ACQUITY UPLC® System Hexane / Tetrahydrofuran Compatibility Kits

Why are there two versions?

There are two ACQUITY UPLC System Hexane/Tetrahydrofuran kits: one supporting ACQUITY UPLC Binary Solvent Managers with passive check valves and one supporting ACQUITY UPLC Binary Solvent Managers with Intelligent Intake Valves (iValves), as follows:

- Part Number 205000464 for passive check valves
- Part Number 205000551 for iValves

What’s included in these release notes

The ACQUITY UPLC System Hexane/Tetrahydrofuran kit is required for the proper operation of the ACQUITY UPLC System when Hexane and Tetrahydrofuran are used regularly as mobile phase components. There are two kits: one for systems that have an ACQUITY UPLC Binary Solvent Manager with passive check valves and one for systems that have an ACQUITY UPLC Binary Solvent Manager with the Intelligent Intake Valves (iValve).

Supported ACQUITY, ICS, and firmware versions

All existing ACQUITY UPLC hardware and ACQUITY UPLC ICOP (Instrument Control Option Pack) versions 1.30 and higher and ACQUITY UPLC Module firmware versions 1.30 are recommended with the ACQUITY UPLC System Hexane/THF kits. The ACQUITY UPLC System Hexane/THF kits are compatible with the ACQUITY UPLC System 1.20A, 1.23A, 1.23B ICOPs, and the ACQUITY UPLC System 1.30 driver.

Solvent Compatibility

The ACQUITY UPLC System can now support the use of Hexane and Tetrahydrofuran in mobile phases.

Note: Both Hexane and Tetrahydrofuran have low boiling points. Specifically, Hexane = 68.7°C and Tetrahydrofuran = 66°C. The ACQUITY UPLC Column Modules are capable of running up to a maximum of 90°C. It is not recommended to exceed the boiling point of any solvents, including Hexane or Tetrahydrofuran.

The ACQUITY UPLC Instrument Software allows you to set maximum limits for column temperature values within a method. It is recommended that these limits are used when the method uses mobile phases that contain either Hexane or Tetrahydrofuran.
The ACQUITY UPLC System supported Solvents

The following solvents are supported with ACQUITY UPLC Systems:

- Methanol
- Water
- Acetonitrile
- Isopropanol (I.P.A.)
- Tetrahydrofuran (THF)
- Hexane

The ACQUITY UPLC System supported Sample Diluents

The following solvents are supported, in addition to those above with ACQUITY UPLC Systems:

- Dimethyl sulfoxide (DMSO)
- Dimethylformamide (DMF)

The ACQUITY UPLC System supported Mobile Phase Additives or Modifiers

The following additives or modifiers are supported, in addition to those above with ACQUITY UPLC Systems:

- 0.2% Formic Acid
- 0.1% trifluoroacetic acid (TFA)
- 0.1% triethyl amine (TEA)
- 0.1% hexafluorobuteric acid
- 10mM phosphate buffer
- 10mM ammonium bicarbonate
- 50mM ammonium hydroxide
- 50mM ammonium acetate
- 0.1% Ethylenediaminetetraacetic acid (EDTA)

The ACQUITY UPLC System supported Cleaning Agents

The following cleaning agents are supported, in addition to those above with ACQUITY UPLC Systems:

- Phosphoric acid (≈30%)
- Sodium hydroxide (≈1M)
The ACQUITY UPLC System unsupported Solvents

The following solvents are not supported with ACQUITY UPLC Systems:

- Methylene-Chloride
- Chloroform
- Ethyl Acetate
- Toluene
- Chlorinated solvents, including Trichlorobenzene
- Strong acids >5%

**Note:** The use of buffers, acids, and bases should be avoided as needle wash solvents. However, for some samples it may be necessary to address solubility and carryover effects by adding needle wash solvent additives that change pH or ionic strength.

Running Hexane and THF with ACQUITY UPLC Systems

Because both hexane and THF are low viscosity and low surface tension solvents, the following recommendations for general operation should be followed:

- The use of Full loop injection mode
- For Needle and Loop characterization large air gaps (≥ 4µL) are required. The value for the air gaps should be entered in the Sample Manager method loaded prior to beginning the calibration procedure. A zero flow rate method can be created with the appropriate air-gap values and then applied using the “Setup” function. Needle and Loop Characterization can then be initiated.
- For Hexane, the ACQUITY UPLC System backpressure should not be allowed to exceed 12,000 psi.

**Note:** ACQUITY UPLC System performance will be impacted by use of low viscosity solvents, particularly Hexane, as the system was initially designed for use with reversed phase solvents. Lower viscosity solvents may lead to greater dispersion and transfer loss during sample aspiration into the sample loop.

**Note:** Highly volatile solvents such as Tetrahydrofuran and Hexane are supported with the current Closed Waste ACQUITY UPLC system configurations only. This includes:

- ACQUITY UPLC Binary Solvent Managers with serial numbers above J05UPB131M
- ACQUITY UPLC Sample Managers with serial numbers above J05UPS051M.
- ACQUITY UPLC System modules with serial numbers below this cut-off do not have the current closed process waste design and are not supported for use with Tetrahydrofuran, Hexane, or any volatile solvent.

**Note:** For ACQUITY UPLC Sample Manager with serial Numbers below C07UPS695M and for ACQUITY UPLC Autosamplers with serial Numbers below C07UPA335M, it is recommended that the upgrade be performed at a Waters repair depot. This is because the needlewash pump tubing is difficult to replace with Hexane or THF compatible tubing. Instruments after this date have compatible tubing already installed.
Supported Configurations for ACQUITY UPLC Systems Running Hexane and THF with:

- The ACQUITY UPLC with single Column Heater, High Temperature Column Heater, the 30 cm Column Heater/Cooler or Column Heater/Cooler is supported. The Column Manager (Left or Right versions), is NOT supported because the module uses PEEK tubing at the outlet of each column. These outlet lines are required for passive solvent cooling and are not recommended for use with these solvents.

ACQUITY UPLC System Qualification

Note: For ACQUITY UPLC Software versions 1.23B or earlier, the Connections AQT for the Waters ACQUITY UPLC® Systems supports use of the standard PEEK needle only, (30µL PEEK Needle 700002644).

Both the stainless steel needle and the PEEK Needle produce linear calibration curves for caffeine used for the AQT. However the X-intercept may be larger for the stainless steel needle. A more positive x-intercept (SAA) indicates that there is a greater degree of dispersion in the sample as it is drawn through the needle; this has a greater effect on lower volume injections. This results in a decrease in peak areas for low volumes and a potential to fail the test, (to pass the Automated Qualification Test, Injector Accuracy value must be ≤ 200 nL).

To use the stainless steel needle with Connections AQT for the Waters ACQUITY UPLC® System, Waters recommends that the ACQUITY UPLC Sample Manager firmware should be updated to version 1.30 by the Waters Field Service Engineer performing the kit installation. The ACQUITY UPLC Sample Manager Firmware version 1.30 uses an increased Needle Overfill Flush volume, which decreases the X-intercept value.
ACQUITY UPLC System Diagnostics

The ACQUITY UPLC Binary Solvent Manager Diagnostics using Hexane

The ACQUITY UPLC Binary Solvent Manager Diagnostics Tests should be run at 12,000 psi. This value can be set in the ACQUITY UPLC Console software.

![Static Decay Test](image)

![Dynamic Leak Test](image)