

## 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
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 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](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 position1>-b<relative position2>	Cross-link:	TPQIGDKFSSR-VRVLPNEKTLR-a7-b8
		Mono-link:	SLPVDFESSTMTIDKHDIK-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 7<sup>th</sup> 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
...
SADEGATVFYCTCTSCGYKFR-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](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
```