

Seamless Integration of an HPLC System with Most Common MS Platforms

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ABSTRACT

In this poster we present a new approach for integrating HPLC instrument control seamlessly into the most common mass spectrometry platforms. The introduced software tool preserves the familiar environment for MS⁽ⁿ⁾ users when it comes to MS method setup and data analysis. With respect to LC instrument control, the software tool opens a new window dedicated to chromatography that allows the editing of complex HPLC instrument methods in a user-friendly way.

The poster shows how to connect HPLC systems to MS software like Analyst[®] (ABI), Xcalibur[™] (Thermo), and HyStar[™] (Bruker). This concept allows the MS user to control Dionex HPLC front ends without leaving their familiar MS software where they can also process the acquired UV data. Therefore, a significantly better HPLC/MS system integration can be achieved.

THE CHALLENGE: MS Software Has Limited HPLC Control Features, HPLC Software Has Limited MS Data Processing Features

Advanced mass spectrometers, like triple quadrupole, Q-TOF (quadrupole – time of flight), or ion trap devices are for most analytical purposes equipped with an HPLC front end. In fact, the importance of chromatographic separations in the liquid phase prior to MS or MS⁽ⁿ⁾ is increasingly recognized. Chromatographic separation is needed, for example, to overcome:

- Suppression effects, commonly observed with atmospheric pressure MS sources
- Isomeric interferences in samples of high complexity

For many analytical tasks a combination of high resolution chromatography with sophisticated MS techniques is required. Nevertheless, this attractive hyphenation still struggles with the fact that the MS and HPLC worlds are not yet perfectly merged. Available software for instrument control and data analysis is generally focused either on MS or LC interests, with no total solution available.

What Level of HPLC Instrument Control Would Be Optimal?

The MS software Analyst (ABI), Xcalibur (Thermo), and HyStar (Bruker) allows for excellent control of the MS instrumentation. There is almost no limitation for routine applications as well as sophisticated research experiments (e.g., polarity can be switched on the fly) and ion exclusion lists increase throughput.

But to use the HPLC/MS system to full capacity, a similar level of control of the HPLC instrumentation is desired. For example:

- Different autosampler injection routines (full-loop, partial-loop, μ L pick-up) support either highest precision or lowest sample consumption. Therefore the right choice of the injection routine determines the success of the whole HPLC/MS experiment.
- Another example applies to complex samples. In this case column switching techniques (multidimensional HPLC) reduce sample complexity. As a result, lower ion suppression effects result in better MS performance.

THE SOLUTION: DCMS^{Link} – A Software Plug-in for Single-Point Control of HPLC Instruments from Various MS Software

Supported Chromatography Hardware and MS Software

The Dionex Chromatography Mass Spectrometry Link (DCMS^{Link}) provides an interface for controlling a wide range of Dionex chromatography instruments from the following third party mass spectrometry software:

- Analyst from ABI/Sciex
- HyStar from Bruker
- Xcalibur from Thermo

Principle

DCMS^{Link} is based on existing Chromeleon® technology. It installs and uses certain portions of the Chromeleon Chromatography Management System such as the Chromeleon Server Configuration and Program Editor. Installation qualification is also managed via Chromeleon tools.

When DCMS^{Link} is installed, the MS software takes care of:

- Data acquisition
- Data processing
- Reporting

The following easy to use, yet powerful functions for Dionex HPLCs become available from the MS software via DCMS^{Link}:

- Method creation via a DCMS^{Link} Program Wizard
- Method editing via a DCMS^{Link} Program Editor
- Direct Instrument control (such as setting the flow and detector wavelength) through dedicated command dialogs

WORKFLOW EXAMPLE

1. Hardware Configuration

As a first step all HPLC modules must be configured. The Chromeleon Server Configuration editor (Figure 1) allows users to easily add, remove, or reconfigure HPLC modules. Important hardware settings such as autosampler loop size or syringe sizes can be defined (Figure 2). The final version of the hardware configuration is then saved. Changes can easily be made if the hardware configuration changes (e.g., if a different loop size is used).

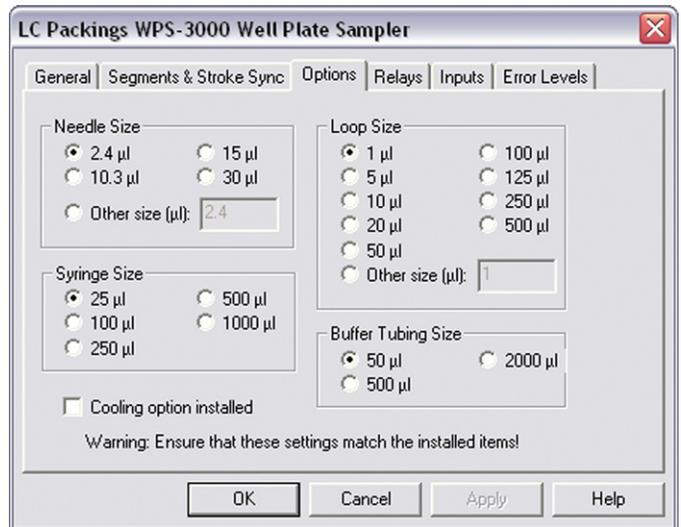


Figure 2. Defining important hardware settings such as autosampler loop size via the corresponding module's Properties dialog.

2. Method Creation

The Program Wizard helps even experienced HPLC users generate new HPLC methods for use with an MS in a convenient way. All important parameters (e.g., gradient profile (Figure 3), total runtime, or injection routines) can be defined and saved afterwards. After finishing the method creation, a dedicated "Ready check" informs users if there are any inconsistencies (Figure 4).

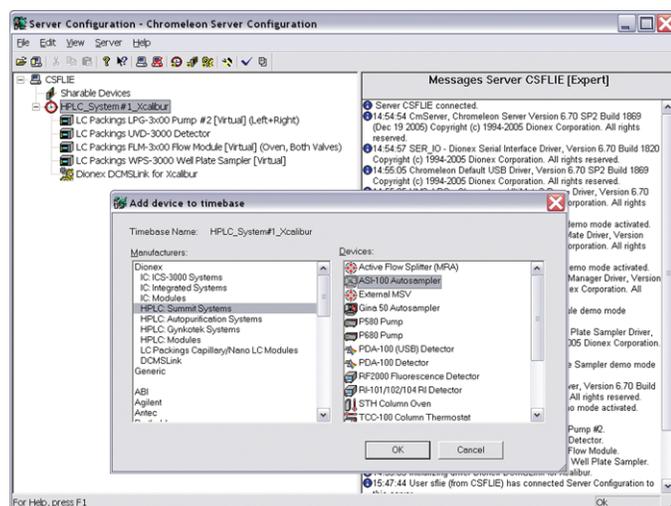


Figure 1. Chromeleon Server Configuration Editor window. DCMS^{Link} supports a wide range of Dionex / LC Packings Chromatography instruments. The example HPLC system consists of four modules plus one of the MS software specific synchronization drivers (i.e., "Dionex DCMS^{Link} for Xcalibur", "Dionex DCMS^{Link} for Analyst", or "Dionex DCMS^{Link} for HyStar"). By double-clicking on one of the modules a corresponding dialog appears for all module settings (Figure 2).

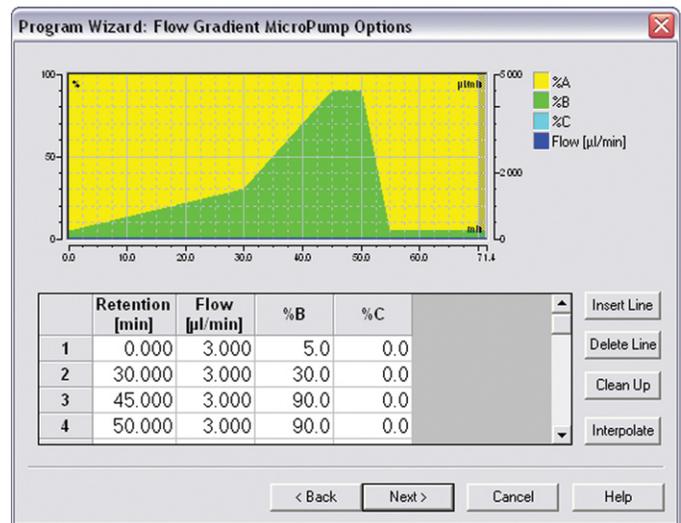


Figure 3. Method creation via the Program Wizard. An intuitive user interface allows for the simple creation of complicated methods.

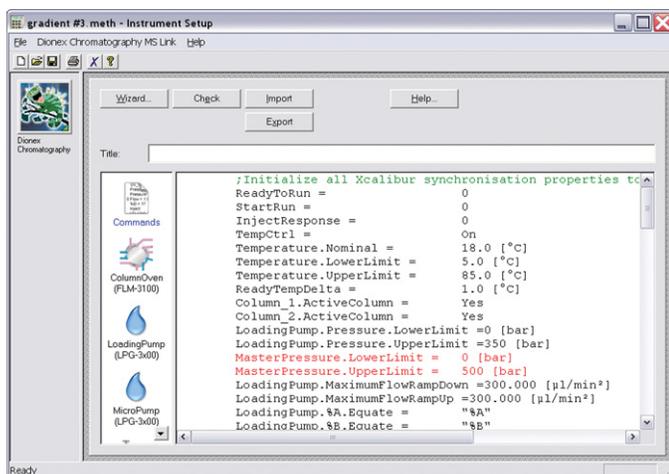


Figure 4. "Ready Check" function for easier method creation and editing. Inconsistencies are detected and indicated in red. In this example the minimum and maximum pressure limits were not set properly by the user. Double-clicking on the relevant command line shows the allowed values in dialogs similar to Figure 6.

3. Method Editing

Saved methods can be easily edited via the Program Editor (Figure 5).

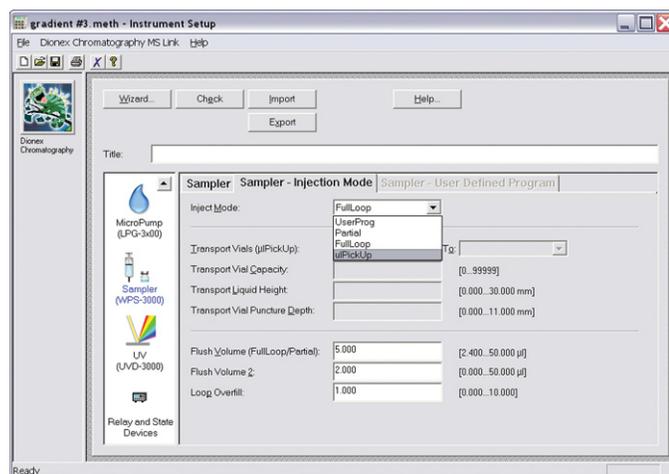


Figure 5. Easy and fast method editing in device specific dialogs. In this example after clicking on the Sampler (WPS-3000) button on the left, a sampler specific dialog with three tabs appeared. Using the pull-down menu it is now possible to change the injection routine (e.g., from full-loop to partial-loop).

4. Direct Control of Instrument Settings

Before starting the HPLC/MS experiments the HPLC system can be directly controlled (e.g., start flow, set eluent composition) via dedicated command dialogs (Figure 6).

HPLC system diagnostic parameters such as UV lamp age, injection valve counter, and cam revolutions, can also be monitored in these dialogs.

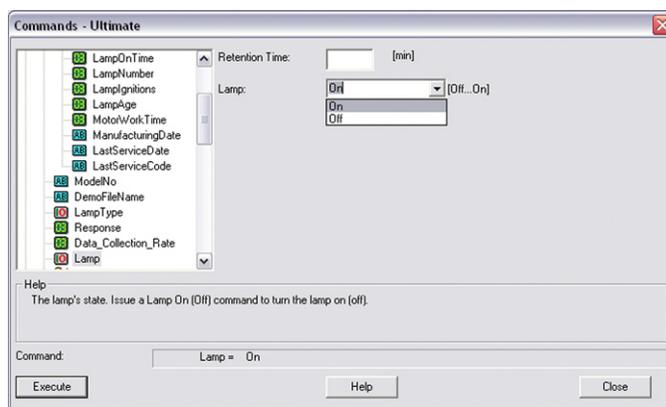


Figure 6. Dedicated command dialogs allow for direct control of instrument settings (such as set eluent composition, start flow, turn on detector lamp). In addition, the user has helpful access to important system diagnostic parameters such as UV lamp age.

5. Data Processing and Documentation

After the data acquisition of an LC-MS run with additional UV detection is finished, the UV chromatograms become available in the MS software for peak integration, quantification, and reporting. For this the user can utilize the complete set of features of the respective MS software.

A log file containing all operational actions of the HPLC instrumentation also becomes available in the MS software. This allows for consistent single point documentation of all relevant information and ensures compliance with regulations.

CONCLUSIONS

Dionex Chromatography Mass Spectrometry Link (DCMSLink) merges the software worlds of both HPLC and MS. The new concept utilizes the HPLC control part of the Dionex Chromatography Management System Chromeleon and incorporates it into the MS software. The following benefits are provided by this approach:

- Chromeleon's advanced HPLC control features are now accessible through Xcalibur, Analyst, and HyStar.
- Single-point control of Dionex HPLC instruments is provided from the MS software without sacrificing the HPLC system functionality.
- With this solution, a significantly better HPLC/MS system integration is achieved.

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Analyst is a registered trademark of Applied Biosystems.
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