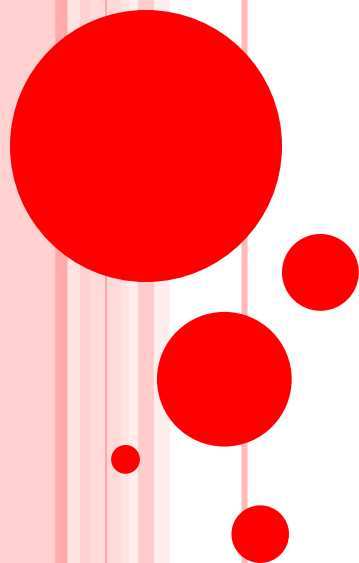


CHEMCART INTEGRATION WITH CHEMAXON

Diana Soto
DeltaSoft, Inc.

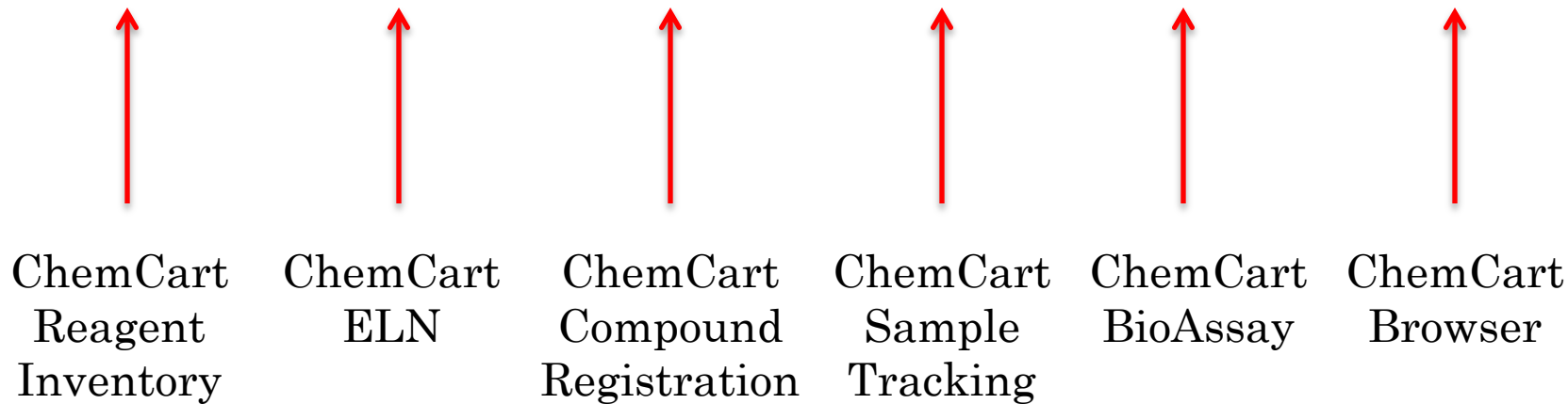




- Specializing in R&D informatics since 1996
- Based in New Jersey, USA
- Commercial Software Applications
 - ChemCart suite of products
- Consulting Services
- ChemAxon Partners since 2005



SUITE OF APPLICATIONS



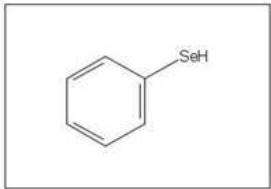
CHEMCART REAGENT INVENTORY

“One Stop Shop”
for commercial
and in-house
reagent sourcing,
inventory and
tracking

File Edit Form List Search Sort Pivot Update Notebook Tools Options Help

Inventory Barcode

Reagent Inventory



Compound ID: MFCD00000001
Formula: C₆ H₅ Se
Mol. Wt.: 157.073 CLogP: 2.29
CAS: 645-96-5

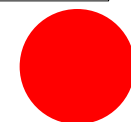
Commercial Sources		Supplier	Catalog #	Quantity	Units	Price	Currency
		Fluka Chemie AG	12595				
		Aldrich Fine Chemicals	375152-1G	1	G	47.7	USD
		ABCR GabH Product List	AB121842-0005.00-GRM	5	G	148	EUR
		ABCR GabH Product List	AB118546-0001.00-GRM	1	G	36.1	EUR
		ABCR GabH Product List	AB118546-0005.00-GRM	5	G	96	EUR
		ABCR GabH Product List	AB121842-0001.00-GRM	1	G	42	EUR
		ABCR GabH Product List	AB118546-0025.00-GRM	25	G	376	EUR
		Aithaca Chemical Corp.	(001425)				
		Alfa Aesar Catalog	A12876-03	1	G	45.3	USD

Chemical Name	Compound Categories	Bottle Categories
BENZENESELENO	Peroxide Foraset	Project A reserve
HYDROSELENOBENZENE		
PHENYLSELENO		
SELENOPHENOL		

In-house Sources

Site	Barcode	Supplier	Catalog#	Curr Amt	Orig Amt	Units	Date Recd	Date Ordered	Owner	Location	Exp Date
Hillsborough	234534	Aldrich Fine Chemicals	375152-250MG	120	250	MG	17-Jun-2011		dianas	Biology Lab 42	
Hillsborough	89223	ABCR GabH Product List	AB118546-0005...	5	5	G	30-Jun-2011	29-Jun-2011	dianas	Biology Lab 42	
Hillsborough	65499654	Fluka Chemie AG	12595			**	30-Jun-2011	29-Jun-2011	cheaca...	Chemistry Lab 34	
Hillsborough	12553	ABCR GabH Product List	AB121842-0001...	1	1	G	11-Jul-2011	11-Jul-2011	cheaca...	Chemistry Lab 34	
Hillsborough	74585	ABCR GabH Product List	AB118546-0025...	25	25	G	11-Jul-2011	11-Jul-2011	dianas	Biology Lab 42	
Hillsborough	96521	ABCR GabH Product List	AB118546-0025...	25	25	G	11-Jul-2011	11-Jul-2011	dianas	Biology Lab 42	
Hillsborough	41258	ABCR GabH Product List	AB118546-0025...	25	25	G	11-Jul-2011	11-Jul-2011	dianas	Biology Lab 42	
Hillsborough	41225	ABCR GabH Product List	AB121842-0005...	5	5	G	11-Jul-2011	11-Jul-2011	dianas	Biology Lab 42	
Hillsborough	223344	ABCR GabH & CO. KG	AB121842-0001...	1	1	G	24-Jun-2011	24-Jun-2011	hank	Main Stock Room	
Hillsborough	4342	ABCR GabH Product List	AB118546-0001...	1	1	G	29-Jun-2011	13-May-2011	dianas	Biology Lab 42	
Hillsborough	234	ABCR GabH Product List	AB118546-0001...	1	1	G	30-Jun-2011	13-May-2011	dianas	Biology Lab 42	
Hillsborough	234A	VWR Scientific	AAAA12876-14	25	25	G	30-Jun-2011	13-May-2011	dianas	Biology Lab 42	
Hillsborough	5	VWR Scientific	AAAA12876-14	25	25	G	30-Jun-2011	13-May-2011	joeche...	Chemistry Lab 34	
Hillsborough	35234	Fluka Chemie AG	12595			**	08-Jul-2011	29-Jun-2011	cheaca...	Chemistry Lab 34	16-Aug-2014
Hillsborough	2346	Fluka Chemie AG	12595			**	30-Jun-2011	29-Jun-2011	cheaca...	Chemistry Lab 34	

Main | History | Supplier Info | Safety | Documents | Product Properties



CHEMCART ELN

Record Experiments

Auto Calculations

Quick pick reagents or text

Query Notebook

Configurable Reporting

Electronic Sign & Witness

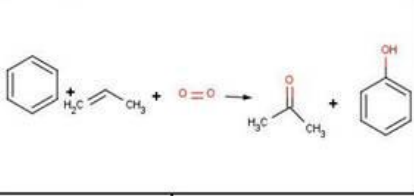
File Edit Form List Search Sort Pivot Update Notebook Tools Options Help

DELTA
SOFT

DeltaBook



Title **Synthesis of Acetone** Scientist Diana Soto Notebook NA10003 Exp#
Date 16-May-2012 Continued from
on

Reaction



Temp 25C Solvent THF


Reagents

Structure	Name	Lot#	MF	LR	MW	Act MW	Eq	Theo Mass	Act Mass	mmol	d	Vol
			C ₃ H ₆	N	42.08	42.08	1	1.08	1.00	23.76		
			O ₂	N	32.00	32.00	1	0.82	2.00	62.50		

Experimental Procedure

To a 500-mL beaker add 50 mL of acetone, then stir in 30 mL of 30% hydrogen peroxide. Place the beaker in a salt-ice bath and cool it to 5° C. After cooling, slowly add 3 mL of 75% sulfuric acid drop by drop with an eye dropper. Stir the mixture continuously while adding the acid, keep the temperature between 5° C to 10° C, stop adding acid if the temperature gets too high. It is very important that you moderate the reaction, high temperatures will lower your yield and cause the formation of the less useful dicyclo isomer. After adding all the acid, continue stirring for 5 minutes. Keep the mixture in the bath for 1 to 3 hours, or even up to 24 hours. After sitting, a white precipitate should have formed. Filter the mixture to collect the crystals, then wash them with 300-500 mL of water. Allow the crystals to dry before using, keep them damp if storing. For increased purity, add the precipitate to ethyl ether and let it dissolve. Place the ethyl ether solution in a separatory funnel and wash by shaking with three portions of cold water. Add the...

Products

Lot#	CORPID	Structure	MF	MW	Act MW	Eq	Theo Mass	Act Mass	Purity	mmol
			C ₆ H ₆ O	94.11				1.000	100	
								2.000	100	

Lit Ref

Comments

Summary Reagents Products Files Images Index Registration

Hit List: 1 of 1 (Reaction) Selected: 1 of 1 (Reaction) Searching: All (Filtered)

CHEMCART REGISTRATION

Compound, Lot, Sample

- Duplicate structure checking
- Set required / optional fields
- Use picklists for controlled vocabulary

Configurable

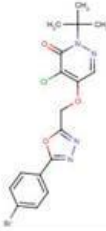
- Fields
- Forms

File Edit Form List Search Sort Pivot Update Tools Options Help

DELTA SOFT

Chemreg

Structure



New Compound New Batch

Batch Count 1

Corp ID	11
Reg. No.	1020631
Batch ID	11-0-1
Mol Formula	C ₁₇ H ₁₆ BrClN ₄ O ₃
Batch Formula	C ₁₇ H ₁₆ BrClN ₄ O ₃
Mol Weight	439.69
MW with Salt	439.69
Exact Mass	438.00
Reg Date	26-Mar-2012
Reg By	JIMB
Alias	

Project	Project-1
Therapeutic Target	
Solvent	
Solubility	
Purity	
Purification Method	
Melting Point (°C)	
Boiling Point (°C)	
Library	LIB1
External Source	
External Reg. #	

Salt Form	No Salt	#
Notebook Ref	D8852	
Amount Submitted	10	Units mg
Submitter	Charles Fleming	
Stereochemistry		
Appearance		

Reference	
Chemical Name	
Comments	

Compound Batch Sample Spectra Components Documents Image Reactions

Hit List: 3 of 20468 (CHEMREG_COMPOUND) Selected: 3 of 20468 (CHEMREG_COMPOUND) Searching: All Filtered

CHEMCART SAMPLE TRACKING

Inventory & Track samples, materials

Track sample workflow

Store documents, images, safety data, properties

Dispense samples

Assay requests

File Edit Form List Search Sort Pivot Update Tools Options Help

DELTA SOFT

Sample Tracking

New Sample

Sample Tracking

Sample ID	1	Container Type	plastic tube	Barcode	100001
Parent Sample ID	12	Original Amount	25	Compound ID	
Sample Type	Formulation	Current Amount	0.25	Batch ID	
Owner	DS	Amount Units	mg	Created By	mike
Sample Date	27-Jul-2011	Tare Weight		Created Date	17-Jul-2011
Expiration Date	30-Jul-2020	Volume	2	Modified By	DIANAS
Source	external	Volume Units	ml	Modified Date	15-Jul-2011
Status	in use	Depletion Limit	0.25		

Sample Name	Saran Resin testing
Comments	

Location	Hillsborough NJ	Location Barcode	1234
----------	-----------------	------------------	------

New

Sample Category	agriculture
-----------------	-------------

New

Type	Name
Vendor Referen...	441252

New

Security Group	1
----------------	---

Sample | Sample Documents | Sample Images | Sample Properties | Sample Substances | Sample Safety | Sample Workflow | Sample Table | Sample Dispense

Hit List: 1 of 103 (SAMPLES) | Selected: 1 of 103 (SAMPLES) | Searching: All (Filtered)

CHEMCART BIOASSAY

Biological Data Entry

- Associate test results with registered samples
- Single point or batch load from Excel, text files, etc.
- Configurable picklists

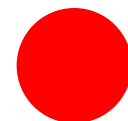
The screenshot displays the CHEMCART BIOASSAY software interface. The main window shows a data entry grid for Plate ID 1, with columns numbered 1 to 12 and rows labeled A to H. The grid contains numerical values, and the cells are color-coded based on their values. To the right of the grid, the DELTASOFT logo is visible, along with the chemical structure of 3-pyridinecarboxylic acid. Below the structure, a table lists sample information: Corp ID (DS-000002), MF (C₆H₅NO₂), MW (123.1094), Hbond Acceptors (3), Hbond Donors (1), and LogP (0.8322).

Plate ID	1	2	3	4	5	6	7	8	9	10	11	12
A		-4.07	-3.43	-3.50	5.17	0.77	4.29	1.04	-6.24	-7.28	-7.29	
B		-2.46	3.80	1.30	7.46	0.90	0.42	3.10	4.16	3.17	5.43	
C		-2.97	-0.08	7.22	2.15	6.99	3.98	1.48	0.58	4.06	-2.93	
D		-2.26	-4.31	4.12	3.62	0.21	5.86	3.72	-6.15	2.40	-0.69	
E		-6.24	-4.08	4.17	6.85	1.84	-0.50	0.15	-2.22	-6.03	2.02	
F		-2.77	-0.14	-5.78	-4.33	-3.05	-2.05	-2.48	-5.33	-0.94	-7.88	
G		-10.81	-7.75	-5.40	-0.26	-6.37	-9.18	-2.15	-4.77	-4.80	-5.21	
H		-7.47	-8.23	-8.52	-6.61	-7.50	-5.20	-11.06	-11.80	-7.78	-8.44	

DELTASOFT

OC(=O)c1ccncc1

Corp ID	DS-000002
MF	C ₆ H ₅ NO ₂
MW	123.1094
Hbond Acceptors	3
Hbond Donors	1
LogP	0.8322



CHEMCART BROWSER

Query by Form for chemical structures, reactions, data, documents, files, and images

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

The screenshot displays the CHEMCART BROWSER software interface. At the top, there is a menu bar with options: File, Edit, Form, List, Search, Sort, Pivot, Update, Tools, Options, Help. Below the menu is a toolbar with various icons. The main window is titled "DELTA SOFT Project Summary Form".

STRUCTURE

CC(=O)N(C)C(=O)c1cccnc1

Table 1: Project Summary

CorpID	NSC	Mol Weight	Formula
DS-000859	34003	208.216	C ₁₀ H ₁₂ N ₂ O ₃

Table 2: LogConc Data

LogConc	Panel	Cell	Panel #	Total #
-4	LNS	NCH-H23	1	1
-4	LNS	NCH-H5	1	1
-4	LNS	A549/AT...	1	1
-4	LNS	EKVX	1	1
-4	LNS	NCH-H3...	1	1
-4	LNS	NCH-H4...	1	1
-4	LNS	HOP-62	1	1
-4	LNS	HOP-92	1	1

Table 3: Date Tested

Date Tested	Point #	Log Conc	Pct Inhib
15-Feb-1988	1	-8	0.016
	2	-6	1.223
	3	-5	10.44
	4	-4.5	25.121
	5	-4.25	35.956
	6	-4	51.271
	7	-3.75	63.006

Table 4: Document List

Document	Description
DataSheet.pdf	PDF doc
Report.xlsx	Excel Doc
ProjectResult...	Project Re...

Table 5: Bar Chart Data

CorpID	Value
DS-000859	200
DS-000778	250
DS-000009	250

Table 6: Scatter Plot Data

Log Conc	Pct Inhib
-8	0.016
-6	1.223
-5	10.44
-4.5	25.121
-4.25	35.956
-4	51.271
-3.75	63.006

Table 7: Pie Chart Data (cell # and nlog)

cell #	nlog
20	1
24	3
23	4
18	8
16	17
19	21
10	26
14	26
13	2

At the bottom of the interface, there are tabs for "Sample Data" and "Structure Grid". The status bar shows: Hit List 1 of 3 (SAMPLEDATA_JCHEM) Selected: 1 of 3 (SAMPLEDATA_JCHEM) Searching: All (Filtered)

DISCOVERY IN A BOX

- Turn key solution
- Preinstalled/preconfigured
- Cloud or Internal hosting
- Provides key software systems to help a lab get up and running quickly
- ChemCart suite of applications
- Powered by ChemAxon Technology



CREATE A CHEMCART APPLICATION, WITH A CHEMAXON BACKEND IN <10 MIN!

The screenshot displays the ChemCart ADMIN web application interface. The main window is titled "ChemCart - CHEMCART_ADMIN - Google Chrome" and shows the "Add Application" dialog box. The dialog box has a tabbed interface with the following tabs: 1. Properties, 2. Sources, 3. Joins, 4. Source Properties, 5. Column Properties, 6. Servers, 7. Users/Roles, 8. Forms, and 9. Picklists. The "Properties" tab is active, showing the following fields:

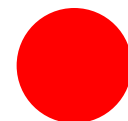
- Application Name:
- Display Name:
- Category:
- Sketcher:
- Renderer:
- Available to Users:
- Buffer Size:
- Database Hint:
- Configuration:

Below these fields is a "Features" table:

Feature	Enabled
Spolfire DecisionSite	<input type="checkbox"/>
ChemCart Administration	<input type="checkbox"/>
Update Mode	<input type="checkbox"/>
Export to ISIS For Excel	<input type="checkbox"/>
Export to Accord For Excel	<input type="checkbox"/>
Jasper Reports	<input type="checkbox"/>
Registrar	<input type="checkbox"/>
Export to JChem For Excel	<input type="checkbox"/>

At the bottom of the dialog box, there is a "Description" text area and a set of buttons: Help, Previous, Next, Validate, Save, and Close.

The background interface shows a sidebar with "Applications" and "Servers Assigned" sections, and a main content area with a table for "Add Application". The table has columns for "App ID" and "Application Name".



Create a ChemCart application with a ChemAxon
back end in ~~<10 min ?!~~

< 5 MIN.

A

CONTACT US!

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908.595.9777

www.deltasoftinc.com

