DayBook
An Electronic Laboratory Notebook for DayCart

Yvonne C. Shimshock, Ph.D.
Manager, Business Development

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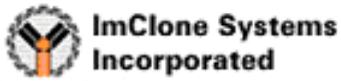
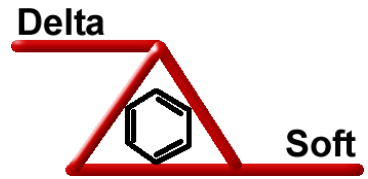
DeltaSoft, Inc.

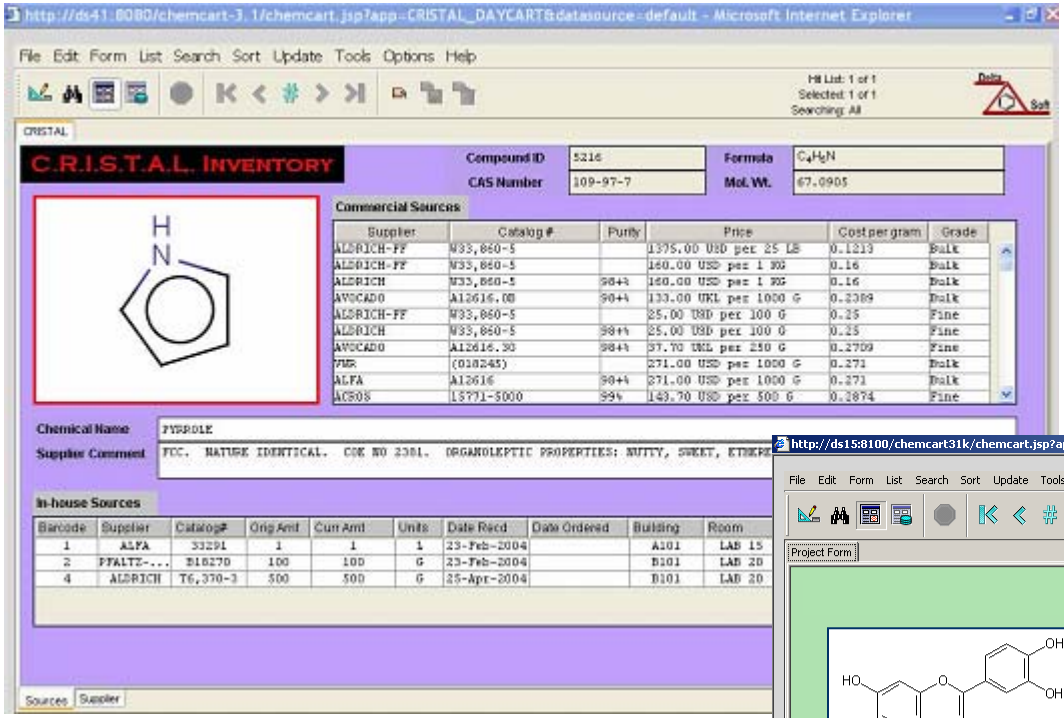
- Research systems consulting company since 1996
- Specialize in Discovery Informatics
- Solution focused software applications
  - Custom solutions and services
  - Multi-vendor integrated solutions
  - 'Out-of-the-Box' solutions
    - ChemCart
    - DeltaBook
    - CRISTAL

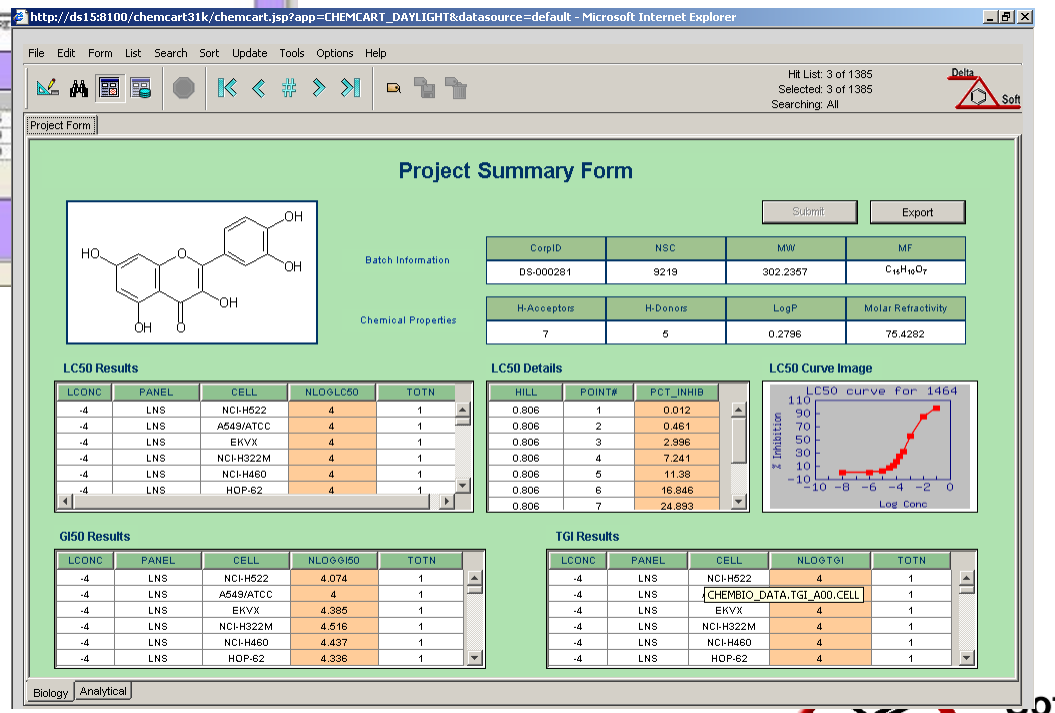
DeltaSoft Clients





DeltaSoft with Daylight's DayCart

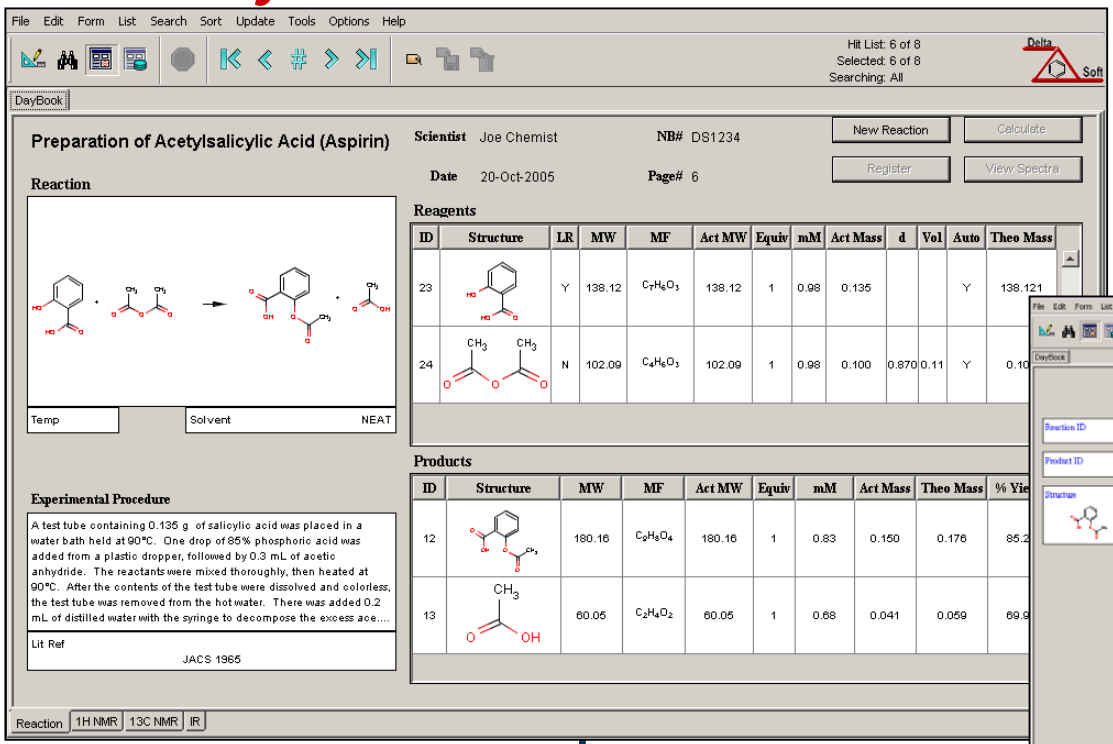


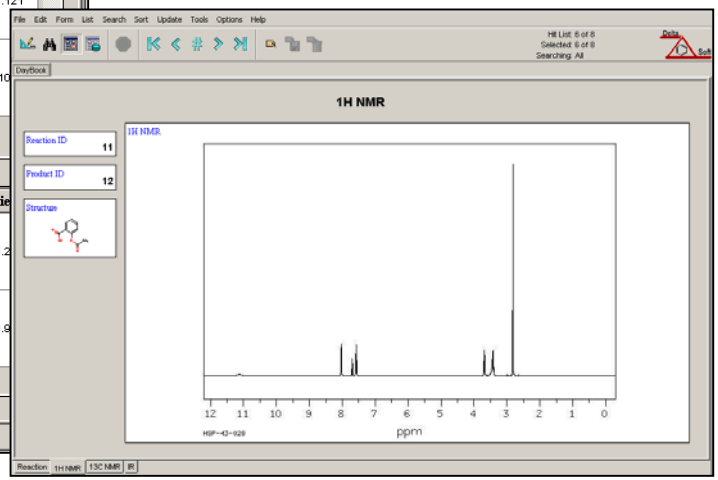


DayBook Basics

- Built on DeltaSoft's ChemCart technology
  - Out-of-the-Box interface to data cartridges
  - Web based
  - Flexible forms interface
  - Search, View, Update chemical structures, data, images
  - List management
  - Platform independent
  - Data model independent
- Developed in collaboration with Medicinal Chemists
- Uses Daylight's DayCart for chemistry support
  - Commercially available DayCart notebook
- Customizable
  - API
  - Link to Chemical Registration
  - Link to Chemical Reagent Inventory

DayBook Architecture





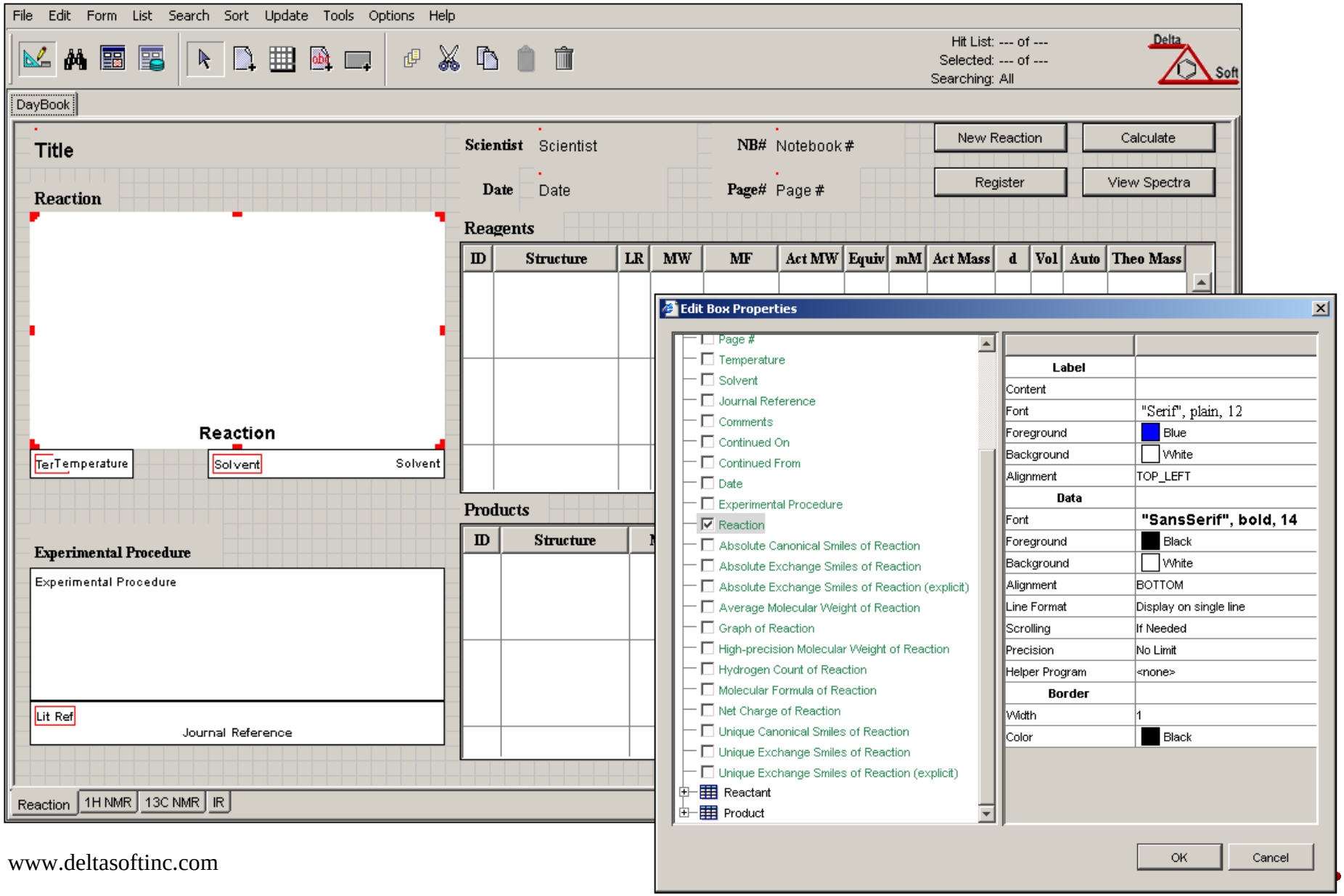
ChemCart Server

ORACLE / DayCart Cartridge

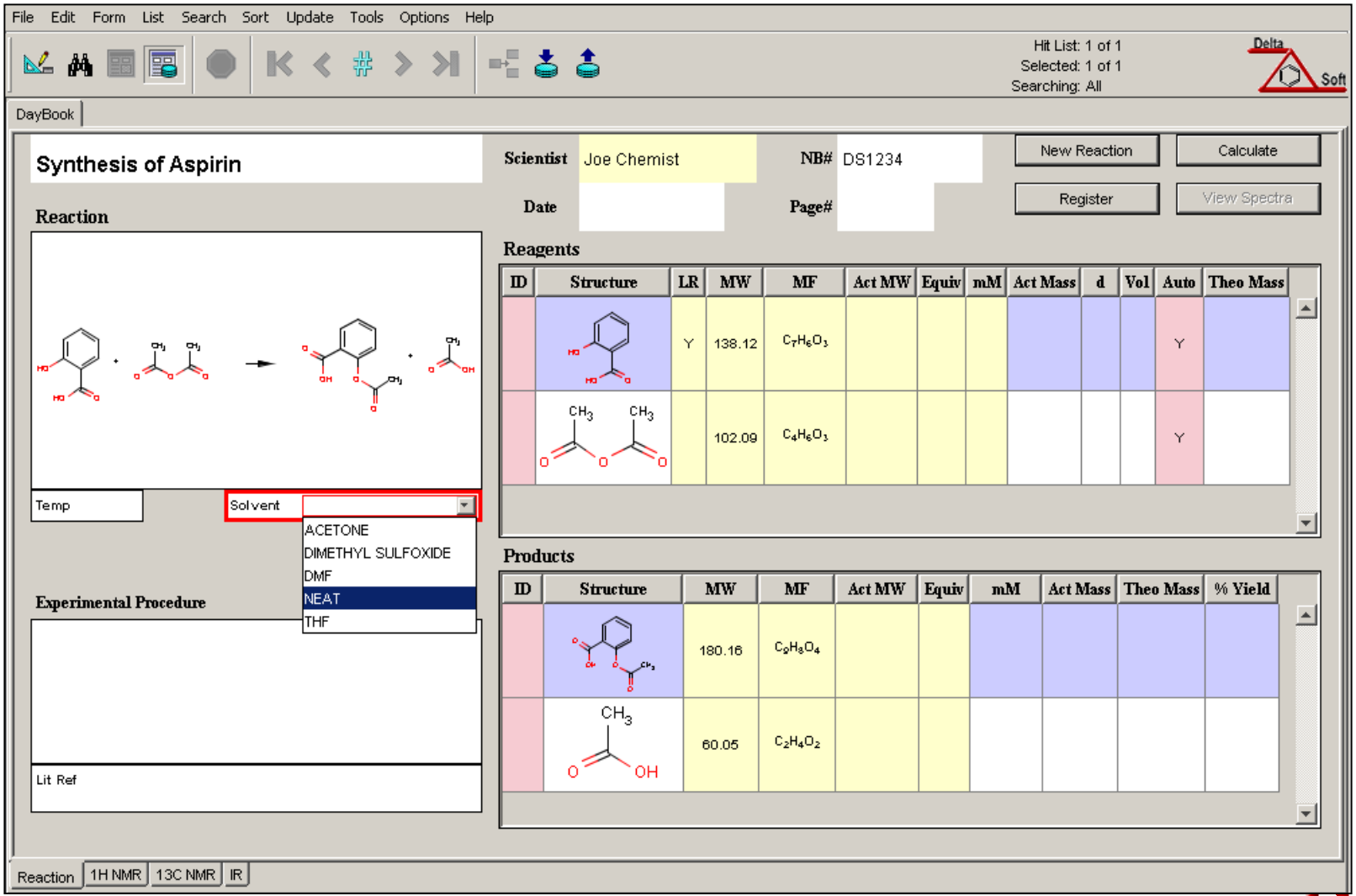
Molecules / Reactions
Experimental detail
Test results (including Images)

Delta Soft

Design Notebook Page (Boxes,Tables,Labels,Buttons,Sheets)



Create Notebook entry

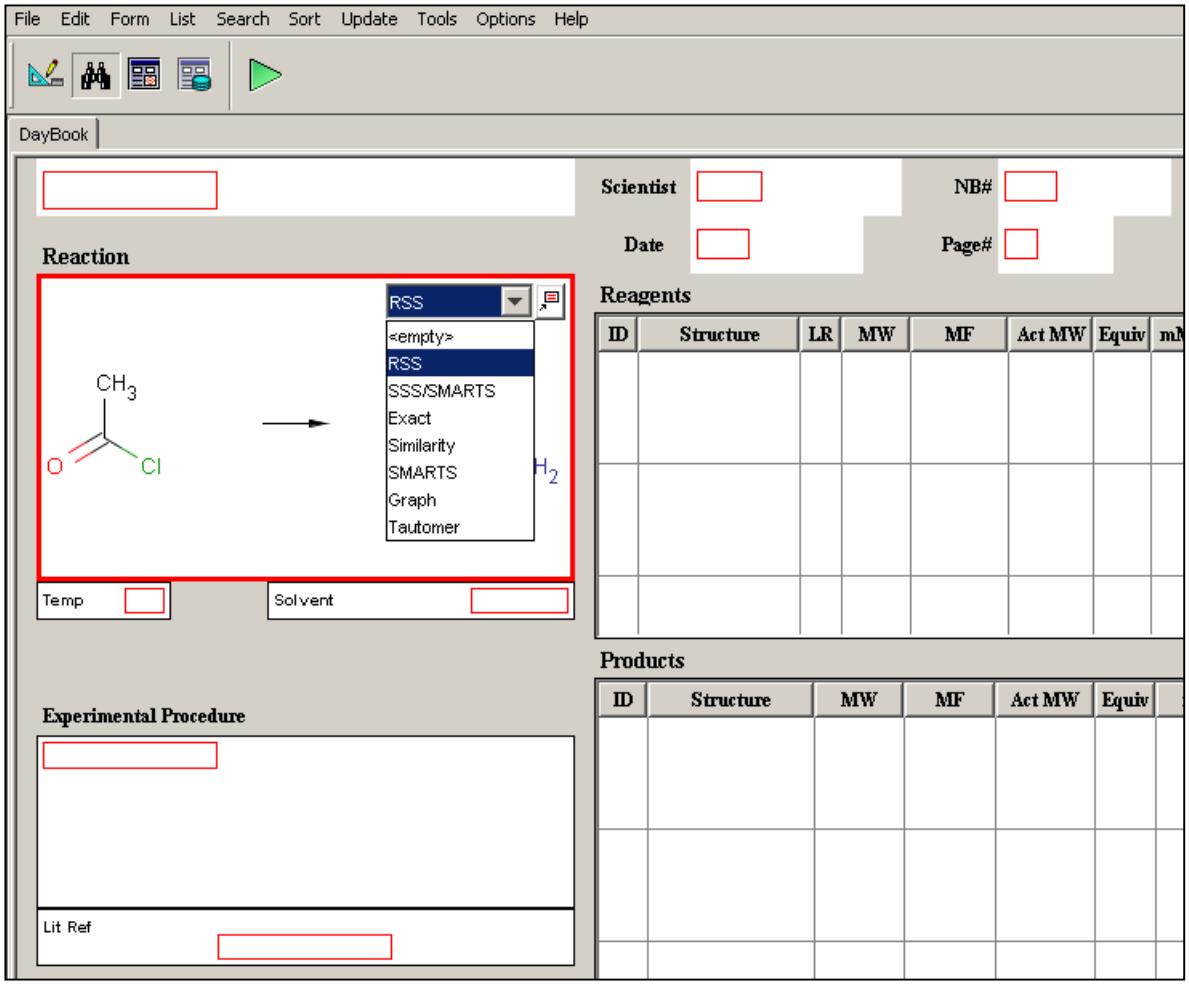


Soft

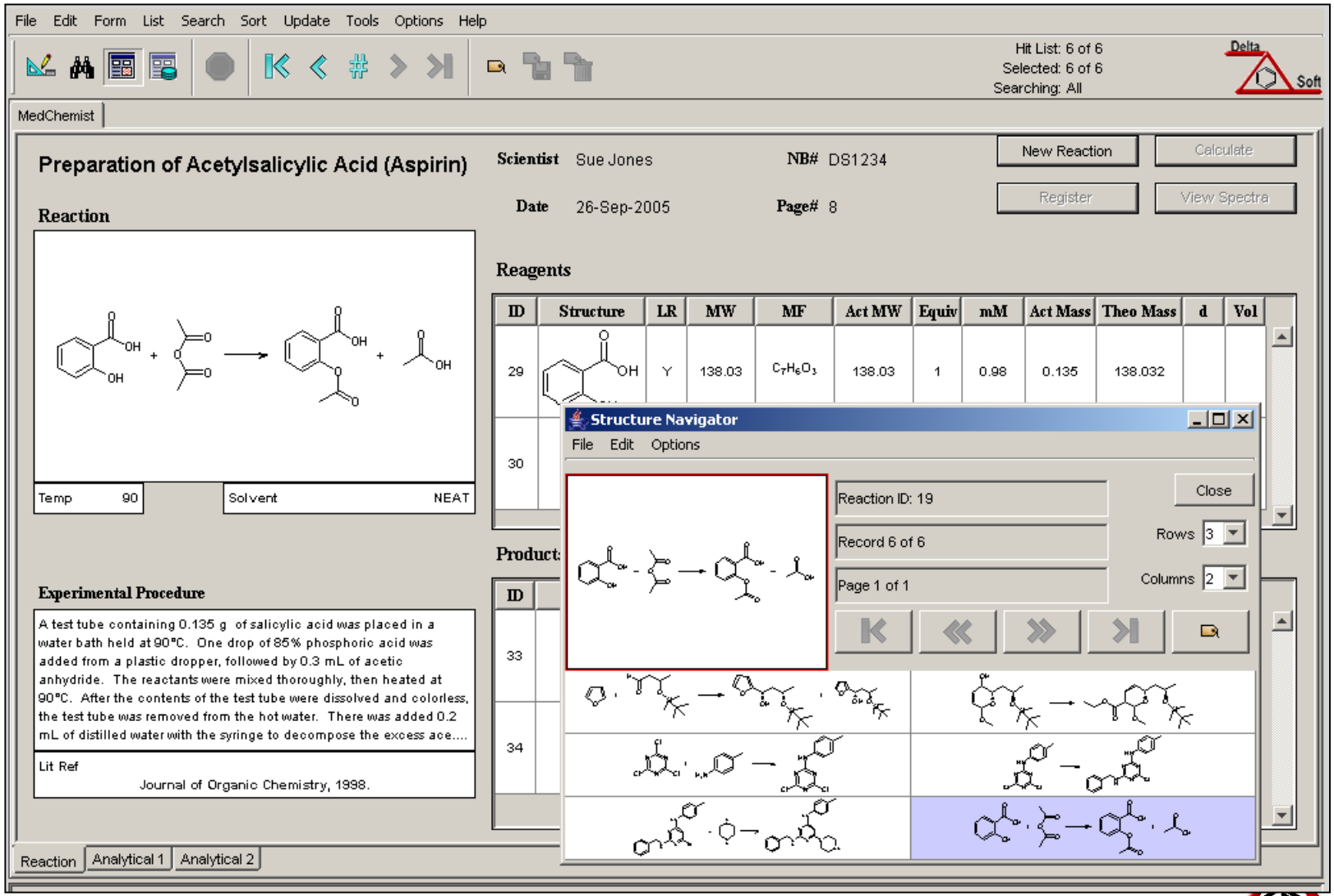
DayBook Features

- Electronically record all aspects of chemical synthesis
  - reaction, reagents, products, experimental detail (including images)
  - enter reaction; reagents and products are generated with cartridge calculation of MF and MW
- Auto limiting reagent
- Auto calculations
  - mmol, vol, theooretical yield, % yield
- Duplicate notebook pages for similar reactions
- Use Picklists to add corporate standard terms
- Use Quick Pick to add reagents or text
- Save drafts, update notebook pages, publish to database
- Batch file upload (.csv, .sdf, .rdf, binary files)
  - field mapper

Search Notebook (Form or Advanced Query Builder)



View Search Results (Form or Structure Navigator)



Manipulate Hit Lists

- Add
- Remove
- Perform operations (AND, OR, NOT, XOR)
- Share
  - Public
  - Private
  - Role
- Save & Manage
  - For All DayBook Objects
    - Forms
    - Search Criteria
    - Hit Lists
    - Sort Criteria
    - Print Layouts

Export

- Forms
- Lists
- Files
  - CSV
  - SDFile
  - RDFile
  - XDFile
  - ISIS for Excel
  - Accord forExcel
- Copy/Copy As Image
- Save as Rxnfile/Molfile

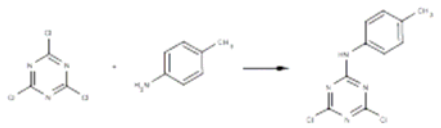
Generate Reports

Project: First Project
Notebook: The First Notebook
Scientist: T.. Joe

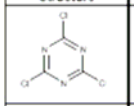
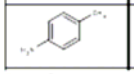
Experiment: Synthesis of Tri-amino Triazine
Temperature(°C): 0
Date: 10/4/2005
Reference: JOC 1995, 31-34.
Comments:
Experimental Procedure:
A solution of aniline in acetone was added dropwise to a 0°C solution of cyanuric chloride. The cold bath was removed and the reaction stirred at room temp for 3 hr. Solvent was removed in vacuo and the resulting solid was washed with hexane then dried under high vacuum.

Reaction: Step 1
Solvent: Acetone

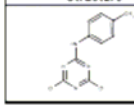
Reaction Diagram:



Reagents:

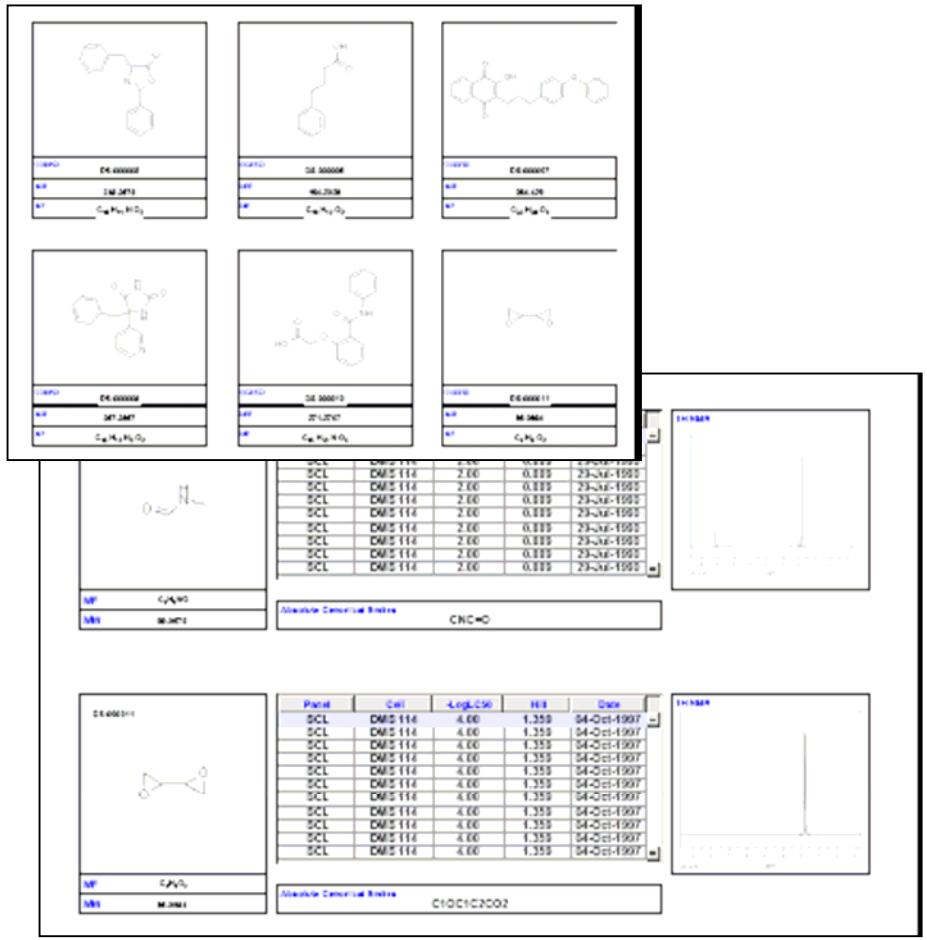
Structure	Formula	Mol. Wt.	Theo. Mass	Act. Mass	Equiv.	Density	Volume	Stock
	$C_3Cl_3N_3$	184.41	10.412	9.396	1.1	1	9.396	50.952
	C_7H_9N	107.153	107.153	5.5	1	1	5.5	51.328

Products:

Structure	Formula	Mol. Wt.	Theo. Mass	Act. Mass	Equiv.	% Yield
	$C_{10}H_8Cl_2N_4$	255.103	13.094	12.5	1	95.463

Signature _____ Date _____

Witness _____ Date _____



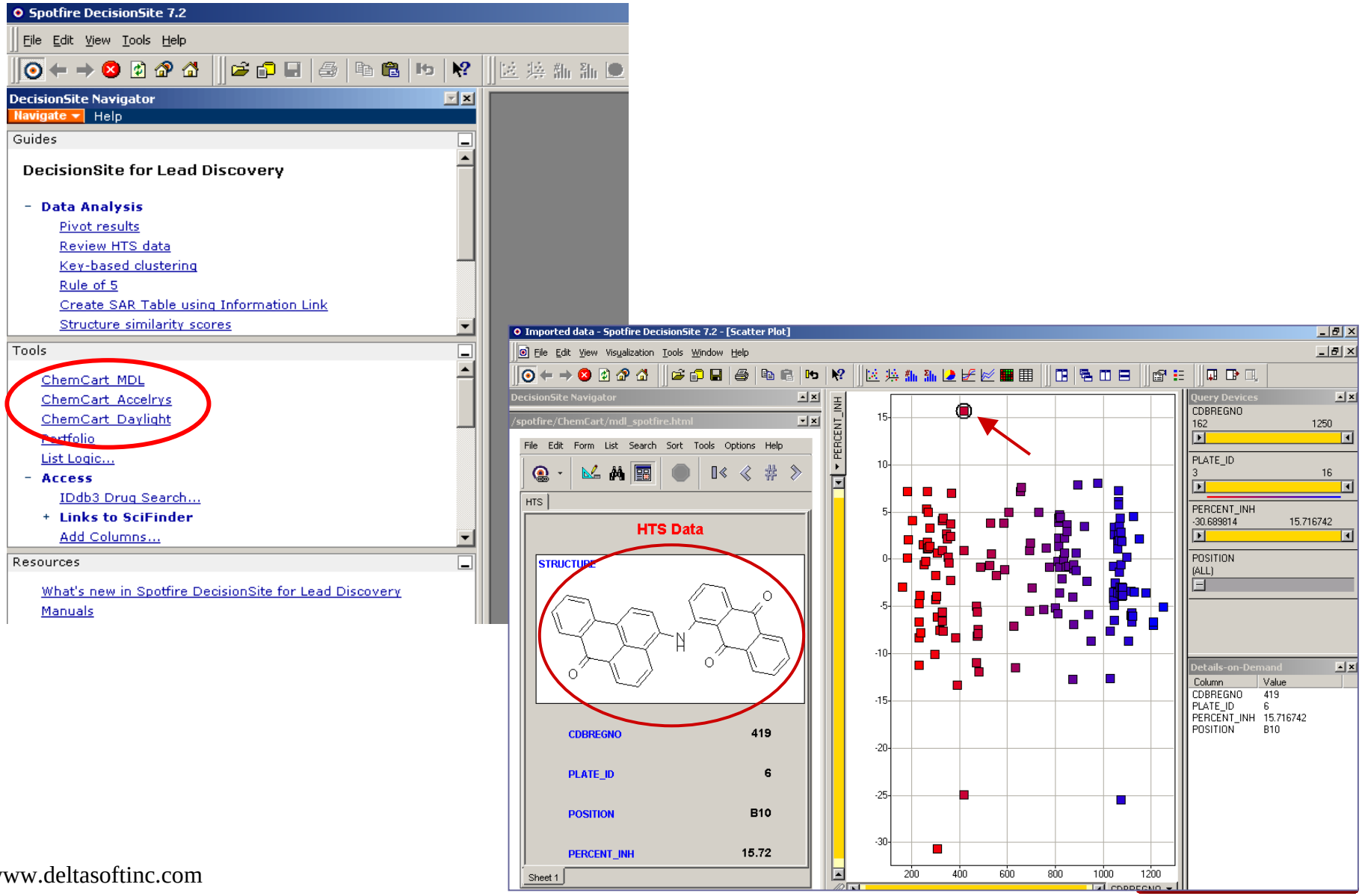
www.deltasoftinc.com

Delta Soft

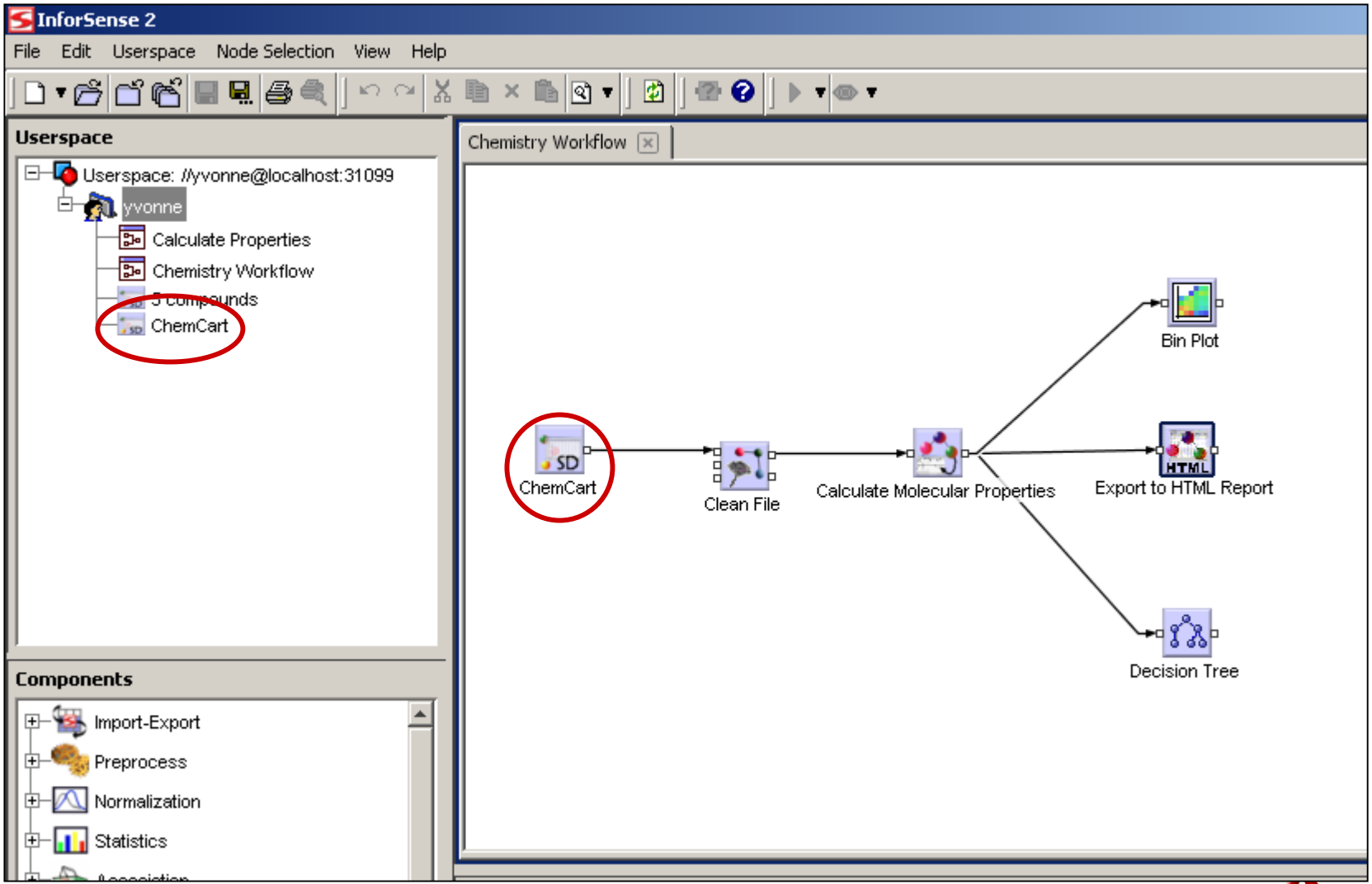
Optional Integrations

- Accelrys Accord for Excel
- IBM InsightLink
- IBM DiscoveryLink (Information Integrator)
- InforSense KDE
- MDL ISIS for Excel
- Spotfire DecisionSite

Integration with Spotfire



Analyze data in KDE workflow



DayBook Summary

- An interface to research experiments using DayCart cartridge
  - Web based
  - Configurable forms
  - UI designed for scientists
    - Auto calculate
    - Picklists
    - Quick Picks
    - Duplicate reactions
    - Searching by Form or Advanced
- Customize
  - **Buttons**
- Link to other systems
  - Internal (Registration, Inventory)
  - 3rd party