

DeltaSoft's ChemCart

An integrated suite of
applications using ChemAxon
components

DeltaSoft, Inc.

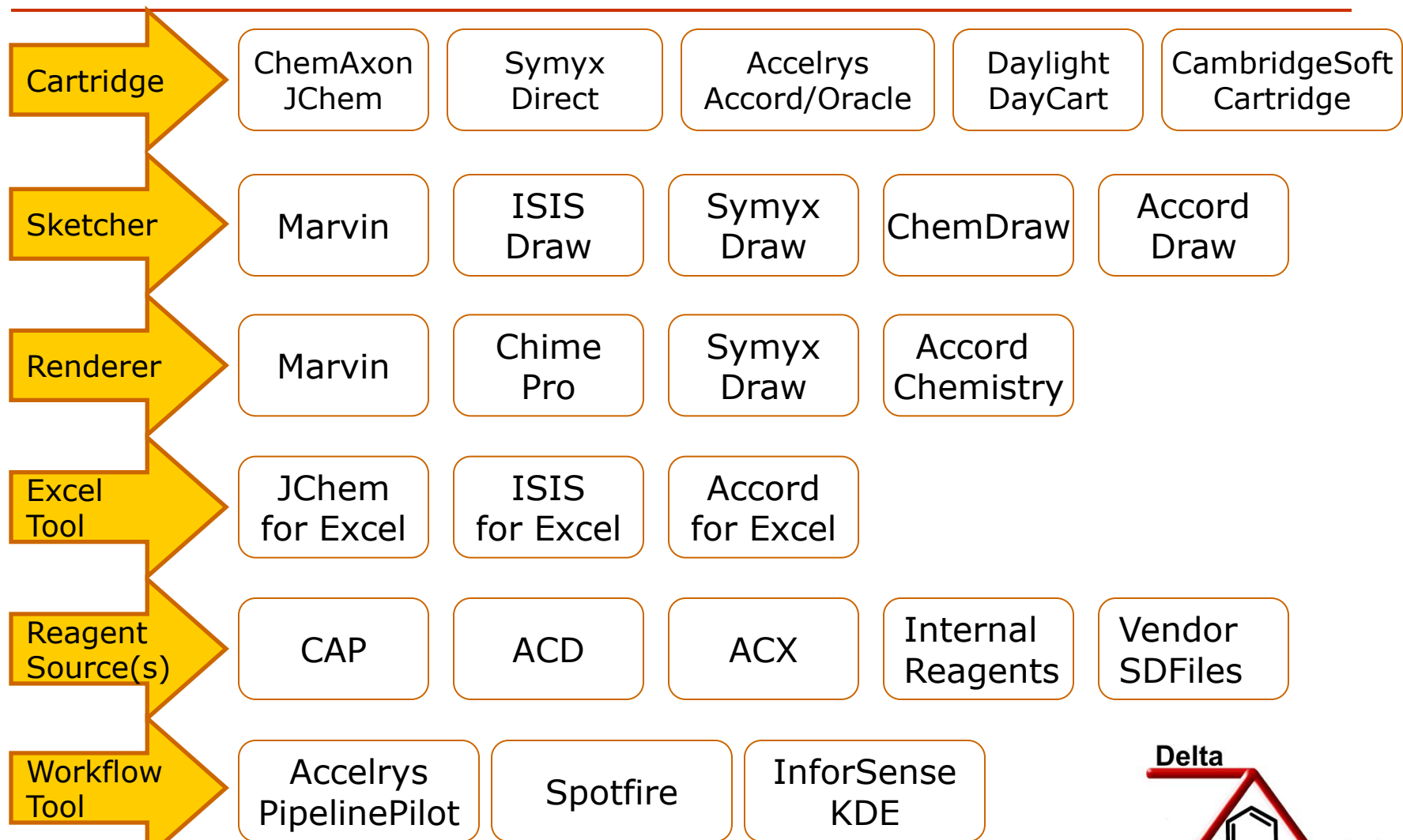
- ❑ Specializing in R&D Informatics since 1996
- ❑ Commercial software applications
 - ChemCart
 - ❑ web interface to research data
 - ChemCart Applications
 - ❑ Compound Registration
 - ❑ Reagent Inventory
 - ❑ Sample Inventory
 - ❑ Electronic Laboratory Notebook
 - ❑ BioAssay
 - ❑ Structure Activity Browser
 - ❑ Custom Synthesis Tracker
- ❑ Services

DeltaSoft's Discovery Informatics Expertise

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



Component Approach – Choice!



ChemCart

The screenshot displays the ChemCart software interface. At the top is a menu bar with options: File, Edit, Form, List, Search, Sort, Update, Tools, Options, Help. Below the menu is a toolbar with various icons. The main window is titled "Project Summary Form" and contains a chemical structure of a benzamide derivative. To the right of the structure are fields for "CompID" (DS-00001), "MW" (177.2455), and "MF" (C₁₄H₁₆N₂O). Below these are fields for "H-Acceptor" (2), "H-Donor" (0), and "LogP" (1.403). There are buttons for "Add to List", "Pipeline Tool", and "Print Report".

The "LC50 Results" table lists various panels and their corresponding cell lines and aLogLC50 values:

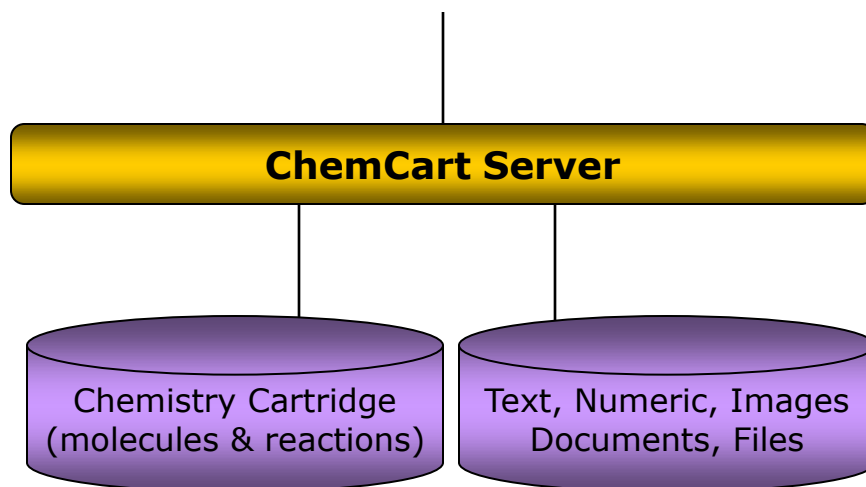
Panel	Cell	aLogLC50
LNS	NCI-H23	4.09
LNS	NCI-H522	4.99
LNS	A549/ATCC	4.00
LNS	BRVX	4.07
LNS	NCI-H226	4.00
LNS	NCI-H222M	4.00
LNS	NCI-M460	4.04
LNS	HDP-62	4.00
LNS	HDP-19	4.08
LNS	HDP-92	4.09
LNS	LSP-529	4.17
SEL	DMS 114	4.09
SEL	DMS 273	4.00
COL	HT29	4.02
COL	HCC-2998	4.08
COL	NCI-116	4.08
COL	SW620	4.21
COL	CDLO 206	4.12
COL	BLD-1	4.08
COL	NCI-15	4.46

The "LC50 Details" table shows the following data points:

Point #	LogConc	% Inh
1	-5	0.00
2	-5	0.21
3	-5	4.64
4	-4.5	17.02
5	-4.25	32.56
6	-4	50.16
7	-3.75	66.23
8	-3.5	81.59
9	-3	94.08
10	-2	101.43
11	-1	98.00

A graph titled "Conc. vs. % Inh" plots the percentage of inhibition against the concentration of the compound. The x-axis is labeled "Concentration" and ranges from -8 to -1. The y-axis is labeled "% Inh" and ranges from 0 to 100. The data points from the LC50 Details table are plotted, showing a sigmoidal curve that levels off at approximately 98% inhibition at a concentration of -1.

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



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 displays the 'Compound Registration' window in ChemAxon JChem. On the left, a chemical structure of N,N-dimethylbenzylamine is shown. The right side contains a registration form with the following data:

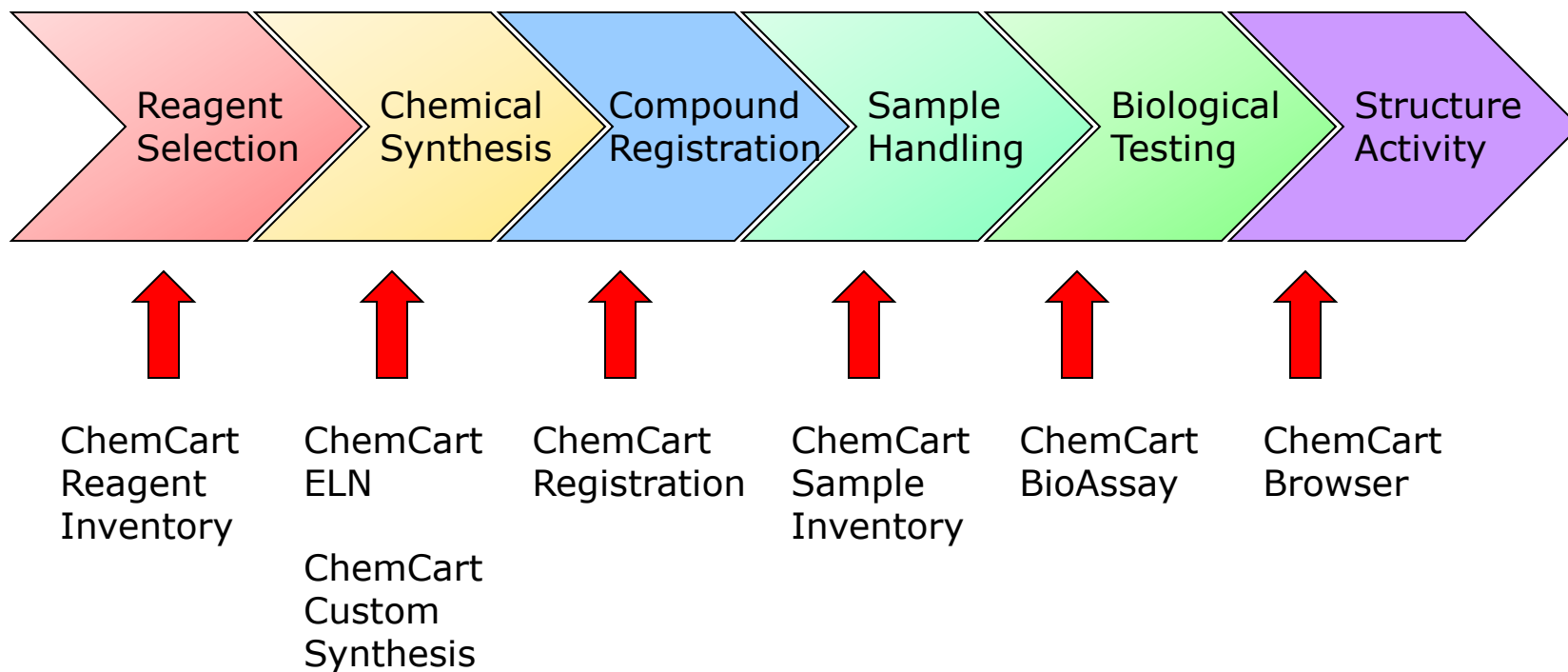
Corp ID	DS1000007	Project	PROJECT1
Reg. No.	1000007	Therapeutic Target	TARGET1
Batch ID	DS1000007-0-1	Solvent	
Mol Formula	C ₁₁ H ₁₅ N O	Solubility	DMSO
Batch Formula	C ₁₁ H ₁₅ N O	Purity	>90%
Mol Weight	177.24	Purification Method	Crystallization
MW with Salt	177.24	Melting Point (°C)	110-111
Exact Mass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

Below the registration form, there are fields for Reference (JACS, 2006), Chemical Name (amine), and Comments (reserved for Project 1, keep in cold storage).

- Partnered since 2006
- Fully integrated, supporting latest version
- Joint customers using Registration, Search & Browse, Inventory in production



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: MFCD0000653
CAS Number: 98-88-4
Formula: C₇H₅ClO
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. The main window is titled "Synthesis of Aspirin". It features a central reaction diagram showing the synthesis of aspirin from salicylic acid and acetic anhydride. Below the reaction, there are fields for "Temp" (90) and "Solvent" (NEAT). The interface is divided into several sections: "Reagents" and "Products" tables, an "Experimental Procedure" text area, and a "Comments" field. The "Reagents" table lists salicylic acid and acetic anhydride with their respective molecular formulas and weights. The "Products" table lists aspirin and acetic acid. The "Experimental Procedure" section contains a detailed description of the synthesis process. The "Comments" field contains the text "use in Project 236".

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		

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			

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

Registration

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

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

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 shows the 'Biological Test Results' window in the ChemCart BioAssay software. The window title is 'Test Results' and it contains the following information:

Test Results

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 window also features a 'Result Image' section with a microscopic image of a cell culture plate, a 'Document Description' table, and a 'Structure' section with a chemical structure diagram.

Document Description	Document
uv spectra	UV.pdf
assay protocol	Protocol.doc
reader file	RawData.txt
excel data	RawData.xls

The chemical structure shown is CN(C)CC(=O)c1ccccc1.

ChemCart Structure Activity Browser

- Query by Form for chemical structures, reactions, data, documents, files, and images
- Run multiple queries simultaneously with each having different search criteria
- Build customizable forms, or use pre-defined forms to view results
- Search by substructure, similarity, exact, and more
- Generate custom report printouts of search results
- Extensive result list handling

Project Summary Form

CompID	MW	SM
DS-00001	177.2455	C ₁₄ H ₁₆ N ₂ O

H-Acceptors	H-Donors	LogP
2	0	1.403

LC50 Results

Panel	Cell	aLogLC50
LNS	NCI-H223	4.05
LNS	NCI-H522	4.98
LNS	A549/ATCC	4.00
LNS	ERVX	4.07
LNS	NCI-H226	4.00
LNS	NCI-H322M	4.00
LNS	NCI-H460	4.04
LNS	HDP-62	4.00
LNS	HDP-19	4.08
LNS	HDP-92	4.09
LNS	LXFL 529	4.17
SCL	DMS 114	4.09
SCL	DMS 273	4.00
CDL	HT29	4.02
CDL	HCC-2998	4.08
CDL	HCT-116	4.06
CDL	SW620	4.21
CDL	COLO 205	4.12
CDL	DLD-1	4.08
CDL	HTC-156	4.16

LC50 Details

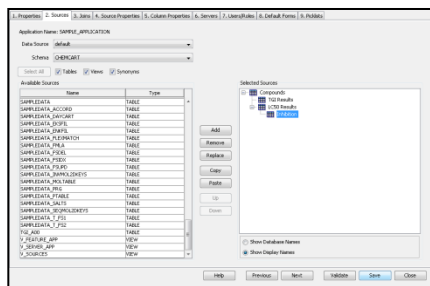
Point#	LogConc	% Inh
1	-8	0.00
2	-6	0.21
3	-5	4.84
4	-4.5	17.02
5	-4.25	32.56
6	-4	50.16
7	-3.75	66.23
8	-3.5	81.59
9	-3	94.09
10	-2	101.43
11	-1	99.50

Conc. vs % Inh

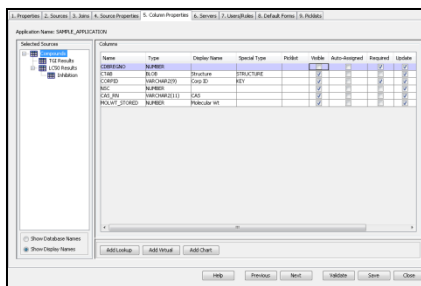
File Details

File	Details
bio\data.csv	raw data
MSI.pdf	mass spec
Protocol.doc	assay protocol

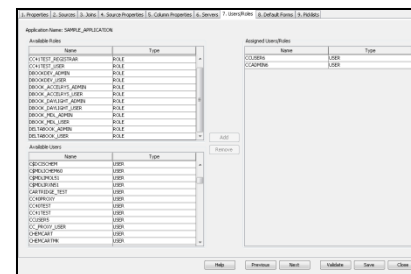
Create a rich user interface & deploy worldwide in less than 5 minutes!



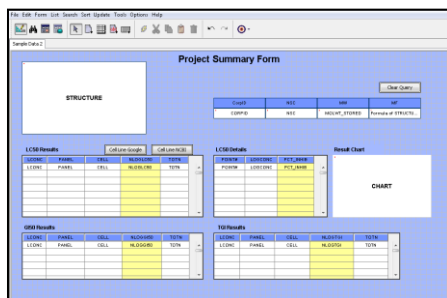
Select Data Sources
Define joins



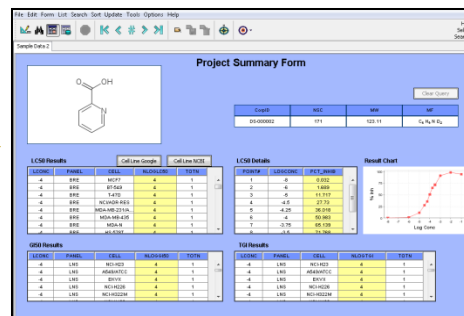
Set friendly column names.
Set pick lists



Set user access



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



Search worldwide!

ChemCart Integrations & API

Imported data - Spotfire DecisionSite 7.2 - [Scatter Plot]

DecisionSite Navigator
/spotfire/ChemCart/mol_spotfire.html

HTS

HTS Data

STRUCTURE

O=C1C=CC(=O)Nc2ccc3c(c1)ccc(O)c3

CDBREGNO	419
PLATE_ID	6
POSITION	B10
PERCENT_INH	15.72

Sheet 1

Query Devices

CDBREGNO	162
PLATE_ID	3
PERCENT_INH	-30.689814
POSITION	(ALL)

Details-on-Demand

Column	Value
CDBREGNO	419
PLATE_ID	6
PERCENT_INH	15.716742
POSITION	B10

Operations

Services (Private)

- Apply
- Calculate Molecular Properties
- Convert Molecular Properties to 2D
- Similarity Filter
- Substructure Filter
- Vector(s) to Columns
- SVMModel
- Custom Lipinski calculator
- cdk2 tracker
- fingerprints
- lip_angles
- top_lipinski
- rottable_bonds
- test_cs_add_bo
- test_cs_dune_group
- test_services_evaluation
- tox_reference_database

Parameter Editor - test

Name	Value
Path	...
Method	...
Batch	...
Index	...

Apply Node Reset

<DataSet> 8 / 40 rows selected

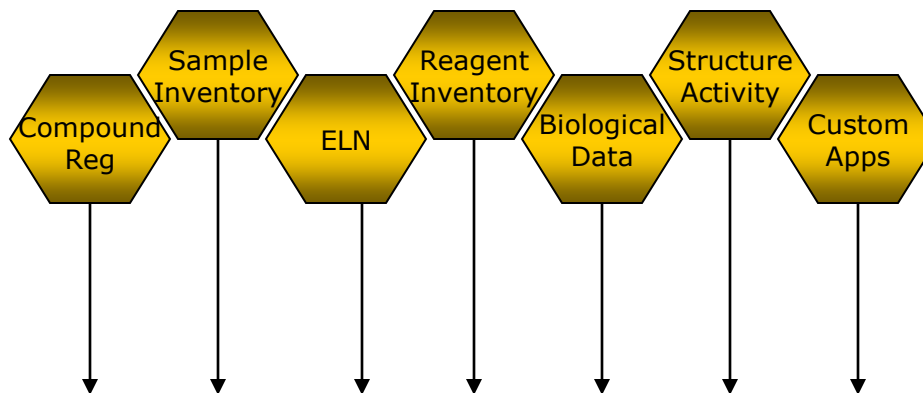
Charts

1 - Parallel Plot

2 - Box Plot

ChemCart Informatics Solution

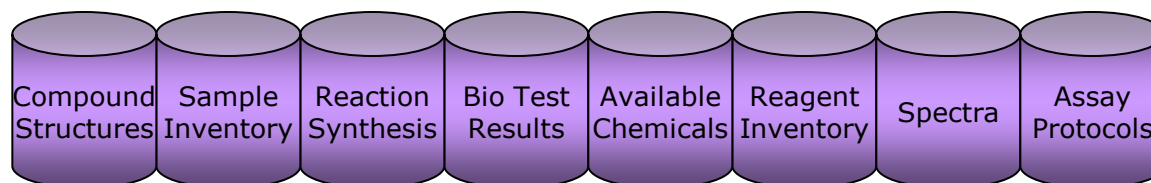
Web Served Applications



Middle Tier



Oracle & Data Cartridge



ChemCart Summary

- Web-based, configurable forms interface to Oracle
 - Benefit to Scientist
 - Provides easy access to data necessary for decision making
 - Enhances communication & collaboration by use of sharable objects (forms, searches, hit lists, etc.)
 - Facilitates acceptance by integration with scientist-familiar chemical sketchers/renderers, search engines
 - Benefit to IT
 - Reduces deployment & maintenance overhead
 - Provides Rapid Application Development capabilities that do not require programming
 - Integrates with corporate standards (chemistry cartridge, sketcher/renderer, platform)
- Integrates with 3rd party software for data analysis

Contact Us

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Please stop by the partner table to see more!

