

Analytical Studio Professional for High-Throughput Purification

Turn HTP Data Overload into Swift Decisions and
Actions with Analytical Studio-Professional

In today's fast-paced drug discovery environment, the bottleneck is no longer sample preparation or data acquisition; it's making rapid, confident decisions from complex chromatographic and mass spectrometry data. Virscidian's Analytical Studio Professional (AS-Pro) transforms your high-throughput purification (HTP) workflow by automating method selection, fraction collection trigger optimization, and data integration across instruments and modalities. AS-Pro enables you to process hundreds to thousands of compounds weekly with higher purity, fewer re-runs, and faster turnaround times, all while reducing manual data review and minimizing operator intervention. Backed by substance-centric workflows and vendor-agnostic flexibility, AS-Pro delivers reliable, actionable results that accelerate your projects and improve lab productivity.

As a refresher, an HTP workflow is outlined below:

Crude screening – Each plate of samples is injected on one or more orthogonal liquid chromatography (LC) or supercritical fluid chromatography (SFC) methods to discover which separation gives the best balance of purity, yield, and runtime.



Building prep runs – Analysts assemble complex sample lists that mix column chemistries, pH, gradients, and extra equilibration steps. Selecting the “right” method for every sample can be overwhelming.



Fraction-collection triggers – For each target you still must decide: UV or MS (mass spectrometry) triggers? Which mass or wavelength? What retention time window?



Post-run decisions – Pool, dry-down, or QC every fraction? Each choice generates more data to review.

Without automated processing, this decision-heavy workflow can overwhelm scientists and limit throughput.

This is where Analytical Studio Professional (AS-Pro) comes in. AS-Pro addresses the data challenges of HTP by automating method selection, sample list creation, and review by exception workflows. Used by labs worldwide, AS-Pro enables you to go from samples to results, allowing labs to achieve throughput goals of purifying hundreds to thousands of samples weekly.

Key Features

UNIFIED RESULTS FROM CRUDE SCREEN TO FINAL QC

AS-Pro organizes every LC, SFC, and MS analysis around the compound, not the instrument. All results for a sample, no matter the method, appear in one view, giving scientists instant context across the entire HTP workflow.

- End-to-end automation from crude screening to final QC confirmation and compound registration
- Integrated data across all methods, fraction plates, pooling/dry-down steps, and final QC, regardless of vendor platform
- Seamless metadata flow from LIMS, ELNs, and schedulers across the workflow
- Sample-centric organization streamlines any manual data review

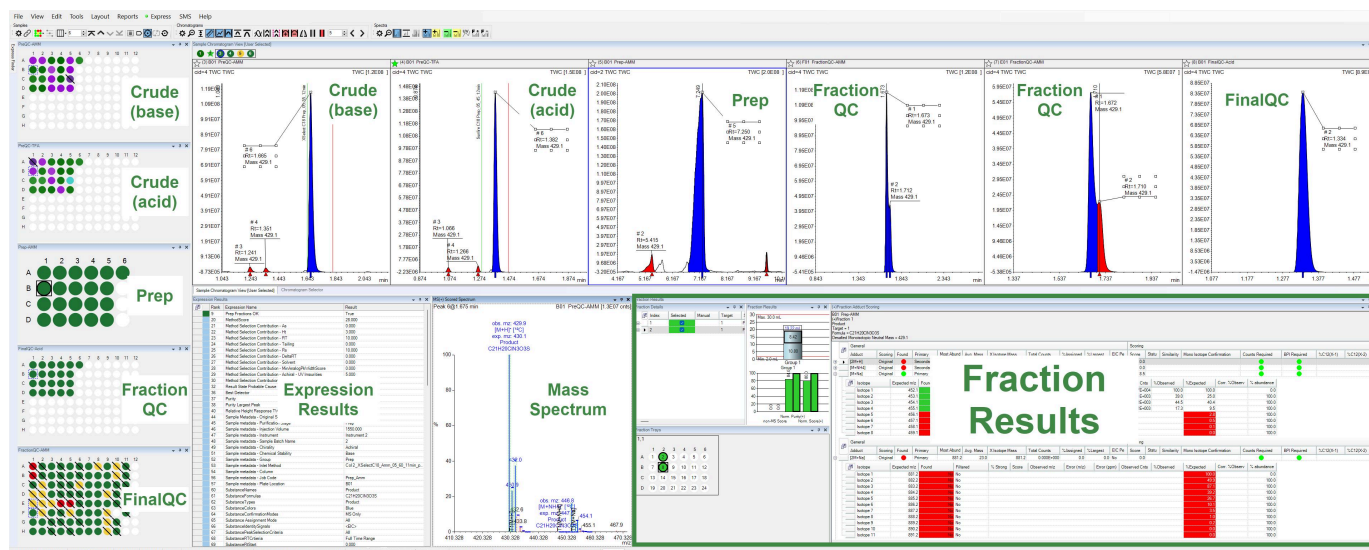


Figure 1

Selecting a sample or peak in one pane automatically highlights the corresponding data across the other stages of the workflow. This substance-centric data handling simplifies any manual data review that you decide to perform.

FLEXIBLE SCREENING STRATEGIES WITH COMPREHENSIVE OR FIRST-METHOD-FOUND SCREENING WORKFLOWS

Evaluate multiple chromatographic methods using traditional **comprehensive** workflows or AS-Pro's unique **first-acceptable-method** approach

AS-Pro lets you evaluate multiple screening chromatography conditions using either the traditional *comprehensive* approach, or switch to a *first-acceptable-method* workflow that initiates preparative chromatography and fraction collection as soon as a suitable screening method is confirmed.¹ Both methods provide automated method selection along with the optimized sample lists complete with fraction collection parameters.

Comprehensive Mode

Screen all samples by all screening methods. AS-Pro analyzes results, selects the best method for each sample, and builds prep sample lists. Screening samples using the comprehensive mode maximize purity and provide more comprehensive method evaluation.

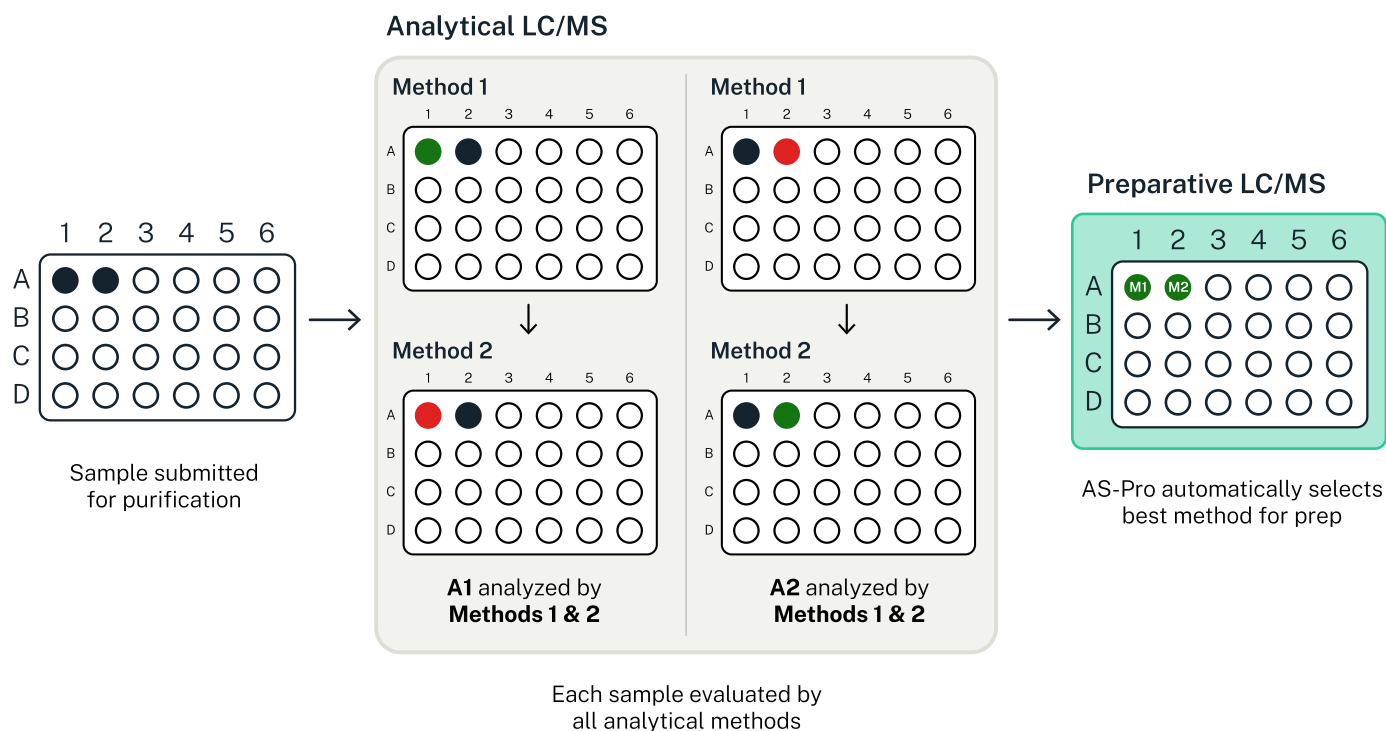


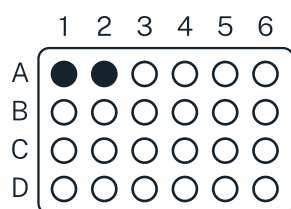
Figure 2

Screening phase, comprehensive approach. All samples are analyzed by all chromatography-MS methods and then the data are processed in AS-Pro to select the best separation technique for prep.

¹ Requires use of Waters LC/MS instrumentation with AutoLynx.

First-Acceptable-Method

Run sample by screening Method A only. If sufficient separation is achieved, sample proceeds to prep. If not, AS-Pro adds sample to the Method B sample list. The first-acceptable-method approach can maximize throughput while reducing operator and instrument time as well as solvent and sample use.

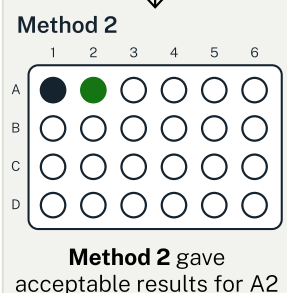
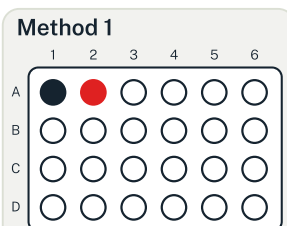
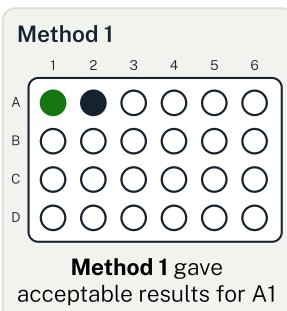


Sample submitted for purification

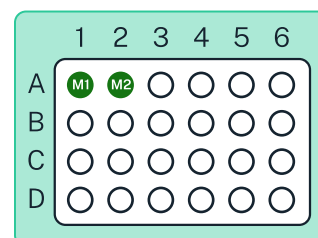
Figure 3

In the first-acceptable-method screening mode, a sample is run by one screening method and then processed. If the results show that the method provides sufficient purity for fraction collection, the sample is then run on the prep instrument and fractions are collected. If the data from screening show the method doesn't yield adequate separation, the sample is re-run by an alternative screening chromatographic technique as originally planned.

Analytical LC/MS



Preparative LC/MS

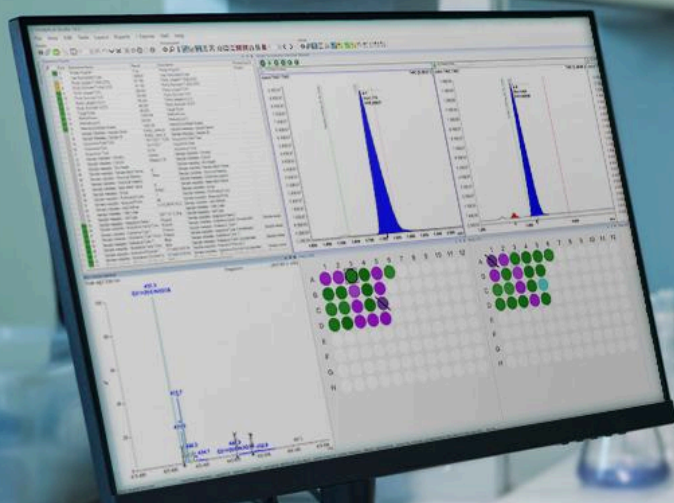


Samples run by **Method 2 only if not separated by Method 1**

TURN ISOTOPIC DETAIL INTO CONFIDENT COMPOUND IDS WITH AS-PRO

HTP generates mountains of MS data, yet most data analysis software ignores some of the most important information, the isotopic patterns. AS-Pro doesn't. AS-Pro features a substance-driven workflow where:

- Theoretical isotope patterns compared to experimental spectra to verify compound presence
- Hits must match both expected retention time (if known), and isotopic pattern to be considered "found"
- Reduces false positives and unnecessary manual review



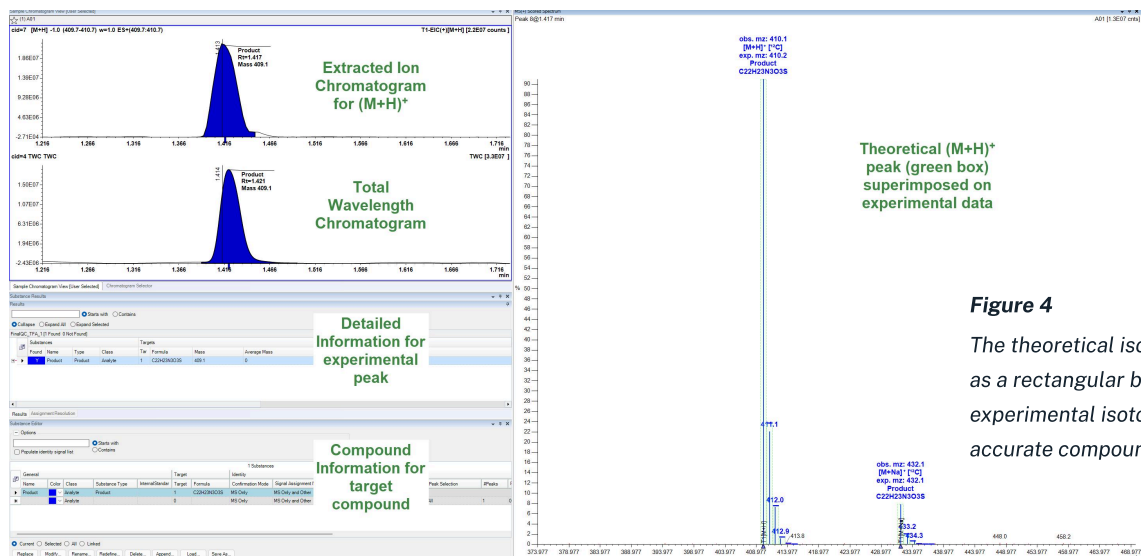


Figure 4

The theoretical isotopic pattern is shown as a rectangular box overlaid on the experimental isotope pattern, confirming accurate compound identification

FIND HIDDEN IMPURITIES WITH AS-PRO'S COMPOSITE CHROMATOGRAMS AND PEAK COMPONENTS

Selecting the best separation method during crude screening is essential for delivering clean fractions. AS-Pro enhances this process with built-in chemical intelligence, creating two “pseudo-chromatograms”:

- **COI composite chromatogram:** Combines the extracted ion chromatograms (EICs) of the compound of interest's related adducts into a single chromatogram
- **Unknown composite chromatogram:** Sums all unrelated ions within a defined retention time window and intensity threshold, revealing co-eluting impurities

For additional information, AS-Pro includes a Peak Components view, which inspects ions eluting near the compound of interest. By plotting all these ions together, it becomes straightforward for AS-Pro to distinguish impurities from the target compound and its adducts. AS-Pro leverages these composite profiles to compare methods and rank separation quality, ultimately selecting the method most likely to produce high-purity fractions. The result is fewer re-runs, higher-purity collections, and a high-throughput workflow you can rely on to run automatically.

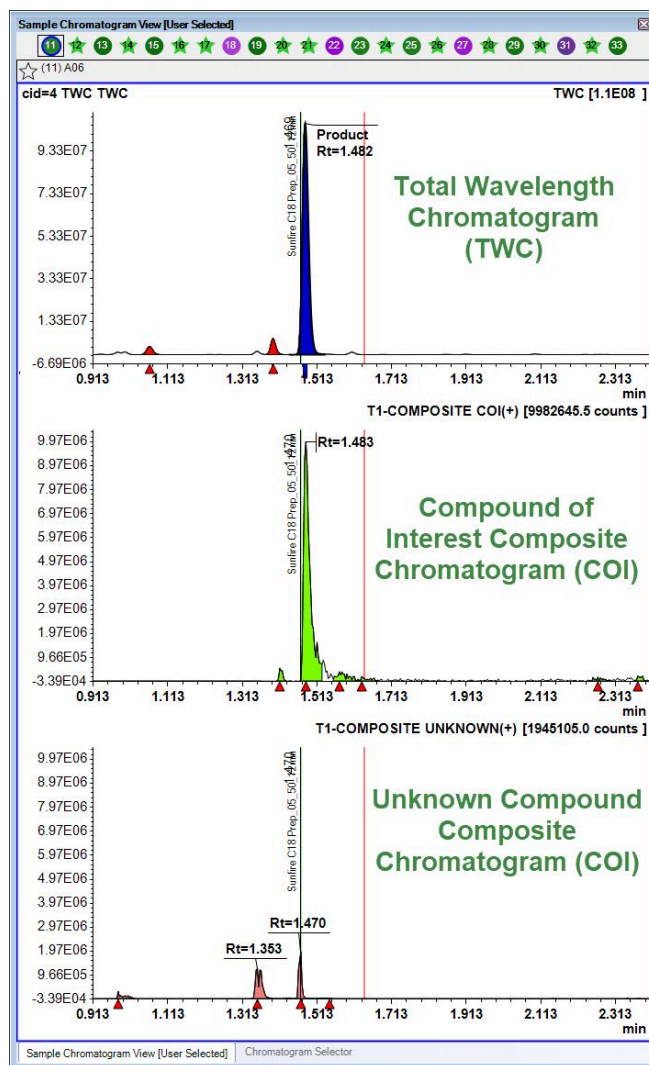


Figure 5

“Pseudo-chromatograms” help determine whether any unknowns will co-elute with your compound of interest

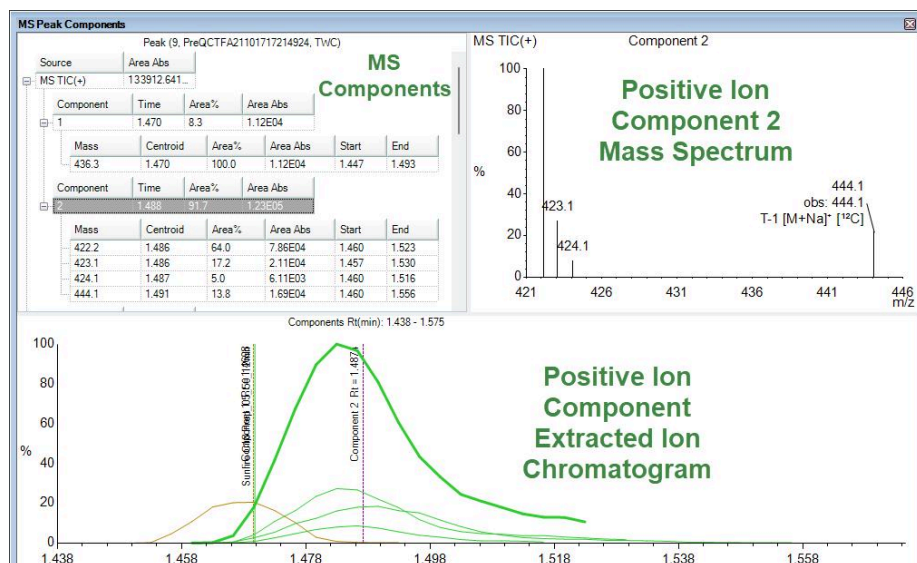


Figure 6

Peak Components display shows compounds eluting near your compound of interest.

AUTOMATICALLY OPTIMIZE FRACTION COLLECTION TRIGGERS FOR EACH COMPOUND

AS-Pro doesn't stop after choosing the best prep method; it also automatically provides additional fraction-collection trigger metadata and information that helps correctly set or select appropriate fraction trigger thresholds, minimizing false negative and false positive fractions, no matter how much (or how little) of your target compound is present.

- Automatically selects the best detector and trigger threshold
- Supports splitting and pooling fractions to maximize purity
- Calculates MS-based purity estimates which can be used to minimize unnecessary fraction QC
- Maximizes target compound collection while minimizing mobile phase and impurity collection

If you run Waters LC/MS instruments and FractionLynx™ with Analytical Studio software, you have the following additional functionality and benefits:

- Fraction collection thresholds determined for each compound individually, maximizing the volume and concentration of the target of interest collected
- Best detector (MS, UV, other) and signal (molecular ion, adduct, specific UV wavelength) for triggering automatically selected for each compound separately
- Multiple triggers can be combined, for example triggering based on the UV signal but only after target ion is seen by the MS

The fraction collection capabilities in AS-Pro ensure that higher purity compounds are delivered faster with reduced dry-down time, lower costs, and less waste.

For more details on Analytical Studio's advanced fraction collection capabilities, see our Application Note, [“Virscidian’s Analytical Studio software combined with Waters FractionLynx Increases Fraction Purity.”](#)

On Screen Report

Sample Attributes	Substances	Expressions	Fraction Trigger Logic Lo	Generic-Prep-Wavelength-Lo
Sample Name	Product Mass	PreQC-PrepOK	Generic-Prep-Lo Trigger	
		<input checked="" type="checkbox"/>	3Tube_MIT_Hi_Med	Mass A and UVA
		<input checked="" type="checkbox"/>	3Tube_MIT_Hi_Med	Mass (A or B) and UVA
		<input checked="" type="checkbox"/>	3Tube_MIT_Hi_Med	Mass (A or B) and UVA
		<input checked="" type="checkbox"/>	3Tube_MIT_Hi_Med	Mass A and UVA
				Mass A and UVA
				Mass (A or B) and UVA
				Mass A
				Mass A and UVA
				Mass A and UVA
				Mass A and UVA
Demo5016303-1.raw	499.21	<input checked="" type="checkbox"/>	3Tube_MIT_Med_Hi	Mass A and UVA
Demo5016311-1.raw	583.24	<input checked="" type="checkbox"/>	3T	VA
Demo5016319-1.raw	585.31	<input checked="" type="checkbox"/>	3T	and UVA
Demo5016304-1.raw	546.26	<input checked="" type="checkbox"/>	3T	and UVA
Demo5016312-1.raw	536.24	<input checked="" type="checkbox"/>	3T	VA
Demo5016320-1.raw	553.29	<input checked="" type="checkbox"/>	3T	and UVA
Demo5016305-1.raw	513.23	<input checked="" type="checkbox"/>	3T	and UVA
Demo5016313-1.raw	523.28	<input checked="" type="checkbox"/>	3Tube_MIT_Hi_Med	Mass (A or B) and UVA
Demo5016321-1.raw	500.01	<input checked="" type="checkbox"/>	3Tube_MIT_Hi_Med	Mass A and UVA
Demo5016306-1.raw		<input checked="" type="checkbox"/>	3Tube_MIT_Med_Med	Mass (A or B) and UVA
Demo5016314-1.raw		<input checked="" type="checkbox"/>	3Tube_MIT_Hi_Med	Mass (A or B) and UVA
Demo5016322-1.raw		<input checked="" type="checkbox"/>	3Tube_MIT_Hi_Hi	Mass A and UVA
Demo5016307-1.raw		<input checked="" type="checkbox"/>	3Tube_MIT_Hi_Hi	Mass A and UVA
Demo5016315-1.raw	515.24	<input checked="" type="checkbox"/>	3Tube_MIT_Med_Med	Mass (A or B) and UVA
Demo5016323-1.raw	559.21	<input type="checkbox"/>		
Demo5016300-1.raw	557.30	<input type="checkbox"/>		

Annotations:

- Fraction collection begins if UV signal reaches Hi threshold and MS reaches Medium threshold** (points to 3Tube_MIT_Hi_Med)
- Both specified mass and UV required for fraction collection** (points to 3Tube_MIT_Hi_Med)
- UV wavelength used for fraction triggering** (points to VA)
- Either of two masses and the UV signal needed** (points to 3Tube_MIT_Med_Med)

Figure 7

Analytical Studio automatically determines the best fraction triggers on a sample-by-sample basis when running Analytical Studio along with Waters FractionLynx software.

ONE-CLICK, END-TO-END REPORTING THAT FITS YOUR LAB'S STYLE

AS-Pro provides a myriad of reporting options, allowing you to have data formatted and reported to match your unique specifications. AS-Pro can use pre-selected templates without user intervention

- Generates unified reports that include screening, prep, fraction collection, and final QC across multiple instruments and vendors
- Customizable templates support internal SOPs or sponsor formats
- Reports can summarize entire runs or offer detailed traceability per sample
- Focused summaries can be created while reviewing flagged results

VENDOR-AGNOSTIC INTEGRATION FOR TRULY FLEXIBLE WORKFLOWS

Virscidian believes that you should have the freedom and flexibility to select the best instruments for your workflow. That's why our software is vendor-agnostic.

- Imports raw files from all major chromatography, MS, and detector platforms, allowing you to choose the best-in-class hardware for your workflow
- Works with enterprise LIMS/ELN systems, local databases, or simple spreadsheet uploads
- Shares metadata bidirectionally for flawless sample tracking, automated processing, and global report publishing

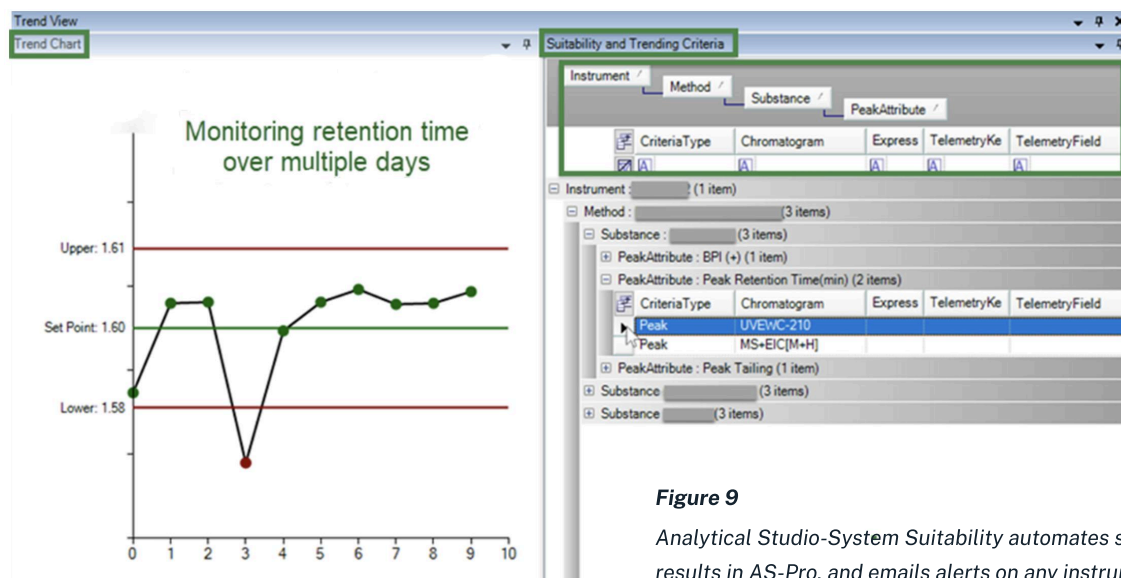


Figure 9

Analytical Studio-System Suitability automates suitability checks, saves results in AS-Pro, and emails alerts on any instrument issues.

Summary

Analytical Studio Professional brings order and speed to the most demanding high-throughput purification campaigns. By unifying every LC, SFC, and MS result around the compound, and not the instrument, it replaces manual data wrangling with intelligent automation. Method selection, focused-gradient prep runs, compound-specific fraction triggers, and one-click reporting all flow from the same platform, reducing re-runs, solvent, and analyst time. Add optional modules for fraction-weight mapping and system suitability, and AS-Pro becomes the single data spine for your entire purification lab. The outcome is consistent, high-purity material delivered days, or even weeks, faster than legacy workflows, freeing your scientists to focus on discovery rather than data management.



Ready to see how AS-Pro can turn your HTP backlog into a streamlined, automated pipeline?

Contact Virscidian today for a live demonstration or workflow consultation and discover how quickly your lab can move from samples to confirmed, high-purity compounds.

