Virscidian

Sample Management Capabilities

Analytical Studio Sample Management Services
Analytical Studio Sample List Builder

Managing metadata and generating instrument-ready sample lists are key challenges for high-throughput chromatography-mass spectrometry labs. Virscidian's Sample Management informatics solutions include two integrated products that simplify these processes:

- **Analytical Studio Sample Management Services (AS-SMS):** Centralizes metadata storage and enables ELNs, LIMS, and other lab informatics systems to be integrated into Analytical Studio
- **Analytical Studio Sample List Builder (AS-Sample List Builder):** A wizard-driven interface that automates the creation of instrument-ready sample lists (chromatography-MS, liquid handling, solid dosing, etc.), reducing manual entry and improving efficiency

Together, these tools enhance lab productivity, minimize errors, enforce SOPs, and maintain the highest data integrity standards.

Key Challenges & Solutions

METADATA CAPTURE & MANAGEMENT

Metadata ensures traceability and reproducibility in workflows and includes:

- Sample Identification – Unique IDs, batch codes, plate positions
- Composition & Origin – Chemical structures, raw materials, expected products
- Preparation & Handling – Sample synthesis, purification, storage details
- Method Parameters – Solvents, reaction environments, chromatography settings
- Collection Data – Timestamps, user IDs, instrument details

Most chromatography and mass spectrometry systems are unable to provide sufficient metadata storage volume necessary for processing when multiple substances and specific workflow information is required. AS-SMS solves this by storing unlimited metadata while seamlessly integrating with other informatics systems for API-based electronic sharing of information.

AUTOMATED SAMPLE LIST GENERATION

AS-SMS can connect with your ELN, LIMS, or other lab systems, capturing experimental metadata while ensuring necessary metadata are passed to the appropriate instruments and/or robotics. AS-Sample List Builder provides a wizard-driven interface for submitting samples to instrumentation, allowing:

- Automated instrument-ready sample list creation for major commercial chromatography-MS instrument, liquid handlers, and a range of solid dosing robots
- Submission from third-party informatics systems or Excel uploads via a csv import
- Better enforcement of standardized workflows for both automated and manual labs
- Allows users to create, optimize, and maintain all samples, standards, blanks, and QC injections that make up the analytical instrument protocols

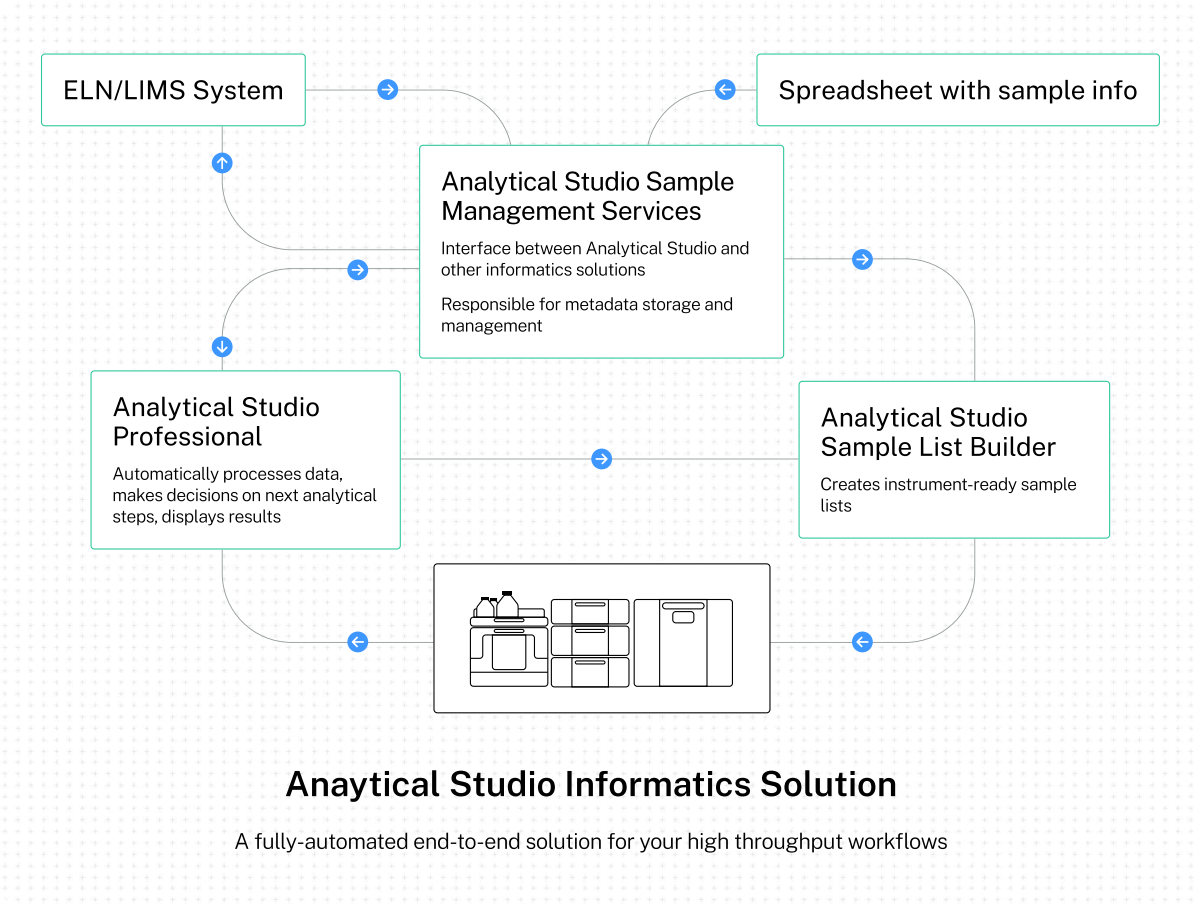


Figure 1

AS-SMS and AS-SLB are integral components of Analytical Studio, responsible for managing metadata and generating instrument-ready sample lists

Analytical Studio Sample Management Services (AS-SMS)

KEY FEATURES

- ELN/LIMS Integration – Enables bi-directional communication with informatics systems
- Centralized Metadata Storage – Stores unlimited metadata (structures, formulae, conditions) and passes only relevant details to AS-Sample List Builder

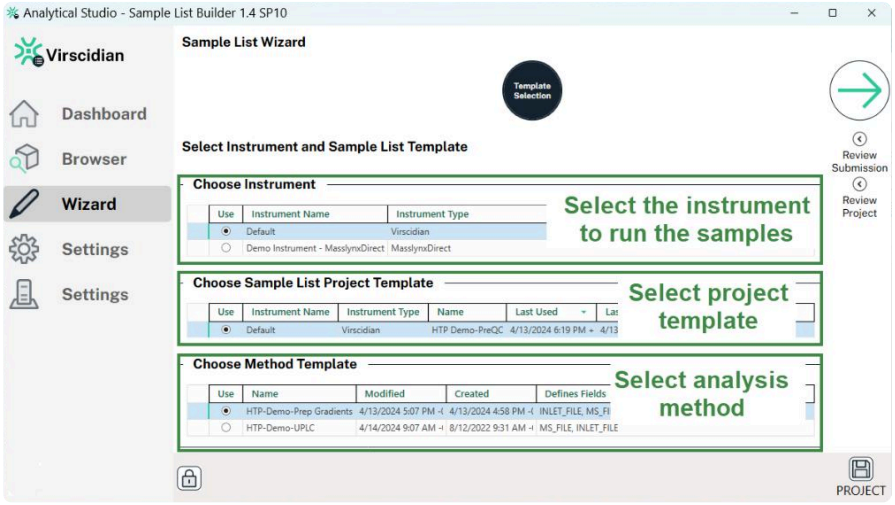
BENEFITS

- Efficiency & Time Savings – One-click sample submissions eliminate manual data entry, reducing errors and saving time
- Data Integrity & Compliance – Ensures all samples run with validated metadata, supporting QA/QC
- Scalable to a wide range of multi-modal workflows – Handles complex high-throughput operations while remaining flexible for smaller labs
- Enhanced Collaboration – Smooth integration with third-party software and hardware ensures streamlined operations

Analytical Studio Sample List Builder (AS-Sample List Builder)

KEY FEATURES

- Instrument-Ready Sample Lists – Automatically generates lists for all major LC/MS, solid dosing robots, and liquid handler systems
- Wizard-Driven Interface – Guides users through setup, method assignment, and external controls
- Allows programmatic sample-list generation when used with scheduling and/or orchestration software
- Reusable Templates – Saves and reuses templates for common workflows (e.g. acidic vs. basic conditions)
- Filtering & Selective Re-Runs – Easily re-run only failed QC samples without rebuilding lists
- Inter-System Connectivity – Integrates with all major chromatography and mass spectrometry software



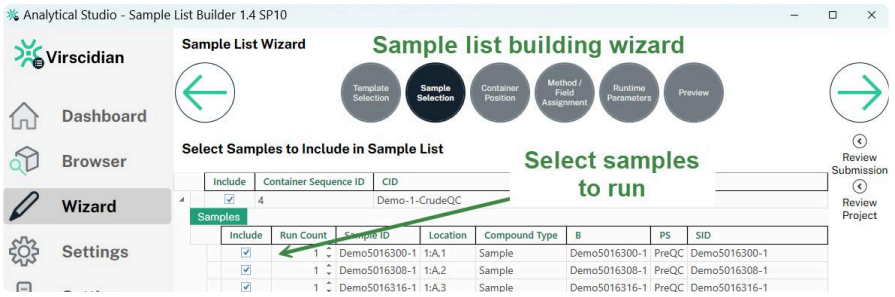


Figure 2

Building an instrument-ready sample list is streamlined with AS-Sample List Builder's wizard walking you through the process step-by-step

BENEFITS

- Intuitive, Step-by-Step Workflow – Eliminates guesswork, ensuring correct field mapping and method assignments
- Error Reduction – Automated metadata capture minimizes manual entry mistakes
- Simplifies use of multivendor chromatography-MS platforms – Eliminates need for specialized training on multiple instrument platforms
- Consistent Method Enforcement – Ensures SOPs are followed with automatic QA/QC sample insertion (e.g. blanks, calibration samples, standards)
- Scalability – Supports both small-scale and high-throughput workflows

WHY CHOOSE VIRSCIDIAN'S SAMPLE MANAGEMENT TOOLS?

- Integration with existing ELNs, LIMS, and instruments
- Stores unlimited amounts of metadata
- Eliminates manual file handling and redundant data entry
- Ensures sample traceability, compliance, and accuracy
- Scalable and flexible for any lab workflow

THE NEXT-GENERATION SOLUTION FOR SAMPLE MANAGEMENT

Virscidian's Sample Management informatics tools are the next-generation solution for labs seeking an automated, submission-centric, and wizard-driven approach to managing samples. AS-SMS can store all experimental metadata while AS-Sample List Builder provides a clear, step-by-step workflow for creating robust sample lists. Combined, these informatics solutions help labs optimize throughput, reduce manual data entry mistakes, enforce SOPs, and maintain the highest data integrity standards.

Ready to streamline sample list creation?

Experience simplified submissions and rock-solid metadata integrity with Virscidian's Analytical Studio Sample Management tools. Contact us to learn more today!

Dotmatics