

# **Quantum Nuclear Magnetic Resonance Spectrometer**

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## **SpinStudioJ Installation Manual**

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# Chapter 1 Overview

## 1.1 Introduction

SpinStudioJ is a professional software package for NMR data acquisition and processing in the products of Zhongke-niujin. The software contains two programs, namely the interface program SpinStudioJ and the experiment control program nmrexpctrl. This document will give a detailed introduction to the installation and uninstallation of these two programs, obtaining the license, and software configuration.

## 1.2 Software version and Conventions

The name of the released software version contains information such as the software name and version number, separated by "\_". For example, SpinStudioJ-1.6.7, where 1.6.7 represents the version number. This manual is written for the software SpinStudioJ\_1.6.7.

In order to make the text in the manual more clear and easier to be understood by users, following conventions are used in this manual:

1. Commands to be entered are all in ***bold italic***, e.g. ***syscf***.
2. Menus, buttons are all in **bold**, e.g. **File, Acquire**.

## 1.3 Hardware and software requirements

### 1.3.1 Supported operating system

Support for Windows 7 and Windows 10 with 64-bit operating systems, this article mainly introduces the operation in Windows 7, the operation in Windows 10 is slightly different from Windows 7.

### 1.3.2 Hardware Environment

Computer: PC and compatible;

CPU: 2.0 GHz or higher;

RAM: 16G or more;

Monitor: Recommend 1600×900 or higher resolution, 24-bit color or more;

Other peripherals: Standard keyboard, mouse, serial ports, network interface;

Software distribution media: CD-ROM.

### 1.3.3 Supported spectrometer

SpinStudioJ\_1.6.7 supports BIXI-I, Quantum-I and Quantum-I<sup>plus</sup>, and needs to be configured according to different hardware.

### 1.3.4 Configuration before installation

1. Set to disable standby. Right-click on the computer desktop and select **Personalization> Screen Saver> Change Power Settings> Change Computer Sleep Time** and change it to "Never", as shown in Figure 1.1.

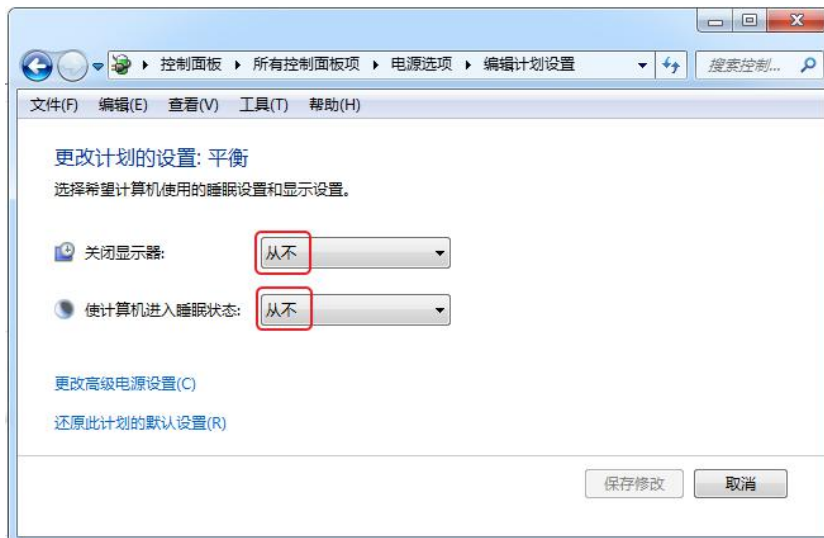


Figure 1.1 Choose installation language

2. Check the configuration values of temperature, auto sample changer, level

gauge and other data in *emc.conf*. The specific method is as follows.

Open **Fterm**, click the **F link** in the menu bar, and choose **open the address book**, as shown in Figure 1.2.



Figure 1.2 Menu Bar of Fterm

Select the address of the master and click **Connect**, as shown in Figure 1.3.



Figure 1.3 Connect master

After entering the main interface of the master, click the Enter key, type *fsrw* after the # character, and the "file system property has been set to readwrite" pops up, and the readwrite mode is successfully changed. Then type *vi /etc/emc.conf* to open the emc configuration file, as shown in Figure 1.4.

```
[root@master_21 ~]# cd /home/nmr/EMC
[root@master_21 EMC]# fsw
file system property has been set to readwrite
[root@master_21 EMC]# vi /etc/emc.conf
```

Figure 1.4 Change to read-write mode

After the interface is refreshed, click the letter E on the keyboard to enter the editable mode, as shown in Figure 1.5.

```
E325: ATTENTION
Found a swap file by the name "/etc/.emc.conf.swp"
  owned by: root   dated: Wed Jan 22 16:33:31 2014
  file name: /etc/emc.conf
  modified: no
  user name: root  host name: master_21
  process ID: 3661 (still running)
While opening file "/etc/emc.conf"
  dated: Tue Jun 9 14:50:20 2020
  NEWER than swap file!

(1) Another program may be editing the same file.
    If this is the case, be careful not to end up with two
    different instances of the same file when making changes.
    Quit, or continue with caution.

(2) An edit session for this file crashed.
    If this is the case, use ":recover" or "vim -r /etc/emc.conf"
    to recover the changes (see ":help recovery").
    If you did this already, delete the swap file "/etc/.emc.conf.swp"
    to avoid this message.

Swap file "/etc/.emc.conf.swp" already exists!
[O]pen Read-Only, (E)dit anyway, (R)ecover, (Q)uit, (A)bort:█
```

Figure 1.5 Enter edit mode

At this time, "-- INSERT --" appears at the bottom, as shown in Figure 1.6.

```

#only for MASTER
[MASTER]
#lock data send gap - unit:ms
LockGapLine1=100
LockGapLine2=200
LockGapLine3=400
LockGapLine4=1000

#Temperature data send gap - unit:ms
TempGapLine = 1000
#heating wait time,32 bits value
TempRadCounter = 15000
#ignore heating over temp
IgnoreTempProtect = 0
#Spin rate data send gap - unit:ms
SpinRateGateLine = 500
#use 2:0,0me Spinner and Varian spinner,4:Bruker Spinner
SpinRatioCtrl = 4
#Tune data send gap - unit:ms
TuneGapLine=100
#tune source:1:BB transmitter,2:BB transmitter
TuneXnrMo=1

#Sample down air pressure, 12bits value
SampleDownPressure = 5000
#close gas counter,set it at the end of sample down
SampleDownCounter = 200

##High temperature protect value(degree Celsius)
TempProtectVoltage = 150

##High temperature precision, SpinStudioJ only support 1
TempHighPrecision=1

#Temperature data send to periphery: 0--SpinStudioJ, 1--SpinStudio
TempDataToPeriphery=0

#Mixer Channel switch by frequency range - unit:MHz
HFreqLowest = 230
DFreqLowest = 70
DFreqHighest = 80

#only for XMTR
[XMTR]
LowBand = 100

#1:pts0
#2:pts1
-- INSERT --

```

Figure 1.6 Enter parameter modification state

Find the four relevant parameters and check whether the values are correct. If it needs to be modified, use the arrow keys on the keyboard to move the cursor to the parameter value position for modification.

- ① TempHighPrecision = 1, which means that the temperature uses high precision. 1 means high precision, 0 means non-high precision, SpinStudioJ only supports high precision.
- ② TempDataToPeriphery = 0, indicating that the temperature is not sent through the peripheral thread. SpinStudioJ needs to be set to 0 and SpinStudio is set to 1.
- ③ HeN2DataToPeriphery=0, indicating that the level gauge data is not sent through the peripheral thread. SpinStudioJ needs to be set to 0 and SpinStudio is set to 1.
- ④ ASCDataToPeriphery=0, indicating that the auto sample changer data is not sent through the peripheral thread. SpinStudioJ needs to be set to 0 and SpinStudio is set to 1.

```

#High temperature precision, SpinStudioJ only support 1
TempHighPrecision=1

#Temperature data send to periphery: 0--SpinStudioJ, 1--SpinStudio
TempDataToPeriphery=0

[PERIPHERY]
#Send Level Meter Data to: 0--SpinStudioJ, 1--SpinStudio
HeN2DataToPeriphery=0
#Send Auto sample changer Data to: 0--SpinStudioJ, 1--SpinStudio
ASCDDataToPeriphery=0

```

Figure 1.7 Parameters to be checked

After all modifications are completed, press **Esc** on the keyboard to exit the parameter modification state. Regardless of the cursor position, directly enter **:wq** to save this modification. The word "...written" will pop up at this time. Type **fsro** and reset it to read-only mode, as shown in Figure 1.8. If you find that no parameters need to be modified after checking, you can enter: **q!** to exit the current mode without saving any changes, and then type **fsro** to set it to read-only mode.

```

"/etc/emc.conf" [dos] 143L, 2983C written
[root@master_21 ~]# fsro
file system property has been set to readonly
[root@master_21 ~]#

```

Figure 1.8 Set to read-only mode

## Chapter 2 Install SpinStudioJ

SpinStudioJ contains two programs, the interface layer and the experimental control layer. The installation process of the two programs will be introduced below.

### 2.1 Install SpinStudioJ

1. Insert the software CD into the workstation's CD-ROM drive, open the SpinStudioJ folder, and double-click the interface program installation file SpinStudioJ\_\*.exe, and the installation language selection dialog will pop up (Figure 2.1). There are two options: English and Chinese (Simplified). In this manual, English is selected as an example.



Figure 2.1 Choose installation language

2. After selecting the language, click **OK**, and a dialog as shown in Figure 2.2 will pop up. Click **Next** to start the installation.



Figure 2.2 Start installation

3. Please read the software license agreement and related terms of use carefully, check "I accept..." and click **Next**.

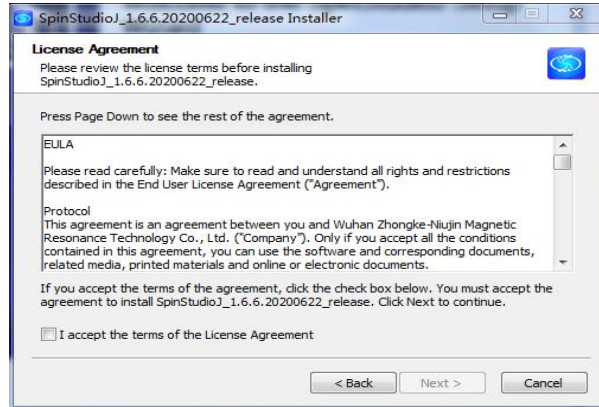


Figure 2.3 License agreement

4. Select the target path for installation. Generally use the default path, as shown in Figure 2.4, and then click **Next**. The installation path can only be in English, and there can be no space characters. If the conditions are not met, the next step cannot be performed.

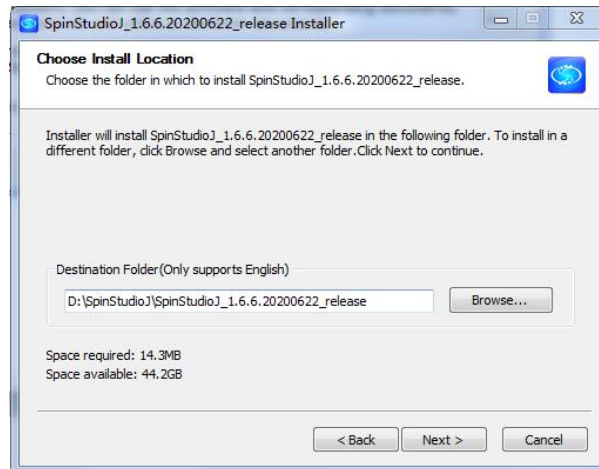


Figure 2.4 Installation path

5. Set the folder name of SpinStudioJ in the start menu bar of the computer, and click **Install** without modifying it.

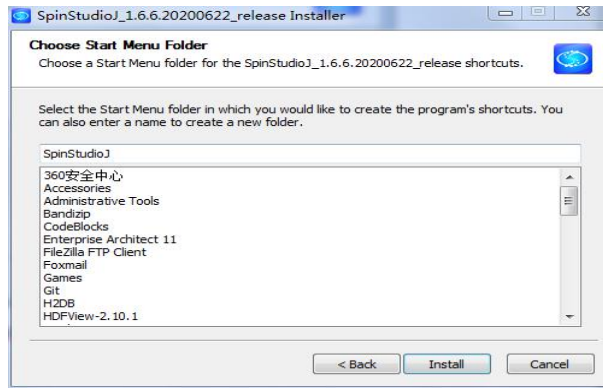


Figure 2.5 Set the folder name of SpinStudioJ in the start menu bar of the computer

6. The installation process takes 2~3 minutes (Figure 2.6). After the installation is complete, "Open release\_notes" is checked by default (Figure 2.7), and clicking Finish will automatically open the release notes. If unchecked, after the installation is complete, you need to go to the installation directory to view the release notes.

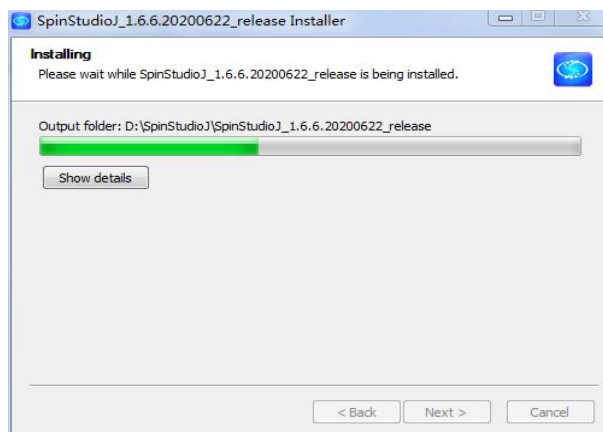


Figure 2.6 Installing

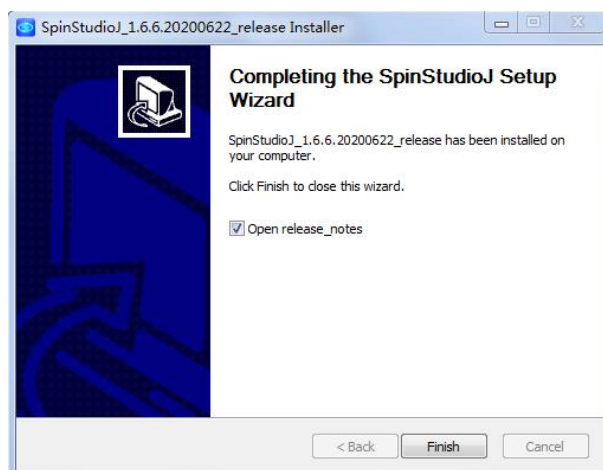


Figure 2.7 Finish installation

7. After the installation is complete, release\_notes will pop up (Figure 2.8). So far, the SpinStudioJ interface package is installed, and the SpinStudioJ shortcut icon is generated on the desktop.

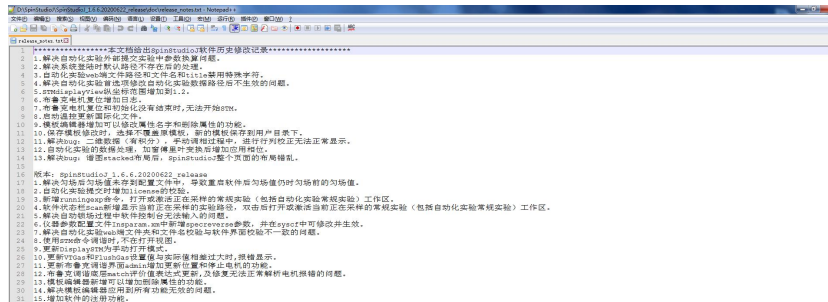


Figure 2.8 Release notes

## 2.2 Install nmrexpctrl

1. Return to the software folder in the CD, double-click nmrexpctrl\_\*.exe to install the experiment control program, the process is the same as the interface program installation. The first is to select the installation language, also take English as an example, as shown in Figure 2.9.



Figure 2.9 Choose installation language

2. After selecting the language, click **OK**, and a dialog as shown in Figure 2.10 will pop up. Click **Next** to start the installation.



Figure 2.10 Start installation

3. Please read the software license agreement and related terms of use carefully, check "I accept..." and click **Next**.



Figure 2.11 License agreement

4. Select the installation directory. If the default installation directory is not modified when the interface program is installed, click **Next** directly; if the installation directory of the interface program is changed, you must ensure that the two are in the same directory.

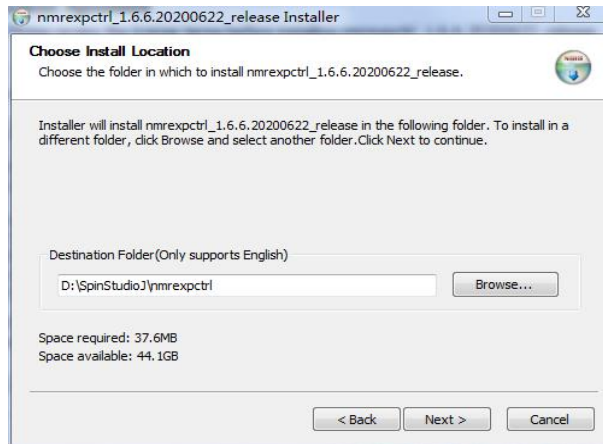


Figure 2.12 Installation path

5. Wait for the installation to complete, click **Finish** to complete the installation.

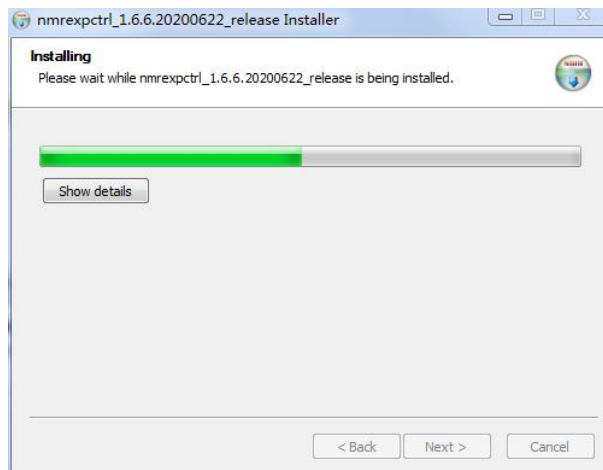


Figure 2.13 Installing

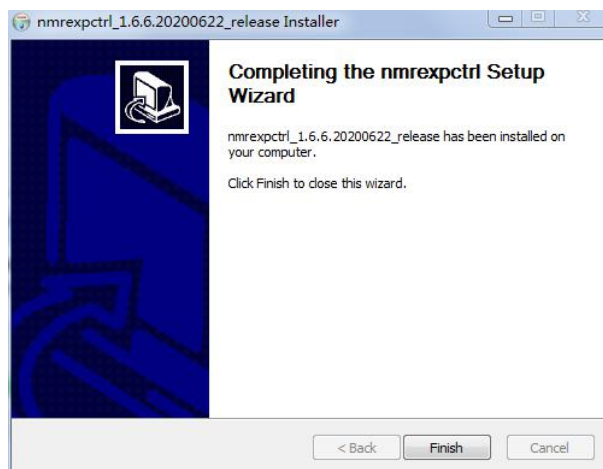


Figure 2.14 Finish installation

6. After the installation is complete, return to the desktop, double-click the shortcut icon to open the software (Figure 2.15).



Figure 2.15 Desktop shortcut

## Chapter 3 SpinStudioJ License

### 3.1 Register in SpinStudioJ

After SpinStudioJ is installed, double-click the desktop shortcut to open SpinStudioJ software. In the main menu(Figure 3.1), click **Help> Register**, and the software registration dialog box will pop up, as shown in Figure 3.2.

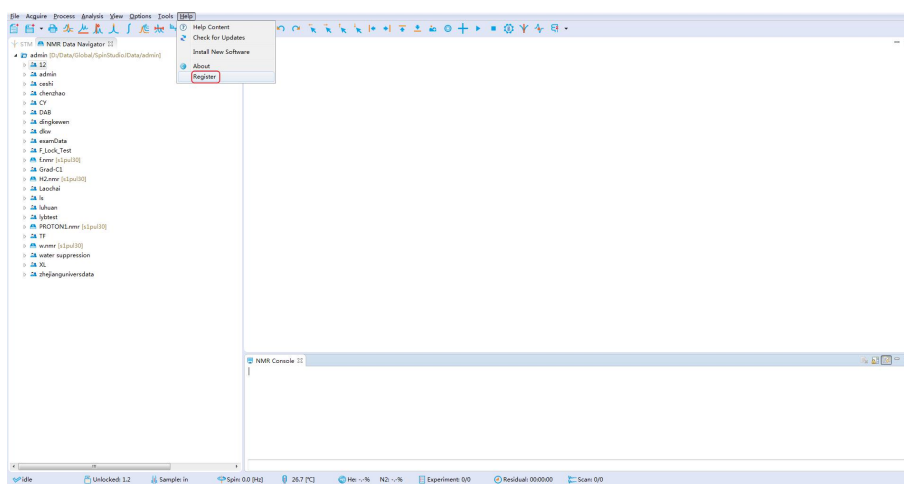


Figure 3.1 main interface of SpinStudioJ

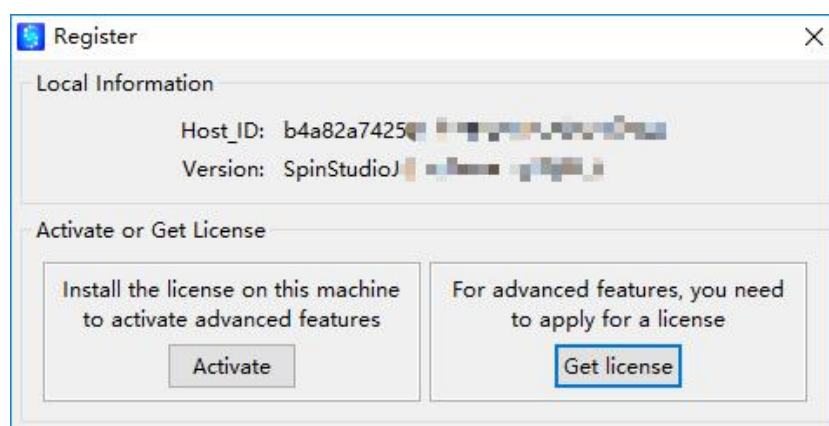


Figure 3.2 Registration dialog

Click **Get license** to automatically go to the registration page, as shown in Figure 3.3. The Host\_ID and Version in the webpage are the physical address of the

workstation and the current software version that has been obtained automatically. After filling in other relevant information, click **Submit** to complete the application.

SpinStudioJ —NMR software based on plug-in architecture

To get the license  
Please! Fill in the form

Salutation \*  
Please select...

Name \*  
Surname \*

Email \*  
Phone \*  
Organization \*

Sector \*  
Please select...

Market \*  
Please select...

Country \*  
Please select...

Version \*  
spinstudioj\_1.6.7.20200703\_r

Please, To check the Module

Basic Module

Advanced Module (the Advance Module is not free,and the staff will contact you.)

Your license needs Host ID to generate

Host ID\*  
b4e82a742541268a4dfdaae206663ad

Yes, I accept the SpinStudioJ's policy\*

SUBMIT

Figure 3.3 Registration page

If you submit it without filling in all the required fields, a pop-up prompt will appear (Figure 3.4). Click **OK** and continue to fill in.

localhost:8080 显示  
Please You have Required field!

确定

Salutation \* Required field\*  
Please select...

Name \* Required field\*  
Surname \*

Email \* Required field\*  
Phone \* Required field\*  
Organization \*

Sector \* Required field\*  
Please select...

Market \* Required field\*  
Please select...

Country \* Required field\*  
Please select...

Version \* Required field\*  
Please select...

Please, To check the Module

Basic Module

Advanced Module (the Advance Module is not free,and the staff will contact you.)

Your license needs Host ID to generate

Host ID \* Required field\*  
Please select...

Yes, I accept the SpinStudioJ's policy\* [Uncheck the policy\\*](#)

SUBMIT

Contact  
•Email: linzao@qone-inst.com  
•Tel: +86-027-81773999  
•Address: No. 128 Guanggu 7th Road, East Lake High-Technology Zone, Wuhan, Hubei, China

Figure 3.4 registration failed

After submitting the application, you will receive the license file by email. Copy it to the workstation, open the dialog shown in Figure 3.2 again, and click **Activate** to

select the license file. After activation, a successful registration dialog will pop up (Figure 3.5). Click **OK**, and the registration dialog is updated to the state shown in Figure 3.6.

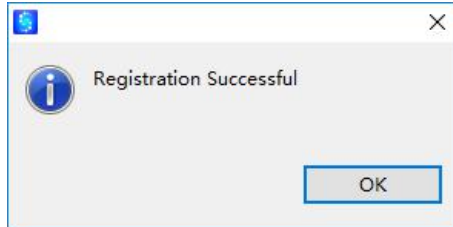


Figure 3.5 Successful registration dialog

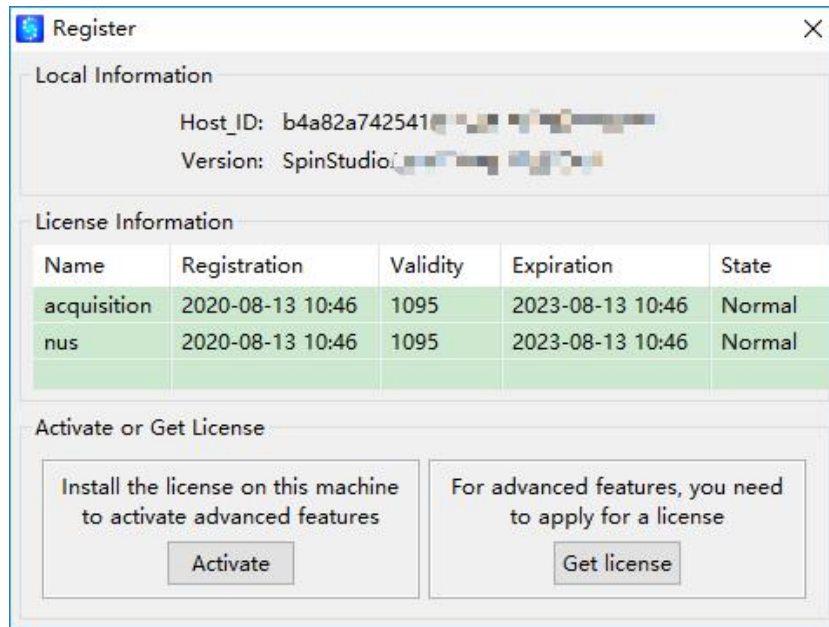


Figure 3.6 Successful registration interface

## 3.2 Website registration

You can also register through the website, the registration website is [www.spinstudioj.net/license/register.do](http://www.spinstudioj.net/license/register.do). Note that you need to fill in the Host\_ID of the workstation and select the correct software version. The other processes are the same as the activation from SpinStudioJ.

## Chapter 4 Installation of plug-ins

In the main menu bar, click **Help** to open the drop-down menu, then click **Install New Software**, to pop-up a dialog.

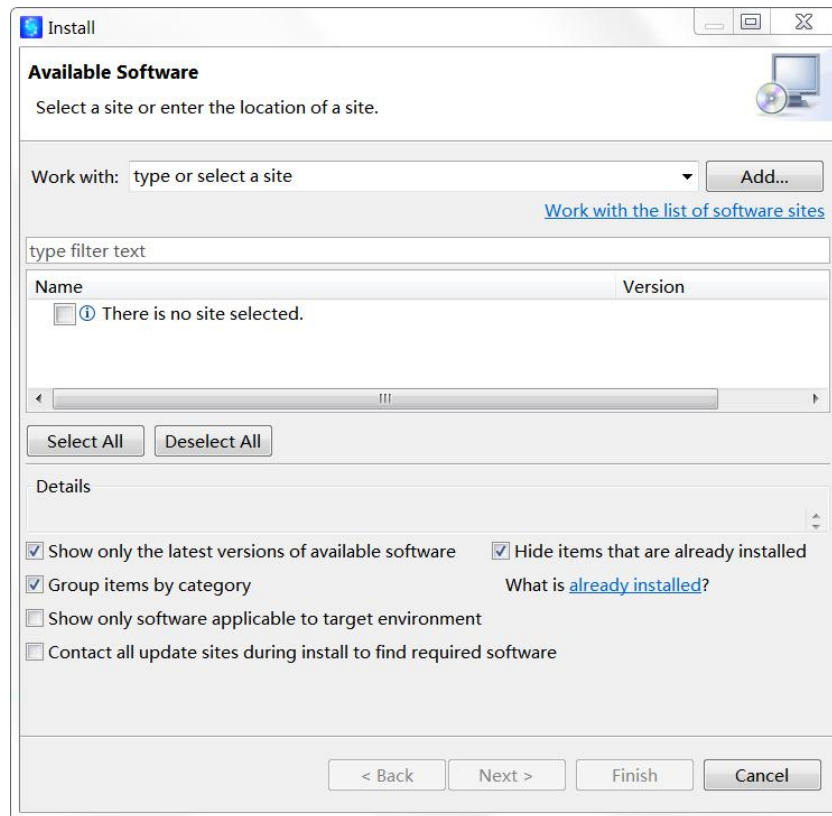


Figure 4.1 Installation wizard dialog

1. Click the hyperlink Work with the list of software sites below **Add** button to open a dialog box (Figure 4.2):

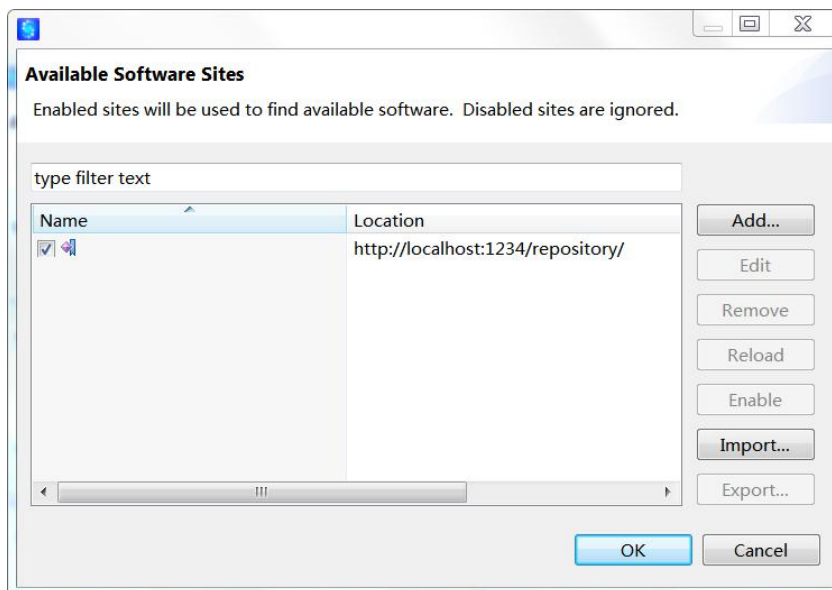


Figure 4.2 Plugin address management dialog

2. Click **Add** in Figure 4.2 to open a new box (Figure 4.3), then click **Local** to find the local directory where plug-ins are located (e.g. F:/Git/Features/repository), and click **OK** to return to the above dialog box (Figure 4.4).

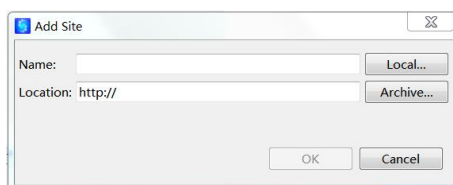


Figure 4.3 Add plugin address dialog

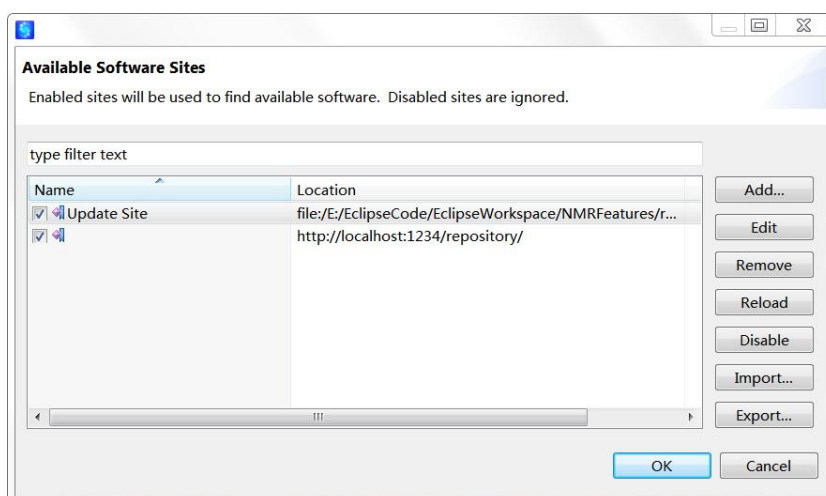


Figure 4.4 Plugin address management dialog

Click **OK** to return to the initial dialog box (Figure 4.1), then open the drop-down menu right to **Work with**, select the added directory, a list of plug-ins will be displayed (Figure 4.5).

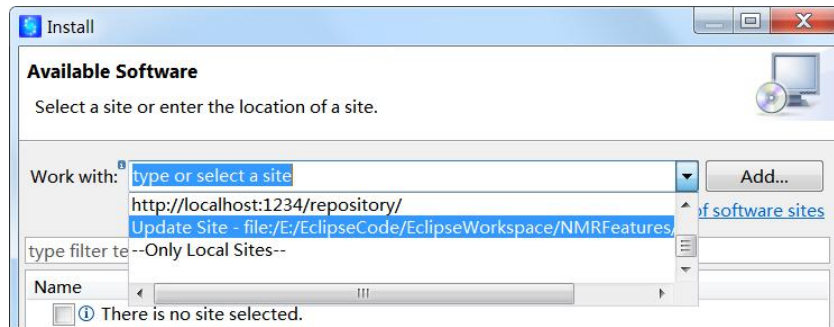


Figure 4.5 Installation dialog

As shown in Figure 4.6, if the path is blank or the updated features are not displayed, uncheck the “Group items by category” and the updated features should be displayed.

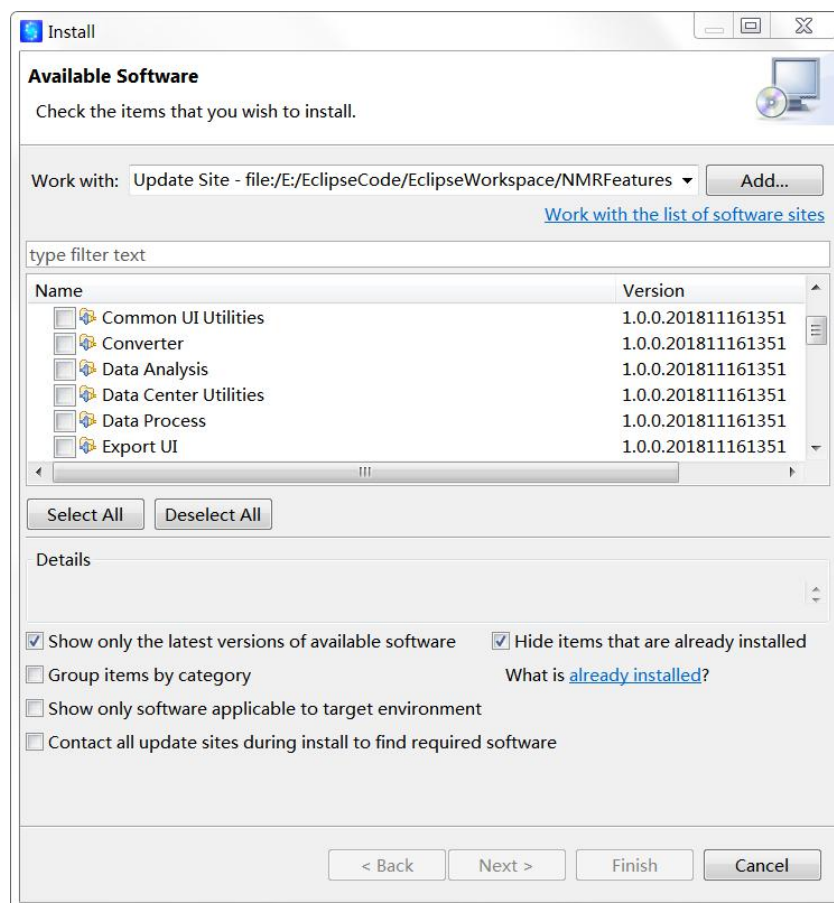


Figure 4.6 Show updated features window

Click **Select All**→**Next**→**Finish**, then click **OK**, **Yes** according to the hint to restart SpinStudioJ.

## Chapter 5 System Configuration

After the software is started, enter the *syscf* command in the software command line to pop up the password verification dialog (Figure 5.1).



Figure 5.1 System configuration password check

Only the system administrator has the right to configure the system. Therefore, only the system administrator password can be used to configure the system. The initial password is “zhongkeMR”, and the administrator can modify it. After the password verification is passed, the system configuration directory is entered, including “Component”, “Automation”, and “Others”, as shown in Figure 5.2.

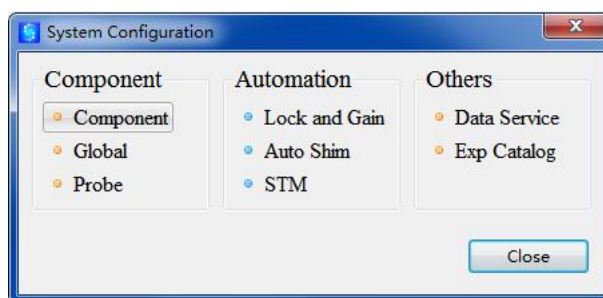


Figure 5.2 System configuration directory

### 5.1 Component

Component consists of three parts: ① Component: parameters related to each component of the system, such magnet, RF system, console, Autosampler; ② Global: global and fundamental parameters; ③ Probe: probe specific parameters.

## 5.1.1 Component

### 1. Basic parameters

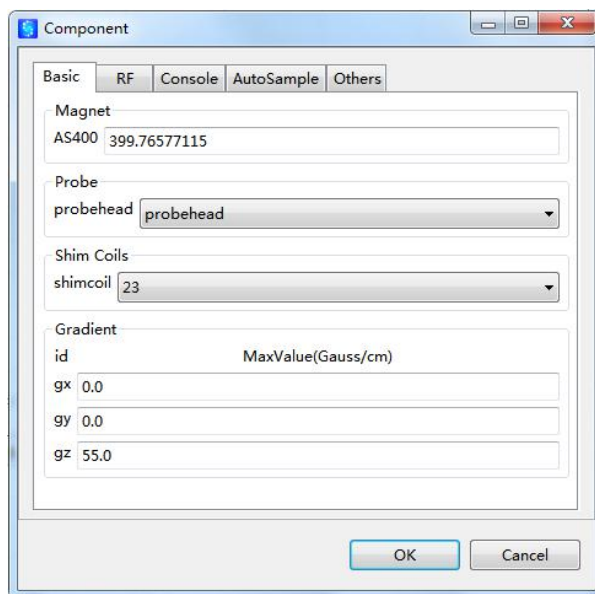


Figure 5.3 Basic configuration

**Magnet:** Magnet model.

**Probe:** File name corresponding to the specific probe. The options are based on the existing files in the directory for system configuration, which were created by engineer before delivering.

**Shim coils:** Number of shim coils, choose according to the system, e.g., 23 for 400MHz and 40 for 600MHz.

**Gradient:** The gradient field strength of the probe in x, y, z directions, the unit is Gauss/cm. Generally, the probe only has a gradient in the z direction, and the engineer will fill in the value after testing the gradient field strength.

### 2. RF parameters

This part is the configuration of the RF power amplifier and preamplifier, as shown in Figure 5.4.

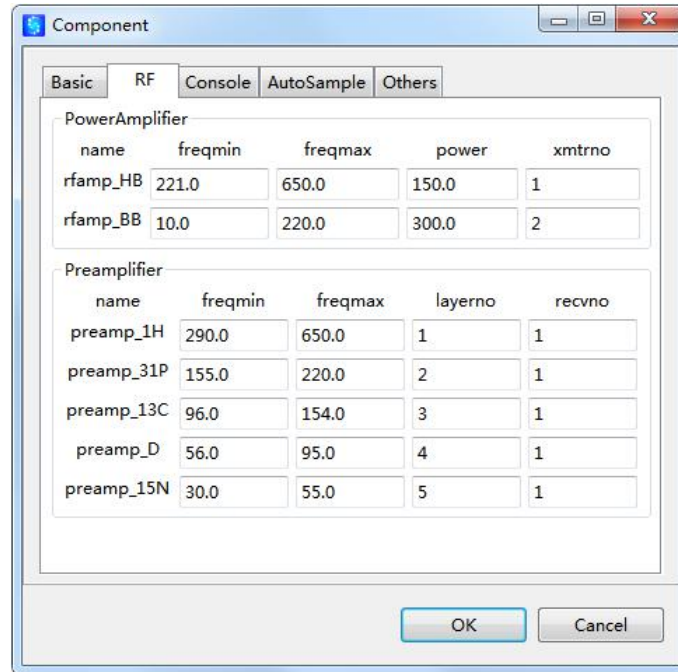


Figure 5.4 RF configuration

**PowerAmplifier:** RF power amplifier configuration information. Set the frequency range (MHz) of the high-band power amplifier (rfamp\_HB) and broadband power amplifier (rfamp\_BB). Set the minimum frequency (freqmin), maximum frequency (freqmax), maximum power (W), and transmitter number (xmtrno) of the power amplifier respectively.

**Preamplifier:** Preamplifier configuration information. Configure the frequency range of the preamplifier of each layer, including the lowest frequency (freqmin) and the highest frequency (freqmax) (MHz), and the corresponding preamplifier layer number (layerno) and transmitter number (recvno).

Generally, use the default frequency range in Figure 5.4. If there are special configurations, such as two high-band power amplifiers or two broadband power amplifiers, engineers need to edit the configuration in the software directory `nmrexpctrl\system\config\components`.

### 3. Console parameter

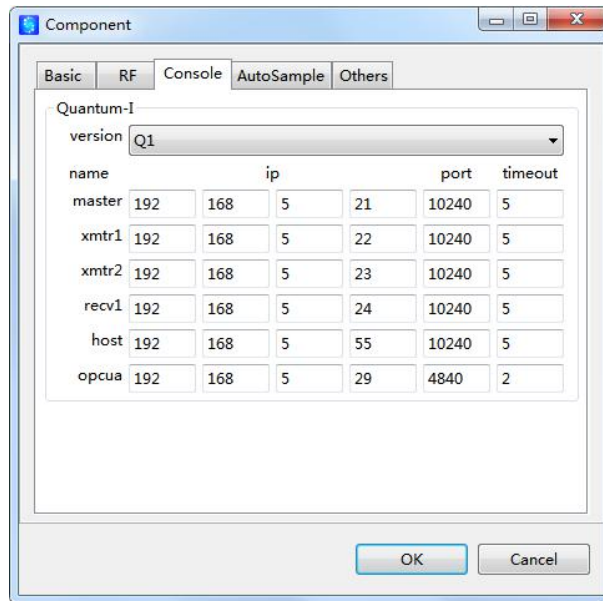


Figure 5.5 Console configuration

This section will set the console model and the network parameters of each main component.

Version represents the console model. Q1 means the first generation console (discontinued), Q1P means the upgraded version of the first generation console (in mass production), both of which need to configure the IP address and port number corresponding to master, xmtr1, xmtr2 and recv1; Q2 Indicates that the second generation console (under development) does not need to configure the IP address and port number corresponding to master, xmtr1, xmtr2, and recv1. But all console models need to configure the IP address and port number of the host and OPCUA.

The default IP addresses of master computer, first and second transmitters, receiver and local host are sequentially set from 192.168.5.21 to 192.168.5.24, while their port number are all set to 10240.

The default IP address of local host is 192.168.5.55, and port number 10240.

The default IP address of OPCUA is 192.168.5.29 and port number is 4840. OPC UA (OPC Unified Architecture) is a service based, cross-platform communication solution. Computer can send instructions to hardware through OPCUA.

Timeout is used to define the response time (s) from IP address. The connection will be considered failed without response over this time period. Use default values.

#### 4. Auto Sample changer parameter

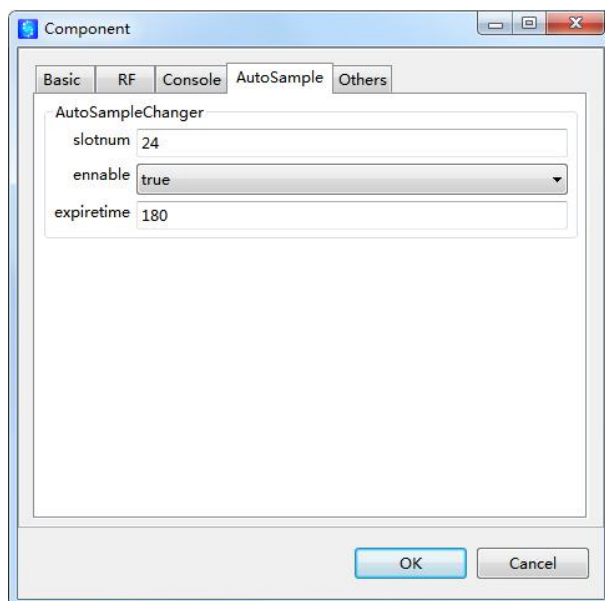


Figure 5.6 Auto Sample Change configuration

Set the slot number of sample changer, only two selections for **slotnum**, i.e., 24 or 60. You can also decide if to use it by setting the value of **enable** to true or false.

**expiretime**: Time used for the judgement of sample changer status. If the sample changer dose not respond to an instruction over this time period, an error message will be popped up.

#### 5. Others parameters

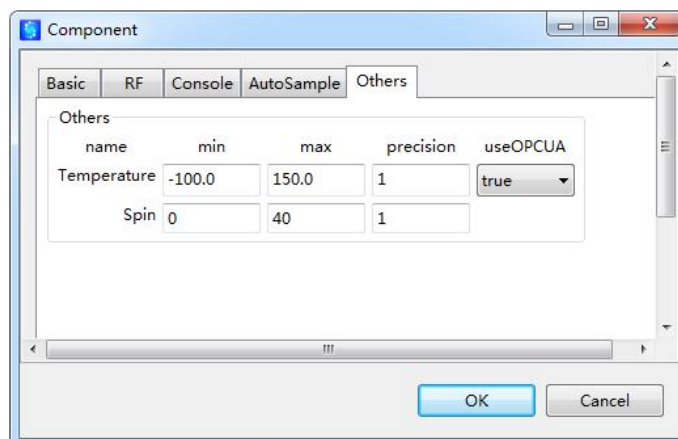


Figure 5.7 Others configuration in Component

**temperature:** VT control parameters. Set the minimum temperature (min) and maximum temperature (max) supported by the probe, as well as the temperature control precision (decimal numbers). useOPCUA indicates whether to use OPCUA for temperature control, true for yes and false for no.

**spin:** Sample rotating parameter. Set the minimum and maximum spinning rates allowed by the console, and the spinning precision (decimal numbers).

### 5.1.2 Global Parameters

(1) **Global:**

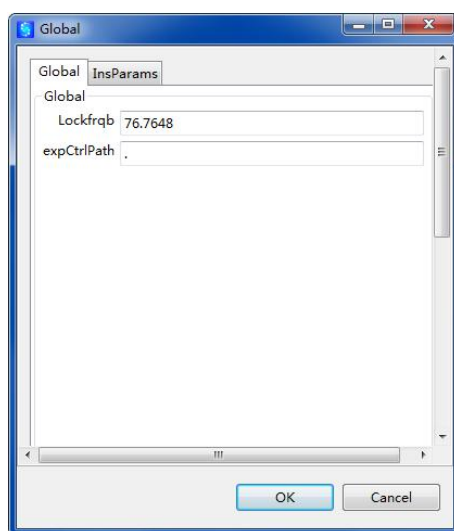


Figure 5.8 Global configuration

**Lockfrqb:** The base lock field frequency.

**expCtrlPath:** The relative path of the experiment control program and the interface program. "." means that they are at the same level of the folder in the workstation. Modifications will cause the software to fail to start normally.

(2) **InsParams:**

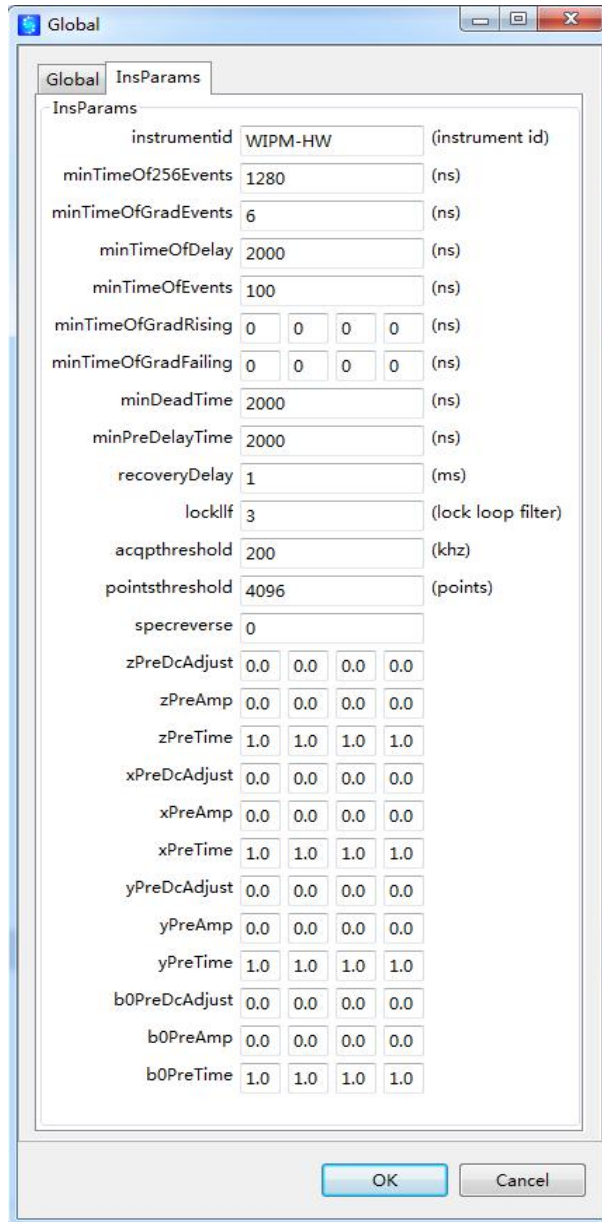


Figure 5.9 Instrument parameter configuration

Basic parameters about the time events and others of the instrument, set by engineer before delivering and not allowed to change.

### 5.1.3 Probe related parameters

#### 1. Main:

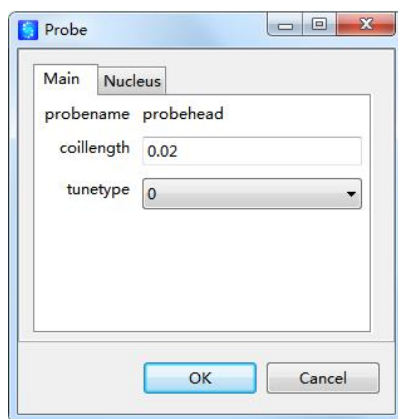


Figure 5.10 Probe configuration

Basic parameters for probe setting.

**probename:** The name of currently used probe, corresponding to the probe filename in **Basic**. All parameters of the probe are retrieved from the file with the same name.

**coilength:** The length of RF coil of specified probe.

**tunetype:** The tuning type of the probe. 0 for manual and 1 for automatic.

## 2. Nucleus:

Configure the pulse widths for observe, decoupling and spinlock and corresponding powers for each nucleus (Figure 5.11).

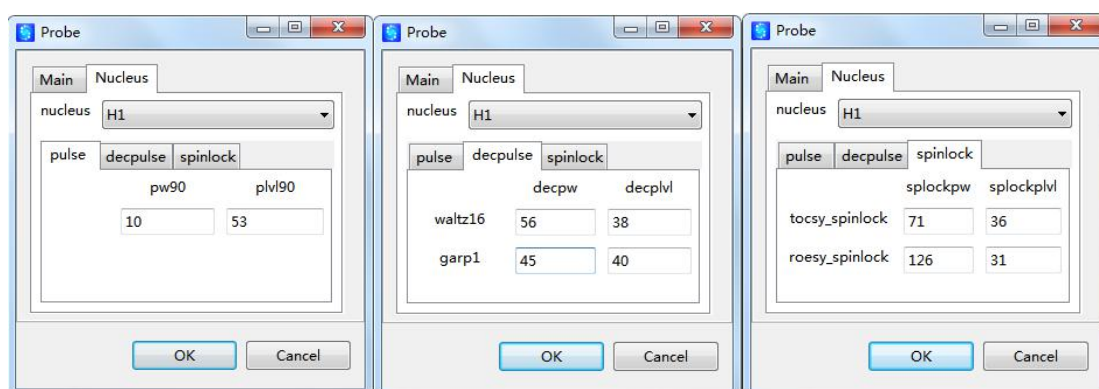


Figure 5.11 Nuclear related configuration

## 5.2 Automation

Configuration for Automation experiments (Figure 5.12), which includes three

components ①Lock and Gain; ②Auto Shim; ③STM.

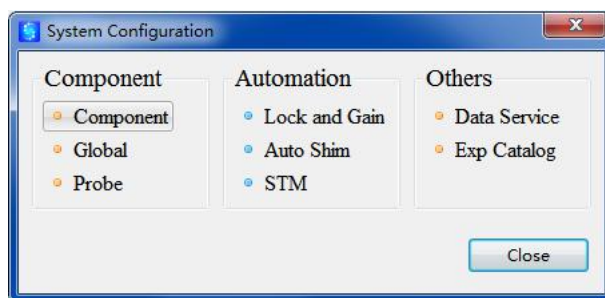


Figure 5.12 System configuration directory

## 5.2.1 Lock and Gain

### 1. autoGain

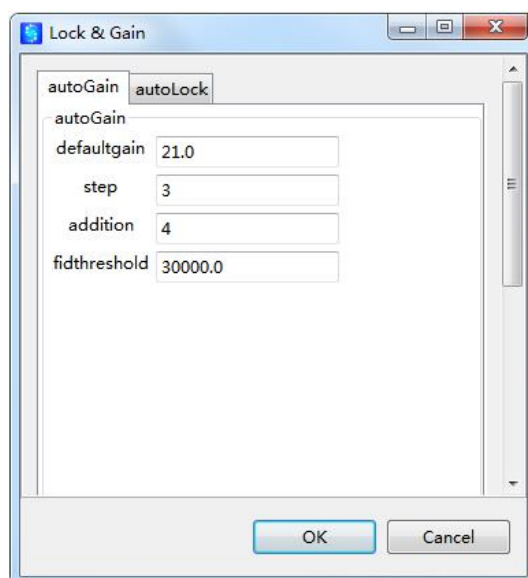


Figure 5.13 Automatic gain parameter configuration

**defaultgain:** Initial value for gain calculation, with a default value of 21;

**step:** Increment for gain adjustment, with a default value of 3.

**addition:** Value to be deducted from calculated gain value, set according to specific instrument (2~10), with a default value of 3.

**fidthreshold:** Maximum FID intensity used for automatic gain calculation. The maximum value for FID is 32768, but 30000 is recommended.

## 2. autoLock

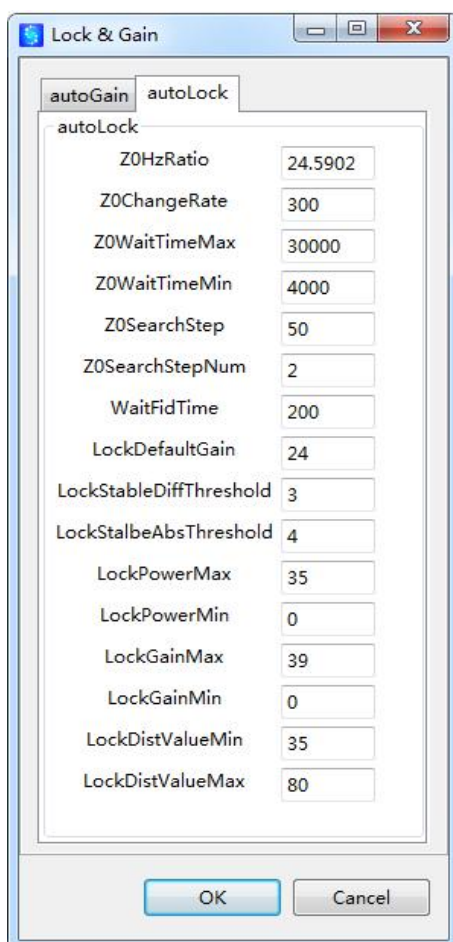


Figure 5.14 Automatic lock parameter configuration

Z0HzRatio: Conversion value between Z0 and Hz, set by engineer.

Z0ChangeRate: Change rate of Z0, set by engineer.

Z0WaitTimeMax: Maximum time for Z0 stabilization, set by engineer.

Z0WaitTimeMin: Minimum time for Z0 stabilization, default value being 4000.

Z0SearchStep: Increment for Z0 searching, default value being 50.

Z0SearchStepNum: Steps for Z0 searching, default value being 2. Used to determine whether the correct Z0 is searched in right way.

WaitFidTime: Waiting time for acquiring FID (ms), default value being 200.

LockDefaultGain: Value for lock gain (dB), using 21 by default.

LockStableDiffThreshold: Threshold of lock level fluctuation, using 3 by default.

The lock is defined as stable when fluctuation is smaller than this value.

LockStalbeAbsThreshold: Absolute fluctuation threshold for stable lock, using 3 be default.

LockPowerMax: Maximum lock power (dB), using 35 by default.

LockPowerMin: Minimum lock power (dB), using 0 by default.

LockGainMax: Maximum lock gain (dB), using 39 by default.

LockGainMin: Minimum lock gain (dB), using 0 by default.

LockDistValueMin: Minimum value of final lock level, using 35 by default.

LockDistValueMax: Maximum value of final lock level, using 80 by default.

## 5.2.2 Auto Shim

### 1. AutoGain

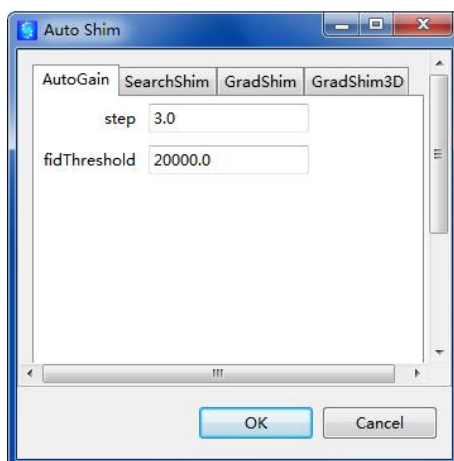


Figure 5.15 AutoGain configuration for SearchShim

step: Increment of gain optimization for **SearchShim**, with a default value of 3.

fidThreshold: Maximum FID intensity used for automatic gain calculation for SearchShim. The maximum value for FID is 32768, but 20000 is recommend.

### 2. SearchShim

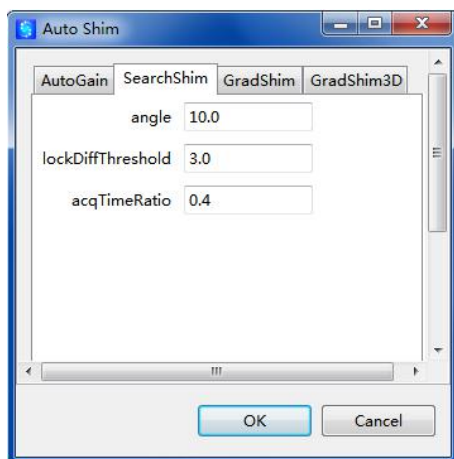


Figure 5.16 SearchShim configuration

angle: Pulse angle for acquisition. Small angle is normally used, with  $50^\circ$  as default.

lockDiff Threshold: Threshold of lock level fluctuation, using 3 by default. When the evaluation method for SearchShim is Locklevel, the fluctuation of lock level must be smaller than this value before starting shimming.

acqTimeRatio: The scale value used to optimize acqtime, usually ranges from 0.2 to 0.7, and the default value is 0.4. The final acqtime is set to the time that the FID fully decays multiplied by  $(1+acqTimeRatio)$ .

### 3. GradShim

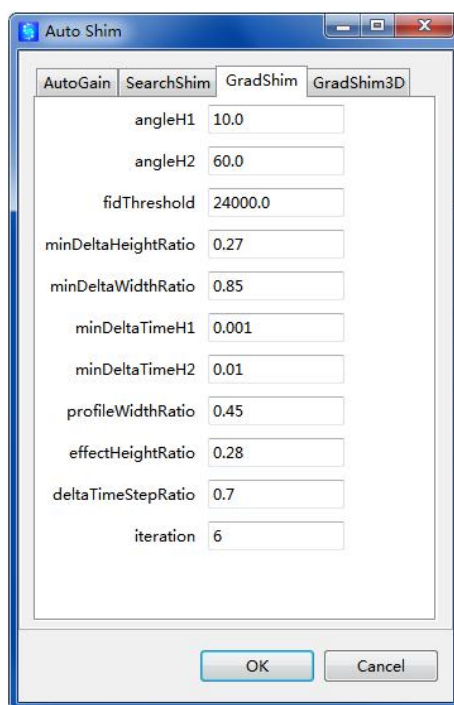


Figure 5.17 GradShim parameter configuration

angleH1: Pulse angle for acquisition when using proton GradShim. Small angle is normally used, with  $20^\circ$  as default.

angleH2: Pulse angle for acquisition when using deuterium GradShim. Small angle is normally used, with  $60^\circ$  as default.

fidThreshold: Maximum FID intensity used for automatic gain calculation for GradShim. The maximum value for FID is 32768, but 24000 is recommended.

minDeltaHeightRatio: Minimum height ratio of profile for deltatime optimization, recommending 0.27.

minDeltaWidthRatio: Minimum width ratio of profile for deltatime optimization, recommending 0.85.

minDeltaTimeH1: Minimum deltatime for proton GradShim.

minDeltaTimeH2: Minimum deltatime for deuterium GradShim.

profileWidthRatio: Targeting width ratio of profile for gzlevel optimization, recommending 0.45.

effectHeightRatio: The effective ratio of the range of points when calculating the field map is recommended to use the default value of 0.28.

deltaTimeStepRatio: When optimizing the adjustment ratio of deltatime, it is recommended to use the default value of 0.7, that is, multiply the value based on the current value when optimizing deltatime.

iteration: The number of iterations, that is, the maximum number of iterations when using the field map shimming, is recommended to use the default value of 4.

#### 4. GradShim3D

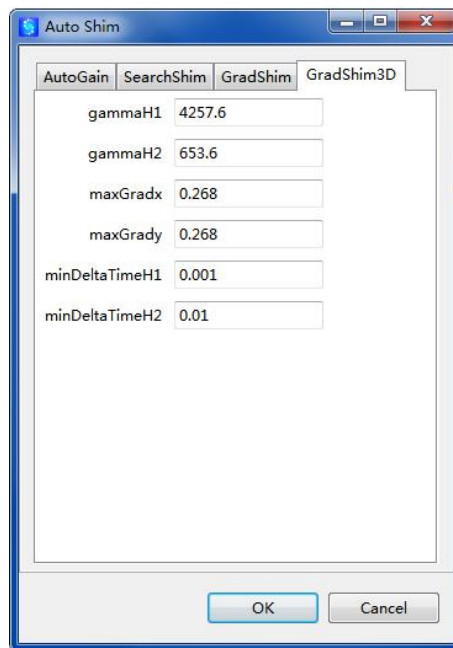


Figure 5.18 GradShim3D parameter configuration

GammaH1: Gyromagnetic ratio of proton (Hz/G).

GammaH2: Gyromagnetic ratio of deuterium (Hz/G).

maxGradx: Maximum gradient generated by x1 coil of room temperature shim set, configured according to the type of shim set. The default value is 0.268.

maxGrady: Maximum gradient generated by y1 coil of room temperature shim set, configured according to the type of shim set. The default value is 0.268.

minDeltaTimeH1: Minimum deltatime for proton 3D GradShim.

minDeltaTimeH2: Minimum deltatime for deuterium 3D GradShim.

### 5.2.3 STM

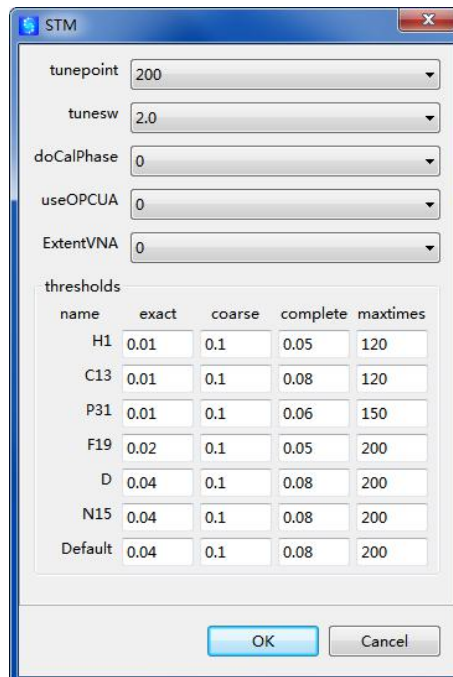


Figure 5.19 STM parameter configuration

tunepoint: Sweep points, default value is 200.

tunesw: Bandwidth for tuning (MHz), recommended as 2.0.

doCalPhase: Whether to do phase calculation. 0 for no (non-version E preamp), 1 for yes (version E preamp).

use OPCUA: Whether to use OPCUA for tuning control. 0 for no, 1 for yes.

thresholds: Automatic tuning threshold settings.

name: The tune nucleus name.

exact: The convergence value of the fine tuning, generally with the default value.

coarse: The convergence value of coarse tuning, generally with the default value.

complete: Convergence value in actual use, generally with the default value.

maxtimes: The maximum number of iterations to calculate, usually with the default value.

default: The tuning-related parameter value of the nucleus that is not in the list.

## 5.3 Others

This part mainly includes Data Service and experiment directory configuration.

### 5.3.1 Data Service

Data Service includes the management of regular experimental data and automated experimental data, mainly to configure data format conversion and related parameters for uploading data using FTP. To use the FTP file upload function, you must first configure the corresponding user name and password on the FTP server, and set the file access path for the user. Otherwise, the file upload function cannot be used. Then configure the corresponding FTP server address and user name and password in the software system configuration.

#### 1. Global:

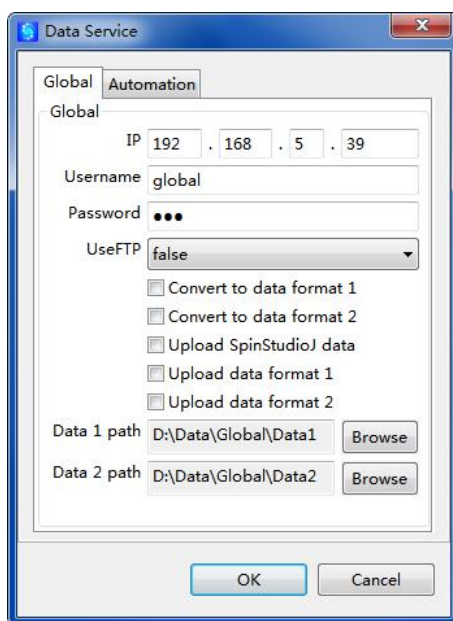


Figure 5.20 Global experimental data conversion and upload configuration

IP: IP address of FTP server.

Username: User name set by the FTP server (must be the same as the FTP server user name).

Password: The login password corresponding to the FTP server user name. (It

must be the same as the corresponding username and password in the FTP server, otherwise the file cannot be uploaded).

**UseFTP:** Whether to use FTP server for file upload. True means use, after the automated experiment is completed, the system will automatically upload the file corresponding to the current experiment to the root directory corresponding to the username of the FTP server; false means not to use, that is, the file is not automatically uploaded using the FTP server.

**Convert to data format 1:** Convert to data format 1, which is converted to Varian format data.

**Convert to data format 2:** Convert to data format 2, which is converted into Bruker format data.

**Upload SpinStudioJ Data:** Upload data in SpinStudioJ format.

**Upload data format 1:** Upload data of format 1.

**Upload data format 2:** Upload data of format 2.

**Format 1 path:** Format 1 data storage path. It is recommended to use the default path or click **Browse** to modify it.

**Format 2 path:** Format 2 data storage path, it is recommended to use the default path, or click **Browse** to modify.

## 2. Automation:

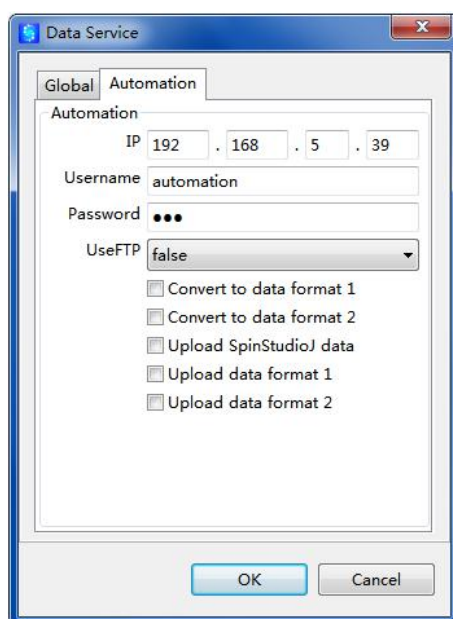


Figure 5.21 Automated experimental data conversion and upload related configuration

Same as Global file upload configuration.

### 5.3.2 Experiment Catalog

The directory structure of NMR Data Navigator is configured in **Experiment Catalog**, with three options for **College**, **Test Center** and **Pharmaceutical Factory**. User can select one of them according to your requirement, referring to Figure 5.22 for details. The default option is **College**.

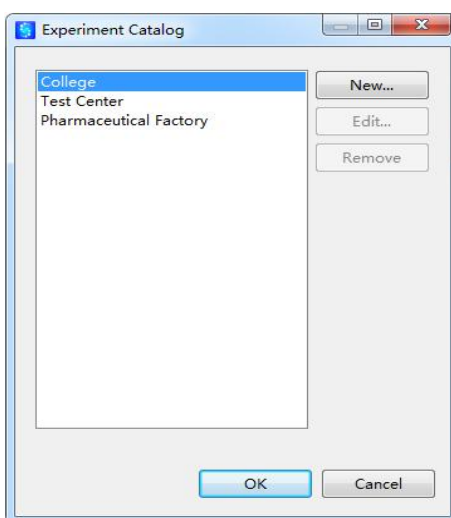


Figure 5.22 Data navigation directory structure configuration

In addition to the three existing directory structures of the software, the user can also click the button  to create a new directory structure, or click the button  or  to edit or delete the new directory structure.

Clicking  button will open a window for creating new category (Figure 5.23) by entering the name for new category. Select guest, then click **New** to pop up a dialog box (Figure 5.24). Enter a name to create a new directory under guest. You can further create new directory under it.

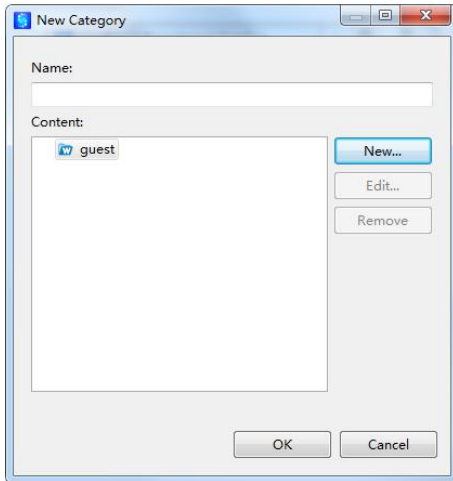


Figure 5.23 New Directory Structure dialog

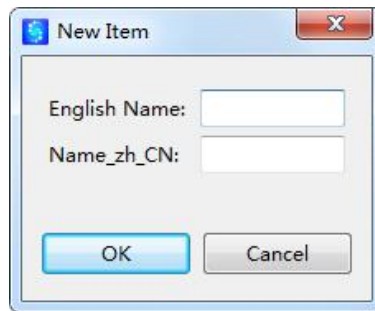



Figure 5.24 Edit the new directory name dialog under the guest

## Chapter 6 Uninstall SpinStudioJ

Find the shortcut of SpinStudioJ on the computer desktop, right-click and select “Open the location of the file”. Go to the software installation file and double-click  to pop up the uninstall dialog (Figure 6.1). Click **Yes** to start uninstalling (Figure 6.2).

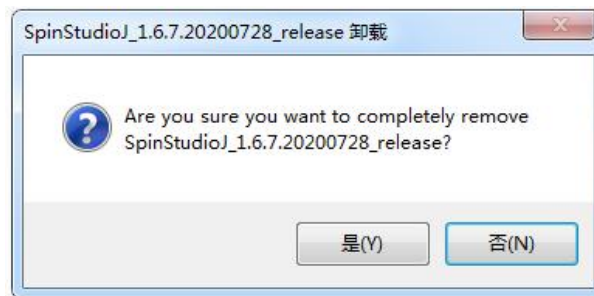


Figure 6.1 Uninstallation dialog

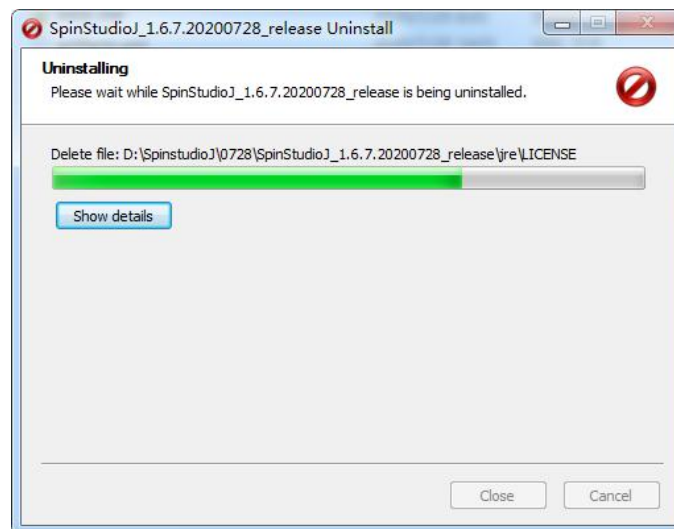


Figure 6.2 Uninstalling

After uninstalling, a dialog of successful uninstallation pops up (Figure 6.3), and the desktop shortcut is deleted at the same time.

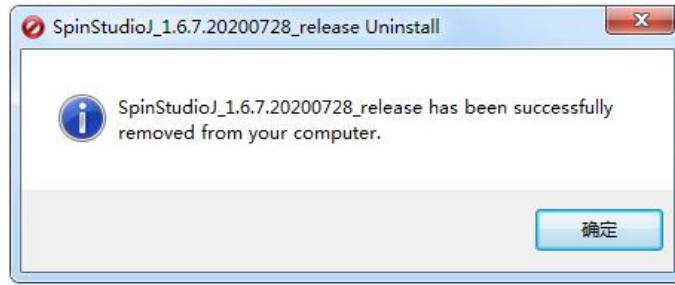


Figure 6.3 Uninstall successfully

Then uninstall the experimental control layer. Open the nmrexpctrl folder, double-click and the uninstall dialog will pop up (Figure 6.4). Click Yes to start the uninstallation (Figure 6.5). After the uninstallation is complete, the uninstallation success dialog pops up (Figure 6.6). At this point, SpinStudioJ is completely uninstalled.

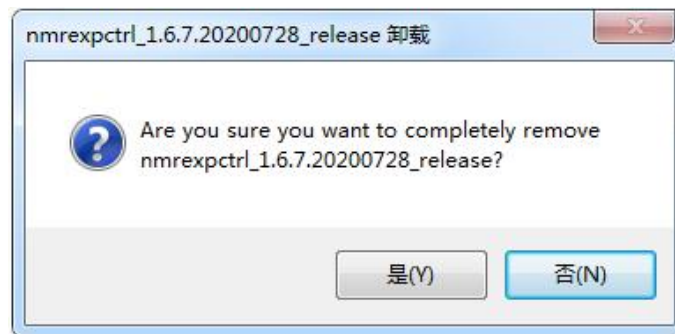


Figure 6.4 Uninstallation dialog

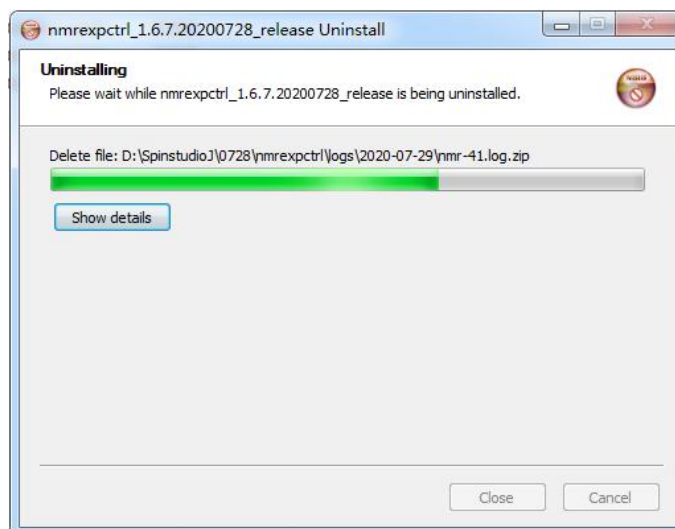


Figure 6.5 Uninstalling

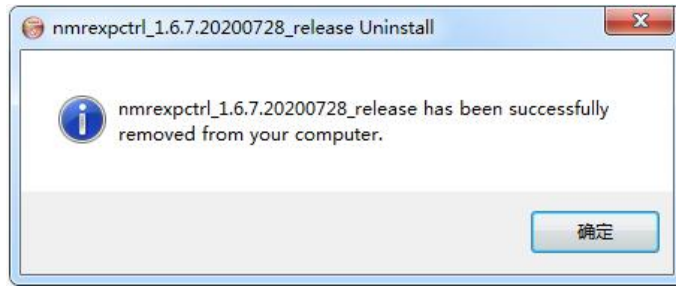


Figure 6.6 Uninstall successfully