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Processing Step A: Workflow

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Result name: clnsn1457\_3

Result file: D:\Jana\Creatics\cr01\_001\_1\clnsn1457\_3-(02).msf

Description: Typical RT 30 Minimum RT 3

Workflow based on template: LFQProfiler\_processing\_30\_3\_SN2

Creation date: 1/26/2016 3:07:16 PM

Created with Discoverer version: 2.1.0.81

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The pipeline tree:

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|-(0) Spectrum Files

|-(1) Spectrum Selector

|-(2) Sequest HT

|-(3) Percolator

|-(4) LFQProfiler FF

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Processing node 0: Spectrum Files

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Input Data:

- File Name(s): D:\cl\_data\adenoma\_control\clnsn1457\_3.RAW

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Processing node 1: Spectrum Selector

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1. General Settings:

- Precursor Selection: Use MS1 Precursor

- Use New Precursor Reevaluation: True

- Use Isotope Pattern in Precursor Reevaluation: True

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: 400 Da

- Max. Precursor Mass: 2000 Da

- Total Intensity Threshold: 0

- Minimum Peak Count: 1

3. Scan Event Filters:

- Mass Analyzer: Any

- MS Order: Any

- Min. Collision Energy: 0

- Max. Collision Energy: 1000

- Scan Type: Is Full

- Polarity Mode: Any

4. Peak Filters:

- S/N Threshold (FT-only): 2

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

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Processing node 2: Sequest HT

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1. Input Data:

- Protein Database: RefNCBInr\_human\_120814\_base.fasta

- Enzyme Name: <Enzyme Version="1" Name="Trypsin" CleavageSites="KR" CleavageInhibitors="P" Offset="1" CleavageSpecificity="SpecificAtBothEnds" />

- 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: 0.6 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

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Processing node 3: Percolator

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1. Input Data:

- Maximum Delta Cn: 0.05

- Maximum Rank: 0

2. Decoy Database Search:

- Target FDR (Strict): 0.01

- Target FDR (Relaxed): 0.05

- Validation based on: q-Value

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Processing node 4: LFQProfiler FF

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1. Feature Finding:

- Mass tolerance: 10 ppm

- Charge Low: 1

- Charge High: 5

- Typical RT: 30

- Minimum RT: 3

- Averagine similarity: 0.3