

DayBook

An Electronic Laboratory Notebook for DayCart

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

Daylight Euro-MUG
5-7 October 2005
Cambridge, England

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

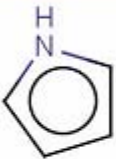
http://ds-41:8080/chemcart-3.1/chemcart.jsp?app=CRISTAL_DAYCART&datasource=default - Microsoft Internet Explorer

File Edit Form List Search Sort Update Tools Options Help

CRISTAL

C.R.I.S.T.A.L. INVENTORY

Compound ID: 5216 Formula: C₄H₅N
 CAS Number: 109-97-7 Mol. Wt.: 67.0905



Commercial Sources

Supplier	Catalog #	Purity	Price	Cost per gram	Grade
ALDRICH-FF	N33,860-5		1375.00 USD per 25 LB	0.1213	Bulk
ALDRICH-FF	N33,860-5		160.00 USD per 1 KG	0.16	Bulk
ALDRICH	N33,860-5	98+%	160.00 USD per 1 KG	0.16	Bulk
AVOCADO	A12616.00	90+%	133.00 UKL per 1000 G	0.2369	Bulk
ALDRICH-FF	N33,860-5		25.00 USD per 100 G	0.25	Fine
ALDRICH	N33,860-5	98+%	25.00 USD per 100 G	0.25	Fine
AVOCADO	A12616.30	98+%	37.70 UKL per 250 G	0.2709	Fine
7MR	(010245)		271.00 USD per 1000 G	0.271	Bulk
ALFA	A12616	90+%	271.00 USD per 1000 G	0.271	Bulk
ACSOS	LS771-5000	99%	143.70 USD per 500 G	0.2874	Fine

Chemical Name: PYRROLE
 Supplier Comment: FCC. NATURE IDENTICAL. CDE NO 2361. ORGANOLEPTIC PROPERTIES: BUTTY, SWEET, ETHERAL

In-house Sources

Barcode	Supplier	Catalog#	Orig Amt	Cur Amt	Units	Date Recd	Draw Ordered	Building	Room
1	ALFA	33291	1	1	1	23-Feb-2004		A101	LAB 15
2	PFALZE...	B10270	100	100	G	23-Feb-2004		B101	LAB 20
4	ALDRICH	T6,370-3	500	500	G	25-Apr-2004		B101	LAB 20

Sources Supplier

http://ds-8100/chemcart31/chemcart.jsp?app=CHEMART_DAYLIGHT&datasource=default - Microsoft Internet Explorer

File Edit Form List Search Sort Update Tools Options Help

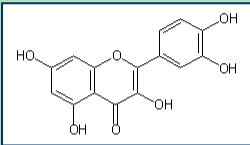
Project Form

Batch Information

CorpID	NSC	MW	MF
DS-000281	9219	302.2357	C ₁₄ H ₁₀ O ₇

Chemical Properties

H-Acceptors	H-Donors	LogP	Molar Refractivity
7	5	0.2796	75.4282



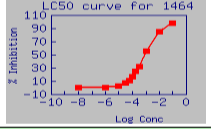
LC50 Results

LC50C	PANEL	CELL	NLOG50	TOTN
-4	LNS	NCI-H522	4	1
-4	LNS	A549/ATCC	4	1
-4	LNS	EKVX	4	1
-4	LNS	NCI-H322M	4	1
-4	LNS	NCI-H460	4	1
-4	LNS	HOP-62	4	1

LC50 Details

HILL	POINT#	PCT_INHIB
0.806	1	0.012
0.806	2	0.461
0.806	3	2.996
0.806	4	7.241
0.806	5	11.38
0.806	6	16.846
0.806	7	24.893

LC50 Curve Image



LC50 curve for 1464

GI50 Results

LC50C	PANEL	CELL	NLOG50	TOTN
-4	LNS	NCI-H522	4.074	1
-4	LNS	A549/ATCC	4	1
-4	LNS	EKVX	4.385	1
-4	LNS	NCI-H322M	4.516	1
-4	LNS	NCI-H460	4.437	1
-4	LNS	HOP-62	4.338	1

TGI Results

LC50C	PANEL	CELL	NLOG50	TOTN
-4	LNS	NCI-H522	4	1
-4	LNS	CHEMBO_DATA.TGI_A00.CELL	4	1
-4	LNS	EKVX	4	1
-4	LNS	NCI-H322M	4	1
-4	LNS	NCI-H460	4	1
-4	LNS	HOP-62	4	1

Biology Analytical

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

File Edit Form List Search Sort Update Tools Options Help

Hit List: 6 of 8
Selected: 6 of 8
Searching: All

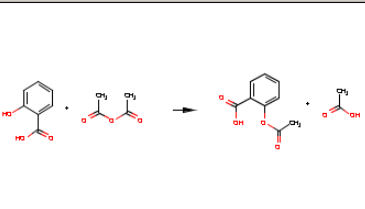
DayBook

Preparation of Acetylsalicylic Acid (Aspirin)

Scientist: Joe Chemist NB#: DS1234 [New Reaction] [Calculate]



Date: 20-Oct-2005 Page#: 6 [Register] [View Spectra]

Reaction





Temp: Solvent: NEAT

Reagents

ID	Structure	LR	MW	MF	Act MW	Equiv	mM	Act Mass	d	Vol	Auto	Theo Mass
23		Y	138.12	C ₇ H ₆ O ₃	138.12	1	0.98	0.135			Y	138.121
24		N	102.09	C ₄ H ₆ O ₃	102.09	1	0.98	0.100	0.870	0.11	Y	0.10

Products

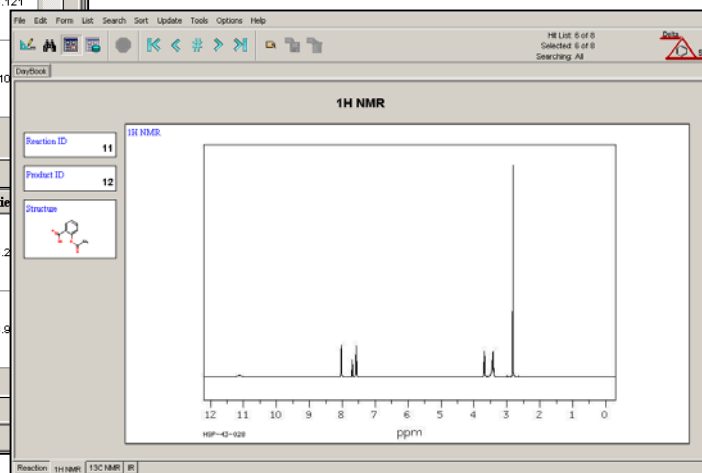
ID	Structure	MW	MF	Act MW	Equiv	mM	Act Mass	Theo Mass	% Yie
12		180.16	C ₉ H ₈ O ₄	180.16	1	0.83	0.150	0.176	85.2
13		60.05	C ₂ H ₄ O ₂	60.05	1	0.88	0.041	0.059	69.9

Experimental Procedure

A test tube containing 0.135 g of salicylic acid was placed in a water bath held at 90°C. One drop of 85% phosphoric acid was added from a plastic dropper, followed by 0.3 mL of acetic anhydride. The reactants were mixed thoroughly, then heated at 90°C. After the contents of the test tube were dissolved and colorless, the test tube was removed from the hot water. There was added 0.2 mL of distilled water with the syringe to decompose the excess ac...

Lit Ref: JACS 1965

Reaction: 1H NMR 13C NMR IR



ChemCart Server

ORACLE / DayCart Cartridge

Molecules / Reactions
Experimental detail
Test results (including Images)



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

The screenshot displays the Delta software interface for creating a design notebook page. The main window is titled "DayBook" and contains several sections:

- Title:** Scientist Scientist, NB# Notebook #, Page# Page #
- Reaction:** A large white box with a red border, containing a reaction scheme. Below it are labels for "Temperature" and "Solvent".
- Reagents:** A table with columns: ID, Structure, LR, MW, MF, Act MW, Equiv, mM, Act Mass, d, Vol, Auto, Theo Mass.
- Products:** A table with columns: ID, Structure, MW, MF, Act MW, Equiv, mM, Act Mass, d, Vol, Auto, Theo Mass.
- Experimental Procedure:** A text area containing "Experimental Procedure" and "Lit Ref" (Journal Reference).

An "Edit Box Properties" dialog box is open in the foreground, showing a list of checkboxes for various data fields. The "Reaction" checkbox is checked. The dialog also shows settings for the selected box, including font and border options.

Edit Box Properties

- Page #
- Temperature
- Solvent
- Journal Reference
- Comments
- Continued On
- Continued From
- Date
- Experimental Procedure
- Reaction**
- Absolute Canonical Smiles of Reaction
- Absolute Exchange Smiles of Reaction
- Absolute Exchange Smiles of Reaction (explicit)
- Average Molecular Weight of Reaction
- Graph of Reaction
- High-precision Molecular Weight of Reaction
- Hydrogen Count of Reaction
- Molecular Formula of Reaction
- Net Charge of Reaction
- Unique Canonical Smiles of Reaction
- Unique Exchange Smiles of Reaction
- Unique Exchange Smiles of Reaction (explicit)

Label

Content	
Font	"Serif", plain, 12
Foreground	<input checked="" type="checkbox"/> Blue
Background	<input type="checkbox"/> White
Alignment	TOP_LEFT

Data

Font	"SansSerif", bold, 14
Foreground	<input checked="" type="checkbox"/> Black
Background	<input type="checkbox"/> White
Alignment	BOTTOM
Line Format	Display on single line
Scrolling	If Needed
Precision	No Limit
Helper Program	<none>

Border

Width	1
Color	<input checked="" type="checkbox"/> Black

OK Cancel

Create Notebook entry

File Edit Form List Search Sort Update Tools Options Help

Hit List: 1 of 1
Selected: 1 of 1
Searching: All

DayBook

Synthesis of Aspirin

Scientist: Joe Chemist NB#: DS1234
Date: Page#

New Reaction Calculate
Register View Spectra

Reaction

Temp Solvent

- ACETONE
- DIMETHYL SULFOXIDE
- DMF
- NEAT
- THF

Reagents

ID	Structure	LR	MW	MF	Act MW	Equiv	mM	Act Mass	d	Vol	Auto	Theo Mass
		Y	138.12	C ₇ H ₆ O ₃							Y	
			102.09	C ₄ H ₆ O ₃							Y	

Products

ID	Structure	MW	MF	Act MW	Equiv	mM	Act Mass	Theo Mass	% Yield
		180.16	C ₉ H ₈ O ₄						
		60.05	C ₂ H ₄ O ₂						

Reaction 1H NMR 13C NMR IR

Delta 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, theoretical 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)

File Edit Form List Search Sort Update Tools Options Help

DayBook

Reaction

CH₃
O=C-Cl

→

H₂

Temp Solvent

Scientist NB#

Date Page#

Reagents

ID	Structure	LR	MW	MF	Act MW	Equiv	mM

Products

ID	Structure	MW	MF	Act MW	Equiv

Experimental Procedure

Lit Ref

Dropdown menu: RSS, <empty>, RSS, SSS/SMARTS, Exact, Similarity, SMARTS, Graph, Tautomer

View Search Results (Form or Structure Navigator)

File Edit Form List Search Sort Update Tools Options Help

Hit List: 6 of 6
Selected: 6 of 6
Searching: All

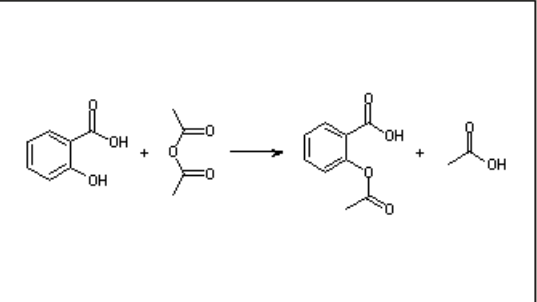
MedChemist

Preparation of Acetylsalicylic Acid (Aspirin)

Scientist Sue Jones NB# DS1234
Date 26-Sep-2005 Page# 8

New Reaction Calculate
Register View Spectra

Reaction



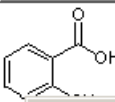
Temp 90 Solvent NEAT

Experimental Procedure

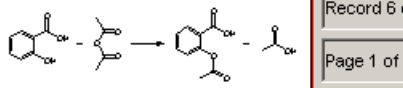
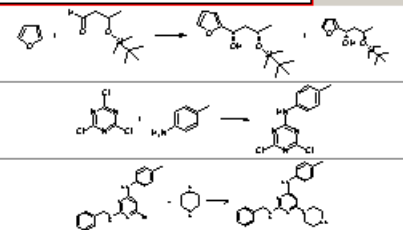
A test tube containing 0.135 g of salicylic acid was placed in a water bath held at 90°C. One drop of 85% phosphoric acid was added from a plastic dropper, followed by 0.3 mL of acetic anhydride. The reactants were mixed thoroughly, then heated at 90°C. After the contents of the test tube were dissolved and colorless, the test tube was removed from the hot water. There was added 0.2 mL of distilled water with the syringe to decompose the excess ace....

Lit Ref
Journal of Organic Chemistry, 1998.

Reagents

ID	Structure	LR	MW	MF	Act MW	Equiv	mM	Act Mass	Theo Mass	d	Vol
29		Y	138.03	C ₇ H ₆ O ₃	138.03	1	0.98	0.135	138.032		

Product

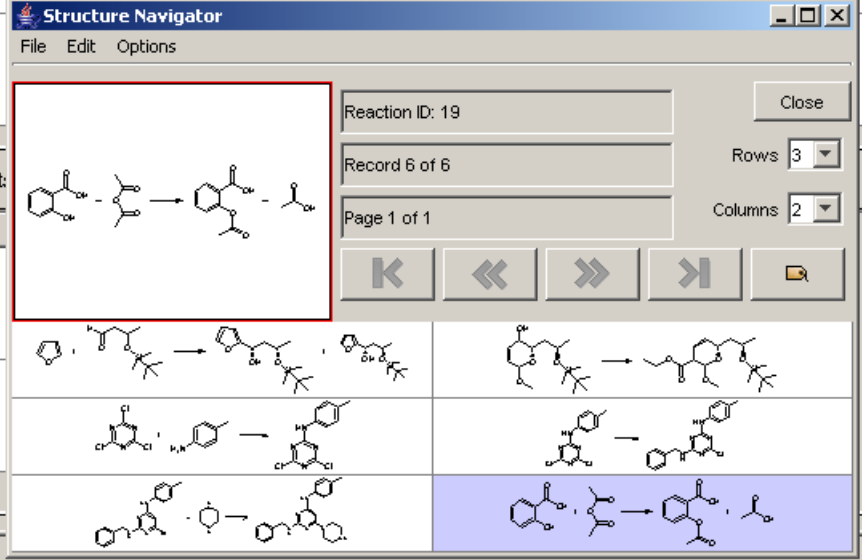
33											
34											

Structure Navigator

File Edit Options

Reaction ID: 19
Record 6 of 6
Page 1 of 1

Close
Rows 3
Columns 2



Reaction Analytical 1 Analytical 2

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
 - SDFfile
 - RDFfile
 - XDFfile
 - 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 Reaction: Step 1
 Temperature(°C): 0 Solvent: Acetone
 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 Diagram:

Reagents:

Structure	Formula	Mol. Wt.	Theo. Mass	Act. Mass	Equiv.	Density	Volume	Stock
	C ₃ Cl ₃ N ₃	184.41	10.412	9.396	1.1	1	9.396	50.952
	C ₇ H ₇ N	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 ₃ Cl ₂ N ₄	255.103	13.094	12.5	1	95.463

Signature _____ Date _____
 Witness _____ Date _____

Grid of chemical structures and data tables:

- Top row: Three chemical structures with associated data tables (e.g., EI 00007, SE 00006, EI 00007).
- Middle row: Three chemical structures with associated data tables (e.g., EI 00008, SE 00003, EI 00011).
- Bottom row: Two chemical structures with associated data tables (e.g., C₄H₉NO, M 00012).

Below the grid are two chromatograms (CHROM) and two data tables:

Peak	Cell	Log ₁₀ CSF	HS	Date
SCL	DMS 114	4.00	1.355	04-Oct-1997
SCL	DMS 114	4.00	0.000	23-Jul-1995
SCL	DMS 114	4.00	0.000	23-Jul-1995
SCL	DMS 114	4.00	0.000	23-Jul-1995
SCL	DMS 114	4.00	0.000	23-Jul-1995
SCL	DMS 114	4.00	0.000	23-Jul-1995
SCL	DMS 114	4.00	0.000	23-Jul-1995
SCL	DMS 114	4.00	0.000	23-Jul-1995

Mobile Chemical Index: CNC=O

Peak	Cell	Log ₁₀ CSF	HS	Date
SCL	DMS 114	4.00	1.355	04-Oct-1997
SCL	DMS 114	4.00	1.355	04-Oct-1997
SCL	DMS 114	4.00	1.355	04-Oct-1997
SCL	DMS 114	4.00	1.355	04-Oct-1997
SCL	DMS 114	4.00	1.355	04-Oct-1997
SCL	DMS 114	4.00	1.355	04-Oct-1997
SCL	DMS 114	4.00	1.355	04-Oct-1997
SCL	DMS 114	4.00	1.355	04-Oct-1997
SCL	DMS 114	4.00	1.355	04-Oct-1997
SCL	DMS 114	4.00	1.355	04-Oct-1997

Mobile Chemical Index: ClOC1C2O2



Optional Integrations

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

Integration with Spotfire

Spotfire DecisionSite 7.2

File Edit View Tools Help

DecisionSite Navigator

Navigate Help

Guides

DecisionSite for Lead Discovery

- Data Analysis
 - Pivot results
 - Review HTS data
 - Key-based clustering
 - Rule of 5
 - Create SAR Table using Information Link
 - Structure similarity scores

Tools

- [ChemCart MDL](#)
- [ChemCart Accelrys](#)
- [ChemCart Daylight](#)
- Portfolio
- List Logic...
- Access
 - IDdb3 Drug Search...
 - + Links to SciFinder
 - Add Columns...

Resources

- [What's new in Spotfire DecisionSite for Lead Discovery](#)
- [Manuals](#)

Imported data - Spotfire DecisionSite 7.2 - [Scatter Plot]

File Edit View Visualization Tools Window Help

DecisionSite Navigator

/spotfire/ChemCart/mdl_spotfire.html

File Edit Form List Search Sort Tools Options Help

HTS

HTS Data

STRUCTURE

O=C1C=CC(=O)N(C1)c2ccc3c(c2)C(=O)N3

CDBREGNO 419

PLATE_ID 6

POSITION B10

PERCENT_INH 15.72

Sheet 1

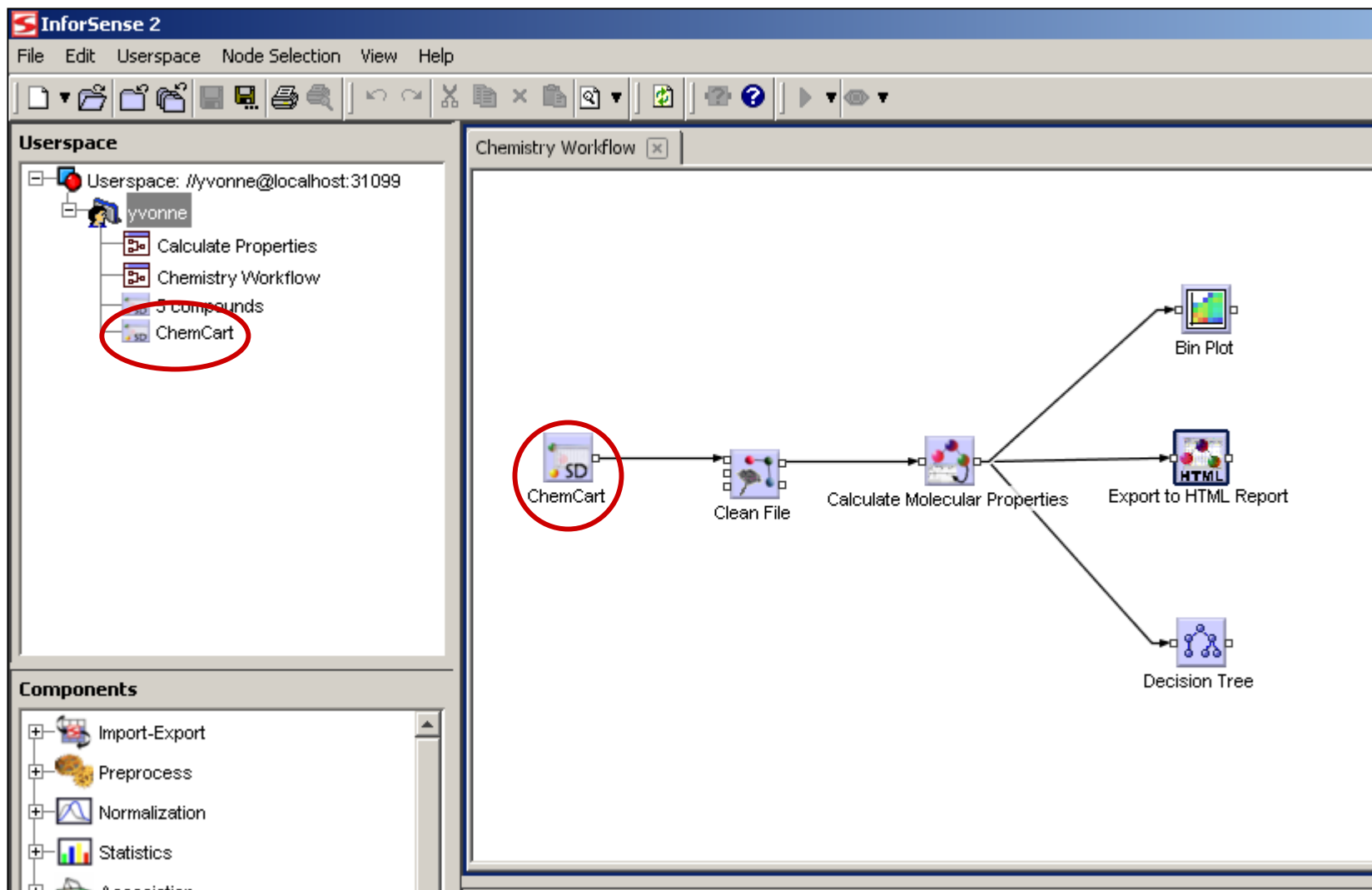
Query Devices

CDBREGNO	1250
PLATE_ID	16
PERCENT_INH	15.716742
POSITION (ALL)	B10

Details-on-Demand

Column	Value
CDBREGNO	419
PLATE_ID	6
PERCENT_INH	15.716742
POSITION	B10

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