QUANT_NP_Genedata_Workflow

This is the root workflow

depke

Software Version: 7.6
Report Creation Date: 02.09.2013 08:46:15

Summary

QUANT_NP_Genedata_Workflow

Description: This is the root workflow

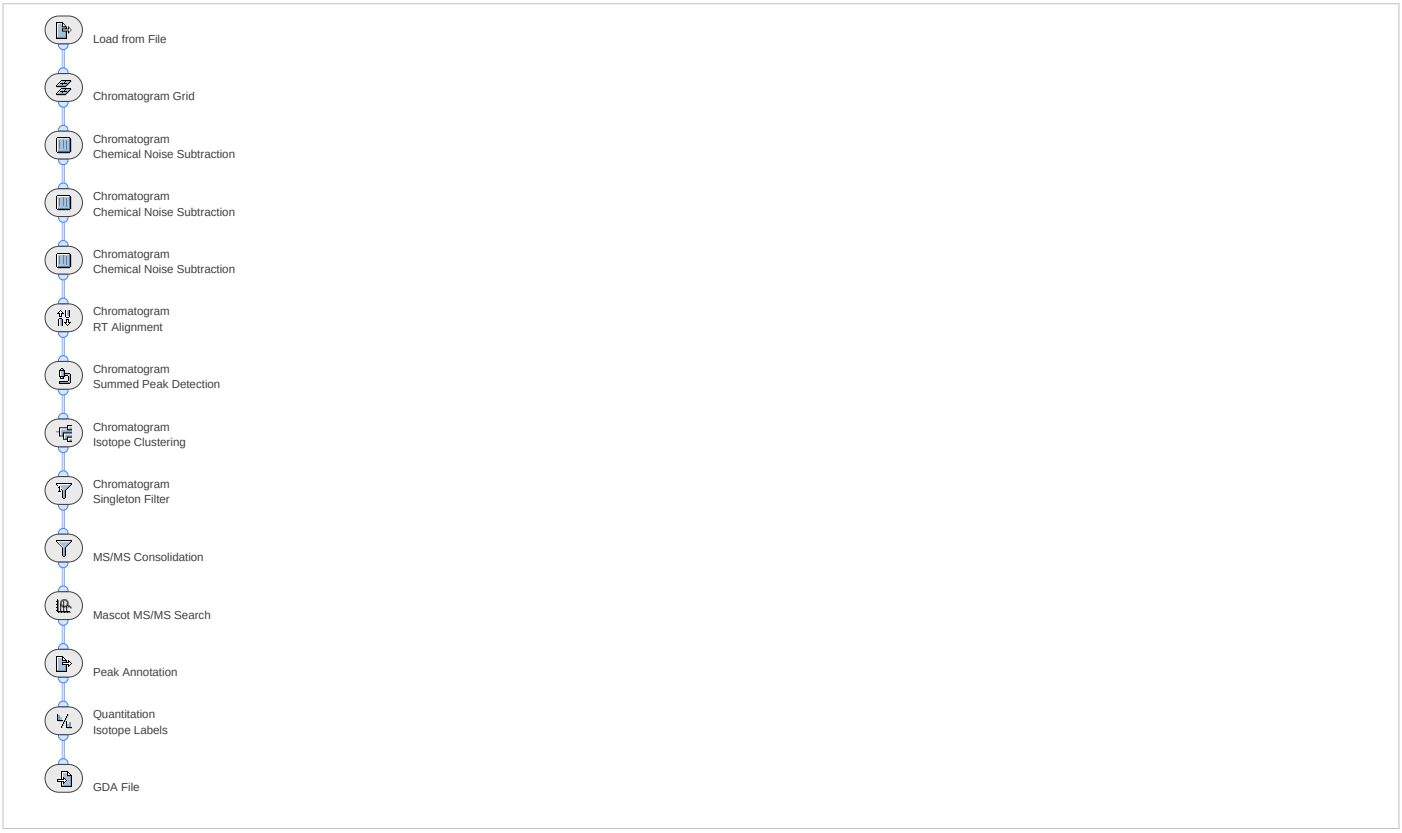
Settings:

Activity	Settings
QUANT_NP_Genedata_Workflow	Name: *QUANT_NP_Genedata_Workflow*
	Description: *This is the root workflow*
	Last Saved: *by depke at 02.09.2013 08:45:11*
Load from File	Name: *New MS Data Set*
	Format: *auto_detect_parser*
	Files/Folders: */Shared/AG_Voelker/QExactive/2012/120704_MD_NP_24h_SILAC_Ju2011_3BR: 120704_BR1_AuNP_Ko_SILAC_Ju2011_10_10_susp.raw, 120704_BR1_FeOxNP_Ko_SILAC_Ju2011_10_10_susp.raw, 120704_BR2_AuNP_Ko_SILAC_Ju2011_10_10_susp.raw, 120704_BR2_FeOxNP_Ko_SILAC_Ju2011_10_10_susp.raw, 120704_BR3_AuNP_Ko_SILAC_Ju2011_10_10_susp.raw, 120704_BR3_FeOxNP_Ko_SILAC_Ju2011_10_10_susp.raw*
	Profile Data Cutoff: *1 [Intensity]*
	Centroid Data Cutoff: *0 [Intensity]*
	Restrict Range: *true*
	m/z Minimum: *300 Da*
	m/z Maximum: *Da*
	RT Minimum: *[Time]*
	RT Maximum: *[Time]*
Chromatogram Grid	m/z Grid Method: *Adaptive Grid*
	Scan Count: *10*
	ΔRT Smoothing: *0*
Chromatogram Chemical Noise Subtraction	RT Structure Removal: *true*
	Minimum RT Length: *6 Scans*
Chromatogram Chemical Noise Subtraction	Chromatogram Smoothing: *true*
	RT Window: *5 Scans*
	Estimator: *Moving Average*
	Chemical Noise Subtraction: *true*
	RT Window: *251 Scans*
	Quantile: *51*
	Threshold: *5000 [Intensity]*
Chromatogram Chemical Noise Subtraction	RT Structure Removal: *true*
	Minimum RT Length: *6 Scans*
	m/z Structure Removal: *true*
	Minimum m/z Length: *4 Points*
Chromatogram RT Alignment	m/z Window: *5 Points*
	RT Window: *5 Scans*
	Gap Penalty: *1*
	RT Search Interval: *50 Scans*
	Alignment Scheme: *Pairwise Alignment Based Tree*

Activity	Settings
Chromatogram Summed Peak Detection	Summation Window: *3 Scans*
	Overlap: *50*
	Minimum Peak Size: *6 Scans*
	Maximum Merge Distance: *3 Points*
	Use Peak RT Splitting: *true*
	Intensity Profiling: *Integral*
	Gap/Peak Ratio: *30*
	Curvature-based Peak Detection
	Export Summed Chromatogram *false*
Chromatogram Isotope Clustering	RT Tolerance: *0.2 [Time]*
	m/z Tolerance: *0.03 Da*
	peptide
	Ionization: *Protonation*
	Minimum Charge: *1*
	Maximum Charge: *10*
	Shape Tolerance: *0.5*
	Recompute Mono-Isotopic Peak *true*
	Restrict Cluster Size: *true*
	Minimum Cluster Size Ratio: *0.62*
	Keep Existing Clusters *false*
	Export Summed Chromatogram *false*
Chromatogram Singleton Filter	*No settings.*
MS/MS Consolidation	m/z Window: *0.0 Da*
	RT Window: *0.0 [Time]*
	Method: *nearest*
	Filter: *filter_clusters*
	Consolidation: *highest_tic*
	One Per Cluster *true*
	Across Chromatograms *false*
Mascot MS/MS Search	Ionization: *positive*
	Merged Search *false*
	Annotate Spectra *true*
	Accept: *By Property*
	Score > 10.0 AND Rank = 1
	Export Folder: *true*
	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=1;MODS=;IT_MODS=Label:13C(6) (K),Label:13C(6) (R),Oxidation (M);QUANTITATION=None;TOL=20;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;ErrTolRepeat=0;SHOWALLMODS=

Activity	Settings
Peak Annotation	m/z Window: *0 Da*
	RT Window: *0 [Time]*
	Use Available Cluster Charges *false*
	Take MS/MS Data from Reference Chromatograms *false*
Quantitation Isotope Labels	Labels: *lysine_6 : arginine_6*
	RT Tolerance: *0.5 [Time]*
	m/z Tolerance: *0.02 Da*
	Observable: *Intensity*
	Include matched by mass only *true*
	Include unmatched *false*
	Group by Protein: *true*
	Condensing Method: *arithmetic_mean*
	Include ungrouped *false*
GDA File	Export: *Cluster Groups*
	Observable: *Ratio*
	Export Experiment Annotation *true*
	Export Item Annotation *true*
	Custom Destination: *true*
	Export File: */Home:* *20130826_QUANT_SILAC_HG001_24h_NP_Au_FeOx_score10.gda*
	Export Annotations and Data as a Single File *true*
	Keep Duplicated Item Annotations *false*

Graphics:


Load from File
Chromatogram Grid
Chromatogram
Chemical Noise Subtraction
Chromatogram
Chemical Noise Subtraction
Chromatogram
Chemical Noise Subtraction
Chromatogram
RT Alignment
Chromatogram
Summed Peak Detection
Chromatogram
Isotope Clustering
Chromatogram
Singleton Filter
MS/MS Consolidation
Mascot MS/MS Search
Peak Annotation
Quantitation
Isotope Labels
GDA File