JUST ANOTHER CHEMICAL QUERY TOOL OR NOT

ChemQ POC to Implementation
How does innovation get started?

- “Necessity is the mother of invention”
- Opportunity and circumstance
- “Straw man proposal”
- Proof-of-concept

Utilizing ChemAxon’s example database query tool as a “Proof-of-concept”, we developed a generic chemical structure tool, that can be used stand alone or as a building block for larger solutions that require structure searching.
Generic Chemical Query System

- **User Demand & Need**
  - Explosion of chemical databases (PubChem, ChemNavigator, ACD)
  - Security issues and concerns sending search structures across internet
  - Logistics & Intellectual Property “seeding”

- **System Requirements**
  - [Admin] Quickly create, configure and deploy new data source
  - [Admin] Update data for data source without disruption in service
  - [User] Query data source with chemical structure and attributes
  - [User] View & export hit results from a query
  - [User] “Cherry pick” hit results across queries

- **System module**
  - Utilize query system as a module and integrate into existing systems and workflows
  - Utilize query system as a building block for new systems that require structure searching and extend the capability
Why ChemAxon?

- **ChemAxon – JChem**
  - Existing license across multiple affiliates
  - Mature and leading cheminformatics vendor
  - Strong vendor relationship with Takeda
  - Takeda possess significant expertise in JChem

- **JChem Example Database Query Tool**
  - 50 – 60% required functionality already exists within JChem
  - No requirement for cartridge or Oracle (open source databases)
  - Web-based example inline with Takeda informatics strategy

- **TCAL Proof of concept (POC) complete**
  - Informatics goal for FY2011
  - Load 5.3M in <8 hours; query response acceptable for 5.3M records
  - Two days effort to complete POC
  - User “buy in” (tangible example)
ChemQ: Proof-of-Concept

Query

Importing

Results

Exporting
Gap Analysis of POC

- Takeda standard UI layout (no frames)
- Authentication & access control
- Internationalization support
- Configurable query input (select, autocomplete, checkbox, radio)
- Fields administration hiding, labeling, tool tips, searchable, exportable (date importing)
- User auditing (login, search, export)
- Cherry picking records across search results and exporting
- Administration capabilities (cache/active tables, importing, reconfiguring)
- Record detail view and printing
- Result sorting
ChemQ Navigation

As part of Aldrich Chemistry Services, AldrichCPR brings over 15 years of experience in sourcing and custom packaging of synthetic building blocks and screening compounds for research organizations around the world. Over that time, we have gained valuable experience in working with hundreds of chemical suppliers serving this market. This experience has given us insight into the capability and performance metrics for our global supply chain. Our new Aldrich Market Select Collections include not only the products from suppliers that we have found achieve high performance in quality, delivery, and pricing.

To request a quotation, please email your list of STRUCTURE IDs to cnc_orders@sial.com. Don't forget to provide your full company name and contact information. Please remember to also include the target quantity you require for each substance and the critical packaging that is required.

Datasource description

Link to browse all records

Click structure for quick view

Display selected fields

Search page link

Link to record details
Search Interface & Options

- Quick structure retrieval
- Search by defined key identifier (one/line)
- Defined custom Marvin toolbar template based upon user feedback
- Structure drawing area
- Select fields to display on results page
- Field input hints and tool tips
- Input search conditions using customized form widgets
Search Interface & Options

- Select structure searching type
- Input results display
- Saved searches
- Search within previous results
- Input sorting conditions
- Save and activate previous searches for repeated use
- History of last 50 searches
Results Interface & Options

- Export search results
- Hit alignment and highlighting
- "Cherry pick" records
- Navigation buttons
- Sort search results
- Clear or View “cherry picked” records
- Name & Save search
Technology Stack & Components

- **Client (Web)**
  - **YUI**: Yahoo web UI components
  - **Marvin**: Client view both applets and images
  - **JChemManager**: Table creation and data importing
  - **WebMacro**: Java view middle tier for rendering html templates

- **Middle Tier (Java)**
  - **J2EE/Java Servlets**: application logic and data access
  - **WebMacro**: Java view middle tier for rendering html templates
  - **JChemBase**: Cheminformatics model and controller
  - **Tomcat**: Clustered Java application server
  - **Apache**: Various libraries & tools httpd, Log4j, Commons (Lang, IO, Collections, etc.)
  - **Jespa**: Single sign-on authentication and access control across Active Directory domains
  - **JSON**: Configuration and AJAX messaging (JSON.org, Jackson JSON)

- **Database Persistence**
  - **Oracle/PostgreSQL**: Data persistence
  - **JSON**: User preferences and audit information (MongoDB)

* **Not required**
** Administration
1. User authenticates via windows log in

2. User accesses ChemQ via browser

3. Application server delegates to Jespa/AD to authenticate user and lookup permissions

4. User actions audited (log in, query, export)


Proper AD trust configuration is critical
Data Sources

- Takeda Global Compound Collection
- Aldrich ChemNavigator Market Select
- PubChem Compound Database
- Top 500 Brand Name Prescription Drugs
- UCSF Zinc Screening Compound Collection

More to be added…
Summary & Closing

- Open Source & Collaboration
- Roadmap
  - Support child tables
  - Federated searching across data sources
  - Collaboration capabilities (sharing searches, wiki)
  - HTML5 (ExtJS)
  - Datasource configuration utility
  - noSQL database support (MongoDB)
  - Webservice interface & support (REST)
- Future Modules
  - Shipment Request & Tracking
  - Reagent Stockroom Operations (check in/out, dispose)
  - Reagent Procurement (shopping chart, ordering)
  - Data Warehouse Query Tool
Acknowledgements

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