

DeltaSoft's ChemCart

A web-based, integrated suite of applications for
discovery research

ChemAxon US UGM
September 14-15, 2010
Boston, MA



DeltaSoft, Inc.

- ❑ Specializing in R&D Informatics since 1996
- ❑ Based in New Jersey, USA
- ❑ Commercial software applications
 - ChemCart
 - ❑ web interface to research data
 - ChemCart Applications
 - ❑ Compound Registration
 - ❑ Reagent Inventory
 - ❑ Electronic Laboratory Notebook
 - ❑ BioAssay
 - ❑ Sample Inventory
 - ❑ Structure Activity Browser
 - ❑ Custom Synthesis Tracking
 - ❑ ChemCart for Excel
- ❑ Services

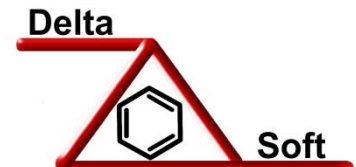
DeltaSoft's Discovery Informatics Expertise

- ❑ Cheminformatics & Bioinformatics
- ❑ Application Design and Development
- ❑ Chemistry Cartridge Evaluation and Tuning
- ❑ Data Model Design / Oracle Optimization and Support
- ❑ Strategic Planning
- ❑ Software Integration

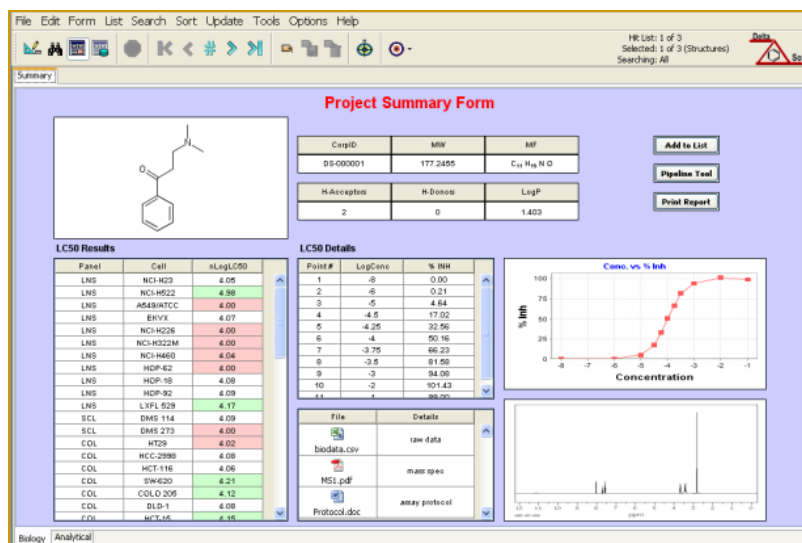
Our partners:



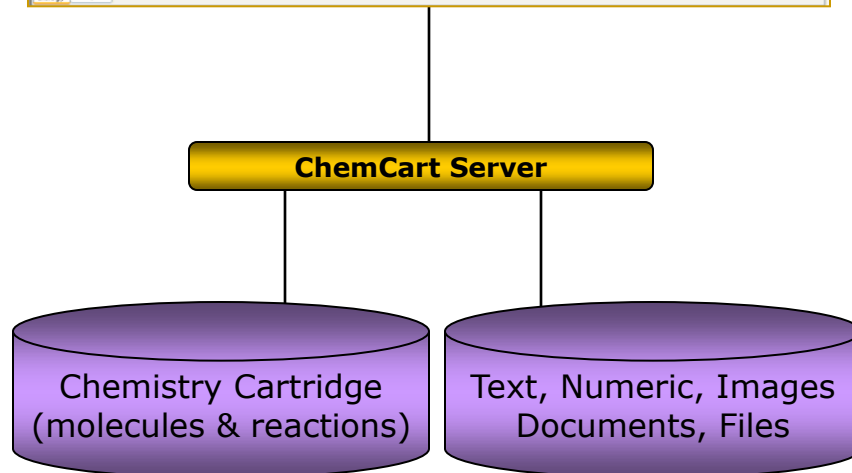
Our Clients



ChemCart



Dynamic web forms interface to research information; including structures/reactions, data, images, files

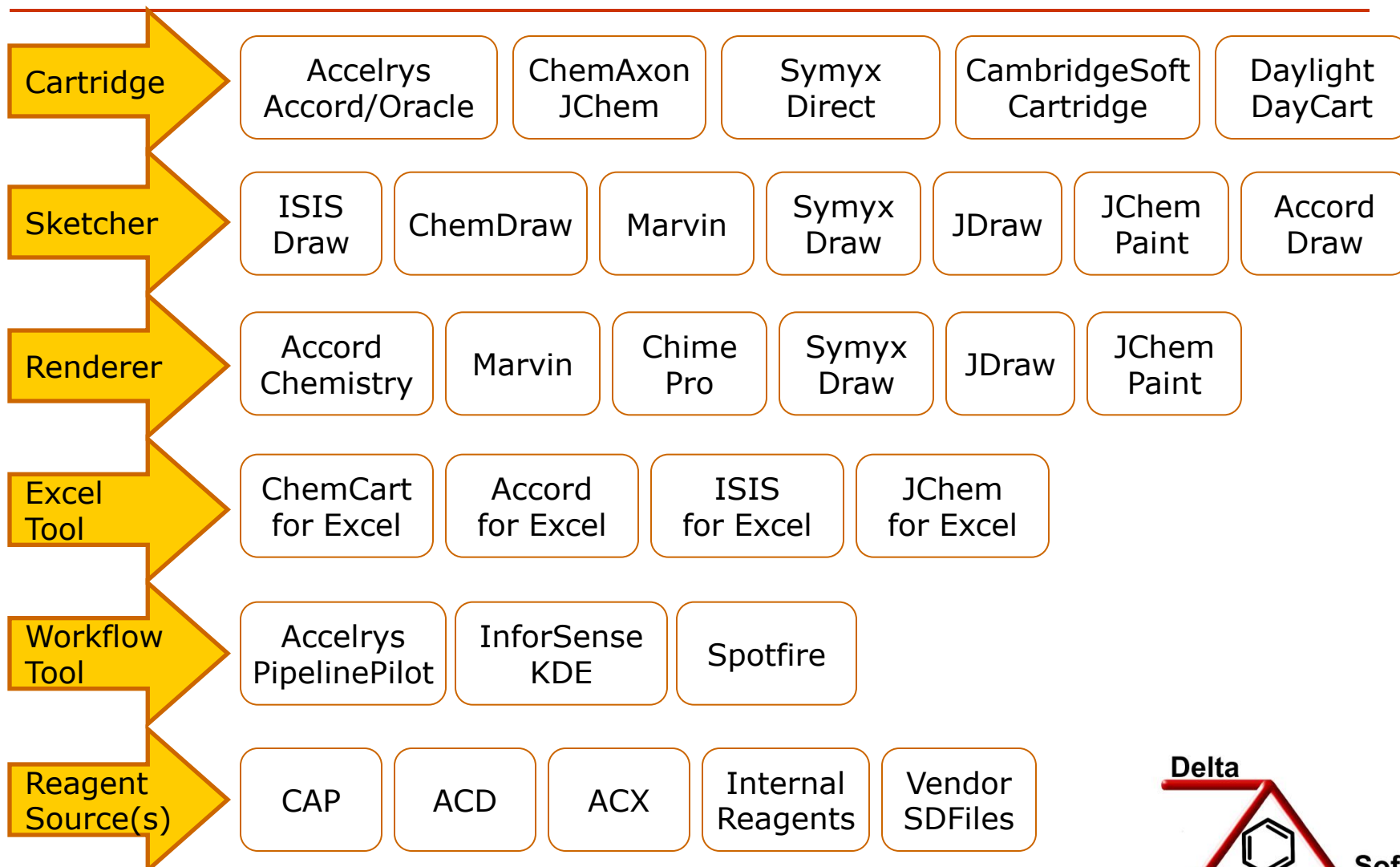


ChemCart – ‘Next Generation’

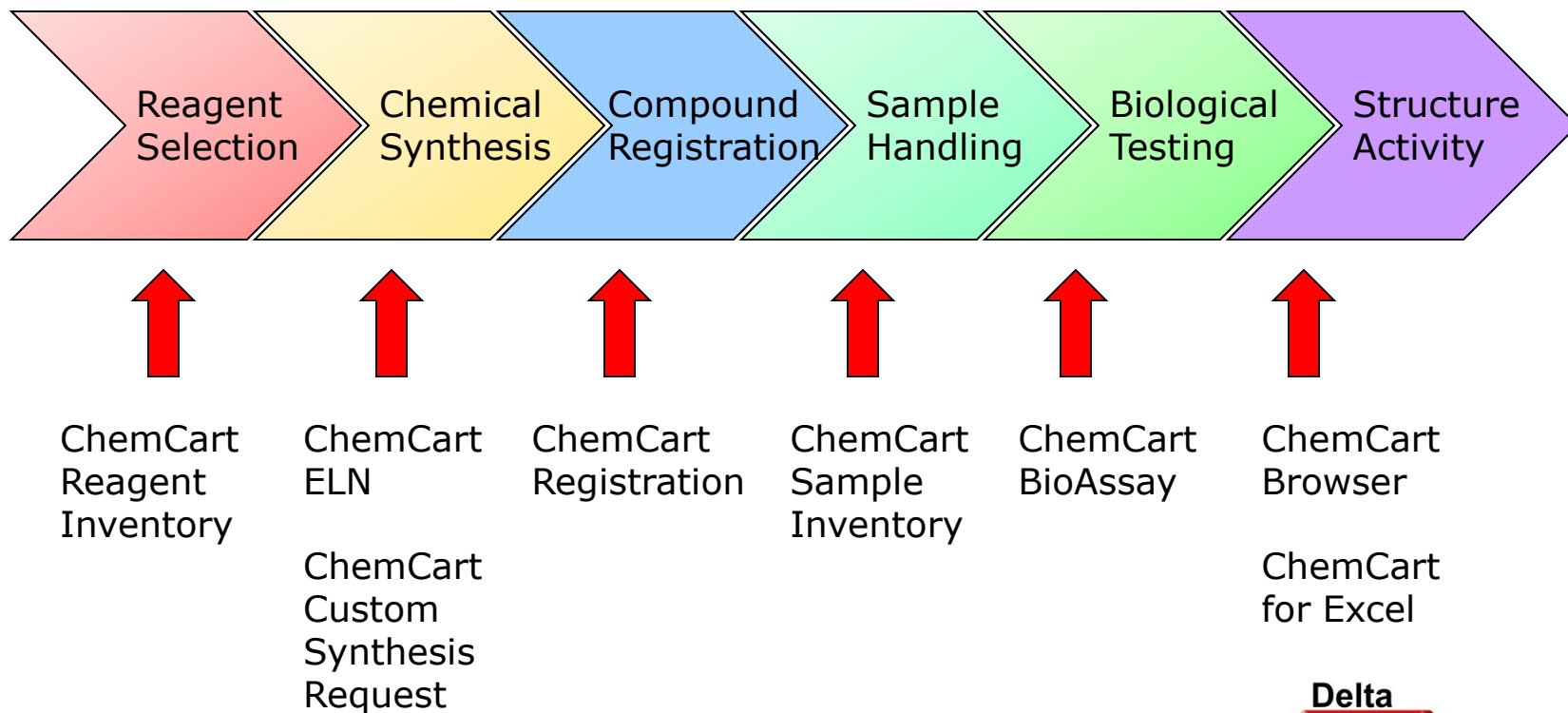
- ❑ Configurable forms interface
 - Structures / Reactions, Data, Images, Documents & Files
- ❑ Web-based, no client install
- ❑ Accesses chemistry data cartridge databases
- ❑ Utilizes any chemical sketcher / renderer
- ❑ Integrates with pipelining and analysis tools
- ❑ Links to multiple Oracle databases, any data model
- ❑ Use Out-of-the-Box Applications or for Rapid Application Development
- ❑ Deployable on internal servers, hosted, or in the ‘Cloud’



Component Approach – Choice!



ChemCart Applications



ChemCart Reagent Inventory

- ❑ “One Stop Shop” for commercial and in-house reagent sourcing
 - Vendor, pricing, supplier info
 - Location, amount, barcode info
 - Compound & Bottle Categories
 - Health & Safety
- ❑ Shopping Cart
 - Internal
 - Supplier
- ❑ Track bottle history from cradle to grave
- ❑ Link to Purchasing

Reagent Inventory

Compound ID: MFCD00000653
CAS Number: 98-88-4
Formula: C₇ H₅ Cl O
Mol. Wt.: 140.568

Chemical Name: BENZOYL CHLORIDE
Supplier Comment: CORROSIVE; LACHRYMATORY; MOISTURE-SENSITIVE; TOXIC

Compound Categories: CORROSIVE
Bottle Categories: reserved

Commercial Sources		Add to Cart	MSDS				
Supplier	Catalog #	Pkg Size	Units	Price	Currency	Purity	Conc.
BAYER	16.18	0		0.00	UNK		100
BDH	10054 3J	100	ML	0.00	UNK	99.0%	100
BDH	27349 4B	500	ML	0.00	UKL	>99%	100
BDH	27349 4B	500	ML	0.00	UKL	>99%	100
BDH	27349 1S	2.5	L	0.00	UKL	>99%	100
E-MERCK	8.01804.0100	100	ML	9.36	EUR	>99%	100
E-MERCK	8.01804.0106	100	ML	0.00	UNK	>99%	100
E-MERCK	8.01804.1000	1	L	16.05	EUR	>99%	100

In-house Sources		Add to Cart									
Barcode	Supplier	Catalog#	Lot No	Orig Amt	Curr.Amt	Units	Date Recd	Date Ordered	Owner	Location	Exp Date
262	LANCASTER	3317	1-1	1000	1000	ML	17-Nov-2006	31-Jul-2006	CHEMCART	US Lab 2	20-Jan-2015
825146	ALDRICH	B1,269-5		25	25	ML	26-Jun-2007	26-Jun-2007	CHEMCART	US Store 1	
3001	FLUKA	RDH-15215	22-04-99	100	100	ML	25-Jul-2006	25-Jul-2006	CRISTAL33	US Lab 2	30-Jan-2010
258	JANSSEN	10.575.02	1-1	50	50	KG	17-Nov-2006	25-Jul-2006	CRISTAL33	UK Store 1	20-Jan-2015
259	JANSSEN	10.575.02	1-1	50	50	KG	17-Nov-2006	25-Jul-2006	CRISTAL33	UK Store 1	20-Jan-2015
3004	ACROS	10575-0010	8-1-77	1	1	L	25-Jul-2006	25-Jul-2006	CRISTAL33	US Lab 2	15-Mar-2009
3005	ACROS	10575-0010	8-1-77	1	1	L	25-Jul-2006	25-Jul-2006	CRISTAL33	US Lab 2	15-Mar-2009
3006	ACROS	10575-0010	8-1-77	1	1	L	25-Jul-2006	25-Jul-2006	CRISTAL33	US Store 2	15-Mar-2009
260	ACROS	10575-0010	1-1	1	1	L	17-Nov-2006	25-Jul-2006	CRISTAL33	UK Store 1	20-Jan-2015

ChemCart ELN

- Record experiments
 - Reaction, reagents, products,
 - Text, images, documents & files
- Auto calculations
 - limiting reagent
 - mmol, vol, theo yield, % yield
- Quick Pick reagents or text
- Duplicate pages
- Lock experiment & audit changes
- Print notebook pages
- Query own ELN or all
- Link to Registration, Inventory

The screenshot displays the ChemCart ELN software interface for a synthesis experiment titled "Synthesis of Aspirin". The interface includes a menu bar (File, Edit, Form, List, Search, Sort, Update, DeltaBook, Tools, Options, Help), a toolbar with various icons, and a status bar at the top right showing "HR List: 10 of 31", "Selected: 10 of 31 (Reaction)", and "Searching: All".

The main workspace is divided into several sections:

- Title:** Synthesis of Aspirin
- Scientist:** Med Chemist
- Notebook:** DS003
- Exp#:** 10
- Date:** 09-Nov-2007
- Continued from:** 16
- on:** 18

The **Reaction** section shows a chemical reaction diagram for the synthesis of aspirin, with a "New Reaction" button. Below the diagram, the temperature is set to 90 and the solvent is NEAT.

The **Reagents** section includes a table with columns: Structure, Name, Lot#, MF, LR, MW, Act MW, Eq, Theo Mass, Act Mass, mmol, d, Vol. Two reagents are listed:

Structure	Name	Lot#	MF	LR	MW	Act MW	Eq	Theo Mass	Act Mass	mmol	d	Vol
	acid	1-1	C ₇ H ₆ O ₃	Y	138.12	138.12	1	138.12	2.50	18.10		
	anhydride	21-3-4	C ₄ H ₆ O ₃	N	102.09	102.09	1	1.85	1.85	18.10		

The **Products** section includes a table with columns: Lot#, ID, Structure, MF, MW, Act MW, Eq, Theo Mass, Act Mass, Purity, mmol, % Yield. Two products are listed:

Lot#	ID	Structure	MF	MW	Act MW	Eq	Theo Mass	Act Mass	Purity	mmol	% Yield
17-1			C ₉ H ₈ O ₄	180.16	180.16	1	3.261	3.000	100	16.66	92.0
			C ₂ H ₄ O ₂	80.05	80.05	1	1.087	0.000			

The **Experimental Procedure** section contains a "Quick Pick Text" button and a text area with the following text: "A test tube containing salicylic acid was placed in a water bath 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 and heated at 90 C. When the contents of the test tube were dissolved and colorless, H₂O was added, and the test tube was cooled in an ice bath. The crystalline product was collected in a Hirsch funnel."

The **LR Ref** section shows "Journal Article". The **Comments** section shows "use in Project 236".

The bottom of the interface features a navigation bar with tabs: Summary, Reagents, Products, Files, Images, Index, ChemReg.

ChemCart Custom Synthesis

- Request custom synthesis, internal or external
- Provide experimental details, including image of reaction scheme and supporting documents
- Create RFQs
- Track and browse synthesis progress
- Generate reports

Custom Synthesis Request Form

Request #	REQ-27	Request Type	Library	Structure	
Request Date	23-Apr-2009	Project	Project 1		
Requester	MikeD	Initials	MD	Date Needed By	14-May-2009
Project Leader	YvonneS	Amt. Needed	500 mgs		
Desired Chemical Purity	95%	Is it Chiral	N	Chiral Purity	

Synthetic Scheme

Reaction Steps

Reaction Step	Yield
1	80
2	80
3	70

Supplier: ChemDiv

Chemical Name: Modafinil

Starting Materials / Intermediates:

Special Handling Instructions:

Analytical Methods: HPLC, LCMS, NMR, C, H, N

ChemCart Registration

- Compound, Lot, Sample
 - Duplicate structure checking
 - Set required / optional fields
 - Use picklists for controlled vocabulary
- Configurable
 - Fields
 - Forms
- Sample Inventory
 - Track sample location
 - Sample request

File Edit Form List Search Sort Update Tools Options Help

HR List: 7 of 7
Selected: 7 of 7 (CHEMREG_COMPOUND)
Searching: All

Registration

Structure

Chemical structure: CN(C)CC(=O)c1ccccc1

Compound Registration

New Compound New Batch

Corp ID	DS1000007	Project	PROJECT1
Reg. No.	1000007	Therapeutic Target	TARGET1
Batch ID	DS1000007-0-1	Solvate	
Mol Formula	C ₁₁ H ₁₅ N O	Solubility	DMSO
Batch Formula	C ₁₁ H ₁₅ N O	Purity	>90%
Mol Weight	177.24	Purification Method	Crystallization
MW with Salt	177.24	Melting Point (°C)	110-111
Exact Mass		Boiling Point (°C)	
Reg Date	21-Apr-2008	Library	Library 105
Reg By	CCADMIN6	External Source	
Alias		External Reg. #	ER 3726

Salt Form	No Salt	#	
Notebook Ref	268-1		
Amount Submitted	57	Units	mg
Submitter	CCUSER6		
Stereochemistry			
Appearance	white solid		

Reference	JACS, 2006
Chemical Name	amine
Comments	reserved for Project 1, keep in cold storage

Compound Batch Sample Spectra

Integration with ChemAxon

ChemAxon JChem
Cartridge for Structure
Storage/Searching

ChemAxon JChem
Cartridge for Structure
Calculations (MW, MF)

ChemAxon Marvin for
Structure
Sketching/Rendering

The screenshot shows the 'Registration' window of ChemAxon JChem. It features a 'Structure' panel on the left displaying a chemical structure of a tertiary amine. Below this is a table of properties including Salt Form, Notebook Ref, Amount Submitted, Submitter, Stereochemistry, Appearance, Reference, Chemical Name, and Comments. On the right, there are buttons for 'New Compound' and 'New Batch', followed by two tables: one for compound identification (Corp ID, Reg. No., Batch ID, Mol Formula, Batch Formula, Mol Weight, MW with Salt, Exact Mass, Reg Date, Reg By, Alias) and another for project details (Project, Therapeutic Target, Solvate, Solubility, Purity, Purification Method, Melting Point, Boiling Point, Library, External Source, External Reg. #). Three yellow arrows point from external text labels to the Structure panel, the 'New Compound' button, and the compound identification table.

Corp ID	DS100000
Reg. No.	1000007
Batch ID	DS1000007-0-1
Mol Formula	C ₁₁ H ₁₅ N O
Batch Formula	C ₁₁ H ₁₅ N O
Mol Weight	177.24
MW with Salt	177.24
Exact Mass	
Reg Date	21-Apr-2008
Reg By	CCADMIN6
Alias	

Project	PROJECT1
Therapeutic Target	TARGET1
Solvate	
Solubility	DMSO
Purity	>90%
Purification Method	Crystallization
Melting Point (°C)	110-111
Boiling Point (°C)	
Library	Library 105
External Source	
External Reg. #	ER 3726

ChemCart BioAssay

- ❑ Biological Data entry
 - Associate test results with registered samples
 - Single point entry
 - Batch load from Excel, text files, etc.
 - Configurable pick lists
- ❑ Load image results
 - Paste single images
 - Batch load
- ❑ Attach supporting documents
 - Original Excel files
 - Raw data

The screenshot displays the 'Test Results' window in the ChemCart BioAssay software. The window title is 'Test Results' and it includes a menu bar (File, Edit, Form, List, Search, Sort, Update, Tools, Options, Help) and a toolbar. The main content area is titled 'Biological Test Results' and contains the following information:

Comp ID: DS-5615
Lot: 43-1
Sample (barcode): 100012

Project	Assay Name	Version	Notebook	Page	Cell Line	Result Type	Qualifier	Result Value	Units	Date Created	Entered By
CytoTox	CT-1	1	15-1	23	AD38	IC50	=	0.5	uM	21-Apr-2008	CHEMCART
CytoTox	CT-2	1	15-2	34	AD38	IC50	=	0.4	uM	21-Apr-2008	CHEMCART
MitoTox	MT-1	1	16-3	65	MTL	EC90	=	1.4	uM	21-Apr-2008	CHEMCART
Enzyme	E1	1	16-6	14	CEM	IC50	=	10	uM	21-Apr-2008	CHEMCART
Enzyme	E1	1	19-5	45	CEM	IC50	=	11	uM	21-Apr-2008	CHEMCART
Enzyme	E2	1	19-7	37	CEM	IC50	=	8.6	uM	21-Apr-2008	CHEMCART

The interface also features a 'Result Image' section showing a microplate image, a 'Document Description' section with a list of files (uv spectra, assay protocol, reader file, excel data) and their corresponding document types (UV.pdf, Protocol.doc, RawData.txt, RawData.xls), and a 'Structure' section displaying the chemical structure of a compound.

ChemCart for Excel

The screenshot shows the ChemCart for Excel-SAR_BROWSER dialog box overlaid on a Microsoft Excel spreadsheet. The spreadsheet contains a table with columns labeled A through O. Row 1 has headers: A: STRUCTURE, B: CORPID, C: MOLWT_STORED. Rows 2-6 contain chemical structures and their corresponding CORPID and MOLWT_STORED values.

The ChemCart for Excel-SAR_BROWSER dialog box is open, showing the following options:

- Export From ChemCart:** List | Search |
- Fields:** A tree view showing various fields. The following fields are selected:
 - Structures
 - CDBREGNO
 - STRUCTURE
 - Formula of STRUCTURE
 - Mol. Wt. of STRUCTURE
 - CORPID
 - NSC
 - CAS_RN
 - MOLWT_STORED
 - PROJECT_ID
 - PROJECT_ID_LOOKI
- Export Order and Display Name:** A table with columns: Add, Field, Export Name.

Add	Field	Export Name
	Structures.STRUCTURE	STRUCTURE
	Structures.CORPID	CORPID
	Structures.MOLWT_STORED	MOLWT_STORED
- Display Repeating Data:** Display Repeating Data
- Export Name Format:** <field> (Display Name)
- Date Format:** dd-MMM-yyyy
- Decimal Places:** No Limit
- Column Width:** 0
- Auto-Fit:** Auto-Fit
- Alignment:** TOP
- Font:** Arial, plain, 12
- Workbook Export Options:**
 - Starting Cell:** A1
 - Create New Sheet (Name: ChemCartExport)
 - Use Existing Sheet
 - Show Structures on Export
 - Exclude Header
- Limit to:** 5000 hits, 20000 rows
- Export:** Load, Save, Clear
- List Sheet:** Sheet1
- List Selection:** \$A\$1
- Run Now** and **Cancel** buttons.

Design Form

- ❑ Use Default
- ❑ Create ad hoc
- ❑ Sheets
- ❑ Export / Import forms
- ❑ Fields added to database are automatically available

The screenshot displays the ChemCart software interface. The main window is titled 'ChemCart - CHEMCART_ACCELRY'S - Windows Internet Explorer'. The menu bar includes File, Edit, Form, List, Search, Sort, Update, Tools, Options, and Help. The toolbar contains various icons for file operations and editing. The main workspace shows a 'Project Summary Form' design area with a grid background. A large white box labeled 'STRUCTURE' is positioned in the upper left. Below it, there are tabs for 'LC50 Results', 'Cell Line Google', and 'Cell Line NCBI'. The 'LC50 Results' tab is active, showing a table with columns: PANEL, CELL, NLOGLC50, and LC50C. The table contains several rows of data. An 'Edit Box Properties' dialog is open, showing a list of fields under 'SAMPLEDATA_ACCORD'. The 'STRUCTURE' field is selected and checked. The dialog also shows formatting options for the selected field, including Label, Content, Font (Arial, bold, 12), Foreground (Blue), Background (White), Alignment (TOP_LEFT), Data, Font (Arial, plain, 12), Foreground (Black), Background (White), Conditional Format (Off), Alignment (BOTTOM), Line Format (Display on single line), Is Data HTML (False), Scrolling (IF Needed), Precision (No Limit), Helper Program (<none>), Element, Border Width (2), Border Color (Custom (0,51,102)), Tab Order (10000), and Tag.

Query

- Methods
 - Form
 - Advanced Query Builder
 - StructA AND NOT StructB
 - SQL Editor
- Cartridge operators
 - Substructure
 - Exact
 - Similarity
 - Equals
 - Etc.

The screenshot displays the Delta Software interface. The main window is the 'Project Summary Form' for project 'SAR 2v4'. A red box highlights a 'Similarity' dropdown menu. An 'Edit Term' dialog is open, showing a search for 'STRUCTURE' with a similarity search type. The 'Options' section includes a similarity value of 0.5 and a list of match options, all of which are checked. A 'Query Builder' dialog is also open, showing a field selector on the left and a term editor on the right. The term editor shows two terms, A and B, both of type 'STRUCTURE'. The composer shows the query 'A and not (B)'. The query viewer shows the resulting SQL query:

```
SSS (STRUCTURE, <structure>)  
and  
not (SSS (STRUCTURE, <structure>))
```

View Results

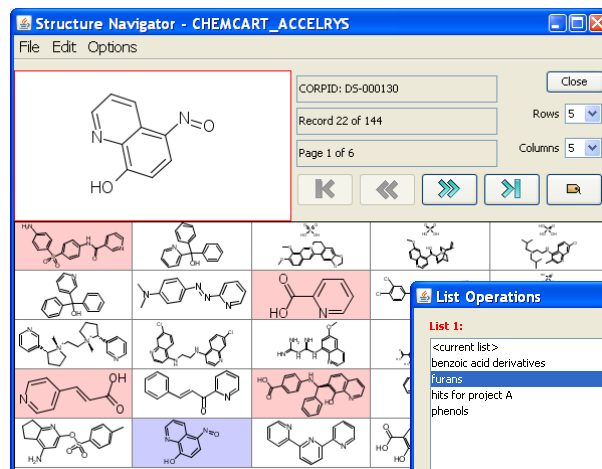
- ❑ Navigate hit list by chemical structure
- ❑ Tag and keep or remove

The screenshot displays the ChemCart software interface within a Windows Internet Explorer browser window. The main window title is "ChemCart - CHEMCART_ACCELRY5". The interface includes a menu bar (File, Edit, Form, List, Search, Sort, Update, Tools, Options, Help) and a toolbar with navigation icons. The "Project Summary Form" is visible, showing details for "CORPID: DS-000002", "NSC: 171", and "MF: C₆H₅NO₂". Below this, a table lists properties: H-Acceptors (3), H-Donors (1), LogP (0.8922), and MW (123.110). A "Pipeline Pilot Protocols" panel on the right offers buttons for Properties, SAR Table, and Heatmap. The "LC50 Results" table is shown below, with columns for PANEL, CELL, NLOG₁₀LC50, and LC50. The table contains 18 rows of data, with the row for NCI-H460 highlighted in red. A "Structure Navigator" window is open in the foreground, displaying a grid of chemical structures. The selected structure is 4-pyridylacetic acid, with its SMILES string CC(=O)OCC1=CC=NC=C1. The navigator window also shows navigation controls and a "Close" button. A small graph titled "vs. % Inh" is visible in the background of the navigator window.

PANEL	CELL	NLOG ₁₀ LC50	LC50
LNS	NCI-H23	4	
LNS	A549/ATCC	4.14	
LNS	EKVX	4	
LNS	NCI-H226	4.18	
LNS	NCI-H322M	4	
LNS	NCI-H460	5.2	
LNS	HOP-62	4	
LNS	HOP-92	4	
COL	HT29	4	
COL	HCT-116	4	
COL	SW-620	4	
COL	COLO 205	4	
COL	HCT-15	4	
COL	KM12	4	

Manipulate Hit Lists

- ❑ Add Items
- ❑ Cherry Pick
- ❑ Perform Boolean Operations
- ❑ Maintain List History
- ❑ Import / Export
- ❑ Save, Manage, Share



List Operations

List 1:

- <current list>
- benzoic acid derivatives
- furans
- hits for project A
- phenols

List 2:

- <current list>
- benzoic acid derivatives
- furans
- hits for project A
- phenols

Boolean operations: AND, OR, NOT, XOR

Read Access: Owner Only

Write Access: Owner Only

Hit Count: 384

Created By: YVONNE

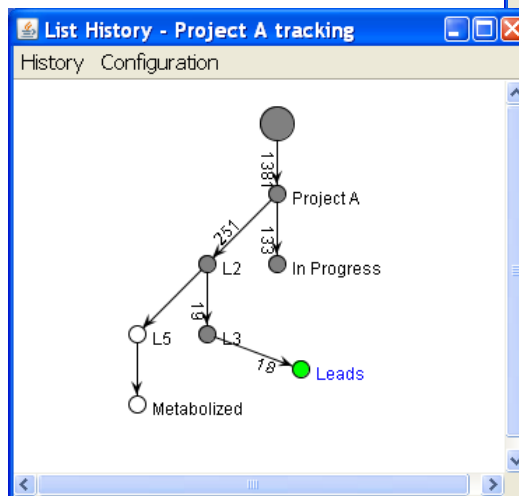
Created: 20-Mar-2007 10:07 AM

Modified By: YVONNE

Modified: 03-Apr-2007 12:04 PM

Show Content

Execute Logic Save Export Load To Form



Report

- Print forms
- Create ad hoc reports
- Save / Share standard reports
- Export to file
 - CSV
 - SDF
 - RDF
 - XDF
 - Excel
 - Accord for Excel
 - ISIS for Excel
 - JChem for Excel
 - ChemCart for Excel
- Export to pivot

The image displays three overlapping windows from the ChemCart software interface:

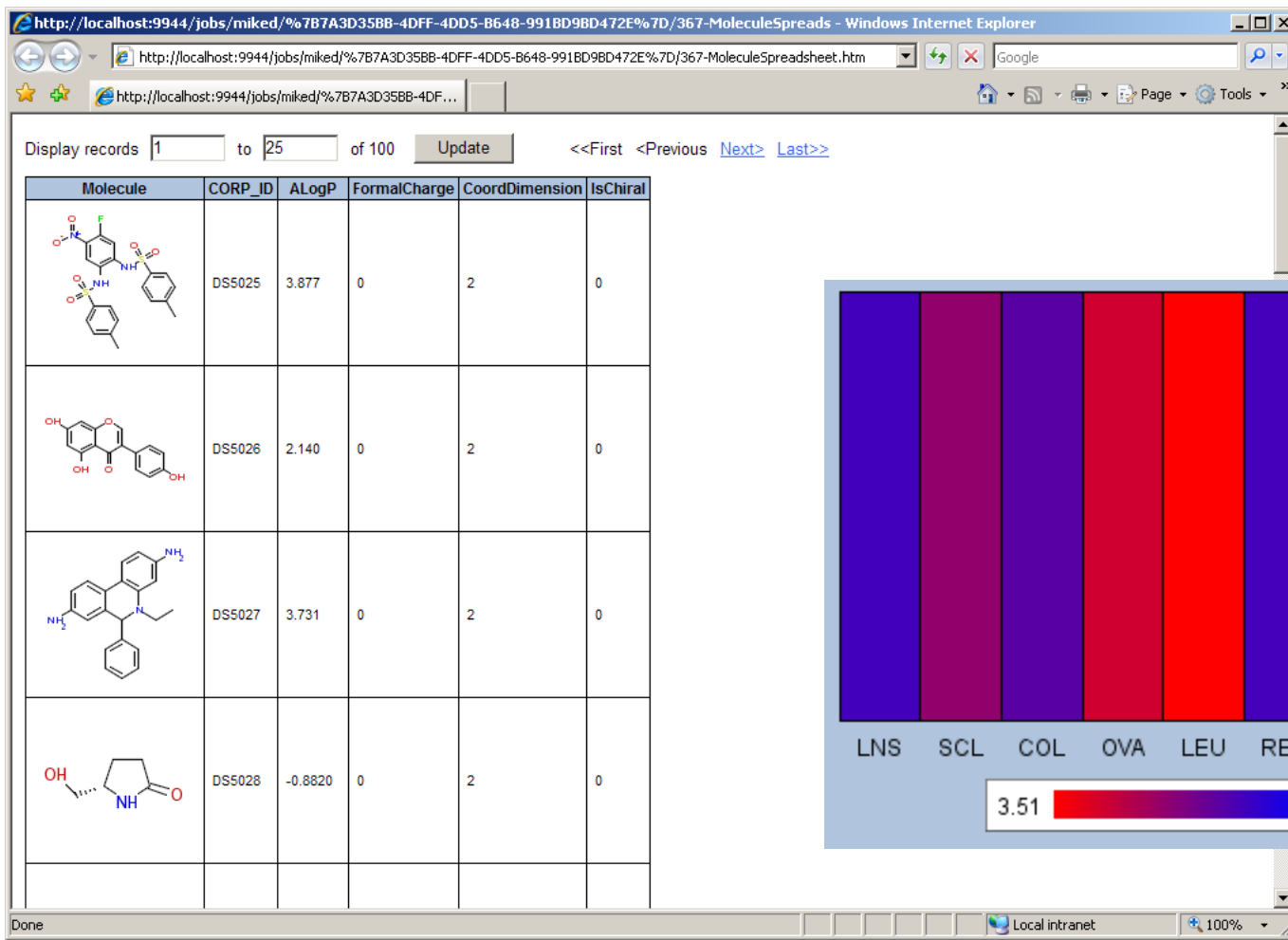
- Top Window (Compound Summary Form):** A table listing compounds with their structures, molecular formulas, molecular weights, and other properties.
- Middle Window (Grid of Structures):** A grid of eight chemical structures, each with a label and an average LC50 value.
- Bottom Window (Pivot Table):** A pivot table showing data for various compounds across multiple assays.

COMPID	Structure	MF	MF	%NH	CAS_IN
DS-000041	<chem>C1=NC2=C(N1)N=CN=C2</chem>	C ₁₀ H ₈ N ₂ O	215.22	-6.24	41-215-1
DS-000070	<chem>C1=CC=C(C=C1)C=C</chem>	C ₈ H ₈ O ₂	122.12	-5.21	623-30-3
DS-000541	<chem>C1=CC=C(C=C1)C=C</chem>	C ₁₀ H ₁₄ N ₂ O	208.35	-6.24	541-288-1
		C ₁₀ H ₈ O ₂	208.22	-0.31	479-13-0
		C ₁₂ H ₁₄ N ₂ O	202.26	-3.02	6313-00-1
		C ₁₂ H ₁₀ O ₄	216.19	-4.64	298-81-7

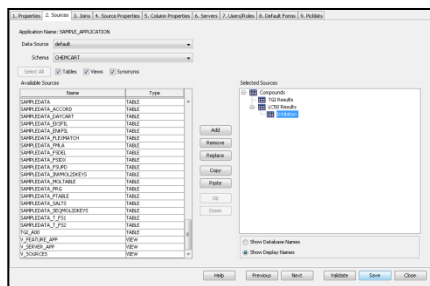
Structure	Avg LC50
<chem>C1=CC=C(C=C1)C=C</chem>	4.00
<chem>C1=CC=C(C=C1)C=C</chem>	4.00
<chem>C1=CC=C(C=C1)C=C</chem>	4.00
<chem>C1=CC=C(C=C1)C=C</chem>	4.13
<chem>C1=CC=C(C=C1)C=C</chem>	4.00
<chem>C1=CC=C(C=C1)C=C</chem>	4.00
<chem>C1=CC=C(C=C1)C=C</chem>	4.00
<chem>C1=CC=C(C=C1)C=C</chem>	4.00

COMPID	STRUCTURE	AVG	AVG	AVG	AVG	AVG	AVG	AVG	AVG	AVG	AVG	AVG	AVG	AVG	AVG
DS-000009	<chem>C1=CC=C(C=C1)C=C</chem>	4	4.18	4	4.14	4	2.1	5.18	4	4	4	4	4	4	4
DS-000001	<chem>C1=CC=C(C=C1)C=C</chem>	4.00	4.978	4	4.07	4	5.04	4.036	4	4.091	4.023	4.079	4.097	4.097	4.306
DS-000066	<chem>C1=CC=C(C=C1)C=C</chem>	4	5.205	4	4	4	4.17	4	4	4.12	4	4	4	4	4
DS-000002	<chem>C1=CC=C(C=C1)C=C</chem>	4		4.14	4	4.18	4	5.2	4	4	4		4	4	4
DS-000086	<chem>C1=CC=C(C=C1)C=C</chem>	4		4	4	4	4	4	4	4	4	4	4	4	4

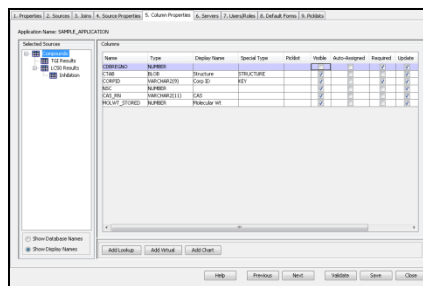
Analyze & Report: InforSense, Pipeline Pilot, Spotfire



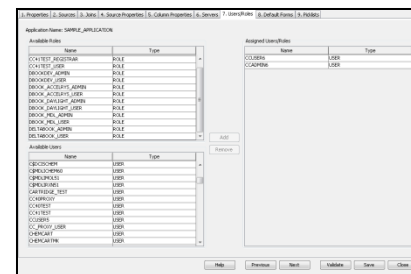
Create a rich user interface & deploy worldwide in less than 5 minutes!



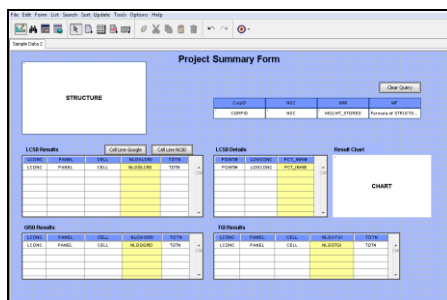
Select data sources.
Define joins.



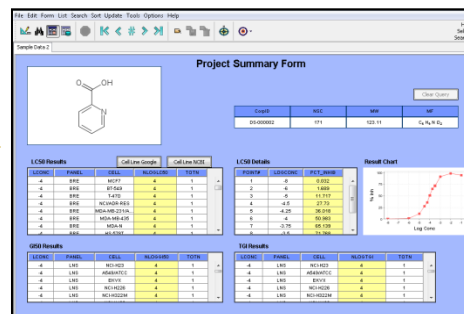
Set friendly column names.
Set picklists.



Set user access.



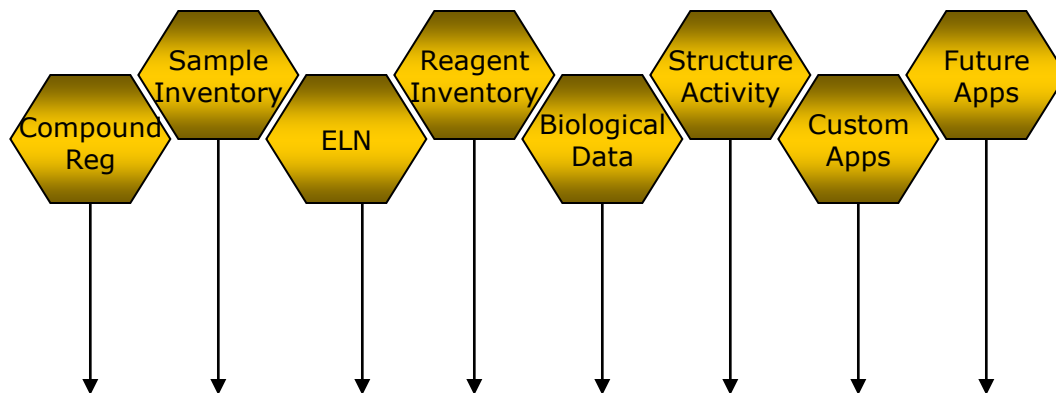
Draw a form with boxes,
tables, labels, and
buttons.
Save publicly.



Search worldwide!

ChemCart Informatics Solution

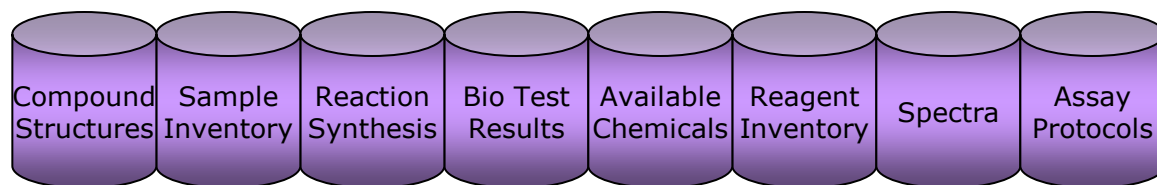
Web Served Applications



Middle Tier



Oracle & Data Cartridge



ChemCart Summary

- ❑ Web-based, configurable forms interface
 - Benefit to Scientist
 - ❑ Ad hoc access to any research data
 - ❑ Sharable objects for communication (e.g. forms, hit lists)
 - ❑ Scientist-familiar chemical sketchers/renderers, search engines
 - Benefit to IT
 - ❑ Minimal deployment & maintenance overhead
 - ❑ Rapid Application Development environment, no programming
 - ❑ Corporate standards (chemistry cartridge, sketcher/renderer, platform)
- ❑ Integrates with best-of-breed 3rd party software for analysis and data integration
- ❑ Provides API for customer-specific workflow implementation

Contact Us

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