

The xpy3-tools tutorial

Oleg V. Petrov | KFNT MFF | Univerzita Karlova

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1 Introduction

`xpy3-tools` is a collection of Python scripts for NMR data processing, designed to be suitable for use with Bruker Topspin program. As such `xpy3-tools` rely on Bruker Python API available in Topspin version 4.1.3 or newer [1]. Since version 4.2, the Python scripts can be run directly from the Topspin command line as `xpy3 <script name>`, in a way similar to conventional Jython scripts and AU programs.

The scripts primarily target the author's own practice but surely could be of interest to other NMR practitioners. The present version of `xpy3-tools` (v1.5) comprises 14 scripts (see Table 1), which number is meant to be extended in newer versions, as time goes on and a to-do list tend to grow.

Although sharing a workspace with Topspin means, among other things, the access to the Topspin's GUI, many scripts have their own windows popping up for interactive parameter optimization and visual control. The graphical functionality is implemented using `matplotlib` / `Tkinter` methods. Input/output functionality is supported by the Python module `BrukerIO` from the package `JUtils` (<https://github.com/jtrebosc/JUtils>).

None of `xpy3-tools` will modify in place `fid`, `ser`, `acqu(123)` and other files that store raw NMR data. When a script is programmed to write into those files, as *e.g.* in case of de-noising, the entire dataset will be copied under a new EXPNO thus preserving the original raw signal. Otherwise the data are processed in-place, the files of processed data being saved in `pdata` under the same EXPNO from whence the script has been called.

2 List of scripts

<i>Script name</i>	<i>Function</i>	<i>Comments</i>
baseline	Baseline correction in 1D	Uses rolling standard deviation distribution method to identify baseline points [4] and Whittaker method for their interpolation [5].
baseline2	baseline applied to individual spectra in a pseudo-2D data set.	Enables navigation across 2D dataset for baseline adjustment of individual spectra.
cpmg_fp	Whole-echo processing for a CPMG echo train.	Relies on zero points in a CPMG signal when splitting into echoes. To have such zeros, consider using a op_qcpmg pulse program.
cpmg_recursive	T_2 relaxation analysis of a CPMG echo train using mono-exponential recursive model.	Quantifies individual echoes, plots their cumulative sum vs time and fits with a recursive model [6].
cpmg_relaxation	T_2 relaxation analysis of a CPMG echo train using mono- or stretched-exponential model.	Plot 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.	Uses a Toeplitz matrix format to convert FID to 2D; the SVD threshold value is computed according to [7].
denoise2	Approximation of a 2D signal in time domain using noise-adaptive principal components.	Run NUS on acquired data to randomize the principal components and thereby average their noise-related content in order to use them in data approximation [8].
icoshift	Peak alignment over a series of spectra stacked in a pseudo-2D dataset or mutually related via multi display.	A number of peak regions can be selected for individual alignment, or one can rely on a particular peak to shift the entire spectrum.
phase_fid	Zero-order phasing of time domain signals (1D).	Handy for maximizing the Re-part of a signal prior to quantitation.
rotsync	Replication of a rotor-synchronized MAS spectrum out of an arbitrarily sampled FID signal.	Useful in quantitation of different chemical shift components through direct integration; handy for line shape analysis.
rotsync_plus	Employs a more involved echo quantitation than in rotsync.	In theory should provides better SNR than rotsync.
sino_fid	Hand-free signal-to-noise ratio (SNR) calculator for time-domain signals (1D).	SNR is defined as the ratio of FID amplitude to $2 * \text{std}$ of noise per channel.
symmetrize	MAS sideband symmetrization for 1D quadrupolar spectra of half-integer spins.	Facilitates the fitting of 1 st -order quadrupolar model to MAS spinning sidebands; handy for good-looking presentations of spectra.
t1t2	Basic relaxation analysis	Interactive integration of pseudo 2D spectra with exponential fits; accounts for baselines.

utils	Contains common utility functions and classes.	Ever growing collection of <code>defs</code> .
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3 Installation

3.1 Python environment setup

Topspin 4.1.4+ comes with a preinstalled Python 3 environment in <topspin>/python/lib/python3.x/ which includes Bruker Python API and other packages necessary for running demo scripts. To use another Python environment available in the system, you have to specify a proper path to the Python 3 interpreter. In Topspin 4.2+, you can do that on Topspin's preferences page, Preferences → Python 3+ → Select Python 3+ Environment. In Topspin 4.1.x, you are bound to the prefix <topspin>/python/... unless you backported 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's command line, otherwise you are to call them as regular Python modules – from a system's command line (CLI) or from a dedicated IDE such as Spyder or VSCode.

Imagine you have chosen a Python 3.x interpreter installed in /usr/local/bin on your Linux machine. Imagine also that your package installer is pip, namely pip3.x. Then open the terminal (CLI), change the directory to /usr/local/bin and run the command

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

where the configuration file requirements.txt is taken from the xpy3-tools repository. This will install all dependencies required for Table 1. Next you have to provide a search path for the Bruker Python API packages. It can be done by means of a .pth text file containing a path to a site-package (or dist-package) folder from the Topspin's prefix, e.g.

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

which must be placed in a namesake of site-package in your Python 3 environment. Alternatively, you may install those packages from .whl files usually available from <topspin>/python/examples:

```
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 must be taken of the module BrukerIO. The package JTutils that contains this module cannot be installed via pip. To get the module, copy brukerIO.py directly from the JTutils project page at <https://github.com/jtrebosc/JTutils/blob/master/CpyLib/> and place the file in the folder where xpy3-tools scripts are kept (see the next paragraph).

Installation on a Windows machine is supposed to be similar, though it has not been tested yet.

3.2 Placement of scripts

Running xpy3-tools scripts from the Topspin's command line requires a proper script location. A search path for Python 3 scripts is hard-coded via the xpy3.py file to <topspin>/python/examples. The simplest way to make it work is, therefore, to move the xpy3-tools scripts along with brukerIO.py into that folder. Should you prefer another location, add a path. 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 following lines (mind indents):

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

You may add as many paths in `extras` as you want, separating them by a comma. As mentioned in paragraph 3.1, `xpy3-tools` can be run as regular console (CLI) scripts, *i.e.* as `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` in Topspin 4.1.3).

4 Usage examples

4.1 baseline

This script implements interactive baseline correction in 1D. For the baseline classification part, it employs a function `std_distribution()` from the package `pybaselines` [2]. The function identifies baseline points by analyzing a rolling standard deviation distribution across a spectrum. It is controlled by two parameters – `half_window` and `num_std` – to adjust, respectively, the number of points involved in the rolling standard deviation calculation and the number of standard deviations for baseline points thresholding. For the baseline interpolation part, it employs a Whittaker smoother `ws2d()` from the package `vam.whittaker` [3]. This adds the third adjustable parameter – `lambda` – to control the interpolation smoothness. In the Topspin command line, you run `xpy3 baseline` (Fig. 1), which 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 baseline thus estimated.

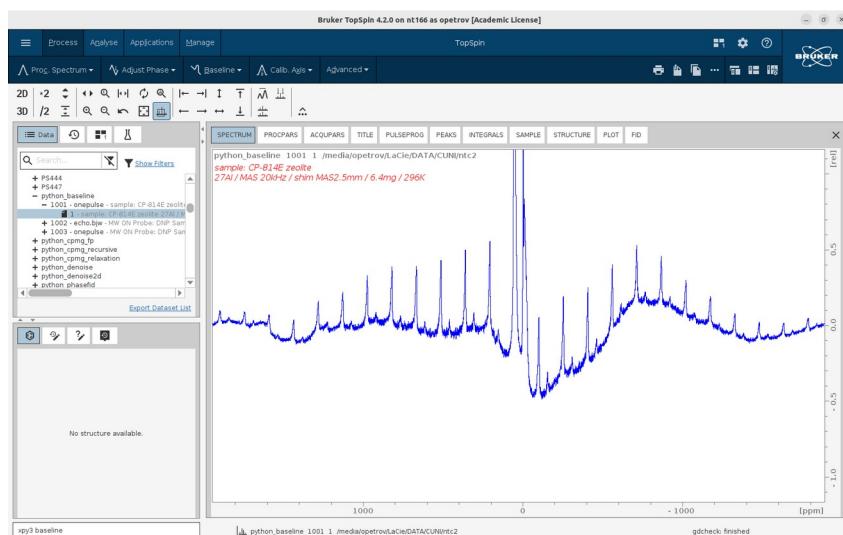


Fig. 1

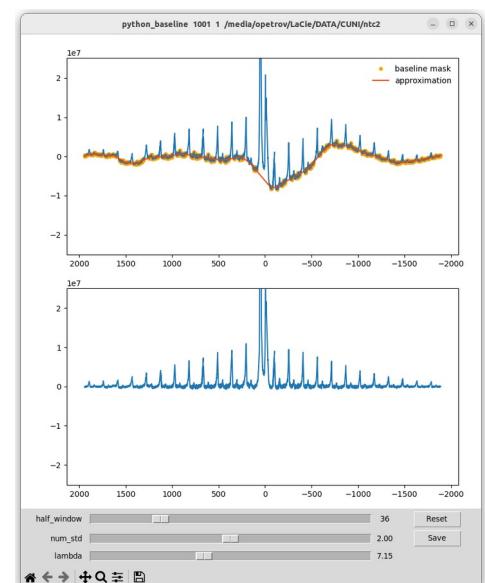


Fig. 2

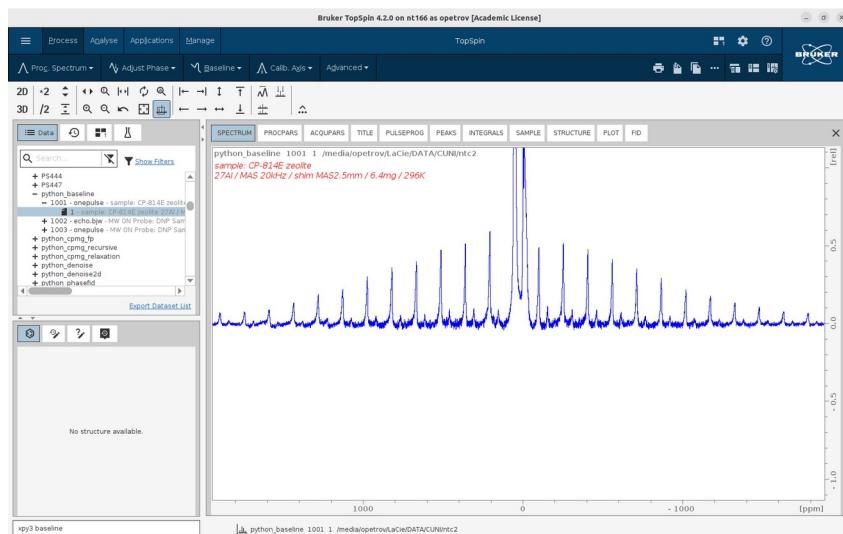


Fig. 3

The baseline estimate can be improved using sliders. Clicking **Reset** will restore the automatic estimate. Clicking **Save** writes the spectrum shown on the bottom graph to the pdata folder and updates the Topspin window (Fig. 3). It can be used to perform multiple additive baseline corrections, to remove multiple frequency baseline distortions. When modification times of **1r** and **1i** files coincide (meaning Re and Im parts of processed data are still coherent), baseline correction applies to both Re and Im parts of a spectrum. This seems useful if you wish to process the spectrum any further using both these parts (phasing, conversion to magnitude mode, inverse FT, etc.). It is applicable to datasets with **1i** file missing, i.e. to magnitude spectra.

4.2 baseline2

The command `xpy3 baseline2` performs a series of baseline corrections on individual spectra stored in pseudo-2D datasets, that is, in **2rr** and **2ii** files (but not in **2ir** or **2ri** files). For instance, Fig. 4 shows a series of 24 spectra from a T_1 inversion-recovery experiment on methane compressed inside MOF powder.

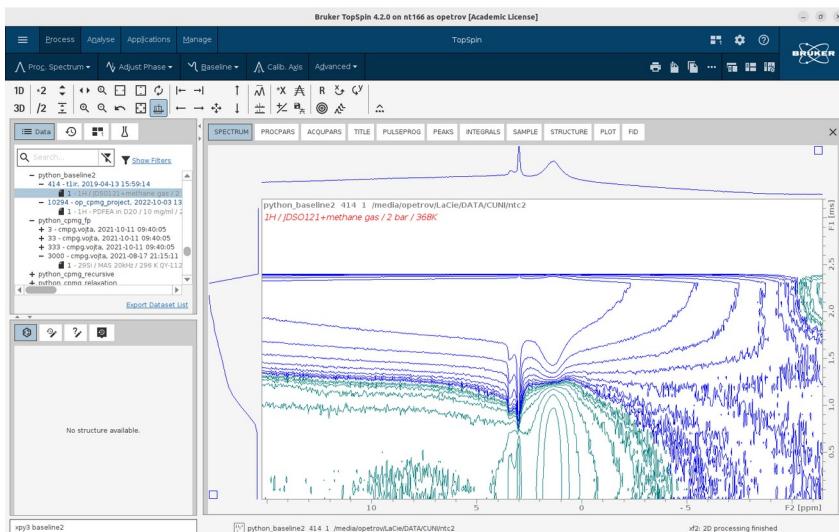


Fig. 4

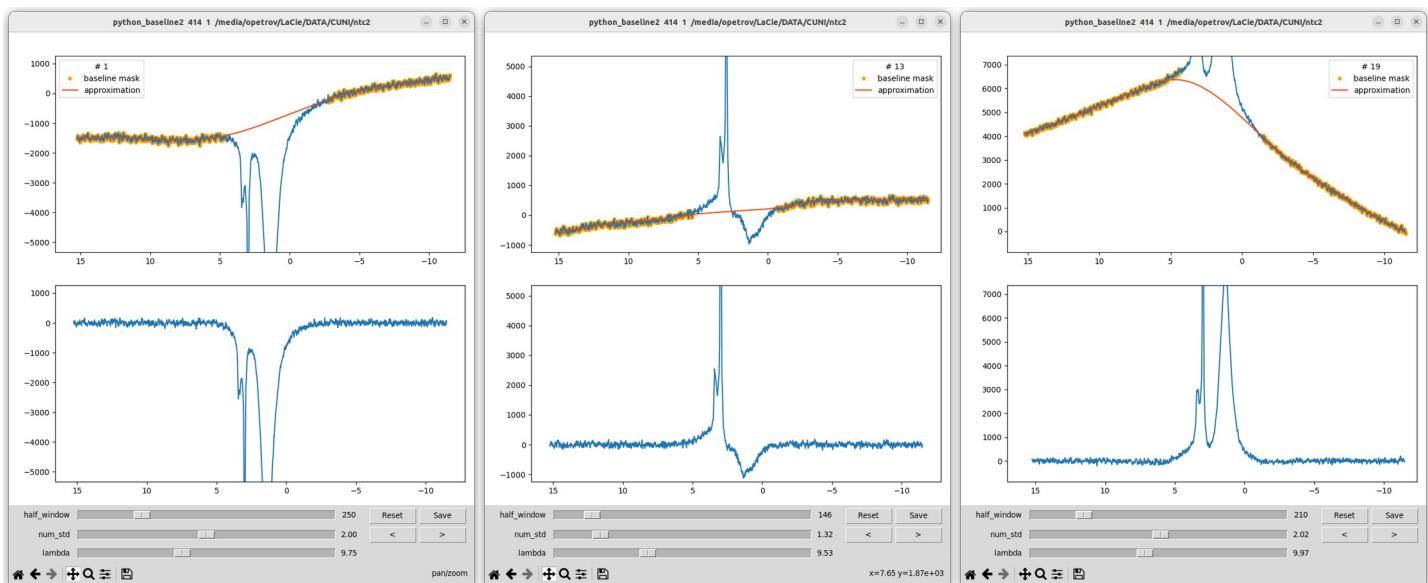


Fig. 5

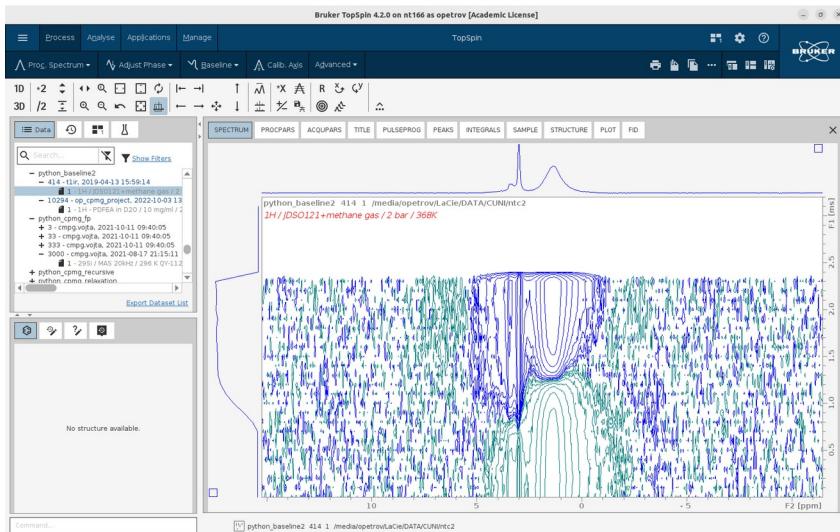


Fig. 6

Running the `xpy3 baseline2` command brings about a pop-up window identical to Fig. 2 but with the option to navigate across spectra using the buttons ">" and "<". By default, the first spectrum of a series is displayed. Once you inspect and optimize, if needed, the baseline estimate, you switch to another spectrum, and so on (Fig. 5). Eventually you click `Save` to write the entire series to the disk (Fig. 6).

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

4.3 `cpmg_fp`

This script applies to `qcpmg` type pulse programs that generate continuously sampled echo decays (aka echo trains). When processing such an echo decay as a regular fid – *i.e.* with the command `fp` (FT + phase correction) – it results in a discrete ‘spikelet’ spectrum. To get a more conventional continuous spectrum instead, you have first to collapse the echo train into a single echo (sum of echoes) and follow the whole-echo processing steps, *i.e.*, split the echo in the middle, swap the halves and then FT. This is essentially what `cpmg_fp` does, plus the first-order phase correction to maximize the Re part of the resultant spectrum.

Fig. 7 shows a train of 256 spin echoes from a zeolite sample (^{29}Si NMR). Typing `xpy3 cpmg_fp` brings about a two-graph window (Fig. 8) with the top graph showing the echo decay signal (same as in a Topspin window), while the bottom graph shows the average echo (sum of echoes) after first splitting the signal into individual echo segments. By default, all echo segments are included in the sum, but you can change this with the slider (# echoes). Changing # echoes affects both SNR and the lineshape of the spectrum provided it comprises differently relaxing components (different T_2 's). Once you are certain about # echoes, click `OK` to get the spectrum (Fig. 9).

For the script to work, the echoes in the train must be separated by one or more zero data points. A pulse program `op_qcpmg` attached to the `xpy3-tools` package is a special modification of a standard Topspin `qcpmg` program introducing such zeroes into a CPMG echo decay.

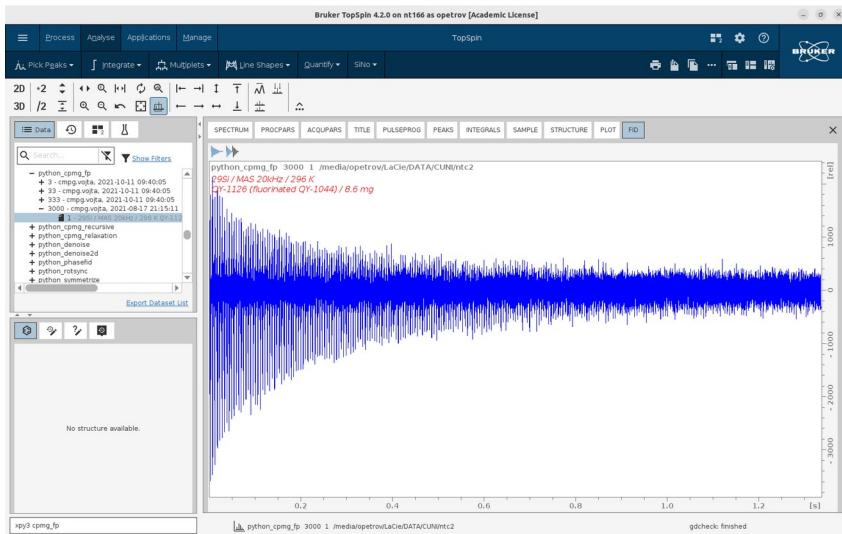


Fig. 7

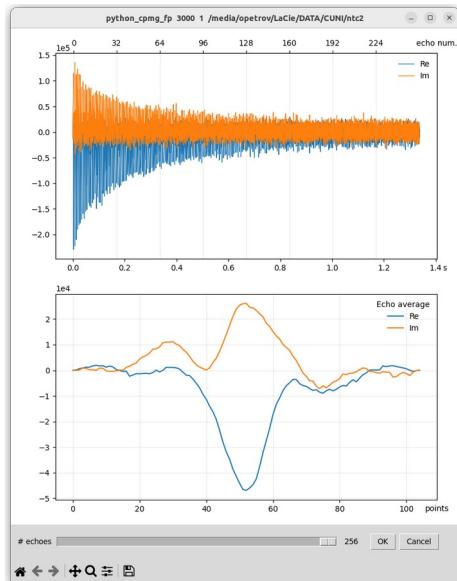


Fig. 8

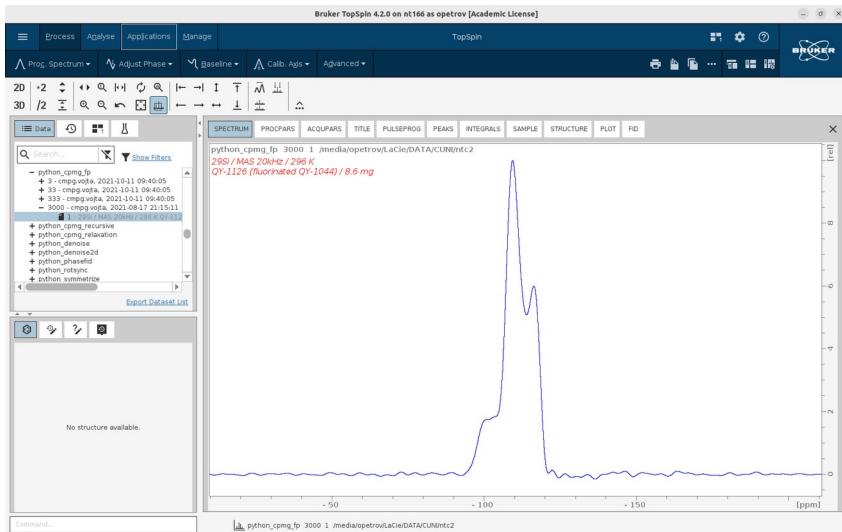


Fig. 9

4.4 cpmg_relaxation

This script again is intended for qcpmg type pulse programs generating continuous trains of zero-separated echoes. Given the zero positions, the script splits the train into individual echoes and quantifies them using either the midpoint intensity or integral intensity. The resultant echo decay curve – echo signal vs. echo time – can be fitted with either mono or stretched exponential model.

Fig. 10 shows an example 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. 11). The top graph shows the experimental signal, with detected echo positions marked with asterisks, and the bottom graph shows the echo decay curve, on a semi-log scale, measured by default from echo midpoints (with the option to switch to echo integrals). Clicking `Fit Me!` fits a mono-exponential model to the curve, the best-fit parameters being annotated (Fig. 12). In case of pronounced non-exponential decay,

there is an option to use a stretched exponential model with a mean relaxation time reported (Fig. 13). 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 will not be saved, so mind that you write them down before clicking **Save&Quit**.

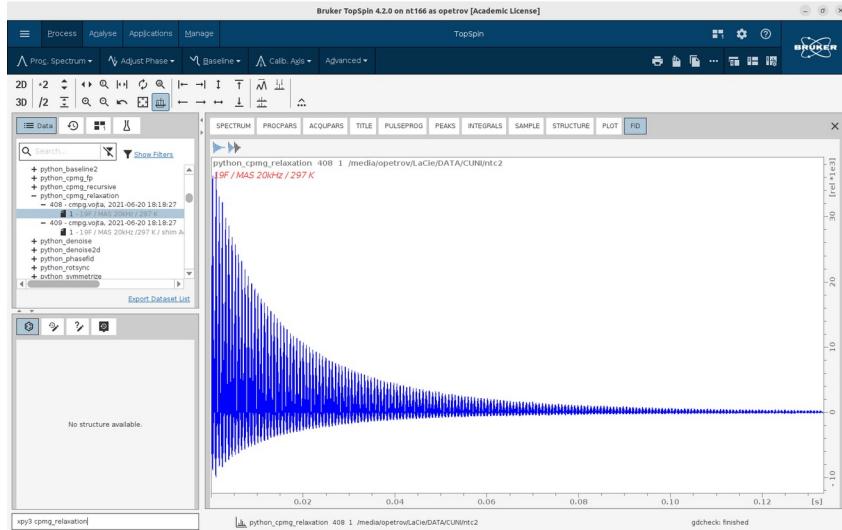


Fig. 10

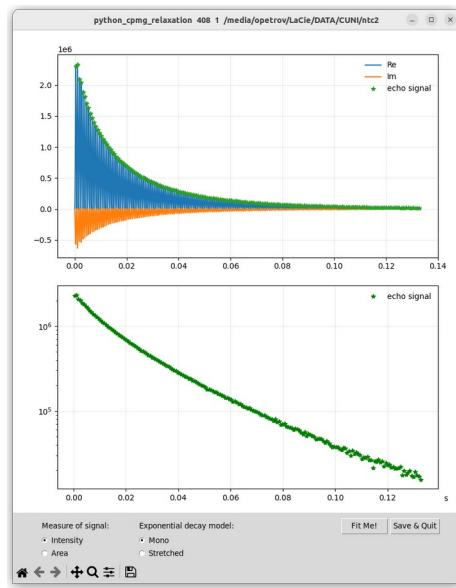


Fig. 11

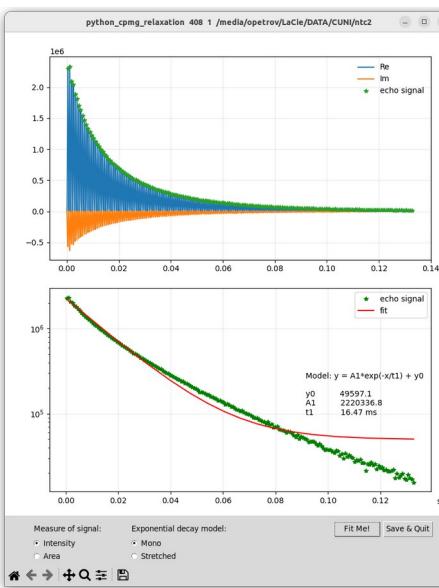


Fig. 12

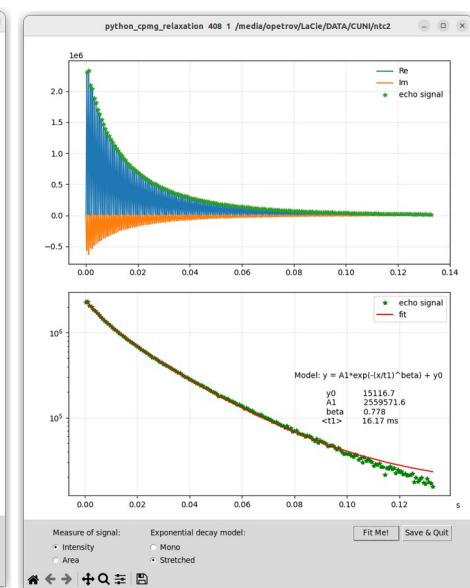


Fig. 13

4.5 cpmg_recursive

The functionality of this script is identical to `cpmg_relaxation` except for its using a cumulative sum of consecutive echoes as the measure of relaxation instead of individual echoes' intensity. The cumulative sum of echoes is fitted with a recursive mono-exponential relaxation model [6]. The advantage of this approach is two-fold: (i) the summation decreases a scatter in points on longer relaxation times; (ii) the best-fit parameters are less sensitive to the initial, fast-relaxing data points and thus better capture the overall relaxation trend. Fig. 14

shows the performance of `cpmg_recursive` on the same data as in Fig. 10. The GUI controls are analogous to `cpmg_relaxation`.

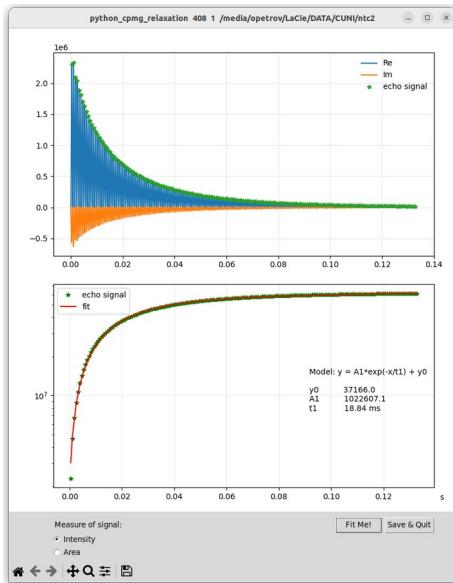


Fig. 14

4.6 denoise

This script carries out a Cadzow-like noise removal from 1D signals in time domain. The Cadzow's method [10] is based on a low-rank decomposition of a data matrix, hence at the first step the signal is to be converted into a matrix, specifically into a Toeplitz matrix where each row is a shifted version of the signal. Next, the matrix is subjected to a singular value decomposition (SVD) and only some largest singular values are retained. Then, the retained terms are employed to reconstruct (approximate) the matrix, which is finally re-arranged in a 1D array. To avoid dealing with group delay's points preceding the actual data points, the script automatically converts the signal to an AMX type ('analog filter' type) prior to denoising, using the Topspin command `convdta`.

The script does not have a GUI for interactive parameter optimization. To tackle performance issues, if any, the user may try and truncate the FID signal as much as possible by setting the Topspin's proc. parameter `TDef f` somewhere between `TD` and the value at which truncation artifacts ('sinc wiggles') become visible. Another parameter the user can play with is the number of the largest singular values involved in the Toeplitz matrix approximation. This number is set automatically using a Gavish-Donoho's (G.-D.) thresholding rule [7] but you can adjust it running the script with an optional argument `offset`,

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

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

Fig. 15 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. 16), in which case `denoise` leaves two noisy spikes at 47 and 170 ppm. As a rule, such spikes appear 'off-phase' wrt real peaks and hence are readily recognizable as noise-related artifacts.

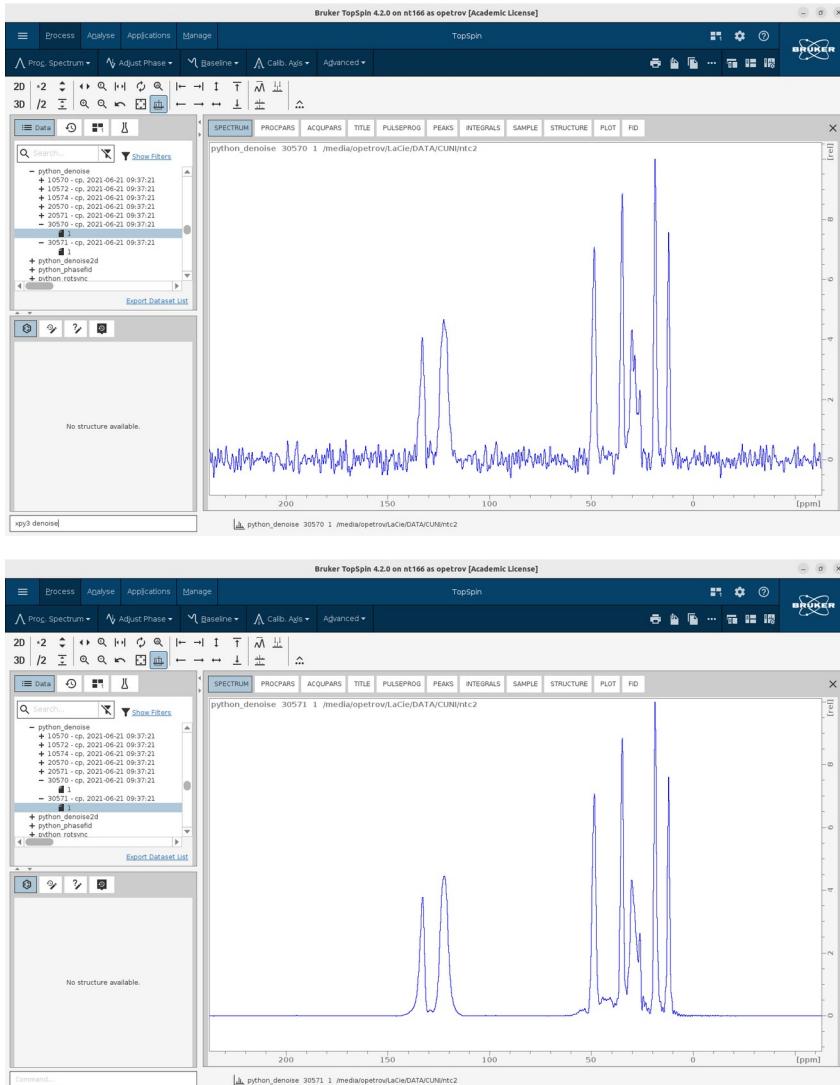


Fig. 15

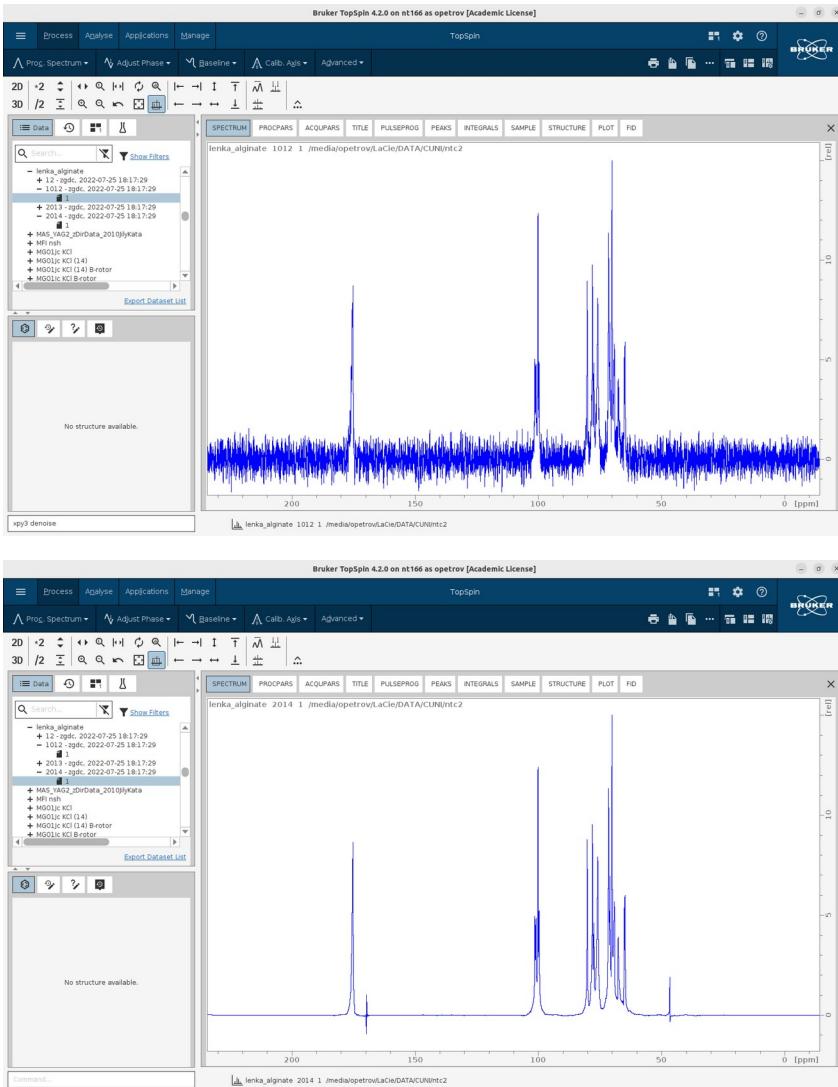


Fig. 16

4.7 denoise2

This script implements noise removal in 2D by an original method (see [8]). In brief, it is a variant of the PCA-based de-noising where the principal components (PCs) constituting a basis for signal approximation are attenuated proportionally to their noise-related content. You can think of it as a regularized SVD approximation, contrary to the conventional low-rank SVD approximation used in the 1D version `denoise`. The PC attenuation is achieved through ‘averaging’ same-rank PCs in a repetitive SVD of randomly chosen data samples. The size of the samples is controlled by a parameter `nus` in the range of 0.25 to 1.0 and the number of samples by the parameter `samples`. Both of these parameters can be passed through external arguments as below (the square brackets indicate that these arguments are optional):

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

Given no arguments, the script estimates `nus` automatically and `samples` is defaulted to 20.

Fig. 17 shows a phase-sensitive 2D INADEQUATE spectrum of strychnine in CDCl_3 (from Bruker's example dataset /examdata/exam_CMCse_3/). Beneath it is the same spectrum but after applying denoise2, demonstrating a factor of 2.3 improvement in SNR.

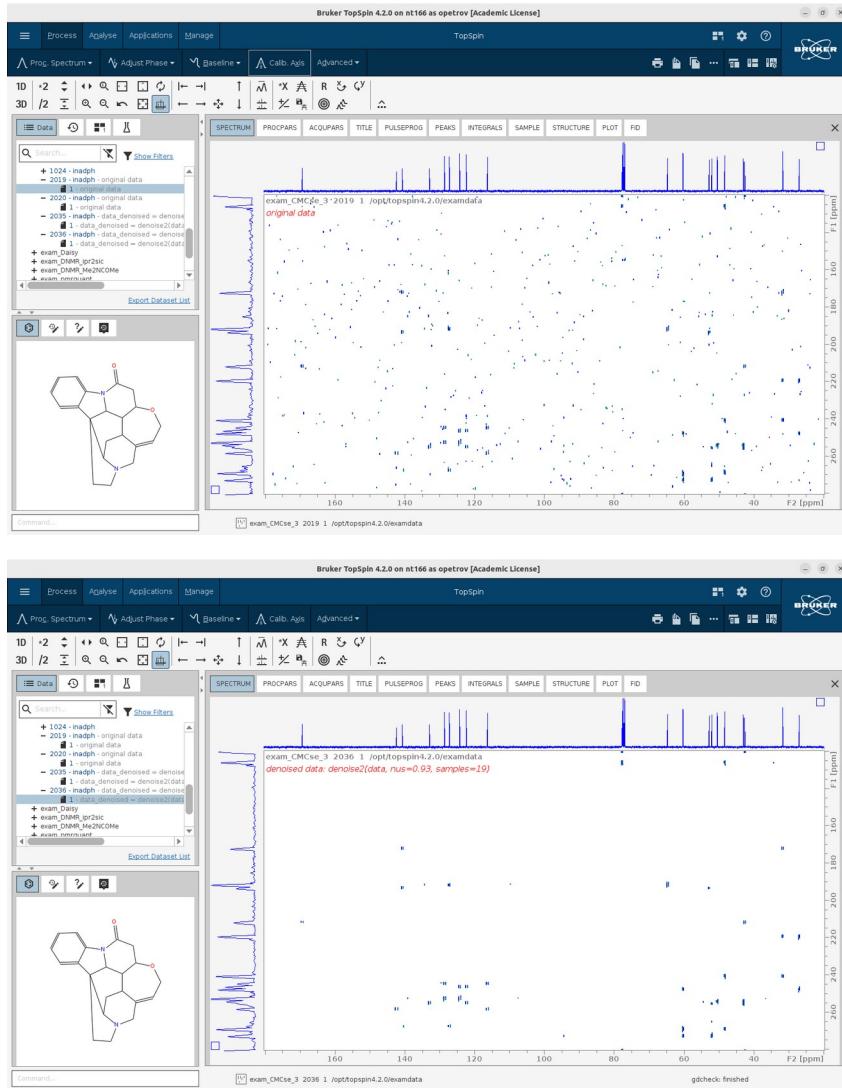


Fig. 17

Running denoise2 on large datasets and with the number of samples greater than the default 20 may take a painfully long time (longer than a minute). Should you not want to wait, you could interrupt the script by closing the accompanying progress bar widget and then restart it with a less number of samples. Like its 1D counterpart, denoise2 copies the whole data set to a nearest available EXPNO prior to de-noising.

4.8 icoshift

This is a frontend to utility functions of `pyicoshift` [9] – a Python implementation of the *icoshift*, which stands for an ‘*interval correlation optimized shifting*’ algorithm for peak alignment. It applies to spectra of the same peak pattern but with the peak positions prone to fluctuations in pH, ion content, temperature etc., or

shifted due to instrumental factors. The `icoshift` script can be run either on a pseudo-2D dataset or on 1D spectra related to each other via multi-display (`.md`) mode, provided they are of the same size.

Fig. 18 shows spectra of a polyacrylamide hydrogel in D₂O from a variable-temperature experiment, opened in a Topspin's multi-display window (`.md`). Typing `xpy3 icoshift` brings about a two-graph GUI (Fig. 19). 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. 20 and 21, 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" [9]), 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.

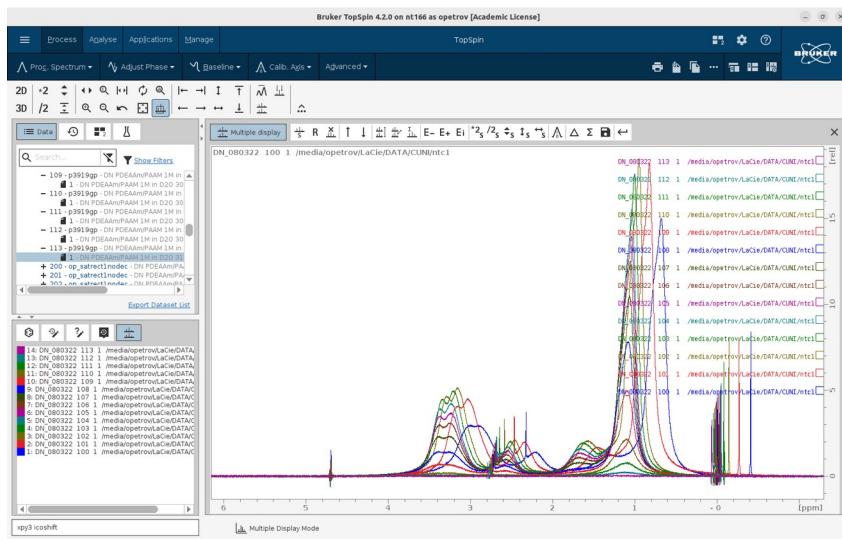


Fig. 18

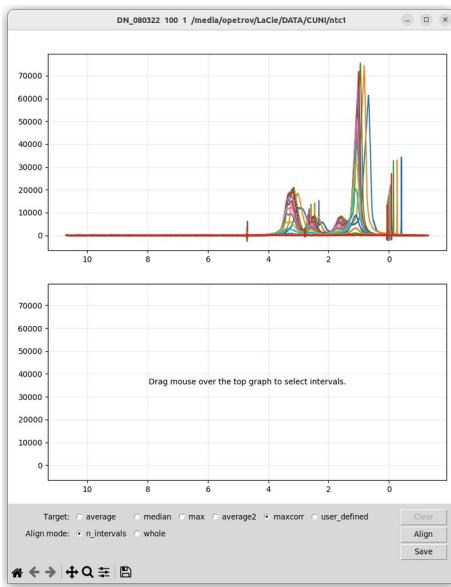


Fig. 19

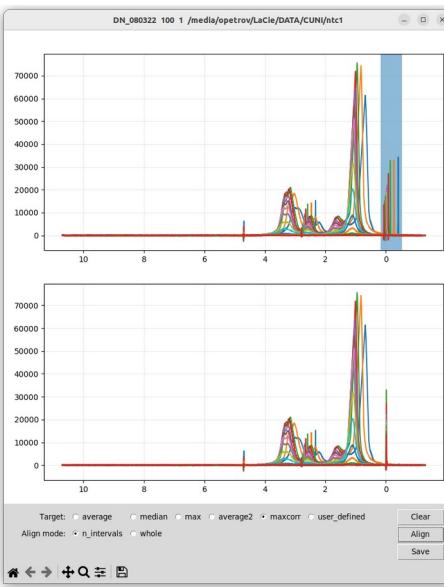


Fig. 20

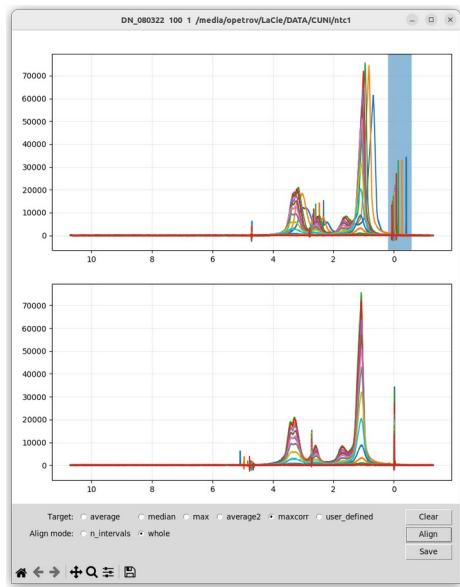


Fig. 21

4.9 phase_fid

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

Figs. 23 shows rotation of a CPMG echo train from Fig. 22 in order to maximize the real part of the echoes. The `phase_fid` saves the rotation under a new EXPNO, as it should when raw data are modified (Fig. 24). There is an option `Zero Im` to nullify the imaginary part of the rotated signal, which is a convenient and easy way to obtain a symmetric Fourier transform of the signal (the approach often employed in ^2H lineshape analysis). The value of the `PH_ref` slider can be written down and used to correct the homonymous Topspin's parameter for subsequent experiments.

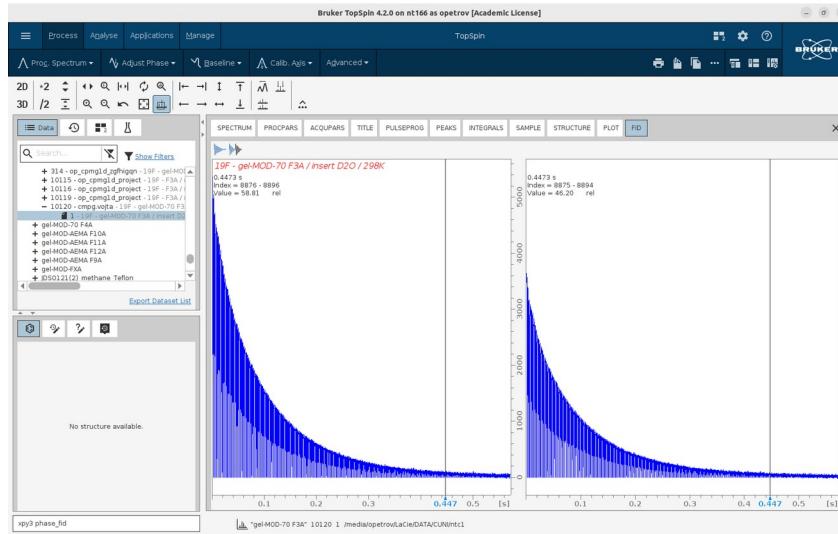


Fig. 22

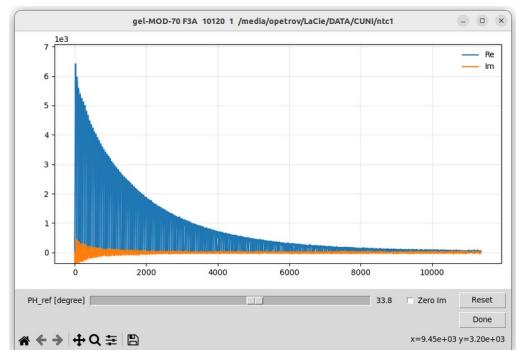


Fig. 23

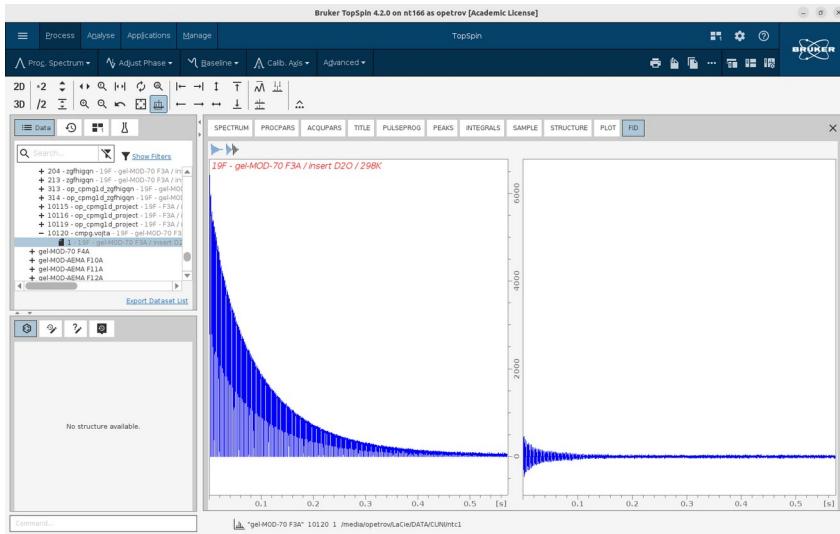


Fig. 24

4.10 rotsync

This tool is specific to magic angle spinning (MAS) NMR. What it does is, it positions rotary echoes in a 1D MAS signal and re-samples the signal down to these positions, thus rendering it a ‘rotor synchronized’ signal. The rotor-synchronized signal is one without spinning sidebands (ssb) in the spectrum, with satellite transitions intensity all falling into the centerband where it superimposes the central transition peaks. Thus, when it comes to quantitation of spectral components with different chemical shifts, it can be done directly through integration over the centerband. The line shape of the rotor-synchronized spectrum is equivalent to the case of the infinite MAS rate, which is convenient for the line shape analysis.

Usually, rotor synchronization is implemented on the fly during signal acquisition. This, however, requires thorough adjustment of both sampling period and sampling offset as acquisition parameters. Since it is tedious and difficult to control, one might prefer this post-acquisition synchronization instead. Of course, it would require for the rotary echoes be well defined (detectable) over a few rotor periods.

Fig. 25 shows the centerband of a MAS spectrum of Al(acac)₃ acquired under a 20 kHz MAS (²⁷Al NMR). Running `xpy3 rotsync` brings about a window (Fig. 26) showing the given FID signal, 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 next available EXPNO and process it with `efp` command (Fig. 27).

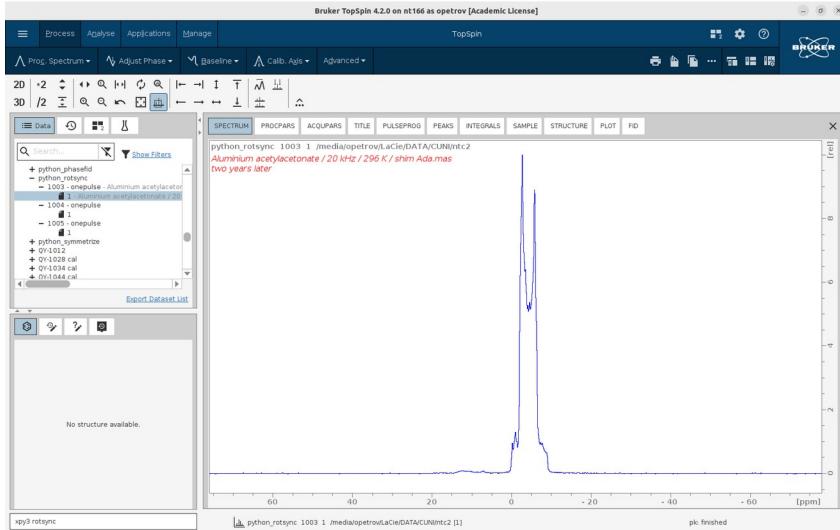


Fig. 25

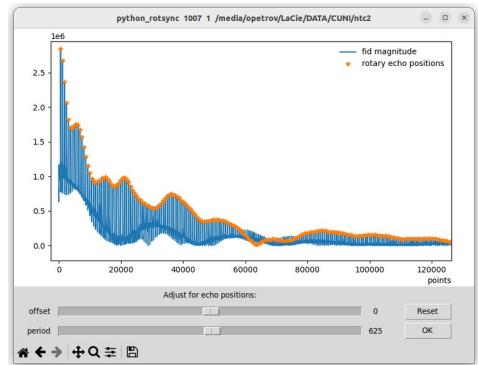


Fig. 26

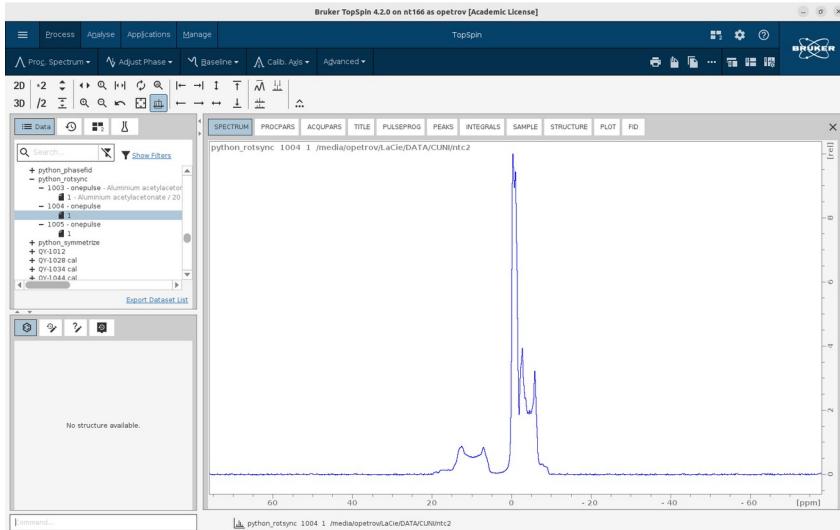


Fig. 27

4.11 rotsync_plus

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

4.12 sino_fid

This is an extension of Topspin's `sino` towards time domain. With this script you can measure the ratio of the highest intensity in a fid, or an echo, to its noise level. The latter is defined as 2 times standard deviation of the noise, in accord to the Topspin's definition of SNR. The noise component is extracted from the fid by means of principal component analysis, the procedure being similar to that used in `denoise` in paragraph 4.6. It particularly means that the signal may be truncated and thus have no pure noise region. The measurement is hand free – just type `xpy3 sino_fid` and it will report SINO (FID) in a message.

4.13 symmetrize

This, again, applies to MAS NMR data, namely to quadrupolar MAS spectra of half-integer spins. The spinning sideband (ssb) manifolds in such spectra may appear highly asymmetric with respect to the central band, even when the first-order quadrupolar interactions prevail meaning a high degree of symmetry. The observed ssb intensity distributions are skewed both positively and negatively, suggesting there being several competing factors of such asymmetry. These factors include magic angle misadjustment, uneven probe response as a function of frequency, a noneligible second-order quadrupolar term, and maybe others. Fig. 28 is an example of ssb distribution with positive skewness (^{27}Al NMR). If you really need it appear symmetric, e.g. to see how ssb manifolds from different samples compare, or to fit the first-order quadrupolar model to the ssb pattern, or simply to present the spectrum at its best (i.e., without instrument factors engaged), then use this script.

Typing `xpy3 symmetrize` brings about a two-graph window (Fig. 29). On the top graph you can 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 the sliders. The cb recognition relies on a Topspin's auto-integration method (see `int auto`), namely 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 by assigning `mode = 'mean'`. If needed, this 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 Topspin (Fig. 30).

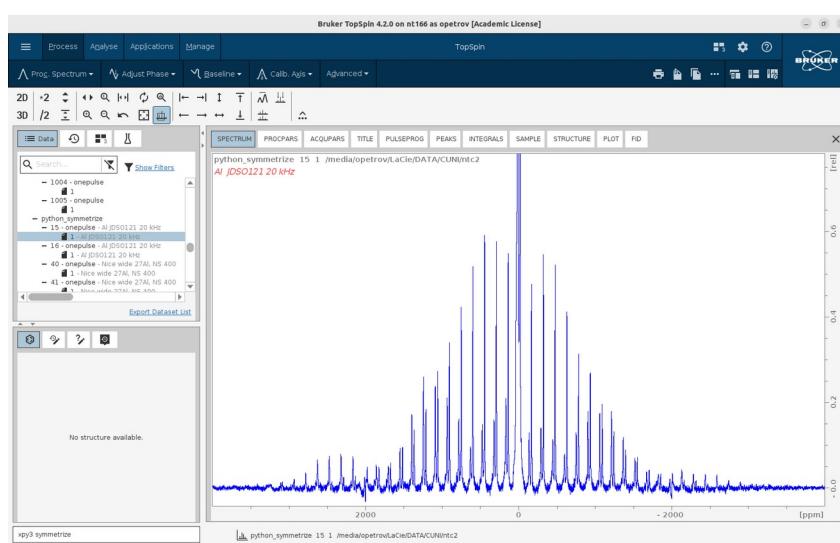


Fig. 28

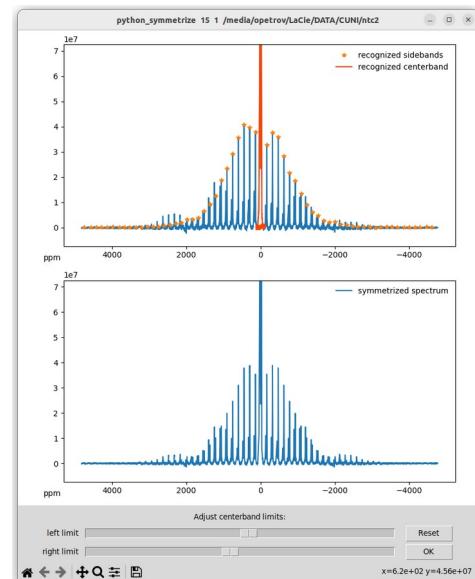


Fig. 29

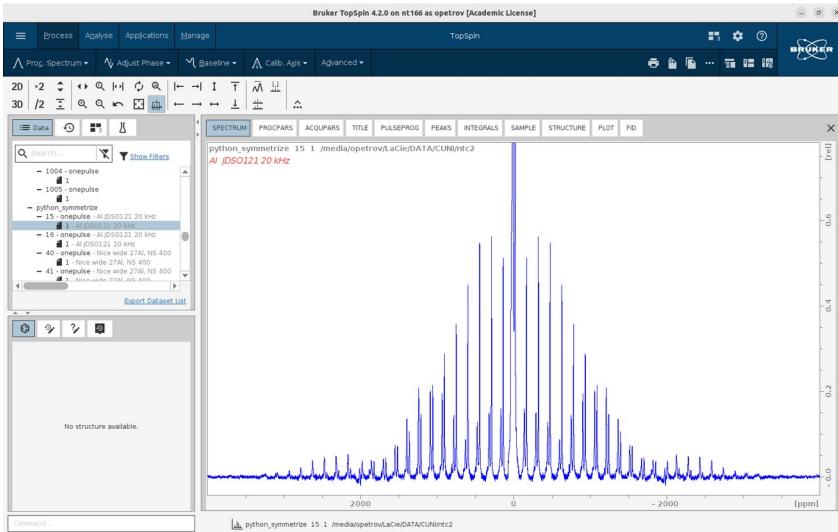


Fig. 30

4.14 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 FIDs. Besides, it doesn't seek the biggest peak in the integration region, plotting only the integral itself. The relaxation models used are mono-, two-, and stretched exponentials. The relaxation delays are read from a VDLIST file, sorted in ascending order. If a VDLIST file is not found, the integrals are plotted against their index numbers, in which case the fitting functionality is disabled.

The script has an option for signal denoising based on SVD threshold method, thereby decreasing a scatter in points in the plots. Another option which is useful for spectra with non-zero baselines is automatic subtraction of a baseline shift contribution from the plots. (Apparently, this option needs more testing. Should it fail, use `baseline2` instead in order to correct spectra for their baselines in the first place.)

Fig. 31 shows a two-graph GUI popped up after typing in a command `xpy3 t1t2` for the dataset shown in Fig. 4, which is 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. 32), with a live updating upon new selections. In this example, an intrinsic mono-exponential relaxation of the selected peak is obscured by non-zero baseline shift. To fix it, you can check a Baseline corrector checkbox, then fit a mono-exponential model normally via `Fit Me!` (Fig. 33).

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

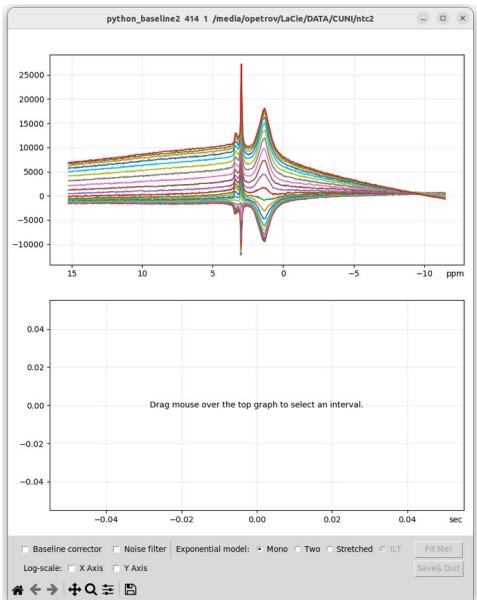


Fig. 31

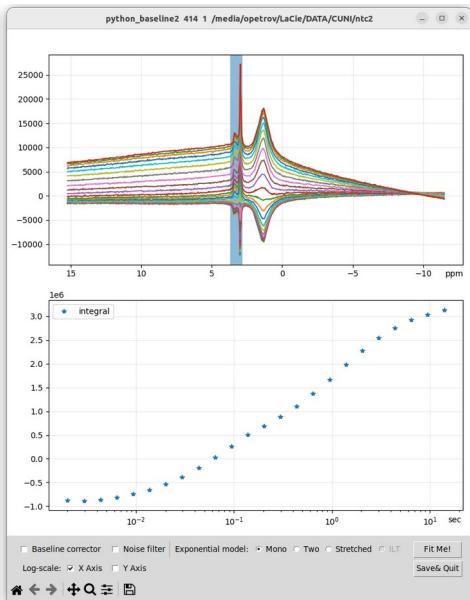


Fig. 32

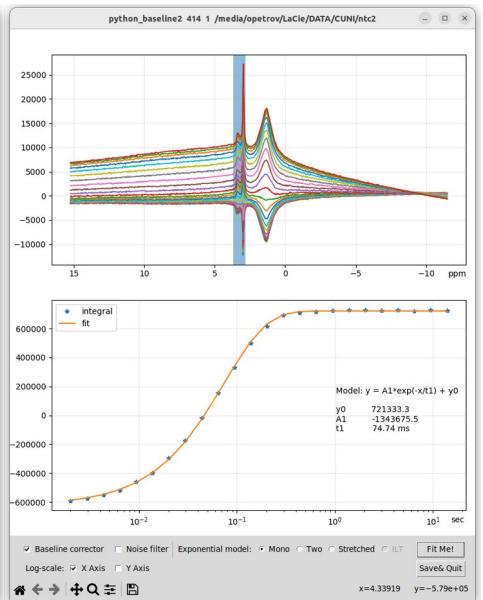


Fig. 33

5 Final remarks

The Bruker API for Python added to recent versions of Topspin [1] is a tempting option for those who used to write their own Python scripts for NMR data processing. The `xpy3-tools` is a small collection of such formerly standalone scripts used by the author turned into Topspin add-ons, decorated in one style. The tasks performed by the `xpy3-tools` may seem too diverse or, on the contrary, too specific, and thereby make an impression that `xpy3-tools` will not find its use. But then AU programs and Jython scripts from the Topspin library are diverse yet used by many. Anyway, this version of `xpy3-tools` is just a base for a greater collection of scripts. The experienced NMR users who tend to write their own scripts might consider it a template / building blocks / complement to their own efforts.

6 References

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