



PURE SHIFT IMPLEMENTATION

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JEOL

Basics

$$H \psi = E \times \psi$$

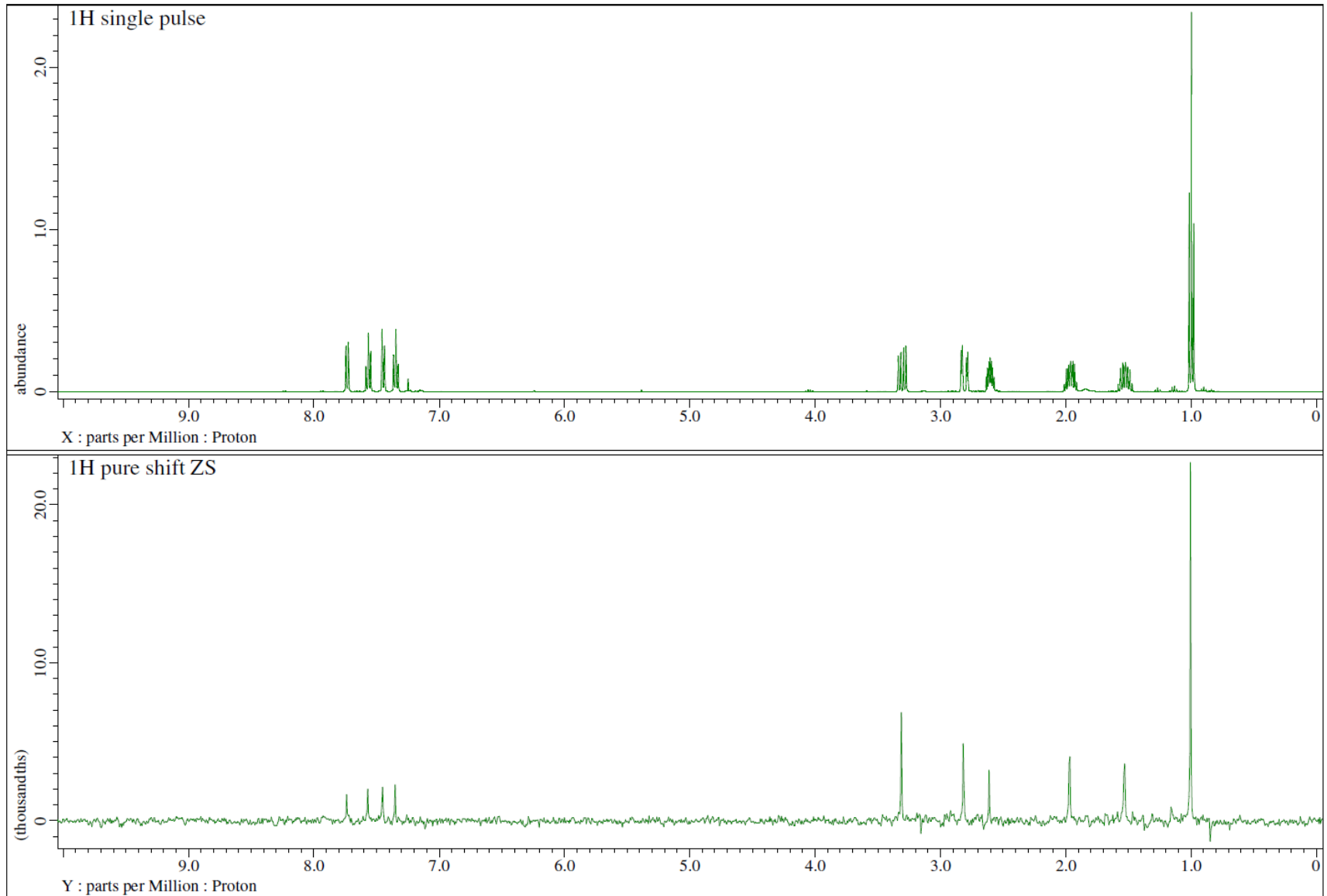
Experiment submission

The screenshot displays the JEOL NMR software interface. At the top, the menu bar includes Connection, Tools, Config, Shims, Samples, Jobs, and Queue. The main window is divided into several sections:

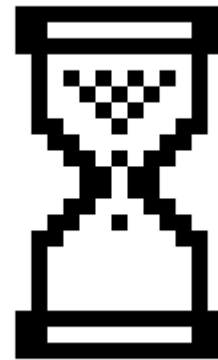
- Activity Panel:** Shows the current sample as 'Ethyldanone (5)' with a status of 'Idle'. It includes a 'Monitor' button and a 'Status' button.
- Sample Control:** Features 'Load' and 'Interactive' buttons.
- Table:** A table with columns for No., Sample Name, Solvent, Slot, and Comment. The fourth row, 'EI' in slot 0, is highlighted in green and marked with a red '1'.
- Job Panel:** Shows the selected job 'EI' with a duration of 0:08. It lists sub-jobs: 'Proton' (0:02) and 'Experiment 1' (pure_shift_ZS, 0:07).
- Method Selection:** A grid of buttons for various NMR methods. The 'pure_shift_ZS' button is highlighted with a red '2'.
- Queue:** A table for managing the job queue with columns for Job #, Status, User, Job title, Scheduling, and Est End Time.
- Job Parameters:** Includes settings for 'allow printing' (set to 'to PDF') and 'project'.
- Submit Button:** A large green button with a play icon, marked with a red '3'.
- Bottom Status Bar:** Displays system parameters: Receiver Gain: 50, Spin: 0[Hz], Lock: 588, Temp: 20.9[dC], Helium: 83[%], Nitrogen: 57[%], and Queue Length: 0.

Automated acquisition and processing

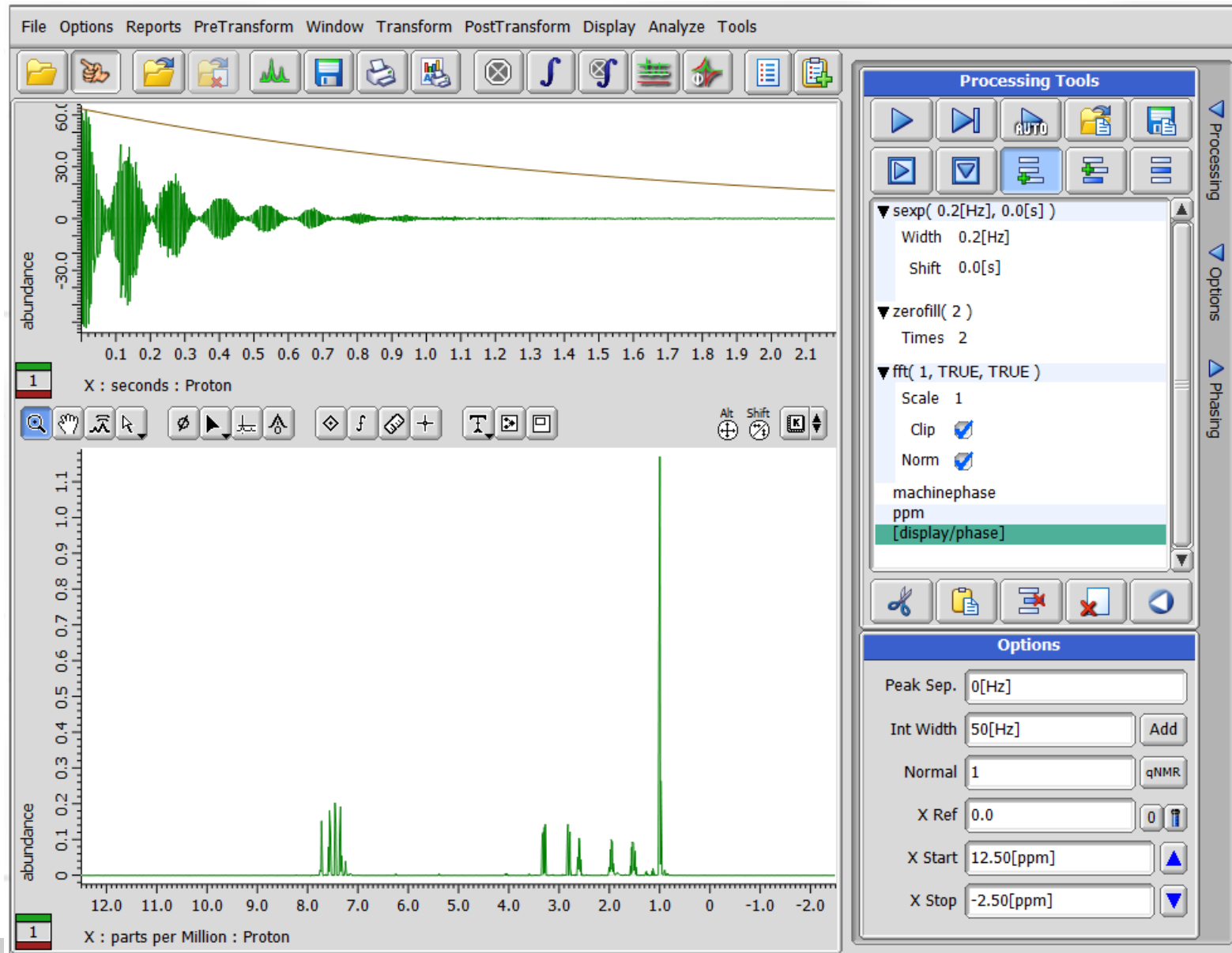
Proton vs Pure shift (ZS)



Processing



Typical processing of single pulse



1D from 2D interferogram (old)

File Options PreTransform Window Transform PostTransform Display Analyze Tools

1D

AXES

X

- ▶trapezoid3(0[pnt], 82[pnt], 82[pnt])
- ▶shift(-19[pnt], TRUE, FALSE)
- ▶shift(0.242[s], TRUE, FALSE)
- ▶tilt(-45[deg], FALSE)

[transpose]

Y

- sum_plane
- [transpose]

1

View

2

3

4

Levels

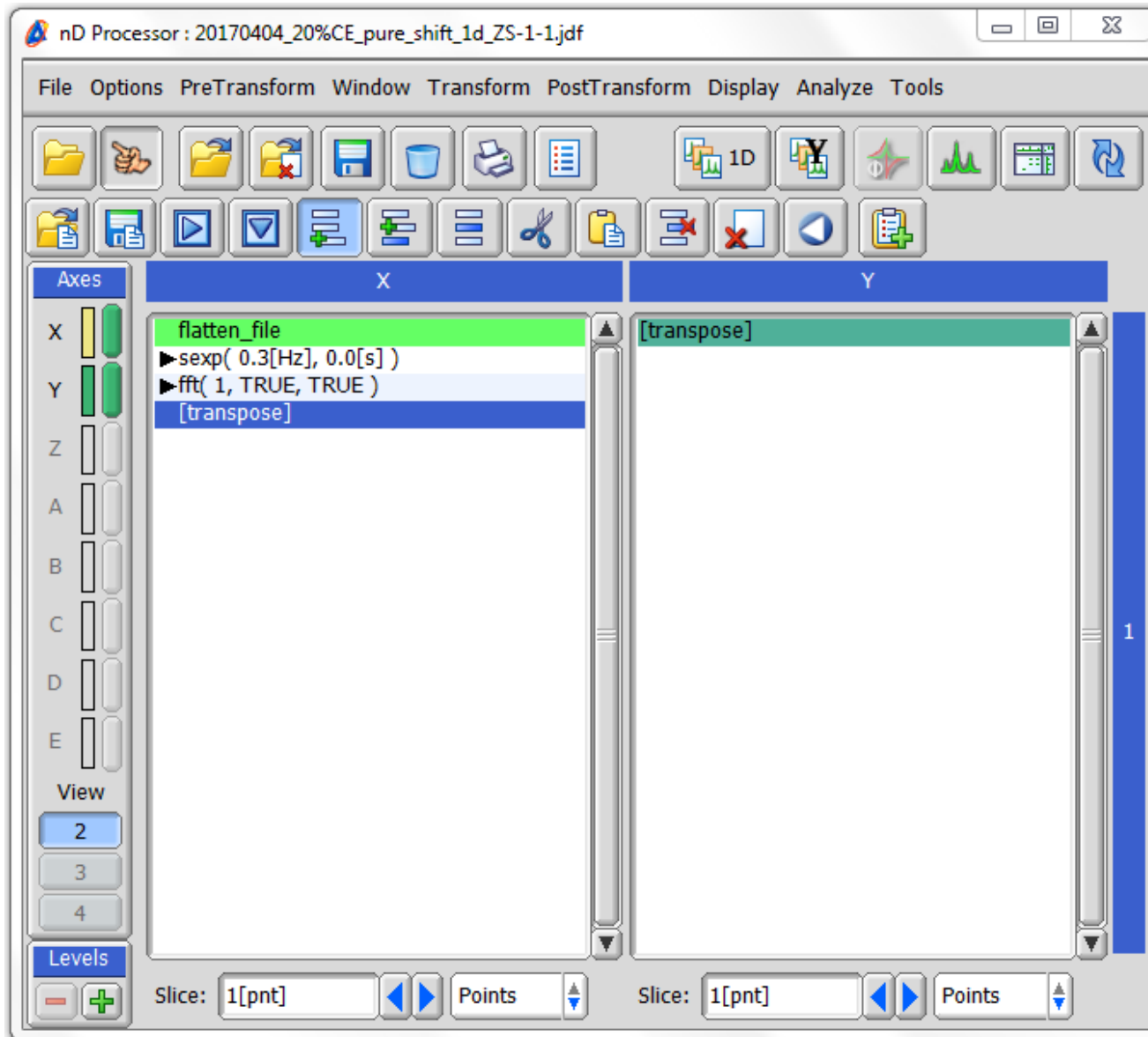
[-] [+]

X Slice: 1[pnt] Points

Y Slice: 1[pnt] Points

2

1D from 2D interferogram (new)



Next Delta
release:
2D from 3D
interferograms

Covariance processing

The screenshot shows the nD Processor software interface. The title bar reads "nD Processor : southampton_cosy_reduced-to-1kpts-1-1.jdf". The menu bar includes "File", "Options", "PreTransform", "Window", "Transform", "PostTransform", "Display", "Analyze", and "Tools". A toolbar with various icons is located below the menu bar. The main workspace is divided into two columns, X and Y, under the heading "Axes".

X Column:

- sinbell_auto
- ▶fft(1, TRUE, TRUE)
- ppm
- [transpose]

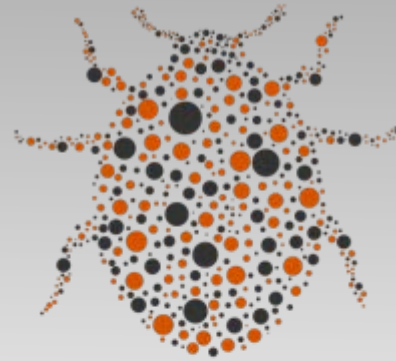
Y Column:

- sinbell_auto
- ▶fft(1, TRUE, TRUE)
- ppm
- abs
- ▼indirect_covar(X)
- Dim
- [transpose]

At the bottom, there are "Slice" controls for both X and Y, both set to "1[pnt]".



Pulse sequence coding



IT'S NOT A
BUG
IT'S A
FEATURE

Basics (ZS)

header

```
process = "pureshift.list";  
include "header";
```

```
end header;
```

instrument

```
include "instrument";
```

```
end instrument;
```

acquisition

```
x_domain      => "Proton";
```

```
x_offset      => 5[ppm];
```

```
x_sweep       => 10[ppm];
```

```
x_points      => 2000;
```

```
scans         => 8;
```

```
[...]
```

```
end acquisition;
```

pulse

```
collect COMPLEX,OBS REAL;
```

```
x_pulse => x90, help "90deg pulse width";
```

```
x_atn   =? xatn;
```

```
relaxation_delay => 2[s], help "inter-pulse  
delay";
```

```
[...]
```

```
phase_1 = {0, 180, 180, 0, 90, 270,  
270, 90};
```

```
phase_2 = {0, 0, 180, 180};
```

```
phase_3 = {0};
```

```
phase_4 = {90};
```

```
phase_slice = {0, 0, 180, 180};
```

```
phase_acq = {0, 180, 180, 0, 90, 270,  
270, 90};
```

```
[...]
```

Basics (ZS)

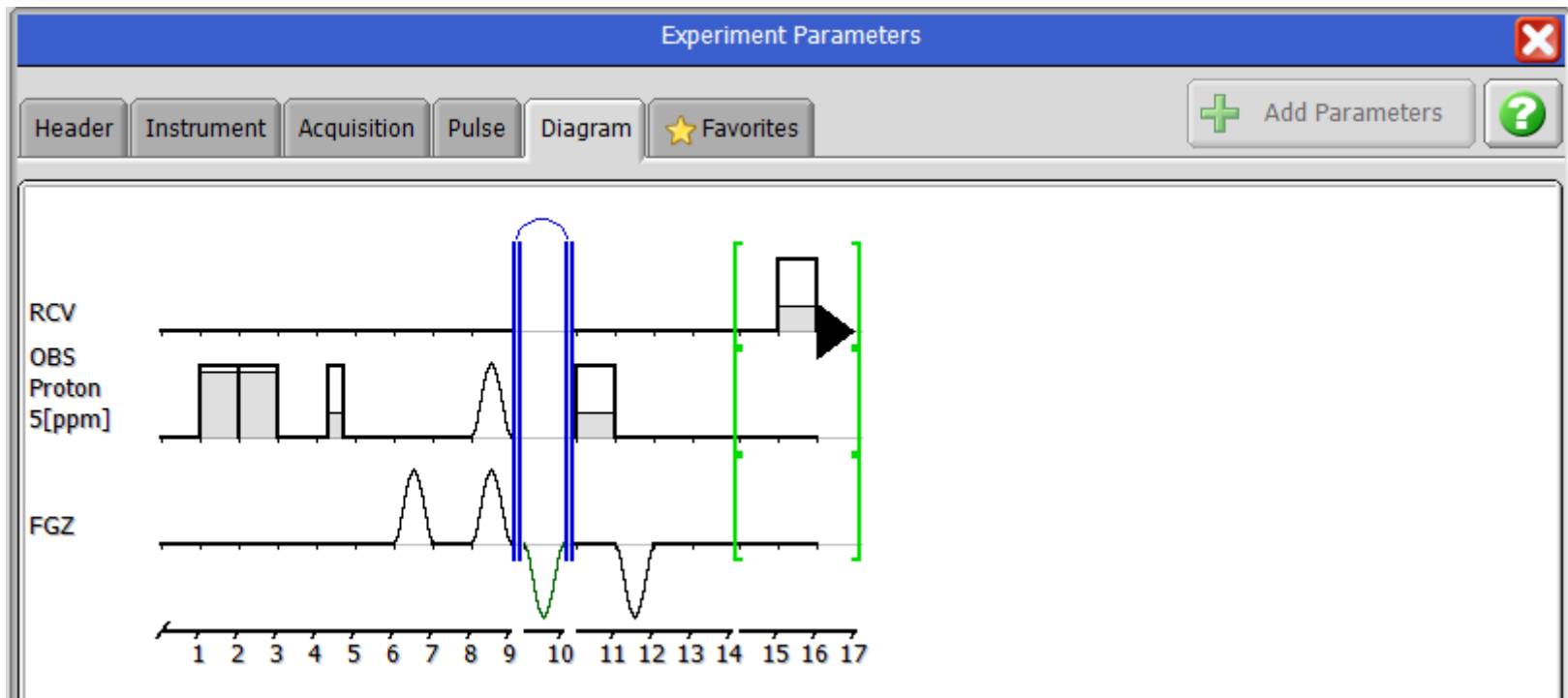
Experiment Parameters

Header Instrument Acquisition Pulse Diagram ★ Favorites + Add Parameters ?

x_domain Proton

x_offset 5[ppm]

x_sweep 10[ppm]



Basics (ZS)

```
begin
  relaxation_delay;
  x_pulse, (obs.gate, obs.phs.phase_1, obs.atn.x_atn);
  t1 ystep 1/(2*y_sweep);
  grad_1, (fgz.gate, fgz.shape.grad_1_shape, fgz.amp.grad_1_amp);
  tau_a - grad_1;
  obs_sel_180, (obs.gate, obs.phs.phase_slice, obs.atn.obs_sel_atn180,
obs.shape.obs_sel_shape, fgz.gate, fgz.shape.grad_slice_shape,
fgz.amp.grad_slice_amp);
  parallel
    begin
      (tau_a + tau_b);
      justify center
        grad_2, (fgz.gate, fgz.shape.grad_2_shape, fgz.amp.grad_2_amp);
    end parallel;
  x_pulse * 2, (obs.gate, obs.phs.phase_2, obs.atn.x_atn);
  grad_3, (fgz.gate, fgz.shape.grad_3_shape, fgz.amp.grad_3_amp);
  tau_b - grad_3;
  t1 ystep 1/(2*y_sweep);
  acq( dead_time, delay, phase_acq );
end pulse;
```

Pulse shape calculations (PSYCHE)

$b1_attn = 20[dB] * \log(\sqrt{0.5 * band_width / chirp_pulse * q}) * 4 * chirp_pulse$;
 $chirp_atn_calc = hard_square_atn - b1_attn$, help "attenuator for 180 chirp pulse";
 $chirp_atn = chirp_atn_calc + 24[dB]$, help "20deg pulse (chirp +24dB)";

Experiment Parameters

Header Instrument Acquisition **Pulse** Diagram Favorites

+ Add Parameters ?

Pulse

x_pulse 6[us] x90

x_atn 0.3[dB]

Adiabatic Pulse

chirp_shape_up chirp_fc_gen

chirp_shape_down chirp_fc_gep

band_width 12[kHz]

chirp_smooth 10[%]

q 5

chirp_pulse 15[ms]

hard_square_atn 67.89804[dB]

b1_atn 38.57332[dB]

chirp_atn_calc 29.32471[dB]

chirp_atn 53.32471[dB] chirp_atn_calc + 24[dB]

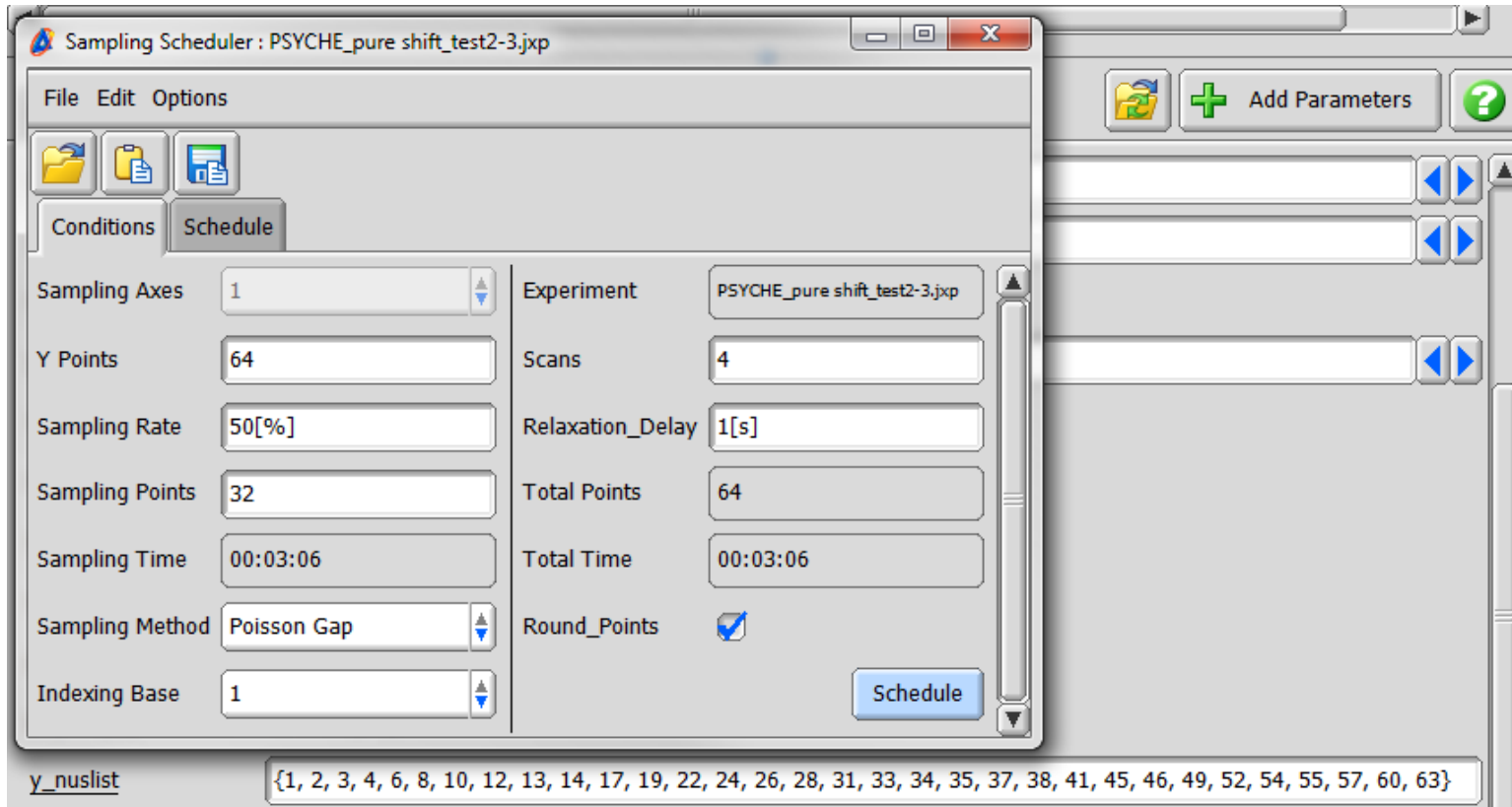
Acquire parameter

interval_sampling 0.16676[ms]

delta_acq 0.16156[ms]

cycle_time 0.16676[ms]

NUS with pure shift



Setup as in any other 2D experiment

Real time pure shift

module_config = "continuous_fid"; (concatenate acquisitions in one file instead of separate files)

loop n times

[...]

*x_pulse*2,(obs.gate,obs.phs.phase_y,obs.atn.x_atn);*

when irr_decoupling do

on (irr.gate, irr.noise.irr_noise, irr.atn.irr_atn_dec);

end when;

acquire begin

[...]

end acquire;

when irr_decoupling do

off (irr.gate, irr.noise.irr_noise, irr.atn.irr_atn_dec);

end when;

[...]

end loop;

Thank you

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