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PURE SHIFT IMPLEMENTATION

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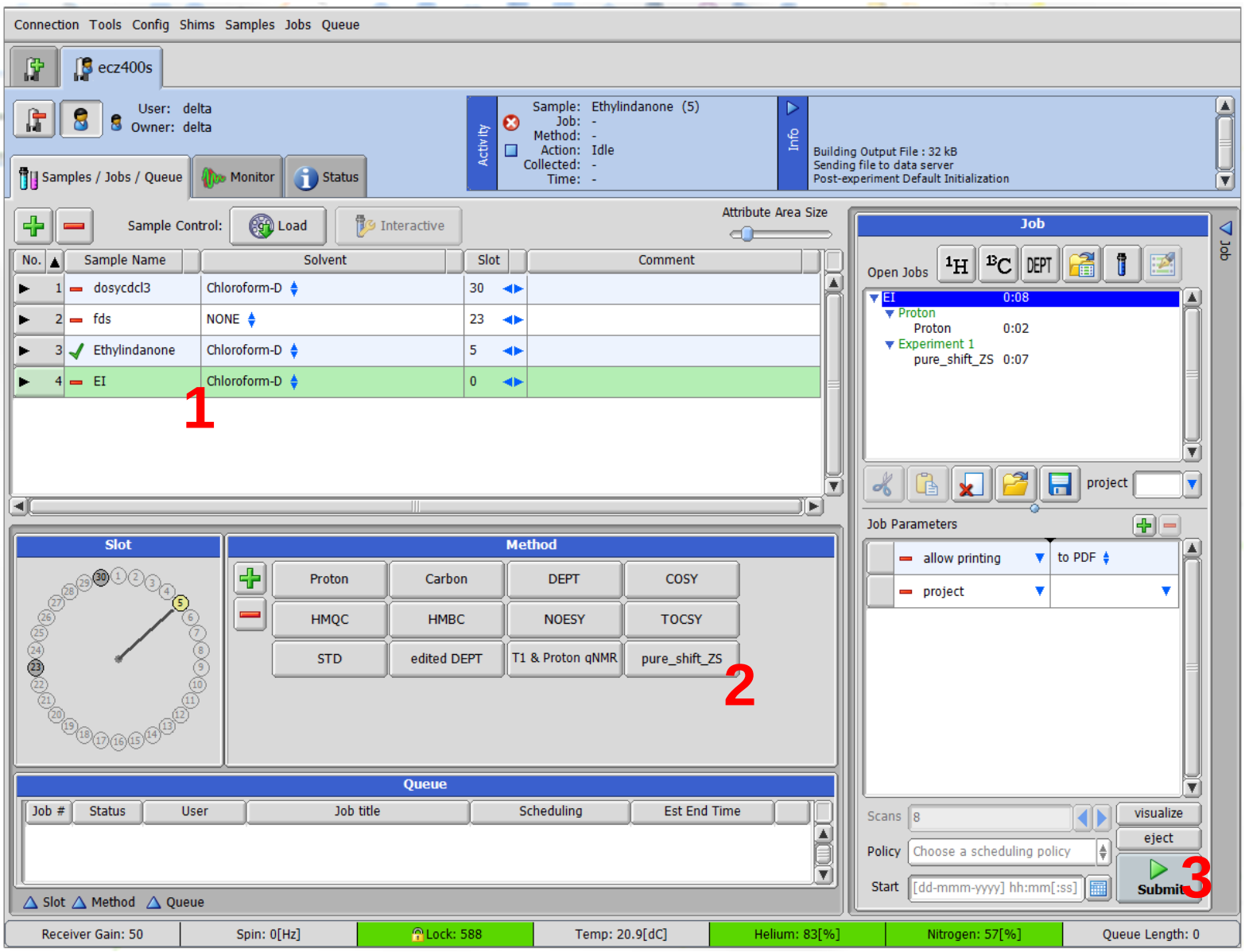
Basics

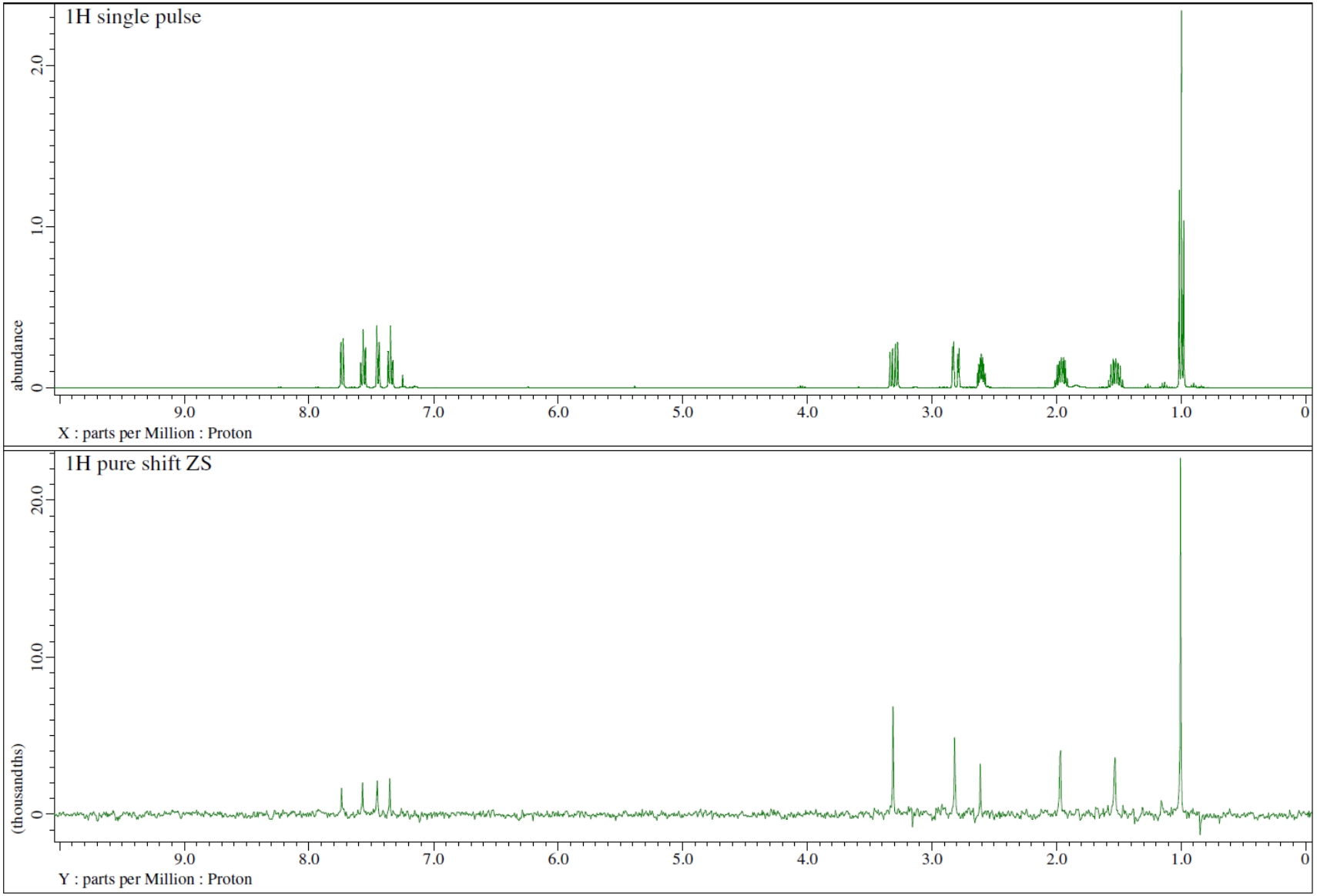
$$H\psi = E \times \psi$$

Experiment submission

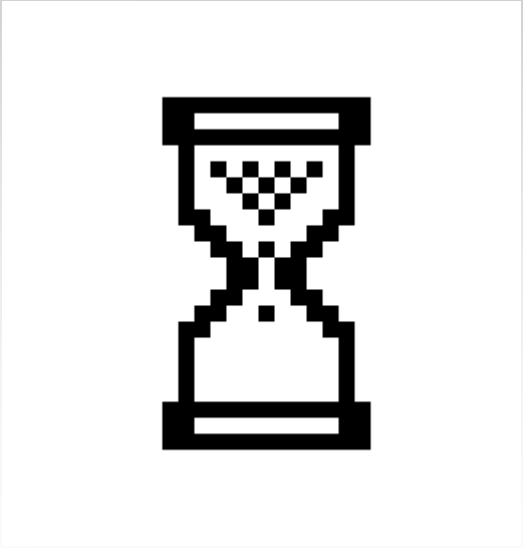


Automated acquisition and processing

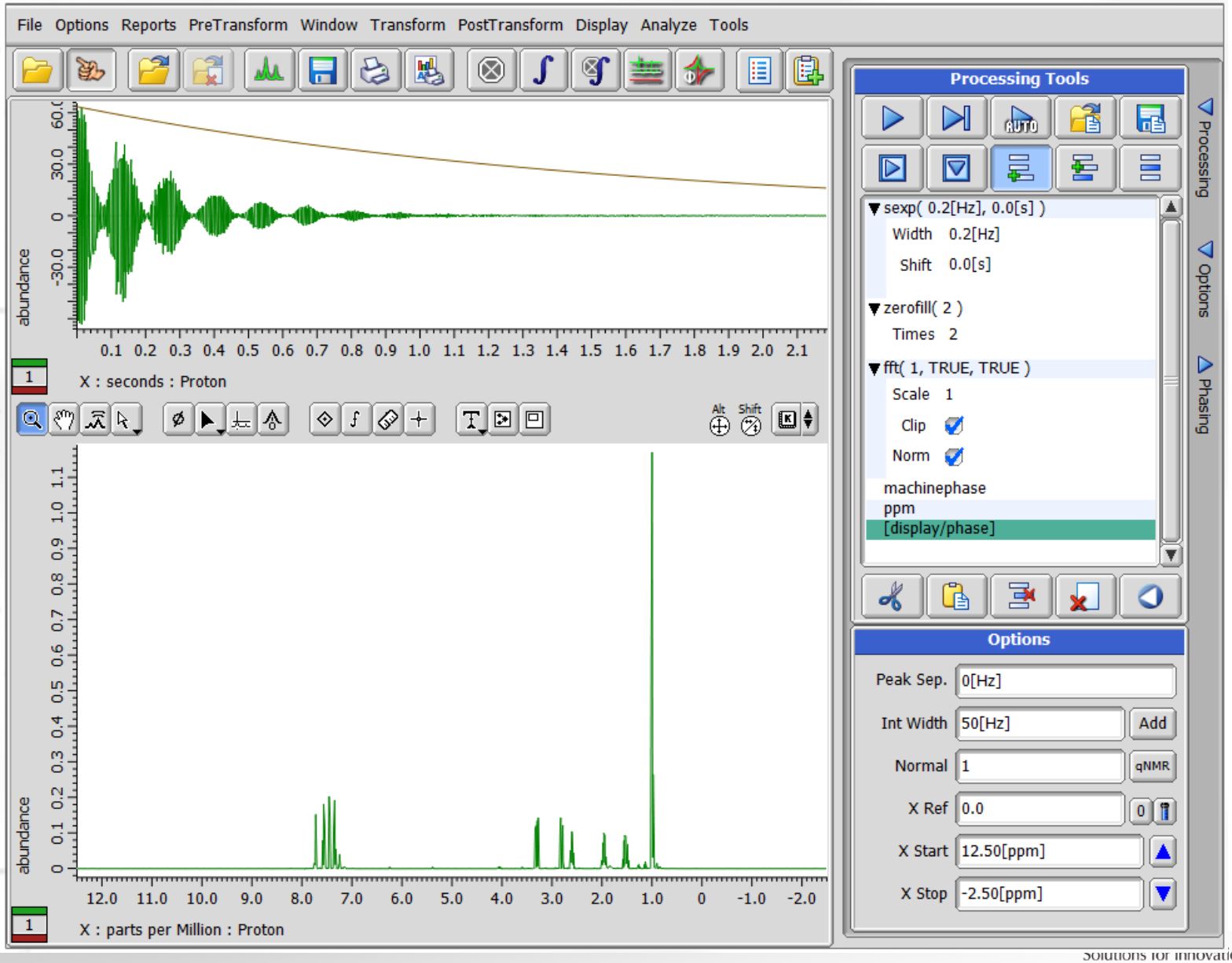
Proton vs Pure shift (ZS)



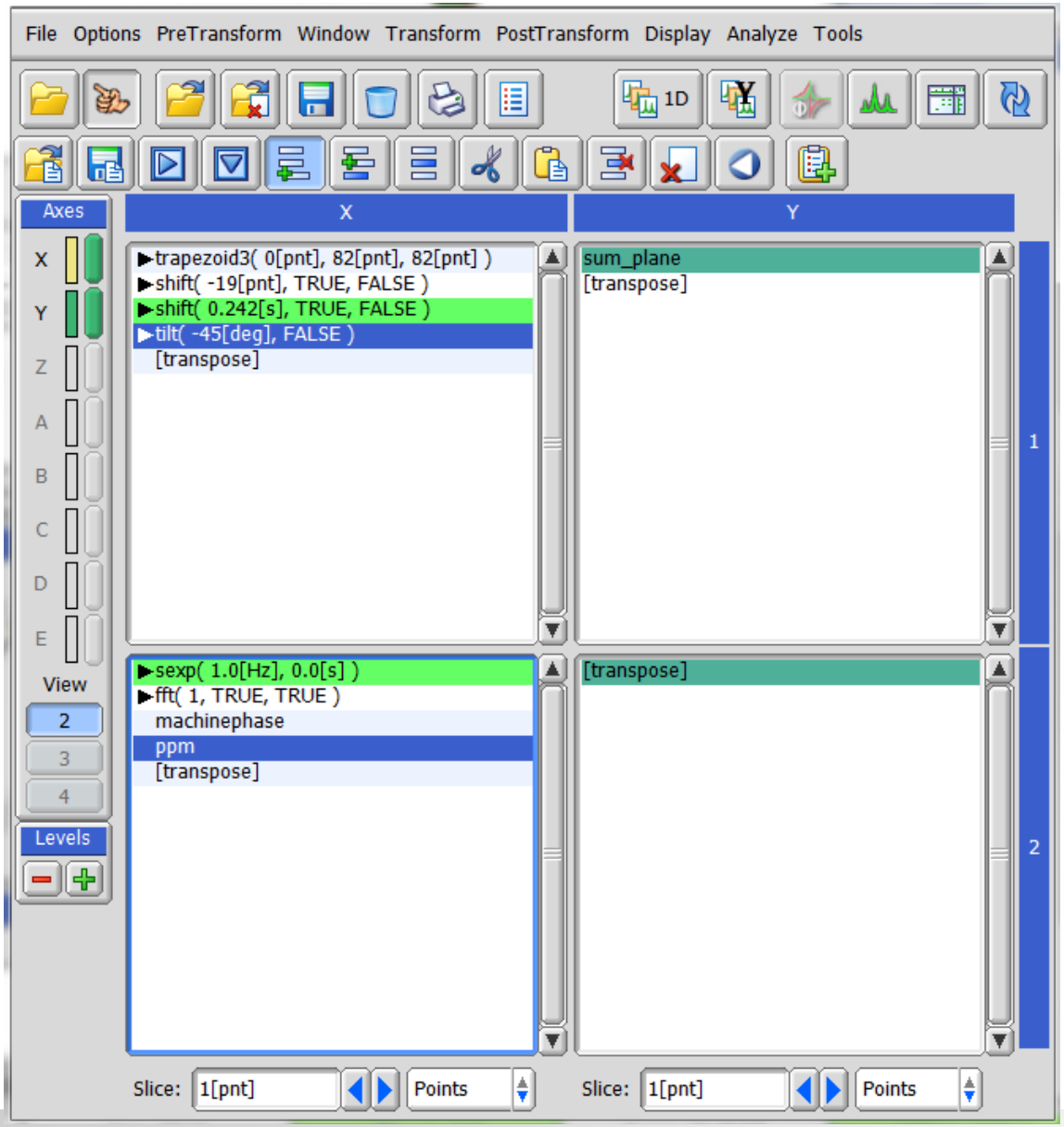
Processing



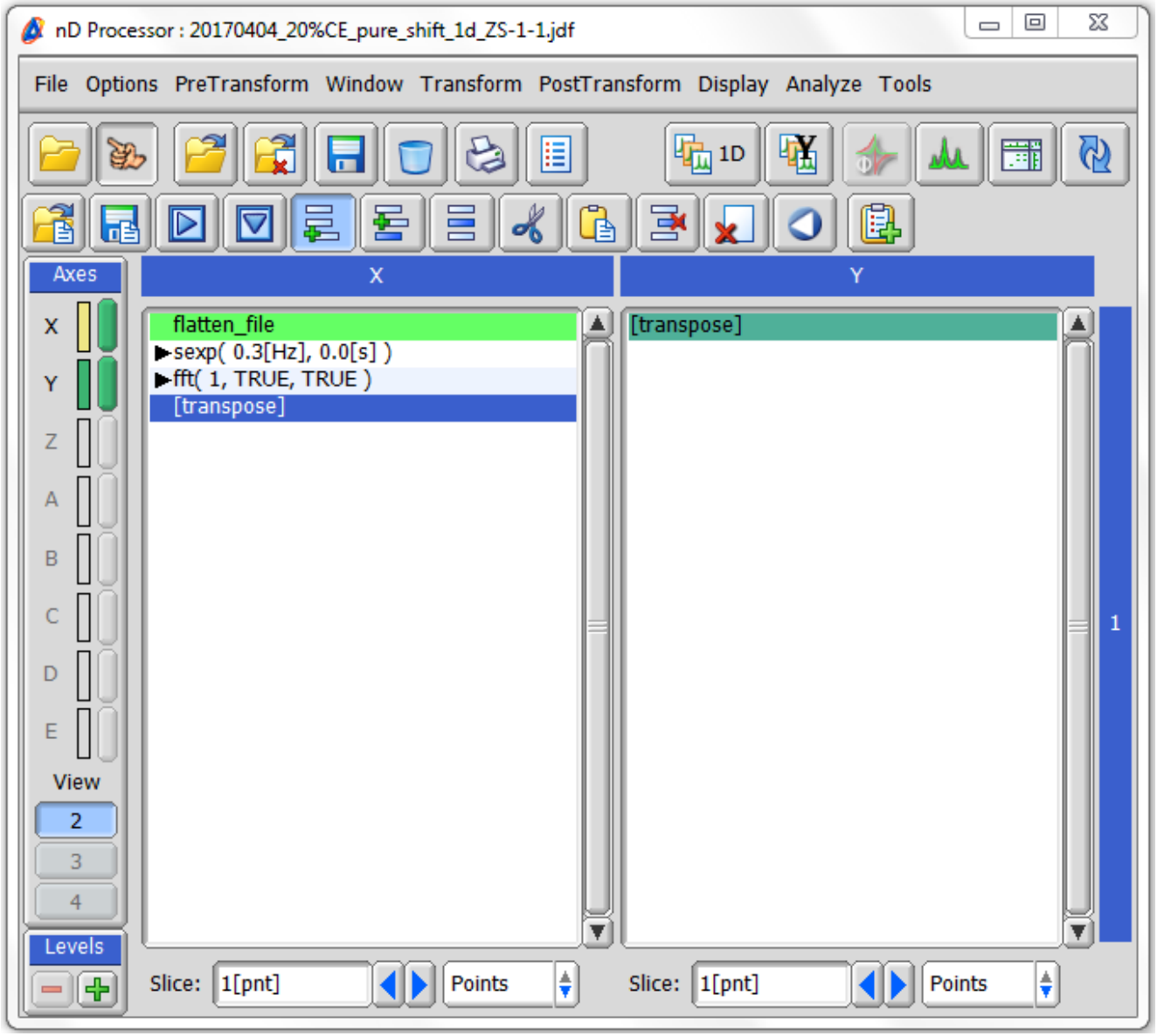
Typical processing of single pulse



1D from 2D interferogram (old)

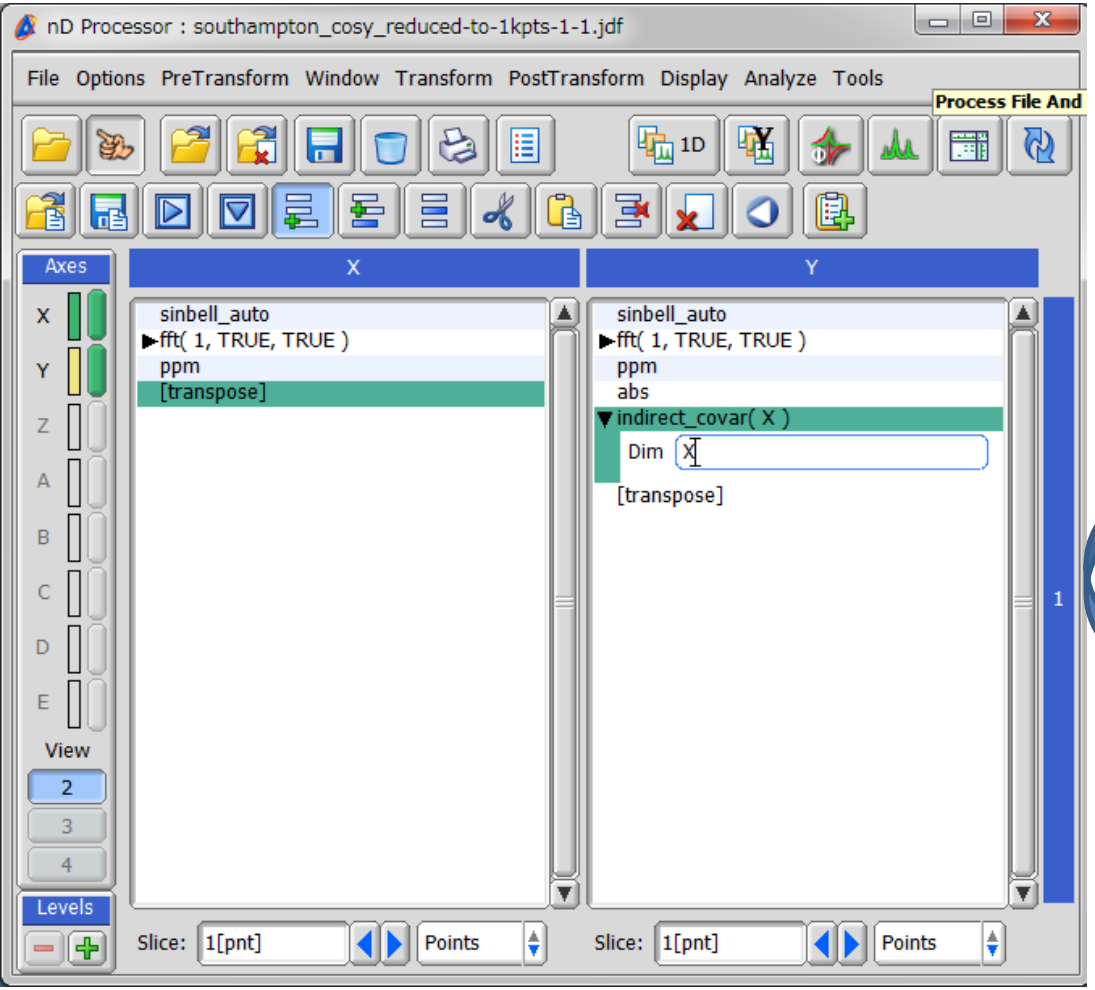


1D from 2D interferogram (new)



Next Delta release:
2D from 3D interferograms

Covariance processing



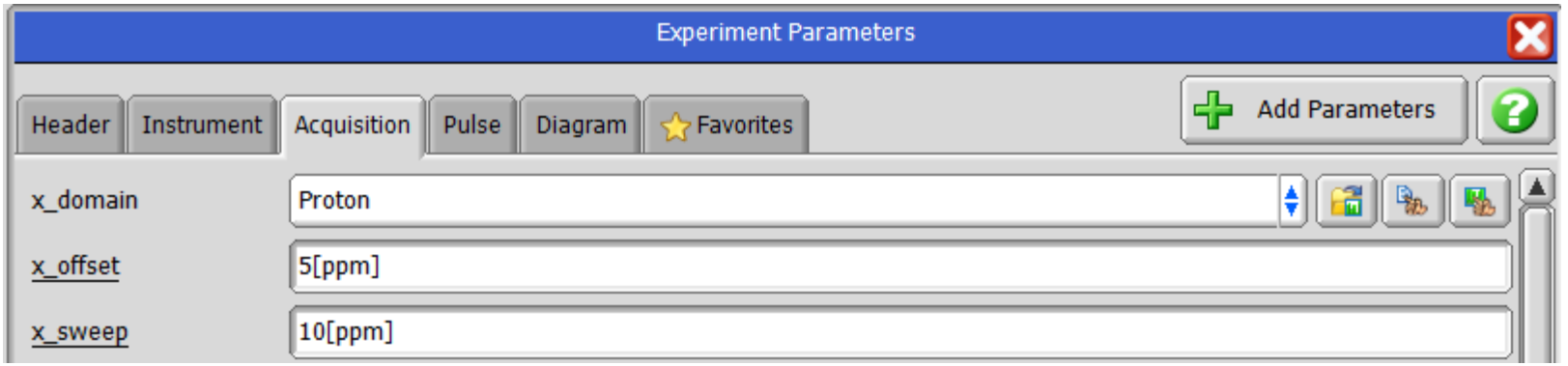
Pulse sequence coding

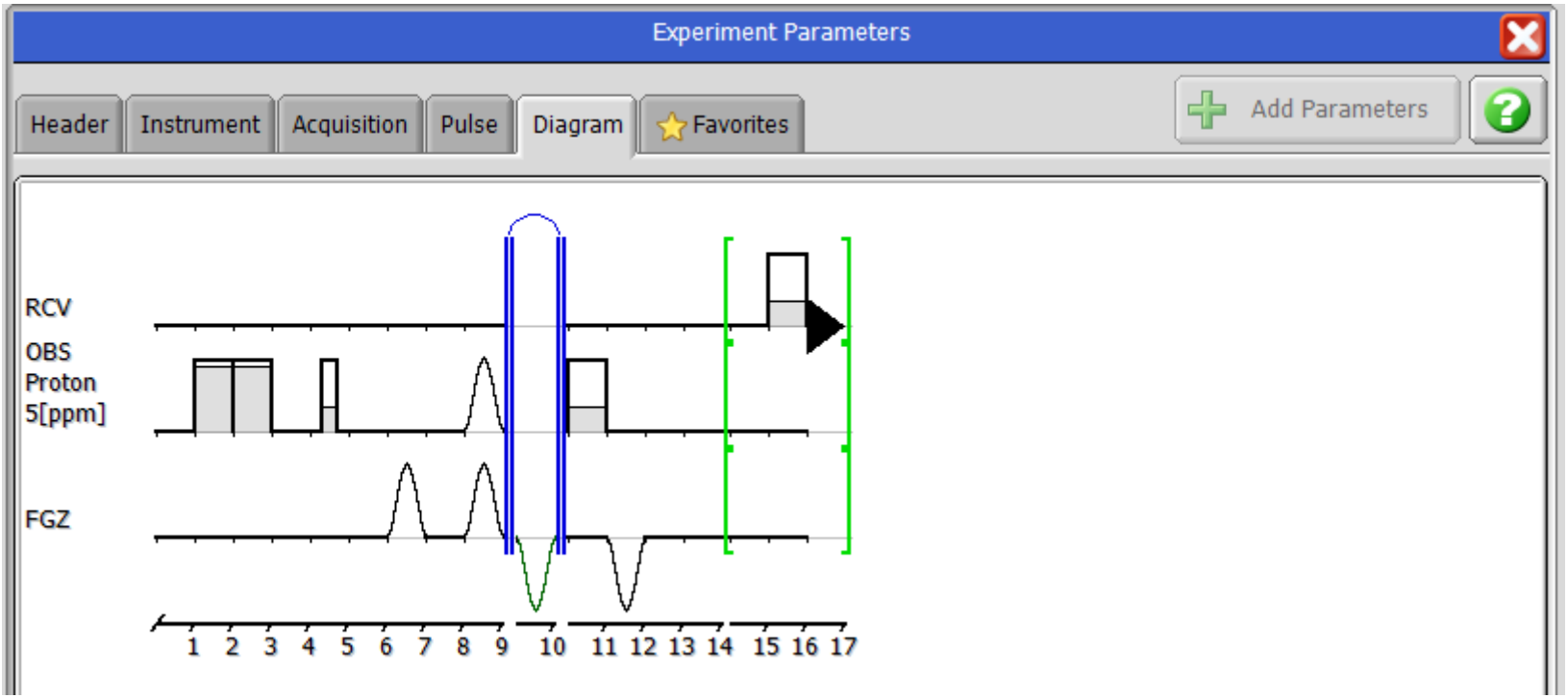
Basics (ZS)

```
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)



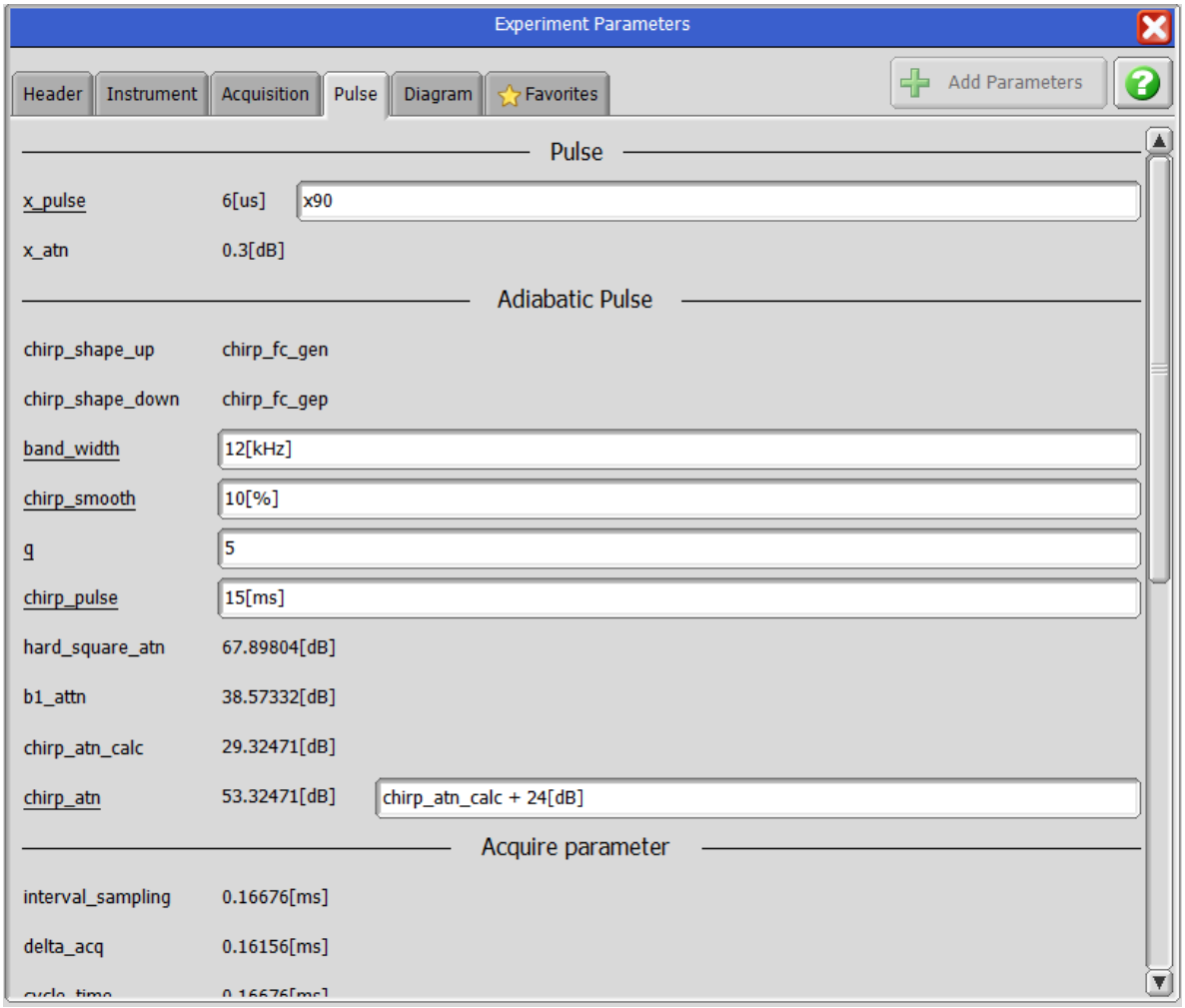


Basics (ZS)

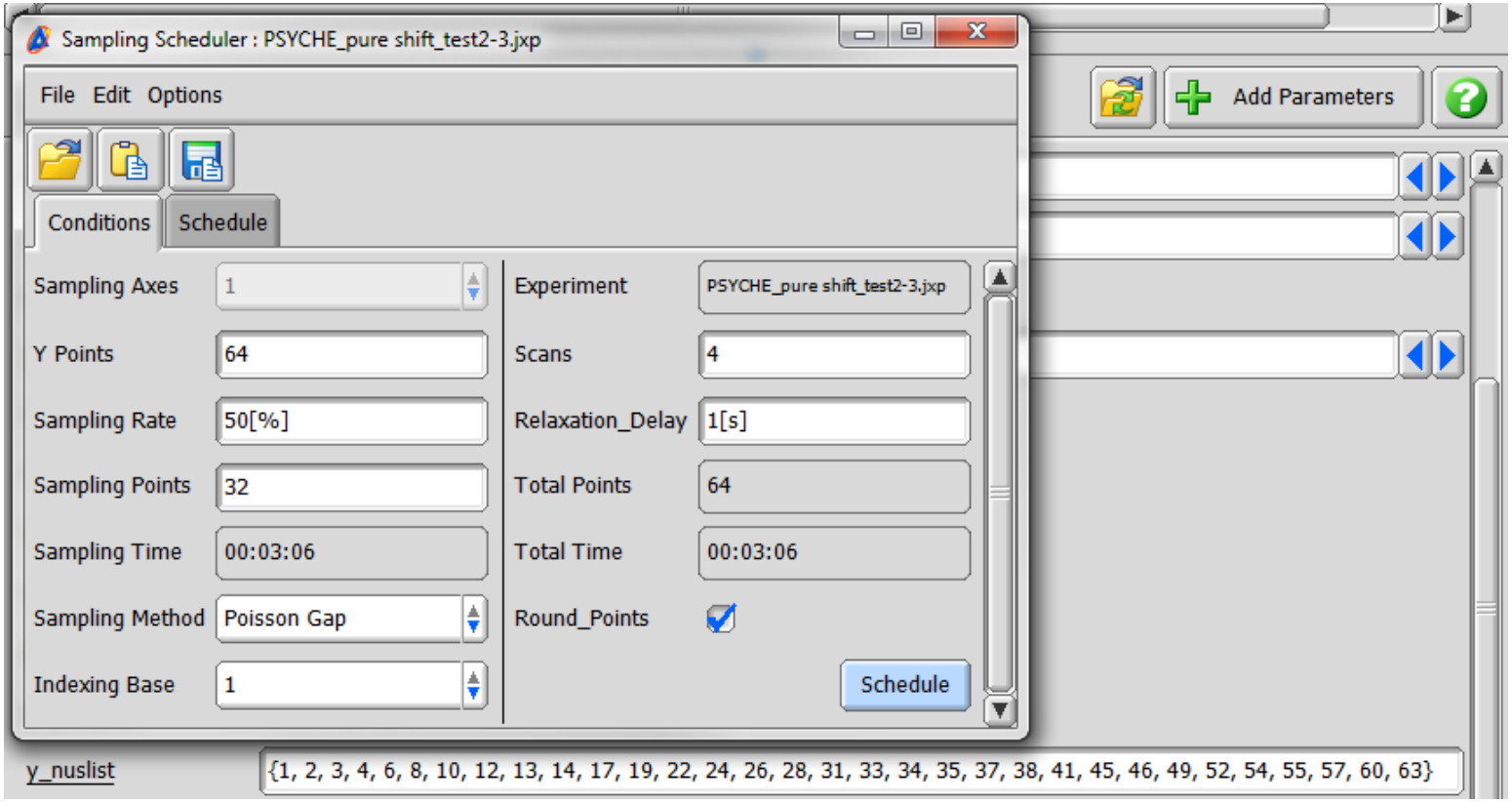
```
begin
   relaxation_delay;
   x_pulse, (obs.gate, obs.phs.phase_1, obs.atn.x_atn);
   t1 ystep 1/(2*y_sweep);
   grad_1, (fgz.gate, fgz.shape.grad_1_shape, fgz.amp.grad_1_amp);
   tau_a - grad_1;
   obs_sel_180, (obs.gate, obs.phs.phase_slice, obs.atn.obs_sel_atn180,
obs.shape.obs_sel_shape, fgz.gate, 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)";



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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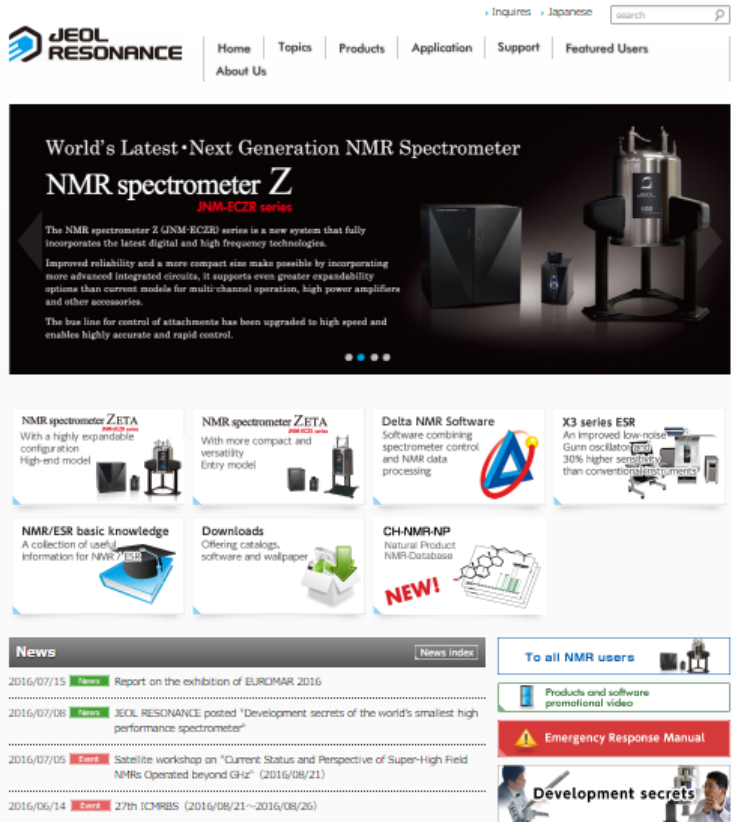
  - Description of our products
  - Free processing software
  - Free natural products database
  - Application notes
  - Events
  - And more



- **http://nmrsupport.jeol.com/ (for our users)**