

# LC control software for maximum flexibility and rapid automation of new mode of operation

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## Overview

- Full automation for high throughput data analysis
- Rapid separation method development
- Fast hardware integration and configuration
- Plug-in device architecture and automation for flexibility
- Integration with laboratory information system (LIMS) for provenance tracking

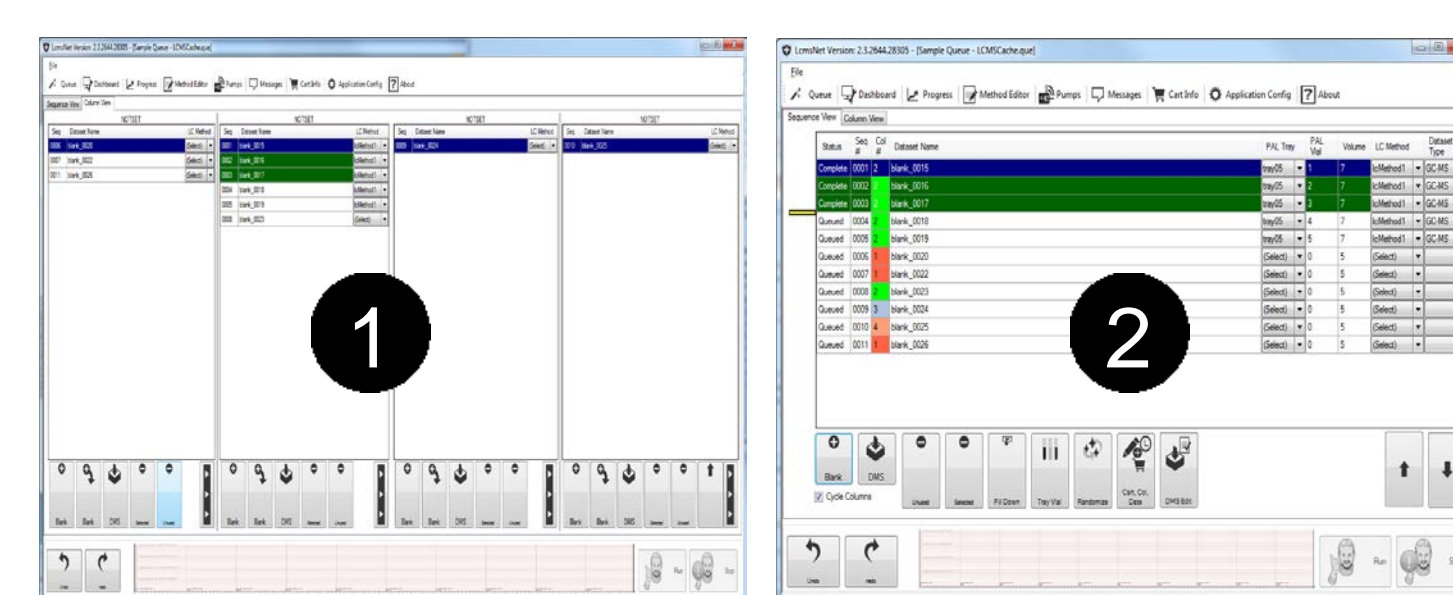
## Introduction

- Addressing instrument flexibility is critical as online sample processing and separation configuration provide opportunities for new or improved capabilities.
- Researchers are currently faced with either buying a packaged solution (if available) or investing considerable time and effort into customizing existing equipment. Here, we present a new approach, where flexibility is designed into the system software allowing for rapid implementation of new configurations
- A flexible device abstraction framework is used as the control architecture to address these needs and the software package is now known as LCMSNet®

## Software Overview

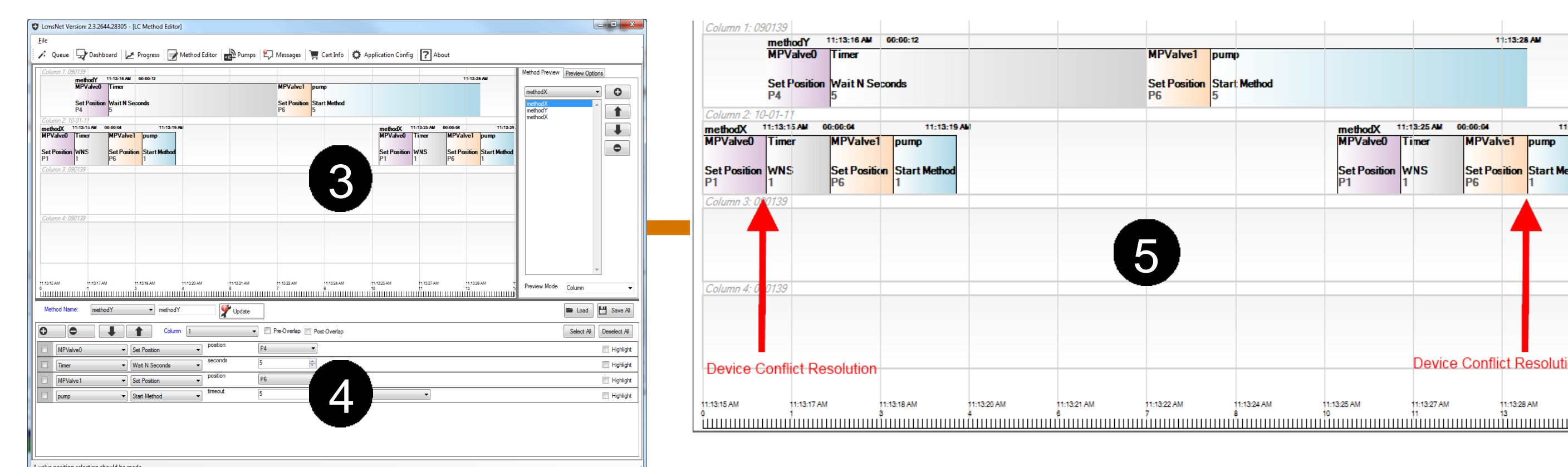
### Sample queue

- The sample queue allows the user to define run characteristics
- Can be represented in column (1) or sequence (2) view
- Sample meta-data is downloaded from the LIMS for provenance tracking purposes



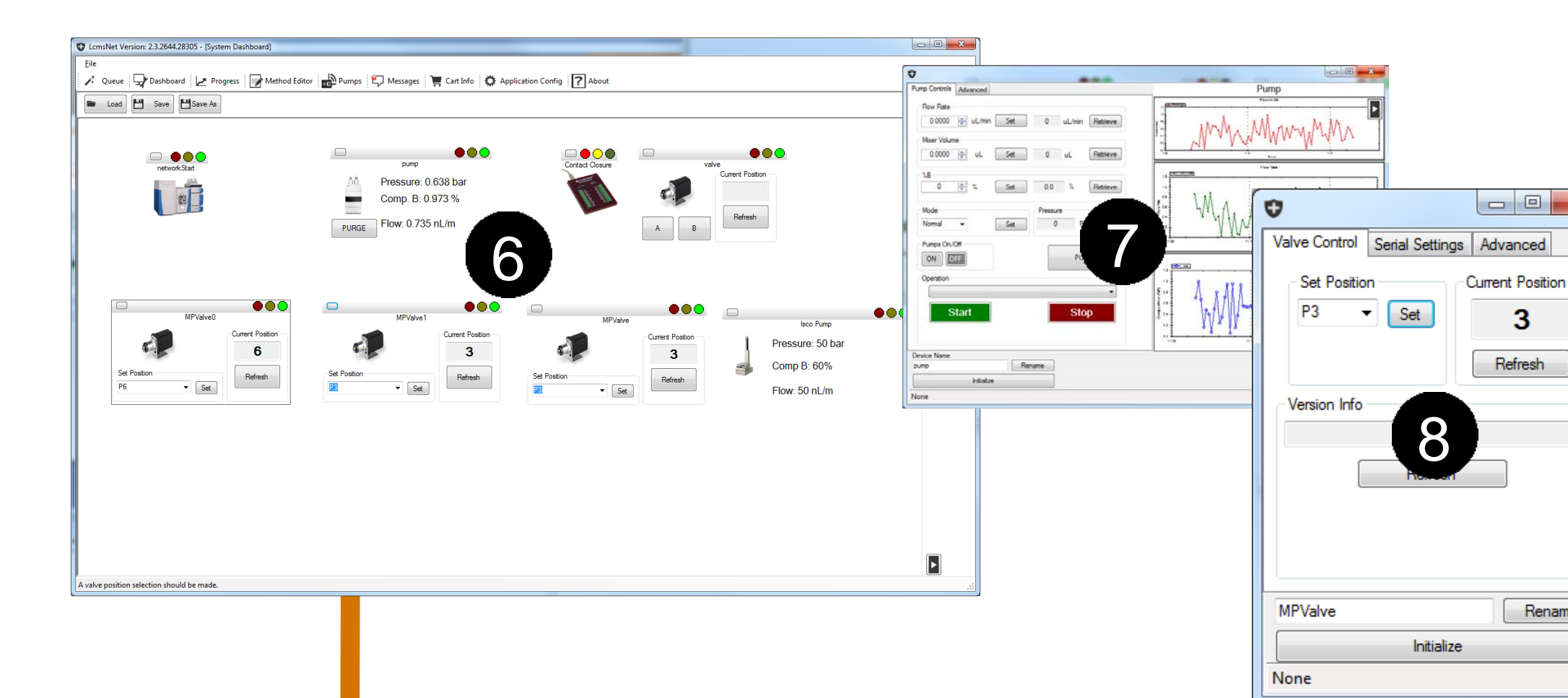
### Separation Method Editor

- The Method Editor (3 and 4) allows the user to define LC-separations as a time-table of device control events (4)
- Different separations can be constructed and visually compared (3) to maximize instrument duty cycle
- Every device registered through the HAL is accessible from the timetable editor (4)
- Methods are optimized using a method alignment algorithm (5) to avoid event overlap



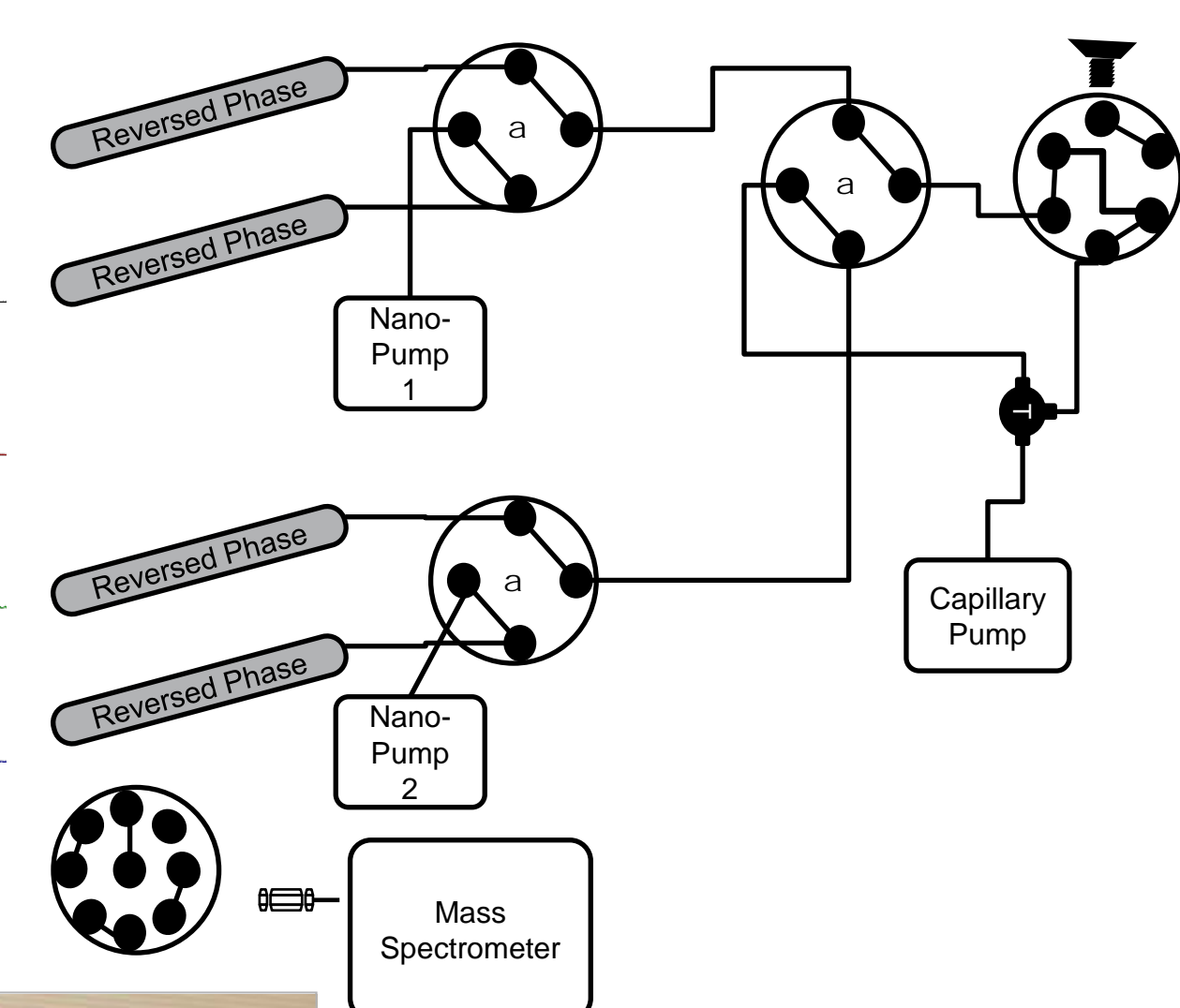
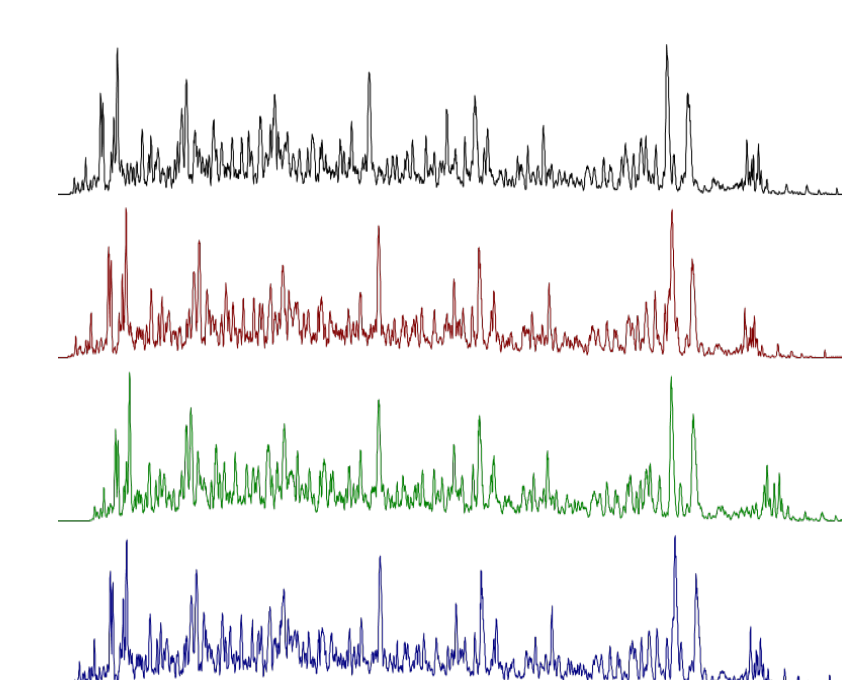
### Hardware configuration and integration

- The system dashboard (6) allows the researcher to dynamically add devices at run-time via plug-ins
- Device configuration (7, 8)
- Integrated hardware: LEAP HTS PAL, Agilent 1200 series Nano Pump, Teledyne ISCO D-series pumps, VICI Valco valves, Labjack U12 for contact closure, Bruker and Thermo MS connectivity

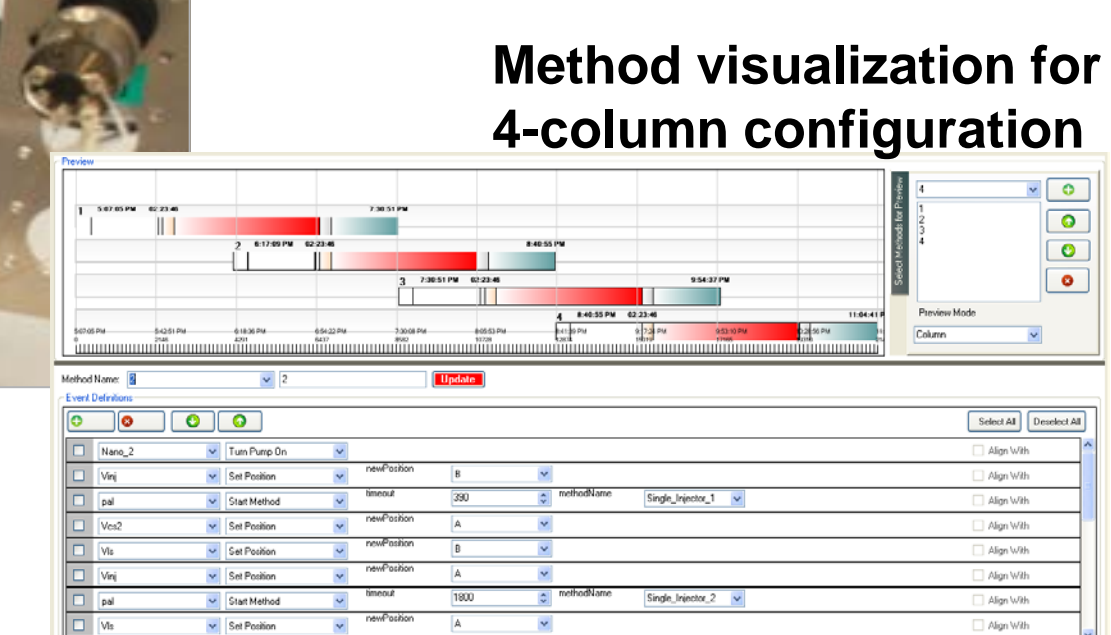


## Example Separation Configurations

### Parallel 4-column<sup>1</sup>

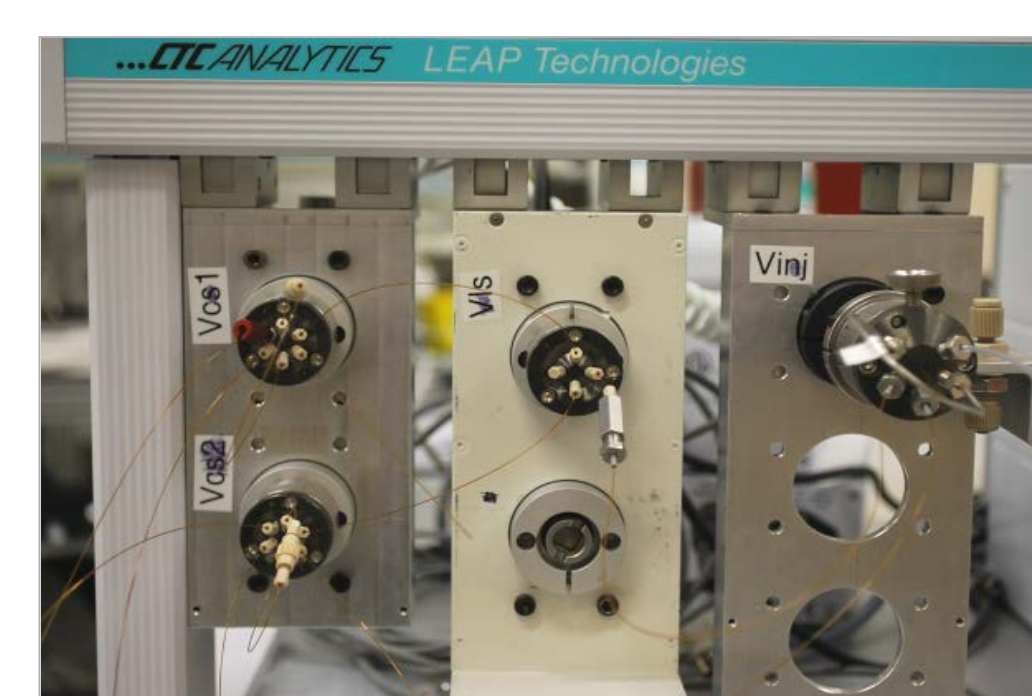
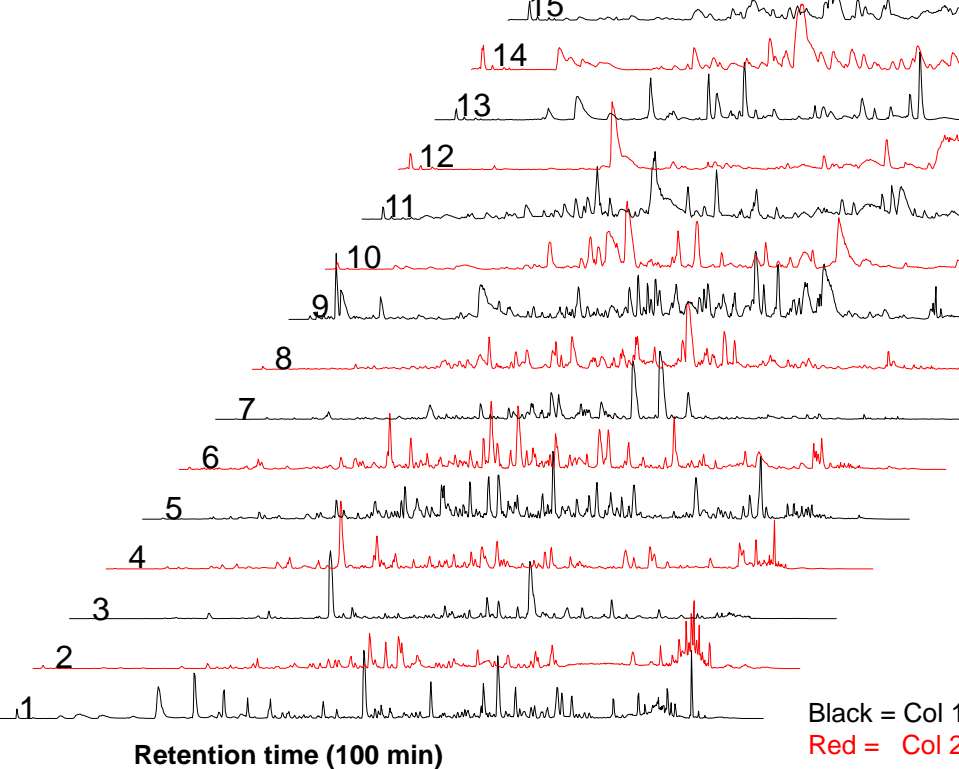


4-column fluidic configuration with ~100% MS duty cycle

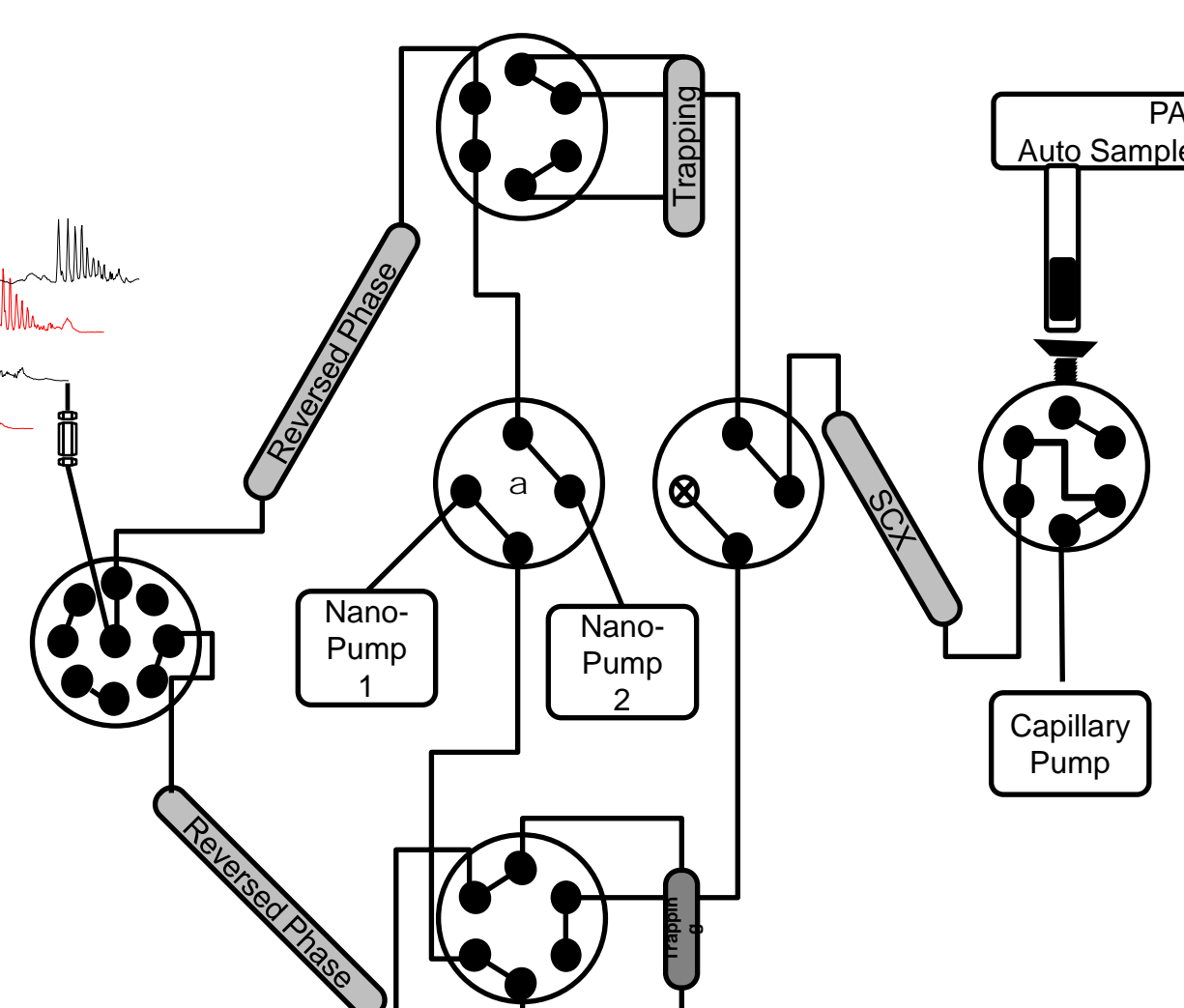


### 2-column 2D

#### Base peak chromatograms of 15 fractions

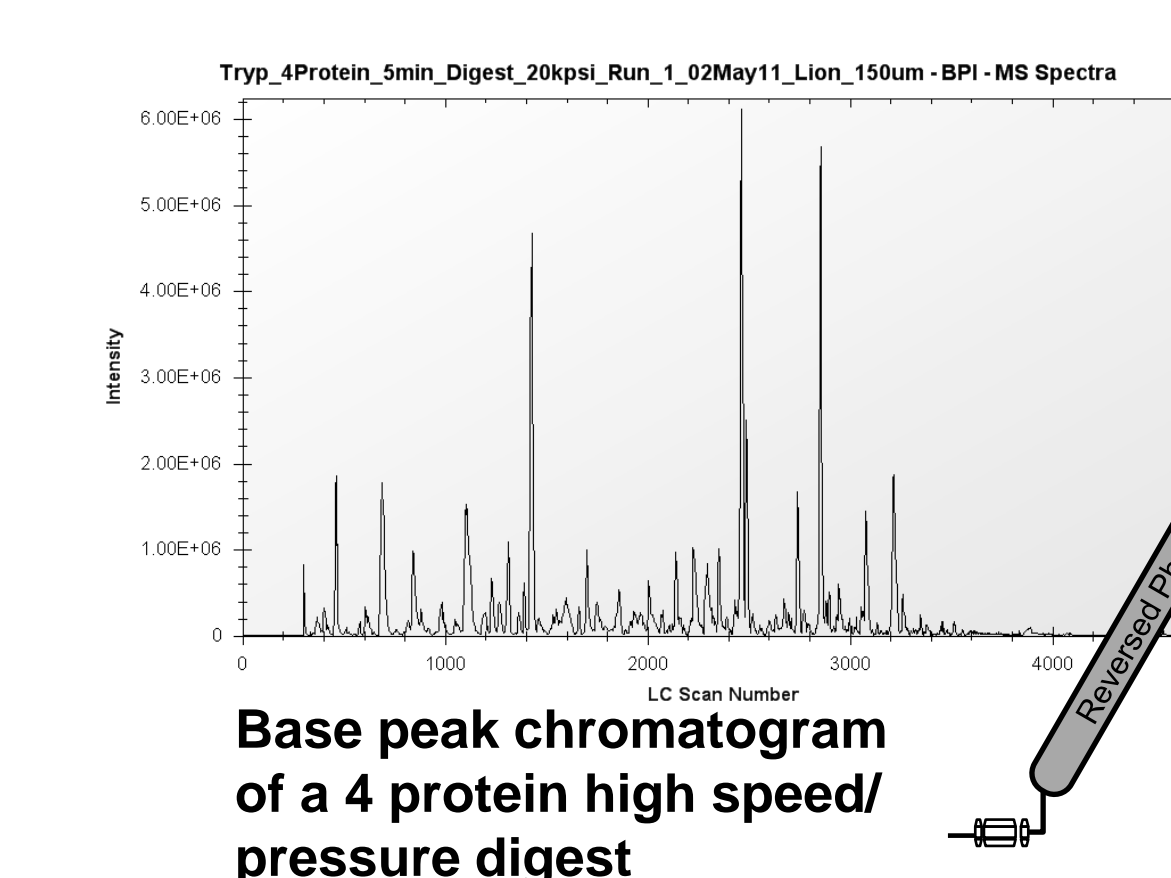


2D fluidic configuration with ~100% MS duty cycle



Fully automated online 2D-LC system

### Online digestion



Online Digestion System: Rapid integration of a third party high pressure digestion module (XstreamPCT(tm), Pressure BioSciences Inc.).

## Conclusions

- Software supports dynamic hardware configuration changes at run time and automation of drastically different hardware configurations
- Separation method development can be done quickly
- Visualization techniques provide instrument duty cycle feedback
- Automated parallel column operation without sample overlap risk and reduced instrument effective dead time

## Acknowledgements

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## Reference

1. Livesay, E. A.; Tang K. Q.; Taylor B. K.; Buschback M. A.; Hopkins D. F.; LaMarche B. L.; Zhao R.; Shen Y. F.; Orton D. J.; Moore R. J.; Kelly R. T.; Udseth H. R.; Smith R. D. Fully automated four-column LC-MS system for maximizing throughput in proteomic analyses. *Anal. Chem.* 80:294-302 (2008).

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