Note: This is Supplementary Document S1 of Rossouw S, Bendou H, Bell L, Rigby J, Christoffels A. Effect of polyethylene glycol 20 000 on protein extraction efficiency of formalin-fixed paraffin-embedded tissues in South Africa. Afr J Lab Med. 2021;10(1), a1122. <https://doi.org/10.4102/ajlm.v10i1.1122>

Supporting Information

File S1 – Certificates of analyses for all samples

1.1 Pellet_noPEG_HILIC_1

Project Details

- 1: PeptideShaker Version: 1.16.31
- 2: Date: Sat Dec 15 10:59:09 CAT 2018
- 3: Experiment: 1068_Pellet_noPEG_HILIC_1_PEG-pilot-study
- 4: Sample: 1068_Pellet_noPEG_HILIC_1_PEG-pilot-study
- 5: Replicate Number: 0
- 6: Identification Algorithms: X!Tandem, MS Amanda and MS-GF+

Database Search Parameters

- 1: Precursor Tolerance Unit: ppm
- 2: Precursor Ion m/z Tolerance: 10.0
- 3: Fragment Ion Tolerance Unit: Da
- 4: Fragment Ion m/z Tolerance: 0.02
- 5: Cleavage: Enzyme
- 6: Enzyme: Trypsin
- 7: Missed Cleavages: 2
- 8: Specificity: Specific
- 9: Database: uniprot-human-ref-proteome-trypsin-Oct2018_concatenated_target_decoy.fasta
- 10: Forward Ion: b
- 11: Rewind Ion: y
- 12: Fixed Modifications: Methylthio of C
- 13: Variable Modifications: Oxidation of M, Deamidation of N, Deamidation of Q
- 14: Refinement Variable Modifications: Acetylation of protein N-term, Pyrolidone from E, Pyrolidone from Q, Pyrolidone from carbamidomethylated C
- 15: Refinement Fixed Modifications: Methylthio of C

Input Filters

- 1: Minimal Peptide Length: 8
- 2: Maximal Peptide Length: 30
- 3: Precursor m/z Tolerance: 10.0
- 4: Precursor m/z Tolerance Unit: Yes
- 5: Unrecognized Modifications Discarded: Yes

Validation Summary

- 1: Proteins: #Validated: 2431.0
- 2: Proteins: Total Possible TP: 2953.17
- 3: Proteins: FDR Limit [%]: 0.99

4: Proteins: FNR Limit [%]: 18.75
5: Proteins: Confidence Limit [%]: 77.32
6: Proteins: PEP Limit [%]: 22.68
7: Proteins: Confidence Accuracy [%]: 0.13
8: Peptides (Unmodified): #Validated: 8061.0
9: Peptides (Other): #Validated: 919.0
10: Peptides (Unmodified): Total Possible TP: 8925.99
11: Peptides (Other): Total Possible TP: 1604.24
12: Peptides (Unmodified): FDR Limit [%]: 0.98
13: Peptides (Other): FDR Limit [%]: 0.87
14: Peptides (Unmodified): FNR Limit [%]: 10.75
15: Peptides (Other): FNR Limit [%]: 43.25
16: Peptides (Unmodified): Confidence Limit [%]: 79.63
17: Peptides (Other): Confidence Limit [%]: 91.62
18: Peptides (Unmodified): PEP Limit [%]: 20.37
19: Peptides (Other): PEP Limit [%]: 8.38
20: Peptides (Unmodified): Confidence Accuracy [%]: 0.1
21: Peptides (Other): Confidence Accuracy [%]: 0.53
22: PSMs (Charge 2): #Validated PSM: 6715.0
23: PSMs (Charge 3): #Validated PSM: 2897.0
24: PSMs (Charge 4 and Charge 5, 6): #Validated PSM: 364.0
25: PSMs (Charge 2): Total Possible TP: 8150.28
26: PSMs (Charge 3): Total Possible TP: 3445.06
27: PSMs (Charge 4 and Charge 5, 6): Total Possible TP: 393.55
28: PSMs (Charge 2): FDR Limit [%]: 1.0
29: PSMs (Charge 3): FDR Limit [%]: 0.97
30: PSMs (Charge 4 and Charge 5, 6): FDR Limit [%]: 0.82
31: PSMs (Charge 2): FNR Limit [%]: 18.53
32: PSMs (Charge 3): FNR Limit [%]: 16.89
33: PSMs (Charge 4 and Charge 5, 6): FNR Limit [%]: 8.42
34: PSMs (Charge 2): Confidence Limit [%]: 78.64
35: PSMs (Charge 3): Confidence Limit [%]: 79.11
36: PSMs (Charge 4 and Charge 5, 6): Confidence Limit [%]: 83.33
37: PSMs (Charge 2): PEP Limit [%]: 21.36
38: PSMs (Charge 3): PEP Limit [%]: 20.89
39: PSMs (Charge 4 and Charge 5, 6): PEP Limit [%]: 16.67
40: PSMs (Charge 2): Confidence Accuracy [%]: 0.19
41: PSMs (Charge 3): Confidence Accuracy [%]: 0.45
42: PSMs (Charge 4 and Charge 5, 6): Confidence Accuracy [%]: 9.09

PTM Scoring Settings

1: Probabilistic Score: PhosphoRS
2: Accounting for Neutral Losses: No
3: Threshold: 95.0

Spectrum Counting Parameters

1: Method: NSAF
2: Validated Matches Only: No

Annotation Settings

1: Intensity Limit: 0.75
2: Automatic Annotation: Yes

3: Selected Ions: b, y
4: Neutral Losses: H₂O, CH₄OS, NH₃
5: Neutral Losses Sequence Dependence: Yes
6: Fragment Ion m/z Tolerance: 0.02

1.2 Pellet_noPEG_HILIC_2

Project Details

1: PeptideShaker Version: 1.16.31
2: Date: Sat Dec 15 11:10:38 CAT 2018
3: Experiment: 1068_Pellet_noPEG_HILIC_2_PEG-pilot-study
4: Sample: 1068_Pellet_noPEG_HILIC_2_PEG-pilot-study
5: Replicate Number: 0
6: Identification Algorithms: X!Tandem, MS Amanda and MS-GF+

Database Search Parameters

1: Precursor Tolerance Unit: ppm
2: Precursor Ion m/z Tolerance: 10.0
3: Fragment Ion Tolerance Unit: Da
4: Fragment Ion m/z Tolerance: 0.02
5: Cleavage: Enzyme
6: Enzyme: Trypsin
7: Missed Cleavages: 2
8: Specificity: Specific
9: Database: uniprot-human-ref-proteome-trypsin-Oct2018_concatenated_target_decoy.fasta
10: Forward Ion: b
11: Rewind Ion: y
12: Fixed Modifications: Methylthio of C
13: Variable Modifications: Oxidation of M, Deamidation of N, Deamidation of Q
14: Refinement Variable Modifications: Acetylation of protein N-term, Pyrolidone from E, Pyrolidone from Q, Pyrolidone from carbamidomethylated C
15: Refinement Fixed Modifications: Methylthio of C

Input Filters

1: Minimal Peptide Length: 8
2: Maximal Peptide Length: 30
3: Precursor m/z Tolerance: 10.0
4: Precursor m/z Tolerance Unit: Yes
5: Unrecognized Modifications Discarded: Yes

Validation Summary

1: Proteins: #Validated: 1924.0
2: Proteins: Total Possible TP: 2355.68
3: Proteins: FDR Limit [%]: 0.94
4: Proteins: FNR Limit [%]: 19.08
5: Proteins: Confidence Limit [%]: 90.63
6: Proteins: PEP Limit [%]: 9.38
7: Proteins: Confidence Accuracy [%]: 0.11
8: Peptides (Unmodified): #Validated: 6211.0
9: Peptides (Deamidation of N): #Validated: 418.0

10: Peptides (Other): #Validated: 326.0
11: Peptides (Unmodified): Total Possible TP: 7279.69
12: Peptides (Deamidation of N): Total Possible TP: 605.56
13: Peptides (Other): Total Possible TP: 544.42
14: Peptides (Unmodified): FDR Limit [%]: 1.0
15: Peptides (Deamidation of N): FDR Limit [%]: 0.96
16: Peptides (Other): FDR Limit [%]: 0.92
17: Peptides (Unmodified): FNR Limit [%]: 15.51
18: Peptides (Deamidation of N): FNR Limit [%]: 31.55
19: Peptides (Other): FNR Limit [%]: 40.26
20: Peptides (Unmodified): Confidence Limit [%]: 88.11
21: Peptides (Deamidation of N): Confidence Limit [%]: 85.82
22: Peptides (Other): Confidence Limit [%]: 97.77
23: Peptides (Unmodified): PEP Limit [%]: 11.89
24: Peptides (Deamidation of N): PEP Limit [%]: 14.18
25: Peptides (Other): PEP Limit [%]: 2.23
26: Peptides (Unmodified): Confidence Accuracy [%]: 0.26
27: Peptides (Deamidation of N): Confidence Accuracy [%]: 0.75
28: Peptides (Other): Confidence Accuracy [%]: 0.64
29: PSMs (Charge 2): #Validated PSM: 5222.0
30: PSMs (Charge 3 and Charge 4, 5, 6): #Validated PSM: 2590.0
31: PSMs (Charge 2): Total Possible TP: 6660.32
32: PSMs (Charge 3 and Charge 4, 5, 6): Total Possible TP: 2889.72
33: PSMs (Charge 2): FDR Limit [%]: 1.0
34: PSMs (Charge 3 and Charge 4, 5, 6): FDR Limit [%]: 0.97
35: PSMs (Charge 2): FNR Limit [%]: 22.54
36: PSMs (Charge 3 and Charge 4, 5, 6): FNR Limit [%]: 11.27
37: PSMs (Charge 2): Confidence Limit [%]: 84.33
38: PSMs (Charge 3 and Charge 4, 5, 6): Confidence Limit [%]: 75.32
39: PSMs (Charge 2): PEP Limit [%]: 15.67
40: PSMs (Charge 3 and Charge 4, 5, 6): PEP Limit [%]: 24.68
41: PSMs (Charge 2): Confidence Accuracy [%]: 0.13
42: PSMs (Charge 3 and Charge 4, 5, 6): Confidence Accuracy [%]: 1.3

PTM Scoring Settings

1: Probabilistic Score: PhosphoRS
2: Accounting for Neutral Losses: No
3: Threshold: 95.0

Spectrum Counting Parameters

1: Method: NSAF
2: Validated Matches Only: No

Annotation Settings

1: Intensity Limit: 0.75
2: Automatic Annotation: Yes
3: Selected Ions: b, y
4: Neutral Losses: H₂O, CH₄OS, NH₃
5: Neutral Losses Sequence Dependence: Yes
6: Fragment Ion m/z Tolerance: 0.02

1.3 Pellet_noPEG_HILIC_3

Project Details

- 1: PeptideShaker Version: 1.16.31
- 2: Date: Sat Dec 15 11:28:58 CAT 2018
- 3: Experiment: 1068_Pellet_noPEG_HILIC_3_PEG-pilot-study
- 4: Sample: 1068_Pellet_noPEG_HILIC_3_PEG-pilot-study
- 5: Replicate Number: 0
- 6: Identification Algorithms: X!Tandem, MS Amanda and MS-GF+

Database Search Parameters

- 1: Precursor Tolerance Unit: ppm
- 2: Precursor Ion m/z Tolerance: 10.0
- 3: Fragment Ion Tolerance Unit: Da
- 4: Fragment Ion m/z Tolerance: 0.02
- 5: Cleavage: Enzyme
- 6: Enzyme: Trypsin
- 7: Missed Cleavages: 2
- 8: Specificity: Specific
- 9: Database: uniprot-human-ref-proteome-trypsin-Oct2018_concatenated_target_decoy.fasta
- 10: Forward Ion: b
- 11: Rewind Ion: y
- 12: Fixed Modifications: Methylthio of C
- 13: Variable Modifications: Oxidation of M, Deamidation of N, Deamidation of Q
- 14: Refinement Variable Modifications: Acetylation of protein N-term, Pyroglutamine from E, Pyroglutamine from Q, Pyroglutamine from carbamidomethylated C
- 15: Refinement Fixed Modifications: Methylthio of C

Input Filters

- 1: Minimal Peptide Length: 8
- 2: Maximal Peptide Length: 30
- 3: Precursor m/z Tolerance: 10.0
- 4: Precursor m/z Tolerance Unit: Yes
- 5: Unrecognized Modifications Discarded: Yes

Validation Summary

- 1: Proteins: #Validated: 1323.0
- 2: Proteins: Total Possible TP: 1736.24
- 3: Proteins: FDR Limit [%]: 0.91
- 4: Proteins: FNR Limit [%]: 24.59
- 5: Proteins: Confidence Limit [%]: 89.74
- 6: Proteins: PEP Limit [%]: 10.26
- 7: Proteins: Confidence Accuracy [%]: 0.12
- 8: Peptides (Unmodified): #Validated: 3725.0
- 9: Peptides (Deamidation of N): #Validated: 189.0
- 10: Peptides (Other): #Validated: 179.0
- 11: Peptides (Unmodified): Total Possible TP: 4918.08
- 12: Peptides (Deamidation of N): Total Possible TP: 251.6
- 13: Peptides (Other): Total Possible TP: 443.23
- 14: Peptides (Unmodified): FDR Limit [%]: 0.99
- 15: Peptides (Deamidation of N): FDR Limit [%]: 0.53

16: Peptides (Other): FDR Limit [%]: 0.56
17: Peptides (Unmodified): FNR Limit [%]: 25.06
18: Peptides (Deamidation of N): FNR Limit [%]: 27.79
19: Peptides (Other): FNR Limit [%]: 60.16
20: Peptides (Unmodified): Confidence Limit [%]: 87.77
21: Peptides (Deamidation of N): Confidence Limit [%]: 81.23
22: Peptides (Other): Confidence Limit [%]: 93.53
23: Peptides (Unmodified): PEP Limit [%]: 12.23
24: Peptides (Deamidation of N): PEP Limit [%]: 18.77
25: Peptides (Other): PEP Limit [%]: 6.47
26: Peptides (Unmodified): Confidence Accuracy [%]: 0.2
27: Peptides (Deamidation of N): Confidence Accuracy [%]: 0.48
28: Peptides (Other): Confidence Accuracy [%]: 0.5
29: PSMs (Charge 2): #Validated PSM: 2847.0
30: PSMs (Charge 3 and Charge 4, 5, 6): #Validated PSM: 1502.0
31: PSMs (Charge 2): Total Possible TP: 4364.54
32: PSMs (Charge 3 and Charge 4, 5, 6): Total Possible TP: 1803.61
33: PSMs (Charge 2): FDR Limit [%]: 0.98
34: PSMs (Charge 3 and Charge 4, 5, 6): FDR Limit [%]: 1.0
35: PSMs (Charge 2): FNR Limit [%]: 35.36
36: PSMs (Charge 3 and Charge 4, 5, 6): FNR Limit [%]: 17.64
37: PSMs (Charge 2): Confidence Limit [%]: 89.2
38: PSMs (Charge 3 and Charge 4, 5, 6): Confidence Limit [%]: 81.82
39: PSMs (Charge 2): PEP Limit [%]: 10.8
40: PSMs (Charge 3 and Charge 4, 5, 6): PEP Limit [%]: 18.18
41: PSMs (Charge 2): Confidence Accuracy [%]: 0.28
42: PSMs (Charge 3 and Charge 4, 5, 6): Confidence Accuracy [%]: 3.13

PTM Scoring Settings

1: Probabilistic Score: PhosphoRS
2: Accounting for Neutral Losses: No
3: Threshold: 95.0

Spectrum Counting Parameters

1: Method: NSAF
2: Validated Matches Only: No

Annotation Settings

1: Intensity Limit: 0.75
2: Automatic Annotation: Yes
3: Selected Ions: b, y
4: Neutral Losses: H₂O, CH₄OS, NH₃
5: Neutral Losses Sequence Dependence: Yes
6: Fragment Ion m/z Tolerance: 0.02

1.4 Pellet_PEG_HILIC_1

Project Details

1: PeptideShaker Version: 1.16.31
2: Date: Sat Dec 15 12:52:23 CAT 2018

3: Experiment: 1068_Pellet_PEG_HILIC_1_PEG-pilot-study
4: Sample: 1068_Pellet_PEG_HILIC_1_PEG-pilot-study
5: Replicate Number: 0
6: Identification Algorithms: X!Tandem, MS Amanda and MS-GF+

Database Search Parameters

1: Precursor Tolerance Unit: ppm
2: Precursor Ion m/z Tolerance: 10.0
3: Fragment Ion Tolerance Unit: Da
4: Fragment Ion m/z Tolerance: 0.02
5: Cleavage: Enzyme
6: Enzyme: Trypsin
7: Missed Cleavages: 2
8: Specificity: Specific
9: Database: uniprot-human-ref-proteome-trypsin-Oct2018_concatenated_target_decoy.fasta
10: Forward Ion: b
11: Rewind Ion: y
12: Fixed Modifications: Methylthio of C
13: Variable Modifications: Oxidation of M, Deamidation of N, Deamidation of Q
14: Refinement Variable Modifications: Acetylation of protein N-term, Pyrolidone from E, Pyrolidone from Q, Pyrolidone from carbamidomethylated C
15: Refinement Fixed Modifications: Methylthio of C

Input Filters

1: Minimal Peptide Length: 8
2: Maximal Peptide Length: 30
3: Precursor m/z Tolerance: 10.0
4: Precursor m/z Tolerance Unit: Yes
5: Unrecognized Modifications Discarded: Yes

Validation Summary

1: Proteins: #Validated: 1957.0
2: Proteins: Total Possible TP: 2580.94
3: Proteins: FDR Limit [%]: 0.97
4: Proteins: FNR Limit [%]: 24.84
5: Proteins: Confidence Limit [%]: 91.76
6: Proteins: PEP Limit [%]: 8.24
7: Proteins: Confidence Accuracy [%]: 0.12
8: Peptides (Unmodified): #Validated: 6269.0
9: Peptides (Deamidation of N): #Validated: 337.0
10: Peptides (Other): #Validated: 269.0
11: Peptides (Unmodified): Total Possible TP: 7266.08
12: Peptides (Deamidation of N): Total Possible TP: 536.86
13: Peptides (Other): Total Possible TP: 406.01
14: Peptides (Unmodified): FDR Limit [%]: 0.99
15: Peptides (Deamidation of N): FDR Limit [%]: 0.89
16: Peptides (Other): FDR Limit [%]: 0.74
17: Peptides (Unmodified): FNR Limit [%]: 14.55
18: Peptides (Deamidation of N): FNR Limit [%]: 37.64
19: Peptides (Other): FNR Limit [%]: 33.93
20: Peptides (Unmodified): Confidence Limit [%]: 87.7
21: Peptides (Deamidation of N): Confidence Limit [%]: 87.61

22: Peptides (Other): Confidence Limit [%]: 97.19
23: Peptides (Unmodified): PEP Limit [%]: 12.3
24: Peptides (Deamidation of N): PEP Limit [%]: 12.39
25: Peptides (Other): PEP Limit [%]: 2.81
26: Peptides (Unmodified): Confidence Accuracy [%]: 0.27
27: Peptides (Deamidation of N): Confidence Accuracy [%]: 0.91
28: Peptides (Other): Confidence Accuracy [%]: 0.91
29: PSMs (Charge 2): #Validated PSM: 5044.0
30: PSMs (Charge 3 and Charge 4, 5, 6): #Validated PSM: 2377.0
31: PSMs (Charge 2): Total Possible TP: 6558.44
32: PSMs (Charge 3 and Charge 4, 5, 6): Total Possible TP: 2834.7
33: PSMs (Charge 2): FDR Limit [%]: 0.99
34: PSMs (Charge 3 and Charge 4, 5, 6): FDR Limit [%]: 0.97
35: PSMs (Charge 2): FNR Limit [%]: 23.9
36: PSMs (Charge 3 and Charge 4, 5, 6): FNR Limit [%]: 17.0
37: PSMs (Charge 2): Confidence Limit [%]: 85.83
38: PSMs (Charge 3 and Charge 4, 5, 6): Confidence Limit [%]: 90.77
39: PSMs (Charge 2): PEP Limit [%]: 14.17
40: PSMs (Charge 3 and Charge 4, 5, 6): PEP Limit [%]: 9.23
41: PSMs (Charge 2): Confidence Accuracy [%]: 0.41
42: PSMs (Charge 3 and Charge 4, 5, 6): Confidence Accuracy [%]: 1.54

PTM Scoring Settings

1: Probabilistic Score: PhosphoRS
2: Accounting for Neutral Losses: No
3: Threshold: 95.0

Spectrum Counting Parameters

1: Method: NSAF
2: Validated Matches Only: No

Annotation Settings

1: Intensity Limit: 0.75
2: Automatic Annotation: Yes
3: Selected Ions: b, y
4: Neutral Losses: H₂O, CH₄OS, NH₃
5: Neutral Losses Sequence Dependence: Yes
6: Fragment Ion m/z Tolerance: 0.02

1.5 Pellet_PEG_HILIC_2

Project Details

1: PeptideShaker Version: 1.16.31
2: Date: Sat Dec 15 13:18:32 CAT 2018
3: Experiment: 1068_Pellet_PEG_HILIC_2_PEG-pilot-study
4: Sample: 1068_Pellet_PEG_HILIC_2_PEG-pilot-study
5: Replicate Number: 0
6: Identification Algorithms: X!Tandem, MS Amanda and MS-GF+

Database Search Parameters

1: Precursor Tolerance Unit: ppm
2: Precursor Ion m/z Tolerance: 10.0
3: Fragment Ion Tolerance Unit: Da
4: Fragment Ion m/z Tolerance: 0.02
5: Cleavage: Enzyme
6: Enzyme: Trypsin
7: Missed Cleavages: 2
8: Specificity: Specific
9: Database: uniprot-human-ref-proteome-trypsin-Oct2018_concatenated_target_decoy.fasta
10: Forward Ion: b
11: Rewind Ion: y
12: Fixed Modifications: Methylthio of C
13: Variable Modifications: Oxidation of M, Deamidation of N, Deamidation of Q
14: Refinement Variable Modifications: Acetylation of protein N-term, Pyroglutamine from E, Pyroglutamine from Q, Pyroglutamine from carbamidomethylated C
15: Refinement Fixed Modifications: Methylthio of C

Input Filters

1: Minimal Peptide Length: 8
2: Maximal Peptide Length: 30
3: Precursor m/z Tolerance: 10.0
4: Precursor m/z Tolerance Unit: Yes
5: Unrecognized Modifications Discarded: Yes

Validation Summary

1: Proteins: #Validated: 1672.0
2: Proteins: Total Possible TP: 2237.92
3: Proteins: FDR Limit [%]: 0.96
4: Proteins: FNR Limit [%]: 25.97
5: Proteins: Confidence Limit [%]: 90.22
6: Proteins: PEP Limit [%]: 9.78
7: Proteins: Confidence Accuracy [%]: 0.13
8: Peptides (Unmodified): #Validated: 5234.0
9: Peptides (Deamidation of N): #Validated: 338.0
10: Peptides (Other): #Validated: 259.0
11: Peptides (Unmodified): Total Possible TP: 6178.49
12: Peptides (Deamidation of N): Total Possible TP: 517.02
13: Peptides (Other): Total Possible TP: 558.91
14: Peptides (Unmodified): FDR Limit [%]: 0.99
15: Peptides (Deamidation of N): FDR Limit [%]: 0.59
16: Peptides (Other): FDR Limit [%]: 0.77
17: Peptides (Unmodified): FNR Limit [%]: 16.19
18: Peptides (Deamidation of N): FNR Limit [%]: 35.81
19: Peptides (Other): FNR Limit [%]: 54.18
20: Peptides (Unmodified): Confidence Limit [%]: 79.74
21: Peptides (Deamidation of N): Confidence Limit [%]: 77.42
22: Peptides (Other): Confidence Limit [%]: 90.07
23: Peptides (Unmodified): PEP Limit [%]: 20.26
24: Peptides (Deamidation of N): PEP Limit [%]: 22.58
25: Peptides (Other): PEP Limit [%]: 9.93
26: Peptides (Unmodified): Confidence Accuracy [%]: 0.26
27: Peptides (Deamidation of N): Confidence Accuracy [%]: 0.66

28: Peptides (Other): Confidence Accuracy [%]: 0.71
29: PSMs (Charge 2): #Validated PSM: 4237.0
30: PSMs (Charge 3 and Charge 4, 5, 6): #Validated PSM: 2124.0
31: PSMs (Charge 2): Total Possible TP: 5613.89
32: PSMs (Charge 3 and Charge 4, 5, 6): Total Possible TP: 2474.32
33: PSMs (Charge 2): FDR Limit [%]: 0.99
34: PSMs (Charge 3 and Charge 4, 5, 6): FDR Limit [%]: 0.99
35: PSMs (Charge 2): FNR Limit [%]: 25.51
36: PSMs (Charge 3 and Charge 4, 5, 6): FNR Limit [%]: 15.07
37: PSMs (Charge 2): Confidence Limit [%]: 84.77
38: PSMs (Charge 3 and Charge 4, 5, 6): Confidence Limit [%]: 82.35
39: PSMs (Charge 2): PEP Limit [%]: 15.23
40: PSMs (Charge 3 and Charge 4, 5, 6): PEP Limit [%]: 17.65
41: PSMs (Charge 2): Confidence Accuracy [%]: 0.13
42: PSMs (Charge 3 and Charge 4, 5, 6): Confidence Accuracy [%]: 1.22

PTM Scoring Settings

1: Probabilistic Score: PhosphoRS
2: Accounting for Neutral Losses: No
3: Threshold: 95.0

Spectrum Counting Parameters

1: Method: NSAF
2: Validated Matches Only: No

Annotation Settings

1: Intensity Limit: 0.75
2: Automatic Annotation: Yes
3: Selected Ions: b, y
4: Neutral Losses: H₂O, CH₄OS, NH₃
5: Neutral Losses Sequence Dependence: Yes
6: Fragment Ion m/z Tolerance: 0.02

1.6 Pellet_PEG_HILIC_3

Project Details

1: PeptideShaker Version: 1.16.31
2: Date: Sat Dec 15 13:31:17 CAT 2018
3: Experiment: 1068_Pellet_PEG_HILIC_3_PEG-pilot-study
4: Sample: 1068_Pellet_PEG_HILIC_3_PEG-pilot-study
5: Replicate Number: 0
6: Identification Algorithms: X!Tandem, MS Amanda and MS-GF+

Database Search Parameters

1: Precursor Tolerance Unit: ppm
2: Precursor Ion m/z Tolerance: 10.0
3: Fragment Ion Tolerance Unit: Da
4: Fragment Ion m/z Tolerance: 0.02
5: Cleavage: Enzyme

6: Enzyme: Trypsin
7: Missed Cleavages: 2
8: Specificity: Specific
9: Database: uniprot-human-ref-proteome-trypsin-Oct2018_concatenated_target_decoy.fasta
10: Forward Ion: b
11: Rewind Ion: y
12: Fixed Modifications: Methylthio of C
13: Variable Modifications: Oxidation of M, Deamidation of N, Deamidation of Q
14: Refinement Variable Modifications: Acetylation of protein N-term, Pyroglutamine from E, Pyroglutamine from Q, Pyroglutamine from carbamidomethylated C
15: Refinement Fixed Modifications: Methylthio of C

Input Filters

1: Minimal Peptide Length: 8
2: Maximal Peptide Length: 30
3: Precursor m/z Tolerance: 10.0
4: Precursor m/z Tolerance Unit: Yes
5: Unrecognized Modifications Discarded: Yes

Validation Summary

1: Proteins: #Validated: 1064.0
2: Proteins: Total Possible TP: 1559.1
3: Proteins: FDR Limit [%]: 0.94
4: Proteins: FNR Limit [%]: 32.41
5: Proteins: Confidence Limit [%]: 90.52
6: Proteins: PEP Limit [%]: 9.48
7: Proteins: Confidence Accuracy [%]: 0.19
8: Peptides (Unmodified): #Validated: 2831.0
9: Peptides (Deamidation of N): #Validated: 127.0
10: Peptides (Other): #Validated: 152.0
11: Peptides (Unmodified): Total Possible TP: 4015.39
12: Peptides (Deamidation of N): Total Possible TP: 274.36
13: Peptides (Other): Total Possible TP: 212.73
14: Peptides (Unmodified): FDR Limit [%]: 0.99
15: Peptides (Deamidation of N): FDR Limit [%]: 0.79
16: Peptides (Other): FDR Limit [%]: 0.66
17: Peptides (Unmodified): FNR Limit [%]: 30.25
18: Peptides (Deamidation of N): FNR Limit [%]: 55.79
19: Peptides (Other): FNR Limit [%]: 31.35
20: Peptides (Unmodified): Confidence Limit [%]: 87.96
21: Peptides (Deamidation of N): Confidence Limit [%]: 80.38
22: Peptides (Other): Confidence Limit [%]: 79.65
23: Peptides (Unmodified): PEP Limit [%]: 12.04
24: Peptides (Deamidation of N): PEP Limit [%]: 19.62
25: Peptides (Other): PEP Limit [%]: 20.35
26: Peptides (Unmodified): Confidence Accuracy [%]: 0.23
27: Peptides (Deamidation of N): Confidence Accuracy [%]: 0.62
28: Peptides (Other): Confidence Accuracy [%]: 0.63
29: PSMs (Charge 2): #Validated PSM: 2075.0
30: PSMs (Charge 3 and Charge 4, 5, 6): #Validated PSM: 1198.0
31: PSMs (Charge 2): Total Possible TP: 3511.31
32: PSMs (Charge 3 and Charge 4, 5, 6): Total Possible TP: 1648.76
33: PSMs (Charge 2): FDR Limit [%]: 0.96

34: PSMs (Charge 3 and Charge 4, 5, 6): FDR Limit [%]: 0.83
35: PSMs (Charge 2): FNR Limit [%]: 41.55
36: PSMs (Charge 3 and Charge 4, 5, 6): FNR Limit [%]: 28.18
37: PSMs (Charge 2): Confidence Limit [%]: 86.73
38: PSMs (Charge 3 and Charge 4, 5, 6): Confidence Limit [%]: 76.7
39: PSMs (Charge 2): PEP Limit [%]: 13.27
40: PSMs (Charge 3 and Charge 4, 5, 6): PEP Limit [%]: 23.3
41: PSMs (Charge 2): Confidence Accuracy [%]: 0.29
42: PSMs (Charge 3 and Charge 4, 5, 6): Confidence Accuracy [%]: 0.97

PTM Scoring Settings

1: Probabilistic Score: PhosphoRS
2: Accounting for Neutral Losses: No
3: Threshold: 95.0

Spectrum Counting Parameters

1: Method: NSAF
2: Validated Matches Only: No

Annotation Settings

1: Intensity Limit: 0.75
2: Automatic Annotation: Yes
3: Selected Ions: b, y
4: Neutral Losses: H2O, CH4OS, NH3
5: Neutral Losses Sequence Dependence: Yes
6: Fragment Ion m/z Tolerance: 0.02

1.7 WCPL_noPEG_HILIC_1

Project Details

1: PeptideShaker Version: 1.16.31
2: Date: Sat Dec 15 15:42:13 CAT 2018
3: Experiment: 1068_WCPL_noPEG_HILIC_1_PEG-pilot-study
4: Sample: 1068_WCPL_noPEG_HILIC_1_PEG-pilot-study
5: Replicate Number: 0
6: Identification Algorithms: X!Tandem, MS Amanda and MS-GF+

Database Search Parameters

1: Precursor Tolerance Unit: ppm
2: Precursor Ion m/z Tolerance: 10.0
3: Fragment Ion Tolerance Unit: Da
4: Fragment Ion m/z Tolerance: 0.02
5: Cleavage: Enzyme
6: Enzyme: Trypsin
7: Missed Cleavages: 2
8: Specificity: Specific
9: Database: uniprot-human-ref-proteome-trypsin-Oct2018_concatenated_target_decoy.fasta
10: Forward Ion: b
11: Rewind Ion: y

- 12: Fixed Modifications: Methylthio of C
- 13: Variable Modifications: Oxidation of M, Deamidation of N, Deamidation of Q
- 14: Refinement Variable Modifications: Acetylation of protein N-term, Pyrolidone from E, Pyrolidone from Q, Pyrolidone from carbamidomethylated C
- 15: Refinement Fixed Modifications: Methylthio of C

Input Filters

- 1: Minimal Peptide Length: 8
- 2: Maximal Peptide Length: 30
- 3: Precursor m/z Tolerance: 10.0
- 4: Precursor m/z Tolerance Unit: Yes
- 5: Unrecognized Modifications Discarded: Yes

Validation Summary

- 1: Proteins: #Validated: 2501.0
- 2: Proteins: Total Possible TP: 2921.72
- 3: Proteins: FDR Limit [%]: 1.0
- 4: Proteins: FNR Limit [%]: 15.28
- 5: Proteins: Confidence Limit [%]: 87.35
- 6: Proteins: PEP Limit [%]: 12.65
- 7: Proteins: Confidence Accuracy [%]: 0.08
- 8: Peptides (Unmodified): #Validated: 7736.0
- 9: Peptides (Deamidation of N): #Validated: 565.0
- 10: Peptides (Other): #Validated: 412.0
- 11: Peptides (Unmodified): Total Possible TP: 8214.35
- 12: Peptides (Deamidation of N): Total Possible TP: 826.03
- 13: Peptides (Other): Total Possible TP: 685.06
- 14: Peptides (Unmodified): FDR Limit [%]: 0.97
- 15: Peptides (Deamidation of N): FDR Limit [%]: 0.88
- 16: Peptides (Other): FDR Limit [%]: 0.97
- 17: Peptides (Unmodified): FNR Limit [%]: 6.8
- 18: Peptides (Deamidation of N): FNR Limit [%]: 32.08
- 19: Peptides (Other): FNR Limit [%]: 40.17
- 20: Peptides (Unmodified): Confidence Limit [%]: 75.53
- 21: Peptides (Deamidation of N): Confidence Limit [%]: 86.29
- 22: Peptides (Other): Confidence Limit [%]: 88.89
- 23: Peptides (Unmodified): PEP Limit [%]: 24.47
- 24: Peptides (Deamidation of N): PEP Limit [%]: 13.71
- 25: Peptides (Other): PEP Limit [%]: 11.11
- 26: Peptides (Unmodified): Confidence Accuracy [%]: 0.26
- 27: Peptides (Deamidation of N): Confidence Accuracy [%]: 0.82
- 28: Peptides (Other): Confidence Accuracy [%]: 0.77
- 29: PSMs (Charge 2): #Validated PSM: 6806.0
- 30: PSMs (Charge 3 and Charge 4, 5, 6): #Validated PSM: 3253.0
- 31: PSMs (Charge 2): Total Possible TP: 8003.91
- 32: PSMs (Charge 3 and Charge 4, 5, 6): Total Possible TP: 3451.35
- 33: PSMs (Charge 2): FDR Limit [%]: 0.98
- 34: PSMs (Charge 3 and Charge 4, 5, 6): FDR Limit [%]: 0.98
- 35: PSMs (Charge 2): FNR Limit [%]: 15.91
- 36: PSMs (Charge 3 and Charge 4, 5, 6): FNR Limit [%]: 6.76
- 37: PSMs (Charge 2): Confidence Limit [%]: 80.28
- 38: PSMs (Charge 3 and Charge 4, 5, 6): Confidence Limit [%]: 78.48
- 39: PSMs (Charge 2): PEP Limit [%]: 19.72

40: PSMs (Charge 3 and Charge 4, 5, 6): PEP Limit [%]: 21.52
41: PSMs (Charge 2): Confidence Accuracy [%]: 0.15
42: PSMs (Charge 3 and Charge 4, 5, 6): Confidence Accuracy [%]: 1.28

PTM Scoring Settings

1: Probabilistic Score: PhosphoRS
2: Accounting for Neutral Losses: No
3: Threshold: 95.0

Spectrum Counting Parameters

1: Method: NSAF
2: Validated Matches Only: No

Annotation Settings

1: Intensity Limit: 0.75
2: Automatic Annotation: Yes
3: Selected Ions: b, y
4: Neutral Losses: H₂O, CH₄OS, NH₃
5: Neutral Losses Sequence Dependence: Yes
6: Fragment Ion m/z Tolerance: 0.02

1.8 WCPL_noPEG_HILIC_2

Project Details

1: PeptideShaker Version: 1.16.31
2: Date: Sat Dec 15 15:51:09 CAT 2018
3: Experiment: 1068_WCPL_noPEG_HILIC_2_PEG-pilot-study
4: Sample: 1068_WCPL_noPEG_HILIC_2_PEG-pilot-study
5: Replicate Number: 0
6: Identification Algorithms: X!Tandem, MS Amanda and MS-GF+

Database Search Parameters

1: Precursor Tolerance Unit: ppm
2: Precursor Ion m/z Tolerance: 10.0
3: Fragment Ion Tolerance Unit: Da
4: Fragment Ion m/z Tolerance: 0.02
5: Cleavage: Enzyme
6: Enzyme: Trypsin
7: Missed Cleavages: 2
8: Specificity: Specific
9: Database: uniprot-human-ref-proteome-trypsin-Oct2018_concatenated_target_decoy.fasta
10: Forward Ion: b
11: Rewind Ion: y
12: Fixed Modifications: Methylthio of C
13: Variable Modifications: Oxidation of M, Deamidation of N, Deamidation of Q
14: Refinement Variable Modifications: Acetylation of protein N-term, Pyroglutamine from E, Pyroglutamine from Q, Pyroglutamine from carbamidomethylated C
15: Refinement Fixed Modifications: Methylthio of C

Input Filters

- 1: Minimal Peptide Length: 8
- 2: Maximal Peptide Length: 30
- 3: Precursor m/z Tolerance: 10.0
- 4: Precursor m/z Tolerance Unit: Yes
- 5: Unrecognized Modifications Discarded: Yes

Validation Summary

- 1: Proteins: #Validated: 2057.0
- 2: Proteins: Total Possible TP: 2648.48
- 3: Proteins: FDR Limit [%]: 0.88
- 4: Proteins: FNR Limit [%]: 22.85
- 5: Proteins: Confidence Limit [%]: 91.1
- 6: Proteins: PEP Limit [%]: 8.9
- 7: Proteins: Confidence Accuracy [%]: 0.11
- 8: Peptides (Unmodified): #Validated: 6442.0
- 9: Peptides (Other): #Validated: 751.0
- 10: Peptides (Unmodified): Total Possible TP: 7009.47
- 11: Peptides (Other): Total Possible TP: 1368.81
- 12: Peptides (Unmodified): FDR Limit [%]: 0.99
- 13: Peptides (Other): FDR Limit [%]: 0.93
- 14: Peptides (Unmodified): FNR Limit [%]: 9.07
- 15: Peptides (Other): FNR Limit [%]: 45.52
- 16: Peptides (Unmodified): Confidence Limit [%]: 79.43
- 17: Peptides (Other): Confidence Limit [%]: 88.95
- 18: Peptides (Unmodified): PEP Limit [%]: 20.57
- 19: Peptides (Other): PEP Limit [%]: 11.05
- 20: Peptides (Unmodified): Confidence Accuracy [%]: 0.24
- 21: Peptides (Other): Confidence Accuracy [%]: 0.56
- 22: PSMs (Charge 2): #Validated PSM: 5359.0
- 23: PSMs (Charge 3 and Charge 4, 5, 6): #Validated PSM: 2677.0
- 24: PSMs (Charge 2): Total Possible TP: 6758.4
- 25: PSMs (Charge 3 and Charge 4, 5, 6): Total Possible TP: 3085.87
- 26: PSMs (Charge 2): FDR Limit [%]: 0.99
- 27: PSMs (Charge 3 and Charge 4, 5, 6): FDR Limit [%]: 0.97
- 28: PSMs (Charge 2): FNR Limit [%]: 21.55
- 29: PSMs (Charge 3 and Charge 4, 5, 6): FNR Limit [%]: 14.13
- 30: PSMs (Charge 2): Confidence Limit [%]: 84.22
- 31: PSMs (Charge 3 and Charge 4, 5, 6): Confidence Limit [%]: 77.32
- 32: PSMs (Charge 2): PEP Limit [%]: 15.78
- 33: PSMs (Charge 3 and Charge 4, 5, 6): PEP Limit [%]: 22.68
- 34: PSMs (Charge 2): Confidence Accuracy [%]: 0.14
- 35: PSMs (Charge 3 and Charge 4, 5, 6): Confidence Accuracy [%]: 1.03

PTM Scoring Settings

- 1: Probabilistic Score: PhosphoRS
- 2: Accounting for Neutral Losses: No
- 3: Threshold: 95.0

Spectrum Counting Parameters

- 1: Method: NSAF

2: Validated Matches Only: No

Annotation Settings

- 1: Intensity Limit: 0.75
- 2: Automatic Annotation: Yes
- 3: Selected Ions: b, y
- 4: Neutral Losses: H₂O, CH₄OS, NH₃
- 5: Neutral Losses Sequence Dependence: Yes
- 6: Fragment Ion m/z Tolerance: 0.02

1.9 WCPL_noPEG_HILIC_3

Project Details

- 1: PeptideShaker Version: 1.16.31
- 2: Date: Sat Dec 15 16:00:50 CAT 2018
- 3: Experiment: 1068_WCPL_noPEG_HILIC_3_PEG-pilot-study
- 4: Sample: 1068_WCPL_noPEG_HILIC_3_PEG-pilot-study
- 5: Replicate Number: 0
- 6: Identification Algorithms: X!Tandem, MS Amanda and MS-GF+

Database Search Parameters

- 1: Precursor Tolerance Unit: ppm
- 2: Precursor Ion m/z Tolerance: 10.0
- 3: Fragment Ion Tolerance Unit: Da
- 4: Fragment Ion m/z Tolerance: 0.02
- 5: Cleavage: Enzyme
- 6: Enzyme: Trypsin
- 7: Missed Cleavages: 2
- 8: Specificity: Specific
- 9: Database: uniprot-human-ref-proteome-trypsin-Oct2018_concatenated_target_decoy.fasta
- 10: Forward Ion: b
- 11: Rewind Ion: y
- 12: Fixed Modifications: Methylthio of C
- 13: Variable Modifications: Oxidation of M, Deamidation of N, Deamidation of Q
- 14: Refinement Variable Modifications: Acetylation of protein N-term, Pyroglutamine from E, Pyroglutamine from Q, Pyroglutamine from carbamidomethylated C
- 15: Refinement Fixed Modifications: Methylthio of C

Input Filters

- 1: Minimal Peptide Length: 8
- 2: Maximal Peptide Length: 30
- 3: Precursor m/z Tolerance: 10.0
- 4: Precursor m/z Tolerance Unit: Yes
- 5: Unrecognized Modifications Discarded: Yes

Validation Summary

- 1: Proteins: #Validated: 2384.0
- 2: Proteins: Total Possible TP: 2810.55
- 3: Proteins: FDR Limit [%]: 0.92

4: Proteins: FNR Limit [%]: 16.25
5: Proteins: Confidence Limit [%]: 87.69
6: Proteins: PEP Limit [%]: 12.31
7: Proteins: Confidence Accuracy [%]: 0.09
8: Peptides (Unmodified): #Validated: 6996.0
9: Peptides (Deamidation of N): #Validated: 540.0
10: Peptides (Other): #Validated: 506.0
11: Peptides (Unmodified): Total Possible TP: 7757.03
12: Peptides (Deamidation of N): Total Possible TP: 880.04
13: Peptides (Other): Total Possible TP: 1026.32
14: Peptides (Unmodified): FDR Limit [%]: 0.99
15: Peptides (Deamidation of N): FDR Limit [%]: 0.93
16: Peptides (Other): FDR Limit [%]: 0.99
17: Peptides (Unmodified): FNR Limit [%]: 10.77
18: Peptides (Deamidation of N): FNR Limit [%]: 38.99
19: Peptides (Other): FNR Limit [%]: 51.17
20: Peptides (Unmodified): Confidence Limit [%]: 77.15
21: Peptides (Deamidation of N): Confidence Limit [%]: 93.91
22: Peptides (Other): Confidence Limit [%]: 90.65
23: Peptides (Unmodified): PEP Limit [%]: 22.85
24: Peptides (Deamidation of N): PEP Limit [%]: 6.09
25: Peptides (Other): PEP Limit [%]: 9.35
26: Peptides (Unmodified): Confidence Accuracy [%]: 0.18
27: Peptides (Deamidation of N): Confidence Accuracy [%]: 0.42
28: Peptides (Other): Confidence Accuracy [%]: 0.4
29: PSMs (Charge 2): #Validated PSM: 6256.0
30: PSMs (Charge 3): #Validated PSM: 2712.0
31: PSMs (Charge 4 and Charge 5, 6): #Validated PSM: 356.0
32: PSMs (Charge 2): Total Possible TP: 7599.86
33: PSMs (Charge 3): Total Possible TP: 3019.42
34: PSMs (Charge 4 and Charge 5, 6): Total Possible TP: 364.46
35: PSMs (Charge 2): FDR Limit [%]: 0.99
36: PSMs (Charge 3): FDR Limit [%]: 1.0
37: PSMs (Charge 4 and Charge 5, 6): FDR Limit [%]: 0.84
38: PSMs (Charge 2): FNR Limit [%]: 18.54
39: PSMs (Charge 3): FNR Limit [%]: 11.34
40: PSMs (Charge 4 and Charge 5, 6): FNR Limit [%]: 3.66
41: PSMs (Charge 2): Confidence Limit [%]: 78.67
42: PSMs (Charge 3): Confidence Limit [%]: 73.68
43: PSMs (Charge 4 and Charge 5, 6): Confidence Limit [%]: 63.16
44: PSMs (Charge 2): PEP Limit [%]: 21.33
45: PSMs (Charge 3): PEP Limit [%]: 26.32
46: PSMs (Charge 4 and Charge 5, 6): PEP Limit [%]: 36.84
47: PSMs (Charge 2): Confidence Accuracy [%]: 0.47
48: PSMs (Charge 3): Confidence Accuracy [%]: 0.35
49: PSMs (Charge 4 and Charge 5, 6): Confidence Accuracy [%]: 5.26

PTM Scoring Settings

1: Probabilistic Score: PhosphoRS
2: Accounting for Neutral Losses: No
3: Threshold: 95.0

Spectrum Counting Parameters

- 1: Method: NSAF
- 2: Validated Matches Only: No

Annotation Settings

- 1: Intensity Limit: 0.75
- 2: Automatic Annotation: Yes
- 3: Selected Ions: b, y
- 4: Neutral Losses: H₂O, CH₄OS, NH₃
- 5: Neutral Losses Sequence Dependence: Yes
- 6: Fragment Ion m/z Tolerance: 0.02

1.10 WCPL_PEG_HILIC_1

Project Details

- 1: PeptideShaker Version: 1.16.31
- 2: Date: Sat Dec 15 17:12:11 CAT 2018
- 3: Experiment: 1068_WCPL_PEG_HILIC_1_PEG-pilot-study
- 4: Sample: 1068_WCPL_PEG_HILIC_1_PEG-pilot-study
- 5: Replicate Number: 0
- 6: Identification Algorithms: X!Tandem, MS Amanda and MS-GF+

Database Search Parameters

- 1: Precursor Tolerance Unit: ppm
- 2: Precursor Ion m/z Tolerance: 10.0
- 3: Fragment Ion Tolerance Unit: Da
- 4: Fragment Ion m/z Tolerance: 0.02
- 5: Cleavage: Enzyme
- 6: Enzyme: Trypsin
- 7: Missed Cleavages: 2
- 8: Specificity: Specific
- 9: Database: uniprot-human-ref-proteome-trypsin-Oct2018_concatenated_target_decoy.fasta
- 10: Forward Ion: b
- 11: Rewind Ion: y
- 12: Fixed Modifications: Methylthio of C
- 13: Variable Modifications: Oxidation of M, Deamidation of N, Deamidation of Q
- 14: Refinement Variable Modifications: Acetylation of protein N-term, Pyrolidone from E, Pyrolidone from Q, Pyrolidone from carbamidomethylated C
- 15: Refinement Fixed Modifications: Methylthio of C

Input Filters

- 1: Minimal Peptide Length: 8
- 2: Maximal Peptide Length: 30
- 3: Precursor m/z Tolerance: 10.0
- 4: Precursor m/z Tolerance Unit: Yes
- 5: Unrecognized Modifications Discarded: Yes

Validation Summary

- 1: Proteins: #Validated: 2329.0

2: Proteins: Total Possible TP: 2667.93
3: Proteins: FDR Limit [%]: 0.99
4: Proteins: FNR Limit [%]: 14.39
5: Proteins: Confidence Limit [%]: 71.84
6: Proteins: PEP Limit [%]: 28.16
7: Proteins: Confidence Accuracy [%]: 0.13
8: Peptides (Unmodified): #Validated: 6688.0
9: Peptides (Other): #Validated: 813.0
10: Peptides (Unmodified): Total Possible TP: 7530.3
11: Peptides (Other): Total Possible TP: 1016.01
12: Peptides (Unmodified): FDR Limit [%]: 0.99
13: Peptides (Other): FDR Limit [%]: 0.74
14: Peptides (Unmodified): FNR Limit [%]: 12.2
15: Peptides (Other): FNR Limit [%]: 20.76
16: Peptides (Unmodified): Confidence Limit [%]: 77.85
17: Peptides (Other): Confidence Limit [%]: 84.47
18: Peptides (Unmodified): PEP Limit [%]: 22.15
19: Peptides (Other): PEP Limit [%]: 15.53
20: Peptides (Unmodified): Confidence Accuracy [%]: 0.14
21: Peptides (Other): Confidence Accuracy [%]: 1.01
22: PSMs (Charge 2): #Validated PSM: 5582.0
23: PSMs (Charge 3 and Charge 4, 5, 6): #Validated PSM: 2763.0
24: PSMs (Charge 2): Total Possible TP: 6993.26
25: PSMs (Charge 3 and Charge 4, 5, 6): Total Possible TP: 2982.18
26: PSMs (Charge 2): FDR Limit [%]: 0.99
27: PSMs (Charge 3 and Charge 4, 5, 6): FDR Limit [%]: 0.94
28: PSMs (Charge 2): FNR Limit [%]: 21.15
29: PSMs (Charge 3 and Charge 4, 5, 6): FNR Limit [%]: 8.22
30: PSMs (Charge 2): Confidence Limit [%]: 81.68
31: PSMs (Charge 3 and Charge 4, 5, 6): Confidence Limit [%]: 82.22
32: PSMs (Charge 2): PEP Limit [%]: 18.32
33: PSMs (Charge 3 and Charge 4, 5, 6): PEP Limit [%]: 17.78
34: PSMs (Charge 2): Confidence Accuracy [%]: 0.12
35: PSMs (Charge 3 and Charge 4, 5, 6): Confidence Accuracy [%]: 2.27

PTM Scoring Settings

1: Probabilistic Score: PhosphoRS
2: Accounting for Neutral Losses: No
3: Threshold: 95.0

Spectrum Counting Parameters

1: Method: NSAF
2: Validated Matches Only: No

Annotation Settings

1: Intensity Limit: 0.75
2: Automatic Annotation: Yes
3: Selected Ions: b, y
4: Neutral Losses: H₂O, CH₄OS, NH₃
5: Neutral Losses Sequence Dependence: Yes
6: Fragment Ion m/z Tolerance: 0.02

1.11 WCPL_PEG_HILIC_2

Project Details

- 1: PeptideShaker Version: 1.16.31
- 2: Date: Sat Dec 15 17:19:56 CAT 2018
- 3: Experiment: 1068_WCPL_PEG_HILIC_2_PEG-pilot-study
- 4: Sample: 1068_WCPL_PEG_HILIC_2_PEG-pilot-study
- 5: Replicate Number: 0
- 6: Identification Algorithms: X!Tandem, MS Amanda and MS-GF+

Database Search Parameters

- 1: Precursor Tolerance Unit: ppm
- 2: Precursor Ion m/z Tolerance: 10.0
- 3: Fragment Ion Tolerance Unit: Da
- 4: Fragment Ion m/z Tolerance: 0.02
- 5: Cleavage: Enzyme
- 6: Enzyme: Trypsin
- 7: Missed Cleavages: 2
- 8: Specificity: Specific
- 9: Database: uniprot-human-ref-proteome-trypsin-Oct2018_concatenated_target_decoy.fasta
- 10: Forward Ion: b
- 11: Rewind Ion: y
- 12: Fixed Modifications: Methylthio of C
- 13: Variable Modifications: Oxidation of M, Deamidation of N, Deamidation of Q
- 14: Refinement Variable Modifications: Acetylation of protein N-term, Pyrolidone from E, Pyrolidone from Q, Pyrolidone from carbamidomethylated C
- 15: Refinement Fixed Modifications: Methylthio of C

Input Filters

- 1: Minimal Peptide Length: 8
- 2: Maximal Peptide Length: 30
- 3: Precursor m/z Tolerance: 10.0
- 4: Precursor m/z Tolerance Unit: Yes
- 5: Unrecognized Modifications Discarded: Yes

Validation Summary

- 1: Proteins: #Validated: 2413.0
- 2: Proteins: Total Possible TP: 2829.69
- 3: Proteins: FDR Limit [%]: 0.99
- 4: Proteins: FNR Limit [%]: 15.34
- 5: Proteins: Confidence Limit [%]: 91.26
- 6: Proteins: PEP Limit [%]: 8.74
- 7: Proteins: Confidence Accuracy [%]: 0.12
- 8: Peptides (Unmodified): #Validated: 7489.0
- 9: Peptides (Deamidation of N): #Validated: 577.0
- 10: Peptides (Other): #Validated: 411.0
- 11: Peptides (Unmodified): Total Possible TP: 8079.0
- 12: Peptides (Deamidation of N): Total Possible TP: 853.27

13: Peptides (Other): Total Possible TP: 744.46
14: Peptides (Unmodified): FDR Limit [%]: 0.99
15: Peptides (Deamidation of N): FDR Limit [%]: 0.87
16: Peptides (Other): FDR Limit [%]: 0.97
17: Peptides (Unmodified): FNR Limit [%]: 8.5
18: Peptides (Deamidation of N): FNR Limit [%]: 33.02
19: Peptides (Other): FNR Limit [%]: 45.26
20: Peptides (Unmodified): Confidence Limit [%]: 69.16
21: Peptides (Deamidation of N): Confidence Limit [%]: 80.95
22: Peptides (Other): Confidence Limit [%]: 84.27
23: Peptides (Unmodified): PEP Limit [%]: 30.84
24: Peptides (Deamidation of N): PEP Limit [%]: 19.05
25: Peptides (Other): PEP Limit [%]: 15.73
26: Peptides (Unmodified): Confidence Accuracy [%]: 0.15
27: Peptides (Deamidation of N): Confidence Accuracy [%]: 0.97
28: Peptides (Other): Confidence Accuracy [%]: 1.15
29: PSMs (Charge 2): #Validated PSM: 6668.0
30: PSMs (Charge 3 and Charge 4, 5, 6): #Validated PSM: 3165.0
31: PSMs (Charge 2): Total Possible TP: 8010.99
32: PSMs (Charge 3 and Charge 4, 5, 6): Total Possible TP: 3449.93
33: PSMs (Charge 2): FDR Limit [%]: 0.99
34: PSMs (Charge 3 and Charge 4, 5, 6): FDR Limit [%]: 0.98
35: PSMs (Charge 2): FNR Limit [%]: 17.61
36: PSMs (Charge 3 and Charge 4, 5, 6): FNR Limit [%]: 9.23
37: PSMs (Charge 2): Confidence Limit [%]: 80.43
38: PSMs (Charge 3 and Charge 4, 5, 6): Confidence Limit [%]: 75.56
39: PSMs (Charge 2): PEP Limit [%]: 19.57
40: PSMs (Charge 3 and Charge 4, 5, 6): PEP Limit [%]: 24.44
41: PSMs (Charge 2): Confidence Accuracy [%]: 0.22
42: PSMs (Charge 3 and Charge 4, 5, 6): Confidence Accuracy [%]: 0.74

PTM Scoring Settings

1: Probabilistic Score: PhosphoRS
2: Accounting for Neutral Losses: No
3: Threshold: 95.0

Spectrum Counting Parameters

1: Method: NSAF
2: Validated Matches Only: No

Annotation Settings

1: Intensity Limit: 0.75
2: Automatic Annotation: Yes
3: Selected Ions: b, y
4: Neutral Losses: H₂O, CH₄OS, NH₃
5: Neutral Losses Sequence Dependence: Yes
6: Fragment Ion m/z Tolerance: 0.02

1.12 WCPL_PEG_HILIC_3

Project Details

1: PeptideShaker Version: 1.16.31
2: Date: Sat Dec 15 17:31:14 CAT 2018
3: Experiment: 1068_WCPL_PEG_HILIC_3_PEG-pilot-study
4: Sample: 1068_WCPL_PEG_HILIC_3_PEG-pilot-study
5: Replicate Number: 0
6: Identification Algorithms: X!Tandem, MS Amanda and MS-GF+

Database Search Parameters

1: Precursor Tolerance Unit: ppm
2: Precursor Ion m/z Tolerance: 10.0
3: Fragment Ion Tolerance Unit: Da
4: Fragment Ion m/z Tolerance: 0.02
5: Cleavage: Enzyme
6: Enzyme: Trypsin
7: Missed Cleavages: 2
8: Specificity: Specific
9: Database: uniprot-human-ref-proteome-trypsin-Oct2018_concatenated_target_decoy.fasta
10: Forward Ion: b
11: Rewind Ion: y
12: Fixed Modifications: Methylthio of C
13: Variable Modifications: Oxidation of M, Deamidation of N, Deamidation of Q
14: Refinement Variable Modifications: Acetylation of protein N-term, Pyrolidone from E, Pyrolidone from Q, Pyrolidone from carbamidomethylated C
15: Refinement Fixed Modifications: Methylthio of C

Input Filters

1: Minimal Peptide Length: 8
2: Maximal Peptide Length: 30
3: Precursor m/z Tolerance: 10.0
4: Precursor m/z Tolerance Unit: Yes
5: Unrecognized Modifications Discarded: Yes

Validation Summary

1: Proteins: #Validated: 2163.0
2: Proteins: Total Possible TP: 2635.99
3: Proteins: FDR Limit [%]: 0.97
4: Proteins: FNR Limit [%]: 18.76
5: Proteins: Confidence Limit [%]: 89.79
6: Proteins: PEP Limit [%]: 10.21
7: Proteins: Confidence Accuracy [%]: 0.1
8: Peptides (Unmodified): #Validated: 6344.0
9: Peptides (Deamidation of N): #Validated: 456.0
10: Peptides (Other): #Validated: 436.0
11: Peptides (Unmodified): Total Possible TP: 7005.45
12: Peptides (Deamidation of N): Total Possible TP: 653.73
13: Peptides (Other): Total Possible TP: 668.62
14: Peptides (Unmodified): FDR Limit [%]: 0.98
15: Peptides (Deamidation of N): FDR Limit [%]: 0.88
16: Peptides (Other): FDR Limit [%]: 0.92
17: Peptides (Unmodified): FNR Limit [%]: 10.46
18: Peptides (Deamidation of N): FNR Limit [%]: 31.11

19: Peptides (Other): FNR Limit [%]: 35.27
20: Peptides (Unmodified): Confidence Limit [%]: 78.32
21: Peptides (Deamidation of N): Confidence Limit [%]: 79.41
22: Peptides (Other): Confidence Limit [%]: 88.82
23: Peptides (Unmodified): PEP Limit [%]: 21.68
24: Peptides (Deamidation of N): PEP Limit [%]: 20.59
25: Peptides (Other): PEP Limit [%]: 11.18
26: Peptides (Unmodified): Confidence Accuracy [%]: 0.23
27: Peptides (Deamidation of N): Confidence Accuracy [%]: 0.66
28: Peptides (Other): Confidence Accuracy [%]: 0.7
29: PSMs (Charge 2): #Validated PSM: 5546.0
30: PSMs (Charge 3): #Validated PSM: 2314.0
31: PSMs (Charge 4 and Charge 5, 6): #Validated PSM: 328.0
32: PSMs (Charge 2): Total Possible TP: 6770.42
33: PSMs (Charge 3): Total Possible TP: 2577.66
34: PSMs (Charge 4 and Charge 5, 6): Total Possible TP: 344.01
35: PSMs (Charge 2): FDR Limit [%]: 0.99
36: PSMs (Charge 3): FDR Limit [%]: 0.99
37: PSMs (Charge 4 and Charge 5, 6): FDR Limit [%]: 0.61
38: PSMs (Charge 2): FNR Limit [%]: 18.93
39: PSMs (Charge 3): FNR Limit [%]: 11.3
40: PSMs (Charge 4 and Charge 5, 6): FNR Limit [%]: 5.72
41: PSMs (Charge 2): Confidence Limit [%]: 81.82
42: PSMs (Charge 3): Confidence Limit [%]: 67.23
43: PSMs (Charge 4 and Charge 5, 6): Confidence Limit [%]: 45.45
44: PSMs (Charge 2): PEP Limit [%]: 18.18
45: PSMs (Charge 3): PEP Limit [%]: 32.77
46: PSMs (Charge 4 and Charge 5, 6): PEP Limit [%]: 54.55
47: PSMs (Charge 2): Confidence Accuracy [%]: 0.28
48: PSMs (Charge 3): Confidence Accuracy [%]: 0.85
49: PSMs (Charge 4 and Charge 5, 6): Confidence Accuracy [%]: 10.0

PTM Scoring Settings

1: Probabilistic Score: PhosphoRS
2: Accounting for Neutral Losses: No
3: Threshold: 95.0

Spectrum Counting Parameters

1: Method: NSAF
2: Validated Matches Only: No

Annotation Settings

1: Intensity Limit: 0.75
2: Automatic Annotation: Yes
3: Selected Ions: b, y
4: Neutral Losses: H₂O, CH₄OS, NH₃
5: Neutral Losses Sequence Dependence: Yes
6: Fragment Ion m/z Tolerance: 0.02