Delta Tips

NMR data processing software

1/2

🗩 JEOL RESONANCE

NMDT_0072 How to automatically reflect the measurement parameters in the saved file name.

Have you ever been confused by forgetting to change the file name when you changed measurement conditions?

In Delta, you can automatically reflect the parameters used in the measurements to the filename. The automatic input can prevent file name entry errors and facilitate data sorting.

The measurement filename is specified by "storage_filename" on the "Header" tab of the experiment file. By default, the "storage_filename" is "\$(SAMPLE)_\$(EXP. filename)". At this time, the sample name and the text entered in "filename" are automatically reflected in the saved file name as "sample name_filename". When the sample name is "sampleA" and the filename is "proton", the file is saved as "sampleA_proton".

Header Instrument	Acquisition Pulse	Diagram 👷 Favorites	Add Parameters				
storage_filename	sampleA_proton	\$(SAMPLE)_\$(EXP.filename)					
filename	proton						

Editing the saved filename

By editing the "storage_filename", sample parameters and experimental parameters can be automatically reflected in the saved filename. There are three types of character strings that can be reflected: (1) Sample attributes, (2) Experiment parameters, and (3)Date. (1) Sample attributes are associated with samples, such as set temperatures (temp_set) and MAS frequencies (MAS_spin_set). To reflect them automatically, insert "SAMPLE." in front of the parameter you want to enter, such as \$(SAMPLE.temp_set) or \$(SAMPLE.MAS_spin_set).

(2) Experiment parameters are ones in experiment files, such as the observation center (x_offset) and the number of scans (scans).

To reflect them automatically, insert "EXP." in front of the parameter you want to enter, for example \$(EXP.x_offset) or \$(EXP. scans). (3) Measurement date can be reflected by inserting \$(YEAR)\$(MONTH_NUM)\$(DAY_NUM).(See NMDT_0003 for details) As an example, we will show how to automatically reflect the set temperature and the number of scans into the saved file name in addition to

the default sample name and file name.

1. Automatic reflection of sample attributes

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+	- 4		Samp	le Control:	🏠 Eject	P	Interac	tive						At
No. 🔺	Sample	Nan	ne		Solvent			Kind		Shared	Verified	Error	Owner	Last Load
V 1	▼ 1 🔿 sampleA NONE 🛊					Liquids	\$	0	Ø		kyazawa	Yesterday		
	Attributes		- spin_s	set			15[Hz	:]						•
	- spin_state		state		•			▼ SPIN ON 🛊						
🕒 🖶 💻 temp_set		_set	v			80[dC]								
			- temp	_state		•	TEMP	ON 🛊						

Set the temperature by "temp_set" in the sample attribute as shown in the figure above.

Therefore, if you add "_\$(SAMPLE. temp_set)" to the "storage_filename" column, the setting value of "temp_set" will be automatically reflected into the storage_filename as shown in the figure below.

Header	Instrument	Acquisition	Pulse	Diagram	☆ Favorites	2+	Add Parameters	
storage_filename sample			oton_80	[dC] \$(P.filename)_\$(SAMPLE.temp_set)	1		
filename		proton						

Delta Tips



2. Automatic reflection of Experiment parameters

The number of scans is set by "scans" of the Experiment file.

Header Instrument	Acquisition Pulse Diagram 🏠 Favorites	Add Parameters
x_domain	Proton	+ 🖀 🕾 🔺
x_offset	[5[ppm]	
x_sweep	[15[ppm]	
x_points	16384	
scans	64	
x_prescans	1	
mod_return	1	
x_acq_time	2.73215[s]	V

If you add "_\$(EXP. scans)" to the "storage_filename" column, the setting value of "scans" will be automatically reflected as shown below.

Header Instrument	Acquisition Pulse Diagram 🏠 Favorites	Add Parameters				
storage_filename	sampleA_proton_80[dC]_64 \$(SAMPLE)_\$(EXP.filename)_\$(SAMPLE.temp_set)_\$(EXP.scans)					
filename	proton					

Since there is no unit for the number of scans, only numbers are entered, making it difficult to understand as a filename. In such a case, it is recommended to directly enter the character string "scans" as shown below.

	Header Instrument	Acquisition Pulse Diagram ☆ Favorites	0
storage_filename		sampleA_proton_80[dC]_64scans \$\(SAMPLE)_\$(EXP.filename)_\$(SAMPLE.temp_set)_\$(EXP.scans)scans	
	filename	proton	

