

Connecting Systems Across Experimental Workflows

	Katalyst D2D	ELN/LIMS*	Third-Party Analytical Data Software* (e.g. Virscidian, MestreLab)	Experiment Execution Systems* (e.g. Chemspeed, Unchained Labs)
Primary focus	Experimental workflow orchestration & data management	Documentation, sample & results management	Analytical data processing & interpretation	Automated experiment execution
Experiment design/reaction planning	Integrated. Optional AI plug-in ✓	Vendor and experiment-dependent	Out of scope	Vendor-dependent
Workflow execution	Coordinates entire workflow ✓	Limited	Handles analytical workflows	Experiment execution workflows
Analytical data processing	Results connected to experiment(s) ✓	Limited	Core strength ✓	Limited
Multi-step workflow continuity	Across DMTA cycle ✓	Partial	Partial	Partial
Hardware integration	Vendor-agnostic for analytical and experiment hardware ✓	Limited/Add-ons	Analytical instruments	Automation hardware
Structured AI-ready data	Contextualized experimental and analytical results ✓	Vendor and experiment-dependent	Analytical results	Experiment logs
Best suited for	HTE, automated experimentation, materials workflows ✓	Compliance and record keeping	High-volume analytical data processing	Automated material handling
Core competency	Central orchestration layer Connected experimental workflows and contextualized data	Scientific record-keeping and compliance	Analytical processing and interpretation	Experiment execution platform

* Complementary to Katalyst D2D