Peakjuggler Manual

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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
- **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`

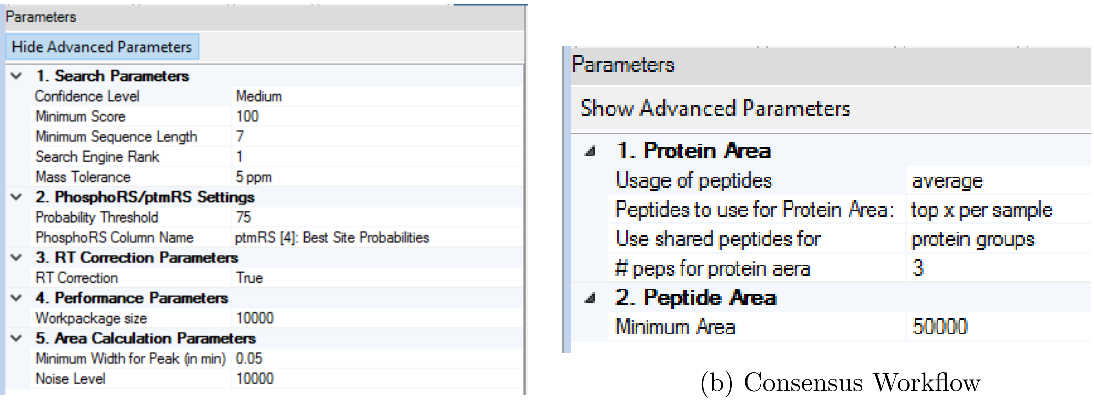
Peakjuggler consists of two nodes, one for the processing workflow and one for the consensus workflow.

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



Parameters

Hide Advanced Parameters

1. Search Parameters	
Confidence Level	Medium
Minimum Score	100
Minimum Sequence Length	7
Search Engine Rank	1
Mass Tolerance	5 ppm
2. PhosphoRS/ptmRS Settings	
Probability Threshold	75
PhosphoRS Column Name	ptmRS [4]: Best Site Probabilities
3. RT Correction Parameters	
RT Correction	True
4. Performance Parameters	
Workpackage size	10000
5. Area Calculation Parameters	
Minimum Width for Peak (in min)	0.05
Noise Level	10000

(a) Processing Workflow

Parameters

Show Advanced Parameters

1. Protein Area	
Usage of peptides	average
Peptides to use for Protein Area:	top x per sample
Use shared peptides for	protein groups
# peps for protein aera	3
2. Peptide Area	
Minimum Area	50000

(b) Consensus Workflow

Figure 1: Node Parameters

- **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

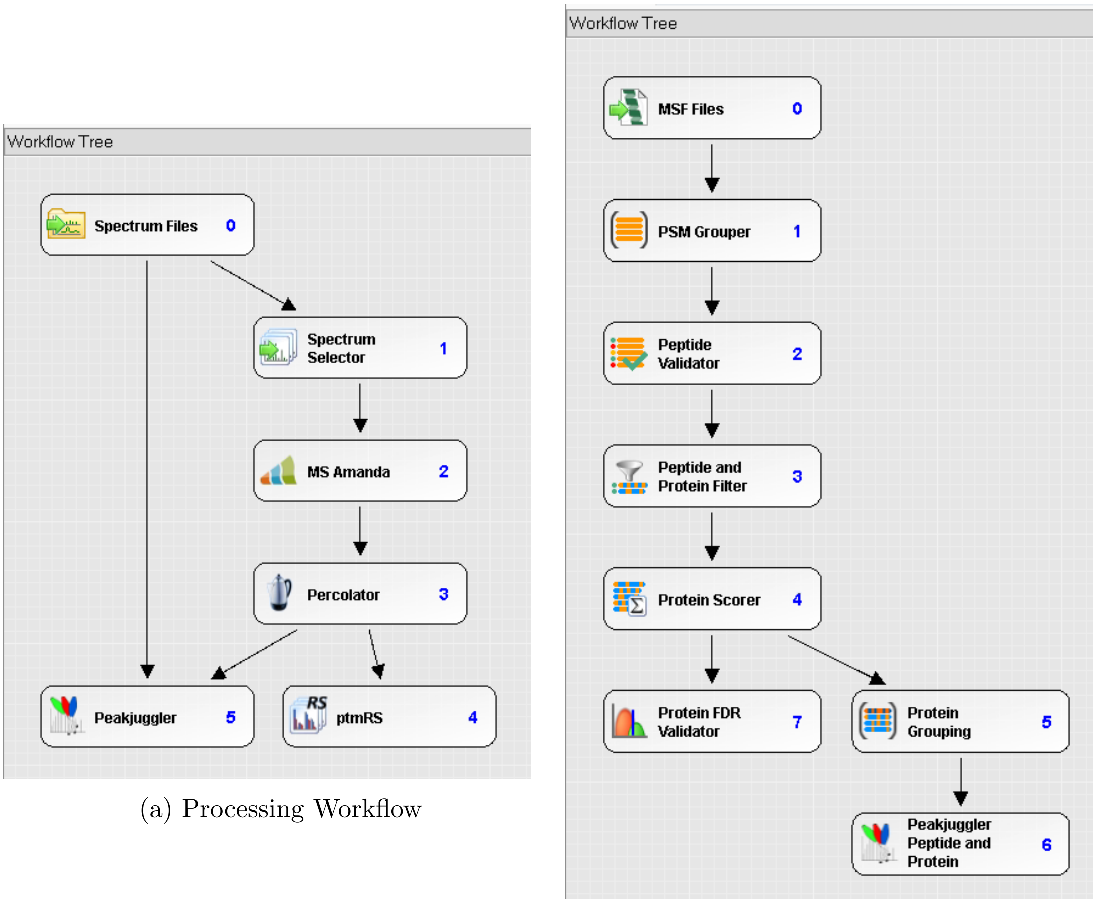
The consensus node needs to be connected to the *Protein Grouping* node.

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

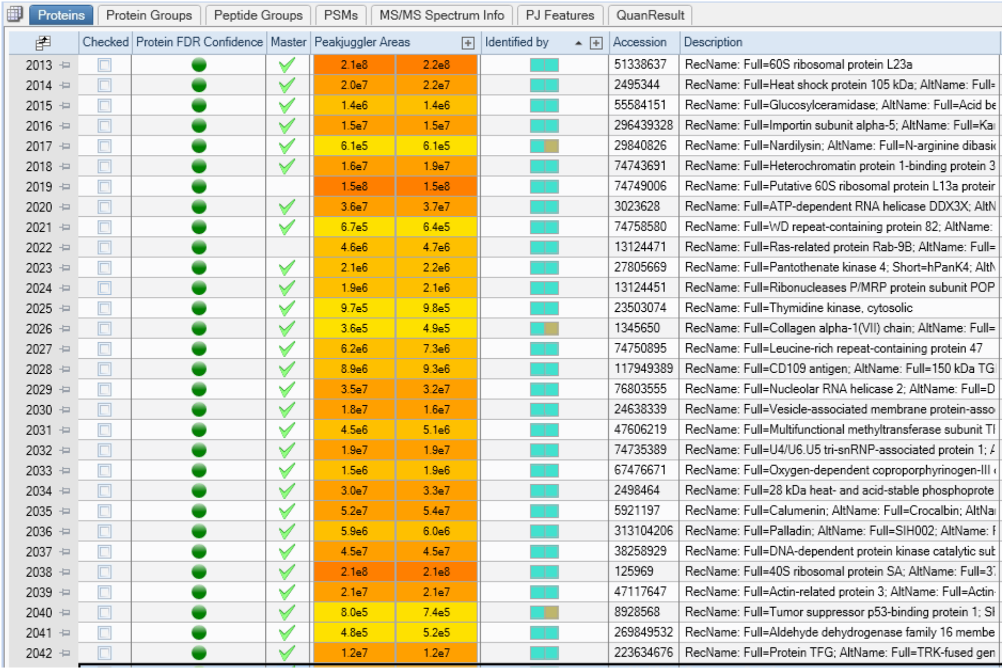


(a) Processing Workflow

(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



	Checked	Protein FDR Confidence	Master	Peakjuggler Areas		Identified by	Accession	Description
2013	☐	●	✓	2.1e8	2.2e8	🟦🟦	51338637	RecName: Full=60S ribosomal protein L23a
2014	☐	●	✓	2.0e7	2.2e7	🟦🟦	2495344	RecName: Full=Heat shock protein 105 kDa; AltName: Full=
2015	☐	●	✓	1.4e6	1.4e6	🟦🟦	55584151	RecName: Full=Glucosylceramidase; AltName: Full=Acid b
2016	☐	●	✓	1.5e7	1.5e7	🟦🟦	296439328	RecName: Full=Importin subunit alpha-5; AltName: Full=Ka
2017	☐	●	✓	6.1e5	6.1e5	🟦🟫	29840826	RecName: Full=Nardilysin; AltName: Full=N-arginine dibasi
2018	☐	●	✓	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 protei
2020	☐	●	✓	3.6e7	3.7e7	🟦🟦	3023628	RecName: Full=ATP-dependent RNA helicase DDX3X; AltN
2021	☐	●	✓	6.7e5	6.4e5	🟦🟦	74758580	RecName: Full=WD repeat-containing protein 82; AltName:
2022	☐	●		4.6e6	4.7e6	🟦🟦	13124471	RecName: Full=Ras-related protein Rab-9B; AltName: Full=
2023	☐	●	✓	2.1e6	2.2e6	🟦🟦	27805669	RecName: Full=Pantothenate kinase 4; Short=hPanK4; Alt
2024	☐	●	✓	1.9e6	2.1e6	🟦🟦	13124451	RecName: Full=Ribonucleases P/MRP protein subunit POP
2025	☐	●	✓	9.7e5	9.8e5	🟦🟦	23503074	RecName: Full=Thymidine kinase, cytosolic
2026	☐	●	✓	3.6e5	4.9e5	🟦🟫	1345650	RecName: Full=Collagen alpha-1(VII) chain; AltName: Full=
2027	☐	●	✓	6.2e6	7.3e6	🟦🟦	74750895	RecName: Full=Leucine-rich repeat-containing protein 47
2028	☐	●	✓	8.9e6	9.3e6	🟦🟦	117949389	RecName: Full=CD109 antigen; AltName: Full=150 kDa TG
2029	☐	●	✓	3.5e7	3.2e7	🟦🟦	76803555	RecName: Full=Nucleolar RNA helicase 2; AltName: Full=D
2030	☐	●	✓	1.8e7	1.6e7	🟦🟦	24638339	RecName: Full=Vesicle-associated membrane protein-asso
2031	☐	●	✓	4.5e6	5.1e6	🟦🟦	47606219	RecName: Full=Multifunctional methyltransferase subunit T
2032	☐	●	✓	1.9e7	1.9e7	🟦🟦	74735389	RecName: Full=U4/U6.U5 tri-snRNP-associated protein 1;
2033	☐	●	✓	1.5e6	1.9e6	🟦🟦	67476671	RecName: Full=Oxygen-dependent coproporphyrinogen-III
2034	☐	●	✓	3.0e7	3.3e7	🟦🟦	2498464	RecName: Full=28 kDa heat- and acid-stable phosphoprote
2035	☐	●	✓	5.2e7	5.4e7	🟦🟦	5921197	RecName: Full=Calumenin; AltName: Full=Crocalbin; AltNa
2036	☐	●	✓	5.9e6	6.0e6	🟦🟦	313104206	RecName: Full=Palladin; AltName: Full=SIH002; AltName:
2037	☐	●	✓	4.5e7	4.5e7	🟦🟦	38258929	RecName: Full=DNA-dependent protein kinase catalytic su
2038	☐	●	✓	2.1e8	2.1e8	🟦🟦	125969	RecName: Full=40S ribosomal protein SA; AltName: Full=3
2039	☐	●	✓	2.1e7	2.1e7	🟦🟦	47117647	RecName: Full=Actin-related protein 3; AltName: Full=Actin
2040	☐	●	✓	8.0e5	7.4e5	🟦🟫	8928568	RecName: Full=Tumor suppressor p53-binding protein 1; S
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

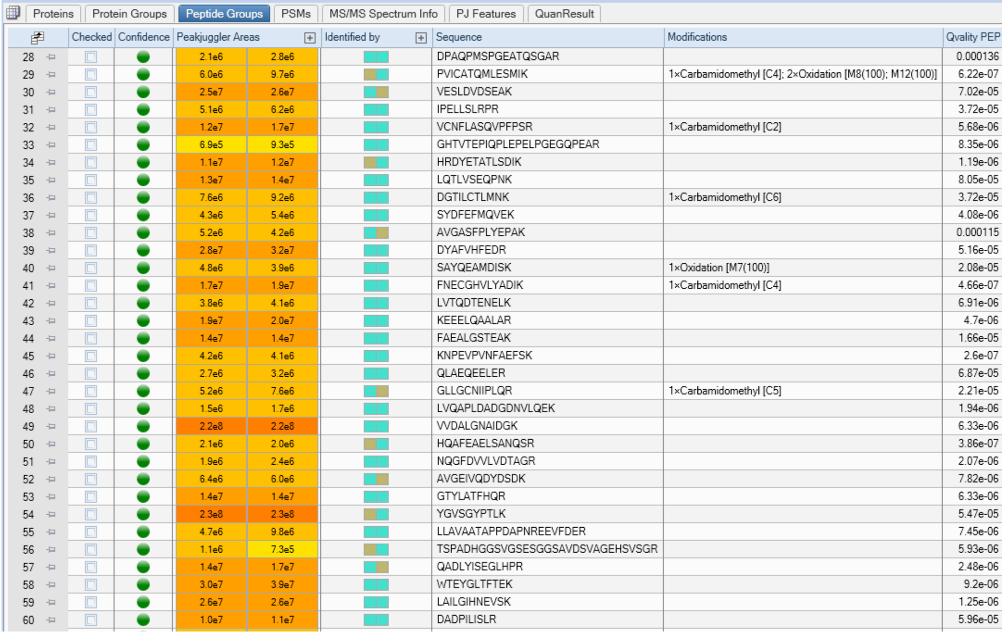
3.2.1 PjFeatures

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)

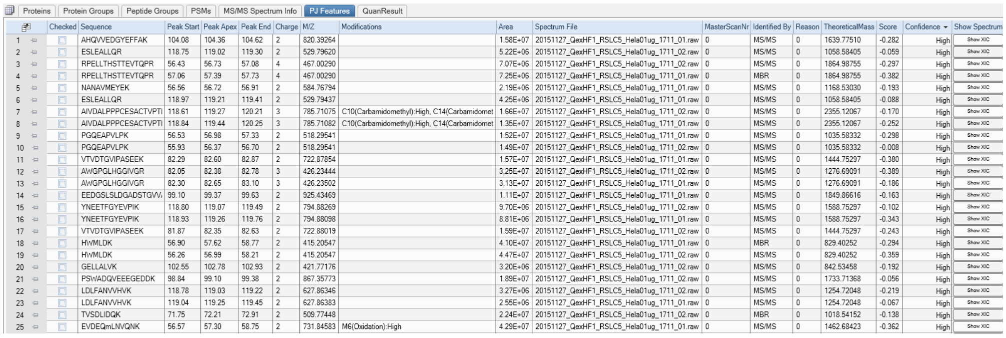
3.2.2 PjQuanResult

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)



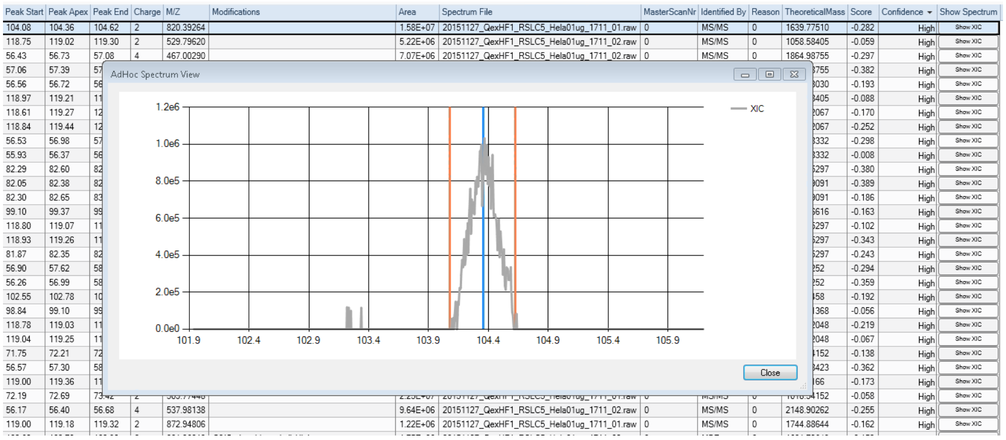
	Checked	Confidence	Peakjuggler Areas		Identified by	Sequence	Modifications	Qvality PEP
28	☐	●	2.1e6	2.8e6	🟦🟦	DPAQPMSPGEATQSGAR		0.000136
29	☐	●	6.0e6	9.7e6	🟫🟦	PVICATQMLESMIK	1×Carbamidomethyl [C4]; 2×Oxidation [M8(100); M12(100)]	6.22e-07
30	☐	●	2.5e7	2.6e7	🟦🟫	VESLDVDSEAK		7.02e-05
31	☐	●	5.1e6	6.2e6	🟦🟦	IPELLSLRPR		3.72e-05
32	☐	●	1.2e7	1.7e7	🟦🟦	VCNFLASQVPFPSR	1×Carbamidomethyl [C2]	5.68e-06
33	☐	●	6.9e5	9.3e5	🟦🟦	GHTVTEPIQPLEPELPGEGQPEAR		8.35e-06
34	☐	●	1.1e7	1.2e7	🟫🟦	HRDYETATLSDIK		1.19e-06
35	☐	●	1.3e7	1.4e7	🟦🟦	LQTLVSEQPNK		8.05e-05
36	☐	●	7.6e6	9.2e6	🟦🟦	DGTILCTLMNK	1×Carbamidomethyl [C6]	3.72e-05
37	☐	●	4.3e6	5.4e6	🟦🟦	SYDFEFMQVEK		4.08e-06
38	☐	●	5.2e6	4.2e6	🟦🟫	AVGASFPLYEPAK		0.000115
39	☐	●	2.8e7	3.2e7	🟦🟦	DYAFVHFEDR		5.16e-05
40	☐	●	4.8e6	3.9e6	🟦🟦	SAYQEAMDISK	1×Oxidation [M7(100)]	2.08e-05
41	☐	●	1.7e7	1.9e7	🟦🟦	FNECGHVLYADIK	1×Carbamidomethyl [C4]	4.66e-07
42	☐	●	3.8e6	4.1e6	🟦🟦	LVTQDTENELK		6.91e-06
43	☐	●	1.9e7	2.0e7	🟦🟦	KEEELQAALAR		4.7e-06
44	☐	●	1.4e7	1.4e7	🟦🟦	FAEALGSTEAK		1.66e-05
45	☐	●	4.2e6	4.1e6	🟦🟦	KNPEVPVNFAEFSK		2.6e-07
46	☐	●	2.7e6	3.2e6	🟦🟦	QLAEQEELER		6.87e-05
47	☐	●	5.2e6	7.6e6	🟦🟫	GLLGCNIIPLQR	1×Carbamidomethyl [C5]	2.21e-05
48	☐	●	1.5e6	1.7e6	🟦🟦	LVQAPLDADGDNVLQEK		1.94e-06
49	☐	●	2.2e8	2.2e8	🟦🟦	VVDALGNAIDGK		6.33e-06
50	☐	●	2.1e6	2.0e6	🟫🟦	HQAFEAELSANQSR		3.86e-07
51	☐	●	1.9e6	2.4e6	🟦🟦	NQGFDVVLVDTAGR		2.07e-06
52	☐	●	6.4e6	6.0e6	🟦🟫	AVGEIVQDYDSDK		7.82e-06
53	☐	●	1.4e7	1.4e7	🟦🟦	GTYLATFHQR		6.33e-06
54	☐	●	2.3e8	2.3e8	🟫🟦	YGVSGYPTLK		5.47e-05
55	☐	●	4.7e6	9.8e6	🟦🟦	LLAVAATAPPDAPNREEVFDER		7.45e-06
56	☐	●	1.1e6	7.3e5	🟫🟦	TSPADHGGSVGSESGGSAVDSVAGEHSVSGR		5.93e-06
57	☐	●	1.4e7	1.7e7	🟦🟫	QADLYISEGLHPR		2.48e-06
58	☐	●	3.0e7	3.9e7	🟦🟦	WTEYGLTFTEK		9.2e-06
59	☐	●	2.6e7	2.6e7	🟦🟦	LAILGIHNEVSK		1.25e-06
60	☐	●	1.0e7	1.1e7	🟦🟦	DADPILISLR		5.96e-05

Figure 4: Peptide Groups table



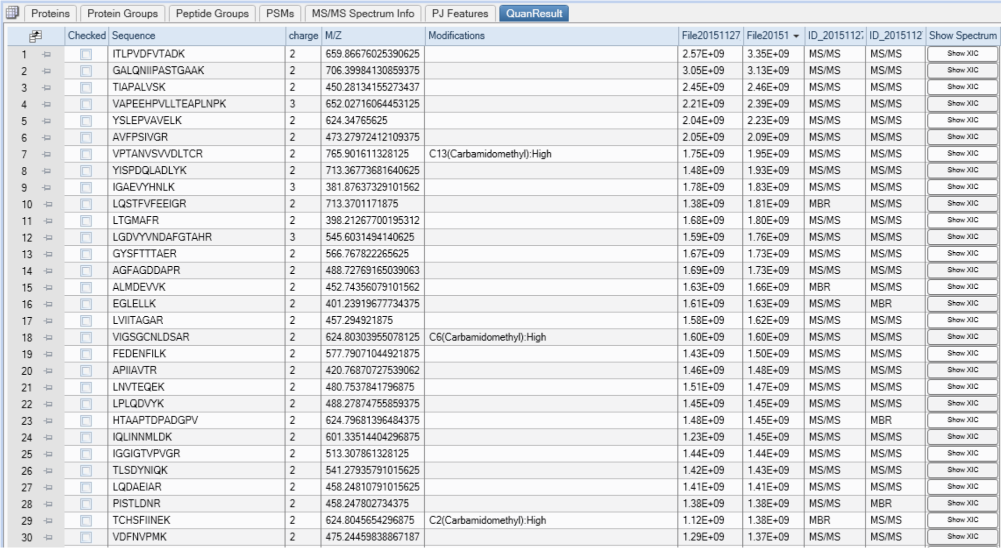
	Checked	Sequence	Peak Start	Peak Apex	Peak End	Charge	M/Z	Modifications	Area	Spectrum File	MasterScanNr	Identified By	Reason	TheoreticalMass	Score	Confidence	Show Spectrum
1	☐	AHQVVEDGYEFFAK	104.08	104.36	104.62	2	820.39264		1.58E+07	20151127_QexHF1_RSLC5_Hela01ug_1711_01.raw	0	MS/MS	0	1639.77510	-0.282	High	Show XIC
2	☐	ESLEALLQR	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	Show 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	Show 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	☐	ESLEALLQR	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	Show 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	Show 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	Show XIC
12	☐	AWGPGLHGGIVGR	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	Show XIC
13	☐	AWGPGLHGGIVGR	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	Show 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	Show 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	Show 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	Show 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	Show 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	Show 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	Show 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	Show 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_QexHF1_RSLC5_Hela01ug_1711_01.raw	0	MS/MS	0	1462.68423	-0.362	High	Show XIC

Figure 5: Feature table



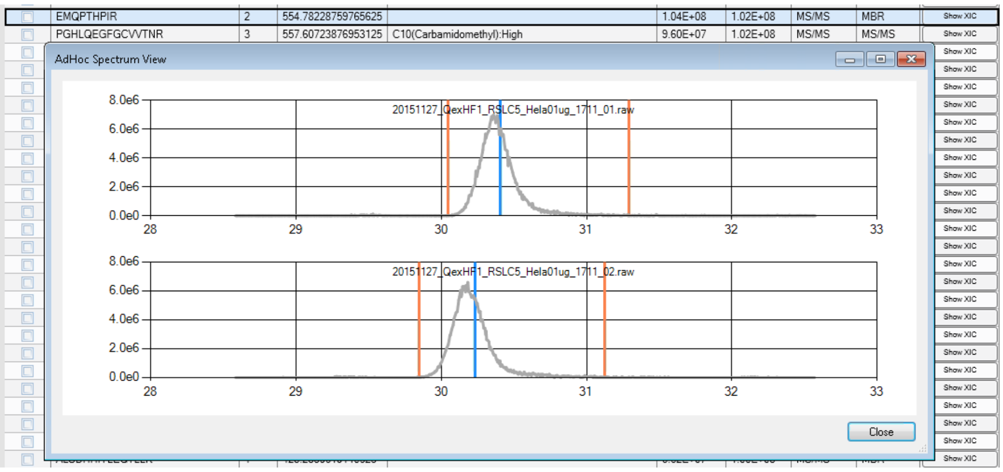
Peak Start	Peak Apex	Peak End	Charge	M/Z	Modifications	Area	Spectrum File	MasterScanNr	Identified By	Reason	TheoreticalMass	Score	Confidence	Show Spectrum
104.08	104.36	104.62	2	820.39264		1.58E+07	20151127_QexHF1_RSLC5_Hela01ug_1711_01.raw	0	MS/MS	0	1639.77510	-0.282	High	Show XIC
118.75	119.02	119.30	2	529.79620		5.22E+06	20151127_QexHF1_RSLC5_Hela01ug_1711_02.raw	0	MS/MS	0	1058.58405	-0.059	High	Show XIC
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	Show XIC
57.06	57.39	57									3755	-0.382	High	Show XIC
56.56	56.72	56									3030	-0.193	High	Show XIC
118.97	119.21	11									3405	-0.088	High	Show XIC
118.61	119.27	12									2067	-0.170	High	Show XIC
118.84	119.44	12									2067	-0.252	High	Show XIC
56.53	56.98	57									3332	-0.298	High	Show XIC
55.93	56.37	56									3332	-0.008	High	Show XIC
82.29	82.60	82									5297	-0.380	High	Show XIC
82.05	82.38	82									9091	-0.389	High	Show XIC
82.30	82.65	83									9091	-0.186	High	Show XIC
99.10	99.37	99									6616	-0.163	High	Show XIC
118.80	119.07	11									5297	-0.102	High	Show XIC
118.93	119.26	11									5297	-0.343	High	Show XIC
81.87	82.35	82									5297	-0.243	High	Show XIC
56.90	57.62	58									252	-0.294	High	Show XIC
56.26	56.99	58									252	-0.359	High	Show XIC
102.55	102.78	10									458	-0.192	High	Show XIC
98.84	99.10	99									1368	-0.056	High	Show XIC
118.78	119.03	11									2048	-0.219	High	Show XIC
119.04	119.25	11									2048	-0.067	High	Show XIC
71.75	72.21	72									4152	-0.138	High	Show XIC
56.57	57.30	58									3423	-0.362	High	Show XIC
119.00	119.36	11									166	-0.173	High	Show XIC
72.19	72.69	73.42	2									-0.058	High	Show XIC
56.17	56.40	56.68	4	537.98138		9.64E+06	20151127_QexHF1_RSLC5_Hela01ug_1711_02.raw	0	MS/MS	0	2148.90262	-0.255	High	Show XIC
119.00	119.18	119.32	2	872.94806		1.22E+06	20151127_QexHF1_RSLC5_Hela01ug_1711_01.raw	0	MS/MS	0	1744.88644	-0.162	High	Show XIC

Figure 6: XIC of a single PjFeature



	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	☐	GALQNIIPASTGAAK	2	706.39984130859375		3.05E+09	3.13E+09	MS/MS	MS/MS	Show XIC
3	☐	TIAPALVSK	2	450.28134155273437		2.45E+09	2.46E+09	MS/MS	MS/MS	Show XIC
4	☐	VAPEEHPVLLTEAPLNPK	3	652.02716064453125		2.21E+09	2.39E+09	MS/MS	MS/MS	Show XIC
5	☐	YSLEPVAVELK	2	624.34765625		2.04E+09	2.23E+09	MS/MS	MS/MS	Show XIC
6	☐	AVFPSIVGR	2	473.27972412109375		2.05E+09	2.09E+09	MS/MS	MS/MS	Show XIC
7	☐	VPTANVSVVDLTCR	2	765.901611328125	C13(Carbamidomethyl):High	1.75E+09	1.95E+09	MS/MS	MS/MS	Show XIC
8	☐	YISPDQLADLYK	2	713.36773681640625		1.48E+09	1.93E+09	MS/MS	MS/MS	Show XIC
9	☐	IGAEVYHNLK	3	381.87637329101562		1.78E+09	1.83E+09	MS/MS	MS/MS	Show XIC
10	☐	LQSTFVFEEIGR	2	713.3701171875		1.38E+09	1.81E+09	MBR	MS/MS	Show XIC
11	☐	LTGMAFR	2	398.21267700195312		1.68E+09	1.80E+09	MS/MS	MS/MS	Show XIC
12	☐	LGDVYVNDAFGTAHR	3	545.6031494140625		1.59E+09	1.76E+09	MS/MS	MS/MS	Show XIC
13	☐	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	☐	ALMDEVVK	2	452.74356079101562		1.63E+09	1.66E+09	MBR	MS/MS	Show XIC
16	☐	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	☐	VIGSGCNLDSAR	2	624.80303955078125	C6(Carbamidomethyl):High	1.60E+09	1.60E+09	MS/MS	MS/MS	Show XIC
19	☐	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	☐	LNVTEQEK	2	480.7537841796875		1.51E+09	1.47E+09	MS/MS	MS/MS	Show XIC
22	☐	LPLQDVYK	2	488.27874755859375		1.45E+09	1.45E+09	MS/MS	MS/MS	Show XIC
23	☐	HTAAPTDPADGPV	2	624.79681396484375		1.48E+09	1.45E+09	MS/MS	MBR	Show XIC
24	☐	IQLINNMLDK	2	601.33514404296875		1.23E+09	1.45E+09	MS/MS	MS/MS	Show XIC
25	☐	IGGIGTVPVGR	2	513.307861328125		1.44E+09	1.44E+09	MS/MS	MS/MS	Show XIC
26	☐	TLSDYNIQK	2	541.27935791015625		1.42E+09	1.43E+09	MS/MS	MS/MS	Show XIC
27	☐	LQDAEIAR	2	458.24810791015625		1.41E+09	1.41E+09	MS/MS	MS/MS	Show XIC
28	☐	PISTLDNR	2	458.247802734375		1.38E+09	1.38E+09	MS/MS	MBR	Show XIC
29	☐	TCHSFIINEK	2	624.8045654296875	C2(Carbamidomethyl):High	1.12E+09	1.38E+09	MBR	MS/MS	Show XIC
30	☐	VDFNVPMK	2	475.24459838867187		1.29E+09	1.37E+09	MS/MS	MS/MS	Show XIC

Figure 7: QuanResult table



☐	EMQPTHPIR	2	554.78228759765625		1.04E+08	1.02E+08	MS/MS	MBR	Show XIC
☐	PGHLQEGFGCVVTNR	3	557.60723876953125	C10(Carbamidomethyl):High	9.60E+07	1.02E+08	MS/MS	MS/MS	Show XIC

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.[1] Peakjuggler also performs a target-decoy quantification and assigns confidences to the Features. **This feature is still under development!**

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[1] 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