

***Q3 technologies***

## Data Curation Services creating reusable knowledgebase for bioinformatics companies

Q3's global sourcing model gives the maximum benefit to customers in terms of cost savings, improved quality, access to highly talented professionals, flexibility of operations and reduced time to market.

## Case Study - Client based in Boston, MA

The client is the industry leading supplier of internet browser and web server based chemical databases consulting services to biotechnological and pharmaceutical and chemical industries.

### Company Profile

### Business Situation

Modern Biology, chemistry techniques and practices generate outsized amount of data and huge number of chemical compounds. As a consequence, one of the biggest challenges is to tag all of the available information so they can analyze and generate knowledge from it.

As a major contributor to the ongoing life sciences research and development, you must be dealing with several tera- bytes of scientific data.

Research indicates that the modern day pharmaceutical and biotechnology companies have about 3-40 tera bytes of data depending on their business size. The wealth of this scientific data can only be unleashed when it is intelligently integrated and computed.

Our data curation services are focused to create reusable knowledgebase. The following table indicates the key parameters that we identified with respect to chemical, biological, pharmacology and bibliographic databases:

#### Key Parameters

<b>Chemistry</b>	2D structure, molecular weight, molecular formula, IUPAC name, SMILE notation etc,
<b>Biology</b>	Therapeutic indication, target information, assay, and activity information
<b>Pharmacology</b>	ADMET parameters
<b>Bibliography</b>	Patent/Article number, Approval/expiry dates, Author names etc.,
<b>Annotations and ontology</b>	

We have identified some of the important databases that we can curate:

- Small molecule databases with biological, pharmacological activities
- Known drugs database
- Reaction databases
- Toxicology database
- Clinical, pre-clinical database

- Protein-protein interactions, QTLs, gene/protein families, biomarkers, expression/toxicology profiling and synteny databases to understand the conservation across different systems
- Metabolic pathway databases - support with microarray-analyzed expression profiling, custom tool development for drawing pathways and link them to various sources

## How is it useful?

Database	Usage
<ul style="list-style-type: none"> <li>• All compounds studied against a class of protein</li> <li>• Compounds active against a particular Target or set of Targets.</li> <li>• Compounds with ADMET data</li> <li>• Compounds with only pre-clinical and clinical data</li> <li>• Appending data for a given compound / set of compounds from various sources into a unique structure library database</li> <li>• FDA approved Drug database</li> </ul>	<ul style="list-style-type: none"> <li>• Identify scaffolds associated with a biological activity</li> <li>• Categorize large structure data sets using the chemical diversity</li> <li>• Identify structural fragments responsible for activity/toxicity</li> <li>• Compare compounds with toxicity and known drug databases</li> <li>• Search &amp; analyze combinatorial libraries using scaffolds</li> <li>• Identify scaffolds and subject the set of structures for R-Group deconvolution studies</li> <li>• Recognize the activity, or selectivity, relationship of structure fragments and R-Group analysis</li> <li>• Generate pharmacophores from set of active structures against a target or class of targets</li> <li>• Identify compounds for screening</li> </ul>

## Solution

Q3 has identified the importance of data management and offers following curation and database services.

Q3 helps you in curation of Chemical, Biological, Pre-Clinical, Clinical and ADME/Toxicology databases. We use multiple source including, patents, journals and other sources of literature. These Databases can add value to the ongoing target identification, lead identification and lead optimization in your drug discovery programs.

Databases can also be customized as per your requirements. We have identified some of your critical needs and recommend using the following database services: Q3 set up a dedicated team consisting of a team lead and database developers with Internal program managers to monitor and guide the client-vendor partnership.

Q3 ensured a transparent and flexible relationship by putting the right combination of people and technology under detailed consultation with technical managers at client site.

Semi-detailed specifications were provided by client's and Q3's system architects worked extensively with peers both at Q3 and at client site for building a state of the art data base structure and detailed functional and design specifications.

Automated testing tools like Winrunner were used by experienced QA professionals to ensure bug free, application milestones delivery within deadlines.