

# DeltaSoft's ChemCart

An integrated suite of applications that leverage  
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

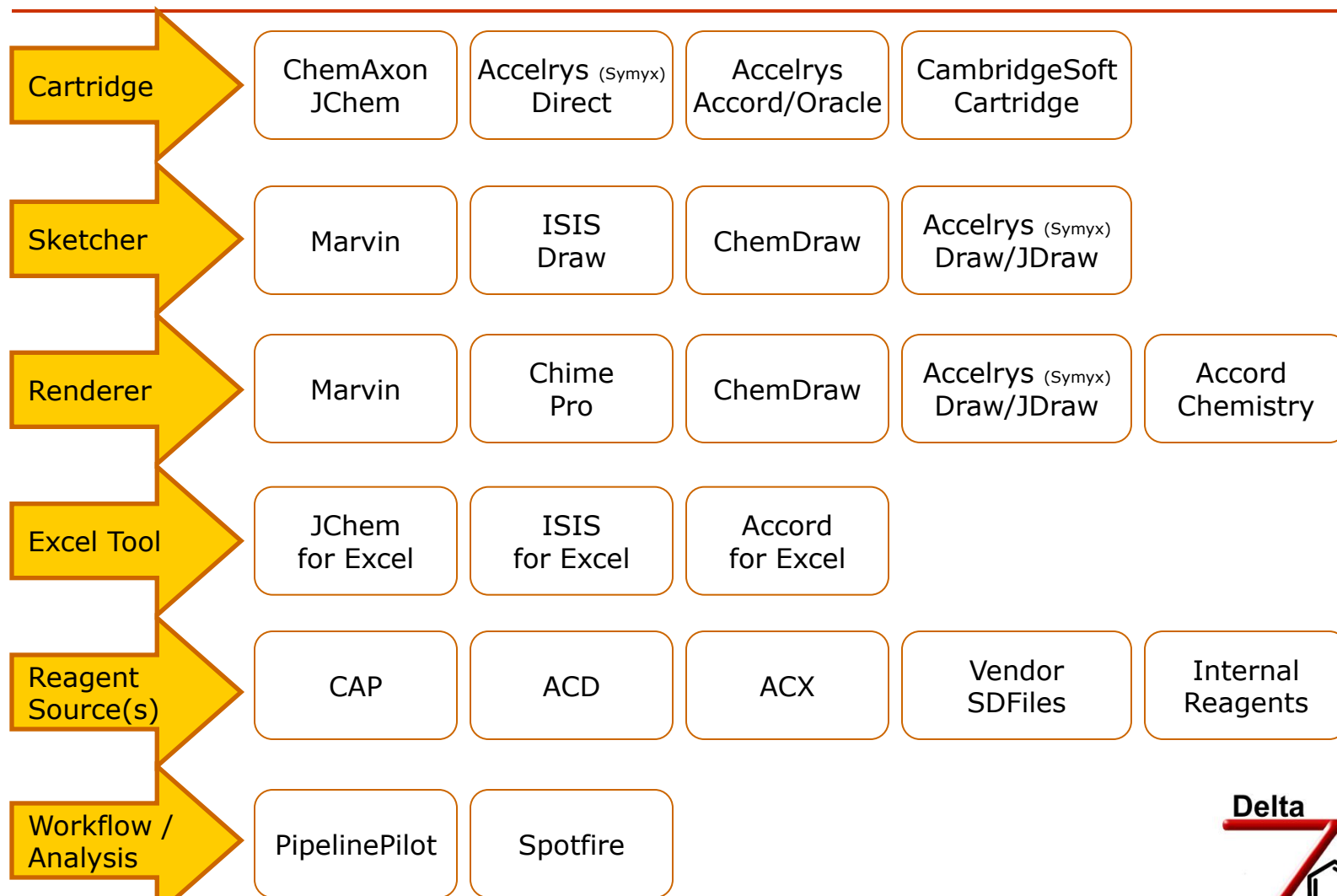
# DeltaSoft's Discovery Informatics Expertise

---

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



# Component Approach – Choice!



# ChemCart

**Project Summary Form**

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

CompID	MW	MF
DS-00001	177.2455	C <sub>11</sub> H <sub>16</sub> N <sub>2</sub> O

H-Acceptor	H-Donor	LogP
2	0	1.403

**LC50 Results**

Panel	Cell	IC50
LNS	NCI-H23	4.09
LNS	NCI-H22	4.98
LNS	A549/ATCC	4.00
LNS	ERVX	4.07
LNS	NCI-H226	4.00
LNS	NCI-H223M	4.00
LNS	NCI-H460	4.04
LNS	HDP-62	4.00
LNS	HDP-19	4.08
LNS	HDP-92	4.09
LNS	L5178	4.17
SCL	DMS 114	4.09
SCL	DMS 273	4.00
CDL	HT29	4.02
CDL	HCC-2998	4.08
CDL	NCI-116	4.06
CDL	SW620	4.21
CDL	COLO 205	4.12
CDL	BLD-1	4.08
F-DL	HT-10	4.16

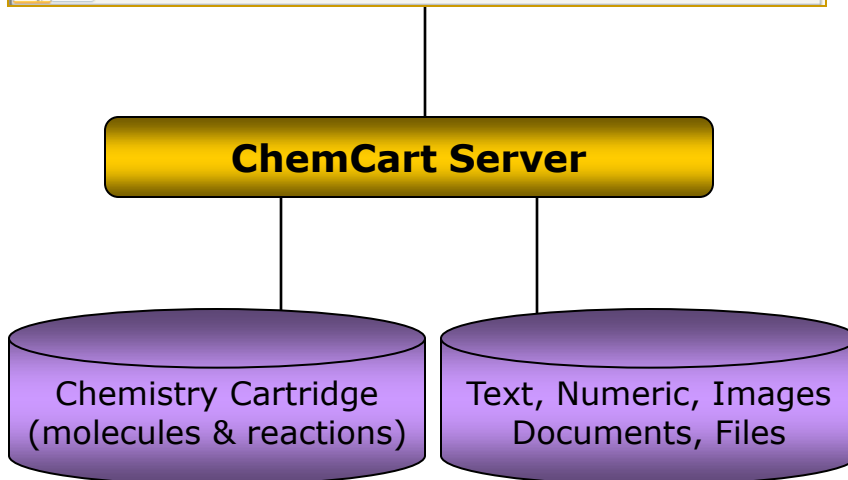
**LC50 Details**

Point#	LogConc	% Inh
1	-6	0.00
2	-5	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	81.58
9	-3	94.09
10	-2	101.43
11	-1	99.00

**Conc. vs % Inh**

**Mass Spectrum**

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

ChemAxon Structure  
Standardizer / Structure Checker

The screenshot shows the 'Compound Registration' window in ChemAxon JChem. On the left, a chemical structure is displayed: a benzene ring attached to a carbonyl group, which is further attached to a propyl chain ending in a dimethylamino group. Below the structure are fields for 'Salt Form' (No Salt), 'Notebook Ref' (268-1), 'Amount Submitted' (57 mg), 'Submitter' (CCUSER6), 'Stereochemistry', and 'Appearance' (white solid). On the right, a table lists registration details:

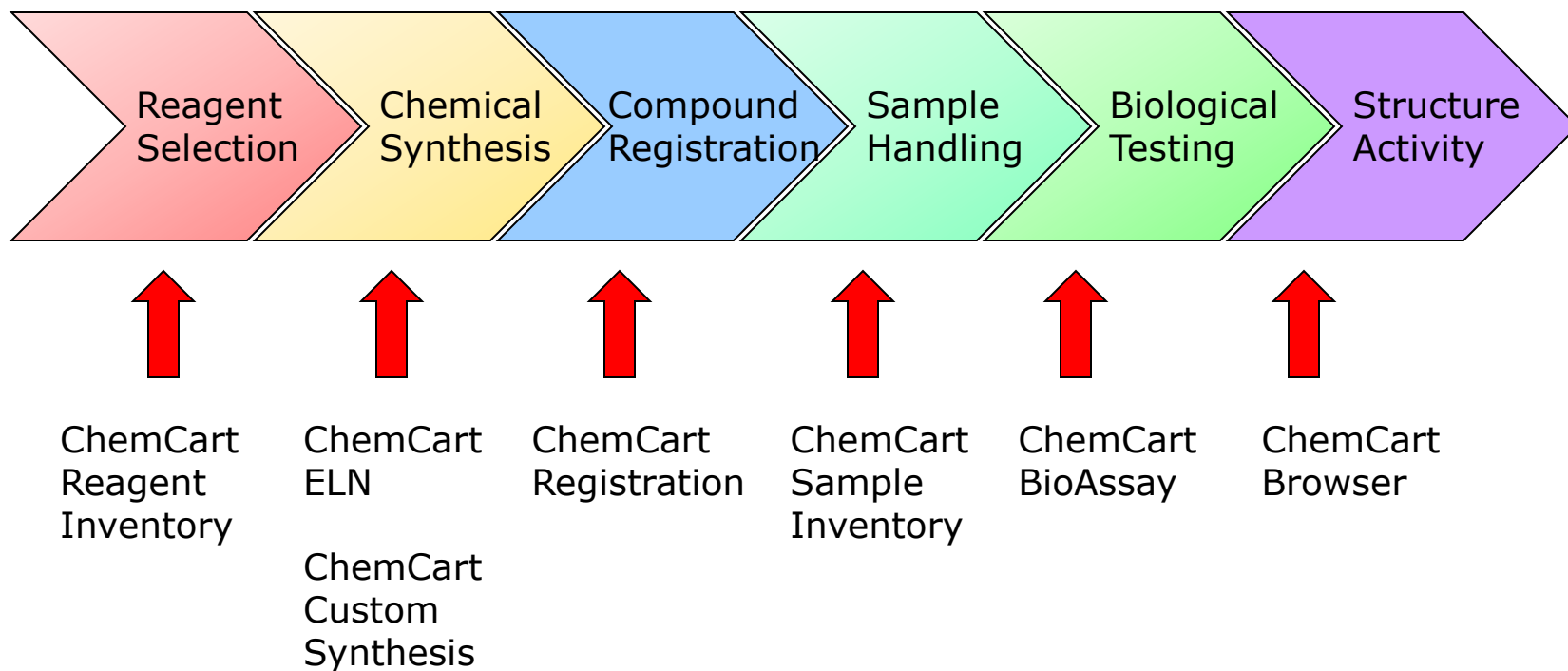
Corp ID	DS1000007	Project	PROJECT1
Reg. No.	1000007	Therapeutic Target	TARGET1
Batch ID	DS1000007-0-1	Solvent	
Mol Formula	C <sub>11</sub> H <sub>15</sub> N O	Solubility	DMSO
Batch Formula	C <sub>11</sub> H <sub>15</sub> N O	Purity	>90%
Mol Weight	177.24	Purification Method	Crystallization
MW with Salt	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

At the bottom of the window, 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 ELN, Registration, BioAssay, Inventory, Search & Browse, Inventory in production



# ChemCart Applications



# Case #1: Registration

- ❑ Problem: Large chemical company needed to replace aging compound registration system used by several thousand scientists.
- ❑ Solution: ChemCart Registration, JChem Cartridge, Marvin
- ❑ Project Details
  - Standardized and migrated structures from another chemistry engine to JChem
  - Mapped and migrated legacy data to ChemCart Registration
  - Implemented customer specific business rules
    - ❑ Required/optional fields
    - ❑ Controlled vocabulary picklists
  - Integrated with LDAP
  - Configured user interface
- ❑ Application Key Features
  - Registration of parent compounds
    - ❑ and components
  - Duplicate structure checking
  - Validation of field formats
  - Registration reports

The screenshot displays the 'Compound Registration' window in ChemCart. It features a chemical structure editor on the left showing a tertiary amine derivative (N,N-dimethyl-2-phenylacetamide). The main area contains a data entry form with the following fields:

Corp ID	DS1000007	Project	PROJECT1
Reg. No.	1000007	Therapeutic Target	TARGET1
Batch ID	DS1000007-0-1	Solvent	
Mol Formula	C <sub>11</sub> H <sub>15</sub> N O	Solubility	DMSO
Batch Formula	C <sub>11</sub> H <sub>15</sub> 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

Additional fields include Salt Form (No Salt), Notebook Ref (268-1), Amount Submitted (57 units), Submitter (CCUSER6), Stereochemistry, and Appearance (white solid). A 'Reference' field is filled with 'JACS, 2006', and 'Chemical Name' is 'amine'. The 'Comments' field contains 'reserved for Project 1, keep in cold storage'.

# Case #2: Reagent Inventory

- ❑ Problem: Multi-site pharmaceutical company needed to streamline reagent inventory tracking processes.
- ❑ Solution: ChemCart Reagent Inventory, JChem Cartridge, Marvin
- ❑ Project Details
  - Loaded supplier catalog information into JChem
  - Mapped and migrated legacy bottle data to ChemCart Reagent Inventory
  - Integrated with existing stockroom request application
  - Configured with barcode readers
  - Integrated with LDAP
- ❑ Application Key Features
  - Access supplier and in-house data
  - Structure searching
  - Configurable categories
    - ❑ Compound
    - ❑ Bottle
  - Safety reports
  - Phase 2: link to purchasing

The screenshot displays the 'Reagent Inventory' application window. At the top, there is a menu bar (File, Edit, Form, List, Search, Sort, Cart, Commercial, In-house, Tools, Options, Help) and a toolbar with navigation icons. The main content area is divided into several sections:

- Compound Information:** Compound ID: MFCD00006653, Formula: C<sub>7</sub>H<sub>5</sub>ClO, CAS Number: 98-88-4, Mol. Wt.: 140.568.
- Chemical Structure:** A chemical structure of Benzoyl Chloride is shown.
- Commercial Sources:** A table listing suppliers, catalog numbers, package sizes, units, prices, currencies, purities, and concentrations.
- In-house Sources:** A table listing internal inventory with columns for Barcode, Supplier, Catalog#, Lot No, Orig Amt, Curr Amt, Units, Date Recd, Date Ordered, Owner, Location, and Exp Date.
- Chemical Name:** BENZOYL CHLORIDE
- Supplier Comment:** CORROSIVE; LACHRYMATORY; MOISTURE-SENSITIVE; TOXIC
- Compound Categories:** corrosive
- Bottle Categories:** reserved

At the bottom of the window, there is a status bar with 'Main History Supplier Info Safety' and a 'Delta' icon.

# Case #3: Cloud Implementation

- ❑ Problem: University needed to track experiments, register compounds and associated biological test results, manage compound samples and chemical reagents. No dedicated IT support.
- ❑ Solution: ChemCart Suite (ELN, Reagent Inventory, Registration, Sample Inventory, BioAssay, Browser), JChem Cartridge, Marvin, Amazon Cloud
- ❑ Project Details
  - Installed ChemCart Suite and ChemAxon components in the cloud
  - Migrated structures and biology from local database to enterprise JChem
- ❑ Application Key Features
  - Register from ELN
    - ❑ Record reaction, reagents, products
    - ❑ Track experimental detail
    - ❑ Add documents and images
    - ❑ Submit new compounds / batches

The screenshot displays the ChemCart Suite interface for a reaction record titled "Synthesis of Aspirin". The interface includes a menu bar (File, Edit, Form, List, Search, Sort, Update, DeltaBook, Tools, Options, Help) and a toolbar with navigation icons. The main content area is divided into several sections:

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

The **Reaction** section shows a chemical reaction scheme for the synthesis of aspirin, with a "New Reaction" button. Below the reaction, there are fields for **Temp:** 90 and **Solvent:** NEAT.

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

Structure	Name	Lot#	MF	LR	MW	Act MW	Eq	Theo Mass	Act Mass	mmol	d	Vol
	acid	1-1	C <sub>7</sub> H <sub>6</sub> O <sub>3</sub>	Y	138.12	138.12	1	138.12	2.90	18.10		
	anhydride	21-3-4	C <sub>4</sub> H <sub>6</sub> O <sub>3</sub>	N	102.09	102.09	1	1.85	1.85	18.10		

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

Lot#	ID	Structure	MF	MW	Act MW	Eq	Theo Mass	Act Mass	Purity	mmol	% Yield
17-1			C <sub>9</sub> H <sub>8</sub> O <sub>4</sub>	180.16	180.16	1	3.261	3.000	100	18.05	92.0
			C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	80.05	80.05	1	1.087	0.000			

The **Experimental Procedure** section contains a text box 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 cooled, NaCl was added, and the test tube was cooled in an ice bath. The crystalline product was collected in a Hirsch funnel."

The **Comments** section contains the text: "use in Project 236".

At the bottom, there are tabs for Summary, Reagents, Products, Files, Images, Index, and ChemReg.

# Case #4: External Collaborator

- ❑ Problem: Mid-size US pharmaceutical company needed an informatics system that could be accessed in a limited way by external collaborator located in Europe.
- ❑ Solution: ChemCart Suite (ELN, Reagent Inventory, Registration, Sample Inventory, BioAssay, Browser), JChem Cartridge, Marvin
- ❑ Project Details
  - Migrated data from Excel spreadsheets to enterprise JChem
  - Configurable categories Created collaborator-specific applications
    - ❑ ChemCart application level security
    - ❑ Oracle roles and data views
- ❑ Application Key Features
  - BioAssay
    - ❑ Binding, functional, in vivo, DMPK
    - ❑ Documents
    - ❑ Images
    - ❑ Insert from Excel
    - ❑ Bulk loading from CSV

The screenshot displays the 'Biological Test Results' window in the ChemCart Suite. At the top, there is a menu bar with options like File, Edit, Form, List, Search, Sort, Update, Tools, Options, and Help. Below the menu, there are navigation icons and a status bar indicating 'Hit List: 1 of 1', 'Selected: 1 of 1 (Compounds)', and 'Searching: All'. The main area is divided into several sections:

- Test Results:** A table with columns for Project, Assay Name, Version, Notebook, Page, Cell Line, Result Type, Qualifier, Result Value, Units, Date Created, and Entered By. The data rows are as follows:

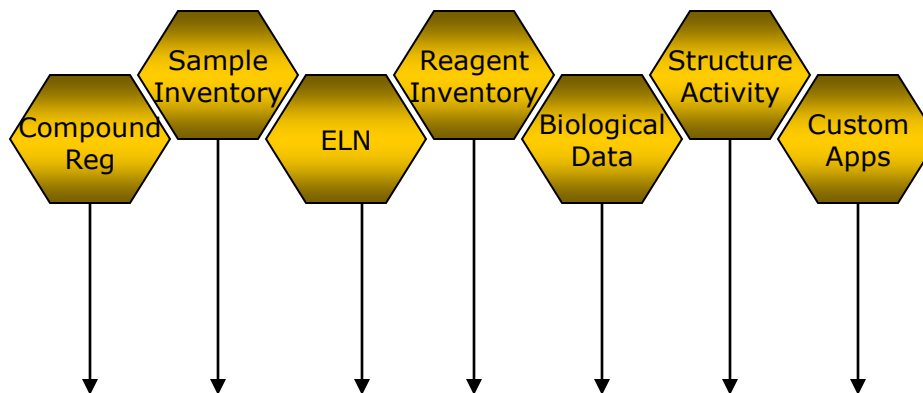
Project	Assay Name	Version	Notebook	Page	Cell Line	Result Type	Qualifier	Result Value	Units	Date Created	Entered By
CytoTox	CT-1	1	15-1	23	AD38	IC50	=	0.5	uM	21-Apr-2008	CHEMCART
CytoTox	CT-2	1	15-2	34	AD38	IC50	=	0.4	uM	21-Apr-2008	CHEMCART
MitoTox	MT-1	1	16-3	65	MTL	EC90	=	1.4	uM	21-Apr-2008	CHEMCART
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

Below the table, there are three panels:

- Result Image:** A circular image showing a cell-based assay with blue fluorescence spots.
- Document Description:** A table listing documents such as 'uv spectra', 'assay protocol', 'reader file', and 'excel data', each with a corresponding document icon.
- Structure:** A chemical structure diagram of a compound, specifically a benzamide derivative.

# ChemCart Informatics Solution

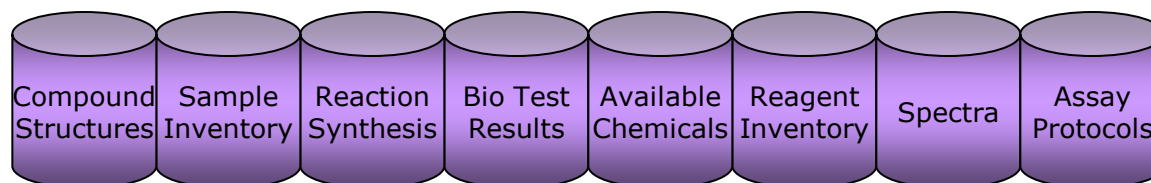
## Web Served Applications



## 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...)
    - 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 pipelining and analysis tools

# Contact Us

---

Michael A. Dippolito  
President  
miked@deltasoftinc.com

Yvonne C. Shimshock, PhD, PMP  
Director, Bus Dev  
yvonne@deltasoftinc.com

DeltaSoft, Inc.  
624 Courtyard Drive  
Hillsborough, NJ 08844  
Tel:908-595-9777

Please stop by the partner table to see more!

