

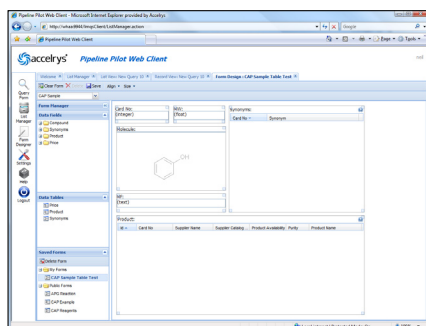
High performance web service-based search and data retrieval for Pipeline Pilot

Search across many different data sources regardless of search engine & schema design

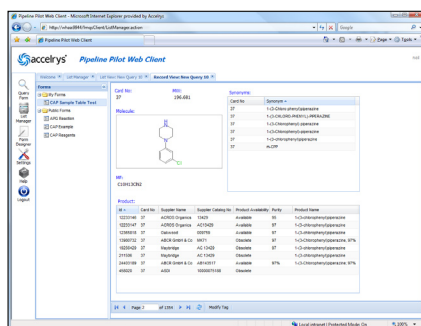
Support for generic SQL, Symyx, IDBS and Accord chemistry cartridges out-of-the-box

Cheminformatics Collection

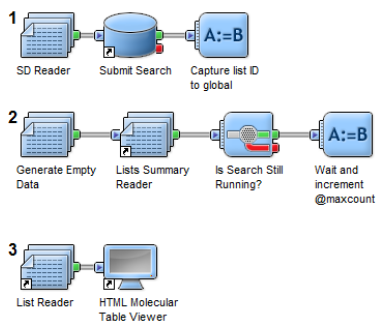
The Cheminformatics Collection is an infrastructure collection designed to support the development of enterprise cheminformatics systems and applications using Pipeline Pilot. The collection includes the List Management and Query Services (LMQS) system to bring high performance chemistry-focused search and hit list management capabilities to Pipeline Pilot. LMQS uses a metadata-driven design to enable you to rapidly search multiple data sources that may utilize a variety of different database search engines and schemas. Together with a drag and drop forms-based web interface and dedicated component collection, LMQS provides you with a complete search infrastructure to support a variety of enterprise informatics applications.



Building a query form for a data source in the LMQS Web Interface



Browsing the results of a search in the LMQS Web Interface



Protocol that imports a structure from an SDF file to use in a substructure search against a reagent database. In this example, search results are stored in a new list and displayed in an HTML table

With the Cheminformatics Collection you can:

- Search a diverse range of data sources from a single web browser based client or Web Port application, regardless of underlying chemistry format, database design, or search engine
- Easily integrate new and existing data sources for searching in Pipeline Pilot through LMQS without needing to modify underlying database designs or migrate data
- Build high-performance, information-centric, Web Port and Pipeline Pilot based data search and browse applications more easily and efficiently by using LMQS query and list management capabilities to simply protocol building and design
- Take advantage of intrinsic list management capabilities in the Pipeline Pilot ecosystem to build protocols to visualize, analyze, and report on search results from almost any data source
- Use the LMQS Web Interface to provide an easy to use, forms-based 'one-stop-shop' interface to bench scientists for searching, organizing and reporting on their data
- Build flexible, SOA-based scientific informatics systems and applications based on existing data sources quickly and efficiently by utilizing LMQS' metadata-driven approach, component collection and web service API

Flexible Search and Data Retrieval

Traditional database systems require data to be loaded into specific schemas, with each system typically having its own client. As the availability of external data increases and new systems are introduced, the number of database systems grows and data becomes difficult to manage and access across multiple systems. LMQS is designed to solve this challenge by providing a set of flexible web services that enable searching across different data sources.

Cheminformatics Collection

Metadata mapping of individual data sources to descriptive field names presented through LMQS web services enables users to query disparate data sources using a common set of query terms accessible through the LMQS Web Interface, Pipeline Pilot Web Port or by users building protocols with the Pipeline Pilot Professional Client.

By using metadata, LMQS eliminates the need to migrate or modify database schemas to make individual data sources available to users for searching. It also provides the flexibility to modify data sources without recompiling code and makes it possible to replace database search engines. For example, LMQS makes it possible for you to switch from one chemistry cartridge to another without needing to make changes to business logic or clients.

List Management

One of the key capabilities that LMQS provides is the ability to organize search results into lists. When a user runs a search against a particular data source, for example against a corporate chemistry database, any resulting hits are organized and stored in a list, generated upon completion of the query. Lists may be browsed, sorted, edited and deleted by users through the LMQS Web Interface. Lists can also be consumed and processed directly within Pipeline Pilot, making it possible for you to store a list of molecules generated from a user search for reference and process it through protocols for additional analysis, reporting, or for export to other applications.

LMQS Web Interface

An integral part of the LMQS system is the LMQS Web Interface, a thin, AJAX-based client interface that provides drag and drop forms building for querying and data browsing from within a standard web browser. Easy to use and deploy with zero footprint, the LMQS Web Interface enables users to design forms that can be associated with individual data sources to enable them to run searches and browse results lists. The Interface also provides a List Manager view that enables users to manage and browse any of their results lists and generate reports, calculate descriptors or export to other applications by calling

Pipeline Pilot protocols directly. Views of lists can be shared with other users by generating a link to a given list which can be copied into an email and sent to colleagues for viewing on their own desktop in a web browser or from within a portal environment.

Component Collection

The LMQS Component Collection offers a number of components to maximize the utility of LMQS services within Pipeline Pilot and make data browse and search applications built from protocols faster, simpler to assemble and easier to maintain. The collection offers two reader components for returning individual list members or list status information into protocols along with a List Viewer component for displaying list contents in an LMQS Web Client list view grid. For searching data sources, a Submit Search component enables queries to be constructed and executed using LMQS services from within Pipeline Pilot protocols. Any lists generated by protocols are viewable from within the LMQS Web Interface.

A Boon for SOA Development

LMQS is built on open, industry standard technologies that include Simple Object Access Protocol (SOAP), Web Services Definition Language (WSDL) and XML Schema Definition Language (XSD). As well as being callable from within Pipeline Pilot protocols through a dedicated component collection, LMQS offers a full web service API for use within SOA system development. LMQS supports all Pipeline Pilot security and authentication methods including Active Directory and LDAP, making it possible for you to build highly secure but accessible search systems for the end user. By enabling system developers to support many different data sources or reconfigure underlying data sources and search engines without having to impact the end user, LMQS further augments the already powerful web service development environment that Pipeline Pilot provides.