

VION使用手册



Administration 界面

主要用于仪器,文件夹,科学数据库,GxP等相关设置

打开administration/Consumable

进行溶剂，色谱柱等的设置，
设置后可在方法中进行选择使用

Administrative Links

Recent Tasks

- Security
- Search libraries
- Recent library item details
- Manage the Scientific Library
- Licensing

Consumables
Define and manage consumables used with instrument systems

Solvents Buffer systems Column definitions Sample plates

Printer Method Management
View or create methods to print documents into UNIFI and extract data from UNIFI reports.

Manage printer methods Manage report extraction methods

Software Management
Change the database password, record UNIFI software information, and manage diagnostic log settings

Manage disk drives Change database password Record UNIFI information
Define diagnostic log settings

Device Management
View and manage device configurations

Create Instrument Systems

Event Log
Search Event Log and edit Event Properties

Event Browser System Audit Trail Data Audit Trail Imported Events Event Properties

Explorer Management
Define and manage synonyms and categories used in Explorer

Manage Categories Define Synonyms

LIMS Configuration
Manage LIMS configurations

Licensing
Register, activate, assign, and view product licenses

Manage Custom Fields and Formulas
Define and manage custom fields for storing data and calculating analysis results

Offline Storage Management
Manage offline storage configurations

Qualification and Maintenance
Qualify system components and manage qualification methods, licenses, results and maintenance logs

Qualify Maintain Manage

Scientific Library
View and manage Scientific Library information

Search libraries Manage libraries Create library items

Security
Manage users and roles, define policies and access, and create reasons for user actions

Access Management Roles Users Global Policies Folder Policies Predefined Reasons

Signature Methods
Manage signature methods used for signing reports

Manage Methods Predefined Meanings Predefined Comments

System Monitor
View and manage the sample lists in the queue for an instrument system

Task Monitor
View and manage system tasks

Monitor current tasks View schedules View task properties

Consumable/Solvent界面可定义不同的溶剂，可在分析方法中进行选择使用。

点击“Create”进行溶剂的定义

UNIFI自带常用的溶剂，如需要，可自己设置

Solvent name	Solvent type	Concentration (mmol/L)	Description
1 Acetic Acid	Acid	10	
2 Acetonitrile	General		
3 Ammonium Acetate	Salt	30	
4 Ammonium Bicarbonate	Salt	30	
5 Ammonium Formate	Salt	30	
6 Chloroform	General		
7 Dibasic Sodium Phosphate	Base	100	
8 Ethanol	General		
9 Ethyl Acetate	General		
10 Formic Acid	Acid	10	
11 Hexane	General		
12 Isopropanol	General		
13 Methanol	General		
14 Monobasic Sodium Phosphate	Acid	100	
15 Potassium Phosphate	Salt	30	
16 Sodium Chloride	Salt	1000	
17 Sodium Citrate	Salt	30	
18 Sodium Formate	Salt	30	
19 Sodium Phosphate	Salt	30	
20 Tetrahydrofuran	General		
21 Triethylamine	Base	20	
22 Trifluoroacetic Acid	Acid	10	
23 TRIS	Salt	30	
24 Tris Base	Base	100	
25 Tris-HCl	Acid	100	
26 Water	Aqueous		

Consumable/Buffer界面可定义不同的缓冲盐系统，
可在分析方法中进行选择使用。

Consumables

Welcome to UNIFI

LCMS System

Administration

Consumables

Search folders...

Home > Buffer systems

Tasks

Buffer systems

Create Modify Remove Refresh

点击“Create”进行缓冲盐系统的定义

Consumables

Home

Solvents

Buffer systems

Column definitions

Sample plates

Buffer systems list

	Buffer system name	Comment	Concentration to deliver (mmol/L)	Acid	Base	Salt	Aqueous
1	Neutral Phosphate	Neutral Phosphate - Buffer System	20	Monobasic Sodium Phosphate	Dibasic Sodium Phosphate	Sodium Chloride	Water
2	Tris-TrisCl	Tris-TrisCl - Buffer System	20	Tris-HCl	Tris Base	Sodium Chloride	Water

Consumable/Column Definition界面可定义不同的色谱柱，可在分析方法中进行选择使用。

UNIFI已经包含大部分Waters的UPLC色谱柱，可点击Create进行新色谱柱定义

Column	Column name	Part number	Dimensions	Particle size (µm)	Comments	Vendor	User Created
1	ACQUITY UPLC-HSS T3	186003537	1 mm * 150 mm	1.8	ACQUITY UPLC Column	Waters	<input type="checkbox"/>
2	ACQUITY UPLC-BEH C8	186002876	1 mm * 100 mm	1.7	ACQUITY UPLC Column	Waters	<input type="checkbox"/>
3	ACQUITY UPLC-BEH C18	186002350	2.1 mm * 50 mm	1.7	ACQUITY UPLC Column	Waters	<input type="checkbox"/>
4	ACQUITY UPLC-BEH300 C4	186004495	2.1 mm * 50 mm	1.7	ACQUITY UPLC Column	Waters	<input type="checkbox"/>
5	ACQUITY UPLC-OST C18	186003950	2.1 mm * 100 mm	1.7	ACQUITY UPLC Column	Waters	<input type="checkbox"/>
6	ACQUITY UPLC-HSS C18 SB	186004117	2.1 mm * 30 mm	1.8	ACQUITY UPLC Column	Waters	<input type="checkbox"/>
7	ACQUITY UPLC-BEH HILIC	186003458	1 mm * 100 mm	1.7	ACQUITY UPLC Column	Waters	<input type="checkbox"/>
8	ACQUITY UPLC-BEH C18	186002344	1 mm * 50 mm	1.7	ACQUITY UPLC Column	Waters	<input type="checkbox"/>
9	ACQUITY UPLC-HSS C18	186003534	2.1 mm * 150 mm	1.8	ACQUITY UPLC Column	Waters	<input type="checkbox"/>
10	ACQUITY UPLC-HSS T3	186003539	2.1 mm * 100 mm	1.8	ACQUITY UPLC Column	Waters	<input type="checkbox"/>
11	ACQUITY UPLC-HSS C18 SB	186004119	2.1 mm * 100 mm	1.8	ACQUITY UPLC Column	Waters	<input type="checkbox"/>
12	ACQUITY UPLC-BEH300 C18	186005594	1 mm * 150 mm	1.7	ACQUITY UPLC Column	Waters	<input type="checkbox"/>
13	ACQUITY UPLC-HSS T3	186003540	2.1 mm * 150 mm	1.8	ACQUITY UPLC Column	Waters	<input type="checkbox"/>
14	ACQUITY UPLC-HSS C18	186003533	2.1 mm * 100 mm	1.8	ACQUITY UPLC Column	Waters	<input type="checkbox"/>
15	ACQUITY UPLC-BEH Phenyl	186003378	2.1 mm * 150 mm	1.7	ACQUITY UPLC Column	Waters	<input type="checkbox"/>
16	ACQUITY UPLC-BEH300 C18	186003687	2.1 mm * 150 mm	1.7	ACQUITY UPLC Column	Waters	<input type="checkbox"/>
17	ACQUITY UPLC-BEH130 C18	186003686	2.1 mm * 100 mm	1.7	ACQUITY UPLC Column	Waters	<input type="checkbox"/>
18	ACQUITY UPLC-BEH300 C4	186004497	2.1 mm * 150 mm	1.7	ACQUITY UPLC Column	Waters	<input type="checkbox"/>
19	ACQUITY UPLC-BEH HILIC	186003460	2.1 mm * 50 mm	1.7	ACQUITY UPLC Column	Waters	<input type="checkbox"/>
20	ACQUITY UPLC-BEH300 C4	186004496	2.1 mm * 100 mm	1.7	ACQUITY UPLC Column	Waters	<input type="checkbox"/>
21	ACQUITY UPLC-HSS C18 SB	186004118	2.1 mm * 50 mm	1.8	ACQUITY UPLC Column	Waters	<input type="checkbox"/>
22	ACQUITY UPLC-BEH C18	186002346	1 mm * 100 mm	1.7	ACQUITY UPLC Column	Waters	<input type="checkbox"/>
23	ACCQ-Tag Ultra UPLC	186003837	2.1 mm * 100 mm	1.7	ACQUITY UPLC Column	Waters	<input type="checkbox"/>
24	ACQUITY UPLC-HSS C18 SB	186004115	1 mm * 100 mm	1.8	ACQUITY UPLC Column	Waters	<input type="checkbox"/>
25	ACQUITY UPLC-BEH Shield RP18	186002854	2.1 mm * 100 mm	1.7	ACQUITY UPLC Column	Waters	<input type="checkbox"/>
26	ACQUITY UPLC-BEH Shield RP18	186003909	2.1 mm * 30 mm	1.7	ACQUITY UPLC Column	Waters	<input type="checkbox"/>
27	ACQUITY UPLC-HSS C18 SB	186004114	1 mm * 50 mm	1.8	ACQUITY UPLC Column	Waters	<input type="checkbox"/>
28	ACQUITY UPLC-HSS C18	186003529	1 mm * 50 mm	1.8	ACQUITY UPLC Column	Waters	<input type="checkbox"/>
29	ACQUITY UPLC-BEH130 C18	186003554	2.1 mm * 50 mm	1.7	ACQUITY UPLC Column	Waters	<input type="checkbox"/>
30	ACQUITY UPLC-BEH HILIC	186003457	1 mm * 50 mm	1.7	ACQUITY UPLC Column	Waters	<input type="checkbox"/>

Consumable/Sample Plate界面可定义不同的样品盘，可在分析方法中进行选择使用。

Consumables

Home > Sample plates

Tasks

Consumables

- Home
- Solvents
- Buffer systems
- Column definitions
- Sample plates

Sample plates

Sample plates list

	Sample tray	Plate format	Number of wells	Comment
1	ANSI - 96 well 350 µL	ANSIMicrotiter	96	96 Well 350 µL Holder
2	ANSI - 96 well 700 µL Glass Insert	ANSIMicrotiter	96	96 Well 700 µL Glass Insert Holder
3	ANSI - 48 Tube 0.65 mL Holder	ANSIMicrotiter	48	48 Tube 0.65 mL Holder
4	ANSI - 24 Vial 4 mL Holder	ANSIMicrotiter	24	24 Vial 4 mL Holder
5	ANSI - 384 well 250 µL	ANSIMicrotiter	384	384 Well 250 µL Holder
6	ANSI - 96 well 2 mL	ANSIMicrotiter	96	96 Well 2 mL Holder
7	ANSI - 96 well 1 mL	ANSIMicrotiter	96	96 Well 1 mL Holder
8	ANSI - 96 well 1 mL Glass Insert	ANSIMicrotiter	96	96 Well 1 mL Glass Insert Holder
9	ANSI - 48 Vial 2 mL Holder	ANSIMicrotiter	48	48 Vial 2 mL Holder
10	ANSI - 384 well 100 µL	ANSIMicrotiter	384	384 Well 100 µL Holder
11	ANSI - 24 Tube 1.5 mL Holder	ANSIMicrotiter	24	24 Well 1.5 mL Tubes Holder

UNIFI软件中可选择的样品盘

打开administration/Device Management

The screenshot displays the Waters UNIFI Administration web interface. The browser title is "Waters UNIFI - Administration". The interface includes a top navigation bar with "My Work", "Welcome to UNIFI", "LCMS System", and "Administration" tabs. A search bar is located in the top right corner. The main content area is titled "Areas of Administration" and contains a grid of administrative tasks. A red box highlights the "Device Management" section, which includes the sub-option "Create Instrument Systems".

Administrative Links

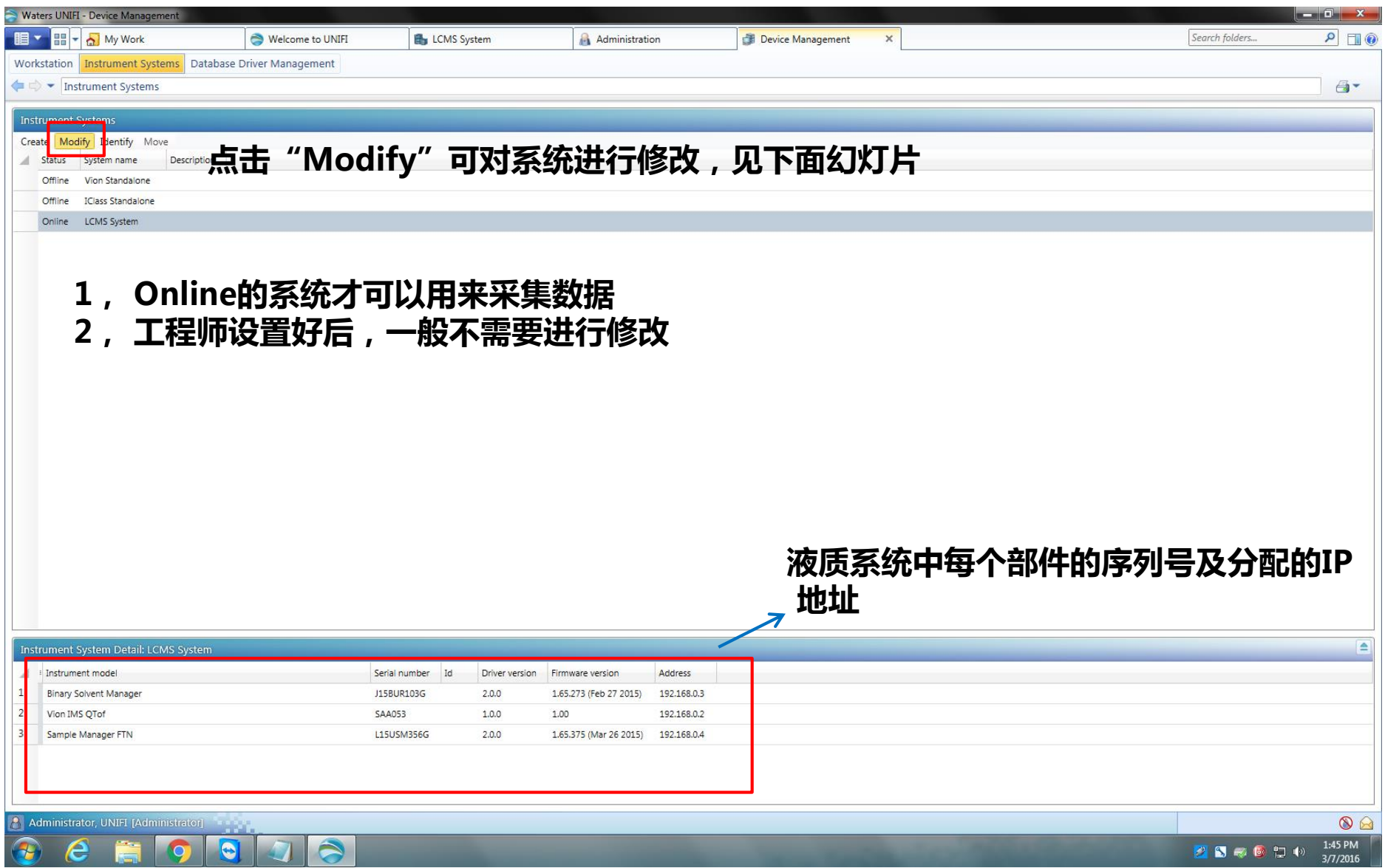
- Recent Tasks
- Security
- Search libraries
- Recent library item details
- Manage the Scientific Library
- Licensing

Administrative Tasks:

- Consumables**: Define and manage consumables used with instrument systems. Sub-options: Solvents, Buffer systems, Column definitions, Sample plates.
- Printer Method Management**: View or create methods to print documents into UNIFI and extract data from UNIFI reports. Sub-options: Manage printer methods, Manage report extraction methods.
- Software Management**: Change the database password, record UNIFI software information, and manage diagnostic log settings. Sub-options: Manage disk drives, Change database password, Record UNIFI information, Define diagnostic log settings.
- Device Management**: View and manage device configurations. Sub-option: Create Instrument Systems.
- Event Log**: Search Event Log and edit Event Properties. Sub-options: Event Browser, System Audit Trail, Data Audit Trail, Imported Events, Event Properties.
- Explorer Management**: Define and manage synonyms and categories used in Explorer. Sub-options: Manage Categories, Define Synonyms.
- LIMS Configuration**: Manage LIMS configurations.
- Licensing**: Register, activate, assign, and view product licenses.
- Manage Custom Fields and Formulas**: Define and manage custom fields for storing data and calculating analysis results.
- Offline Storage Management**: Manage offline storage configurations.
- Qualification and Maintenance**: Qualify system components and manage qualification methods, licenses, results and maintenance logs. Sub-options: Qualify, Maintain, Manage.
- Scientific Library**: View and manage Scientific Library information. Sub-options: Search libraries, Manage libraries, Create library items.
- Security**: Manage users and roles, define policies and access, and create reasons for user actions. Sub-options: Access Management, Roles, Users, Global Policies, Folder Policies, Predefined Reasons.
- Signature Methods**: Manage signature methods used for signing reports. Sub-options: Manage Methods, Predefined Meanings, Predefined Comments.
- System Monitor**: View and manage the sample lists in the queue for an instrument system.
- Task Monitor**: View and manage system tasks. Sub-options: Monitor current tasks, View schedules, View task properties.

可进行系统的设置

Device Management/Instrument System可进行所用液质系统的设置



点击“Modify”可对系统进行修改，见下面幻灯片

- 1, Online的系统才可以用来采集数据
- 2, 工程师设置好后，一般不需要进行修改

液质系统中每个部件的序列号及分配的IP地址

Instrument System/Modify界面可进行进样完毕后自动Standby，节约溶剂及气体等

The screenshot displays the Waters Instrument System configuration interface. The top navigation bar includes 'My Work', 'Welcome to UNIFI', 'LCMS System', 'Administration', and 'Device Management'. The main content area is titled 'Instrument System' and contains fields for 'System Name' (LCMS System), 'Description', 'Primary pump name' (Binary Solvent Manager), and 'Primary pump serial number' (J15BUR103G). A red box highlights the 'Save' icon in the top right corner. Below this, the 'Startup Shutdown' configuration section is shown, with a red box around the 'Startup Shutdown' tab. The 'Configuration' section includes a dropdown for 'shutdown method' and a 'Settings' button. The 'Enable Startup and Shutdown' section has checkboxes for 'Enable Startup' and 'Enable Shutdown (Error shutdown is always enabled)'. The 'Time before Shutdown to Standby' section has a checked checkbox for 'Enable automatic shutdown after period of time of system being idle' and an 'Idle time' field set to 01 hours and 00 minutes. The 'Schedule' section has checkboxes for 'Run startup' and 'Run shutdown', with 'Run shutdown' selected. The 'Time' field is set to 09:00, and the 'Schedule' section has checkboxes for 'Monday', 'Tuesday', 'Wednesday', 'Thursday', 'Friday', 'Saturday', and 'Sunday', with 'Wednesday', 'Thursday', and 'Friday' selected. The 'Details' section at the bottom shows 'Description', 'Folder' (Company/Vion Installation LCMS), 'Last modified by' (administrator), 'Last modified' (Mar 07, 2016 13:38:31 China Standard Time), and 'Version' (2).

点击“保存”完成设置

点击“Start up/Shutdown”，对系统自动关机进行设置

选择已经建立好的shutdown method

选择“Enable Shutdown(error shutdown is always enabled)”

选择时间(比如1小时)，意思是系统报错后或最后一针样品进完后，在设定时间会将仪器按照设定的方法自动关机

A1 dministration/Scientific Library,可进行数据库的编辑,导入等.UNIFI有中药数据库,农残兽残数据库,毒物数据库等,需要购买Lisence才能使用

The screenshot shows the Waters UNIFI Administration web interface. The browser address bar displays "Waters UNIFI - Administration" and the page title is "Areas of Administration". The interface includes a navigation menu on the left with "Administrative Links" and "Recent Tasks". The main content area is divided into two columns of administrative tasks. The "Scientific Library" section, which includes "View and manage Scientific Library information" and sub-links for "Search libraries", "Manage libraries", and "Create library items", is highlighted with a red rectangular box. Other sections include Consumables, Printer Method Management, Software Management, Device Management, Event Log, Explorer Management, LIMS Configuration, Licensing, Manage Custom Fields and Formulas, Offline Storage Management, Qualification and Maintenance, Security, Signature Methods, System Monitor, and Task Monitor.

The screenshot displays the Waters Scientific Library software interface. The top navigation bar includes tabs for 'My Work', 'Welcome to UNIFI', 'LCMS System', 'Administration', and 'Scientific Library'. The main window is titled 'Scientific Library' and shows a search criteria table with one entry: 'Name equals *'. Below the table, the search options are set to 'Spec, Default Custom Library' and '100 Results'. A red box highlights the search criteria table and the search options. The search results section is currently empty.

Search criteria	Operator	Search value
1 Name	equals	*

Search in: Spec, Default Custom Library Show: 100 Results Search

Name	Library name
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可对已有数据库进行搜索

The screenshot displays the Waters Scientific Library software interface. The main window is titled "Library Item Editor" and shows a form for editing a library item. The form includes fields for "Item type" (Compound), "Item description", "IUPAC name", "Formula", "Hill formula", "Average molar mass", "Monoisotopic mass", "Item tag", and "InChI". A "Tools" menu is highlighted in the top right corner. A "Create Library Item" dialog box is open in the foreground, prompting for "Item name" and "Library" (Default Custom Library). The dialog box has "OK" and "Cancel" buttons. The background interface also shows a "Results" panel on the left and "Synonyms" and "Physical properties" sections at the bottom.

也可自己导入数据库（此处为单个导入）

Administrator/ Security 可以进行数据安全性的相关设置, 比如建立文件夹, 建立角色, 用户等

The screenshot displays the Waters UNIFI Administration web interface. The top navigation bar includes 'My Work', 'Welcome to UNIFI', 'LCMS System', and 'Administration'. The main content area is titled 'Areas of Administration' and lists various management tasks. The 'Security' section is highlighted with a red border and contains buttons for 'Access Management', 'Roles', 'Users', 'Global Policies', 'Folder Policies', and 'Predefined Reasons'. A blue arrow points from the 'Access Management' button to a blue text overlay that reads '通过Access可以建立文件夹' (Through Access, folders can be created). Other sections include Consumables, Printer Method Management, Software Management, Device Management, Event Log, Explorer Management, LIMS Configuration, and Licensing. The bottom of the screen shows the Windows taskbar with the system clock at 2:00 PM on 3/7/2016.

通过Access可以建立文件夹

建立Shut Down的方法

主要目的是当仪器采集完最后一针样品后,根据设定的程序,自动关机

在 shutdown 方法界面, 在shutdown进行液相,进样器和质谱等的设置

The screenshot displays the Waters software interface for configuring a shutdown method. The left sidebar shows the 'Shutdown' method selected, with 'Binary Solvent Manager' highlighted. The main panel is titled 'Shutdown to standby' and contains several sections:

- Prime Solvents:** Includes checkboxes for 'Prime Solvents', 'Pump A, Lines: A1 A2', and 'Pump B, Lines: B1 B2'. The 'Run time' is set to 5 min.
- Prime Seal Wash:** Includes a checkbox for 'Prime Seal Wash' and a 'Run time' of 5 min.
- Set How:** A section highlighted with a red box, containing:
 - Set Flow
 - Flow rate: 0 mL/min
 - Solvent configuration:
 - A: A1 50 %
 - B: B1 50 %

将流速设置为0mL/min,
这就意味着进样最后一针结束,将流速设置为0

在 shutdown 方法界面, 在shutdown进行液相,进样器和质谱等设置

Startup Shutdown Error

My Work Welcome to UNIFI LCMS System Administration shutdown method:Startu... x Search folders...

Shutdown

Instruments

Binary Solvent Manager

Sample Manager FTN

Vion IMS QToF

Transitions

Shutdown to standby

Shutdown to maintenance

Shutdown to standby

Prime Syringes

Prime Syringes

Prime Wash solvent for: 5 sec

Prime Purge solvent for: 1 Cycles

Characterize Needle Seal

Characterize Needle Seal

Should perform if seal is replaced.

The following properties are set whether starting up or shutting down

Column Temperature

Column Temperature

Has column

Off

Setpoint: Off °C

Sample Temperature

Sample Temperature

Off

Setpoint: Off °C

将色谱柱的温度设置为off,
将样品管理室的温度设置为off

意味着进样最后一针结束后,柱温和样品管理室温度
关掉

在 shutdown 方法界面, 在shutdown进行液相,进样器和质谱等设置

The screenshot displays the 'Shutdown to standby' configuration window in the Waters UNIFI software. The window title is 'Shutdown to standby'. Below the title, it states 'The following properties are set whether starting up or shutting down'. The 'MS Instrument' section is highlighted with a red box and contains the following options:

- MS Instrument
- Operate/standby
 - Switch to operate
 - Switch to instrument standby
 - Switch to source standby
- Instrument setup
 - Run instrument setup

The left sidebar shows the 'Shutdown' method selected, and the 'Vion IMS QTof' instrument is highlighted in the 'Instruments' list. The text on the right side of the image provides instructions on how to configure the MS Instrument settings.

选中MS Instrument,

选择Switch to instrument standby

意味着进样最后一针结束后,将质谱设置为Standby状态

在 shutdown 方法界面, 在error界面下进行液相, 进样器和质谱等设置

The screenshot displays the Waters UNIFI software interface. At the top, there are tabs for 'Startup', 'Shutdown', and 'Error', with 'Error' selected and highlighted by a red box. Below the tabs, a navigation pane on the left shows 'Instruments' and 'Transitions'. Under 'Instruments', 'Binary Solvent Manager' is highlighted with a red box and a blue arrow pointing to it. The main window shows the 'Error shutdown' configuration. A red box highlights the 'Set Flow' section, which includes a checked 'Set Flow' checkbox, a 'Flow rate' field set to '0 mL/min', and a 'Solvent configuration' section with two rows: 'A: A1' at '50 %' and 'B: B1' at '50 %'.

**将流速设置为0mL/min,
这就意味着当系统出现报错后,流速将设置为0**

在 shutdown 方法界面, 在error界面下进行液相, 进样器和质谱等设置

将色谱柱的温度设置为off,
将样品管理室的温度设置为off

意味着系统报错后, 将会把柱温和样品管理室温度
关掉

在 shutdown 方法界面, 在error界面下进行液相,进样器和质谱等设置

选中MS Instrument,

选择Switch to instrument standby

意味着系统报错后,将把质谱设置为Standby状态

My Work 界面

主要用于分析方法的建立,分析的建立及分析数据的采集及处理

以下操作用于打开液质系统,进行液质系统的准备,为采集数据做好准备

点击“ My Work” 界面,点击“ Instrument System” 进行设置

Instrument Systems

Instrument System (3)

- Vion Standalone [Offline]
- Iclass Standalone [Offline]
- LCMS System [Online]**

选择“ online” 的系统,双击后进入液质系统的控制界面

Administrator, UNIFI [Administrator]

点击后,进入仪器控制界面,

两个界面都可以进行系统的设置

液质系统的控制界面

液质系统的快捷方式

System Activity: Idle

Summary: LCMS System, Status: Idle, System: Idle, Startup: Maintenance, Current method: [blank]

Pressure and flow: 53 psi, 0.000 mL/min

Delta pressure: 0 psi

Solvents: A1: 50.0%, B1: 50.0%

Sample Manager FTN: Idle, Temperatures (°C): Sample: 10.1, 10.0; Column: 45.0, 45.0

Vion IMS QTof: Idle, Source: ESI, Sample: Idle, Reference: Idle

在LC/MS界面下的设置

The screenshot displays the Waters LC/MS software interface. On the left, the 'Console Navigation' pane is visible, with a red box highlighting the 'LCMS System' folder and its sub-items: 'Binary Solvent Manager', 'Vion IMS QTof', and 'Sample Manager FTN'. Another red box highlights the 'Summary' sub-item under 'LCMS System'. A blue arrow points from the 'LCMS System' folder to the main content area. The main content area shows the 'Instrument System Summary' page, which includes the 'Waters' logo and the text 'THE SCIENCE OF WHAT'S POSSIBLE™'. Below this, the 'Instrument System' section displays three modules: 'Solvent Delivery' (Binary Solvent Manager), 'Sample Management' (Sample Manager FTN), and 'Mass Spectrometer' (Vion IMS QTof). At the bottom, the 'System Activity' section shows a green bar with a checkmark and the word 'Idle'. On the right side, there are three panels: 'Summary' (showing 'LCMS System' status as 'Idle'), 'Instruments' (showing 'Binary Solvent Manager' and 'Sample Manager FTN' status), and 'Vion IMS QTof' (showing 'Vion IMS QTof' status as 'Idle').

LC/MS及LC/MS界面下包含的三个模块

LC/MS system下包含以下几项：

Solvent Delivery

Binary Solvent Manager

Sample Management

Sample Manager FTN

Mass Spectrometer

Vion IMS QTof

System Activity

Idle

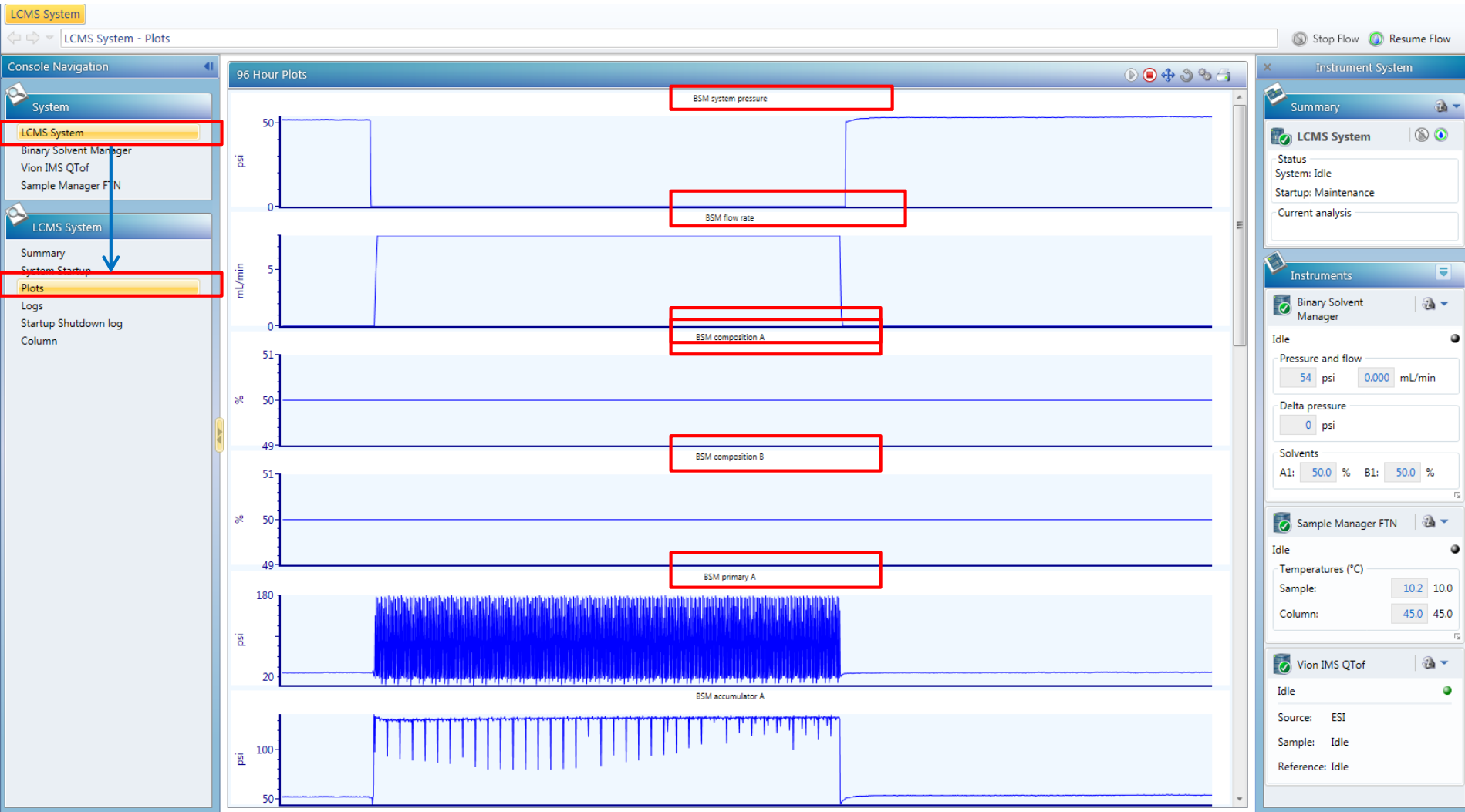
LCMS System/Summary , 主要显示整个系统的状态

**显示仪器的状态,
绿色代表系统状态OK
红色代表系统有报错**

泵系统 进样系统 质谱系统

System Activity: **Idle**

LCMS System/Plots , 主要显示整个系统的压力等反馈情况



LCMS System/Logs , 主要显示整个系统状态的反馈情况

The screenshot displays the Waters LCMS System interface. The main window shows a list of system logs. The left sidebar contains navigation options, with 'LCMS System' and 'Logs' highlighted. The right sidebar shows the 'Instrument System' summary, including status (Idle), startup (Maintenance), and current analysis. The 'Instruments' section shows 'Binary Solvent Manager' and 'Sample Manager FTN' with their respective parameters.

Type	Date	Device unique name	Instrument type	Category	User	Action
			Sample Manager FTN			
42	Mar 02, 2016 09:32:11 China Standard Time	L15USM356G	Sample Manager FTN	FTN Prime Syringe	Administrator, UNIFI	Prime Syringe
43	Mar 02, 2016 09:28:08 China Standard Time	L15USM356G	Sample Manager FTN	Calibration	Administrator, UNIFI	Z-axis calibration
44	Mar 02, 2016 09:19:50 China Standard Time	L15USM356G	Sample Manager FTN	FTN Needle Seal Readiness Test	Administrator, UNIFI	Needle Seal Readiness
45	Mar 02, 2016 09:15:43 China Standard Time	L15USM356G	Sample Manager FTN	Sample Manager FTN Leak Test	Administrator, UNIFI	Leak Test
46	Mar 02, 2016 09:14:57 China Standard Time	L15USM356G	Sample Manager FTN	FTN Characterize Needle Seal	Administrator, UNIFI	Characterize Needle Seal
47	Mar 01, 2016 19:15:32 China Standard Time	L15USM356G	Sample Manager FTN	FTN Wash Needle test	Administrator, UNIFI	Wash Needle
48	Mar 01, 2016 15:30:39 China Standard Time	L15USM356G	Sample Manager FTN	System Event	System,	Sample Manager FTN: eCord connected
49	Mar 01, 2016 14:52:06 China Standard Time	L15USM356G	Sample Manager FTN	System Event	System,	Sample Manager FTN: eCord disconnected
50	Mar 01, 2016 14:47:15 China Standard Time	L15USM356G	Sample Manager FTN	System Event	System,	Sample Manager FTN: eCord connected
51	Feb 24, 2016 15:24:14 China Standard Time	L15USM356G	Sample Manager FTN	System Event	System,	Sample Manager FTN: Communication Failure
52	Feb 24, 2016 09:41:07 China Standard Time	L15USM356G	Sample Manager FTN	FTN Wash Needle test	Administrator, UNIFI	Wash Needle
53	Feb 24, 2016 09:40:21 China Standard Time	L15USM356G	Sample Manager FTN	FTN Wash Needle test	Administrator, UNIFI	Wash Needle
54	Feb 24, 2016 09:37:35 China Standard Time	L15USM356G	Sample Manager FTN	FTN Prime Syringe	Administrator, UNIFI	Prime Syringe
55	Feb 23, 2016 18:07:27 China Standard Time	L15USM356G	Sample Manager FTN	FTN Wash Needle test	Administrator, UNIFI	Wash Needle
56	Feb 23, 2016 18:05:21 China Standard Time	L15USM356G	Sample Manager FTN	FTN Prime Syringe	Administrator, UNIFI	Prime Syringe

Details

Instrument system: LCMS System

Summary: Characterize Needle Seal

Description: Navigate to instrument specific log to see the details

Category: FTN Characterize Needle Seal

Instrument type: Sample Manager FTN

Serial number: L15USM356G

Instrument System Summary

LCMS System

Status: Idle

System: Idle

Startup: Maintenance

Current analysis

Instruments

Binary Solvent Manager

Idle

Pressure and flow: 54 psi, 0.000 mL/min

Delta pressure: 0 psi

Solvents: A1: 50.0 %, B1: 50.0 %

Sample Manager FTN

Idle

Temperatures (°C): Sample: 10.2 10.0, Column: 45.0 45.0

Vion IMS QTof

Idle

Source: ESI

Sample: Idle

Reference: Idle

LCMS System/startup shutdown log , 主要显示整个系统 startup shutdown状态的操作记录

The screenshot displays the Waters LCMS System software interface. The main window shows the 'Startup Shutdown Log Entries' table, which records system status changes, errors, and manual operations. The table includes columns for Status, Date/Time, Cause, and Message. A console navigation pane on the left highlights the 'Startup Shutdown log' option. On the right, the 'Instrument System' summary panel shows the current status of the LCMS System as 'Idle' and provides details for the Binary Solvent Manager and Sample Manager FTN instruments.

#	Status	Date/Time	Cause	Message
1	✓	Mar 07, 2016 10:10:19 China Standard Time	Cleared Instrument System Error	The system error has been cleared
2	✓	Mar 04, 2016 23:16:17 China Standard Time	Cause Of Error Cleared	The error that caused the system to shutdown has been cleared, the system can continue by performing a startup or shutdown.
3	✓	Mar 04, 2016 23:16:09 China Standard Time	Instrument System Error	An error on one of the Instruments caused the system to shutdown
4	✓	Mar 04, 2016 17:15:09 China Standard Time	Cleared Instrument System Error	The system error has been cleared
5	✓	Mar 04, 2016 17:14:11 China Standard Time	Cause Of Error Cleared	The error that caused the system to shutdown has been cleared, the system can continue by performing a startup or shutdown.
6	✓	Mar 04, 2016 17:12:57 China Standard Time	Instrument System Error	An error on one of the Instruments caused the system to shutdown
7	✓	Mar 04, 2016 13:21:37 China Standard Time	Instrument System Error	An error on one of the Instruments caused the system to shutdown
8	✓	Mar 04, 2016 12:08:10 China Standard Time	Instrument System Error	An error on one of the Instruments caused the system to shutdown
9	✓	Mar 04, 2016 11:36:19 China Standard Time	Cause Of Error Cleared	The error that caused the system to shutdown has been cleared, the system can continue by performing a startup or shutdown.
10	✓	Mar 04, 2016 11:36:19 China Standard Time	Tasklist Failed	An error during a tasklist caused the system to shutdown
11	✓	Mar 04, 2016 11:34:42 China Standard Time	Manual Startup or Shutdown	User requested startup or shutdown from Maintenance to Ready
12	✓	Mar 04, 2016 10:58:16 China Standard Time	Acquisition Started	An Acquisition was started causing the system to startup.
13	✓	Mar 04, 2016 10:58:16 China Standard Time	Cleared Instrument System Error	The system error has been cleared
14	✓	Mar 04, 2016 10:57:59 China Standard Time	Cause Of Error Cleared	The error that caused the system to shutdown has been cleared, the system can continue by performing a startup or shutdown.
15	✓	Mar 04, 2016 10:57:56 China Standard Time	Instrument System Error	An error on one of the Instruments caused the system to shutdown
16	✓	Mar 04, 2016 10:29:46 China Standard Time	Cleared Instrument System Error	The system error has been cleared
17	✓	Mar 04, 2016 10:25:22 China Standard Time	Cause Of Error Cleared	The error that caused the system to shutdown has been cleared, the system can continue by performing a startup or shutdown.
18	✓	Mar 04, 2016 10:23:56 China Standard Time	Instrument System Error	An error on one of the Instruments caused the system to shutdown

Binary Solvent Manager 界面下的操作

Binary Solvent Manager/Summary界面下，看到整个液相系统的状态

The screenshot displays the Waters Binary Solvent Manager (BSM) Summary interface. The main window shows the system is in an 'Idle' state. Key parameters are visible in the 'Flow Conditions' section:

- Flow rate: 0.000 mL/min
- Pressure: 54 psi
- Degasser: 0.43 psi
- Composition: Solvent A1: 50.0 %, Solvent B1: 50.0 %

An 'Edit settings' dialog box is open, allowing for adjustments to the flow rate and solvent configuration. The 'Flow conditions' section of the dialog shows the flow rate set to 0.000 mL/min. The 'Solvent configuration' section shows Solvent A1 at 50.0% and Solvent B1 at 50.0%.

At the bottom of the interface, there are two plots:

- BSM system pressure:** A line graph showing pressure fluctuations over time, with values ranging from approximately 53.4 psi to 53.8 psi.
- BSM composition A:** A line graph showing the percentage of solvent A over time, which remains constant at 50%.

Annotations in Chinese provide additional context:

- 液相状态** (Liquid phase status) points to the 'I-Class Binary Solvent Manager' status indicator.
- 点击可进行流速的设置** (Click to set flow rate) points to the 'Edit settings' dialog box.
- 目前系统的流速及压力** (Current system flow rate and pressure) points to the 'Flow Conditions' section.

Binary Solvent Manager/Setup界面，可进行流动相的灌注

Prime A/B Solvents

Prime: Solvent A, A1 Solvent B, B1

Run time: 5.0 min

Start Stop

Progress

Status and progress

Test status: Idle

0.0 5 min

Reset Binary Solvent Manager

Are you sure you want to reset the instrument?

Yes No

点击“prime A/B solvent”
进行流动相的灌注

图是错误的

Binary Solvent Manager/Setup界面，可进行泵系统的测试及维护

Current configuration
Leak detection: Enabled

Prime seal wash
Do you want to start priming seal wash?
Yes No

Click "yes" to proceed with the seal wash, which is used to clean the piston rod. It is generally performed with a 90/10 (water/acetonitrile or methanol) solvent mixture.

点击“yes”后进行柱塞杆的灌注，

Seal wash是用来洗柱塞杆的，一般常用90/10（水/乙腈或甲醇）

Binary Solvent Manager/Setup界面，可进行液相系统的重启

The screenshot displays the Waters Binary Solvent Manager/Setup interface. The main window is titled "Prime A/B Solvents" and shows settings for Solvent A (A1) and Solvent B (B1) with a run time of 5.0 min. A "Progress" section indicates the test status is "Idle" with a progress bar from 0.0 to 5 min. A "Reset Binary Solvent Manager" dialog box is open, asking "Are you sure you want to reset the instrument?" with "Yes" and "No" buttons. The dialog box is highlighted with a red border. In the left sidebar, the "Binary Solvent Manager" section is expanded, and the "Setup" sub-section is selected. The "Reset instrument..." option is highlighted with a red border, and a blue arrow points from it to the dialog box. The right sidebar shows the "Instrument System" summary, including status (Idle), pressure (54 psi), and solvent percentages (A1: 50.0%, B1: 50.0%).

Binary Solvent Manager/Maintain界面，可进行泵系统的测试及维护

The screenshot displays the Waters Binary Solvent Manager/Maintain software interface. The main window is titled "Instrument Information" and contains the following data:

Instrument	
Serial number:	J15BUR103G
Firmware version:	1.65.273 (Feb 27 2015)
Firmware checksum:	0x3462a3f3
Software version:	2.0.0

The text "泵的序列号及软件版本号" (Pump serial number and software version number) is overlaid on the right side of the instrument information panel. The interface also includes a left-hand navigation pane with sections for "System", "Binary Solvent Manager", and "Maintain". The "Maintain" section is expanded to show "Instrument Information". On the right side, there are panels for "Instrument System" (Summary) and "Instruments" (Binary Solvent Manager, Sample Manager FTN, Vion IMS QToF) with various operational parameters like pressure, flow, and temperatures.

Binary Solvent Manager/Maintain界面，可查看泵的流路设计

The screenshot displays the Waters LCMS System software interface. The main window is titled "Interactive Display" and shows a detailed flow diagram of the pump system. The diagram includes two primary pumps (29psi and -1psi) and two accumulators (54psi and 2psi). It also shows solvent select valves (A1, B1), a degasser (0.40 psi), a vent valve system, a sample manager, and a waste container. The flow is set to 0.000 mL/min at 50.0% solvent concentration. The interface includes a console navigation pane on the left with "Binary Solvent Manager" and "Maintain" highlighted, and a summary pane on the right showing system status and instrument details.

泵的流路图

Binary Solvent Manager/Maintain界面，可查看泵的流路设计

Click "start" to perform leak test

Leak Test Configuration:

- Parameters: Accumulator pressure: 14000 psi, Pump: A
- Fluidics end point: Vent valve end point, Column end point, Include needle and seal
- Options: Prime, Automatically retry the test if it fails, Retry attempts: 0

Progress:

- Status and progress: Test status: Ready, 0.0 / 8 min
- Leak rate (nL/min): Accumulator: 0.0, Primary: 0.0
- Pressure (psi): Accumulator: 2011, Primary: 9

96 Hour Plots:

- BSM system pressure: Pressure (psi) vs. Time (min)
- BSM composition A: Composition (%) vs. Time (min)

Console Navigation:

- System: Binary Solvent Manager, Vion IMS QTof, Sample Manager FTN
- Binary Solvent Manager: Summary, Setup, Maintain, Troubleshoot
- Maintain: Instrument Information, Interactive Display, Performance, Heads, Leak Test, Reset Pumped Volume...

Instrument System Summary:

- Summary: Icims (Status: Error, System: Error, Startup: Error, Current analysis)
- Instruments: Binary Solvent Manager (Idle), Sample Manager FTN (Idle), Vion IMS QTof (Detector setup negative polarity required)

Sample Manager FTN 的界面下的操作

Sample Manager FTN /Summary界面，可看到进样系统的操作记录

The screenshot displays the Waters UNIFI software interface. The main window shows the 'Sample Manager FTN' Summary page. On the left, the 'Console Navigation' pane has 'Sample Manager FTN' selected, with arrows pointing to the 'Summary' and 'Logs' sub-items. The central 'Logs' window is highlighted with a red border and contains the following data:

Type	Date	Category	User	Action
5	Mar 04, 2016 11:36:19 China Standard Time	System Event	System,	Sample Manager FTN: Zp-axis move h/w fault
6	Mar 04, 2016 11:29:12 China Standard Time	FTN Needle Seal Readiness Test	Administrator, UNIFI	Needle Seal Readiness
7	Mar 04, 2016 11:23:38 China Standard Time	FTN Characterize Needle Seal	Administrator, UNIFI	Characterize Needle Seal
8	Mar 04, 2016 11:22:04 China Standard Time	FTN Wash Needle test	Administrator, UNIFI	Wash Needle
9	Mar 04, 2016 11:16:32 China Standard Time	FTN Wash Needle test	Administrator, UNIFI	Wash Needle
10	Mar 04, 2016 11:16:26 China Standard Time	FTN Wash Needle test	Administrator, UNIFI	Wash Needle
11	Mar 04, 2016 11:10:56 China Standard Time	FTN Prime Syringe	Administrator, UNIFI	Prime Syringe
12	Mar 04, 2016 10:47:10 China Standard Time	FTN Needle Seal Readiness Test	Administrator, UNIFI	Needle Seal Readiness
13	Mar 04, 2016 10:45:08 China Standard Time	Sample Manager FTN Leak Test	Administrator, UNIFI	Leak Test
14	Mar 04, 2016 10:44:11 China Standard Time	FTN Prime Syringe	Administrator, UNIFI	Prime Syringe
15	Mar 04, 2016 10:31:34 China Standard Time	FTN Needle Seal Readiness Test	Administrator, UNIFI	Needle Seal Readiness
16	Mar 04, 2016 10:30:59 China Standard Time	FTN Characterize Needle Seal	Administrator, UNIFI	Characterize Needle Seal
17	Mar 04, 2016 10:29:45 China Standard Time	FTN Needle Seal Readiness Test	Administrator, UNIFI	Needle Seal Readiness

Below the logs table, the 'Details' pane shows the following information:

Result details
 Pass/Fail: Pass
 Pressure: 7 psi
 Offset: 0.6 mm

On the right side of the interface, the 'Instrument System' summary shows the 'LCMS System' status as 'Idle' and 'Startup: Maintenance'. Below this, the 'Instruments' section shows 'Binary Solvent Manager' and 'Sample Manager FTN' both in 'Idle' status. The 'Sample Manager FTN' section displays 'Temperatures (°C)' for the Sample (10.1) and Column (45.0).

进样系统的
操作记录

Sample Manager FTN /Setup界面，可对进样系统进行设置

**点击可进行修改
(除非添加loop环。
否则不要修改)**

进样针的标准设置

Extended loop size: 0 μL
 Needle size: 15 μL
 Sample syringe size: 100 μL

漏液监控设置

When vial is missing: Fail On Error
 When door is opened: The light will turn on
 Upper leak detector: Enabled
 Lower leak detector: Enabled
 When e-cord is missing: Allow acquisition list operations

预加热器的设置

Active column pre-heater is: Present
 Column pre-heater configuration is: Active

**样品管理器的设置
(可以进9块板自动进样装置，须额外购买)**

Note: when you change the SO configuration...

Sample Organizer: None configured

Edit settings

Sample Manager FTN

Extended loop size: Standard 0 μL
 Custom 0.0 μL
 Needle size: Standard 15 μL
 Custom 15 μL
 Sample syringe size: 100 μL

OK Cancel

Once started, and using the default time and cycles, this process will take about 2 minutes to complete.

Prime wash solvent for: 15 sec

Prime purge solvent for: 5 cycles

Start Stop

Progress

Status and progress

Test status: Ready

0.0 2 min

设置灌注的时间，即可开始灌注

Purge solvent 的灌注是保证注射器内部没有气体，保证进样的准确性；

Wash solvent 是用于进样针的外部，常用溶液为90%的有机相溶液，可根据实际情况调节；

Sample Manager FTN /Setup界面，可进行进样针的清洗

The screenshot displays the Waters Sample Manager FTN software interface. The main window is titled "Wash Needle" and contains the following elements:

- A message: "Once started, the needle wash process will take an additional 30 seconds to complete."
- A "Wash time:" field set to "6 sec".
- "Start" and "Stop" buttons.

The left-hand "Console Navigation" pane shows a tree view with the following items:

- System
 - LCMS System
 - Binary Solvent Manager
 - Vion IMS QToF
 - Sample Manager FTN
- Sample Manager FTN
 - Summary
 - Setup
 - Maintain
- Setup
 - Configure
 - Prime Syringe
 - Wash Needle
 - Reset instrument...

The right-hand "Instrument System" pane shows a summary of the system status:

- LCMS System:** Status: Idle, System: Idle, Startup: Maintenance, Current analysis: [empty]
- Binary Solvent Manager:** Idle, Pressure and flow: 48 psi, 0.000 mL/min, Delta pressure: 4 psi, Solvents: A1: 50.0 %, B1: 50.0 %
- Sample Manager FTN:** Idle, Temperatures (°C): Sample: 10.2 / 10.0, Column: 45.0 / 45.0
- Vion IMS QToF:** Idle, Source: ESI, Sample: Idle, Reference: Idle

A red box highlights the "Wash Needle" window, and a blue arrow points to the "Start" button. The text "点击“Start”开始" is overlaid on the image.

Sample Manager FTN /Setup界面，可进行进样针的清洗

The screenshot displays the Waters Sample Manager FTN software interface. The main window is titled 'Wash Needle' and contains the following elements:

- Wash Needle Section:** A text box stating 'Once started, the needle wash process will take an additional 30 seconds to complete.' Below it, a 'Wash time:' field is set to '6 sec'. 'Start' and 'Stop' buttons are visible on the right.
- Progress Section:** A 'Status and progress' area showing 'Test status: Ready' and a progress bar from 0.0 to 1 min.
- Reset Dialog Box:** A modal dialog box titled 'Reset Sample Manager FTN' is centered on the screen. It contains the question 'Are you sure you want to reset the instrument?' and 'Yes' and 'No' buttons. A red box highlights this dialog, and a blue arrow points from the 'Reset Instrument...' option in the left-hand navigation pane to it.

The left-hand navigation pane shows a tree structure with the following items:

- System
 - LCMS System
 - Binary Solvent Manager
 - Vion IMS QToF
 - Sample Manager FTN (highlighted with a red box)
- Sample Manager FTN
 - Summary
 - Setup (highlighted with a red box)
 - Maintain
- Setup
 - Configure
 - Prime Syringe
 - Wash Needle (highlighted with a red box)
 - Reset Instrument... (highlighted with a red box)

The right-hand pane shows the 'Instrument System' summary, including status (Idle), pressure and flow (48 psi, 0.000 mL/min), delta pressure (1 psi), solvents (A1: 50.0%, B1: 50.0%), and temperatures for the Sample Manager FTN and Vion IMS QToF.

当仪器报错时，可点击“reset”让仪器恢复正常状态

Sample Manager FTN /Maintain界面，可对进样系统进行诊断或维护

The screenshot displays the Waters Sample Manager FTN software interface. The main window is titled 'Instrument Information' and contains the following data:

Instrument	
Serial number:	L15USM356G
Firmware version:	1.65.375 (Mar 26 2015)
Firmware checksum:	0x34728d7d
Software version:	2.0.0

Maintenance Information	
Counters	
Power on time:	225.2 hours
Last power on:	7.2 hours
Power cycles:	9
Injection count:	80
Injection count threshold:	0
Trap valve actuations:	0
Solenoids	
Wash solvent actuations:	16
Sample Syringe	
Sample syringe volume dispensed:	0.05 L
Sample syringe lost steps checks:	346
Sample syringe times lost steps:	0
Rotary Valves	
Inject valve actuations:	260
Sample valve actuations:	2629
Axes	
Theta axis actuations:	901
Theta axis rehome:	0
R Axis actuations:	804
Z Axis actuations:	7686
Zn Axis actuations:	1737

The interface also features a left-hand navigation pane with 'Sample Manager FTN' and 'Maintain' sections, and a right-hand 'Instrument System' summary panel. A large red box highlights the central 'Instrument Information' and 'Maintenance Information' sections. A blue arrow points from the 'Maintain' section to the 'Instrument Information' section. The text '进样系统的相关信息' (Information about the injection system) is overlaid in the center of the screenshot.

Sample Manager FTN /Maintain界面，可对进样系统进行漏液测试

The screenshot displays the Waters Sample Manager FTN software interface. The main window is titled "Leak Test" and contains a "Start" button. A red box highlights the text: "Once started, the Leak test will automatically stop upon completion or upon error." Below this, the "Progress" section shows "Test status: Ready" and a progress bar at 0.0 / 2.2 min. The "Results" section states "Test results are not available at the moment." The left sidebar shows the "Maintain" menu with "Leak Test" selected. The right sidebar shows the "Instrument System" summary, including "Binary Solvent Manager" (Idle) and "Vion IMS QToF" (Desolvation gas flow error).

Click "start" to perform the leak test of the sample system.

Vion IMS TOF 界面下的操作

VION IMS QTof /Summary界面，可查看VION质谱的状态

The screenshot displays the Waters VION IMS QTof Summary interface. The main window is titled "Instrument Summary" and shows the instrument is "Idle". The interface is divided into several sections:

- Instrument Summary:** Shows the instrument name "Vion IMS QTof" and its status "Idle".
- Instrument Status:** A table of status indicators:

Status	
Vacuum:	OK - Pumped
Operate:	Operate
Instrument:	Idle
Setup (standard):	Passed - Mar 04, 2016 17:40:38 CST
Setup (high mass):	Not run
Sample fluidics:	Idle
Reference fluidics:	Idle
- ESI Parameters:**

Source temperature:	99.96 °C
Desolvation temperature:	279.79 °C
Cone gas:	0.00 L/h
Desolvation gas:	794.43 L/h

The interface also includes a left-hand navigation pane with "Vion IMS QTof" and "Summary" highlighted, and a right-hand pane showing system-level details like "LCMS System" and "Binary Solvent Manager".

质谱的状态



VION IMS QToF /Summary界面，可查看VION质谱的操作记录

The screenshot displays the Waters VION IMS QToF Summary interface. The central pane shows a log of system events with the following data:

Type	Date	Category	User	Action
Warning	Mar 04, 2016 23:22:37 China Standard Time	System Event	System	Pump override enabled.
Error	Mar 04, 2016 23:21:15 China Standard Time	System Event	System	IMS Pressure Lock Failure.
Warning	Mar 04, 2016 23:17:57 China Standard Time	System Event	System	Pump override enabled.
Error	Mar 04, 2016 23:17:53 China Standard Time	System Event	System	IMS Pressure Lock Failure.
Error	Mar 04, 2016 23:17:26 China Standard Time	System Event	System	IMS Pressure Setup Failure.
Error	Mar 04, 2016 23:16:31 China Standard Time	System Event	System	IMS Pressure Lock Failure.
Warning	Mar 04, 2016 23:16:17 China Standard Time	System Event	System	Pump override enabled.
Error	Mar 04, 2016 23:16:09 China Standard Time	System Event	System	IMS Pressure Lock Failure.
Info	Mar 04, 2016 17:40:38 China Standard Time	System Event	System	Instrument setup completed
Info	Mar 04, 2016 17:27:08 China Standard Time	System Event	System	Instrument setup started
Warning	Mar 04, 2016 17:14:18 China Standard Time	System Event	System	Pump override enabled.
Warning	Mar 04, 2016 17:14:17 China Standard Time	System Event	System	System connection restored
Warning	Mar 04, 2016 17:14:16 China Standard Time	System Event	System	Source Temperature settle.

The interface also includes a 'Console Navigation' pane on the left with 'Vion IMS QToF' and 'Summary' highlighted, and an 'Instrument System' pane on the right showing system status (Idle) and solvents (A1: 50.0%, B1: 50.0%). A large red box highlights the log table, and the text 'VION质谱的操作记录' is overlaid on it.

VION IMS QToF /Setup界面，可对质谱进行校正及质谱重新启动

Instrument Setup

Start Stop **Complete**
Instrument Setup Complete

Please ensure that the low mass calibration standard is present in vial C and Leucine enkephalin lockmass standard is present in vial B

Fluidics setup completed
Sample Fluidics Setup started
Fluidics setup completed
Lock Mass Correction Started.
Lock Mass Correction detected masses : 554.26.
Lock Mass Correction detected masses : 554.26.
Lock Mass Correction detected masses : 554.26.
Lock Mass Correction detected masses : 554.26.
Lock Mass Correction detected masses : 554.26.
Lock Mass Correction complete.
CCS Calibration - Acquiring data 1% complete
CCS Calibration - Acquiring data 8% complete
CCS Calibration - Acquiring data 16% complete
CCS Calibration - Acquiring data 25% complete
CCS Calibration - Acquiring data 33% complete
CCS Calibration - Acquiring data 41% complete
CCS Calibration - Acquiring data 50% complete
CCS Calibration - Acquiring data 58% complete
CCS Calibration - Acquiring data 66% complete
CCS Calibration - Acquiring data 75% complete
CCS Calibration - Acquiring data 83% complete
CCS Calibration - Acquiring data 91% complete
CCS Calibration - Acquiring data 100% complete
CCS Calibration successful.
CCS Calibration Complete
Instrument Setup Complete
Nothing to run. Instrument Setup has detected that it does not need to run any tasks at this time.
Instrument Setup Complete

Plot Data

0.00 0 0.000e+0

530.0 540.0 550.0 560.0 570.0
Mass (m/z)

Reset instrument
Are you sure you want to reset the instrument?
Yes No

Instrument System

Summary

LCMS System

Status
System: Idle
Startup: Maintenance
Current analysis

Instruments

Binary Solvent Manager

Idle

Pressure and flow
52 psi 0.000 mL/min

Delta pressure
0 psi

Solvents
A1: 50.0 % B1: 50.0 %

Sample Manager FTN

Idle

Temperatures (°C)
Sample: 10.1 10.0
Column: 45.0 45.0

Vion IMS QToF

Idle

Source: ESI
Sample: Idle
Reference: Idle

VION IMS QToF /Setup界面，可对质谱进行校正及质谱重新启动

1, 点击“start”开始自动校正后，在此界面会出现时时校正的情况

2, setup会优化以下参数：
双通道ADC比值的精确测量，Detector setup, 优化质谱的分辨率
在非淌度模式下进行质量数的校正, 1000, 2000
在淌度模式下进行CCS值的校正, 1000, 2000

VION IMS QTof /Setup界面，可对质谱进行校正及质谱重新启动

当通讯失去连接时，可点击“reset”可对质谱进行重启

Instrument Setup Complete

Please ensure that the low mass calibration standard is present in vial C and Leucine enkephalin lockmass standard is present in vial B

Fluidics setup completed
 Sample Fluidics Setup started
 Fluidics setup completed
 Lock Mass Correction Started.
 Lock Mass Correction detected masses : 554.26.
 Lock Mass Correction detected masses : 554.26.
 Lock Mass Correction detected masses : 554.26.
 Lock Mass Correction detected masses : 554.26.
 Lock Mass Correction detected masses : 554.26.
 Lock Mass Correction complete.
 CCS Calibration - Acquiring data 1% complete
 CCS Calibration - Acquiring data 8% complete
 CCS Calibration - Acquiring data 16% complete
 CCS Calibration - Acquiring data 25% complete
 CCS Calibration - Acquiring data 33% complete
 CCS Calibration - Acquiring data 41% complete
 CCS Calibration - Acquiring data 50% complete
 CCS Calibration - Acquiring data 58% complete
 CCS Calibration - Acquiring data 66% complete
 CCS Calibration - Acquiring data 75% complete
 CCS Calibration - Acquiring data 83% complete
 CCS Calibration - Acquiring data 91% complete
 CCS Calibration - Acquiring data 100% complete
 CCS Calibration successful.
 CCS Calibration Complete
 Instrument Setup Complete
 Nothing to run. Instrument Setup has detected that it does not need to run any tasks at this time.
 Instrument Setup Complete

Reset instrument

Are you sure you want to reset the instrument?

Yes No

Plot Data

Mass (m/z)

530.0 540.0 550.0 560.0 570.0

52 psi 0.000 mL/min

Delta pressure 0 psi

Solvents A1: 50.0 % B1: 50.0 %

Temperatures (°C) Sample: 10.1 10.0 Column: 45.0 45.0

Source: ESI Sample: Idle Reference: Idle

VION IMS QTof /Maintain 界面，可对检查质谱的一些性能

VION质谱的相关信息

Package	Version	Build Date
Instrument Client	1155	Nov 18, 2015 11:52:00 China Standard Time (+08:00)
Instrument	1269	Nov 25, 2015 15:19:00 China Standard Time (+08:00)
Instrument VxWorks	1288	Nov 18, 2015 12:36:56 China Standard Time (+08:00)
Vion IMS QTof	1.0.0	Nov 25, 2015 00:00:00 China Standard Time (+08:00)

VION IMS QTof /Maintain 界面，可对检查质谱的一些性能

The screenshot displays the 'Fluidics' control panel in the Waters VION IMS QTof /Maintain software. The interface is divided into two main sections: 'Sample Fluidics' and 'Reference Fluidics'. Both sections include buttons for 'Start infusion', 'Refill', 'Purge', 'Wash', and 'Reset'. The 'Sample Fluidics' section shows a reservoir set to 'C', an infusion flow rate of 10.0 µl/min, and a fill volume of 250 µl. The 'Reference Fluidics' section shows a reservoir set to 'B', an infusion flow rate of 10.00 µl/min, and a baffle position set to 'Sample'. The 'Baffle position' dropdown is highlighted with a red box and an arrow pointing to the explanatory text below. The right side of the interface shows a 'Summary' panel for the LCMS System, an 'Instruments' panel for the Binary Solvent Manager, and a 'Sample Manager FTN' panel. The 'Sample Manager FTN' panel shows the sample and column temperatures.

样品流路

Start infusion : 开始进样
 Refill: 管路充满液体
 Purge: 灌注管路,主要目的是排除管路中的气泡,让要进样的液体充满管路

校正液流路

在这里可以选择“ sample” 或者是“ reference”

选择“ sample” 意味着sample流路中的液体进入质谱

反之，“reference” 流路的溶液进入质谱

VION IMS QToF /Maintain 界面，可对检查质谱的一些性能

The screenshot displays the Waters VION IMS QToF software interface. The main window is titled "Vacuum" and shows the system status as "OK - Pumped". A "Vent" button is visible. The interface includes a left-hand navigation pane with "Maintain" and "Vacuum" highlighted. The right-hand pane shows the "Instrument System" summary, including status, instruments, and solvents.

Ok , 代表质谱系统的真空度是正常的
点击“vent”将质谱泄真空。

所以，请不要点击，除非你真的要泄掉质谱的真空

Pressure	
Backing:	3.27e0 mbar
Trap:	3.42e0 mbar
IMS:	3.31e0 mbar
IonGuide:	6.56e-3 mbar
Cell1:	7.71e-3 mbar
Cell2:	7.85e-3 mbar
TOF:	2.81e-7 mbar

Turbo speed	
Source:	100.76 %
TOF:	100.76 %

Turbo operation time	
Source:	1,045 hours
TOF:	1,066 hours

VION IMS QToF /Tools/Mannual optimization 界面，可进行质谱参数的设置

Manual Optimization 进行仪器的参数设置

选择“正或负离子模式” (Positive/Negative)
选择“淌度模式或非淌度模式” (Sensitivity/Resolution)
仪器状态“operate”、“source standby”、“关机” (Operate/Source Standby)
选择“灵敏度或分辨率模式” (TOF/Mobility)
打开“气体”其中API气体为氮气 (API Gas)
Collision Gas 气体为氩气 (Collision Gas)
扫描的质量范围及扫描时间 (Scan range and time)

ESL LockSpray Instrument Fluidics StepWave Trap/IMS System2 MS Purif RF

Capillary (kV):	3.00	3.06
Sampling Cone (V):	80	
Source Offset (V):	80	94
Source Temperature (°C):	100	100
Desolvation Temperature (°C):	280	280
Cone Gas (L/hour):	0	0
Desolvation Gas (L/hour):	800	796

VION IMS QToF /Tools/Mannual optimization 界面，可进行质谱参数的设置

Manual Optimization

Plot Data

0.00 0 0.000e+0

553.5 554.0 554.5 555.0 555.5 556.0 556.5 557.0 557.5 558.0 558.5 559.0 559.5 560.0 560.5 561.0 561.5

Positive Negative **Sensitivity** Resolution TOF Mobility API Gas Collision Gas 1000 1.0 Operate Source Standby

Controls

ESI LockSpray	Instrument	Fluidics	StepWave	Trap/IMS	System2	MS Profile	RF
Capillary (kV):	3.00	3.06					
Sampling Cone (V):	80						
Source Offset (V):	80	94					
Source Temperature (°C):	100	100					
Desolvation Temperature (°C):	280	280					
Cone Gas (L/hour):	0	0					
Desolvation Gas (L/hour):	800	790					

离子源参数设置

VION IMS QToF /Tools/Mannual optimization 界面，可进行质谱参数的设置

Manual Optimization

Mass (m/z)

MZ DT BPI TIC Clear Normalise On

Positive Negative Sensitivity Resolution TOF Mobility API Gas Collision Gas 1000 1.0 Operate Source Standby

Controls

ESI LockSpray	Instrument	Fluidics	StepWave	Trap/IMS	System2	MS Profile	RF
Collision Energy (V):	6						
Ion Guide Gradient (V):	3.0	-154.7					
Aperture 2 (V):	0.0	-157.2					
LM Resolution (low):	4.7						
HM Resolution (high):	15.0						
Pre-filter (V):	10	-167					
Ion Energy (V):	0.2						

Instrument 界面下，一般使用默认参数。

VION IMS QToF /Tools/Mannual optimization 界面，可进行质谱参数的设置

Fluidics 界面下，可以进行A, B和C 管路的相关操作

管路灌满 将原来的溶剂排空并充满所需溶剂

开始进样

不同的流路进入质谱

可以选择Sample或Reference 流路进入质谱

VION IMS QToF /Tools/Mannual optimization 界面，可进行 质谱参数的设置

Manual Optimization

Mass (m/z)

MZ DT BPI TIC Clear

Normalise On

Positive Negative Sensitivity Resolution TOF Mobility API Gas Collision Gas 1000 1.0 Operate Source Standby

Controls	
ESI LockSpray	Instrument
SW 1 Offset (V):	20
SW 2 Offset (V):	30
SW 1 Velocity (m/s):	300
SW 1 Pulse Height (V):	15.0
SW 2 Velocity (m/s):	300
SW 2 Pulse Height (V):	15.0

**Stepwave 参数的设置
一般为默认值**

VION IMS QTof /Tools/Mannual optimization 界面，可进行 质谱参数的设置

Manual Optimization

Mass (m/z)

Trap/MS参数的设置，一般使用默认值

1, 可以改变波高
此参数会影响到淌度的分离

2, 改变淌度的参数后，需要重新进行
仪器的CCS值校正

Parameter	Value
Trap Entrance (V)	0
Trap Stopper (V)	0
Stopper Height (V)	0
Trap Bias (V)	40
Gate Offset (V)	0
Gate Height (V)	40
Aperture 1 (V)	0.0
Trap Wave Velocity (m/s)	100
Trap Pulse Height 'A' (V)	40.0
Trap Pulse Height 'B' (V)	5.0
IMS Wave Velocity (m/s)	250
IMS Pulse Height (V)	50.0
Gate Release (ms)	2.00
Gate Delay (ms)	0
Wave Delay (# pushes)	20

VION IMS QToF /Tools/Mannual optimization 界面，可进行质谱参数的设置

Waters
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Manual Optimization

Mass (m/z)

MZ DT BPI TIC Clear

Normalise On

Positive Negative Sensitivity Resolution TOF Mobility API Gas Collision Gas 1000 1.0 Operate Source Standby

Controls

ESI LockSpray Instrument Fluidics StepWave Trap/IMS System2 MS Profile RF

pDRE Attenuate: Off

pDRE Transmission (%): 50.0

pDRE HD Attenuate: Off

pDRE HD Transmission (%): 20.0

使用默认值

Instrument System

Summary

LCMS System

Status: System: Idle

Startup: Maintenance

Current analysis

Instruments

Binary Solvent Manager

Idle

Pressure and flow: 51 psi, 0.000 mL/min

Delta pressure: 0 psi

Solvents: A1: 50.0 % B1: 50.0 %

Sample Manager FTN

Idle

Temperatures (°C): Sample: 10.1 10.0 Column: 45.0 45.0

Vion IMS QToF

Source Temperature settle.

Source: ESI

Sample: Idle

Reference: Idle

VION IMS QTof /Tools/Mannual optimization 界面，可进行 质谱参数的设置

Mass Profile 主要是用来调节四极杆的通过率的，

一般默认为是Automatic的设置

VION IMS QToF /Tools/Mannual optimization 界面， 可进行质谱参数的设置

Mass Profile 主要是用来调节四极杆的通过率的，

当需要设定四极杆对某些离子的通过率或进行大分子的实验时，可以使用Manual profile

VION IMS QToF /Tools/Mannual optimization 界面，可进行质谱参数的设置

The screenshot displays the 'Manual Optimization' window in the Waters VION IMS QToF software. The main area features a mass spectrum grid with the x-axis labeled 'Mass (m/z)' ranging from 553.5 to 615.0. Below the grid, a text overlay reads: **RF的界面下，采用默认参数** (In the RF interface, use default parameters). A red box highlights the 'Controls' panel, which includes the following parameters:

Parameter	Value	Target/Range
StepWave RF (V)	250	250
Trap/IMS RF (V)	250	250
Ion Guide RF Offset (V)	200	263
Ion Guide RF Gain	5	
Cell1 RF (V)	300	301
Cell2 RF Offset (V)	100	165
Cell2 RF Gain	5	

Additional parameters shown in the 'Controls' panel include MS/MS Ramp Mode (Automatic), MS/MS Ramp Initial (25), and MS/MS Ramp Final (275). The interface also includes a 'Tools' sidebar on the left and an 'Instrument System' sidebar on the right showing system status and solvents.

VION IMS QTof /Tools/Mannual optimization 界面，可在此界面查看LE的情况来查看仪器的响应等情况

Manual Optimization

Plot Data

Pop Out Save Set Load Set Tune Abort

1, 质谱参数优化后, 可点击“save set”对参数进行保存
 2, 点击“load set”可调用之前保存好的参数
 3, 点击“Tune”, 可进行时时数据的数据纪录
 4, 点击“abort”, 停止数据的时时纪录

Mass (m/z)

MZ DT BPI TIC Clear Normalise On

Positive Negative Sensitivity Resolution TOF Mobility API Gas Collision Gas 1000 1.0 Operate Source Standby

Controls

ESI LockSpray	Instrument	Fluidics	StepWave	Trap/IMS	System2	MS Profile	RF
Capillary (kV):		3.00	3.06				
Sampling Cone (V):		80					
Source Offset (V):		80	94				
Source Temperature (°C):		100	100				
Desolvation Temperature (°C):		280	280				
Cone Gas (L/hour):		0	0				
Desolvation Gas (l/hour):		800	798				

通过快捷方式进行VION系统的操作

The screenshot shows the Waters UNIFI LCMS System interface. The main window displays the 'I-Class Binary Solvent Manager' in 'Idle' status. The interface is divided into several sections:

- Console Navigation (Left):** Lists system components like 'System', 'Binary Solvent Manager', and 'Sample Manager FTN'.
- Instrument Summary (Top Center):** Shows 'I-Class Binary Solvent Manager' with 'Idle' status and 'Power' and 'Flow' indicators.
- Flow Conditions (Middle Left):** Displays flow rate (0.000 ml/min), pressure (52 psi), degasser (0.40 psi), and vent valve (System).
- Composition (Middle Right):** Shows solvent percentages: Solvent A1: 50.0%, Solvent B1: 50.0%.
- Performance (Middle Right):** Shows total volume pumped (0 L) and pressure ripple (51 psi).
- Summary (Right Panel):** Provides a quick overview of system status, including 'System: Idle' and 'Startup: Ready'.
- Instruments (Right Panel):** Lists available instruments like 'Binary Solvent' and 'Sample Manager FTN'.
- Sample Manager FTN (Right Panel):** Shows sample and column temperatures (e.g., 10.1, 10.0, 45.0, 45.0).
- Vion IMS QTof (Right Panel):** Shows instrument source (ESI) and sample status (Idle).

Annotations in Chinese provide instructions on how to interact with the system:

- 关于系统的操作 (System Operation):** Points to the 'Summary' and 'Instruments' panels on the right.
- 关于泵的相关操作 (Pump-related operations):** Points to the 'Performance' section in the middle right.
- 关于自动进样器的相关操作 (Autosampler-related operations):** Points to the 'Sample Manager FTN' panel on the right.
- 关于质谱的相关操作 (Mass Spectrometry-related operations):** Points to the 'Vion IMS QTof' panel on the right.

A red checkmark and text at the bottom left state: **点击 (绿色的对号) 可以进入快捷方式, 进入系统, 可以分别对系统里的各个模块进行操作** (Clicking the green checkmark can enter shortcuts, enter the system, and perform operations on various modules in the system).

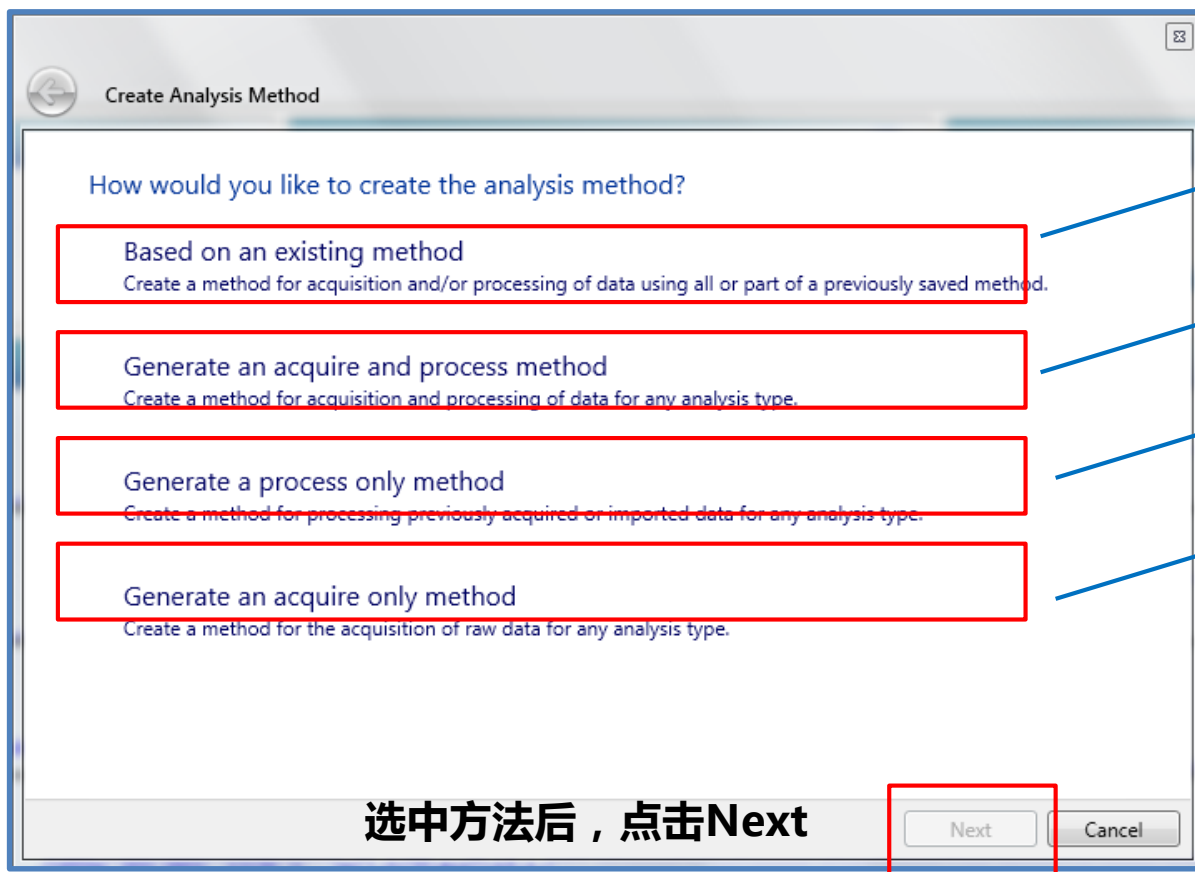
The bottom of the screen shows the Windows taskbar with the system clock at 11:52 AM on 5/11/2010.

建立分析方法及分析,用于采集数据

建立分析方法

在建立采集数据/处理数据的方法，根据需要选择合适的方法类型：

选中方法类型后，点击Next



用以前建立好的方法

建立采集并处理的方法

建立只数据处理的方法

建立采集数据的方法

选中方法后，点击Next

Next

Cancel

在建立采集数据/处理数据的方法，根据需要选择合适的方法类型：

给建立的方法命名及所保存的位置：

Create Analysis Method

Please Enter the Analysis Method Details

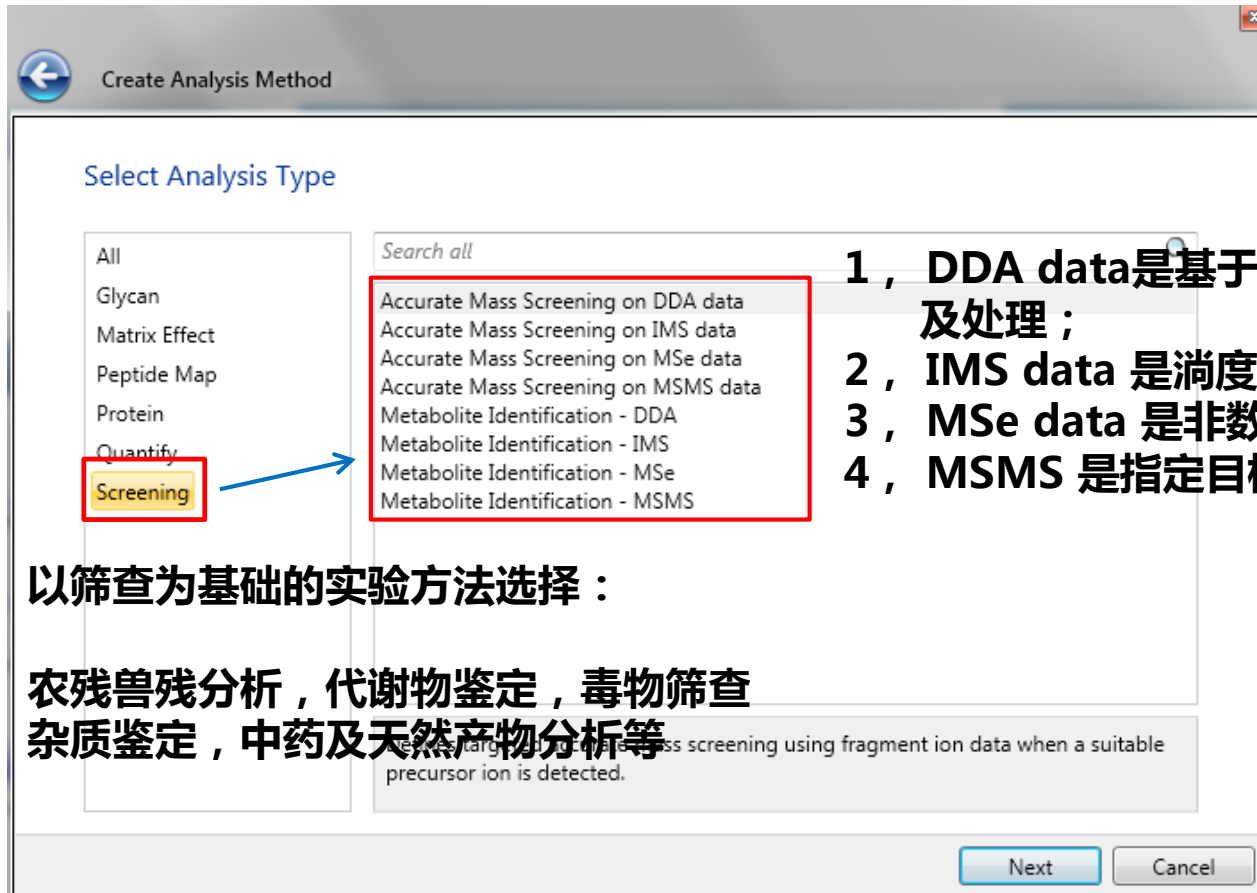
Name: test 命名 *

Description:

Folder: Company/Dan Diagnostics 文件夹存放的位置 *

Next Cancel

选择好合适方法类型后,根据应用选择不同的方法:



- 1, DDA data是基于数据依赖性的数据采集及处理;
- 2, IMS data 是淌度模式的数据采集及处理;
- 3, MSe data 是非数据依赖性的数据采集及处理
- 4, MSMS 是指定目标离子的二级碎片采集及处理

以筛查为基础的实验方法选择：

农残兽残分析，代谢物鉴定，毒物筛查
杂质鉴定，中药及天然产物分析等

Use as target ion for accurate mass screening using fragment ion data when a suitable precursor ion is detected.

选择好合适方法类型后,根据应用选择不同的方法:

选中方法类型后 , 点击Next

The screenshot shows the 'Create Analysis Method' dialog box. On the left, a sidebar lists analysis types: All, Glycan, Matrix Effect, Peptide Map, Protein, Quantify, and Screening (highlighted in yellow). The main area has a search bar and a list of methods. 'Accurate Mass Screening on MSe data' is selected and highlighted in blue. A tooltip is visible over 'Accurate Mass Screening on MSMS data'. Below the list, a description reads: 'Defines accurate mass screening on full scan MS or MSe data for identification, discovery and quantification.' At the bottom, the 'Next' button is highlighted with a red box, and the 'Cancel' button is visible to its right.

选中方法类型后 , 点击Next

选择采集数据所用的系统

Create Analysis Method

Select Instrument System

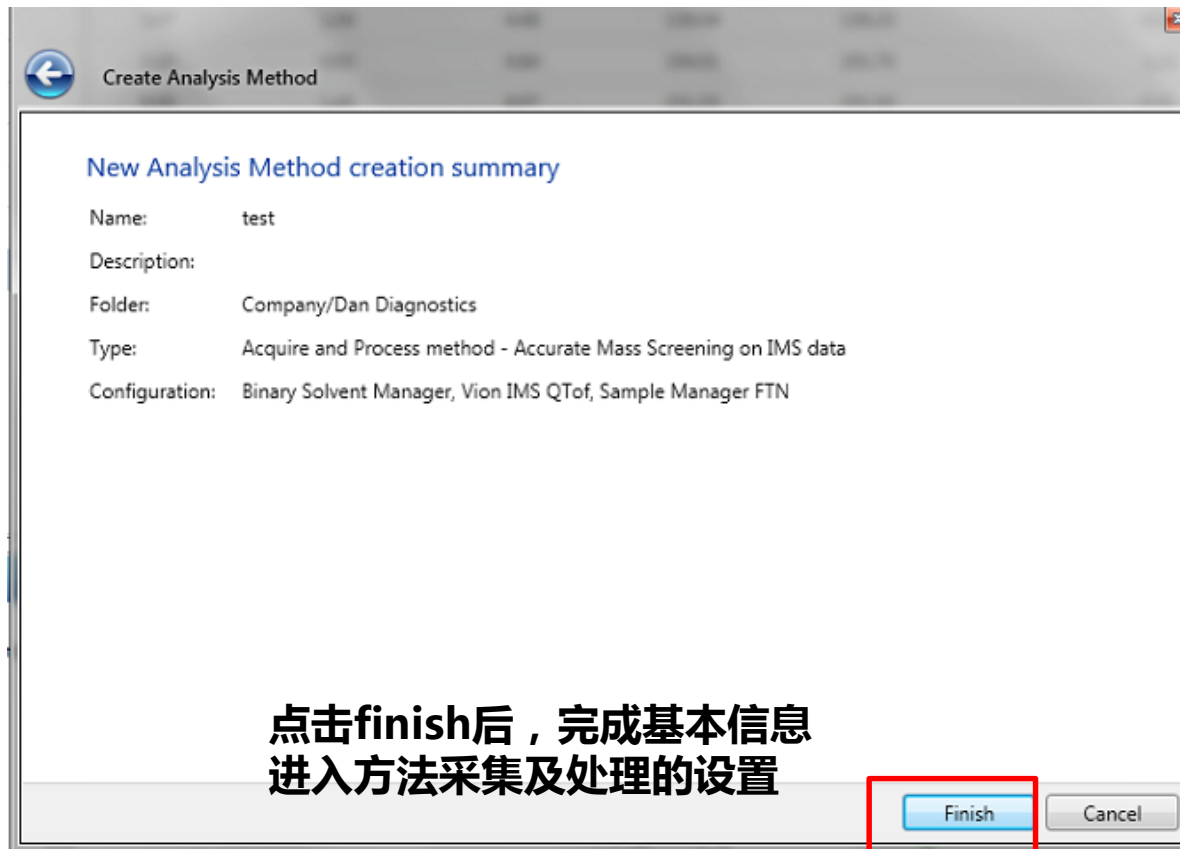
	System name	Status	Description
1	IClass Standalone	Offline	
2	LCMS System	Online	
3	Vion Standalone	Offline	

选择采集数据所用的系统没，所选择的系统必须是online
Offline的系统必须online后才能使用

选中后，单击 Next

Next Cancel

点击“Finish”完成方法的基本信息的建立



采集方法的方法设置

关于质量范围的设置：

VION的仪器校正是自动校正的，目前校正的质量范围是1000，2000和4000。

因此，在方法设置中关于高端质量数的设置，请选择1000，2000 或4000

HDMS或MS的方法

HDMS和MS的方法设置-1

Settings Experiment Options Events

Settings ESI + -

General

Analyzer mode: Sensitivity

Voltages

Capillary voltage: kV

Temperatures

Source temperature: °C

Desolvation temperature: °C

Gas flow

Cone gas: L/h

Desolvation gas: L/h

HDMS和MS的方法设置-2

选择MS模式或High Definition MS 模式

Settings Experiment Options Events

MS Experiment

Mode

- MS
- High Definition MS

Acquisition time

- Use analysis method run time
- Use custom run time

Start time: (Automatic) min End time: (Automatic) min

Scan settings

Low mass: 50 m/z

High mass: 1000 m/z

Scan time: 0.300 s

Collision energy

Collision energy mode: Off

Data reduction

Enable data reduction on acquired data

Expected peak width: 2.00 s

Intensity threshold: 20000 counts

Experiment Type

- MS - Single MS experiment
- MSⁿ - Single MSⁿ experiment
- Function Table - One or more MS, MSMS or MRM functions
- DDA - Data Directed Analysis

A method can only contain parameters for a single experiment type. Changing the experiment type will reset experiment settings to default values.

Ok Cancel

设置采集时间：
1，根据梯度的时间
2，根据需要，可以自行设置扫描时间

设置采集的质量范围及扫描时间

点击“experiment” 选择“MS” 模式

HDMS和MS的方法设置-3

Settings Experiment Options Events 关于LE的设置

Lock correction

Lock correction Mode: Automatic

Automatic lock correction

Automatic Interval (5 min)

Custom Interval 0.50 min

Automatic lock correction requires the Waters LockSpray standard to be placed in the LockSpray reservoir.

Automatic lock correction will sample lock reference periodically as well as at the start and end of each acquisition.

The lock correction interval and sample time will be validated when the analysis method is run.

Options

Pre acquisition checks

Acquisition check failure: Continue with lock correction

Detector check

Automatic detector check: Disabled

Detector check

Automatic detector check: Enabled

1, 可以使用Automatic

2, Custom interval 设置采集时间间隔, 要设置大于0.2min, 一般设置为0.5min

在淌度模式下, 最高质量是2000时, 选择 "Disabled"

其他情况下, 可以选择 "Enabled"

HDMS和MS的方法设置-4

Settings Experiment Options Events

Lock correction

Lock correction
Mode: Custom

Custom lock correction
Single reference mass: 554.2620 m/z
Dual reference mass: 130.0874 m/z Enable dual point correction

Interval: 0.50 min
Application: Use Lock Sprayer Reference

Sample time: 2.00 s
Attenuation: 80.0 %
Collision energy: 18.00 eV
Flow rate: 10.00 µl/min

The lock correction interval and sample time will be validated when the analysis method is run.

Options

Pre acquisition checks
Acquisition check failure: Continue with lock correction

Detector check
Automatic detector check: Disabled

校正液的设置也可以选择“custom”
根据自己需要进行设置

设置 reference 离子的质荷比，可以使用一个离子
或两个离子

设置采集间隔时间，一般设置为0.5min

Sample time，采集时间，一般设置为0.3s
Attenuation：离子强度压缩到 80%（如果设置为80）
Collision energy: 碰撞能量的设置，
Flow rate：流速的设置

HDMS和MS的方法设置-5

Events 的设置相对简单，只需要如下设置即可

Events Table

点击“Enable”

Time (min)	Event	Action	System
1	Initial Flow State	LC	Sample

选择“trigger”时，有三个选项

Triggers

Trigger type: Network

- None
- Network
- Hardware

None，指的是不做前端分离的触发

Network的trigger，UNIFI能控制的分离

Hardware是指UNIFI不能控制的前端分离或第三方的液相

HDMS^E或MS^E的方法设置

HDMS^E和MS^E的方法设置-1

Settings Experiment Options Events

Settings ESI + -

General

Analyzer mode: Sensitivity

Voltages

Capillary voltage: kV

Temperatures

Source temperature: °C

Desolvation temperature: °C

Gas flow

Cone gas: L/h

Desolvation gas: L/h

HDMS^E和MS^E的方法设置-2

Settings Experiment Options Events

MS^E Experiment

MS^E

Mode

- MS^E
- High Definition MS^E
- Perform product ion confirmation

Acquisition time

- Use analysis method run time
- Use custom run time

Start time: (Automatic) min End time: (Automatic) min

Scan settings

Low mass: 50 m/z

High mass: 1000 m/z

Scan time: 0.2 s

Collision energy

Low energy: 6.00 eV

High energy ramp: 20.00 eV to: 30.00

Enable data reduction on acquired data

Expected peak width: 2.00 s

Intensity threshold: 20000 counts

Experiment Type

- MS - Single MS experiment
- MS^E - Single MS^E experiment
- Function Table - One or more MS, MSMS or MRM functions
- DDA - Data Directed Analysis

A method can only contain parameters for a single experiment type. Changing the experiment type will reset experiment settings to default values.

Ok Cancel

需要多设置一个高能量，一般为20-40eV

DDA的方法设置

MS to MSMS 由全扫描触发的二级碎片扫描

主要的目的是：选择全扫描模式中响应强的前几个离子大打碎片

DDA方法设置-1

The screenshot displays the Waters software interface for configuring an experiment. The 'Settings' window is open to the 'Experiment' tab. The 'General' section shows 'Analyzer mode' set to 'Sensitivity'. The 'Voltages' section shows 'Capillary voltage' at 0.50 kV. The 'Temperatures' section shows 'Source temperature' at 120 °C and 'Desolvation temperature' at 550 °C. The 'Gas flow' section shows 'Cone gas' at 50 L/h and 'Desolvation gas' at 800 L/h. The 'Experiment Type' dialog box is open, showing four options: 'MS - Single MS experiment', 'MSⁿ - Single MSⁿ experiment', 'Function Table - One or more MS, MSMS or MRM functions', and 'DDA - Data Directed Analysis'. The 'DDA - Data Directed Analysis' option is selected and highlighted with a red box. A red arrow points from the 'Experiment' tab to the 'Experiment Type' dialog box. The 'ESI' dropdown menu is also highlighted with a red box.

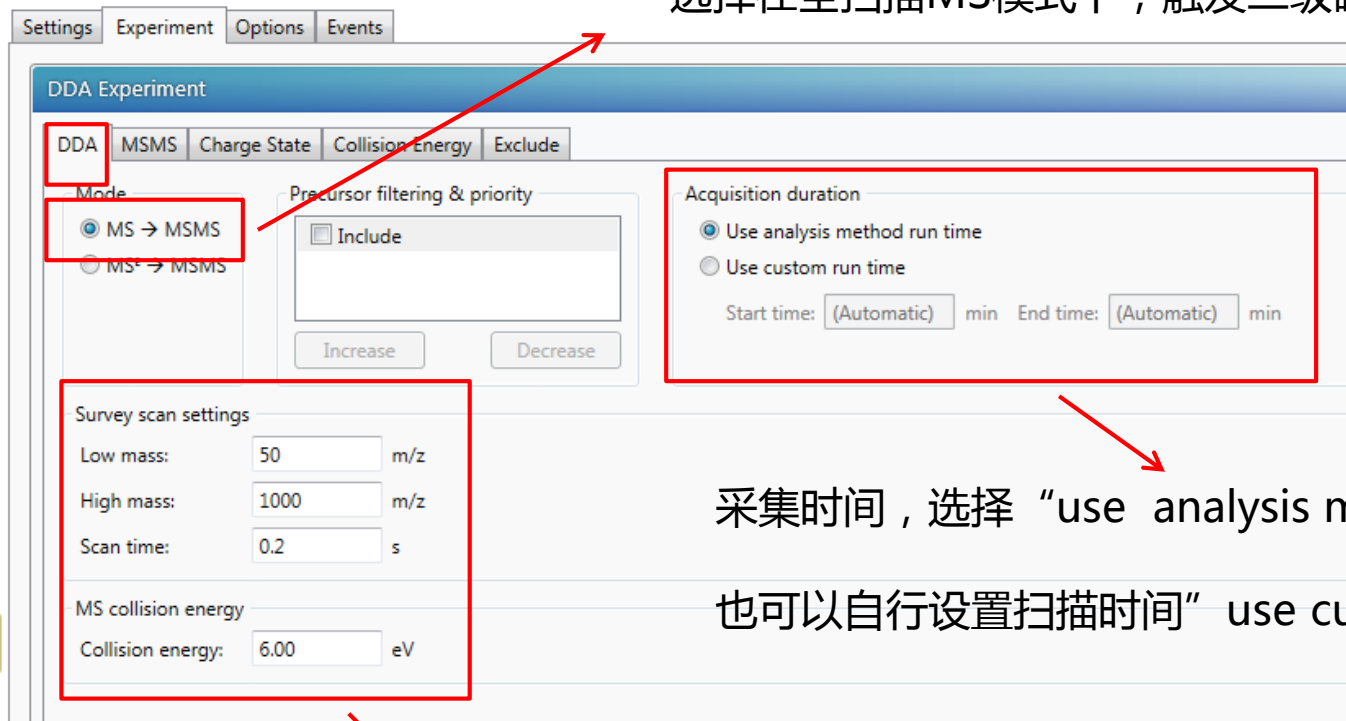
选择“采集数据的模式”

选择“离子化”的模式

点击“experiment”
选择“采集数据的模式”

DDA的方法设置-2

选择在全扫描MS模式下，触发二级碎片采集



采集时间，选择“use analysis method”，根据梯度的时间
也可以自行设置扫描时间“use custom run time”

全扫模MS的设置：质量范围的设置，扫描时间的设置，一级能量的设置

VION的校正质量数1000，2000或4000，因此在设置high Mass时，

选择与校正范围相同的质量数

DDA方法设置-3

设置触发二级扫描的条件
当全扫描中一级质谱图的响应大于某一设定值时，
开始触发二级扫描。

Trigger MSMS acquisition
Acquire when intensity exceeds: 5000 counts

Stop MSMS acquisition
 Acquire until TIC exceeds: 100 counts
 Acquire until timeout expires: 0.2 s

MSMS settings
Maximum simultaneous MSMS acquisitions: 5

Use survey scan settings
 Use custom settings

Scan time: 0.100 s
Low mass: 50 m/z
High mass: 1000 m/z

选择采集“响应前几强的离子”进行二级碎片的扫描

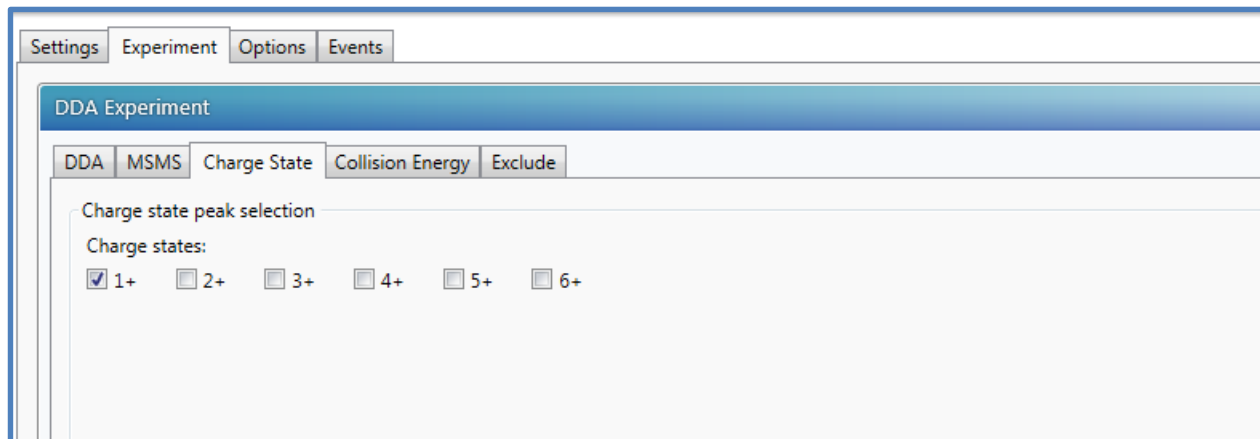
每个母离子采集二级碎片的时间

- 1, 当强度低于一定阈值时,停止采集二级碎片
- 2, 采集一定时间后停止,一般采集1个 scan 或2个Scan 后停止.
- 3, 一般采用第二种方式

二级采集的方法设置：

“use survey scan setting” 是使用一级全扫描的采集的方法
“use custom setting” 可以设置扫描时间和扫描的质量范围

DDA方法设置-4



选择**母离子**的“价态”进行打碎，小分子一般选择“单电荷”

在进行多肽等化合物分析时，可选择带多电荷的母离子

DDA方法设置-5

The screenshot shows the 'DDA Experiment' configuration window. The 'Collision Energy' tab is active, with 'Mode' set to 'Mass dependent ramp'. The 'Low mass ramp settings' are: Low mass: 50 m/z, Ramp: 10.00 eV to 30.00 eV. The 'High mass ramp settings' are: High mass: 1000 m/z, Ramp: 20.00 eV to 50.00 eV. A 'Preview' section shows a graph of 'Collision energy ramp (eV)' vs 'Ramp during scan' for m/z 525. The graph displays three lines: 'High mass ramp' (grey), 'Low mass ramp' (grey), and 'Example ramp' (purple). A red box highlights a point on the graph labeled '15 to 40 eV at m/z 525'.

选择“二级碎片扫描时的碰撞能量”

一般选择
“Mass Dependent ramp”
质量数越大,所需要的碰撞能量越大

选择“能量的范围”

可以通过此按钮
查看不同质量数的能量范围,
并进行能量的调整

Settings Experiment Options Events

DDA Experiment

DDA MSMS Charge State Collision Energy Exclude

Add Delete Delete All Copy Paste Import

There are no rows defined.
Please add a new row using the toolbar.

MSMS dynamic peak exclusion

- Acquire once then always exclude for the rest of the acquisition
- Acquire and then exclude for a duration of: s

排出离子的规则：

第一个选项：采集一次后，就不会再采集此离子的二级碎片；

第二个选项：采集一次后，在采集后的一段时间内不再采集；

一般选择第二个选项，采集间隔时间一般为色谱峰的峰宽，4S

DDA的方法设置

MS^E to MSMS 由MS^E触发的二级碎片扫描 (product ion confirmation)

MS^E to MSMS的目的

主要有两种触发模式：

1, **特定子离子的触发，对可能产生某一个特定子离子的母离子进行确认**

- MS^E 采集低能和高能两个通道，当在 高能通道中发现有设定的母离子存在时，就会
- 触发二级扫描。触发二级扫描时，根据一级扫描中离子的响应的前几强进行触发。
- 参考方法进行设置

2, **中性丢失的触发，对可能产生某一个特定的中性丢失的母离子进行确认**

- MS^E 采集低能和高能两个通道，当通过低能通道和高能通道中发现特定中性丢失的中性物质存在时，就会触发二级扫描。
- 触发二级扫描时，根据一级扫描中离子的响应的前几强触发。
- 参考方法进行设置

DDA方法设置-1

Settings | Experiment | Options | Events

Settings

General

Analyzer mode: Sensitivity

选择“采集数据的模式”

选择“离子化”的模式

ESI

Voltages

Capillary voltage: 0.50 kV

Temperatures

Source temperature: 120 °C

Desolvation temperature: 550 °C

Gas flow

Cone gas: 50 L/h

Desolvation gas: 800 L/h

Experiment Type

Experiment Type

- MS - Single MS experiment
- MS^E - Single MS^E experiment
- Function Table - One or more MS, MSMS or MRM functions
- DDA - Data Directed Analysis

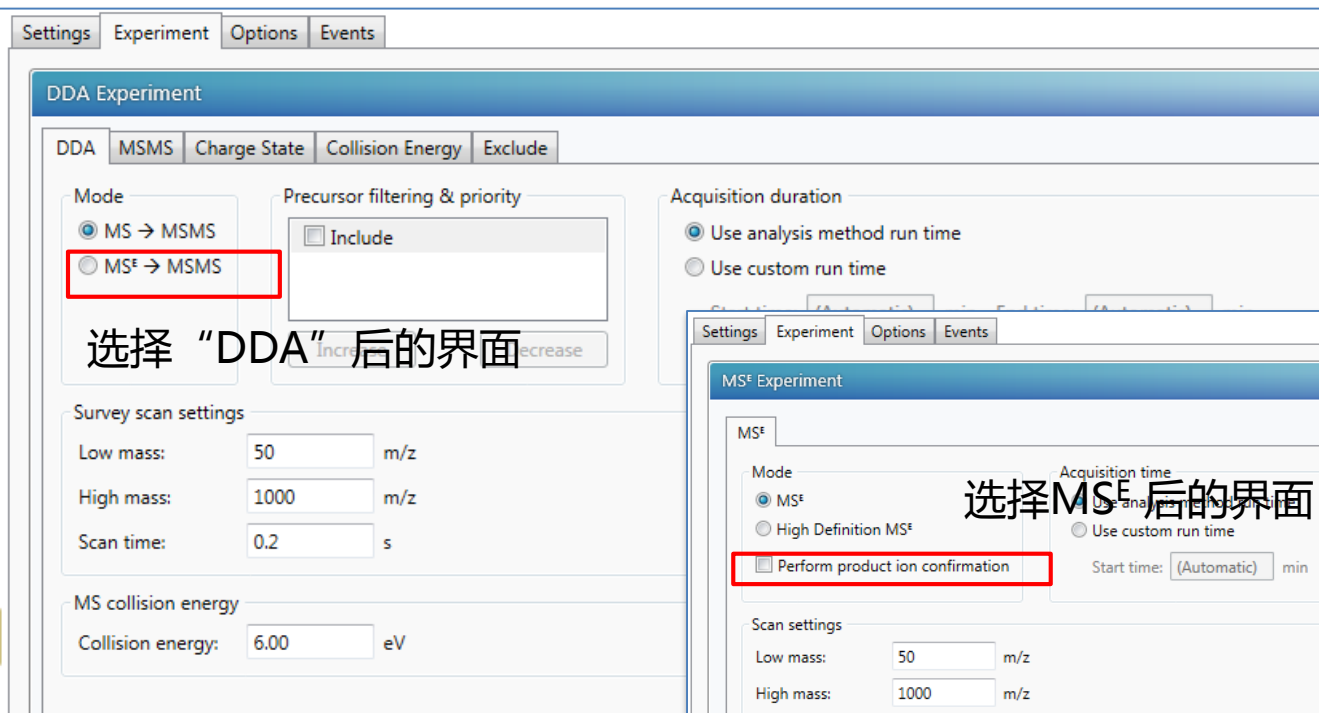
A method can only contain parameters for a single experiment type. Changing the experiment type will reset experiment settings to default values.

Ok Cancel

点击“experiment”
选择“采集数据的模式”

选择MS^E或DDA模式都可以
进入MSE-MSMS

DDA方法设置-2



Settings Experiment Options Events

DDA Experiment

DDA MSMS Charge State Collision Energy Exclude

Mode

- MS → MSMS
- MS^E → MSMS

Precursor filtering & priority

Include

Acquisition duration

- Use analysis method run time
- Use custom run time

Survey scan settings

Low mass: 50 m/z

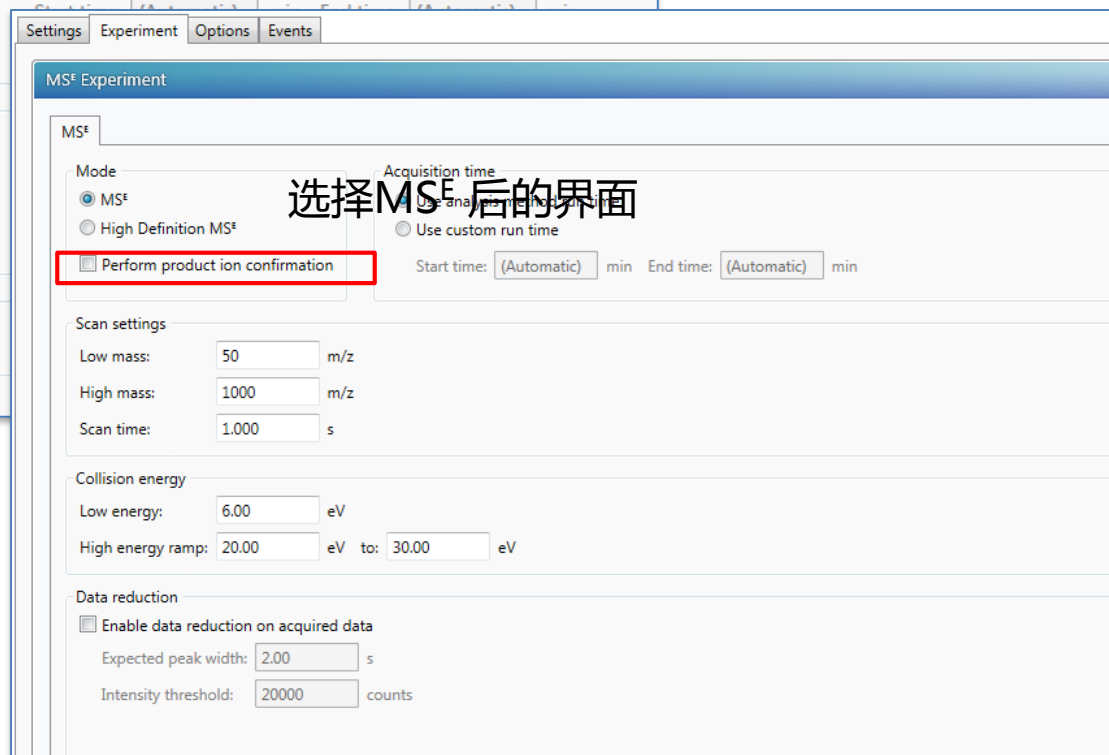
High mass: 1000 m/z

Scan time: 0.2 s

MS collision energy

Collision energy: 6.00 eV

选择“DDA”后的界面



Settings Experiment Options Events

MS^E Experiment

MS^E

Mode

- MS^E
- High Definition MS^E

Acquisition time

- Use analysis method run time
- Use custom run time

Perform product ion confirmation

Start time: (Automatic) min End time: (Automatic) min

Scan settings

Low mass: 50 m/z

High mass: 1000 m/z

Scan time: 1.000 s

Collision energy

Low energy: 6.00 eV

High energy ramp: 20.00 eV to: 30.00 eV

Data reduction

Enable data reduction on acquired data

Expected peak width: 2.00 s

Intensity threshold: 20000 counts

选择MS^E后的界面

DDA方法设置-3

The screenshot shows the 'MSF Experiment' configuration window. The 'Options' tab is selected. The 'MSF' sub-tab is active. The 'Mode' section has 'MSF' selected and 'Perform product ion confirmation' checked. The 'Precursor filtering & priority' section has 'Product Ion' checked. The 'Acquisition time' section has 'Use analysis method run time' selected. The 'Scan settings' section shows 'Low mass: 50 m/z', 'High mass: 1000 m/z', and 'Scan time: 1.000 s'. The 'Collision energy' section shows 'Low energy: 6.00 eV' and 'High energy ramp: 20.00 eV to: 30.00 eV'. Red boxes highlight these sections, with arrows pointing to Chinese annotations.

采集时间的设置

选择“product ion” 或 “Neutral loss” 进行二级的触发

设置“MSF的扫描的质量窗口”及“扫描时间”扫描时间可设置为0.1 或0.2s

•VION的校正质量数1000，2000或4000，因此在设置high Mass时，选择与校正范围相同的质量数

设置“MSF的扫描低能和高能的碰撞能量”

当低能通道的质谱的响应大于某一阈值时,进行二级碎片的扫描

MS^E Experiment

MS^E MSMS Charge State Collision Energy Exclude Product Ion

Trigger MSMS acquisition
Acquire when intensity exceeds: 1000 counts

Stop MSMS acquisition
 Acquire until TIC exceeds: 100 counts
 Acquire until timeout expires: 10.00 s

MSMS settings
Maximum simultaneous MSMS acquisitions: 1

Use survey scan settings
 Use custom settings

Scan time: 1.000 s
Low mass: 50 m/z
High mass: 1000 m/z

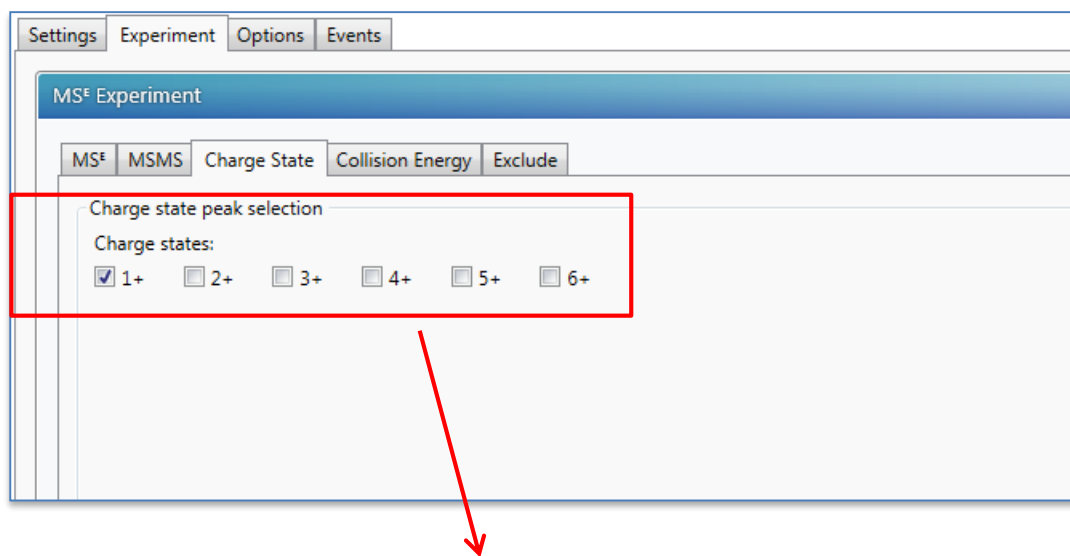
每个母离子采集二级碎片的时间
1, 当强度低于一定阈值时,停止采集二级碎片
2, 采集一定时间后停止, 一般采集1个 scan 或2个Scan 后停止.
3, 一般采用第二种方式

采集响应前几强的母离子的二级碎片

二级采集的方法设置：

“use survey scan setting” 是使用MS^E全扫描的采集的方法
“use custom setting” 可以设置扫描时间和扫描的质量范围

DDA方法设置-5



选择低能量通道的母离子的“价态”进行打碎，小分子一般选择“单电荷”

在进行多肽等化合物分析时，可选择带多电荷的母离子

DDA方法设置-6

Settings Experiment Options Events

MS^E Experiment Experiment Type

MS^E MSMS Charge State Collision Energy Exclude Product Ion

Collision energy
Mode: Mass dependent ramp

Mass dependent ramp
Define a mass-dependent collision energy ramp based on interpolation between a low-mass and a high-mass ramp.

Low mass ramp settings
Low mass: 50 m/z
Ramp: 10.00 eV to: 30.00 eV

High mass ramp settings
High mass: 1000 m/z
Ramp: 20.00 eV to: 50.00 eV

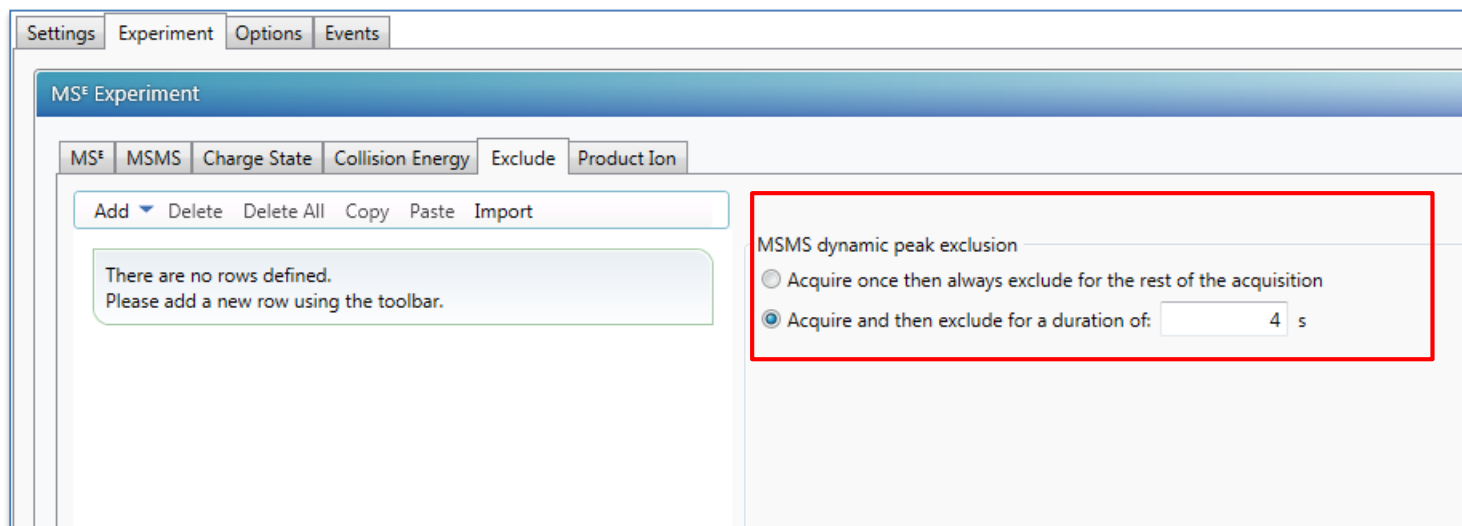
选择“二级碎片扫描时的碰撞能量”
一般选择“Mass Dependent ramp”
质量数越大,所需要的碰撞能量越大

选择“能量的范围”

可以通过此按钮查看不同质量数的能量范围,并进行能量的调整

15 to 40 eV at m/z 525

The screenshot shows the 'Collision Energy' settings in the Waters software. A red box highlights the 'Collision energy' dropdown menu set to 'Mass dependent ramp'. Another red box highlights the 'Low mass ramp settings' and 'High mass ramp settings' input fields. A red arrow points from the text '选择“能量的范围”' to the 'Ramp' input fields. A third red box highlights a button with a downward arrow, with a red arrow pointing to it from the text '可以通过此按钮查看不同质量数的能量范围,并进行能量的调整'. A fourth red box highlights a data point on the graph: '15 to 40 eV at m/z 525'. The graph shows 'Collision energy ramp (eV)' on the y-axis (0 to 40) and 'm/z' on the x-axis. It features three lines: a grey line for 'High mass ramp', a grey line for 'Low mass ramp', and a purple line for 'Example ramp'. The 'Example ramp' is a straight line starting at approximately 15 eV at m/z 150 and ending at 40 eV at m/z 525.



排出离子的规则：

第一个选项：采集一次后，就不会再采集此离子的二级碎片；

第二个选项：采集一次后，在采集后的一段时间内不再采集；

一般选择第二个选项，采集间隔时间一般为色谱峰的峰宽，4S

DDA方法设置-8

Settings Experiment Options Events

MS² Experiment

MS² MSMS Charge State Collision Energy Exclude Product Ion

Add Delete Delete All Copy Paste Import

	Description	Mass (m/z)	Threshold
1		238.2345	5,000

Settings

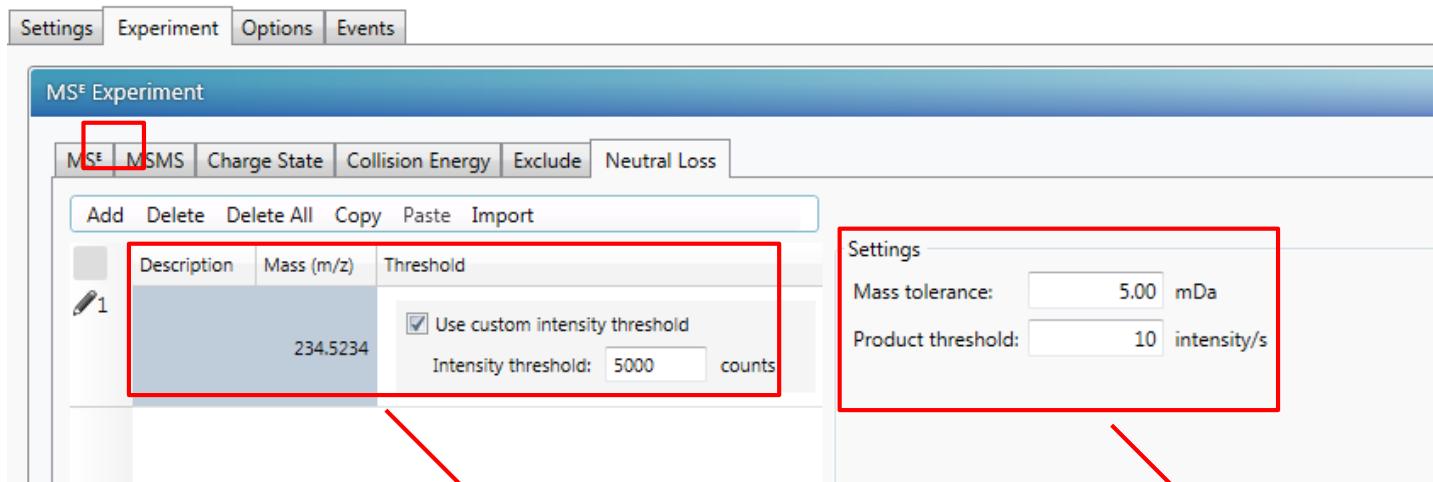
Mass tolerance: mDa

Product threshold: intensity/s

点击“ add” 后,添加“ 子离子” 及“ 阈值” ,

设置子离子的质量数的偏差
及子离子相应的阈值

DDA方法设置-9



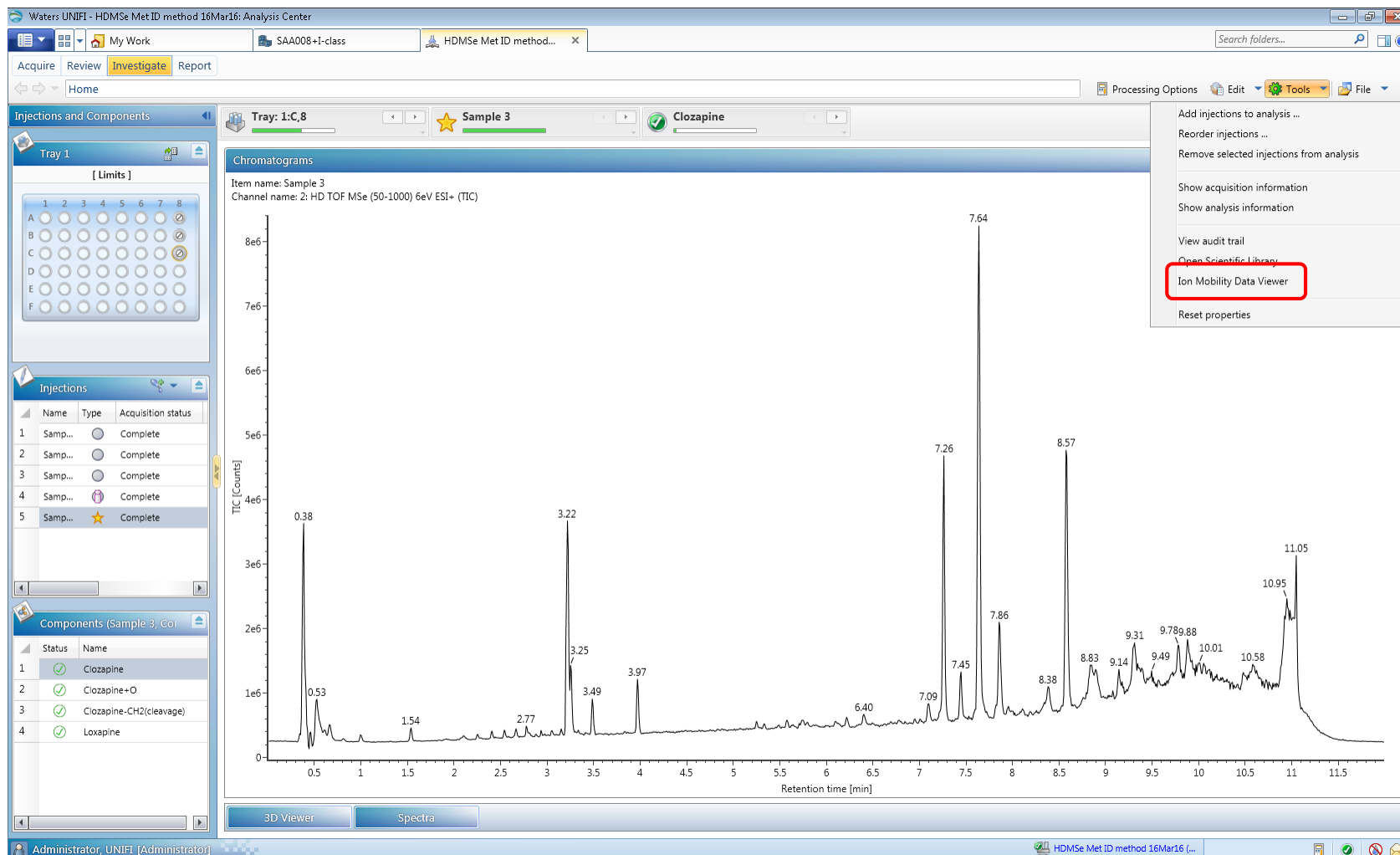
点击“add”后,添加“Neutral loss”及“阈值”,

设置neutral loss 的质量数的偏差
及子离子相应的阈值

Ion Mobility Data Viewer

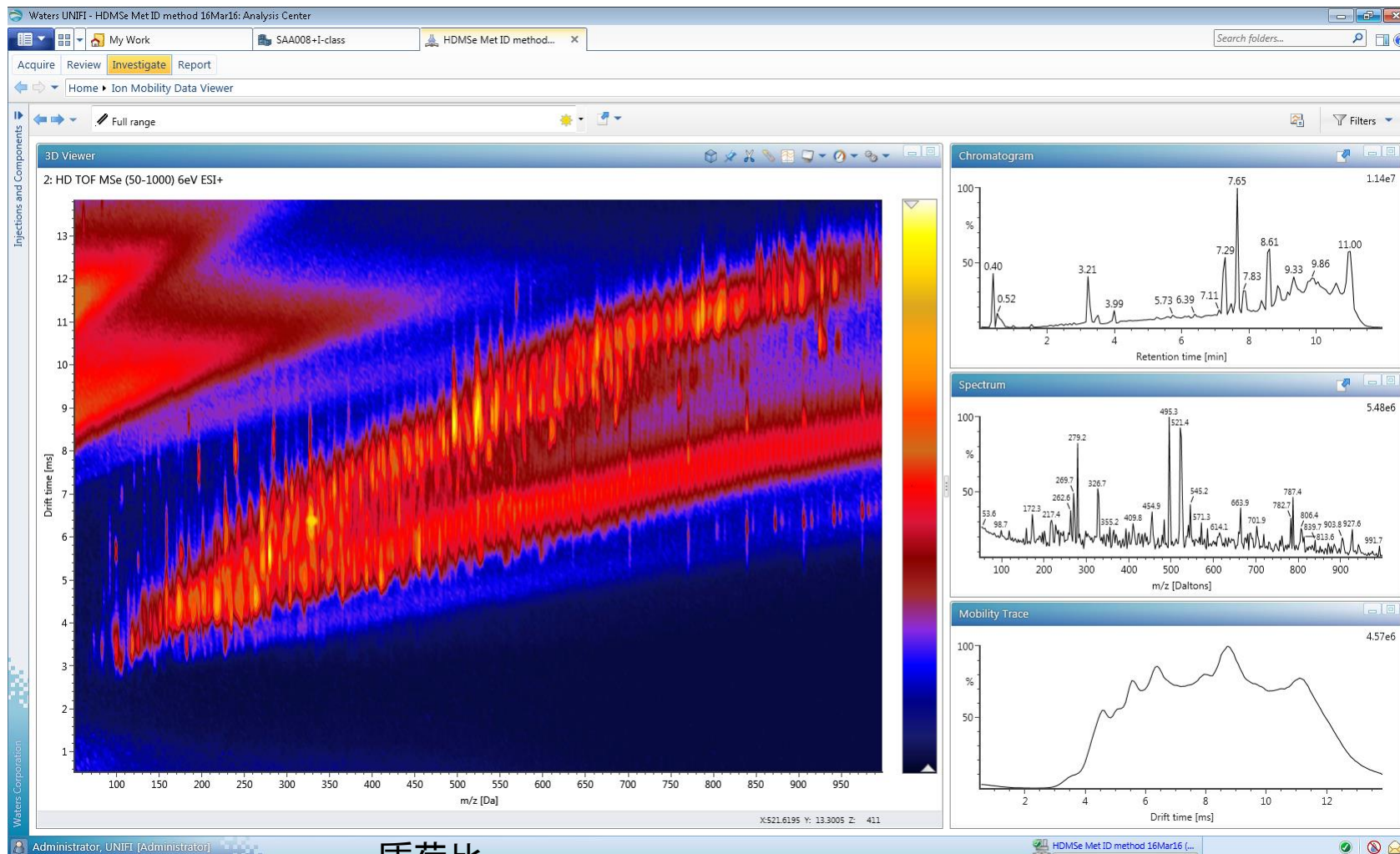
手动进行淌度数据的处理

Ion Mobility Data Viewer



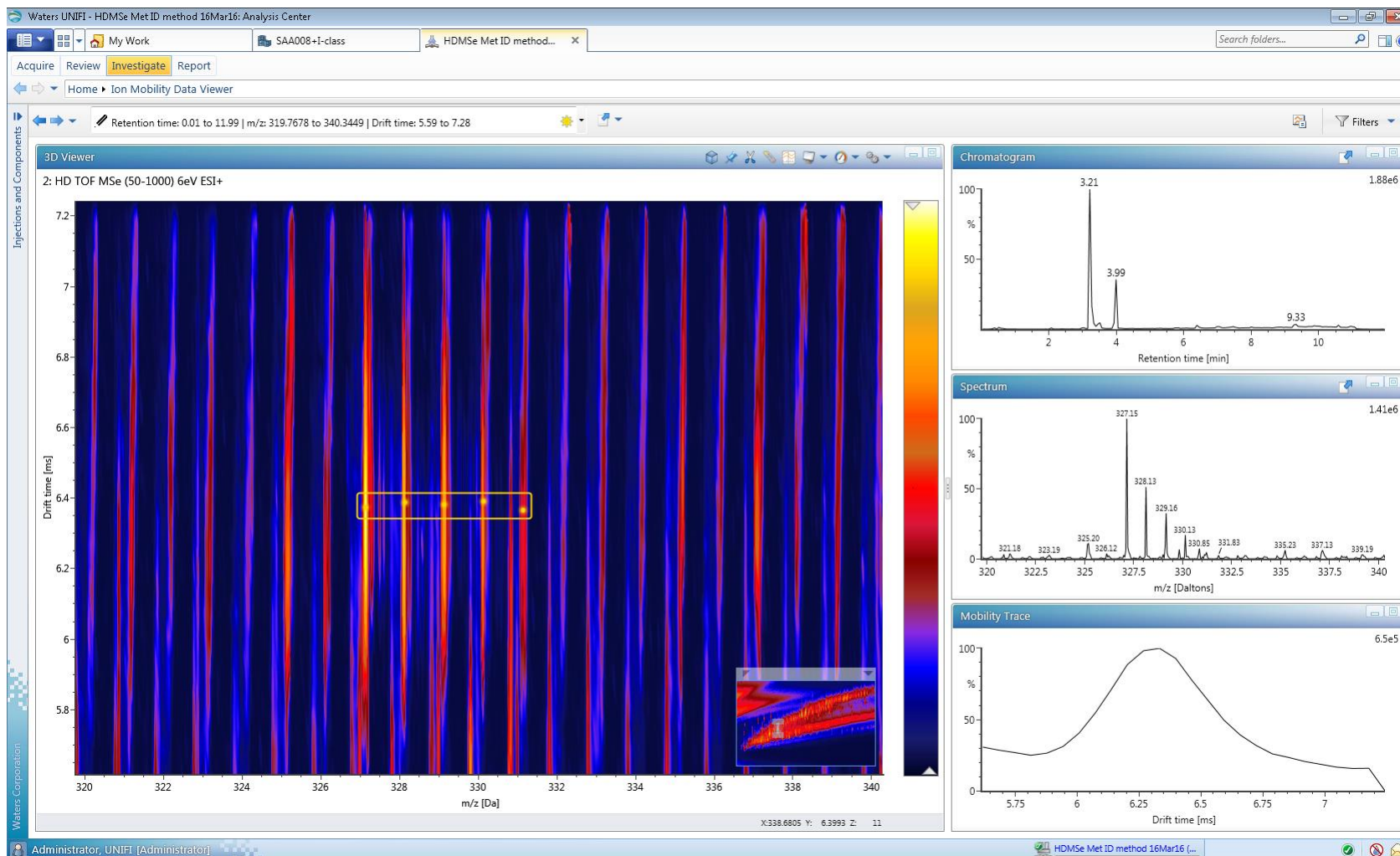
Ion Mobility Data Viewer

漂移时间

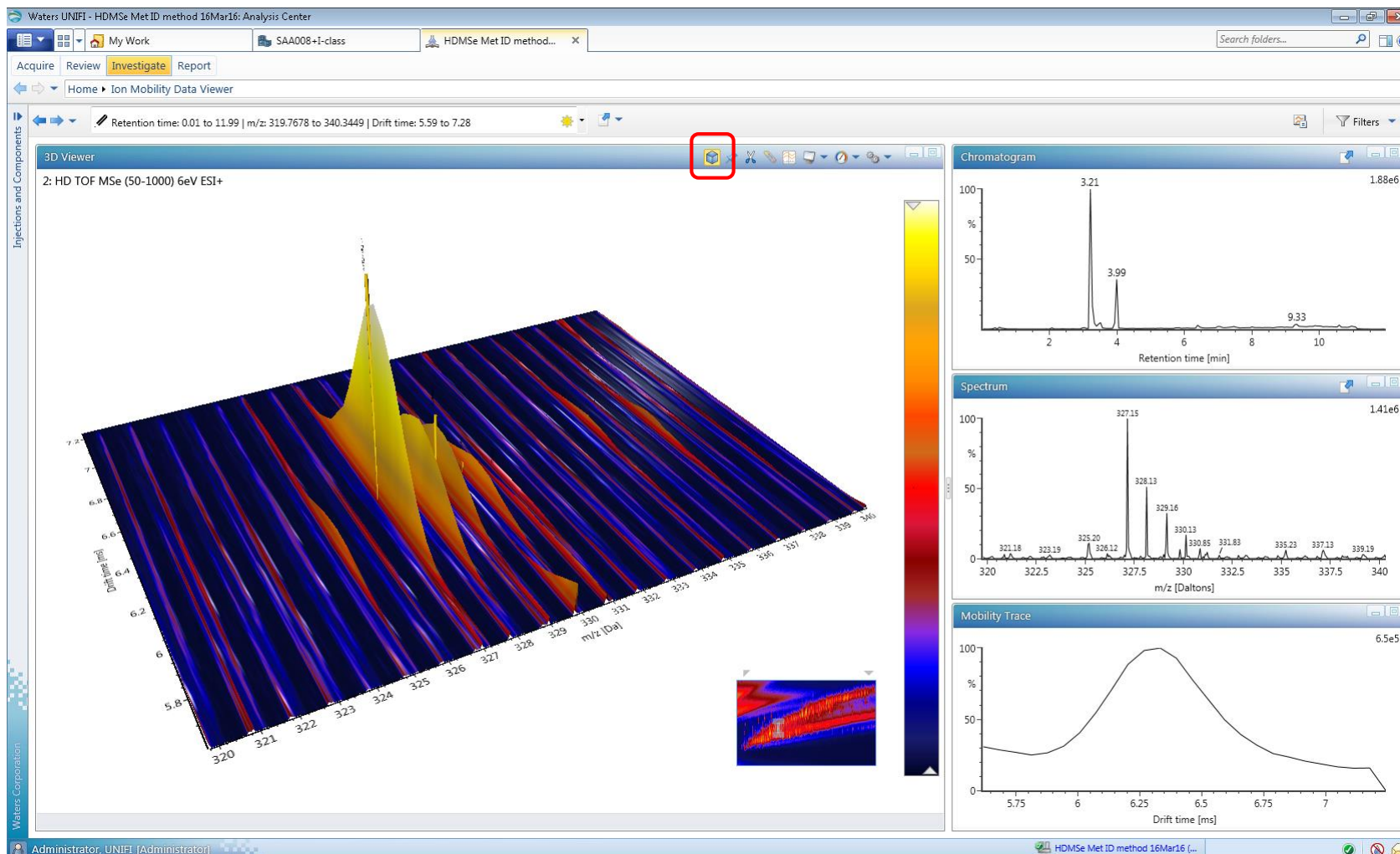


质荷比

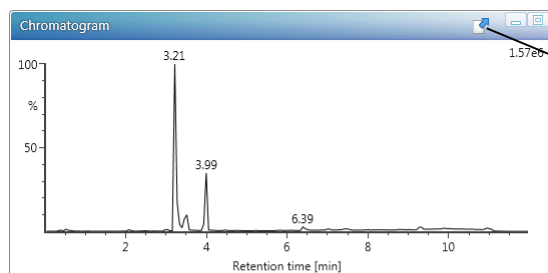
Ion Mobility Data Viewer



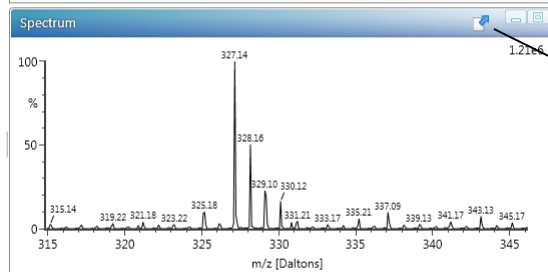
Ion Mobility Data



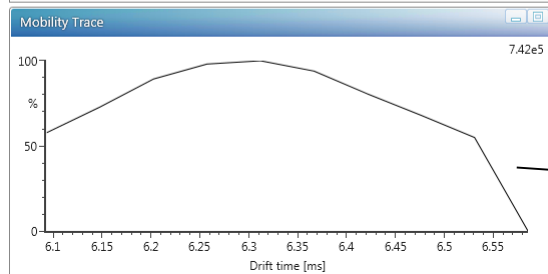
Ion Mobility Viewer



Select to generate extracted mass chromatogram in Investigate

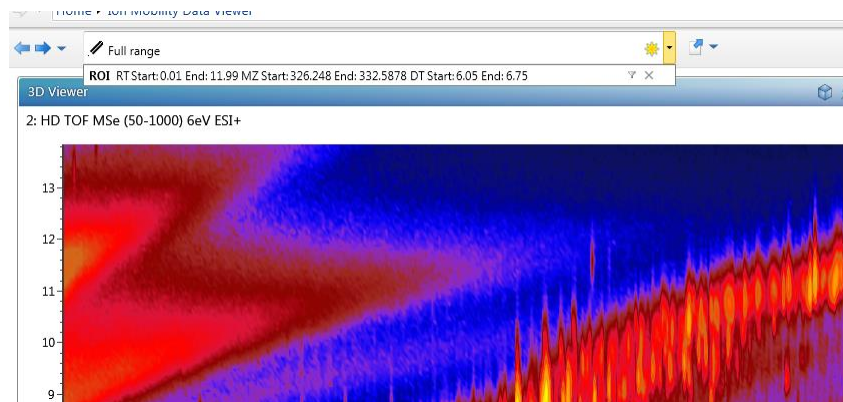
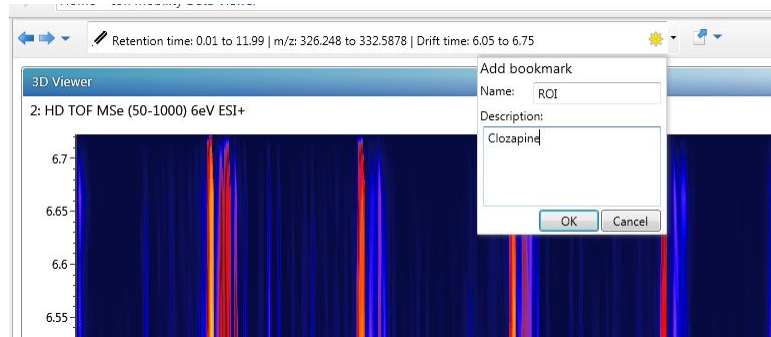
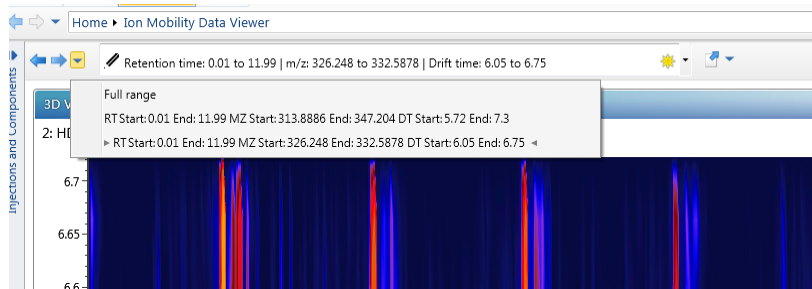


Select to combine mass spectra in Investigate



Select drift time region of interest

Ion Mobility Viewer - using bookmarks



- Whenever you zoom into data in the ion mobility viewer a bookmark history is created
- These bookmarks can be saved and exported
- Bookmarks can also be imported into other Analyses

Ion Mobility Data Viewer – exporting bookmarks

The screenshot displays the Waters UNIFI software interface. The main window is titled "Waters: UNIFI - HDMSe Met.ID method 16Mar16: Analysis Center" and shows the "Ion Mobility Data Viewer" section. A red box highlights a bookmark icon in the top toolbar. A "Save As" dialog box is open, showing the file path "Computer > New Volume (F:) > Unifi UEPs > MS Driver v1.1". The file name is "Clozapine" and the save type is "XML file (.xml) (*.xml)".

The background interface includes several data visualization panels:

- 3D Viewer:** A 2D plot of Drift time [ms] (y-axis, 1-13) versus m/z [Da] (x-axis, 100-950). The plot shows a color-coded distribution of ions, with a prominent red region at higher drift times and lower m/z values.
- Chromatogram:** A plot of Retention time [min] (x-axis, 2-12) versus intensity. The plot shows several peaks with retention times labeled: 3.21, 3.99, 5.73, 6.39, 7.11, 7.29, 7.65, 7.83, 8.61, 9.33, 9.86, and 11.00.
- Mobility Trace:** A plot of Drift time [ms] (x-axis, 2-12) versus relative intensity (%). The plot shows a broad peak centered around 8-10 ms drift time.

The status bar at the bottom indicates the user is "Administrator, UNIFI [Administrator]" and the current method is "HDMSe Met.ID method 16Mar16".

Ion Mobility Viewer Comparison Mode - alignment

Waters UNIFI - HDMSe Met ID method 16Mar16: Analysis Center

My Work SAA008+1-class HDMSe Met ID method...

Acquire Review Investigate Report

Home Ion Mobility Data Viewer

Chromatographic window:

3D Viewer

Chromatogram

Comparison Settings

Data

Reference data: Sample 2

Comparison data: Sample 3 Align

Parameters

Chromatographic windows: Start: 0.01 End: 11.99

Start

Align Sample Replicates (Sample 2 to Sample 3)

Intensity [Counts]

Retention time [min]

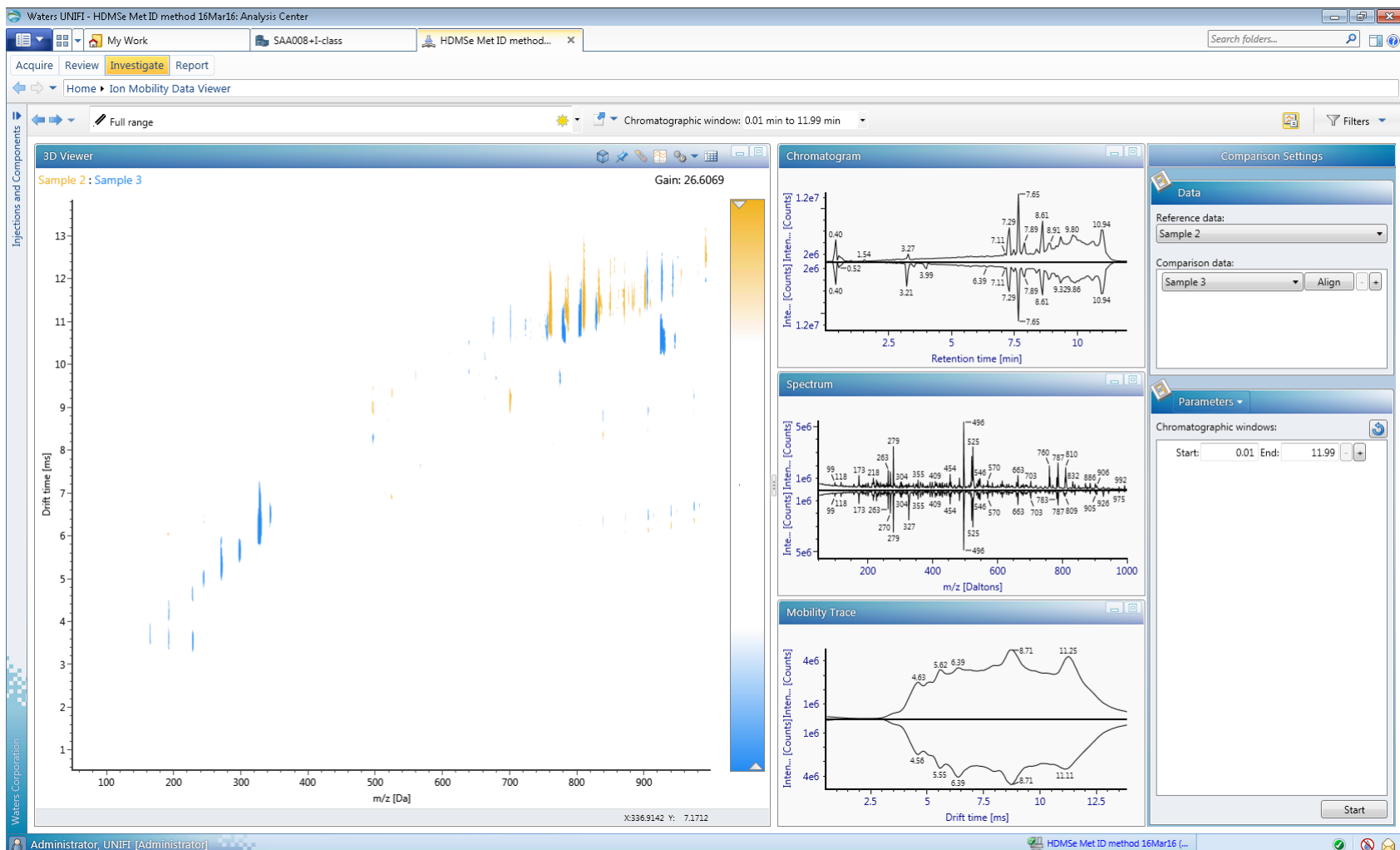
Injection Name	Start RT (min)	End RT (min)	Scale RT	Shift RT	Include
1 Sample 2	0.01	11.99	1.00	0.00	<input checked="" type="checkbox"/>
2 Sample 3	0.01	11.99	1.00	0.00	<input checked="" type="checkbox"/>

OK Cancel

X:336.9142 Y: 7.1712

Administrator, UNIFI [Administrator] HDMSe Met ID method 16Mar16 [...]

Ion Mobility Viewer Comparison Mode



Ion Mobility Viewer Comparison Mode

