

NUS实验设定及数据处理



1. NUS设定

▶ 添加二维实验→点开实验参数编辑 🛃



(此处以HSQC实验为例,其他二维实验设定步骤相同)

➤ 在Acquisition项中打开添加参数①→在弹出的小窗口中选择y_nuslist②→参数中出现y_nuslist选项,点击y_nuslist③



▶ 在弹出的窗口中输入非均匀采样的点数→Schedule→Apply

Sampling Sch	eduler : Poisson Gap				_		
File Edit Options							
(Condition			Schedule			
Sampling Axes	1		No. Y	tota	l : 32[pnt]		
Y Points	128	•	一 ³ Y轴总点数	,增大点数,	可提高Y	袖分辨率	卒
Sampling Rate	25[%]	-		工任不通共	书名时间	すいる	5小为75%
Sampling Points	32		7 1		며따다	,	ヒク 川23%
Total Points	[128		> 实际采样,	点数			
Sampling Method	Poisson Gap		11 17 12 20 13 22				
Sine Weight	2		14 24 = 15 28				
Tolerance	1[%]		16 34 17 39			1.1.1	
Indexing Base	1		19 46 20 50				
Experiment	hsqc_auto.jxp		21 57 22 61				
Scans	2		23 68 24 77 25 78				
Relaxation Delay	1.5[s]		26 82 27 86				
Sampling Time	00:04:04		28 95 29 105				
		Ы					
			Sampling points returned:	1	64 65	128 Y	
	Schedule)	32		A	pply	

▶ 设置完成出现以下界面,其他测试参数设定与普通二维谱参数设定相同

	Experiment Parameters	3
Header Instrument	Acquisition Pulse Diagram 🏠 Favorites	
x_prescans	8	
y_domain	Carbon13	
y_offset	85[ppm]	
y_sweep	[170[ppm]	
y_points	128	
x_acq_time	0.17076[s]	
x_resolution	5.85618[Hz]	
y_acq_time	7.49007[ms]	
y_resolution	133.51017[Hz]	
y_nuslist	, 5, 6, 8, 9, 10, 13, 15, 17, 20, 22, 24, 28, 34, 39, 43, 46, 50, 57, 61, 68, 77, 78, 82, 86, 95, 105, 112, 116, 125}	
nuslist_idx_base	1	

2. NUS数据处理

> 实验测试完成,弹出以下界面→点击翻转按钮①回到数据处理界面
 →调入NUS处理方法②



▶ 调入的处理方法为测试使用的<u>脉冲序列中对应的处理方法</u>加nus的list:

①在底下File Filter中输入nus筛选(如下图所示)

②窗口中若没有出现File Filter选项,打开左上角Options,勾选Show File Filter

🖉 Open Process List — 🗆					×	
File Options Go 😁	Recent 숡 Favo	orite Files				
proc O Show Recom	mended Files		•			
Group Directories		nus.list				
Show Places		_nus.list hase_nus.list				
Show Device	s	e_abs_nus.list e_phase_nus.list e_pn_nus.list				
Documents	2d_inverse_ 2d_inverse_	abs_nus.list phase_nus.list				
✓ DEVICES ▲ Disk Drives	2d_inverse_ cbcaconh_nu	pn_nus.list is.list ius.list				
Spectrometers	noah_hmbc_ noah_hsqc_r	nus.list nus.list			Ļ	
▼ FAVORITES						
	Processing List	File				
	File Filter: *n	us.list	1			

比如常用的HSQC脉冲序列中对应处理方法为: 2d_inverse_pn.list NUS数据处理方法应该使用: 2d_inverse_pn_nus.list

▶ 如何查看<u>脉冲序列中对应的处理方法</u>: Header→process

	Experiment Parameters
Header Instrument	Acquisition Pulse Diagram 🕎 Favorites
storage_filename	CHCI3_HSQC \$(SAMPLE)_HSQC
filename	hsqc
storage_comment	hsqc \$(SAMPLE.comment) \$(EXP.comment)
comment	hsqc 加里此处没有显示process
process	2d_inverse_pn.list
auto_gain	□ 点开右上角问号 / / □
filter_limit	16 Sexperiment Viewer - hsqc_auto
	header filename => "hsgc"; sample_id => ""; comment => "hsgc"; process => "2d inverse_pn.list"; include "header pd";
	force_tune = FALSE; 在此义件中可找到初
	force_dual_mode = FALSE; end header; 应的process
	<pre>instrument include "instrument"; SPIN_STATE => "SPIN OFF"; end instrument; acquisition x_domain =? "Proton"; x_offset = 5[ppm]; x_sweep => 12[ppm];</pre>

▶ 调入处理方法后,点击2D Viewer按钮 🛅 即可查看谱图



