# ACQUITY UPLC I-Class IVD System Guide

715003736IVD / Revision C

# THE SCIENCE OF WHAT'S POSSIBLE."

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## **General Information**

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## Safety considerations

Some reagents and samples used with Waters instruments and devices can pose chemical, biological, or radiological hazards (or any combination thereof). You must know the potentially hazardous effects of all substances you work with. Always follow good laboratory practice, and consult your organization's standard operating procedures.

## Considerations specific to the ACQUITY UPLC I-Class IVD instruments

Warning: To avoid injury, if the ACQUITY UPLC I-Class IVD system must be relocated, drain and remove all liquids, including solvents and waste, from the system.



**Warning:** To avoid injury, if the ACQUITY UPLC I-Class IVD system must be relocated, disconnect the power cord and all cables.



Warning: To prevent incorrect reporting of results, verify proper sample vial placement and positioning against the sample list, prior to sample injection.

**See also:** For safety considerations regarding specific system modules, consult the appropriate information on the user documentation CD (part number 715003740IVD).

#### FCC radiation emissions notice

Changes or modifications not expressly approved by the party responsible for compliance, could void the users authority to operate the equipment. This device complies with Part 15 of the FCC Rules. Operation is subject to the following two conditions: (1) this device may not cause harmful interference, and (2) this device must accept any interference received, including interference that may cause undesired operation.

#### Canada spectrum management emissions notice

This class A digital product apparatus complies with Canadian ICES-001.

Cet appareil numérique de la classe A est conforme à la norme NMB-001.

## **Electrical power safety notice**

Do not position the instrument so that it is difficult to operate the disconnecting device.

### Safety hazard symbol notice

Documentation needs to be consulted in all cases where the A symbol is used to find out the nature of the potential hazard and any actions which have to be taken.

#### **Equipment misuse notice**

If the equipment is used in a manner not specified by the manufacturer, the protection provided by the equipment may be impaired.

#### Safety advisories

Consult Appendix A for a comprehensive list of warning and caution advisories.

## **Operating the ACQUITY UPLC I-Class IVD system**

When operating the ACQUITY UPLC I-Class IVD system, follow standard quality control (QC) procedures and the guidelines presented in this section.

#### **Applicable symbols**

Symbol	Definition
	Indicates the medical device manufacturer as defined in EU Directive 98/79/EC
EC REP	Indicates the authorized representative in the European Community
CE	Confirms that a manufactured product complies with all applicable European Community directives
ABN 49 065 444 751	Australia C-Tick EMC compliant

Symbol	Definition
c C used Us	Confirms that a manufactured product complies with all applicable United States and Canadian safety requirements
i	Consult instructions for use
	Electrical and electronic equipment with this symbol may contain hazardous substances and should not be disposed of as general waste. For compliance with the Waste Electrical and Electronic Equipment Directive (WEEE) 2012/19/EU, contact Waters Corporation for the correct disposal and recycling instructions.
IVD	For in vitro diagnostic use

### Audience and purpose

This guide is intended only for professionally trained and qualified laboratory personnel who install, operate, and maintain ACQUITY UPLC I-Class IVD system modules. It gives an overview of the system's technology and operation.

## Intended use of the ACQUITY UPLC I-Class IVD system



The Waters ACQUITY UPLC I-Class IVD system is CE-marked according to the European Union In Vitro Diagnostic Device Directive 98/79/EC.

The ACQUITY UPLC I-Class IVD system is a general purpose in vitro diagnostic instrument used to quantify and qualify of a wide variety of compounds in biological sample matrices. The system is intended to be used only by qualified operators.

## Calibrating

To calibrate LC systems, follow acceptable calibration methods using at least five standards to generate a standard curve. The concentration range for

standards should include the entire range of QC samples, typical specimens, and atypical specimens.

When calibrating mass spectrometers, consult the instrument's online Help system for instructions.

## **Quality control**

Routinely run three QC samples that represent subnormal, normal, and above-normal levels of a compound. If sample trays are the same or very similar, vary the location of the QC samples in the trays.

Ensure that QC sample results fall within an acceptable range, and evaluate precision from day to day and run to run. Data collected when QC samples are out of range might not be valid. Do not report these data until you are certain that the instrument performs satisfactorily.

You can use TargetLynx software to set quality parameters that incorporate a range of confirmatory checks to identify samples outside of user-specified or regulatory thresholds. See the TargetLynx Online help topic "QC Monitor properties." Data should also be manually inspected prior to the reporting of any results.

When analyzing samples from a complex matrix such as soil, tissue, serum/plasma, whole blood, and other sources, note that the matrix components can adversely affect LC/MS results, enhancing or suppressing ionization. To minimize these matrix effects, Waters recommends you adopt the following measures:

- Prior to the instrumental analysis, use appropriate sample pretreatment such as protein precipitation, liquid/liquid extraction (LLE), or solid phase extraction (SPE) to remove matrix interferences.
- Whenever possible, verify method accuracy and precision using matrix-matched calibrators and QC samples.
- Use one or more internal standard compounds, preferably isotopically labeled analytes.
- To ensure data integrity, Waters recommends you run QC samples before and after test samples within a single analysis. Additionally, you can periodically run known samples as unknowns to verify assay results for a single analysis.

### ISM Classification: ISM Group 1 Class B

This classification has been assigned in accordance with IEC CISPR 11 Industrial Scientific and Medical (ISM) instruments requirements. Group 1 products apply to intentionally generated and/or used conductively coupled radio-frequency energy that is necessary for the internal functioning of the equipment. Class B products are suitable for use in both commercial and residential locations and can be directly connected to a low voltage, power-supply network.

## EC authorized representative



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# 1 ACQUITY UPLC I-Class IVD System

The ACQUITY UPLC I-Class IVD system is a general purpose, in vitro, tool for quantifying and qualifying diverse compounds in biological sample matrices. The system is intended to be used by only highly qualified operators.

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## System components

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#### Major components of the ACQUITY UPLC I-Class IVD System:



The ACQUITY UPLC I-Class IVD system includes the following components:

- ACQUITY UPLC I-Class Binary Solvent Manager (BSM)
- ACQUITY UPLC I-Class Sample Manager Flow-Through-Needle (SM FTN)
- $50 \ \mu L \ extension \ loop \ for \ SM-FTN$
- Column Heater with active pre-heating (CH-A) and tubing
- · Column Heater (CH-A) extension kit for mass spectrometer
- Xevo TQ-S IVD mass spectrometer
- ACQUITY UPLC I-Class System Startup kit, including solvent tray module
- Leak sensors
- ACQUITY UPLC BEH C<sub>18</sub> column, 1.7 μm, 2.1 x 50 mm, IVD
- ACQUITY UPLC I-Class IVD system documentation CD, part number 715003740IVD
- Workstation and MassLynx, ACQUITY UPLC Console software, and Connections INSIGHT software
- FlexCart, optional

#### **Binary solvent manager**

The Waters ACQUITY UPLC I-Class IVD Binary Solvent Manager (BSM) delivers solvent compositions for isocratic and binary gradient methods at flow rates of between 0.01 and 2.0 mL per minute. Its features include in-line filters upstream of a primary check valve, the Waters<sup>®</sup> Intelligent Intake Valve ( $i^2Valve$ ), automated priming functions, and daily system-setup routines.

The design of the binary solvent manager is optimized for sub-2- $\mu$ m particle liquid chromatography. The upper pressure limit is set at 124,106 kPa (1241 bar, 18,000 psi) per pump. A maximum flow rate of 1 mL/min is permitted at system backpressures to 124,106 kPa (1241 bar, 18,000 psi), which falls within the range of optimal linear velocity for sub-2- $\mu$ m particle columns of ID 1.0 mm to 3.0 mm.

**See also:** The ACQUITY UPLC I-Class IVD Binary Solvent Manager Overview and Maintenance Guide (part number 715003739IVD) for more details.

#### Sample manager-flow through needle

The ACQUITY UPLC I-Class IVD Sample Manager - Flow Through Needle (SM - FTN) incorporates a flow-through-needle mechanism. The mechanism aspirates a sample from plates and vials and holds it in the sample needle in preparation for injecting the sample onto the column. The needle serves as part of the injection flow path when the sample is pushed onto the column.

A 50-µL extension loop (installed between the sample needle and the injection valve) can increase the injection volume beyond that of the sample needle.

The flow-through-needle mechanism operates similarly to most traditional HPLC systems.

**See also:** The ACQUITY UPLC I-Class IVD Sample Manager - Flow Through Needle Overview and Maintenance Guide (part number 715003737IVD) for more details.

#### Column heater with active preheater

The ACQUITY UPLC I-Class IVD column heater (CH-A) controls the column temperature independent of flow rate.

The column heater (CH-A) heats the column compartment to any temperature between 20 °C and 90 °C that is at least 5 °C above the ambient temperature. For example, if the ambient temperature is 25 °C, the range is 30 to 90 °C. A low dispersion, active preheating device heats the incoming solvent to match the temperature of the column before the solvent enters the column. The column compartment can accommodate columns of up to 4.6 mm I.D. and up to 150 mm length.

**See also:** The ACQUITY UPLC I-Class IVD Column Heater Overview and Maintenance Guide (part number 715003738IVD) for more details.

#### Xevo TQ-S IVD mass spectrometer

The Waters<sup>®</sup> Xevo<sup>®</sup> TQ-S is a tandem quadrupole, atmospheric-pressure ionization (API) mass spectrometer. Designed for routine HPLC/MS/MS and UPLC<sup>®</sup>/MS/MS analyses in quantitative and qualitative applications, it can operate at fast acquisition speeds compatible with UltraPerformance LC<sup>®</sup>.

**See also:** The Xevo TQ-S IVD Mass Spectrometry System Operator's Overview and Maintenance Guide for more details.

## **Column technology**

ACQUITY UPLC IVD columns are packed with sub-2- $\mu$ m, bridged, ethylsiloxane, hybrid or 1.8- $\mu$ m high-strength silica particles that can mechanically endure high-pressure conditions. The column hardware can withstand as much as 124,106 kPa (1241 bar, 18,000 psi). The column dimensions allow optimal MS-compatible flow rates, and matched outlet tubing minimizes the effect of extra-column volume.

#### eCord technology

ACQUITY UPLC columns include an eCord<sup>™</sup> column chip that tracks the usage history of the column. The eCord column chip interacts with the system software, recording information for as many as 50 sample queues run on the column. The eCord column chip provides documentation of the column used for each chromatographic run and records the following information:

- Number of injections onto the column
- Number of samples injected onto the column
- The highest pressure that the column has experienced (and the date)
- The highest temperature the column has experienced (and the date)

In addition to the variable column usage data, the eCord column chip also stores these fixed, column-manufacturing data:

- Unique column identification
- Certificate of Analysis
- QC test data

When you attach the eCord column chip to a receptacle on the column heater or column manager, information is automatically recorded by the system. No user action is required.

#### Software and data system

MassLynx software, which includes the TargetLynx<sup>™</sup> application manager, controls the mass spectrometer and analyzes, manages, and distributes its data.

You perform these procedures using the MassLynx software:

- Configuring the system
- Creating LC and MS/MS methods that define operating parameters for a run
- Tuning and mass calibrating the mass spectrometer automatically
- Running samples
- Monitoring the run
- Acquiring data
- Processing data
- Reviewing data
- Printing data

The ACQUITY UPLC Console is a software application that you use to configure settings, monitor performance, run diagnostic tests, and maintain the system and its modules.

Connections INSIGHT software monitors the system's operational characteristics. It securely transmits system usage, performance parameters, and diagnostic information to the Waters technical service team.

#### **Optional columns**

The standard column used with the ACQUITY UPLC I-Class IVD system is the ACQUITY UPLC BEH  $C_{18}$  column, 1.7 µm, 2.1 × 50 mm, IVD. The following additional columns may be used:

- ACQUITY UPLC BEH  $C_{18}$  column, 1.7 µm, 2.1 × 100 mm IVD
- ACQUITY UPLC BEH  $C_{18}$  column, 1.7 µm, 2.1 × 150 mm IVD
- ACQUITY UPLC HSS T3 column, 1.8 μm, 2.1 × 50 mm IVD
- ACQUITY UPLC BEH Phenyl column, 1.7 μm, 2.1 × 50 mm IVD

## Vials, plates, and seals

For information on vials, plates, and seals, refer to the following:

- Waters Autosampler Vials, Plates, and Seals for use with the ACQUITY UPLC Systems Family (part number 720004278).
- Sample Vials and Accessories (part number 720001818).

Note: All Waters plates meet ANSI/SBS standards.

## For additional information

On the system documentation CD, you can find this additional information about the ACQUITY UPLC I-Class IVD system (715003740IVD):

- ACQUITY UPLC I-Class IVD Binary Solvent Manager Overview and Maintenance Guide (part number 715003739IVD)
- ACQUITY UPLC I-Class IVD Sample Manager Flow Through Needle Overview and Maintenance Guide (part number 715003737IVD)
- ACQUITY UPLC I-Class IVD Column Heater Overview and Maintenance Guide (part number 715003738IVD)
- Xevo TQ-S IVD Mass Spectrometry System Operator's Overview and Maintenance Guide
- Controlling Contamination in Ultra Performance LC/MS and HPLC/MS Systems (part number 715001307)
- Additional helpful documents

# **2** Optimizing Performance

Follow the advice and guidelines in this chapter to help ensure optimum performance from your ACQUITY UPLC I-Class IVD system.

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## **General guidelines**

ACQUITY UPLC I-Class system guidelines differ from those governing standard HPLC practices primarily because a chromatography that uses small (less than 2  $\mu$ m) particles places certain constraints on the system. Chromatography performed on a UPLC system is of a much smaller-scale than that performed using an HPLC system, yet it gives a higher resolution. Moreover, analysis time for UPLC is shorter, and solvent and sample consumption are significantly reduced.

The ACQUITY UPLC I-Class chromatograph requires optimum performance from the sample manager because sample dispersion is more evident when using smaller columns. The reduction in chromatographic run time also makes efficient management of cycle time essential.

When performing fast UPLC analyses, note that a peak of interest can be less than 0.5 seconds wide. Waters recommends a sampling rate of 25 to 50 points across a peak, which provides good quantitation. Sampling rates faster than

#### 2 Optimizing Performance

20 points per second yield higher baseline noise, requiring you to adjust filter time constants accordingly.

The optimal ACQUITY UPLC flow rate differs from that of a typical HPLC column. The table below offers operating guidelines for ACQUITY UPLC columns under both isocratic and gradient conditions. Note that the values provided are approximations and that optimum performance for your molecule or separation can occur at a different flow rate.

Column size	Molecular weight	Flow rate
$2.1 \times 50 \text{ mm}$	<500	600 μL/min
$2.1 \times 50 \text{ mm}$	1000	300 µL/min
$2.1 \times 50 \text{ mm}$	1500	150 μL/min
$2.1 \times 50 \text{ mm}$	2000	100 µL/min

Optimal flow rates for molecular weight range:

Follow these general recommendations when performing a UPLC analysis:

- Use high quality solvents, buffers, and additives (MS-grade, prefiltered with a 2  $\mu m$  filter).
- Use high quality water (ultrapure, prefiltered with a 2  $\mu$ m filter).
- Always use solvent filters on tubing lines in solvent bottles.
- Filter buffers with a 0.2-µm filter membrane.
- Keep concentrated stock solutions, to use when preparing working solutions.
- Do not add fresh buffer to old, which can promote microbial growth.
- Make fresh buffer solutions daily.
- Do not block the degasser vent line. Trim the tubing, if necessary.
- Do not submerge the waste or degasser vent lines in liquid.

**See also:** For details about how to route the tubing, see the *ACQUITY UPLC I-Class IVD Binary Solvent Manager Overview and Maintenance Guide* (part number 715003739IVD.)

- Flush buffers from the system, using water, immediately after you are done with them.
- Use 10-20% organic solvent in water as a storage solvent, if you keep the system idle for extended periods (longer than 24 hours).

- Keep the seal-wash line primed.
- Prime solvent lines during system startup.
- Keep all solvent lines primed.
- Monitor the waste level, to ensure that it is never too high.
- When starting the binary solvent manager, ensure solvent flows through pump A and pump B. Do not specify a 0 mL/min flow rate at startup for either pump.
- Use the Load Ahead option when you desire a shorter cycle time and *only when* the conditions specified in the methods for two consecutive samples are identical.
- If you experience problems with carryover, do not use the Load Ahead or Loop Offline options while you are troubleshooting.
- When installing or removing a column, always hold the active preheater's reusable compression fitting in place. Rotate the column or optional in-line filter to install or remove it. Do *not* tighten using a wrench.

## Carryover

You observe carryover in chromatographic systems when a previously injected analyte appears as a peak in the chromatogram of subsequent samples. Carryover tends to occur when a small amount of analyte remains in the system after a sample is injected. You can measure carryover by observing analyte peaks that appear when you run a blank sample immediately after an analytical sample.

**See also:** For details about carryover performance, see Appendix B, "Specifications".

A common cause of carryover is inadequate washing of the system. Choosing an appropriate wash solvent can minimize carryover for a particular analysis. The wash solvent must be strong enough to dissolve any remaining sample and the wash duration must be long enough to remove the residue from the system.

Method conditions also affect carryover. Too short a hold-time at the final conditions of a gradient, especially if the gradient is steep, can fail to remove all analytes from the system. It is important to completely flush the system and reequilibrate the column before proceeding to a subsequent analysis. Use caution when choosing the Load Ahead and Loop Offline options. Initiating them before the highly organic part of the gradient reaches the needle can leave sample residue in the system. Thus you can forfeit to system downtime whatever time you gained using the options as you clean the system of the accumulated residue.

The hydrophobicity and solubility of samples are additional factors to consider when trying to minimize carryover.

**Tip:** Use additional valve cycles (actuate the valve) if you suspect that sample residue in the valve is causing carryover problems.

## Contamination

To minimize contamination, ensure cleanliness during sample preparation. For example, verify that sample preparation tools are cleaned thoroughly.

**See also:** Controlling Contamination in Ultra Performance LC/MS and HPLC/MS Systems (part number 715001307).

## Temperature

Waters recommends you set sample temperature limits when configuring a method in the data application. Always ensure that your temperature limits are set in accordance with your analysis method. (Refer to online Help for instructions.)

## Reproducibility

The precision (area reproducibility) is less than 0.5% RSD for injection volumes between 2.0 and 10.0  $\mu$ L (see Appendix B, "Specifications").

## Cycle time (between injections)

The short run time of a UPLC separation requires efficient use of the time between analyses.

The Load Ahead and Loop Offline options of the ACQUITY UPLC I-Class IVD SM-FTN help decrease cycle time. See the ACQUITY UPLC Console online Help for details on how to use these features.

**Caution:** To prevent the loss of sample, note that the Load Ahead option does not operate for the first injection of a sample set or for injection sets whose methods differ.

Consider these attributes of the Load Ahead option carefully before deciding to use it:

- Load Ahead is designed for two consecutive samples whose conditions, as specified in their respective methods, are identical. If you run consecutive samples for which different methods are specified, the first method will be applied to all samples aspirated.
- MassLynx software does not operate in Load Ahead mode across batches.

## **Preventing leaks**

Preventing leaks ensures that the system maintains adequate pressure and sample integrity throughout the analysis.

Leaks can potentially occur at any tubing connection, gasket, or seal but are most common at tubing connections. Low pressure leaks (on the intake side of the solvent manager's pump) cause solvent loss and air introduction during

the intake cycle. Leaks at high pressure fittings (downstream of the  $i^2Valves$ ) can leak solvent but do not introduce air.

To prevent leaks, follow Waters' recommendations for the proper tightening of system fittings. Note specifically that different techniques apply to retightening fittings versus installing them for the first time.

#### See also:

- The user documentation for the modules included in your system for more details on leak detection.
- The ACQUITY UPLC I-Class IVD Column Heater Overview and Maintenance Guide (part number 715003738) for details on connecting active preheaters.

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## Sample preparation

UPLC analysis places some additional restrictions on sample preparation.

### **Particulates**

The small column frit size  $(0.2 \ \mu\text{m})$  can become blocked more easily than larger HPLC column frits  $(2.0 \ \mu\text{m})$ . Particle-free mobile phase solvents and sample solutions are therefore essential for UPLC analysis. See "General guidelines" on page 23 for recommendations on choosing and handling solvents.

## Matching sample diluents

When you use the auto-dilution option on the SM-FTN, the purge solvent serves as the sample diluent. Ensure that your sample solution is soluble and miscible in your chosen purge solvent.

**Caution:** To avoid broad peaks and poor peak shape, ensure that your sample diluents match the initial conditions of your gradient.

# **3** Preparing the System

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## Preparing system hardware

### Powering-on the system

Powering-on the system entails starting the ACQUITY UPLC I-Class IVD system workstation, system modules, and MassLynx software. Each device or instrument beeps three times and runs a series of startup tests. See "Status LEDs" on page 30 and "Power LED" on page 30, for information on how to interpret indicator LED modes for device or instrument flow status and whether the units are powered-on.

**Tip:** The column heater is automatically powered-on when you power-on the sample manager.

For mass spectrometer power-on instructions, refer to the Xevo TQ-S IVD Mass Spectrometry System Operator's Overview and Maintenance Guide.

#### To power-on the system:

- 1. Power-on the ACQUITY UPLC I-Class IVD system's workstation.
- 2. Power-on the binary solvent manager and sample manager by pressing the power switch on the top, left-hand side of each devices' door.

**See also:** "Status LEDs" on page 30 and "Power LED" on page 30 for information on how to interpret LED modes for device or instrument flow status and whether the units are powered-on.

3. Start MassLynx software.

**Tip:** You can monitor the ACQUITY UPLC Console for messages and LED indications.

## Monitoring system module LEDs

LEDs on each system module indicate the module's state of functioning. The LEDs are specific to their modules, so the significance of their various colors and modes can differ from one module to another.

### **Power LED**

The power LED, on the left-hand side of a module's front panel, indicates the power-on or power-off status of the module. This LED is green when power is applied to the unit and unlit when power is not applied.

**Tip:** To provide adequate ventilation, the sample manager fans run continuously, even when the power switch is in the "off" position. These fans switch off only when you disconnect the power cable from the back of the module.

## **Status LEDs**

#### Flow LED (binary solvent manager)

The flow LED, on the right-hand side of the power LED on the binary solvent manager's front panel, indicates the flow status. A steady green flow LED indicates flow through the binary solvent manager.

#### Run LED (sample manager)

The run LED, on the right-hand side of the power LED on the sample manager's front panel, indicates the run status. A steady-green run LED indicates that injections are being run.

LED mode and color	Description
Unlit	Binary solvent manager and sample manager – Indicates the device is currently idle.
Steady green	<ul> <li>Binary solvent manager – Indicates solvent is flowing.</li> <li>Sample manager – Indicates the sample manager is operating normally, attempting to complete any outstanding samples or diagnostic function requests. When sample and diagnostic function requests are finished, the LED reverts to the unlit mode.</li> </ul>
Flashing green	Binary solvent manager and sample manager – Indicates that the module is initializing.
Flashing red	Indicates that an error stopped the instrument or device. Refer to the ACQUITY UPLC Console for information regarding the error.
Steady red	Indicates a module's failure that prevents its further operation. Power-off the module, and then power-on. If the LED is still steady red, contact your Waters service representative.

#### **Status LED indications:**

#### Enabling the leak sensors

**Rule:** When you power-on the system, the leak sensors default to disabled status unless previously enabled.

#### To enable the leak sensors:

1. In the ACQUITY UPLC Console, select Control > Leak Sensors.

2. To enable the leak sensor for an individual module, click the status on the left-hand side of the module's description.

Tip: To enable all leak sensors, click Enable All.

#### Starting the system

Use the Start up system function after the system has been idle a short period of time (as much as 12 hours) and when you plan to use the same solvents that you used during the previous run.

Start the "Start up system" function from the control panel.

#### **BSM Recommendations:**

- Prime the binary solvent manager for 1 minute for each solvent when the system has been idle for four or more hours, and you intend to use the solvents already in the system.
- Prime the binary solvent manager for four minutes for each solvent when you intend to use fresh solvents of the same composition as those already in the system.

#### SM - FTN recommendations:

- If you are changing solvents, prime the wash syringes and sample syringe for 35–50 cycles.
- If you are using the same solvent, prime the wash syringes and sample syringe for 20 cycles.
- Ensure the seal is characterized upon startup, and repeat the characterization periodically.

#### To refresh the system:

- 1. In the ACQUITY UPLC Console, click Control > Start up system.
- 2. In the Start up system dialog box, review the settings, and select a different option, if needed.
  - Solvent line A only (default)
  - Solvent line B only
  - Both A and B

3. Click OK.

**Result:** The system primes the selected solvents, primes the sample manager with one weak-wash prime (using the wash and sample syringes), and ignites the lamp in the detector.

## **Configuring MassLynx software**

Configure the MassLynx system software, for use with ACQUITY:

- Start MassLynx and log in.
- Select system modules, and name the system (see MassLynx Help for details).
- Open the ACQUITY Console and control panels.

## **ACQUITY control panels**

You can monitor control panels for the binary solvent manager, sample manager, and detector from MassLynx software. The control panels appear on the Additional Status tab of the Inlet Editor window.

#### **Binary solvent manager control panel**

The binary solvent manager control panel displays flow status, system pressure, total flow rate, and solvent composition parameters.

**Rule:** You can edit these parameters when the system is idle by clicking the underlined value. You cannot edit binary solvent manager parameters while the system is running samples.

#### Binary solvent manager control panel:



The following table describes the items in the binary solvent manager control panel:

Control panel item	Description
Flow LED	Displays the actual flow LED on the front panel of the binary solvent manager unless communications with the binary solvent manager are lost.
Status	Displays the status of the current operation.
System Pressure	Displays system pressure, in kPa, bar, or psi. You can customize pressure units via the ACQUITY UPLC Console.
Flow Rate	Displays the total flow rate of the binary solvent manager, from 0.000 to 2.000 mL/min under normal operation and 0.000 to 8.000 mL/min when priming.
Solvent Composition	Displays the percentage of solvent to be drawn from the solvent lines (A and B). Composition values range from 0.0 to 100.0%.
🔇 (Stop Flow)	Immediately stops all flow from the binary solvent manager.

#### Binary solvent manager control panel items:

You can access these additional functions by right-clicking anywhere in the binary solvent manager control panel:

Control panel function	Description
Start up system	Brings the system to operational conditions after an extended idle period or when switching to different solvents.
	See "Starting up the system" in the <i>Binary</i> Solvent Manager Operator's Overview and Maintenance Information.
Prime solvents	Displays the Prime Solvents dialog box.
	See "Priming the binary solvent manager" in the Binary Solvent Manager Operator's Overview and Maintenance Information.
Prime seal wash	Starts priming the seal wash.
	See "Priming the seal wash system" in the Binary Solvent Manager Operator's Overview and Maintenance Information.
Wash plungers	Initiates the plunger wash sequence, which fills and then slowly empties the primary and accumulator chambers (with the current solvent composition) while performing a high speed/volume seal wash. This action helps prevent the buildup of precipitates on the pump plungers which can damage the high pressure seals.
Launch ACQUITY UPLC Console	Launches the ACQUITY UPLC Console.
Reset BSM	Resets the binary solvent manager after an error condition.
Help	Displays the ACQUITY UPLC Console online Help.

#### Additional functions in the binary solvent manager control panel:

## Sample manager control panel

The sample manager control panel displays current sample compartment and column heater temperatures and set points. You can edit these values when the system is idle by clicking the underlined value. You cannot edit sample manager set points while the system is running samples.

Tips:

- To keep the sample compartment at a constant temperature, open its door only when necessary.
- The sample manager's fans stop circulating air whenever the sample compartment door is open.

#### Run LED Status . Sample Manager FTN Run Current sample Current column heater compartment 26.5 °C -0.2 temperature Sample Column temperature 35.0 0ff Sample **Display ACQUITY UPLC** Column heater set compartment set Console point point

#### Sample manager control panel:

The following table describes the items in the sample manager's control panel:

Sample	manager	control	panel	items:
--------	---------	---------	-------	--------

Control panel item	Description
Run LED	Displays the actual run LED on the front panel, unless communications are lost.
Status	Displays the status of the current operation.
Current Sample Compartment Temperature	Displays the current sample compartment temperature, to 0.1 °C resolution, even when active temperature control is disabled.
Sample Compartment Set Point	Displays the current sample compartment set point, to 0.1 °C resolution. When active temperature control is disabled, this field displays "Off".
Control panel item	Description
--------------------------------------	--
Current Column Heater Temperature	Displays the current column heater temperature to 0.1 °C resolution, even when active temperature control is disabled.
Column Heater Set Point	Displays the current column heater set point, to 0.1 °C resolution. When active temperature control is disabled, this field displays "Off".
(Display Console)	Displays the ACQUITY UPLC Console.

#### Sample manager control panel items: (Continued)

You can access these additional functions by right-clicking anywhere in the sample manager control panel.

Control panel function	Description
Prime	Displays the Prime dialog box.
	See "Priming the SM-FTN" in the Sample Manager - Flow Through Needle Operator's Overview and Maintenance Guide, (part number 715003737IVD)
Wash needle	Displays the Wash Needle dialog box.
	See "Washing the SM-FTN needle" in the Sample Manager - Flow Through Needle Operator's Overview and Maintenance Guide, (part number 715003737IVD)
Reset SM	Resets the sample manager following an error condition.
Help	Displays the ACQUITY UPLC Console online Help.

#### Additional functions in the sample manager control panel:

# Starting the ACQUITY UPLC Console

The ACQUITY UPLC Console software provides a way to configure settings, monitor performance, run diagnostic tests, and maintain the system and its modules. It replaces the keypads and small-screen displays traditionally found on the fronts of system modules. The ACQUITY UPLC Console functions independently of data applications and does not recognize or control them.

From the ACQUITY UPLC Console's interface, you can quickly navigate to visual representations of each module and its components. You can also navigate to interactive diagrams, which show interconnections and provide diagnostic tools for troubleshooting problems.

#### To start the ACQUITY UPLC Console from MassLynx software:

- 1. In the MassLynx window, click Inlet Method.
- 2. In the Inlet Method window, click the ACQUITY Additional Status tab.
- 3. Click Display Console 🚺.

# **4** Maintenance Procedures

Keep to a maintenance schedule, and perform maintenance as required and described in this chapter.

#### **Contents:**

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# Maintenance schedule

The following tables list periodic maintenance schedules that ensure optimum instrument performance of the ACQUITY UPLC I-Class IVD system.

The maintenance frequencies shown apply to instruments that normally receive moderate use. When using the system throughout the day (and on nights and weekends), or when using aggressive solvents such as buffers, perform these maintenance tasks more frequently.

#### See also:

- For complete procedures, refer to the component's Overview and Maintenance Guide on your ACQUITY UPLC I-Class IVD system documentation CD (part number 715003740IVD).
- For information on how to schedule routine preventative maintenance based on system usage, see page 48.

Maintenance procedure	Frequency
Replace the leak sensor on the column heater	As needed. For example, when the leak sensor is damaged or an error message states the leak sensor is not detected.
Replace the column	<ul> <li>As needed. The typical failure modes are as follows:</li> <li>High backpressure. The column causes a high pressure shutdown.</li> <li>Method requirements are not attained. This can be exhibited by poor peak shape, resolution between peaks lost, tailing, etc. Perform a plate count to establish column efficiency.</li> </ul>
Replace the active preheater assembly	<ul> <li>As needed. The typical failure modes are as follows:</li> <li>Error message. Any active preheater error messages, including messages indicating the active preheater is not detected or connected or has a temperature sensor error.</li> <li>Leak. This can be detected visibly, using the leak sensor or by noticing that peak retention times vary.</li> <li>Carryover. Reseat the active preheater assembly connections and/or replace the ferrules.</li> <li>Split peaks. Reseat the active preheater assembly connections and/or replace the ferrules.</li> </ul>
Replace the column stabilizer assembly	<ul> <li>As needed. The typical failure modes are as follows:</li> <li>Leak. This can be detected visibly, using the leak sensor or by noticing the peak retention times vary.</li> <li>Carryover. Reseat the column stabilizer assembly connections and/or replace the ferrules.</li> <li>Split peaks. Reseat the column stabilizer assembly connections and/or replace the ferrules.</li> </ul>

#### Column Manager maintenance procedures:

Maintenance procedure	Frequency
Replace the column in-line filter frit	Replace as part of the annual scheduled routine maintenance and, thereafter, as needed. The typical failure modes are as follows:
	• High back pressure. The column in-line filter causes a high pressure shutdown. In this case, disconnect the column. If the system exhibits pressure decay, check the system pressure at known conditions. Replace the frit.
	• Leak. The system exhibits low back pressure or shorter retention times.
Replace the column in-line filter unit	<ul> <li>As needed. The typical failure modes are as follows:</li> <li>High back pressure. The column in-line causes a high pressure shutdown. In this case, disconnect the in-line filter. If the system exhibits pressure decay, check the system pressure at known conditions. Replace the frit or entire in-line filter assembly.</li> <li>Leak. This can be detected visibly, using the leak sensor or by noticing the peak retention times vary.</li> <li>Split peaks. Replace the filter frit.</li> </ul>
Clean the device's exterior with a soft, lint-free cloth, or paper dampened with water	Perform as part of your annual routine scheduled maintenance and when solvent or dust accumulates.

#### Column Manager maintenance procedures: (Continued)

Maintenance procedure	Frequency
Clean the instrument with a soft, lint-free cloth, or paper dampened with water	Perform as part of your annual routine scheduled maintenance and when solvent or dust accumulates.
Replace the leak sensor	As needed. For example, when the leak sensor is damaged or an error message states the leak sensor is not detected.
Replace the needle seal	Replace as part of the annual scheduled routine maintenance and, thereafter, as needed. The typical failure modes are as follows:
	• The dynamic leak test fails.
	• The needle seal readiness test fails.
	• Peaks do not appear on your chromatogram.
	• Peak areas are lower than expected.
Replace the sample needle	Replace when the needle breaks, when the error message "Drawing sample rate excessive <value>" appears, or the needle seal readiness test is failed.</value>
Replace the sample syringe	Replace as part of the annual scheduled routine maintenance and, thereafter, as needed. The typical failure modes are as follows:
	• The sample syringe leak test fails.
	<ul> <li>Air bubbles are in the syringe.</li> <li>A sample syringe hardware error message appears.</li> </ul>
Replace the injection valve cartridge	Perform as part of your annual routine scheduled maintenance and if the system shows erratic system pressure from run to run.
Clean the injection port	Perform as part of your annual routine scheduled maintenance and if you see sample or particulate accumulation.

#### Sample Manager Flow-Through-Needle maintenance procedures:

Maintenance procedure	Frequency
Replace the leak sensor	As needed. For example, when the leak sensor is damaged or an error message states the leak sensor is not detected.
Replace the mixer	Replace as part of the annual scheduled routine maintenance and, thereafter, as needed. The typical failure modes are as follows:
	• You see a visible leak.
	• You see erratic retention times.
	• The mixer assembly causes a high pressure shutdown.
Replace the pump interconnect tubing	Replace as part of the annual scheduled routine maintenance and, thereafter, as needed. The typical failure modes are as follows:
	• You see a visible leak
	• The system exhibits a high pressure shutdown and the pressure decays when the connection after the tubing is broken.
Replace the $i^2 Valve$ cartridge	Replace as part of the annual scheduled routine maintenance and, thereafter, as needed. The typical failure modes are as follows:
	• Late eluting peaks are exhibited and/or after a dynamic leak test was performed where the leak rate is above the acceptable limit.
	• The solvent manager exhibits a low or erratic flow rate/ pressure pulsations.
	• An intelligent intake valve error message occurs.

### Binary Solvent Manager maintenance procedures:

Maintenance procedure	Frequency
Replace the in-line	As needed. The typical failure modes are as follows:
filter	• High back pressure. The in-line filter causes a high pressure shutdown. In this case, disconnect the in-line filter. If the system exhibits pressure decay, check the system pressure at known conditions. Replace the frit or entire check valve assembly.
	• Leak. This can be detected visibly, using the leak sensor, or by noticing that peak retention times vary.
Replace the accumulator check valve	Replace as part of the annual scheduled routine maintenance and, thereafter, as needed. The typical failure modes are as follows:
	• Late eluting peaks are exhibited and/or after a dynamic leak test was performed where the leak rate is above the acceptable limit.
	• The solvent manager exhibits a low or erratic flow rate/ pressure pulsations.
Replace solvent reservoir filters	Replace as part of the annual scheduled routine maintenance and, thereafter, as needed. The typical failure modes are as follows:
	• Slow baseline drift is exhibited.
	• Retention times are increasing.
	• The system exhibits low erratic system pressure.
Clean the air filter in the door	Perform as part of your annual routine scheduled maintenance and when solvent or dust accumulates.
Replace the air filter in the door	Replace annually.

### **Binary Solvent Manager maintenance procedures: (Continued)**

Maintenance procedure	Frequency
Replace the plunger and seals	Replace as part of the annual scheduled routine maintenance and, thereafter, as needed. The typical failure modes are as follows:
	• Late eluting peaks are exhibited and/or after a dynamic leak test was performed where the leak rate is above the acceptable limit.
	• There is flow from the seal wash effluent during the high pressure dynamic leak test.
	• The solvent manager exhibits low or erratic flow rate/ pressure pulsations.
Replace the vent valve cartridge	Replace as part of your annual routine scheduled maintenance and if the dynamic leak test fails during the accumulator portion.
Clean the device's exterior with a soft, lint-free cloth, or paper dampened with water	Perform as part of your annual routine scheduled maintenance and when solvent or dust accumulates.

#### **Binary Solvent Manager maintenance procedures: (Continued)**

# **Spare parts**

Warning: To ensure that your system operates as designed, produces accurate results, and is not damaged, use only Waters Quality Parts®. Visit www.waters.com/wqp for information about Waters Quality Parts, including how to order them

Listed below are parts you may want to keep on hand for repairs and maintenance:

- BSM PM kit
- SM PM kit
- ESI probe spares kit
- Source spares kit
- APH IVD
- Needle, 50 µL

- Kit, ACQUITY UPLC I-Class MS PEEK 17 inch
- ACQUITY UPLC BEH C18 1.7 μm 2.1 50 mm IVD
- ACQUITY UPLC BEH C18 1.7 μm 2.1 100 mm IVD
- ACQUITY UPLC BEH C18 1.7 µm 2.1 150 mm IVD
- ACQUITY UPLC BEH C18 1.7 µm 2.1 50 mm IVD, 3-pack
- ACQUITY UPLC BEH C18 1.7 μm 2.1 100 mm IVD, 3-pack
- ACQUITY UPLC BEH C18 1.7 µm 2.1 150 mm IVD, 3-pack
- ACQUITY UPLC HSS T3 1.8 µm 2.1 50 mm IVD
- ACQUITY UPLC HSS T3 1.8 µm 2.1 50 mm IVD, 3-pack
- ACQUITY UPLC BEH Phenyl 1.7 μm 2.1 50 mm, IVD 3-pack

# **Troubleshooting with Connections INSIGHT**

Connections INSIGHT<sup>®</sup> is an "intelligent" device management (IDM) Web service that enables Waters to provide proactive service and support for the ACQUITY UPLC system. To use Connections INSIGHT, you must install its service agent software on your MassLynx workstation. In a client/server system, you must also install the service agent, on the computer from which you control the system. The service agent software automatically and securely captures and sends information about the support needs of your system directly to Waters.

If you encounter a performance issue when using the ACQUITY UPLC Console software, you can manually submit a Connections Insight request to Waters customer support. Alternatively, you can use Remote Desktop, a real-time collaboration option that controls the two-way connection with the ACQUITY UPLC system by enabling the Connections INSIGHT iAssist service level.

These sources, which are available on the Waters' web site, provide more information about Connections INSIGHT and Connections INSIGHT iAssist:

- Connections INSIGHT User's Guide (part number 715003036)
- Connections INSIGHT Quick Start Guide (part number 715003037)

#### To submit a Connections Insight request:

- 1. Select Troubleshoot > Submit Connections Insight request.
- 2. In the Connections Insight Request dialog box, type your name, telephone number, e-mail address, and a description of the problem.
- 3. Click Submit, and allow approximately 5 minutes to save the service profile.

**Result:** A .zip file containing your Connections Insight profile is forwarded to Waters customer support for review.

**Tip:** Saving a service profile or plot file from the Instrument Console can require as much as 150 MB of file space.

# Safety and handling

Bear in mind the following safety considerations when performing maintenance procedures on the mass spectrometer:



**Warning:** To avoid personal contamination with biohazards, toxic compounds, or their residues, wear clean, chemical-resistant, powder-free gloves when handling the components.



**Warning:** To prevent injury, always observe Good Laboratory Practice when handling solvents, changing tubing, or operating the instrument. Know the physical and chemical properties of the solvents used (see the Material Safety Data Sheets for the solvents in use).



**Warning:** To avoid electric shock, do not remove the instrument's panels. The panels cover components that are serviceable only by Waters technicians.



**Warning:** To avoid electric shock, ensure that the instrument is in Standby mode before beginning any maintenance operation.



**Warning:** To avoid burn injuries, ensure that the probe and mass spectrometer source are not hot before working on them.



**Caution:** When performing maintenance inside the source enclosure of the mass spectrometer, ensure that the following criteria are met:

- Instrument is in Standby mode.
- LC flow is diverted to waste or set to off.
- Desolvation gas is turned off.

See Appendix A for safety advisory information.

# **Configuring maintenance warnings**

Maintenance counters provide real-time usage status information that can help you determine when to schedule routine maintenance for specific components. You can set usage thresholds and maintenance warnings that alert you when a component reaches the designated threshold limit. By setting threshold limits and monitoring these usage counters regularly, you can minimize unexpected failures and unscheduled downtime during important work. For information on setting maintenance warnings, consult the ACQUITY UPLC Console online Help.

# A Safety Advisories

Waters instruments display hazard symbols designed to alert you to the dangers of operating and maintaining the instruments. Their corresponding user guides also include the hazard symbols, with accompanying text statements describing the hazards and telling you how to avoid them. This appendix presents all the safety symbols and statements that apply to the entire line of Waters products.

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# Warning symbols

Warning symbols alert you to the risk of death, injury, or seriously adverse physiological reactions associated with an instrument's use or misuse. Heed all warnings when you install, repair, and operate Waters instruments. Waters assumes no liability for the failure of those who install, repair, or operate its instruments to comply with any safety precaution.

# Task-specific hazard warnings

The following warning symbols alert you to risks that can arise when you operate or maintain an instrument or instrument component. Such risks include burn injuries, electric shocks, ultraviolet radiation exposures, and others.

When the following symbols appear in a manual's narratives or procedures, their accompanying text identifies the specific risk and explains how to avoid it.

Warning: (Risk of danger. When this symbol appears on an instrument, consult the instrument's user documentation for important safety-related information before you use the instrument.)

Warning: (Risk of hot surfaces.)



Warning: (Risk of fire.)

Warning: (Risk of sharp-point puncture injury.)

Warning: (Moving machinery.)

Warning: (Risk of exposure to ultraviolet radiation.)



Warning: (Risk of contacting corrosive substances.)



Warning: (Risk of exposure to a toxic substance.)



Warning: (Risk of personal exposure to laser radiation.)

Warning: (Risk of exposure to biological agents that can pose a serious health threat.)

Warning: (Risk of tipping.)



Warning: (Risk of explosion.)

Warning: (Use eye protection.)

# **Specific warnings**

The following warnings can appear in the user manuals of particular instruments and on labels affixed to them or their component parts.

#### **Burst warning**

This warning applies to Waters instruments fitted with nonmetallic tubing.



- Wear eye protection.
- Extinguish all nearby flames.
- Do not use tubing that is, or has been, stressed or kinked.
- Do not expose nonmetallic tubing to incompatible compounds like tetrahydrofuran (THF) and nitric or sulfuric acids.
- Be aware that some compounds, like methylene chloride and dimethyl sulfoxide, can cause nonmetallic tubing to swell, which significantly reduces the pressure at which the tubing can rupture.

#### Mass spectrometer flammable solvents warning

This warning applies to instruments operated with flammable solvents.

Warning: Where significant quantities of flammable solvents are involved, a continuous flow of nitrogen into the ion source is required to prevent possible ignition in that enclosed space.

Ensure that the nitrogen supply pressure never falls below 690 kPa (6.9 bar, 100 psi) during an analysis in which flammable solvents are used. Also ensure a gas-fail connection is connected to the LC system so that the LC solvent flow stops if the nitrogen supply fails.

#### Mass spectrometer shock hazard

This warning applies to all Waters mass spectrometers.

Warning: To avoid electric shock, do not remove the mass spectrometer's protective panels. The components they cover are not user-serviceable.

This warning applies to certain instruments when they are in Operate mode.

Warning: High voltages can be present at certain external surfaces of the mass spectrometer when the instrument is in Operate mode. To avoid nonlethal electric shock, make sure the instrument is in Standby mode before touching areas marked with this high voltage warning symbol.

### **Biohazard warning**

This warning applies to Waters instruments that can be used to process material that can contain biohazards: substances that contain biological agents capable of producing harmful effects in humans.

Warning: Waters instruments and software can be used to analyze or process potentially infectious human-sourced products, inactivated microorganisms, and other biological materials. To avoid infection with these agents, assume that all biological fluids are infectious, observe Good Laboratory Practice, and consult your organization's biohazard safety representative regarding their proper use and handling. Specific precautions appear in the latest edition of the US National Institutes of Health (NIH) publication, *Biosafety in Microbiological and Biomedical Laboratories* (BMBL).

### **Chemical hazard warning**

This warning applies to Waters instruments that can process corrosive, toxic, flammable, or other types of hazardous material.



**Warning:** Waters instruments can be used to analyze or process potentially hazardous substances. To avoid injury with any of these materials, familiarize yourself with the materials and their hazards, observe Good Laboratory Practice (GLP), and consult your organization's safety representative regarding proper use and handling. Guidelines are provided in the latest edition of the National Research Council's publication, *Prudent Practices in the Laboratory: Handling and Disposal of Chemicals*.

# **Caution advisory**

Caution advisories appear where an instrument or device can be subject to use or misuse capable of damaging it or compromising a sample's integrity. The exclamation point symbol and its associated statement alert you to such risk.



**Caution:** To avoid damaging the instrument's case, do not clean it with abrasives or solvents.

# Warnings that apply to all Waters instruments

When operating this device, follow standard quality-control procedures and the equipment guidelines in this section.

Attention: Changes or modifications to this unit not expressly approved by the party responsible for compliance could void the user's authority to operate the equipment.

**Important:** Toute modification sur cette unité n'ayant pas été expressément approuvée par l'autorité responsable de la conformité à la réglementation peut annuler le droit de l'utilisateur à exploiter l'équipement.

Achtung: Jedwede Änderungen oder Modifikationen an dem Gerät ohne die ausdrückliche Genehmigung der für die ordnungsgemäße Funktionstüchtigkeit verantwortlichen Personen kann zum Entzug der Bedienungsbefugnis des Systems führen.

**Avvertenza:** qualsiasi modifica o alterazione apportata a questa unità e non espressamente autorizzata dai responsabili per la conformità fa decadere il diritto all'utilizzo dell'apparecchiatura da parte dell'utente.

**Atencion:** cualquier cambio o modificación efectuado en esta unidad que no haya sido expresamente aprobado por la parte responsable del cumplimiento puede anular la autorización del usuario para utilizar el equipo.

**注意**:未經有關法規認證部門允許對本設備進行的改變或修改,可能會使使用者喪失操作該設備的權利。

**注意**?未经有关法规认证部门明确允许对本设备进行的改变或改装,可能会使使用者 丧失操作该设备的合法性。

주의: 규정 준수를 책임지는 당사자의 명백한 승인 없이 이 장치를 개조 또는 변경할 경우,

이 장치를 운용할 수 있는 사용자 권한의 효력을 상실할 수 있습니다.

**注意**:規制機関から明確な承認を受けずに本装置の変更や改造を行うと、本装置のユーザーとしての承認が無効になる可能性があります。

Warning: Use caution when working with any polymer tubing under pressure:

- Always wear eye protection when near pressurized polymer tubing.
  - Extinguish all nearby flames.
  - Do not use tubing that has been severely stressed or kinked.
  - Do not use nonmetallic tubing with tetrahydrofuran (THF) or concentrated nitric or sulfuric acids.
  - Be aware that methylene chloride and dimethyl sulfoxide cause nonmetallic tubing to swell, which greatly reduces the rupture pressure of the tubing.

Attention: Manipulez les tubes en polymère sous pression avec precaution:

- Portez systématiquement des lunettes de protection lorsque vous vous trouvez à proximité de tubes en polymère pressurisés.
- Eteignez toute flamme se trouvant à proximité de l'instrument.
- Evitez d'utiliser des tubes sévèrement déformés ou endommagés.
- Evitez d'utiliser des tubes non métalliques avec du tétrahydrofurane (THF) ou de l'acide sulfurique ou nitrique concentré.
- Sachez que le chlorure de méthylène et le diméthylesulfoxyde entraînent le gonflement des tuyaux non métalliques, ce qui réduit considérablement leur pression de rupture.

**Vorsicht**: Bei der Arbeit mit Polymerschläuchen unter Druck ist besondere Vorsicht angebracht:

- In der Nähe von unter Druck stehenden Polymerschläuchen stets Schutzbrille tragen.
- · Alle offenen Flammen in der Nähe löschen.
- Keine Schläuche verwenden, die stark geknickt oder überbeansprucht sind.
- Nichtmetallische Schläuche nicht für Tetrahydrofuran (THF) oder konzentrierte Salpeter- oder Schwefelsäure verwenden.
- Durch Methylenchlorid und Dimethylsulfoxid können nichtmetallische Schläuche quellen; dadurch wird der Berstdruck des Schlauches erheblich reduziert.

Attenzione: fare attenzione quando si utilizzano tubi in materiale polimerico sotto pressione:

- Indossare sempre occhiali da lavoro protettivi nei pressi di tubi di polimero pressurizzati.
- Spegnere tutte le fiamme vive nell'ambiente circostante.
- Non utilizzare tubi eccessivamente logorati o piegati.
- Non utilizzare tubi non metallici con tetraidrofurano (THF) o acido solforico o nitrico concentrati.
- Tenere presente che il cloruro di metilene e il dimetilsolfossido provocano rigonfiamenti nei tubi non metallici, riducendo notevolmente la pressione di rottura dei tubi stessi.

Advertencia: se recomienda precaución cuando se trabaje con tubos de polímero sometidos a presión:

- El usuario deberá protegerse siempre los ojos cuando trabaje cerca de tubos de polímero sometidos a presión.
- Si hubiera alguna llama las proximidades.
- No se debe trabajar con tubos que se hayan doblado o sometido a altas presiones.
- Es necesario utilizar tubos de metal cuando se trabaje con tetrahidrofurano (THF) o ácidos nítrico o sulfúrico concentrados.
- Hay que tener en cuenta que el cloruro de metileno y el sulfóxido de dimetilo dilatan los tubos no metálicos, lo que reduce la presión de ruptura de los tubos.

警告: 當在有壓力的情況下使用聚合物管線時, 小心注意以下幾點。

- 當接近有壓力的聚合物管線時一定要戴防護眼鏡。
- 熄滅附近所有的火焰。
- 不要使用已經被壓癟或嚴重彎曲管線。
- 不要在非金屬管線中使用四氫呋喃或濃硝酸或濃硫酸。
- 要了解使用二氯甲烷及二甲基亞楓會導致非金屬管線膨脹,大大降低管線的耐壓 能力。

▲ 警告: 当有压力的情况下使用管线时,小心注意以下几点:

- ▲・ 当接近有压力的聚合物管线时一定要戴防护眼镜。
  - 熄灭附近所有的火焰。
  - 不要使用已经被压瘪或严重弯曲的管线。
  - 不要在非金属管线中使用四氢呋喃或浓硝酸或浓硫酸。
  - 要了解使用二氯甲烷及二甲基亚枫会导致非金属管线膨胀,大大降低管线的耐压能力。

경고: 가압 폴리머 튜브로 작업할 경우에는 주의하십시오.

- 가압 폴리머 튜브 근처에서는 항상 보호 안경을 착용하십시오.
- 근처의 화기를 모두 끄십시오.
- 심하게 변형되거나 꼬인 튜브는 사용하지 마십시오.
- 비금속 (Nonmetallic) 튜브를 테트라히드로푸란 (Tetrahydrofuran: THF) 또는 농축 질산 또는 황산과 함께 사용하지 마십시오.
- 염화 메틸렌 (Methylene chloride) 및 디메틸술폭시드 (Dimethyl sulfoxide) 는 비금속 튜브를 부풀려 튜브의 파열 압력을 크게 감소시킬 수 있으므로 유의하십 시오.

警告: 圧力のかかったポリマーチューブを扱うときは、注意してください。

- 加圧されたポリマーチューブの付近では、必ず保護メガネを着用してください。
- ・ 近くにある火を消してください。
- 著しく変形した、または折れ曲がったチューブは使用しないでください。
- ・ 非金属チューブには、テトラヒドロフラン (THF) や高濃度の硝酸または硫酸 などを流さないでください。
- ・ 塩化メチレンやジメチルスルホキシドは、非金属チューブの膨張を引き起こ す場合があり、その場合、チューブは極めて低い圧力で破裂します。

Warning: The user shall be made aware that if the equipment is used in a manner not specified by the manufacturer, the protection provided by the equipment may be impaired.

**Attention:** L'utilisateur doit être informé que si le matériel est utilisé d'une façon non spécifiée par le fabricant, la protection assurée par le matériel risque d'être défectueuses.

**Vorsicht:** Der Benutzer wird darauf aufmerksam gemacht, dass bei unsachgemäßer Verwenddung des Gerätes die eingebauten Sicherheitseinrichtungen unter Umständen nicht ordnungsgemäß funktionieren.

**Attenzione:** si rende noto all'utente che l'eventuale utilizzo dell'apparecchiatura secondo modalità non previste dal produttore può compromettere la protezione offerta dall'apparecchiatura.

**Advertencia:** el usuario deberá saber que si el equipo se utiliza de forma distinta a la especificada por el fabricante, las medidas de protección del equipo podrían ser insuficientes.

警告: 使用者必須非常清楚如果設備不是按照製造廠商指定的方式使用, 那麼該設備所提供的保護將被消弱。

警告: 使用者必须非常清楚如果设备不是按照制造厂商指定的方式使用, 那么该设备所提供的保护将被削弱。

경고: 제조업체가 명시하지 않은 방식으로 장비를 사용할 경우 장비가 제공하는 보호 수단이 제대로 작동하지 않을 수 있다는 점을 사용자에게 반드시 인식시켜야 합니다.

**警告**: ユーザーは、製造元により指定されていない方法で機器を使用すると、機器が提供している保証が無効になる可能性があることに注意して下さい。

# **Electrical and handling symbols**

# **Electrical symbols**

These can appear in instrument user manuals and on the instrument's front or rear panels.

	Electrical power on
0	Electrical power off
$\bigcirc$	Standby
	Direct current
$\sim$	Alternating current (single phase)
	Protective earth terminal
m	Frame or chassis ground
	Fuse

# Handling symbols

These handling symbols and their associated text can appear on labels affixed to the outer packaging of Waters instrument and component shipments.

<u> </u>	Keep upright!
×	Keep dry!
¥	Fragile!
Ж	Use no hooks!

# **B** Specifications

These system specifications depend on the conditions in individual laboratories. Refer to the *ACQUITY UPLC I-Class (IVD) System Site Preparation Guide* (part number 715003724), or contact Waters Technical Service for details.

**Note:** For specifications on the mass spectrometer, see the Xevo TQ-S IVD Mass Spectrometry System Operator's Overview and Maintenance Guide.

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# **Physical specifications**

# **Binary solvent manager**

The following table lists the physical specifications for the ACQUITY UPLC I-Class IVD BSM:

Attribute	Specification
Height	22.9 cm (9.0 inches)
Width	34.3 cm (13.5 inches)
Depth	66.0 cm (26.0 inches)
Weight	26.3 kg (58.0 pounds)

#### **BSM** physical specifications:

# Sample manager - FTN

The following table lists the physical specifications for the ACQUITY UPLC I-Class IVD SM-FTN:

#### Sample manager - FTN physical specifications:

Attribute	Specification
Height	27.1 cm (10.7 inches)
Width	34.3 cm (13.5 inches)
Depth	71.2 cm (28.0 inches)
Weight	26.1 kg (57.5 pounds)

# **Column heater**

The following table lists the physical specifications for the ACQUITY UPLC I-Class IVD column heater-A:

#### **CH-A physical specifications:**

Attribute	Specification
Height	7.6 cm (3.0 inches)
Width	34.3 cm (13.5 inches)
Depth	62.9 cm (24.8 inches)
Weight	5.7 kg (12.5 pounds)

# **TQ-S** mass spectrometer

The following table lists the physical specifications for the Xevo TQ-S mass spectrometer:

#### **CH-A physical specifications:**

Attribute	Specification
Height	71.1 cm (28 inches)
Width	61.0 cm (24 inches)
Length	99.5 cm (39 inches)
Weight, with two scroll pumps	352 kg (777 pounds)
Weight, with two rotary pumps	408 kg (899 pounds)

# **Environmental specifications**

The following table lists the environmental specifications for the ACQUITY UPLC I-Class IVD system:

Warning: To prevent inaccurate results, do not operate the instrument outside the operating temperature and humidity specified.

#### ACQUITY UPLC I-Class IVD system environmental specifications:

Attribute	Specification
Acoustic noise	<65 dBA, system: binary solvent manager, sample manager (SM-FTN), CH-A
Operating temperature	15 to 28°C (59 to 82 °F) Short-term (1.5 h) variations must be no more than ±2 °C (3.5 °F)
Operating humidity	20 to 80%, noncondensing
Shipping and storage temperature	0 to 40 °C
Shipping and storage humidity	20 to 80%, noncondensing

The following table lists the electrical specifications for the ACQUITY UPLC I-Class IVD system:

Attribute	Specification
Protection class <sup>1</sup>	Class I
Overvoltage category <sup>2</sup>	II
Pollution degree <sup>3</sup>	2
Moisture protection <sup>4</sup>	Normal (IPX0)
Line voltages, nominal	Grounded AC
Voltage range	100 to 240 Vac
Frequency	50/60 Hz
Maximum power draw	BSM: 360 VA
	SM-FTN: 400 VA

### ACQUITY UPLC I-Class IVD system electrical specifications:

- 1. **Protection Class I** The insulating scheme used in the instrument to protect from electrical shock. Class I identifies a single level of insulation between live parts (wires) and exposed conductive parts (metal panels), in which the exposed conductive parts are connected to a grounding system. In turn, this grounding system is connected to the third pin (ground pin) on the electrical power cord plug.
- 2. **Overvoltage Category II** Pertains to instruments that receive their electrical power from a local level such as an electrical wall outlet.
- 3. **Pollution Degree 2** A measure of pollution on electrical circuits that can produce a reduction of dielectric strength or surface resistivity. Degree 2 refers only to normally nonconductive pollution. Occasionally, however, expect a temporary conductivity caused by condensation.
- 4. **Moisture Protection** Normal (IPX0) IPX0 means that no Ingress Protection against any type of dripping or sprayed water exists. The "X" is a placeholder that identifies protection against dust, if applicable.

# Binary solvent manager input/output specifications

The following table lists the input/output specifications for the ACQUITY UPLC I-Class IVD BSM:

Attribute	Specification
Contact closure	Maximum voltage: 30 VDC
outputs (SW1 to SW3)	Maximum current: 0.5 A
	Maximum VA rating: 10 W
	Contact resistance (nominal): 0.2 ohms
	Screw terminal connector
Run stopped output	Maximum voltage: 30 VDC
	Maximum current: 0.5 A
	Maximum VA rating: 10 W
	Contact resistance (nominal): 0.2 ohms
	Screw terminal connector
	Behavior: If an error message exists, switch is closed and then opened when the error is cleared.
Stop flow input	TTL signal or contact closure:
	Input voltage range: ±30 VDC
	Logic High: ≥3.0 VDC
	Logic Low: ≤1.9 VDC
	Minimum pulse width: 100 msec
	Screw terminal connector
Start gradient input	TTL signal or contact closure:
	Input voltage range: ±30 VDC
	Logic High: ≥3.0 VDC
	Logic Low: ≤1.9 VDC
	Minimum pulse width: 100 msec
	Screw terminal connector

#### **BSM** input/output specifications:

Attribute	Specification
Auxiliary input 1	TTL signal or contact closure:
	Input voltage range: ±30 VDC
	Logic High: ≥3.0 VDC
	Logic Low: ≤1.9 VDC
	Minimum pulse width: 100 msec
	Screw terminal connector
Auxiliary input 2	TTL signal or contact closure:
	Input voltage range: ±30 VDC
	Logic High: ≥3.0 VDC
	Logic Low: ≤1.9 VDC
	Minimum pulse width: 100 msec
	Screw terminal connector
Analog outputs (1 and 2)	0 to 2 volts full scale, screw terminal (digital to analog converter range is -0.1 to 2.1 to allow for offsets)

### BSM input/output specifications: (Continued)

# Sample manager - FTN input/output specifications

The following table lists the input/output specifications for the ACQUITY UPLC I-Class IVD SM - FTN:

Sample manager	- FTN	input/output	specifications:
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Attribute	Specification
Event output relay	Maximum voltage: 30 VDC
(Inject Start Out)	Maximum current: 0.5 A
	Contact resistance (nominal): 0.2 ohms
Digital input signal	Maximum input voltage: 30 VDC
(Inject Hold In)	Logic High: ≥3.0 VDC
	Logic Low: ≤1.9 VDC

# Xevo TQ-S input/output specifications

The following table lists the input/output specifications for the Xevo TQ-S mass spectrometer:

#### Xevo TQ-S input/output specifications:

Attribute	Specification
Xevo TQ-S	200-240 V, 50/60 Hz, 2 kW maximum
XDS 46i scroll pump	200-230 V, 50/60 Hz
XDS 100B scroll pump	200-230 V, 50/60 Hz
SV65 BI rotary pump (two included)	200-240 V, 50/60 Hz

# Wetted materials of construction

# **Binary solvent manager**

The following table lists the wetted materials of construction for the ACQUITY UPLC I-Class IVD BSM:

#### BSM wetted materials of construction:

Description	Specification
Wetted materials	316L stainless steel, UHMWPE blend, MP35N, titanium alloy, gold, sapphire, ruby, zirconia, Nitronic 60, DLC, fluoropolymer, PEEK™ and PEEK blend

# Sample manager - FTN

The following table lists the wetted materials of construction for the sample ACQUITY UPLC I-Class IVD SM-FTN:

#### Sample manager - FTN wetted materials of construction:

Description	Specification
Wetted materials	316L stainless steel, polymide, PEEK blend, DLC, PPS

# **Column Heater**

The following table lists the wetted materials of construction for the ACQUITY UPLC I-Class IVD column heater:

#### Wetted materials of construction:

Description	Specification
Wetted materials	316L stainless steel

# C External Connections

A Waters technical service representative unpacks and installs your ACQUITY UPLC I-Class IVD system modules.



**Caution:** To avoid damaging system modules, Contact Waters Technical Service (see page iv). If you must transport a system component or remove it from service, contact Waters Technical Service for recommended cleaning, flushing, and packaging procedures.



Warning: To avoid back injuries, do not attempt to lift the system modules without assistance.

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# System tubing connections

The system's external tubing connections for solvent flow and drainage are shown below:

Solvent flow for ACQUITY UPLC I-Class IVD system with an SM-FTN:



\*The mass spectrometer is located on the right-hand side of the BSM, SM-FTN, and CH.

# **External wiring connections**

# ACQUITY UPLC I-Class IVD instrument external wiring connections

The rear panel connections for ACQUITY UPLC I-Class IVD system modules are shown below



# **Ethernet connections**

The sample manager provides communications using an internal 10/100/1000 megabit Ethernet switch that accommodates the PC (workstation) and as many as five other Ethernet devices. Connect the shielded Ethernet cables from each module to the electronic connections on the rear panel of the sample manager. The sample manager is connected internally to the Ethernet switch.

**Requirement:** To ensure optimum performance and signal integrity, use only approved (or Waters supplied), shielded, CAT 5 ethernet cables.

**See also:** *Ethernet Instrument Getting Started Guide*, part number 71500074403.

# **Column heater connection**

The sample manager powers and communicates with the column heater. The external communication cable must be connected to the rear of the column heater and the sample manager.

To make column heater connections:

**Caution:** To avoid damaging electrical parts, never disconnect an electrical assembly while power is applied to a system module. To interrupt power to a module, set the power switch to Off, and then unplug the power cord from the AC outlet. After power is removed, wait 10 seconds thereafter before you disconnect an assembly.

- 1. Ensure the sample manager and the column heater are powered-off.
- 2. Connect the external communication cable to the High Density (HD) port on the rear of the column heater.
- 3. Connect the other end of the external communication cable to the QSPI port on the rear of the sample manager.
# **Signal connections**

# **Connecting signal cables**

Refer to the signal connection location shown on the silk-screened label affixed to the rear panel of each system module.

## **Required materials**

- 9/32-inch nut driver
- Flat-blade screwdriver
- Connector
- Signal cable

#### To connect signal cables:

1. Insert the connector into the connector port on the back of the system module.



2. Using the flat-blade screwdriver, attach the positive and negative leads of the signal cable to the connector.



3. Fit the grounding cable's fork terminal on the rear panel grounding stud, and secure the terminal with the locking nut.

**Tip:** Use the 9/32-inch nut driver to tighten the locking nut until the fork terminal does not move.



## Binary solvent manager I/O signal connectors

The rear panel of the binary solvent manager includes two removable connectors that hold the screw terminals for I/O signal cables. These connectors are keyed so that they can be inserted only one way.

#### Binary solvent manager I/O signal connectors:



For electrical specifications, see Appendix C, "System Specifications".

Signal connection	Description
Auxiliary 1 In	Reserved for future use.
Auxiliary 2 In	Reserved for future use.
Run Stopped Out	Indicates (with a contact closure) the binary solvent manager has ceased operation because of an error condition or operator request.
Switch 1 Out	Used to send time-based contact closure signals to external devices.

#### Binary solvent manager analog-out/event-in connections:

Signal connection	Description
0–2V Analog 1 Out	<ul> <li>Outputs the analog signal to a device such as an integrator or strip-chart recorder. Via the MassLynx software, you can select one of the following signals as the chart out signal:</li> <li>Flow rate</li> <li>System pressure</li> <li>Composition (%A %B)</li> </ul>
Gradient In	Initiates the pumps to begin gradient operation
	by contact closure input or 0-volt input.
Stop Flow In	Allows you to stop the flow from the binary solvent manager when an error condition or hardware failure occurs on another system module.
Switch 2 Out	Used to send time-based contact closure signals to external devices.
Switch 3 Out	Used to send time-based contact closure signals to external devices.
0–2V Analog 2 Out	<ul> <li>Outputs the analog signal to a device such as an integrator or strip-chart recorder. Via the MassLynx software, you can select one of the following signals as the chart out signal:</li> <li>Flow rate</li> <li>System pressure</li> <li>Composition (%A, %B)</li> </ul>

## Binary solvent manager analog-out/event-in connections: (Continued)

Signal	Parameter Setting at 0 Volts (Minimum)	Parameter Setting at 2.000 Volts (Maximum)
Flow Rate	0.000 mL/min	2 mL/min
System Pressure	–345 kPa (–3.45 bar, –50 psi)	124,106 kPa (1241 bar, 18,000 psi)
Composition	0.0%	100.0%

#### **Chart-out signal conditions:**

## Sample manager I/O signal connectors

The rear panel of the sample manager includes a removable connector that holds the screw terminals for I/O signal cables. This connector is keyed so that it can receive a signal cable inserted only one way.

**Requirement:** A contact closure output connection (Inject Start Out) from the sample manager is required to trigger a mass spectrometer.

#### Sample manager I/O signal connectors:

$\llbracket$					
1	2	3	4	5	6
Inject Start Out +	Inject Start Out -	Ground	Ground	Inject Hold In +	Inject Hold In -

For electrical specifications, see Appendix B.

Signal connections	Description
Inject Start Out	Indicates (with a contact closure output) that an injection has started.
Inject Hold In	Delays the next injection when the sample manager receives a contact closure input (from another system module, for example).

## Sample manager event-out/event-in connections:

# Connecting to the electricity source

Each system module requires a separate, grounded power source. The ground connection in all power outlets must be common and physically close to the system.



Warning: To avoid electrical shock, do as follows:

- Use only authorized power cords that are shipped with your instrument or supplied from your local Water's distributor.
- Power-off and unplug each system module before performing any maintenance operation on the module.
- Connect each system module to a common ground.

#### To connect to the electricity source:

**Recommendation:** Use a line conditioner and uninterruptible power supply (UPS) for optimum, long-term, input voltage stability. For sizing and selection of the UPS or line conditioner, contact Waters technical support.

- 1. Connect the female end of the power cord to the receptacle on the rear panel of each module.
- 2. Connect the male end of the power cord to a suitable wall outlet.

**Alternative:** If your system includes the optional FlexCart, connect the female end of the FlexCart's electrical cables (included in the startup kit) to the receptacle on the rear panel of each system module. Connect the hooded, male end of the FlexCart's electrical cables to the power strips on the back of the cart. Finally, connect each power strip's cable to a wall outlet operating on its own circuit.



#### FlexCart power connections (optional):

#### C External Connections

# **D** Solvent Considerations

This information applies to the ACQUITY UPLC I-Class IVD system modules.

Warning: To avoid injury, familiarize yourself with materials and their hazards, observe Good Laboratory Practice (GLP), and consult your organization's safety representative regarding proper use and handling. See the Material Safety Data Sheets for the solvents you use. Guidelines are provided in the latest edition of the National Research Council's publication, *Prudent Practices in the Laboratory: Handling and Disposal of Chemicals*.

**See also:** Controlling Contamination in Ultra Performance LC/MS and HPLC/MS Systems (part number 715001307).

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#### **Contents:**

# **Solvent guidelines**

# **Clean solvents**

Clean solvents ensure reproducible results and permit you to operate with minimal instrument maintenance.

Dirty solvents can cause baseline noise and drift, and they can clog solvent reservoir filters, inlet filters, and capillary lines.

# **Solvent quality**

Use MS-grade solvents for the best possible results. Filter solvents through a 0.2-µm membrane filter. Small particles can permanently block a system's capillary lines. Filtering solvents also improves check-valve performance.

**Recommendation:** Ensure that you choose solvents and membrane filters that are compatible with each other and that you follow the manufacturers' recommendations.

# Solvent preparation

Proper solvent preparation, primarily filtration, can prevent many pumping problems.

Store mobile phases in borosilicate glass reservoirs type 1, class  $A^2$  or type  $3.3^3$ . Use brown-stained glassware to inhibit microbial growth. Use aluminum foil or Waters caps to cover the reservoirs.

## Water

Use water only from a high-quality water purification system. If the water system does not deliver filtered water, filter the water through a  $0.2\mathchar`\mu m$  membrane filter.

Recommendation: Use MS-quality (or better) water.

**Caution:** To prevent the proliferation of microbial colonies that clog system filters and capillary lines, add a small amount (less than 10%) of an organic solvent, such as acetonitrile or methanol, and completely replace the mobile phase daily. Pure aqueous solvents must not remain in a shut-down system because they serve as a substrate for microbial growth.

## **Using buffers**

Adjust the pH of aqueous buffers. Filter them to remove insoluble material, and then blend them with appropriate organic modifiers. After you finish

using a buffer, flush it from the pump by running a wet-prime with at least five system volumes of HPLC-grade, distilled or deionized water.

To prevent microbial growth during shutdowns lasting longer than 24 h, flush the pump and solvent lines with a solution of organic solvent/water in which the organic component is greater than 20%.

**Caution:** To avoid damaging a mass spectrometer by unwittingly introducing incompatible buffers, consult the instrument's accompanying documentation to determine what buffers are compatible.

**Tip:** To avoid salt precipitation, nonvolatile buffer concentrations must not exceed 100 mM.

# Solvent recommendations

The ACQUITY UPLC I-Class IVD system was designed for reversed-phase chromatography and ACQUITY UPLC BEH column chemistries. Waters evaluated the system's reliability using traditional reversed-phase solvents.

This section lists solvents recommended for the ACQUITY UPLC I-Class IVD system. Contact Waters Customer Service to determine whether you can use solvents that do not appear in the list without adversely affecting instrument or system performance.

# **Recommended solvents**

- Acetonitrile
- Acetonitrile/water mixtures
- Isopropanol
- Methanol
- Methanol/water mixtures
- Water

# Solvents to avoid

Avoid these solvents:

- Solvents that contain halogens: chlorine, fluorine, bromine, or iodine.
- Strong acids. (Use them only in weak concentration, less than 5%, unless using them as cleaning agents. Avoid using acids as mobile phases when their pH is less than 2.0.)
- Solutions that contain strong concentrations (greater than 0.1% wt.) of complexing agents like ethylenediaminetetraacetic acid (EDTA).
- Compounds that form peroxides, such as UV-grade ethers, dioxane, and diisopropylether.

# **Recommended additives/modifiers**

- $\leq 0.3\%$  vol. acetic acid
- $\leq 50 \text{ mM}$  ammonium acetate
- $\leq 10 \text{ mM}$  ammonium bicarbonate
- ≤50 mM ammonium hydroxide
- ≤0.1% wt. ethylenediaminetetraacetic acid (EDTA)
- $\leq 0.2\%$  vol. formic acid
- ≤0.1% vol. heptafluorobutyric acid
- \* 1% to 4% aqueous solutions of hexafluorois opropanol (HFIP) for oligonucleotide applications



**Warning:** To avoid contact with corrosive material that can be present on instrument components HFIP damages, do not use HFIP in wash solvents.



**Caution:** To avoid damaging the instrument, do not use HFIP in wash solvents.

- $\leq 10 \text{ mM phosphate buffer}$
- $\leq 0.1\%$  vol. triethyl amine (TEA)
- ≤0.1% vol. trifluoroacetic acid (TFA)

## **Recommended sample diluents**

- Acetonitrile
- Acetonitrile/water mixtures
- Chloroform
- Dimethylformamide (DMF)
- Dimethyl sulfoxide (DMSO)
- Isooctane
- Isopropanol
- Methanol
- Methanol/water mixtures
- Methylene chloride
- Water

## **Recommended cleaning agents**

You may use these cleaning agents:

- Formic acid ( $\leq 10\%$ )
- Phosphoric acid ( $\leq 30\%$ )
- Sodium hydroxide ( $\leq 1$  M)

# System recommendations

# **ACQUITY UPLC I-Class IVD system recommendations**

- **Caution:** To prevent the proliferation of microbial colonies that clog system filters and capillary lines, add a small amount (less than 10%) of an organic solvent, such as acetonitrile or methanol, and completely replace the mobile phase daily. Aqueous solvents must not remain in a shut-down system because they serve as a substrate for microbial growth.
- Contact Waters for recommended system cleaning and flushing procedures.
- Contact your Waters sales representative or local technical support organization to determine the typical chromatography conditions and/or instrument operating parameters suitable for the ACQUITY I-Class IVD system.
- Chloroform, methylene chloride, halogenated solvents, and toluene can be used in weak dilutions (less than 10% vol.) as additives, modifiers, or sample diluents.
- Methanesulfonic acid is *not* recommended for use in ACQUITY UPLC I-Class IVD systems.
- Always use properly cleaned and maintained glassware.

## **Binary solvent manager recommendations**

- The seal wash system must never run dry, particularly during separations that use a polar mobile phase.
- For reversed-phase applications, use aqueous seal wash solutions with a weak organic component (for example 1:9 methanol/water).
- Do not use nonvolatile buffers as seal wash solvents.
- Ensure that the mobile phase is completely soluble in and compatible with all of the solvents in use on the system.

## Sample manager recommendations

- Typical organic sample diluents such as dimethylsulfoxide (DMSO) and dimethylformamide (DMF) are supported.
- Do not use buffers as needle wash solvents. You can use acids and bases.

# **Properties of common solvents**

The following table lists the properties for some common chromatographic solvents:

Solvent	Vapor Pressure mm Hg (Torr)	Boiling Point (°C)	Flash Point (°C)
Acetonitrile	88.8 at 25 °C	81.6	6
<i>n</i> -butyl acetate	7.8 at 20 °C	126.11	22
<i>n</i> -butyl alcohol	4.4 at 20 °C	117.5	37
<i>n</i> -butyl chloride	80.1 at 20 °C	78.44	-9
Chlorobenzene	8.8 at 20 °C	131.69	28
Chloroform	158.4 at 20 °C	61.15	none
Cyclohexane	77.5 at 20 °C	80.72	-20
Cyclopentane	400 at 20 °C	49.26	-7
o-Dichlorobenzene	1.2 at 20 °C	180.48	66
Dichloromethane	350 at 20 °C	39.75	none
Dimethyl acetamide	1.3 at 25 °C	166.1	70
N,N-Dimethylformamide	2.7 at 20 °C	153.0	58
Dimethyl sulfoxide	0.6 at 25 °C	189.0	88
1,4-Dioxane	29 at 20 °C	101.32	12
Ethyl alcohol	43.9 at 20 °C	78.32	15
Ethyl ether	442 at 20°C	34.55	-45
Ethylene dichloride	83.35 at 20 °C	83.48	13
Heptane	35.5 at 20 °C	98.43	-4
Iso-octane	41 at 20 °C	99.24	-12

#### **Properties of common solvents:**

Solvent	Vapor Pressure mm Hg (Torr)	Boiling Point (°C)	Flash Point (°C)
Isobutyl alcohol	8.8 at 20 °C	107.7	28
Isopropyl alcohol	32.4 at 20 °C	82.26	12
Isopropyl myristate	<1 at 20 °C	192.6	164
Methanol	97 at 20 °C	64.7	11
Methyl <i>t</i> -butyl ether	240 at 20 °C	55.2	-28
Methyl ethyl ketone	74 at 20 °C	79.64	-9
Methyl isobutyl ketone	16 at 20 °C	117.4	18
N-Methylpyrrolidone	0.33 at 25 °C	202.0	86
Pentane	420 at 20 °C	36.07	-49
<i>n</i> -Propyl alcohol	15 at 20 °C	97.2	23
Propylene carbonate	0.13 at 20 °C	241.7	135
Pyridine	18 at 25 °C	115.25	20
Toluene	28.5 at 20 °C	110.62	4
1,2,4-Trichlorobenzene	1 at 20 °C	213.5	106
Triethylamine	57 at 25 °C	89.5	-9
Trifluoroacetic acid	97.5 at 20 °C	71.8	-3
Water	17.54 at 20 °C	100.0	
o-xylene	6 at 20 °C	144.41	17

#### **Properties of common solvents: (Continued)**

# **Solvent miscibility**

Before you change solvents, refer to the table below to determine solvent miscibility. Be aware of these effects:

- Changes involving two miscible solvents can be made directly. Changes involving two solvents that are not totally miscible (for example, from chloroform to water) require an intermediate solvent like *n*-propanol.
- When you switch from a strong buffer to an organic solvent, thoroughly flush the system using water before you add the organic solvent (see "Water" on page 82).

- Temperature affects solvent miscibility. If you are running a high-temperature application, consider the effect of the higher temperature on solvent solubility.
- Buffers dissolved in water can precipitate when mixed with organic solvents.

Polarity index	Solvent	Viscosity cP, 20 °C (@1 atm)	Boiling point °C (@1 atm)	Miscibility number (M)	$\lambda$ Cutoff (nm)
0.0	N-hexane	0.313	68.7	29	—
1.8	Triethylamine	0.38	89.5	26	—
4.3	1-propanol	2.30	97.2	15	210
4.3	2-propanol	2.35	117.7	15	—
5.2	Ethanol	1.20	78.3	14	210
5.5	Benzyl alcohol	5.80	205.5	13	—
5.7	Methoxyethanol	1.72	124.6	13	—
6.2	Acetonitrile	0.37	81.6	11, 17	190
6.2	Acetic acid	1.26	117.9	14	—
6.4	Dimethylformamide	0.90	153.0	12	—
6.5	Dimethylsulfoxide	2.24	189.0	9	—
6.6	Methanol	0.60	64.7	12	210
9.0	Water	1.00	100.0	_	_

#### Solvent miscibility:

## Using miscibility numbers (M-numbers)

Use miscibility numbers (M-numbers) to predict the miscibility of a liquid with a standard solvent.

To predict the miscibility of two liquids, subtract the smaller M-number value from the larger M-number value.

- When the difference between the two M-numbers is 15 or less, the two liquids are miscible, in all proportions, at 15°C.
- A difference of 16 indicates a critical solution temperature from 25 to 75 °C, with 50 °C as the optimal temperature.

• When the difference is 17 or greater, the liquids are immiscible, or their critical solution temperature is above 75  $^{\circ}$ C.

Some solvents prove immiscible with solvents at both ends of the lipophilicity scale. These solvents receive a dual M-number:

- The first number, always lower than 16, indicates the degree of miscibility with highly lipophilic solvents.
- The second number applies to the opposite end of the scale. A large difference between these two numbers indicates a limited range of miscibility.

For example, some fluorocarbons are immiscible with all the standard solvents and have M-numbers of 0 and 32. Two liquids with dual M-numbers are usually miscible with each other.

A liquid is classified in the M-number system by testing for miscibility with a sequence of standard solvents. A correction term of 15 units is then either added or subtracted from the cutoff point for miscibility.

# **Solvent viscosity**

Generally, viscosity is not a consideration when you operate with a single solvent or under low pressure. However, with gradient chromatography, the viscosity changes that occur as the solvents are mixed in different proportions can effect pressure changes during the run. For example, a 1:1 water/methanol mixture produces twice the pressure of either water or methanol alone.

If you do not know the extent to which pressure changes affect the analysis, monitor the pressure during the run.

# E FlexCart Assembly

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# Assembling the FlexCart

If your system includes the optional FlexCart, follow the procedure below to unpack and assemble it.

**Recommendation:** Because the assembled system weighs at least 140.6 kg, Waters recommends that you assemble the instruments and components on the FlexCart.

#### To assemble the FlexCart

1. Remove the contents from the box packaged in the FlexCart.

**Tip:** The box contains the monitor arm, the bolts used to attach the monitor arm to the base, and an IBM instruction book for converting the monitor from stand-alone to arm-mounted.

#### **FlexCart components:**



2. Remove the 4 Phillips screws from the support plate at the rear of the monitor, and mount the monitor onto the movable arm assembly. Refer to the IBM instruction book, if necessary.



- 3. Loosen the 2 T25 TORX screws, at the bottom left-hand side of the cart, that secure the bracket for the CPU.
- 4. Attach the power and video cables to the CPU, and place it in position on the bottom shelf of the cart.
- 5. Route the monitor's power and video cables through the plastic channel provided, and plug them into the monitor. Refer to the IBM instruction book, if necessary.
- 6. Insert the keyboard shelf's 2 captive thumbscrews into slots on the cart's front panel at a level that affords comfortable and safe operation. Turn the thumbscrews 1/4-turn clockwise to lock the position of the shelf.



# Adjusting the FlexCart's height

## To adjust the cart's height:

- 1. Loosen the side lock knobs before raising or lowering the top portion of the cart.
- 2. Remove the crank handle from its storage brackets on the lower right-hand side of the cart.

3. Insert the crank handle into the bottom front of the cart, and turn it to raise or lower the cart.



**Tip:** If your system includes a mass spectrometer and it is positioned on the right-hand side of the system stack, set the cart to a height that minimizes the length of tubing needed between the instruments stacked on the cart and the mass spectrometer.

- 4. Tighten the side lock knobs after reaching the desired height.
- 5. Loosen the keyboard shelf's 2 captive thumbscrews on the cart's front panel.
- 6. Move the keyboard to a level that provides comfortable and safe operation. Turn the thumbscrews 1/4-turn clockwise to lock the position of the shelf.

# Locking the FlexCart in place

#### To lock the FlexCart in place:

Lock the cart by depressing the lock pedal located at the front of the cart.

## To release the FlexCart floor lock brake:

Release the cart by depressing the brake release bar located at the front of the cart.



# Moving the assembled FlexCart

**Caution:** To avoid spills of damaging solvent, remove all solvent reservoirs from the solvent tray before moving the cart.



**Caution:** To avoid striking low doorways, lower the cart fully before moving it.



**Caution:** To avoid toppling the instruments stacked on the cart, do not move the cart by pushing on them.

Once it is assembled, you can move the cart to other areas of a lab to minimize tubing runs between the ACQUITY UPLC instruments and a mass spectrometer. Use the lip on top of the cart to pull it.



## E FlexCart Assembly