

LabSolutions (LCMSMS)简易操作流程



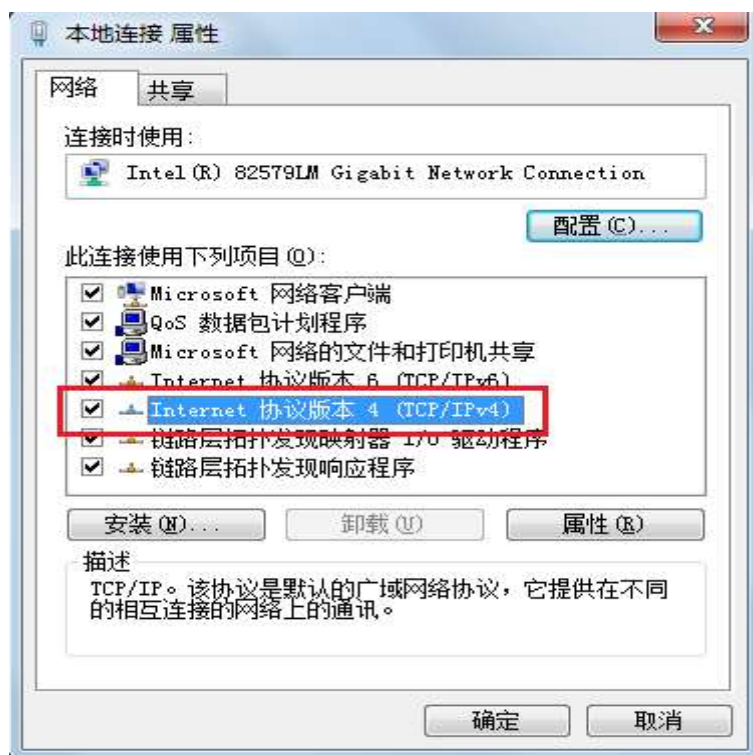
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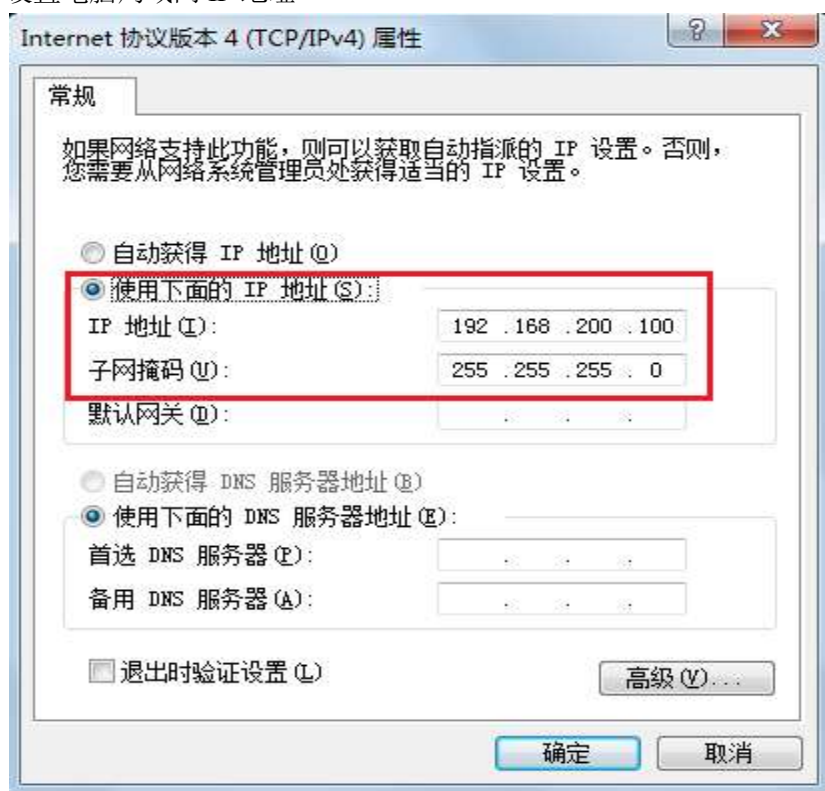
1. 联机设置与系统配置

1.1 CBM-20A/Alite 电脑 IP 地址设定

电脑网络“本地连接” “属性”



设置电脑局域网 IP 地址



1.2 LabSolutions 系统配置

LabSolutions 状态确认

电脑开机完毕后，确认电脑右下方的相关图标为**绿色**。【注：“黄色”说明系统正在启动，请稍等片刻；“红色”表示有错误产生，请重启电脑。如电脑重启后故障依旧，请联系岛津客服。】

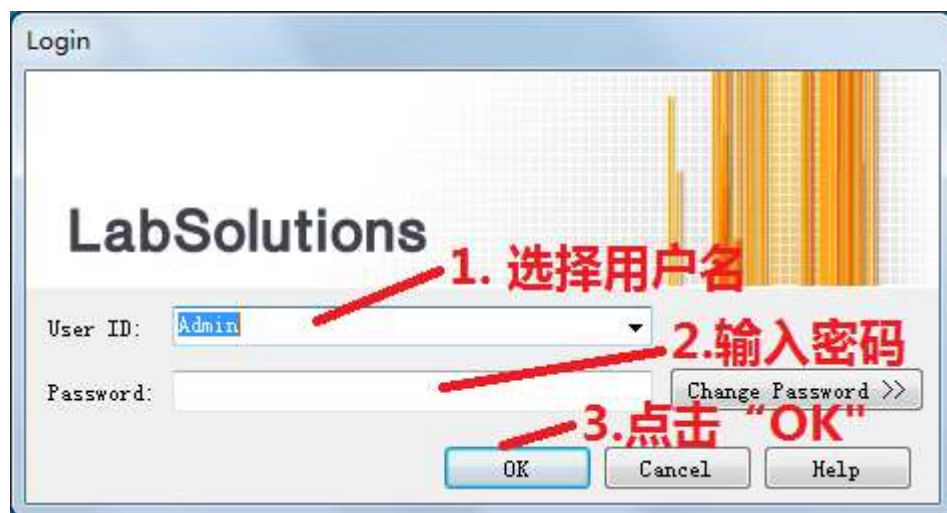


LabSolutions 软件启动



双击电脑桌面的 LabSolutions 启动 LabSolutions

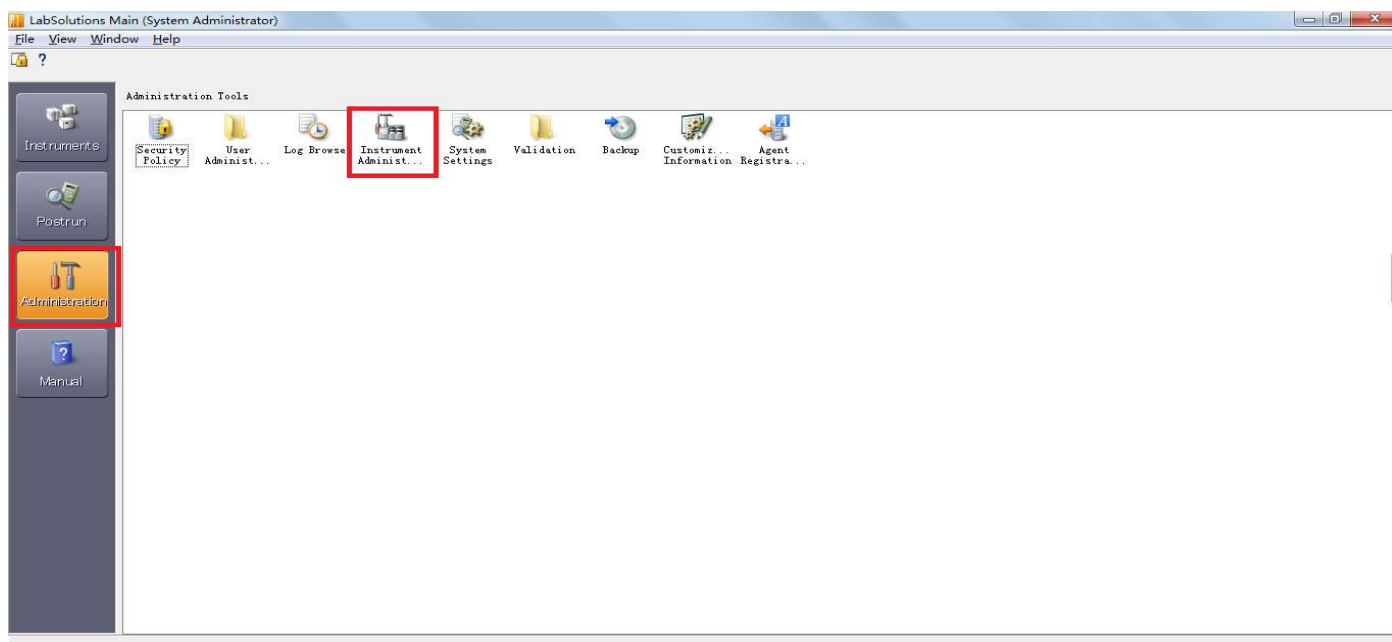
软件登录



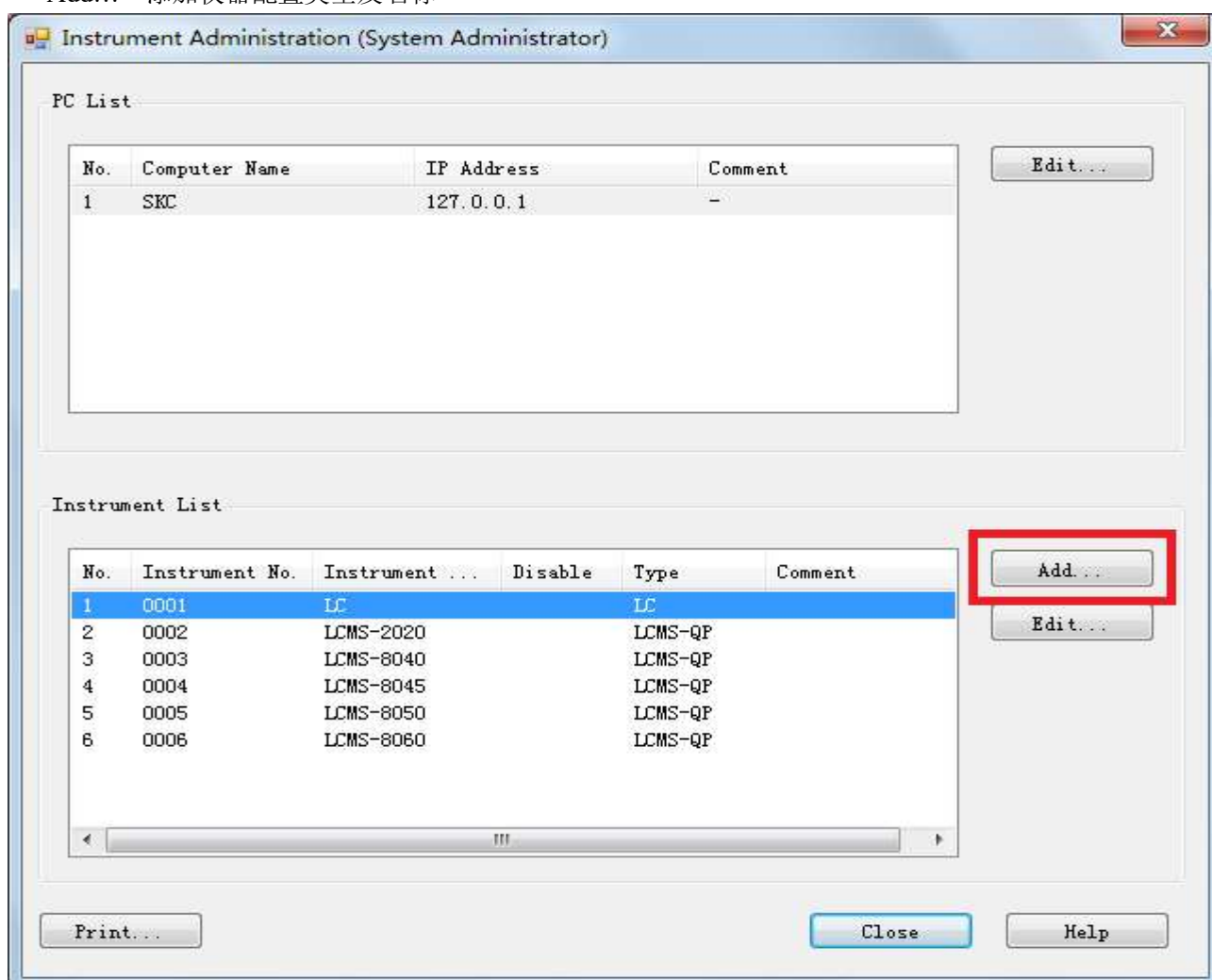
- ◆ User ID: 默认为“Admin”
- ◆ Password: 默认为“空”

创建仪器硬件配置名

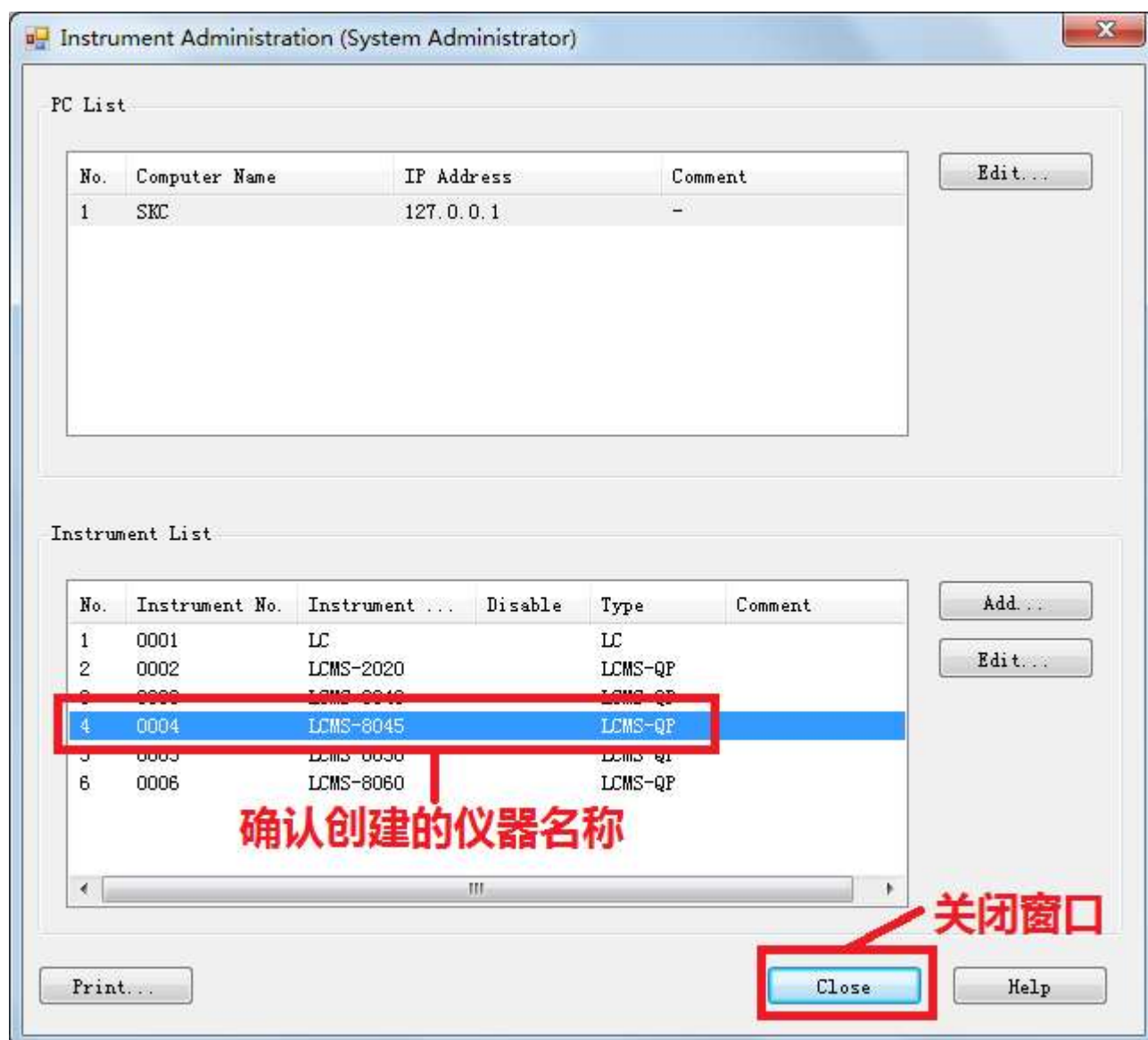
“Administration”窗口，双击“Instrument Administration”



“Add...” 添加仪器配置类型及名称



选择“仪器类型” 创建“仪器名称”

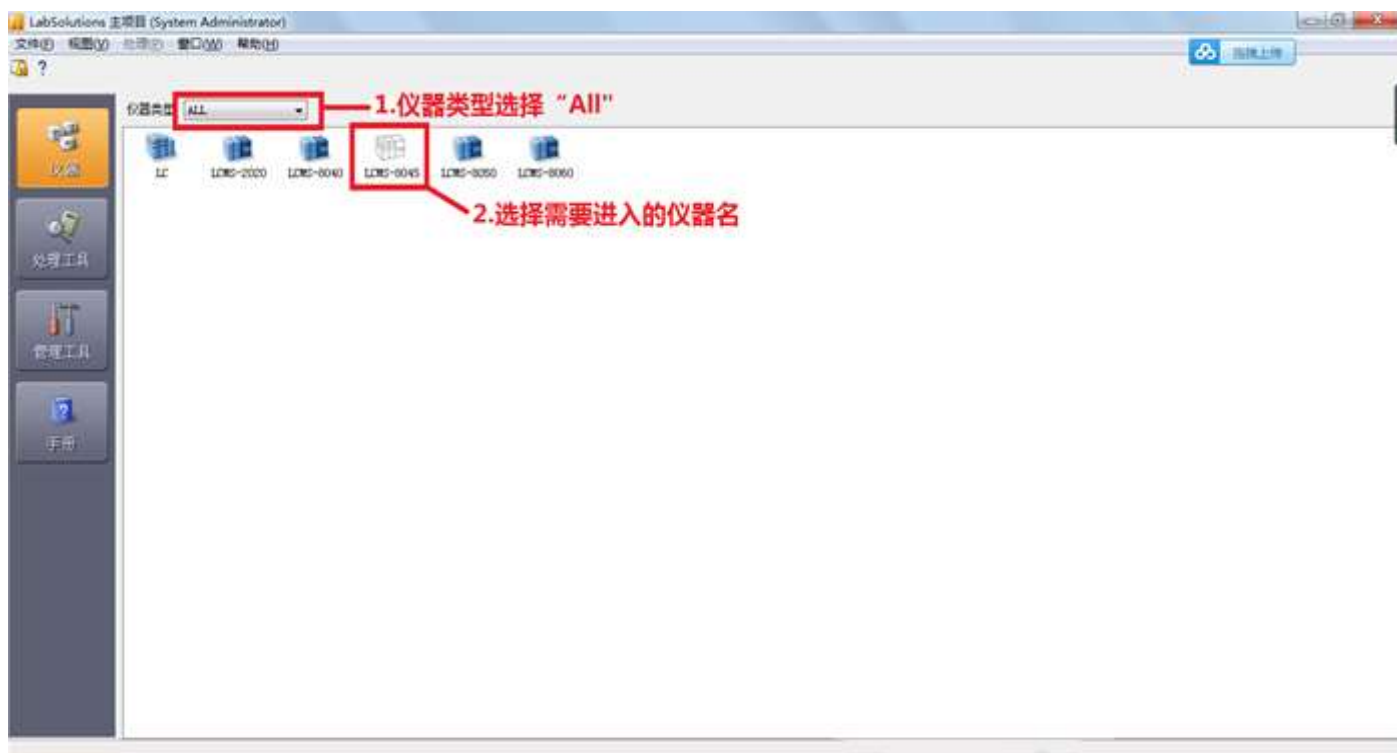


1.3 通讯设置

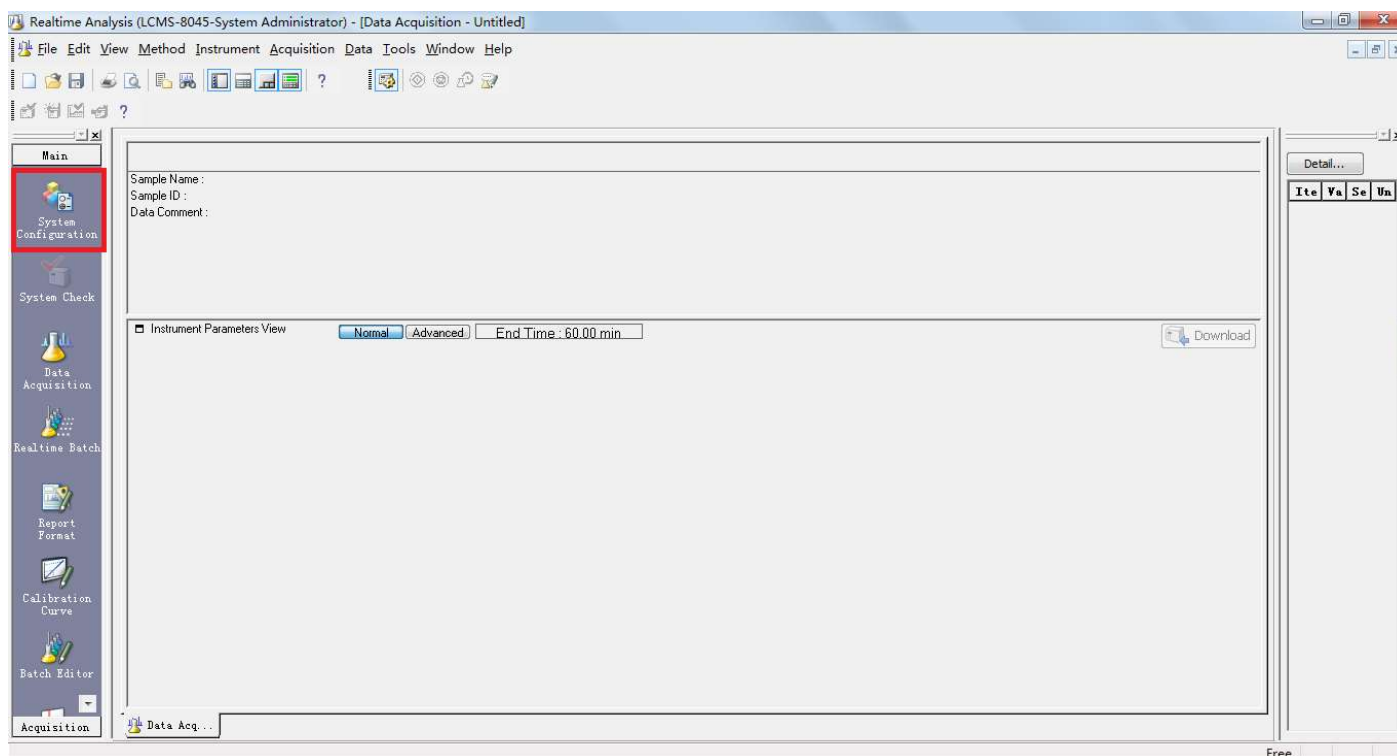
依次打开 LC、MS、电脑电源开关

LC 通讯设置

双击需要运行的“仪器名称”打开实时分析窗口



助手栏下“主项目（Main）”快捷菜单栏，打开“系统配置（System Configuration）”窗口



LC 选择相应的“CBM”类型，打开“Settings”窗口刷新 CBM 的 IP 地址

Instrument

Instrument Name: LCMS-8045

Instrument Type: LCMS-QP

Comment:

Communication:

选择相应的LC型号

Instrument	Model	Communication	Settings	Settings
LC	None	None	None	Settings
PDA	None	None	None	Settings
ELSD	SCL-10Avp	None	None	Settings
MWD	SCL-10Asp	None	None	Settings
LCMS	CBM-20A	None	None	Settings
Gilson/CTC	CBM-20Alite	None	None	Settings
APV	LC-2030	None	None	Settings
ADC	LC-2040	None	None	Settings

OK Cancel Help

Instrument

Instrument Name: LCMS-8045

Instrument Type: LCMS-QP

Comment:

点击 "Settings..." 打开通讯设置窗口

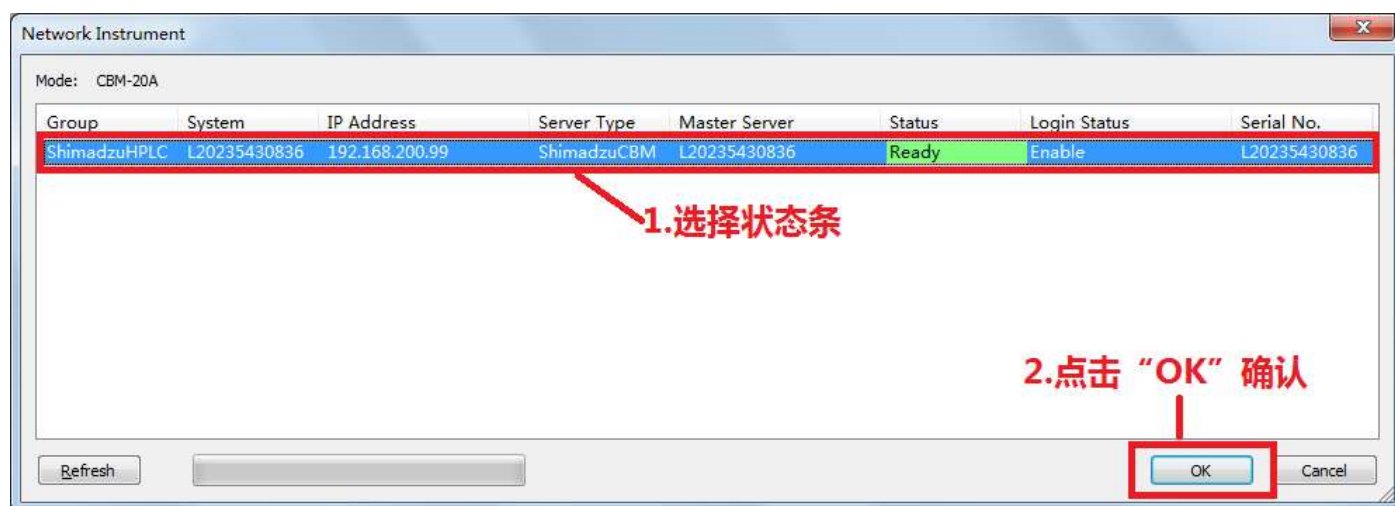
Instrument	Model	Communication	Settings	Settings
LC	CBM-20A	Ethernet	0.0.0.0	Settings...
PDA	None	None	None	Settings
ELSD	None	None	None	Settings
MWD	None	None	None	Settings
LCMS	None	None	None	Settings
Gilson/CTC	None	None	None	Settings
APV	None	None	None	Settings
ADC	None	None	None	Settings

OK Cancel Help

选择“Ethernet”，点击“List”进入“Network Instrument”窗口进行 IP 地址刷新

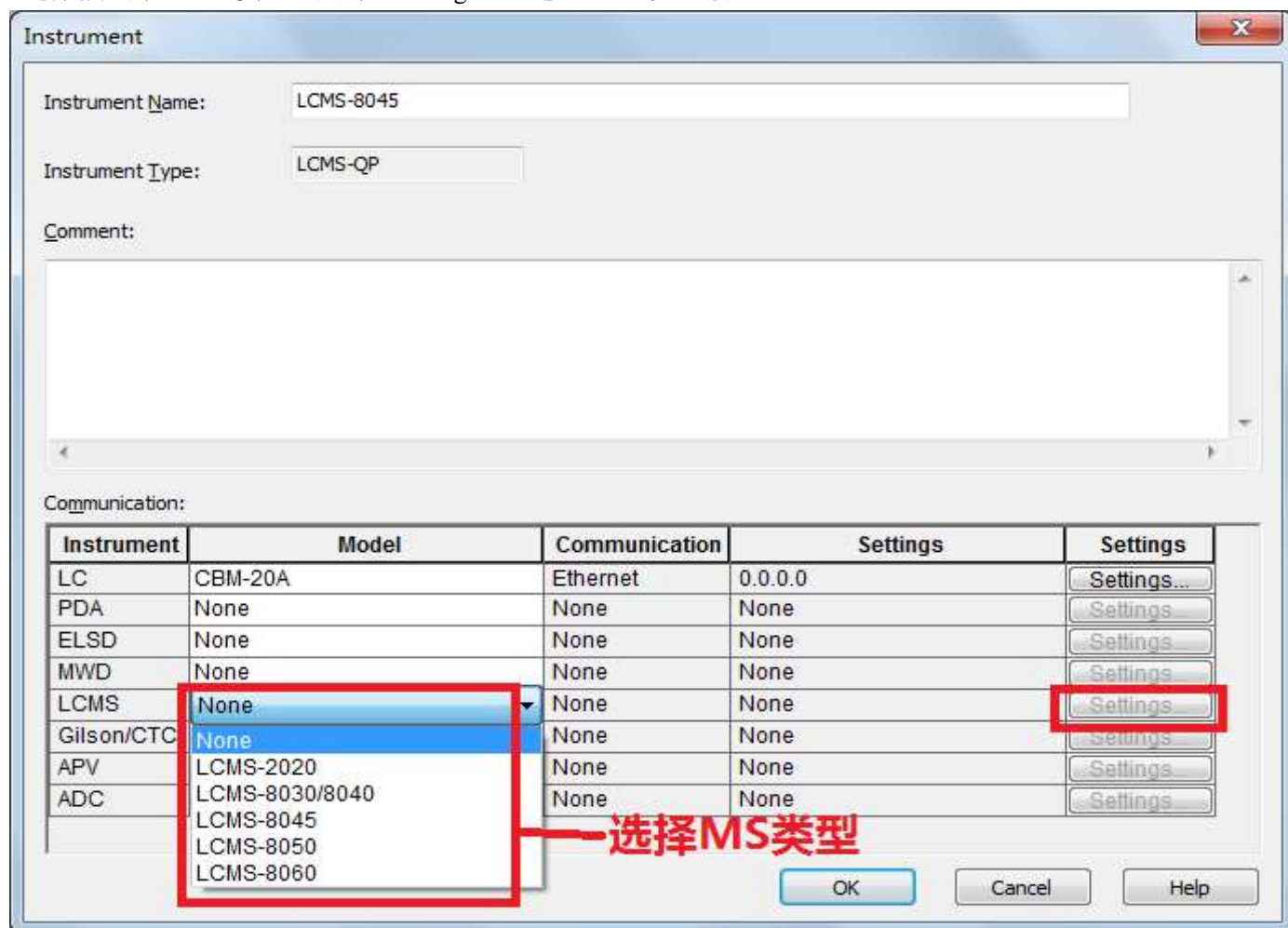


确认如下界面中能够刷新出链接状态条，选择状态条后点击 OK 退出。



MS 通讯设置

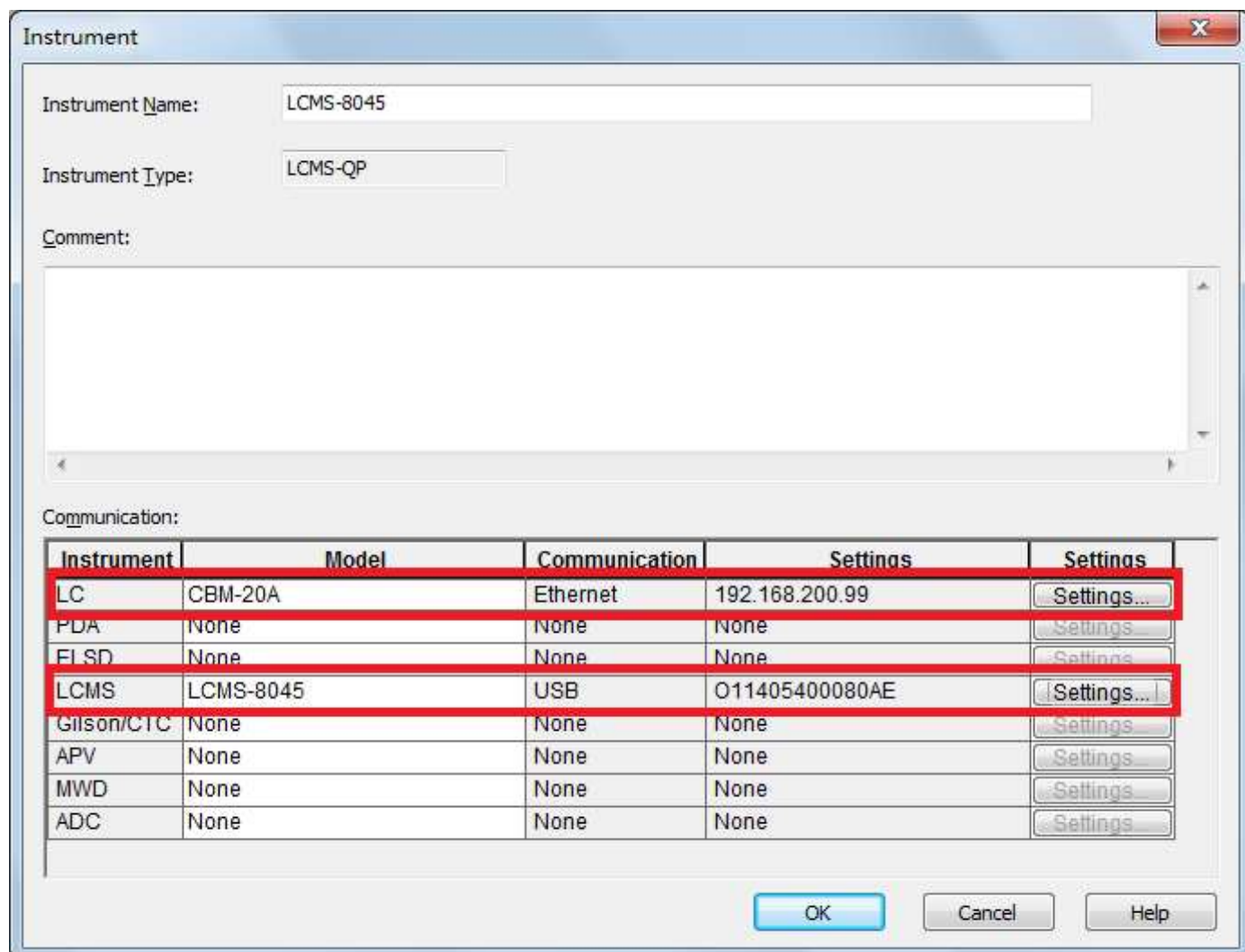
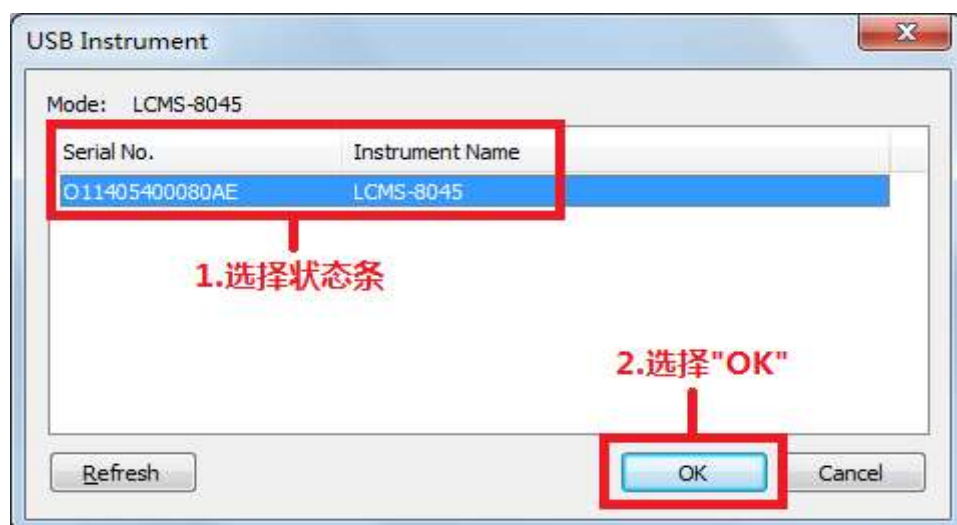
选择相应的 LCMS 类型，点击 “Settings...” 进入“通讯设置”窗口



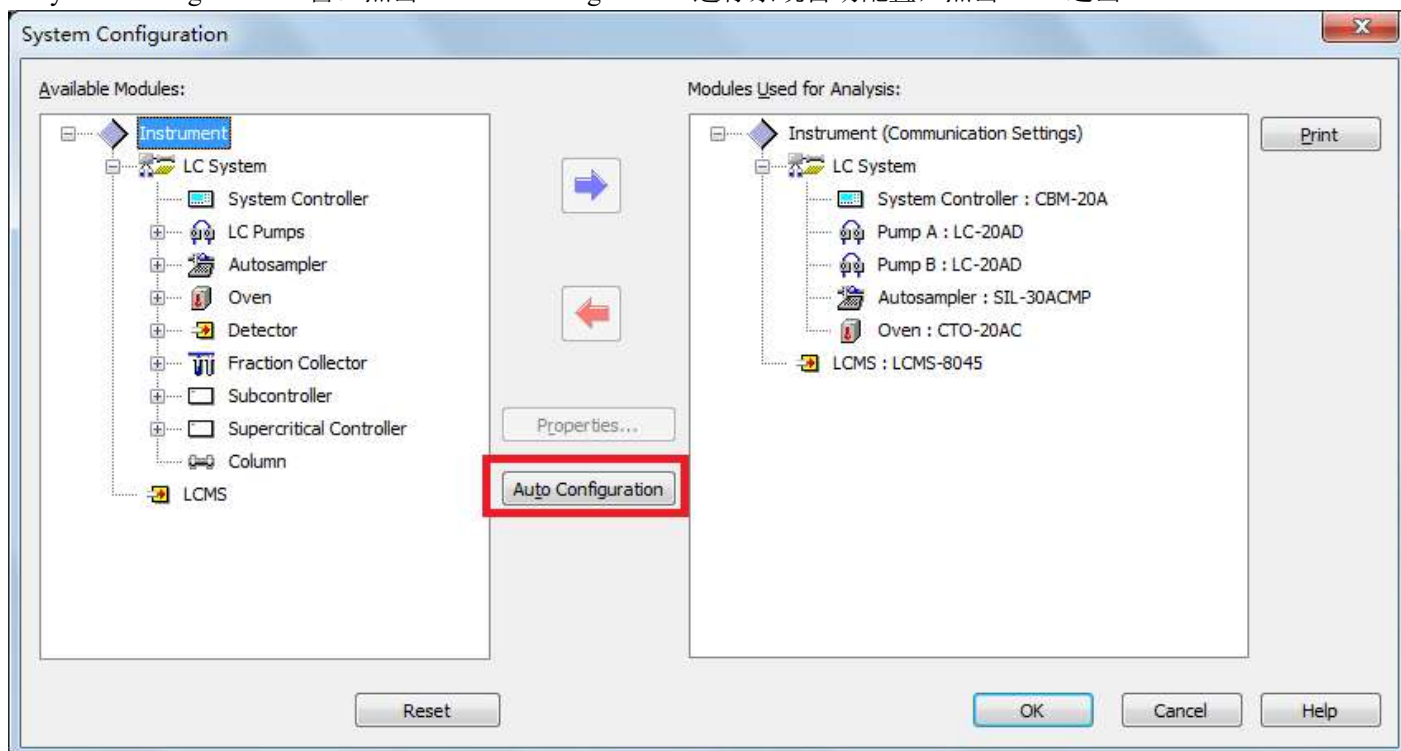
选择连接类型 “USB”, 点击 “List...” 打开 “USB Instrument”



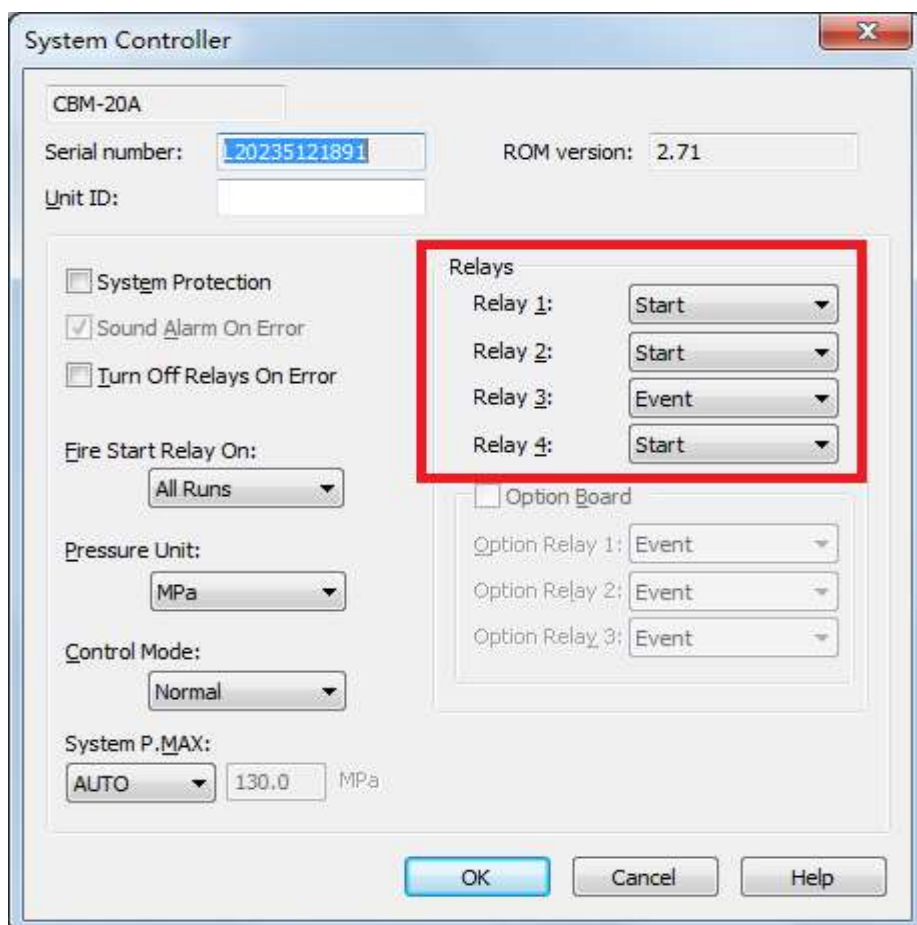
确认“USB Instrument”窗口能够刷新出相应的仪器类型和设备序列号



“System Configuration” 窗口点击 “Auto Configuration”进行系统自动配置，点击“OK”退出



设置 CBM 与 MS 触发信号类型



MS Detector

Detector Name:

LCMS-8045

Serial number:

Unit ID:

Interface: Valve:

Analog Output:

Event Input/Output

Input Terminal1:	START	Output Terminal1:	EVENT
Input Terminal2:	None	Output Terminal2:	EVENT
Input Terminal3:	None		
Input Terminal4:	None		
Input Terminal5:	None		
Input Terminal6:	None		

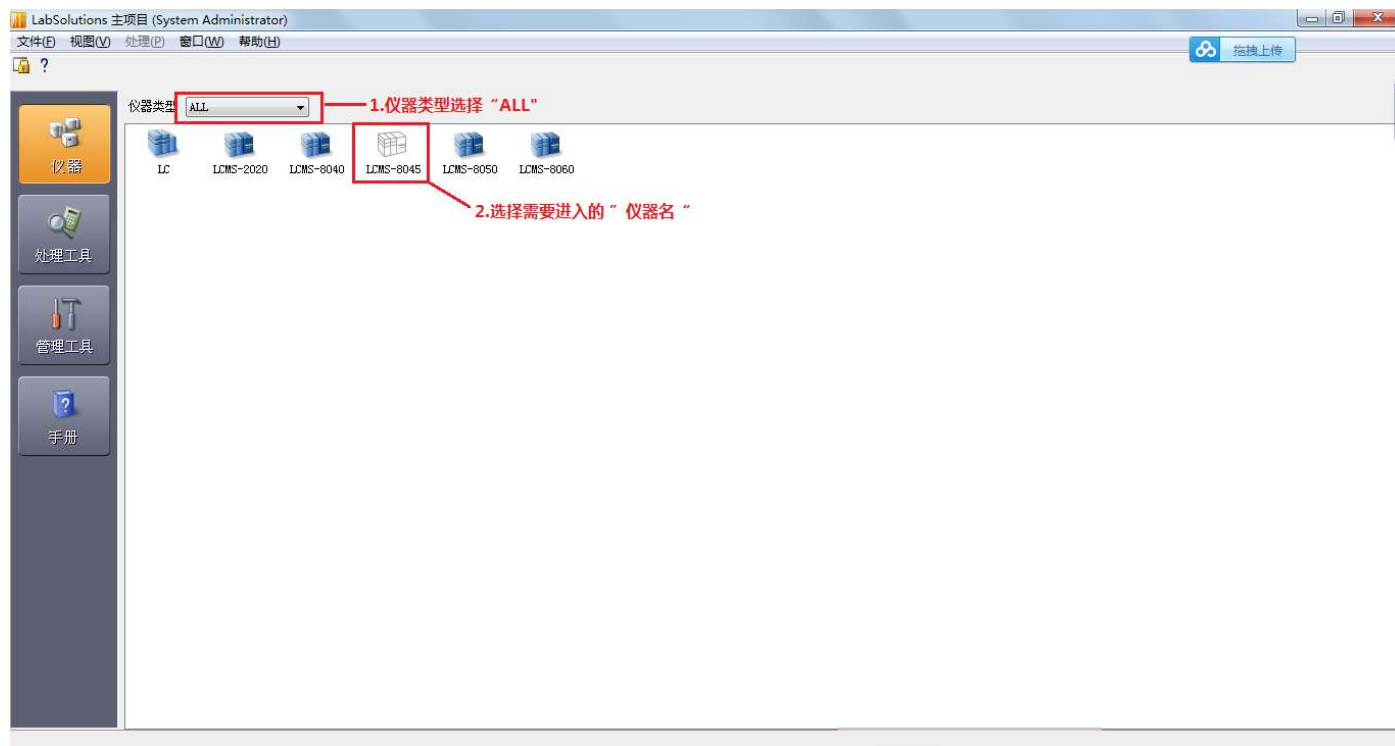
System Check...

OK Cancel Help

2. 开机

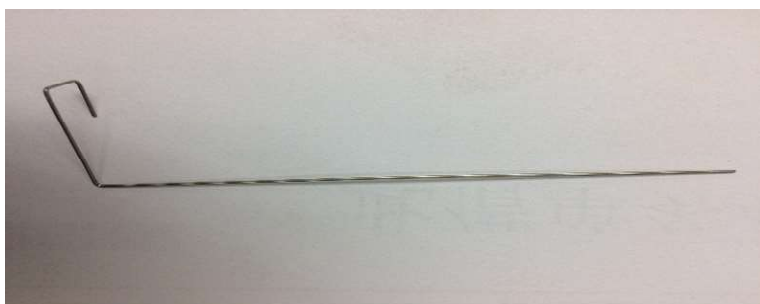
- ◆ 确认所有设备的电源已打开（质谱电源开关位于仪器右后方红色按钮）。
- ◆ 确认氮气（690-800KPa）、氩气（500-800KPa）、零级空气（8045/8050/8060）(700-800KPa) 已接入仪器，输出压力正确。

2.1 启动实时分析程序



2.2 启动真空系统

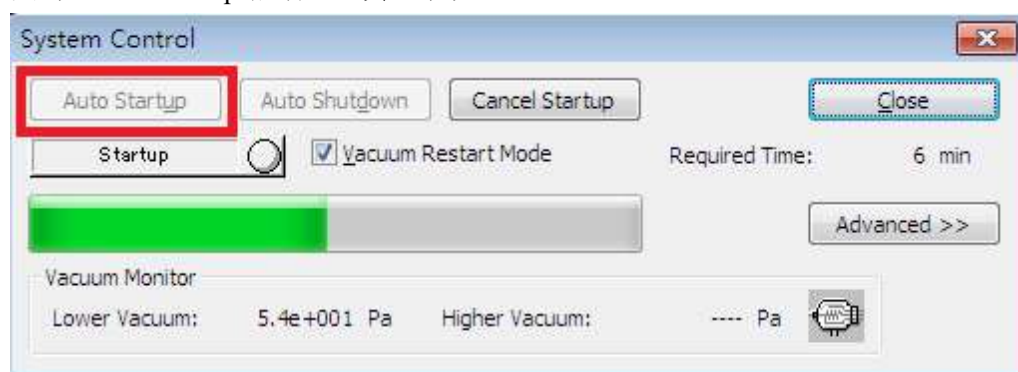
注：请使用堵针将离子通道入口堵塞。



打开“System Control”窗口



点击“Auto Startup”启动 MS 真空系统



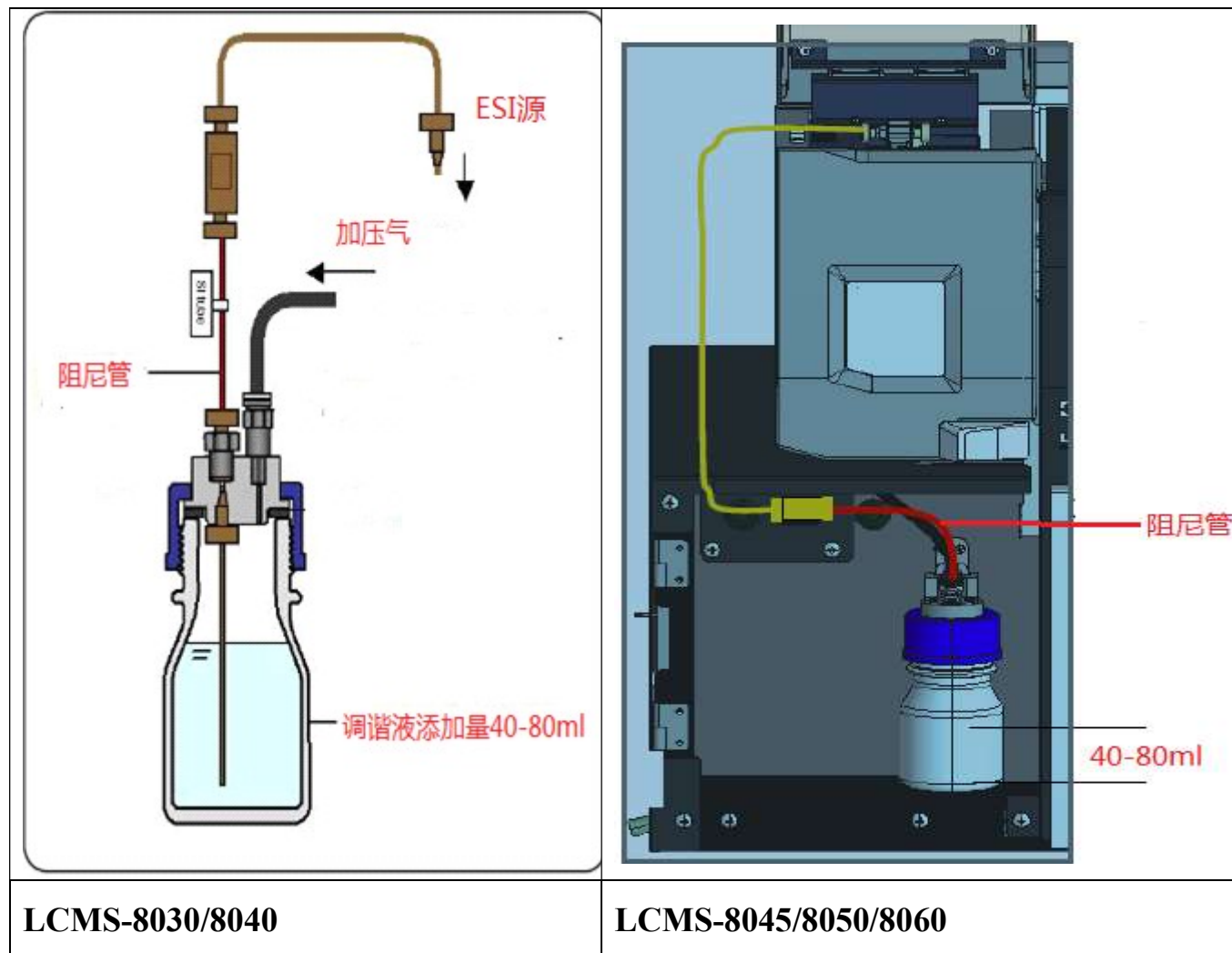
- ◆ 点击“Auto Startup”按钮后，通常 30 分钟后真空系统启动完成，此时，质谱主机上的“STATUS”指示灯亮起为绿色常亮。
- ◆ 当 $IG < 3.0 \times 10^{-3} \text{pa}$ (LCMS8030/40/45), $IG < 6.0 \times 10^{-3} \text{pa}$ (LCMS8050/60) 时 MS 显示“准备就绪”可进行样品分析。
- ◆ 如果需得到稳定的测试结果，至少需要抽真空 12h 以上再进行测试。
- ◆ 点击“Advanced”按钮，确认 CID GAS 右侧的“Open”按钮已打开。

3. 调谐

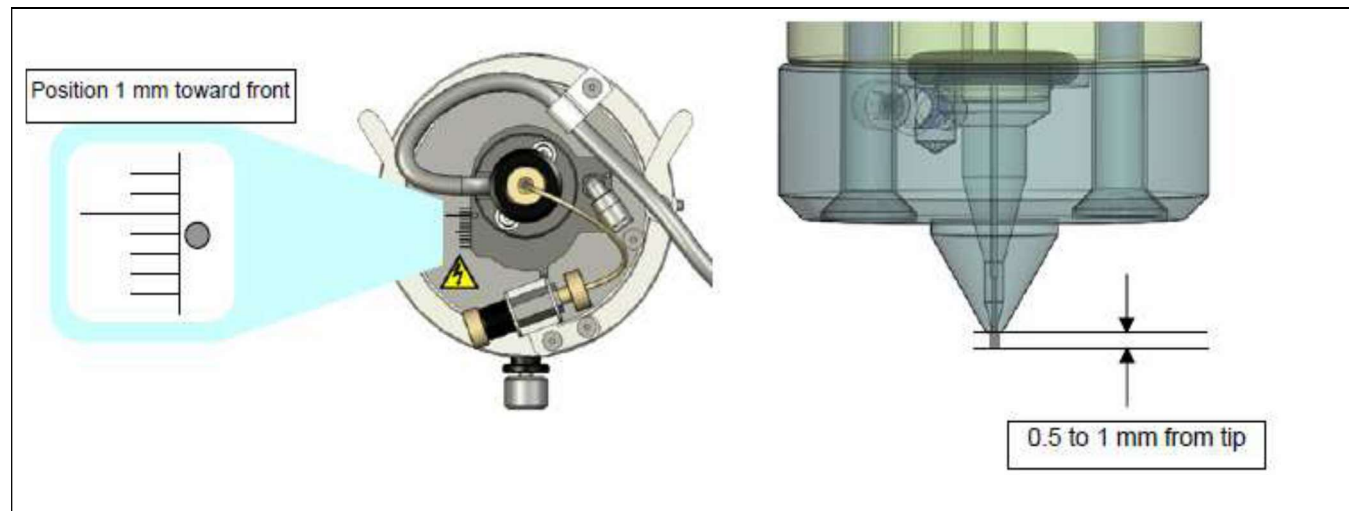
请依照仪器使用说明书的要求正确添加调谐液及连接调谐液传送管路，设置 ESI 离子源位置

3.1 调谐前准备

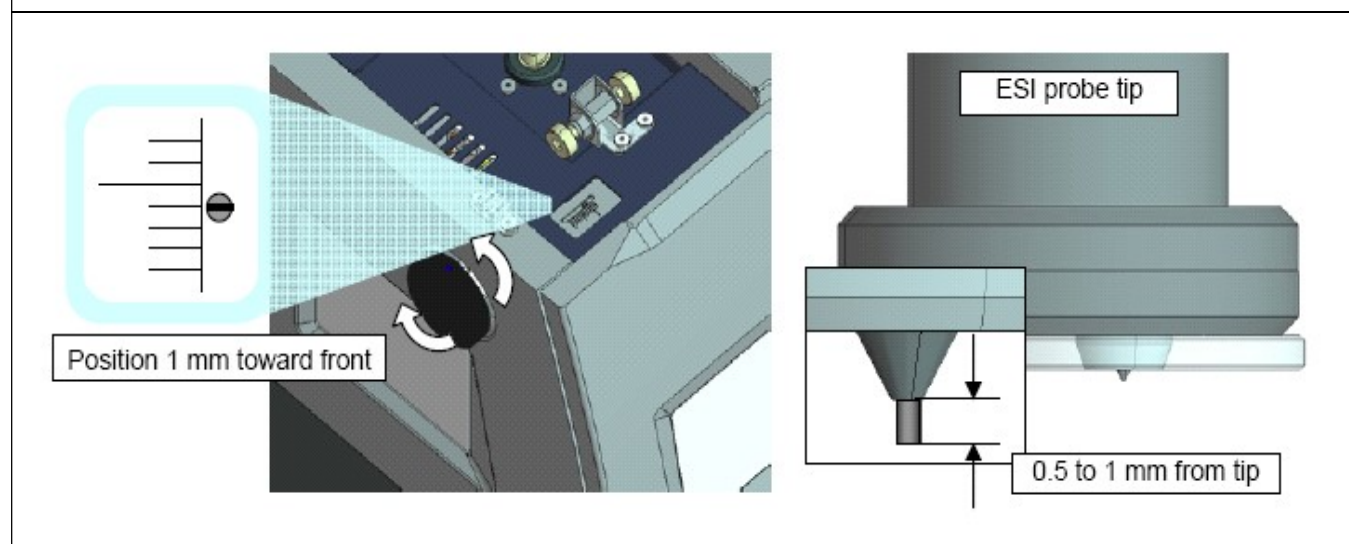
注：确认调谐液有效期



ESI 源位置设置



LCMS-8030/8040



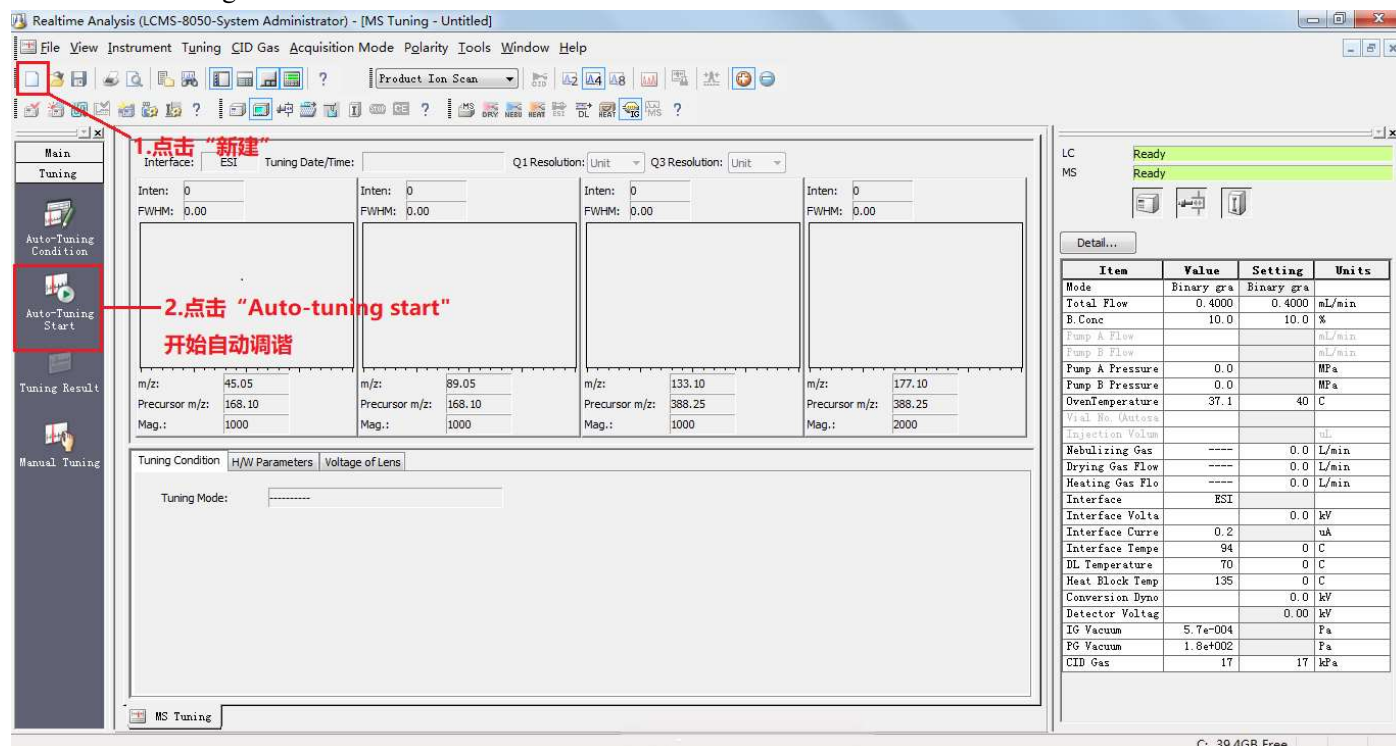
LCMS-8045/8050/8060

3.2 开始自动调谐

点击 “Tuning” 打开调谐窗口



点击“Auto-Tuning Start”开始自动调谐



等待自动调谐完成

Auto-Tuning

Interface: Time: sec

Total: **Q1 Scan-Positive - 6 %**

Step: **Calibrating m/z - 22 %**

#: 12/216

Auto-Tuning Condition

☒ Positive

☒ Negative

☒ Detector Adjustment

☒ Sensitivity Adjustment

☒ Resolution Adjustment

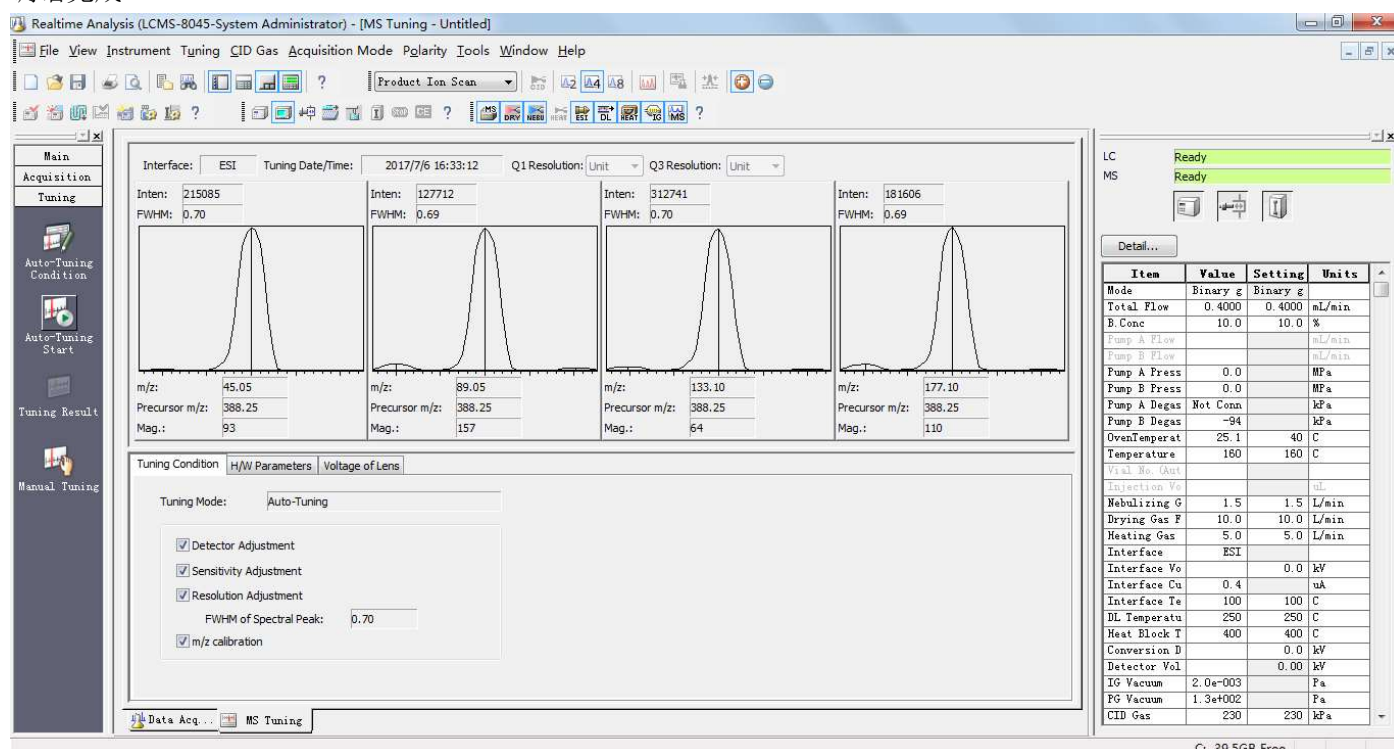
FWHM of Spectral Peak: 0.70

☒ m/z Calibration

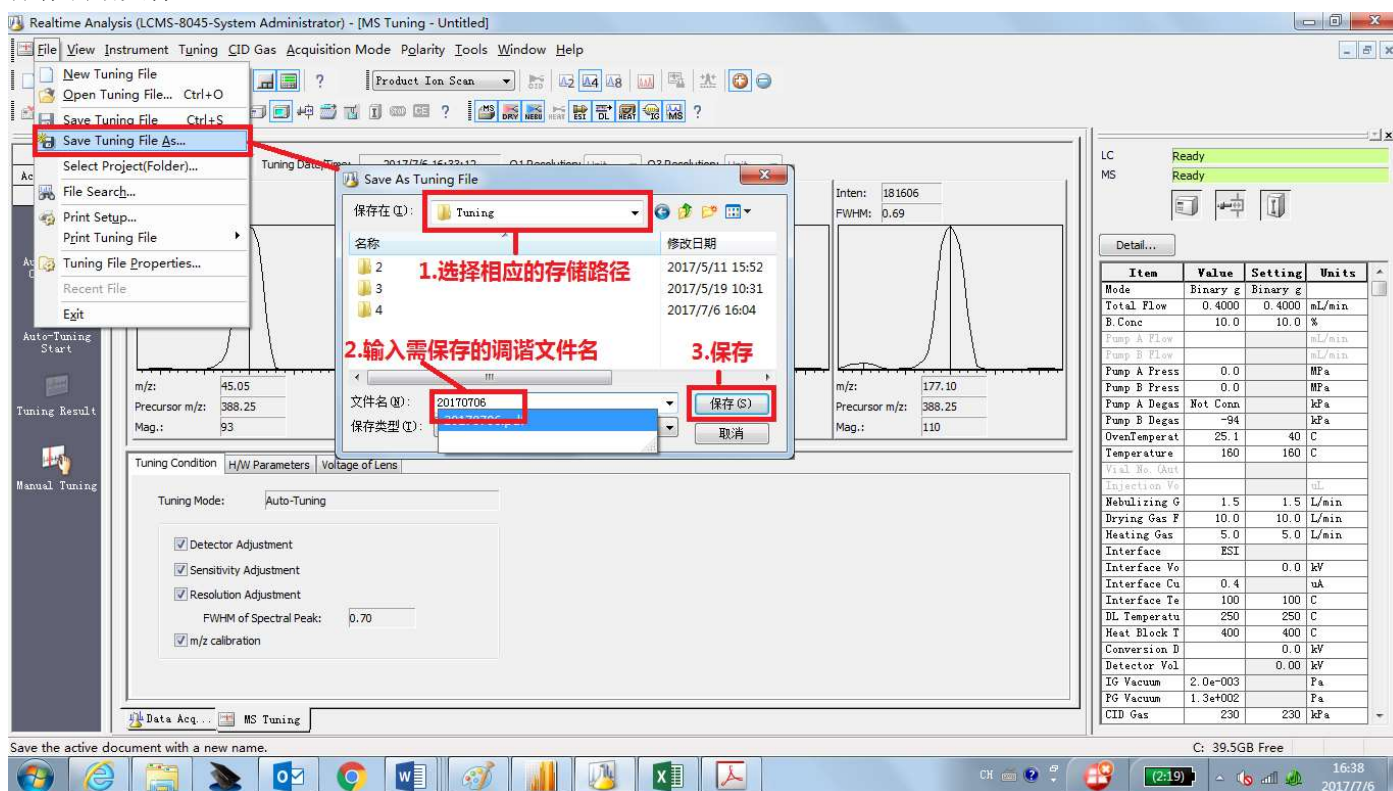
H/W Parameters

Nebulizing Gas:	1.50	L/min	DL:	250	C
Mon.:	1.50	L/min	Mon Temp.:	250	C
Drying Gas:	10.00	L/min	Heat Block:	400	C
Mon.:	----	L/min	Mon Temp.:	400	C
Heating Gas:	5.00	L/min	CID Gas.:	230	kPa
Mon.:	5.01	L/min	Mon.:	230	kPa
Interface:	4.00	kV	Conversion Dynode:	5.00	kV
Mon Current:	0.63	uA	Detector:	2.26	kV
Set Temp.:	100	C	PG Vacuum:	1.2e+002	Pa
Mon Temp.:	100	C	IG Vacuum:	2.0e-003	Pa

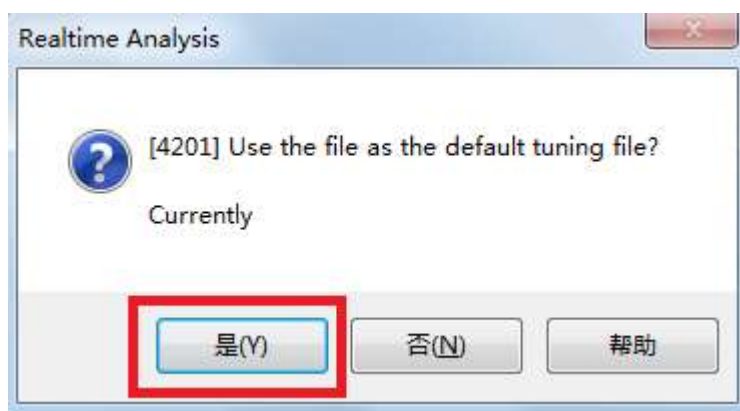
调谐完成



保存调谐文件



保存为当前缺省的调谐文件



- ◆ 自动调谐完成通常约需 40min，如自动调谐失败请记录错误信息并联系岛津工程师。自动调谐结果评价,请参考相关的仪器使用说明书。

4. 仪器方法参数编辑和 MRM 优化

4.1 仪器方法参数编辑

Data acquisition 窗口，参考标准方法设置相关的方法参数。

设置 MS 相关的采集参数

1. 选择新建

2. 选择“正、负”离子极性类型

3. 选择相应的扫描方式

4. “Event”列表

6. 设置每个“Event”相应的采集时间、化合物名

5. 设置每个“Event”相应的通道参数

Type	Event#	+	-	Compound Name	m/z	Time (0.000 min - 10.000 min)
MRM	1			100.00>100.00		

Ch	Precursor m/z	Product m/z	Dwell Time (msec)	CE
Ch1	100.00	100.00	100.0	-35.0
Ch2				
Ch3				
Ch4				

设置 MS 相关的离子源参数(使用默认参数)

设置MS相关的离子源参数

Item	Value	Setting	Units
Mode	Binary g	Binary g	
Total Flow	0.4000	0.4000	mL/min
B Conc	10.0	10.0	%
Pump A Flow			mL/min
Pump B Flow			mL/min
Pump A Press	0.0		MPa
Pump B Press	0.0		MPa
Pump A Degas	Not Conn		kPa
Pump B Degas	-94		kPa
Oven Temperat	25.0	40	C
Temperature	160	160	C
Vial No. Aut			
Injection Vol			μL
Nebulizing G	1.5	1.5	L/min
Drying Gas F	10.0	10.0	L/min
Heating Gas	5.0	5.0	L/min
Interface	ESI		
Interface Vo	0.0		kV
Interface Cu	0.4		uA
Interface Te	100	100	C
DL Temperatu	250	250	C
Heat Block T	400	400	C
Conversion D	0.0		kV
Detector Vol	0.00		kV
IG Vacuum	2.0e+003		Pa
PG Vacuum	1.3e+002		Pa
CID Gas	230	230	kPa

设置 LC 泵参数

Realtime Analysis (LCMS-8045-System Administrator) - [Data Acquisition - Method1.lcm]

LCReady MSReady

Instrument Parameters View

Mode: Binary gradient

Configured Pumps

Pump A: LC-30AD

Pump B: LC-30AD

Pressure Limits (Pump A, B)

Maximum: 60.0 MPa

Minimum: 0.0 MPa

Total Flow: 0.4000 mL/min

Pump B Conc.: 8.0 %

Pump B Curv.: 0

End Time: 3.00 min

Download

LC MS Ready

Item	Value	Setting	Units
Mode	Binary g	Binary g	
Total Flow	0.4000	0.4000	mL/min
B. Conc	10.0	10.0	%
Pump A Flow			mL/min
Pump B Flow			mL/min
Pump A Press	0.0		MPa
Pump B Press	0.0		MPa
Pump A Degas	Not Conn		kPa
Pump B Degas	-94		kPa
OvenTemperat	25.0	40	C
Temperature	160	160	C
Vial No. Aut			
Injection Vo			nL
Nebulizing G	1.5	1.5	L/min
Drying Gas F	10.0	10.0	L/min
Heating Gas	5.0	5.0	L/min
Interface	ESI		
Interface Vo		0.0	kV
Interface Cu	0.4		uA
Interface Te	100	100	C
DL Temperatu	250	250	C
Heat Block T	400	400	C
Conversion D		0.0	kV
Detector Vol		0.00	kV
IG Vacuum	2.0e+003		Pa
FG Vacuum	1.3e+002		Pa
CID Gas	230	230	kPa

C: 39.5GB Free

设置 LC 时间程序

Realtime Analysis (LCMS-8045-System Administrator) - [Data Acquisition - Method1.lcm]

LCReady MSReady

Instrument Parameters View

LC Time Prog

Max Intensity: 0 %

Time	Module	Command	Value
1.50	Pumps	Pump B Conc.	95
1.51	Pumps	Pump B Conc.	8
3.00	Controller	Stop	
4.00			
5.00			
6.00			
7.00			
8.00			
9.00			

End Time: 3.00 min

Download

LC MS Ready

Item	Value	Setting	Units
Mode	Binary g	Binary g	
Total Flow	0.4000	0.4000	mL/min
B. Conc	10.0	10.0	%
Pump A Flow			mL/min
Pump B Flow			mL/min
Pump A Press	0.0		MPa
Pump B Press	0.0		MPa
Pump A Degas	Not Conn		kPa
Pump B Degas	-94		kPa
OvenTemperat	25.0	40	C
Temperature	160	160	C
Vial No. Aut			
Injection Vo			nL
Nebulizing G	1.5	1.5	L/min
Drying Gas F	10.0	10.0	L/min
Heating Gas	5.0	5.0	L/min
Interface	ESI		
Interface Vo		0.0	kV
Interface Cu	0.4		uA
Interface Te	100	100	C
DL Temperatu	250	250	C
Heat Block T	400	400	C
Conversion D		0.0	kV
Detector Vol		0.00	kV
IG Vacuum	2.0e+003		Pa
FG Vacuum	1.3e+002		Pa
CID Gas	230	230	kPa

C: 39.5GB Free

设置 LC 程序停止时间(与“Controller Stop”时间相同)

Realtime Analysis (LCMS-8045-System Administrator) - [Data Acquisition - method1.lcm]

File Edit View Method Instrument Acquisition Data Tools Window Help

LCReady MSReady

Sample Name:
Sample ID:
Data Comment:

LC MS ALL

Max Intensity: 0
Time 15.886 Inten. 0.000

Instrument Parameters View

Normal Advanced End Time: 10.00 min

MS Interface Data Acquisition LC Time Prog. Pump Column Oven Controller Autosampler AutoPurge

LC Time Program

LC Stop Time: 3:00 min

Apply to All acquisition time

设置LC停止时间

Detail...

Item	Value	Setting	Units
Mode	Binary	Binary	
Total Flo	0.4000	0.4000	mL/min
B Conc	70.0	70.0	%
Pump A Pr	1.0		MPa
Pump B Pr	1.0		MPa
Pump A De	Not Co		kPa
Injection			μL
Nebulizin	3.0	3.0	L/min
Drying Ga	10.0	10.0	L/min
Heating G	10.0	10.0	L/min
Interface	ESI		
Interface	0.0	0.0	kV
Interface	299	300	C
DL Temper	250	250	C
Heat Bloc	400	400	C
Conversio	0.0	0.0	kV
Detector	0.00		kV
IG Vacuum	1.7e-0		Pa
PG Vacuum	1.1e+0		Pa
CID Gas	230	230	kPa

C: 40.4GB Free

设置柱温箱温度

Realtime Analysis (LCMS-8045-System Administrator) - [Data Acquisition - Method1.lcm]

File Edit View Method Instrument Acquisition Data Tools Window Help

LCReady MSReady

Instrument Parameters View

Normal Advanced End Time: 3:00 min

MS Interface Data Acquisition LC Time Prog. Pump Column Oven Controller Autosampler AutoPurge

Model: CTO-30A

Oven Temperature: 40 C

Temperature: 90 C

Heat Compensation: AUTO

Heat Compensation Flow: 0.4000 mL/min

Ready Check: On

Ready Check...

1.设置柱温箱温度上限

2.设置合适的柱温箱温度

Detail...

Item	Value	Setting	Units
Mode	Binary	Binary	
Total Flow	0.4000	0.4000	mL/min
B Conc	10.0	10.0	%
Pump A Flow			mL/min
Pump B Flow			mL/min
Pump A Press	0.0		MPa
Pump B Press	0.0		MPa
Pump A Degas	Not Conn		kPa
Pump B Degas	-94		kPa
Oven Temperat	25.0	40	C
Temperature	160	160	C
Injection Vo			μL
Nebulizing G	1.5	1.5	L/min
Drying Gas F	10.0	10.0	L/min
Heating Gas	5.0	5.0	L/min
Interface	ESI		
Interface Vo	0.0	0.0	kV
Interface Cu	0.4		uA
Interface Te	100	100	C
DL Temperatu	250	250	C
Heat Block T	400	400	C
Conversion D	0.0	0.0	kV
Detector Vol	0.00		kV
IG Vacuum	2.0e-003		Pa
PG Vacuum	1.3e+002		Pa
CID Gas	230	230	kPa

C: 39.5GB Free

设置自动进样器参数（默认参数）

Realtime Analysis (LCMS-8045-System Administrator) - [Data Acquisition - Method1.lcm]

File Edit View Method Instrument Acquisition Data Tools Window Help

LCReady MSReady

Instrument Parameters View

Model: SIL-30AC Autosampler

Injection Settings

Sample Rack: Rack 1.5 mL 105 vials

Needle Stroke: 52 mm

Control Yial Needle St: 52 mm

Sampling Speed: 15.0 uL/sec

✓ Cooler Temperature: 4 C

Measuring Line Purge Volume: 100 uL

Air Gap Volume: 0.1 uL

Rinse Settings

Rinse: External only

Rinsing Speed: 35 uL/sec

Rinsing Volume: 500 uL

Rinse Mode: Before and after aspira

Rinse Di Time: 2 sec

Rinse Pump: Rinse port only

Purge Settings

Purge Time: 10.0 min

Purge Port: ging with Default RO 10.0 min

Measuring Line ging with Default RO 10.0 min

Pre-treatment...

Detail...

Item	Value	Setting	Units
Mode	Binary g	Binary g	
Total Flow	0.4000	0.4000	mL/min
B. Conc	10.0	10.0	%
Pump A Flow			mL/min
Pump B Flow			mL/min
Pump A Press	0.0		MPa
Pump B Press	0.0		MPa
Pump A Degas	Not Conn		kPa
Pump B Degas	-94		kPa
Oven Temperat	25.0	40	C
Temperature	160	160	C
Vial No. Out			
Injection Vo			uL
Nebulizing G	1.5	1.5	L/min
Drying Gas F	10.0	10.0	L/min
Heating Gas	5.0	5.0	L/min
Interface	ESI		
Interface Vo		0.0	kV
Interface Cu	0.4		uA
Interface Te	100	100	C
DL Temperatu	250	250	C
Heat Block T	400	400	C
Conversion D		0.0	kV
Detector Vol		0.00	kV
IG Vacuum	2.0e+003		Pa
PG Vacuum	1.3e+002		Pa
CID Gas	230	230	kPa

C: 39.5GB Free

设置自动排液参数

Realtime Analysis (LCMS-8045-System Administrator) - [Data Acquisition - Method1.lcm]

File Edit View Method Instrument Acquisition Data Tools Window Help

LCReady MSReady

Instrument Parameters View

Model: SIL-30AC Autosampler

Purge

1st: Mobile Phase A

2nd: Mobile Phase B

3rd: None

4th: None

Autosampler:

Measuring: Default RO

Rinse Port: R1

R2

Default RO

Init. Conc.-Replace: 5 min

Warm up

Exit: 0 min

Total Flow: 0.0000 mL/min

✓ Activate system after AutoPu

Purging Pump

Pump A: LC-30AD

Pump B: LC-30AD

Detail...

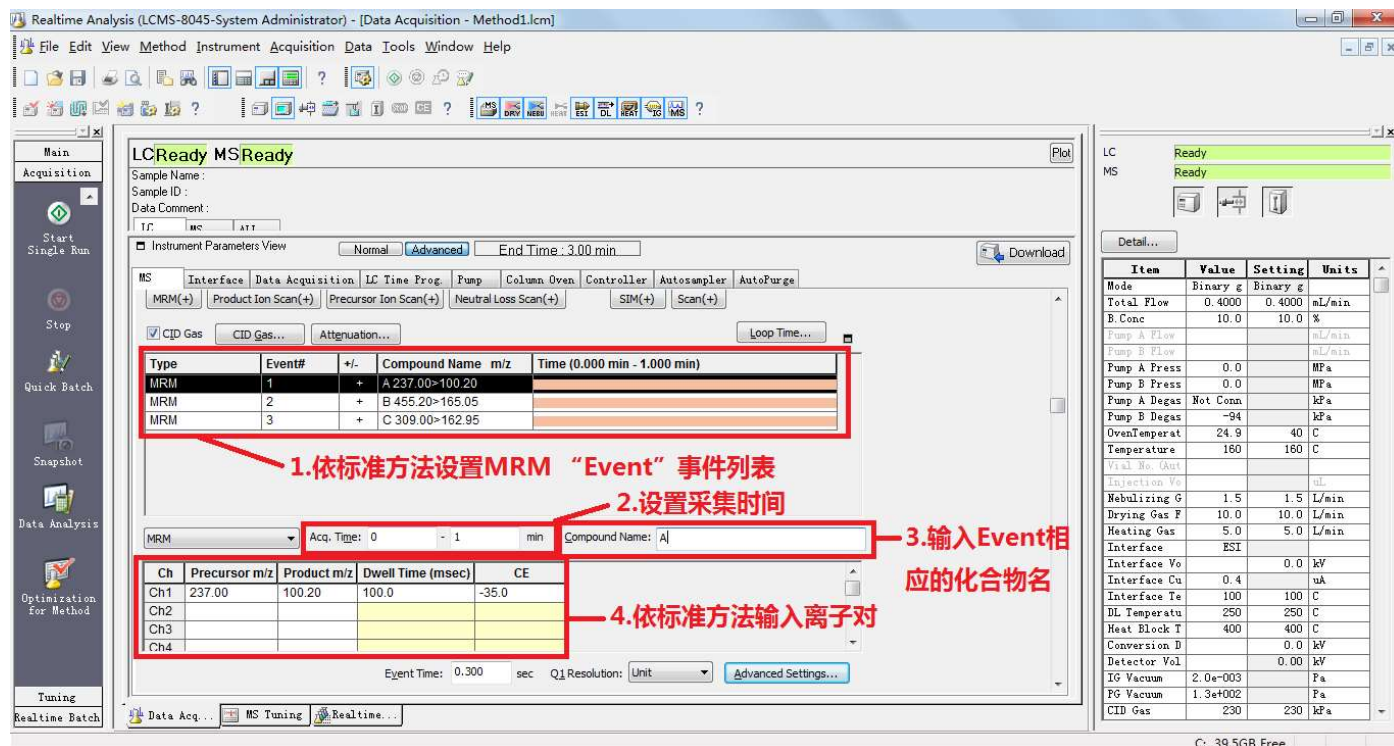
Item	Value	Setting	Units
Mode	Binary g	Binary g	
Total Flow	0.4000	0.4000	mL/min
B. Conc	10.0	10.0	%
Pump A Flow			mL/min
Pump B Flow			mL/min
Pump A Press	0.0		MPa
Pump B Press	0.0		MPa
Pump A Degas	Not Conn		kPa
Pump B Degas	-94		kPa
Oven Temperat	25.0	40	C
Temperature	160	160	C
Vial No. Out			
Injection Vo			uL
Nebulizing G	1.5	1.5	L/min
Drying Gas F	10.0	10.0	L/min
Heating Gas	5.0	5.0	L/min
Interface	ESI		
Interface Vo		0.0	kV
Interface Cu	0.4		uA
Interface Te	100	100	C
DL Temperatu	250	250	C
Heat Block T	400	400	C
Conversion D		0.0	kV
Detector Vol		0.00	kV
IG Vacuum	2.0e+003		Pa
PG Vacuum	1.3e+002		Pa
CID Gas	230	230	kPa

C: 39.5GB Free

4.2 MRM 优化

- ◆ 指定离子优化方法参考如下程序，不指定离子优化方法请参考仪器使用说明书。
- ◆ 参考相应的标准方法设置 LC 及 MS 参数。
- ◆ MRM 优化使用标准样品量 LCMS8030/8040 约为 1ng (1ug/mL,进样 1uL), LCMS-8045/8050/8060 约为 0.1ng (0.1ug/mL,进样 1uL) (相关浓度与离子化效率相关)。采用 LC 自动进样器进样，二通代替色谱柱。

创建“Event”，依标准方法输入相关的离子对信息



1. 依标准方法设置MRM “Event” 事件列表

2. 设置采集时间

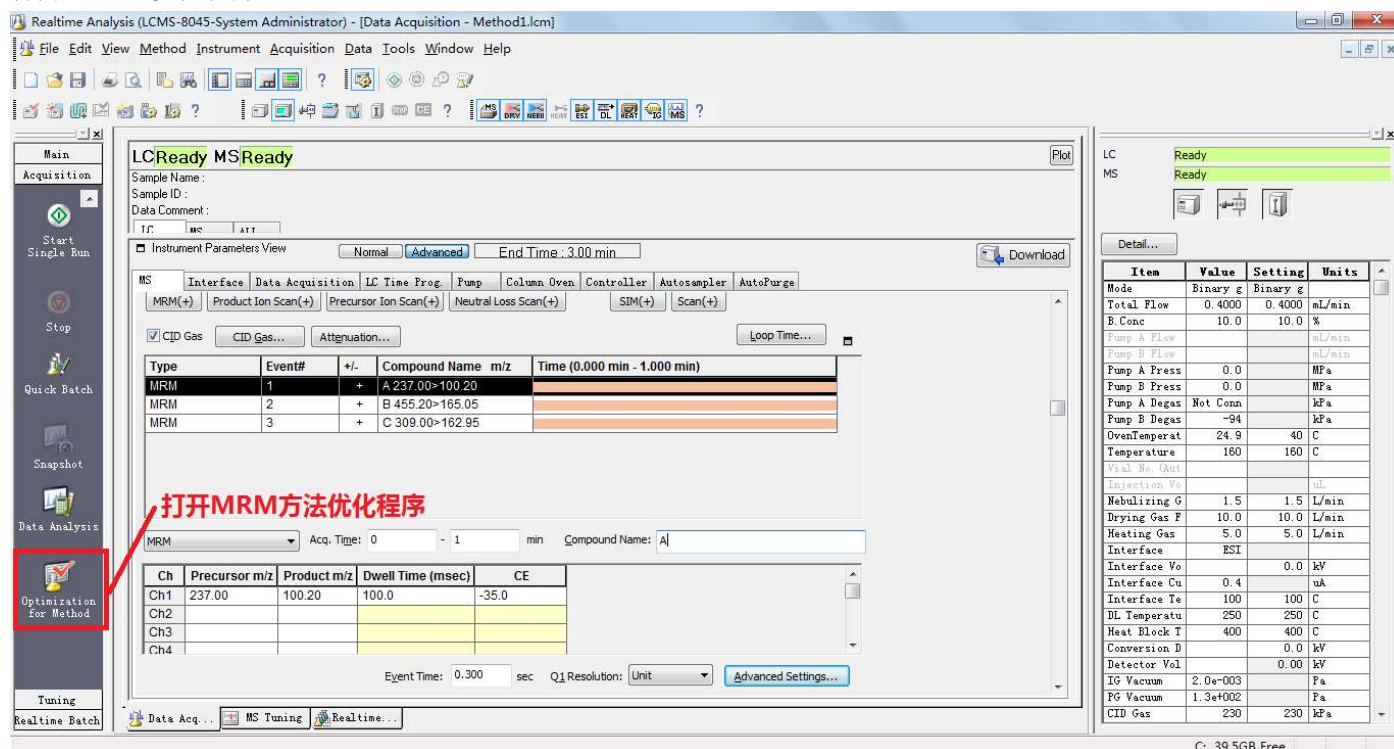
3. 输入Event相应的化合物名

4. 依标准方法输入离子对

Type	Event#	+/-	Compound Name	m/z	Time (0.000 min - 1.000 min)
MRM	1	+	A	237.00-100.20	
MRM	2	+	B	455.20-165.05	
MRM	3	+	C	309.00-162.95	

Ch	Precursor m/z	Product m/z	Dwell Time (msec)	CE
Ch1	237.00	100.20	100.0	-35.0
Ch2				
Ch3				
Ch4				

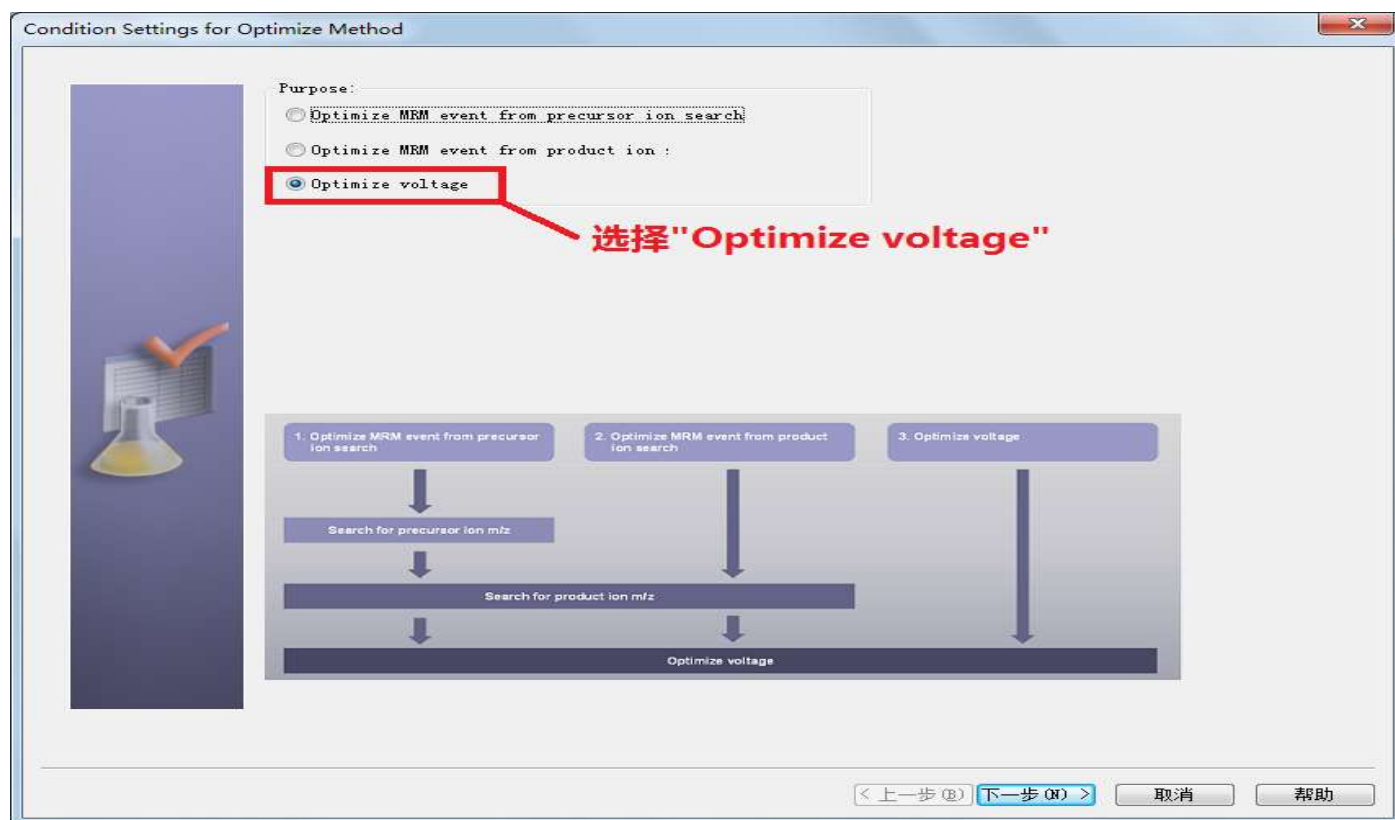
打开 MRM 优化程序



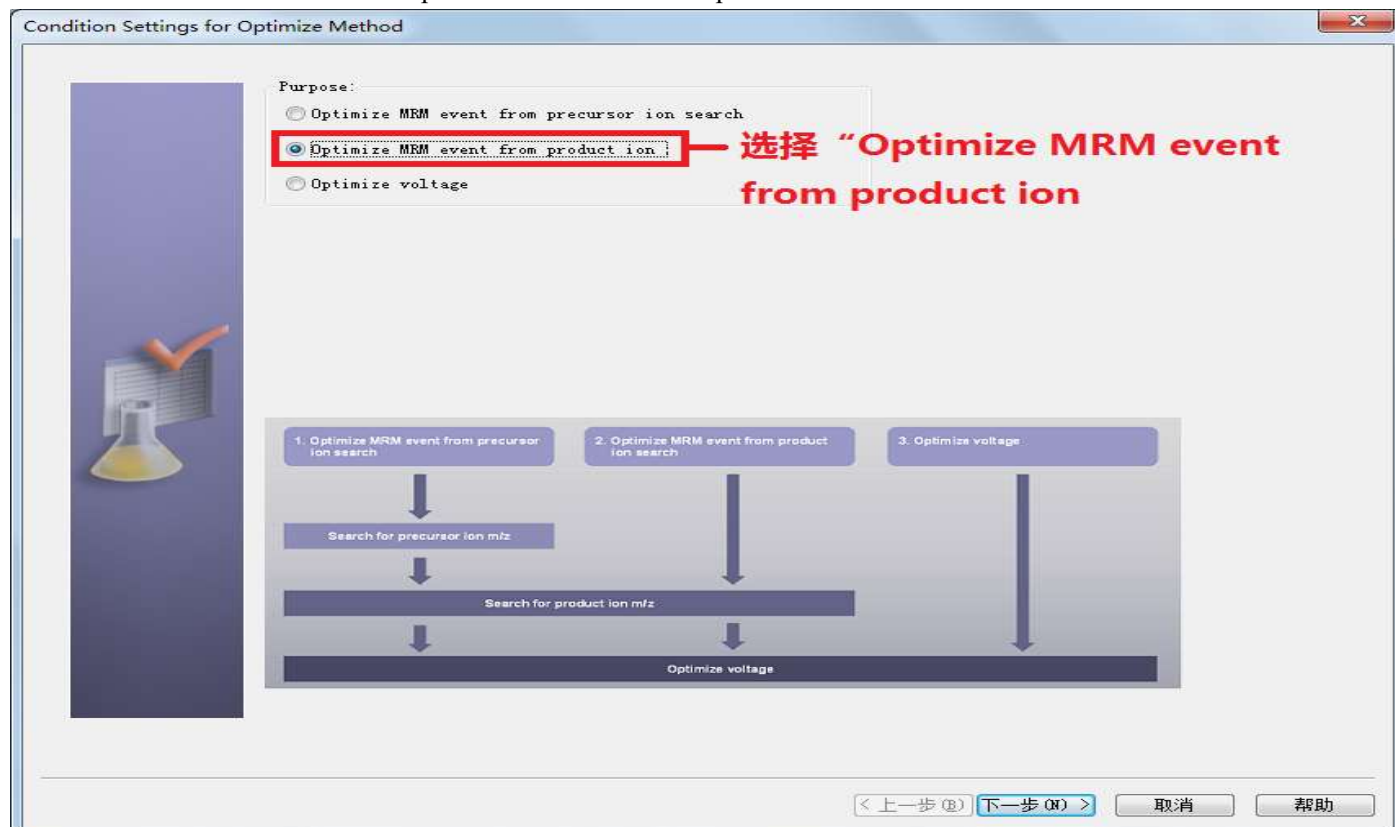
打开MRM方法优化程序

选择相应的 MRM 优化方式

指定离子对选择“Optimize voltage”



指定母离子不指定子离子选择 “Optimize MRM event from product ion”



指定离子对方法优化参数

Condition Settings for Optimize Method

Method File: Method1.lcm Max Loop 0.27 sec Predicted end 12.00 min

☐ Adjust Precursor m/z

☒ Optimize Voltage **1.选择 "Optimize Voltage"**

☐ Adjust Product m/z

ID	Target	Description	Sample ID	Vial#	Tray	In
1	☒	MRM (+) A 237.00>100.20		1	1	1.0
2	☒	MRM (+) B 455.20>165.05		1	1	1.0
3	☒	MRM (+) C 309.00>162.95		1	1	1.0

2.设置相应的样品进样信息

Output Folder: C:\LabSolutions\Data\Project1\ **3.优化方法及数据存储路径**

☒ Apply to method file **4.优化结果应用于当前方法**

☐ Create new method files by every eve

C:\LabSolutions\Data\Project1\

☐ Shutdown after optimizati **5.优化完成后是否关闭LCMS系统**

< 上一步(B) Start 取消 帮助

指定母离子不指定子离子方法参数优化

Condition Settings for Optimize Method

Method File: Method1-mrm.lcm Max Loop Time 0.82 sec Predicted end 12.00 min

☐ Check for Precursor :

☐ Adjust Precursor m/z

☒ Optimize Voltage **1.选择 "Optimize Voltage"**

☒ Auto select product

☐ Adjust Product m/z

at same time...

#	Target	Compound Name	Precursor m/z	+/-	Start (min)	End (min)	Sample ID	Vial#	Tray	In
1	☒	A	237.00	+	0.000	1.000		1	1	1.0
2	☒	B	455.20	+	0.000	1.000		1	1	1.0
3	☒	C	309.00	+	0.000	1.000		1	1	1.0

2.设置相应的样品进样信息

Output Folder: C:\LabSolutions\Data\Project1\ **3.优化方法及数据文件存储路径**

☒ Apply to method fi **4.优化结果应用于当前方法**

☐ Save new method fil

C:\LabSolutions\Data\Project1\Method1-mrm_201707061717.lcm

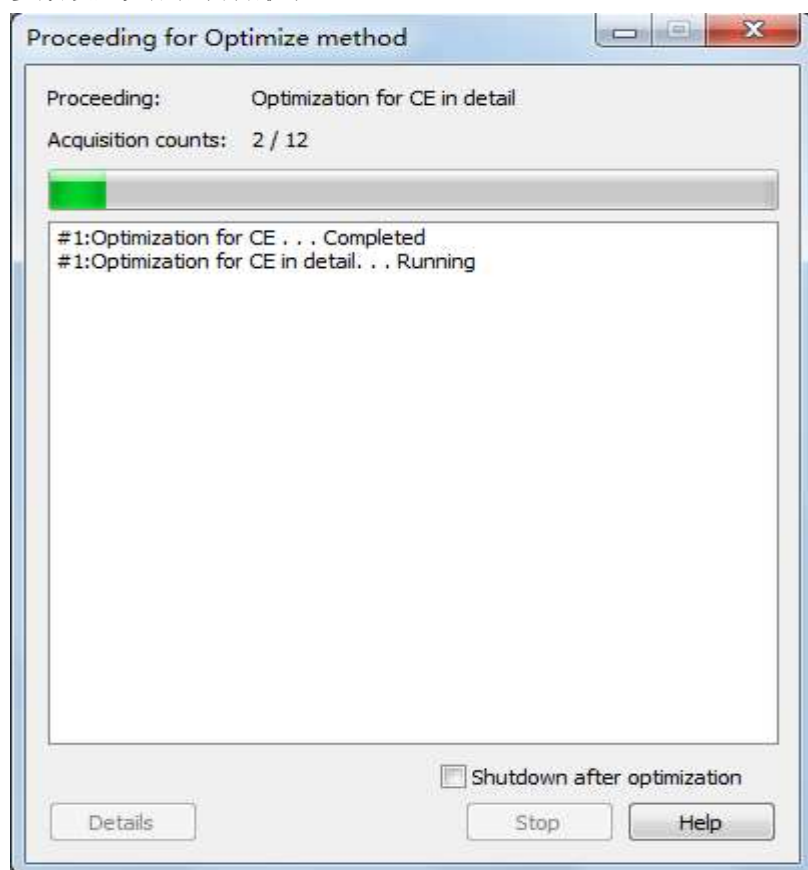
☐ Create new method files by every event

C:\LabSolutions\Data\Project1\ ☐ The setting is reflected without opti

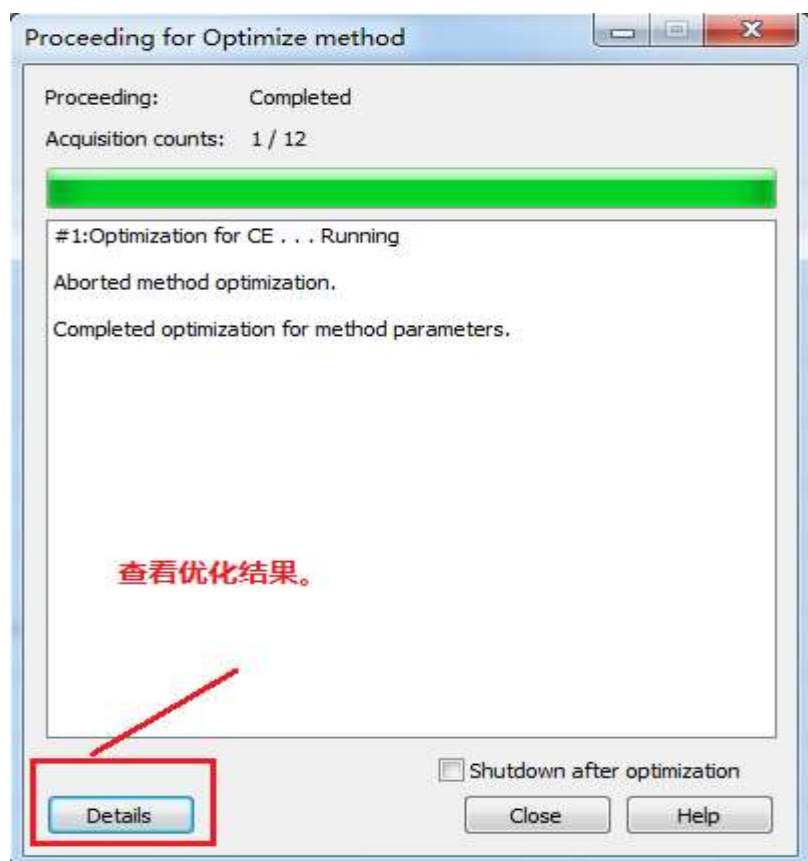
☐ Shutdown after optimizati **5.优化完成后是否关闭LCMS系统**

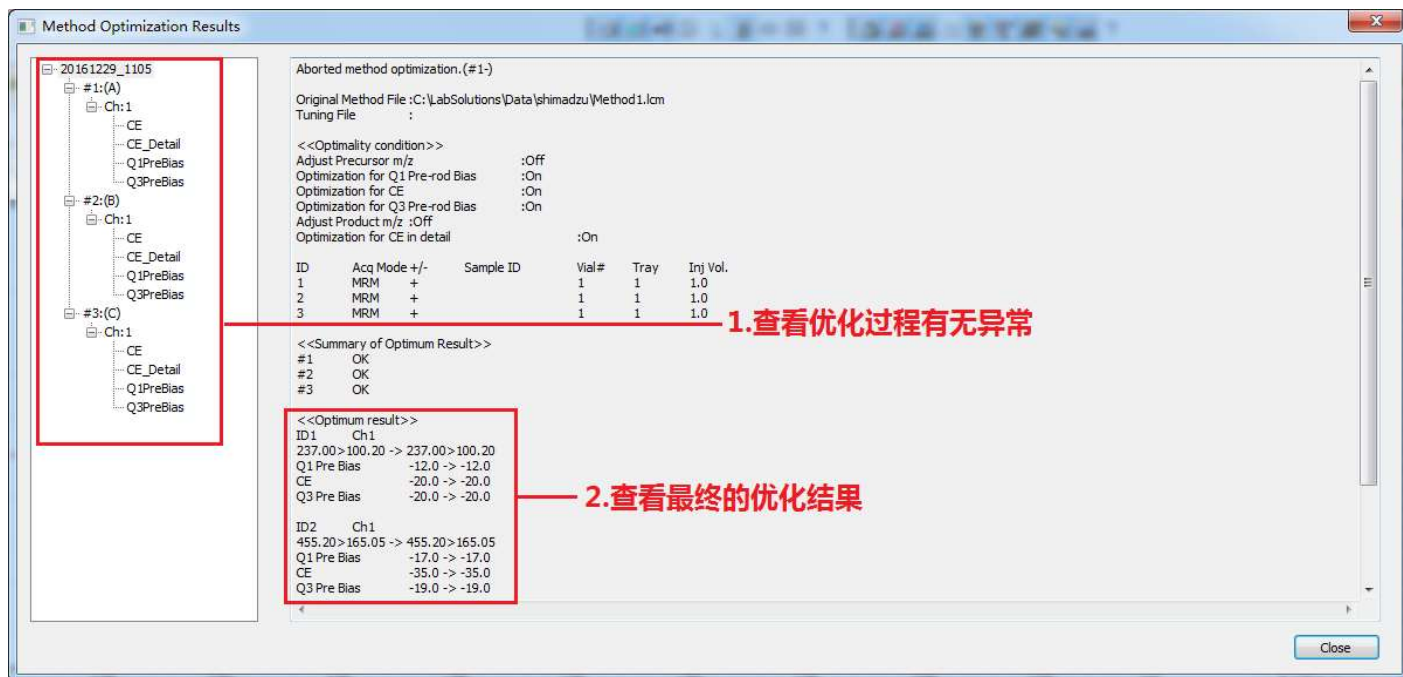
< 上一步(B) Start 取消 帮助

参数设置完成后开始优化



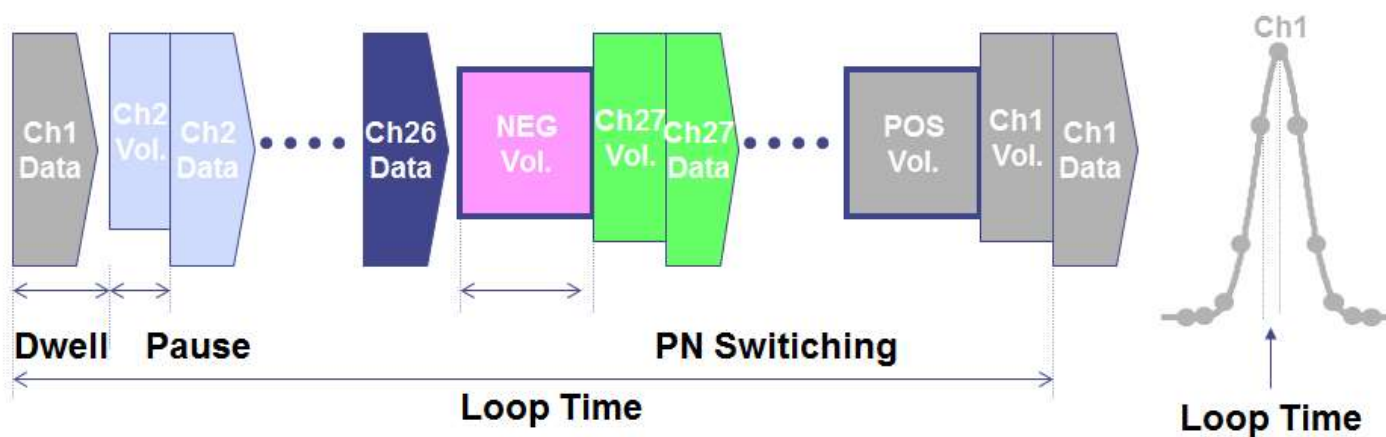
优化完成后查看结果





4.3 Loop Time 参数优化

Loop Time 含义



打开 Dwell Time Calculation/Loop Time 窗口

Realtime Analysis (LCMS-8045-System Administrator) - [Data Acquisition - Method1.lcm, 1_A_CE_Select.lcd]

File Edit View Method Instrument Acquisition Data Tools Window Help

Main Acquisition

Start Single Run

Stop

Quick Batch

Snapshot

Data Analysis

Optimization For Method

Tuning

Realtime Batch

LCReady MSReady

Sample Name: CE_Select #1 CE:50.000to10.00

Sample ID:

Data Comment:

LC MS ALL

0.015 Inten. 2.5 0.000 5.0 7.5 10.0 12.5 15.0 17.5 min

Instrument Parameters View

Normal Advanced End Time: 3.00 min

Download

MS Interface Data Acquisition LC Time Prog. Pump Column Oven Controller Autosampler AutoPurge

Positive Negative End Time: 2.500 min MS Program Edit Valve and MS Program...

MRM(+), Product Ion Scan(+), Precursor Ion Scan(+), Neutral Loss Scan(+), SIM(+), Scan(+)

CID Gas CID Gas... Attenuation...

Loop Time...

Type Event# +/- Compound Name m/z Time (0.000 min - 2.500 min)

Type	Event#	+/-	Compound Name	m/z	Time (0.000 min - 2.500 min)
MRM	1	+	A 237.00>100.20		
MRM	2	+	B 455.20>165.05		
MRM	3	+	C 309.00>162.95		

MRM Acq. Time: 0 - 2.5 min Compound Name: A

Ch	Precursor m/z	Product m/z	Dwell Time (msec)	Q1 Pre Bias(V)	CE	Q3 Pre Bias(V)
Ch1	237.00	100.20	100.0	-12.0	-20.0	-20.0
Ch2						

LC MS Ready

Detail...

Item	Value	Setting	Units
Mode	Binary g	Binary g	
Total Flow	0.4000	0.4000	mL/min
B. Conc	8.0	8.0	%
Pump A Flow			mL/min
Pump B Flow			mL/min
Pump A Press	24.0		MPa
Pump B Press	23.9		MPa
Pump A Degas	Not Conn		kPa
Pump B Degas	-94		kPa
OvenTemperat	40.0	40	C
Temperature	90	90	C
Vial Se. Gask			
Injection Va			nl
Nebulizing G	3.0	3.0	L/min
Drying Gas F	10.0	10.0	L/min
Heating Gas	10.0	10.0	L/min
Interface	ESI		
Interface Vo		4.0	kV
Interface Cu	12.8		uA
Interface Te	300	300	C
DL Temperatu	250	250	C
Heat Block T	400	400	C
Conversion D		10.0	kV
Detector Vol		2.28	kV
IG Vacuum	2.0e+003		Fa
FG Vacuum	1.3e+002		Fa
CID Gas	230	230	kPa

C: 39.5GB Free

输入合适的 Loop Time 计算 Dwell Time

Dwell Time Calculation/Loop Time

Maximum Loop Time

Target Value: 0.309 sec

Calculate Dwell Time

1.依据峰宽设置Loop time, 保障每个色谱有15-20个扫描点。

Start - End Time(min)	Event	Loop Time(sec)	Dwell Time(msec)
0.000 - 2.500	3	0.309	100.0

2.点击计算最新dwell time。

Maximum Event: 3 Maximum Loop Time(sec): 0.309

Minimum Dwell Time(msec): 100.0

Maximum Dwell Time(msec): 100.0

3.应用于方法。

Apply to Method Close

更新方法组分表，保存 MRM 方法

Realtime Analysis (LCMS-8050-System Administrator) - [Data Acquisition - Method1.lcm]

File Edit View Method Instrument Acquisition Data Tools Window Help

Instrument Parameters

- Baseline Check Parameters...
- Data Processing Parameters(MS)...
- MS Data View Parameters...
- QA/QC Parameters(MS)...
- System Suitability Settings...
- Optimization for Method...
- Optimization Result...
- Add MRM event...
- Update MRM event time by compound table...
- Update compound table m/z by MRM event...
- Update display sequence by compound table...
- Export Compound Table...
- Import Compound Table...

2.保存方法文件。

1.通过MRM event更新组分表。

End Time: 3.00 min

Column Oven Controller Autosampler AutoPurge

min MS Program Edit Valve and MS Program...

MRM(+), Product Ion Scan(+), Precursor Ion Scan(+), Neutral Loss Scan(+), SIM(+), Scan(+)

☒ CID Gas CID Gas... Attenuation... Loop Time...

Type	Event#	+/-	Compound Name	m/z	Time (0.000 min - 2.500 min)
MRM	1	+	A	237.00>100.20	
MRM	2	+	B	455.20>165.05	
MRM	3	+	C	309.00>162.95	

MRM Acq. Time: 0 - 2.5 min Compound Name: A

Ch Precursor m/z Product m/z Dwell Time (sec) A1 Dwell A1 CF A3 Dwell A3

Update compound table m/z by MRM/SIM event.

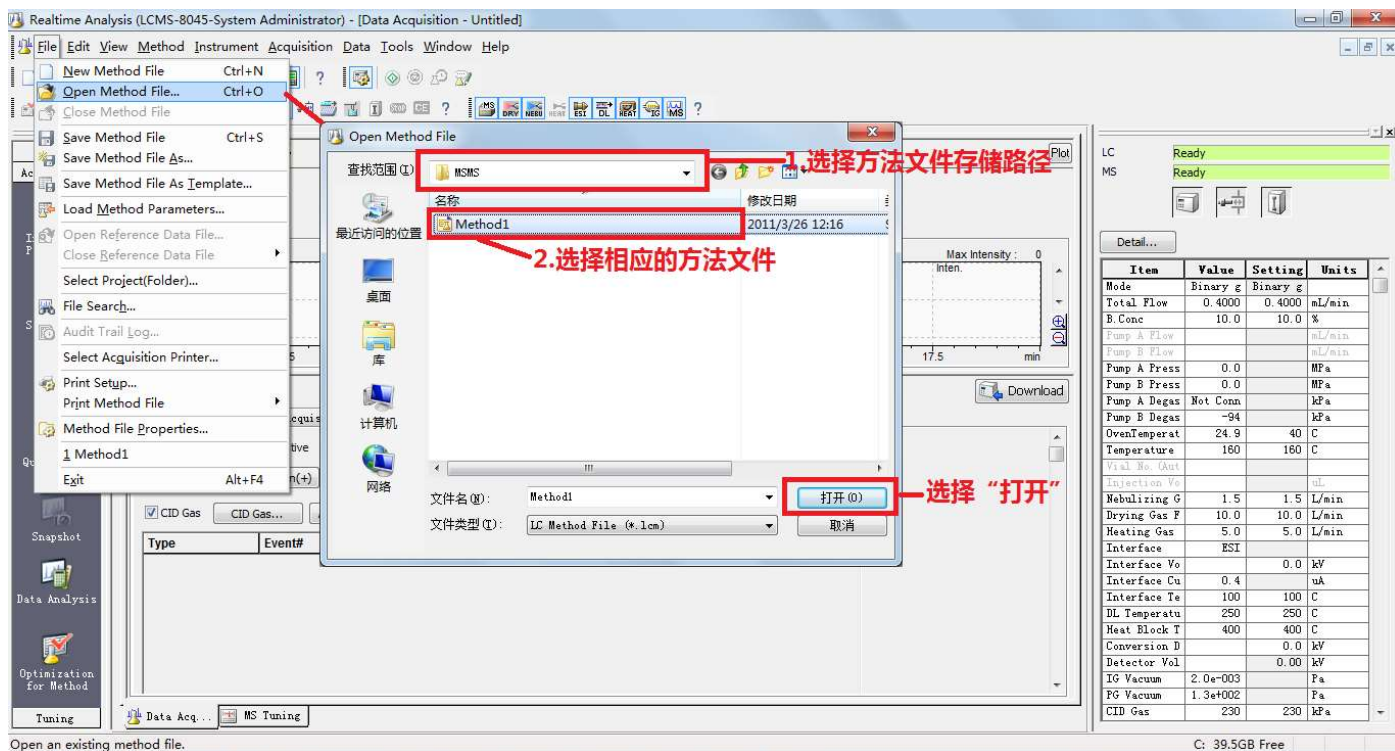
LC Not Connected
MS Not Connected

Detail...

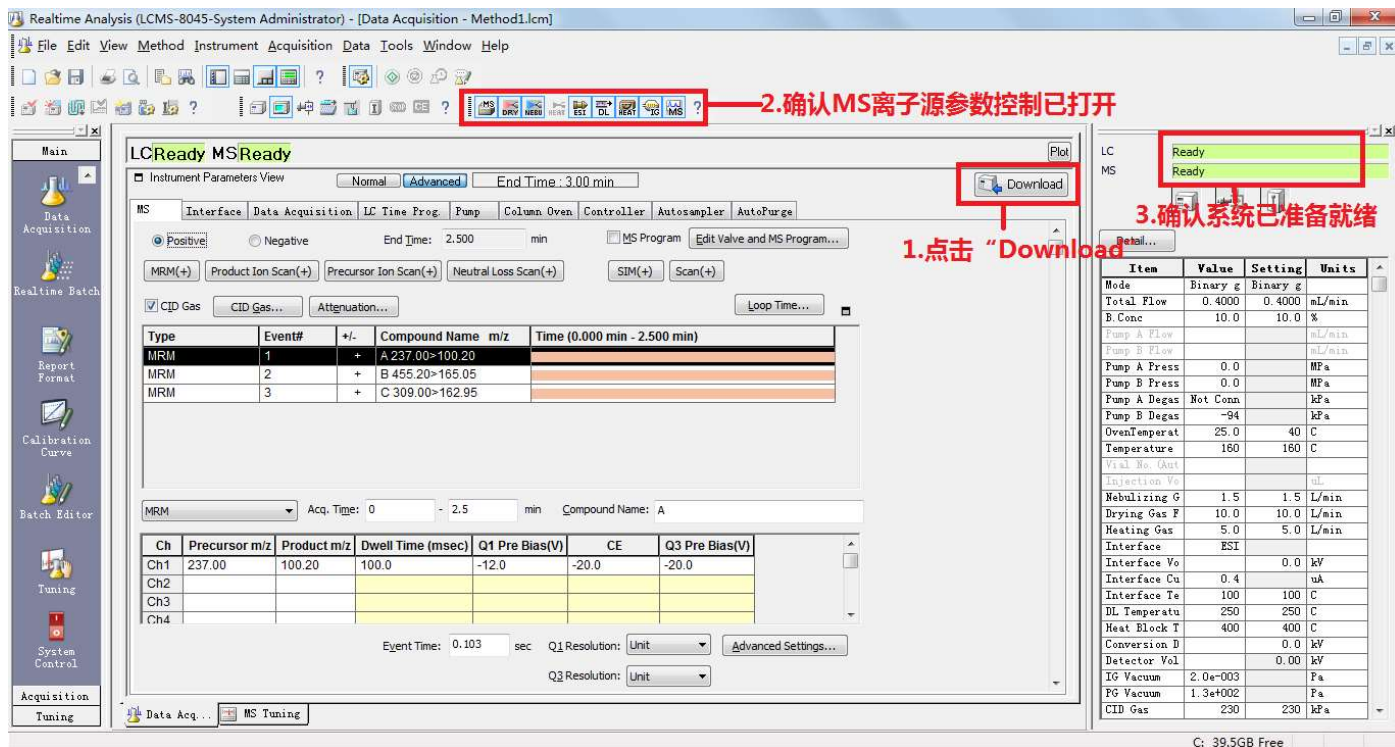
Item	Value	Setti	Units
Mode			
Total Flow			sL/min
B Conc			%
Pump A Flow			sL/min
Pump B Flow			sL/min
Pump A Pressure			MPa
Pump B Pressure			MPa
Pump A Temperature			°C
Pump B Temperature			°C
Injection			sL
Reboiler			L/min
Drying Gas			L/min
Heating Gas			L/min
Interface			
Interface			kV
Interface			mA
Interface			°C
DL Temper			°C
Heat Elec			°C
Conversion			kV
Detector			kV
IG Vacuum			Ts
FG Vacuum			Ts
CID Gas			MPa

5. 样品测试

打开相应的方法文件

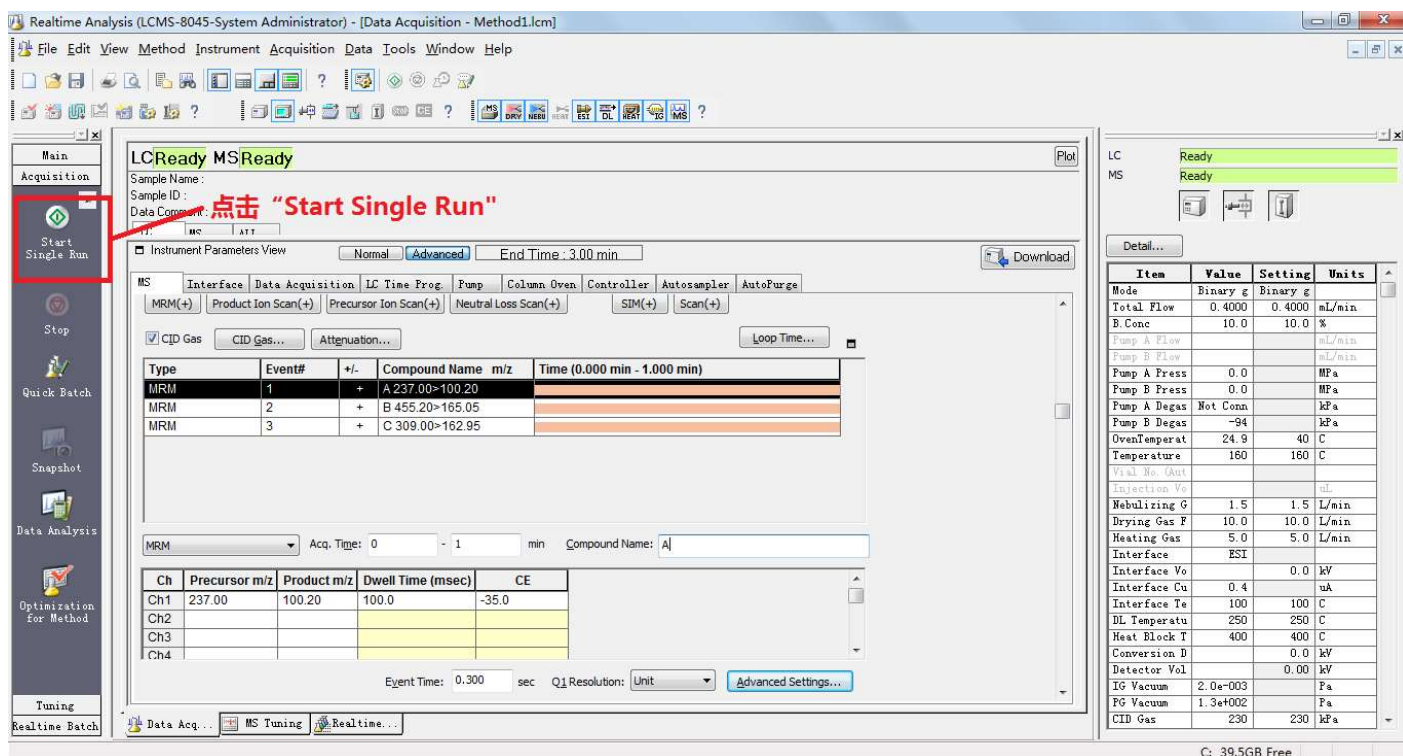


等待系统准备就绪

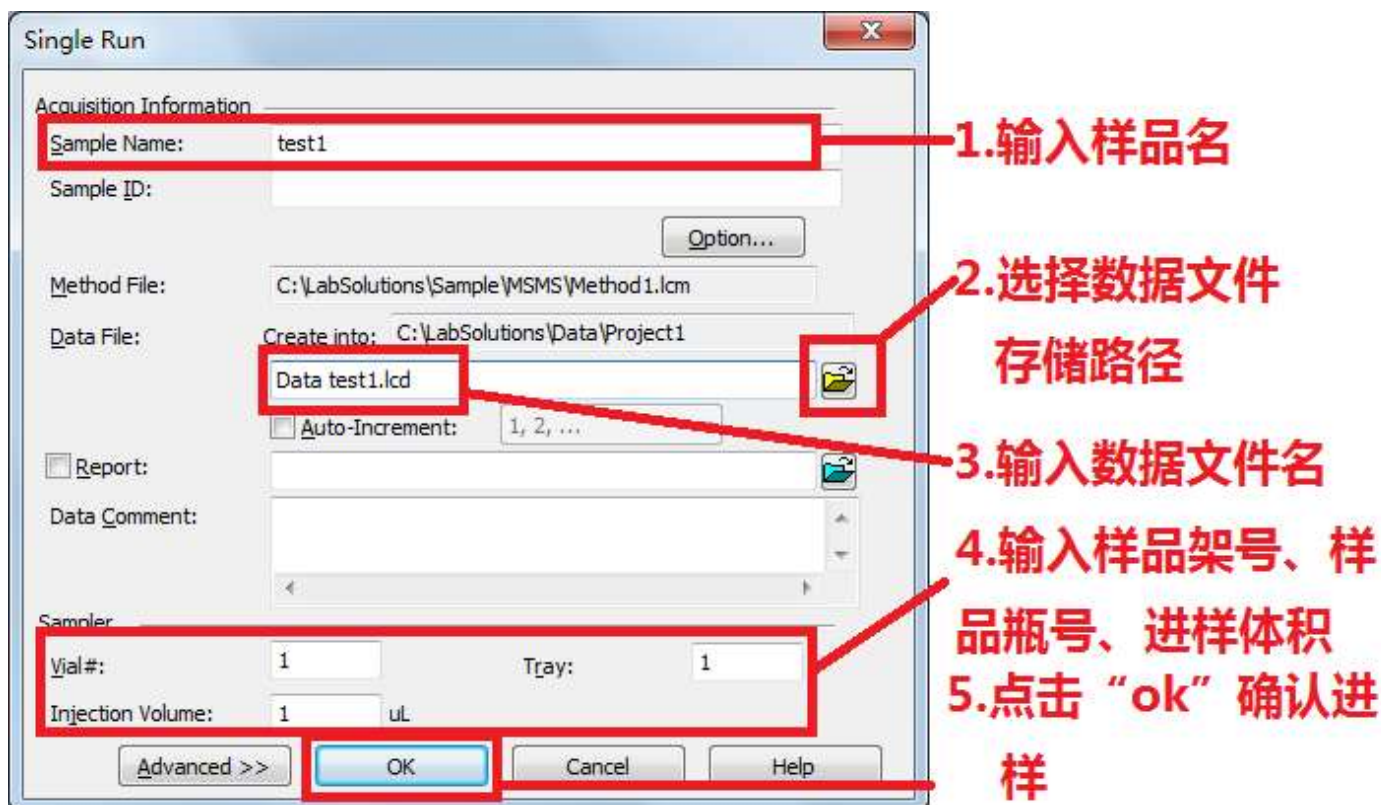


5.1 单次分析

打开单次分析登录窗口



样品信息输入

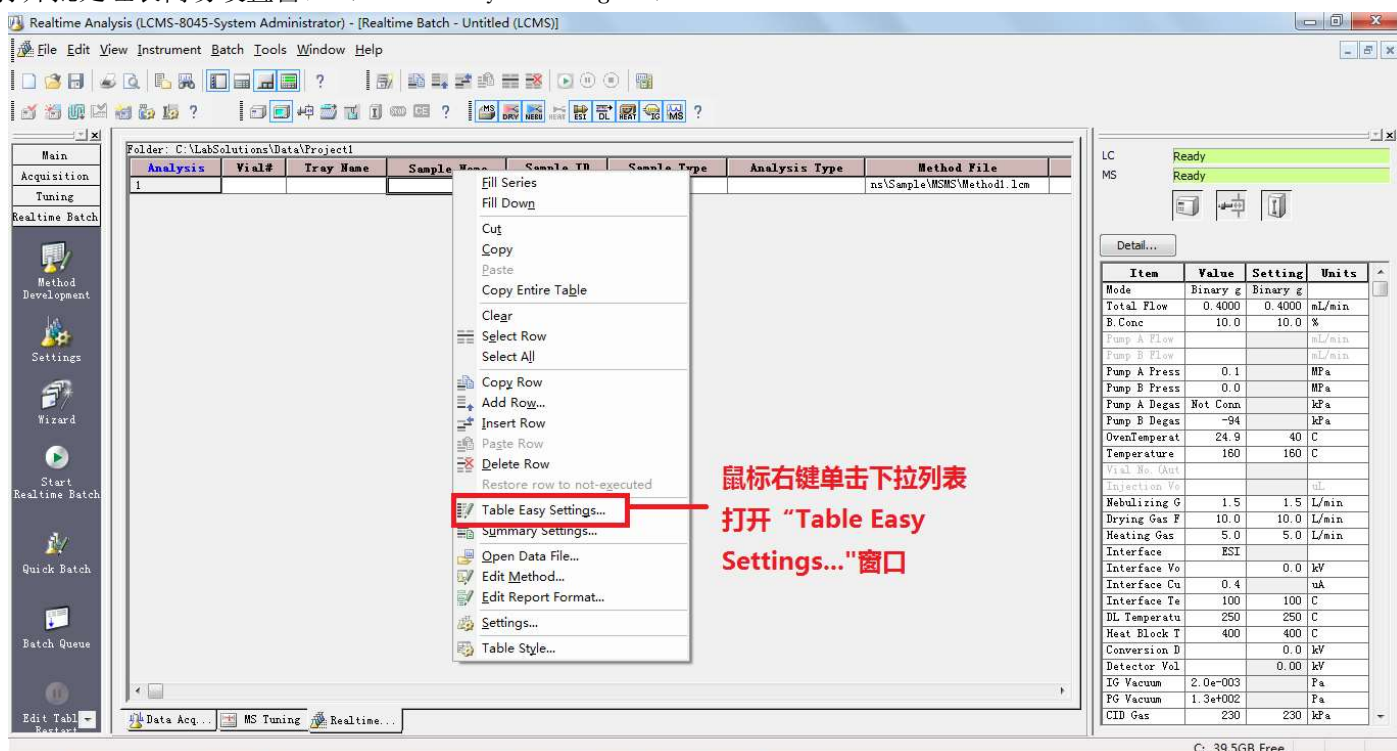


5.2 批处理分析

打开批处理窗口

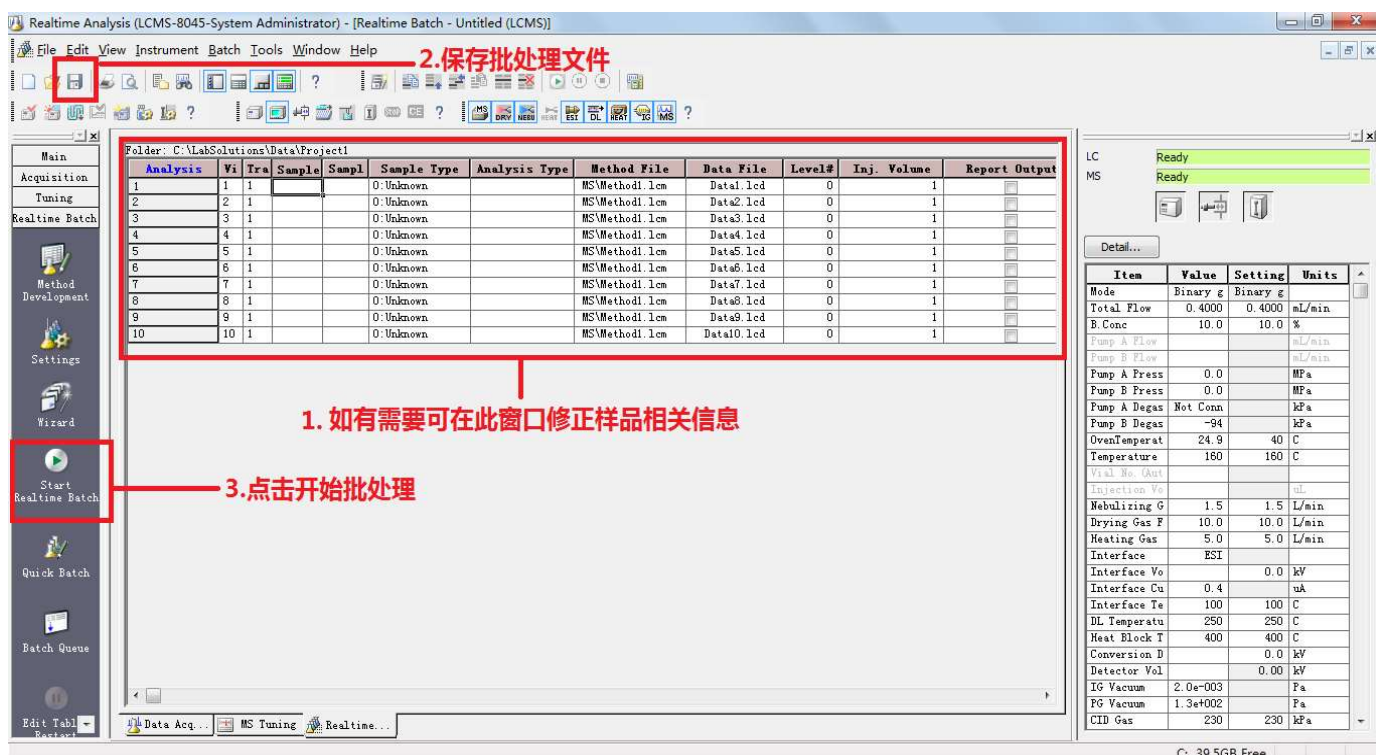


打开批处理表简易设置窗口 (Table Easy Settings...)





在如下窗口中可再次编辑相应的样品信息

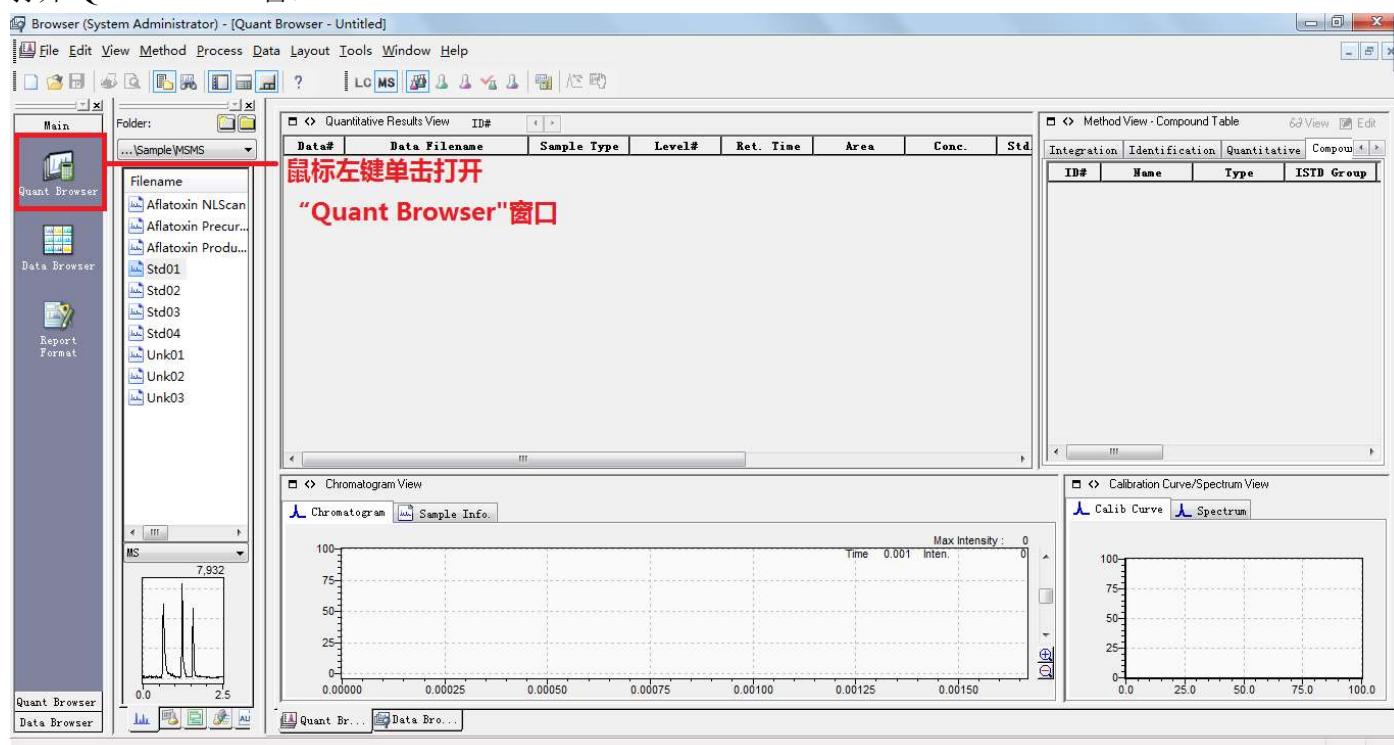


6. 标准曲线的建立

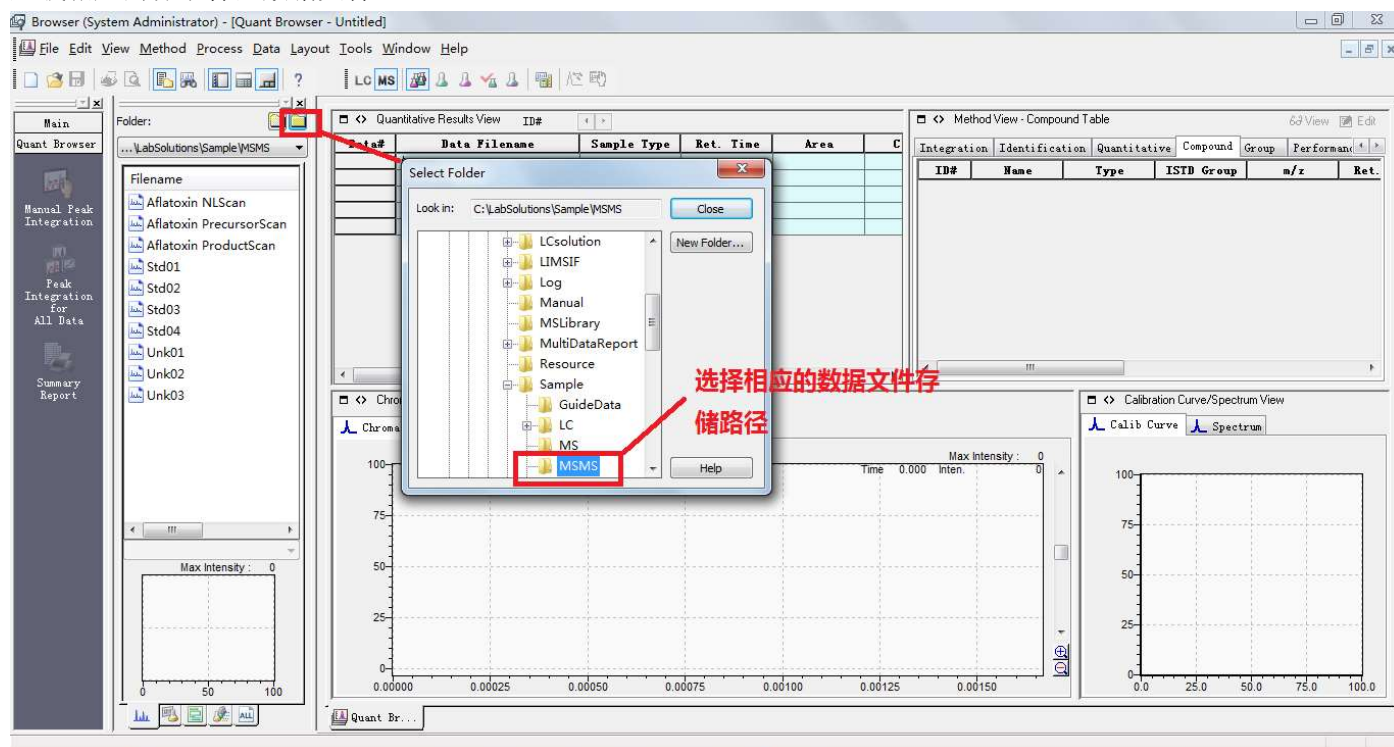
打开“Browser”窗口：



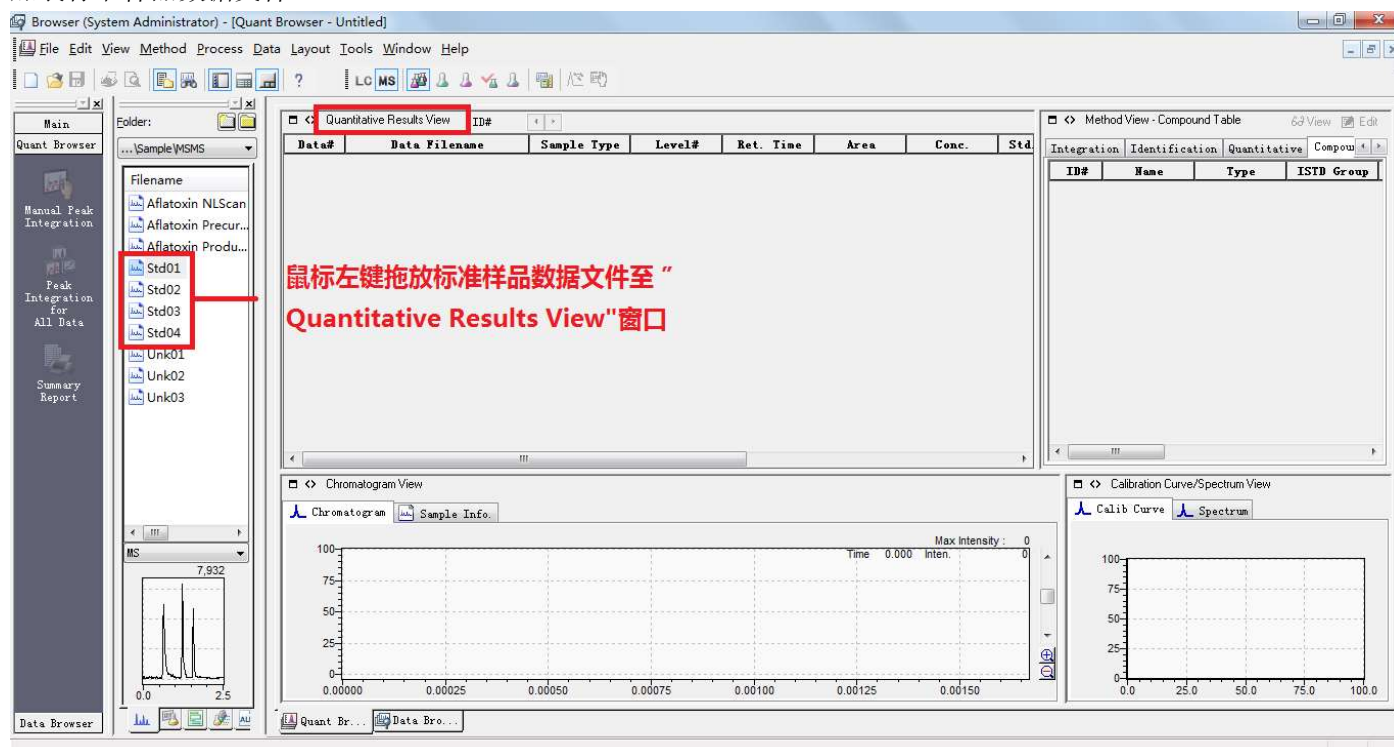
打开“Quant Browser”窗口



加载相应的标准样品数据文件



加装标准样品数据文件



设置积分参数

1. 点击 "Edit"

在 "Integration" 窗口设置合适的积分参数，使目标化合物能够被正确积分

设置定性参数

在 "Identification" 窗口输入合适的定性参数

设置定量参数

Browser (System Administrator) - [Quant Browser - Method1.lcm]

File Edit View Method Process Data Layout Tools Window Help

LC MS

Folder: ...LabSolutions\Sample\MSMS

Filename

- Aflatoxin NLSan
- Aflatoxin PrecursorScan
- Aflatoxin ProductScan
- Std01
- Std02
- Std03
- Std04
- Unk01
- Unk02
- Unk03

Manual Peak Integration

Peak Integration For All Data

Summary Report

Quantitative Results View

Data#	Data Filename	Sample Type	Ret. Time
1	Std01.lcd	Unknown	-----
2	Std02.lcd	Unknown	-----
3	Std03.lcd	Unknown	-----
4	Std04.lcd	Unknown	-----
	Average		-----
	Maximum		-----
	Minimum		-----
	Std. Dev.		-----

在“Quantitative”窗口
输入合适的定量参数

Method View - Quantitative Parameters

Integration Identification Quantitative Compound Group Performance Spectrum Custom

Quantitative Method: External Standard

Unit: ppm

Calculated by: ☒ Area ☐ Height

Calibration Curve

of Calib. Levels: 4

Curve Fit Type: Linear

Zero: Not Forced

Weighting Method: 1/C²

Format of Concentration: ☐ Decimal Digits ☒ Significant Digits

Grouping Type: Not Used

Chromatogram View

Chromatogram Sample Info.

Max Intensity: 14,183

Time: 1.599 Inten. 77

Calibration Curve/Spectrum View

Calib Curve Spectrum

编辑化合物表信息

Browser (System Administrator) - [Quant Browser - Method1.lcm]

File Edit View Method Process Data Layout Tools Window Help

LC MS

Folder: ...LabSolutions\Sample\MSMS

Filename

- Aflatoxin NLSan
- Aflatoxin PrecursorScan
- Aflatoxin ProductScan
- Std01
- Std02
- Std03
- Std04
- Unk01
- Unk02
- Unk03

Manual Peak Integration

Peak Integration For All Data

Summary Report

Quantitative Results View

Data#	Data
1	Std01.lcd
2	Std02.lcd
3	Std03.lcd
4	Std04.lcd
	Average
	Maximum
	Minimum
	Std. Dev.

Method View - Compound Table

Integration	Identification	Quantitative	Compound	Group	Performance	Spectrum	Custom	QC Check
ID#	Name	Type	m/z	Ret. Time	Conc. (1)	Conc. (2)	Conc. (3)	Conc. (4)
1	A	Target	IC	0.001	1	1	1	1
2		Target	IC	0.001	1	1	1	1

1.输入化合物名 2.选择化合物类型 3.选择相应的“Event”

4.选择相应的定量离子对 5.输入相应的保留时间 6.输入相应的标准样品浓度

Chromatogram View

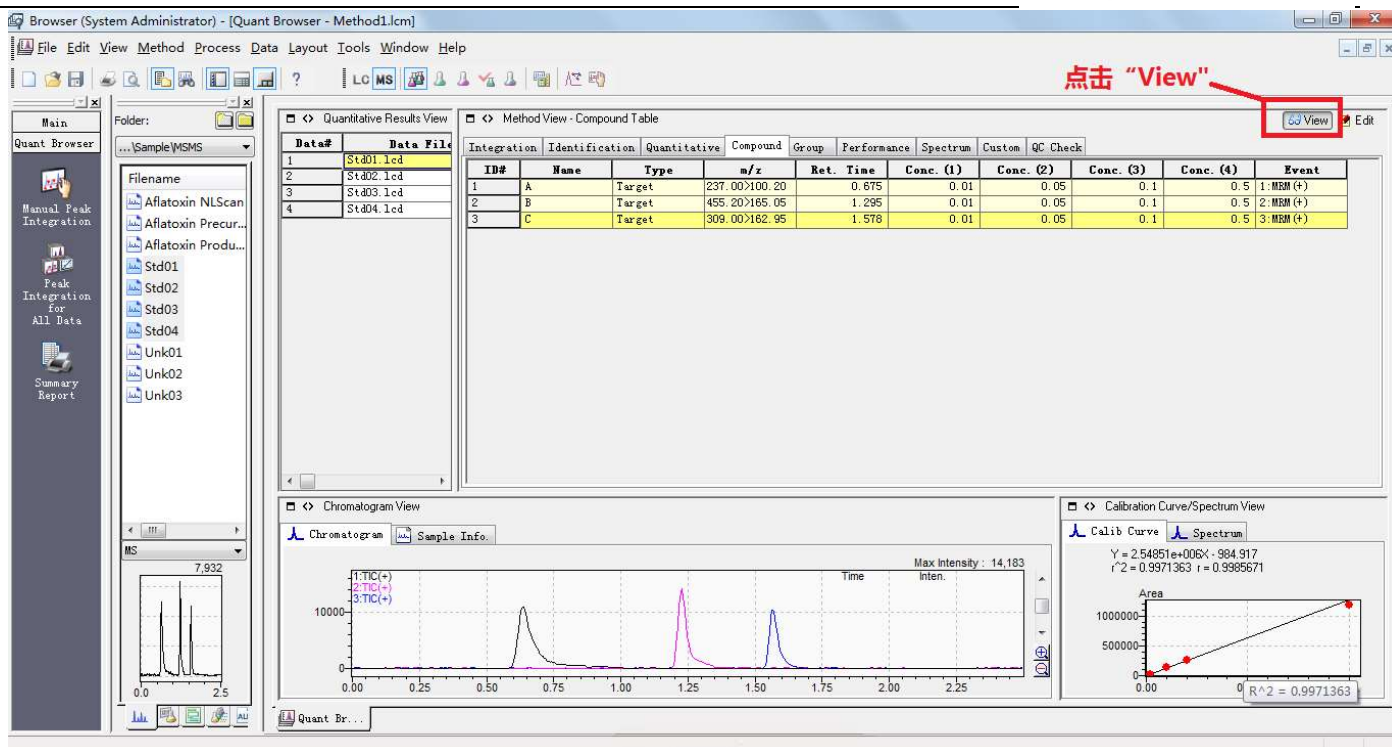
Chromatogram Sample Info.

Max Intensity: 14,183

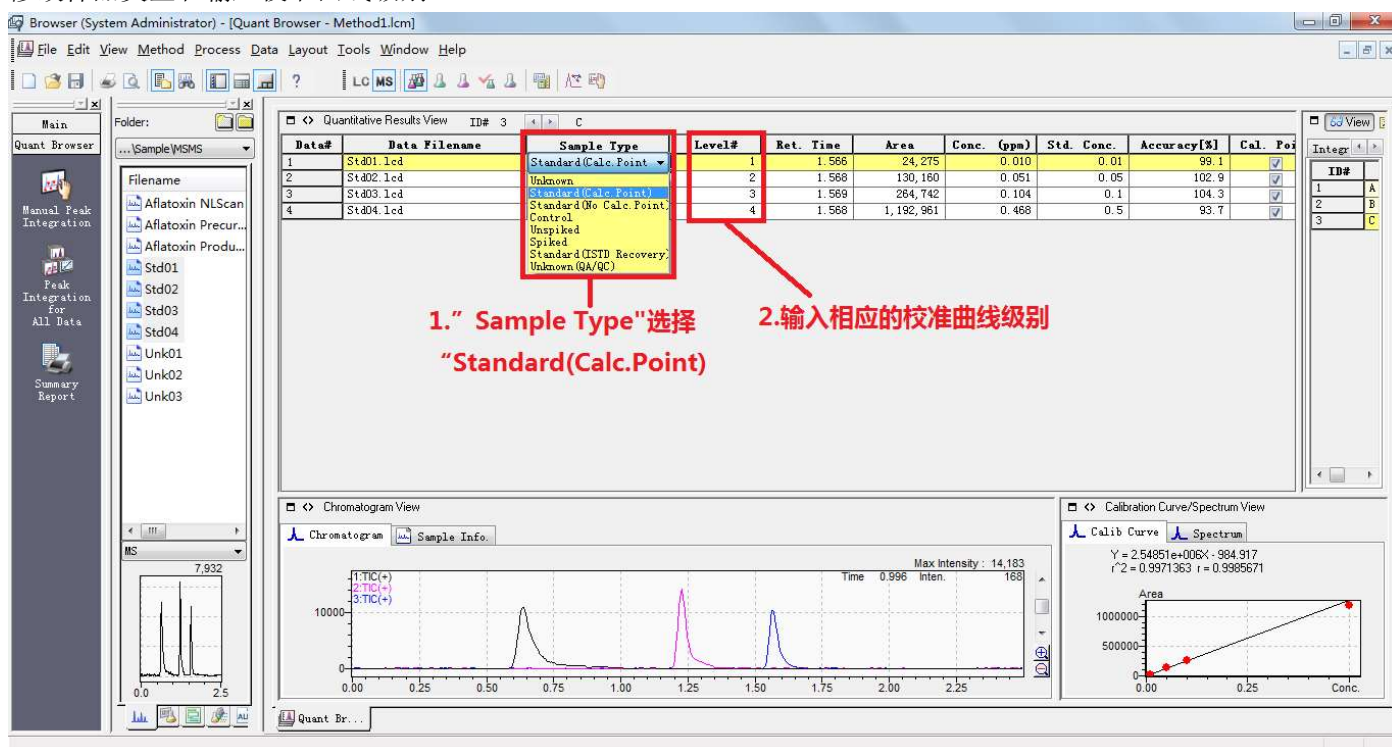
Time: 1.599 Inten. 77

Calibration Curve/Spectrum View

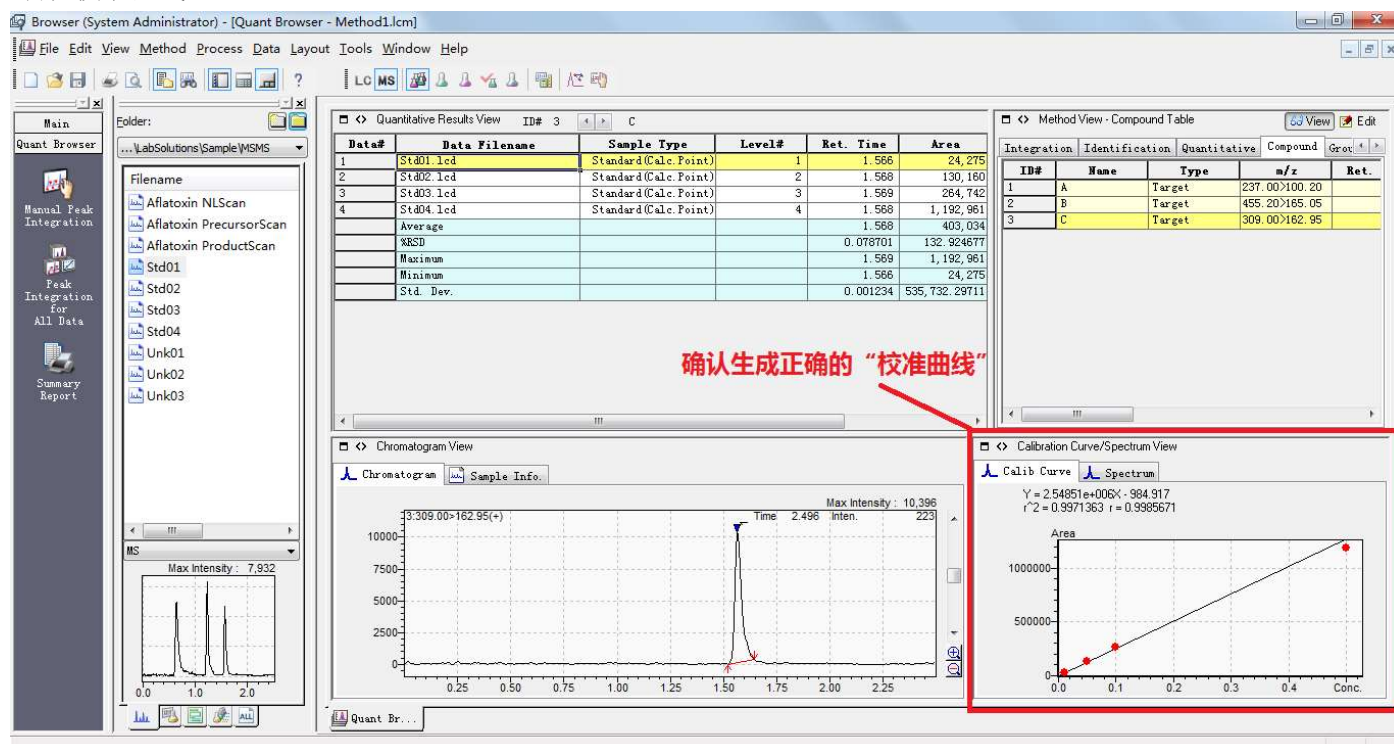
Calib Curve Spectrum



修改样品类型和输入校准曲线级别



确认校准曲线



7. 样品定量结果计算

Browser (System Administrator) - [Quant Browser - Method1.lcm]

File Edit View Method Process Data Layout Tools Window Help

LC MS

9. 点击保存

1. 鼠标左键拖放未知样品数据文件至 "Quantitative Results View" 窗口

2. 查看定量结果

Quantitative Results View ID# 1 A

Data#	Data File	Sample Type	Level#	Ret. Time	Area	Conc. (ppm)	Std. Conc.
1	Std01.lcd	Standard Calc. Poi	1	0.637	36,195	0.010	0.01
2	Std02.lcd	Standard Calc. Poi	2	0.646	187,076	0.048	0.05
3	Std03.lcd	Standard Calc. Poi	3	0.654	385,310	0.098	0.1
4	Std04.lcd	Standard Calc. Poi	4	0.649	2,095,553	0.527	0.5
5	Unk01.lcd	Unknown	0	---	---	---	---
6	Unk02.lcd	Unknown	0	0.670	109,936	0.029	---
7	Unk03.lcd	Unknown	0	0.631	1,333,401	0.336	---

Method View - Compound Table

ID#	Name	Type	m/z	Ret. Ti
1	A	Target	237.00>100.20	0
2	B	Target	455.20>165.05	1
3	C	Target	309.00>162.95	1

Chromatogram View

Chromatogram Sample Info

79,634

1.237.00>100.20(+)

25000

0.00 0.25 0.50 0.75 1.00 1.25 1.50 1.75 2.00 2.25

Time

Max Intensity: 31,530

Inten.

Calibration Curve/Spectrum View

Calib Curve Spectrum

Y = 3.98377e+006X - 4.014.10

r^2 = 0.9977929 r = 0.9988958

Area

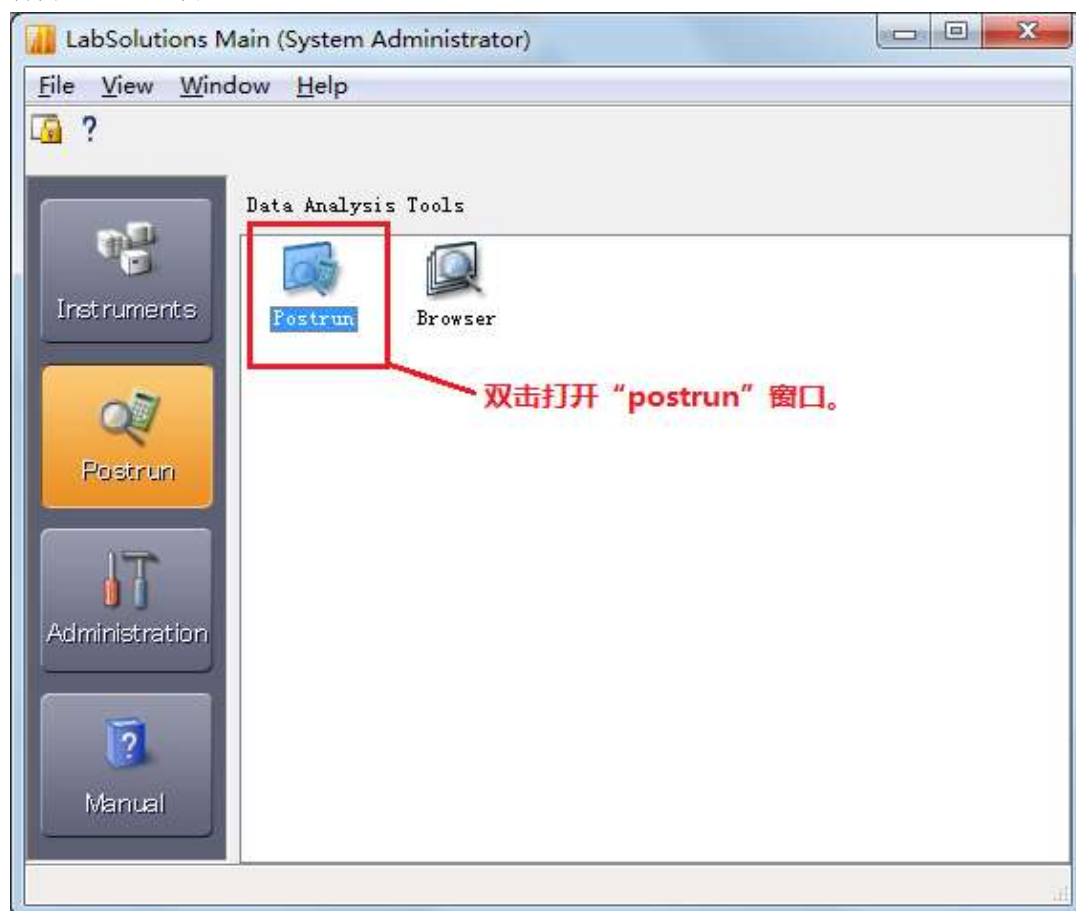
2000000

1000000

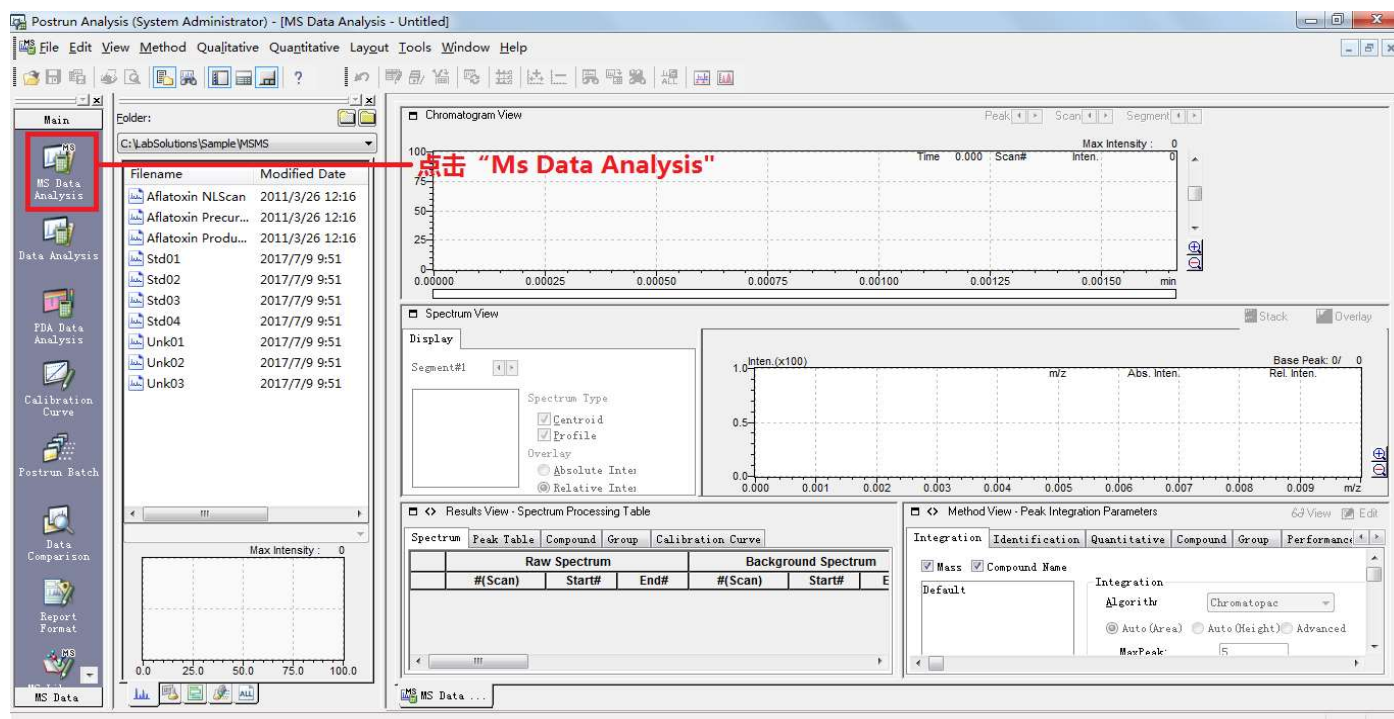
0.00 0.25 Conc.

8. 报告模板编辑

打开“Postrun”窗口



打开 “Ms Data Analysis”窗口



打开数据文件存储路径

打开数据文件存储路径

选择相应的数据文件储存文件夹

打开数据文件

1. 双击打开数据文件

2. 点击“Data Report”

Peak	Top Time	Start Time	End Time	Top Time	Start Time	End Time
1	---	0.381	0.391	0.386	0.340	---
2	---	1.217	1.227	1.222	1.181	---
3	---	1.569	1.579	1.574	1.523	---

选择需要输出的报告项目

1.选择需要在报告中显示的项目

2.鼠标左键空白处拖放合适大小窗口

保存报告模板

1.输入报告模板名

2.保存

Save the active report format file with a new name.

打印报告

Postrun Analysis (System Administrator) - [MS Data Analysis - Unk03.lcd]

File Edit View Method Qualitative Quantitative Layout Tools Window Help

Folder: C:\LabSolutions\Sample\MSMS

Filename	Modified Date
Aflatoxin NLSan	2011/3/26 12:16
Aflatoxin Precur...	2011/3/26 12:16
Aflatoxin Produ...	2011/3/26 12:16
Std01	2017/7/9 9:51
Std02	2017/7/9 9:51
Std03	2017/7/9 9:51
Std04	2017/7/9 9:51
Unk01	2017/7/9 9:51
Unk02	2017/7/9 9:51
Unk03	2017/7/9 9:51

1. 鼠标左键双击打开需要输出报告的数据文件

2. 点击 "Data Report"

Chromatogram View Segment#1

Max Intensity: 463,946

Spectrum View

Event# 1 MRM(D+) Ret. Time: [0.623>0.633][0.567<>0.932] Scan#: [364>370][331<>544]

Event# 2 MRM(D+) Ret. Time: [0.625>0.635][0.568<>0.934] Scan#: [365>371][332<>545]

Event# 3 MRM(D+) Ret. Time: [0.627>0.637][0.570<>0.936] Scan#: [366>372][333<>546]

Results View - Spectrum Processing Table

Spectrum	Raw Spectrum			Background Spectrum		
	Top Time	Start Time	End Time	Top Time	Start Time	End Time
1	---	0.623	0.633	0.628	0.567	---
2	---	1.217	1.227	1.222	1.181	---
3	---	1.564	1.574	1.569	1.523	---

Method View - Peak Integration Parameters

Integration Identification Quantitative Compound Group Performance

Mass Compound Name

Default

Algorithm Chromatopac

Auto (Area) Auto (Height) Advanced

MaxPeak: 5

Postrun Analysis (System Administrator) - [Data Report - Unk03.lcd(Report in Data File)]

File Edit View Item Layout Page Tools Window Help

Folder: C:\LabSolutions\Sample\MSMS

Filename	Modified Date
Report sample	2017/7/9 10:22
Report1	2011/3/26 12:16
Sample	2011/3/26 12:16
Summary1	2011/3/26 12:16

1. 鼠标左键拖放报告模板至空白处

2. 点击打印报告

2017/7/9 10:33:56 1/1

==== Shimadzu LabSolutions Analysis Report ====

Acquired by: 1

Sample Name: 7

Sample ID: 1

Injection Volume: 1

Data File: C:\LabSolutions\Sample\MSMS\Unk03.lcd

Method File: C:\LabSolutions\Sample\MSMS\Method1.lcm

Report Format File: C:\LabSolutions\System\DEFAULT.rsr

Month-Day Acquired: 2010/5/25

Month-Day Processed: 2017/7/9

<Chromatogram>

MS Chromatogram

(x100,000)

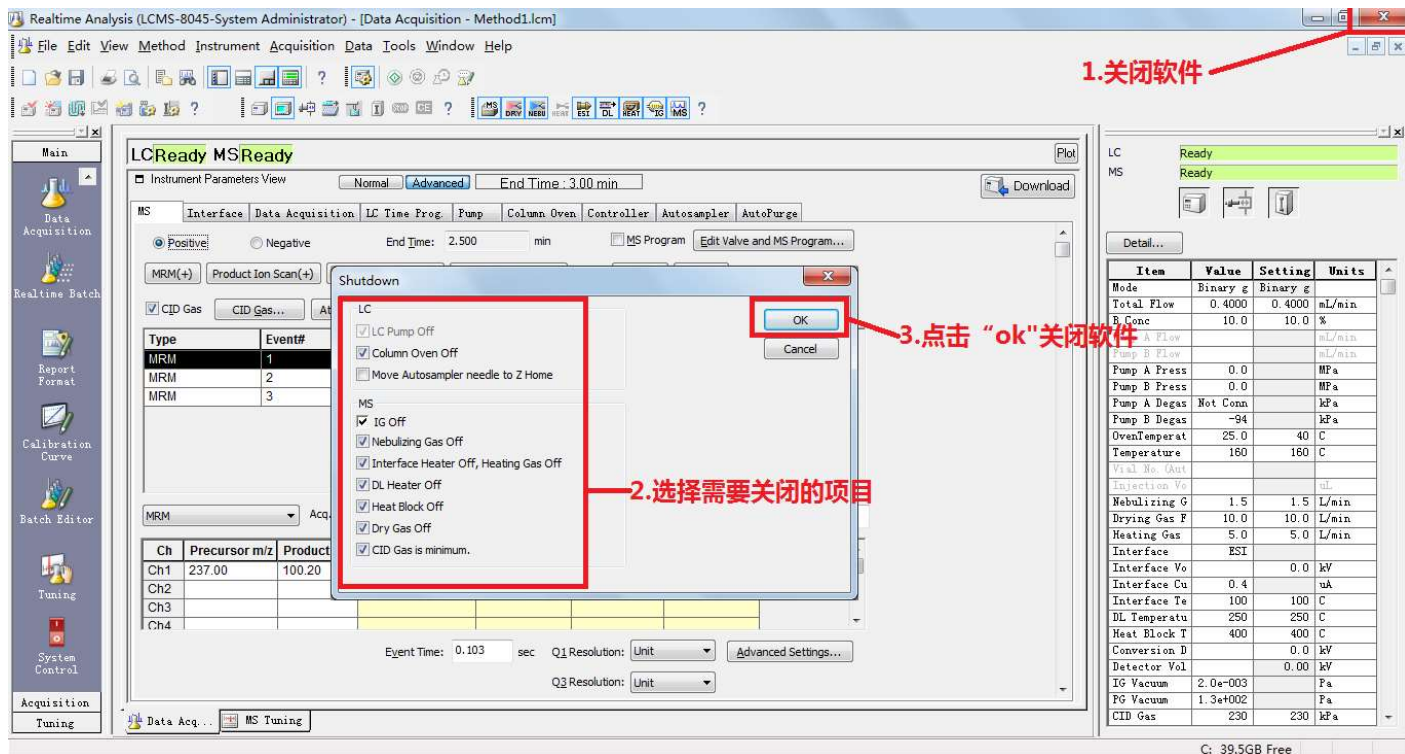
489,720

TIC(+):@1/TIC(+):@2/TIC(+):@3

9. 关机

9.1 日常关机

关闭“Realtime Analysis”软件，弹出窗口勾选需要关闭的项目，关闭软件后，DLPlung 堵上 DL



9.2 完全关机

打开“System Control”窗口，操作方法同 2.1 “启动真空系统”，然后点击“Auto Shutdown”



- ◆ 等待进度条完成，即可关闭所有软件窗口
- ◆ 最后关闭液相色谱各单元和质谱单元电源
- ◆ 关闭氮气、空气发生器电源开关，氩气阀开关