

## ISQ EC and ISQ EM

## **Mass Spectrometer**

## **Operating Manual**

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**Original Operating Manual** 

The hardware descriptions in this manual revision refer to the ISQ EC mass spectrometer. For the manual release history, see page 227.

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# **1 Using this Manual**

This chapter provides information about this manual, the conventions used throughout the manual, and the reference documentation that is available in addition to this manual.

## 1.1 About this Manual

This manual describes the functional features and operating principle of your Thermo Scientific<sup>™</sup> ISQ<sup>™</sup> EC and ISQ<sup>™</sup> EM mass spectrometers and provides instructions for installation, set up, start up, shut down, operation, maintenance, and troubleshooting.

The layout of this manual is designed to provide quick reference to the sections of interest to the user. To obtain a full understanding of your detector, read this manual thoroughly.

This manual also contains safety messages, precautionary statements, and special notices that can prevent personal injury, damage to the detector, or loss of data when followed properly.

Note the following:

- The detector configuration may vary; therefore, not all descriptions necessarily apply to your particular detector.
- If some detail applies to only one model or variant, the model or variant is identified by name.
- Illustrations in this manual are provided for basic understanding. They can vary from the actual model of the detector or component. However, this does not influence the descriptions. No claims can be derived from the illustrations in this manual.

### **1.2** Conventions

This section describes the conventions that are used throughout this manual.

#### 1.2.1 Safety Messages

The safety messages and precautionary statements in this manual appear as follows:

- Safety messages or precautionary statements that apply to the entire manual and all procedures in this manual are grouped in the Safety chapter.
- Safety messages or precautionary statements that apply to an entire section or to multiple procedures in a section appear at the beginning of the section to which they apply.
- Safety messages that apply to only a particular section or procedure appear in the section or procedure to which they apply. They appear different from the main flow of text.

Safety messages are often preceded by an alert symbol and/or alert word. The alert word appears in uppercase letters and in bold type.

Make sure that you understand and follow all safety messages presented in this manual.

#### **1.2.2** Special Notices and Informational Notes

Special notices and informational notes in this manual appear different from the main flow of text. They appear in boxes and a note label identifies them. The label text appears in uppercase letters and in bold type.

**WARNING** Indicates that failure to take note of the accompanying information may result in personal injury.

**AVERTISSEMENT** Indique que ne pas tenir compte de l'information jointe peut entraîner des blessures corporelles.

**NOTICE** Indicates that failure to take note of the accompanying information could cause wrong results or may result in damage to the device.

**ATTENTION** Indique que ne pas tenir compte de l'information jointe peut conduire aux résultats faux ou endommager l'appareil.

**TIP** Highlights information of general interest or helpful information that can make a task easier or optimize the performance of the detector.

**TIP** *Veuillez noter Signale des informations d'intérêt général ou utiles qui peuvent simplifier l'exécution d'une tâche ou optimiser le fonctionnement du détecteur.* 

#### **1.2.3** Typographical Conventions

These typographical conventions apply to the descriptions in this manual:

Data Input and Output

- The following appears in **bold** type:
  - Input that you enter by the keyboard or that you select with the mouse
  - Buttons that you click on the screen
  - Commands that you enter by the keyboard
  - Names of, for example, dialog boxes, properties, and parameters

 For brevity, long expressions and paths appear in the condensed form, for example: Click Start > All Programs > Thermo Chromeleon 7 > Services Manager > Start Instrument Controller.

#### References and Messages

- References to additional documentation appear *italicized*.
- Messages that appear on the screen are identified by quotation marks.

#### Viewpoint

If not otherwise stated, the expressions *left* and *right* in this manual always refer to the viewpoint of a person that is facing the detector from the front.

#### Particularly Important Words

Particularly important words in the main flow of text appear *italicized*.

#### Electronic Manual Version (PDF)

The electronic version (PDF) of the manual contains numerous links that you can click to go to other locations within the manual. These include:

- Table of contents entries
- Index entries
- Cross-references (in blue text), for example, to sections and figures

### **1.3** Reference Documentation

In addition to this operating manual, other documentation is available for reference.

Hardware Documentation

Additional hardware documentation includes the following:

Operating manuals for the other modules of the LC or IC system

• Instrument Installation Qualification Operating Instructions

**TIP** Electronic versions of these manuals are available as PDF (Portable Document Format) files. To open and read the PDF files, Adobe<sup>™</sup> Reader<sup>™</sup> or Adobe<sup>™</sup> Acrobat<sup>™</sup> is required.

#### Software Documentation

Additional software documentation includes the following:

Chromeleon™ 7 Help and documents

The *Chromeleon 7 Help* provides extensive information and comprehensive reference material for all aspects of the software. For basic information about device installation and configuration, refer to the *Installation Guide*; for specific information about a certain device, refer to the *Instrument Configuration Manager Help*. In Chromeleon 7, devices are called modules.

For information about the main elements of the user interface and stepby-step guidance through the most important workflows, refer to the *Quick Start Guide*.

For a concise overview of the most important workflows, refer to the *Reference Card*.

Chromeleon™ 6.8 Help

The *Chromeleon 6.8 Help* provides extensive information for all aspects of the software, including device installation and configuration.

**TIP** The *Chromeleon* Help and documents are included in the software shipment.

Third-Party Documentation

Refer also to the user documentation provided by the manufacturers of third-party components and materials, for example, Safety Data Sheets (SDSs).

Third-party documentation includes the user documentation for the gas supply, as applicable:

• User documentation for the nitrogen generator

# 2 Safety

This chapter provides general and specific safety information and informs about the intended use of the detector.

## 2.1 Safety Symbols and Signal Words

# 2.1.1 Safety Symbols and Signal Words in This Manual (Symboles de sécurité et mentions d'avertissement utilisés dans ce manuel)

This manual contains safety messages to prevent injury of the persons using the detector. The safety symbols and signal words in this manual include the following:



Always be aware of the safety information. Do not proceed until you have fully understood the information and consider the consequences of what you are doing.



**CAUTION** Indicates a hazardous situation that, if not avoided, could result in minor or moderate injury.



**WARNING** Indicates a hazardous situation that, if not avoided, could result in serious injury.

*Ce manuel contient des messages de sécurité visant à prévenir les blessures chez les utilisateurs du détecteur. Les symboles de sécurité et les mentions d'avertissement utilisés dans ce manuel sont les suivants :* 



Soyez toujours au fait des informations de sécurité. N'entreprenez rien avant d'avoir bien compris toutes les informations et considéré les conséquences de vos actes.



**ATTENTION** Indique une situation dangereuse qui, si elle n'est pas évitée, peut aboutir à des blessures mineures à modérées.



**AVERTISSEMENT** Indique une situation dangereuse qui, si elle n'est pas évitée, peut entraîner de graves blessures.

#### 2.1.2 Observing this Manual

Observe the following:

- Before installing or operating the instrument, read this manual carefully to be familiar with the instrument and this manual. The manual contains important information with regard to user safety as well as use and care of the instrument.
- Always keep the manual near the instrument for quick reference.
- Save this manual and pass it on to any subsequent user.



Read, understand, and comply with all safety messages and precautionary statements presented in this manual.



*Il est important de lire, de comprendre et de respecter tous les messages et consignes de sécurité présentés dans ce manuel.* 

#### 2.1.3 Safety Symbols on the Instrument

The table lists the safety symbols that appear on the instrument or on labels affixed to the instrument. Follow the safety notices in this manual to prevent the risk of operator injury or damage to the instrument.

Symbol	Description
	Indicates a potential hazard. Refer to this manual to avoid the risk of personal injury and/or to prevent damage to the device.
ΙΟ	Power supply is on
	Power supply is off
~	Indicates alternating current.
	Indicates a terminal for protective grounding.
	Indicates that an electrical shock could or might occur
	Alerts you to the presence of a hot surface that <i>could</i> or <i>might</i> cause burn injuries.
	Indicates that eye damage <i>could</i> or <i>might</i> occur.
8	Alerts you to carefully read your instrument's documentation to ensure your safety and the instrument's operation ability. Failing to carefully read the documentation <i>could</i> or <i>might</i> put you at risk for a physical injury.
	Indicates that physical injury <i>could</i> or <i>might</i> occur if two or more people do not lift an object.

Symbole	La description
	Indique un danger potentiel. Référez-vous à ce manuel pour prévenir les risques de blessures et/ou éviter d'endommager l'appareil.
ΙΟ	L'instrument est mis sous tension. L'instrument est mis hors tension.
~	Indique un courant alternatif.
	Indique une borne de mise à la terre.
4	Indique un risque de choc électrique.
	Vous avertit de la présence d'une surface chaude présentant un risque de blessure par brûlure.
	Indique un risque de lésion oculaire.
	Vous avertit qu'il est important de lire attentivement la documentation de l'instrument afin de garantir votre sécurité et la capacité opérationnelle de l'instrument. Si vous ne lisez pas attentivement la documentation, vous vous exposez à des risques de blessure.
	Indique un risque de blessure si un objet n'est pas soulevé par deux personnes ou plus.

## 2.2 Intended Use

The instrument is intended for use in liquid chromatography (LC) and ion chromatography (IC) mass spectrometry (MS) applications. The system is for use by qualified personnel and in laboratory environment only.

The instrument is intended for laboratory research use only. It is not intended for use in diagnostic procedures.

#### Laboratory Practice

Thermo Fisher Scientific recommends that the laboratory in which the MS system is used follow best practices for LC-MS and IC-MS analyses. This includes among others:

- Using appropriate standards
- Regularly running calibration
- Establishing shelf life limits and following them for all consumables used with the system
- Running the system according to the laboratory's verified and validated 'lab developed test' protocol

## 2.3 Safety Precautions

#### 2.3.1 General Safety Information (Consignes Générales de Sécurité)

All users must observe the general safety information presented in this section and all specific safety messages and precautionary statements elsewhere in this manual during all phases of installation, operation, troubleshooting, maintenance, shutdown, and transport of the detector.

Tous les utilisateurs doivent respecter les consignes générales de sécurité présentées dans cette section ainsi que tous les messages et consignes de sécurité spécifiques exposés dans ce manuel, pendant toutes les phases d'installation, de fonctionnement, de dépannage, d'entretien, d'arrêt et de transport du détecteur.



If the instrument is used in a manner not specified by Thermo Fisher Scientific, the protection provided by the detector could be impaired. Observe the following:

- Operate the instrument only within its technical specifications.
- Use only the replacement parts and additional components, options, and peripherals specifically authorized and qualified for the detector by Thermo Fisher Scientific.
- Perform only the procedures that are described in this operating manual and in supporting documents for the detector.
   Follow all instructions step-by-step and use the tools recommended for the procedure.
- Open the enclosure of the detector and other components only if specifically instructed to do so in this manual.
- Thermo Fisher Scientific cannot be held liable for any damage, material or otherwise, resulting from inappropriate or improper use of the detector. If there is any question regarding appropriate usage, contact Thermo Fisher Scientific before proceeding.



*Si l'instrument est utilisé de façon non spécifiée par Thermo Fisher Scientific, la protection prévue par le détecteur pourrait être altérée. Veillez à respecter les consignes suivantes :* 

- Faites fonctionner l'instrument en respectant ses caractéristiques techniques.
- Utilisez uniquement les pièces de rechange, composants, options et périphériques supplémentaires spécifiquement autorisés et qualifiés pour le détecteur par Thermo Fisher Scientific.
- Suivez uniquement les procédures décrites dans ce manuel d'utilisation et dans les documents connexes du détecteur.
- Ouvrez le boîtier du détecteur et les autres composants uniquement si cela est spécifiquement indiqué dans ce manuel.
- Thermo Fisher Scientific ne peut être tenu pour responsable des dommages, matériels ou autres, résultant de l'utilisation inappropriée ou incorrecte du détecteur. En cas de questions concernant l'usage approprié, contactez Thermo Fisher Scientific avant de poursuivre.

#### Safety Standard

This device is a Safety Class I instrument (provided with terminal for protective grounding). The device has been manufactured and tested according to international safety standards.

#### Norme de sécurité

Cet instrument appartient à la classe de protection I (fourni avec une borne de mise à la terre). Il a été fabriqué et testé selon les normes de sécurité internationales.

#### 2.3.2 Qualification of the Personnel

Observe the information below on the proper qualification of the personnel installing and/or operating the detector.

Respectez les informations ci-dessous concernant la qualification appropriée du personnel chargé d'installer ou d'utiliser le détecteur.



#### Installation

Only skilled personnel are permitted to install the instrument and to establish the electrical connections according to the appropriate regulations. Thermo Fisher Scientific recommends always having service personnel certified by Thermo Fisher Scientific perform the installation (for brevity, referred to as Thermo Fisher Scientific service engineer).

If a person other than a Thermo Fisher Scientific service engineer installs and sets up the module, the installer is responsible for ensuring the safety of the module and system.

#### **General Operation**

The instrument is designed to be operated only by trained and qualified personnel in a laboratory environment.

All users must know the hazards presented by the detector and the substances they are using. All users should observe the related Safety Data Sheets (SDSs).



#### Installation

Seul du personnel qualifié est autorisé à installer l'instrument et à effectuer les branchements électriques selon les réglementations appropriées. Thermo Fisher Scientific recommande que l'installation soit toujours effectuée par du personnel d'entretien certifié par Thermo Fisher Scientific (appelé, par souci de brièveté, ingénieur d'entretien Thermo Fisher Scientific).

*Si une personne autre qu'un ingénieur d'entretien Thermo Fisher Scientific installe et configure le module, cet installateur est responsable de la sécurité du module et du système.* 

#### Fonctionnement général

L'instrument est conçu pour être utilisé en laboratoire par du personnel formé et qualifié.

Tous les utilisateurs doivent connaître les risques inhérents au détecteur et aux substances utilisées. Ils doivent également respecter les fiches techniques santé-sécurité (FTSS).

#### 2.3.3 Personal Protective Equipment

Wear personal protective equipment and follow good laboratory practice to protect you from hazardous substances. The appropriate equipment depends on the hazard. For advice on the hazards and the equipment required for the substances you are using, refer to the material handling and safety data sheet provided by the vendor.

Portez un équipement de protection individuelle et respectez les bonnes pratiques de laboratoire pour vous protéger des substances dangereuses. L'équipement approprié dépend du risque. Pour obtenir des conseils sur les risques et l'équipement requis en fonction des substances utilisées, reportezvous à la fiche de manutention et à la fiche technique santé-sécurité fournies par le fournisseur.



An eyewash facility and a sink should be available nearby. If any substance contacts your skin or eyes, wash the affected area and seek medical attention.



Une installation permettant de se laver les yeux ainsi qu'un lavabo doivent se trouver à proximité du système. Si une substance entre en contact avec la peau ou les yeux, lavez la zone touchée et consultez un médecin.

#### Protective Clothing

To protect you from chemical splashes, harmful liquids, or other contamination, when performing any work on or near the LC-MS or IC-MS system put on appropriate protective clothing, such as a lab coat. For information about the proper handling of a particular substance and for advice on specific hazards, refer to the safety data sheet (SDS) for the substance you are using.

#### Vêtements de protection

Pour vous protéger des projections chimiques, des liquides dangereux ou d'autres contaminants lors d'une intervention sur le système LC-MS ou IC-MS, ou à proximité de ce dernier, portez des vêtements de protection appropriés comme une blouse de laboratoire. Pour obtenir des renseignements sur la manipulation correcte d'une substance particulière ainsi que des conseils concernant certains dangers spécifiques, reportez-vous à la fiche technique santé-sécurité (FTSS) de la substance utilisée.

#### Protective Eyewear

To prevent liquids from striking your eyes, put on appropriate protective eyewear, such as safety glasses with side shields. If there is a risk of splashing liquids, put on goggles.

#### Lunettes de protection

Pour éviter les éclaboussures de liquides dans les yeux, portez des lunettes de protection appropriées, comme des lunettes de sécurité à écrans latéraux. En cas de risque de projections de liquide, portez des lunettes de protection.

Gloves	
	To protect you from harmful liquids and avoid personal injury during maintenance or service, put on appropriate protective gloves.
Gants	Pour vous protéger des liquides dangereux et éviter les blessures au cours d'une activité de maintenance ou d'entretien, portez des lunettes de protection appropriées.

#### 2.3.4 Electrical Safety Precautions



#### WARNING— Electric Shock or Damage to the Device

High voltages are present inside the device that could cause an electric shock or damage to the device.

- Do not make any changes to the electrical or grounding connections.
- If you suspect any kind of electrical damage, disconnect the power cord and contact Thermo Fisher Scientific Technical Support for assistance.
- Do not open the housing or remove protective panels unless specifically instructed to do so in this manual.
- Do not place liquid reservoirs directly upon the device. Liquid might leak into the device and get into contact with electronic components causing a short circuit. Instead, place liquid reservoirs in the solvent rack that is available for the HPLC system.



AVERTISSEMENT—Risque de choc électrique ou d'endommagement de l'appareil

Les hautes tensions présentes à l'intérieur du dispositif peuvent provoquer un choc électrique ou endommager le dispositif.

- Ne modifiez ni les branchements électriques ni les connexions de mise à la terre.
- Si vous soupçonnez un dysfonctionnement électrique, débranchez le cordon d'alimentation et contactez l'assistance technique de Thermo Fisher Scientific.
- Sauf instruction contraire dans ce manuel, n'ouvrez pas le boîtier et ne retirez pas les panneaux de protection.
- Ne placez pas de réservoir de liquide directement sur l'appareil. En cas de fuite, le liquide peut pénétrer dans l'appareil, entrer en contact avec les composants électriques et provoquer un courtcircuit. Placez plutôt les réservoirs de liquide dans le support pour solvant disponible avec le système HPLC.

#### 2.3.5 General Residual Hazards

Pay attention to the following general residual hazards when working with the instrument:



#### WARNING—Hazardous Substances

Many organic solvents, mobile phases, and samples are harmful to health. Be sure that you know the toxic and infectious properties of all substances that you are using. You may not know the toxic or infectious properties of many substances that you are using. If you have any doubt about a substance, treat it as if it contains a potentially harmful substance. For advice on the proper handling of a particular substance, refer to the Safety Data Sheet (SDS) of the manufacturer. Observe the guidelines of Good Laboratory Practice (GLP).

- Be sure that you know the properties of all substances that you are using. Avoid exposure to harmful substances. If you have any doubt about a substance, handle the substance as if it is potentially harmful.
- Wear personal protective equipment as required by the hazard and follow good laboratory practice.
- Reduce the volume of substances to the minimum volume required for sample analysis.
- Do not operate the detector in a potentially flammable environment.
- Avoid accumulation of harmful substances. Make sure that the installation site is well ventilated.
- Dispose of hazardous waste in an environmentally safe manner that is consistent with local regulations. Follow a regulated, approved waste disposal program.



#### **AVERTISSEMENT—Substances dangereuses**

De nombreux solvants, phases mobiles et échantillons organiques sont dangereux pour la santé. Veillez à bien connaître les propriétés toxiques et infectieuses de toutes les substances utilisées. Il est possible que vous ne connaissiez pas les propriétés toxiques ou infectieuses de nombreuses substances que vous utilisez. Au moindre doute concernant un échantillon, traitez-le comme s'il contenait une substance potentiellement dangereuse. Pour obtenir des conseils sur la manipulation correcte d'une substance particulière, reportez-vous à la fiche technique santé-sécurité (FTSS) du fabricant.

- Veillez à bien connaître les propriétés de toutes les substances utilisées. Évitez toute exposition à des substances nocives. En cas de doute sur une substance, manipulez-la comme si elle était potentiellement dangereuse.
- Portez l'équipement de protection individuelle requis en fonction du risque et respectez les bonnes pratiques de laboratoire.
- *Réduisez le volume des substances au minimum requis pour l'analyse de l'échantillon.*
- N'utilisez pas le détecteur dans un environnement potentiellement inflammable.
- Évitez toute accumulation de substances nocives. Assurez-vous que le site d'installation est bien ventilé.
- Débarrassez-vous des déchets dangereux de manière écologique, conformément à la réglementation en vigueur au niveau local. Suivez un programme d'élimination des déchets réglementé et approuvé.



#### WARNING—Biohazard

Biohazardous material, for example microorganisms, cell cultures, tissues, body fluids, and other biological agents can transmit infectious diseases. To avoid infections with these agents:

- Assume that all biological substances are at least potentially infectious.
- Wear personal protective equipment as required by the hazard and follow good laboratory practice.
- Dispose of biohazardous waste in an environmentally safe manner that is consistent with local regulations. Follow a regulated, approved waste disposal program.



#### AVERTISSEMENT—Risque biologique

Les matières dangereuses, par exemple les microorganismes, les cultures cellulaires, les tissus, les fluides corporels et autres agents biologiques, peuvent transmettre des maladies infectieuses. Pour éviter toute infection avec ces agents :

- Considérez toute substance biologique comme étant au moins potentiellement infectieuse.
- Portez l'équipement de protection individuelle requis en fonction du risque et respectez les bonnes pratiques de laboratoire.
- Débarrassez-vous des déchets d'activités de soins à risques infectieux de manière écologique, conformément à la réglementation en vigueur au niveau local. Suivez un programme d'élimination des déchets réglementé et approuvé.



#### WARNING—Self-Ignition of Solvents

Solvents with a self-ignition temperature below 150 °C might ignite when in contact with a hot surface (for example, due to leakage in the chromatography system). Avoid the use of these solvents.



#### AVERTISSEMENT—Auto-inflammation des solvants

Les solvants dont la température d'auto-inflammation est inférieure à 150 °C peuvent s'enflammer en cas de contact avec une surface chaude (par exemple, lors d'une fuite du système de chromatographie). Évitez d'utiliser ces solvants.



#### WARNING—Hazardous Vapors

Install the LC-MS or IC-MS system in a well-ventilated laboratory. If the mobile phase or sample includes volatile or flammable solvents, do not allow them to enter the workspace. If the mobile phase or sample includes volatile or flammable solvents, avoid open flames and sparks.

- The exhaust gas may contain hazardous fumes. To avoid an accumulation of the exhaust gasses, ensure that the exhaust gas is absorbed by a fume hood or other ventilating device. Maintain a well-ventilated laboratory. Do not vent directly into the laboratory.
- Avoid open flames and sparks. Do not operate the detector in the presence of flammable gases or fumes.



#### AVERTISSEMENT—Vapeurs dangereuses

Installez le système LC-MS ou IC-MS dans un laboratoire bien ventilé. Si la phase mobile ou l'échantillon contient des solvants volatils ou inflammables, empêchez qu'ils ne pénètrent dans l'espace de travail. Si la phase mobile ou l'échantillon contient des solvants volatils ou inflammables, évitez les flammes nues et les sources d'étincelles à proximité.

- Les gaz d'échappement peuvent contenir des fumées dangereuses.
  Pour éviter l'accumulation des gaz d'échappement, assurez-vous que ces derniers sont bien absorbés par une hotte aspirante ou un autre dispositif de ventilation. Assurez une ventilation adéquate dans le laboratoire. N'évacuez pas directement dans le laboratoire.
- Évitez les flammes nues et les sources d'étincelles à proximité. N'utilisez pas le détecteur en présence de gaz ou de fumées inflammables.



#### CAUTION—Escape of Hazardous Substances from PEEK Capillaries

In the LC or IC system, capillaries made of PEEK may be used. Swelling or attack by acids can cause PEEK capillaries to start leaking or to burst.

- Certain chemicals, for example, trichlormethane (CHCl<sub>3</sub>), dimethyl sulfoxide (DMSO), or tetrahydrofuran (THF) can cause PEEK to swell.
- Concentrated acids, such as sulfuric acid and nitric acid, or a mixture of hexane, ethyl acetate, and methanol, can attack PEEK.
- Swelling or attack is not a problem with brief flushing procedures.
- For more information, refer to the technical literature on the chemical resistance of PEEK.



## ATTENTION—Rejet de substances dangereuses par les capillaires en PEEK

Dans le système LC ou IC, il est possible d'utiliser des capillaires en PEEK. Le gonflement ou l'attaque provoqué par les acides peut entraîner des fuites ou des brisements des capillaires en PEEK.

- Certaines substances chimiques comme le trichlorométhane (CHCl3), le diméthyl sulfoxide ou le tétrahydrofurane ont pour effet de faire gonfler le PEEK.
- Des acides concentrés tels que l'acide sulfurique et l'acide nitrique ou un mélange hexane, acétate d'éthyle et méthanol peuvent attaquer le PEEK.
- L'exposition brève dans le cadre de procédures de nettoyage n'entraîne pas le gonflement ni l'attaque du matériel en PEEK.
- Pour obtenir plus d'informations, consultez la documentation technique sur la résistance chimique du PEEK.



#### CAUTION

Fused silica is used in flow cells and capillaries. To avoid personal injury always wear safety glasses when handling fused silica tubing, for example, when cutting fused silica tubing to length.



#### ATTENTION

Les cuves à circulation et les capillaires sont constitués de silice fondue. Pour éviter les blessures, portez toujours des lunettes de sécurité lorsque vous manipulez des tubes en silice fondue, par exemple, pour les couper à la bonne longueur.



#### **CAUTION**—Allergic Reaction

Some capillaries in the HPLC system are made of MP35N<sup>™</sup>, a nickelcobalt based alloy. Individuals with sensitivity to nickel/cobalt may show an allergic reaction from skin contact.



#### ATTENTION—Réaction allergique

Certains capillaires du système HPLC sont composés de MP35N™, un alliage nickel-cobalt. En cas de contact avec la peau, celui-ci peut provoquer une réaction allergique chez les personnes sensibles au nickel/cobalt.



#### CAUTION—Sparking due to Electrostatic Discharge

Liquid flowing through capillaries can generate static electricity. This effect is particularly present with insulating capillaries and non-conductive solvents (for example, pure acetonitrile). Discharge of electrostatic energy might lead to sparking, which could constitute a fire hazard. Prevent the generation of static electricity near the chromatography system.



#### ATTENTION—Étincelles dues aux décharges électrostatiques

Le liquide circulant dans les capillaires peut générer de l'électricité statique, en particulier en présence de capillaires isolants et de solvants non conducteurs (par exemple, l'acétonitrile pur). Les décharges électrostatiques peuvent provoquer des étincelles et présentent donc un risque d'incendie. Évitez la formation d'électricité statique à proximité du système de chromatographie.
# 2.4 Solvent and Additive Information

To protect optimal functionality of the instrument observe these recommendations on the use of solvents and additives:

- Use only solvents and additives that are compatible with all parts in the flow path.
- Follow any specific recommendations presented in other sections of this manual. Refer also to the *operating manuals for all modules in the LC or IC system*. They may provide additional guidelines and information.
- Some of the cleaning procedures in this manual call for the use of methanol. If methanol is unavailable or prohibited for use in cleaning procedures, substitute LCMS-grade ethanol.

# 2.5 Compliance Information

Thermo Fisher Scientific performs complete testing and evaluation of its products to ensure full compliance with applicable domestic and international regulations. When the device is delivered to you, it meets all pertinent electromagnetic compatibility (EMC) and safety standards as described in this manual. For details, see section 11.1, page 222.

Changes that you make to the device may void compliance with one or more of these EMC and safety standards. Changes to the device include replacing a part or adding components, options, or peripherals not specifically authorized and qualified for the product by Thermo Fisher Scientific. To ensure continued compliance with EMC and safety standards, replacement parts and additional components, options, and peripherals must be ordered from Thermo Fisher Scientific or one of its authorized representatives.

The device has been shipped from the manufacturing site in a safe condition.

# **3 Instrument Overview**

This chapter introduces you to the mass spectrometer and the main components.

# **3.1** Mass Spectrometer Operating Principle

The ISQ EC and ISQ EM mass spectrometers have been specifically designed and engineered for liquid chromatography (LC) or ion chromatography (IC) combined with mass spectrometry (MS). These technologies can provide sensitive and selective detection of organic molecules. Interfacing High Performance Liquid Chromatography (HPLC or LC) or Ion Chromatography (IC) and MS provides the separation scientist with one of the most powerful analytical tools available. Both LC or IC and MS have developed to a point whereby they represent two of the most important techniques in characterizing and detecting organic compounds.

Mass spectrometry is a very powerful analytical technique used in a number of fields, including:

- Identification of unknown compounds
- Quantitation of known compounds
- Determination of chemical structure

The basic function of an MS detector is to measure the mass-to-charge ratio of ions. The unit of mass used is the Dalton (Da). One Dalton is equal to 1/12of the mass of a single atom of carbon-12. This follows the accepted convention that an atom of carbon-12 has exactly 12 atomic mass units (amu). The MS detector does not directly measure molecular mass, but the mass-to-charge ratio of the ions. Electrical charge is a quantized property and so can exist only as an integer; that is, 1, 2, 3, and so on. The unit of charge used here (z) is that which is on an electron (negative) or a proton (positive). Therefore, the mass-to-charge ratio measured can be denoted by m/z. Most ions encountered in mass detection have just one charge. In this case, the mass-to-charge ratio is often referred to as the "mass" of the ion.

# 3.2 Overview of an LC/MS or IC/MS Analysis

In a typical LC/MS or IC/MS analysis, the liquid chromatograph (LC) or ion chromatograph (IC) portion of the system separates a mixture into its chemical components. The LC/IC pump produces a solvent stream (the mobile phase) that passes through an LC/IC column (containing the stationary phase) under high pressure. An autosampler introduces a measured quantity of sample into this solvent stream.

As the solvent stream passes through the LC/IC column, the sample separates into its chemical components. The rate at which the components of the sample elute from the column depends on their relative affinities to the mobile phase and the solid particles that make up the column packing. As the separated chemical components exit the LC/IC column, they enter the mass spectrometer for ionization and analysis. As the mass spectrometer analyzes the ionized components and determines each mass-to-charge ratio (m/z) and relative intensity, it sends a data stream to the data system computer. When the system setup includes a syringe pump and divert/inject valve, there are three additional ways to introduce a sample into the mass spectrometer, as described in *Table 1*.

Method	Description
Direct infusion	Connect a syringe pump directly to the atmospheric pressure ionization (API) source of the mass spectrometer.
High-flow infusion	Use a union tee to combine the flow from a syringe pump with the flow from an LC or IC pump.
Manual loop injection	Connect a sample loop, a needle port fitting, and an LC/IC pump to an external divert/inject valve. After you fill the sample loop with sample, switch the position of the divert/inject valve, which places the contents of the sample loop in the path of the solvent flow produced by the LC or IC pump.

Table 1: Methods of sample introduction into the mass spectrometer

The ISQ EC and ISQ EM Single Quadrupole Mass Spectrometers consist of an atmospheric pressure ion (API) source, ion optics, a single-stage mass analyzer, and an ion detection system. The ion optics, mass analyzer, ion detection system, and part of the API source are enclosed in a vacuum manifold. Ionization of the sample takes place in the API source. The specific method used to ionize the sample is referred to as the ionization technique. The ion optics transmit the ions produced in the API source into the mass analyzer to determine the mass-to-charge ratio (m/z) (of the ions produced in the API source). The polarity of the electric potentials applied to the API source and ion optics determines whether positively charged ions or

negatively charged ions are transmitted to the mass analyzer. You can set up data acquisition methods for the mass spectrometer to analyze positively or negatively charged ions or to switch between these polarity modes during a single run. See Figure 1 for an overview of the ISQ EC and ISQ EM systems.



Figure 1: Diagram of ISQ EC and ISQ EM systems.

The ISQ EC and ISQ EM Single Quadrupole Mass Spectrometers each operate as a conventional mass spectrometer with one stage of mass analysis. The ion source ionizes the sample, ion optics transfer the created ions through the vacuum system, mass analysis of the ion products occurs in the quadrupole assembly, and the resulting mass-selected ions are then transferred to the ion detection system.

# 3.3 Software Operation

The mass spectromter is designed to be operated from a computer configured with Chromeleon software. Chromeleon software provides complete instrument control, data acquisition, and data management.

The data system serves as the user interface to the mass spectrometer, autosampler, LC pump, and syringe pump. Refer to the Chromeleon Help for more information about the ISQ EC and ISQ EM Single Quadrupole Mass Spectrometer data processing and instrument control. Each sequence of loading a mass analyzer with ions followed by mass analysis of the ions is called a scan. The mass spectrometer utilizes both a full scan type and/or selected ion monitoring (SIM) scan type to create, fragment, and detect ions. The ability to vary not only the ionization and ion polarity modes, but the scan mode and scan type, provides greater flexibility in the instrumentation for solving complex analytical problems.

The method editor in Chromeleon allows the user to set up scans in a variety of ways, combining both full scans and SIM scans. The user can also call for scans of either or both polarities. Simplified ion source controls and a simplified method editor make setting up an instrument method easier than ever, while the ability to switch to manual controls means that users who wish to control each device independently do not lose that freedom. For more information on the method editor, please see the help file in the Chromeleon data system. Users can set up full scans to get a picture of the entire mass spectrum as well as set up SIM scans to monitor for the presence of specific ions. The ability to apply source collision induced dissociation (sCID) gives the user the capability to reduce the presence of adducts, or to create confirmation ions via fragmentation in the ion optics of the system.



This chapter provides information for unpacking the system and informs you about the scope of delivery.

# 4.1 Unpacking

## Damaged Packaging, Defective on Arrival

Inspect the shipping container for signs of external damage and, after unpacking, inspect the instrument for any signs of mechanical damage that might have occurred during shipment.

If you suspect that the instrument may have been damaged during shipment, immediately notify the incoming carrier and Thermo Fisher Scientific about the damage. Shipping insurance will compensate for the damage only if reported immediately.

### Unpacking the Instrument



### CAUTION—Heavy Load, Bulky Device

The instrument is too heavy or bulky for one person alone to handle safely. A minimum of two people are required to lift the instrument from the shipping crate to the lab bench. To avoid personal injury or damage to the instrument, observe the following guidelines:

- Physical handling of the instrument, including lifting or moving, requires a team effort of two persons.
- A team effort is in particular required when lifting the instrument into the system stack or when removing it.
- To lift or move the instrument, grasp the instrument by the sides. Do not move or lift the instrument by the front bezel. This will damage the bezel or the instrument.



### ATTENTION—Charge lourde, appareil volumineux

L'instrument est trop lourd ou encombrant pour être soulevé ou déplacé par une personne seule. Au moins deux personnes doivent le soulever pour le transférer de la caisse d'expédition à la paillasse. Pour éviter les blessures et les dommages à l'instrument, respectez les consignes suivantes :

- Deux personnes sont nécessaires pour manipuler physiquement l'instrument, notamment pour le soulever et le déplacer.
- Ce travail d'équipe est tout particulièrement nécessaire pour soulever l'instrument et l'installer sur l'empilage du système ou pour l'en retirer.
- Pour soulever ou déplacer l'instrument, saisissez-le par les côtés. Ne saisissez pas l'instrument par le cadran frontal pour le soulever ou le déplacer. Vous risqueriez d'endommager le cadran ou l'instrument.

#### Tools required

Screwdriver, Torx<sup>™</sup> T20

#### Follow these steps

- 1) Place the shipping container on the floor and open it.
- Remove the accessory kit from the shipping container as shown in Figure 2.
- 3) Remove the cardboard inner tray from the shipping container.
- 4) Remove the outer cardboard box
- 5) Remove the mechanical pump box.
- 6) Remove the foam under the mass spectrometer.



Figure 2: Shipping Container

- 4) Grasp the mass spectrometer by the sides. Slowly and carefully, lift the detector out of the shipping container and place it on a stable surface.
- 5) Transport the mass spectrometer to the installation site, if it is not already there, and place it in the system stack.

**TIP** Keep the shipping container and all packing material. These items will be needed if the detector is transported to a new location or shipped.



### CAUTION—Instrument Damage

The foam shipping insert that keeps the glass top of the quadrupole manifold assembly in-place must be removed prior to turning on the instrument.



### ATTENTION—Risque d'endommagement de l'instrument

La pièce en mousse qui maintient en place la partie supérieure en verre de l'ensemble collecteur quadripolaire pendant le transport doit être retirée avant la mise sous tension de l'instrument.

# 4.2 Scope of Delivery

The following items are included in the delivery:

- Mass spectrometer
- Accessory Kit For details about the kit content, see section 10.2 Ship Kit, page 215.
- Foreline pump
- Operating manual

**NOTICE** The delivery scope is limited to the ISC EC or ISQ EM system. Refer to the HPLC, IC, or other accessory manuals for their delivery inventory.

# **5** Installation

This chapter specifies the requirements for the installation site and describes how to set up, install, and configure the mass spectrometer.

# 5.1 Safety Guidelines for Installation

Pay attention to the following safety guidelines:



Observe all warning messages and precautionary statements presented in section 2.3 Safety Precautions (see page 23).



Respectez tous les messages d'avertissement et les consignes présentés dans la section 2.3 Safety Precautions (voir page 23).



### CAUTION—Heavy Load, Bulky Device

The instrument is too heavy or bulky for one person alone to handle safely. A minimum of two people are required to lift the instrument from the shipping crate to the lab bench. To avoid personal injury or damage to the instrument, observe the following guidelines:

- Physical handling of the instrument, including lifting or moving, requires a team effort of two persons.
- A team effort is in particular required when lifting the instrument into the system stack or when removing it.
- To lift or move the instrument, grasp the instrument by the sides. Do not move or lift the instrument by the front bezel. This will damage the bezel or the instrument.



### ATTENTION—Charge lourde, appareil volumineux

L'instrument est trop lourd ou encombrant pour être soulevé ou déplacé par une personne seule. Au moins deux personnes doivent le soulever pour le transférer de la caisse d'expédition à la paillasse. Pour éviter les blessures et les dommages à l'instrument, respectez les consignes suivantes :

- Deux personnes sont nécessaires pour manipuler physiquement l'instrument, notamment pour le soulever et le déplacer.
- Ce travail d'équipe est tout particulièrement nécessaire pour soulever l'instrument et l'installer sur l'empilage du système ou pour l'en retirer.
- Pour soulever ou déplacer l'instrument, saisissez-le par les côtés. Ne saisissez pas l'instrument par le cadran frontal pour le soulever ou le déplacer. Vous risqueriez d'endommager le cadran ou l'instrument.

#### CAUTION—INSTRUMENT DAMAGE

Clean tubing cutters with methanol prior to use. Otherwise, tubing may be contaminated with oil and grease from packing material. For more information, please refer to the ship kit on page 215.

### ATTENTION-RISQUE D'ENDOMMAGEMENT DE L'INSTRUMENT

Nettoyez les coupe-tubes avec du méthanol avant utilisation. Sinon, les tubes risquent d'être contaminés par l'huile et la graisse provenant du matériel d'emballage. Pour plus d'informations, consultez le kit d'expédition à la page 215.

# 5.2 Installing the Mass Spectrometer

The mass spectrometer is installed and set up by a Thermo Fisher Scientific service engineer or representative. The service engineer checks that the installation is correct and that the detector operates as specified. The engineer also demonstrates the basic operation and main features.

If the instrument is moved or reinstalled later by personnel other than Thermo Fisher Scientific service engineer, follow the steps below.

- Pay attention to the safety guidelines and observe all site requirements. For the safety guidelines when installing the instrument, see section 5.1, page 51. For the site requirements, see section 5.3, page 55.
- 2) Set up the mass spectrometer hardware. See section 5.5, page 68.
- 3) Set up the flow connections. See section 5.6, page 113.
- 4) Turn on the system. See section 5.7, page 115.Adjust the display brightness and date and time as required.
- 5) Installation in the Chromeleon software (optional) When the display shows the Main Menu after the self-test, set up the detector in the software. See section 6.4, page 123.

**TIP** Before turning on the power to the instrument for the first time, verify that the chromatography software is installed on the data system computer. Verify that the network card is properly configured to communicate to the mass spectrometer. When the power is turned on, the required USB drivers for the LC or IC are automatically found and the Windows<sup>™</sup> operating system can detect the device.

6) Recommended:

Perform Instrument Installation Qualification.

In Chromeleon, a wizard is available to guide you through the qualification process:

On the Chromeleon 7.2 Console: Click Tools > Instrument
Qualification > Installation Qualification.

Follow the instructions in the *Instruments Installation Qualification Operating Instructions*. The manual provides information about the required materials and detailed instructions.

7) *Recommended:* Perform Operational Qualification.

The qualification kit includes all materials required for the qualification and detailed instructions.

# 5.3 Site Requirements

The operating environment is important to ensure optimal performance of the detector. This section provides important requirements for the installation site. Note the following:

# 5.3.1 Workbench

The system is designed to be placed on a workbench. If the workbench holds a complete mass spectrometer and possibly other instruments, the bench must be capable to bear the weight of all devices and instruments, including solvents.

For dimensions and weight of the detector, see chapter 9 Specifications, page 211.

Provide a sturdy workbench of a height that ensures convenient access to the interior of each device in the system. The workbench must stand in a secure and level position that is free of vibrations. The bench top must be dry, clean, and resistant to chemicals.

Allow sufficient free space on the sides for gas connections and for proper air circulation. Allow at least 5 cm of clearance on the rear, at least 5 cm of clearance on the right side.

Make sure that the power switch and power cord can be easily reached at any time.

# 5.3.2 Power Considerations

The power supply of the device has wide-ranging capability, accepting any line voltage in the range specified for the device.

To avoid power fluctuations, the use of an uninterruptible power supply (UPS) is recommended.

A common ground for all system modules will avoid ground loops, which can create erratic results (for example, high baseline noise).



### CAUTION—Electric Shock or Damage to the Device

- Connecting the device to a line voltage higher or lower than specified could result in personal injury or damage to the device. Therefore, connect the device to the specified line voltage only.
- Never connect the device to a power socket that is shared with other equipment (for example, multiple sockets).
- Do not use defective multiple socket or extensions cords, as they could result in personal injury or damage to the device.
- After the power to the device is turned off, the device is still energized as long as the power cord is connected. Repair work on the device while the device is connected to power could lead to personal injury. Therefore, always unplug the power cord before starting repair work inside the device. If you were instructed to remove any covers or panels, do not connect the power cord to the device while the cover or panels are removed.



ATTENTION—Risque de choc électrique ou d'endommagement de l'appareil

- Le branchement de l'appareil sur une tension plus élevée ou plus basse que celle spécifiée pourrait blesser le personnel ou endommager l'appareil. Par conséquent, ne branchez l'appareil que sur la tension de ligne spécifiée.
- Ne branchez jamais l'appareil sur une prise partagée avec un autre équipement (par exemple, une multiprise).
- N'utilisez pas de multiprise ou de rallonge défectueuse, sous peine de blesser le personnel ou d'endommager l'appareil.
- Après la mise hors tension de l'appareil, ce dernier est toujours alimenté tant que le cordon d'alimentation est raccordé au secteur. Les réparations effectuées sur l'appareil alors que ce dernier est toujours raccordé au secteur pourraient blesser le personnel. Par conséquent, débranchez toujours le cordon d'alimentation avant de procéder à des réparations à l'intérieur de l'appareil. Si vous avez reçu pour consigne de retirer des couvercles ou panneaux, ne branchez pas le cordon d'alimentation tant que les couvercles ou panneaux ne sont pas remis en place.

# 5.3.3 Power Cord

The power cords are designed to match the wall socket requirements of the country in which they are used. The end of the power cords that plugs into the power socket on the device is identical for all power cords. The end of the power cords that plugs into the wall socket is different.

The ISQ EC and ISQ EM instruments come with the required type of power cord for your region. Use Table 2 to identify the correct power cord for your region. If you need to replace your power cord or buy an additional cord, you may use any brand of power cord, as long as it is appropriate for your region.

Region	Thermo Scientific Part Number C13 (for PC, monitors, and autosamplers)	Thermo Scientific Part Number C19 (for LC, IC, and MS)
North America 120V		
North America 250V		
Japan 125V		
Switzerland 250V		
Australia 250V		
China 250V		

Region	Thermo Scientific Part Number C13 (for PC, monitors, and autosamplers)	Thermo Scientific Part Number C19 (for LC, IC, and MS)
Europe- Schuko 250V		
United Kingdom 250V		
Denmark 250V		
Italy 250V		
Israel 250V	F. L. L. D.	
India 250V		



Table 2: Power Cord Identification by Region



### WARNING—Electric Shock or Damage to the Device

- Never use a power cord other than the power cords provided by Thermo Fisher Scientific for the device.
- Only use a power cord that is designed for the country in which you use the device.
- Do not use defective multiple socket or extensions cords, as they could result in personal injury or damage to the device.
- Never plug the power cord to a power socket that is shared with other equipment (for example, multiple sockets).
- Operate the device only from a power outlet that has a protective ground connection.
- In case of emergency, it must be possible to reach the power cord easily at any time to disconnect the device from the power line.



AVERTISSEMENT—Risque de choc électrique ou d'endommagement de l'appareil

- N'utilisez jamais un autre cordon d'alimentation que ceux fournis par Thermo Fisher Scientific pour l'appareil.
- Utilisez uniquement un cordon d'alimentation adapté au pays dans lequel vous utilisez l'appareil.
- N'utilisez pas de multiprise ou de rallonge défectueuse, sous peine de blesser le personnel ou d'endommager l'appareil.
- Ne branchez jamais le cordon d'alimentation sur une prise partagée avec un autre équipement (par exemple, une multiprise).
- L'appareil ne doit fonctionner qu'avec une prise électrique mise à la terre.
- En cas d'urgence, le cordon d'alimentation doit être facilement accessible à tout moment pour pouvoir débrancher l'appareil.



## WARNING—Electric Shock or Damage to a Product

Misuse of the power cords could cause personal injury or damage the instrument. Use the power cords provided by Thermo Fisher Scientific only for the purpose for which they are intended. Do not use them for any other purpose, for example, for connecting other instruments.



# AVERTISSEMENT—Risque de choc électrique ou d'endommagement d'un produit

L'utilisation incorrecte des cordons d'alimentation risque de blesser le personnel ou d'endommager l'instrument. Utilisez les cordons d'alimentation fournis par Thermo Fisher Scientific uniquement pour l'usage auquel ils sont destinés. Ne les utilisez pas à d'autres fins, par exemple, pour raccorder d'autres instruments.

# 5.3.4 Condensation

**NOTICE** Condensation in the device can damage the electronics. Therefore, when using, shipping, or storing the device, avoid or minimize conditions that can lead to a build-up of condensation in the device. For example, avoid significant or fast changes in environmental conditions. If you suspect that condensation is present, allow the device to warm up to room temperature. This may take several hours. Wait until the condensation is gone completely before connecting the detector to the power line.

# 5.3.5 Operating Conditions

When operating the instrument, make sure that the installation site meets these general environmental and operating conditions:

Temperature

Temperature fluctuations can affect the performance of the detector. Avoid locations with significant changes in temperature and strong air drafts. For example, do not place the detector in the direct sunlight, near heating or cooling sources, or under an air duct.

#### Humidity

The relative humidity of the operating environment is important for the performance of the detector. Operate the detector in the specified humidity range, with no condensation.

When the humidity is too high, condensation may occur, causing damage to the electronic components in the detector. When the humidity is too low, static electricity may accumulate and discharge, shortening the life of the electronic components.

### Ventilation

Make sure that the installation site is well ventilated at any time to avoid potential health hazards and safety risks, which may be caused by handling hazardous substances, volatiles or gases.

#### Vibration

Vibrations may affect the performance of the instrument. Therefore, the installation site should be free of vibrations. Avoid placing the instrument in locations where vibrations are caused by other instruments.

# 5.3.6 Gas Ventilation



#### CAUTION—Hazardous Fumes

The exhaust gas of the instrument may contain hazardous fumes that pose health and safety risks. Avoid an accumulation of gas. The exhaust gas must always be removed by proper ventilation. Make sure that the installation site is well ventilated. Do not vent directly into the laboratory.



#### **ATTENTION**—Fumées dangereuses

Les gaz d'échappement de l'instrument peuvent contenir des fumées dangereuses qui représentent un risque pour la santé et la sécurité. Évitez toute accumulation de gaz. Les gaz d'échappement doivent toujours être évacués par une ventilation appropriée. Assurez-vous que le site d'installation est bien ventilé. N'évacuez pas directement dans le laboratoire.

Make sure that the location fulfills the following requirements:

- Operate the instrument near the gas supply and ventilation sources.
- Ventilation must be at atmospheric pressure with no vacuum or negative pressure applied.
- Install the instrument in a well-ventilated laboratory. Both the source exhaust and the foreline pump must be connected to a suitable exhaust. Direct the gas exhaust tubing to a fume hood or connect it to another ventilation device.

# 5.3.7 Nitrogen Gas Supply

#### **NOTICE**—Gas Specifications

The requirements and specifications for the gas supplied to the instrument have major impact on the instrument performance. Observe the following notes:

- If the gas supply pressure is varying or dropping below the specified pressure range, it can impair the performance of the instrument.
- Non-volatile hydrocarbons, such as compressor oils, in the gas supplied to the system can cause permanent damage to the instrument.
- If the supply gas is contaminated with particles (size ≥ 0.1 µm), water vapor or other non-volatile substances, it can impair the performance or even damage the instrument.
- Observe all requirements and specifications for the supply gas in this manual to avoid damage to the detector.

Make sure that the location fulfils the following requirements:

 Make sure that the gas supply is regulated to a stable gas pressure that is within the specified gas pressure range. (95–110 psig or 655–760 kPa)

**TIP**—For sheath gas settings at or below 65 psig, nitrogen gas supply pressure of 90–100 psig (620–690 kPa) is sufficient.

**TIP**—If operating the ISQ EC and ISQ EM at maximum source gas settings, it is recommended that  $\geq$  100 psig ( $\geq$  690 kPa) input pressure is used.

 Nitrogen gas (typically ≥ 99% nitrogen purity) is recommended for most applications.

- Each instrument requires up to 30 L/min of nitrogen
- In standby, the instrument consumes ~15 L/min of nitrogen.
- ¼ in. OD Teflon tubing should be used to connect to each instrument. 760 cm is provided in the installation kit.

**NOTICE**—Do not use 6 mm tubing. This can damage the fittings. Use only ¼ in. OD Teflon tubing.

- If connecting multiple instruments to one nitrogen line, ensure the minimum pressure is delivered to each instrument when all are consuming the maximum amount of gas.
- The system should be placed close to the nitrogen gas source since gas pressure decreases as the length of tubing increases.
- Options for delivering nitrogen are (in order of convenience):
  - A nitrogen generator: These are available in larger units that may be remotely located or as point-of-use systems. Work with the specific vendor in order to determine output purity via an oxygen sensor. Point-of-use systems require compressor maintenance every 3,000 hrs.
  - Facility size Dewar: These are large globes located outside a facility. They are filled as needed.
  - Portable Dewar: These are roll around Dewars. Be sure to get one capable of outputting 100 psig. The 35 and 80 psig models do not provide sufficient gas pressure. There can be problems with them not boiling off nitrogen fast enough at high flow rates. Plan to change Dewars more often than you think, especially when not using much gas. At low, or no, consumption, the Dewar must still vent off nitrogen during the day to prevent it from going too high in pressure. This boil off rate is a function of the ambient temperature. In our experience, a Dewar will go empty in 2-3 weeks even if not used.

# 5.4 Unpacking the Instrument

It is crucial to remove the black foam insert that is wedged between the power supply module and the manifold. The foam insert keeps the glass top of the manifold in-place during shipping. In order to remove the shipping foam, please follow the instructions below:

- 1) Be sure the instrument is unplugged.
- 2) Using the provided tool kit, remove the top panel and right-hand side panel of the instrument.
- 3) Unscrew the power supply.
- 4) Lift up the power supply module as shown in Figure 3.
- 5) Remove the black foam insert.
- 6) Swing the power supply module back in place and secure it with the screw.
- 7) Replace the side and top panels.





Figure 3: Power supply module and location of manifold foam insert

# 5.5 Setting Up the Hardware

This section describes how to set up the hardware and provides information about the instrument connectors and cables.

# 5.5.1 Installing the Foreline Pump

The external mechanical pump as shown in Figure 4 is placed near the instrument and it is quiet at only 48 dB (A).

The pump size is 470 mm (length) x 158 mm (width) x 229 mm (height), and weighs 28 kg.

It should be placed on the floor or located somewhere where its vibration will not adversely affect instrument performance.



Figure 4: Foreline Pump

Check the foreline pump voltage setting as indicated in Figure 5. It shows a pump configured for 110 V operation. The voltage must match that of the supplied voltage to the MS instrument. For example, if the MS instrument is using 110 V, it is important that the foreline pump voltage is also set to 110 V.

If you are using 230 V, you must remove the two screws and flip the cover over so the blue label indicating 230 V is at the top.



### WARNING—Electric Shock or Damage to a Product

The pump voltage must match that of the power supplied to the MS instrument. Failure to match the voltage may result in pump and/or instrument damage.



## AVERTISSEMENT—Risque de choc électrique ou d'endommagement d'un produit

La tension de la pompe doit correspondre à celle fournie au spectromètre de masse. Dans le cas contraire, la pompe ou l'instrument risque d'être endommagé.



Figure 5: Foreline Edwards pump voltage setting

Then, check that the pump is set to high vacuum mode. The mode selector knob on the side of the system should be turned to the very right (towards the small droplets).

Next, install the oil mist filter assembly and oil return kit.

The EMF oil mist filter is used to separate and trap oil mist and odors discharged with the exhaust from oil sealed rotary vacuum pumps. They are a two-part filtration system consisting of a composite oil mist filter and an activated carbon odor filter. As the exhaust gases travel into the filter housing, and through the two-stage filter elements, oil droplets that are trapped by the composite filter travel into a collection reservoir located at the base of the housing. The oil is then returned to the pump through the oil return kit.

Follow the steps below to install the oil return kit.

- The gas ballast adapter has two parts: a metal adapter and a plastic adapter. First, assemble the metal gas ballast adapter by following the steps below. All the necessary parts are shipped with the Edwards pump.
  - a. Add the smaller O-ring so that it seals radially on the metal adapter. See Figure 6.



Gas Ballast Adapter



Figure 6: Adding the small O-ring to the gas ballast adapter

b. Use a gloved finger to apply a small amount of Apezion vacuum grease to the O-ring. If Apezion vacuum grease is unavailable, use a drop of vacuum pump oil instead. See Figure 7.



Figure 7: Applying oil to the small O-ring on the metal gas ballast adapter

c. Add the large O-ring to the base of the metal adapter. See Figure 8.



Figure 8: Attaching the large O-ring to the metal gas ballast adapter

2) Attach the metal O-ring to the black plastic adapter and the black O-ring on the metal adapter. See Figure 9.



*Figure 9: Installing the metal O-ring on the plastic gas ballast adapter* 

3) Screw the black adapter into the metal adapter. See Figure 10.



Figure 10: Screwing the adapters together

4) Remove the gas ballast knob from the top of the foreline pump by pushing down and turning it. See Figure 11.


Figure 11: Removing the gas ballast knob

**NOTICE**—Be sure the spring inside the inlet port stays in the inlet. If it comes out when you remove the cover, put it back in the inlet before adding the gas ballast adapter.

5) Locate the pins on the gas ballast adapter and the mating notches on the inlet port on the foreline pump. See Figure 12.



Figure 12: Finding the mating pins and notches

6) Insert the adapter assembly into the inlet port using the matching notches. See Figure 13.



Figure 13: Installing the adapter into the inlet

7) Push down on the adapter and turn it to the right to secure it to the inlet port. See Figure 14.



Figure 14: Securing the adapter

8) Turn the adapter so the flats are positioned as shown. One of the flats should face towards the number II on the pump. It should now be properly installed in the inlet port. See Figure 15.



Figure 15: Correctly installed adapter



9) Install the brass restrictor bushing into the small black hose for the oil mist filter. See Figure 16.

Figure 16: Installing the brass restrictor bushing into the oil mist filter hose

10) Push the bushing all the way into the hose. See Figure 17.



Figure 17: Correctly installed bushing



11) Attach the hose from the oil mist filter to the adapter using the included clamp. Push the hose all the way down on the adapter. This will push the restrictor bushing up into the hose. See Figure 18.

Figure 18: Attaching the oil mist filter hose to the adapter



12) Tighten the clamp, using a tool if necessary. Be sure the clamp is flush against the top of the adapter. See Figure 19.

Figure 19: Tightening the clamp with a tool



13) Install the foreline hose from the back of the mass spectrometer to the inlet port on the foreline pump. See Figure 20.

Figure 20: Installing the foreline hose to the foreline pump



14) Install and tighten the clamp to secure the foreline hose in place. See Figure 21.

Figure 21: Installing the clamp for the exhaust hose

**NOTICE**—Be sure to attach the foreline hose from the rear of the MS instrument to the inlet port of the foreline pump as shown on in Figure 41.

**TIP**—The instrument can be pushed completely against the back wall of the laboratory counter. The hose can bend to either side.



### WARNING—Electric Shock or Damage to a Product

The pump voltage must match that of the power supplied to the MS instrument. Failure to match the voltage may result in pump and/or instrument damage



### AVERTISSEMENT—Risque de choc électrique ou d'endommagement d'un produit

La tension de la pompe doit correspondre à celle fournie au spectromètre de masse. Dans le cas contraire, la pompe ou l'instrument risque d'être endommagé.



#### WARNING—Instrument Damage

The foreline hose length cannot be extended because it will adversely affect the pressure in the vacuum manifold.



### AVERTISSEMENT—Risque d'endommagement de l'instrument

*Le tuyau foreline ne peut pas être allongé, car cela aurait une incidence négative sur la pression dans le collecteur à vide.* 

# 5.5.2 Installing the Oil Mist Filter

To install the oil mist filter:

1) Remove the plug rom the oil mist filter. Leave the metal O-ring in place See Figure 22.



Figure 22: Removing the plug from the oil mist filter

2) Install the skinny hose adapter. Ensure it is hand tight. See Figure 23.



*Figure 23: Installing the skinny hose adapter* 

3) Install the oil mist filter adapter on the gray exhaust port adapter on the pump. See Figure 24



Figure 24: Installing the oil mist filter adapter on the gray exhaust port adapter

 Tighten the gray exhaust port adapter on the pump using an adjustable wrench. It is important that this is tight to prevent oil from leaking. See Figure 25.



Figure 25: Tightening the gray exhaust port adapter

**NOTICE**—Install the oil mist filter into the installed gray adapter. Do NOT replace the gray adapter with the black one that ships with the Edwards pump.

5) Place the oil mist filter onto the adapter. See Figure 26.



Figure 26: Installing the oil mist filter onto the adapter

**NOTICE**— The oil mist filter must be installed in the same direction as the exhaust flow as indicated by the arrow on the lower housing.

6) Use the included clamp to attach secure the oil mist filter to the adapter. Do not loosen the gray exhaust port adapter when installing the oil mist filter. See Figure 27.



Figure 27: Securing the oil mist filter with a clamp

7) Trim the hose to remove extra length. The hose should not be so short that it kinks. It should not be so long that it extends above the fitting on the oil mist filter. The orientation should be approximately horizontal so that oil does not collect in the hose. See Figure 28.



Figure 28: Trimming the hose

8) Attach the small black hose to the front of the oil mist filter to connect it to the pump exhaust. First, slide a clamp over the hose, then attach it to the oil mist filter. See Figure 29.



Figure 29: Attaching the pump exhaust hose to the oil mist filter assembly



9) Tighten the clamp with a tool. See Figure 30.

Figure 30: Tightening the oil mist filter assembly small hose clamp

**NOTICE**—Do not loosen the gray exhaust port adapter when installing the oil mist filter.

- 10) Now, install the top exhaust adapter to the oil mist filter. First, unscrew the cap at the top of the oil mist filter and discard.
- 11) Add the oil mist filter top O-ring. See Figure 31.



Figure 31: Installing the oil mist filter top O-ring

12) Add the top adapter. See Figure 32.



*Figure 32: Installing the oil mist filter top adapter* 



13) Install and secure the clamp that attaches the top adapter and O-ring to the oil mist filter. See Figure 33.

Figure 33: Securing the top adapter and O-ring with a clamp



14) Install the exhaust hose clamp and hose on the adapter. See Figure 34.

Figure 34: Installing the hose clamp and hose to the top adapter

15) Secure the clamp with a nut driver or flat handled screwdriver. See Figure 35.



Figure 35: Tightening the clamp with a nut driver

**NOTICE**—As you run the exhaust line to the house exhaust, do not let it unscrew or ben the exhaust port adapter.

Figure 36 shows a close-up picture of a correctly installed oil mist filter with the clear white bottom housing connected directly to the pump exhaust manifold. Be sure to attach the included gas ballast oil drain kit tubing from the bottom of the housing back to the pump ballast manifold.





Figure 36: Foreline pump oil mist filter assembly and oil return kit

# 5.5.3 Adding Oil to the Foreline Pump

This section contains instructions for adding oil to your foreline pump.

1) Use only the same type of Edwards pump oil that ships with the foreline pump. See Figure 37.



Figure 37: Edwards's foreline pump oil



2) Unscrew the cap on the oil reservoir and set aside. See Figure 38.

Figure 38: Unscrewing the oil reservoir cap



3) Add pump oil into the reservoir. Fill the pump a little over the halfway mark on the sight glass. See Figure 39.

Figure 39: Adding oil to the foreline pump

4) Close and tighten the reservoir cap. See Figure 40.

**NOTICE**—After tuning on the pump, the oil level might drop. If the oil level goes below halfway on the sight glass, vent the mass spectrometer and add oil.



Figure 40: Closing and tightening the oil reservoir cap

5) The power cord from the pump should be plugged directly into the back of the MS instrument as shown in Figure 41.



Figure 41: Rear side of instrument

## 5.5.4 Installing the Solvent Trap

A 4 L solvent trap bottle is also provided with the instrument. This tubing can be cut to connect the front, right of the instrument to the bottle and then from the bottle to the exhaust. Two 90° elbows are included to make bends around the edge of the table if desired. This tubing can be cut to any length required. See Figure 42.

The outlet of the solvent trap bottle must be connected to a suitable exhaust.



#### WARNING—Hazardous Vapors

The solvent gas may contain hazardous fumes. Maintain a wellventilated laboratory.



#### **AVERTISSEMENT—Vapeurs dangereuses**

Les gaz miscibles peuvent contenir des fumées dangereuses. Assurez une ventilation adéquate dans le laboratoire.



Figure 42: Instrument solvent trap

## 5.5.5 Installing the Source Housing Drain Insert and Sweep cone

Your instrument ships with the source housing drain insert and sweep cone uninstalled due to risk of shipping damage to sensitive parts. Please follow this step-by-step guide prior to turning on the power.



### WARNING—Instrument Damage

Wear gloves and eye protection to avoid contamination of sensitive parts.



AVERTISSEMENT—Risque d'endommagement de l'instrument

*Portez des gants et des lunettes de protection pour éviter de contaminer les parties sensibles.* 

- 1) Open the front bezel by grasping the door on the left edge.
- 2) Lift up the top hatch of the instrument to provide sufficient space to remove the source housing as shown in Figure 43.





Figure 43: Removal of the source housing

3) Remove PEEK capillary fitting connection at grounding union as shown in Figure 44.



Figure 44: Disconnect PEEK capillary connection of source at grounding union

4) Pull-up on the two cam levers located on the lower right and lefthand side of the source housing. As the cams rotate, the source housing will come away from the bulkhead and will slide off the two metal guide rods as shown in Figure 46.





Figure 45: Removal of source housing

5) Slowly remove the source housing as shown in *Figure 46*, taking care to avoid damage to the ESI probe and capillary connection.



Figure 46: Removing the source housing

6) Place the source housing in a safe location and install the sweep cone as shown in *Figure 47*.





Figure 47: Installation of sweep cone

- 7) The cone should snap in place and make a snug seal against the Teflon collar.
- Re-install the source housing in the reverse order as shown in Figure 48 with special care taken to be sure to slide the source housing onto the metal guide rods.



Figure 48: Reinstalling the Source Housing

9) Re-attach the PEEK capillary tubing to the grounding union. See *Figure 49*.



Figure 49: Reattaching the PEEK tubing to the grounding union



### WARNING—Instrument Damage

To ensure safe operation, the metal grounding union must always be securely fastened in the grounding clamp, which is attached to the metal housing of the ion source. Ensure the thumbscrew is tightened when reinstalling the probe ground connections. Damage to LC or IC might occur if the system is not properly grounded.



### AVERTISSEMENT—Risque d'endommagement de l'instrument

Pour assurer un fonctionnement sûr, la jonction de mise à la terre métallique doit toujours être solidement fixée au raccord de mise à la terre qui est attaché au boîtier métallique de la source d'ions. Vérifiez que les vis à oreilles sont serrées lors de la réinstallation des conducteurs de terre de la sonde. Les systèmes LC ou IC pourraient être endommagés si le système n'est pas correctement mis à la terre.

## 5.5.6 Switching Between HESI and APCI Modes on the ISQ EM Source Housing

Your ISQ EM source housing has a switch on the side of the source housing that must be aligned with the installed probe (HESI or APCI) for your system to work properly. Please follow the instructions in this section before starting your analysis.

 If you want to use the HESI probe on your ISQ EM, ensure that the probe switch on the side of the source housing is turned to the side. The HESI label will show clearly. Ensure the probe switch on the left side of the source housing faces up so that the needle is positioned correctly for analyzing samples. See *Figure 50*.



Figure 50: Ensuring the ISQ EM Source Housing is in HESI mode

2) If you want to use APCI mode, ensure the probe switch on the side of the source housing faces up so that the needle is positioned correctly for analyzing samples. See *Figure 51*.



Figure 51: Ensuring the ISQ EM Source Housing is in APCI mode

**TIP**—Before removing the APCI source housing, turn the APCI switch so that it is horizontal. This moves the APCI needle to a more secure position in at the top of source housing for transport.

# 5.5.7 Installing the Internal Calibration Solution

Your instrument ships with an empty bottle in-place of the internal calibration solution. It will be necessary to remove this shipping bottle and replace it with the labeled version as shown in *Figure 52*.

**TIP**—The instrument ships with two bottles of calibration solution. Each bottle contains over 250 mL of liquid and is stable at room temperature for up to one year.

TIP—Ideally, the spare bottle should be stored at 4 °C.



Figure 52: Labeled internal calibration solution for Autotune



#### WARNING—Instrument Damage

Wear protective clothing, eyewear and gloves during the calibrant bottle installation procedure.



### AVERTISSEMENT—Risque d'endommagement de l'instrument

*Portez des vêtements, des lunettes et des gants de protection lors de la procédure d'installation de la bouteille d'étalonnage.* 

- 1) Remove the cap from the empty bottle at the front of the instrument, taking care not to damage the capillaries and gas lines that are present.
- 2) Unscrew one of the labeled calibrant bottles and attach to existing cap located on the instrument as shown in *Figure 53*.



Figure 53: Location to install internal calibrant

**TIP**—Each autotune experiment uses approximately 10mL of calibrant solution. Please be sure to check liquid level of the bottle prior to performing any autotune experiment.

**TIP**—If any liquid spills unto the drain area located directly below the bottle, be sure to clean and dry the liquid leak sensor as shown in Figure 16.

### 5.5.8 Connecting the IC or LC to the MS Inlet

This section provides instructions for connecting the LC or IC to the ISQ EC inlet.

Figure 54 shows the various fluidic connections for the MS instrument. See Table 3 for descriptions of the MS fluidics.



Figure 54: ISQ EC and ISQ EM MS fluidics overview

Letter	Description
А	Instrument inlet
В	Inlet to valve
С	Valve to grounding union
D	Grounding union to source (probe)
E	Reference calibrant to valve

Table 3: MS Instrument Fluidics

The LC to MS inlet or instrument inlet connection can be rotated 90° to face upwards in the event that the user wishes to connect to the MS instrument from the top hatch. Using the tool kit provided with the instrument, remove the external cover on the left side of the instrument (if facing the instrument). Next, remove the lock screw located on the outside of the left side panel (if facing the instrument), directly opposite of the inlet. Once the retaining screw is removed, the inlet assembly can be freely moved to the other set of two holes. The inlet has a tapped hole and a pin to position it and can be conveniently positioned as required for the application as shown in Figure 55.





Figure 55: LC to MS inlet assembly

## 5.5.9 Flushing the Calibration Solution

This section provides instructions for flushing the calibration solution. The instrument must be completely connected and running before calibrant solution can be flushed.

1) In the **Detector-More Options** box, toggle the valve position to **Load** using the dropdown menu. See Figure 56.
| Detector - More Options   | - 🗆 X                    |  |  |
|---|--------------------------|--|--|
| More Options: Detector Vanquish ISQ Family<br>Instrument: DESKTOP-2PMSODN_1 |                          |  |  |
| Maintenance mode  | Calibration gas valve    |  |  |
| Enter Maintenance Mode  | Six port valve position: |  |  |
| Exit Maintenance Mode   | Calibration valve pre    |  |  |
| Overall status: Off   | Tum On Standby Mode      |  |  |
|   | Close                    |  |  |

Figure 56: Flushing the calibrant

2) Check the Calibration Valve Pressurization box. See Figure 57.

Detector - More Options	- 🗆 X		
More Options: Detector Vanquish ISQ Family Instrument: DESKTOP-2PMSODN_1			
Maintenance mode	Calibration gas valve		
Enter Maintenance Mode	Six port valve position: Load ~		
Exit Maintenance Mode	Calibration valve pressurization		
Overall status: Off	Tum On Standby Mode		
	Close		

Figure 57: Checking the calibration valve pressurization box

- 3) Watch for liquid entering the clear drain line (behind the bulkhead union).
- 4) Let the calibration solution flush for approximately 30 sec.

5) Uncheck the Calibration Valve Pressurization box. See Figure 58.

Detector - More Options More Options: Detector Instrument: DESKTOP-3	- □ × Vanquish ISQ Family 2PMSODN_1
Maintenance mode Enter Maintenance Mode Exit Maintenance Mode	Calibration gas valve Six port valve position: Load Calibration valve pressurization
Overall status: Off	Tum On Standby Mode

*Figure 58: Disabling the calibration valve pressurization* 

# 5.5.10 Connecting the System to the PC

This section provides instructions for connecting all parts of the LC-MS or IC-MS system to the PC.

### 5.5.10.1 Connecting the ISQ EC and EM Mass Spectrometer to the PC

The mass spectrometer requires a local LAN connection 10Base-T connection. The cabling has been provided to connect directly to the PC. The PC has two LAN connections located on the rear of the PC. Plug the 10Base-T cable into the PC card as shown in Figure 59 by the red cable. For Internet and local IT infrastructure, please use the location as indicated by the blue cable as shown in Figure 59.



Figure 59: Connecting the ISQ EC MS to the PC

### 5.5.10.2 Connecting the LC or IC Instrument to the PC

Please follow the manufacturer's recommended guidelines on how to connect the PC to the front-end chromatograph instrument. Refer to the "Unpacking" chapter for more information regarding the preinstalled software.

# 5.5.10.3 Configuring the LAN

If you purchased a PC with the mass spectrometer, the network settings will be configured for you. If you purchased a PC independently, please follow

the instructions on page 125 to configure the IPv4 settings on the appropriate LAN.

## 5.5.10.4 Connecting the Fluidics System to the Mass Spectrometer

The instrument ships with various PEEK capillaries to assist in the connection to front-end chromatograph. Do not bypass or alter PEEK capillaries that are internal to the MS instrument. These connect the internal reference inlet system and valve to the ion source.

# 5.6 Summary of Hardware Installation

This section provides a step-by-step overview of the hardware installation procedure for your mass spectrometer. Refer to previous sections for details for each step.

- 1) Locate and place the mass spectrometer on the lab bench, next to IC or LC chromatograph instrument.
- 2) Allow sufficient space for the PC workstation and monitor.
- 3) Follow the Site Requirements section of this manual which include instructions and guidelines for power, ventilation and nitrogen.
- Wear appropriate personal protective gear, including lab coat, safety glasses and gloves.
- 5) Attach the nitrogen supply line.



#### CAUTION—Gas Supply Safety

The nitrogen supply line should not be delivering gas or set to the "on" position for a generator or source valve and set to "open". Failure may result in personal injury. Wait until the supply line is firmly attached to the instrument prior to turning on the gas.



#### ATTENTION—Sécurité de l'alimentation en gaz

La conduite d'alimentation en azote ne doit pas distribuer de gaz ou être réglée sur la position « on » (marche) pour une vanne de générateur ou de source et être réglée sur « open » (ouverte). Le non-respect de cette consigne peut entraîner des blessures corporelles. Attendez que la conduite d'alimentation soit solidement raccordée à l'instrument avant d'activer l'alimentation en gaz.

- 6) Install the foreline pump.
- 7) Remove the capillaries attached to the source housing.

- 8) Remove PEEK capillaries and source housing as shown in *Figure 44* and *Figure 45*.
- 9) Install sweep cone as shown in Figure 47.
- 10) Check that source drain collar is correctly installed as shown in Figure 48.
- 11) Install source housing and re-attach capillaries.
- 12) Verify correct voltage on foreline pump matches lab/building power supply.
- 13) Connect foreline pump power cord to pump and MS instrument.
- 14) Verify MS instrument power switch is set to the "off" position.
- 15) Connect MS instrument power cord to wall outlet.
- 16) Switch on the MS instrument.
- 17) The MS instrument will automatically turn on the foreline pump and the system will begin to achieve nominal vacuum.

**TIP**—The mass spectrometer typically takes an hour before it can be used in normal operation. If possible, allow the system to achieve stable vacuum overnight

# 5.7 Powering Up the System

The power switch is located at the rear of the instrument's top right corner as shown in Figure 60 below. The instrument will power on when the switch is in the up-right position as shown. The MS instrument will automatically switch between 110V and 230V. There is no manual adjustment required.



Figure 60: Location of power switch

Check the foreline pump voltage setting as indicated in *Figure 61*. The voltage must match that of the supplied voltage to the MS instrument. For example, if the MS instrument is using 110V, it is important that the foreline pump voltage is also set to 110V.



Figure 61: Foreline Edwards pump voltage setting

# **6 Operation**

This chapter describes the elements for instrument control, provides information for routine operation and for shutdown.

# 6.1 Introduction to this Chapter

The information in this chapter assumes that the initial setup of the system has already been completed. If this is not the case, refer to the instructions in chapter 5 Installation before proceeding (see page 50).

For a basic description of instrument control and automated sample analysis with the Chromeleon software, see section 6.4. Details on control and operation of the detector are available in the *Chromeleon Help*.

# 6.2 Safety Guidelines for Operation

When operating the detector, pay attention to the following safety guidelines:



Observe all warning messages and precautionary statements presented in section 2.3 Safety Precautions (see page 23).



#### CAUTION—Explosion Hazard or Damage to the Detector

When using tetrahydrofuran (THF), the use of air as supplied gas may pose an explosion hazard. This can pose a safety and health risk and damage the detector. Always use nitrogen with tetrahydrofuran or other highly combustible solvents.



#### ATTENTION-Risque d'explosion ou d'endommagement du détecteur

Lors de l'utilisation de tétrahydrofurane (THF), il y a un risque d'explosion si le gaz d'alimentation est l'air. Cela peut représenter un risque pour la sécurité et la santé et endommager le détecteur. Utilisez toujours de l'azote avec le tétrahydrofurane ou d'autres solvants hautement inflammables.

**NOTICE** Pay attention also to the following guidelines:

- When operating the chromatography system, always set the upper pressure limit for the pump. This prevents damage resulting from leakage or from running the pump dry.
- If there is evidence of leakage in the detector, turn off the pump flow and remedy the situation immediately.

- Verify that the detector gas flow is turned on always before you turn on the pump flow to the detector. Do not direct pump flow to the detector without gas flow being turned on.
- When turning on detector gas flow and pump flow Turn on the detector gas flow first, wait at least 5 minutes and only then turn on the pump flow.
- When turning off pump flow and detector gas flow
   Turn off the pump flow first, wait at least 5 minutes and only then
   turn off the detector gas flow. During the waiting period, the drain
   pump drains any remaining mobile phase to waste before it
   automatically turns off.
- Observe the requirements for gas supply and ventilation. See section 5.3 Site Requirements, page 55.
- Observe the specifications for operation. See Specifications 211.

# 6.3 MS Instrument Overview

This section provides an overview of the MS instrument. Figure 62 shows the various fluidic connections for the MS instrument. See Table 4 for descriptions of the MS fluidics



Figure 62: ISQ EC and ISQ EM MS fluidics overview

Letter	Description	
А	Instrument inlet	
В	Inlet to valve	
С	Valve to grounding union	

Letter	Description
D	Grounding union to source (probe)
E	Reference calibrant to valve

Table 4: MS Instrument Fluidics

# 6.4 Configuring the MS in Chromeleon

Your MS instrument utilizes the first native MS driver for Chromeleon 7.2 chromatography data systems (CDS). Unlike other MS instruments, there is no other auxiliary software required to directly control the MS.

#### Configuring the MS

- 1) Please follow the steps as outlined below to configure the MS within Chromeleon 7.2.
- 2) The MS instrument should be powered "On", under vacuum and supplied with nitrogen gas.
- Open Chromeleon Service Manager and select the "Configure Instruments" option. Follow documented Chromeleon procedures to create a new instrument within Chromeleon 7 to add either an IC or LC system.
- 4) Once the front-end LC or IC is configured select "Add module to instrument" as shown in Figure 63.
- 5) The MS can be found in either one of several locations
  - 1) Thermo Scientific >Mass Spectrometry> ISQ LCMS Family
  - 2) Thermo Scientific> Mass Spectrometry> ISQ ICMS Family

🍰 Add module to instrument		×
Instrument Name: Vanquish Manufacturers: Thermo Scientific IC: Dionex ICS-3000 Systems IC: Dionex ICS-3000 Systems IC: Dionex ICS-6000 Systems IC: Dionex ICS-6000 Systems IC: Dionex ICS-6000 Systems IC: Dionex Modules IC: Dionex Modules HPLC: Dionex Utilitate 3000 HPLC: Vanquish HPLC: Opinex Utilitate 3000 HPLC: Vanquish HPLC: Opinex Utilitate 3000 HPLC: Wodules ESA Modules ESA Modules Extraction Modules Mass Spectrometry Generic ABI Agilent Berhold Dostmonn	Modules: ISO ICMS Family Legacy Mass Spectrom Wass Spectrometer Vanquish ISO Family	eter
	OK	Cancel

Figure 63: Location of ISQ EC or ISQ EM instrument module

6) If you purchased a PC with your mass spectrometer, the instrument will configure automatically and display an IP address. See *Figure 64*.

Vanquish ISQ Family Configuration X				
General Maintenance A	sociate pump	info		
Device name:				
Remote start: ActiveHigh				
Hardware inject sync	hronization			
Split flow	Γ	1	00 %	
✓ Fraction Collection				
✓ Warn on source chan	ge			
Simulation mode				
Vacuum Pressure Units: Torr				
Source Gas Pressure Units: psig 💌				
Communication settings				
IP address: 192.168.1.234 Edit				
TCP port: 30				
ок с	ancel	Help		

Figure 64: ISQ MS Family Configuration - General tab

- 7) If you purchased a PC independently, please follow the instructions below to configure the IPv4 settings on the appropriate LAN.
- 8) Turn on the computer and allow it to complete its boot processes.
- Select Start > Control Panel > Network and Internet > Network and Sharing Center to open the Network Connections window.
- 10) Configure the network card that will connect to the mass spectrometer.

- a. Right-click on the card and select **Rename** to rename this connection. Rename it to **ISQ EC** or **ISQ EM**.
- b. Right-click on the **ISQ EC** or **ISQ EM** connection and select **Properties** to set the IP address.
- c. Disable all the protocol except the **Internet Protocol (TCP/IP) Version 4**, by unchecking the boxes.
- Under Communication Settings, click the Edit button next to the IP address. The Local Area Connection Status window opens. See Figure 65.

4	Local Area Connection Status	J
	General	
	Connection	
	IPv4 Connectivity: No Internet access	L
	IPv6 Connectivity: No network access	
	Media State: Enabled	
	Duration: 15 days 04:53:18	
	Speed: 100.0 Mbps	
	D <u>e</u> tails	
	Activity	
	Sent — 駴 — Received	
	Bytes: 469,728,460 24,029,705,501	
	Properties Diagnose Diagnose	
	Qlose	

*Figure 65: Local area connection status window* 

- 12) Click Properties to open the local area network properties.
- 13) Under the Networking tab lot the Local Area Connection Properties window, double-click the Internet Protocol Version 4 (TCP/IPv4) connection item or click Properties. See Figure 66

Local Area Connection Properties			
Networking Sharing			
Connect using:			
Broadcom NetXtreme Gigabit Ethernet			
Configure			
This connection uses the following items:			
Client for Microsoft Networks			
Gos Facker Scheduler			
Broadcom Advanced Server Program Driver			
□ → Internet Protocol Version 6 (TCP/IPv6)			
Internet Protocol Version 4 (TCP/IPv4)			
Link-Layer Topology Discovery Mapper I/O Driver			
Install Uninstall Properties			
Description			
Transmission Control Protocol/Internet Protocol. The default wide area network protocol that provides communication across diverse interconnected networks.			
OK Cancel			

Figure 66: Selecting the network connection

14) Configure the IP Address and Subnet as shown in Figure 67.

'ou can get IP settings assigned a his capability. Otherwise, you nee	utomatically if your network supports ed to ask your network administrator
or the appropriate IP settings.	
Obtain an IP address automa	tically
Use the following IP address:	
IP address:	192.168.1.1
Subnet mask:	255.255.255.0
Default gateway:	
Obtain DNS server address au	utomatically
Use the following DNS server	addresses:
Preferred DNS server:	
Alternate DNS server:	• • •
🔲 Validate settings upon exit	Advanced

Figure 67: Configuring the IP address and subnet mask

**NOTICE** If using the supplied USB to Ethernet adapter to connect the instrument, transferring large data files using the USB hub that the adapter is installed in while simultaneously collecting data on the instrument can cause occasional communication issues.

15) Click **OK** and return to the General tab on the Chromeleon configuration pane. See Figure 68.

Vanquish ISQ Family Configuration X				
General Maintenance A	ssociate pump info			
Device model: ISQ EM				
Device name:	ISQEM			
Remote start:	ActiveHigh 💌			
Hardware inject sync	chronization			
Split flow 100 %				
✓ Fraction Collection				
Warn on source chan	nge			
Simulation mode				
Vacuum Pressure Units:	Torr			
Source Gas Pressure Units: psig 💌				
Communication settings				
IP address: 192.168.1.234 Edit				
TCP port: 30				
ок с	ancel Help			

Figure 68: ISQ Family Configuration-General Tab

- 16) Set the **Device Model** to ISQ EC or ISQ EM, depending on which instrument you are using.
- 17) The **Device Name** is the name used to identify the ISQ EC or ISQ EC MS in Chromeleon. In most cases, you should accept the default name. If you enter a different name, you may have re-link controls on the ePanels or edit the name in the instrument methods.
- 18) If you want to connect the MS directly to an autosampler, check Hardware Inject Synchronization. Otherwise, the ISQ EC will be controlled by Chromeleon software. This mode is normally not used.

**IMPORTANT**—Generally, **Hardware Inject Synchronization** should not be used. See 164 for additional information about remote start cables.

- 19) If Hardware Inject Synchronization is checked, set Remote Start to Active Low or Active High. The selection should be the same as the setting on the autosampler.
- To set the split flow multiplier, check Split Flow. The split flow multiplier can be set from 1–100%
- 21) If you would like to perform mass-directed fraction collection, check **Fraction Collection**.
- 22) If you would like the instrument to remind you to select the correct position for the APCI discharge pin when swapping between HESI and APCI probes, check Warn on Source Change.
- 23) Normally, the Simulation Mode box is not checked. Checking the Simulation Mode box allows users to work in Chromeleon software without interacting with the instrument or analyzing real data. Simulation Mode is mostly used for training purposes.

IMPORTANT—Usually, Hardware Inject Synchronization and Simulation Mode should both be left unchecked.

24) Select the **Maintenance** tab and verify that all entries are enabled as shown in Figure 69.

Vanquish ISQ EC Configuration			
General Maintenance Associate pump info			
	Enable	Days	
Foreline pump oil:		125	
Turbo pump oil/bearing: 🔽 729		729	
Multiplier:		1000	
	Re	set all	
ОК	Cancel H	elp	

Figure 69: ISQ EC or ISQ EM MS configuration - Maintenance tab

Use the **Maintenance** tab to set maintenance intervals for the foreline pump oil, turbo pump oil and bearing, and the electron multiplier. To view usage times for these items, open the Chromeleon Console and go to **ISQ EC (ISQ EM)** > **Wellness**. See

	and the second	The Provide Contract Contract Contract	(101) 401
Black Create File Edit View Too	s Help		
istruments «	Launch eWorldlow • Smart Startup?	utation • 🙀 Release Control 🛬 Monitor Baseline • 😑 Concurringities • 🖂 CAutogenerated • • 🖂 🕼 ۵۰۰	
V Her Y	Bome PumpModule SamplerModule	ColumiCorp ISOEC Bitr Audi Statup Queue	
op local instrument Controller a running rale.	Module Status Settings		
ASERU	Corrected	Detector - Wellness	
PE-ASBRU_2 🔅	ReadyToDownized Shooth gas p		
	Aux ges press	Wellness: Detector Vanquish ISQ EC	
	Retention Time	Instrument: PE-ASBRU 2	
	Vacuum read-		
		Dataset Model Manager 190	
	21456795-	Instance D	
	20300000	Versions Serui Numbers Pro-	
		Controller interface many files Leng show board 195045299	
	More Options	Controller Herdinan PPGA fitmane 54 Lans draw HV/board 1004/39/5	
	Welness	PC communications ferrouse: 233.72.99.28 Pressure controller loard: 164310A9	
	Seatre	Presure controller fermane: 18 Presure manifold board: 17270000 Spectral plot could not be created.	
	10300000	Lens driver firmware: 20 Vaporter board: 17/11700F No spectra selected.	
	-	REferences	
	Scanning/Tuning \$200000	Instrument driver version: 1.0.0.46	
	Real Time Scan	Mantenance	
		Active? Usage Time Time in Use min	
		Foreine pump of: Yes 125 (days) 2.77 (days) (2.23) Reset Counter 10.00	
		Turbo pump: Yes 725 [days] 2.77 [days] (0.4%) Reset Counter	
	Adde man	Multipler: Yes 1000 (dow) 0.00 (dow) (0.01) Reset Counter	
	Date Time		
	0 1000017 2.3136 AM 9300	a detue.	
	0 //20/2017 9:25:38 AM -05:00	Calibration Compound: 250.0 (ni) Available (0.0%) Liked)	
	0 7/20/2017 9:25:34 AM -05:00	Core	
	0 7/20/2017 9.25.32 AM -05.00		
	0 7/20/2017 9:25:28 AM -05:00	ISGEC Trying to connect	
	(B) 7/20/2017 9.25.28 AM -05:00	ISQEC This driver does not have a valid final certification.	
	7/20/2017 9:25:27 AM -05:00	Instalizing driver Varquish ISQ EC	
instruments	7/20/2017 9:25:27 AM -05:00	ThermoFisher ISOEC LCDvive - ThermoFisher ISOEC LCDvive, Venion 1.8.0.46 Couvrient ® Thermo Fisher Scientific 2017. All rights reserved.	
Data			

Figure 70: Viewing maintenance intervals In the Chromeleon Console

- 25) Click **OK** when you have finished setting the maintenance intervals.
- 26) Select the **Associate Pump Info** tab to associate a pump or change pump types. See *Figure 71*.

Vanquish ISQ EC	Configuration	
General Maintenance Associate pump info		
Associate a pump		
Manufacturer:	HPLC:Vanquish	
Model:	Vanquish Binary Pump 💌	
Main Device	PumpModule	
Pump Device	Pump	
Note: The names of the main device and pump device (if applicable) must match exactly what you have named them when you configured the pumps.		
ОК	Cancel Help	

Figure 71: MS configuration – Associate Pump Info Tab

- 27) If you want to associate a pump with the MS, check the Associate a Pump box. If this box is not checked, you must set the pump flow in the instrument method editor for each method. The software will also prompt you to check the pump flow before tuning the instrument if you have not associated a pump.
- 28) Use the drop-down menus for **Manufacturer** and **Model** to choose the proper settings for the pump installed on the system. See *Figure 72*.

Associate	a pump	Associate	a pump
Manufacturer: Model: Main Device Pump Device	HPLC:Vanguish	Manufacturer: Model: Main Device Pump Device	HPLC:Vanquish
Note: The nam if applicable) n named them wh	es of the main device and pump device nust match exactly what you have en you configured the pumps.	Note: The name (if applicable) m named them wh	es of the main device and pump device nust match exactly what you have en you configured the pumps.

Figure 72: MS configuration – Adding pump information

29) Enter the **Main Device** and **Pump Device** names. The names must match the ones for the pump. See Figure 73.

Vanquish ISQ EC Configuration		
General Maintenance Associate pump info		
🔽 Associate a pump		
Manufacturer: HPLC:Vanquish		
Model: Vanquish Binary Pump		
Main Device PumpModule		
Pump Device Pump		
Note: The names of the main device and pump device (if applicable) must match exactly what you have named them when you configured the pumps.		
OK Cancel Help		

*Figure 73: MS configuration— Entering the device names* 

30) Select the **OK** button and Chromeleon will attempt initial communication with the MS instrument. A successful attempt will provide several entries in the instrument configuration audit trail window as shown in Figure 74 below.



Figure 74: MS instrument audit trail information

# 6.5 User Operation

The **Run Mode** starts sample analysis and turns on the gas flow automatically if the gas flow was turned off.

### 6.5.1 Chromeleon User Interface

The **Diagnostics** screen displays real-time information and values with a default ePanel may be displayed once Chromeleon 7.2 is launched and connects with the configured system. This ePanel is termed "ISQ EC" or "ISQ EM". If the ePanel is missing, please follow the instructions under **Adding the MS instrument ePanel** below.

### 6.5.1.1 Chromeleon ePanel

You should see a user interface similar to what is shown in Figure 75 and Figure 76, depending on whether the MS is attached to a HPLC or IC instrument.



Figure 75 : HPLC MS Instrument Panel



Figure 76: IC MS Instrument Panel

Parameter	Description
Status window	Indicates whether the system is ready to operate. Status window will show as "busy" while the instrument is in acquisition mode
Instrument connect	Enables direct software control over the MS instrument. This can be toggled "on" or "off" with the slide bar.
Real time scan	Feature that allows user to immediately trigger acquisition mode. A new window will appear with real-time scanning data and ability to adjust instrument parameters.
Manual tune	This mode is for service engineers to set up the instrument. Do not use this mode for other purposes.
Sheath gas pressure status	Displays the main nitrogen gas pressure used for desolvation/ nebulization.
Sweep gas pressure status	Counter-flow gas pressure coming out of sweep cone. Used for dirtier sample matrices and more complex mobile-phase compositions
Aux gas pressure status	Gas flow around the outside of the spray needle. This gas can be heated to aid in desolvation
Vaporizer temp status	Heat applied to aux gas to aid in desolvation
Ion transfer tube temp status	Heat applied to the ion transfer tube, which carries ions into the ion optics. Used to further desolvate the ions
Source voltage status	Voltage applied to ESI capillary for ionization
Source current status	Current of the source voltage
Chromatogram window	This window will activate with the real-time data display during acquisition mode or during an automated batch sequence
Foreline pressure status	Foreline pump pressure

Table 5: MS Instrument ePanel functions

Table 5 lists the various ePanel features and their respective description and function. Once the instrument has been configured and connected to Chromeleon software, please take note of the foreline pressure status.

**TIP**—Instrument voltages will not be applied to the source until nominal vacuum has been achieved.

The ePanel will allow the user to select an ESI positive or negative autotune, and ESI diagnostic-only tune, or a manual tune.

**IMPORTANT**—Manual tune should only be used by Thermo Fisher Scientific service engineers.

The system will automatically optimize the instrument based on the internal reference solution (calibrant) and provide a result in the Chromeleon audit trail similar to what is shown in Table 6.

Parameter	Enables direct software control over the MS instrument. This can be toggled "on" or "off" with the slide bar.
Tune status	Indicates the overall status of the tune experiment
Current tune task name	Indicates the sub-task name currently being performed
Current tune task action	Indicates the current status of the sub-task being performed
ESI Positive Tune	Run autotune for ESI positive modes of operation
ESI Negative Tune	Run autotune for ESI negative modes of operation
ESI Diagnostic- only Tune	Runs a series of hardware checks to ensure that the ISQ EC MS is operating as anticipated
Manual Tune	Allows users to change tuning settings on selected analyzer components.

Table 6: AutoTune ePanel feature descriptions

### 6.5.1.2 Real Time Scanning

When selecting the **Real Time Scan** option from the ePanel, a new window will appear as shown in Figure 77 and the instrument will be ready enter acquisition mode and allow the user the ability to modify certain instrument settings.



Figure 77: Real Time Scanning Window

This feature is designed for real-time instrument optimization of an analyte or group of analytes. The feature is designed to work based on injection or direct infusion of the analyte(s) into the MS instrument. In order to enter into acquisition mode, select the "Play" button at the top left-hand corner of the real-time scanning window. Once the "Play" button is pressed, the system will allow the user to modify the instrument settings in real-time. See Table 7 for a list of real-time scanning features.

**TIP**— Ensure the **Use Calibrant** box is unchecked if you wish to analyze anything other than the internal reference calibrant solution. Checking the box will initiate the calibrant infusion process.

**TIP**— Scan masses must be entered into the **Mass Table** before real-time scanning will initiate.

**TIP**—Once the **Play** button has been pressed, the instrument settings can be changed in real-time.

Parameter	Description
Play button	Initiates real time scanning
Stop button	Ends real-time scanning
Real time data display	Shows the real-time data acquisition once the Play button has been selected. The X ( $m/z$ mass range) and Y (relative signal intensity) are displayed.
Status window	Displays the current source type and instrument status
Scan type	User selectable for full scan and SIM modes of operation
Spectrum Type	Select the spectrum type: profile or centroid For SIM methods, select profile mode only.
Polarity	Select the probe polarity
Use calibrant	A check in this box will actuate the internal valve and initiate an internal calibrant infusion into the MS instrument
Use tune value	Use to enter a custom value for the tube lens
lon transfer tube temp	Select the heat applied to transfer tube after the exit cone
Vaporizer temp	Select the heat applied to the ESI probe out of the manifold for aiding in desolvation
Source voltage	Select the voltage applied to the ESI capillary for ionization
Source CID voltage	Voltage applied within the source to induce collisional dissociation
Tube lens voltage	Select the voltage applied to the tube lens
Sheath gas pressure	Select the main nitrogen gas pressure used for desolvation / nebulization.
Aux gas pressure	Select the gas flow around the probe outer manifold
Sweep gas pressure	Select the counter-flow gas pressure coming out of sweep cone
Load calibration masses	Button that automatically provides pre-selected full-scan masses for internal calibrant.
Mass Table	Enter selected mass and/or mass range of interest. Real-time data display will auto update with selection

Table 7: Real time scanning list of features and descriptions

Entering analyte masses of interest into the **Mass Table** will automatically update the real time data display for the given mass or mass range of interest.

### 6.5.1.3 Autotune Procedure

**IMPORTANT**—The ESI source housing must be installed and configured before tuning the ISQ EM. The instrument cannot be tuned with the APCI source installed.

The reference solution delivery system as shown in Figure 78 includes a 6port valve plumbed between the chromatograph and the ion source. The valve allows for automated switching between the flow paths originating from the chromatographic effluent or the reference solution.



Figure 78: Reference Inlet System

To deliver the reference solution to the ion source, a 500  $\mu$ L calibrant loop is first filled by setting the 6-port valve to load and pressurizing a bottle of reference solution. Then, the 6-port valve is switched back to inject so the flow from the chromatograph pushes the reference solution into the ion source.

**IMPORTANT**—It is critical that the solvent delivery pump is set for 50  $\mu$ L/min during the automated autotune process.

**IMPORTANT**—Before running your first autotune, it is critical that the valve and sample loop are flushed with calibrant. Please follow the step-by-step instructions below.

- 1) Follow all steps as indicated in this chapter so far and Section 5.5.
- The MS instrument should be connected to the PC, configured in Chromeleon, and in a ready state with nitrogen gas flow set to **On** and nominal vacuum status.
- Fill an LC or IC reservoir with a standard LC or IC solvent. Example solvents are: 100% Fisher Scientific Water Optima LC/MS Grade (PN W6-4) or 18.2 DI MΩ water type 1.
- 4) Set pump to flow 50  $\mu$ L/min.
- 5) From the ISQ EC instrument ePanel, select Real Time Scanning.
- 6) Check the **Use Calibrant** box and press the **Play** button to initiate infusion of the internal reference solution.
- 7) Flush the system with the mobile phase for 5 min.
- 8) Turn on the calibrant.

**TIP**— Liquid should be exiting from the valve into the instrument waste stream for several minutes after pressing **Play**.

- 9) Press **Stop**. The valve and injection loop are now flushed.
- 10) Exit Real Time Scanning mode. The applet window closes.
- 11) Press the **Tune** button to open the Tune window. Select **Positive Autotune**.
- 12) The system will now initiate an autotune. Once completed, a summary of the tune result appears in the Chromeleon audit trail.

# 6.6 Running Your First Sample

This section provides information about running samples on the ISQ EC mass spectrometer. This MS instrument is designed for seamless incorporation into the Chromeleon run control workflows. As a result, the instrument method editor follows the same rules and logic as other modules and detectors for either ion or liquid chromatography instruments.

Once the MS instrument is properly connected and controlled by Chromeleon, the user may create an instrument method. Select create a new method in Chromeleon 7.2 and follow the automated prompts. The method editor is divided into two sections, source settings (top) and scan settings (bottom). Each section has different modes based upon user preference and workflows.

### 6.6.1 Getting Started

The ISQ EC and ISQ EM instrument method editor features an easy and advanced mode,

There are three main elements the ISQ EC MS instrument method editor: the Source Parameters pane, the Scans pane, and Fraction Collection Channels pane. See Figure 79.

SIGEN Mass Detector for ISOEM (Nanquish 160 Fereily)	4
Can fra defector Can fra defe	
cans San time Man (af an Andre Source Co Angre and Andre Source Co Scans Pane	Napadon He Min bandro peak width: 30 a Dealerd scare peak: 6 Dealerd scare peak: 20 He
radion Collection Channels and Tope Name Tope Name and Tope Name and Tope Name and To	

Figure 79: ISQ EC and ISQ EM method editor

### 6.6.2 Method Editor—Source Settings, Easy View

The ISQ EC and ISQ EM instrument method editor features an easy and advanced mode for setting the source parameters. In the easy mode, all relevant source settings are calculated automatically based upon the pump flow value. This value is automatically derived if the front-end pump is associated in the instrument configuration. See Section 6.4: Configuring the MS in Chromeleon.

If the pump is not associated, the user must manually enter a pump flow value to calculate all the necessary source values. These parameters are calculated into three (for HESI methods) or four (for APCI methods) separate slider bars that control different aspects of source functions. The user can hover over each slider bar to see the actual values that are applied. As the sliders are moved up and down, the underlying algorithms calculate new iterative values from the default setting. See Table 8.

Parameter	Description
Use This Detector	Select the check box to enable the currently installed detector.
Installed Probe Type	Indicates the installed probe type. For an ISQ EC MS, the only choice is HESI, for an ISQ EM MS, the choices are HESI and APCI.
Method Source Type	Set this to the source type for the method you are developing. This does not need to be the installed source type, although you can only run methods for the installed source type.
More Robustness – More Sensitivity	Selects whether more sensitivity or more robustness is desired.
Less Volatile Mobile Phase – Highly Volatile Mobile Phase	Slider is used to select whether the mobile phase is volatile or nonvolatile
Thermally Stabile Analyte – Thermally Labile Analyte	Slider is used to select whether analyte is stable or labile (unstable).
Total Pump Flow	Amount of liquid that flows from the LC (mL/min)
Instrument Flow	Percentage of the total pump flow that goes to the MS. This can be changed by using the Split Flow parameter in Instrument Configuration.

Table 8: HESI Source parameters: Easy view
Parameter	Description
Use This Detector	Select the check box to enable the currently installed detector.
Installed Probe Type	Indicates the installed probe type. For an ISQ EC MS, the only choice is HESI, for an ISQ EM MS, the choices are HESI and APCI.
Method Source Type	Set this to the source type for the method you are developing. This does not need to be the installed source type, although you can only run methods for the installed source type.
More Robustness – More Sensitivity	Selects whether more sensitivity or more robustness is desired.
Less Volatile Mobile Phase – Highly Volatile Mobile Phase	Slider is used to select whether the mobile phase is volatile or nonvolatile
Thermally Stabile Analyte – Thermally Labile Analyte	Slider is used to select whether analyte is stable or labile (unstable).
Ionic Analyte in Mobile Phase – Non-Ionic Analyte in Mobile Phase	Slider is used to indicate if analytes are ionized in the mobile phase.
Total Pump Flow	Amount of liquid that flows from the LC (mL/min)
Instrument Flow	Percentage of the total pump flow that goes to the MS. This can be changed by using the Split Flow parameter in Instrument Configuration.

Table 9: APCI Source parameters: Easy view

The MS instrument method editor will look similar to Figure 80 below. The bottom pane is only available if fraction collection mode is selected in the instrument configuration.

2020Hees benchr	
Scans	Acquisition rate
Ear New May (a) In Factor Under	No bandro park with 18 = Corent score par park, 6 = Arguellon else 2.0 He
Tractor Collocation Crant Has 5	
Fraction Collection Channels Pane	

Figure 80: MS instrument method editor - Source settings, easy view

# 6.6.3 Method Editor—Source Settings, Advanced View

To make fine-tuned adjustments for the best optimization of the source parameters, the user can select the advanced view. This will carry over the set values from the easy mode. Using the easy mode default settings allows for a convenient starting point for optimization in the advanced mode. See Figure 81.

**TIP**—Once adjustments are made in the advanced view, if the user switches back to the easy settings, the closest slider values will be selected.

ISQEM-I	Mass Detecto	x									
				installed probe typ	e: APCI						
Use Use	this detector			Method source typ	HESI	~ (	) Easy 🛞 Advanc	bed			
Source	settings										
Vaport	zer temperatu	re:	117 'C Sheath	gas pressure:	28.8	psig					
lon tree	nafer tube tem	sperature:	300 °C Aux ge	e preseure:	3.2	peig					
Source	voitage post	tive ions:	3000 V Sweep	gas pressure:	0.5	peig					
Source	e voltage nega	ative ions:	2000 V								
Meth	od type: Sc	can mode	~ Transfer	scans							
Scans	5									E (	Groups
	Time (nin)	Scan Name	Mass List or Rance (amu)	Dwell or Scan Times (s)	SIM Widths (amu)	Ion Polarity	Spectrum Type	Source CID Voitage	Tube Lens Votage		Time Total Scan Orrom, Filter Time (s) Peak Width (s) Detector Gain
•	0.00	) test	100-300	0,4959		Positive	Centroid ~		LastTune		0.00 0.500 3.000 LastTune
•							Profile		LastTune		
Fracti	on Collec	tion Channels									
	Name	Scan Filter				Target M	ass (min) Target M	ass (max)		-	
•								_			

Figure 81: MS instrument method editor – Source settings, advanced view

Additional features of the advanced source settings are shown in Table 10 below.

Parameter	Description
Vaporizer temperature	Heat applied the auxiliary gas for desolvation. 0 °C – 550 °C
Ion transfer tube	Heat applied to the transfer tube at the source to aid in desolvation
temperature	and transmission. 150 °C – 400 °C
Sheath gas pressure	Primary gas flow for liquid nebulization. 0 psig – 80 psig
Aux gas pressure	Auxiliary heated gas that aids in desolvation. 0 psig – 15 psig
Sweep gas pressure	Counter-current gas flow at the sweep cone to improve robustness. 0 psig – 2 psig
Source voltage positive ions	HESI capillary voltage for positive ionization. 0 V – 8000 V
Source voltage negative ions	HESI capillary voltage for negative ionization -8000V – 0 V

Table 10: HESI source parameters: Advanced view

Parameter	Description
Vaporizer temperature	Heat applied the auxiliary gas for desolvation. 0 °C – 550 °C
Ion transfer tube	Heat applied to the transfer tube at the source to aid in desolvation
temperature	and transmission. 150 °C – 400 °C
Sheath gas pressure	Primary gas flow for liquid nebulization. 0 psig – 80 psig
Aux gas pressure	Auxiliary heated gas that aids in desolvation. 0 psig – 15 psig
	(Recommended range: 0 – 10 psig)
<b>6</b>	Counter-current gas flow at the sweep cone to improve robustness.
Sweep gas pressure	0 psig – 2 psig
Source current positive	APCI corona discharge needle current for positive ionization. 0 $\mu$ A –
ions	50 μA (Recommended range: 0 – 8 μA)
Source current negative	APCI corona discharge needle current for negative ionization. 0 $\mu$ A –
ions	50 μA (Recommended range: 0 – 8 μA)

Table 11: APCI source parameters: Advanced view

# 6.6.4 Method Editor—Scan Settings,

The basic mode scan table is designed to be minimalistic for easy method creation. To enter a full scan or selected ion monitoring (SIM) scan, simply enter the desired mass of interest and the preferred polarity. The scan name and Source CID values are optional (defaults to 0.0 V). Scan and dwell times are automatically calculated based upon the inputted acquisition rate. Enter the minimum peak width value and scans per peak desired, and the sampling rate will be calculated in Hz. If the minimum peak width value is unknown, adjust the values until the desired rate is selected. The sampling rate is applied to each scan line item entered in the scan table. See Figure 82.

攭 Instrument Method Wizard - ISQEM (Vanguish ISQ Family): ISQEM-Mass Detector	×
ISQEM-Mass Detector for ISQEM (Vanquish ISQ Family).	4
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Figure 82: Method Editor—Basic Mode

Parameters and descriptions of the method editor basic mode settings are in .

Parameter	Description
Scan name	The name of the compound being scanned
Mass list or range (amu)	The masses the system will scan. Full-scan mode: Start and end mass are separated by a dash. SIM mode: Individual masses or multiple values separated by a comma.
Ion Polarity	Indicates whether positive or negative ions are generated
Source CID voltage	Accelerates ions into the background gas to aid in desolvation. Can increase sensitivity or reduce noise for some analytes. Range: 0-100 V, default: 0 V (no source CID)
Transfer scans	Select button to transfer scan information typed in Basic Mode to Scan Mode

Table 12: Scan parameters: Basic Mode

Parameter	Description
Name	The name of the channel for fraction collection
Scan Filter	Based on the scan information entered into the Scans pane
Target Mass (min)	The minimum mass scanned within the scans range
Target Mass (max)	The maximum mass scanned within the scans range
Table 12. Frantian a	allastian shannala nannnastana. Daois Mada

 Table 13: Fraction collection channels parameters: Basic Mode

# 6.6.5 Method Editor—Component Mode

The component mode offers advanced features over the basic mode and is designed for already defined methods where the analytes of interest are known. All scans entered in the table are SIM entries which correspond to a component. This table can be exported into the Chromeleon studio into a corresponding processing method. Likewise, a component table from the processing method can be imported into the instrument method scan table allowing the simplified method creation. In addition, users can also define the acquisition times based upon start and end times. Based on the start and end times, the instrument will optimize the dwell time for each SIM entry to maximize ion detection.

On the right pane, there are advanced options. Acquisition rates are still determined by the peak width and desired scan per peak entries, however, this value is now calculated into the corresponding scan/dwell times for the table. A single full scan is added to the method if the full scan check box is selected. Another feature of component mode is a dwell time priority feature that uses a multiplier to assign more or less dwell time to a certain component. Selecting **High** increases the dwell time of that ion by the High priority multiplier factor. This can improve the limit of quantitation (LOQ). Set confirming ions to **Normal** when the LOQ is less important. See Figure 83.

TIP—Minimizing overlapping acquisition times allows for best performance.



Figure 83: Method editor—Component mode

Parameters and descriptions of the method editor component mode settings are found in .

Parameter	Description				
Name	Description of the scan, perhaps the name of the compound being				
	scanneu				
Start time (min)	The time the system I	begins scanning			
End time (min)	The time the system s	stops scanning			
Mass	The mass the system	scans			
Ion polarity	Indicates whether po	sitive or negative ions are generated			
Spectrum type	Indicates whether the spectrum shown is profile or centroid. For SIM methods, select centroid mode only.				
Source CID voltage	Accelerates ions into the background gas to aid in desolvation. Can increase sensitivity or reduce noise for some analytes. Range: 0-100 V, default: 0 V (no source CID)				
Tube lens voltage	Voltage applied to tube lens after the ion transfer tube. $0 V - 300 V$ . Higher values can aid in desolvation. Lower values can reduce fragmentation. Can increase sensitivity or reduce noise for some analytes. Note: Use 0 to 300 V for positive ions. Use 0 to -300 V for negative ions. Use higher values for higher masses. If <b>Last Tune</b> is input, the tube lens will be run with the values stored in the tune file. <b>Last</b>				
Acquisition rate	Min. baseline peak width Desired Scans per	Minimum expected chromatographic peak width. Must be a positive number from 0.1 — 60 s Number of scans desired across the peak.			
	peak	Range is 1 – 20			

	÷			
	Acquisition Rate	Effective acquisition rate in Hz. Calculated automatically from Min. Baseline Peak Width and Desired Scans per Peak.		
Time summary				
Resulting total scan	The baseline peak width divided by the number of points desired			
time	across the peak.	· · · · · · · · · · · · · · · · · · ·		
SIM time	Total length of all SIN the total scan time u	A scans for each compound in the list. Equal to nless the method also contains a full scan event		
	Use full scan with	Specifies if full scan is to be added to		
	mass range	acquisition		
	Scan time	The time spent on the full scan event		
	Start time	The time the system begins scanning		
	Source CID	Accelerates ions into the background gas to aid in desolvation. Can increase sensitivity or reduce noise for some analytes. Range: 0-100 V, default: 0 V (no source CID)		
	Use last tune tube	Voltage applied to tube lens after the ion		
Full Scan	lens voltage	transfer tube. 0 V – 300 V. Higher values can aid in desolvation. Lower values can reduce fragmentation. Can increase sensitivity or reduce noise for some analytes. Note: Use 0 to 300 V for positive ions. Use 0 to -300 V for negative ions. Use higher values for higher masses. If <b>Last Tune</b> is input, the tube lens will be run with the values stored in the tune file. <b>Last Tune</b> is the standard way to		
Fraction Collection	Name	The name of the channel for fraction collection		
	Scan Filter	Based on the scan information entered into the Scans pane		
	Target Mass (min)	The minimum mass scanned within the scans range		
	Target Mass (max)	The maximum mass scanned within the scans range		
Acquisition Ontions	SIM Scan Widths	Set the SIM scan widths from 0.1 – 10 amu.		
Acquisition Options	Allow Dwell Time	Increases the dwell times for selected scans.		
	Prioritization	The choices for each scan are Normal or High.		
	High Priority Multiplier	If using a high dwell time prioritization, set the		
	multiplier			

Table 14: Scan Parameters—Component mode

# 6.6.6 Method Editor—Scan Mode

The most advanced method of entering scans, Scan Mode gives the user complete control over all relevant scan settings. Scans from basic and

component modes can be transferred to scan mode. Acquisition times are entered sequentially, where each new time entry defines the end of the previous scans and the start of the subsequent scans entries. The dwell or scan times can be entered manually, since they are completely defined by the user. SIM widths are also user settable unlike basic and scan modes. See Figure 84.



Figure 84: Method editor—Scan Mode

Please refer to Table 15 and Table 16 for more information on the scan mode settings.

Parameter	Description
Time (min)	The time the system begins scanning
Scan name	Description of the scan, perhaps the name of the compound being scanned
Mass list or range (amu)	The masses the system will scan. Full-scan mode: Start and end mass are separated by a dash. SIM mode: Individual masses or multiple values separated by a comma.
Dwell or scan times (sec)	SIM mode: the amount of time (in seconds) that the MS scans the SIM ion mass. Full-scan mode: determines the amount of time for each individual scan.
SIM widths (amu)	Sets the width range of the SIM column. 0.1 – 10 amu
Ion polarity	Indicates whether positive or negative ions are generated
Spectrum Type	Indicates whether the spectrum is in profile or centroid mode. For SIM methods, select centroid mode only.

Source CID voltage	Accelerates ions into the background gas to aid in desolvation. Can increase sensitivity or reduce noise for some analytes. Range: 0-100 V, default: 0 V (no source CID)
Tube lens voltage	Voltage applied to tube lens after the ion transfer tube. $0 V - 300 V$ . Higher values can aid in desolvation. Lower values can reduce fragmentation. Can increase sensitivity or reduce noise for some analytes. Note: Use 0 to 300 V for positive ions. Use 0 to -300 V for negative ions. Use higher values for higher masses. If <b>Last Tune</b> is input, the tube lens will be run with the values stored in the tune file. <b>Last Tune</b> is the standard way to run the tube lens.

Table 15: Scan mode parameters: Scans Pane

Parameter	Description		
Time (min)	Time that the MS begins to acquire this particular group of scans		
Total scan time (sec)	Sum of all the scans in each segment		
Chrom. filter peak width (sec)	Sets the peak width to match the width of the HPLC or IC peak		
Detector gain	Sets the detector gain to the one in the previous tune file or may be set manually		
Table 16: Scan mode parameters: Groups Pape			

 Table 16: Scan mode parameters: Groups Pane

Parameter	Description		
Name	The name of the channel for fraction collection		
Scan Filter	Based on the scan information entered into the Scans pane		
Target mass (min)	The minimum mass scanned within the scans range		
Target mass (max)	The maximum mass scanned within the scans range		
Table 17: Company and a parameters. Function Collection Champels Dans			

Table 17: Scan mode parameters: Fraction Collection Channels Pane

## 6.6.7 Method Development

Often, a method needs to be optimized for enhanced sensitivity or improved qualitative detection. Whether starting from a fresh method or transferring a protocol from a different system, it is important to take a diligent approach to obtaining the proper source and scan parameters. Some things to consider: mass-to-charge ratio, polarity, adduct formation, mobile phase composition, mobile phase flow rate, etc. It is always important to verify the m/z being detected versus assuming an  $[M+H]^+$  or  $[M-H]^-$  ion as there are many possible adduct formations. Polarity is another important consideration as some molecules favor protonation or deprotonation due to their chemistry, and can have significantly different responses for a given polarity.

All new methods, including method transfer, should start with a full scan to confirm the primary *m/z*. As the source on the ISQ EC and ISQ EM is different than other mass spectrometers, there could be a different profile of adducts or clusters being formed. It is always wise to start with a higher concentration to confidently detect and confirm your analyte of interest rather than starting low. For a quick analysis, an optional syringe drive pump can be paired with your MS and directly infused or teed into your mobile phase. As the sample is delivered, it can be monitored in real time using the Real Time Scan feature on the instrument ePanel. This allows you to quickly adjust scan and source settings on the fly without waiting on injection cycles or chromatography. Keep in mind, as the mass range of the full scan increases, the total ion counts/chromatogram (TIC) will increase as well, leading to a higher baseline. It can be more informative to have narrower mass ranges to start with rather than a scan over the entire mass range of the instrument.

Some methods require optimal sensitivity. There are many factors that can be optimized and will improve instrument sensitivity. Selected Ion Monitoring or SIM will give the best performance by increasing the number of analyte ions detected compared to a full scan. Source settings can improve both ionization and the efficiency of desolvation. These parameters are dependent on the application conditions, as solvent chemistry and flow rates have dramatic effects on performance. The instrument method editor offers the easy mode source settings that output good starting default values based upon flow rate. These values can then be adjusted based upon application particulars such as high aqueous or high organic content, sample matrix, and even analyte lability. Source parameters can also be adjusted using the Real Time Scan feature to quickly optimize and speed up method development. Some source settings are interdependent (temperature/auxiliary gas) and should be adjusted in conjunction. It is always better to make incremental adjustments versus optimizing each source setting to its maximum value one at a time.

# 6.6.8 MS Instrument Data Signal Channels

To monitor data acquisition in real time, go to the instrument console and select the filter tab. Up to eight filter channels can be selected and monitored in real time in the Chromeleon ISQ EC ePanel.

## 6.6.9 Custom Variables

The ISQ EC and ISQ EM support custom variables. The variables must match in the sequence and the method. See the Chromeleon Help for instructions on setting up custom variables in the instrument method.

# 6.6.10 Chromeleon Audit Trail

The Chromeleon audit trail will log numerous informational events for all of the modules in your instrument configuration. In the event of an error or warning, check the audit trail for more information.

# 6.7 Shutting Down the MS Instrument

If the instrument will not be operated for some time, follow the instructions on enabling standby for detector in this section.

# 6.7.1 Short-Term Standby

If the instrument is unused for a few days, allow it to remain connected to the system, and for the system to remain powered on.

To interrupt operation of the instrument for a short period (short-term shutdown), for example, overnight, observe these guidelines for the detector:

- Keep the instrument connected to the system flow path.
- Turn off the pump flow.
- If you operate the instrument from a chromatography data system, keep the detector connected to the data system.

When resuming operation, let the flow equilibrate and verify that the operating parameters for the other system modules are set as required before proceeding.

To set Smart Standby parameters, go to the Chromatography Studio and select Smart Standby. Set the standby parameters for the MS using the check boxes. See Figure 85.



Figure 85: Smart Standby Parameters

# 6.7.2 Long-Term Shutdown

Use the information in this section to prepare the system for high-level maintenance and repair.

Powering Off the Instrument

**TIP** Shutting down the mass spectrometer affects the operation of the system. When shutting down the MS, also observe the shutdown instructions for the other system modules and take appropriate action (refer to the *Operating Manuals* for the modules).

To power off, follow the instructions below.

- Flush the system with an appropriate, pure solvent (minimum LC/MSgrade) that does not contain any salts. Make sure that residual sample components, impurities from the column, or buffers are completely removed from the detector.
- 2) Cool down the vaporizer.

- 3) Turn off the pump flow and then the gas flow:
  - a) Turn off the pump flow to the detector. Wait at least 5 minutes. During the waiting period, the detector drains any remaining mobile phase to waste.
  - b) Turn off the gas flow on the system.
  - c) Wait until the system pressure is down to zero before you continue.
  - d) Turn off the gas supply to the system.
- 4) Turn off the system with its main power switch.

#### Setting Smart Shutdown Parameters

To set Smart Shutdown parameters, go to the Chromatography Studio and select Smart shutdown. Set the shutdown parameters for the MS using the check boxes. See Figure 86.

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Figure 86: Smart Shutdown Parameters

Restarting the Mass Spectrometer

To restart the detector, follow these steps:

1) Prepare and restart the other modules in the system, following the instructions in the *Operating Manuals* for the modules.

- 2) Flush the components in the flow path before the detector before you connect the detector to the system flow path.
- 3) Verify that gas is supplied to the MS.
- 4) Turn on the instrument with its main power switch.
- 5) Before starting an analysis, let the system equilibrate and be sure that it is ready for operation.

#### Setting Smart Start Up Parameters

To set Smart Start Up parameters, go to the Chromatography Studio and select Smart Start Up. Set the start up parameters for the MS using the check boxes. See Figure 87.

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Figure 87: Smart Start Up Parameters

#### Using the Chromeleon Queue

You can set the post-run instrument state for the ISQ EC in the queue. In the Chromeleon Console, select **Queue**. In the **After Running the Queue** drop-down menu, select the action you want for the MS. See Figure 88.



Figure 88: Setting the MS state in the Chromeleon queue

# 6.7.3 Venting the Mass Spectrometer

Follow the procedure below to vent the mass spectrometer.

- 1) Disconnect the data system from the instrument in Chromeleon software.
- 2) Push the power button at the back of the instrument down to the off position to power off the mass spectrometer. See Figure 89.



*Figure 89: Powering off the mass spectrometer* 

- 3) Wait 5 minutes.
- 4) Loosen the vent valve knob inside the front door of the instrument next to the source housing. See Figure 90.



Figure 90: Venting the mass spectrometer

# 6.8 Remote Start Cable

Remote start cables are used with Hardware Inject Synchronization. This allows the autosampler or another modules to send a hardware signal to the MS to tell it to start acquiring at the beginning of a run. Hardware Inject Synchronization is optional and not used by default.

The MS includes an "LC/IC Start" port that can be used for hardware synchronization of the run start.



Figure 91: View of the LC/IC Start Port on the MS

The Start Port consists of a 6-pin mini DIN connector. The pins are used as described in Table 18.

Pin Number	Used for
1	Not Used
2	Not Used
3	Ground
4	Inhibit Ready Out
5	Ground
6	Remote Start In

Table 18: Correct use of connection pins

The MS default polarity is to start on an active low signal (pulled to ground to indicate start of run). In instrument configuration, this can be changed to active high. You must configure the autosampler or other modules to output the start signal with the same polarity. Be sure to set the duration of the start signal to 2 s or so.

## 6.8.1 Vanquish HPLC-Autosampler

- Remote start cable part number: 1R76396-1060 (grey cable)
- Connect to
  - MS LC/IC Start port

• Vanquish Autosampler **Dig I/O 1** port

## 6.8.2 UltiMate 3000

- Remote start cable part number: 1R76396-1061 (black cable)
- Connect to
  - MS LC/IC Start port
  - UltiMate AS Autosampler Digital I/O 4 port

### 6.8.3 AS-AP Autosampler

- Remote start cable part number: 1R76396-1062 (grey pigtail cable)
- Attach remote start cable to a 12-port phoenix connector (PN 923686, part of IC ship kit)
  - Wiring: MS <-> AS-AP
    - Pin 6 <-> Pin 10 (RLY 4, Port NO)
    - Pin 5 <-> Pin 11 (RLY 4, Port COM)
- Connect to
  - MS LC/IC Start port
  - AS-AP RLY port

# 6.8.4 Integrion Autosampler (no AS-AP)

- Remote start cable part number: 1R76396-1062 (grey pigtail cable)
- Attach remote start cable to a 12-port phoenix connector (PN 923686, part of IC ship kit)
  - Wiring: MS <-> Integrion
    - Pin 6 <-> Pin 3 (RLY 2, Port NO)
    - Pin 5 <-> Pin 2 (RLY 2, Port COM)
- Connect to

- MS LC/IC Start port
- Integrion **RLY** port

# 7 Maintenance and Service

This chapter describes the routine maintenance and the service procedures that the user may perform.

# 7.1 Introduction to Maintenance and Service

This chapter describes the routine maintenance and service and repair procedures that the user may perform.



Additional maintenance or service procedures must be performed only by service personnel certified by Thermo Fisher Scientific (for brevity, referred to as Thermo Fisher Scientific service personnel).

The instrument is designed for easy maintenance and service. The userserviceable parts can be accessed from the front. If not stated otherwise, the maintenance procedures do not require that you remove the mass spectrometer from the system.

# 7.2 Safety Guidelines for Maintenance and Service

When performing maintenance or service procedures, pay attention to the following safety guidelines:



Observe all warning messages and precautionary statements presented in section 2.3 Safety Precautions, page 23.



#### WARNING—High Voltage

High voltages are present inside the instrument that could cause an electric shock. Do not open the housing or remove protective panels unless the instrument is unplugged.



#### AVERTISSEMENT—Haute tension

Les hautes tensions présentes à l'intérieur de l'instrument peuvent provoquer un choc électrique. N'ouvrez le boîtier et ne retirez les panneaux de protection que si l'instrument est débranché.



#### WARNING—Escape of Hazardous Substances from Flow Connections

Flow and capillary connections can be filled with substances that can pose health risks. Solvent can spray when capillaries burst, slip out of their fittings, or are not properly tightened or when capillary connections are otherwise open.

- Wear appropriate protective equipment and follow good laboratory practice.
- Before starting maintenance or repair procedures, flush out harmful substances with an appropriate solvent.



#### AVERTISSEMENT—Rejet de substances dangereuses par les raccords d'écoulement

Les raccords d'écoulement et les connexions capillaires peuvent contenir des substances susceptibles de constituer un risque pour la santé. Les solvants peuvent jaillir lorsque les capillaires éclatent, glissent hors des raccords ou ne sont pas correctement serrés, ou lorsque les connexions capillaires sont ouvertes.

- Portez un équipement de protection approprié et respectez les bonnes pratiques de laboratoire.
- Avant de démarrer les procédures d'entretien ou de réparation, éliminez les substances dangereuses avec un solvant approprié.



#### **CAUTION**—Spraying Solvent

Solvents can spray when under high pressure.

- Stop the pump flow prior to opening the flow path.
- Wait until the system pressure is down to zero.
- Wear appropriate protective equipment.



#### ATTENTION—Projections de solvant

Les solvants peuvent jaillir sous haute pression.

- Arrêtez la pompe avant d'ouvrir le circuit d'écoulement.
- Attendez que la pression du système redescende à zéro.
- Portez un équipement de protection approprié.

#### NOTICE—Detector Gas Flow and Pump flow

Improper handling of detector gas flow and pump flow start and stop can damage the detector. When turning on detector gas flow and pump flow, turn on the detector gas flow first, wait at least 5 minutes and only then turn on the pump flow.

# 7.3 General Rules for Maintenance and Service

For successful maintenance and service procedures, follow these rules and recommendations:

- Before starting maintenance or service procedures, shut down the instrument when instructed to do so.
- Use only the replacement parts specifically authorized and qualified for the detector by Thermo Fisher Scientific. For ordering information, see Section 10.3, page 217.
- Follow all instructions systematically and use the tools recommended for the procedure.
- Before opening the flow path to replace capillaries in the system, turn off the pump flow and wait until the system pressure is down to zero.
- Dirty components can contaminate the system. Contamination leads to poor performance of the modules and entire system or can even cause damage to the modules and system. Therefore:
  - Always wear appropriate gloves.
  - Place the components only on a clean, lint-free surface.
  - Keep your tools clean.
  - Use only lint-free cloth for cleaning.
- When disconnecting capillaries, protect open flow connections with plugs.

# 7.4 Routine and Preventive Maintenance

Optimum instrument performance, maximum uptime of the system, and accurate results can be obtained only if the instrument is in good condition and properly maintained.

# 7.4.1 Maintenance Plan

Perform the maintenance procedures in the table on a regular basis. The frequency given in the table is a suggestion. The optimum frequency for maintenance depends on several factors, such as the types and amounts of samples and solvents used with the detector.

Frequency	What you should do
Daily	Inspect the connections for signs of leakage or blockage.
Regularly	Inspect the connections for damage, such as cracks, nicks, cuts, or blockage.
	Check that all warning labels are still present on the detector and clearly legible. If they are not, contact Thermo Fisher Scientific for replacement.
	Check the drain tubes:
	<ul> <li>Check that the drain tubes properly connect to the drain ports on the bottom right side of the detector.</li> </ul>
	<ul> <li>Make sure that the tubes are unclogged and routed below the level of the drain ports.</li> </ul>
	<ul> <li>Check the volume of the liquid in the waste container.</li> <li>Empty the container as needed.</li> </ul>
	Check all electrical connections to ensure that they are properly seated.
Annually	Have Thermo Fisher Scientific service personnel perform preventive maintenance once a year.
	For details on the service interval, see section 7.4.2, page 174.

Frequency	What you should do
	Perform the gas filter replacement annually according to the service interval on the display.
	For details on the service interval, see section 7.4.2, page 174.
L	Table 19: Maintenance Frequency

**TIP** The mass spectrometer is just one component of an IC-MS or LC-MS system. To maintain optimal analytical performance, perform routine maintenance on each of the various system modules, such as pump, autosampler, etc.

# 7.4.2 Preventive Maintenance Schedule

The preventive maintenance features of the detector provide information about internal parameters and service intervals.

If a date is expired, it appears in red.

# 7.4.3 Cleaning or Decontaminating the Instrument

Cleaning and decontamination must be performed by qualified personnel wearing suitable personal protective equipment. Always observe national and local regulations.

**NOTICE** Wipe up all liquids spilled onto the system immediately. If surfaces are exposed for longer periods, these liquids can cause damage.

#### Decontamination

Decontamination is required, for example, when leakage or spillage has occurred, or before service or transport of the detector. Use a suitable cleaning detergent or disinfectant to ensure that the treatment renders the detector safe to handle. Parts required

- Suitable cleaning detergent (or disinfectant)
- Purified water
- Lint-free cloths or wipes



CAUTION—Explosive Gas Mixtures from Alcoholic Cleaning Detergents

Alcohol-containing cleaning detergents may form flammable and explosive gas mixtures when exposed to air.

- Use such cleaning detergents only when required and only in adequately ventilated rooms.
- Avoid open flames or exposure to excessive heat during the cleaning process.
- Wipe the cleaned components thoroughly dry after cleaning. Do not operate the detector before it is completely dry.



ATTENTION—Mélanges gazeux explosifs provenant des détergents de nettoyage à base d'alcool

Les détergents de nettoyage à base d'alcool peuvent former des mélanges gazeux explosifs et inflammables lorsqu'ils sont exposés à l'air.

- N'utilisez ce type de détergents qu'en cas de nécessité et uniquement dans des pièces suffisamment ventilées.
- Lors du nettoyage, évitez les flammes nues ou l'exposition à une chaleur excessive.
- Après le nettoyage, essuyez soigneusement tous les composants nettoyés. N'utilisez pas le détecteur tant qu'il n'est pas complètement sec.

**NOTICE** Observe the following:

- Only use cleaning detergents that will not damage the surfaces of the system.
- Never use sharp tools or brushes for cleaning any surfaces.
- Do not use sprays for cleaning.
- Prevent cleaning detergent from entering the flow path.
- Do not use excessively wetted cloth or wipes for cleaning. Prevent any liquids from entering the functional components of the detector. Liquids can cause a short circuit when getting in contact with the electronic components.

#### Preparations

Turn off the power to the mass spectrometer and disconnect the power cord from the power source.

#### Follow these steps

- Wipe the surfaces clean with a clean, dry, soft, lint-free cloth or wipe. If necessary, slightly dampen the cloth or wipe with a solution of lukewarm water and a suitable cleaning detergent.
- 2) Allow the cleaning detergent to react as recommended by the manufacturer.
- 3) Wipe the cleaned surfaces with purified water to ensure that all cleaning detergent residues have been removed.
- 4) Wipe the surfaces dry using a soft, lint-free cloth or wipe.

## 7.4.4 Replacing the ESI Probe Capillaries for the ISQ EC and ISQ EM

Follow the instructions in this section to replace the probe capillaries.



#### CAUTION—Eye Damage

Please be sure to wear protective eyewear during the probe replacement procedure due to exposure to elevated levels of nitrogen gas originating from the source housing.



#### ATTENTION—Lésions oculaires

Lors de la procédure de remplacement de la sonde, veillez à porter des lunettes de protection pour éviter d'être exposé aux niveaux élevés d'azote du boîtier de la source.



#### **CAUTION**—Excessive Heat

Turn off the probe temperature prior to capillary replacement and allow at least 5 minutes for cool down prior to capillary removal. Failure to do so may result in physical injury.



#### ATTENTION—Chaleur excessive

Avant de retirer le capillaire pour le remplacer, désactivez le chauffage de la sonde, puis laissez-la refroidir au moins 5 minutes. Le non-respect de cette consigne peut entraîner des blessures corporelles.

**NOTICE** Be sure to wear gloves during the probe replacement procedure in order to avoid contamination of the capillary and ESI probe assembly.

Please follow the following procedure in the event that the probe must be replaced.

- 1) Follow all safety precautions as outlined above and in the Safety section of this manual.
- 2) Stop all automated runs and batch sequences.

- 3) Turn gas flows down to standby state prior to cooling probe.
- 4) Turn-off probe temperature and allow a minimum of 5 minutes to cool down the probe.
- 5) Verify probe temperature on Chromeleon ePanel.
- 6) Stop liquid flow of the front-end chromatograph.
- 7) Open the front door and top-hatch of the MS instrument.
- 8) Disconnect the PEEK capillary going from the probe to the grounding union as shown in Figure 100.
- 9) Locate the black plastic knob of the ESI probe assembly and slowly turn counter-clockwise to remove from the source spray chamber housing as shown in Figure 100.



Figure 92: Removal of ESI probe assembly

**TIP** The source chamber housing does not need to be removed in order to replace the probe assembly.

**IMPORTANT** As the ESI probe assembly is removed from the source chamber housing, there will be an audible sound along with a physical change as nitrogen gas escapes into the atmosphere.

10) To remove the capillary from the ESI probe assembly, it will be necessary to push down on a spring-loaded retaining knob, while at the same time removing the probe capillary by turning the PEEK knurled fitting counter-clockwise as shown in Figure 100.





Figure 93: Removing the capillary from the ESI probe assembly

**TIP** The old probe is made out of stainless steel and will be discolored from previous use under high temperature conditions. This is normal.

- 11) Place the old probe aside and replace with a new probe that ships in the instrument accessory kit.
- 12) During replacement, it is important to carefully thread the capillary back into the ESI assembly body.
- 13) Hand-tighten the probe to where the capillary barely protrudes from the probe as shown in Figure 1Figure 94.
- 14) Adjust the protrusion depth of the capillary by turning the PEEK knurled fitting until the spray probe tip aligns with the top hash mark on the source housing and the needle aligns with the second hash



mark. The correct adjustment is shown in Figure is shown in Figure 94.

Figure 94: Capillary assembly alignment marks on source housing

15) Once the length is correctly adjusted, lock the needle in place by turning the top of the probe so it lines up with the square in the spring on the spray probe. See Figure 95.



Figure 95: Correct needle adjustment

16) Align the pin on the capillary assembly with the slot in the source housing and screw the needle in place. See Figure 96.


Figure 96: Aligning the pin on the spray probe with the source housing

17) Screw the probe into the source housing and reconnect the liquid line.

**TIP** There can be some variation between electrospray needles and spray probes. A ¼ turn in or out from the pictured penetration could be correct, depending on the tolerances of the probe itself. If the beam is unstable, try both directions.

## 7.4.5 Replacing the APCI Probe Capillaries for the ISQ EM

Follow the instructions in this section to replace the APCI probe capillaries.



## CAUTION—Eye Damage

Please be sure to wear protective eyewear during the probe replacement procedure due to exposure to elevated levels of nitrogen gas originating from the source housing.



### ATTENTION—Lésions oculaires

Lors de la procédure de remplacement de la sonde, veillez à porter des lunettes de protection pour éviter d'être exposé aux niveaux élevés d'azote du boîtier de la source.



### **CAUTION**—Excessive Heat

Turn off the probe temperature prior to capillary replacement and allow at least 5 minutes for cool down prior to capillary removal. Failure to do so may result in physical injury.



### ATTENTION—Chaleur excessive

Avant de retirer le capillaire pour le remplacer, désactivez le chauffage de la sonde, puis laissez-la refroidir au moins 5 minutes. Le non-respect de cette consigne peut entraîner des blessures corporelles.

**NOTICE** Be sure to wear gloves during the probe replacement procedure in order to avoid contamination of the capillary and ESI probe assembly.

Please follow the following procedure in the event that the probe must be replaced.

- 1) Follow all safety precautions as outlined above and in the Safety section of this manual.
- 2) Stop all automated runs and batch sequences.
- 3) Turn gas flows down to standby state prior to cooling probe.
- 4) Turn-off probe temperature and allow a minimum of 5 minutes to cool down the probe.
- 5) Verify probe temperature on Chromeleon ePanel.
- 6) Stop liquid flow of the front-end chromatograph.
- 7) Open the front door and top-hatch of the MS instrument.



8) Disconnect the PEEK capillary going from the probe to the grounding union as shown in Figure 97.

Figure 97: Disconnecting PEEK capillary connection of source at grounding union

9) Locate the black plastic knob of the APCI probe assembly and slowly turn counter-clockwise to remove from the source spray chamber



housing as shown in Figure 98.

Figure 98: Removal of APCI probe assembly

**TIP** The source chamber housing does not need to be removed in order to replace the probe assembly.

**IMPORTANT** As the APCI probe assembly is removed from the source chamber housing, there will be an audible sound along with a physical change as nitrogen gas escapes into the atmosphere.



10) To remove the capillary from the APCI probe assembly, loosen the top of the APCI probe with a 3/8" wrench. See Figure 99.

Figure 99: Loosening the nut on the APCI probe

11) Use 3/16" wrench to loosen the nut and then unscrew the PEEK fitting. See Figure 101.



Figure 100: Removing the capillary from the APCI probe assembly

12) Remove the PEEK fitting. See Figure 101.



Figure 101: Removing the PEEK fitting

 Remove the capillary and clear ferrule from the stainless-steel nut. See Figure 102.



Figure 102: Removing the clear ferrule and PEEK capillary

- 14) Discard the used silica tubing and install new silica tubing cut to the length of the probe.
- 15) Add the clear ferrule and reinsert the PEEK capillary until it bottom into the stainless steel nut.
- 16) Use the 3/16" wrench to tighten the PEEK fitting.
- 17) Reinsert the capillary into the APCI probe and tighten it with the 3/8" wrench.
- 18) During replacement, it is important to carefully thread the capillary back into the APCI assembly body. See



Figure 103: Threading capillary assembly into APCI probe

19) Align the pin on the APCI probe assembly with the slot in the source housing and screw the probe in place. See Figure 104.



Figure 104: Aligning the pin on the APCI probe with the source housing

20) Screw the probe into the source housing and reconnect the liquid line.

## 7.4.6 Replacing the APCI Needle

Follow the steps below to replace the APCI needle.

- 1) Follow the instructions for removing the APCI probe in Section 7.4.5.
- 2) Ensure the APCI needle is down so that it can be accessed. See Figure 105.



Figure 105: Locating the APCI Needle

3) With gloved hands, pull the APCI needle out of the source housing and install a new needle. See Figure 106.



Figure 106: Removing and reinstalling the APCI needle

4) Reinstall the source housing as detailed in Section 7.4.6985.5.5.

## 7.4.7 Cleaning the Front Optics

Follow the procedure below to remove and clean the front optics of the ISQ EC and ISQ EM mass spectrometers.

- 1) Turn the power off on the mass spectrometer. See Section 6.7.2.
- 2) Vent the mass spectrometer. See Section 6.7.3.
- 3) Allow the ion transfer tube to cool to a safe temperature.
- 4) Remove the six source housing screws as shown in Figure 107.



Figure 107: Removing source housing screws

5) Use a 2.5 mm hex key to gently screw in the three set screws as shown in Figure 108: Screwing in the set screws. The set screws will push the cone assembly out of the instrument



Figure 108: Screwing in the set screws

6) The cone should move out enough to break the internal seal. Once that occurs, remove the cone and front optics by hand. See Figure 109: View of front optics with seal broken



Figure 109: View of front optics with seal broken

 Set in on a piece of aluminum foil or other sterile surface. See Figure 110.



Figure 110: View of removed optics

8) Remove the ion transfer tube. See Figure 111: Removing the ion transfer tube.



Figure 111: Removing the ion transfer tube

9) Remove the three screws that hold the Q00/L0 assembly to the PEEK piece. Then remove the Q00/L0 assembly. See Figure 112.



*Figure 112: Removing the Q00/L0 assembly* 

10) Insert the pegs on the LO removal tool (included in the accessory kit) into the two holes on LO. See Figure 113: LO with removal tool in place.



Figure 113: L0 with removal tool in place

11) Turn LO using the tool until the rectangular slots line up with the beryllium-copper fingers. Turn the Q00/LO assembly upside down, and LO should come off the assembly. See Figure 114: LO separated from assembly.



Figure 114: LO separated from assembly

12) Using your thumb, push on the tapered side of Q00 to remove it from the cage holding it. See Figure 115: Removing Q00 from cage assembly. This step takes a fair bit of force. Do not drop Q00.



Figure 115: Removing Q00 from cage assembly

 Q00 and L0 should now be separate from the cage assembly. See Figure 116.



Figure 116: Q00 and L0

14) Using a small Allen key, unscrew the PEEK piece between the jumper wires. Remove the piece. See Figure 117



Figure 117: Removing the PEEK piece between the jumper wires

15) Very carefully unplug the two jumper wires that connect to the skimmer and tube lens. See Figure 118: Removing the Jumper Wires.



Figure 118: Removing the Jumper Wires

16) Press on the electrical pin through the hole where the first jumper wire was just unplugged to remove the skimmer cone. All that holds the skimmer cone in place are the Q00 assembly and its electrical connection, so if you unplugged the wire in the previous step, it should just take a little bit of force to remove it. See Figure 119.



Figure 119: Removing the Skimmer Cone

17) Remove the three screws holding the tube lens in place. To remove the tube lens, press on the electrical pin through the second hole where the jumper was unplugged using a tool like an Allen wrench. See Figure 120.



Figure 120: Removing Tube Lens Screws

18) Now you should have removed all of the optics for cleaning. See Figure 121: Optics parts.



Figure 121: Optics parts

- 19) To clean the optics:
- a. Using water and Liquinox, scrub the optics using a soft toothbrush.
- b. Sonicate the optics in water and Liquinox for 5 to 10 minutes.
- c. Rinse the optics parts using 18  $M\Omega$  or Optima LCMS grade water.
- d. Sonicate the optics parts in 18  $M\Omega$  or Optima LCMS grade water for 5 to 10 minutes.
- e. Rinse the optics parts using Optima LCMS grade methanol.
- f. Sonicate the optics parts in Optima LCMS grade methanol.
- g. Blow the optics parts dry with nitrogen gas.
- h. Reverse the steps above to reassemble the optics and reinstall the assembly into the MS.

## 7.5 Removing the Instrument from the System Stack



### CAUTION—Heavy Load, Bulky Device

The instrument is too heavy or bulky for one person alone to handle safely. A minimum of two people are required to lift the instrument from the shipping crate to the lab bench. To avoid personal injury or damage to the instrument, observe the following guidelines:

- Physical handling of the instrument, including lifting or moving, requires a team effort of two persons.
- A team effort is in particular required when lifting the instrument into the system stack or when removing it.
- To lift or move the instrument, grasp the instrument by the sides. Do not move or lift the instrument by the front bezel. This will damage the bezel or the instrument.



### ATTENTION—Charge lourde, appareil volumineux

L'instrument est trop lourd ou encombrant pour être soulevé ou déplacé par une personne seule. Au moins deux personnes doivent le soulever pour le transférer de la caisse d'expédition à la paillasse. Pour éviter les blessures et les dommages à l'instrument, respectez les consignes suivantes :

- Deux personnes sont nécessaires pour manipuler physiquement l'instrument, notamment pour le soulever et le déplacer.
- Ce travail d'équipe est tout particulièrement nécessaire pour soulever l'instrument et l'installer sur l'empilage du système ou pour l'en retirer.
- Pour soulever ou déplacer l'instrument, saisissez-le par les côtés. Ne saisissez pas l'instrument par le cadran frontal pour le soulever ou le déplacer. Vous risqueriez d'endommager le cadran ou l'instrument.

**NOTICE** Make sure that you do not pull on any tubes, capillaries or cables of the other system modules when you remove the detector from the stack.

Follow these steps

- 1) *If applicable:* Remove any modules that stand on top of the detector in the system stack.
- 2) Remove the mass spectrometer from the system stack. The following steps require a team effort:
  - a) Take the mass spectrometer on both sides and lift it slightly.
  - b) Grasp the mass spectrometer from below and lift it from the stack.
  - c) Place the mass spectrometer on a clean and stable surface.

## 7.6 Updating the Mass Spectrometer Firmware

The mass spectrometer is shipped with the most recent firmware version.

To update the instrument firmware, a chromatography data system, such as the Chromeleon Chromatography Management System, is required. The following update description refers to the Chromeleon software.

When				
	Updating the instrument firmware might be required, for example, when a new firmware version is released that adds functionality or solves problems of a previous version.			
Items required				
	Firmware version/Chromeleon Service Release as appropriate			
	<b>TIP</b> When a new firmware version is released, the new version will be included in the next available Chromeleon Service Release. The new firmware will <i>not</i> be transferred automatically to the device when you install the Chromeleon Service Release.			
Preparations				
	<ul> <li>Read the release notes provided with the firmware and/or Chromeleon Service release.</li> </ul>			
	<ul> <li>Verify the following:</li> </ul>			
	• The instrument is connected in Chromeleon.			
	<ul> <li>All operations on the instrument (Chromeleon 7) or timebase (Chromeleon 6.8) that includes the mass spectrometer have been stopped. The instrument or timebase is idle.</li> </ul>			
Check the currently installed fir	mware version in the instrument:			

• On the Main Menu of the instrument display

-or-

 On the General tab page in the Chromeleon 7 Instrument Configuration Manager or the Chromeleon 6.8 Server Configuration program

### Follow these steps

- 1) Start the Chromeleon 7 Instrument Configuration Manager or the Chromeleon 6.8 Server Configuration program.
- 2) Perform a firmware update from the **General** tab page in the configuration dialog box for the mass spectrometer. For details, refer to the *Chromeleon Help*.

**NOTICE** A firmware downgrade or incomplete firmware update may result in loss of functionality or malfunctioning of the mass spectrometer.

- Do not interrupt communication between the Chromeleon software and the MS at any time during the procedure.
- At the beginning of the update process, a message appears showing the firmware version currently installed in the detector and the version that will be transferred from the Chromeleon software. If the firmware installed in the detector is a later version than the version in Chromeleon, cancel the download.

The firmware update may take several minutes.

- Monitor the Audit Trail of the Chromeleon Instrument Configuration Manager (or Server Configuration program) to see whether the firmware update was successful or failed.
- If the firmware update failed, turn the device off and on again and repeat the firmware update.
- If the firmware update fails repeatedly, contact Thermo Fisher Scientific Technical Support for assistance.
- 3) After a successful firmware update, requalification of the instrument may be required. See the release notes for a recommendation.

## 8 Troubleshooting

This chapter is a guide to troubleshooting issues that may arise during operation of the instrument.

## 8.1 General Information about Troubleshooting

The following features help you to identify and eliminate the source for problems that may arise during operation of the instrument.

If you are unable to resolve a problem following the instructions given here or if you experience problems that are not covered in this section, contact Thermo Fisher Scientific Technical Support for assistance. See the contact information at the beginning of this manual.

To facilitate device identification have the serial number and technical name available when communicating with Thermo Fisher Scientific.

#### Status Indicator on the Instrument Display

The instrument display provides an overview of the instrument status. If no warnings are active, the **Status** is **Normal**.

### Troubleshooting Check

If a problem occurs with the instrument, performing a troubleshooting check helps identifying and isolating the cause of the problem.

#### Warning and Error Codes

If a problem occurs during operation of the detector, a warning or error code and a message on the detector appear. Certain soft key functions become available. Depending on the severity of the code, a running sequence is continued or interrupted.

**TIP** If you operate the instrument from a chromatography data system, the problem is also reported to the software and a message appears in the audit trail of the software. In case of Chromeleon, a related message for the problem appears in the Chromeleon Audit Trail.

### **Operating Issues**

Leaks are a potential safety issue. Therefore, if a leak sensor detects leakage, beeping starts to alert you beeping starts to alert you in addition to the warning code and a message on the display. Follow the instructions in this manual to find and eliminate the source for the leakage.

For information on all operating issues that may occur and affect detector performance, see Chapter 6, "Operation."

**TIP** The **Diagnostics** screen provides helpful information for troubleshooting if a problem occurs in the mass spectrometer. If other values are subject to fluctuations or outside of a range, contact

Technical Support.

## 8.2 Troubleshooting Problems with Autotune

Use Table 20 below to diagnose and solve problems with Autotune.

Symptom	Cause		
Autotune fails at beginning	Chromatograph not set to 50 $\mu L/min.$ If there is no liquid flow from the chromatograph to push the calibrant into the ion source, the autotune will fail.		
Autotune runs for a while but then fails	Chromatograph not set to 50 $\mu$ L/min. If the calibrant is pushed to the ion source more quickly, the loop will run out before the instrument refills it. If it is pushed too slowly, the electrospray may not be stable.		
Autotune runs for a while but then fails	If the system is failing autotune with a message that the spray stability check has failed, check the liquid connections for leaks.		
Autotune runs for a while but then fails	An incorrectly adjusted electrospray needle. Adjust electrospray needle.		
Autotune runs for a while but then fails	The flow rate out of the liquid pump is unstable. AXP pumps in particular require high back pressures to provide a stable flow. When using an AXP pump, backpressure coils should be installed between the pump and the instrument to allow the pump to run at a stable flow rate.		
Reference solution not flowing down the drain during fill time	Out of calibrant. Replace the calibrant bottle.		
Reference solution not flowing down the drain during fill time	Green PEEK tube in the bottle may be above the liquid level. Adjust the position of the tubing so it is near the bottom of the bottle. It should not touch the bottom or it may pick up particulates and clog the tubing.		
Reference solution not flowing down the drain during fill time	No nitrogen to the instrument		
Reference solution not flowing down the drain or flowing too slowly during fill time	The clear plastic pressurization line, green PEEK, or calibrant loop may be kinked. Alternatively, the ferrules on the green PEEK tubing may be overtightened.		

Symptom	Cause
Reference solution not flowing down the drain or flowing too slowly during fill time	The small orifice on the top of the calibrant bottle may be clogged.
Reference solution does not stop flowing after fill time	The bottle is not depressurizing. The frit on the valve of the calibrant delivery system may be clogged. This valve is located on the gas control module under the main power supply inside of the instrument.
Reference solution does not stop flowing after fill time	The waste line may be inserted too far down the drain tube. This will cause the liquid to be siphoned from the bottle.

Table 20: Autotune problems

**TIP** If you are unable to resolve a problem following the instructions given here or if you experience problems that are not covered in this section, contact Thermo Fisher Scientific Technical Support for assistance.

## 8.3 Troubleshooting Leaky Source Gases

If the ISQ EC or ISQ EM is having problems with leaky source gases, try tightening the spray chamber pins.

- 1) Shut down and vent the instrument as described in Section 6.7.
- 2) Remove the source housing as described in Section 5.5.5.
- Check if the spray chamber pins are tight. If they are loose, use a T10 screwdriver to tighten the spray chamber guide pins as shown in Figure 122.



Figure 122: Tightening spray chamber pins

## **9** Specifications

This chapter provides the physical and performance specifications, including information about the materials used in the flow path of the detector.

## 9.1 Physical Specifications

The physical conditions of the detector are specified as shown below in Table 21.

Туре	Specification
Range of use	Indoor use only
Ambient temperature	15 – 35 °C
Ambient humidity	20 – 80% relative humidity (non-condensing)
Pollution degree	2
Power requirements	230 ± 10% or 120 +6% -10% V AC; 50/60 Hz, 15A
Overvoltage category	Н
Emission sound pressure level	<70 dB(A)
Dimensions (height x width x depth)	52 x 42 x 91 cm (20.5 x 16.5 x 36 in.)
Weight	Approx. 71 kg (156 lbs.)

Table 21: Physical Specifications of the ISQ EC and ISQ EM Mass Spectrometers

# 10 Accessories, Consumables and Replacement Parts

This chapter describes the standard accessories that are shipped with the detector and the accessories that are available as an option. This chapter also provides information for reordering consumables and replacement parts.

## **10.1** General Information

The instrument must be operated only with the replacement parts and additional components, options, and peripherals specifically authorized and qualified by Thermo Fisher Scientific.

Accessories, consumables, and replacement parts are always maintained at the latest technical standard. Therefore, part numbers are subject to change. If not otherwise stated, updated parts will be compatible with the parts they replace.

## 10.2 Ship Kit

The ship kit includes the items listed in the table. The kit content is subject to change and may vary from the information in this manual. See the content list included in the kit for the most recent information about the kit content at the time when the instrument is shipped. See Table 22 for a list of parts included in the ship kit.

ltem	Part Number	Quantity in shipment
	1R120590-6205	1
Waste bottle and tubing kit		
Waste bottle with stand		1
Tubing, source exhaust		10 ft.
Tubing, 1/4 in, FEP (nitrogen)		25 ft.
Tubing, foreline pump exhaust		10 ft.
Source exhaust 90° elbow connector	1R78001-0026	1
Cable, Ethernet cable from PC to instrument (15 ft.)	1R76396-0052	1
Fuse kit	1R120458-0001	1
Grounding union	1R76256-0090	1
Cotton tipped swabs	A0301-0200	1 pack
PEEK tubing, red, 1/16 in OD, 0.005 in ID (5 ft.)	1R76433-3006S	1
PEEK tubing, green, 1/16 in OD, 0.030 in ID (5 ft.)	1R76433-3007S	1
Nut, 1/4 in, brass	1R4038-0004	2
Ferrule, 1/4 in, back, brass	1R4039-0015	2
Ferrule, 1/4 in, front, brass	1R4039-0004	2
Fitting, fingertight, 1 piece	1R4034-0020	4
Fitting, fingertight, 2 piece	1R4034-0010	4
Replacement calibrant solution lid and tubing	1R120590-3002	1
Cable, remote start for Vanquish	1R76396-1060	1
Cable, remote start for UltiMate 3000	1R76396-1061	1
Cable, remote start for IC and other instruments	1R76396-1062	1
Gloves, clean nitrile, large	1R23827-0009	6
Gloves, clean nitrile, medium	1R723827-0008	6
Tool kit	1R120590-6203	1
Wrench, T10 hex key		1
Wrench, T20 hex key		1
Wrench, 2 mm hex key		1
Wrench, 2.5 mm hex key		1
Wrench, 1/4-5/16 open end		1
Wrench, 3/8-7/16 open end		1
Wrench, 1/2-9/16 open end		1
Driver, T10		1

Item	Part Number	Quantity in shipment
Driver, T25		1
Driver, Phillips		1
Tubing cutter, 1/16 PEEK		1
Tubing cutter, 1/8 plastic		1
Tubing cutter, large hose		1
Tool, ion transfer tube removal		1
Tool, lens 0 removal		1
Ion transfer tube	1R120590-4502	1
Power cable, foreline pump to instrument	1R96000-98161	1
USB 3.0 to Ethernet adapter	1R76322-0401	1
Spray Needle, HESI II	80000-60317	1
Foreline pump tray	1R7800-0032	1
Bulkhead, LC/IC Input, PEEK	1R4035-0600	1
Oil mist filter (connects to oil return kit)	1R76505-0037	1
Oil return kit (connects to oil mist filter)	1R76505-0022	1
Vacuum hose clamp, NW25	1R76505-2002	2
O-ring with centering ring, NW25	1R76505-2001	2
Hose adapter, NW25 to 1 in	1R76505-5004	2
Hose clamp, 21-38 mm	1R4120-0003	2
Sweep cone	1R120590-2041	1
Drain insert for spray chamber	1R120590-2144	1
ISQ EC/EM manual CD	1R120591-0010	1
ISQ EM with HESI/APCI source only		
Corona APCI Needle	70005-98033	1
Fused silica capillary, 150 μm x 88 mm	1R120590-3007	1

Table 22: Parts Included in Ship Kit
# **10.3 Replacement Parts**

The parts in the table below may be ordered and installed by the user. See Chapter 7, Maintenance and Service for information about installing the parts listed in Table 23.

Part Number	Description		
1R120590-4502	Ion Transfer Tube (spare included in installation kit)		
	PEEK Tubing and Fittings Kit		
	Grounding union (spare included in installation kit)		
	Fitting, Fingertight, 1 piece		
1R120590-6220	Fitting, Fingertight, 2 piece		
	PEEK Tubing, Green, 1/16 in. OD × 0.03 in. ID (5 ft.)		
	PEEK Tubing, Red, 1/16 in. OD × 0.003 in. ID (5 ft.)		
	Replacement Rubber Slit, Top Left Corner of Instrument		
80000-60317	Spray Needle, HESI II (spare included in installation kit)		
80000-60321	Spray Probe, HESI II		
1R120590-0032	HESI Spray Chamber (full assembly)		
1R120590-0024	HESI/APCI Spray Chamber Assembly (ISQ EM only)		
80000-60165	Spray Probe, APCI (ISQ EM only)		
1R76022-14633	Replacement Electron Multiplier (multiplier only)		
1R4035-0600	Bulkhead, LC/IC Input, PEEK		
1R76256-0090	Grounding Union (spare included in installation kit)		
1R120590-6221	Calibrant Valve Rotor Rebuild Kit		
1R120590-3002	Replacement Calibrant Solution Lid and Tubing		
1R76433-0060	Calibrant Valve Sampler Loop, 500 μL		
1R120590-6204	Calibrant Solution, 250 mL		

Part Number	Description			
	ISQ EC and ISQ EM Tool Kit			
	Wrench, T10 Hex Key			
	Wrench, T20 Hex Key			
	Wrench, 2 mm Hex Key			
	Wrench, 2.5 mm Hex Key			
	Wrench, 3/8 – 7/16 in. Open End			
	Wrench, 1/4 – 5/16 in. Open End			
	Wrench, 1/2 – 9/16 in. Open End			
1R120590-6203	Driver, T10			
	Driver, T20			
	Driver, T25			
	Driver, Phillips			
	Tubing Cutter, 1/16 PEEK			
	Tubing Cutter, 1/8 Plastic			
	Tubing Cutter, Large Hose			
	Tool, Ion Transfer Tube Removal			
	Tool, Lens 0 Removal			
1R120554-0010	Fan Filter, for Electronics Fan (Left Side)			
1R76475-5002	Fan Filter, for Turbomolecular Pump Fan (right side)			
1R120590-6063	Front Lower Bezel (with front LED board)			
1R120590-6064	ISQ EC Front Door			
1R120590-6085	ISQ EM Front Door			
1R120590-0007	Top Hatch			
1R120590-0021	Top Cover			
1R120590-0022	Right Side Cover			
1R120590-0023	Left Side Cover			
1R3814-110	O-ring, Vent Valve			
1R120590-6034	Source Drain With Spring			
1R120590-2041	Sweep Cone			
1R120590-2144	Drain Insert for Spray Chamber			

Part Number	Description		
	Nitrogen Fittings Rebuild Kit		
	Nitrogen Pressure Relief Valve		
	Nitrogen Bulkhead Fitting, One-touch		
	Tee, ¼ in., One-touch		
1K120590-6223	Tubing, ¼ in., FEP		
	Nut, ¼ in., Brass		
	Ferrule, ¼ in., Back, Brass		
	Ferrule, ¼ in., Front, Brass		
1R120590-6205	Waste Bottle and Tubing Kit		
	Waste Bottle with Stand		
10120500 6201	Tubing, Source Exhaust		
16120390-0201	Tubing, ¼ in., FEP (nitrogen)		
	Tubing, Foreline Pump Exhaust		
1R78001-0026	Source Exhaust 90 ° Elbow Connector		
	Communications Cable Kit		
	Cable, Shielded 10 Base-T Crossover, 15 ft.		
	Cable Remote Start for Vanquish		
1R120590-6226	Cable Remote Start for Ultimate 3000		
	Cable Remote Start for IC or other module		
	USB 3.0 to Gigabit Ethernet Adapter		
	Cable, Internal Ethernet Patch Cable, 15 in.		
1R120590-6040	Front Cone and Q00 Assembly		
1R120590-2071	Tube Lens		
1R120590-2215	Graphite Seal		
1R120590-6017	Q00 Assembly		
1R120590-6041	Front Receiver Assembly with Q0		
1R120590-6312	Wire, Q0 Jumper 1		
1R120590-6313	Wire, Q0 Jumper 2		
1R120595-0640	Board, Baffle Cone		
1R120590-2184	Bushing, Spray Chamber Cam Pin, Left-hand		

Part Number	Description			
1R120590-2185	Bushing, Spray Chamber Cam Pin, Right-hand			
1R120590-2092	Guide Pin, Spray Chamber			
1R76412-0110	Seal, Teflon 50 i.d.			
1R76412-0111	Seal, Teflon 77.65 i.d.			
1R120590-6066	Q0 Assembly			
1R120379-0001	Ion Detector Assembly with Electron Multiplier and Leads			
1R120590-2161	Top Glass cover			
1R120590-2178	Skimmer Cone			
1R76505-0022	Oil Return Kit (Connects to oil mist filter)			
70005-98033	Corona APCI Needle (ISQ EM only)			
1R120590-2809	APCI Needle Switch Knob (ISQ EM only)			
1R120590-6207	APCI Kit (ISQ EM only)			
1R120590-6208	APCI Spare Parts Kit (ISQ EM only)			
1R76505-0037	Oil Mist Filter (Connects to oil return kit)			
A0301-15101	Vacuum Pump Oil			
1R76505-3010	Foreline Pump			
	Foreline Pump Connection Kit			
	Tubing, turbo pump to foreline pump			
1R120590-6227	Hose clamp 21–38 mm			
	O-ring with centering ring, NW16			
	O-ring with centering ring, NW25			
	Vacuum hose clamp NW25			
	Hose adapter, NW25 to 1 in.			

Table 23: Spare Parts List

# **11 Appendix**

This chapter provides additional information about compliance.

# **11.1** Compliance Information

#### 11.1.1 Declarations of Conformity

CE Declaration of Conformity

The device has satisfied the requirements for the CE mark and is compliant with the applicable requirements.

#### **RoHS** Compliance

This product complies with the RoHS (Restrictions of Hazardous Substances) directives:

*European RoHS Directive* Directive on the restriction of the use of certain hazardous substances in electrical and electronic equipment

The CE mark on the device indicates that the product is compliant with the directive.

 China RoHS regulations
Measures for Administration of the Pollution Control of Electronic Information Products

One of following logos may be present on the device if applicable:



## 11.1.2 WEEE Compliance

This product is required to comply with the European Union's Waste Electrical & Electronic Equipment (WEEE) Directive 2002/96/EC. It is marked with the following symbol:



Figure 123: WEEE symbol

Thermo Fisher Scientific has contracted with one or more recycling or disposal companies in each European Union (EU) Member State, and these companies should dispose of or recycle this product. For further information, contact Thermo Fisher Scientific.

#### **11.1.3 FCC Compliance**

This equipment has been tested and found to comply with the limits for a Class A digital device, pursuant to part 15 of the U.S. FCC Rules.

These limits are designed to provide reasonable protection against harmful interference when the equipment is operated in a commercial environment. This equipment generates, uses, and can radiate radio frequency energy and, if not installed and used in accordance with the instructions, may cause harmful interference to radio communications. Operation of this equipment in a residential area is likely to cause harmful interference, in which case the user will be required to correct the interference at his expense.

### 11.1.4 Regulatory Compliance

Thermo Fisher Scientific performs complete testing and evaluation of its products to ensure full compliance with applicable domestic and international regulations. When the system is delivered to you, it meets all pertinent electromagnetic compatibility (EMC) and safety standards as EMC EN 61326-1:2013. Safety IEC 61010-1:2010, IEC 61010-2-010:2014, IEC 61010-2-081:2015. Restriction of Hazardous Substances Directive (2011/65/EU).

Changes that you make to your system may void compliance with one or more of these EMC and safety standards. Changes to your system include replacing a part or adding components, options, or peripherals not specifically authorized and qualified by Thermo Fisher Scientific. To ensure continued compliance with EMC and safety standards, replacement parts and additional components, options, and peripherals must be ordered from Thermo Fisher Scientific or one of its authorized representatives.

#### 11.1.5 Low Voltage Safety Compliance

This device complies with Low Voltage Directive 2014/35/EU and harmonized standard EN 61010-1:2001.

### **11.1.6** Notice on Lifting and Handling of Thermo Scientific Instruments

For your safety, and in compliance with international regulations, the physical handling of this Thermo Fisher Scientific instrument requires a team effort to lift and/or move the instrument. This instrument is too heavy and/or bulky for one person alone to handle safely.

### 11.1.7 Notice on the Proper Use of Thermo Scientific Instruments

In compliance with international regulations: Use of this instrument in a manner not specified by Thermo Fisher Scientific could impair any protection provided by the instrument.

### 11.1.8 Notice on the Susceptibility to Electromagnetic Transmissions

Your instrument is designed to work in a controlled electromagnetic environment. Do not use radio frequency transmitters, such as mobile

phones, in close proximity to the instrument. For manufacturing location, see the label on the instrument.

# 11.1.9 Manual Release History

Revision	Released	Covering
А	August 2017	ISQ EC MS
В	December 2017	ISQ EC MS
С	October 2018	ISQ EC MS; ISQ EM MS
D	December 2018	ISQ EC MS; ISQ EM MS
E	February 2019	ISQ EC MS; ISQ EM MS

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www.thermofisher.com

Thermo Fisher Scientific Inc. 168 Third Avenue Waltham Massachusetts 02451 USA

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