

Quick Start Guide

Welcome to the ProteoIQ quick start guide. This guide describes the basic steps for setting up your first project in ProteoIQ. For more detailed information not covered in this document please see the ProteoIQ tutorials and help manual. Prior to creating the first ProteoIQ project please read the tutorials provided in the ProteoIQ installation path:

C:\Program Files\ProteoIQ\docs

System Requirements

! ProteoIQ **MUST** be installed on a computer with **minimum of 2 GB** of physical memory (RAM). It is also recommended that the computer have at least 4 GB of free disk space on the harddrive containing the ProteoIQ installation. !

What You Need To Get Started

- Protein sequence database in FASTA format

ProteoIQ comes preloaded with the following databases:

<u>Organism</u>	<u>Source</u>
<i>Homo sapiens</i>	Swiss-Prot and GenBank
<i>Mus musculus</i>	GenBank
<i>Saccharomyces cerevisiae</i>	Swiss-Prot

If your database search results were generated using a database that is not included in ProteoIQ you will need to locate your sequence database (in FASTA format) and run the **Modify Database** wizard to enable its use in ProteoIQ.

- Database search results

You will need to locate your database search results. Supported formats include the following:

Mascot (.dat), SEQUEST (.out and .dta or .srf), Proteome Discoverer (.msf), X!Tandem (.xml), and pepXML. **NOTE:** When using the SEQUEST .out format, the **sequest.params** file must be present in each SEQUEST results folder, as this is required for determining the parameters used in the database search.

Please read the remainder of this Quick Start Guide for more help on setting up ProteoIQ and tutorials are also provided as a guide to creating new ProteoIQ projects.

Software Requirements

This release of ProteoIQ requires Java version 1.6.14 or higher. ProteoIQ will not work on earlier versions of Java. For Windows users, if Java version 1.6.14 is not installed, ProteoIQ will automatically install it during the installation process.

Installing ProteoIQ

Double click on the ProteoIQ installer and follow the instructions to install ProteoIQ. For Windows Vista users, you may need to right click on the ProteoIQ installer and select “Run as administrator”.

Licensing

From the ProteoIQ navigation panel select View License. To enter a new license type the license code into the fields available and select submit. **Note:** Your computer must have an active internet connection. For unlimited licenses this will be the only time ProteoIQ has to confirm the license so your computer can be removed from the internet once the license has been activated. If you are using the ProteoIQ 40 or 200 versions the license key must be confirmed each time ProteoIQ is opened so the computer must always have access to the internet.

If your license has expired or you are using the ProteoIQ viewer select Open Viewer Only. This will allow you to access previously processed ProteoIQ data files without the need for an active license key.

Creating your first project - what you will need to get started

1. Database search results – either
 - a. Mascot (.dat),
 - b. SEQUEST
 - i. Folder of .out and .dta files
 - ii. Zipped (.zip) file of .out and .dta files
 - iii. BioWorks output (.srf file)
 - c. Proteome Discoverer (displayed as “Sequest .msf”)
 - d. X!Tandem (.xml),
 - e. or pepXML.
2. FASTA database

Database search results

Mascot (.dat)

Mascot renders results in two formats: its native data format (**.dat**) and an HTML view. The HTML files should NOT be used in ProteoIQ. The (.dat) files are typically located in the directory **Inetpub\Mascot\data** and are organized by an assigned number which is generated when the search is performed. We recommend copying the search results into another directory prior to running ProteoIQ. This will ensure that the data may be easily accessed for multiple analyses at a later date. There is also no need to rename your (.dat) files. When you select the file in the **Available Results Files** viewer, ProteoIQ extracts the name of the peak list from the (.dat) file and renders it in the window

SEQUEST (.out)

SEQUEST folders often contain very large numbers of (.out) (SEQUEST search result) and (.dta) (Thermo peak list format) files that will slow access to the files. For this reason, we recommend copying these folders to a separate directory or compressing (zipping) the .out and .dta files into a .zip file prior to running ProteoIQ.

NOTE: The user needs to ensure that **sequest.params** file is present in each SEQUEST results folder, as this is required for determining the parameters used in the database search.

SEQUEST (.srf format)

BioWorks versions 3.2 and greater support the creation of **.srf** files. ProteoIQ currently supports parsing of **.srf** files generated natively during the SEQUEST search or **.srf** files created by conversion of .out and .dta files.

Proteome Discoverer (.msf)

ProteoIQ currently supports parsing of **.msf** files generated natively during the Proteome Discoverer search or converted from **.srf** files.

Locating your FASTA database

ProteoIQ uses the FASTA database that corresponds to the database search results you are loading into the software. The database is used to correlate peptides (from your database search results) to proteins in the FASTA database. ProteoIQ comes preloaded with several databases however we recommend using the same database that was used for database searching. For Mascot users, the databases are located in the **Inetpub\Mascot\database** directory. For SEQUEST/BioWorks and Proteome Discoverer users you can find your FASTA database in the **Xcalibur\database** directory.