



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

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

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

Takeda CRQ Web

Admin Search Request List Tools Help

0 items mpustelnik

Search > Chemical

File Edit View Insert Atom Bond Structure Tools Help

Search Clear

Search Clear

Dynamic tips

- 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 Directory (ACD).



Results display options

# Structure Search Results Interface

List management

Search results

Sorting

Exporting

Pagination

AJAX list handling

Link product detail

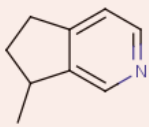
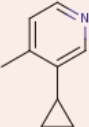
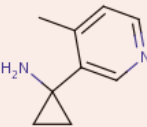
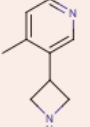
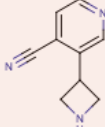
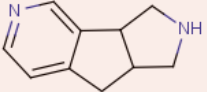
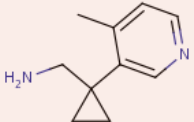
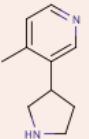
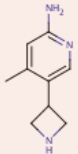
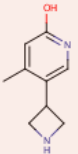
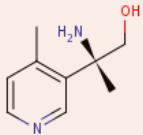
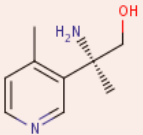
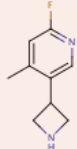
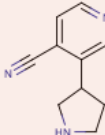
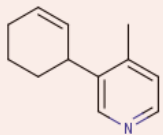
Inventory system link

Search > Chemical > Results

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

Sort By: MW [Export] [Refresh]

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

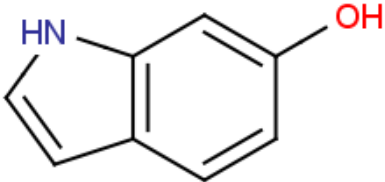
Pagination

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	<b>Data Analysis with Open Source Tools</b> - Philipp K. Janert; <b>Paperback</b>	<b>\$24.60</b> You Save: \$15.39 (38%)	1
<a href="#">Save for later</a> <a href="#">Delete</a>	Eligible for FREE Super Saver Shipping <input type="checkbox"/> <b>This will be a Gift</b> <a href="#">(Learn more)</a>		
Item added on September 14, 2011 Condition: New In Stock	<b>R in Action</b> - Robert Kabacoff; <b>Paperback</b>	<b>\$35.91</b> You Save: \$24.08 (40%)	1
<a href="#">Save for later</a> <a href="#">Delete</a>	Eligible for FREE Super Saver Shipping <input type="checkbox"/> <b>This will be a Gift</b> <a href="#">(Learn more)</a>		

**Saved Items--To Buy Later** **Price:**

Item added on December 14, 2010	<b>Colorbok Learn To Crochet Kit, Hat and Scarf</b> - Colorbok	See other <a href="#">new offers</a> from \$8.28
	This item is no longer available from the seller you selected.	

**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

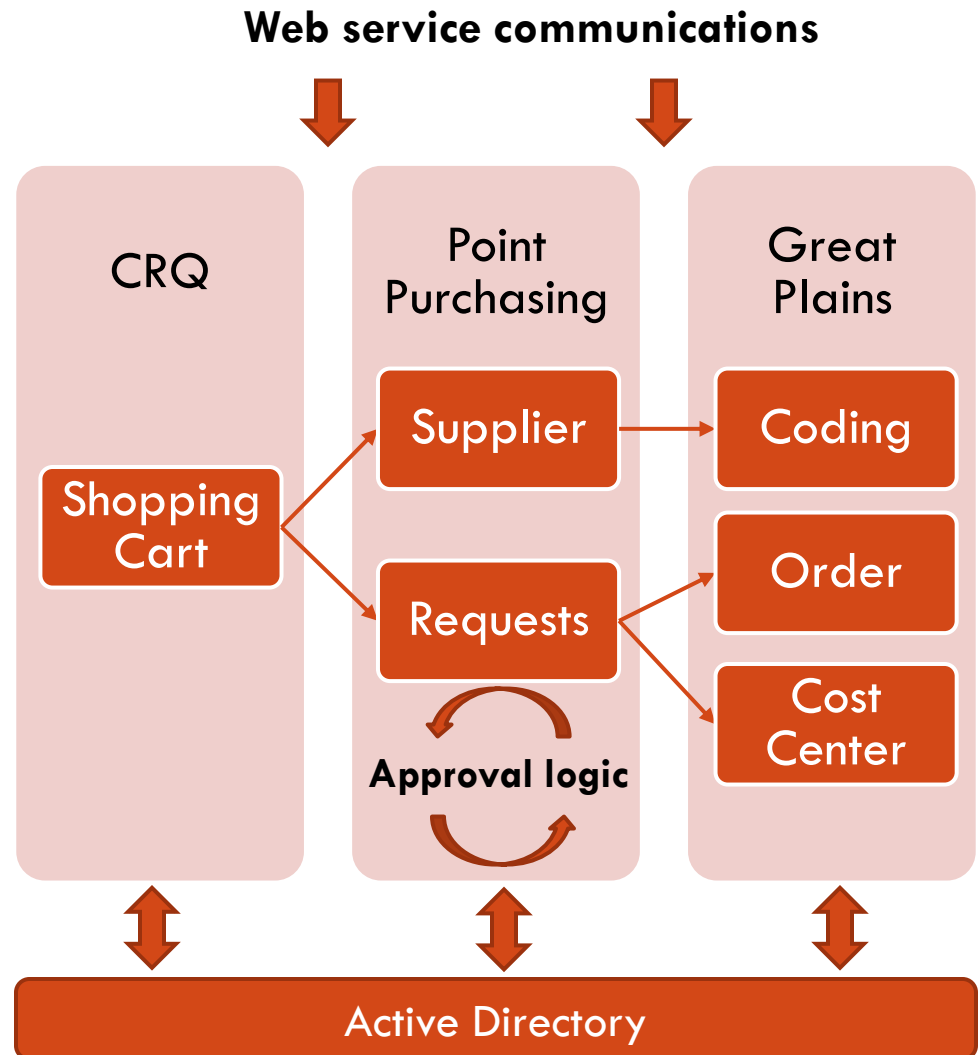
The screenshot shows a shopping cart interface titled "Request > Shopping Cart" with a "Confirm" button in the top right. The interface is divided into several sections:

- Project Association:** A dropdown menu labeled "\*Project:" with "-- Select --" is highlighted by a red box and an arrow from the "Project association" label.
- Request Name:** A text field containing "7-AZAINDOLE" is located next to the project dropdown.
- Shipping Options:** A dropdown menu labeled "\*Shipping Options:" with "Overnight" selected is highlighted by a red box and an arrow from the "Shipping options" label.
- Table of Items:** The main area contains a table with three rows, each representing a chemical compound. Each row has a checkbox, a structure image, a "Details" column, and a "Comments" column.
  - Item 1:** 7-AZAINDOLE. Supplier: ACROS, Catalog Id: 105100050, UOM: 5 G, Cost: \$65.5, Quantity: 1, Purpose: None. A red box highlights the text "submitted [ 2010/02/04 ] - nscorah, COMBI-BLOCKS, 100 G" in the comments column, with an arrow from the "Pending request" label.
  - Item 2:** 6-HYDROXYINDOLE. Supplier: ALDRICH, Catalog Id: 18805-1G-F, UOM: 1 G, Cost: \$203.5, Quantity: 1, Purpose: None. A red box highlights the text "CIS110370" in the comments column, with an arrow from the "Exists in inventory" label.
  - Item 3:** 1H-PYRROLO[2,3-B]PYRIDINE-5-CARBONITRILE. Supplier: ALFA, Catalog Id: H30237-MD, UOM: 250 MG, Cost: \$74.6, Quantity: 1, Purpose: None. A red box highlights the empty comments field, with an arrow from the "Notes to purchasing and supplier" label.
- Advanced Options:** At the bottom, there is a section titled "Advanced Options" containing:
  - A dropdown menu labeled "Wish List:" with "[ new ]" selected, highlighted by a red box and an arrow from the "Save cart to Wish list" label. Next to it is a "Save & Clear" button.
  - A checkbox labeled "Sample Management" highlighted by a red box and an arrow from the "Sample management delivery option" label.
  - A button labeled "[ Export to Excel ]".

At the bottom left, the Takeda logo is visible.

# 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

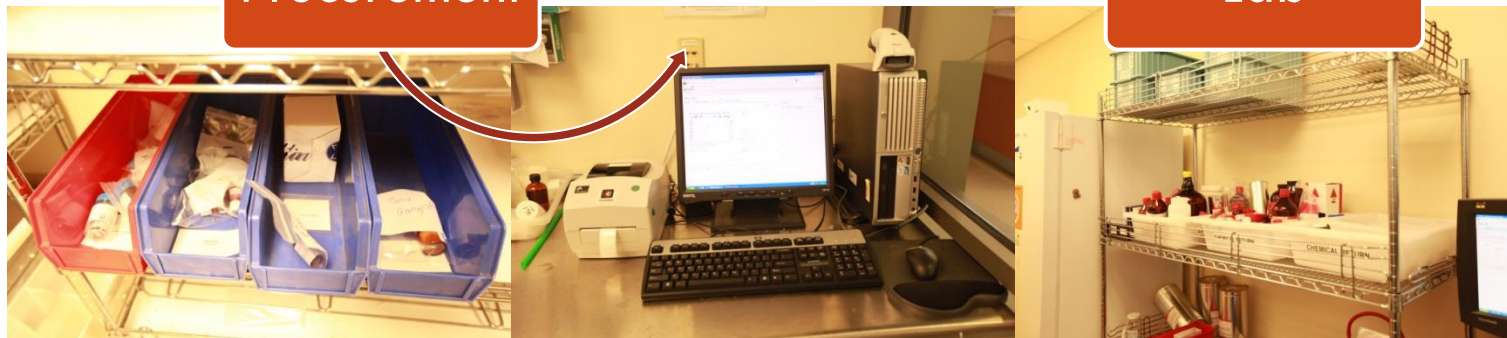
- Ordered
- Received
- Chemist

## 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 | >> ]

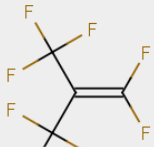
MFC00012788	Mol. Wt.: 224.2	Supplier	Catalog Id	Quantity	Purity	Cost	Status
<input type="checkbox"/>		ADVTECHIND	1045178	5 G	99%	248 USD	✖
<input type="checkbox"/>		ADVTECHIND	1048298	5 G		179.55 USD	✖
<input type="checkbox"/>		ADVTECHIND	1048298	5 G		179.55 USD	✖
<input type="checkbox"/>		ADVTECHIND	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	✔
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<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 [ << | < | > | >> ]

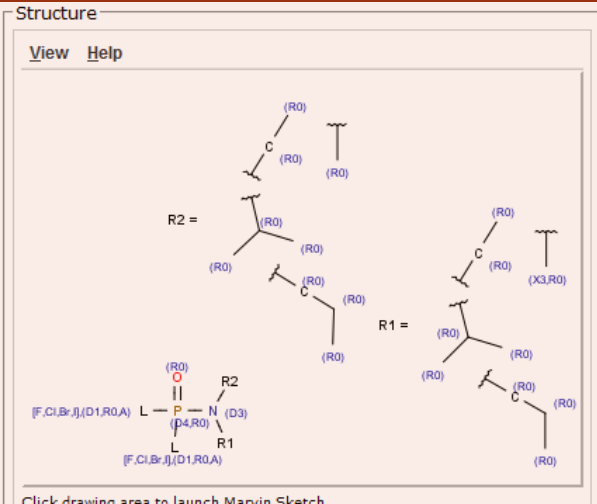
Code	*Name	Category	Type	Status	Date (YYYY/MM/DD)
1. a.1.a	1,1,3,3,3-Pentafluoro-2-(trifluoromethyl)-1-propene 	Weapons	Exact	Enabled	2007/08/09

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

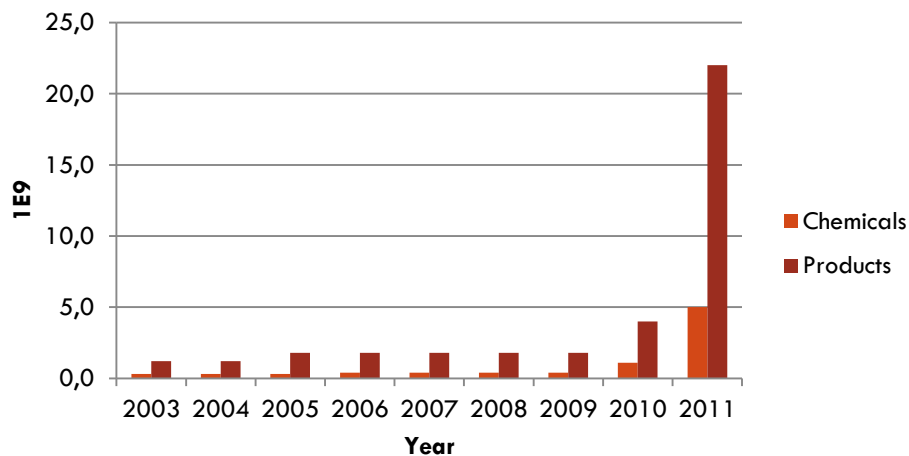




# History

- 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)

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Thank You!