Over the last 25 years pharmaceutical R&D organizations have invested in high throughput methodologies, automation, and informatics assets with the intention to increase overall productivity. These assets are typically not integrated from initial experimental design through to decision making. This lack of integration creates a significant impediment to the productivity objectives of organizations.

Katalyst D2D empowers scientists to easily and efficiently design, plan, execute, analyze, and make decisions about high-throughput and parallel experiments in a single integrated interface.

From Design to Decide
Katalyst D2D is purpose-built to support a wide variety of experimental workflows. While Katalyst is delivered with a default set-up, the application can be configured to support custom workflows in a facile manner. Fundamentally, the application is built from discrete functional units (widgets) that can be used to create desired user interface (UI) layouts. These may be arranged by the user to meet their workflow requirements.

The first step of any parallel or high throughput experiment is to design a set of reactions to be executed. The inputs to such a design are:

1. Target reaction product(s) of interest
2. Process route for each reaction product, including machine-initiated or scientist-initiated operations (and parameters for ranges)
3. Starting materials, reagents, and any related material classes required for the process route to be executed

Katalyst allows users to design a parallel experiment by defining material classes specified by the process route in the Reaction Design widget. The process route is visually represented by a reaction scheme that allows users to associate material classes to a location relative to the reaction arrow.

Katalyst D2D supports your entire experimental design.
Materials may be selected and associated with the Reaction Scheme in the following ways:

1. Use the Material Query widget to search both internal and external data sources to associate (via drag-and-drop) a material to the appropriate position and specify the material class for that group.

2. Simply double-click at the appropriate position in the reaction scheme to manually add a structure using the ‘structure drawing pop-up window’.

Drag and drop materials into the reaction scheme to populate your design in Katalyst D2D.

Use the embedded structure drawing widget to populate the reaction scheme.
Pop-up forms enable you to define material amounts and locations. Once a material has been assigned to a location in the reaction scheme, you can define whether it should be added neat, or from stock solution.

The stock solution calculator in Katalyst D2D allows you to define concentrations, total recipe amounts, and excess.

Based on the design envisioned by the scientist, Katalyst supports physical execution of the high throughput or parallel experiment by allowing users to specify the following:

1) Physical arrangement of parallel experiments in a variety of reaction vessels

2) Physical layout of materials to be dispensed into reaction vessels

3) Physical amounts required for each material with the capability to support volumetric, gravimetric, and molarity values, as necessary

4) Operations and procedures along with the specific parameters for each operation required for experiment execution
Katalyst offers the capability to generate both human-readable and machine-readable procedures for experiment execution.

Machine readable instructions allows the user to avoid the effort of configuring the execution and analysis instrumentation by providing the ability to export formatted procedure files that are easily imported into specific instrument software interfaces.

Human-readable instructions may be generated as a report for procedural steps that require manual effort (e.g., weighing and preparation of reagent stock solutions).
Katalyst is built upon ACD/Labs’ established Spectrus Platform—delivering a proven, industry leading solution for vendor agnostic, multi-technique analytical data handling. Katalyst empowers users with the capability to create samples and execute analyses for various experiment types (LC/UV/MS, NMR, IR, etc.) from most major instrument vendors. Data processing and analysis is also carried out in the same system. All relevant analytical data is automatically associated with each individual well in an array.

**Sampling**

The sampling of reaction vessels is supported by the following workflow:

1. Define sample vessels for every analytical experiment (e.g., HPLC vials, 96-well microtiter plates, etc.)
2. Designate the method by which the reaction vessels will be sampled (e.g., aspirate and dispense)
3. Specify the volume of reaction material to be sampled for analysis, as well as volume of any analytical sample diluent. Additional analytical sample preparation operations may also be defined
4. Assign the analysis technique(s) for the resultant analytical samples

Katalyst D2D supports the automated preparation of analytical samples and procedures.
Execution of Analytical Experiments

Once samples and analyses are defined, Katalyst will generate a formatted procedure list for a variety of instrument types.

Analytical Data Processing

Katalyst allows users to establish association of analytical results to samples in two ways:

**Automated**—instruments acquiring analytical results (as specified in the design and planning phase) may be monitored by ACD/Labs technology that will automatically sweep the instrument for new data at user-defined time periods. Once acquisition for each individual sample is complete, fully automated processing, analysis, and association to Katalyst records is performed.

**Manual**—alternatively, users may choose to manually process, analyze, and associate analytical data to Katalyst records, for either a single dataset or a batch of analytical data—using a fully-functional desktop application add-on (ACD/Spectrus Processor for Katalyst D2D).
Once analytical data processing and analysis is complete, Katalyst automatically assembles and associates the results for each individual well in the experimental array. Spectra may be compared easily within the same interface for various parallel reaction variants. Live analytical data provides the capability to conveniently reprocess and/or reanalyze, should the need arise. Graphing and plotting tools within the interface empower the user to visualize trends and support fast, effective decision-making.

Stacked chromatograms of the 10 reactions with the best product yield by peak area. Live data enables facile review and analysis with capabilities to zoom and reprocess or re-analyze at will.

LC/MS results for a 96 well plate visualized as a dynamic stacked plot of assigned chromatograms. Rapidly assess the quality of their chromatography, data processing, and data analysis in one display.

The ‘Plotting Workspace’ empowers you to easily spot trends in your results.

From Design to Decide in one application for efficient, collaborative high throughput experimentation