

IDENT_NP_Genedata_Workflow

This is the root workflow

depke

Software Version: 7.6

Report Creation Date: 02.09.2013 09:07:56

Summary

IDENT_NP_Genedata_Workflow

Description: This is the root workflow

Settings:

Activity	Settings
IDENT_NP_Genedata_Workflow	Name: <i>IDENT_NP_Genedata_Workflow</i>
	Description: <i>This is the root workflow</i>
	Last Saved: <i>by depke at 02.09.2013 09:07:30</i>
Load from File	Name: <i>New MS Data Set</i>
	Format: <i>auto_detect_parser</i>
	Files/Folders: <i>/Shared/AG_Voelker/QExactive/130131_MDKSFS_NP_co_int_capt: 130130_RN1HGpJL74_FeOxNP_intS9_2h_MagCapt_130117.raw, 130130_RN1HGpJL74_FeOxNP_intS9_4h_MagCapt_130117.raw</i>
	Profile Data Cutoff: <i>1 [Intensity]</i>
	Centroid Data Cutoff: <i>0 [Intensity]</i>
Load from File	Name: <i>New MS Data Set</i>
	Format: <i>auto_detect_parser</i>
	Files/Folders: <i>/Shared/AG_Voelker/QExactive/130328_MDKSFS_NP_Au_int: 130328_RN1HG_AuNP_intS9_2h_FACS_130320.raw, 130328_RN1HG_AuNP_intS9_4h_FACS_130320.raw</i>
	Profile Data Cutoff: <i>1 [Intensity]</i>
	Centroid Data Cutoff: <i>0 [Intensity]</i>
Chromatogram Grid	m/z Grid Method: <i>Adaptive Grid</i>
	Scan Count: <i>10</i>
	Δ RT Smoothing: <i>0</i>
Chromatogram Grid	m/z Grid Method: <i>Adaptive Grid</i>
	Scan Count: <i>10</i>
	Δ RT Smoothing: <i>0</i>
Chromatogram Chemical Noise Subtraction	RT Structure Removal: <i>true</i>
	Minimum RT Length: <i>6 Scans</i>
Chromatogram Chemical Noise Subtraction	RT Structure Removal: <i>true</i>
	Minimum RT Length: <i>6 Scans</i>
Chromatogram Chemical Noise Subtraction	Chromatogram Smoothing: <i>true</i>
	RT Window: <i>5 Scans</i>
	Estimator: <i>Moving Average</i>
	Chemical Noise Subtraction: <i>true</i>
	RT Window: <i>251 Scans</i>
	Quantile: <i>51</i>
	Threshold: <i>5000 [Intensity]</i>

Activity	Settings
Chromatogram Chemical Noise Subtraction	Chromatogram Smoothing: <i>true</i>
	RT Window: <i>5 Scans</i>
	Estimator: <i>Moving Average</i>
	Chemical Noise Subtraction: <i>true</i>
	RT Window: <i>251 Scans</i>
	Quantile: <i>51</i>
	Threshold: <i>5000 [Intensity]</i>
Chromatogram Chemical Noise Subtraction	RT Structure Removal: <i>true</i>
	Minimum RT Length: <i>6 Scans</i>
	m/z Structure Removal: <i>true</i>
	Minimum m/z Length: <i>4 Points</i>
Chromatogram Chemical Noise Subtraction	RT Structure Removal: <i>true</i>
	Minimum RT Length: <i>6 Scans</i>
	m/z Structure Removal: <i>true</i>
	Minimum m/z Length: <i>4 Points</i>
Chromatogram RT Alignment	m/z Window: <i>5 Points</i>
	RT Window: <i>5 Scans</i>
	Gap Penalty: <i>1</i>
	RT Search Interval: <i>50 Scans</i>
	Alignment Scheme: <i>Pairwise Alignment Based Tree</i>
Chromatogram RT Alignment	m/z Window: <i>5 Points</i>
	RT Window: <i>5 Scans</i>
	Gap Penalty: <i>1</i>
	RT Search Interval: <i>50 Scans</i>
	Alignment Scheme: <i>Pairwise Alignment Based Tree</i>
Chromatogram Summed Peak Detection	Summation Window: <i>3 Scans</i>
	Overlap: <i>50</i>
	Minimum Peak Size: <i>6 Scans</i>
	Maximum Merge Distance: <i>3 Points</i>
	Use Peak RT Splitting: <i>true</i>
	Intensity Profiling: <i>Integral</i>
	Gap/Peak Ratio: <i>30</i>
	<i>Curvature-based Peak Detection</i>
	Export Summed Chromatogram <i>false</i>
Chromatogram Summed Peak Detection	Summation Window: <i>3 Scans</i>
	Overlap: <i>50</i>
	Minimum Peak Size: <i>6 Scans</i>
	Maximum Merge Distance: <i>3 Points</i>
	Use Peak RT Splitting: <i>true</i>
	Intensity Profiling: <i>Integral</i>
	Gap/Peak Ratio: <i>30</i>
	<i>Curvature-based Peak Detection</i>
	Export Summed Chromatogram <i>false</i>

Activity	Settings
Chromatogram Isotope Clustering	RT Tolerance: <i>0.2 [Time]</i>
	m/z Tolerance: <i>0.03 Da</i>
	<i>peptide</i>
	Ionization: <i>Protonation</i>
	Minimum Charge: <i>1</i>
	Maximum Charge: <i>10</i>
	Shape Tolerance: <i>0.5</i>
	Recompute Mono-Isotopic Peak <i>true</i>
	Restrict Cluster Size: <i>true</i>
	Minimum Cluster Size Ratio: <i>0.62</i>
	Keep Existing Clusters <i>false</i>
	Export Summed Chromatogram <i>false</i>
Chromatogram Isotope Clustering	RT Tolerance: <i>0.2 [Time]</i>
	m/z Tolerance: <i>0.03 Da</i>
	<i>peptide</i>
	Ionization: <i>Protonation</i>
	Minimum Charge: <i>1</i>
	Maximum Charge: <i>10</i>
	Shape Tolerance: <i>0.5</i>
	Recompute Mono-Isotopic Peak <i>true</i>
	Restrict Cluster Size: <i>true</i>
	Minimum Cluster Size Ratio: <i>0.62</i>
	Keep Existing Clusters <i>false</i>
	Export Summed Chromatogram <i>false</i>
Chromatogram Singleton Filter	<i>No settings.</i>
Chromatogram Singleton Filter	<i>No settings.</i>
MS/MS Consolidation	m/z Window: <i>0.0 Da</i>
	RT Window: <i>0.0 [Time]</i>
	Method: <i>nearest</i>
	Filter: <i>filter_clusters</i>
	Consolidation: <i>highest_tic</i>
	One Per Cluster <i>true</i>
	Across Chromatograms <i>false</i>
MS/MS Consolidation	m/z Window: <i>0.0 Da</i>
	RT Window: <i>0.0 [Time]</i>
	Method: <i>nearest</i>
	Filter: <i>filter_clusters</i>
	Consolidation: <i>highest_tic</i>
	One Per Cluster <i>true</i>
	Across Chromatograms <i>false</i>

Activity	Settings
Mascot MS/MS Search	Ionization: <i>positive</i>
	Merged Search <i>false</i>
	Annotate Spectra <i>true</i>
	Accept: <i>By Property</i>
	Score > 10.0 AND Rank = 1
	Export Folder: <i>true</i>
	Export Folder: /Home: Mascot
Mascot MS/MS Search	FILE=;FORMAT=Mascot generic;USERNAME=MD;USEREMAIL=depke@uni-greifswald.de;COM=search;DB=Sau_8325_BLAST_HGW;TAXONOMY=All entries;CLE=Trypsin;PFA=0;MODS=;IT_MODS=Carbamidomethyl (C), Oxidation (M);QUANTITATION=None;TOL=10;TOLU=ppm;PEP_ISOTOPE_ERROR=1;ITOL=0.05;ITOLU=Da;CHARGE=2+, 3+ and 4+;MASS=Monoisotopic;PRECURSOR=;INSTRUMENT=ESI-TRAP;ERRORTOLERANT=;DECOY=;REPORT=AUTO;INTERMEDIATE=;FORMVER=1.01;SEARCH=MIS;PEAK=AUTO;REPTYPE=peptide;ErrToRepeat=0;SHOWALLMODS=
	Ionization: <i>positive</i>
	Merged Search <i>false</i>
	Annotate Spectra <i>true</i>
	Accept: <i>By Property</i>
	Score > 10.0 AND Rank = 1
	Export Folder: <i>true</i>
Peak Annotation	Export Folder: /Home: Mascot
	FILE=;FORMAT=Mascot generic;USERNAME=MD;USEREMAIL=depke@uni-greifswald.de;COM=search;DB=Sau_8325_BLAST_HGW;TAXONOMY=All entries;CLE=Trypsin;PFA=0;MODS=;IT_MODS=Carbamidomethyl (C), Oxidation (M);QUANTITATION=None;TOL=10;TOLU=ppm;PEP_ISOTOPE_ERROR=1;ITOL=0.05;ITOLU=Da;CHARGE=2+, 3+ and 4+;MASS=Monoisotopic;PRECURSOR=;INSTRUMENT=ESI-TRAP;ERRORTOLERANT=;DECOY=;REPORT=AUTO;INTERMEDIATE=;FORMVER=1.01;SEARCH=MIS;PEAK=AUTO;REPTYPE=peptide;ErrToRepeat=0;SHOWALLMODS=
	m/z Window: 0 Da
	RT Window: 0 [Time]
	Use Available Cluster Charges <i>false</i>
	Take MS/MS Data from Reference Chromatograms <i>false</i>
	Consolidate Peptides: <i>true</i>
Peak Annotation	Show Top: 1
	Use MS/MS TIC <i>false</i>
	Use Search Score <i>true</i>
	m/z Window: 0 Da
	RT Window: 0 [Time]
	Use Available Cluster Charges <i>false</i>
	Take MS/MS Data from Reference Chromatograms <i>false</i>
Group by Protein	Consolidate Peptides: <i>true</i>
	Show Top: 1
	Use MS/MS TIC <i>false</i>
	Use Search Score <i>true</i>
	Include ungrouped <i>true</i>
	Include ungrouped <i>true</i>
	Include ungrouped <i>true</i>

Activity	Settings
GDA File	Export: <i>Cluster Groups</i>
	Observable: <i>Intensity</i>
	Export Experiment Annotation <i>false</i>
	Export Item Annotation <i>true</i>
	Custom Destination: <i>true</i>
	Export File: <i>/Home:</i> <i>20130826_IDENT_NP_HG001_S9int_2h4h_FeOx_Mag_score10</i>
	Export Annotations and Data as a Single File <i>true</i>
	Keep Duplicated Item Annotations <i>false</i>
Excel File	Export: <i>Cluster Groups</i>
	Observable: <i>Max. Intensity</i>
	Export Experiment Annotation <i>true</i>
	Export Item Annotation <i>true</i>
	Custom Destination: <i>true</i>
	Export File: <i>/Home:</i> <i>20130826_IDENT_NP_HG001_S9int_2h4h_FeOx_Mag_score10</i>
	Add MH+ Column <i>false</i>
	Add Orig. RT Column <i>false</i>
	Export Annotations and Data as a Single File <i>true</i>
	Keep Duplicated Item Annotations <i>false</i>
GDA File	Export: <i>Cluster Groups</i>
	Observable: <i>Intensity</i>
	Export Experiment Annotation <i>false</i>
	Export Item Annotation <i>true</i>
	Custom Destination: <i>true</i>
	Export File: <i>/Home:</i> <i>20130826_IDENT_NP_HG001_S9int_2h4h_Au_FACS_score10</i>
	Export Annotations and Data as a Single File <i>true</i>
	Keep Duplicated Item Annotations <i>false</i>
Excel File	Export: <i>Cluster Groups</i>
	Observable: <i>Max. Intensity</i>
	Export Experiment Annotation <i>true</i>
	Export Item Annotation <i>true</i>
	Custom Destination: <i>true</i>
	Export File: <i>/Home:</i> <i>20130826_IDENT_NP_HG001_S9int_2h4h_Au_FACS_score10</i>
	Add MH+ Column <i>false</i>
	Add Orig. RT Column <i>false</i>
	Export Annotations and Data as a Single File <i>true</i>
	Keep Duplicated Item Annotations <i>false</i>

Graphics:

