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Samples & Files  
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Factors  
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NTU\_phospho

Options: WT10, WT, Cnal, Cnal10

Study variable(s) for grouping:

File;NTU\_phospho

Groups sorted by:

File (Ascending);NTU\_phospho (Ascending)

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Quan Methods  
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None

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Files  
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[F5] 110710\_WT10\_NTU\_20211126

F:\MS DATA\A227\NTU\_B305\110710-110713\110710\_WT10\_NTU\_20211126.raw

[F6] 110711\_WT\_NTU\_20211126

F:\MS DATA\A227\NTU\_B305\110710-110713\110711\_WT\_NTU\_20211126.raw

[F7] 110712\_Cnal10\_NTU\_20211126

F:\MS DATA\A227\NTU\_B305\110710-110713\110712\_Cnal10\_NTU\_20211126.raw

[F8] 110713\_Cnal\_NTU\_20211126

F:\MS DATA\A227\NTU\_B305\110710-110713\110713\_Cnal\_NTU\_20211126.raw

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Sample Groups  
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Study variable(s) for grouping:

File;NTU\_phospho

Groups sorted by:

File (Ascending);NTU\_phospho (Ascending)

F5, WT10

[S5] 110710\_WT10\_NTU\_20211126

NTU\_phospho=WT10

F6, WT

[S6] 110711\_WT\_NTU\_20211126

NTU\_phospho=WT

F7, Cnal10

[S7] 110712\_Cnal10\_NTU\_20211126

NTU\_phospho=Cnal10

F8, Cnal

[S8] 110713\_Cnal\_NTU\_20211126

NTU\_phospho=Cnal

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Samples  
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[S5] 110710\_WT10\_NTU\_20211126

NTU\_phospho=WT10

[S6] 110711\_WT\_NTU\_20211126

NTU\_phospho=WT

[S7] 110712\_Cnal10\_NTU\_20211126

NTU\_phospho=Cnal10

[S8] 110713\_Cnal\_NTU\_20211126

NTU\_phospho=Cnal

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Files to Samples  
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[F5] 110710\_WT10\_NTU\_20211126

[S5] 110710\_WT10\_NTU\_20211126

NTU\_phospho=WT10

[F6] 110711\_WT\_NTU\_20211126

[S6] 110711\_WT\_NTU\_20211126

NTU\_phospho=WT

[F7] 110712\_Cnal10\_NTU\_20211126

[S7] 110712\_Cnal10\_NTU\_20211126

NTU\_phospho=Cnal10

[F8] 110713\_Cnal\_NTU\_20211126

[S8] 110713\_Cnal\_NTU\_20211126

NTU\_phospho=Cnal

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Analysis Settings  
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Consensus Step : Workflow  
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Result name: 110491-110494\_NTU305\_20210909

Result file: F:\MS DATA\A227\NTU\_B305\NTU\_R305\110491-110494\_NTU305\_20210909-(2).pdResult

Description: -

Workflow based on template: 110491-110494\_NTU305\_20210909

Creation date: 11/29/2021 9:48:57 AM

Created with Discoverer version: 2.5.0.400

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The workflow tree:  
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- |-(0) MSF Files
- |-(9) Feature Mapper
- |-(10) Precursor Ions Quantifier
- |-(1) PSM Grouper
- |-(2) Peptide Validator
- |-(3) Peptide and Protein Filter
- |-(4) Protein Scorer
- |-(5) Protein FDR Validator
- |-(6) Protein Grouping
- |-(7) Peptide in Protein Annotation

Post-processing nodes:  
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|-(8) Display Settings

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Processing node 0: MSF Files

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1. Storage Settings:

- Spectra to Store: Identified or Quantified
- Feature Traces to Store: All

2. Merging of Identified Peptide and Proteins:

- Merge Mode: Globally by Search Engine Type

3. FASTA Title Line Display:

- Reported FASTA Title Lines: Best match
- Title Line Rule: standard

4. PSM Filters:

- Maximum Delta Cn: 0.05
- Maximum Rank: 0
- Maximum Delta Mass: 0 ppm

Hidden Parameters:

- MSF File(s): F:\MS DATA\A227\NTU\_B305\NTU\_R305\110491-110494\_NTU305\_20210909-(1).msf

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Processing node 9: Feature Mapper

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1. Chromatographic Alignment:

- Perform RT Alignment: True
- Maximum RT Shift [min]: 10
- Mass Tolerance: 10 ppm
- Parameter Tuning: Coarse

## 2. Feature Linking and Mapping:

- RT Tolerance [min]: 0
- Mass Tolerance: 0 ppm
- Min. S/N Threshold: 5

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Processing node 10: Precursor Ions Quantifier  
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### 1. General Quantification Settings:

- Peptides to Use: Unique + Razor
- Consider Protein Groups for Peptide Uniqueness: True
- Use Shared Quan Results: True
- Reject Quan Results with Missing Channels: False

### 2. Precursor Quantification:

- Precursor Abundance Based On: Intensity
- Min. # Replicate Features [%]: 0

### 3. Normalization and Scaling:

- Normalization Mode: None
- Scaling Mode: None

### 4. Exclude Peptides from Protein Quantification:

- For Normalization: Use All Peptides
- For Protein Roll-Up: Use All Peptides
- For Pairwise Ratios: Exclude Modified

### 5. Quan Rollup and Hypothesis Testing:

- Protein Abundance Calculation: Summed Abundances
- N for Top N: 3
- Protein Ratio Calculation: Pairwise Ratio Based
- Maximum Allowed Fold Change: 100
- Imputation Mode: None

- Hypothesis Test: t-test (Background Based)

6. Quan Ratio Distributions:

- 1st Fold Change Threshold: 2
- 2nd Fold Change Threshold: 4
- 3rd Fold Change Threshold: 6
- 4th Fold Change Threshold: 8
- 5th Fold Change Threshold: 10

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Processing node 1: PSM Grouper

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1. Peptide Group Modifications:

- Site Probability Threshold: 75

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Processing node 2: Peptide Validator

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1. General Validation Settings:

- Validation Mode: Automatic (Control peptide level error rate if possible)
- Target FDR (Strict) for PSMs: 0.01
- Target FDR (Relaxed) for PSMs: 0.05
- Target FDR (Strict) for Peptides: 0.01
- Target FDR (Relaxed) for Peptides: 0.05

2. Specific Validation Settings:

- Validation Based on: q-Value
- Target/Decoy Selection for PSM Level FDR Calculation Based on Score: Automatic
- Reset Confidences for Nodes without Decoy Search (Fixed score thresholds): False

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Processing node 3: Peptide and Protein Filter

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1. Peptide Filters:

- Peptide Confidence At Least: High
- Keep Lower Confident PSMs: False
- Minimum Peptide Length: 6
- Remove Peptides Without Protein Reference: False

2. Protein Filters:

- Minimum Number of Peptide Sequences: 1
- Count Only Rank 1 Peptides: False
- Count Peptides Only for Top Scored Protein: False

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Processing node 4: Protein Scorer

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No parameters

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Processing node 5: Protein FDR Validator

1. Confidence Thresholds:

- Target FDR (Strict): 0.01
- Target FDR (Relaxed): 0.05

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Processing node 6: Protein Grouping

1. Protein Grouping:

- Apply strict parsimony principle: True

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Processing node 7: Peptide in Protein Annotation

1. Flanking Residues:



- Annotate Flanking Residues of the Peptide: True
- Number Flanking Residues in Connection Tables: 1

2. Modifications in Peptide:

- Protein Modifications Reported: Only for Master Proteins

3. Modifications in Protein:

- Modification Sites Reported: All And Specific
- Minimum PSM Confidence: High
- Report Only PTMs: True

4. Positions in Protein:

- Protein Positions for Peptides: Only for Master Proteins

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Processing node 8: Display Settings

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1. General:

- Filter Set:

- ### Master Proteins Default Filter:
- ### Row Filter for TargetProtein:
- ### Master is equal to Master
- ###

'magellan filter set' 1 'MasterFilter.filterset' Filter 'TargetProtein' FilterProperties 1  
'FilterConditionProperties/FilterScope' 'FilterConditionProperties/FilterScopeValueMainGrid' 1 NARY\_AND 1 =  
FilterConditionProperties 1 'NamedComparableFilterCondition/DisplayPropertyHint' 'Master' property  
'Thermo.PD.EntityDataFramework.MasterProteinAssessment, Thermo.Magellan.EntityDataFramework' 'IsMasterProtein'  
constant 'Thermo.PD.EntityDataFramework.MasterProteinAssessment, Thermo.Magellan.EntityDataFramework'  
'IsMasterProtein'

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Workflow messages:  
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11/29/2021 10:09 AM Job Execution: Processing F:\MS DATA\A227\NTU\_B305\NTU\_R305\110491-110494\_NTU305\_20210909-(2).pdResult

11/29/2021 10:09 AM (0) MSF Files: F:\MS DATA\A227\NTU\_B305\NTU\_R305\110491-110494\_NTU305\_20210909-(1).msf

11/29/2021 10:09 AM (0) MSF Files: All 1 files are ready for processing.

11/29/2021 10:09 AM (0) MSF Files: Start transferring results of 1 msf files...

11/29/2021 10:09 AM (0) MSF Files: Transferred 8643 Proteins to result file in 2.6 s.

11/29/2021 10:09 AM (0) MSF Files: Transferred 7889 Decoy Proteins to result file in 2.1 s.

11/29/2021 10:09 AM (0) MSF Files: Added 69493 Mass Spectra to result file.

11/29/2021 10:09 AM (0) MSF Files: Added 743857 traces to result file.

11/29/2021 10:09 AM (0) MSF Files: Added 4 Input Files to result file.

11/29/2021 10:10 AM (0) MSF Files: Added 62416 PSMs to result file.

11/29/2021 10:10 AM (0) MSF Files: Added 21526 Decoy PSMs to result file.

11/29/2021 10:10 AM (0) MSF Files: Added 74695 MS/MS Spectrum Info to result file.

11/29/2021 10:10 AM (0) MSF Files: Added 74695 Precursors to result file.

11/29/2021 10:10 AM (0) MSF Files: Added 12 Specialized Traces to result file.

11/29/2021 10:10 AM (0) MSF Files: Added 212733 LCMS Features to result file.

11/29/2021 10:10 AM (0) MSF Files: Added 1049725 LCMS Peaks to result file.

11/29/2021 10:10 AM (0) MSF Files: Copying data took 1 min 30 s.

11/29/2021 10:10 AM (0) MSF Files: Finding unique sequences took 3.8 s.

11/29/2021 10:10 AM (0) MSF Files: Filtering proteins took 231.4 ms.

11/29/2021 10:11 AM (0) MSF Files: -- Total execution of MSF Files (0) took 1 min 53 s --

11/29/2021 10:11 AM (1) PSM Grouper: Grouping 'PSMs'

11/29/2021 10:11 AM (1) PSM Grouper: Found 19400 Peptide Groups.

11/29/2021 10:11 AM (1) PSM Grouper: Grouping 'Decoy PSMs'

11/29/2021 10:11 AM (1) PSM Grouper: Found 13031 Decoy Peptide Groups.

11/29/2021 10:11 AM (1) PSM Grouper: -- Total execution of PSM Grouper (1) took 40.8 s --

11/29/2021 10:11 AM (2) Peptide Validator: Start PSM and Peptide validation in 'Automatic (Control peptide level error rate if possible)' mode...

11/29/2021 10:11 AM (2) Peptide Validator: Updated PSM confidences in 792.2 ms.

11/29/2021 10:11 AM (2) Peptide Validator: Use svm score for 'peptide' quality run.

11/29/2021 10:11 AM (2) Peptide Validator: Updated peptide confidences using quality in 6.8 s.

11/29/2021 10:11 AM (2) Peptide Validator: Calculating Mascot thresholds.

11/29/2021 10:11 AM (2) Peptide Validator: -- Total execution of Peptide Validator (2) took 7.9 s --

|  |                                 |   |
|--|---------------------------------|---|
| 11/29/2021 10:11 AM                                  | (3) Peptide and Protein Filter: | Filter Peptide Groups   |
| 11/29/2021 10:11 AM                                  | (3) Peptide and Protein Filter: | Filter 5725/19400 Peptide Groups (13675 excluded) and               |
| 35332/62416 PSMs (27084 excluded) took 4.4 s         |                                 |   |
| 11/29/2021 10:11 AM                                  | (3) Peptide and Protein Filter: | Filtering Proteins  |
| 11/29/2021 10:11 AM                                  | (3) Peptide and Protein Filter: | Filter 1959/8643 Proteins (6684 excluded) took 729 ms               |
| 11/29/2021 10:12 AM                                  | (3) Peptide and Protein Filter: | Filter Decoy Peptide Groups   |
| 11/29/2021 10:12 AM                                  | (3) Peptide and Protein Filter: | Filter 56/13031 Decoy Peptide Groups (12975 excluded)               |
| and 163/21526 Decoy PSMs (21363 excluded) took 1.1 s |                                 |   |
| 11/29/2021 10:12 AM                                  | (3) Peptide and Protein Filter: | Filtering Decoy Proteins  |
| 11/29/2021 10:12 AM                                  | (3) Peptide and Protein Filter: | Filter 53/7889 Decoy Proteins (7836 excluded) took 580.8            |
| ms   |                                 |   |
| 11/29/2021 10:12 AM                                  | (3) Peptide and Protein Filter: | Updating counts took 9.7 s.   |
| 11/29/2021 10:12 AM                                  | (3) Peptide and Protein Filter: | -- Total execution of Peptide and Protein Filter (3) took           |
| 17.2 s --  |                                 |   |
| 11/29/2021 10:12 AM                                  | (9) Feature Mapper:             | Extracting features   |
| 11/29/2021 10:12 AM                                  | (9) Feature Mapper:             | Extracting LCMS features  |
| 11/29/2021 10:12 AM                                  | (9) Feature Mapper:             | Extracting feature groups took 10.3 s.                              |
| 11/29/2021 10:12 AM                                  | (9) Feature Mapper:             | Start aligning 3 files ('F5', 'F6', 'F7') to reference file 'F8'... |
| 11/29/2021 10:12 AM                                  | (9) Feature Mapper:             | Calculating RT alignment took 13.2 s                                |
| 11/29/2021 10:12 AM                                  | (9) Feature Mapper:             | Start updating RTs...   |
| 11/29/2021 10:12 AM                                  | (9) Feature Mapper:             | Updating RTs of LCMS Features took 2.5 s.                           |
| 11/29/2021 10:12 AM                                  | (9) Feature Mapper:             | Updating RTs of LCMS Peaks took 11.7 s.                             |
| 11/29/2021 10:12 AM                                  | (9) Feature Mapper:             | Updating RTs of PSMs took 2 s.                                      |
| 11/29/2021 10:12 AM                                  | (9) Feature Mapper:             | Updating RTs of MS/MS Spectrum Info took 809.3 ms.                  |
| 11/29/2021 10:12 AM                                  | (9) Feature Mapper:             | -- Performing retention time alignment took 30.5 s. --              |
| 11/29/2021 10:12 AM                                  | (9) Feature Mapper:             | Extracting feature groups took 0.2 ms.                              |
| 11/29/2021 10:12 AM                                  | (9) Feature Mapper:             | Start aligning 3 files ('F5', 'F6', 'F7') to reference file 'F8'... |
| 11/29/2021 10:12 AM                                  | (9) Feature Mapper:             | Updating m/z values of LCMS Features took 2.2 s.                    |
| 11/29/2021 10:13 AM                                  | (9) Feature Mapper:             | Updating m/z values of LCMS Peaks took 14 s.                        |
| 11/29/2021 10:13 AM                                  | (9) Feature Mapper:             | Updating m/z values of PSMs took 2.9 s.                             |
| 11/29/2021 10:13 AM                                  | (9) Feature Mapper:             | -- Performing mass over charge alignment took 21.5 s. --            |
| 11/29/2021 10:13 AM                                  | (9) Feature Mapper:             | Extracting feature groups took 0.2 ms.                              |
| 11/29/2021 10:13 AM                                  | (9) Feature Mapper:             | Start aligning 3 files ('F5', 'F6', 'F7') to reference file 'F8'... |
| 11/29/2021 10:13 AM                                  | (9) Feature Mapper:             | Updating area values of LCMS Features took 3.4 s.                   |

|                                    |                                 |  |
|------------------------------------|---------------------------------|--|
| 11/29/2021 10:13 AM                | (9) Feature Mapper:             | Updating area values of LCMS Peaks took 16.3 s.                    |
| 11/29/2021 10:13 AM                | (9) Feature Mapper:             | -- Performing abundance alignment took 22.6 s. --                  |
| 11/29/2021 10:13 AM<br>mapping     | (9) Feature Mapper:             | Using RT tolerance of 2.00 min and mass tolerance of 6.3 ppm for   |
| 11/29/2021 10:13 AM                | (9) Feature Mapper:             | Mapping 1 Fraction(s)  |
| 11/29/2021 10:13 AM                | (9) Feature Mapper:             | Mapping Fraction 1 of 1  |
| 11/29/2021 10:15 AM                | (9) Feature Mapper:             | Mapping 1 Fraction(s) took 2 min 11 s                              |
| 11/29/2021 10:15 AM                | (9) Feature Mapper:             | -- Performing cross file mapping took 2 min 11 s. --               |
| 11/29/2021 10:15 AM                | (9) Feature Mapper:             | Storing Top Apex RT for Peptide Groups                             |
| 11/29/2021 10:15 AM                | (9) Feature Mapper:             | Storing Top Apex RT for Peptide Groups took 2.6 s                  |
| 11/29/2021 10:15 AM                | (9) Feature Mapper:             | -- Total execution of Feature Mapper (9) took 3 min 32 s --        |
| 11/29/2021 10:15 AM                | (4) Protein Scorer:             | Calculating Coverage and Counts                                    |
| 11/29/2021 10:15 AM                | (4) Protein Scorer:             | Calculated counts and coverages in 2.9 s.                          |
| 11/29/2021 10:15 AM                | (4) Protein Scorer:             | Scoring target proteins  |
| 11/29/2021 10:15 AM                | (4) Protein Scorer:             | Scored 1959 proteins in 3.5 s.                                     |
| 11/29/2021 10:15 AM                | (4) Protein Scorer:             | Scoring decoy proteins   |
| 11/29/2021 10:15 AM                | (4) Protein Scorer:             | Scored 53 decoy proteins in 226.1 ms.                              |
| 11/29/2021 10:15 AM                | (4) Protein Scorer:             | -- Total execution of Protein Scorer (4) took 6.8 s --             |
| 11/29/2021 10:15 AM                | (5) Protein FDR Validator:      | Apply confidences based on protein scores of 1959 proteins.        |
| 11/29/2021 10:15 AM                | (5) Protein FDR Validator:      | Calculating Sum PEP Score for Proteins                             |
| 11/29/2021 10:15 AM                | (5) Protein FDR Validator:      | Calculating Sum PEP Score for Decoy Proteins                       |
| 11/29/2021 10:15 AM                | (5) Protein FDR Validator:      | -- Total execution of Protein FDR Validator (5) took 3.7 s --      |
| 11/29/2021 10:15 AM                | (6) Protein Grouping:           | Retrieving 1911 protein groups took 76.1 ms.                       |
| 11/29/2021 10:16 AM<br>took 8.4 s. | (6) Protein Grouping:           | Storing, updating and connecting protein groups, PSMs and peptides |
| 11/29/2021 10:16 AM                | (6) Protein Grouping:           | Check 1911 protein groups.   |
| 11/29/2021 10:16 AM                | (6) Protein Grouping:           | Applying strict parsimony took 9.9 s.                              |
| 11/29/2021 10:16 AM                | (6) Protein Grouping:           | Found 1908 protein groups.   |
| 11/29/2021 10:16 AM                | (6) Protein Grouping:           | Retrieving 53 decoy protein groups took 6.3 ms.                    |
| 11/29/2021 10:16 AM<br>took 2 s.   | (6) Protein Grouping:           | Storing, updating and connecting protein groups, PSMs and peptides |
| 11/29/2021 10:16 AM                | (6) Protein Grouping:           | Found 53 decoy protein groups.                                     |
| 11/29/2021 10:16 AM                | (6) Protein Grouping:           | -- Total execution of Protein Grouping (6) took 25.7 s --          |
| 11/29/2021 10:16 AM                | (10) Precursor Ions Quantifier: | Validating LCMS Features   |

|                                     |                                    |  |
|-------------------------------------|------------------------------------|--|
| 11/29/2021 10:16 AM                 | (10) Precursor Ions Quantifier:    | Validating LCMS Features for 332970 items took 3.9 s       |
| 11/29/2021 10:16 AM                 | (10) Precursor Ions Quantifier:    | Validating Consensus Features                              |
| 11/29/2021 10:16 AM                 | (10) Precursor Ions Quantifier:    | Validation of quantification results took 12 s             |
| 11/29/2021 10:16 AM                 | (10) Precursor Ions Quantifier:    | Updating spectrum match areas                              |
| 11/29/2021 10:16 AM                 | (10) Precursor Ions Quantifier:    | Classify quan usage of PSMs                                |
| 11/29/2021 10:16 AM                 | (10) Precursor Ions Quantifier:    | Classifying Peptide Groups quan usage                      |
| 11/29/2021 10:16 AM<br>906.5 ms     | (10) Precursor Ions Quantifier:    | Classifying Peptide Groups quan usage for 5725 items took  |
| 11/29/2021 10:16 AM                 | (10) Precursor Ions Quantifier:    | Calculating Abundances of Peptide Groups                   |
| 11/29/2021 10:16 AM                 | (10) Precursor Ions Quantifier:    | Classifying Peptide Groups quan usage                      |
| 11/29/2021 10:16 AM                 | (10) Precursor Ions Quantifier:    | Counting Razor Peptides                                    |
| 11/29/2021 10:16 AM<br>693.5 ms     | (10) Precursor Ions Quantifier:    | Classifying Peptide Groups quan usage for 5725 items took  |
| 11/29/2021 10:16 AM                 | (10) Precursor Ions Quantifier:    | Calculating Abundances of Proteins                         |
| 11/29/2021 10:16 AM                 | (10) Precursor Ions Quantifier:    | Calculating and applying normalization took 0 ms           |
| 11/29/2021 10:16 AM                 | (10) Precursor Ions Quantifier:    | Calculating ratios for Peptide Groups...                   |
| 11/29/2021 10:16 AM                 | (10) Precursor Ions Quantifier:    | Calculating ratios for Proteins...                         |
| 11/29/2021 10:16 AM<br>Groups...    | (10) Precursor Ions Quantifier:    | Start calculating p-values based on background for Peptide |
| 11/29/2021 10:16 AM                 | (10) Precursor Ions Quantifier:    | Calculating p-values based on background took 11.3 s       |
| 11/29/2021 10:16 AM                 | (10) Precursor Ions Quantifier:    | Calculating p-values for Peptide Groups took 11.4 s.       |
| 11/29/2021 10:16 AM<br>Proteins...  | (10) Precursor Ions Quantifier:    | Start calculating p-values based on background for         |
| 11/29/2021 10:17 AM                 | (10) Precursor Ions Quantifier:    | Calculating p-values based on background took 2.7 s        |
| 11/29/2021 10:17 AM                 | (10) Precursor Ions Quantifier:    | Calculating p-values for Proteins took 2.8 s.              |
| 11/29/2021 10:17 AM                 | (10) Precursor Ions Quantifier:    | Quantification took 40.4 s.                                |
| 11/29/2021 10:17 AM                 | (10) Precursor Ions Quantifier:    | Preparing spectrum visualization took 1.2 s.               |
| 11/29/2021 10:17 AM<br>41.6 s --    | (10) Precursor Ions Quantifier:    | -- Total execution of Precursor Ions Quantifier (10) took  |
| 11/29/2021 10:17 AM                 | (7) Peptide in Protein Annotation: | Start retrieving flanking residues and positions...        |
| 11/29/2021 10:17 AM                 | (7) Peptide in Protein Annotation: | Annotated PSMs/peptides for 1959 proteins.                 |
| 11/29/2021 10:17 AM<br>positions... | (7) Peptide in Protein Annotation: | Start annotating peptide groups with flanking residues and |
| 11/29/2021 10:17 AM                 | (7) Peptide in Protein Annotation: | Annotate Peptide Groups items                              |
| 11/29/2021 10:17 AM                 | (7) Peptide in Protein Annotation: | Start calculating protein coverage...                      |

11/29/2021 10:17 AM (7) Peptide in Protein Annotation: -- Total execution of Peptide in Protein Annotation (7) took 40.9 s --  
11/29/2021 10:17 AM (8) Display Settings:Applying display filter and layout  
11/29/2021 10:17 AM (8) Display Settings:-- Total execution of Display Settings (8) took 56.2 ms --  
11/29/2021 10:17 AM Job Execution: Finalizing file took 13.1 s.  
11/29/2021 10:17 AM Job Execution: Finished F:\MS DATA\A227\NTU\_B305\NTU\_R305\110491-110494\_NTU305\_20210909-(2).pdResult  
11/29/2021 10:17 AM Job Execution: ----- Total Job execution took: 8 min 45 s. -----

=====  
Processing Step A: Workflow  
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Result name: 110491-110494\_NTU305\_20210909  
Result file: F:\MS DATA\A227\NTU\_B305\NTU\_R305\110491-110494\_NTU305\_20210909-(1).msf  
Description: -  
Workflow based on template:  
Creation date: 11/29/2021 9:48:56 AM  
Created with Discoverer version: 2.5.0.400

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The workflow tree:  
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- |-(0) Spectrum Files
- |-(5) Minora Feature Detector
- |-(1) Spectrum Selector
- |-(2) Sequest HT
- |-(3) Percolator
- |-(4) IMP-ptmRS

-----  
Processing node 0: Spectrum Files

-----  
Input Data:

- File Name(s) (Hidden):

F:\MS DATA\A227\NTU\_B305\110710-110713\110710\_WT10\_NTU\_20211126.raw

F:\MS DATA\A227\NTU\_B305\110710-110713\110711\_WT\_NTU\_20211126.raw

F:\MS DATA\A227\NTU\_B305\110710-110713\110712\_Cnal10\_NTU\_20211126.raw

F:\MS DATA\A227\NTU\_B305\110710-110713\110713\_Cnal\_NTU\_20211126.raw

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Processing node 5: Minora Feature Detector

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1. Peak & Feature Detection:

- Min. Trace Length: 5

- S/N Threshold: 1

- Max.  $\Delta$ RT of Isotope Pattern Multiplets [min]: 0.2

2. Feature to ID Linking:

- PSM Confidence At Least: High

-----  
Processing node 1: Spectrum Selector

-----  
1. General Settings:

- Precursor Selection: Use MS1 Precursor

- Use Isotope Pattern in Precursor Reevaluation: True

- Provide Profile Spectra: Automatic

2. Spectrum Properties Filter:

- Lower RT Limit: 0

- Upper RT Limit: 0

- First Scan: 0

- Last Scan: 0

- Lowest Charge State: 0

- Highest Charge State: 0
- Min. Precursor Mass: 350 Da
- Max. Precursor Mass: 5000 Da
- Total Intensity Threshold: 0
- Minimum Peak Count: 1

### 3. Scan Event Filters:

- MS Order: Is Not MS1
- Min. Collision Energy: 0
- Max. Collision Energy: 1000
- Scan Type: Is Full

### 4. Peak Filters:

- S/N Threshold (FT-only): 1.5

### 5. Replacements for Unrecognized Properties:

- Unrecognized Charge Replacements: Automatic
- Unrecognized Mass Analyzer Replacements: ITMS
- Unrecognized MS Order Replacements: MS2
- Unrecognized Activation Type Replacements: CID
- Unrecognized Polarity Replacements: +
- Unrecognized MS Resolution@200 Replacements: 60000
- Unrecognized MSn Resolution@200 Replacements: 30000

### 6. Precursor Pattern Extraction:

- Precursor Clipping Range Before: 2.5 Da
- Precursor Clipping Range After: 5.5 Da

-----  
Processing node 2: Sequest HT  
-----

### 1. Input Data:

- Protein Database: NTU\_R305\_Fusarium oxysporum f.sp lycopersici.fasta



- Enzyme Name: Trypsin (Full)
- Max. Missed Cleavage Sites: 2
- Min. Peptide Length: 6
- Max. Peptide Length: 144
- Max. Number of Peptides Reported: 10

## 2. Tolerances:

- Precursor Mass Tolerance: 10 ppm
- Fragment Mass Tolerance: 0.02 Da
- Use Average Precursor Mass: False
- Use Average Fragment Mass: False

## 3. Spectrum Matching:

- Use Neutral Loss a Ions: True
- Use Neutral Loss b Ions: True
- Use Neutral Loss y Ions: True
- Use Flanking Ions: True
- Weight of a Ions: 0
- Weight of b Ions: 1
- Weight of c Ions: 0
- Weight of x Ions: 0
- Weight of y Ions: 1
- Weight of z Ions: 0

## 4. Dynamic Modifications:

- Max. Equal Modifications Per Peptide: 3
- Max. Dynamic Modifications Per Peptide: 4
- 1. Dynamic Modification: Oxidation / +15.995 Da (M)
- 2. Dynamic Modification: Phospho / +79.966 Da (S, T, Y)

## 6. Dynamic Modifications (protein terminus):

- 1. N-Terminal Modification: Acetyl / +42.011 Da (N-Terminus)

## 7. Static Modifications:

- 1. Static Modification: Carbamidomethyl / +57.021 Da (C)

---

### Processing node 3: Percolator

---

#### 1. Target/Decoy Strategy:

- Target/Decoy Selection: Concatenated
- Validation based on: q-Value

#### 2. Input Data:

- Maximum Delta Cn: 0.05
- Maximum Rank: 0

#### 3. FDR Targets:

- Target FDR (Strict): 0.01
- Target FDR (Relaxed): 0.05

---

### Processing node 4: IMP-ptmRS

---

#### 1. Scoring:

- PhosphoRS Mode: False
- Report Only PTMs: True
- Use Diagnostic Ions: True
- Use Fragment Mass Tolerance of Search Node: True
- Fragment Mass Tolerance: 0.5 Da
- Consider neutral loss peaks for CID, HCD and EThcD: Automatic
- Maximum Peak Depth: 8
- Use a mass accuracy correction: False

#### 2. Performance:

- Maximum Number of Position Isoforms: 500

- Maximum PTMs per peptide: 10

-----  
Workflow messages:  
-----

11/29/2021 09:48 AM Job Execution: Processing F:\MS DATA\A227\NTU\_B305\NTU\_R305\110491-110494\_NTU305\_20210909-(1).msf

11/29/2021 09:49 AM (1) Spectrum Selector: Profile spectra are not sent.

11/29/2021 09:49 AM (1) Spectrum Selector: Reading from file 1 of 4 F5: F:\MS DATA\A227\NTU\_B305\110710-110713\110710\_WT10\_NTU\_20211126.raw (25324 spectra total)

11/29/2021 09:49 AM (2) Sequest HT: Sequence Database: NTU\_R305\_Fusarium oxysporum f.sp lycopersici.fasta

11/29/2021 09:49 AM (1) Spectrum Selector: Sent 16824 spectra from file F5.

11/29/2021 09:49 AM (1) Spectrum Selector: Reading from file 2 of 4 F6: F:\MS DATA\A227\NTU\_B305\110710-110713\110711\_WT\_NTU\_20211126.raw (27172 spectra total)

11/29/2021 09:50 AM (1) Spectrum Selector: Sent 19700 spectra from file F6.

11/29/2021 09:50 AM (1) Spectrum Selector: Reading from file 3 of 4 F7: F:\MS DATA\A227\NTU\_B305\110710-110713\110712\_Cnal10\_NTU\_20211126.raw (26395 spectra total)

11/29/2021 09:50 AM (1) Spectrum Selector: Sent 18470 spectra from file F7.

11/29/2021 09:50 AM (1) Spectrum Selector: Reading from file 4 of 4 F8: F:\MS DATA\A227\NTU\_B305\110710-110713\110713\_Cnal\_NTU\_20211126.raw (27207 spectra total)

11/29/2021 09:51 AM (1) Spectrum Selector: Sent 19701 spectra from file F8.

11/29/2021 09:51 AM (1) Spectrum Selector: Sent 74695 spectra from 4 files (processing time: 1 min 14 s).

11/29/2021 09:51 AM (1) Spectrum Selector: -- Total execution of Spectrum Selector (1) took 2 min 30 s --

11/29/2021 09:51 AM (2) Sequest HT: Storing spectra took 1 min 8 s.

11/29/2021 09:51 AM (2) Sequest HT: There is already an adequate target FASTA index for NTU\_R305\_Fusarium oxysporum f.sp lycopersici(ae889043-7170-45d4-9339-921b061e3358).fasta.

11/29/2021 09:51 AM (2) Sequest HT: Start Sequest HT target search for 74695 spectra (74695 precursors)...

11/29/2021 09:51 AM (2) Sequest HT: lse (2.0.0.24, x64) started at 11/29/2021 9:51:31 AM on A227-20210306 (x64) [20 CPUs] running Microsoft Windows NT 10.0.19042.0 (64bit) [..NET: 4.0.30319.42000]

11/29/2021 09:51 AM (2) Sequest HT: Workload level: #parallel tasks: 10

11/29/2021 09:51 AM (2) Sequest HT: Workload level: #spectra loaded and processed at once: 10000

11/29/2021 09:51 AM (2) Sequest HT: On-Disk search is performed

11/29/2021 09:53 AM (2) Sequest HT: Average search time per spectrum was 1.5 ms.

11/29/2021 09:53 AM (2) Sequest HT: Performing target search took 1 min 52 s.

11/29/2021 09:53 AM (2) Sequest HT: Stored 115091 PSMs for 74695 spectra

11/29/2021 09:53 AM (2) Sequest HT: Discarded 213851 peptide(s) that did not match the conditions for protein terminal modifications.

11/29/2021 09:53 AM (2) Sequest HT: Reading search results took 8.7 s.

11/29/2021 09:53 AM (2) Sequest HT: Saving results took 14.3 s.

11/29/2021 09:53 AM (2) Sequest HT: Saving proteins took 3.7 s.

11/29/2021 09:53 AM (2) Sequest HT: Reading results took 27.2 s.

11/29/2021 09:53 AM (2) Sequest HT: There is already an adequate decoy FASTA index for NTU\_R305\_Fusarium oxysporum f.sp lycopersici(ae889043-7170-45d4-9339-921b061e3358)\_reversed.fasta.

11/29/2021 09:53 AM (2) Sequest HT: Start Sequest HT decoy search for 74695 spectra (74695 precursors)...

11/29/2021 09:53 AM (2) Sequest HT: Ise (2.0.0.24, x64) started at 11/29/2021 9:53:51 AM on A227-20210306 (x64) [20 CPUs] running Microsoft Windows NT 10.0.19042.0 (64bit) [.NET: 4.0.30319.42000]

11/29/2021 09:53 AM (2) Sequest HT: Workload level: #parallel tasks: 10

11/29/2021 09:53 AM (2) Sequest HT: Workload level: #spectra loaded and processed at once: 10000

11/29/2021 09:53 AM (2) Sequest HT: On-Disk search is performed

11/29/2021 09:55 AM (2) Sequest HT: Average search time per spectrum was 1.4 ms.

11/29/2021 09:55 AM (2) Sequest HT: Performing decoy search took 1 min 48 s.

11/29/2021 09:56 AM (2) Sequest HT: Stored 246104 decoy PSMs for 74695 spectra

11/29/2021 09:56 AM (2) Sequest HT: Discarded 248708 peptide(s) that did not match the conditions for protein terminal modifications.

11/29/2021 09:56 AM (2) Sequest HT: Reading search results took 8.6 s.

11/29/2021 09:56 AM (2) Sequest HT: Saving results took 15.3 s.

11/29/2021 09:56 AM (2) Sequest HT: Saving proteins took 3.5 s.

11/29/2021 09:56 AM (2) Sequest HT: Reading results took 27.7 s.

11/29/2021 09:56 AM (2) Sequest HT: Finalizing search results...

11/29/2021 09:57 AM (2) Sequest HT: -- Total search time was 4 min 38 s --

11/29/2021 10:00 AM (3) Percolator: Creating percolator input file with results from Sequest HT (2) took 3 min 0 s.

11/29/2021 10:00 AM (3) Percolator: The input file contains 71735 PSMs, 32084 decoy PSMs and 32 features.

11/29/2021 10:00 AM (3) Percolator: Generated percolator input for concatenated mode

11/29/2021 10:00 AM (3) Percolator: Percolator version 3.05.0, Build Date May 18 2020 02:35:01

11/29/2021 10:00 AM (3) Percolator: Copyright (c) 2006-9 University of Washington. All rights reserved.

11/29/2021 10:00 AM (3) Percolator: Written by Lukas Kříž (lukall@u.washington.edu) in the

11/29/2021 10:00 AM (3) Percolator: Department of Genome Sciences at the University of Washington.

11/29/2021 10:00 AM (3) Percolator: Issued command:

11/29/2021 10:00 AM (3) Percolator: C:\Program Files\Thermo\Proteome Discoverer 2.5\Tools\Percolator\win\percolator.exe --num-threads 12 -s -X C:\ProgramData\Thermo\Proteome Discoverer 2.5\Scratch\Job1721\Percol(3)\output2.xml -N 0 -Z -Y C:\ProgramData\Thermo\Proteome Discoverer 2.5\Scratch\Job1721\Percol(3)\input2.tab

11/29/2021 10:00 AM (3) Percolator: Started Mon Nov 29 10:00:09 2021

11/29/2021 10:00 AM (3) Percolator: Hyperparameters: selectionFdr=0.01, Cpos=0, Cneg=0, maxNiter=10

11/29/2021 10:00 AM (3) Percolator: Reading tab-delimited input from datafile C:\ProgramData\Thermo\Proteome Discoverer 2.5\Scratch\Job1721\Percol(3)\input2.tab

11/29/2021 10:00 AM (3) Percolator: Features:

11/29/2021 10:00 AM (3) Percolator: XCorr Delta Cn From Second PSM Binomial Score Isolation Interference [%] MH+ [Da] Delta Mass [Da] Delta Mass [ppm] Absolute Delta Mass [Da] Absolute Delta Mass [ppm] Peptide Length Is z=1 Is z=2 Is z=3 Is z=4 Is z=5 Is z>5 # Missed Cleavages Log Peptides Matched Log Total Intensity Fraction Matched Intensity [%] Fragment Coverage Series A, B, C [%] Fragment Coverage Series X, Y, Z [%] Log Matched Fragment Series Intensities A, B, C Log Matched Fragment Series Intensities X, Y, Z Longest Sequence Series A, B, C Longest Sequence Series X, Y, Z IQR Fragment Delta Mass [Da] IQR Fragment Delta Mass [ppm] Mean Fragment Delta Mass [Da] Mean Fragment Delta Mass [ppm] Mean Absolute Fragment Delta Mass [Da] Mean Absolute Fragment Delta Mass [ppm]

11/29/2021 10:00 AM (3) Percolator: Found 103819 PSMs

11/29/2021 10:00 AM (3) Percolator: Separate target and decoy search inputs detected, using target-decoy competition on Percolator scores.

11/29/2021 10:00 AM (3) Percolator: Train/test set contains 71735 positives and 32084 negatives, size ratio=2.23585 and pi0=1

11/29/2021 10:00 AM (3) Percolator: Selecting Cpos by cross-validation.

11/29/2021 10:00 AM (3) Percolator: Selecting Cneg by cross-validation.

11/29/2021 10:00 AM (3) Percolator: Split 1: Selected feature 3 as initial direction. Could separate 18590 training set positives with  $q < 0.01$  in that direction.

11/29/2021 10:00 AM (3) Percolator: Split 2: Selected feature 3 as initial direction. Could separate 18382 training set positives with  $q < 0.01$  in that direction.

11/29/2021 10:00 AM (3) Percolator: Split 3: Selected feature 3 as initial direction. Could separate 18411 training set positives with  $q < 0.01$  in that direction.

11/29/2021 10:00 AM (3) Percolator: Found 27674 test set positives with  $q < 0.01$  in initial direction

11/29/2021 10:00 AM (3) Percolator: Reading in data and feature calculation took 2.014 cpu seconds or 2 seconds wall clock time.

11/29/2021 10:00 AM (3) Percolator: ---Training with Cpos selected by cross validation, Cneg selected by cross validation, initial\_fdr=0.01, fdr=0.01

11/29/2021 10:00 AM (3) Percolator: Iteration 1: Estimated 34138 PSMs with  $q < 0.01$

11/29/2021 10:00 AM (3) Percolator: Iteration 2: Estimated 35364 PSMs with  $q < 0.01$

11/29/2021 10:00 AM (3) Percolator: Iteration 3: Estimated 35657 PSMs with  $q < 0.01$

11/29/2021 10:00 AM (3) Percolator: Iteration 4: Estimated 35766 PSMs with  $q < 0.01$

11/29/2021 10:00 AM (3) Percolator: Iteration 5: Estimated 35787 PSMs with  $q < 0.01$

|                     |                 |   |                                  |         |   |
|---------------------|-----------------|---|----------------------------------|---------|---|
| 11/29/2021 10:00 AM | (3) Percolator: | Iteration 6:  | Estimated 35830 PSMs with q<0.01 |         |   |
| 11/29/2021 10:00 AM | (3) Percolator: | Iteration 7:  | Estimated 35851 PSMs with q<0.01 |         |   |
| 11/29/2021 10:00 AM | (3) Percolator: | Iteration 8:  | Estimated 35865 PSMs with q<0.01 |         |   |
| 11/29/2021 10:00 AM | (3) Percolator: | Iteration 9:  | Estimated 35866 PSMs with q<0.01 |         |   |
| 11/29/2021 10:00 AM | (3) Percolator: | Iteration 10:   | Estimated 35871 PSMs with q<0.01 |         |   |
| 11/29/2021 10:00 AM | (3) Percolator: | Learned normalized SVM weights for the 3 cross-validation splits: |                                  |         |   |
| 11/29/2021 10:00 AM | (3) Percolator: | Split1  | Split2                           | Split3  | FeatureName                                     |
| 11/29/2021 10:00 AM | (3) Percolator: | 3.6164  | 2.9267                           | 2.8841  | XCorr   |
| 11/29/2021 10:00 AM | (3) Percolator: | 0.0880  | 0.0928                           | 0.0539  | Delta Cn From Second PSM                        |
| 11/29/2021 10:00 AM | (3) Percolator: | 5.1049  | 4.5524                           | 4.8367  | Binomial Score                                  |
| 11/29/2021 10:00 AM | (3) Percolator: | 0.0198  | 0.0099                           | 0.0279  | Isolation Interference [%]                      |
| 11/29/2021 10:00 AM | (3) Percolator: | -0.7467   | -0.6913                          | -0.4331 | MH+ [Da]  |
| 11/29/2021 10:00 AM | (3) Percolator: | -0.3550   | -0.0864                          | -0.1668 | Delta Mass [Da]                                 |
| 11/29/2021 10:00 AM | (3) Percolator: | 0.4614  | 0.2134                           | 0.2387  | Delta Mass [ppm]                                |
| 11/29/2021 10:00 AM | (3) Percolator: | 1.1442  | 1.1981                           | 1.0450  | Absolute Delta Mass [Da]                        |
| 11/29/2021 10:00 AM | (3) Percolator: | -2.0276   | -2.0464                          | -1.8178 | Absolute Delta Mass [ppm]                       |
| 11/29/2021 10:00 AM | (3) Percolator: | 0.7298  | 0.6370                           | 0.4599  | Peptide Length                                  |
| 11/29/2021 10:00 AM | (3) Percolator: | 0.0000  | 0.0000                           | 0.0000  | Is z=1  |
| 11/29/2021 10:00 AM | (3) Percolator: | -0.0966   | -0.1295                          | -0.1066 | Is z=2  |
| 11/29/2021 10:00 AM | (3) Percolator: | 0.1319  | 0.1321                           | 0.1486  | Is z=3  |
| 11/29/2021 10:00 AM | (3) Percolator: | 0.0357  | 0.0463                           | 0.0119  | Is z=4  |
| 11/29/2021 10:00 AM | (3) Percolator: | -0.1939   | -0.1170                          | -0.1536 | Is z=5  |
| 11/29/2021 10:00 AM | (3) Percolator: | -0.0199   | -0.0478                          | -0.0476 | Is z>5  |
| 11/29/2021 10:00 AM | (3) Percolator: | -0.2116   | -0.1388                          | -0.1617 | # Missed Cleavages                              |
| 11/29/2021 10:00 AM | (3) Percolator: | -0.1547   | -0.1102                          | -0.1406 | Log Peptides Matched                            |
| 11/29/2021 10:00 AM | (3) Percolator: | -0.9523   | -0.8667                          | -0.8856 | Log Total Intensity                             |
| 11/29/2021 10:00 AM | (3) Percolator: | 0.2309  | 0.1432                           | 0.1227  | Fraction Matched Intensity [%]                  |
| 11/29/2021 10:00 AM | (3) Percolator: | -0.2140   | -0.1534                          | -0.2354 | Fragment Coverage Series A, B, C [%]            |
| 11/29/2021 10:00 AM | (3) Percolator: | -0.5426   | -0.2526                          | -0.3650 | Fragment Coverage Series X, Y, Z [%]            |
| 11/29/2021 10:00 AM | (3) Percolator: | -0.7315   | -0.6157                          | -0.5908 | Log Matched Fragment Series Intensities A, B, C |
| 11/29/2021 10:00 AM | (3) Percolator: | -0.4169   | -0.2199                          | -0.2281 | Log Matched Fragment Series Intensities X, Y, Z |
| 11/29/2021 10:00 AM | (3) Percolator: | -0.8979   | -0.8085                          | -0.7390 | Longest Sequence Series A, B, C                 |
| 11/29/2021 10:00 AM | (3) Percolator: | -1.0089   | -1.1422                          | -1.0214 | Longest Sequence Series X, Y, Z                 |

|                     |                              |   |         |         |   |
|---------------------|------------------------------|---|---------|---------|---|
| 11/29/2021 10:00 AM | (3) Percolator:              | -0.0055   | -0.0215 | 0.0127  | IQR Fragment Delta Mass [Da]            |
| 11/29/2021 10:00 AM | (3) Percolator:              | -0.2359   | -0.1703 | -0.1953 | IQR Fragment Delta Mass [ppm]           |
| 11/29/2021 10:00 AM | (3) Percolator:              | 0.2630  | 0.3419  | 0.3294  | Mean Fragment Delta Mass [Da]           |
| 11/29/2021 10:00 AM | (3) Percolator:              | -0.1437   | -0.2700 | -0.1831 | Mean Fragment Delta Mass [ppm]          |
| 11/29/2021 10:00 AM | (3) Percolator:              | -0.2081   | -0.2220 | -0.2613 | Mean Absolute Fragment Delta Mass [Da]  |
| 11/29/2021 10:00 AM | (3) Percolator:              | -0.2781   | -0.3421 | -0.2456 | Mean Absolute Fragment Delta Mass [ppm] |
| 11/29/2021 10:00 AM | (3) Percolator:              | 0.2770  | 0.0158  | 0.1123  | m0                                      |
| 11/29/2021 10:00 AM | (3) Percolator:              | Found 35750 test set PSMs with q<0.01.  |         |         |   |
| 11/29/2021 10:00 AM | (3) Percolator:              | Selected best-scoring PSM per scan+expMass (target-decoy competition):<br>52162 target PSMs and 17331 decoy PSMs. |         |         |   |
| 11/29/2021 10:00 AM | (3) Percolator:              | Tossing out "redundant" PSMs keeping only the best scoring PSM for each<br>unique peptide.                        |         |         |   |
| 11/29/2021 10:00 AM | (3) Percolator:              | Calculating q values.   |         |         |   |
| 11/29/2021 10:00 AM | (3) Percolator:              | Final list yields 4692 target peptides with q<0.01.   |         |         |   |
| 11/29/2021 10:00 AM | (3) Percolator:              | Calculating posterior error probabilities (PEPs).   |         |         |   |
| 11/29/2021 10:00 AM | (3) Percolator:              | PSMId   | score   | q-value | posterior_error_prob peptide            |
| 11/29/2021 10:00 AM | (3) Percolator:              | Processing took 19.48 cpu seconds or 19 seconds wall clock time.  |         |         |   |
| 11/29/2021 10:00 AM | (3) Percolator:              | 36002/362 high confident target/decoy peptides were found for Sequest HT<br>(2).                                  |         |         |   |
| 11/29/2021 10:00 AM | (3) Percolator:              | 4849/1860 medium confident target/decoy peptides were found for Sequest<br>HT (2).                                |         |         |   |
| 11/29/2021 10:00 AM | (3) Percolator:              | -- Total execution of Percolator (64Bit) for Sequest HT (2) took 3 min 36 s --                                    |         |         |   |
| 11/29/2021 10:00 AM | (5) Minora Feature Detector: | Start detecting lcmspeaks...  |         |         |   |
| 11/29/2021 10:00 AM | (5) Minora Feature Detector: | Running 4 jobs with 4 jobs in parallel.   |         |         |   |
| 11/29/2021 10:00 AM | (5) Minora Feature Detector: | Start F5 with 'FTMS + p NSI Full ms [350.0000-1600.0000]'   |         |         |   |
| 11/29/2021 10:00 AM | (5) Minora Feature Detector: | Start F7 with 'FTMS + p NSI Full ms [350.0000-1600.0000]'   |         |         |   |
| 11/29/2021 10:00 AM | (5) Minora Feature Detector: | Start F8 with 'FTMS + p NSI Full ms [350.0000-1600.0000]'   |         |         |   |
| 11/29/2021 10:00 AM | (5) Minora Feature Detector: | Start F6 with 'FTMS + p NSI Full ms [350.0000-1600.0000]'   |         |         |   |
| 11/29/2021 10:02 AM | (5) Minora Feature Detector: | Detecting LcmsPeaks took 1 min 51 s   |         |         |   |
| 11/29/2021 10:02 AM | (5) Minora Feature Detector: | Start processing F5: '110710_WT10_NTU_20211126.raw'.  |         |         |   |
| 11/29/2021 10:02 AM | (5) Minora Feature Detector: | Start processing F6: '110711_WT_NTU_20211126.raw'.  |         |         |   |
| 11/29/2021 10:02 AM | (5) Minora Feature Detector: | Start processing F7: '110712_Cna10_NTU_20211126.raw'.   |         |         |   |
| 11/29/2021 10:02 AM | (5) Minora Feature Detector: | Start processing F8: '110713_Cna1_NTU_20211126.raw'.  |         |         |   |

11/29/2021 10:02 AM (5) Minora Feature Detector: Importing peaks for F5 (scan filter: FTMS + p NSI Full ms [350.0000-1600.0000])...

11/29/2021 10:02 AM (5) Minora Feature Detector: Importing peaks for F6 (scan filter: FTMS + p NSI Full ms [350.0000-1600.0000])...

11/29/2021 10:02 AM (5) Minora Feature Detector: Importing peaks for F7 (scan filter: FTMS + p NSI Full ms [350.0000-1600.0000])...

11/29/2021 10:02 AM (5) Minora Feature Detector: Importing peaks for F8 (scan filter: FTMS + p NSI Full ms [350.0000-1600.0000])...

11/29/2021 10:02 AM (5) Minora Feature Detector: F5: Found 207315 chromatographic peaks.

11/29/2021 10:02 AM (5) Minora Feature Detector: F7: Found 236179 chromatographic peaks.

11/29/2021 10:02 AM (5) Minora Feature Detector: F6: Found 304894 chromatographic peaks.

11/29/2021 10:02 AM (5) Minora Feature Detector: F8: Found 301337 chromatographic peaks.

11/29/2021 10:02 AM (5) Minora Feature Detector: F5: Importing auto traces...

11/29/2021 10:02 AM (5) Minora Feature Detector: F5: Imported 154713 auto traces.

11/29/2021 10:02 AM (5) Minora Feature Detector: F7: Importing auto traces...

11/29/2021 10:02 AM (5) Minora Feature Detector: F7: Imported 161805 auto traces.

11/29/2021 10:02 AM (5) Minora Feature Detector: F6: Importing auto traces...

11/29/2021 10:03 AM (5) Minora Feature Detector: F6: Imported 214718 auto traces.

11/29/2021 10:03 AM (5) Minora Feature Detector: F8: Importing auto traces...

11/29/2021 10:03 AM (5) Minora Feature Detector: F8: Imported 212609 auto traces.

11/29/2021 10:03 AM (5) Minora Feature Detector: Importing peak to spectrum links...

11/29/2021 10:04 AM (5) Minora Feature Detector: Found 16913 features (F7: 3154, F5: 2999, F6: 5265, F8: 5495)

11/29/2021 10:04 AM (5) Minora Feature Detector: Writing data took 5.6 s.

11/29/2021 10:04 AM (5) Minora Feature Detector: Creating features for PSMs took 11.1 s.

11/29/2021 10:04 AM (5) Minora Feature Detector: F5: Unidentified feature detection took 25.9 s

11/29/2021 10:04 AM (5) Minora Feature Detector: F7: Unidentified feature detection took 30 s

11/29/2021 10:04 AM (5) Minora Feature Detector: F8: Unidentified feature detection took 34.2 s

11/29/2021 10:04 AM (5) Minora Feature Detector: F6: Unidentified feature detection took 34.9 s

11/29/2021 10:04 AM (5) Minora Feature Detector: Found 195820 unidentified features (F5 : 37364, F7 : 45368, F8 : 55331, F6 : 57757).

11/29/2021 10:04 AM (5) Minora Feature Detector: -- Total execution of Minora Feature Detector (5) took 3 min 57 s --

11/29/2021 10:04 AM (4) IMP-ptmRS: Starting IMP-ptmRS node 2.0, IMP-ptmRS 1.0.0.0 - based on phosphoRS3 Taus T. et al., J. Proteome Res. 2011, 10, 5354-62

11/29/2021 10:04 AM (4) IMP-ptmRS: More nodes and documentations can be found here <http://ms.imp.ac.at/?goto=pd-nodes>.



11/29/2021 10:04 AM (4) IMP-ptmRS: Scoring with ptmRS (1.0.0.0) for Sequest HT (2) with a fragment ion mass tolerance of 0.02 m/z allowing a maximum of 10 PTMs with neutral loss and 500 isoforms per peptide.

11/29/2021 10:04 AM (4) IMP-ptmRS: (4) Localizing 1xPhospho, elementTarget: S (delta mass: 79.9663, Neutral-losses:H(3) O(4) P - 97.976896)

11/29/2021 10:05 AM (4) IMP-ptmRS: (4) Localizing 1xPhospho, elementTarget: T (delta mass: 79.9663, Neutral-losses:H(3) O(4) P - 97.976896)

11/29/2021 10:05 AM (4) IMP-ptmRS: (4) Localizing 1xPhospho, elementTarget: Y (delta mass: 79.9663, no neutral loss)

11/29/2021 10:05 AM (4) IMP-ptmRS: (4) FITs for CID\_CAD: b, y; FITs with NLs: no

11/29/2021 10:05 AM (4) IMP-ptmRS: (4) FITs for HCD: b, y; FITs with NLs: b, y

11/29/2021 10:05 AM (4) IMP-ptmRS: (4) FITs for ECD\_ETD: c, zRadical, zPrime; FITs with NLs: no

11/29/2021 10:05 AM (4) IMP-ptmRS: (4) FITs for ETHcD: b, y, c, zRadical, zPrime; FITs with NLs: b, y

11/29/2021 10:05 AM (4) IMP-ptmRS: (4) Workload level: #spectra: 74695.

11/29/2021 10:05 AM (4) IMP-ptmRS: (4) Workload level: #spectra per package: 60000.

11/29/2021 10:05 AM (4) IMP-ptmRS: (4) Workload level: #parallel tasks: 20.

11/29/2021 10:06 AM (4) IMP-ptmRS: Writing current ptmRS results to file. Puffer has following size 30000

11/29/2021 10:07 AM (4) IMP-ptmRS: (4) Finished collecting spectra

11/29/2021 10:08 AM (4) IMP-ptmRS: Writing current ptmRS results to file. Puffer has following size 30000

11/29/2021 10:09 AM (4) IMP-ptmRS: Writing current ptmRS results to file. Puffer has following size 7166

11/29/2021 10:09 AM (4) IMP-ptmRS: -- Total execution of IMP-ptmRS (4) took 4 min 27 s --

11/29/2021 10:09 AM Job Execution: Finished F:\MS DATA\A227\NTU\_B305\NTU\_R305\110491-110494\_NTU305\_20210909-(1).msf

11/29/2021 10:09 AM Job Execution: ----- Total Job execution took: 20 min 14 s. -----

=====  
Validation  
=====

=====  
Consensus Step Validation  
=====

Result name: 110491-110494\_NTU305\_20210909  
Result file: F:\MS DATA\A227\NTU\_B305\NTU\_R305\110491-110494\_NTU305\_20210909-(2).pdResult  
Description: -  
Workflow based on template: 110491-110494\_NTU305\_20210909

Creation date: 11/29/2021 9:48:57 AM

Created with Discoverer version: 2.5.0.400

-----  
Peptide Validator nodes:  
-----  
-----

Processing node 2: Peptide Validator  
-----

1. General Validation Settings:

- Validation Mode: Automatic (Control peptide level error rate if possible)
- Target FDR (Strict) for PSMs: 0.01
- Target FDR (Relaxed) for PSMs: 0.05
- Target FDR (Strict) for Peptides: 0.01
- Target FDR (Relaxed) for Peptides: 0.05

2. Specific Validation Settings:

- Validation Based on: q-Value
- Target/Decoy Selection for PSM Level FDR Calculation Based on Score: Automatic
- Reset Confidences for Nodes without Decoy Search (Fixed score thresholds): False

Additional information:  
-----

Used validation mode: 'Automatic (Control peptide level error rate if possible)'.

All PSMs have PEPs. Quality will be used for peptides.

Updated peptide confidences using quality.

-----  
Protein Validator nodes:  
-----  
-----

Processing node 5: Protein FDR Validator

-----  
1. Confidence Thresholds:

- Target FDR (Strict): 0.01
- Target FDR (Relaxed): 0.05

=====  
Processing Step A: Validation  
=====

Result name: 110491-110494\_NTU305\_20210909

Result file: F:\MS DATA\A227\NTU\_B305\NTU\_R305\110491-110494\_NTU305\_20210909-(1).msf

Description: -

Workflow based on template:

Creation date: 11/29/2021 9:48:56 AM

Created with Discoverer version: 2.5.0.400

-----  
Psm Validator nodes:  
-----  
-----

Processing node 3: Percolator  
-----

1. Target/Decoy Strategy:

- Target/Decoy Selection: Concatenated
- Validation based on: q-Value

2. Input Data:

- Maximum Delta Cn: 0.05
- Maximum Rank: 0

3. FDR Targets:

- Target FDR (Strict): 0.01

- Target FDR (Relaxed): 0.05

-----  
Validation for Processing Node: Sequest HT (2)  
-----

Percolator Output:  
-----

Results for Sequest HT (2):

Iteration 1: Estimated 34138 PSMs with  $q < 0.01$   
Iteration 2: Estimated 35364 PSMs with  $q < 0.01$   
Iteration 3: Estimated 35657 PSMs with  $q < 0.01$   
Iteration 4: Estimated 35766 PSMs with  $q < 0.01$   
Iteration 5: Estimated 35787 PSMs with  $q < 0.01$   
Iteration 6: Estimated 35830 PSMs with  $q < 0.01$   
Iteration 7: Estimated 35851 PSMs with  $q < 0.01$   
Iteration 8: Estimated 35865 PSMs with  $q < 0.01$   
Iteration 9: Estimated 35866 PSMs with  $q < 0.01$   
Iteration 10: Estimated 35871 PSMs with  $q < 0.01$

Learned normalized SVM weights for the 3 cross-validation splits:

| Split1  | Split2  | Split3  | FeatureName                |
|---------|---------|---------|----------------------------|
| 3.6164  | 2.9267  | 2.8841  | XCorr                      |
| 0.0880  | 0.0928  | 0.0539  | Delta Cn From Second PSM   |
| 5.1049  | 4.5524  | 4.8367  | Binomial Score             |
| 0.0198  | 0.0099  | 0.0279  | Isolation Interference [%] |
| -0.7467 | -0.6913 | -0.4331 | MH+ [Da]                   |
| -0.3550 | -0.0864 | -0.1668 | Delta Mass [Da]            |
| 0.4614  | 0.2134  | 0.2387  | Delta Mass [ppm]           |
| 1.1442  | 1.1981  | 1.0450  | Absolute Delta Mass [Da]   |
| -2.0276 | -2.0464 | -1.8178 | Absolute Delta Mass [ppm]  |
| 0.7298  | 0.6370  | 0.4599  | Peptide Length             |
| 0.0000  | 0.0000  | 0.0000  | Is z=1                     |

|         |         |         |   |
|---------|---------|---------|---|
| -0.0966 | -0.1295 | -0.1066 | Is z=2  |
| 0.1319  | 0.1321  | 0.1486  | Is z=3  |
| 0.0357  | 0.0463  | 0.0119  | Is z=4  |
| -0.1939 | -0.1170 | -0.1536 | Is z=5  |
| -0.0199 | -0.0478 | -0.0476 | Is z>5  |
| -0.2116 | -0.1388 | -0.1617 | # Missed Cleavages                              |
| -0.1547 | -0.1102 | -0.1406 | Log Peptides Matched                            |
| -0.9523 | -0.8667 | -0.8856 | Log Total Intensity                             |
| 0.2309  | 0.1432  | 0.1227  | Fraction Matched Intensity [%]                  |
| -0.2140 | -0.1534 | -0.2354 | Fragment Coverage Series A, B, C [%]            |
| -0.5426 | -0.2526 | -0.3650 | Fragment Coverage Series X, Y, Z [%]            |
| -0.7315 | -0.6157 | -0.5908 | Log Matched Fragment Series Intensities A, B, C |
| -0.4169 | -0.2199 | -0.2281 | Log Matched Fragment Series Intensities X, Y, Z |
| -0.8979 | -0.8085 | -0.7390 | Longest Sequence Series A, B, C                 |
| -1.0089 | -1.1422 | -1.0214 | Longest Sequence Series X, Y, Z                 |
| -0.0055 | -0.0215 | 0.0127  | IQR Fragment Delta Mass [Da]                    |
| -0.2359 | -0.1703 | -0.1953 | IQR Fragment Delta Mass [ppm]                   |
| 0.2630  | 0.3419  | 0.3294  | Mean Fragment Delta Mass [Da]                   |
| -0.1437 | -0.2700 | -0.1831 | Mean Fragment Delta Mass [ppm]                  |
| -0.2081 | -0.2220 | -0.2613 | Mean Absolute Fragment Delta Mass [Da]          |
| -0.2781 | -0.3421 | -0.2456 | Mean Absolute Fragment Delta Mass [ppm]         |
| 0.2770  | 0.0158  | 0.1123  | m0  |

=====

Filters and Counts

=====

-----

Applied display filters:

-----

This file contains the following filters:

Row Filter for Proteins:

-----

Master is equal to Master

-----

Row Filter for Input Files:

-----

FileName does not end with msf

-----

-----

Number of result items:

-----

Proteins:

1908 filtered / 1959 included / 8643 total

Protein Groups:

1908 included / 1911 total

Peptide Groups:

5725 included / 19400 total

PSMs:

35332 included / 62416 total

MS/MS Spectrum Info:

74695 total

Input Files:

4 filtered / 5 included / 5 total

Study Information:

4 total

Specialized Traces:

12 total

Consensus Features:

128368 total

=====

FDR Values for Entire Result

=====

-----

Actual estimated FDR values (without applied display filters):

-----

These estimated FDR values are based on simple counting of target and decoy items and may divert from the target FDR values you have set in the validation nodes used during workflow processing.

Usually the values will be slightly more conservative than using validation based on linear discriminant analysis or other sophisticated methods.

-----

High confident results:

-----

0.005 (35332 targets, 163 decoys) for Peptide-Spectrum Matches

0.010 (5725 targets, 56 decoys) for Peptide Groups

0.009 (1852 targets, 17 decoys) for Proteins

(No confidence was assigned to Protein Groups)

-----

Medium and High confident results:

-----

0.005 (35332 targets, 163 decoys) for Peptide-Spectrum Matches

0.010 (5725 targets, 56 decoys) for Peptide Groups

0.027 (1959 targets, 53 decoys) for Proteins

(No confidence was assigned to Protein Groups)

-----

Whole dataset:

-----

0.005 (35332 targets, 163 decoys) for Peptide-Spectrum Matches

0.010 (5725 targets, 56 decoys) for Peptide Groups

0.027 (1959 targets, 53 decoys) for Proteins

0.028 (1908 targets, 53 decoys) for Protein Groups

=====

Quantification

=====

=====

Consensus Step Quantification

=====

Result name: 110491-110494\_NTU305\_20210909

Result file: F:\MS DATA\A227\NTU\_B305\NTU\_R305\110491-110494\_NTU305\_20210909-(2).pdResult

Description: -

Workflow based on template: 110491-110494\_NTU305\_20210909

Creation date: 11/29/2021 9:48:57 AM

Created with Discoverer version: 2.5.0.400



-----  
Processing node 10: Precursor Ions Quantifier  
-----

1. General Quantification Settings:

- Peptides to Use: Unique + Razor
- Consider Protein Groups for Peptide Uniqueness: True
- Use Shared Quan Results: True
- Reject Quan Results with Missing Channels: False

2. Precursor Quantification:

- Precursor Abundance Based On: Intensity
- Min. # Replicate Features [%]: 0

3. Normalization and Scaling:

- Normalization Mode: None
- Scaling Mode: None

4. Exclude Peptides from Protein Quantification:

- For Normalization: Use All Peptides
- For Protein Roll-Up: Use All Peptides
- For Pairwise Ratios: Exclude Modified

5. Quan Rollup and Hypothesis Testing:

- Protein Abundance Calculation: Summed Abundances
- N for Top N: 3
- Protein Ratio Calculation: Pairwise Ratio Based
- Maximum Allowed Fold Change: 100
- Imputation Mode: None
- Hypothesis Test: t-test (Background Based)

6. Quan Ratio Distributions:

- 1st Fold Change Threshold: 2
- 2nd Fold Change Threshold: 4

- 3rd Fold Change Threshold: 6
- 4th Fold Change Threshold: 8
- 5th Fold Change Threshold: 10

=====

Processing Step A: Quantification

=====

Result name: 110491-110494\_NTU305\_20210909

Result file: F:\MS DATA\A227\NTU\_B305\NTU\_R305\110491-110494\_NTU305\_20210909-(1).msf

Description: -

Workflow based on template:

Creation date: 11/29/2021 9:48:56 AM

Created with Discoverer version: 2.5.0.400

-----

Processing node 5: Minora Feature Detector

-----

1. Peak & Feature Detection:

- Min. Trace Length: 5
- S/N Threshold: 1
- Max.  $\Delta$ RT of Isotope Pattern Multiplets [min]: 0.2

2. Feature to ID Linking:

- PSM Confidence At Least: High

=====

Derived Quantification Values

=====

-----

Normalization/ Scaling:

-----  
Normalization Mode = None

Protein For Normalization = No FASTA File Selected

Scaling Mode = None

Applied Normalization Values:

-----  
No normalization performed.

=====  
Ratios and Ratio Groups  
=====

-----  
Quantification Group Settings:

-----  
Study variable(s) for grouping: File;NTU\_phospho

Groups sorted by: File (SortAscending);NTU\_phospho (SortAscending)

Quantification Ratios:

-----  
(F7, Cnal10) / (F5, WT10)

(F5, WT10) / (F6, WT)

(F8, Cnal) / (F6, WT)

(F7, Cnal10) / (F8, Cnal)

-----  
Quantification Ratio Coloring:

-----  
Normal space ratio threshold (log2 ratio threshold)

blue (1): < 0.1 (< -3.3)

blue (2): < 0.125 (< -3)

blue (3): < 0.167 (< -2.6)

blue (4): < 0.25 (< -2)

blue (5): < 0.5 (< -1)

white: between 0.5 and 2 (between -1 and 1)

red (5): > 2 (> 1)

red (4): > 4 (> 2)

red (3): > 6 (> 2.6)

red (2): > 8 (> 3)

red (1): > 10 (> 3.3)

=====  
Configuration  
=====

=====  
Consensus Workflow Configuration  
=====

Result name: 110491-110494\_NTU305\_20210909

Result file: F:\MS DATA\A227\NTU\_B305\NTU\_R305\110491-110494\_NTU305\_20210909-(2).pdResult

Description: -

Workflow based on template: 110491-110494\_NTU305\_20210909

Creation date: 11/29/2021 9:48:57 AM

Created with Discoverer version: 2.5.0.400

-----  
Configuration for: MSF Files  
-----

Scores:

- PSM scores (Hidden):

    Mascot: Ions Score

    Sequest HT: XCorr

SEQUEST: XCorr

MS PepSearch: dot Score

MS PepSearch: rev-dot Score

MS PepSearch: MS PepSearch Score

PMI-Byonic: |Log Prob|

PMI-Byonic: Byonic Score

MS Amanda: Amanda Score

---

Configuration for: Protein Scorer

---

Configuration Settings for Protein Score 'SequestSummationScore':

Protein Scoring Options:

- Peptide Relevance Factor: 0.4

---

Configuration for: Display Settings

---

Default Display Filter:

- Default Filter Set (Hidden):

### Master Proteins Default Filter:

### Row Filter for TargetProtein:

### Master is equal to Master

###

'magellan filter set' 1 'MasterFilter.filterset' Filter 'TargetProtein' FilterProperties 1  
'FilterConditionProperties/FilterScope' 'FilterConditionProperties/FilterScopeValueMainGrid' 1 NARY\_AND 1 =  
FilterConditionProperties 1 'NamedComparableFilterCondition/DisplayPropertyHint' 'Master' property  
'Thermo.PD.EntityDataFramework.MasterProteinAssessment, Thermo.Magellan.EntityDataFramework' 'IsMasterProtein'  
constant 'Thermo.PD.EntityDataFramework.MasterProteinAssessment, Thermo.Magellan.EntityDataFramework'  
'IsMasterProtein'

Default Layout:

- Default Layout: (not specified)

=====  
Processing Workflow A: Configuration  
=====

Result name: 110491-110494\_NTU305\_20210909

Result file: F:\MS DATA\A227\NTU\_B305\NTU\_R305\110491-110494\_NTU305\_20210909-(1).msf

Description: -

Workflow based on template:

Creation date: 11/29/2021 9:48:56 AM

Created with Discoverer version: 2.5.0.400

-----  
Configuration for: Sequest HT  
-----

1. Workload Level:

- Automatic: True
- Number of Spectra Processed At Once: 3000
- Number of Parallel Tasks: 0

2. XCorr Confidence Thresholds (low-resolution data):

- z=1: High Confidence XCorr: 1.5
- z=1: Medium Confidence XCorr: 0.7
- z=2: High Confidence XCorr: 2
- z=2: Medium Confidence XCorr: 0.9
- z=3: High Confidence XCorr: 2.5
- z=3: Medium Confidence XCorr: 1.2
- z>=4: High Confidence XCorr: 3
- z>=4: Medium Confidence XCorr: 1.5

3. XCorr Confidence Thresholds (high-resolution data):

- z=1: High Confidence XCorr: 1.2

- z=1: Medium Confidence XCorr: 0.7
- z=2: High Confidence XCorr: 1.9
- z=2: Medium Confidence XCorr: 0.8
- z=3: High Confidence XCorr: 2.3
- z=3: Medium Confidence XCorr: 1
- z>=4: High Confidence XCorr: 2.6
- z>=4: Medium Confidence XCorr: 1.2

-----  
Configuration for: IMP-ptmRS  
-----

1. Scoring:

- Random seed: -2

2. Performance:

- Maximum Search Engine Rank: 5
- Minimum Main Score: 0
- Maximum number of threads: 0

General:

- Modification Configuration (Hidden):

```
<?xml version="1.0" encoding="UTF-8" standalone="yes"?>
<AnyPTM>
<!-- This defines a modifications. The unimodID can be found in (path can be slightly different
C:\ProgramData\Thermo\Proteome Discoverer 2.5\MagellanDBs\unimod_tables.xml
-->
<modification name="Methyl" abbreviation="Methyl" searchdefined="FALSE" mass="14.015650" unimodId="34">
<!-- Targets of the modification -->
<target aminoacid="K"/>
<target aminoacid="R"/>
<!--
```

The modifications below this comment are substituted with the modification above this comment.

Hence, the name of the modifications below have to be identical to the name defined by the search engine.

Trivial substitution (Methyl = 1xMethyl) can also be performed (therefore all modifications will be scored together).

-->

<equivalentmodification name="Methyl" factor="1"/>

<equivalentmodification name="Dimethyl" factor="2"/>

<!--Since arginine does not carry 3 methyls avoid this target-->

<equivalentmodification name="Trimethyl" factor="3" avoidTarget="R"/>

<equivalentmodification name="Methyl (K)" factor="1"/>

<equivalentmodification name="Dimethyl (K)" factor="2"/>

</modification>

<!--EXAMPLE EXAMPLE EXAMPLE EXAMPLE EXAMPLE EXAMPLE EXAMPLE EXAMPLE EXAMPLE EXAMPLE-->

<modification name="ptmRS\_BaseTestModification" abbreviation="baseTestMod" searchdefined="FALSE" mass="69.235469" unimodId="-9999">

<!-- Specifies a modification Test, which will, if on a peptide be used by ptmRS -->

<!-- Specify the targets for current modification. It is important to highlight that this targets are taken for scoring! -->

<target aminoacid="M"/>

<target aminoacid="P"/>

<target aminoacid="E"/>

<!--

Specify neutral losses. This NL will be used while scoring. Also NLs defined by the search engine will

be used. Each <target /> specifies an amino acid (and a number of modification) pair where this NL is possible

-->

<neutralloss abbreviation="NLofM" mass="98.12345">

<target aminoacid="M" factor="3"/>

<target aminoacid="M" factor="2"/>

<target aminoacid="M" factor="1"/>

</neutralloss>

<neutralloss abbreviation="NLofPE" mass="59.3256">

<target aminoacid="P"/>

<target aminoacid="E"/>

</neutralloss>



<!--

Diagnostic ions (DI) can be defined. Currently 3 types of diagnostic ions are supported.

\* First, ions giving evidence for a specific target (e.g. DI found, modification is on Lysine)

\* Second ions giving evidence for the number of modification on a target (e.g. DI found, modification is on any target with the a factor of 2, dimethyl on Lysine/Arginin).

\* Third, combinations of both like in this example

\* Last, just the report it.

-->

<diagnosticion name="Diagnostic Ion1" mass="55" peakdepth="8">

<!-- This diagnostic ions is an evidence that modification is bind to target M -->

<Evidence\_Target>M</Evidence\_Target>

<!-- This diagnostic ions is an evidence for this modification of a factor 3 -->

<Evidence\_Factor>3</Evidence\_Factor>

<!--

Defines the relativity of the given mass:

\* Precursor: DI searched at: precursor + mass

\* ExistingPrecursor (default): DI searched if the precursor was measured in MS2 at: precursor + mass

\* ImoniumIon: The given mass is absolute, therefore here: mass

-->

<Relativity>ExistingPrecursor</Relativity>

</diagnosticion>

<!--

Following modifications are mapped onto the ptmRS\_BaseTestModification:

Modification on PSMs with the name "ptmRS\_SearchengineTestMod1" are mapped onto 1x ptmRS\_BaseTestModification

-->

<equivalentmodification name="ptmRS\_SearchengineTestMod1" factor="1" new="FALSE"/>

<!-- Modification on PSMs with the name "ptmRS\_SearchengineTestMod2" are mapped onto 2x ptmRS\_BaseTestModification (this 2x mod cannot be found on P,E)-->

<equivalentmodification name="ptmRS\_SearchengineTestMod2" factor="2" new="FALSE" avoidTarget="PE"/>

<!-- Modification on PSMs with the name "ptmRS\_SearchengineTestMod3" are mapped onto 3x ptmRS\_BaseTestModification (this 3x mod cannot be found on P,E)-->

<equivalentmodification name="ptmRS\_SearchengineTestMod3" factor="3" new="FALSE" avoidTarget="PE"/>

</modification>

<!-- Defines which fragment ions are used during the scoring in dependence of the activation type -->

<FragmentIonCompositionPreference>

<FragmentIonComposition ActivationType="CID" FragmentIonComposition="b,y"  
NeutralLossFragmentIonComposition=""/>

<FragmentIonComposition ActivationType="HCD" FragmentIonComposition="b,y"  
NeutralLossFragmentIonComposition="b,y"/>

<FragmentIonComposition ActivationType="ETHCD" FragmentIonComposition="b,y,c,zPrime,zRadical"  
NeutralLossFragmentIonComposition="b,y"/>

<FragmentIonComposition ActivationType="ETD" FragmentIonComposition="c,zPrime,zRadical"  
NeutralLossFragmentIonComposition=""/>

</FragmentIonCompositionPreference>

</AnyPTM>

-----  
Configuration for: Minora Feature Detector  
-----

Configuration Settings:

- Number of Parallel Tasks: 0