STRUCTURE OF DELTA

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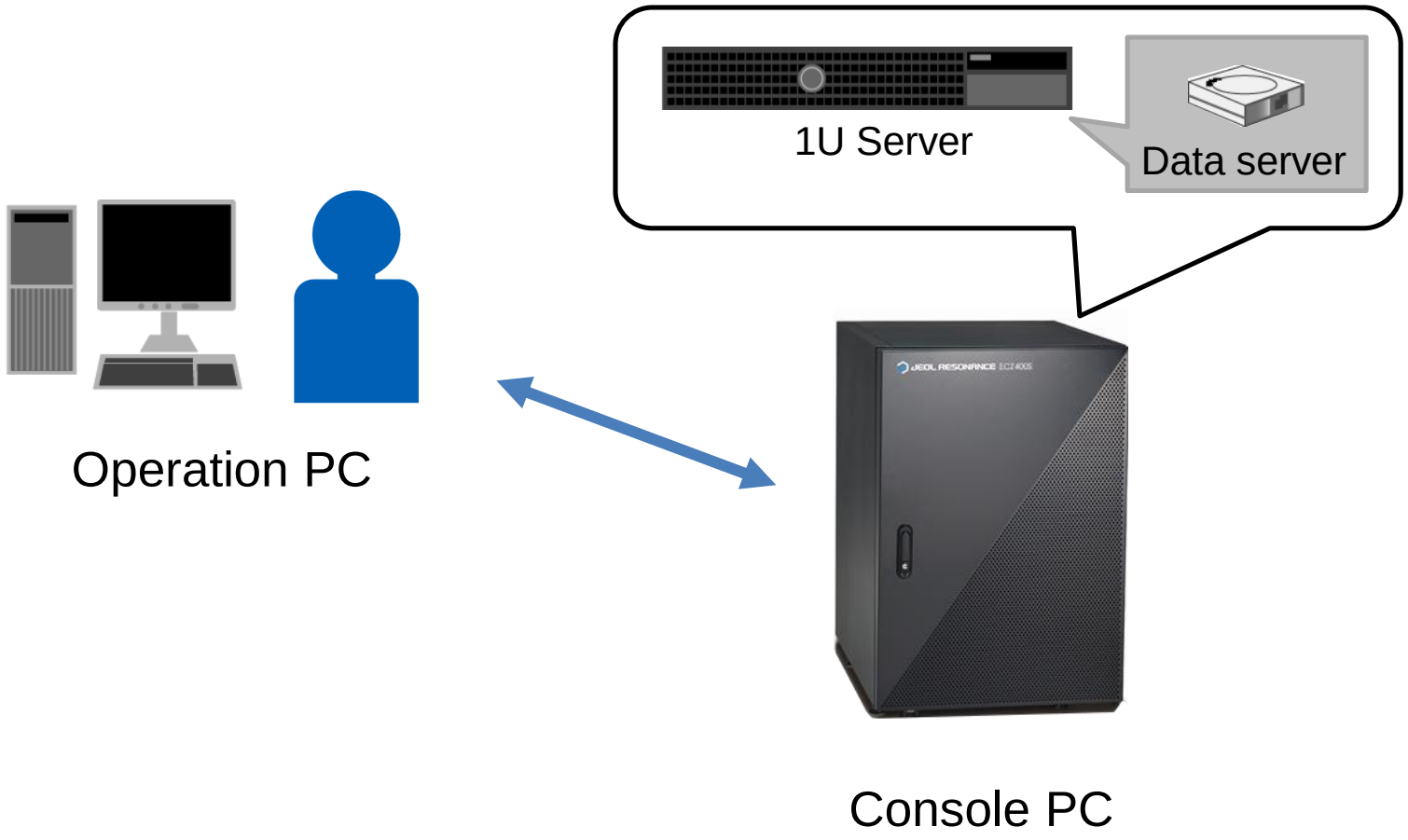
Basics

Operation PC and Console PC

We need to be aware of that both Operation PC and Console PC may store files to operate the system.



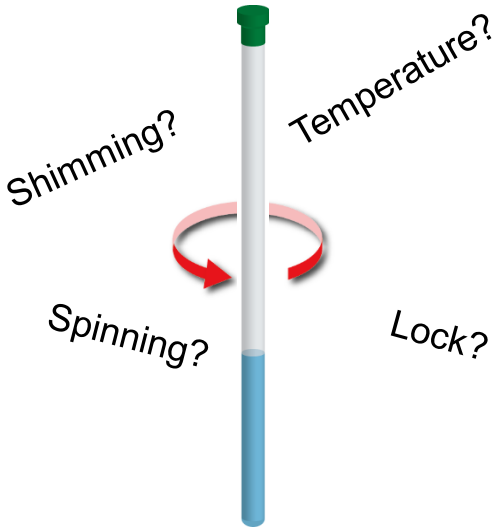
Global folder and Local folder

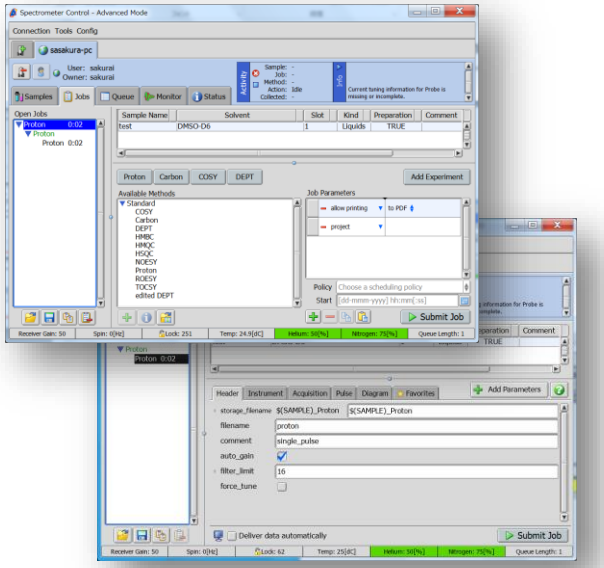
Basic rules of Delta software:

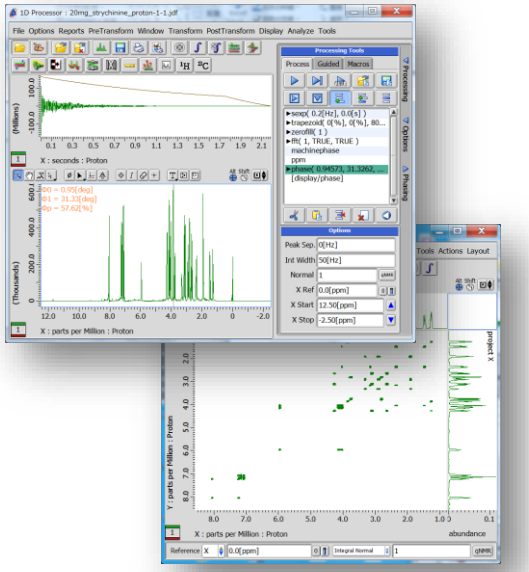
- In the case to use the same file name, the files in local folder (local files) have preference over the files which are stored in global folder (global files).
- The global files can not be directly edited.
- The local files can be customize independently for each Delta user.

Main components

Main components involved in the operation of the system are







Sample conditions

Solvent information

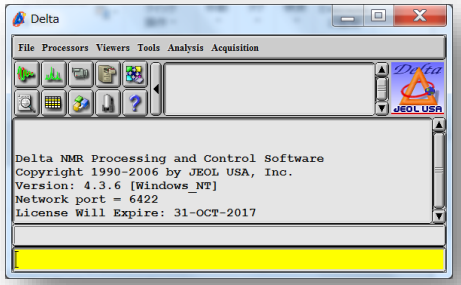
Experimental file

Automation script

Process list

Delta V4

Delta V4 (V3)



Delta V4

Operation PC

Console PC

Global folder
Local folder

Experimental file

Automation script

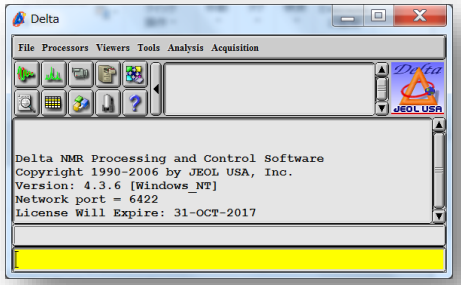
Process list

Solvent information

Sample conditions

Solvent information

Delta V4 (V3)



Delta V4

Operation PC

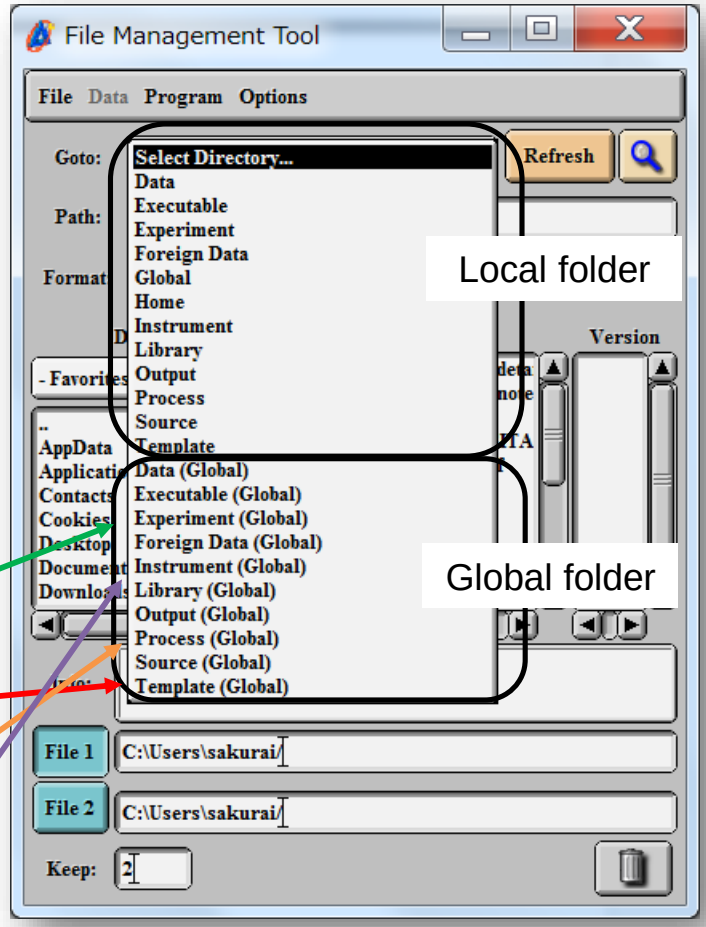
Global folder
Local folder

Experimental file

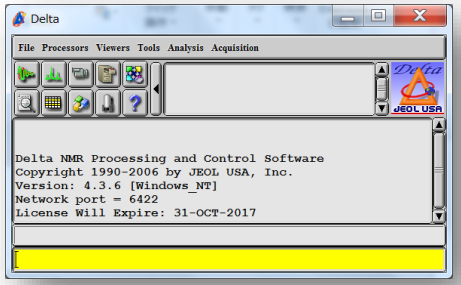
Automation script

Process list

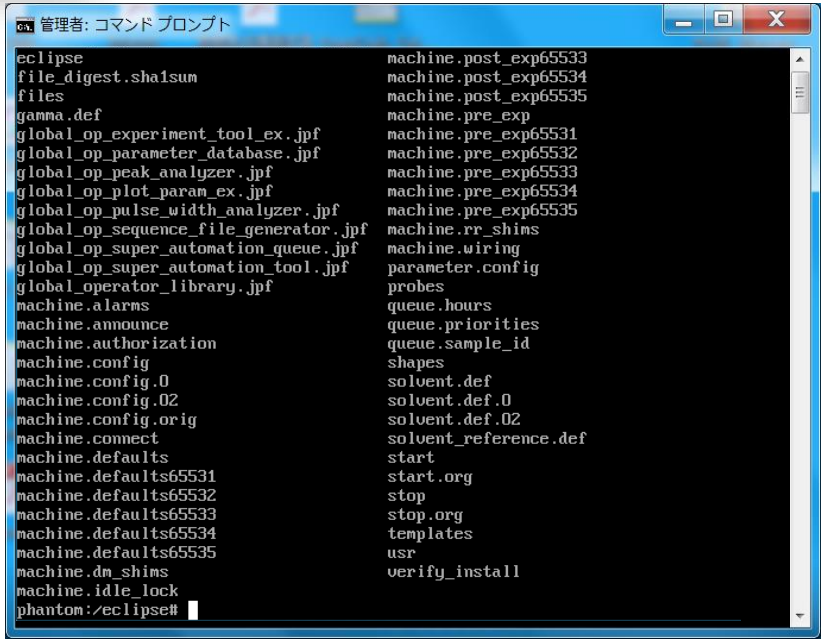
Solvent information



Delta V4 (V3)



Delta V4



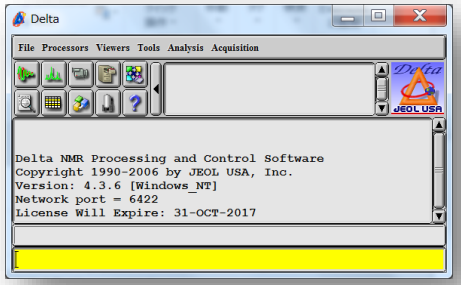
Console PC

Sample conditions

Solvent information

By Command prompt, it is available to modify…

Delta V4 (V3)



Delta V4

Operation PC

Console PC

Global folder
Local folder

Experimental file

Automation script

Process list

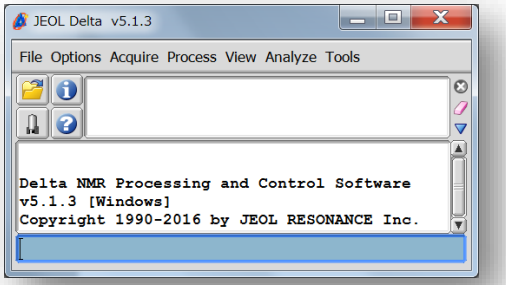
Solvent information

Sample conditions

Solvent information

Delta V5

Delta V5



Delta V5

Operation PC

Console PC

Global folder
Local folder

Experimental file

Automation script

Process list

Global folder
Local folder

Experimental file

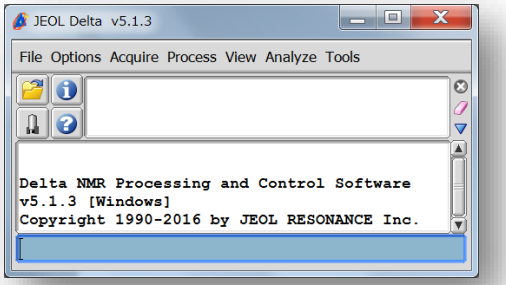
Sample conditions

Automation script

Solvent information

Process list

The merit to use local folder of operation PC



Delta V5

Operation PC

Global folder
Local folder

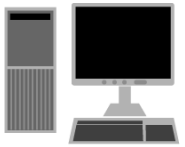
Experimental file

Automation script

Process list

- It is specific for computer.
- It is possible to restrict to Window's account.

The note to use local folder of V5 for operation PC



Operation PC

There are three different “local” folder!!

- “local” 1 (C:¥Users¥”account”¥Documents¥JEOL¥Delta 5.2)

i.e. in the case of “Delta” account,
→ C:¥Users¥Delta¥Documents¥JEOL¥Delta 5.2

Experimental file → C:¥Users¥”account name”¥Documents¥JEOL¥Delta 5.2¥experiments
Automation script → C:¥Users¥”account name”¥Documents¥JEOL¥Delta 5.2¥automation
Process list → C:¥Users¥”account name”¥Documents¥JEOL¥Delta 5.2¥process_lists

It is for personal use.

- “local” 2 (C:¥Users¥”account”¥AppData¥Local¥JEOL¥Delta 5.2)

*AppDta folder is hidden folder.

It is a folder to store the temporal setting file.
For example, when you change the preferences, system.jnv file is stored here.

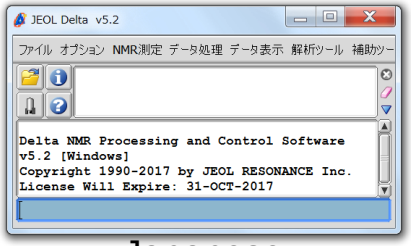
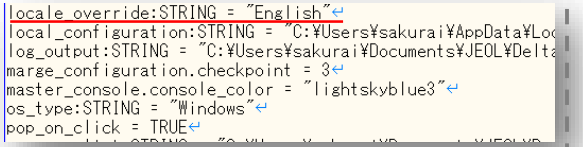
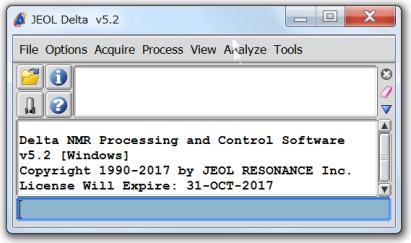
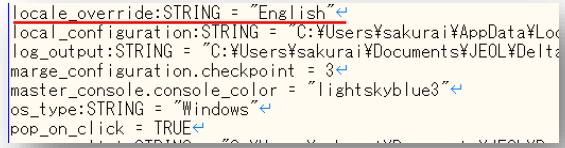
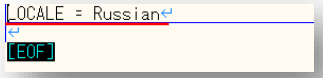
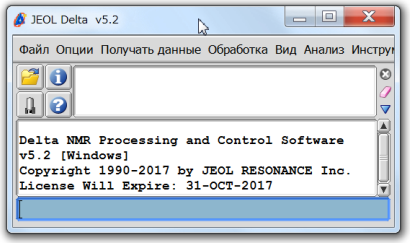
- “local” 3 (C:¥Program Files¥Common Files¥JEOL¥Delta 5.2)

This folder is restricted for administrator account to modify.
It is available to restrict the some setting by making local “.cfg” file here.
→explain more by next slide.

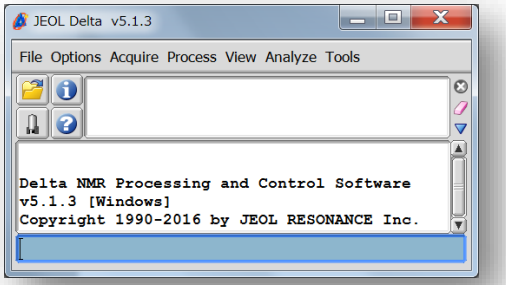
- Ref. Global folder (C:¥Program Files¥JEOL¥Delta 5.2.0.app¥Contents¥Resources¥global)

How does it affect?

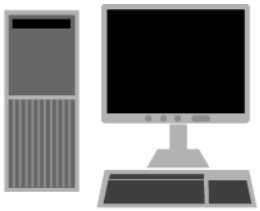
i.e. to restrict the language to “Russian”.

“local” 2 folder	“local” 3 folder	preferences	
none	none	default	 Japanese
 system.jnv	none	English	 English
 system.jnv	 system.cfg	English	 Russian

The merit to use local folder of console PC



Delta V5



Operation PC

2nd operation PC

Console PC

Global folder
Local folder

Experimental file

Automation script

Process list

Sample conditions

Solvent information

- You can use the same files from other computer.
- You can easily share the original files with colleagues.

The note to use local folder of V5 for console PC

There are two different “local” folder!!

Console PC

- “local” 1 (C:¥Program Files¥Common Files¥JEOL¥Control 5.2)

Experimental file → C:¥Program Files¥Common Files¥JEOL¥Control 5.2¥experiments
Automation script → C:¥Program Files¥Common Files¥JEOL¥Control 5.2¥automation
Process list → C:¥Program Files¥Common Files¥JEOL¥Control 5.2¥process_lists
Sample conditions, Solvent information → C:¥Program Files¥Common Files¥JEOL¥Control 5.2¥configuration

It is possible to access by any account

- “local” 2 (C:¥Program Files¥Common Files¥JEOL¥Control 5.2¥users¥”account”)

Experimental file, Automation script, Process list, Solvent information
→ C:¥Program Files¥Common Files¥JEOL¥Control 5.2¥users¥”account”

*It is not valid for sample conditions.

i.e. in the case of “Delta” account,
→ C:¥Program Files¥Common Files¥JEOL¥Control 5.2¥users¥Delta

It is specific for Delta account

- Ref. Global folder (C:¥Program Files¥JEOL¥Control 5.2.0.app¥Contents¥Resources¥global)

How to make local files for Delta V5 (For console PC)

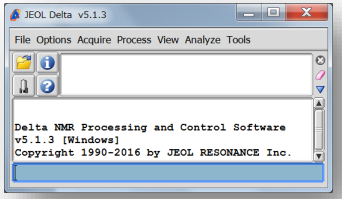
How to make a local file

Experimental file

Automation script

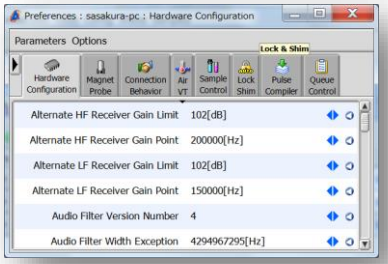
Process list

Upload via file browser of Delta software



Sample conditions

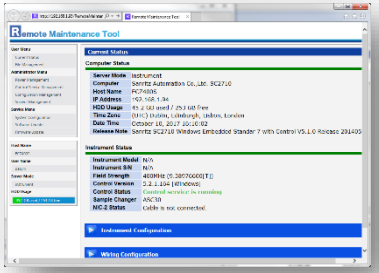
Edit via preference tool of Delta software



Console PC

Solvent information

Edit via Remote Maintenance Tool

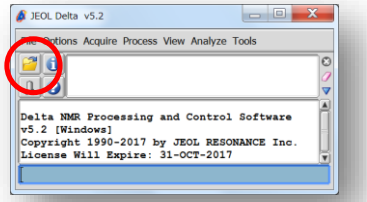


Upload via file browser of Delta software

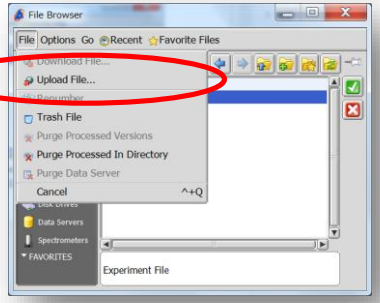
■ “local” 1 (C:¥Program Files¥Common Files¥JEOL¥Control 5.2)

Experimental file | Automation script | Process list

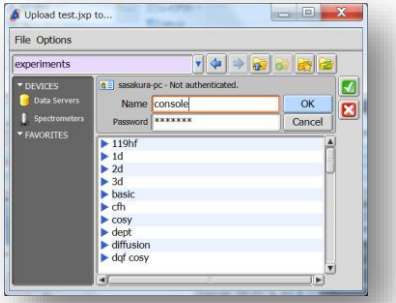
i.e. upload an experimental file.



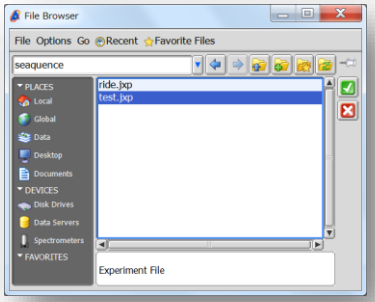
1. Click “Open file and choose tool”.



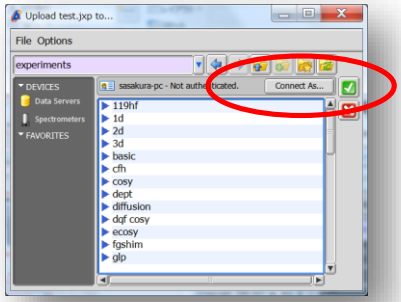
3. Select [File]–[Upload File…].



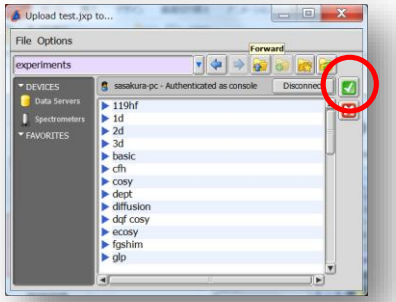
5. Do authentication by “Console”.



2. Select target file.



4. Click “Connect As…” button.



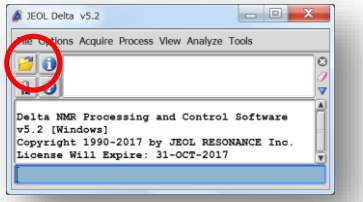
6. Select global folder of experiments.
7. Click “OK” button.

Upload via file browser of Delta software

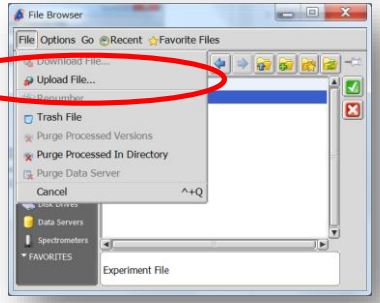
■ “local” 2 (C:¥Program Files¥Common Files¥JEOL¥Control 5.2¥users¥”account”)

Experimental file | Automation script | Process list

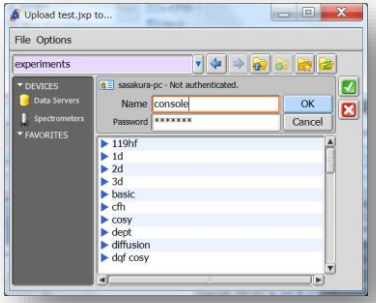
i.e. upload an experimental file for Satoshi account.



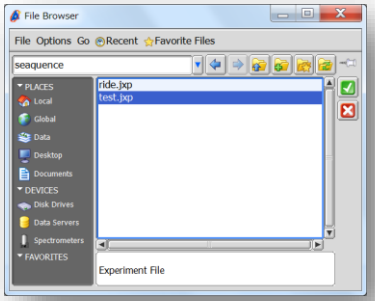
1. Click “Open file and choose tool”.



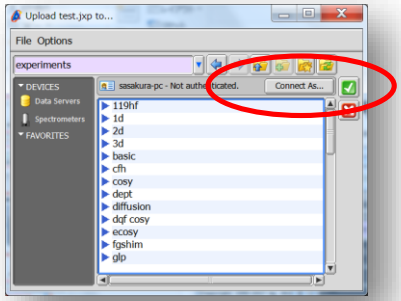
3. Select [File]–[Upload File…].



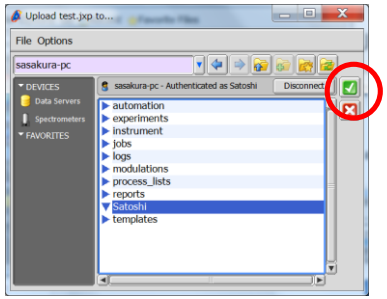
5. Do authentication by “Satoshi”.



2. Select target file.



4. Click “Connect As…” button.



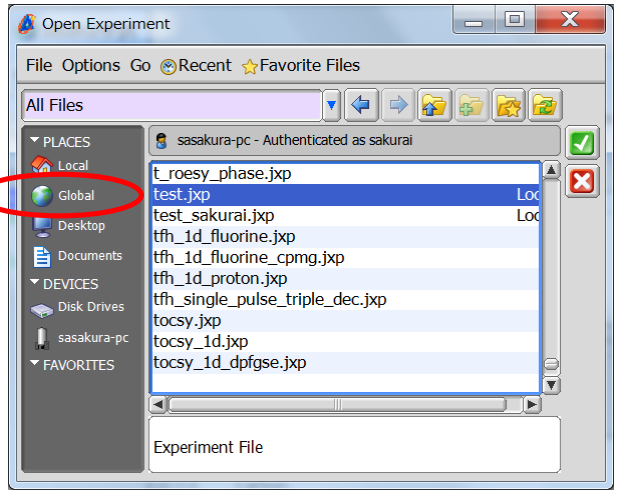
6. Select “Satoshi” folder.
7. Click “OK” button.

How to access to the local file

i.e. access to experimental file.

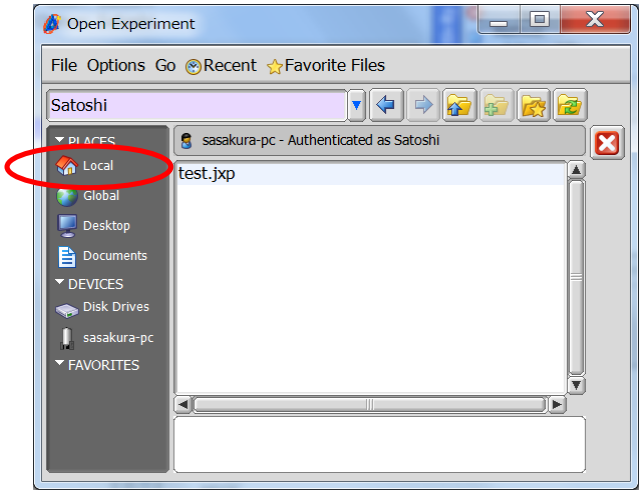
From “local” 1

On “Open Experiment”, select “Global” folder from left box, and develop “all files” folder.
There is uploaded experimental file with description of “Local” there.

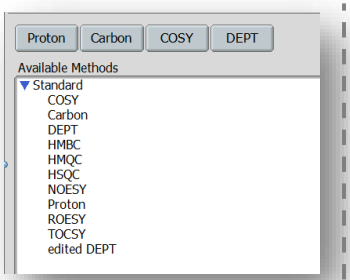
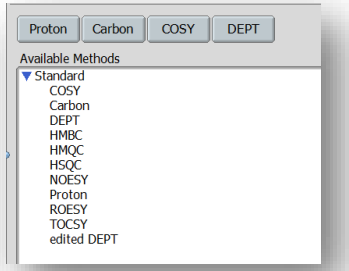
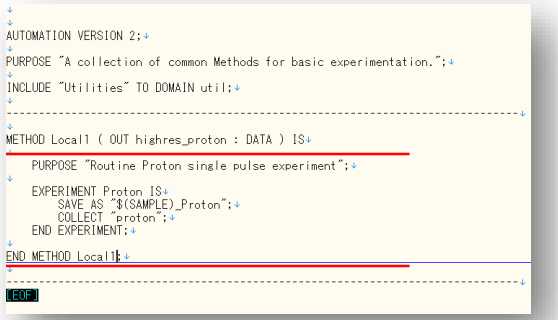
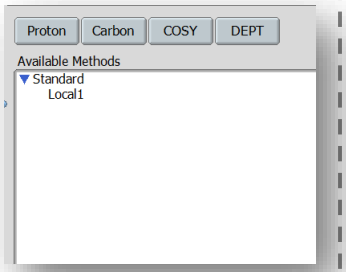
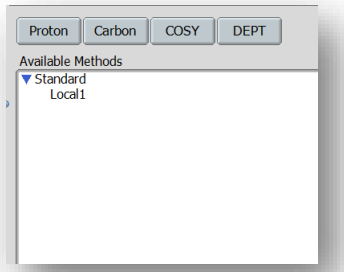
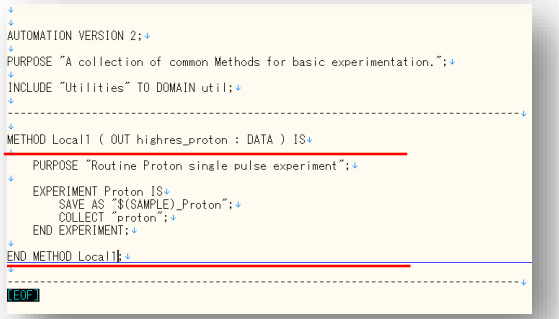
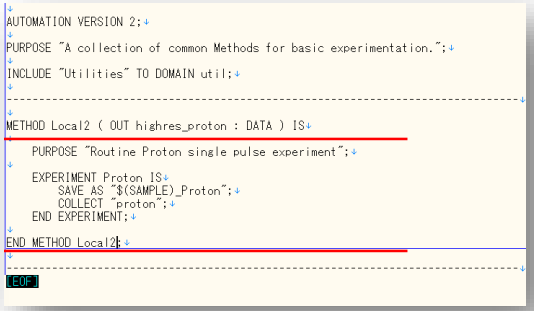
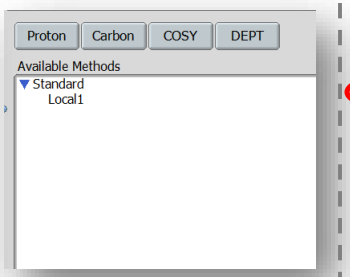
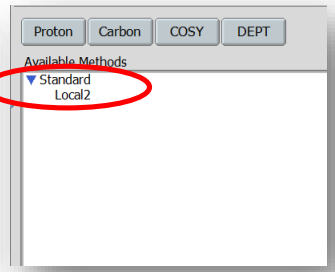


From “local” 2

On “Open Experiment”, select “Local” folder from left box.
There is uploaded experimental file there.



How does it affect?

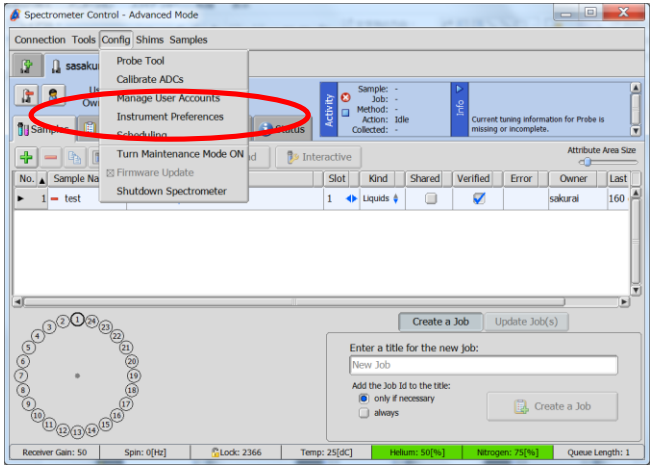
“local” 1 folder	“local” 2 folder (Satoshi)	Delta	Satoshi
none	none		
	none		
			

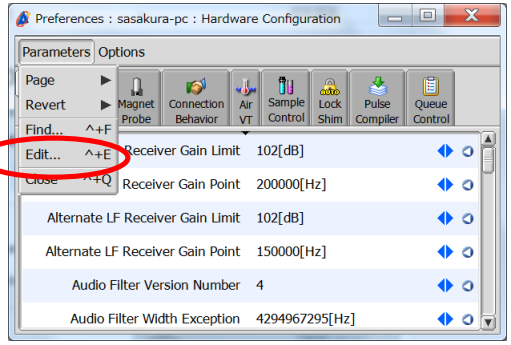
Edit via preference tool of Delta software

- “local” 1 (C:¥Program Files¥Common Files¥JEOL¥Control 5.2)

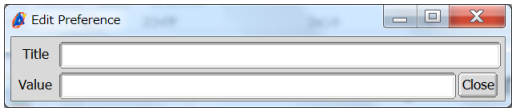
Sample conditions

1. Login to spectrometer by “Console” account.
2. Open the “Hardware Configuration” from [Config]-[Instrument Preferences].
3. On “Hardware Configuration” window, open “Edit Preference” from [Parameters]-[Edit…].





4. Put the commands as next slide.



Edit via preference tool of Delta software

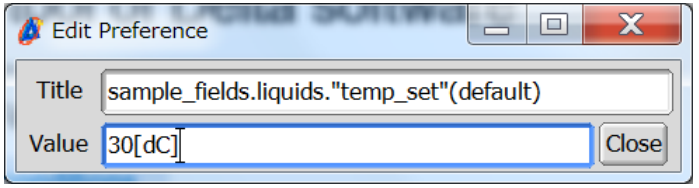
- “local” 1 (C:¥Program Files¥Common Files¥JEOL¥Control 5.2)

Sample conditions

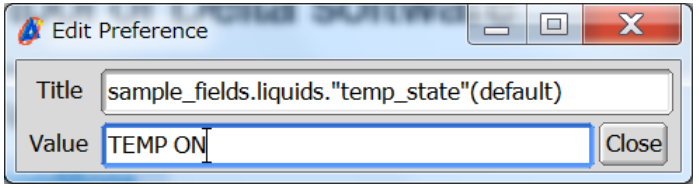
Originally, sample conditions are defined on “sample_fields.jnd” which is in C:¥Program Files¥JEOL¥Control 5.2.0.app¥Contents¥Resources¥global¥configuration.

```
GROUP.GROUP(WIDGET) = "INPUT_BOX"
GROUP.GROUP(CONTAINER_TYPE_INCLUDE) = "NUMBER"

—————————————————————————————————————————————
——
— LIQUIDS
—————————————————————————————————————————————
——

LIQUIDS.TEMP_SET(PRETTY)+PARAMETER.TEMP_SET = "temp_set" —"degrees"
LIQUIDS.TEMP_SET(DEFAULT)     = 25[dC]
LIQUIDS.TEMP_SET(WIDGET)      = "CONSTRAINED_INPUT_BOX"
LIQUIDS.TEMP_SET(ASYNCHRONOUS) = FALSE
LIQUIDS.TEMP_SET(FILTER)      = ""
LIQUIDS.TEMP_SET(AUTOMATIC)   = TRUE

LIQUIDS."SPIN_SET"(PRETTY)+PARAMETER.SPIN_SET = "spin_set" —"spin rate"
LIQUIDS."SPIN_SET"(DEFAULT)     = 15[Hz]
LIQUIDS."SPIN_SET"(WIDGET)      = "CONSTRAINED_INPUT_BOX"
LIQUIDS."SPIN_SET"(ASYNCHRONOUS) = FALSE
LIQUIDS."SPIN_SET"(FILTER)      = ""
LIQUIDS."SPIN_SET"(AUTOMATIC)   = TRUE

LIQUIDS.SPIN_STATE(PRETTY)+PARAMETER.SPIN_STATE = "spin_state" —"spinner"
LIQUIDS.SPIN_STATE(DEFAULT)     = "SPIN ON"
LIQUIDS.SPIN_STATE(WIDGET)      = "SELECT_ENUMERATION"
LIQUIDS.SPIN_STATE(ASYNCHRONOUS) = FALSE
LIQUIDS.SPIN_STATE(FILTER)      = ""
LIQUIDS.SPIN_STATE(AUTOMATIC)   = TRUE
—LIQUIDS.SPIN_STATE(PRETTY) = "spinner"
—LIQUIDS.SPIN_STATE(TYPE)    = "BOOLEAN"
—LIQUIDS.SPIN_STATE(DEFAULT) = TRUE
—LIQUIDS.SPIN_STATE(WIDGET) = "TOGGLE_BUTTON"

LIQUIDS.TEMP_STATE(PRETTY)+PARAMETER.TEMP_STATE = "temp_state"
—"temperature"
LIQUIDS.TEMP_STATE(DEFAULT)     = "TEMP OFF"
LIQUIDS.TEMP_STATE(WIDGET)      = "SELECT_ENUMERATION"
LIQUIDS.TEMP_STATE(ASYNCHRONOUS) = FALSE
LIQUIDS.TEMP_STATE(FILTER)      = ""
LIQUIDS.TEMP_STATE(AUTOMATIC)   = TRUE
```

If I want to set the temperature control with 30 [dC] for all liquid sample as default.



It requires rebooting of Delta software of control.

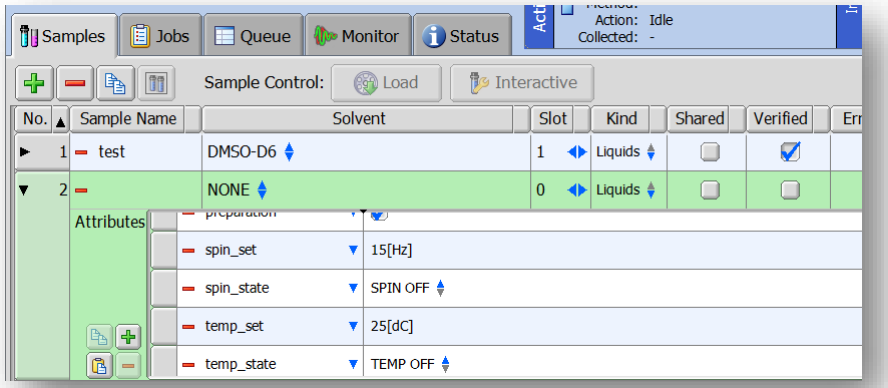


How does it affect?

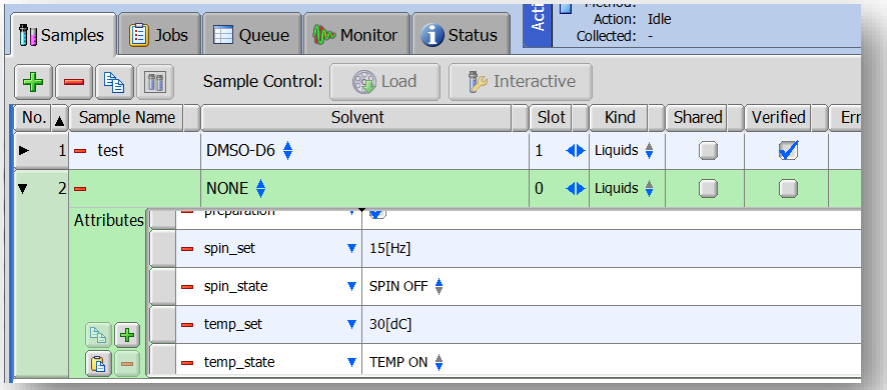
The new “sample_fields.jnv” file was saved in “local”1 folder.

```
— sample_fields
— C:¥Program Files¥Common Files¥JEOL¥Control 5.2¥configuration¥sample_fields.jnv
liquids.spin_state(default) = "SPIN OFF"
liquids.temp_set(default) = 30[dC]
liquids.temp_state(default) = "TEMP ON"
standard."load shims"(automatic) = TRUE
standard."load shims"(default) = "System"
—#Signature 7BF7D06C4A40AFD5402B8CDC79260AA80BE785FD JEOL 10-OCT-2017
17:41:23 GMT 螟乗函髭・
```

Before



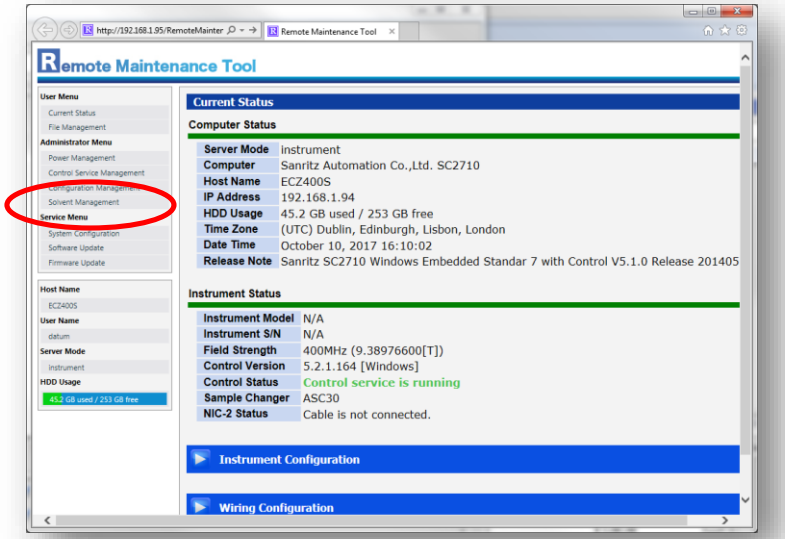
After

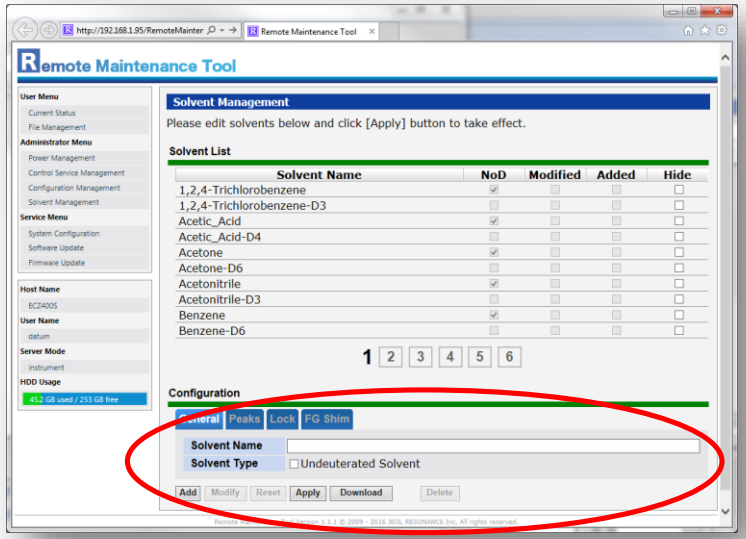


Edit via Remote Maintenance Tool

Solvent information

1. Open the Remote Maintenance Tool (Instrument).
2. Login by console privilege user.
3. Move to “Solvent Management” session.
4. Put in the all information about solvent, like a “Solvent name” and etc.
5. Click the “Add” button.

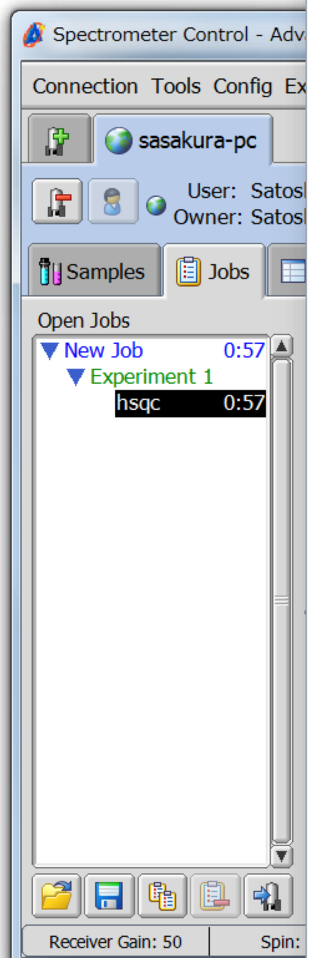




Remote Maintenance Tool

Structure of pulse program

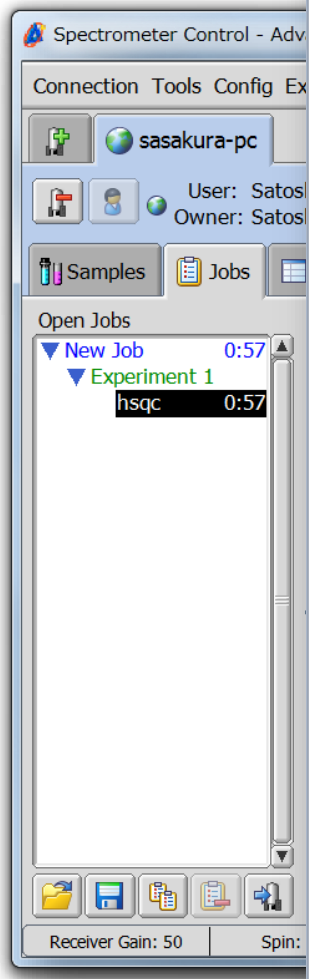
Scrip of Experimental file




```
--
--                                                      --
--                  Experiment Source Code               --
--          Delta NMR Experiment & Machine Control Interface    --
--                                                      --
--                  Copyright (c) 2000 JEOL Ltd              --
--                  All Rights Reserved                 --
--                                                      --
--
-- HELP.eng: absorption pn_hsqc using club with X-decoupling
-- Category: basic, 2D, hsqc, liquids
-- File name : hsqc
--
-- Sequence name :absorption pn_hsqc using club with X-decoupling
--
-- Reference :
-- H.Hu,A.J.Shaka, J.Magn.Reson.,136,54-629(1999)
--
-- V.A.Mandelshtam,H.Hu,A.J.Shaka,Magn.Reson.Chem.,36,S17-S28(1998)
--
-- R.R. Ernst, G. Bodenhausen, A. Wokaun "Principles of Nuclear Magnetic
-- Resonance in One and Two Dimensions" Clarendon Press,
-- Oxford University Press, 1987.
--
-- G.E. Martin, A.S. Zektzer, "Two Dimensional NMR Methods for Establishing
-- NMR Connectivity, VCH, 1988.
--
-- J.K.M Sanders, B Hunter "Modern NMR Spectroscopy, A Guide for Chemists"
-- Oxford University Press, 1987.
--
-- Parameters
-- x_pulse        : 90[deg] obs pulse width
-- x_atn          : attenuator of x_pulse
-- y_pulse        : 90[deg] irr pulse width
-- y_atn          : attenuator of y_pulse
--
--  x_fm_pulse    :  180 deg FM pulse width along x axis
--  x_fm_atn      :  attenuator of x_fm_pulse
--
--  y_fm_pulse    :  180 deg FM pulse width along y axis
--  y_fm_atn      :  attenuator of y_fm_pulse
```

ript

Scrip of Experimental file




```
comment_8 =? "*** Pulse Field Gradient ***";
   grad_selection =? if y_domain = "Carbon13" then "13C = 2.5:1.5:1" else
                     if y_domain = "Nitrogen15" then "15N = 5.94:3.94:1" else
                     if y_domain = "Silicon29" then "29Si = 3.52:1.52:1" else
                     if y_domain = "Phosphorus31" then "31P = 2.24:0.24:1" else
                     "none";

   include "services";
   x_gamma = _get_gamma( x_domain );
   y_gamma = _get_gamma( y_domain );
   temp1   = x_gamma / y_gamma;

   grad_1      => 1[ms], help "duration of grad_1";
   grad_1_amp  => 0.075[T/m], -0.3[T/m] -> 0.3[T/m]:0.0003[T/m], help "amplitude of
grad_1";
   grad_1a_amp =  grad_1_amp/2;
   grad_1b_amp =  -1*grad_1_amp/2;

   grad_2      => grad_1, help "duration of grad_2";
   grad_2_amp  => 0.045[T/m], -0.3[T/m] -> 0.3[T/m]:0.0003[T/m], help "amplitude of
grad_2";
   grad_2a_amp =  -1*grad_2_amp/2;
   grad_2b_amp =  grad_2_amp/2;

   grad_3      => grad_1, help "duration of grad_3";
   grad_3_amp  => (grad_1_amp+grad_2_amp)/temp1, help "amplitude of grad_3";

   grad_shape   => "SINE", fg_shape_names, help "gradient shape";
   grad_recover => 0.1[ms], help "gradient recovery time";

---y_p1_correction =? 360 * ((x_fm_pulse + 1.28*y_pulse+40[us])* y_sweep);

   include "y_dec_param_carbon13";
   include "obs_dante_presat";
   include "obs_presat_time";
   include "tri_presat_homo_dec";
   include "presat_relaxation_delay_calc";
   include "pulse";

   phase_x  = {0};
   phase_y  = {90};
   phase_qd  = {2(0, 180)}.ystep(180%2);
```

ript

.jxi files

By command of “include”, it downloads “.jxi” file from global file (C:¥Program Files¥JEOL¥Control 5.2.0.app¥Contents¥Resources¥global¥experiments).

```
—y_p1_correction =? 360 * ((x_fm_pulse + 1.28*y_pulse+40[us])* y_sweep);

include "y_dec_param_carbon13";
include "obs_dante_presat";
include "obs_presat_time";
include "tri_presat_homo_dec";
include "presat_relaxation_delay_calc";
include "pulse";
```

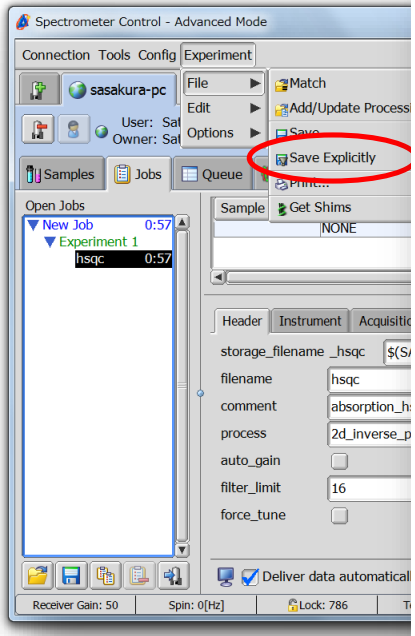
```
—y_dec_param_carbon13.jxi
—
comment_102 =? "*** irr_decoupling ***";

irr_decoupling => TRUE, help "select TRUE or FALSE for decoupling or non_decoupling";

when irr_decoupling do
  irr_noise => "MPF8",("CW","DIPS12","WAUGH","WALTZ","GARP",
               "MPF5","MPF6","MPF7","MPF8","MPF9","MPF10",
               "WURST_30","WURST_40","WURST_50","WURST_70"), help "decoupler
noise modulation";
end when;

include "y_dec_param";
```

y_dec_param_carbon13.jxi

It is necessary to put the .jxi file into the same folder with experimental file in order to include it into experimental file.

Develop the include file into experimental file

When you want to develop the parameters which are defined in include file into experimental file, it is possible by following process.




```
    grad_3_amp              => (grad_1_amp + grad_2_amp) / temp1, help "amplitude of grad_
3";
    grad_shape              => "SINE", fg_shape_names, help "gradient shape";
    grad_recover            => 0.1[ms], help "gradient recovery time";
    comment_102             =? "*** irr_decoupling ***";
    irr_decoupling          => TRUE, help "select TRUE or FALSE for decoupling or
non_decoupling";
    when irr_decoupling do
        irr_noise               => "MPF8", ("CW", "DIPS12", "WAUGH", "WALTZ", "GARP",
"MPF5", "MPF6", "MPF7", "MPF8", "MPF9", "MPF10", "WURST_30", "WURST_40",
"WURST_50", "WURST_70"), help "decoupler noise modulation";
    end when;
    irr_domain              = y_domain;
    when irr_decoupling do
        irr_wurst               = if irr_noise = "WURST_30"
                                then TRUE
                                else if irr_noise = "WURST_40"
                                then TRUE
                                else if irr_noise = "WURST_50"
                                then TRUE
                                else if irr_noise = "WURST_70"
                                then TRUE
                                else FALSE, help "Select TRUE or FALSE for adiabatic
decoupling";
    end when;
    when irr_wurst do
        irr_wurst_b1_default    =? if y_domain = "Fluorine19"
                                then 5[kHz]
                                else 2.5[kHz];
        irr_wurst_b1            => irr_wurst_b1_default;
        irr_wurst_pwidth        = 1 / (4 * irr_wurst_b1);
        irr_dec_merit_factor_value = if x_domain = "Carbon13"
                                then if irr_domain = "Fluorine19"
                                    then 0.7
                                    else 0.9
                                else 0.9;
```

Summary

Structure of operation PC

Operation PC

Console PC

Local folder 1 (account)

- automation — Automation script
- experiments — Experimental file
- process_lists — Process list
- Etc…

Local folder 3 (common)

.cfg file

Global folder

- configuration — Default conditions
- process_lists — Process list
- Etc…

Structure of console PC

Operation PC

1U Server

Data server

Console PC

Local folder

- automation — Automation script
- configuration — Sample conditions, Solvent information
- experiments — Experimental file
- modulations — Noise source, Shaped pulse, FG shaped pulse
- process_lists — Process list
- users
  - console
  - delta
  - Satoshi — Automation script, Process list, Experimental file
  - Etc…
- Etc…

Global folder

- automation — Automation script
- configuration — Sample conditions, Solvent information
- experiments — Experimental file
- modulations — Noise source, Shaped pulse, FG shaped pulse
- process_lists — Process list
- Etc…

Summary

By understanding the file folder structure of the and its priority, it is possible to customize the environment for each account.

Thank you for your kind attention

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