Automated Data Processing for HTE

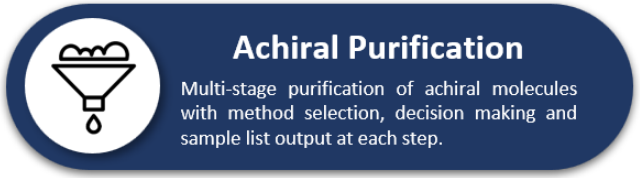
40th ASMS Asilomar Conference 2026

Virscidian

Who is Virscidian?

ABOUT VIRSCIDIAN

- Founded in 2009
- Specialize in analytical chemistry software and automated chromatography / mass spectrometry data processing
- Automate drug discovery workflows where LC-MS data is the primary decision driver
- Produces high-fidelity, AI/ML-ready results for small-molecule research
- Growing team of passionate scientists, developers, integrations specialists, etc.



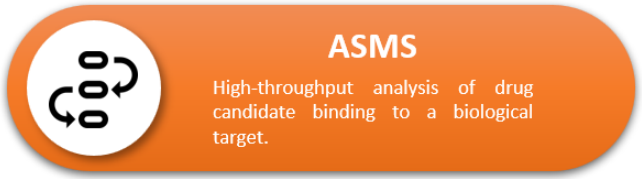
Achiral Purification

Multi-stage purification of achiral molecules with method selection, decision making and sample list output at each step.



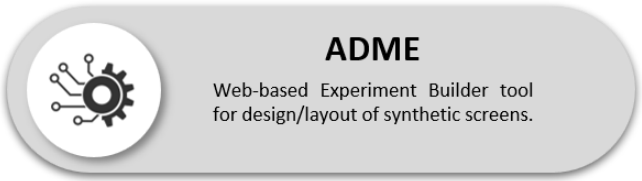
Chiral Purification

Automated method selection and comparison based on tunable criteria



ASMS

High-throughput analysis of drug candidate binding to a biological target.



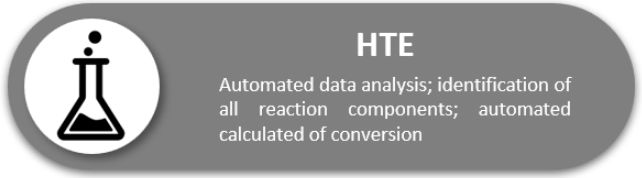
ADME

Web-based Experiment Builder tool for design/layout of synthetic screens.



Compound QC

High-throughput quality control of compound libraries with automated commenting and decision making.



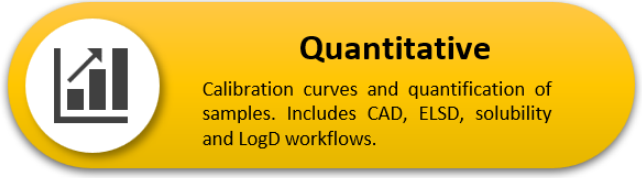
HTE

Automated data analysis; identification of all reaction components; automated calculated of conversion



Instrument Suitability

Monitoring of instrument performance; alerts for failures and trending out-of-spec

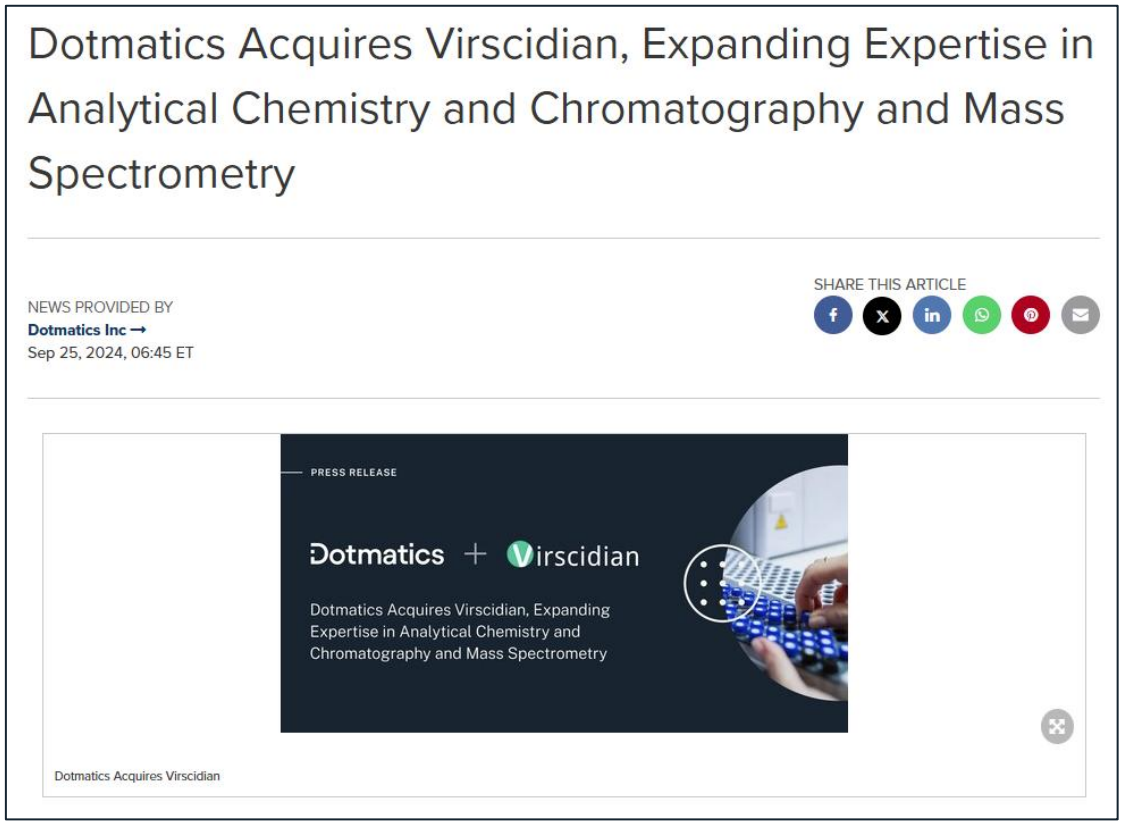


Quantitative

Calibration curves and quantification of samples. Includes CAD, ELSD, solubility and LogD workflows.

DEAL 1

Dotmatics Acquires Virscidian



THE DEAL

15th

acquisition by Dotmatics since 2017

Sept 25, 2024

announcement date; deal terms undisclosed

- Virscidian's Analytical Studio is integrated with Dotmatics' Luma Scientific Intelligence Platform
- Complements Dotmatics' Protein Metrics offering: small-molecule (Virscidian) alongside large-molecule R&D
- Marks Dotmatics' first transaction in North Carolina
- Strengthens automation of complex laboratory data workflows across multimodal R&D

DEAL 2

Siemens Acquires Dotmatics

ENTERPRISE VALUE

$5.1B

Acquired from Insight Partners, Dotmatics' global software-investor backer

SIGNED	CLOSED
Apr 2, 2025	Jul 1, 2025

WHAT IT MEANS

- Dotmatics joins Siemens' Digital Industries Software business, expanding its AI-powered Product Lifecycle Management (PLM) portfolio into Life Sciences
- Positions Siemens to connect scientific R&D through to manufacturing execution, part of the broader Siemens Xcelerator portfolio
- Financed primarily through the sale of shares in listed companies, including Siemens Healthineers
- Expected revenue synergies of roughly $100M per year in the medium term, growing to over $500M per year long-term
- Dotmatics' revenue growth and profitability are expected to be immediately accretive to Siemens' margins and free cash flow

Outline

1

Challenges and Opportunities Facing Commercial Software

2

Core Capabilities That Every Chromatography/Mass Spec Software Must Have

3

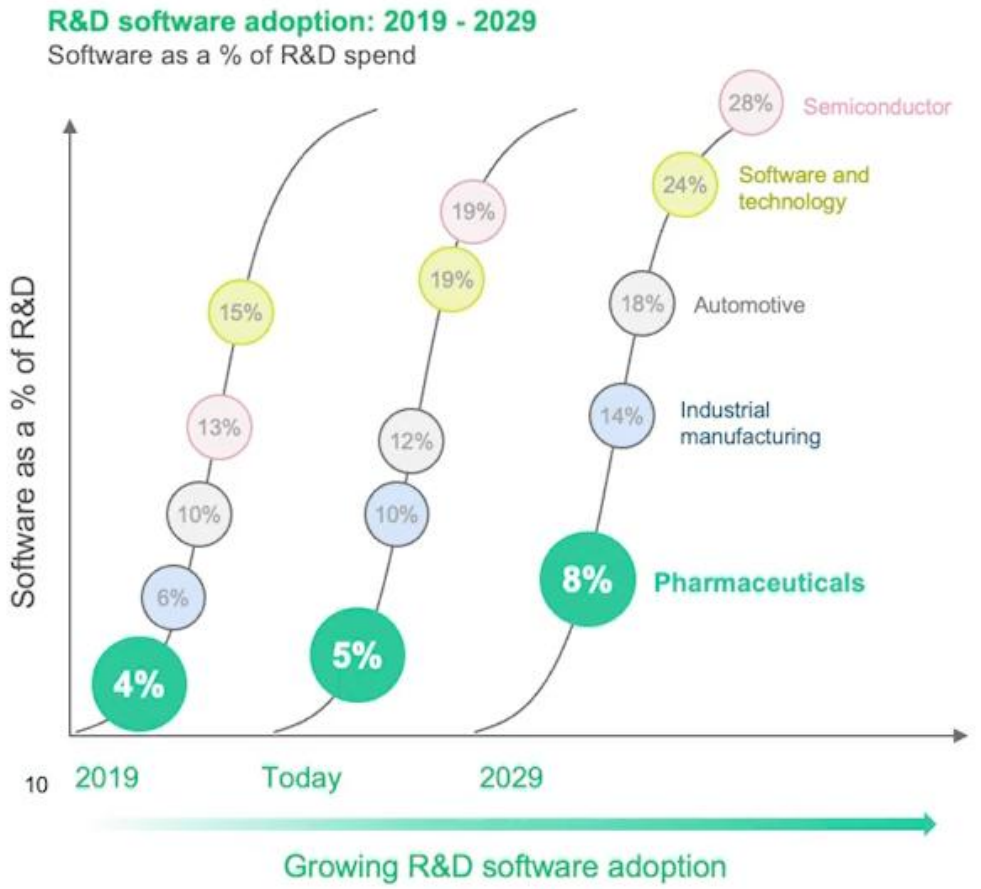
The Vendor's Missing Automation Layer

Commercial Software Faces Many Threats/Challenges/Opportunities

INDUSTRY TREND

Software Spending as % of R&D

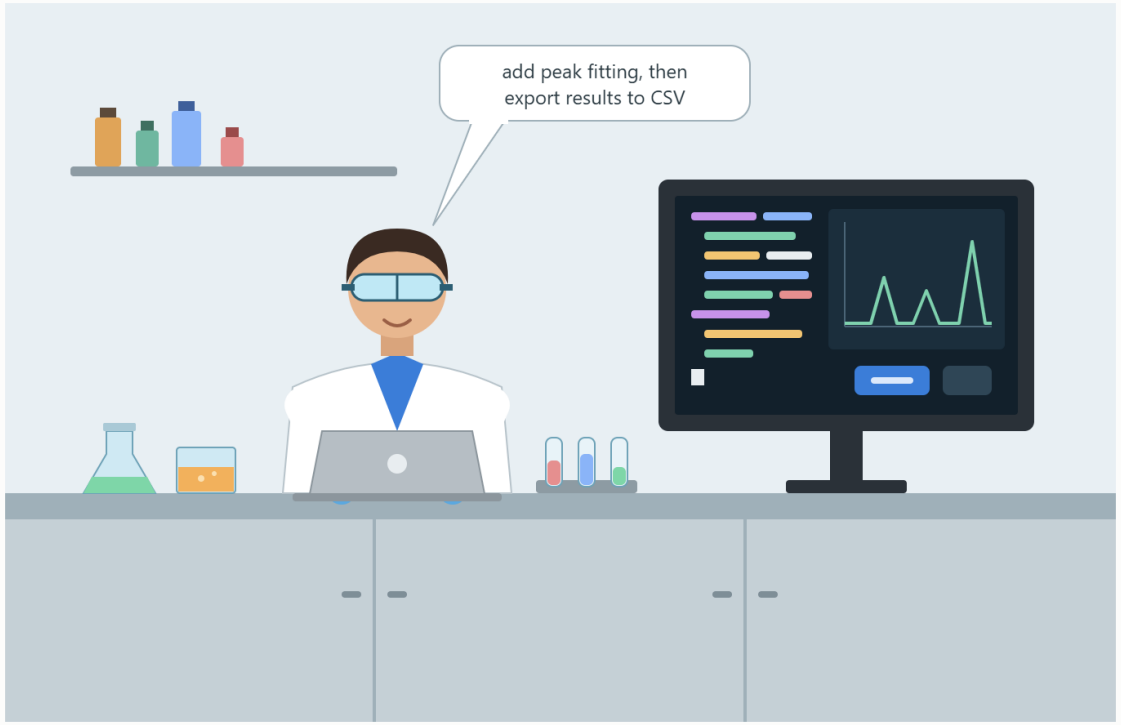
Life sciences has been slower to adopt software solutions than other high-growth, IP-intensive industries…



…but the acceleration of complex R&D workflows is driving the need for technology innovation

Scientific research is pushing into new, more complex modalities and domains	**Specialized applications** for scientific processes and experimentation
Advances in drug research require significant cross-organization collaboration	**In silico drug discovery tools**, such as simulation platforms
Data volumes are increasing as science and research methods advance	**Science-specific data analytics** and management software
Modern workflows require orchestration across many tools and inputs	Cloud-based, shared, **collaborative platforms**

Everyone Is A Software Engineer



- **Everyone now has access to AI tools**
- **AI is increasingly good at making software**
- **Is vibe coding a sustainable path forward?**

Advantages

- Custom solution
- Perfectly suited to your needs
- Under your control
- Low cost

Disadvantages

- Point solution; not general
- No comprehensive data management

AI CONSIDERATIONS

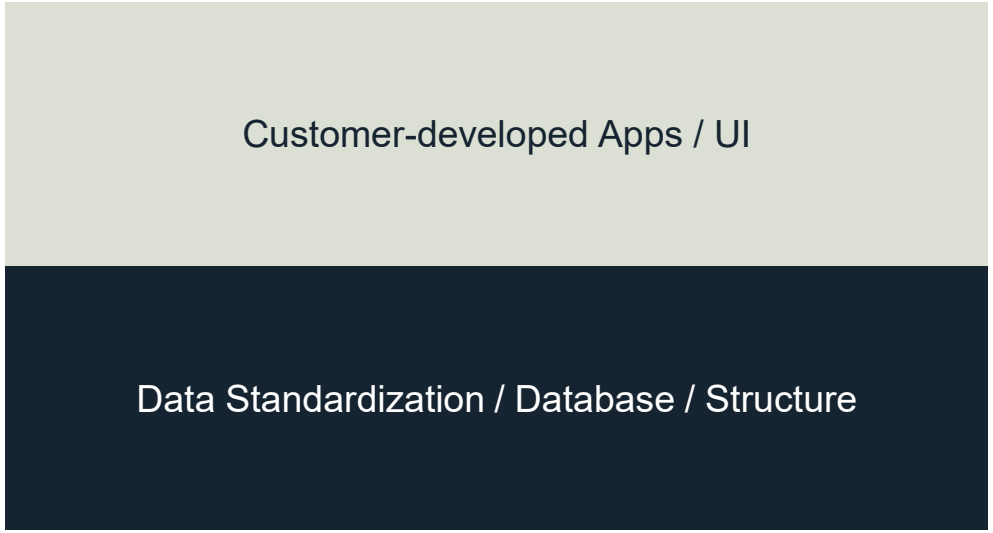
Is Commercial Software Dead?

Short Answer: **Not entirely**

Complicated Answer:

- Many simple, low-complexity applications will be replaced
- “Single-purpose” apps will just be made by AI
- Enterprise apps are safe
- AI is forcing commercial software companies to re-evaluate where their value lies:

Future value in commercial software resides in the data structures and organization



INDUSTRY TREND

Mass Spec Has Gotten Much Faster — Has Data Analysis?

Rough, order-of-magnitude trends in pharma discovery MS over the decades

▲ SAMPLES PROCESSED PER DAY

Rough order of magnitude



1990s	2000s	2010s	2020s
Hundreds	Thousands	Tens of thousands	50,000+

▼ ACQUISITION TIME PER SAMPLE

Rough order of magnitude



1990s	2000s	2010s	2020s
~1–2 min/sample	~30–60 sec/sample	~1–10 sec/sample	<1 sec/sample

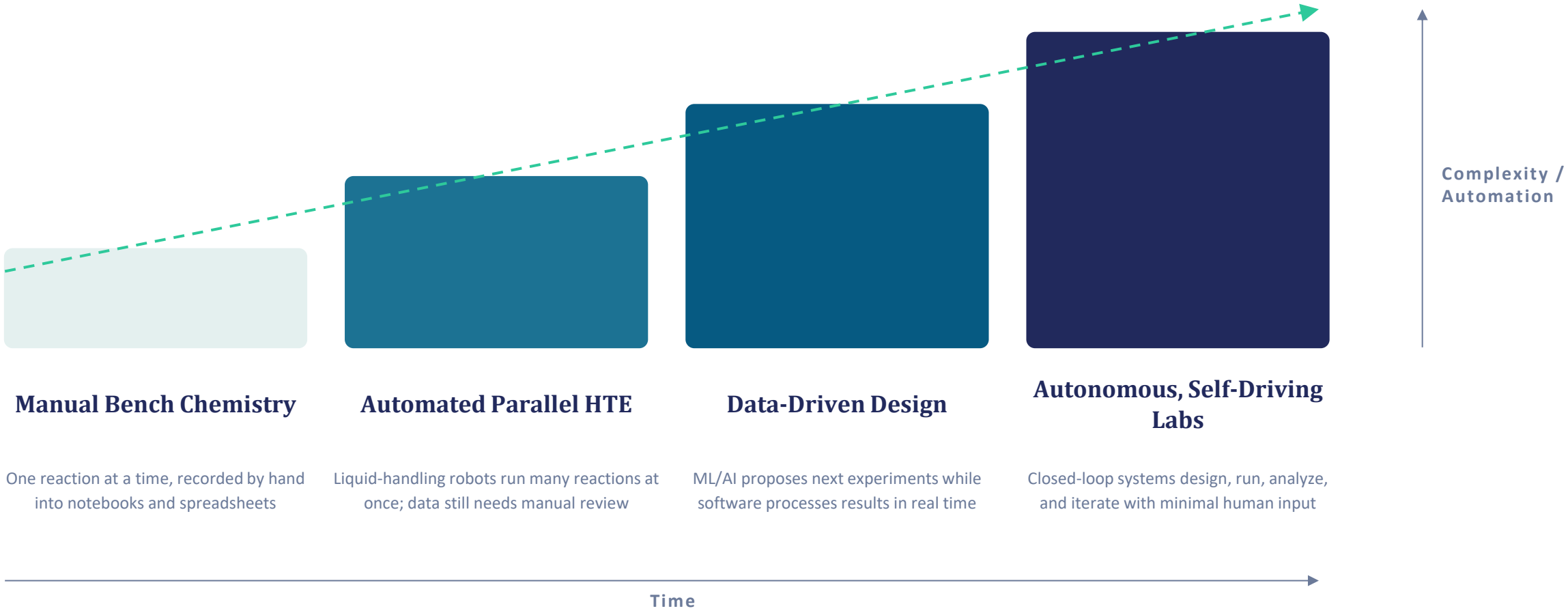
⚠ *Every gain in MS speed multiplies what the data platform must process — turning analysis into the new bottleneck*

Virscidian

INDUSTRY TREND

High Throughput Synthesis Is Moving Toward Full Autonomy

From single manual reactions to closed-loop, self-driving laboratories



Manual Bench Chemistry

One reaction at a time, recorded by hand into notebooks and spreadsheets

Automated Parallel HTE

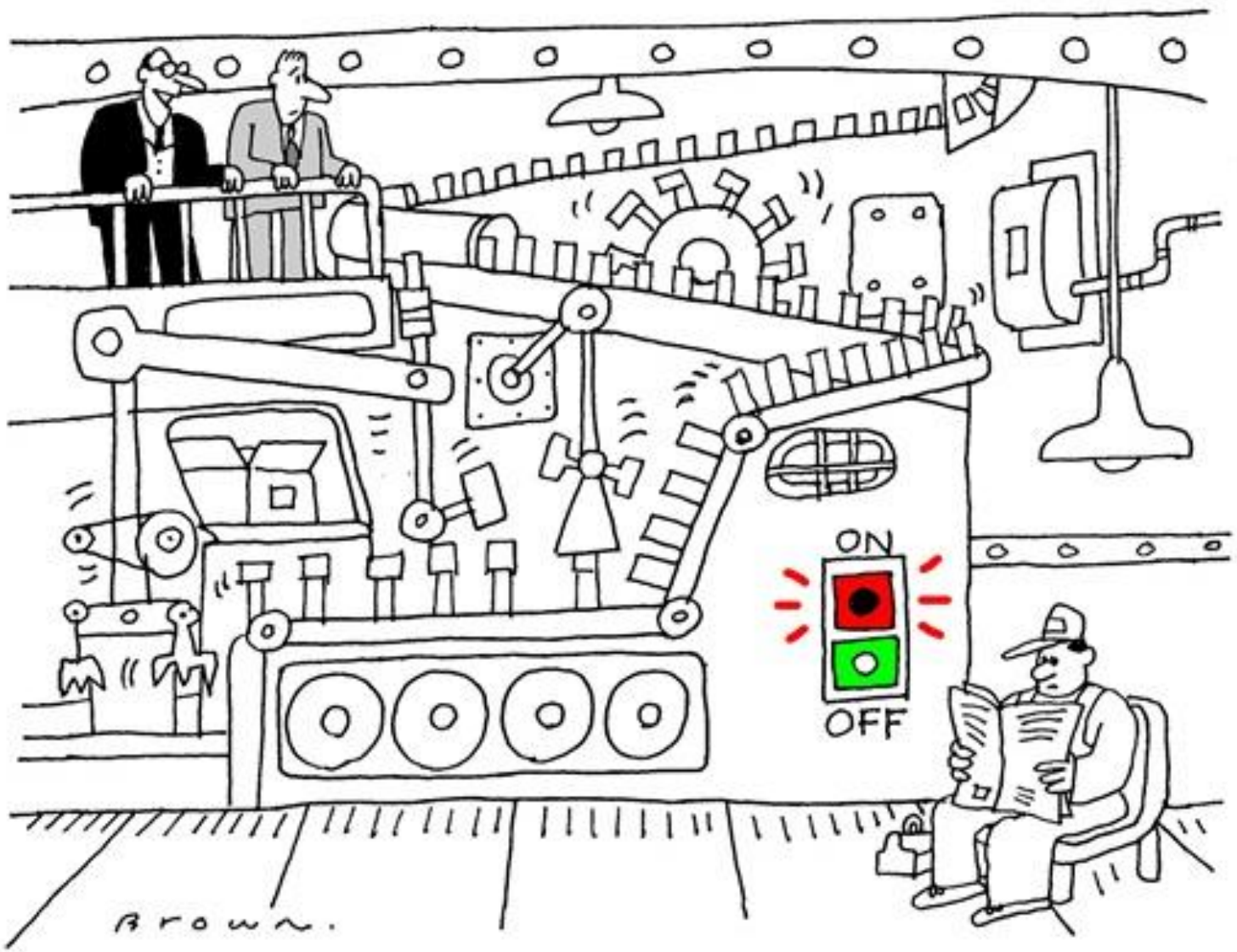
Liquid-handling robots run many reactions at once; data still needs manual review

Data-Driven Design

ML/AI proposes next experiments while software processes results in real time

Autonomous, Self-Driving Labs

Closed-loop systems design, run, analyze, and iterate with minimal human input



"We're almost fully automated now."

Virscidian

Essential software capabilities for chromatography / mass spec

THE DATA SWEEP

From Instrument Run to Structured Record

New files are detected, collected, and structured continuously — no manual export required



LC-MS Instruments

Runs complete; raw result files are written to disk

Watched Folders

Analytical Studio monitors instrument shares in real time

Virscidian Analytical Studio

Parses, validates and normalizes vendor file formats

Data Platform

Clean, AI/ML-ready data is available to scientists

THE DATA SWEEP

Many Data Sources

Many instrument vendors and data formats, each with unique properties

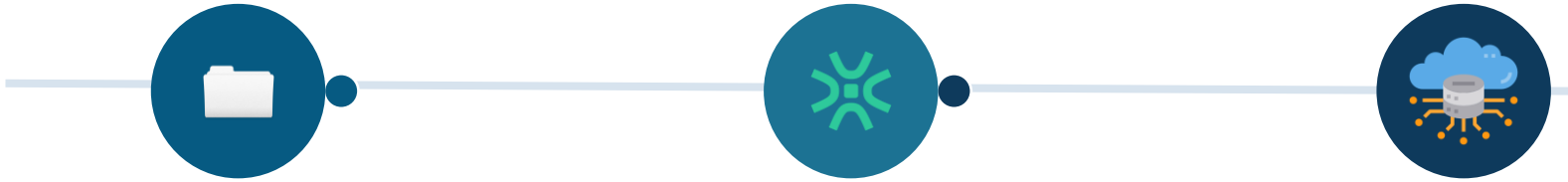
Waters
THE SCIENCE OF WHAT'S POSSIBLE.

SCIEX
The Power of Precision

Agilent

SHIMADZU
Excellence in Science

Thermo SCIENTIFIC



Watched Folders

Analytical Studio monitors instrument shares in real time

Virscidian Analytical Studio

Parses, validates and normalizes vendor file formats

Data Platform

Clean, AI/ML-ready data is available to scientists

SMART PROCESSING

One Instrument, Multiple Processing Paths

Once data is captured, Analytical Studio decides how to process it

CONTEXT-AWARE PROCESSONG METHOD SWITCHING

Processing methods and parameters adjust automatically based on what makes a sample different, such as:

1. **Instrument alignment**

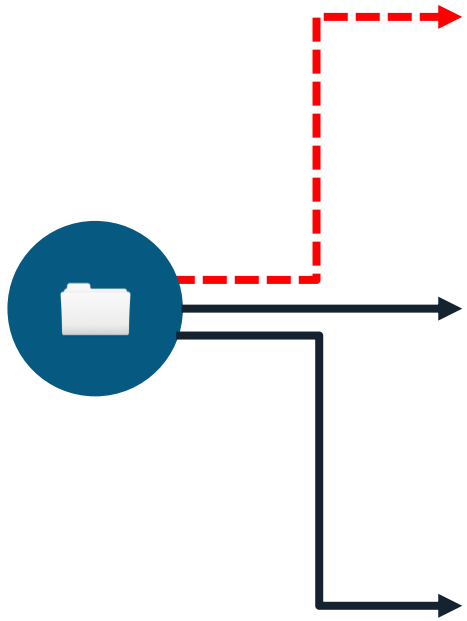
   The method used matches the exact instrument and configuration that generated the data

2. **Experiment / Assay type**

   HTE, HTP, AS-MS, and process-chemistry workflows each apply their own tailored processing logic

3. **Other distinguishing context**

   Substance type, plate position, or any metadata that marks one sample as needing different treatment



EXPRESSIONS

Expressions - Replace Manual Data Manipulation

Live logic, co-located with the data — not a static spreadsheet

~~Manual data manipulation~~ → Expressions — live, co-located, updates in real time

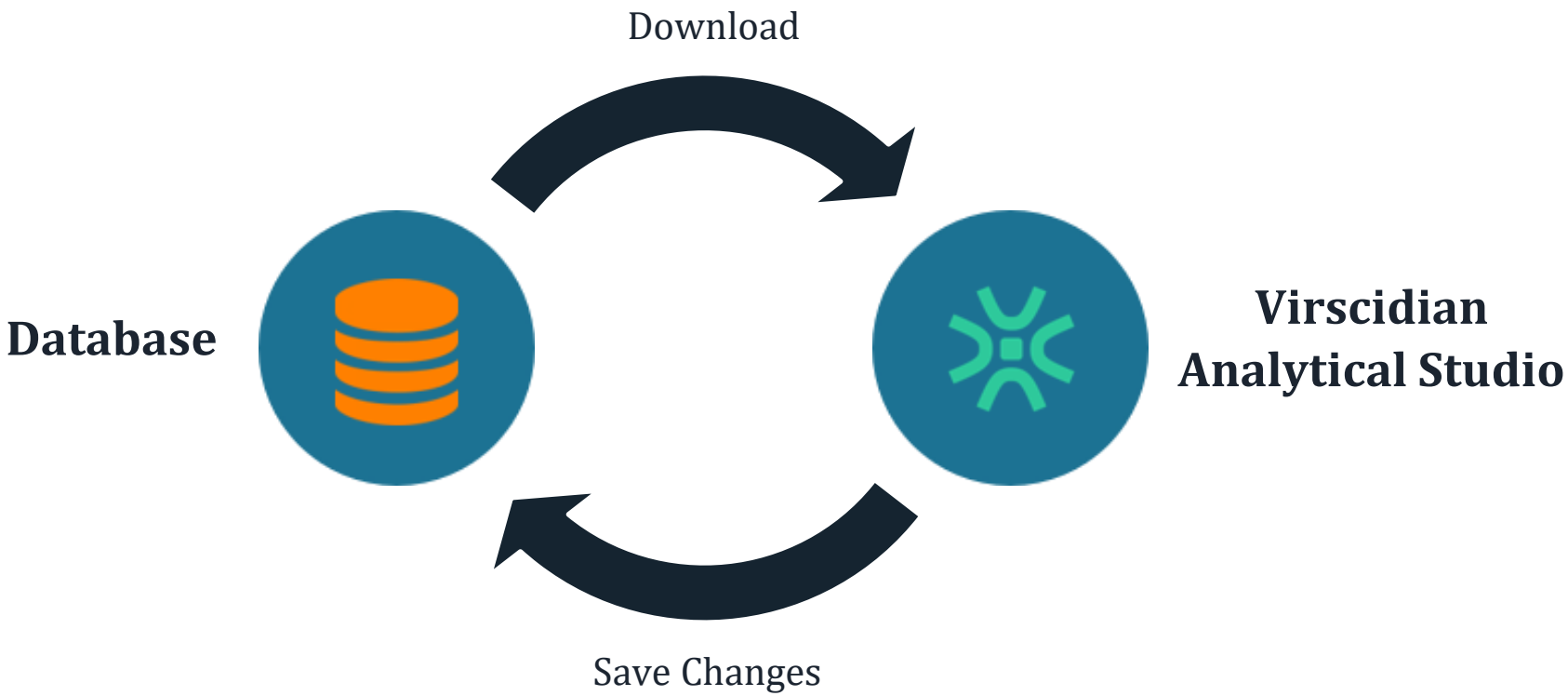
EXPRESSIONS ARE SO MUCH MORE THAN CALCULATIONS

- Substance Results & Peak Attributes
- Customized Calculations
- Reaction/Method Scoring
- Sample Metadata & Reaction Conditions
- Warnings & Review Flags
- Automated Commenting

Virscidian can make automatic decisions for 85-90% of samples; review-by-exception for remainder

Virscidian

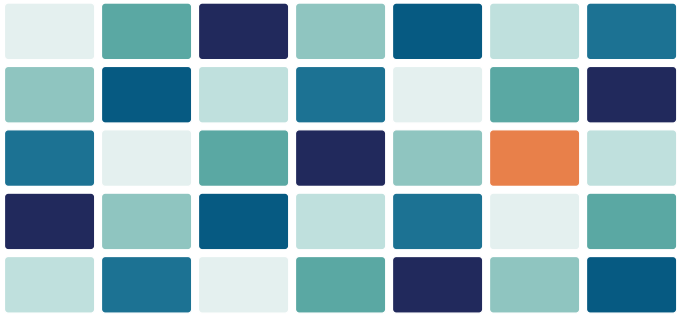
Opportunity for Scientists to Curate Data



SELF-SERVE ANALYSIS

Visualizations and Reports

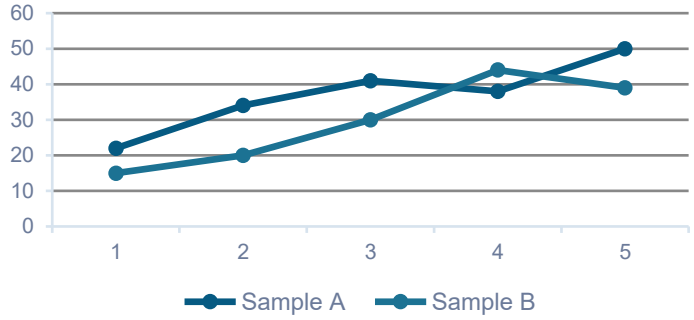
COMPARE SAMPLES AT A GLANCE



Heat Maps

Sample	Purity	Yield
A-2	98.2%	91%
A-3	95.7%	88%
A-4	99.1%	94%
A-5	96.4%	90%

Tables



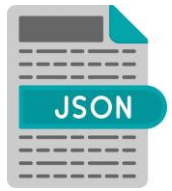
Graphs

PREPARE REPORTS











Key Requirements

Essential Elements of Automated Data Processing

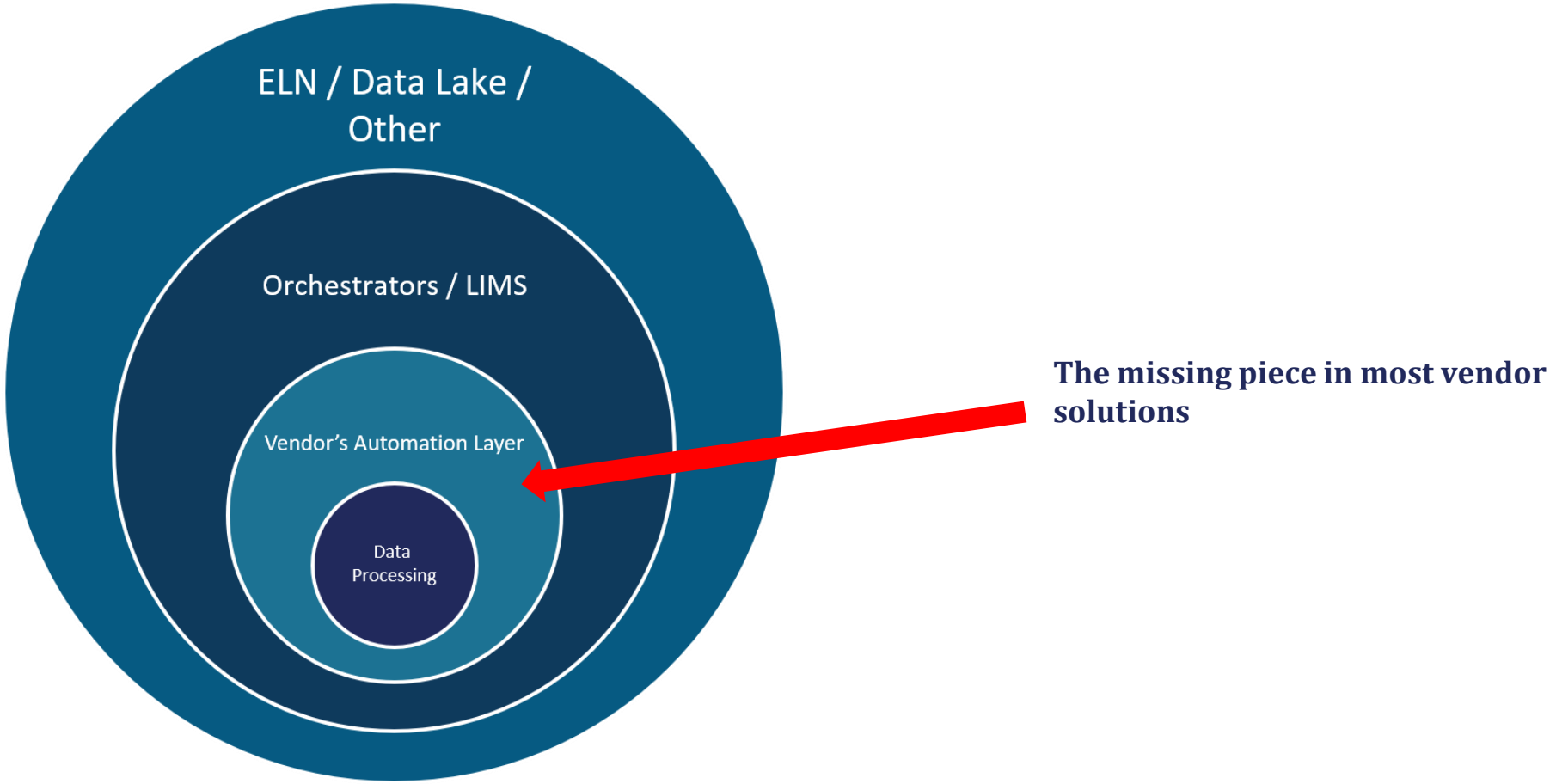
1. Automatically sweep data from instruments of various kinds/formats
2. Automatically process that data with context awareness
3. Automatically apply calculations and business logic to results
4. Make results available for manual curation if desired
5. Provide visualization tools
6. Provide ways to report the data

ECOSYSTEM INTEGRATION

Data Processing Is One Piece of a Much Bigger Picture

A modern vendor doesn't just process data — it speaks the same language as the customer's data platform

CUSTOMER'S DATA MANAGEMENT STRATEGY

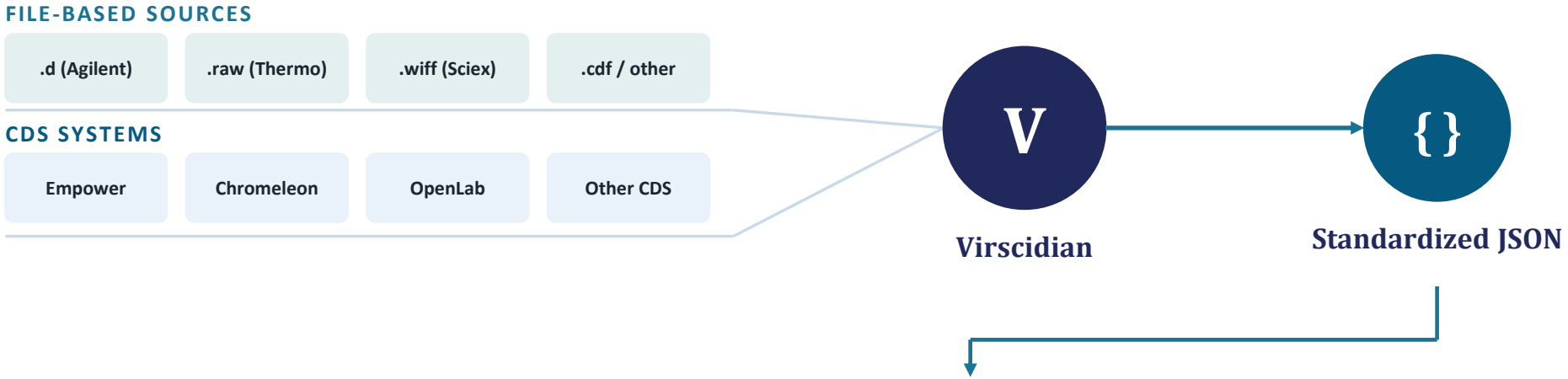


What is Virscidian doing to make the “automation layer”?

DATA HARMONIZATION

One Common Language for Chromatography Data

Every vendor file format and CDS source is harmonized into a single, well-defined JSON representation



WHY STANDARDIZATION MATTERS

One schema for all chromatographic data — regardless of source instrument or CDS

Consistent Processing

The same schema drives identical processing logic, no matter which instrument or CDS the data came from

Cross-Vendor Comparison

Results from different vendors and systems can be compared side-by-side without manual translation

AI/ML-Ready Input

Clean, structured JSON feeds directly into machine learning and AI models — no extra prep required

CDS Extraction Platform

A simple end-to-end flow from a change in CDS to a published standardized package.

1. **Scan CDS** — Monitor configured projects
2. **Detect change** — New / updated injection or result
3. **Create task** — Put durable work on the queue
4. **Extract** — Worker uses vendor SDK/API
5. **Normalize** — Validate + build standard JSON package
6. **Publish** — Send package

What Information can be extracted?

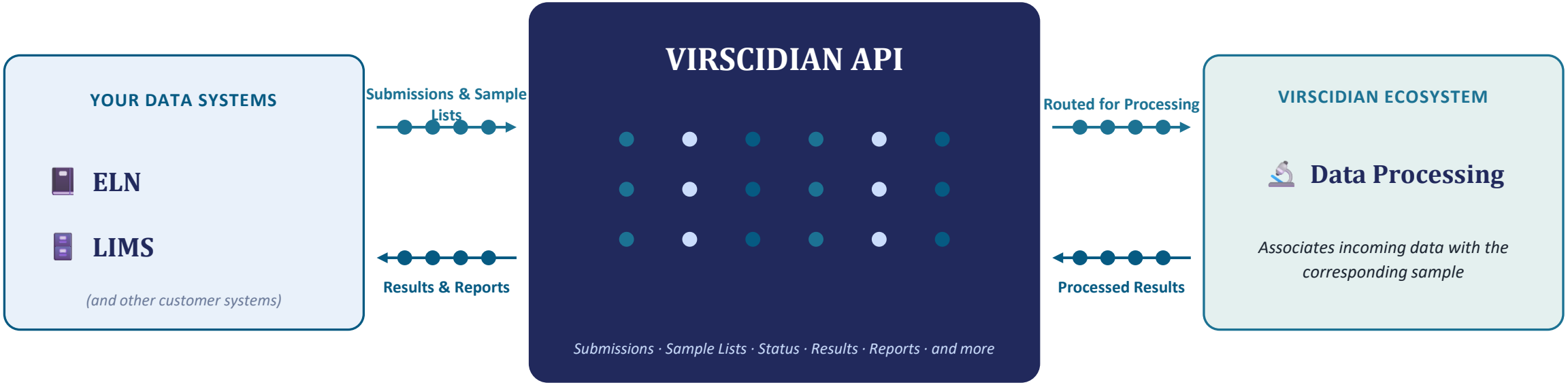
- Projects / entities *the way the CDS organizes data*
- Raw data
- Results *generated by processing within the CDS*
- CDS processing method parameters
- Metadata
- Acquisition method parameters

SUPPORTED CDS ENVIRONMENTS

- Waters Empower
- Agilent OpenLab CDS
- Thermo Chromeleon
- Waters Connect

API INTEGRATION

API – Single Interaction Point In and Out



ORCHESTRATION INTEGRATION

Analytical Decisions Drive the Workflow

Virscidian

Makes the analytical decision

BIDIRECTIONAL API COMMUNICATION

- Sample Tracking
- Event Notifications
- Sample Status
- Results / Artifacts
- Sample Lists

Orchestrator / Scheduler

Executes the workflow logic

Virscidian's results tell the orchestrator / scheduler what to do next

Proceed to Next Step

The sample advances to the next analytical step defined in the workflow

Discard Sample

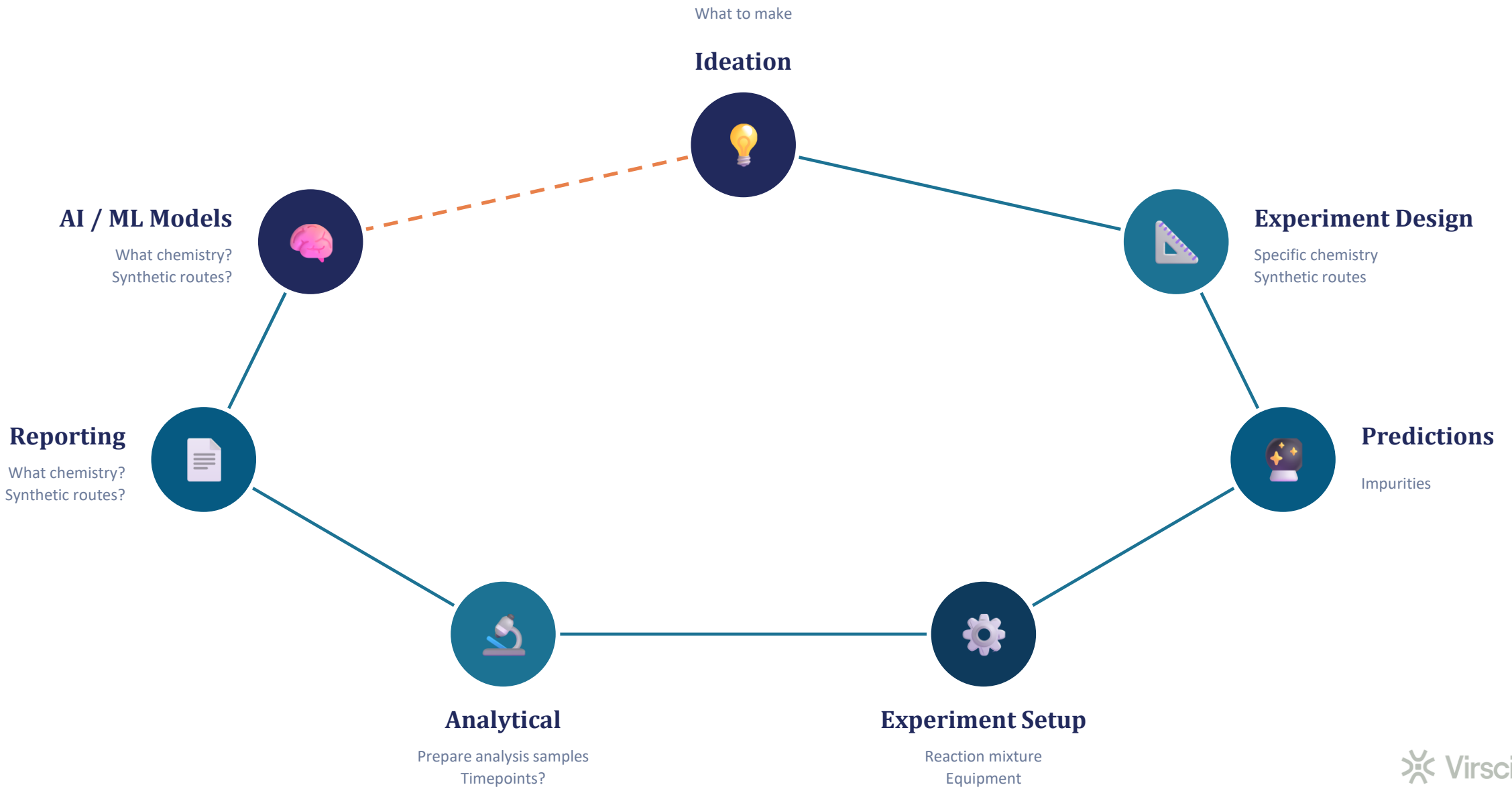
The sample is flagged and removed from the active workflow

Revert to Previous Step

The sample returns to an earlier step for additional analysis

The exact orchestration logic is configurable — these APIs adapt to each customer's unique analytical workflow

Autonomous HTE Labs



Virscidian

Key Requirements

Essential Elements of Automated Data Processing

1. Standardized data from individual files and CDS platforms
2. Formatted and structured for AI and ML
3. APIs for talking to your data systems
4. Integration with lab automation and orchestration software
5. Interact seamlessly in autonomous processes

1

Challenges and Opportunities Facing Commercial Software

2

Core Capabilities That Every Chromatography/Mass Spec Software Must Have

3

The Vendor's Missing Automation Layer

Thank you!