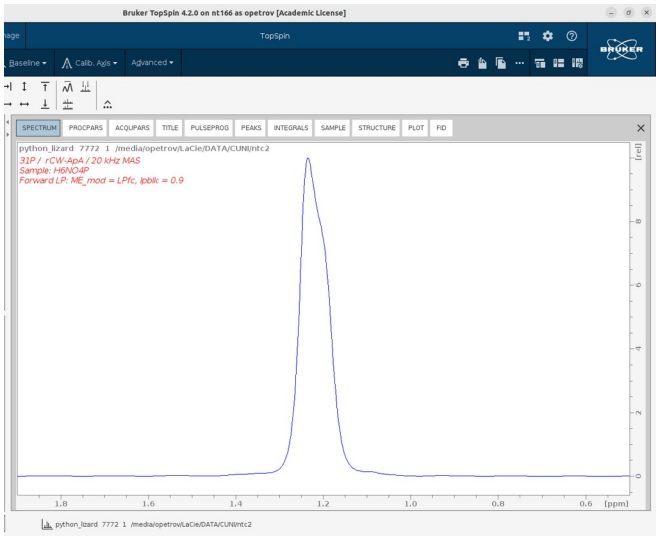
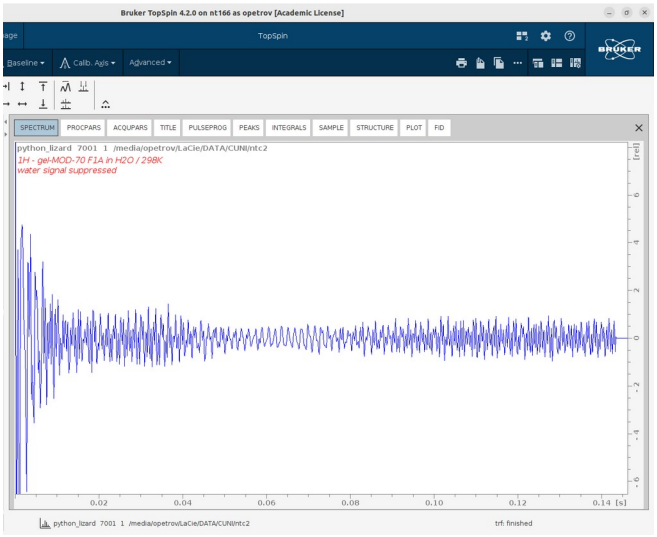


Fig. 23b



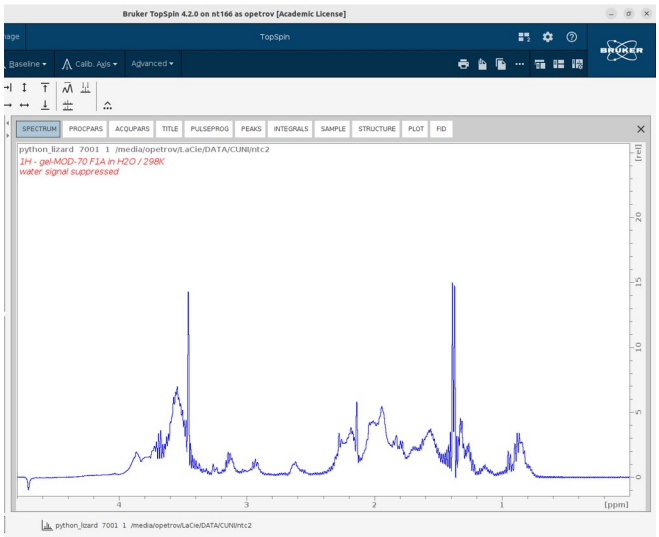
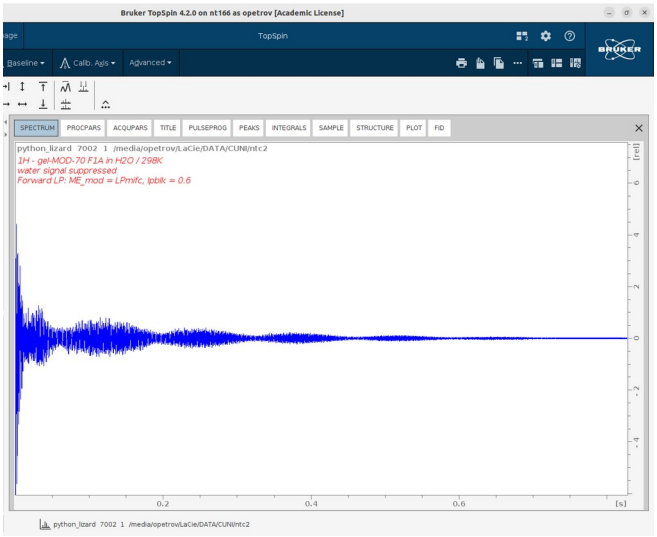


Fig. 24a



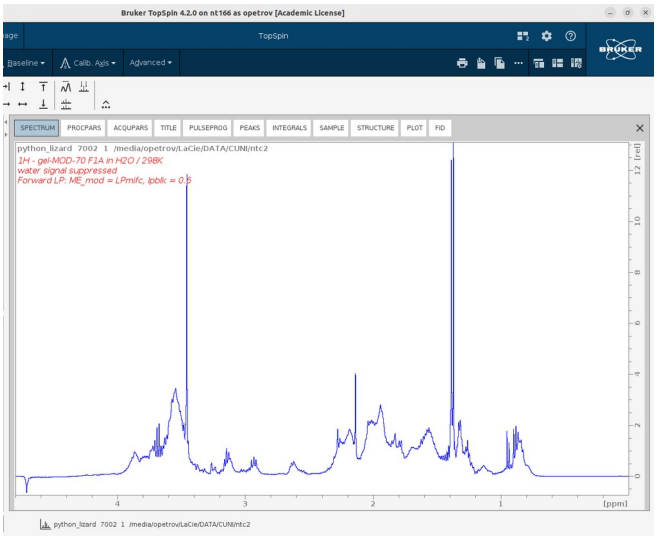


Fig. 24b

4.11 phase_fid

This script implements zero-order phasing (rotation) of a 1D time-domain signal, the first point of the signal being used as a pivot. It is primarily intended for relaxometry where such a rotation may be needed to maximize the Re-part of the signal (for quantitation purposes).

Figs. 26 shows rotation of a CPMG echo train from Fig. 25 that maximizes the real part of the echoes. Like other scripts modifying time-domain data, `phase_fid` will save the rotated signal under a new `EXPNO` (Fig. 27). The option `Zero Im` allows one to nullify the imaginary part of the rotated signal, which comes in handy when a symmetric Fourier transform is required, *e.g.* for ^{2}H NMR line shape analysis. The value of the `PH_ref` slider may be added to Topspin's PROCPARS, for next experiments.

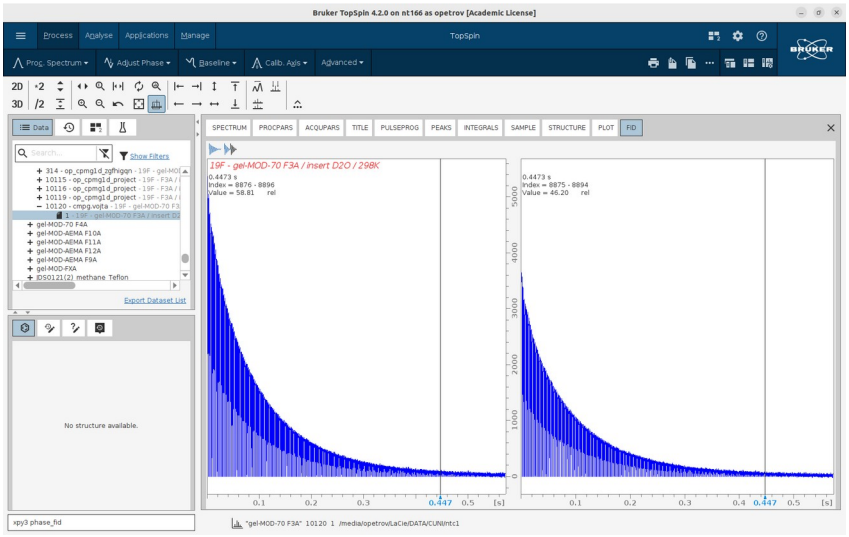


Fig. 25

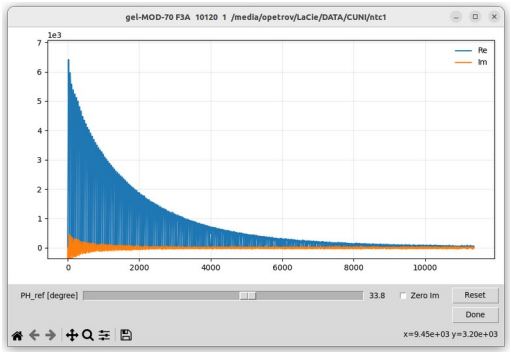


Fig. 26

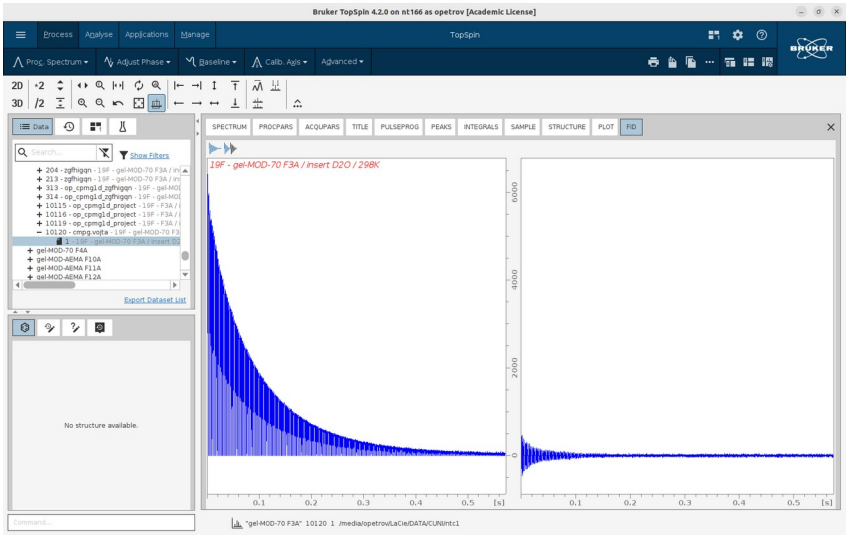


Fig. 27

4.12 rotsync

This tool is relevant to the magic angle spinning (MAS) NMR spectroscopy. What it does is positions rotary echoes in a MAS FID signal and undersamples it to those positions, thereby mimicking a rotor-synchronized FID acquisition. The corresponding FT spectrum will not have spinning sidebands (ssb), as all satellite transitions fall into the centerband where they superimpose a signal of the central transition. As a result, when quantitation of different chemical shift components is required, it can be done through direct integration over the centerband. The line shape of the rotor-synchronized spectrum is equivalent to an infinite MAS rate spectrum, which comes in handy for line shape analysis.

Usually, the rotor synchronization is implemented on the fly during an actual signal acquisition. However it requires thorough adjustment of both the sampling period and the sampling offset as the acquisition parameters. When you find such an adjustment tedious and difficult to control, use this post-acquisition synchronization instead. Of course, it only works if the rotary echoes are well defined (detectable) over a few rotor periods.

Fig. 28 shows the centerband of a MAS spectrum of $Al(acac)_3$ acquired under a 20 kHz MAS (^{27}Al NMR). Running `xpy3 rotsync` brings about a window (Fig. 29) with the given FID, in the magnitude mode, with rotary echo positions marked with asterisks. If needed, you can adjust these positions using the sliders `offset` and `period`. Clicking `OK` saves the echo positions as a new FID signal under nearest available `EXPNO` and process it with `efp` command (Fig. 30).

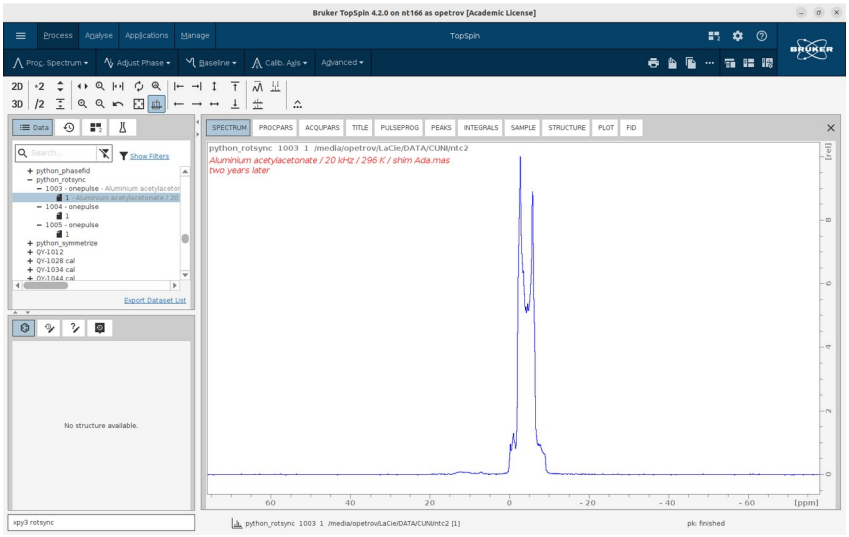


Fig. 28

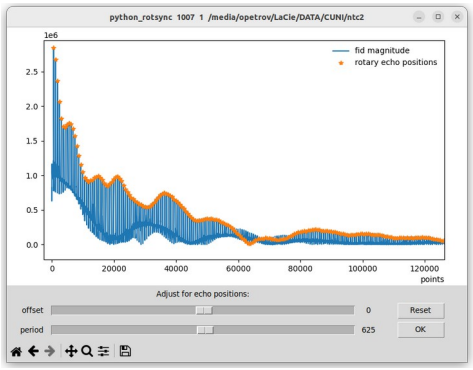


Fig. 29

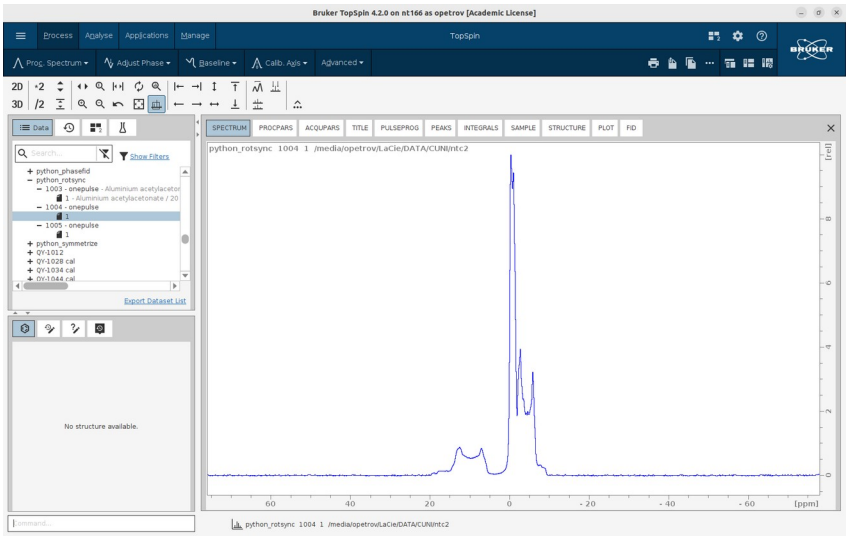


Fig. 30

4.13 rotsync_plus

Identical to `rotsync` except for a more involved echo quantitation procedure, aiming to better SNR.

4.14 sino_fid

It is like Topspin's `sino` but only for time-domain signals. It computes the ratio of the peak intensity of FID to its noise level, the latter being defined as 2 times a standard deviation of the noise, in accord to the Topspin's definition. The noise-related component of FID is extracted using principal component analysis, in the same way as in `denoise`. Consequently, having / specifying pure-noise regions is not necessary. The evaluated SNR is reported in a pop-up message.

4.15 symmetrize

This, again, is relevant to quadrupolar MAS spectra of half-integer spins. The ssb manifolds in such spectra are often asymmetric with respect to the central band, even when the first-order quadrupolar interactions prevail suggesting there must be a good symmetric pattern. The ssb intensity distribution in these cases can be skewed both positively and negatively, indicating contribution of some competing factors. They may be magic angle misadjustment, uneven probe response to frequencies on either sides of central pick, a noneligible contribution of 2nd-order quadrupolar interaction, etc. Fig. 31 is an example of a positively skewed ssb distribution (^{27}Al NMR). If you need it symmetric, *e.g.* to see how ssb manifolds from different samples compare, or to fit the first-order quadrupolar model to ssb, or simply present the spectrum at its best (*i.e.*, without instrument factors engaged), then use this script.

Typing `xpy3 symmetrize` will bring about a two-graph window (Fig. 32). On the top graph you will see the original spectra with ssb's marked with asterisks. In red is shown the recognized centerband (cb) area that is kept intact upon symmetrization. You can re-adjust the cb limits with sliders. The cb recognition relies on a Topspin's auto-integration method (see `int auto`), specifically on the integral regions listed in the `intrng` file. The bottom graph shows a symmetrized spectrum with opposite ssb's equalized using their average intensity. (The averaging is hard-coded in line 105 of the script for `mode='mean'`. If needed, it can be

changed for `mode='maximum'` in which case the ssb of a greater intensity will be placed on either side of the spectrum.) Clicking `OK` will return the symmetrized spectrum to a Topspin's window (Fig. 33).

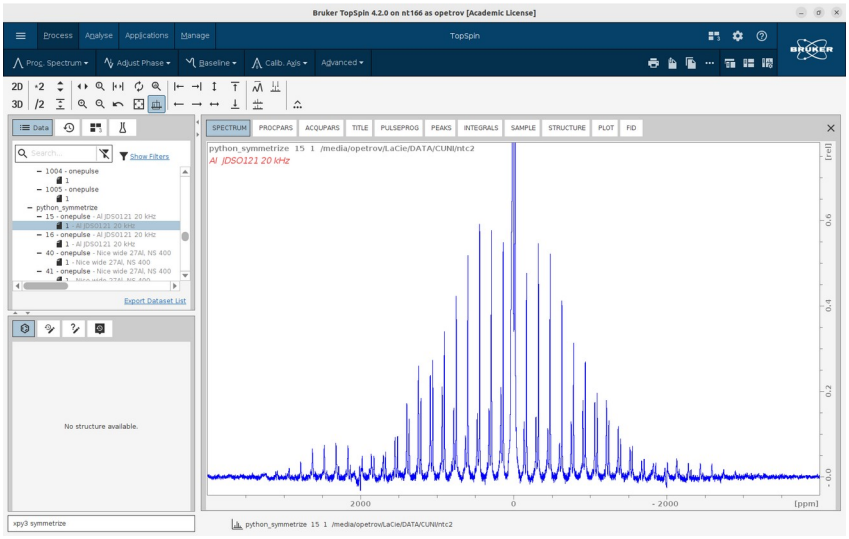


Fig. 31

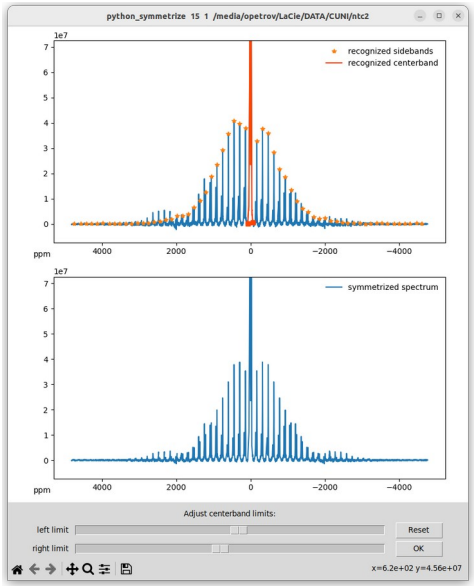


Fig. 32

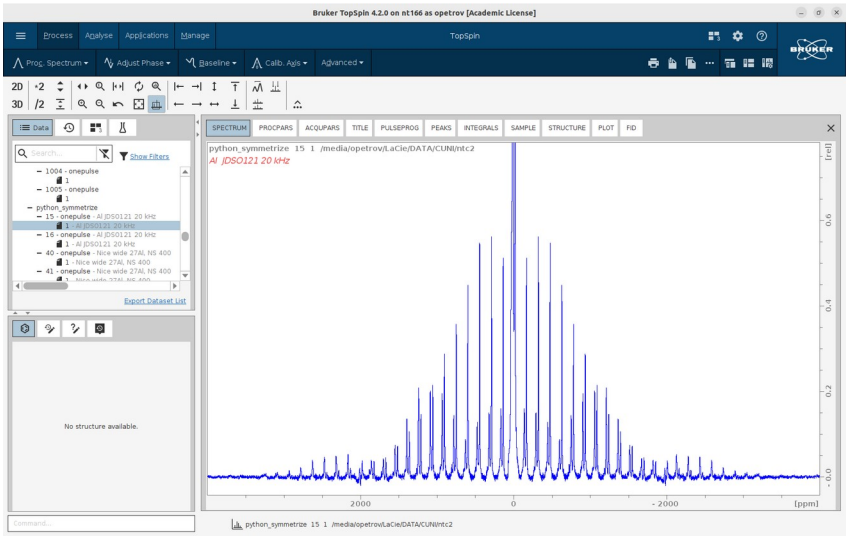


Fig. 33

4.16 t1denoise

It is identical to Bruker AU program `t1noisereduction` by function but quite different in implementation. To identify noise regions along the F1 axis of the given 2D spectrum, `t1denoise` employs a baseline recognition method `std_distribution` [2]. That will lead to noise evaluation over the entirety of F1, not only at periphery. They also differ in how data points classified as noise are treated afterwards. By default, `t1denoise` seeks a column with the smallest standard deviation (std) in the noise regions and then uses this std as a scaling factor to level down noise regions in the rest of the columns. The script can be run with an option at the command line,

```
xpy3 t1denoise [option]
```

where `[option]` may be `--zero`, or shortly `-z`, and `--spline`, or `-s`. The option `-z` implies that data points in the noise regions are set to zero instead of being leveled down. The option `-s` implies that these points are approximated with the Whittaker interpolation [5] and the approximations are subtracted from them. In all the cases, data points outside the noise regions are kept intact, as opposed to Bruker's `t1noisereduction`.

Fig. 34 shows a result of the default behavior of `t1denoise` (*i.e.* when it is run without any option) on the spectrum from Fig. 7 preliminary baseline-corrected with `baseplane`.

It is worth emphasizing the difference between the functions of `baseplane`, `t1denoise`, and `denoise2`. The first script shifts the data leaving all the points as scattered as before. The second script does reduce the scatter but only in those data points that have been classified as a baseline, whereas the points classified as spectral peaks stay as noisy. The third script reduces the scatter in all data points.

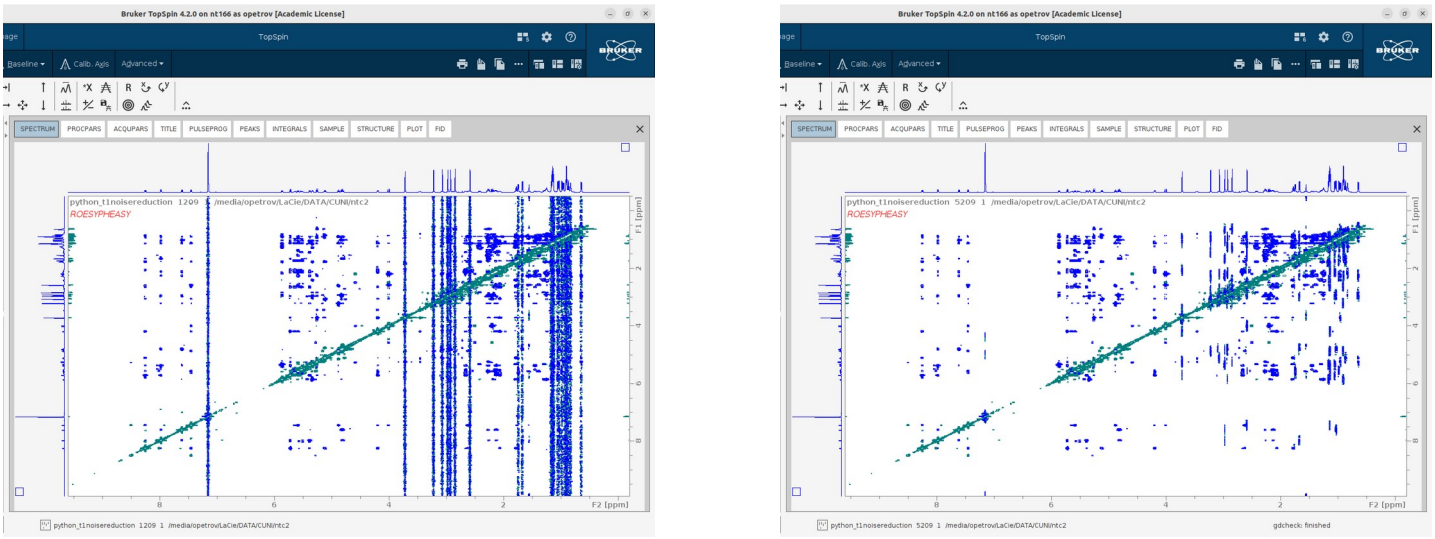


Fig. 34

4.17 t1t2

As the name suggests, `t1t2` is similar in functionality to Topspin's T1T2 relaxation toolbox. What it does is integrates a series of spectra measured at varying delays (pseudo-2D dataset) over an interactively selected region and fits an exponential model to the integral *vs* delay plot. Unlike the Topspin's T1T2, it works only with processed data, not with the FIDs. Moreover, it doesn't seek the biggest peak in the integration region, plotting only the integrals. The relaxation models used are mono-, two-, and stretched exponential ones. Relaxation delay values are read from a VDLIST file, after first being sorted in ascending order. If a VDLIST file is not found, the integrals are plotted against their indices, in which case the fitting functionality is disabled.

The script has an option for signal denoising through SVD thresholding, which is supposed to decrease a scatter in integrals. For spectra with non-zero baselines, there is an option to automatically subtract a baseline shift contribution from the integrals. (Apparently, this option needs more testing. Should it fail, use `baseline2` instead to correct baselines in the first place.)

Fig. 35 shows a two-graph GUI popped up after typing in a command `xpy3 t1t2` for the dataset shown in Fig. 4. These are data from a T_1 inversion-recovery experiment with 24 delays. The top graph displays superimposed spectra where the user can interactively select the desired region. After selection, a T_1 relaxation curve shows up on the lower graph (Fig. 36), with a live updating upon new selections. In this example, the intrinsic mono-exponential relaxation of the selected peak is obscured by a non-zero baseline shift. You can fix it checking a `Baseline corrector` checkbox, then fit a mono-exponential model normally via `Fit Me!` button (Fig. 37).

Clicking `Save&Quit` saves both the experimental and best-fit curves in a `<EXPNO>/pdata/1/ct1t2.001` text file. Note that the annotation text with best-fit model parameters is not saved, so mind writing down the needed values before quitting.

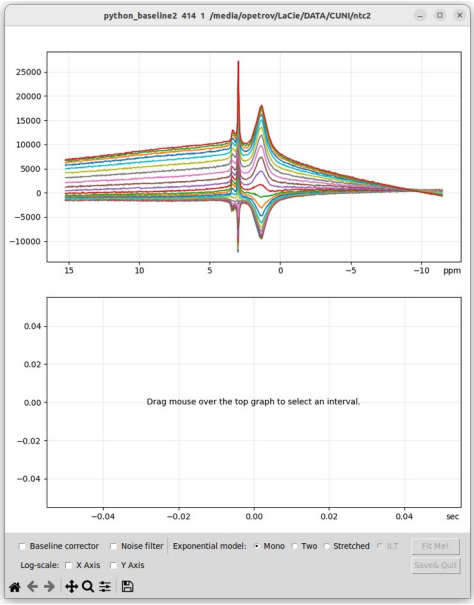


Fig. 35

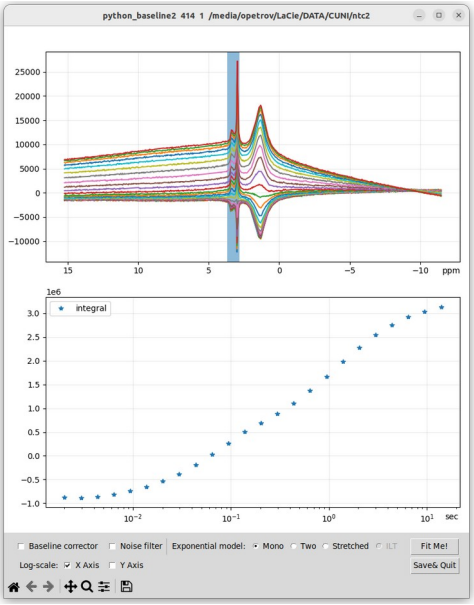


Fig. 36

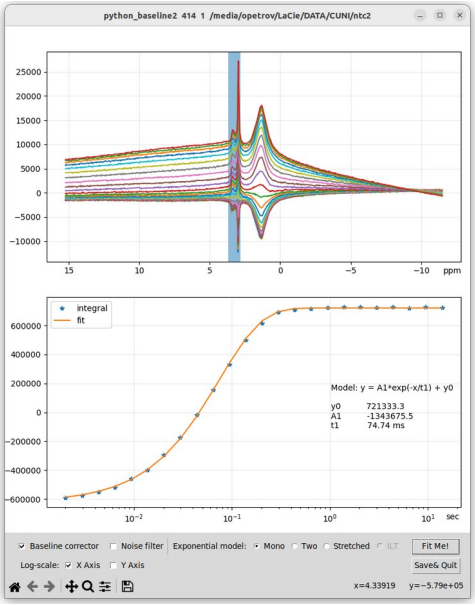


Fig. 37

5 Final remarks

The Python API introduced in Topspin 4.1.3 [1] is a tempting option for those who write their own Python scripts for NMR data processing. The `xpy3-tools` is a small collection of such scripts – formerly standalone, turned into Topspin plugins, decorated in one style. The tasks they solve may seem too diverse, or rather too specific, making impression that `xpy3-tools` will not find its use. But then AU programs and Jython scripts from Topspin's standard library are diverse too, yet they are used by many. Anyway, `xpy3-tools` is meant to to be gradually updated – with new scripts being added, hence higher chances it meets someone's needs. Those who tend to write their own scripts might consider it a template / building blocks / complement to their own efforts.

6 References

[1] https://www.bruker.com/en/products-and-solutions/mr/nmr-software/topspin/topspin-python-interface.html

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