

NMR data processing software

Delta

NMR Software

v5.0



HMBC-J分辨实验测定



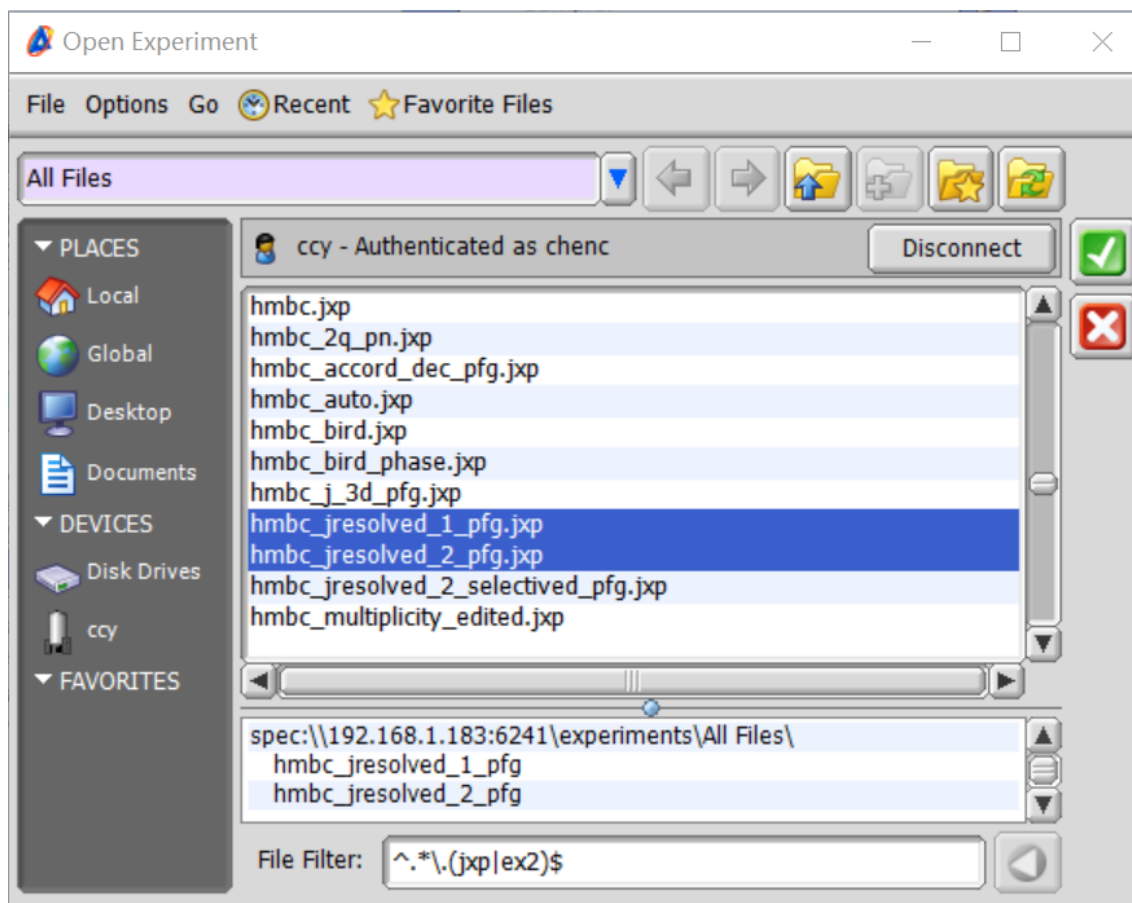
JEOL RESONANCE

1. 实验方法选择

HMBC-J分辨谱是用于测定异核远程耦合常数的方法。

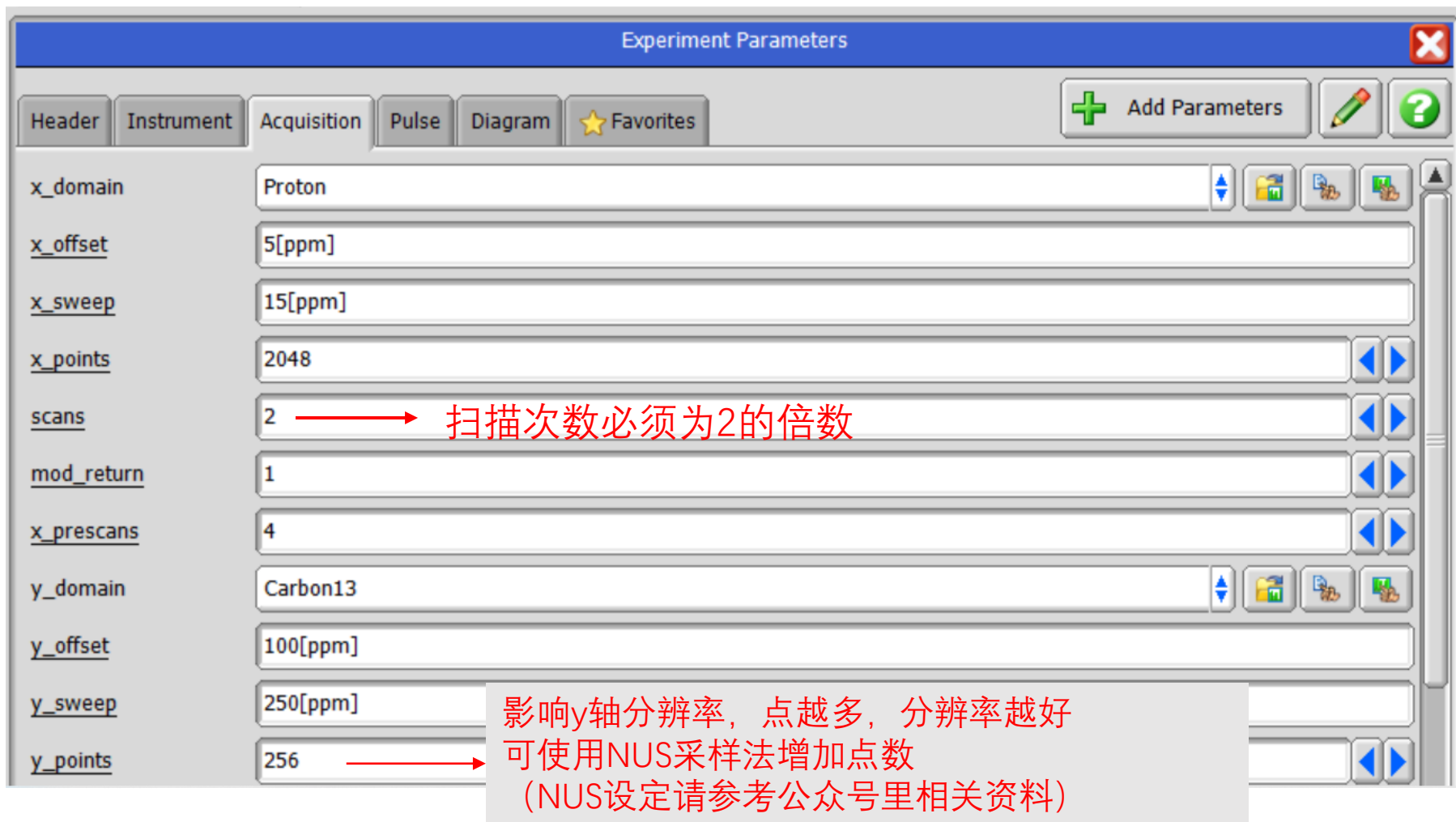
常用的脉冲序列为：

hmbc_jresolved_1_pfg.jxp 或 **hmbc_jresolved_2_pfg.jxp**



2. 实验参数设定（此处以hmbc_jresolved_1_pfg.jxp为例）

➤ 设置Acquisition参数：其他参数与测试HMBC谱图参数设定类似



The screenshot shows the 'Experiment Parameters' window with the following parameters:

Parameter	Value
x_domain	Proton
x_offset	5[ppm]
x_sweep	15[ppm]
x_points	2048
scans	2
mod_return	1
x_prescans	4
y_domain	Carbon13
y_offset	100[ppm]
y_sweep	250[ppm]
y_points	256

Annotations:

- A red arrow points from the text '扫描次数必须为2的倍数' to the 'scans' value of 2.
- A red arrow points from the text '影响y轴分辨率，点越多，分辨率越好 可使用NUS采样法增加点数 (NUS设定请参考公众号里相关资料)' to the 'y_points' value of 256.

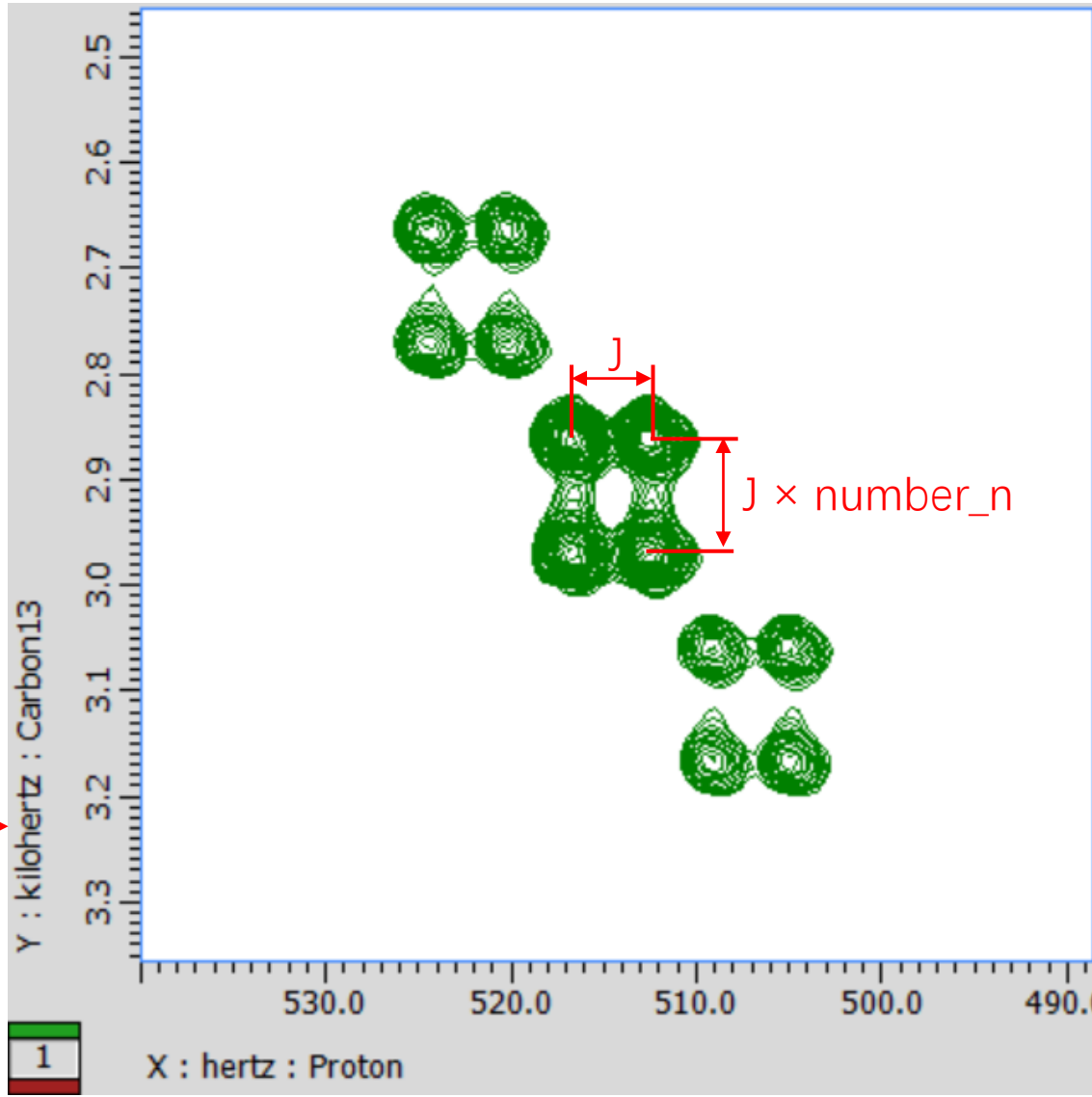
➤ 设置pulse参数：其他参数无需修改

The screenshot shows the 'Experiment Parameters' window with the 'Pulse' tab selected. The window is divided into two sections: 'Pulse' and 'Pulse Delay'. The 'Pulse' section contains parameters for x and y pulses, including pulse width, attenuation, and phase. The 'Pulse Delay' section contains parameters for the coupling constant, number of measurements, maximum time, minimum coupling constant, and relaxation delay. Red arrows point from the parameter values to explanatory text in Chinese.

Parameter	Value	Explanation
x_pulse	9.8[us]	
x_atn	4.6[dB]	
y_pulse	8.5[us]	
y_atn	5[dB]	
j_constant	140[Hz]	CH的J耦合常数
number_n	25	改变n值可调整观测的最小的J值大小
nt1_max	0.25466[s]	
j_min	3.92677[Hz]	
relaxation_delay	1.5[s]	大于T1值

设置完参数，提交实验。

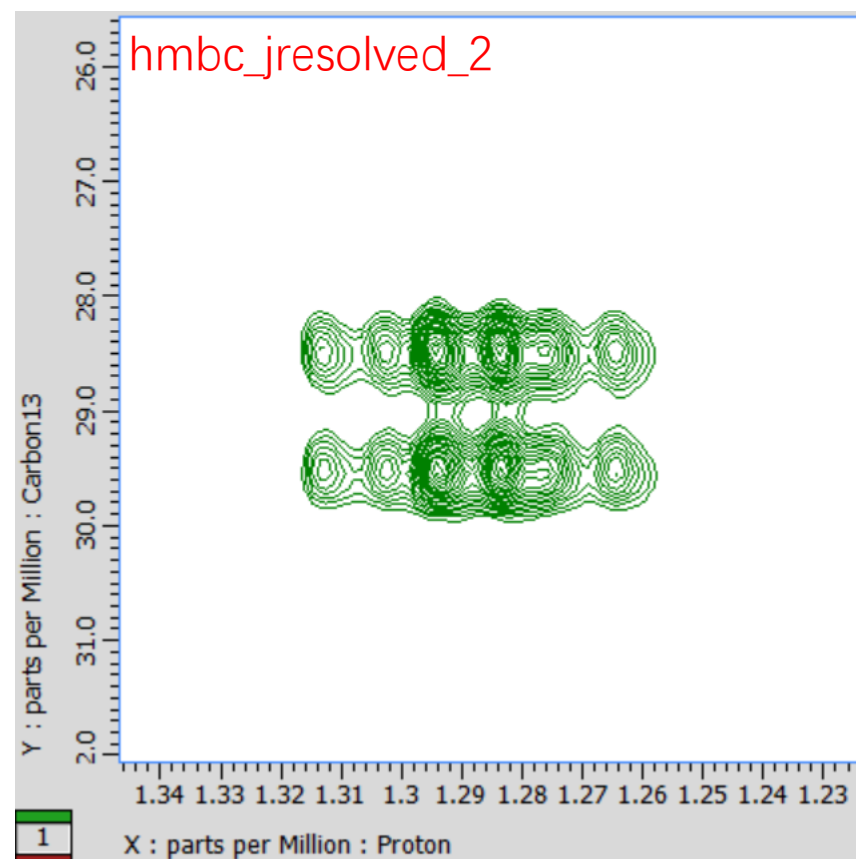
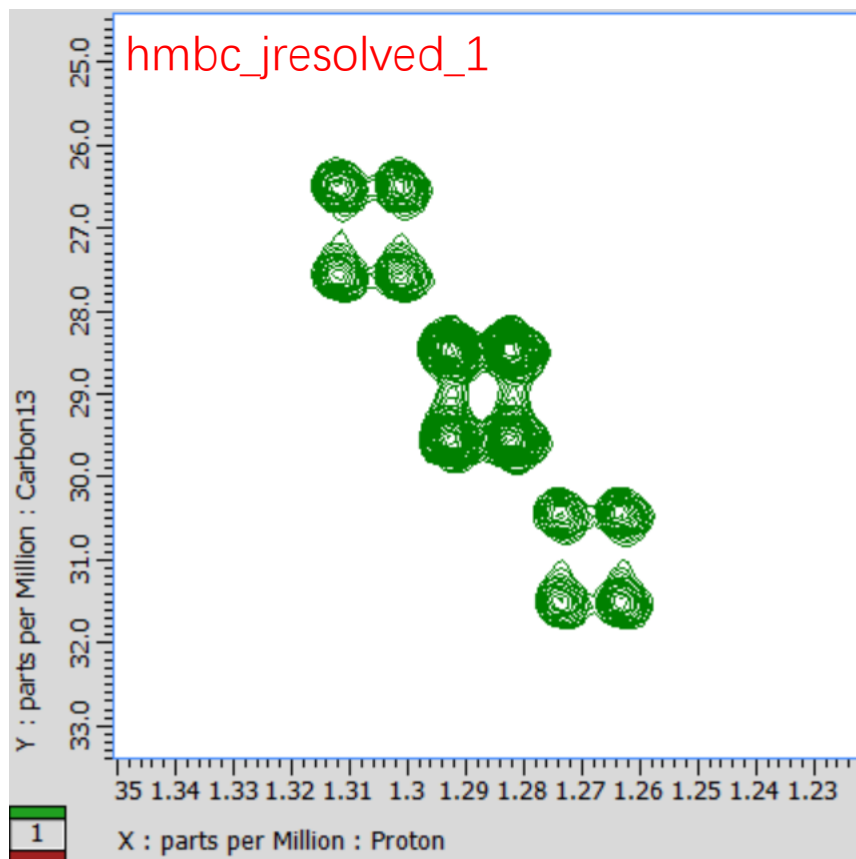
3. 实验结果分析及对比



将坐标轴
的单位换
算为Hz即
可读取



➤ hmbc_jresolved_1_pfg 与 hmbc_jresolved_2_pfg 对比



信号显示不同，J值结果相同
hmbc_jresolved_1信噪比相对更好