

NMR data processing software

Delta

NMR Software

v5.0



氢谱中溶剂峰压制




1. 单个峰压制（以水峰为例）

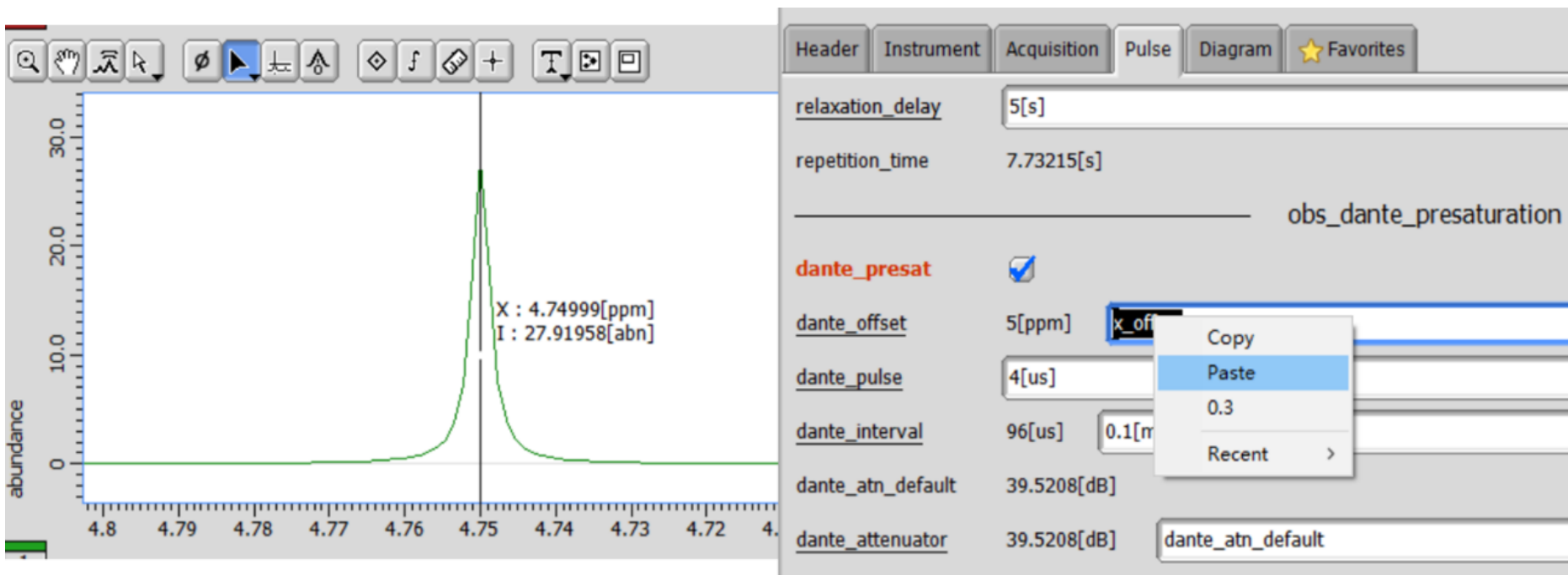
单个溶剂峰压制的主要方法为预饱和，可直接在氢谱中的扩展序列里添加。

1) dante_presat法

①添加氢谱→②打开脉冲编辑→③在pulse里面的扩展序列中勾选dante_presat，在dante_offset处准确输入需要压制的水峰位置。

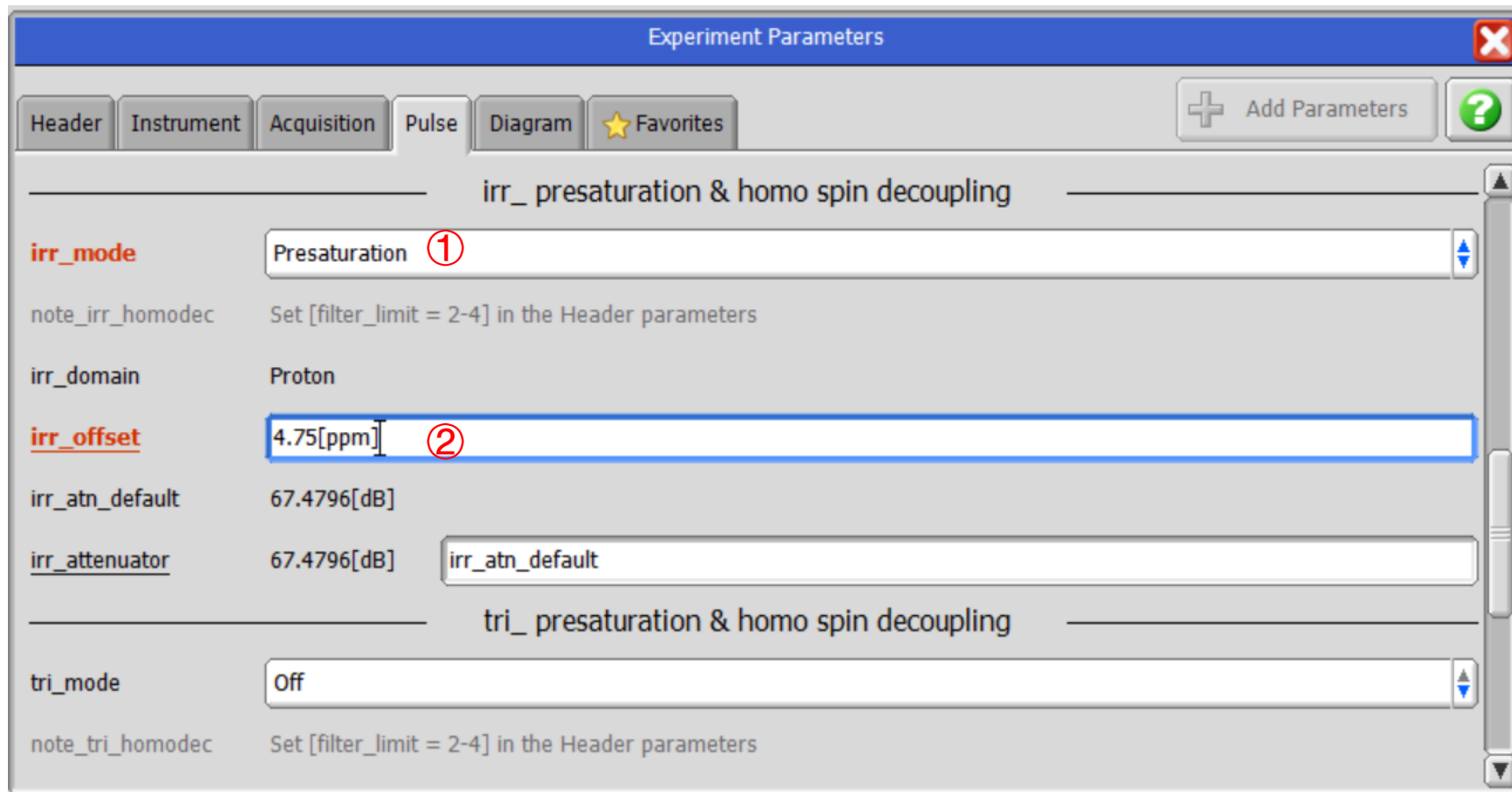
The image shows two windows from a Bruker NMR software interface. The left window is titled "Experiment Parameters" and has tabs for Header, Instrument, Acquisition, Pulse, Diagram, and Favorites. The "Pulse" tab is selected, and a red circle with the number 3 is around it. The "dante_presat" checkbox is checked. The "dante_offset" field contains "4.75[ppm]", with a red arrow pointing to it and the text "直接输入请注意添加单位'[ppm]'" (Direct input, please note to add the unit '[ppm]'). Other parameters include relaxation_delay (5[s]), repetition_time (7.73215[s]), dante_pulse (4[us]), dante_interval (96[us]), dante_atn_default (39.5208[dB]), and dante_attenuator (39.5208[dB]). The right window is titled "Job" and has tabs for 1H, 13C, DEPT, and others. A red circle with the number 1 is around the 1H tab, and a red circle with the number 2 is around the "Pulse" icon. The job list shows a "test" job with a "Proton" sub-job. The "Scans" field is set to 8, and the "Policy" is "Choose a scheduling policy".

水峰位置也可从谱图中复制：选择复制按钮 ，鼠标左键单击选中水峰位置，再在 dante_offset 处选中输入框中内容长按鼠标右键，弹出选项中点粘贴即可。



2) **Presaturation**法（注：此方法可用于单个或两个峰的压制，第二个峰可以在 `tri_mode` 中设置。）

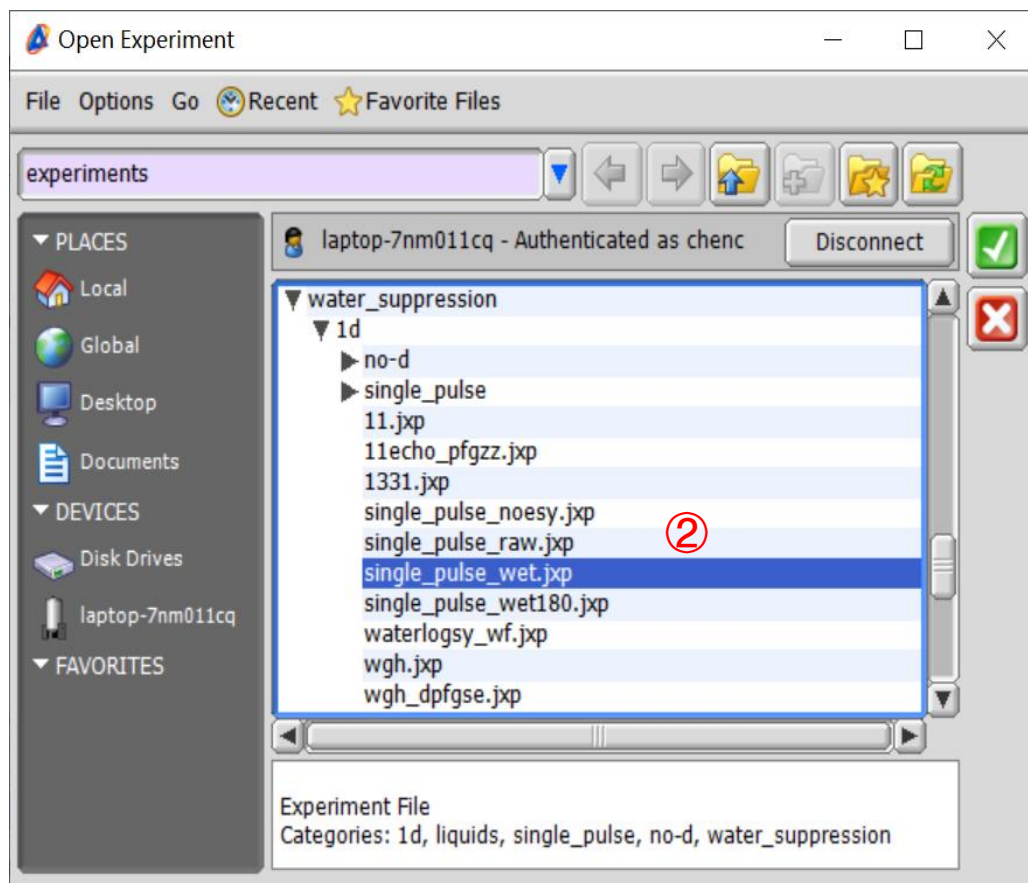
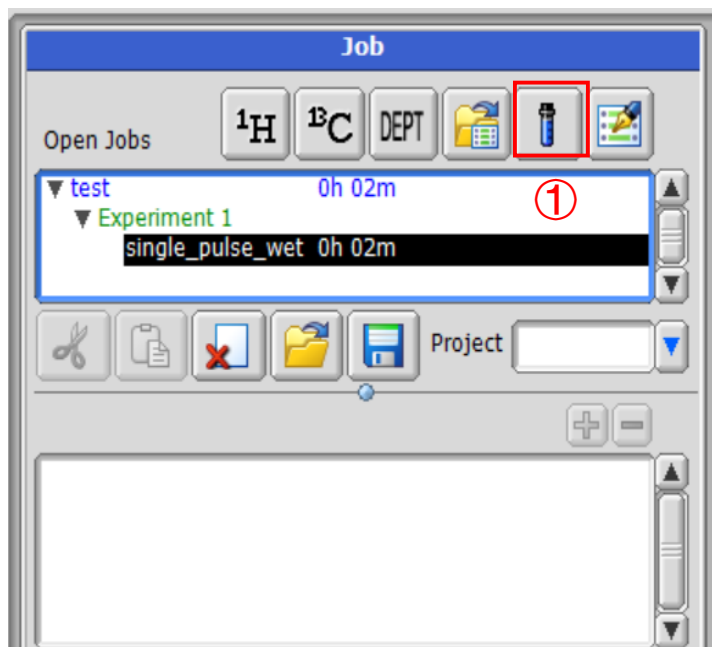
与前一方法步骤类似，在 `pulse` 的扩展序列中添加，①更改 `irr_mode` 为 `Presaturation` 模式→②在 `irr_offset` 处输入待压制水峰的化学位移。



2. 多个溶剂峰压制

如果氢谱中有多个溶剂峰需要压制时，可以选择wet方法，步骤如下：

- ①添加实验→②在Global/water_suppression/1d/single_pulse中选择single_pulse_wet或single_pulse_wet180方法。



③在pulse中设置压制参数

Header Instrument Acquisition **Pulse** Diagram ★ Favorites

③

wet solvent suppression

wet_suppression wet

wet_solvent Chloroform → NoD实验中作为化学位移定标用，如果含有氘代试剂，此项可忽略

wet_shape GAUSS

wet_number 1 → 需要压制的溶剂峰的数量

wet_offset1 5[ppm] x_offset

wet_offset2 0[ppm]

wet_offset3 0[ppm]

wet_offset4 0[ppm]

wet_offset5 0[ppm]

依次输入需要压制的各溶剂峰的化学位移

不同k值的处理效果对比:

