

# Integrated R&D

research, development, scale-up

**Enterprise** Initiatives sites, organizations, time, specialties, applications, markets Execution **Programs**

<b>Innovation</b> Collaboration & Modeling	<b>Risk</b> Standards & Compliance	<b>Cost</b> Lab-to-Plant
---	---------------------------------------	-----------------------------

**Work Groups** Functions chemistry, biology, synthesis, formulations, process, analytical, QA/QC Visibility **Informatics**

<b>Design</b> <i>Imagine, Plan, Setup</i> Hypothesis Formulation Variables Definition Online Literature Public Sources Compound Registry Chemicals & (Materials) Inventory Synthesis planning Project Planning	<b>Execute</b> <i>Schedule, Implement, Track</i> Instrument Control Experiment Control Parameter Selection Data Capture & Store Data Aggregation & Normalization Dynamic Decision Making	<b>Analyze</b> <i>Query, Vizualize, Mine</i> Multi-variable Data Correlation Reaction Pathways Statistical Analysis Spectral clustering Data QC & Curation Simulation and Modeling Curve Fitting Charting	<b>Report</b> <i>Publish, Store, Share</i> Protocols, Procedures, & Results Notebook Storage & AuditTrails Batch Records Document Approvals Cross Project Analysis Automatic Report Generation Report Publication
---	---	--	---

**Users** Tasks materials, samples, instruments, results Throughput **Automation**

<b>Prepare</b> <i>Plan, Dispense, Weigh, Move</i> Solids Dispensing Viscous Liquid and Slurry Handling Solvent Delivery High-Temperature Transfers Volumetric and Gravimetric Dispensing Automated Weighing (High Accuracy) Plate, Vial, Bottle Handling Integrated Off-deck Storage Titrate	<b>Process</b> <i>Mix, Heat, Cool, Equilibrate, Separate</i> Stirred-tank Reactions Temperature Controlled Magnetic Stirring Temperature Controlled Vortexing Powder Mixing (whisking) High Shear Mixing, Viscous Materials Automated Microcompounding High-viscosity Reactive Material Blending (the "A/B Mixer") Film Preparation by Drawdown and Drop Deposition Automated Centrifugation and Phase Separation Materials Deposition and Release Microwashing Powder Agglomeration, Grinding, Sizing Crystallization Sample Filtration for Crystallization	<b>Test</b> <i>Multi-Technique</i> <b>On-Deck</b> pH and Conductivity Mass & Sample Imaging Spectroscopy, Turbidity Color and Gloss Tribology (Friction, Wear, Tack) Chemical Resistance Chromatography Molecular Weight Determination Spectroscopy Thermal Analysis Elemental Analysis & Mass Spectrometry (MS) Light Scattering/Particle Size Mechanical Properties	Surface Energy Permeability Catalyst Activity & Selectivity Viscosity Profilmtry (Thickness)
--	---	--	--

**Materials** Experiments stability, solubility, compatibility, degradability, durability, toxicity, efficacy, manufacturability Properties **Chemistry**

<b>Scale</b> Microgram Milligram Milliliter Mmolar Nanomolar 10's of mg 10's of mL Vials Tubes Flasks Bottles Titre Micro-titre	<b>Materials &amp; Chemistries</b> Materials & Chemistries Hydrogenation (chiral, achiral) Cross Coupling Buchwald-Hartwig Aminations Suzuki-Miyaura Heck Enantioselective transformations Hydroformulation Organometallics Enzymatic Catalysis Polyolefin Polymerization Single site & Ziegler-Natta Halogenated polymers Free-radical polymerization & RAFT Ring-opening polymerization Oxidation & ODH Emissions Ammoxidation/Amination	<b>Analytical Technique</b> <b>Off-Deck</b> Melting Point Static and Dynamic Light Scattering Tribology (Tack, Friction, Wear) Rheometryer GC HPLC LC-MS MS GPC TREF Raman FTIR UV-Vis Optical Microscopy IR Thermography Electron Microscopy Sulfur & Nitrogen Detection	<b>Reaction Technique</b> Batch Pressure Reactions Semi-Continuous/Continuous Pressure Multi-phase reactions (ie Gas/Liquid) Three-Phase Reactor Bulk Polymerizations Emulsion / Suspension Impregnation Co-precipitation
--	--	---	---

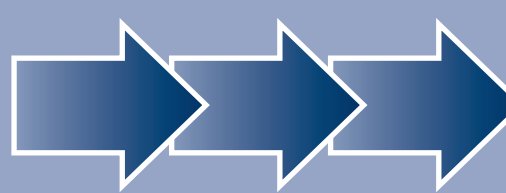
## R&D is under pressure

## Alignment for ROI

Integrate Chemistry, Systems, Software and Scientific Applications

R&D is breaking apart

Symyx integrates R&D



Traditional

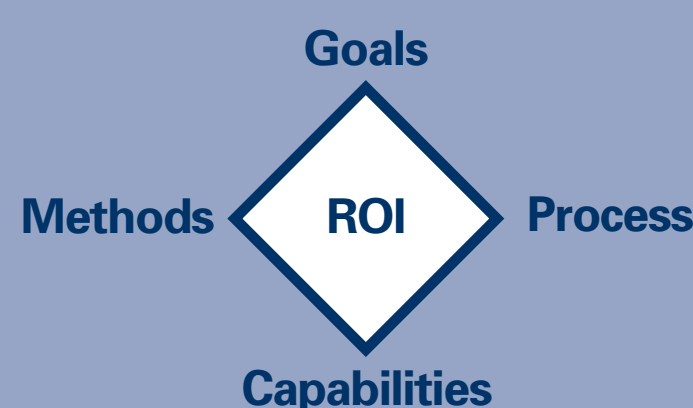
Integrated

Single-dimensional

Paper and File Silos  
Serial, Physical, Manual  
Proprietary, In-House

Multi-dimensional

Digital, Searchable, Unified  
Parallel, Miniaturized, Multivariate  
Open, Platform-based

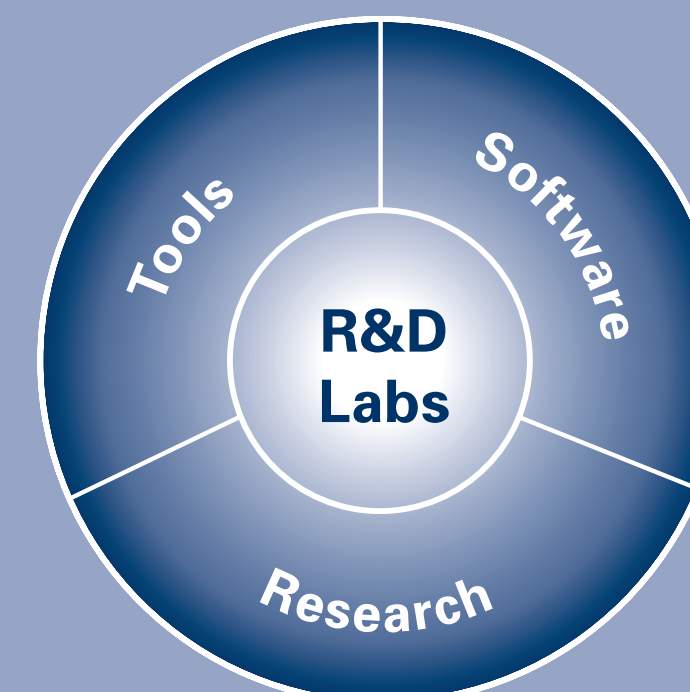


Side A: Value Identification		Side B: Value Realization	
Goals & Initiatives	Process	Capabilities	Methods
Innovation Risk Cost	Design Execute Analyze Report	Prepare Process Test	Scale Materials Analytical Reaction Time
Years to Months	Months to Weeks	Weeks to Days	Days to Minutes
Product Cycle-Time	Project Cycle-Time	Lab Cycle-Time	Experiment Cycle-Time

Reduce Risk and Shorten Cycle-time

## Symyx

Your R&D Integration Partner



Accelerating R&D Certainty



Innovation

Risk

Cost



Value Drivers	Value Opportunities	R&D Execution Initiatives
<p><b>Revenue Growth</b></p> <ul style="list-style-type: none"> <li>Improve Product Performance</li> <li>New Products</li> <li>Grow Young Products</li> <li>Improve Variants</li> <li>Increase Period of Exclusivity</li> <li>Speed Time to Market</li> <li>Other</li> </ul>	<p><b>Product &amp; Process Performance</b></p> <ul style="list-style-type: none"> <li>Technology for new platforms, variants, processes</li> <li>Rapid requirement to materials performance</li> <li>Green attributes</li> <li>Other</li> </ul> <p><b>Knowledge Management</b></p> <ul style="list-style-type: none"> <li>Replace paper notebooks</li> <li>Search across all project documents &amp; databases</li> <li>On-line literature connections</li> <li>Tabulate and correlate published results</li> <li>Search Registration database</li> <li>Document best practices</li> <li>Store searchable experimental results</li> <li>Facilitate 'find-the-expert'</li> <li>Aging workforce</li> <li>CRO exchange</li> <li>Other</li> </ul> <p><b>Patent</b></p> <ul style="list-style-type: none"> <li>Mine datent date</li> <li>Facilitate registrations</li> <li>Facilitate invention disclosures &amp; patent filings</li> <li>Lab records capture and compliance</li> <li>Other</li> </ul>	<p><b>Discovery</b></p> <p><b>Design, Develop &amp; Produce Library</b></p> <ul style="list-style-type: none"> <li>Design chemical synthesis or formulation</li> <li>Synthesize new materials</li> <li>Schedule testing protocol(s) (Analytical or internal)</li> <li>Enter into automation database; reuse and reference</li> <li>Register new and novel materials and compounds</li> <li>Other</li> </ul> <p><b>Screen Library for "Hits"</b></p> <ul style="list-style-type: none"> <li>Execute testing protocol(s); Chemical, Biological, Physical</li> <li>Capture Data into automation database</li> <li>Record Results to notebook entry</li> <li>Rank &amp; evaluate results from many tests; Categorical, Numerical, Complex</li> <li>Capture composition of matter patent information</li> <li>Other</li> </ul> <p><b>Hit to Lead and Lead Validation</b></p> <ul style="list-style-type: none"> <li>Structure-Property-Results Review</li> <li>Design new compounds, materials and synthesis; Synthesize</li> <li>Request Tests from Analytical</li> <li>Request Tests from confirming assays; Biological and Chemical</li> <li>Record to Notebook and Register New Discoveries</li> <li>Other</li> </ul> <p><b>External Sources</b></p> <ul style="list-style-type: none"> <li>Search and review procedures in both internal &amp; external literature</li> <li>Send out technical requests to collaborators</li> <li>Redesign synthesis; property optimization and scale</li> <li>Create new JOC style procedure</li> <li>Other</li> </ul>
<p><b>Safety &amp; Quality</b></p> <ul style="list-style-type: none"> <li>Improve Organizational Predictability</li> <li>Compliance</li> <li>Inherent Product Quality</li> <li>Secure Intellectual Property</li> <li>Fail early Clinical Trials</li> <li>Quality by Design</li> <li>Other</li> </ul>	<p><b>Portfolio Management</b></p> <ul style="list-style-type: none"> <li>Generate product profiles</li> <li>Project information &amp; reports on-line</li> <li>Project resource allocations</li> <li>Workflow routing</li> <li>Manage API/material supply &amp; demand</li> <li>Other</li> </ul> <p><b>Improve Business Process</b></p> <ul style="list-style-type: none"> <li>Standardization to apply quality practices &amp; reduce human error</li> <li>Reduce data collection time</li> <li>Reduce report generation times</li> <li>Track and decrease time per task</li> <li>Improve technology transfer and cross functional decisions</li> <li>Process descriptions</li> <li>Process reviews</li> <li>Support controlled vocabularies</li> <li>Reduce data transcriptions</li> <li>Other</li> </ul> <p><b>Regulatory</b></p> <ul style="list-style-type: none"> <li>21 CFR Part 11</li> <li>GMP processes &amp; documentation</li> <li>Environmental &amp; Global Markets</li> <li>Other</li> </ul>	<p><b>Development</b></p> <p><b>Candidate and Route Selection</b></p> <ul style="list-style-type: none"> <li>Assess development route of Lead/Hit</li> <li>Design Formulation</li> <li>Plan process variable study</li> <li>Schedule testing protocols (Analytical or internal)</li> <li>Evaluate results from both Discovery AND Development</li> <li>Execute Testing to screen and characterize</li> <li>Capture Data into automation database</li> <li>Record Results to notebook entry</li> <li>Capture process patent information</li> <li>Evaluate commercial viability-cost calculations, selectivity &amp; yield</li> <li>Evaluate material and process efficacy and safety</li> <li>Other</li> </ul> <p><b>Process</b></p> <ul style="list-style-type: none"> <li>Develop selected route (ad hoc)</li> <li>Identify critical process parameters and control variables</li> <li>Optimize sub-optimal steps</li> <li>Develop analytical methods and specifications</li> <li>Identify cleaning methods</li> <li>Characterize process yield, selectivity, and safety</li> <li>Produce non-GMP material, identify performance markers</li> <li>Documentation</li> <li>Miniaturize experiments</li> <li>Parallel experimentation</li> <li>Multi-technique analysis</li> <li>Other</li> </ul>
<p><b>Productivity</b></p> <ul style="list-style-type: none"> <li>Shorten Development Cycles</li> <li>Reduce Staff Costs</li> <li>Reduce Materials Costs</li> <li>Improve Yields &amp; Production</li> <li>Asset Utilization</li> <li>Changing Feed Stocks</li> <li>Other</li> </ul>	<p><b>Material Supply Management</b></p> <ul style="list-style-type: none"> <li>Scenario planning for API/materials</li> <li>Multi-step process definitions</li> <li>Characterize &amp; scale the process</li> <li>Validate process &amp; model economics</li> <li>Facilitate technology transfer internally and to third parties</li> <li>Manufacturing materials management</li> <li>Research chemical inventory</li> <li>Other</li> </ul> <p><b>Productivity of Scientist &amp; Engineer</b></p> <ul style="list-style-type: none"> <li>Reuse information</li> <li>Automate experimentation</li> <li>Speed calculations &amp; task execution</li> <li>Register new compounds</li> <li>Improve communication and reporting</li> <li>Searchable consolidated information stores</li> <li>Reduce training</li> <li>Desktop data integration &amp; system access</li> <li>Other</li> </ul>	<p><b>Scale-up &amp; Production</b></p> <p><b>Pilot Plant Route Development</b></p> <ul style="list-style-type: none"> <li>Establish plan to scale or optimize procedure</li> <li>Precise run instruction for operators</li> <li>Rigorous mass and heat balance</li> <li>Schedule QC/QA tests</li> <li>Add to notebook entry</li> <li>Enter into automation database</li> <li>Evaluate results from Discovery AND Development AND Pilot Plant</li> <li>Evaluate process safety</li> <li>Evaluate optimal procedures for manufacturing</li> <li>Other</li> </ul> <p><b>Toxicity, Clinical, Environmental Trials</b></p> <ul style="list-style-type: none"> <li>Generate relevant batch records or documents required by regulatory agencies</li> <li>Add to notebook entry</li> <li>Enter into automation database</li> <li>Cross-analyze trial data with all previous Discovery/Development/ Pilot Plant data</li> <li>Other</li> </ul> <p><b>Registration Batches in Production</b></p> <ul style="list-style-type: none"> <li>Issue batch record sheets (Electronic) Batch approval by regulatory</li> <li>Compliant documentation</li> <li>Other</li> </ul> <p><b>Process Validation &amp; Transfer to Operations</b></p> <ul style="list-style-type: none"> <li>Technology transfer documentation</li> <li>Process validations</li> <li>Qualification runs</li> <li>Issue chemical development report</li> <li>Other</li> </ul> <p><b>Support Manufacturing Operations</b></p> <ul style="list-style-type: none"> <li>Troubleshooting-reverse lookup to Discovery and Development data</li> <li>Continual Optimization</li> <li>Other</li> </ul>

	Design	Execute	Analyze	Report	Software	Systems	Research
<b>Discovery</b>	Design, Develop & Produce Library	Execute testing protocol(s); Chemical, Biological, Physical	Record Results to notebook entry	Rank & evaluate results from many tests; Categorical, Numerical, Complex			
<b>Development</b>	Candidate and Route Selection	Develop selected route (ad hoc)	Identify critical process parameters and control variables	Optimize sub-optimal steps			
<b>Scale-up &amp; Production</b>	Pilot Plant Route Development	Establish plan to scale or optimize procedure	Precise run instruction for operators	Rigorous mass and heat balance			

Solution	Chemistry: materials, catalysts, polymers						Biology: leads, hits, candidates					
	Synthesize	Screen	Develop	Formulate	Characterize	Scale-up	Synthesize	Screen	Develop	Formulate	Characterize	Scale-up
Draw	•	•	•	•	•	•						
MedChem Notebook	•											
Target-ID Notebook		•										
Bio-Screening Notebook		•	•									
Process Notebook						•						
Formulations Notebook					•							
Analytical Notebook					•							
In-vivo Notebook		•										
Registry	•	•		•	•	•						
Materials & Inventory	•	•	•	•	•	•						
Work Requests	•	•	•	•	•	•						
Equipment & Metrology	•		•	•	•							
Library Design	•	•	•	•	•	•						
Instrument Control	•	•	•	•	•	•						
Experiment Control	•	•	•	•	•	•						
Assay Explorer		•	•	•	•	•						
QSAR	•	•	•	•	•	•						
Bio-analysis	•	•										
Genealogy	•	•										
Clustering	•	•										
Synthetic Methodology References	•	•										
Bioactivity References	•	•										
Materials Properties References	•	•	•	•	•	•						
Document Management	•	•	•	•	•	•						
Data Warehousing	•	•	•	•	•	•						
Data Source Query	•	•	•	•	•	•						
Integration Services	•	•	•	•	•	•						
Chemistry Representation	•	•	•	•	•	•						
Powder Dosing			•	•	•							
Parallel Pressure Reactor			•	•	•							
Core Module Robotic Station	•	•	•	•	•	•						
Additives			•	•								
Adhesives, Coatings & Sealants	•	•	•	•	•	•						
Analytical Sample Prep			•	•								
BioCatalysis	•	•	•									
Catalyst Impregnation	•	•										
Coatings & Characterization			•	•								
Gas Phase Catalyst Screening	•	•	•		•							
Excipient Compatibility			•	•								
Forced Degradation			•	•								
Formulations			•	•								
Fuels & BioFeuls & Syngas	•	•	•	•								
Heterogeneous Catalysis	•	•	•	•		•						
Home & Personal Care Formulations & Testing	•	•	•	•								
Liquid Phase Catalyst Screening	•	•	•		•							
Organic Synthesis	•	•	•		•							
Polymerization Formulation			•	•								
Polymer Morph & Salt Selection			•	•								
Polymer Synthesis & Characterization	•	•	•		•							
Polyolefin Catalysis (Single Site, Ziegler-Natta)	•	•	•		•							
Refining (Naptha, Diesel Hydrodesulfurization)	•	•	•		•							
Solubility			•	•								
Viscous Formulations			•	•								

Industry Applications	
<p><b>Chemicals &amp; Energy</b></p> <ul style="list-style-type: none"> <li>Refining &amp; Petrochemicals</li> <li>Polymers (incl. Polyolefins)</li> <li>Base Chemicals</li> <li>Fine &amp; Intermediate Chemicals</li> <li>Paints, Coatings &amp; Inks</li> <li>Lubricants &amp; Oil-Field Chemicals</li> <li>Adhesives</li> <li>Agrochemicals</li> <li>Electronic &amp; Energy Storage</li> </ul>	<p><b>Life Sciences</b></p> <ul style="list-style-type: none"> <li>Small Molecule</li> <li>Large Molecule</li> </ul> <p><b>Consumer Products</b></p> <ul style="list-style-type: none"> <li>Home Personal Care</li> <li>Household Care &amp; Cleaning</li> <li>Food Science</li> <li>Flavors and Fragrances</li> </ul>

	Software	Tools	Research
<b>Enterprise</b>	Decision Support Data Warehouse Workflows	Custom Modules Custom Workflow	Partnerships Collaborative Research
<b>Workgroup</b>	Analysis Logistics Notebooks	Integrated Workflow Benchtop Workflow	Directed Research Technology Development
<b>Desktop &amp; Bench</b>	Content Chemistry	Sample Prep Dispense	Experiment Design Data & Results