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Making UPLC-MS Accessible Through MassLynx Software

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This is an Application Brief and does not contain a detailed Experimental section.

Abstract

This application brief demonstrates that with a few simple steps, Waters' LC-MS instruments, both quadrupoles and TOFs, can be set up and sample schedules run.

Benefits

- IntelliStart's intuitive and easy-to-use software makes Waters LC-MS systems accessible to a wide variety of users.
- The consistent operation across all instruments minimizes training requirements for analysts, and maximizes the flexibility and efficiency with which a laboratory can operate.

Introduction

Waters' instruments and software have been developed with Engineered Simplicity at the core of the design — from the Xevo family's universal source, to the IntelliStart program within MassLynx Software. The simplicity of use however, has not compromised the analytical power, reliability, or sensitivity in any way.

A mass spectrometer is a versatile and powerful detector that can provide quantification, identification, and structural information about an analyte. The utility of mass spectrometry (MS) is further enhanced by coupling the technique with either gas chromatography (GC) or liquid chromatography (LC) for separation prior to detection. While alternative detectors, such as UV, give some structural information they heavily rely on chromatographic separation and retention time for quantification and identification. Retention times can show variability for a variety of reasons, such as sample matrices, mobile phase preparation, and column degradation.

An added consideration when using chromatographic retention time for identification, is different compounds can elute at the same time. This is independent of the detector being used, but the extra identification power of an MS detector significantly reduces the risk of analytes being misidentified.

When using an MS detector it is often possible to deconvolute and quantify by mass, which offers significant benefits. For example, reporting results for routine analysis or quality control may be quicker as less interpretation is required due to the extra selectivity and identification confidence from the MS.

This application brief will demonstrate that with only minimal training, a competent laboratory technician can confidently set up and run many of Waters' mass spectrometers with UltraPerformance LC.

Program Features

IntelliStart – Intuitive software to start up, tune, and calibrate Waters' mass spectrometers.

- Calibration – Step-by-step wizards for fast MS calibration, including LockSpray and mass resolution settings, resulting in a clear pass or fail.
- LC set up – Ideal for QC laboratories and routine analysis. The instrument will switch out of standby, and run check samples to a designated schedule.
- Sample tuning – Automated analyte tuning and MS method building. Project Wizard – Projects contain sample lists and methods and can be saved as templates when necessary, increasing efficiency and reducing potential transcription errors.

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ACQUITY UPLC System with Xevo TQ-S MS.

Results and Discussion

IntelliStart

IntelliStart is a feature within Waters MassLynx Software to aid calibrating the instrument, checking the system, and method development. The program uses wizards to provide simple and intuitive workflows that are consistent across all tasks on quadrupole instruments and Time-of-Flight (TOF) instruments.

Setting up with IntelliStart

From the ACQUITY UPLC Console it is possible to control LC and MS systems; Figure 1 shows the ACQUITY UPLC Console home page. By expanding the options in the top left corner, IntelliStart can be quickly and easily opened. IntelliStart offers several features, such as Instrument Setup (including calibration and resolution settings), Development, and Systems Checks.

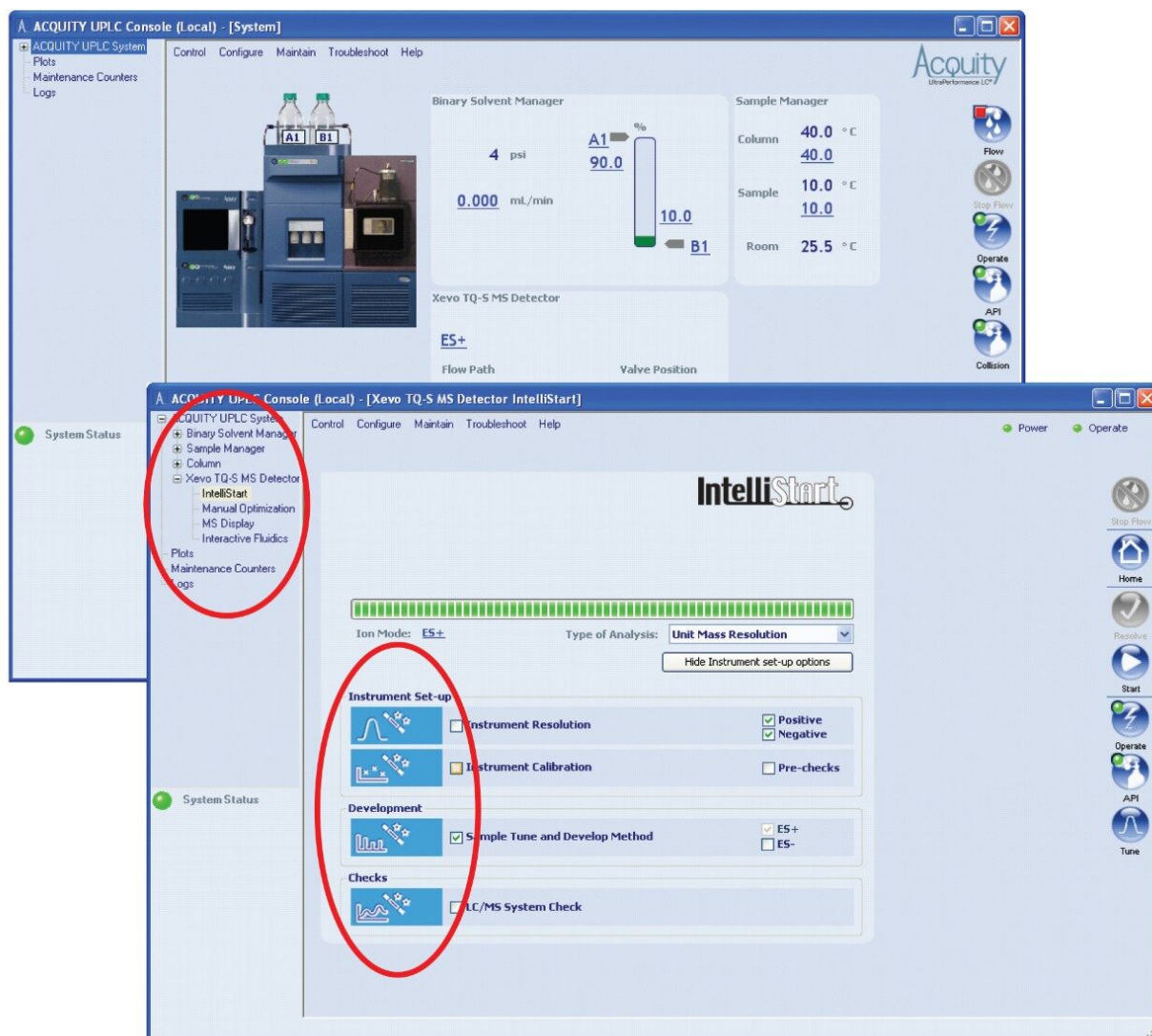


Figure 1. ACQUITY UPLC Console home page and IntelliStart window.

By simply checking the box for the procedure that you wish to carry out and clicking Start on the right side, IntelliStart will open up a wizard. The wizard has the same format for all procedures and all instruments, including single quadrupole (SQ), tandem quadrupole (TQ), TOF, and Q-TOF systems.

The wizard asks just a few questions that are appropriate for the specific mass spectrometer being used and the task, such as ionization mode, Single Ion Recording (SIR), or Multiple Reaction Monitoring (MRM). Figure 2 shows a typical workflow, this example is a Xevo G2 QToF LockSpray calibration – a patented technology enabling automated exact mass measurement on Waters' TOF instruments.

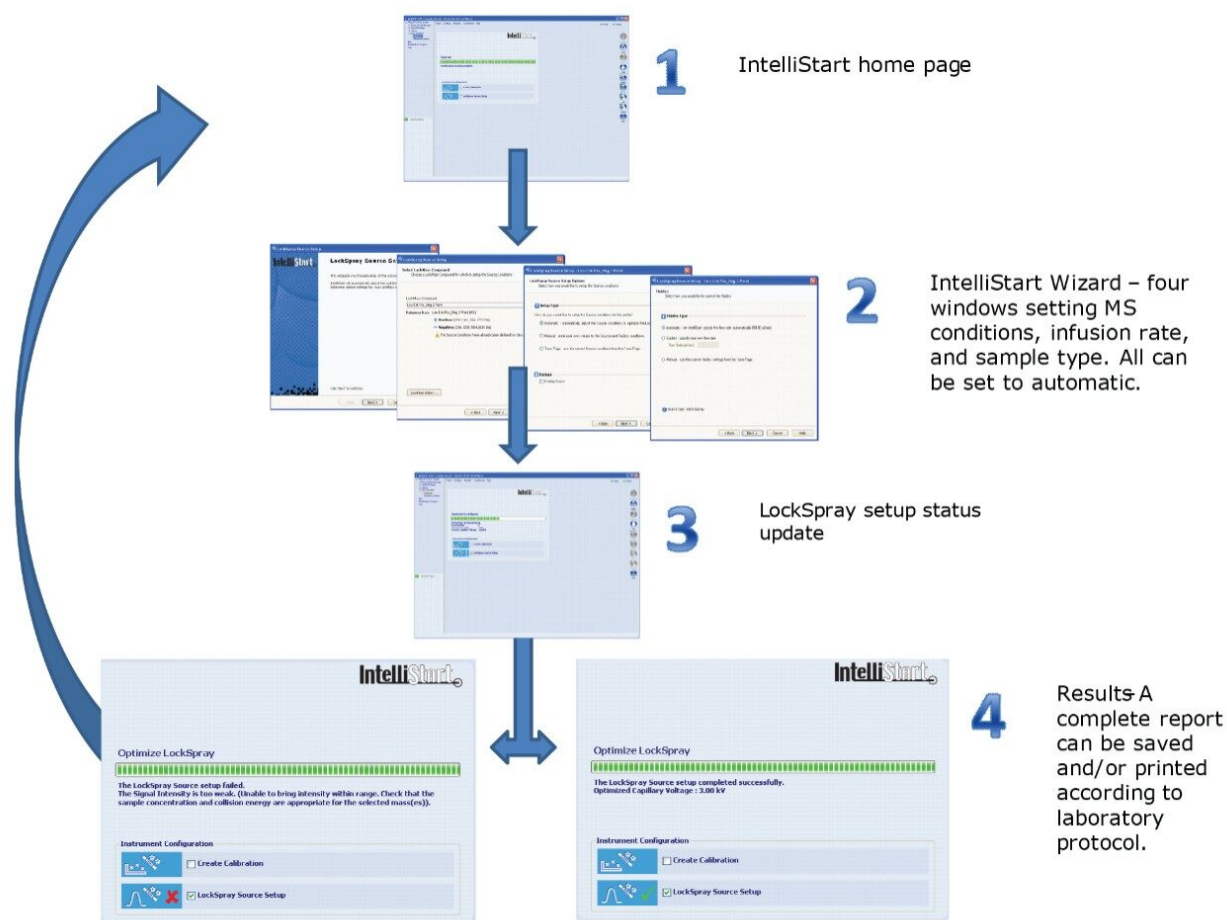


Figure 2. A typical IntelliStart workflow using LockSpray setup on Xevo G2 Q-ToF as an example. The setup that passed was done using automatic conditions. The failed setup was run with a 10-fold decrease in the infusion rate, causing a low response, and hence a fail to be reported.

Running samples using the Project Wizard

MassLynx Software has a wizard that quickly and easily sets up new projects and sample lists. Figure 3 shows the three steps that are required, and the options available to the user.

1. The Project Wizard can be found in the File drop-down menu.
2. The user is then asked for a project name and description of the analysis being carried out to make data as easy as possible to find.
3. The wizard then gives the user three options:
 - Create new project – which will start a blank default project.

- Create using current project as template – with the added option to copy the sample list.
- Create using an existing project.

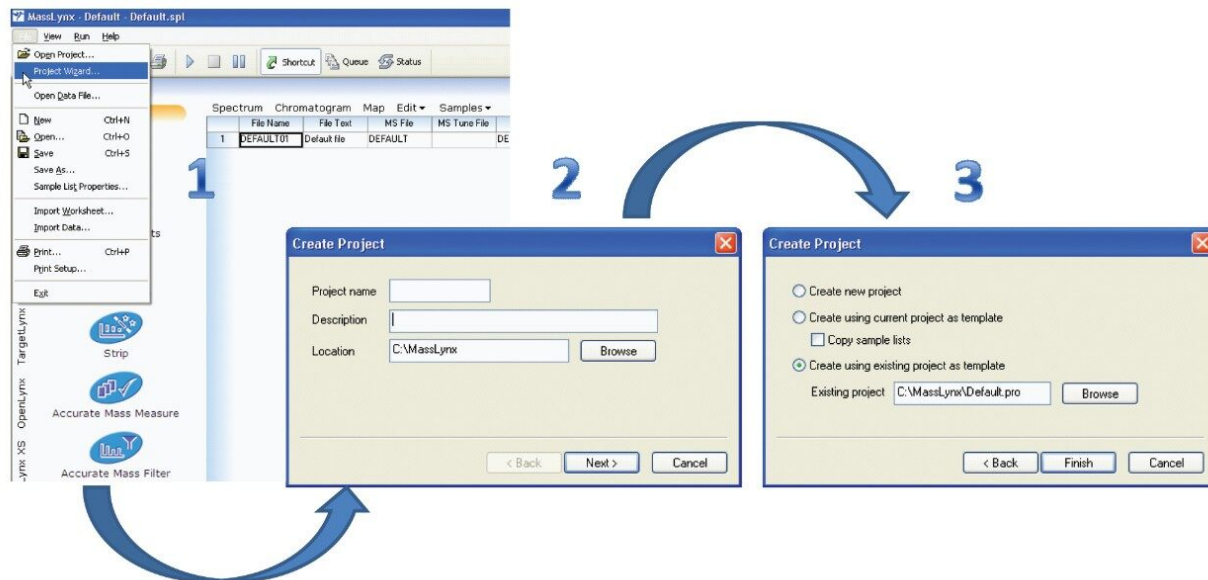


Figure 3. Setting up a project in MassLynx Software.

Step 3 of the Project Wizard is extremely useful for routine analysis and Quality Control laboratories. A project contains LC and MS method conditions and sample list(s). Transferring this information directly into a new project reduces the potential for transcription and method selection errors.

IntelliStart has a System Check function that can automatically run quality control and system check samples at designated intervals. The results can be printed and/or saved according to laboratory protocol. This gives analysts added confidence in the reliability of the results reported and the robustness of the system. Figure 4 shows the IntelliStart window for the System Check Schedule. If the operator decides to use this setting the time of day and the day of the week can be chosen, enabling minimum disruption to the running of samples.

System Check Schedule

LCMS System Check

System Check Type

Pre Run Vial

Run Vial Print Report

Schedule

Run: Time

Off

Daily

Weekly

Figure 4. System Check Schedule.

Using the IntelliStart and the Project Wizard procedures discussed so far, it is possible for an operator to start up an instrument and run a sequence. Assuming that a laboratory has established methods, the initial instrument setup is very similar to an LC system coupled to other detectors, such as a Photodiode Array

(PDA) or a Fluorescence (FLR) detector.

Automated MS method development

IntelliStart's Sample Tuning and Develop Method can tune and optimize a mixture of up to four compounds in a single operation. Once the tuning has successfully completed, a report is generated, and the conditions can be automatically imported into an MS method. This is useful for new users, but also saves valuable time for more experienced mass spectrometrists.

The Waters ACQUITY mass spectrometers along with the Xevo and SYNAPT families have integrated fluidics. Up to three vessels containing sample solutions and calibration solutions can be placed on the system at any one time. This means that calibration solutions can be left on the instrument reducing the likelihood of contamination.

Figure 5 shows three captured screen shots of the Sample Tuning and Develop Method process. The IntelliStart Wizard requires three types of information. Most of the information is entered using check boxes and dropdown lists for ease of use and to limit potential errors. The procedure will optimize cone voltages, search for precursors and fragment ions, and then inform the user that the operation has been successful, indicated by the green check mark.

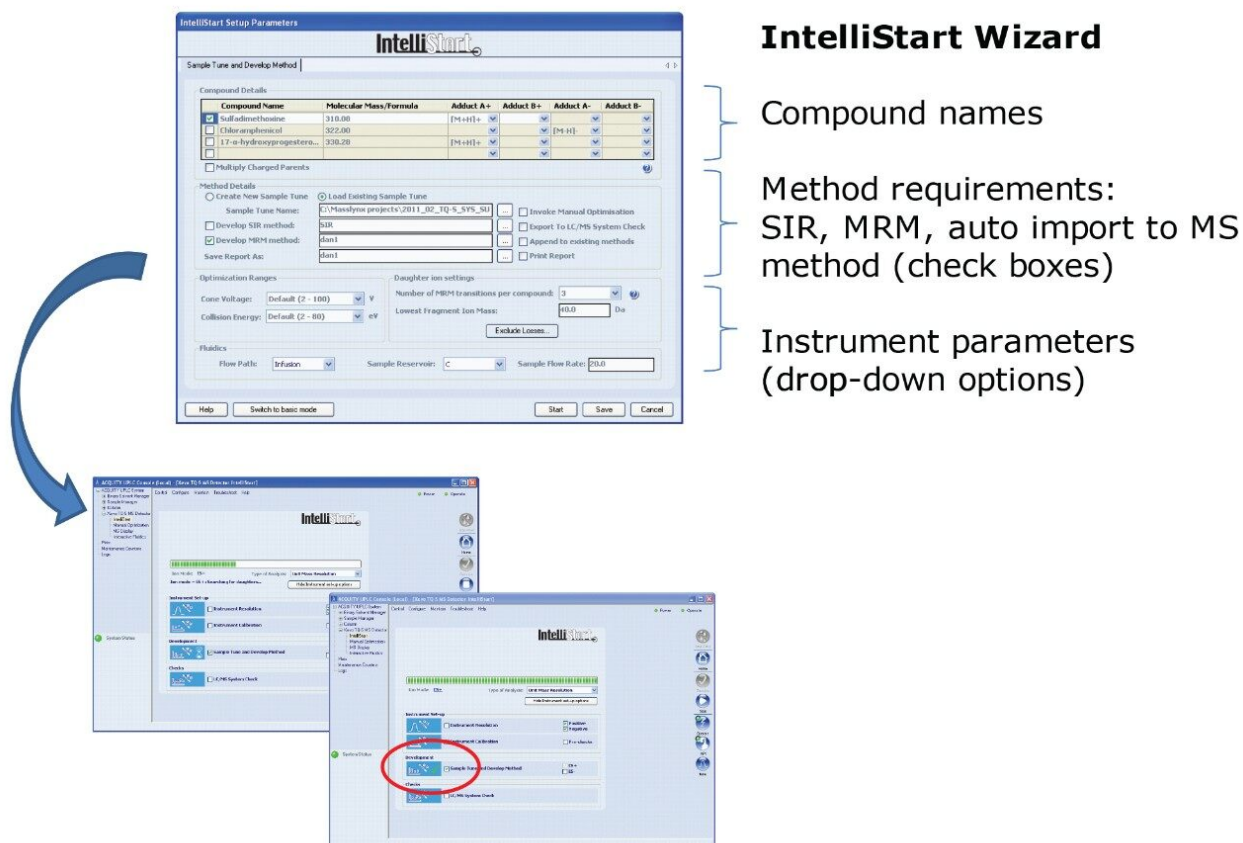


Figure 5. Three captured screen shots for Sample Tuning and Method Development in progress on a Xevo TQ-S.

Conclusion

A mass spectrometer is a very versatile and powerful detector offering quantification, identification, and structural information. IntelliStart within MassLynx Software is designed to make the operation of MS as accessible as possible. This application brief demonstrates that with a few simple steps, Waters' LC-MS instruments, both quadrupoles and TOFs, can be set up and sample schedules run.

Method development steps for the MS detector have been integrated within IntelliStart, and use the same approach as the rest of IntelliStart. For new users it makes compound tuning and optimization a simple task and reproducible from one operator to another. For experienced MS users, this is a valuable time-saving tool.

IntelliStart's intuitive and easy-to-use software makes Waters LC-MS systems accessible to a wide variety of users. The consistent operation across all instruments minimizes training requirements for analysts, and maximizes the flexibility and efficiency with which a laboratory can operate.

Featured Products

[ACQUITY UPLC System <https://www.waters.com/514207>](https://www.waters.com/514207)

[Xevo TQ-S <https://www.waters.com/10160596>](https://www.waters.com/10160596)

[MassLynx MS Software <https://www.waters.com/513662>](https://www.waters.com/513662)

720004087, September 2011