DeltaSoft's ChemCart

An integrated suite of applications using ChemAxon components

ChemAxon 2010 European UGM
May 19, 20 – Budapest, Hungary

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

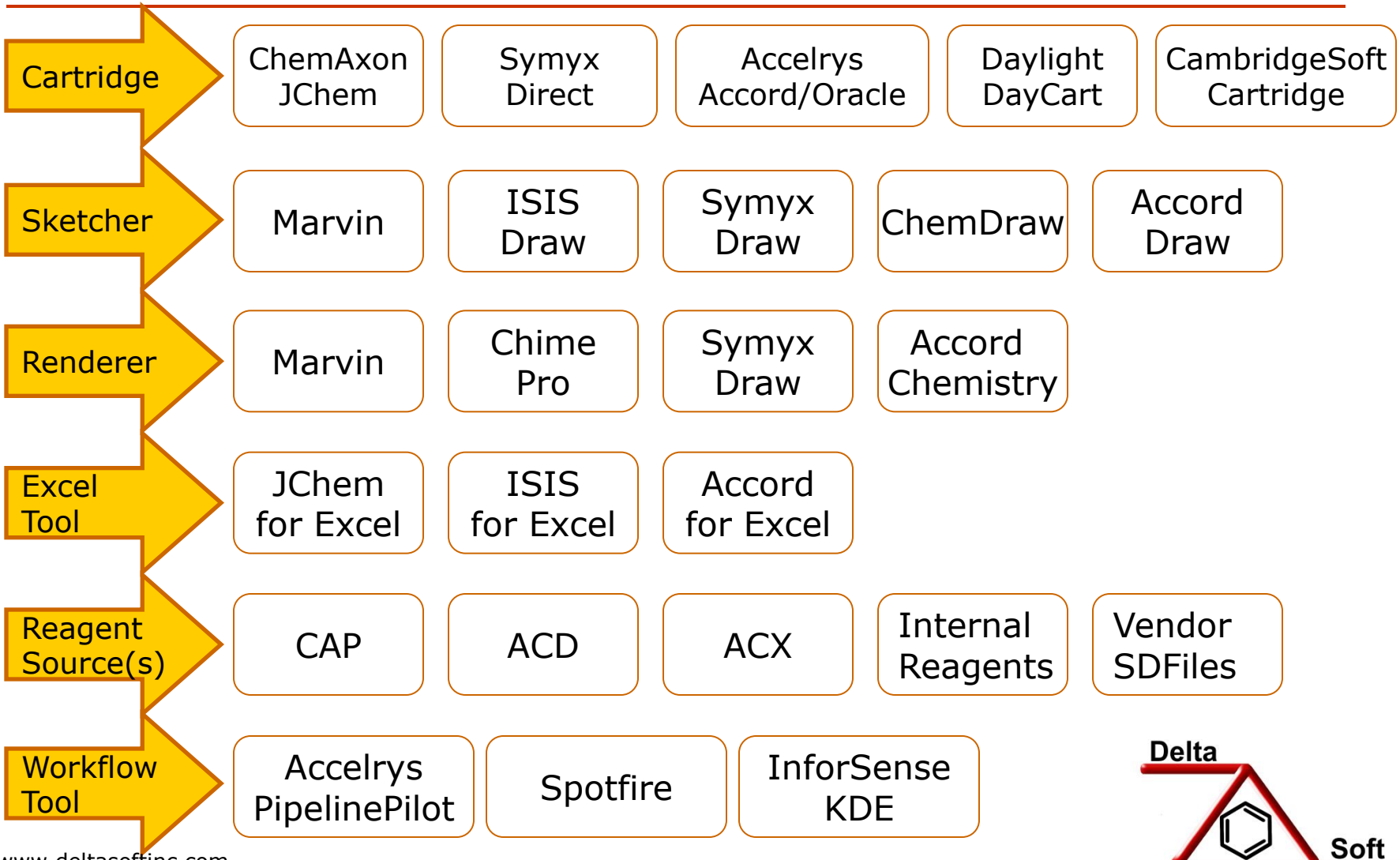
accelrys® CambridgeSoft® Life Science Enterprise Solutions ChemAxon

Daylight Chemical Information Systems, Inc. IBM Business Partner InforSense

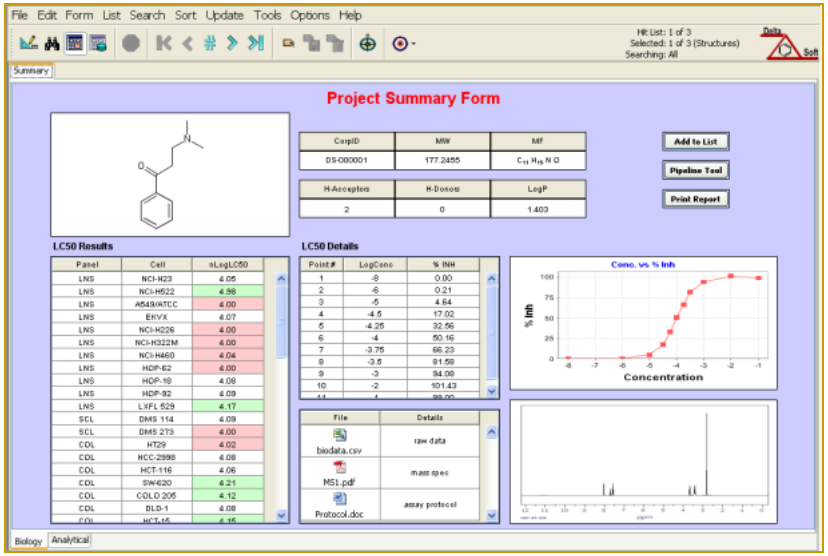
ORACLE PARTNER Spotfire® Symyx®

Delta Soft

Component Approach – Choice!



ChemCart



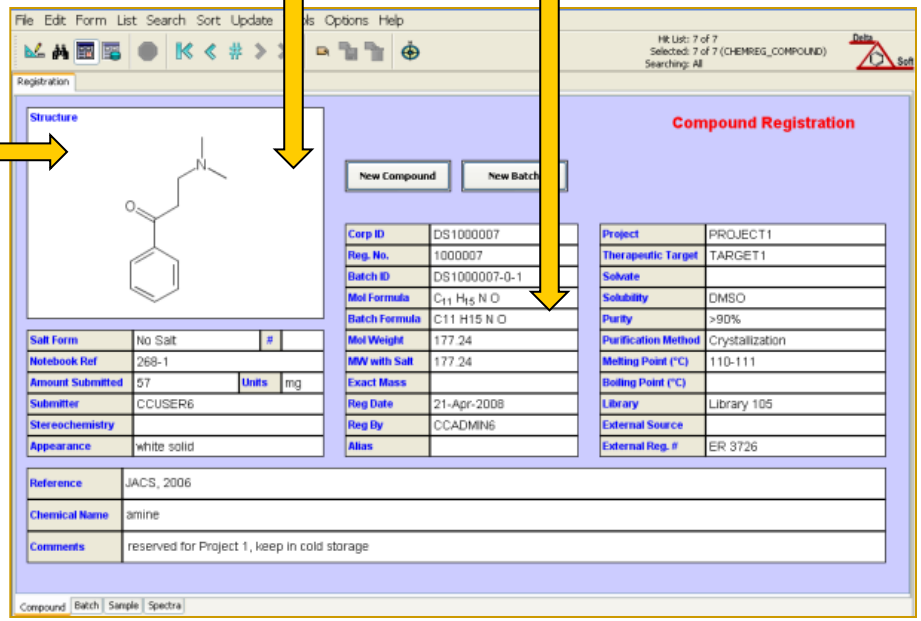
Dynamic web forms interface to research information, including structures/reactions, data, images, documents & files

Integration with ChemAxon

ChemAxon JChem Cartridge for Structure Storage/Searching

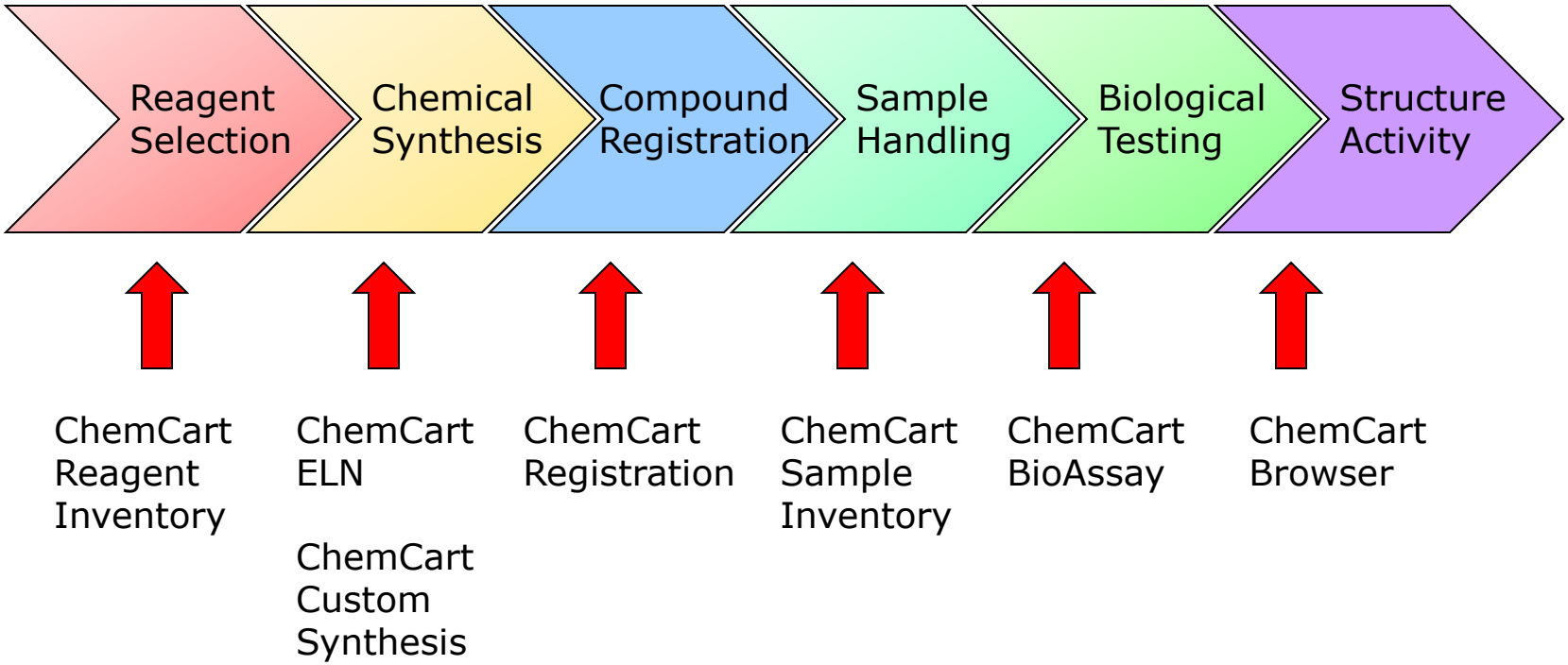
ChemAxon JChem Cartridge for Structure Calculations (MW, MF)

ChemAxon Marvin for Structure Sketching/Rendering



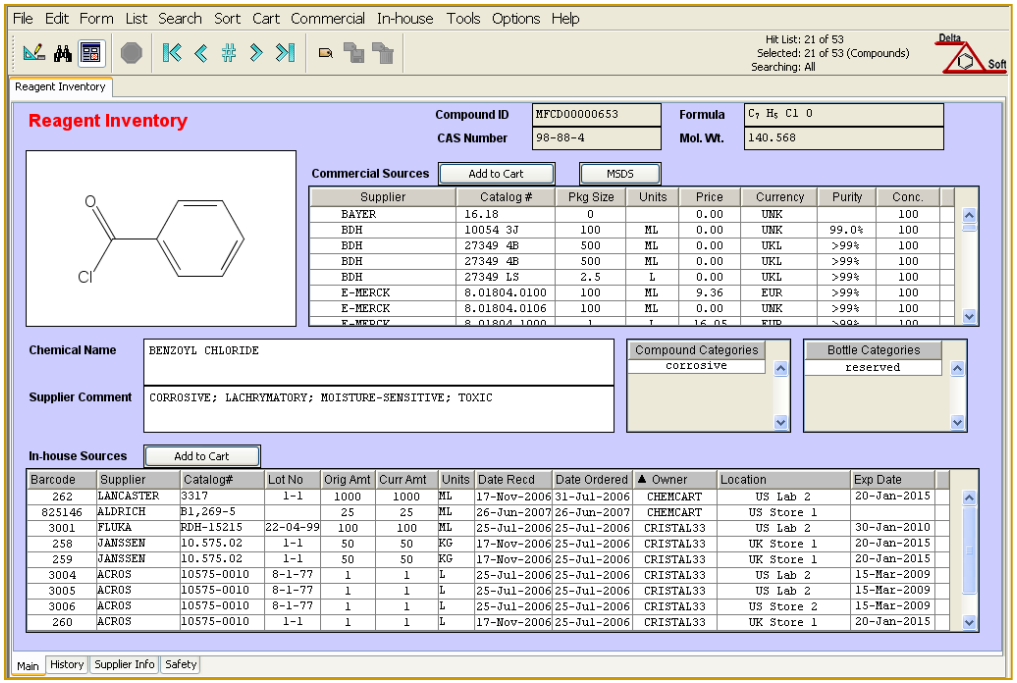
- Partnered since 2006
- Fully integrated, supporting latest version
- Joint customers using Registration, Search & Browse, Inventory in production

ChemCart Applications



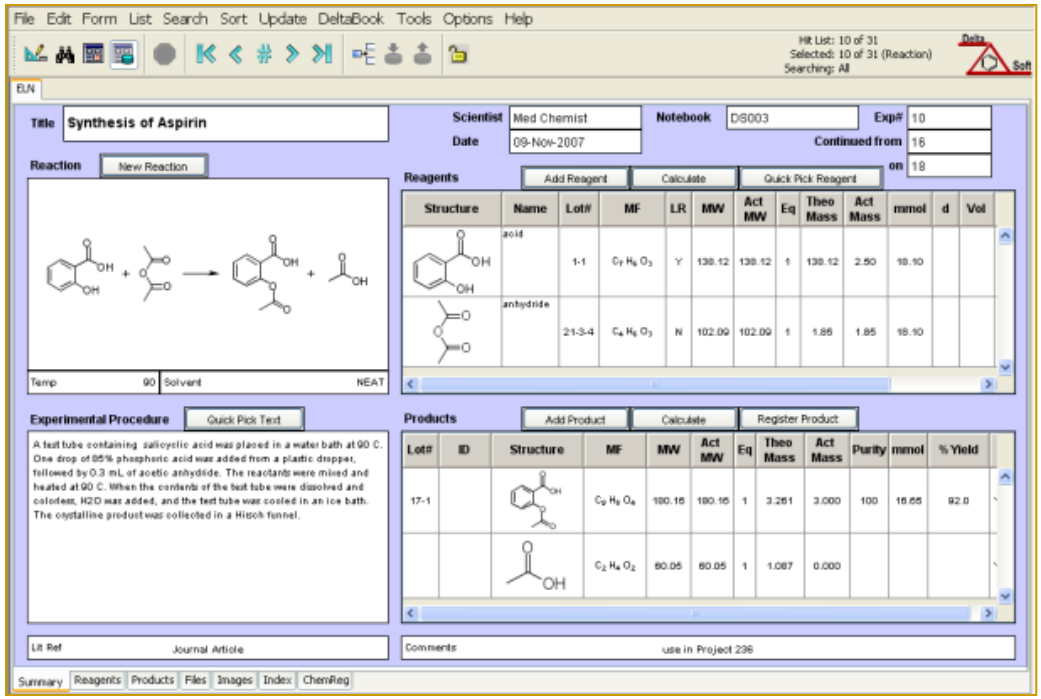
ChemCart Reagent Inventory

- "One stop shop" for Commercial and In-house reagent sourcing
  - Vendor, pricing, supplier info
  - Location, amount, barcode info
  - Compound & bottle categories
  - Health & Safety
- Shopping Cart
  - Internal
  - Supplier
- Track bottle history from cradle to grave
- Link to Purchasing



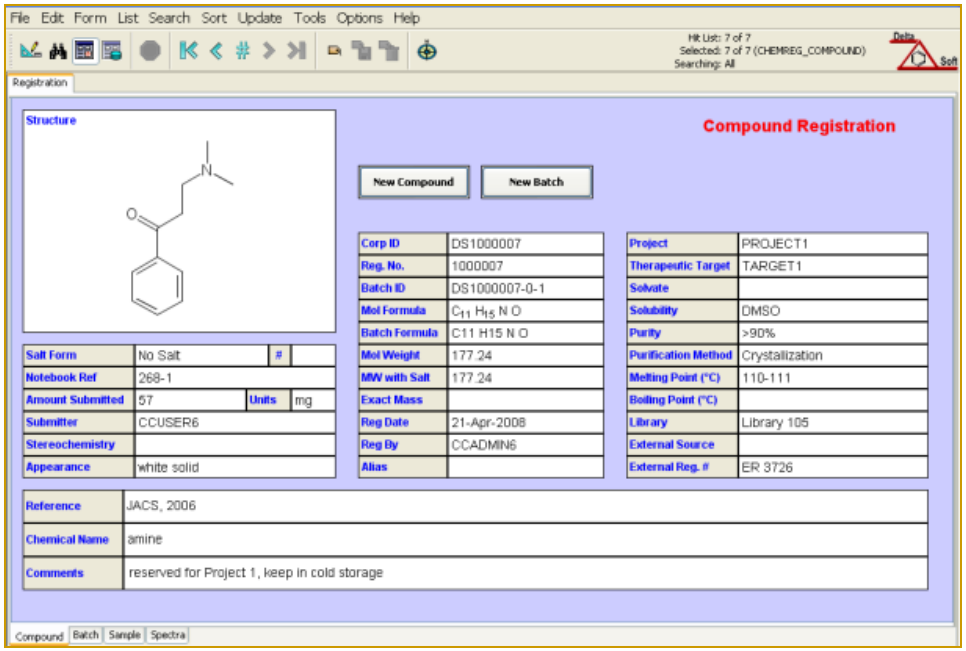
ChemCart ELN

- Record experiments
  - Reaction, reagents, products,
  - Text, images, documents & files
- Auto calculations
  - limiting reagent
  - mmol, vol, theo yield, % yield
- Quick Pick reagents or text
- Duplicate pages
- Lock experiment & audit changes
- Print notebook pages
- Query own ELN or all
- Link to Registration, Inventory



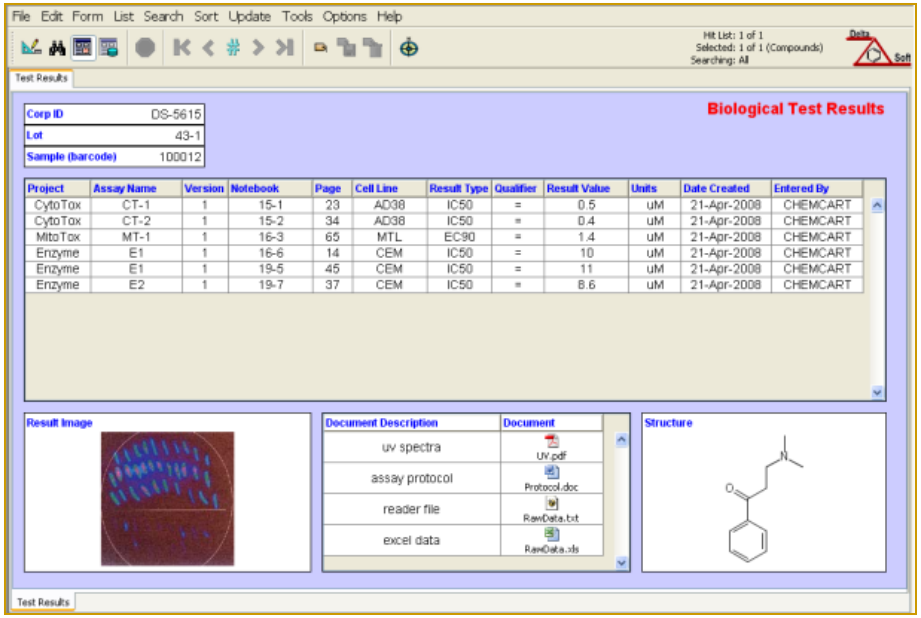
ChemCart Registration

- Compound, Lot, Sample
  - Duplicate structure checking
  - Set required / optional fields
  - Use picklists for controlled vocabulary
- Configurable
  - Fields
  - Forms
- Sample Inventory
  - Track sample location
  - Sample request



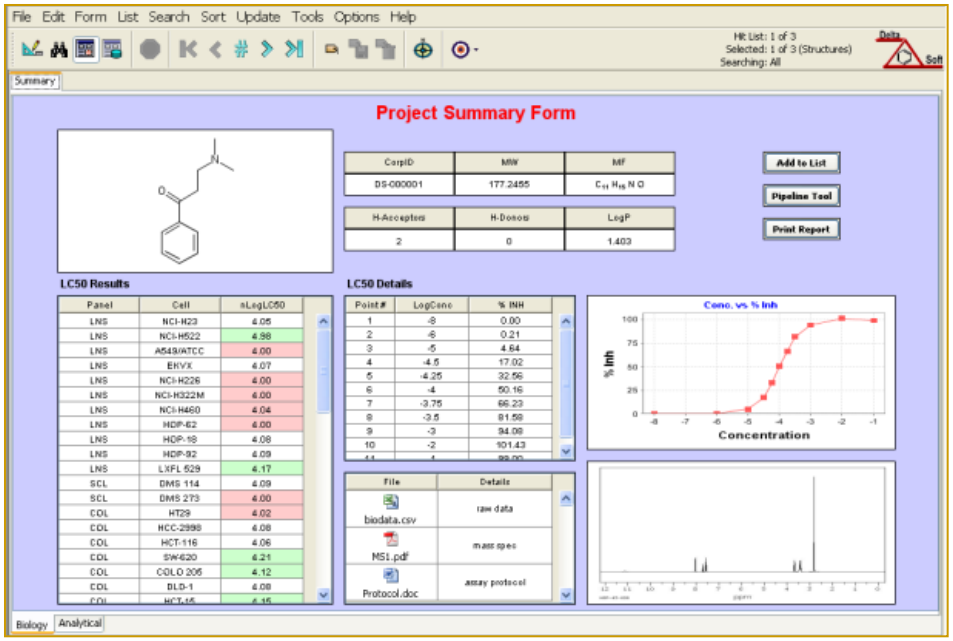
ChemCart BioAssay

- Biological Data entry
  - Associate test results with registered samples
  - Single point entry
  - Batch load from Excel, text files, etc.
  - Configurable pick lists
- Load image results
  - Paste single images
  - Batch load
- Attach supporting documents
  - Original Excel files
  - Raw data

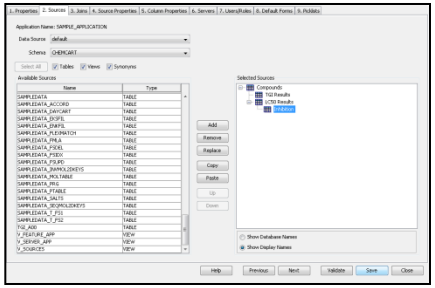


ChemCart Structure Activity Browser

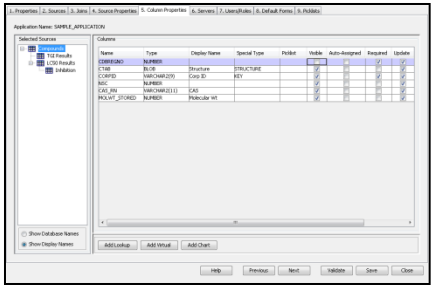
- Query by Form for chemical structures, reactions, data, documents, files, and images
- Run multiple queries simultaneously with each having different search criteria
- Build customizable forms, or use pre-defined forms to view results
- Search by substructure, similarity, exact, and more
- Generate custom report printouts of search results
- Extensive result list handling



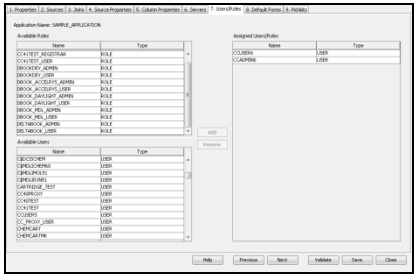
Create a rich user interface & deploy worldwide in less than 5 minutes!



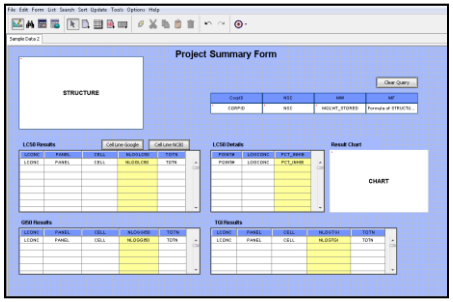
Select Data Sources
Define joins



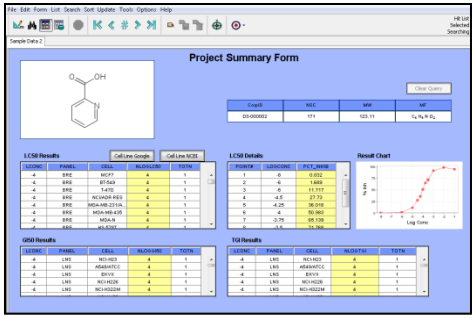
Set friendly column names.
Set pick lists



Set user access



Draw a form with boxes, tables, labels, and buttons.
Save publicly.



Search worldwide!

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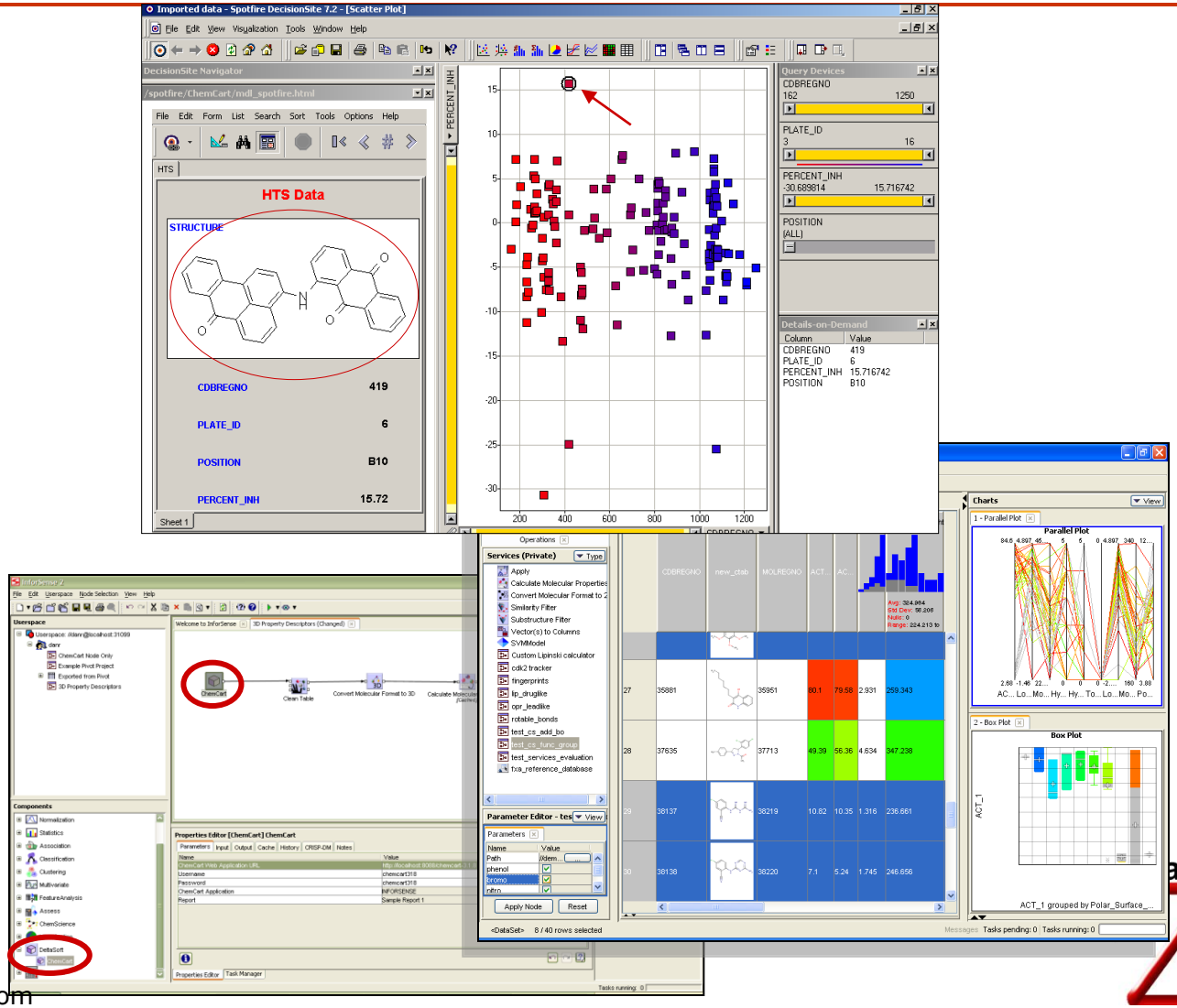
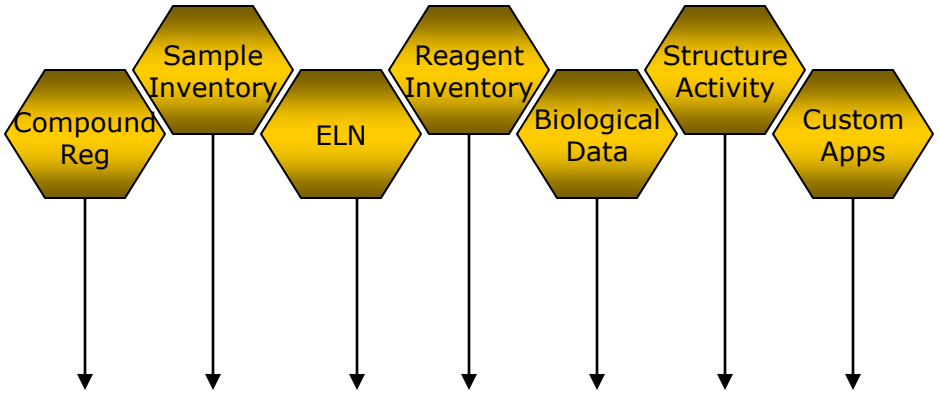
ChemCart Integrations & API



ChemCart Informatics Solution

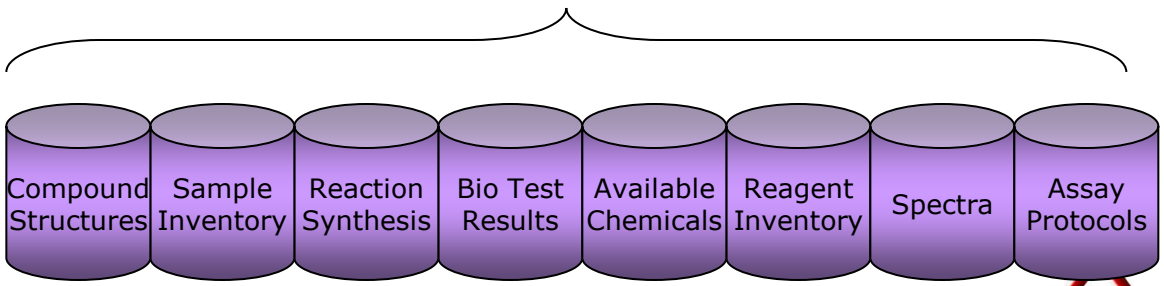
Web Served Applications



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, etc.)
    - 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 3rd party software for data analysis

Contact Us

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Please stop by the partner table to see more!