JEOL

Delta V5 operation

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Connect to spectrometer



- 1. Start Delta V5 (double click 🖉).
- 2. Open Spectrometer Control (click 🔒).
- 3. Select spectrometer on Available Instruments.

🙆 Sp	ectrometer	r Contro	- Adva
Conr	ection T	ools C	onfig
	Available 1	Instrum	ents
JNM	ECS400		

4. Click - connect and login with delta account (click).

	Authentication	
	Please enter your login information	
Name	Account name required	
Password	\frown	
Con	ect Own Cancel	

Name	Password	remarks
delta	delta	For installation account

Sample preparation



- 1. Set sample tube on SCM .
- 2. On Samples tab **1** , you must defined your sample information.
- 3. On Samples tab, click ➡ . You can see new sample definition space on sample list.
- 4. Input sample name.
- 5. Select solvent.
- 6. Click Verified.
- 7. Click sample number. Clicked sample box becomes green color.

No. 🔺 Sample Name	Solvent	Kind	Shared	Verified
▶ 1 -	Chloroform-D 🔶	Liquids 🍦		Ø
No. 🛓 Sample Name	Solvent	Kind	Shared	Verified
▶ 1 🖌 10ETBZ	Chloroform-D 🔶	Liquids 🍦		Ø

8. Click **I** for sample loading.

JNM-ECS400		
User: delta Owner: delta	Sample: - Job: - Method: - □ Action: Idle Collected: - Time: -	
Sample Control: Load 🐉	Interactive	Attribute Area Size

Progress through Synergy



1. Click Create a Job on Samples tab or key in the job name which you want to define your job. You can see the next tab to (Jobs tab).

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Ø Spectrometer Control - Advance	ed Mode					_		
Connection Tools Config Shi	ms Samples							
JNM-ECS400								
User: de S Owner: de	lta Ita Queue ()> Monitor () Sta	S Activity C	Sample: 10 Job: - Method: - Action: Idl ollected: - Time: -	ETBZ e	Info 🔻			
+	Sample Control: 🁔 Eject	Interactive]					Attribute Area Size
No. 🔺 Sample Name	Solvent	Kind	Shared	Verified	Error	Owner	Last Load	
▶ 1 🖌 10ETBZ	Chloroform-D 💠	Liquids 🍦		Ø		delta	Recently	
▶ 2 = 10EtBz 1	Chloroform-D 🔶	Liquids 🍦				delta	Never	
						Create a Job	Update Job(s)]
				Enter	r a title for th	e new job:		
				Add	the Job Id to) only if neces) always	the title: ssary	Creat with th	te a Job is Sample
Receiver Gain: 50	🚯 Spin: 15[Hz] 🔹 🔒 Lock:	650 Tem;	p: 22.5[dC]	Heli	um: 100[%]	Nitroge	n: 76[%]	Queue Length: 1

2. We can choose some experiments which user want to do on Job Parameters box.

3. If user want to do another experiment which is not save in available methods, click Add Experiment for another experiments.

Proton Carbon COSY DEPT	Add Experiment
Available Methods	Job Parameters
COSY Available Methods	A allow printing 🔻 Off 🛊
Carbon DEPT	- project V
HMBC HMQC HSOC	
NOESY Proton	
ROESY TOCSY	
edited DEPT	
	Policy Choose a scheduling policy
	Start [dd-mmm-yyyy] hh:mm[:ss]
+ 1 🗃	Submit Job

4. If you want to change the more detail parameters, select experiment name on Open Jobs list.



5. We can change some experiments parameters on Job Parameters box.

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Open Jobs	Sample Name	Solvent	Kind Preparation	Comment
Vew Job 1	10ETBZ	Chloroform-D	Liquids TRUE	
Proton 0:02				
				Add Parameters
	Header Instrument	Acquisition Pulse Diagram 🕎 Fa	ivorites	
	storage_filename	\$(SAMPLE)_Proton \$(SAMPLE)_	Proton	
	filename	Invoton		
		Comment placed in result file		
	comment	single_pulse		
	auto_filter	Ø		=
	auto gain	Ω		
	<u>-</u> j			
	filter_limit	8		
	force_tune	0		Γ
	save_aborted	7		The second se
	🖳 🗍 Deliver data a	automatically		Submit Job

6. If you first time do this sample, click "Force tune" and "Auto_gain".

, you can see

- 7. If you tick "Deliver data automatically " 🖳 🖉 Deliver data automatically the results on your display.
- 8. The parameters became red word when changed.

Deliver data automatically	Deliver data automatically results	
🥃 🧭 Deliver data automatically	You can see results on your display.	Data Servers (spectrometer) and your workstation
Deliver data automatically	You can't see results on your display.	Data Servers (spectrometer) only

	I IV	× 1×		17	Y		~ 1	
Open Jobs	Sample Name	Solvent	Open Jobs	Sample Name	Solvent	Kind	Preparation	Comment
Vew Job 1	10ETBZ	Chloroform-D	Vew Job 1	10ETBZ	Chloroform-D	Liquids	TRUE	Í 🚺
▼ Proton			▼ Proton					
Proton 0:02			Proton 0:02					Here and the second sec
				4.2/6:		0		
	Header Instrumer	nt Acquisition Pulse Diagram 🕎 Favorites		Header Instrument	Acquisition Pulse Diagram 🏠 Fa	avorites		Add Parameters
	storage_filename	\$(SAMPLE)_Proton \$(SAMPLE)_Proton		storage_filename	\$(SAMPLE)_Proton \$(SAMPLE)_	Proton		In In
	filonamo			filename	Inratan			
	a	Comment placed in result file		inename	procen			
	comment	single_pulse		comment	single_pulse			
					-			
	auto_filter	Ø		auto_filter	V			
	auto gain	0		auto gain	7			
	auto_gain				•			
	filter_limit	8		filter_limit	8			
	No. of Concession, Name				-			
	force_tune			force_tune				
	save aborted	a		save aborted				V
		•	V		-			
	Deliver dat	a automatically		Deliver data	automatically			Submit Job
		a automatically		S Denter data				- Submit Sob

Submit experiment (automation)



9. Click \triangleright submit Job. The experiments are started.

Open Jobs	Sample Name	Solvent	Kind	Preparation	Comment
Vew Job 1	10ETBZ	Chloroform-D	Liquids	TRUE	A
Proton O:02					
	Header	Acquisition Pulse Diagram 🔆 Favo	orites		4dd Parameters
	storage_filename	\$(SAMPLE)_Proton \$(SAMPLE)_Pr	oton		
=	filename	proton			
	comment	single_pulse			
	auto_filter	Ø			=
	auto_gain	Ø			
	filter_limit	8			
	force_tune				U
	save_aborted	Ø			V
	🖳 🏹 Deliver data	automatically			Submit Job

10. If you want to stop experiment, Click 💴





Case A: You have already connected to spectrometer.

1. Click 📴 on Delta Console window.



2.

Click 🥃 Data Servers for downloading from spectrometer. You can select and

download data.



1D processor (open data file)











- 🔍 : Zoom (Zoom view of data)
- Pan View (Pan view of data or slide view)
- 🔝: Amplitude gain (apply amplitude gain)
- Select (To select data of geometry)
- Phase correct (To adjust the phase of spectra)
- Copy position (Copy position to paste buffer)
- : Peak threshold (Adjust the peak threshold)
- Reference (To set a chemical shift reference axis marker)
- ♦ : Peak (Peak picking tool)
- f]: Integral (Integral tool)
- : Measure (To measure distance between peaks)
- +: Cursor (make the horizontal and vertical line)
- T: Annotation (edit annotation in the geometry)
- Second type (To display a structural formula and molecular formula in the geometry)
- PiP (Picture in Picture)

1D processor (open process list)

1. When you open 1D NMR data, you can see 1D processor window.



- 2. If you want to open process_list, click 🔳 .
- 3. When you apply process_list, click 🕨
 - * 🖭 : for 1H process_list, 🖻 : for 13C process_list

1D processor (edit process list)

1. When you want to edit process, you can edit on Processing tool.



2. If you click ►, you can see detail parameters for processing command.

▶dc_balance(0, FALSE)
▼ sexp(1.2[Hz], 0.0[s])
Width (1.2[Hz]
Shift 0.0[s]
▶trapezoid(0[%], 0[%], 90[%], 100
fft(1, TRUE, TRUE)
ppm
[display/phase]

- 3. When you apply process, click .
- 4. If you click o, you can undo your process list.

1D processor (phase correction 1)



- 1. When you click 🕢 (auto phase), the phase of spectrum is adjusted.
- 2. You can see phase correction values on the left upper in spectrum.



3. Those values are inputted in Phasing Tool.



- 4. If you want to adjust those, you can manipulate with Phasing Tool.
- 5. When you finish to adjust, click 🕨 .

(If you can't see Phasing Tool, please click A Phasing on the left.)

1D processor (phase correction 2)

- Click Ø at "Pointer Bar". (Pointer bar i: Ø▶ ⊨ ▲ ◆ f & + T ▷ □ on processor window.)
- 2. You can see the vertical line on you spectrum.



- 3. When your mouse cursor moves to that line, mouse cursor is changed to \Leftrightarrow .
- 4. In that situation, you can change ϕp with dragging.



5. If you want to adjust $\phi 0$ and $\phi 1$, you can manipulate with Phasing Tool.

1D processor (Zoom process)

- 1. Click at "Pointer Bar". (Pointer bar is 🔍 🕅 🔍 on processor window.)
- 2. You can see your mouse cursor became magnifer.



3. When you drag any region or the border, the process window zoom will be changed.



1D processor (Peak threshold)



- Click L at "Pointer Bar". (Pointer bar is
 on processor window.)
- 2. You can see your mouse cursor became peak threshold.



3. You could drag the green line or red line, this process influence peak picking and integral.



1D processor (Peak picking 1)

1. When user decide their peak threshold, click S for auto peak picking





1D processor (Peak picking 2)



- Click at "Pointer Bar". (Pointer bar is 3 + on processor window.)
- 2. You can see your mouse cursor became peak picking.



3. Which peak you want to pick, move the mouse cursor to peak and click left mouse button.





1D processor (Peak integral 1)

1. When user decide their peak threshold, click **f** for auto peak integral.





1D processor (Peak integral 2)



- Click f at "Pointer Bar". (Pointer bar is
 f at "Pointer Bar". (Pointer bar is
- 2. You can see your mouse cursor became peak picking.



3. Which peak you want to integral, move the mouse cursor to peak and drag the region by left mouse button.



1D processor (options)



If you can't see "Options" panel, please click _ Options on the left.

Options				
Peak Sep.	0[Hz]			
Int Width	50[Hz]			
Normal	1			
X Ref	0.0[ppm] 0 👔			
X Start	8.80[ppm]			
X Stop	-1.20[ppm]			

Peak Sep. : The minimum value between peak and peak for peak picking.Int Width : The range of integral.Nomal : Normalize value for integral.X Ref : the value for calibrating chemical shift.X start : the right edge of the spectrum.X Stop : the left edge of the spectrum.

1D processor (Peak reference)

- Click at "Pointer Bar". (Pointer bar is
 processor window.)
- 2. You can see your mouse cursor became reference.



3. Which peak you want to decide reference peak, set the value in X ref on option bar and move the mouse cursor to peak and click by left mouse button.



1D processor (Peak integral normalized)

1. After auto integral, user could see the result about integral.



 Click at "Pointer Bar". (Pointer bar is on processor window.), select the integral and key in the value which user want to normalized on option bar



1D processor (prepare print)

1. After data process, click alt+f for data file name and alt+shift+c for method.





1D processor (prepare print)

1. Click 🖾 For pint data file.



2. If user want to print shim parameters, click delta and tick the print parameters and choose the location



Progress through Synergy

Set up experiment (¹³C automation)

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1. We can click the carbon experiment icon on Job tab.



Set up experiment (¹³C automation)

- 1. If you first time do this sample, click "Force tune" and "Auto_gain".
- 2. If you tick "Deliver data automatically" 📮 🖉 Deliver data automatically the results on your display.
- 3. The parameters became red word when changed.

Deliver data automatically	results	Data is saved to …
🕎 🏹 Deliver data automatically	You can see results on your display.	Data Servers (spectrometer) and your workstation
🖳 🗋 Deliver data automatically	You can't see results on your display.	Data Servers (spectrometer) only

Header Instrument	Acquisition Pulse Diagram 🏠 Favorites	Header Instrument	Acquisition Pulse Diagram 🏠 Favorites	
storage_filename	\$(SAMPLE)_Carbon \$(SAMPLE)_Carbon	storage_filename	\$(SAMPLE)_Carbon \$(SAMPLE)_Carbon	
filename	carbon	filename	carbon	
comment	single pulse decoupled gated NOE	comment	single pulse decoupled gated NOE	
sn_ratio	0	sn_ratio	0	
auto_filter	Ø	auto_filter	Ø	
auto_gain	0	auto_gain	Ø	
filter_limit	8	filter_limit	8	
force_tune	0	force_tune		
save_aborted	ø	save_aborted	Ø	
🖳 🗍 Deliver data a	automatically	🖳 🧭 Deliver data a	automatically	t Job

Progress through Synergy

, you can see

Set up experiment (¹³C automation) The experiments are started. 1. Click > Submit Job Open Jobs Sample Name Solvent Kind Preparation Comment TRUE Vew Job 1 FtBz Chloroform-D Liquids ▼ Proton Proton 0:01 Vew Job 2 ▼ Carbon Carbon 0:53 Add Parameters 0 Header Instrument Acquisition Pulse Diagram Favorites \$(SAMPLE)_Carbon \$(SAMPLE)_Carbon storage_filename filename carbon comment single pulse decoupled gated NOE sn_ratio Ø auto_filter 1 auto_gain 8 filter_limit force_tune save_aborted 1 2 🔒 🔒 🚨 🖳 🧭 Deliver data automatically Submit Job

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2. Wait to collect data.



Set up experiment (¹³C automation)

1. Click Montor , and observed the real time spectrometer.





1. If you want to stop experiment, Click 2.



2. If tick save_aborted (default parameters), stop experiment, the data file will be saved in console

Header Instrument	Acquisition Pulse Diagram 🚼 Favorites			
storage_filename	\$(SAMPLE)_Carbon			
filename	carbon			
comment	single pulse decoupled gated NOE			
sn_ratio				
auto_filter				
auto_gain	Ø			
filter_limit	8			
force_tune				
save_aborted				
👰 🧭 Deliver data a	utomatically Submit Job			



1. When finish your experiment, click and check the Quene tab which is empty.

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🖇 Spectrometer Control - A	Advanced Mode					
Connection Tools Confi	g Queue					
JNM-ECS4	400					
Use Use Own	r: delta er: delta	r 🚺 Status	Sample: EtBz Job: - Method: - Action: Idle Collected: - Time: -	Standard Sta	rting Collection Iding Output File : 512 kB ding file to data server seriment Completed st-experiment Default Initializatio w Job 2 : CANCELLED	n V
Job # Status	User)(ob title	Scheduling		Queue State
			,		Idle Jobs Ready:	0

Finish experiment



- 1. Click and check the Job tab which is empty.
- 2. If not empty, click the Job and click 退 to delete Job.

Spectrometer Control - Advanced Mode		
Connection Tools Config		
JNM-ECS400		
User: delta Dvvner: delta	Sample: Et8z Job: - Method: - Action: Idle Collected: - Time: - Method: - Collected: - Time: -	tion this is a constant of the server of the
Open Jobs	Sample Name Solvent Kind Preparation	Comment
▼ New Job 1 ▼ Proton Proton 0:01 ▼ New Job 2. ▼ Carbon Carbon 0:53	ElBz Chloroform-D Liquids TRUE	×
	Q	
	Proton Carbon COSY DEPT	Add Experiment
	Available Methods Job Parameters	
	V Standard COSY) ▼ Off ‡
•	DEPT project	• •
	HMBL HMQC HSQC NOESY Proton RDESY TOCSY edited DEPT	
	Policy Choose a s	cheduling policy
Delete Alt: Del	the selected Jobs Start [dd-mmm-]	/yyy] hh:mm[:ss]
	+ 0 🖆 🔶 + - % [Submit Job
Receiver Gain: 50 OSpin: 1	15[Hz] @Lock: 532 Temp: 22.1[dC] Helium: 100[%] Nr	trogen: 70[%] Queue Length: 0



DL

- 1. Click **J** and click verified.
- 2. Sample will eject

1 JNM-ECS400				
User: delta S Owner: delta	Sample: EtBz Job: - Method: - Action: Idle Collected: -	Starting Collection Building Output File : 512 kB Sending file to data server Experiment Completed Post-experiment Default Initialization		
Gij Samples Jobs Queue Was Monitor J Status	Time: -	New Job 2 : CANCELLED		
🚽 🗕 🛐 👔 Sample Control: 🍞 Eject 🦻	Interactive		Attribute Area Size	
No. Sample Name Solvent	Kind Shared Verified	Error Owner Last Load		
🕨 1 🚽 EtBz Chloroform-D 🛊	Liquids 🍦 🔲 🧭	delta Recently		
[] INM-ECS400				
User: delta S Owner: delta	Sample: - Job: - Method: - Action: Idle Collected: - Time: -	Starting Collection Building Output File : 512 kB Sending file to data server Experiment Completed Post-experiment Default Initialization New Job 2 : CANCELLED		
Sample Control: 🕞 Load 🚺	Interactive	Sample verified to be in the Sample changer	Attribute Area Size	
No. A Sample Name Solvent	Kind Charod Varified	Error Owner Last Load		
	Kind Shared Vermed	Citor Owner Case Coad		

3. Click – to delete sample for next user to use software.

IP JNM-ECS400	
User: delta S Owner: delta	Are you sure you want to delete this Sample? EtBz
🚺 Samples 📋 Jobs 📄 Queue 🅼 Monitor 🧃	catus Yes No
Sample Contrast. Is Los	Attribute Area Size
No. Sample Marrie Solvent	Kind Shared Verified Error Owner Last Load
► 1 =)Bz Chloroform-D ♦	Liquids 🛊 🔲 🗍 delta Recently



1. Check all your file will be save and click to close delta software.

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