



WEINBERG
COLLEGE OF
ARTS & SCIENCES

Department of
Chemistry

Lunch and Learn

Solvent suppression in three ways: presat, wet, and excitation sculpting (ES)

IMSERC INTEGRATED MOLECULAR STRUCTURE
EDUCATION and RESEARCH CENTER

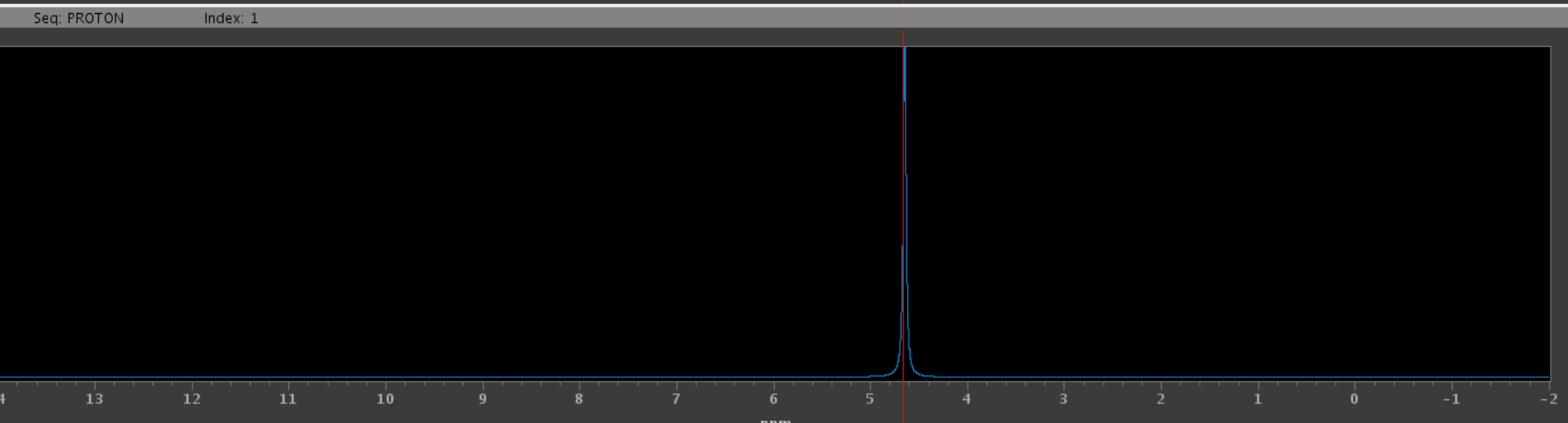
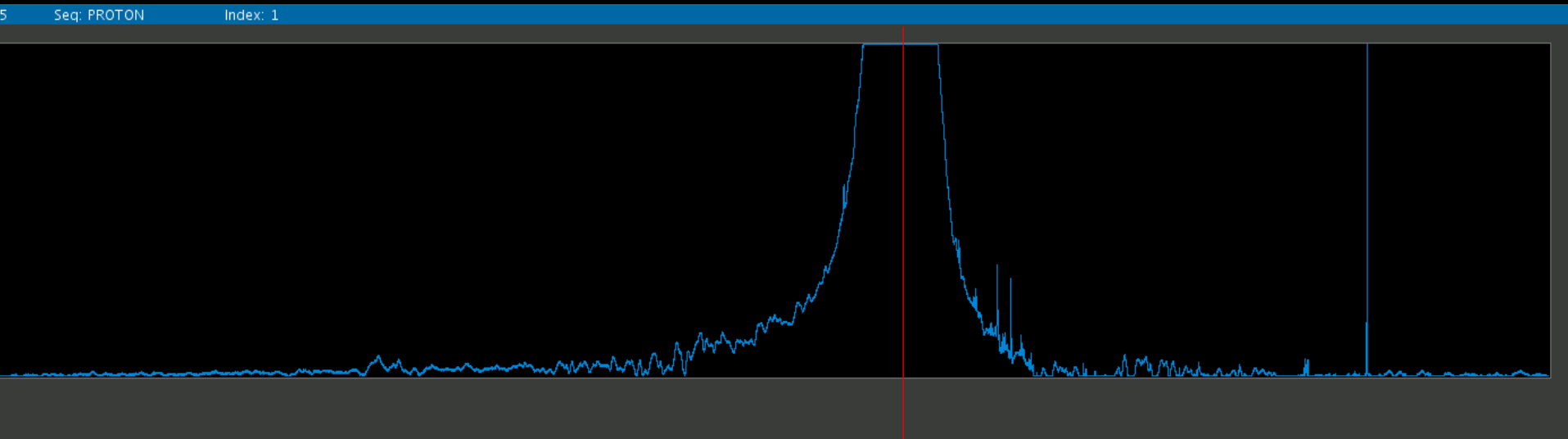


Why?

- **Dynamic range: 16-bit digitizer range +/- 32767**
- Baseline distortion
- Radiation damping
- T1-noise for 2D
- ...

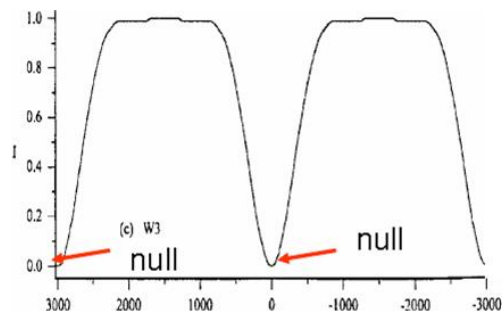


Proton spectrum 2mM sucrose in 90% H₂O/10% D₂O

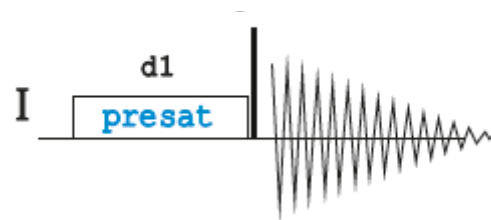


How?

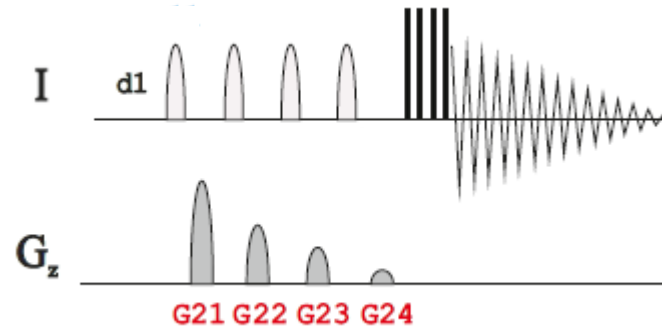
- Saturate the water resonance (presat)
- Destroy the water resonance with pulsed field gradient (PFG) (wet, water gate, dpfgse, ...)
- Produce notch on the water resonance when exciting the protons (jump-return with $90_x-\tau-90_{-x}$, binomial sequences)



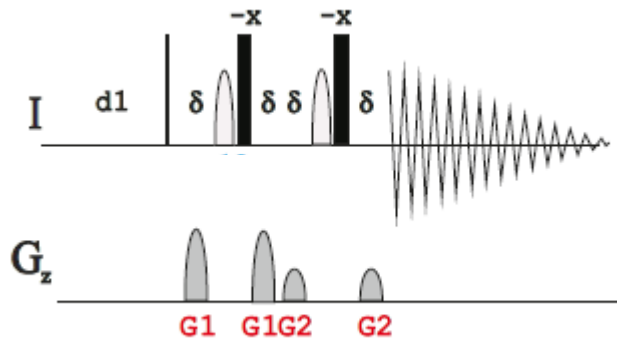
Pulse sequences for three methods on VnmrJ



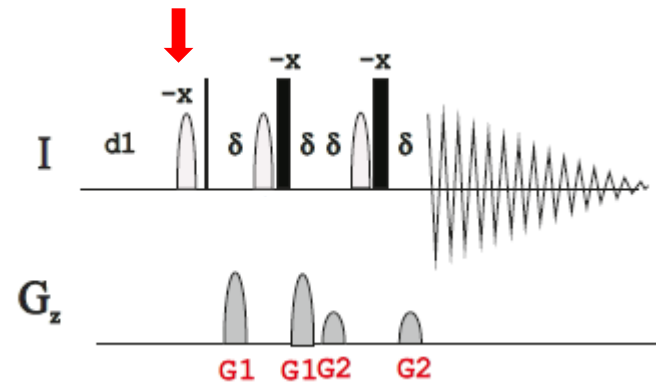
Presat



WET



Excitation Sculpting (ES)



ES w/ water flipback

Interactive Interface after loading presat/wet onto 1d proton

The screenshot shows the NMR software interface for a **PRESAT** experiment. The top navigation bar includes buttons for **Start**, **Acquire**, **Process**, **Show Time**, **Go !**, **Stop**, **MoveSW**, **Sequence**, and **Arrays**. The left sidebar lists menu items: **Default**, **Acquisition**, **Pulse Sequence**, **PRESAT**, **Channels**, **Flags**, **Future Actions**, and **Overview**. The main panel displays the following settings:

- Experiment:** PRESAT **Solvent:** d2o **Observe:** H1 **Decoupler:** C13
- Select Presaturation Band using cursor(s)**
 - Single-Freq PRESAT** **Multi-Freq PRESAT**
 - Buttons: **Box/Cursor**, **Expand/Full**, **Nearest Line**, **CLEAR**, **Select**, **ShowList**
- Number of scans:** 8
- Presaturation Delay:** 2 s
- PURGE**
- Receiver Gain (dB):** 0
- Autogain:**

The screenshot shows the NMR software interface for a **wet1D** experiment. The top navigation bar and left sidebar are identical to the previous screenshot. The main panel displays the following settings:

- Experiment:** wet1D **Solvent:** d2o **Observe:** H1 **Decoupler:** C13
- Select using cursor(s) or threshold**
 - Buttons: **Box/Cursor**, **Expand/Full**, **Nearest Line**, **Threshold**, **CLEAR**, **Show Freqs.**, **Select**, **Select ALL**
- Number of scans:** 8
- Relaxation Delay:** 1.5 s
- C13 decoupling during WET?**
- Receiver Gain (dB):** 0
- Autogain:**

Interface after loading presat/wet into study queue:

Start Acquire Process **Show Time** Save Quit-nosave Default **Go !** Sequence Arrays

Default ProcPlotAdv Acquisition Pulse Sequence **PRESAT** Channels Flags Future Actions Overview

Experiment: PRESAT Solvent: cdcl3 Observe: H1 Decoupler: C13

Spectral Width: -2.0 to 14.0 ppm
Saturate?: Select Later Do Scout
OR H2O peak (offset) 599.8 Hz
OR Suppress... 0 tallest peaks

Minimize SW? Off
Number of scans 8
Presaturation Delay 2 s
 PURGE

Receiver Gain (dB): 30
Autogain:

Before PRESAT acq: Re-shim
After PRESAT acq: Autoplot
Starting with: PROTON
Samplename:
start of Q lock/shim? yes / yes
[More Options: PlotProcAdv page](#)

Start Acquire Process **Show Time** Save Quit-nosave Default **Go !** Sequence Arrays

Default ProcPlotAdv Acquisition Pulse Sequence **WET** Channels Flags Future Actions Overview

Experiment: wet1D Solvent: cdcl3 Observe: H1 Decoupler: C13

Spectral width: -2.0 to 14.0 ppm
WET peaks Define Now Select Later Do Scout
Number of scans 8
Relaxation Delay 1.5 s
Minimize SW? Off
 C13 decoupling during WET? Optimize CF

D2O/H2O H2O CD3CN CH3CN
 DMSO-D6 DMSO-H6 DMSO-wet
 CD3OD CH3OD CD3OH [more...](#)

OR Suppress... 0 tallest peaks
OR Suppress H2O peak (offset) 599.8 Hz

Receiver Gain (dB): 30
Autogain:

Before wet1D acq : Re-shim
After wet1D acq : Autoplot
Starting with: PROTON
Samplename:
start of Q lock/shim? yes / yes
[More Options: PlotProcAdv page](#)

Interface after loading water_ES into study queue

The screenshot shows the Bruker software interface. On the left, the 'Experiment Selector' window is open, displaying a grid of experiment types. The 'DOSY' experiment is selected, and a sub-menu is visible showing 'water_ES', 'STD_ES', and 'wLOGSY_ES'. The main window shows the 'Acquire' tab with a 'Go!' button highlighted in green. The 'Acquisition options' section is expanded, showing parameters for 'water_ES' with solvent 'd2o'. The 'Receiver gain (dB)' is set to 26 with 'Autogain' checked. Other parameters include Spectral width from -2.0 to 14.0 ppm, 16 scans, 1 s relaxation delay, 'Do scout experiment' checked, Water offset 599.8, and 'Optimize powers' checked.

Experiment Selector

Liquids	Calibration	Service
ChemPack	Common	
Std 1D	(HH)Homo2D	
J1(CH)corr	Jn(CH)corr	
(H)Sel1D	Sel2D	
(HC)Crisis2	(HC)HetToxys	
HF_Expts	(CC)corr	
Jspectra	Hadamard	
DOSY	ESuppression	

Study Queue

- Std 1D ▶ water_ES
- Sel 1D ▶ STD_ES
- Homo 2D ▶ wLOGSY_ES

Start Acquire Process Show Time Go! Stop Sequence Arrays Seq. Help

Experiment: water_ES Solvent: d2o Observe: H1 Decoupler: C13

Acquisition options

Receiver gain (dB) 26 Autogain

Spectral width - from -2.0 to 14.0 ppm

Number of scans 16

Relaxation delay 1 s

Do scout experiment

Water offset 599.8

Optimize powers

The screenshot shows the Bruker software interface with the 'water_ES' experiment selected. The 'Acquire' tab is active, and the 'Go!' button is highlighted. The 'Pulse Sequence' section is expanded, showing detailed parameters for 'Excitation Sculpting (DPFGSE)', 'T1rho filter', and 'Solvent Flipback Pulse'. The 'Excitation Sculpting' parameters include Solvent Selective Pulse with width 2500.0 us, power 14.0 dB, fine power 2048.0, and shape W_supp. The 'T1rho filter' parameters include Purge Pulse checked, pulse duration 2.0 ms, and at power 48.0. The 'Steady State' parameters include GRD-90-GRD option checked, Gradient strength 4650, and time 1.6 ms. The 'Solvent Flipback Pulse' parameters include Flipback option unchecked, Keep water along Z checked, width 5.0 ms, power 18.0 dB, fine power 2048.0, shape W_flip, and small angle phase shift 0 deg. A 'Recreate flipback shape' button is visible at the bottom.

Start Acquire Process Show Time Go! Stop Sequence Arrays Seq. Help

water_ES

Excitation Sculpting (DPFGSE)

Solvent Selective Pulse

width 2500.0 us

power 14.0 dB

fine power 2048.0

shape W_supp

Gradient -

strength 7441

time (ms) 1.0 ms

Recovery time 0.5 ms

T1rho filter

Purge Pulse

pulse duration 2.0 ms

at power 48.0

Steady State

GRD-90-GRD option

Gradient -

strength 4650

time 1.6 ms

Solvent Flipback Pulse

Flipback option

Keep water along Z

width 5.0 ms

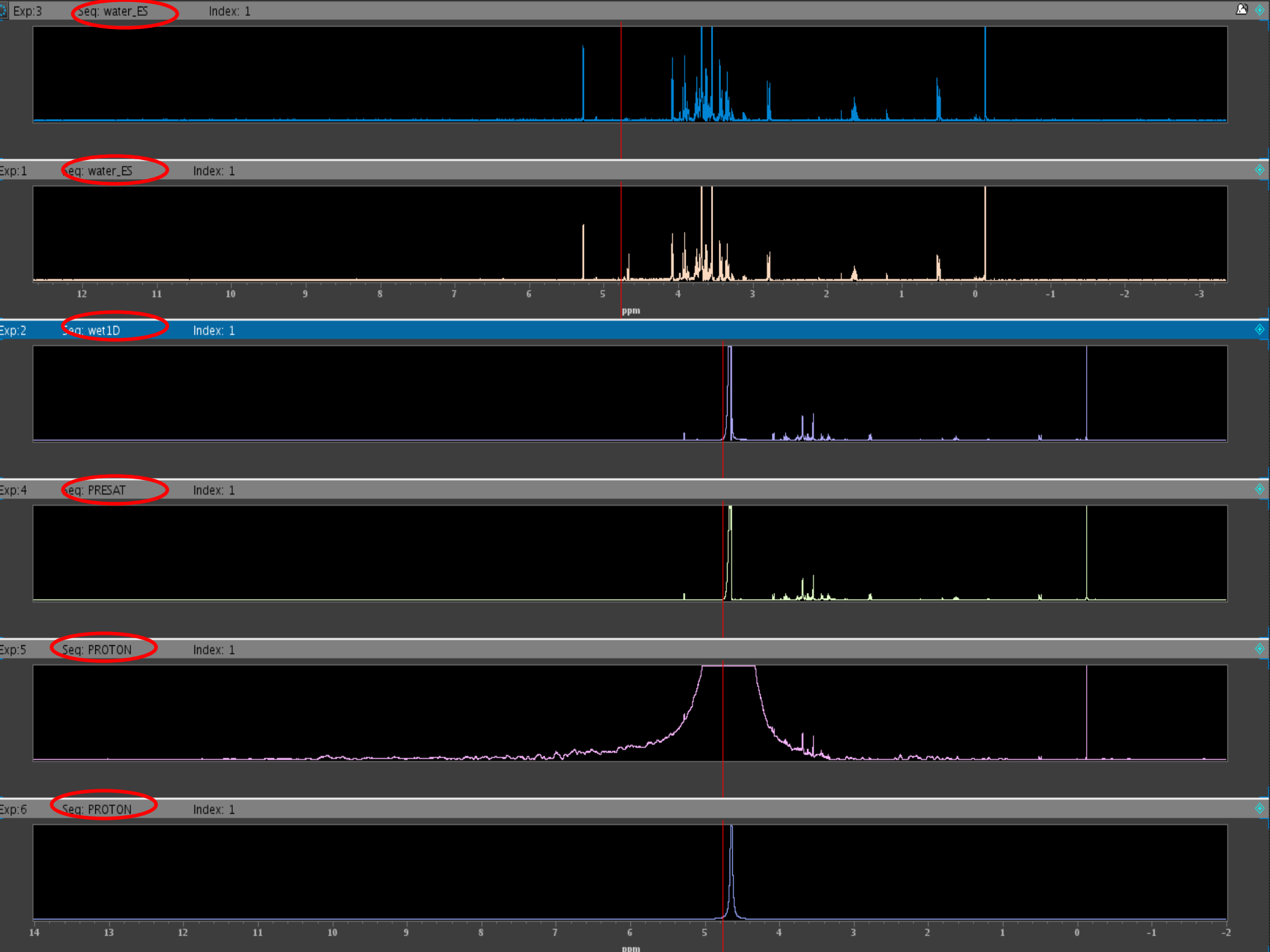
power 18.0 dB

fine power 2048.0

shape W_flip

small angle phase shift 0 deg

Recreate flipback shape



To setup 2D experiments with presat/wet:

- Run a 1d proton with presat/wet first
- Load the 2d either from “experiment selector” or the drop down menu on top of the 1d proton
- DOSY as example to demonstrate

To Summarize (take home message):

- Do I have chemical exchange between solvent and any of my signals?
- The interactive frequency selection interface with presat and wet
- Fully automated ES with study queue/automation runs

