

# Peakjuggler Manual

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May 23, 2016

*Peakjuggler* is a node for Proteome Discoverer that aims to compare areas of peptides over several runs. Additionally it tries to find peptides that aren't identified in all runs.

# **1** Installation

# 1.1 Dependencies

- Proteome Discoverer version 2.0 or 2.1 is required
- ${f R}$  For some parts an R installation is needed. It is included in the installer

# 1.2 Installation

• Download the installer from http://http://ms.imp.ac.at?goto=peakjuggler

Peakjuggler consists of two nodes, one for the processing workflow and one for the consensus workflow.

# 2 Usage

# 2.1 Parameters

# 2.1.1 Processing Node

- 1. Search Parameters
  - Confidence Level: Only use PSMs with at least this confidence
  - **Minimum Score:** The minimum score a PSM needs to be used. This is dependent on the search engine you use

| Pa | rameters                      |                                    |                          |                                   |                |  |  |  |
|----|-------------------------------|------------------------------------|--------------------------|-----------------------------------|----------------|--|--|--|
| Н  | ide Advanced Parameters       |                                    | -                        |                                   |                |  |  |  |
| ~  | 1. Search Parameters          |                                    | Para                     | meters                            |                |  |  |  |
|    | Confidence Level              | Medium                             | CL.                      | A dama d Dama dama                |                |  |  |  |
|    | Minimum Score                 | 100                                | Show Advanced Parameters |                                   |                |  |  |  |
|    | Minimum Sequence Length       | 7                                  |                          |                                   |                |  |  |  |
|    | Search Engine Rank            | 1                                  | 4                        | I. Protein Area                   |                |  |  |  |
|    | Mass Tolerance                | 5 ppm                              |                          | Usage of peptides                 | average        |  |  |  |
| ~  | 2. PhosphoRS/ptmRS Se         | ttings                             |                          | Destides to use for Destain Arres |                |  |  |  |
|    | Probability Threshold         | 75                                 |                          | Peptides to use for Protein Area: | top x per samp |  |  |  |
|    | PhosphoRS Column Name         | ptmRS [4]: Best Site Probabilities |                          | Use shared peptides for           | protein groups |  |  |  |
| ~  | 3. RT Correction Paramet      | ers                                |                          | # pape for protein para           | 2              |  |  |  |
|    | RT Correction                 | True                               |                          | # peps for protein aera           | 3              |  |  |  |
| ~  | 4. Performance Paramete       | rs                                 | 4                        | 2. Peptide Area                   |                |  |  |  |
|    | Workpackage size              | 10000                              |                          | Minimum Area                      | 50000          |  |  |  |
| ~  | 5. Area Calculation Paran     | neters                             |                          |                                   | 00000          |  |  |  |
|    | Minimum Width for Peak (in mi | n) 0.05                            |                          |                                   |                |  |  |  |
|    | Noise Level                   | 10000                              |                          | (b) Consensus We                  | orkflow        |  |  |  |

(a) Processing Workflow



- Minimum Sequence Length: The minimum number of AAs a peptide needs to have to be used
- Search Engine Rank: Up to which search engine rank PSMs are considered
- 2. PhosphoRS/ptmRS Settings
  - **Probability Threshold:** Everything above this threshold is counted as high
  - **PhosphoRS Column:** The name of the phosphoRS/ptmRS column. If this name is not found, PJ tries some standard names, if still no column is found, modifications are taken from the search engine
- 3. RT Correction Parameters
  - **RT Correction:** Peakjuggler can correct retention time shifts. This parameter activates/deactivates this feature.
- 4. Performance Parameters
  - Workpackage size: This regulates the number of spectra that are read into the RAM. If you experience that your RAM is filled up during analysis, it is a good idea to set this parameter lower. Unfortunately with lower package size the analysis will take longer.
- 5. Area Calculation Parameters
  - Minimum Width for Peaks: The minimum time for a peak
  - Noise Level: All signals below this intensity are considered as zero
  - Mass Tolerance: Allowed mass deviation in the XIC

## 2.1.2 Consensus Node

1. Protein Area

- Usage of peptides: Which method should be used to combine peptide areas to the protein area. The possibilities are:
  - sum
  - average
  - median

#### • Peptides to use for Protein Area:

- Top x per sample: Takes the top x peptides per sample and performs the chosen method on their areas.
- Top x over all samples: This method first sums all areas of each peptide in all samples and then takes the top x to calculate the protein area. This ensures that the same peptides are selected in all samples.

#### • Use shared peptides for:

- All proteins: Shared peptides contribute to all proteins they appear in
- Nothing: Shared peptides are ignored
- Protein Groups: If a peptide is only shared within the same protein group use it
- **# peps for protein area:** The maximum number of peptides to combine for the protein area. If a protein has less peptides than this number, all available are used.
- 2. Peptide Area
  - Minimum Area: Peptides with a smaller area are counted as not quantified

# 2.2 Workflow

#### 2.2.1 Processing Node

The processing node needs two connections, one to the *Spectrum Files* node, and another one to the PSM Validation node (e.g. *Percolator* or *Target Decoy PSM Validator*).

#### 2.2.2 Consensus Node

The consensus node needs to be connected to the *Protein Grouping* node.

# 3 Results

#### 3.1 New columns

#### 3.1.1 Protein tab

The protein table receives two new columns: *Peakjuggler Area* and *Identified by*. The areas are colour coded to give a quick overview if the areas are similar in the samples. The



(b) Consensus Workflow

Figure 2: Sample Workflows

Identified by column has one box per sample and indicates the origin of quantification. (MS/MS, MBR or none) See figure 3

| Proteir | ns Prot | ein Groups  | Peptide 0  | Groups       | PSMs       | MS/MS Spectrum | n Info   | PJ Fea | atures | QuanResu  | lt  |
|---------|---------|-------------|------------|--------------|------------|----------------|----------|--------|--------|-----------|---|
| F       | Checked | Protein FDR | Confidence | Master       | Peakjuggle | r Areas 🔹      | Identifi | ed by  | * +    | Accession | Description   |
| 2013 🗇  |         | •           |            | $\checkmark$ | 2.1e8      | 2.2e8          |          |        |        | 51338637  | RecName: Full=60S ribosomal protein L23a                    |
| 2014 🗠  |         | •           |            | $\checkmark$ | 2.0e7      | 2.2e7          |          |        |        | 2495344   | RecName: Full=Heat shock protein 105 kDa; AltName: Full=    |
| 2015 -  |         |             |            | $\checkmark$ | 1.4e6      | 1.4e6          |          |        |        | 55584151  | RecName: Full=Glucosylceramidase; AltName: Full=Acid be     |
| 2016 🗇  |         | •           |            | $\checkmark$ | 1.5e7      | 1.5e7          |          |        |        | 296439328 | RecName: Full=Importin subunit alpha-5; AltName: Full=Ka    |
| 2017 🗠  |         | •           |            | <b>V</b>     | 6.1e5      | 6.1e5          |          |        |        | 29840826  | RecName: Full=Nardilysin; AltName: Full=N-arginine dibasic  |
| 2018 🗠  |         |             |            | $\checkmark$ | 1.6e7      | 1.9e7          |          |        |        | 74743691  | RecName: Full=Heterochromatin protein 1-binding protein 3   |
| 2019 🗇  |         | •           |            |              | 1.5e8      | 1.5e8          |          |        |        | 74749006  | RecName: Full=Putative 60S ribosomal protein L13a proteir   |
| 2020 -  |         |             |            | $\checkmark$ | 3.6e7      | 3.7e7          |          |        |        | 3023628   | RecName: Full=ATP-dependent RNA helicase DDX3X; AltN        |
| 2021 -  |         |             |            | $\checkmark$ | 6.7e5      | 6.4e5          |          |        |        | 74758580  | RecName: Full=W/D repeat-containing protein 82; AltName:    |
| 2022 -  |         | •           |            |              | 4.6e6      | 4.7e6          |          |        |        | 13124471  | RecName: Full=Ras-related protein Rab-9B; AltName: Full=    |
| 2023 -  |         | •           |            | $\checkmark$ | 2.1e6      | 2.2e6          |          |        |        | 27805669  | RecName: Full=Pantothenate kinase 4; Short=hPanK4; Alth     |
| 2024 -  |         | •           |            | $\checkmark$ | 1.9e6      | 2.1e6          |          |        |        | 13124451  | RecName: Full=Ribonucleases P/MRP protein subunit POP       |
| 2025 -  |         | •           |            | $\checkmark$ | 9.7e5      | 9.8e5          |          |        |        | 23503074  | RecName: Full=Thymidine kinase, cytosolic                   |
| 2026 🗇  |         | •           |            | $\checkmark$ | 3.6e5      | 4.9e5          |          |        |        | 1345650   | RecName: Full=Collagen alpha-1(VII) chain; AltName: Full=   |
| 2027 -  |         | •           |            | $\checkmark$ | 6.2e6      | 7.3e6          |          |        |        | 74750895  | RecName: Full=Leucine-rich repeat-containing protein 47     |
| 2028 -  |         |             |            | $\checkmark$ | 8.9e6      | 9.3e6          |          |        |        | 117949389 | RecName: Full=CD109 antigen; AltName: Full=150 kDa TG       |
| 2029 -  |         | •           |            | $\checkmark$ | 3.5e7      | 3.2e7          |          |        |        | 76803555  | RecName: Full=Nucleolar RNA helicase 2; AltName: Full=D     |
| 2030 -  |         | •           |            | $\checkmark$ | 1.8e7      | 1.6e7          |          |        |        | 24638339  | RecName: Full=Vesicle-associated membrane protein-asso      |
| 2031 -  |         |             |            | $\checkmark$ | 4.5e6      | 5.1e6          |          |        |        | 47606219  | RecName: Full=Multifunctional methyltransferase subunit TI  |
| 2032 -  |         | •           |            | $\checkmark$ | 1.9e7      | 1.9e7          |          |        |        | 74735389  | RecName: Full=U4/U6.U5 tri-snRNP-associated protein 1; /    |
| 2033 🗇  |         | •           |            | $\checkmark$ | 1.5e6      | 1.9e6          |          |        |        | 67476671  | RecName: Full=Oxygen-dependent coproporphyrinogen-III (     |
| 2034 -  |         | •           |            | $\checkmark$ | 3.0e7      | 3.3e7          |          |        |        | 2498464   | RecName: Full=28 kDa heat- and acid-stable phosphoprote     |
| 2035 -  |         | •           |            | $\checkmark$ | 5.2e7      | 5.4e7          |          |        |        | 5921197   | RecName: Full=Calumenin; AltName: Full=Crocalbin; AltNa     |
| 2036 😑  |         |             |            | $\checkmark$ | 5.9e6      | 6.0e6          |          |        |        | 313104206 | RecName: Full=Palladin; AltName: Full=SIH002; AltName: F    |
| 2037 🗠  |         | •           |            | $\checkmark$ | 4.5e7      | 4.5e7          |          |        |        | 38258929  | RecName: Full=DNA-dependent protein kinase catalytic sub    |
| 2038 🗠  |         | •           |            | $\checkmark$ | 2.1e8      | 2.1e8          |          |        |        | 125969    | RecName: Full=40S ribosomal protein SA; AltName: Full=3.    |
| 2039 😑  |         | •           |            | $\checkmark$ | 2.1e7      | 2.1e7          |          |        |        | 47117647  | RecName: Full=Actin-related protein 3; AltName: Full=Actin- |
| 2040 -  |         |             |            | V            | 8.0e5      | 7.4e5          |          |        |        | 8928568   | RecName: Full=Tumor suppressor p53-binding protein 1; SI    |
| 2041 -  |         |             |            | ×            | 4.8e5      | 5.2e5          |          |        |        | 269849532 | RecName: Full=Aldehyde dehydrogenase family 16 membe        |
| 2042 🗇  |         |             |            | ×            | 1.2e7      | 1.2e7          |          |        |        | 223634676 | RecName: Full=Protein TFG; AltName: Full=TRK-fused gen      |

Figure 3: Protein Table

## 3.1.2 Peptide Groups tab

Exactly the same as in the protein table. See figure 4

#### 3.2 New tables

#### 3.2.1 PjFeatures

This table is similar to the PSMs table, but not on PSM but on PCM (peptide charge modification) level (see fig 5).

It also provides the user with information regarding the quantification like peak start and end times and a button to show the extracted ion chromatogram (XIC) including the peak boundaries (see fig. 6)

#### 3.2.2 PjQuanResult

The QuanResult is the equivalent to the *Peptide Groups* table for Features. (see fig. 7) It also features an XIC view over all samples (see fig. 8)

| Product     Condence     Peakinger Areas     Methide by     Sequence     Modifications     Qualty PI       28     C     A     2.86     2.86     DPAGPMSPGEATQSGAR     1:Cartamidomethyl [C4];2:ADxidation [M8(100); M12(10)]     622:4       31     C     A     5.86     8.76     VCIVCLATQMLESBIK     1:Cartamidomethyl [C4];2:ADxidation [M8(100); M12(10)]     622:4       31     C     A     5.86     8.264     IPCLATQMLESBIK     1:Cartamidomethyl [C2]     5.686       32     C     A     5.86     8.365     GrtVTEIPQLEPELPCEGOPEAR     1:Cartamidomethyl [C2]     5.686       33     C     A     1.87     1.47     LOTVSEQPNK     1:Sara     1.984       34     C     A     3.86     DGTLCTNMK     1:Carbamidomethyl [C6]     3.7264       35     C     A.86     5.46     DGTLCTNMK     1:Carbamidomethyl [C6]     3.7264       36     C     7.86     9.26     DGTLCTNMK     1:Carbamidomethyl [C6]     3.7264       37     C     A.86     5.464     C  | P  | roteir | ns Prot | ein Groups | Peptide Group     | PSMs  | MS/MS Spe     | ctrum Ini | o PJ Features QuanResult        |   |             |
|--|----|--------|---------|------------|-------------------|-------|---------------|-----------|---------------------------------|---|-------------|
| 8     C     Image: Constraint of the state state of the state of the state of the state of the stat  | Ē  | 9      | Checked | Confidence | Peakjuggler Areas | +     | Identified by | +         | Sequence                        | Modifications   | Qvality PEP |
| 2     -     -     8.0x8     9.7x8     PVICATQMLESMIK     1-Carbamidomethyl[C4]: 2x0xdatoin [M8[100]; M12[100]     6.22e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-       1     -     1.2x7     1.7x7     VESLD/VDSEAK     7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7.02e-<br>7. | 28 | -      |         | •          | 2.1e6             | 2.8e6 |               |           | DPAQPMSPGEATQSGAR               |   | 0.000136    |
| 30   | 29 | -12    |         | •          | 6.0e6             | 9.7e6 |               |           | PVICATQMLESMIK                  | 1×Carbamidomethyl [C4]; 2×Oxidation [M8(100); M12(100)] | 6.22e-07    |
| 31   | 30 | -12    |         | •          | 2.5e7             | 2.6e7 |               |           | VESLDVDSEAK                     |   | 7.02e-05    |
| 32   | 31 | -      |         | •          | 5.1e6             | 6.2e6 |               |           | IPELLSLRPR                      |   | 3.72e-05    |
| 33   | 32 | -12    |         | •          | 1.2e7             | 1.7e7 |               |           | VCNFLASQVPFPSR                  | 1×Carbamidomethyl [C2]                                  | 5.68e-06    |
| 34   | 33 | -12    |         | •          | 6.9e5             | 9.3e5 |               |           | GHTVTEPIQPLEPELPGEGQPEAR        |   | 8.35e-06    |
| 35   | 34 | -      |         | •          | 1.1e7             | 1.2e7 |               |           | HRDYETATLSDIK                   |   | 1.19e-06    |
| 36   | 35 | -12    |         | •          | 1.3e7             | 1.4e7 |               |           | LQTLVSEQPNK                     |   | 8.05e-05    |
| 37   1   4.86   5.46   SVPEFMQVEK   4.064     38   1   5.86   4.26   AVGASFPLYEPAK   0.0001     39   1   2.87   3.27   DYAP/HEDR   0.0001     40   1   2.86   3.26   SAYGEAMDISK   1>Oxidation [M7(100)]   2.084     41   1   1   1.77   1.987   PNECGHVLYADIK   1>Carbamidometryl [C4]   4.664     42   1   3.86   4.166   UTQDTENELK   InCarbamidometryl [C4]   4.664     43   1   1.877   1.987   REEELQAALAR   1.7Carbamidometryl [C4]   4.664     44   1   4.266   4.166   KINPEYPINFAEFSK   2.664   4.664     45   1   4.266   4.166   KINPEYPINFAEFSK   2.664   6.874     47   1   2.286   7.66   GLIGCNIPLQR   1>Carbamidometryl [C5]   2.2144     48   1   1.56   LVQAPLDADGDNVLQEK   1>Carbamidometryl [C5]   2.2144     49   1   1.86   7.66   MGENVLVTAGR   3.866     41 <td< th=""><td>36</td><td>-12</td><th></th><td>•</td><th>7.6e6</th><td>9.2e6</td><td></td><td></td><td>DGTILCTLMNK</td><td>1×Carbamidomethyl [C6]</td><td>3.72e-05</td></td<>   | 36 | -12    |         | •          | 7.6e6             | 9.2e6 |               |           | DGTILCTLMNK                     | 1×Carbamidomethyl [C6]                                  | 3.72e-05    |
| 38   -   5.86   4.86   AVGASPEVYEPAK   0.0001     39   -   2.867   3.287   DYAPVHEDR   5.1664     40   -   2.867   3.287   DYAPVHEDR   1×Cxideion [M7(160)]   2.066     41   -   -   1.77   1.87   FRECGHVLYADIK   1×Carbanidomethyl [C4]   4.664     42   -   3.868   4.168   LVTQDTENELK   1×Carbanidomethyl [C4]   4.664     43   -   -   1.847   1.847   FRECGHVLYADIK   1×Carbanidomethyl [C4]   4.664     44   -   -   1.847   1.847   FRECGHVLYADIK   1×Carbanidomethyl [C5]   2.164     45   -   -   2.864   A.166   KIPEYPYNEAESK   -   2.864     46   -   -   2.864   GLIGCNIPLQR   1×Carbanidomethyl [C5]   2.214     47   -   5.368   7.866   GLIGCNIPLQR   1×Carbanidomethyl [C5]   2.214     48   -   -   1.866   HWAPEYNEAESK   -   Carbanidomethyl [C5]   2.216     59   -   <   | 37 | -      |         | •          | 4.3e6             | 5.4e6 |               |           | SYDFEFMQVEK                     |   | 4.08e-06    |
| 39   -   2.87   3.27   DVAPVHEER   5164-     40   -   -   4.88   3.86   SAYQEAMDISK   1>Oxidation [M7(100)]   2.086-     41   -   -   1.87   INFO   FNECGMUYADIK   1>Carbamidomethyl[C4]   4.66e-     42   -   -   3.86   4.16   IVTQDTENELK   6.91e-     43   -   -   1.87   FAEAGAVAR   7.7e-     44   -   -   1.47   1.47   FAEALGSTEAK   1.66e-     45   -   -   1.867   2.08-   CALCECELER   2.66-     45   -   -   1.867   3.266   GLACECELER   5.86-   3.26-     46   -   -   5.266   GLACECELER   5.86-   1.96-   1.96-     47   -   -   5.266   GLACECELER   1.56-   1.96-   1.96-     48   -   -   1.86   1.96-   1.94-   1.94-   1.94-   1.94-   1.94-     49   -   -   2.282   2.286   1.90- <td>38</td> <td>-12</td> <th></th> <td>•</td> <th>5.2e6</th> <td>4.2e6</td> <td></td> <td></td> <td>AVGASFPLYEPAK</td> <td></td> <td>0.000115</td>  | 38 | -12    |         | •          | 5.2e6             | 4.2e6 |               |           | AVGASFPLYEPAK                   |   | 0.000115    |
| 40   -   +4.66   3.86   SAYQEAMDISK   1xColdation [M7(100])   2.084     41   -   1.777   1.987   FNECGHVLYADIK   1xCarbamidomethyl[Cd]   4.664     42   -   3.86   4.166   LVTQDTRELK   1xCarbamidomethyl[Cd]   4.664     43   -   1.977   1.987   C.877   FAELQANLAR   4.744     44   -   1.977   1.987   C.877   FAELQASTAN   4.744     45   -   1.487   1.487   FAELQSTEAK   1.864   6.874     45   -   4.286   4.166   C.NPVINFAEFSK   C.664   6.874     47   -   5.286   7.866   GLLGCNIIPLQR   1xCarbamidomethyl[C5]   2.2164     48   -   -   1.862   NACEDNULOTAGR   1xCarbamidomethyl[C5]   2.2164     49   -   -   2.886   2.886   NACEDNULOTAGR   1xCarbamidomethyl[C5]   2.2164     51   -   2.186   2.086   MACEDNULVTAGR   2.0764   3.3864     51   -   2.186   2.086   MACG   | 39 | -12    |         | •          | 2.8e7             | 3.2e7 |               |           | DYAFVHFEDR                      |   | 5.16e-05    |
| 41   -   177   197   197   4664     42   -   386   4166   LVTQDTENELK   1xCarbanidomethyl [C4]   4664     43   -   -   386   4166   LVTQDTENELK   651ed     44   -   -   187   2087   KEEELQAALAR   1xCarbanidomethyl [C4]   651ed     44   -   -   4187   1487   1867   77ed   77ed   77ed   77ed     44   -   -   4286   4183   KIPEYPYNFAEESK   22e6   22e6   22e6   22e6   22e6   687ed   687ed   1xCarbanidomethyl [C5]   22te4   22e6   1996   1996   22e6   687ed   1996   1996   22e6   1996   1996   22e6   1996   1996   1996   22e6   1996   <   | 40 | -12    |         | •          | 4.8e6             | 3.9e6 |               |           | SAYQEAMDISK                     | 1×Oxidation [M7(100)]                                   | 2.08e-05    |
| 42   1   3.8.6   4.1.6   L/TQDTENELK   6.914-4     43   1   1.187   2.0.7   KEEELQAALAR   4.7.64     44   1   1.187   2.0.7   KEEELQAALAR   4.7.64     45   1   4.7.64   1.4.7   1.4.7   1.6.6.64     45   1   4.2.86   4.1.68   KNPEVPVNFAEFSK   2.2.6.6     45   1   2.7.86   3.2.6   QLAECEELER   6.876-4     46   1   2.2.86   7.866   GLIC.NIP.QR   1×Carbanidomethyl [C5]   2.2.16     48   1   1.5.66   1.7.66   GLIC.NIP.QR   1×Carbanidomethyl [C5]   2.2.16     49   1   2.2.88   2.2.88   VVDALGNADGK   6.336-4     50   1   2.2.86   2.4.86   NQGFDV/LVDTAGR   2.0.76     51   1   1.9.88   2.4.86   AVGEIVQDYDSDK   7.826-4     51   1   1.9.88   2.4.86   AVGEIVQDYDSDK   7.826-4     52   1   6.4.6   5.9.66   AVGEIVQDYDSDK   7.826-4     54   1   | 41 | -12    |         | •          | 1.7e7             | 1.9e7 |               |           | FNECGHVLYADIK                   | 1×Carbamidomethyl [C4]                                  | 4.66e-07    |
| 43   -   18-7   20-7   KEELQAALAR   4.7-6     44   -   14-7   14-7   FAEALGSTEAK   1.66-4     45   -   4.2-6   4.1-6   KNPEVPNFAEFSK   2.6-6     45   -   2.7-6   3.2-6   GLACGELER   6.87-6     47   -   5.2-6   7.6-6   GLACGELER   6.87-6     47   -   5.2-6   7.6-6   GLACGNIPLQR   1xCarbanidomethyl[C5]   2.21-6     48   -   -   1.5-6   FUCAPLDACGDNVLQEK   1.9-6   1.9-6     49   -   -   2.2-8   2.2-8   1.9-6   1.9-6   3.9-6     51   -   -   2.2-8   2.9-8   1.9-6   1.9-6   3.9-6 <td>42</td> <td>-12</td> <th></th> <td>•</td> <th>3.8e6</th> <td>4.1e6</td> <td></td> <td></td> <td>LVTQDTENELK</td> <td></td> <td>6.91e-06</td>   | 42 | -12    |         | •          | 3.8e6             | 4.1e6 |               |           | LVTQDTENELK                     |   | 6.91e-06    |
| 44   -   -   14-7   14-7   FAELGSTEAK   166-4     45   -   -   42-8   41-8   KNPEVPVNFAEFSK   2.66     45   -   -   42-8   41-8   KNPEVPVNFAEFSK   2.66     47   -   -   52-86   7.66   GLACGELER   1×Carbanidomethyl [C5]   2.21-6     48   -   -   52-86   7.66   GLICCNIPLQR   1×Carbanidomethyl [C5]   2.21-6     49   -   -   2.288   2.288   VVDALGNAIDGK   6.33-4     50   -   2.186   2.066   HQAFEAELSANGSR   3.86-6     51   -   1.966   2.468   NGGFDV/VDTAGR   2.07-6     52   -   6.468   6.066   AVGEIVQDYDSDK   7.82-6     53   -   1.447   1.447   GTYLATHOR   6.33-6     54   -   2.38-8   VVDALGNAIDEK   5.36-6     55   -   -   4.48   9.86   LAVAATAPDAFINEEVDER   7.42-6     55   -   -   1.487   3.86   TSPA   | 43 | -12    |         | •          | 1.9e7             | 2.0e7 |               |           | KEEELQAALAR                     |   | 4.7e-06     |
| 45   -   4.2a6   4.1e6   KIPEYPVINFAEFSK   2.2e4     46   -   2.7a6   3.2a6   QLAEQEELER   6.87e4     47   -   5.2a6   7.8e6   GLIGCNIPLQR   1xCarbanidomethyl[C5]   2.2te4     48   -   -   1.8e6   1.7e6   UVQAPLDADGDNVLQEK   134e4     49   -   2.2a8   2.2a8   VVDALGNAIDGK   6.33e4     50   -   2.1e6   2.0e6   MAGFEDXLVDTAGR   2.0fe4     51   -   1.9e5   2.4e6   NQGFDV/LVDTAGR   2.0fe4     51   -   1.9e5   2.4e6   NQGFDV/LVDTAGR   2.0fe4     52   -   6.4e6   0.9e6   AVGEIVQDYDSDK   7.8e4     53   -   1.4e7   1.4e7   GTVLTFHQR   6.33e4     54   -   -   2.3e8   2.3e8   TSPADHORSVSERSGGSAVDSVAGEHSVSR   5.39e4     54   -   -   1.4e7   1.4e7   QADLYSEGLHPR   2.4e64   5.39e4     55   -   -   1.4e7   1.7e7   QADLYSEGLHPR   2.4e64<   | 44 | -12    |         | •          | 1.4e7             | 1.4e7 |               |           | FAEALGSTEAK                     |   | 1.66e-05    |
| 46   | 45 | -12    |         | •          | 4.2e6             | 4.1e6 |               |           | KNPEVPVNFAEFSK                  |   | 2.6e-07     |
| 47   □   ●   5.86   7.86   GLOCNIFLQR   1xCarbanidomethyl [C5]   2.214     48   □   ●   15.86   17.86   LVQAPLDADGDNVLQEK   1.94e4     49   □   ●   2.286   LVQAPLDADGDNVLQEK   1.94e4     50   □   ●   2.286   ■   HQAFEAELSANGSR   3.86e4     50   □   ●   8.466   0.06 EPW/VDAGR   2.07e4   3.86e4     52   □   ●   8.466   0.06 EPW/VDAGR   2.07e4   6.33e4     52   □   ●   8.466   0.06 EPW/VDAGR   0.07PW/VDAGR   2.07e4     52   □   ●   8.468   8.066   AVGE/VQDYDSDK   7.82e4   6.33e4     53   □   ●   1.447   1.447   GTYLATHAR   6.33e4   6.33e4     54   □   ●   1.487   3.866   MUQAPM/VDYDSDK   7.82e4   6.33e4     55   □   ●   1.487   3.86   TSPADHGSVGSESGGSAVDSVAGEHSVSR   7.82e4   6.33e4     57   □   ●   1.471   1.87  | 46 | -12    |         | •          | 2.7e6             | 3.2e6 |               |           | QLAEQEELER                      |   | 6.87e-05    |
| 48   15.60   17.63   LVQAPLDADGDN/UQEK   1946-4     49   2   2.268   2.268   VVDALGNAIDGK   6.336-4     50   2   2.268   2.268   VVDALGNAIDGK   6.336-4     51   2   1.864   2.268   NQGPDV/LVDTAGR   2.207-4     51   2   6   4.66   0.66   AVGEIVQDYDSDK   7.826-4     51   2   6   4.66   0.66   AVGEIVQDYDSDK   7.826-4     52   2   6   4.66   0.66   AVGEIVQDYDSDK   7.826-4     54   2   6   2.368   2.368   YGVSGYPTLK   5.476-6     55   2   4   1.467   1.477   0.00000000000000000000000000000000000  | 47 | -12    |         | •          | 5.2e6             | 7.6e6 |               |           | GLLGCNIIPLQR                    | 1×Carbamidomethyl [C5]                                  | 2.21e-05    |
| 49   | 48 | -12    |         | •          | 1.5e6             | 1.7e6 |               |           | LVQAPLDADGDNVLQEK               |   | 1.94e-06    |
| 50 +0   •   2 +66   2 4e8   HQAFEAELSANGSR   3 8e4     51 +0   •   1 9e8   2 4e8   NQGFDV/LVDAGR   2 07e4     52 +0   •   6 4e8   8 0e6   AVGEVQDYDSDK   7 82e4     53 +0   •   1 4e7   1 4e7   GTYLATFHQR   6 3ae4     54 +0   •   2 3e8   YOUSGYPTIK   5 47e4     55 +0   •   1 1e8   7 3e5   TSPADHGSVGESGSAUSVAGEHSVSGR   5 39e4     56 +0   •   1 1e8   7 3e5   TSPADHGSVGESGSAUSVAGEHSVSGR   5 39e4     58 +0   •   3 0e7   3 8e7   VTEYGLTPTEK   3 2e4     58 +0   •   2 0e7   2 8e7   LAILGHNEVSK   3 2e4     59 +0   •   2 0e7   2 8e7   LAILGHNEVSK   3 2e4  | 49 | -12    |         | •          | 2.2e8             | 2.2e8 |               |           | VVDALGNAIDGK                    |   | 6.33e-06    |
| 51   Image: Section of the sectin of the section of the section of the section of the section of  | 50 | -12    |         | •          | 2.1e6             | 2.0e6 |               |           | HQAFEAELSANQSR                  |   | 3.86e-07    |
| 52   -   6.4-6   6.0-8   AVGE/VQ/VDSDK   7.82-4     53   -   1.4-7   1.4-7   GTVLATFHQR   6.33-4     54   -   2.3-8   -   GTVLATFHQR   6.33-4     55   -   -   4.7-6   3.8-6   LLAVAATAPDAFINEEVFDER   7.45-4     55   -   -   1.148   7.36-5   TSPADHGSVGSESGGAVDSVAGEHSVSGR   5.93-4     57   -   -   1.148   7.36-5   TSPADHGSVGSESGGAVDSVAGEHSVSGR   5.93-4     58   -   -   3.0-7   3.9-7   QADLYSEGLHPR   2.48-4     58   -   -   2.68-7   -   2.48-7   2.48-4     59   -   -   3.0-7   3.9-7   VIEVGLTFEK   9.2-4     59   -   -   2.68-7   2.8-7   LAIGHNEVSK   1.25-4     60   -   -   1.0-7   LAIGHNEVSK   1.25-4     60   -   1.0-7   LAIGHNEVSK   5.96-4   | 51 | -12    |         | •          | 1.9e6             | 2.4e6 |               |           | NQGFDVVLVDTAGR                  |   | 2.07e-06    |
| 53   Image: Signal Si   | 52 | -12    |         | •          | 6.4e6             | 6.0e6 |               |           | AVGEIVQDYDSDK                   |   | 7.82e-06    |
| 54   Image: Section of the sectin of the section of the section of the section of the section of  | 53 | -12    |         | •          | 1.4e7             | 1.4e7 |               |           | GTYLATFHQR                      |   | 6.33e-06    |
| 55 Image: Constraint of the second  | 54 | -12    |         | •          | 2.3e8             | 2.3e8 |               |           | YGVSGYPTLK                      |   | 5.47e-05    |
| 56   Image: Section of the sectin of the section of the section of the section of the section of  | 55 | -12    |         | •          | 4.7e6             | 9.8e6 |               |           | LLAVAATAPPDAPNREEVFDER          |   | 7.45e-06    |
| 57 Image: Strate Stra   | 56 | -12    |         | •          | 1.1e6             | 7.3e5 |               |           | TSPADHGGSVGSESGGSAVDSVAGEHSVSGR |   | 5.93e-06    |
| 58 ↔     •     3.8-7     V/FFVGLTFEK     9.2-6-7     9.2-6-7     1.25-6       59 ↔     •     2.647     2.647     LAILGIHNEVSK     1.25-6       60 ↔     •     •     1.047     ILDADPILISLR     5.96-6  | 57 | -12    |         | •          | 1.4e7             | 1.7e7 |               |           | QADLYISEGLHPR                   |   | 2.48e-06    |
| 59 ↔     C     2 6e7     2 fe7     LAILGIHNEVSK     125e-4       60 ↔     C     10e7     11e7     DADPILISLR     596e-4  | 58 | -12    |         | •          | 3.0e7             | 3.9e7 |               |           | WTEYGLTFTEK                     |   | 9.2e-06     |
| 60 ⇒ 🖸 🔴 1.0e7 1.1e7 🔲 DADPILISLR 5.96e-0  | 59 | -12    |         | •          | 2.6e7             | 2.6e7 |               |           | LAILGIHNEVSK                    |   | 1.25e-06    |
|  | 60 | -12    |         | •          | 1.0e7             | 1.1e7 |               |           | DADPILISLR                      |   | 5.96e-05    |

Figure 4: Peptide Groups table

| Pible |         | en aloups    Pepide al | oups    Pa | ms max    | ma apecu | uminio | FJ Feau   | Guarinesuit                                 |          |  |              |               |        |                 |        |              |             |
|-------|---------|------------------------|------------|-----------|----------|--------|-----------|---|----------|--|--------------|---------------|--------|-----------------|--------|--------------|-------------|
| i P   | Checked | Sequence               | Peak Start | Peak Apex | Peak End | Charge | M/Z       | Modifications                               | Area     | Spectrum File                              | MasterScanNr | Identified By | Reason | TheoreticalMass | Score  | Confidence + | Show Spects |
| 1 👳   |         | AHQVVEDGYEFFAK         | 104.08     | 104.36    | 104.62   | 2      | 820.39264 |   | 1.58E+07 | 20151127_QexHF1_RSLC5_Hela01ug_1711_01.raw | 0            | MS/MS         | 0      | 1639.77510      | -0.282 | High         | Shav XIC    |
| 2 👳   |         | ESLEALLOR              | 118.75     | 119.02    | 119.30   | 2      | 529.79620 |   | 5.22E+06 | 20151127_QexHF1_RSLC5_Hela01ug_1711_02.raw | 0            | MS/MS         | 0      | 1058.58405      | -0.059 | High         | Shaw XIC    |
| 3 👳   |         | RPELLTHSTTEVTQPR       | 56.43      | 56.73     | 57.08    | 4      | 467.00290 |   | 7.07E+06 | 20151127_QexHF1_RSLC5_Hela01ug_1711_02.raw | 0            | MS/MS         | 0      | 1864.98755      | -0.297 | High         | Shaw XIC    |
| 4 👳   |         | RPELLTHSTTEVTQPR       | 57.06      | 57.39     | 57.73    | 4      | 467.00290 |   | 7.25E+06 | 20151127_QexHF1_RSLC5_Hela01ug_1711_01.raw | 0            | MBR           | 0      | 1864.98755      | -0.382 | High         | Show XIC    |
| 5 👳   |         | NANAVMEYEK             | 56.56      | 56.72     | 56.91    | 2      | 584.76794 |   | 2.19E+06 | 20151127_QexHF1_RSLC5_Hela01ug_1711_01.raw | 0            | MS/MS         | 0      | 1168.53030      | -0.193 | High         | Show XIC    |
| 6 👳   |         | ESLEALLOR              | 118.97     | 119.21    | 119.41   | 2      | 529.79437 |   | 4.25E+06 | 20151127_QexHF1_RSLC5_Hela01ug_1711_01.raw | 0            | MS/MS         | 0      | 1058.58405      | -0.088 | High         | Shaw XIC    |
| 7 👳   |         | AIVDALPPPCESACTVPTI    | 118.61     | 119.27    | 120.21   | 3      | 785.71075 | C10(Carbamidomethyl):High. C14(Carbamidomet | 1.66E+07 | 20151127_QexHF1_RSLC5_Hela01ug_1711_02.raw | 0            | MS/MS         | 0      | 2355.12067      | -0.170 | High         | Shaw XIC    |
| 8 👳   |         | AIVDALPPPCESACTVPTI    | 118.84     | 119.44    | 120.25   | 3      | 785.71082 | C10(Carbamidomethyl):High. C14(Carbamidomet | 1.35E+07 | 20151127_QexHF1_RSLC5_Hela01ug_1711_01.raw | 0            | MS/MS         | 0      | 2355.12067      | -0.252 | High         | Show XIC    |
| 9 👳   |         | PGQEAPVLPK             | 56.53      | 56.98     | 57.33    | 2      | 518.29541 |   | 1.52E+07 | 20151127_QexHF1_RSLC5_Hela01ug_1711_01.raw | 0            | MS/MS         | 0      | 1035.58332      | -0.298 | High         | Show XIC    |
| 10 👳  |         | PGQEAPVLPK             | 55.93      | 56.37     | 56.70    | 2      | 518.29541 |   | 1.49E+07 | 20151127_QexHF1_RSLC5_Hela01ug_1711_02.raw | 0            | MS/MS         | 0      | 1035.58332      | -0.008 | High         | Show XIC    |
| 11 👳  |         | VTVDTGVIPASEEK         | 82.29      | 82.60     | 82.87    | 2      | 722.87854 |   | 1.57E+07 | 20151127_QexHF1_RSLC5_Hela01ug_1711_01.raw | 0            | MS/MS         | 0      | 1444.75297      | -0.380 | High         | Shav XIC    |
| 12 👳  |         | AW/GPGLHGGIVGR         | 82.05      | 82.38     | 82.78    | 3      | 426.23444 |   | 3.25E+07 | 20151127_QexHF1_RSLC5_Hela01ug_1711_02.raw | 0            | MS/MS         | 0      | 1276.69091      | -0.389 | High         | Shav XIC    |
| 13 😐  |         | AW/GPGLHGGIVGR         | 82.30      | 82.65     | 83.10    | 3      | 426.23502 |   | 3.13E+07 | 20151127_QexHF1_RSLC5_Hela01ug_1711_01.raw | 0            | MS/MS         | 0      | 1276.69091      | -0.186 | High         | Shav XIC    |
| 14 😐  |         | EEDGSLSLDGADSTGVV/     | 99.10      | 99.37     | 99.63    | 2      | 925.43469 |   | 1.11E+07 | 20151127_QexHF1_RSLC5_Hela01ug_1711_01.raw | 0            | MS/MS         | 0      | 1849.86616      | -0.163 | High         | Shav XIC    |
| 15 😐  |         | YNEETFGYEVPIK          | 118.80     | 119.07    | 119.49   | 2      | 794.88269 |   | 9.70E+06 | 20151127_QexHF1_RSLC5_Hela01ug_1711_02.raw | 0            | MS/MS         | 0      | 1588.75297      | -0.102 | High         | Shav XIC    |
| 16 🗢  |         | YNEETFGYEVPIK          | 118.93     | 119.26    | 119.76   | 2      | 794.88098 |   | 8.81E+06 | 20151127_QexHF1_RSLC5_Hela01ug_1711_01.raw | 0            | MS/MS         | 0      | 1588.75297      | -0.343 | High         | Shav XIC    |
| 17 😐  |         | VTVDTGVIPASEEK         | 81.87      | 82.35     | 82.63    | 2      | 722.88019 |   | 1.59E+07 | 20151127_QexHF1_RSLC5_Hela01ug_1711_02.raw | 0            | MS/MS         | 0      | 1444.75297      | -0.243 | High         | Shav XIC    |
| 18 👳  |         | HWMLDK                 | 56.90      | 57.62     | 58.77    | 2      | 415.20547 |   | 4.10E+07 | 20151127_QexHF1_RSLC5_Hela01ug_1711_01.raw | 0            | MBR           | 0      | 829.40252       | -0.294 | High         | Shav XIC    |
| 19 👳  |         | HWMLDK                 | 56.26      | 56.99     | 58.21    | 2      | 415.20547 |   | 4.47E+07 | 20151127_QexHF1_RSLC5_Hela01ug_1711_02.raw | 0            | MS/MS         | 0      | 829.40252       | -0.359 | High         | Shav XIC    |
| 20 👳  |         | GELLALVK               | 102.55     | 102.78    | 102.93   | 2      | 421.77176 |   | 3.20E+06 | 20151127_QexHF1_RSLC5_Hela01ug_1711_02.raw | 0            | MS/MS         | 0      | 842.53458       | -0.192 | High         | Shav XIC    |
| 21 👳  |         | PSWADQVEEEGEDDK        | 98.84      | 99.10     | 99.38    | 2      | 867.35773 |   | 1.89E+07 | 20151127_QexHF1_RSLC5_Hela01ug_1711_02.raw | 0            | MS/MS         | 0      | 1733.71368      | -0.056 | High         | Show XIC    |
| 22 🗢  |         | LDLFANVVHVK            | 118.78     | 119.03    | 119.22   | 2      | 627.86346 |   | 3.27E+06 | 20151127_QexHF1_RSLC5_Hela01ug_1711_02.raw | 0            | MS/MS         | 0      | 1254.72048      | -0.219 | High         | Show XIC    |
| 23 🗢  |         | LDLFANVVHVK            | 119.04     | 119.25    | 119.45   | 2      | 627.86383 |   | 2.55E+06 | 20151127_QexHF1_RSLC5_Hela01ug_1711_01.raw | 0            | MS/MS         | 0      | 1254.72048      | -0.067 | High         | Show XIC    |
| 24 😑  |         | TVSDLIDQK              | 71.75      | 72.21     | 72.91    | 2      | 509.77448 |   | 2.24E+07 | 20151127_QexHF1_RSLC5_Hela01ug_1711_02.raw | 0            | MBR           | 0      | 1018.54152      | -0.138 | High         | Show XIC    |
| 25 -= |         | EVDEQmLNVQNK           | 56.57      | 57.30     | 58.75    | 2      | 731 84583 | M6(Oxidation): High                         | 4 29E+07 | 20151127 GexHF1 RSLC5 Hela01ug 1711 01.raw | 0            | MS/MS         | 0      | 1462.68423      | -0.362 | High         | Shaw XIC    |

Figure 5: Feature table



Figure 6: XIC of a single PjFeature

| P  | roteir | ns Pro  | tein Groups Peptide Groups | PSMs M | S/MS Spectrum Info | PJ Features QuanResult    |              |             |             |            |               |
|----|--------|---------|----------------------------|--------|--------------------|---------------------------|--------------|-------------|-------------|------------|---------------|
| đ  | 9      | Checked | Sequence                   | charge | M/Z                | Modifications             | File20151127 | File20151 - | ID_2015112; | ID_2015112 | Show Spectrum |
| 1  |        |         | ITLPVDFVTADK               | 2      | 659.86676025390625 |                           | 2.57E+09     | 3.35E+09    | MS/MS       | MS/MS      | Show XIC      |
| 2  | -122   |         | GALQNIIPASTGAAK            | 2      | 706.39984130859375 |                           | 3.05E+09     | 3.13E+09    | MS/MS       | MS/MS      | Show XIC      |
| 3  | -12    |         | TIAPALVSK                  | 2      | 450.28134155273437 |                           | 2.45E+09     | 2.46E+09    | MS/MS       | MS/MS      | Show XIC      |
| 4  | -122   |         | VAPEEHPVLLTEAPLNPK         | 3      | 652.02716064453125 |                           | 2.21E+09     | 2.39E+09    | MS/MS       | MS/MS      | Show XIC      |
| 5  | -122   |         | YSLEPVAVELK                | 2      | 624.34765625       |                           | 2.04E+09     | 2.23E+09    | MS/MS       | MS/MS      | Show XIC      |
| 6  | -12    |         | AVFPSIVGR                  | 2      | 473.27972412109375 |                           | 2.05E+09     | 2.09E+09    | MS/MS       | MS/MS      | Show XIC      |
| 7  | -122   |         | VPTANVSVVDLTCR             | 2      | 765.901611328125   | C13(Carbamidomethyl):High | 1.75E+09     | 1.95E+09    | MS/MS       | MS/MS      | Show XIC      |
| 8  | -122   |         | YISPDQLADLYK               | 2      | 713.36773681640625 |                           | 1.48E+09     | 1.93E+09    | MS/MS       | MS/MS      | Show XIC      |
| 9  | -12    |         | IGAEVYHNLK                 | 3      | 381.87637329101562 |                           | 1.78E+09     | 1.83E+09    | MS/MS       | MS/MS      | Show XIC      |
| 10 | -122   |         | LQSTFVFEEIGR               | 2      | 713.3701171875     |                           | 1.38E+09     | 1.81E+09    | MBR         | MS/MS      | Show XIC      |
| 11 | -122   |         | LTGMAFR                    | 2      | 398.21267700195312 |                           | 1.68E+09     | 1.80E+09    | MS/MS       | MS/MS      | Show XIC      |
| 12 | -122   |         | LGDVYVNDAFGTAHR            | 3      | 545.6031494140625  |                           | 1.59E+09     | 1.76E+09    | MS/MS       | MS/MS      | Show XIC      |
| 13 | -122   |         | GYSFTTTAER                 | 2      | 566.767822265625   |                           | 1.67E+09     | 1.73E+09    | MS/MS       | MS/MS      | Show XIC      |
| 14 | -      |         | AGFAGDDAPR                 | 2      | 488.72769165039063 |                           | 1.69E+09     | 1.73E+09    | MS/MS       | MS/MS      | Show XIC      |
| 15 | -122   |         | ALMDEVVK                   | 2      | 452.74356079101562 |                           | 1.63E+09     | 1.66E+09    | MBR         | MS/MS      | Show XIC      |
| 16 | -122   |         | EGLELLK                    | 2      | 401.23919677734375 |                           | 1.61E+09     | 1.63E+09    | MS/MS       | MBR        | Show XIC      |
| 17 | -      |         | LVIITAGAR                  | 2      | 457.294921875      |                           | 1.58E+09     | 1.62E+09    | MS/MS       | MS/MS      | Show XIC      |
| 18 | -122   |         | VIGSGCNLDSAR               | 2      | 624.80303955078125 | C6(Carbamidomethyl):High  | 1.60E+09     | 1.60E+09    | MS/MS       | MS/MS      | Show XIC      |
| 19 | -122   |         | FEDENFILK                  | 2      | 577.79071044921875 |                           | 1.43E+09     | 1.50E+09    | MS/MS       | MS/MS      | Show XIC      |
| 20 | -      |         | APIIAVTR                   | 2      | 420.76870727539062 |                           | 1.46E+09     | 1.48E+09    | MS/MS       | MS/MS      | Show XIC      |
| 21 | -122   |         | LNVTEQEK                   | 2      | 480.7537841796875  |                           | 1.51E+09     | 1.47E+09    | MS/MS       | MS/MS      | Show XIC      |
| 22 | -122   |         | LPLQDVYK                   | 2      | 488.27874755859375 |                           | 1.45E+09     | 1.45E+09    | MS/MS       | MS/MS      | Show XIC      |
| 23 | -122   |         | HTAAPTDPADGPV              | 2      | 624.79681396484375 |                           | 1.48E+09     | 1.45E+09    | MS/MS       | MBR        | Show XIC      |
| 24 | -12    |         | IQLINNMLDK                 | 2      | 601.33514404296875 |                           | 1.23E+09     | 1.45E+09    | MS/MS       | MS/MS      | Show XIC      |
| 25 | -12    |         | IGGIGTVPVGR                | 2      | 513.307861328125   |                           | 1.44E+09     | 1.44E+09    | MS/MS       | MS/MS      | Show XIC      |
| 26 | -12    |         | TLSDYNIQK                  | 2      | 541.27935791015625 |                           | 1.42E+09     | 1.43E+09    | MS/MS       | MS/MS      | Show XIC      |
| 27 | -122   |         | LQDAEIAR                   | 2      | 458.24810791015625 |                           | 1.41E+09     | 1.41E+09    | MS/MS       | MS/MS      | Show XIC      |
| 28 | -12    |         | PISTLDNR                   | 2      | 458.247802734375   |                           | 1.38E+09     | 1.38E+09    | MS/MS       | MBR        | Show XIC      |
| 29 | -122   |         | TCHSFIINEK                 | 2      | 624.8045654296875  | C2(Carbamidomethyl):High  | 1.12E+09     | 1.38E+09    | MBR         | MS/MS      | Show XIC      |
| 30 | -00    |         | VDFNVPMK                   | 2      | 475.24459838867187 |                           | 1.29E+09     | 1.37E+09    | MS/MS       | MS/MS      | Show XIC      |

Figure 7: QuanResult table



Figure 8: XIC of a Feature in different samples

# 3.3 Scoring

Peakjuggler also tries to give the quantification a score which indicates how well the integration went. Base for this score was the DeMix-Q paper by Zhang et al.<sup>1</sup> Peakjuggler also performs a target-decoy quantification and assigns confidences to the Features. **This feature is still under development!** 

<sup>1</sup>Bo Zhang, Lukas Kall, and Roman A. Zubarev

DeMix-Q: Quantification-centered Data Processing Workflow Mol Cell Proteomics mcp.O115.055475. First Published on January 4, 2016, doi:10.1074/mcp.O115.055475