



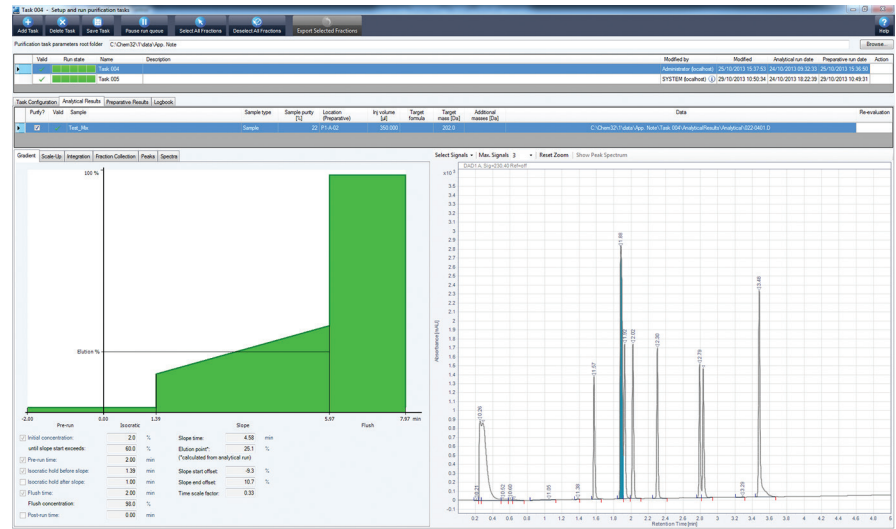
Automated Purification Software for Agilent OpenLAB CDS

Data Sheet

Introduction

Agilent 1260 Infinity LC and LC/MS purification systems offer flexible and easy-to-use solutions for purification of microgram to gram quantities of samples, with maximum levels of recovery and purity. Using combined or dedicated analytical and preparative-scale systems configured to meet the throughput demands of your laboratory, the Agilent Automated Purification Software automates the transfer of data between process steps, streamlining your workflow for highest productivity.

Agilent Automated Purification Software is an easy-to-install add-on for OpenLAB CDS software, and facilitates the automated transfer of purification methodologies from analytical to preparative scale. Algorithms calculate focused gradients on-the-fly for each target compound, ensuring highest purity of fractions collected during preparative-scale purification runs.



Agilent Technologies

Key Benefits

- True “*auto scale-up*” from analytical to preparative scale through mathematical algorithms
- On-the-fly generation of optimized “*focused*” preparative gradients for each sample
- Infinite number of focused gradients to ensure highest purity and recovery
- Highest sample throughput and lowest solvent consumption through focused gradients
- Automated scale-up tool regardless of change in particle size, flow rate, or column dimensions
- Automated Boolean logic of UV and mass signal for fraction triggering

- Support of UV-based purification systems
- Fractions Result Browser displays collected fractions, UV, and mass spectral data at a glance
- Sequence table generator for fast sample reanalysis after results review
- Walk-up and expert modes

Streamline Your Workflow

The Agilent Automated Purification Software is easy to use. The EasyPrep mode provides everything required for occasional purification tasks. With a few clicks, the user can set the desired combination of analytical and preparative columns, upload and process the analytical results, launch the purification run, and review the purification results. Full access to the entire functionality is available through the expert mode, which also provides for configuration of preset methodologies for occasional users.

Agilent Automated Purification Software supports a fully automated purification workflow starting with the import of sample data in *.txt or *.CSV format. It facilitates the generation of sequence tables for analytical scouting. It provides automated target compound confirmation and calculates a focused gradient on the fly for the purification step, ensuring an optimized resolution and minimizing runtime. With the Fractions Result Browser, the position of the collected fractions is quickly and clearly displayed. The purity of each collected fraction can be checked by reviewing UV and mass spectral data from the browser screen. A fraction selection tool permits the export of pure fractions to a liquid handling system, or the generation of a new sequence table for fraction reanalysis within a few mouse clicks.

Figure 1 shows a typical purification workflow that can be automated by deploying the Agilent purification software with a combined analytical and preparative system based on UV or MS detection.

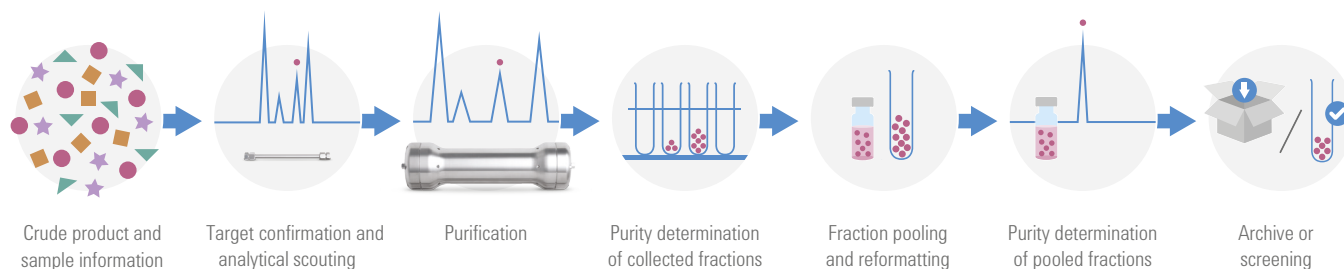


Figure 1. A typical purification workflow that can be automated by deploying the Agilent purification software.

Scaling Up from Analytical UHPLC Columns to Preparative Columns

Scaling up from sub-2 μm analytical UHPLC columns to preparative columns has always been a challenging process for experienced chromatographers, and practically unrealistic for nonexpert users. Agilent Automated Purification Software makes scale-up part of your daily routine work with a few mouse clicks.

A simplified sample submission process on an analytical Agilent 1290 or 1260 Infinity system under OpenLAB CDS ChemStation control with the add-on MassHunter Walk-Up Software guarantees a maximum level of productivity. The data transfer to your 1260 Infinity Preparative Scale Purification System and the analytical result view is straight forward. Separated analytical and preparative systems are the best choice for all high-throughput labs with more than 30 samples per day and for all walk-up purification labs.

Expert Mode—Configuring Analytical and Preparative Systems

The first step of the scale-up process starts by determining the configuration of the analytical and preparative flow paths from both systems. Once logged on to the system in expert mode, all relevant system parameters for the scale-up process can be configured (Figure 2).

The dwell volumes and the dimensions of analytical and preparative columns need to be configured to ensure the correct scale-up from sub-2 μm analytical UHPLC columns to preparative dimensions (Figure 3).

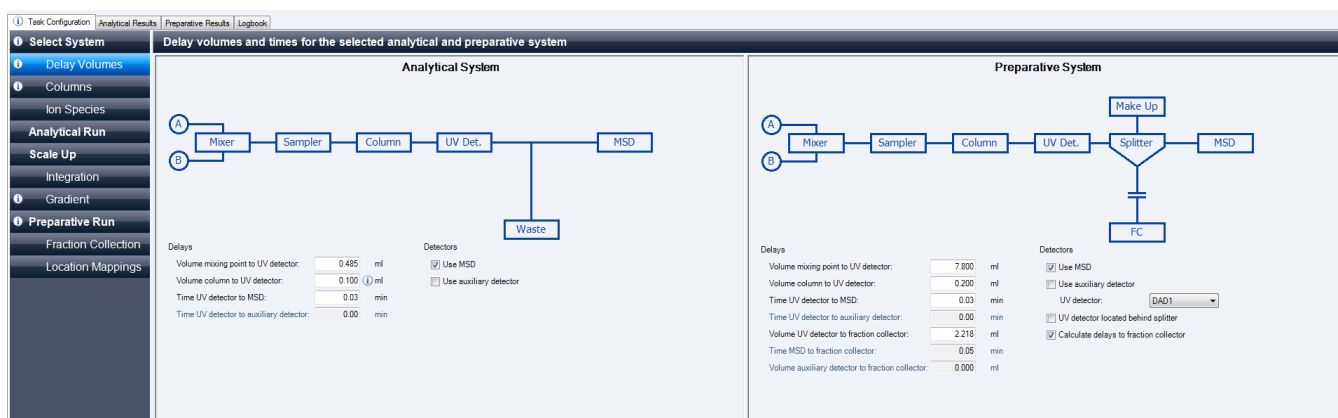


Figure 2. Mapping the hardware characteristics of analytical and preparative LC systems.

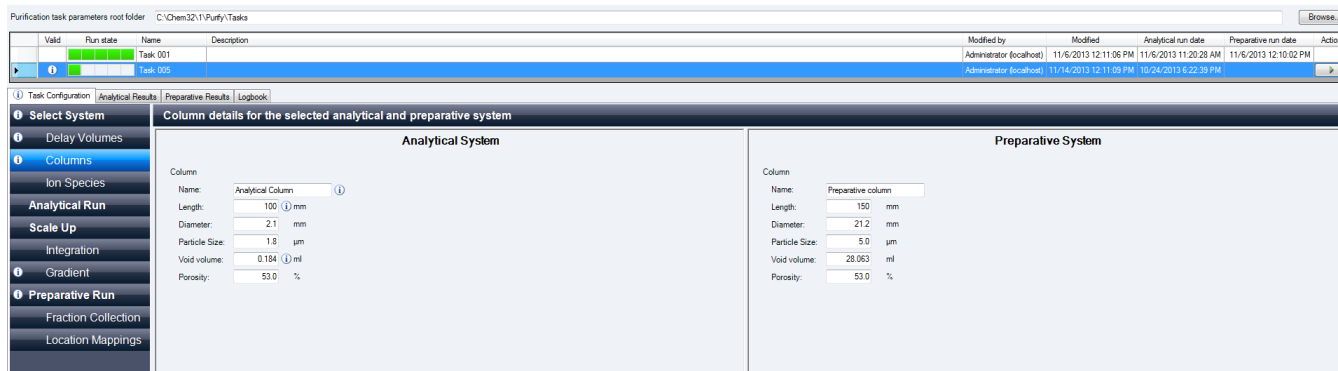


Figure 3. Mapping the dimensions and characteristics of the analytical and preparative columns.

Analytical Scouting and Preparative Performance on a Combined System

Scale-up from analytical to preparative columns can also be achieved with limited analytical performance for flow rates higher than 1 mL/min on a combined analytical-to-prep system. Short analytical scouting runs on 4.6×50 mm columns will provide sample throughput of up to 20 samples per day.

For the expert user, a series of tabs on the configuration page are available to modify all relevant parameters such as column dimensions, ion species, scale-up filtering parameters, integration parameters, and the provided gradient profiles. Modified settings and gradient profiles can be applied as a general setting to purify entire batches of samples (Figure 4).

During the manual review process, target masses can be corrected or additional

triggering compound masses can be entered. Target peaks can be assigned manually with a mouse click (Figure 5).

Any changes in gradient or integration parameters from the analytical result page will be only be applied to the selected sample. This allows the user to optimize general settings for each precious sample.

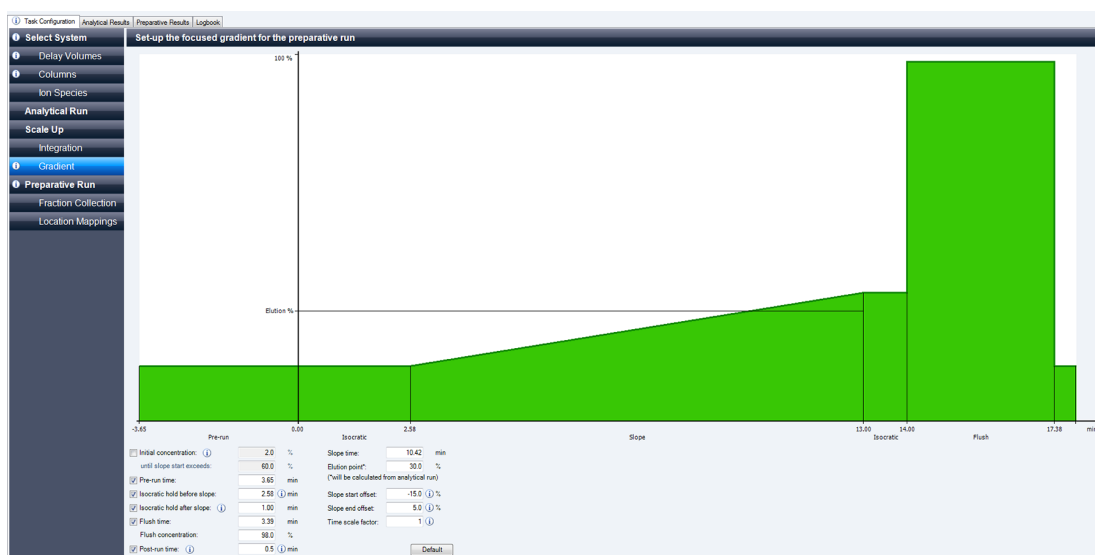


Figure 4. Automated determination of gradient profiles for each target compound. All default parameters can be modified by the user to optimize resolution and efficiency.

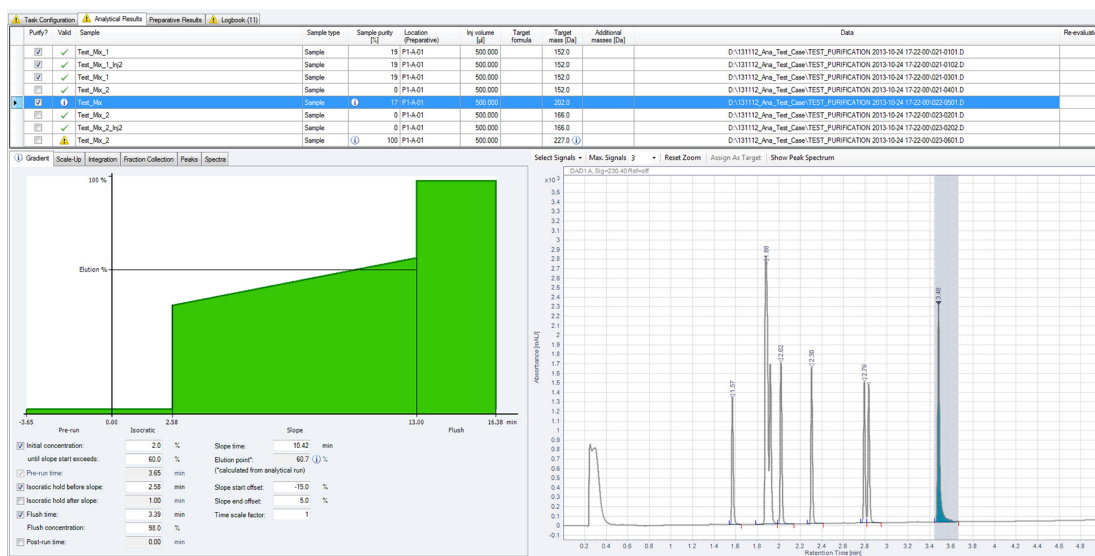


Figure 5. Calculated gradient profile of the detected target compound highlighted in the analytical chromatogram.

EasyPrep User Mode

Walk-up users are often occasional users, and prefer to use a more simplified view of the user interface. The correct number of tabs are available to complete automated purification workflows. With a few mouse clicks, the necessary combination of analytical and preparative columns are selected (Figure 6).

A few mouse clicks later, analytical result sets are uploaded and processed for the purification step. To upload the analytical results, select the folder where the analytical result set has been stored (Figure 7).

The purification process starts automatically, immediately after the download of the result set, or after a manual review step, if required (Figure 8).

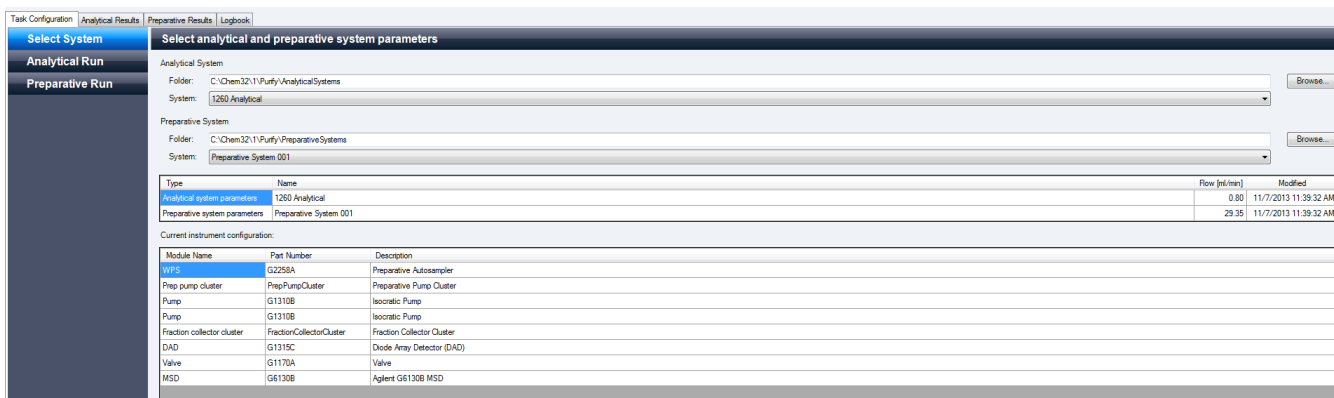


Figure 6. EasyPrep mode has a reduced number tabs for simplified operation by occasional users.

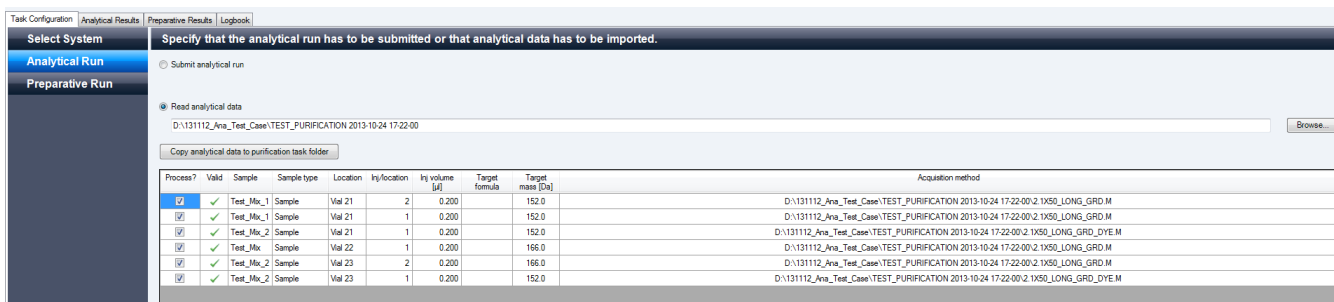


Figure 7. In EasyPrep mode, the walk-up user selects the systems and downloads the results set from a source folder.

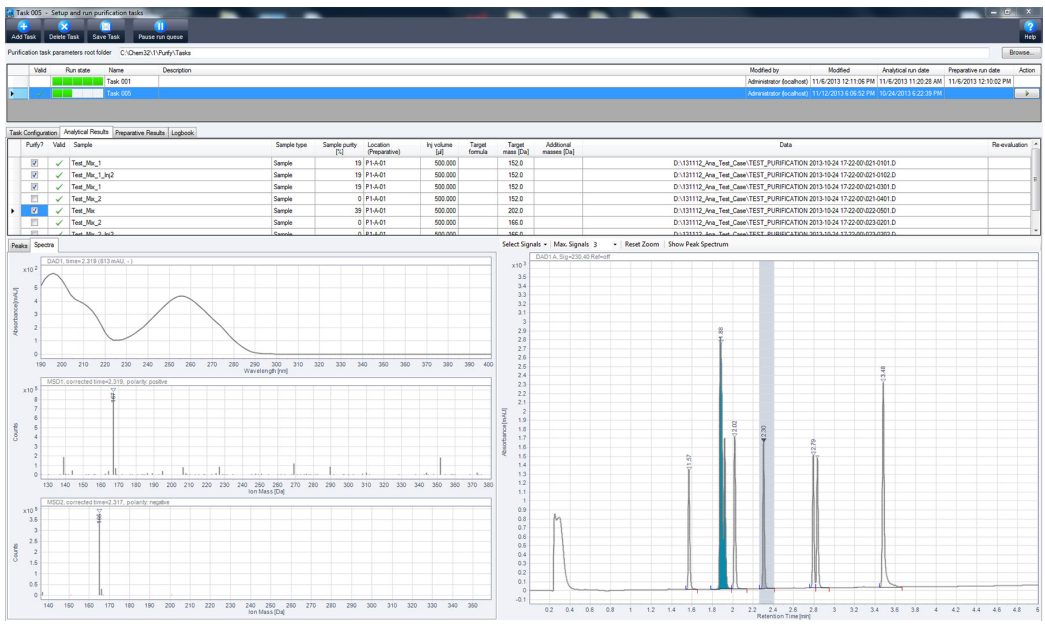


Figure 8. A simple click in the chromatogram displays the spectral data of each peak.

Spectral data from UV and MS detectors, for an unequivocal identification of the target compounds, are available. In routine workflows, the target compound is automatically identified by an

algorithm. Further corrections of the target mass, the addition of compounds for fraction collection, and manual selection of target compounds are completed with a mouse click.

The Fractions Result Browser helps to clearly see the position of the injected sample from the fraction collector, the corresponding collected fractions, and all spectral data (Figure 9).

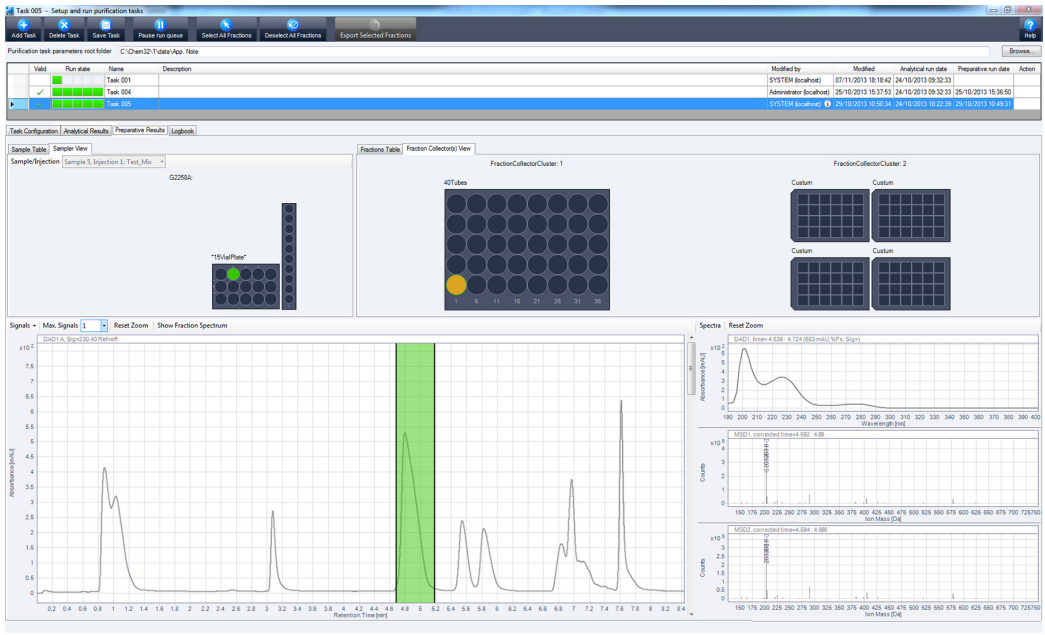


Figure 9. The fraction results browser is an interactive graphical display of the positions of all injected samples and collected fraction tubes. A click on each collected fraction tube displays the position in the chromatogram and all spectral information that was acquired.

Selected fractions can be resubmitted to an analytical Agilent 1290 or 1260 Infinity LC/MS system to determine their purity. The sequence table is generated easily using an export tool within the fractions result browser. The export tool permits the export of information from the collected fractions in *.txt or *.CSV

format to a third party liquid handler for automated pooling processes. A small amount of manual interaction is required to reduce handling mistakes (Figure 10).

Analytical and preparative result sets and purification results can be monitored offline at your desk with the offline

version of the automated purification software. An additional license version of OpenLAB CDS ChemStation is required.

A successful purification work cycle is complete after purity confirmation and quantitation of the desired target compounds (Figure 11).

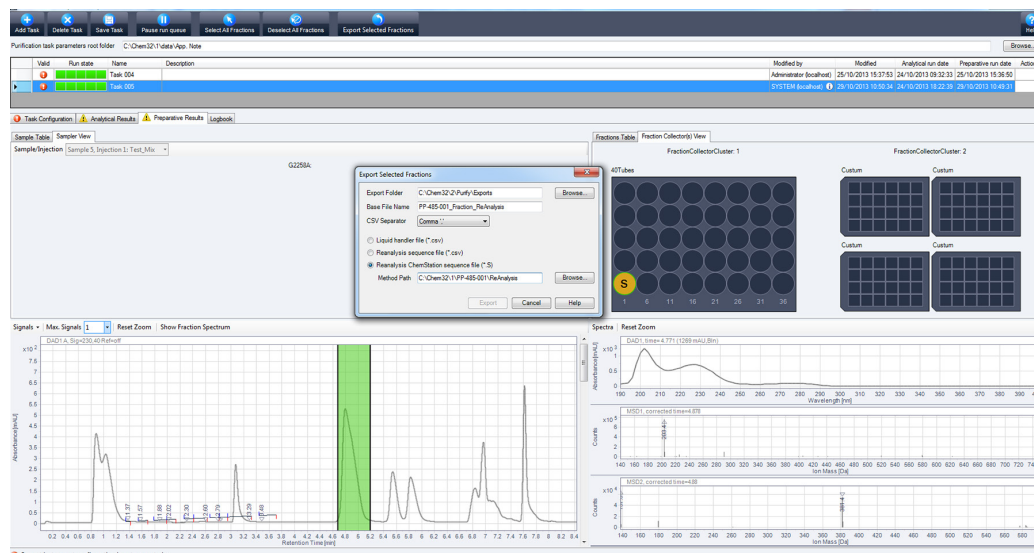


Figure 10. The fractions export tool collects all relevant information for sample reanalysis using liquid handlers. The data can be exported easily through a few clicks.

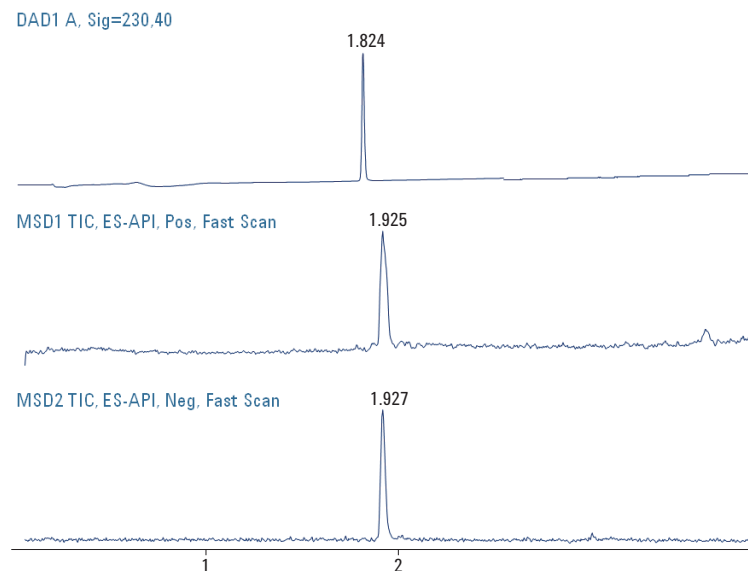


Figure 11. Reanalysis of a collected fraction demonstrating high levels of purity and recovery. The integrated fraction delay sensor in Agilent fraction collectors guarantees the highest purity of collected fractions through exact determination of the capillary delay volume in the preparative flow path.

Ordering Information

Description	Order number
Add-on software Agilent OpenLAB CDS ChemStation Edition, revision C.01.05 or later	
Automated Purification Software online license	M8368AA
Automated Purification Software offline license	M8369AA
Additional software	
MassHunter Walk-Up Software	G2725CA
LabAdvisor Basic Version	M8555AA

www.agilent.com/chem/purification

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