



DEVELOPMENT AND
DEPLOYMENT OF REAGENT
LOGISTICS SOLUTION USING
JCHEMBASE / CARTRIDGE

“Amazon.com” of Reagents

- Business Case
- Catalogue of available products
- Catalogue query tool
- Shopping cart control
- Enterprise Resource Planning (ERP) integration
- Inventory management of reagents
- Miscellaneous

Business Case to Build

- No tool available to fit our needs and requirements
 - ▣ Cost and time constraints
 - ▣ User familiarity with ACD
 - ▣ Point solutions but no end to end solution e.g. CISPro
- Strong desire for flexibility (uncertainty of ERP)
- In-house skill set (Daylight, ChemAxon)
- Build in phases (Show success early on, see history)

Decision Point Q4 2002



Catalogue of Available Products

- Available Chemical Directory (ACD from Accelrys formerly Symyx, Elsevier, MDL)
 - Longest history and vendor familiarity with MFCD IDs
 - Updated quarterly
 - RCG / CPI format
 - ISIS RAF Access/ Isentris / DiscoveryGate / Reagent Logistics
- Import process (1 wk)
 - Import database export (CPI format)
 - Removing records (except records with audit trail, past orders)
 - Inserting new records and suppliers
 - Execute ETL program (incremental, 400K to >5 M structures)
 - Purchasing business rules (removing and remapping of suppliers)
 - Flagging of highly hazardous materials
 - EAR analysis and flagging
 - Utilizing JChem Base
 - Export from development and import to production



Catalogue Query Tool Requirements

- Simple query tool (using JChem Base / Cartridge)
 - ▣ Structure, substructure and similarity searching
 - ▣ Preferred vendors (controlled by purchasing)
 - ▣ List manager (temp, logic, collaborative, public, etc.)
 - ▣ View results (matrix, list) with flag of items in inventory
- Two level hierarchy (Structure over products)
- “Great” search performance (<3 seconds)
- Fulfill any regulatory and policy guidance
 - ▣ Export Administration Regulation (EAR) clearance (foreign nationals)
 - ▣ Limiting hazardous materials (power role)

Focus on SIMPLICITY



Structure Query Interface

Structure drawing palette

Structure search type

Search filters

Dynamic tips

Results display options

Firefox

CRQ Web: Chemical Request System Database, Export, Import icon | Icon S... +

http://webprd2/crq/cpd/hdis/chem/query.html?apptips=true

Takeda CRQ Web

Admin Search Request List Tools Help

0 items mpustelnik

Search > Chemical

Search Clear

File Edit View Insert Atom Bond Structure Tools Help

Structure drawing palette

Structure search type

Type: Substructure

ID: 1/line

Name:

Cas No:

MW: =

cLogP: =

List: -- None --

Preferred Suppliers

Show Inventory First

Display: Matrix List

Sort By: MW

Tips [add]

- Accessing T-Shop [edit]
To access T-shop, go to <http://tshop> and log in with your Windows username/password. For questions about T-shop please contact Purchasing.
- Speeding Up Search [edit]
To increase search performance indicate a **Mwt** range by using the between operator. Remember to put both lower and upper boundaries.
- Searching SCD [edit]
To also search across the Screening Compounds Directory (SCD), place a checkmark in the box marked **SCD**, enter your search criteria, then click **Search**.
- Structure Searching Features [edit]
When querying by structure, you can now use **atom replacement**, **explicit hydrogens**, and **R-groups**.
- ACD Version [edit]
CRQ Web is running the 2011.2 version of the Available Chemicals

Search filters

Dynamic tips

Results display options



Structure Search Results Interface

List management

Search results

Sorting

Exporting

Pagination

AJAX list handling

Link product detail

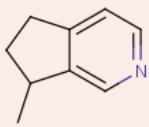
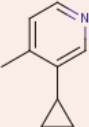
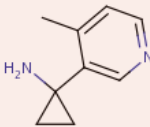
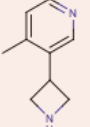
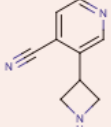
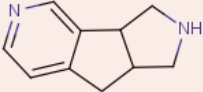
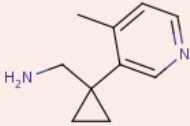
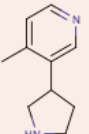
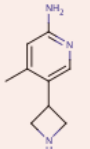
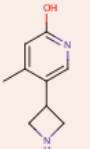
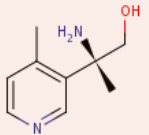
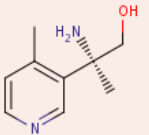
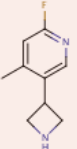
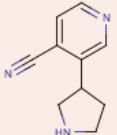
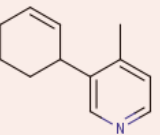
Inventory system link

Search > Chemical > Results

List Options: [TEMP] [check all] [clear all]

Sort By: MW

Result 1 - 50 of 234 [<< | < | > | >>]

1 <input type="checkbox"/> MFCD13175802  45751-96-0 133.2	2 <input type="checkbox"/> MFCD17677322  133.2	3 <input type="checkbox"/> MFCD13189146  148.2	4 <input type="checkbox"/> MFCD17481821  148.2	5 <input type="checkbox"/> MFCD17481772  159.2
6 <input type="checkbox"/> MFCD17215613  160.2	7 <input type="checkbox"/> MFCD13189150  162.2	8 <input type="checkbox"/> MFCD17483903  162.2	9 <input type="checkbox"/> MFCD17482149  163.2	10 <input type="checkbox"/> MFCD17482514  164.2
11 <input type="checkbox"/> MFCD09824066  166.2	12 <input type="checkbox"/> MFCD09824067  166.2	13 <input type="checkbox"/> MFCD17481949  166.2	14 <input type="checkbox"/> MFCD17483855  173.2	15 <input type="checkbox"/> MFCD13152478  173.3

[CIS]




Products Detail Interface

Shopping cart link

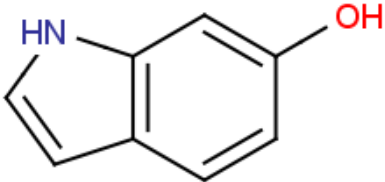
Pagination

Preferred vendor listing

6-HYDROXYINDOLE

2 items 

MFC00152101 Mol. Wt.: 133.1



Chemical: 18 of 2985 [<< | previous | next | >>]

	Supplier	Catalog Id	Quantity	Purity	Cost
<input type="checkbox"/>	ACROS	37901-0010	1 G	98%	88.60 USD
<input type="checkbox"/>	ACROS	37901-0050	5 G	98%	326.90 USD
<input type="checkbox"/>	ACROS	379010010	1 G	97	205.5 USD
<input type="checkbox"/>	ACROS	379010050	5 G	97	811.1 USD
<input checked="" type="checkbox"/>	ALDRICH	18805-1G-F	1 G	99	203.5 USD
<input type="checkbox"/>	COMBI-BLOCKS	IN-0036	1 G	98	60 USD
<input type="checkbox"/>	COMBI-BLOCKS	IN-0036	5 G	97%	240 USD
<input type="checkbox"/>	COMBI-BLOCKS	IN-0036	1 G	97%	60 USD
<input type="checkbox"/>	COMBI-BLOCKS	IN-0036	5 G	98	240 USD
<input type="checkbox"/>	FLUKA	18805-1G-F	1 G	=>99.0%	163.20 USD

[view all]

Note: Indicate amount range for Purchase Order Agreement (POA) items. [view results] | [new query] | [close window]

Add to cart

Link to import into inventory

View non-preferred vendor



Shopping Cart Control



- ❑ Mark and view items in shopping cart
- ❑ Flag items in inventory and pending ordered items
- ❑ Save “abandoned” shopping cart (session listeners)
- ❑ Wish list (persistent shopping cart) for repeated ordering of high turn over reagents
- ❑ “Handoff” to ERP system (Point Purchasing, Microsoft Great Plains) via web service

amazon.com Hello, Matthew Pustelnik. We have [recommendations](#) for you. ([Not Matthew?](#))
Matthew's Amazon.com [Today's Deals](#) [Gifts & Wish Lists](#) [Gift Cards](#) [Your Digital Items](#) [Your Account](#) [Help](#)

Shop All Departments Search All Departments GO [Cart](#) [Wish List](#)

=\$40 Off Instantly Your current subtotal: \$ 60.51
Gift Card savings: - \$ 40.00 [Sign up now](#)
Your cost after savings: \$ 20.51

Shopping Cart for Matthew Pustelnik ([If you're not Matthew Pustelnik, click here.](#))
See more items like those in your Cart **subtotal = \$60.51** Make any changes below? [Update](#)

Shopping Cart Items--To Buy Now		Price:	Qty:
Item added on September 14, 2011 Condition: New In Stock	Data Analysis with Open Source Tools - Philipp K. Janert; Paperback	\$24.60 You Save: \$15.39 (38%)	1
Save for later Delete	Eligible for FREE Super Saver Shipping <input type="checkbox"/> This will be a Gift (Learn more)		
Item added on September 14, 2011 Condition: New In Stock	R in Action - Robert Kabacoff; Paperback	\$35.91 You Save: \$24.08 (40%)	1
Save for later Delete	Eligible for FREE Super Saver Shipping <input type="checkbox"/> This will be a Gift (Learn more)		
Saved Items--To Buy Later		Price:	
Item added on December 14, 2010	Colorbok Learn To Crochet Kit, Hat and Scarf - Colorbok This item is no longer available from the seller you selected.	See other new offers from \$8.28	

READY TO ORDER?
Your order qualifies for free shipping! (Some restrictions apply)
Make sure to select **FREE Super Saver Shipping** as your shipping speed at checkout.
[Proceed to Checkout](#)
[Sign in](#) to turn on 1-Click ordering.
 This will be a Gift [Learn more](#)
Express Checkout with PayPhrase
Matthew's Aggregate Issue [What's this?](#) [Create PayPhrase](#)

Recently Viewed Items
[R in Action](#) by Robert Kabacoff
[The Man Behind the Microchip: Robert Noyce and the Invention of Silicon Valley](#) by Leslie Berlin
[The Chip: How Two Americans Invented the Microchip and Launched a Revolution](#) by T.R. Reid
[View & edit Your Browsing History](#)

Concepts from Amazon.com



Shopping Cart Interface

Project association

Shipping options

Pending request

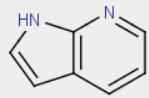
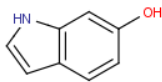
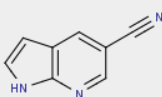
Exists in inventory

Notes to purchasing and supplier

Save cart to Wish list

Sample management delivery option

The screenshot shows a shopping cart interface for chemical reagents. The interface is titled "Request > Shopping Cart" and includes a "Confirm" button in the top right. The main content is organized into three columns: "Structure", "Details", and "Comments".

Structure	Details	Comments
<input checked="" type="checkbox"/> 1. 	Name: 7-AZAINDOLE Supplier: ACROS UOM: 5 G *Quantity: 1 Catalog Id: 105100050 Cost: \$65.5 Purpose: None	
	submitted [2010/02/04] - nscorah, COMBI-BLOCKS, 100 G	
<input checked="" type="checkbox"/> 2. 	Name: 6-HYDROXYINDOLE Supplier: ALDRICH UOM: 1 G *Quantity: 1 Catalog Id: 18805-1G-F Cost: \$203.5 Purpose: None	
	CIS110370	
<input checked="" type="checkbox"/> 3. 	Name: 1H-PYRROLO[2,3-B]PYRIDINE-5-CARBONITRILE Supplier: ALFA UOM: 250 MG *Quantity: 1 Catalog Id: H30237-MD Cost: \$74.6 Purpose: None	

Advanced Options

Wish List: [new] Save & Clear

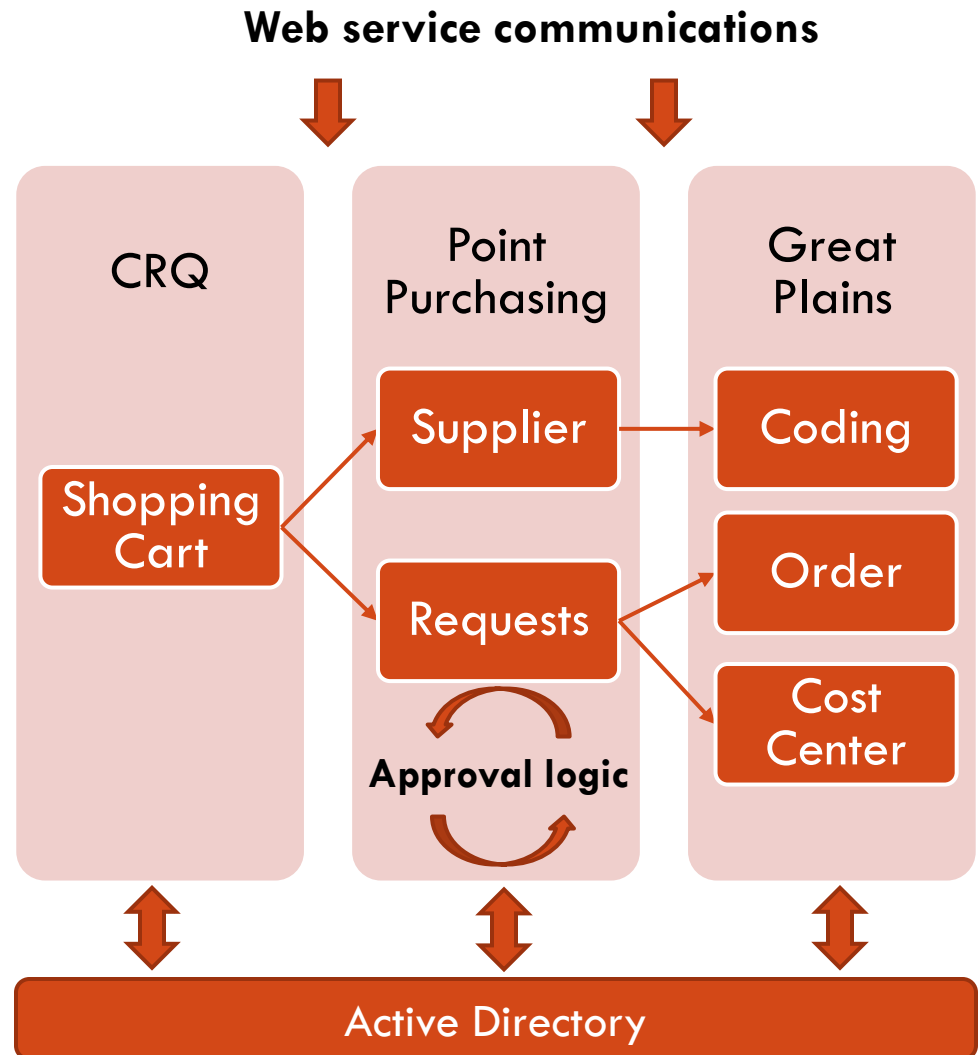
Sample Management [Export to Excel]

The interface also includes control buttons at the bottom: "[check all]", "[clear all]", "[clear cart]", "[hide advanced options]", and "Confirm".



ERP System Integration

- Point Purchasing (mySQL)
 - Purchasing limit with approval (<\$1K/24hr)
 - Approval logic and notification (organization chart in AD)
 - Web service communications
 - Query back to update order status
- Microsoft Great Plains (SQL Server)
 - Cost center definitions
 - Supplier database mapping
 - Web service communications
- Microsoft Active Directory
 - Organization Chart
 - User Information e.g. department



Inventory Management of Reagents

- All containers receive barcode upon delivery to the stockroom
- Containers are checked out / in, disposed, held responsible
- Notification of checked out reagents > 30 days
- Inventory and catalogue system are update asynchronously (15 min.)
- Inventory system operations
 - ▣ Self service reagent check out from the shelves / bins
 - ▣ Reagents are dropped off into a return bin
 - ▣ Location varies based upon reactive groups (streamline returning)
 - ▣ One chemistry intern manages stockroom (inventory baseline 1 year, barcode, etc.)
- Integration into compound registration system (fragment screen)
- Query, results, shopping cart similar to catalogue system

Reagent Lifecycle



Inventory

- Ordered
- Received
- Chemist

Procurement

- Barcoding
- Check In/Out
- Manager

- Reaction
- Disposed
- Chemist

Lab



Inventory Management Components

□ Hardware

- ▣ Industrial rolling shelves
- ▣ Intermec barcode scanner and stand
- ▣ Two computer workstations
- ▣ Intermec thermal transfer barcode printer

□ Locations

- ▣ Marked with alpha numeric code and barcode
- ▣ Any chemical container e.g. bin, shelf, hood

□ Software

- ▣ User interface tailored toward office and lab operations
- ▣ Java web based application build upon JChem Base / Cartridge

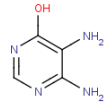



Miscellaneous

- ❑ Hazardous Reagents
 - ❑ List managed by chemists
 - ❑ Chemist is warned when order is placed and email notification to supervisor
- ❑ JChem Base / Cartridge
 - ❑ Marvin View / Sketch (chemical display and input)
 - ❑ Simplified chemical registration system
 - ❑ Updating through admin pages
- ❑ Purchasing
 - ❑ Disabling products (discontinuation)
 - ❑ Remapping suppliers
 - ❑ Setting preferred suppliers
- ❑ Export Administration Regulation (EAR)
 - ❑ All chemicals analyzed and flagged for EAR warnings
 - ❑ EAR flagged reagents do not show up for foreign nationals

4,5-DIAMINO-6-HYDROXYPYRIMIDINE SULFATE
0 items

Chemical: 5 of 89 [<< | previous | next | >>]

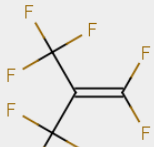
MFCID00012788	Mol. Wt.: 224.2	Supplier	Catalog Id	Quantity	Purity	Cost	Status
		<input type="checkbox"/>	ADVTECHIND 1045178	5 G	99%	248 USD	
		<input type="checkbox"/>	ADVTECHIND 1048298	5 G		179.55 USD	
		<input type="checkbox"/>	ADVTECHIND 1048298	5 G		179.55 USD	
		<input type="checkbox"/>	ADVTECHIND 1048324	5 G		179.55 USD	
		<input type="checkbox"/>	ADVTECHIND 1048324	5 G		179.55 USD	
		<input type="checkbox"/>	AOK-CHEM K9664				
		<input type="checkbox"/>	APAC 551520	1 G		980 USD	
		<input type="checkbox"/>	APIN 23770D			POA USD	
		<input type="checkbox"/>	APIN 23770D			POA USD	
		<input type="checkbox"/>	APIN 23770D			POA USD	
		<input type="checkbox"/>	APIN 23770D			POA USD	
		<input type="checkbox"/>	APIN 23770D			POA USD	
		<input type="checkbox"/>	APIN 23770D			POA USD	
		<input type="checkbox"/>	APIN 23770D			POA USD	
		<input type="checkbox"/>	APIN 23770D			POA USD	
		<input type="checkbox"/>	ARKPHARMINC AK-35480		95		
		<input type="checkbox"/>	ART-CHEM-BB ACB000949				

Export Administration Regulation (EAR)

Search listing by category

Admin > EAR > Search

[A B C D E F G H I J K L M N O P Q R S T U V W X Y Z] 1 - 12 of 12 [<< | < | > | >>]

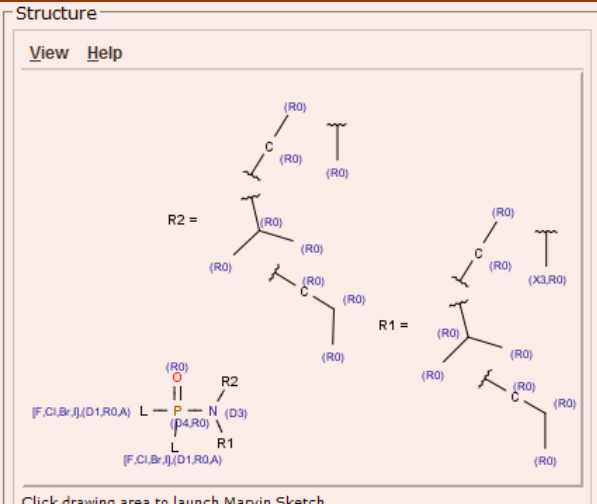
Code	*Name	Category	Type	Status	Date (YYYY/MM/DD)
1. a.1.a	1,1,3,3,3-Pentafluoro-2-(trifluoromethyl)-1-propene 	Weapons	Exact	Enabled	2007/08/09

Admin > EAR > [500063] > Edit

Update Reset

Structure

View Help



Click drawing area to launch Marvin Sketch

Fields

*Code: a.2.b

*Name: N,N-Dialkyl phosphoramidic dihalides

*Category: Weapons

*Type: Substructure

Search: [#6]N([#6])P([F,Cl,Br,I])([F,Cl,Br,I])=O

CAS No.: none

Notes

ECCN 1C355

Update Delete Reset

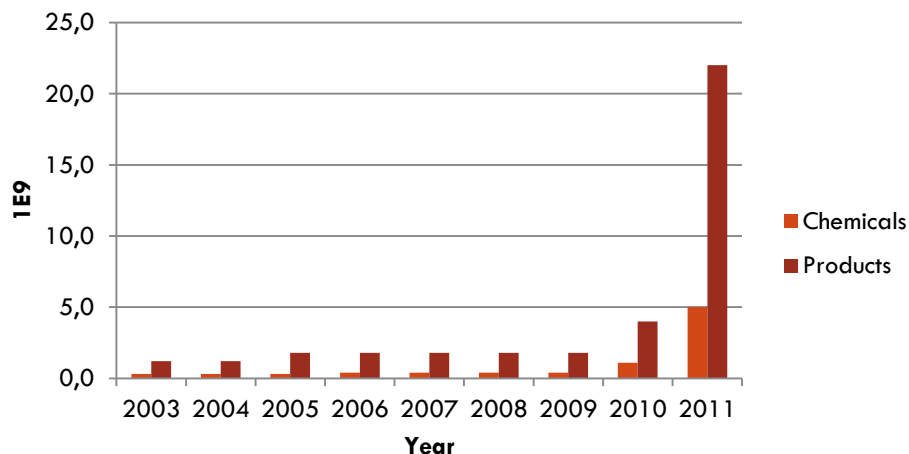
Complex searching



History

- 2003
 - JChem Base middle tier, Daylight Oracle Cartridge
 - >300K chemicals, >1.2 M products
 - Auto-filled Excel export of purchasing request form (No integration into ERP)
- 2004
 - Upgrade to ChemAxon JChem Cartridge
 - Included Screening Compound Directory (SCD)
- 2006
 - Integrated into ERP system
 - >400K chemicals, > 1.8 M products
- 2007
 - Implemented spending limit cap without approval
- 2008
 - Redesigned reagent stockroom
 - Modified stockroom operations
- 2009
 - Added second stockroom
- 2010
 - Switched to CPI from RCG format of ACD
 - > 1.1 M chemicals, > 4 M products
- 2011
 - > 4.2 M chemicals, > 22 M products

ACD Chemicals & Products



Summary

- Refreshed catalogue > 24 times in 8 years of operation
- > 20K orders placed
- > 35K reagents in inventory
- 4 Major upgrades to CIS & CRQ Web (>30 minor updates)
- 4 application server upgrades including a change in vendor (Oracle Weblogic to Apache Tomcat)
- 3 database upgrades (8i, 9i, 10g)
- Supporting 2 stockrooms across 2 buildings
- ACD catalogue growth to >5 M chemicals and >22 M products
- Foundation architecture
 - ▣ J2EE Servlets (WebMacro, AJAX, AppManager)
 - ▣ ChemAxon JChem Base / Cartridge / Marvin
 - ▣ Apache, Tomcat cluster and Oracle



Future Customization & Consideration

- Continued performance enhancement (mixed fingerprint and keys based searching)
- Redesign of user interface e.g. extJS, Dojotoolkit
- Integration to ELN
- Cloud solutions
 - ▣ Alternative content providers e.g. eMolecules
 - ▣ Platform as a Service (PAS)

Acknowledgements

- Christine Clayton – Analyst
- Tamaki Hiratsuka – Analyst
- Yasushi Okubo – Software Engineer
- Steve Wilkens – Computational Scientist
- Erick Co – Chemist
- Jason Brown – Chemist
- Sheldon Cao – Chemist
- Charlie Xiao – Chemist
- Support Staff – ChemAxon



Thank You!