To start the program with a graphical user interface double click the jar file or execute it from the command line with no options.

The program can be executed from command line. Run it with the option "-usage" to get help.

Usage: OPF

-correctproteins <correctproteins>	true / false specifying if the peptides should be grouped into proteins
-file <file>	path to the input file
-MSQuantfile <MSQuantfile>	true / false specifying if the input file is an MSQuant file (if false a generic tab delimited file is expected)
-modfile <modfile>	path to the modifications file
-outfile <outfile>	path to the output file

Example command line execution:
```
java -jar OPF.jar -file c:\testfolder\input\merged_first500.txt -modfile "c:\testfolder\input\mods(with carbidomithyl).txt" -msquantfile true -correctproteins false -outfile c:\testfolder\output2\output.txt
```

The generic tab delimited input file should contain the following set of columns in this exact order:

- Accession number
- Sequence
- Mascot calculated mass [Da]
- Modifications
- XIC 1 [Da*secs]
- 3/1 (of XICs)
- XIC 3 [Da*secs]
- 4/1 (of XICs)
- XIC 4 [Da*secs]
- Used in protein quantitation

The data should be in the same format as in the MSQuant file.

The modfile should contain the following data in this exact order and separated by tabs:

- name of the modification. Round brackets should be escaped if present in the name, e.g. test(testname)name -> test\(testname\)name

- chemical formula of the modification. This should be written using the symbols present in the "elemente" file

- the string "fixed" or "variable" (without quotes) to specify the kind of modification

- the string "residue" or "peptide" to indicate the type of "fixed" modification

- the amino acid symbol if the previous column specified "residue"

There can be multiple records in the modfile. Each record should be on a new line. The program will perform according to the information supplied:

1) Variable modification -> The program will look in the Modifications column of the input file, match the name of the modification, get the number in front of the modification, add the chemical formula of the modification(s) to the chemical formula of the peptide.

2) Fixed modification of an amino acid -> The program will count the number of occurrences of the amino acid in the peptide and add the chemical formula of the modification(s) to the chemical formula of the peptide.

3) Fixed modification of a whole peptide -> The program will add the chemical formula of the modification once to the chemical formula of the peptide.

Example files are included on the website https://trac.nbic.nl/opf