

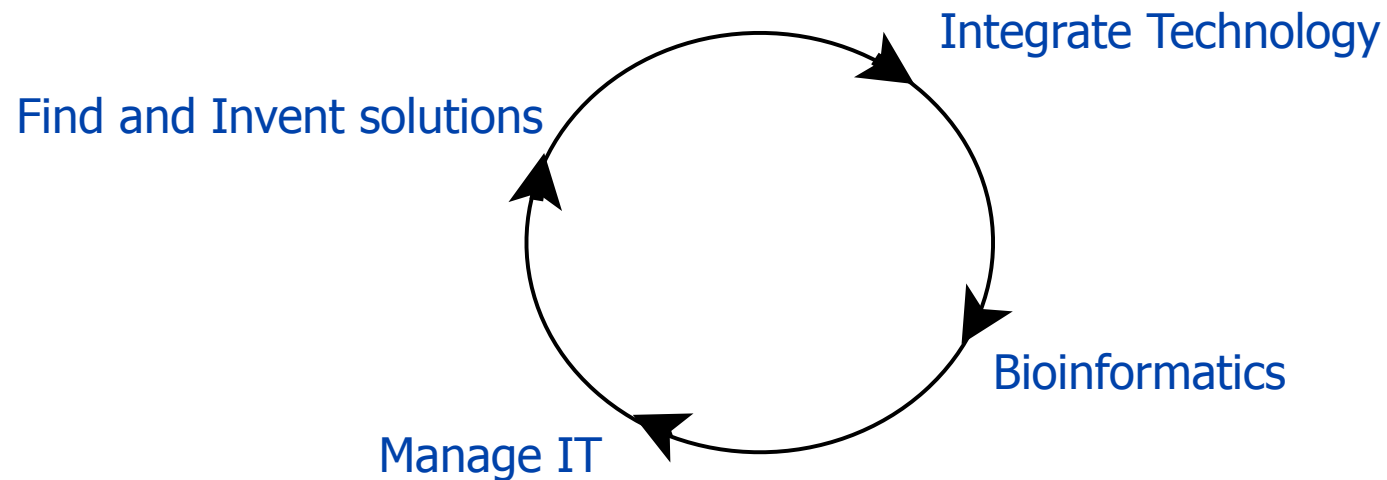
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# **The Right Tool for the Job:** Selecting and Integrating Informatics Tools to Enable Unique Science

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“We make tools to help bench scientists be more productive, efficient, and creative.”



# JOHN McNEIL & Company, Inc.

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- **Founded 2005**
- **Team of eight, most with lab experience**
- **Developers of LabSynch Semantic LIMS**

# Approaching Projects

# Project Planning Process

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- What are the current road blocks and pain points?
- What would enable new science, not just provide incremental improvement?
- What is the project timeline, and how does that compare to requirement change rate?
- If a system is being replaced, did the original fail technically, or in implementation/support?

# Evaluating Tools and Components

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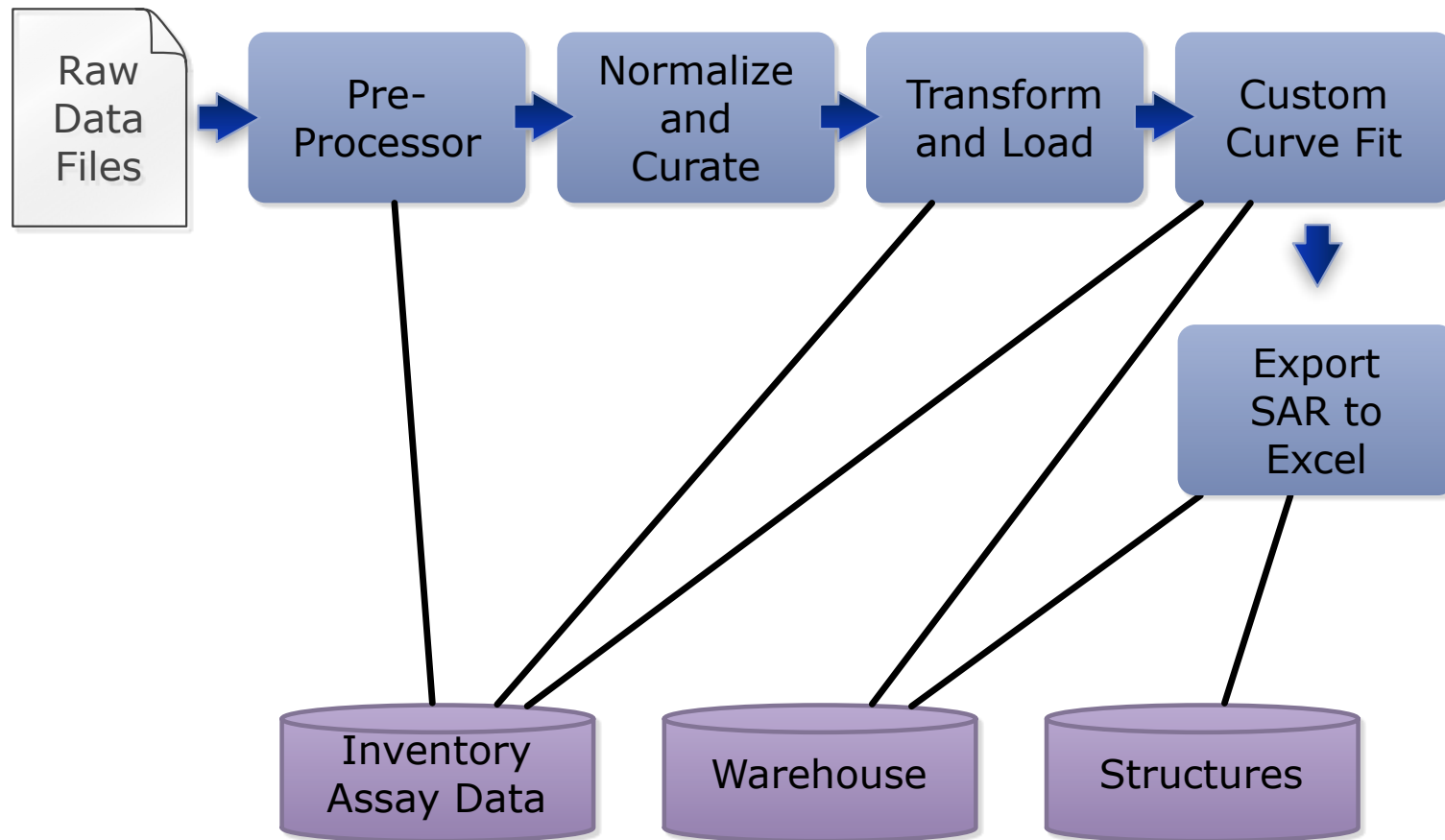
- What is unique to your science?
- What is similar to with other labs?
- What mission-critical software is already deployed?
- What is broken?
  - Identify root cause
- What can be integrated?

# Examples

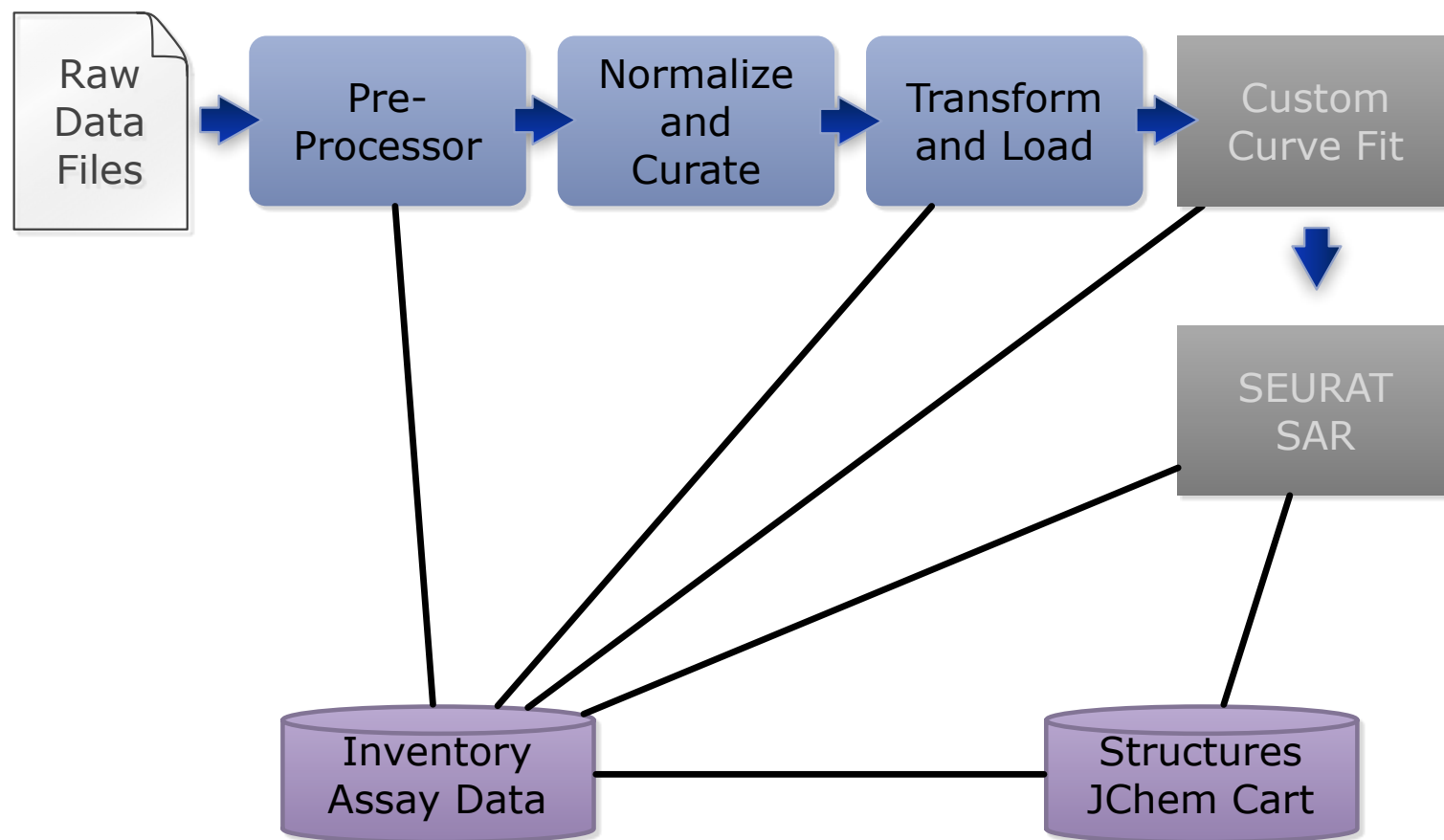
# Case I

- Unique science: practical uHTS allows high volume potency measurement and off-target studies
- Common with other labs: reagent and compound management, Tox/PK, and SAR
- Mission-critical software in place: custom uHTS data processing and curation work-flow
- Root problem: SAR data aggregation rules inconsistent, potency > < lost in Excel format
- Integration tasks: custom curve fit software, SEURAT for SAR, ChemAxon cartridge

# Case I Before



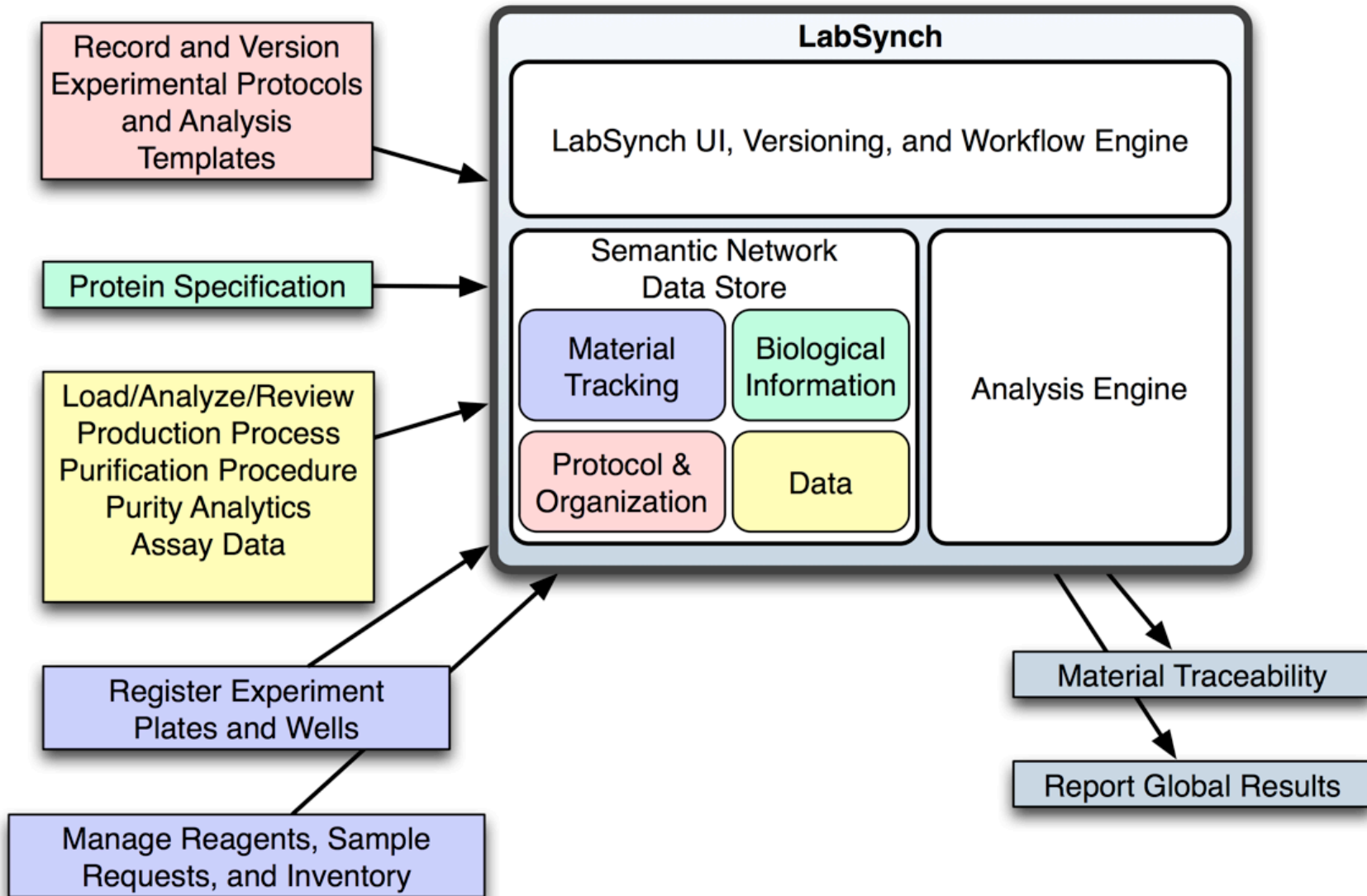
# Case I After



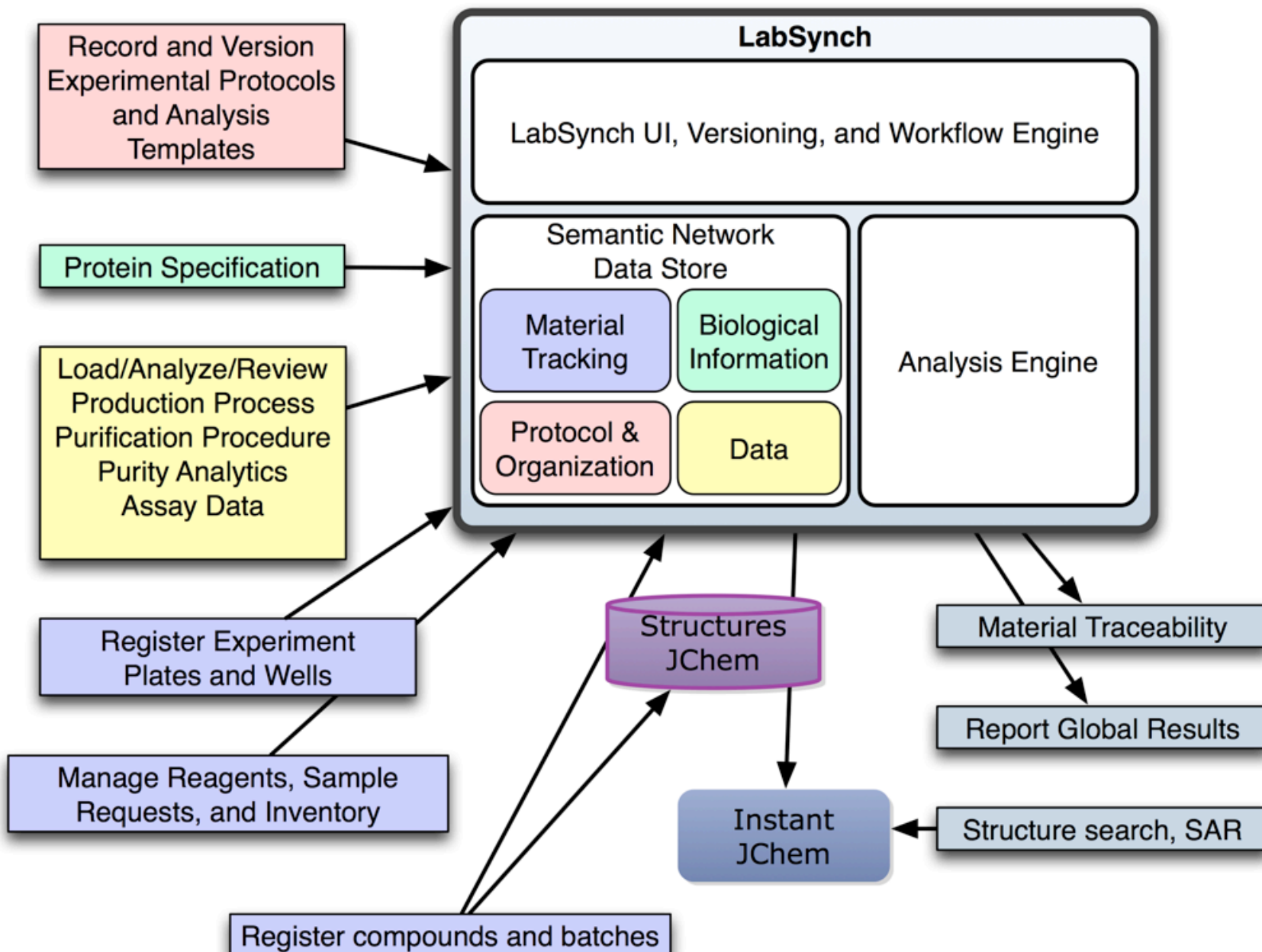
## Case 2

- Unique science: modified proteins with conjugated small molecules
- Common with other labs: protein production, small med-chem team
- Mission-critical software in place: LabSynch Semantic LIMS
- Root problem: small molecules tracked by name, but not batch and structure
- Integration tasks: add structure repository to LabSynch

# Case 2 Before



# Case 2 After



# Single Compound Registration

The screenshot displays the 'Compound Registration' window in the LabSynch software. On the left, a navigation pane shows a tree structure with 'Forms' > 'LabSynch' > 'Compound Registration' selected. The main window has a title bar 'Compound Registration' and a menu bar with 'File', 'Edit', 'View', 'Insert', 'Atom', 'Bond', 'Structure', 'Tools', and 'Help'. Below the menu is a toolbar with icons for selection, erasing, undo, redo, cut, copy, paste, zoom in, zoom out, and a 100% zoom level. The central workspace shows a chemical structure of 5-chloro-2-naphthol, consisting of two fused benzene rings with a chlorine atom (Cl) at the 5-position and a hydroxyl group (OH) at the 2-position. To the right of the workspace is a vertical toolbar with buttons for H, C, N, O, S, F, and P. At the bottom of the workspace are icons for various ring types: a pentagon, a six-membered ring with an N atom, a pentagon, a hexagon, a heptagon, and a fused six-membered ring system. At the bottom right of the window are 'Next' and 'Quit' buttons.

# Compound Batch and Container

Search Inventory **Forms**

- Forms
  - LabSynch
    - Curve Fit Analysis
    - Compound Registration**
    - Container Registration

### Compound Registration

#### Compound Batch Registration

**Compound ID:**  \*

**Created By:** user, admin ▾ \*

**Registration Date:** 4/12/2010 \*

**Notebook Number:**  \*

**Page Number:**  \*

**Page Line Number:**

**Vial Barcode:**  \*

**Current\_Vial\_Weight:**  mg ▾

**Net\_Compound\_Amount:**  \* mg ▾

**Supplier:**  \*

**Supplier Batch ID:**

**Salt Form:**  ▾

**Physical State:**

**Color:**

**Purity:**

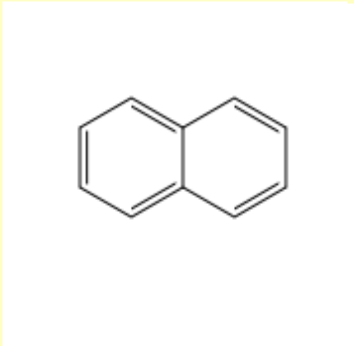
**Comments:**

**Storage Location:**  \*

\* indicates required field

CompoundBatch Saved:

# Compound Detail Page

	<p>Compound Batch ID</p> <p>SS0100001::1</p>	<p>Scientist</p> <p>user, admin</p>
	<p>Registration Date</p> <p>4/8/2010</p>	<p>Vial Barcode</p> <p><a href="#">LV123456</a></p>
	<p>Net Compound Amount</p> <p>133 mg</p>	<p>Storage Location</p> <p><a href="#">Shelf 5</a></p>
<p>Notebook Number</p> <p>notebook</p>	<p>Notebook Page-Line</p> <p>21-21</p>	<p>Physical State</p> <p>state</p>
<p>Color</p> <p>phys</p>	<p>Purity</p> <p>col</p>	<p>Salt Form</p> <p>2 X hcl</p>
<p>Compound Comments</p> <p>pur</p>		<p>Supplier</p> <p>supplier</p>
		<p>Supplier ID</p> <p>23</p>

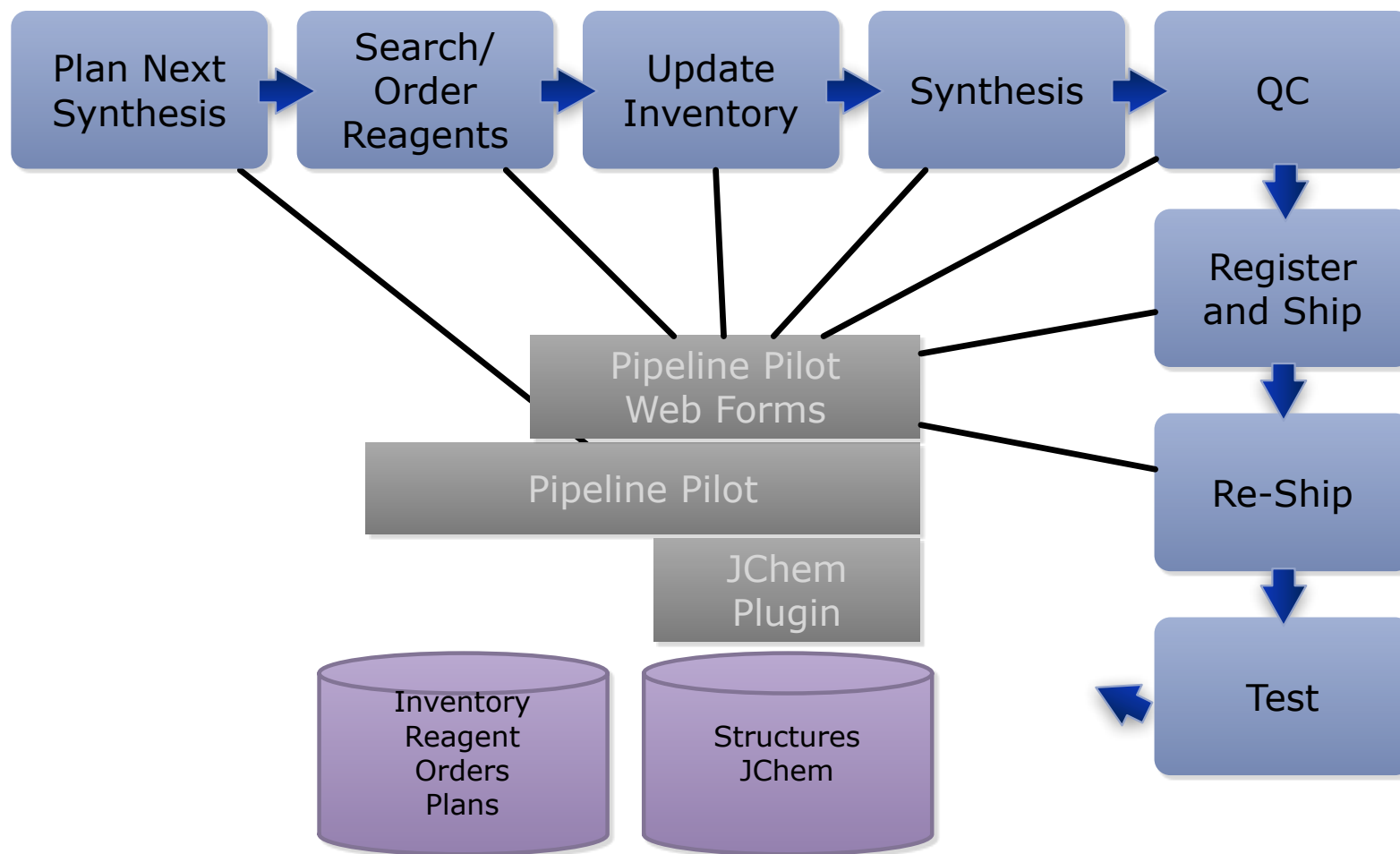
Data: SCRN\_101, D-R\_534

Inventory: Sierra > Reno > Freezer 3 > Shelf 2 > Rack 3 > Location 3

## Case 3

- Unique process: international medicinal chemistry CRO operation running isolated projects in parallel
- Common with other labs: share reagents, track intermediates, manage lead-opt projects
- Mission-critical software in place: Pipeline Pilot
- Root problem: no COTS software available to manage workflow

# Case 3



# Lessons Learned

- Use the best tool for the science and support whatever languages and databases it requires
- Different scientists understand different requirement formats
- Details drive the requirements – get the science right
- Error bars, sig figs,  $<$ ,  $>$ , and  $=$  all matter
- This can be hard; allow time for testing
- Requirements change, this is science

## Services that we provide:

- On site support and training
- Algorithms and custom software for data mining and analysis
- Commercial software selection and integration
- Systems architecture, integration, and development
- Infrastructure architecture and implementation
- IT/Informatics management consulting