DeltaSoft's ChemCart

An integrated suite of applications that leverage ChemAxon components

ChemAxon 2011 US UGM
September 27, 28– San Diego, CA

Delta Soft

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

accelrys®

CambridgeSoft®
Life Science Enterprise Solutions

ChemAxon

Daylight
Chemical Information Systems, Inc.

IBM Business Partner

InforSense

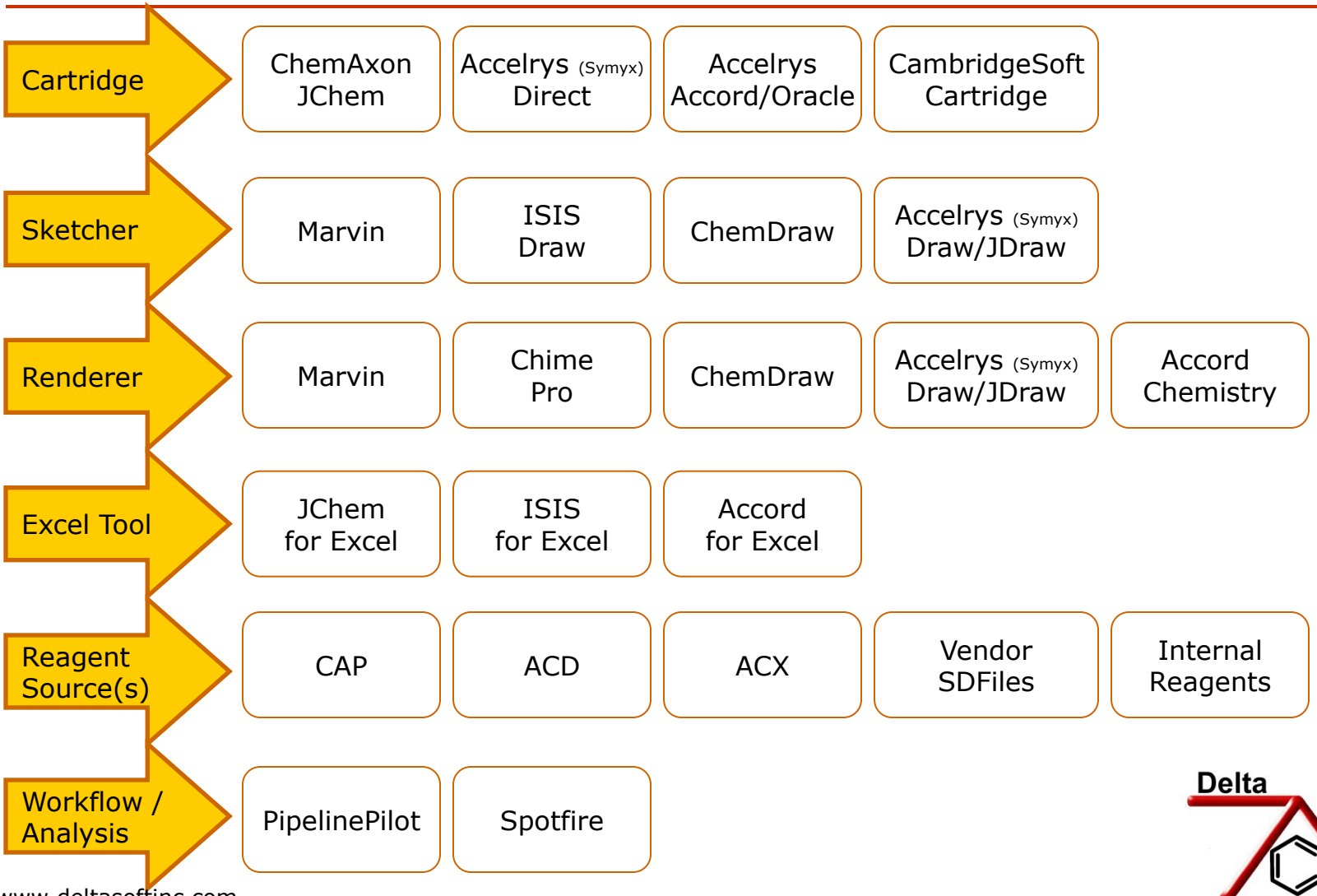
ORACLE PARTNER

Spotfire®

Symyx®

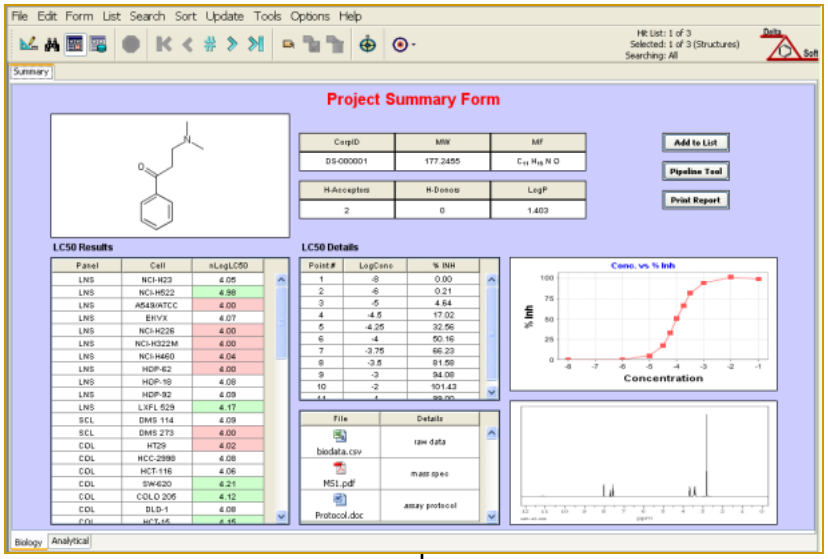
Delta Soft

Component Approach – Choice!



Delta Soft

ChemCart



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

ChemCart Server

Chemistry Cartridge (molecules & reactions)

Text, Numeric, Images Documents, Files

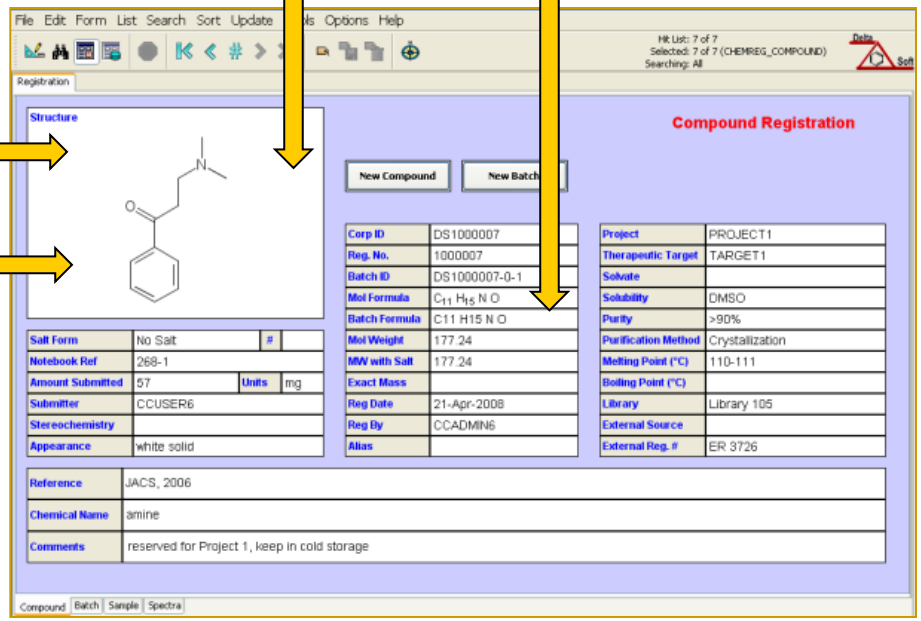
Integration with ChemAxon

ChemAxon JChem Cartridge for Structure Storage/Searching

ChemAxon JChem Cartridge for Structure Calculations (MW, MF)

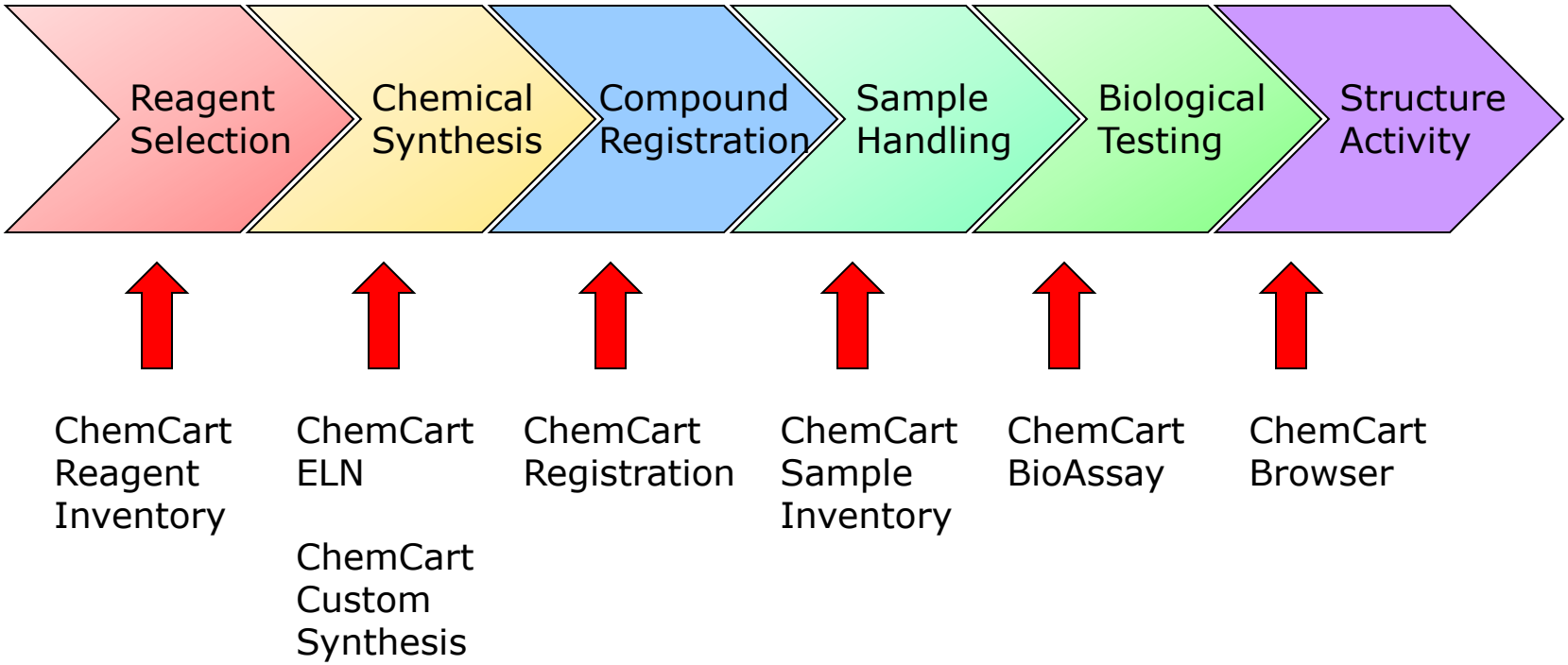
ChemAxon Marvin for Structure Sketching/Rendering

ChemAxon Structure Standardizer / Structure Checker



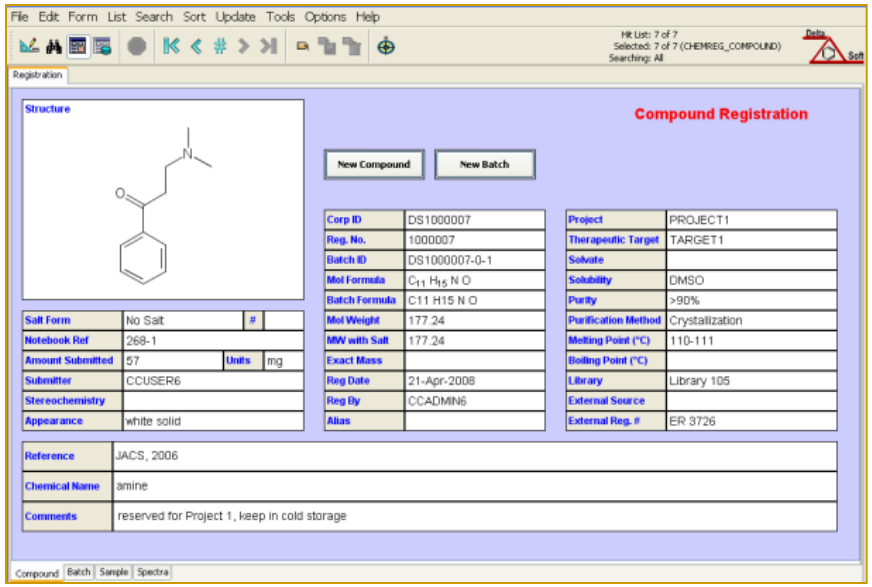
- Partnered since 2006
- Fully integrated, supporting latest version
- Joint customers using ELN, Registration, BioAssay, Inventory, Search & Browse, Inventory in production

ChemCart Applications



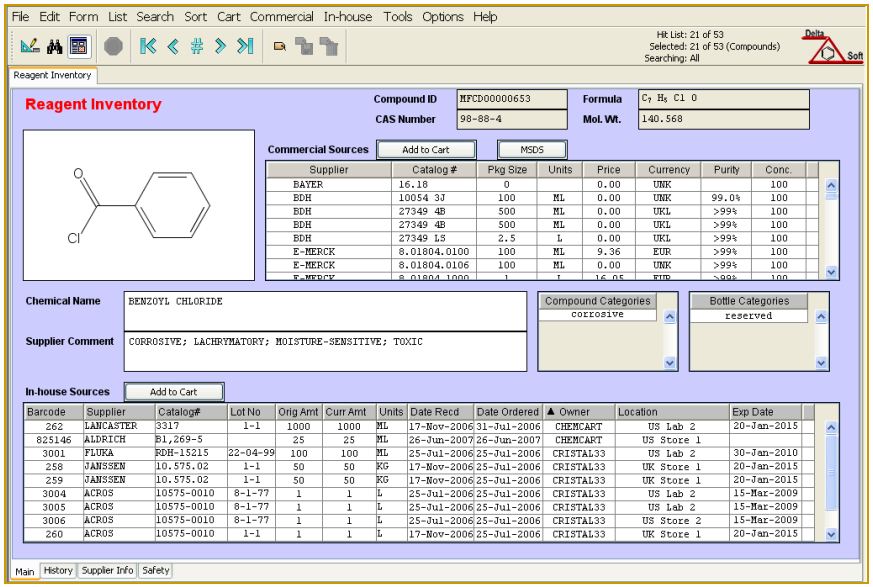
Case #1: Registration

- 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



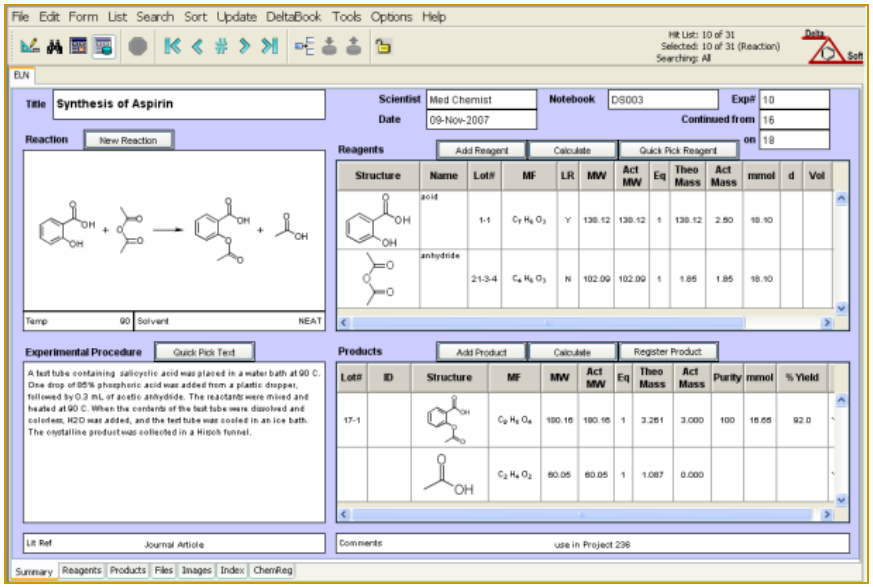
Case #2: Reagent Inventory

- 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



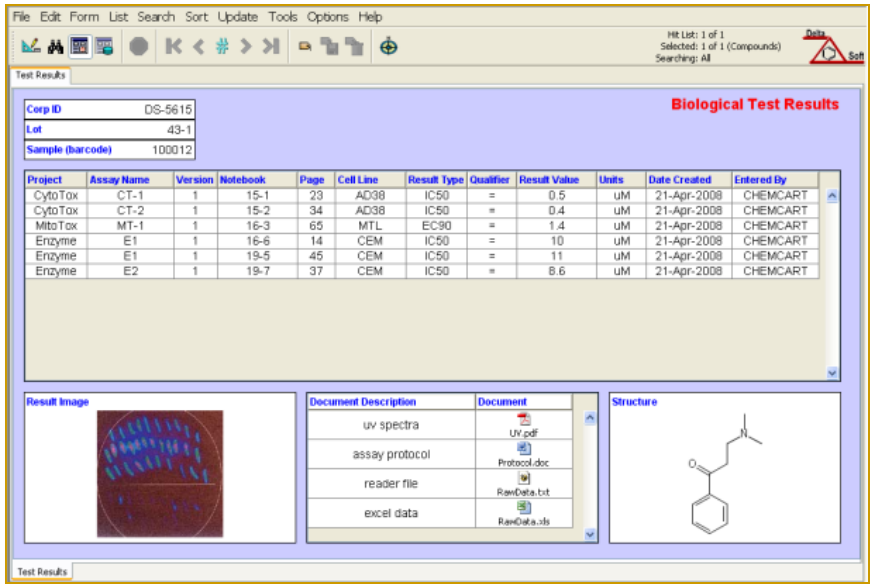
Case #3: Cloud Implementation

- 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



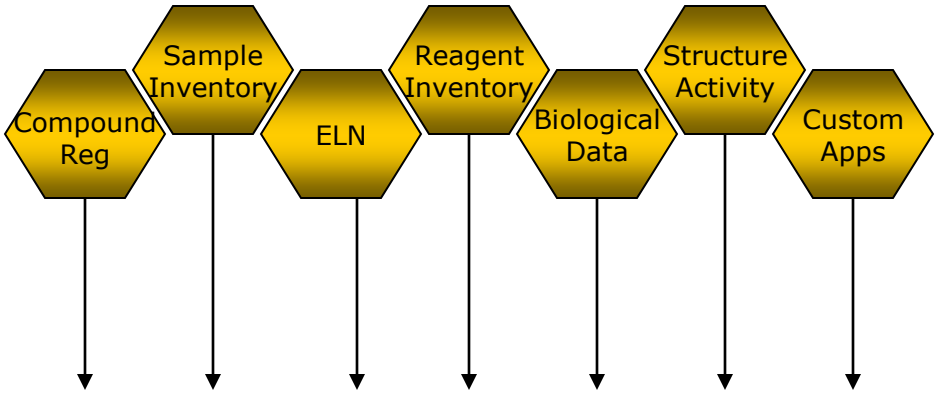
Case #4: External Collaborator

- 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



ChemCart Informatics Solution

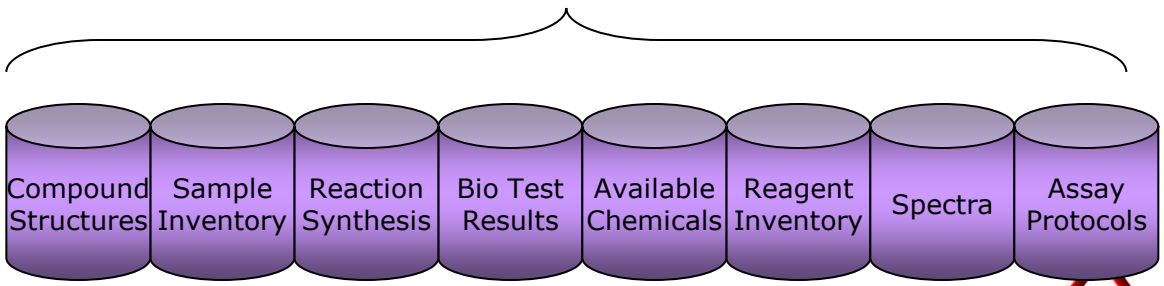
Web Served Applications



Middle Tier

ChemCart Server

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

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Please stop by the partner table to see more!