# Reference manual

## Starting Xlink Analyzer

1. Go to *Menu Tools -> Utilities -> Xlink Analyzer*

## Creating new project

1. Create some directory on your computer. This will be so called “project directory”.   
   You should keep all data files you will use with Xlink Analyzer there.
2. Start Xlink Analyzer
3. Add subunits in the left panel (manually or using Menu File -> Create Project From Structure)
4. Load data in the right panel
5. Save project: navigate to the project directory and save the file with the name of your choice with .json or .txt extension. This file is configuration file of your project.

## Loading existing project

1. Click File -> Load project
2. Choose file with the configuration of your project.

## Input formats

Xlink Analyzer reads files with cross-links and, optionally, protein sequences.

### Cross-links

#### Xlink Analyzer format

A text CSV file (<http://en.wikipedia.org/wiki/Comma-separated_values>) containing the following columns:

|  |  |  |  |
| --- | --- | --- | --- |
| Column Header | Definition | Example | |
| Id | Peptide information in a format: <sequence1>-<sequence2>-a<relative postion1>-b<relative position2> | Cross-link: | TPQIGDKFSSR-VRVLPNEKTLR-a7-b8 |
| Mono-link: | SLPVDFESSTTMTIDKHDYK-a16 |
| Protein1 | Protein name of the first cross-linked residue |  |  |
| Protein2 | Protein name of the second cross-linked residue | Cross-link: | 308 |
| Mono-link: | - |
| AbsPos1 | Residue number of the first cross-linked residue | 125 |  |
| AbsPos2 | Residue number of the second cross-linked residue | Cross-link: | 308 |
| Mono-link: | n/a |
| score | Cross-link confidence score | 30.86 |  |

Only the fields: Protein1, Protein2, AbsPos1, AbsPos2 are required.

* In the Id column, the relative positions correspond to residue index in the peptide. For example, in TPQIGDKFSSR-VRVLPNEKTLR-a7-b8, a7 means 7th residue of the first peptide (lysine)
* AbsPos1 and AbsPos2 must correspond to residue numbering in the PDB files onto which the cross-links will be mapped

Example:

Id,Protein1,Protein2,AbsPos1,AbsPos2,score

TPQIGDKFSSR-VRVLPNEKTLR-a7-b8,RPA2,RPA1,916,612,44.83

…

SADEGATVFYTCTSCGYKFR-a18,RPA12,-,120,n/a,33

…

Example files:

doc/example/PolI/xlinks/Pol1\_4\_XlinkAnalyzer\_format.csv

#### xQuest format

xQuest is a popular software for cross-link identification and its output CSV/XLS files are directly supported by Xlink Analyzer.

Example files:

doc/example/PolI/xlinks/Pol1\_4\_Inter.xls

doc/example/PolI/xlinks/Pol1\_4\_Intra.xls

doc/example/PolI/xlinks/Pol1\_4\_Loop.xls

doc/example/PolI/xlinks/Pol1\_4\_Mono.xls

*Note that although this example has inter-, intra-, loop- and mono-links in separate files, it is not necessary and they may be combined in single file – Xlink Analyzer automatically determines the cross-link type.*

### Sequences

A text file in FASTA format (<http://en.wikipedia.org/wiki/FASTA_format>). This file is optional and only necessary for predicting monolinkable positions (“Modified” tab -> “Not expected to be mono-linked” option). The names of the sequences do not have to be the same as names of the subunits – during project Setup the sequence names can be matched to subunit names interactively.

Example file:

example/PolI/PolI\_sequences.fasta