Proteomics in Galaxy

Galaxy is a web-based platform for data intensive life science research that provides users with a unified, easy-to-use graphical interface to a host of different analysis tools. These tools can be run interactively, one by one, or combined into multi-step workflows that can be executed as a single analysis.

The Norwegian Galaxy server is maintained by ELIXIR Norway and can be accessed at:

https://usegalaxy.no/

Users associated with a Norwegian University can log in using a FEIDE account and will have access to 200 Gb storage space. Galaxy is also directly linked to NeLS (Norwegian e-Infrastructure for Life Sciences) and data within NeLS can be directly analyzed in Galaxy without transfer.

The following list of proteomics software is available through the Norwegian Galaxy node:

(note that there are multiple general tools available also, not listed here)

Protein identification

AccurateMassSearch	Match MS signals to molecules from a database by mass.
CometAdapter	Annotates MS/MS spectra using Comet.
InspectAdapter	Annotates MS/MS spectra using Inspect.
LuciphorAdapter	Modification site localisation using LuciPHOr2.
MascotAdapter	Annotates MS/MS spectra using Mascot.
MascotAdapterOnline	Annotates MS/MS spectra using Mascot.
MaxQuant	Software suite for searching, identification and quantification of proteins
MaxQuant_using_mqpar.xml	Software suite for searching, identification and quantification of proteins
MetaboliteSpectralMatcher	Perform a spectral library search.
Morpheus	database search algorithm for high-resolution tandem mass spectra
MS-GF+	Identifies peptides in tandem mass spectra using the MS-GF+ search engine.
MSGFPlusAdapter	MS/MS database search using MS-GF+.
MyriMatch	Identify peptides in tandem mass spectra.
PepQuery	Peptide-centric search engine for novel peptide identification and validation.
Peptide Shaker	Perform protein identification using various search engines based on results from SearchGUI
Percolator	accurate peptide identification
PhosphoScoring	Scores potential phosphorylation sites in order to localize the most probable sites.
Pout2mzid	add Percolator scoring to mzIdentML
Search engine output to Pin converter	to create Percolator input files
Search GUI	Perform protein identification using various search engines and prepare results for input to Peptide
SimpleSearchEngine	Annotates MS/MS spectra using SimpleSearchEngine.
SpecLibCreator	Creates an MSP formatted spectral library.
SpecLibSearcher	Identifies peptide MS/MS spectra by spectral matching with a searchable spectral library.
SpectraSTSearchAdapter	Interface to the SEARCH Mode of the SpectraST executable
XTandemAdapter	Annotates MS/MS spectra using X! Tandem.

Protein Quantification

FlashLFQ	ultrafast label-free quantification for mass-spectrometry proteomics
IsobaricAnalyzer	Calculates isobaric quantitative values for peptides
moFF	extracts MS1 intensities from spectrum files
ProteinQuantifier	Compute peptide and protein abundances
QuanTP	Correlation between protein and transcript abundances
QuantWiz-IQ	Isobaric Quantitation using QuantWiz-IQ

Statistics and QC

QCCalculator	Calculates basic quality parameters from MS experiments and subsequent analysis data as identificati
QCEmbedder	Attaches a table or an image to a given qc parameter.
QCExporter	Will extract several qp from several run/sets in a tabular format.
QCExtractor	Extracts a table attachment to a given qc parameter.
QCImporter	Imports tables with quality control parameters into qcml files.
QCShrinker	This application is used to remove the verbose table attachments from a qcml file that are not neede
MapStatistics	Extract extended statistics on the features of a map for quality control.
MSstats	statistical relative protein significance analysis in DDA, SRM and DIA Mass Spectrometry
RNPxlXICFilter	Remove MS2 spectra from treatment based on the fold change between control and treatment.

In addition, there are >50 other general statistical tools in Galaxy

Processing

BaselineFilter	Removes the baseline from profile spectra using a top-hat filter.
Decharger	Decharges and merges different feature charge variants of the same peptide.
FeatureFinderMRM	Detects two-dimensional features in LC-MS data.
InternalCalibration	Applies an internal mass recalibration.
LowMemPeakPickerHiRes	Finds mass spectrometric peaks in profile mass spectra.
LowMemPeakPickerHiResRandomAccess	Finds mass spectrometric peaks in profile mass spectra.
MapAlignerIdentification	Corrects retention time distortions between maps based on common peptide identifications.
MapAlignerPoseClustering	Corrects retention time distortions between maps using a pose clustering approach.
MapAlignerSpectrum	Corrects retention time distortions between maps by spectrum alignment.
MapNormalizer	Normalizes peak intensities in an MS run.
MapRTTransformer	Applies retention time transformations to maps.
MassTraceExtractor	Detects mass traces in centroided LC-MS data.
MetaboliteAdductDecharger	Decharges and merges different feature charge variants of the same metabolite.
MRMTransitionGroupPicker	Picks peaks in SRM/MRM chromatograms.
NoiseFilterGaussian	Removes noise from profile spectra by using Gaussian filter (on uniform as well as non-uniform data)
NoiseFilterSGolay	Removes noise from profile spectra by using a Savitzky Golay filter. Requires uniform (equidistant)
PeakPickerHiRes	Finds mass spectrometric peaks in profile mass spectra.
PeakPickerIterative	Finds mass spectrometric peaks in profile mass spectra.

PeakPickerWavelet	Finds mass spectrometric peaks in profile mass spectra.
PeptideIndexer	Refreshes the protein references for all peptide hits.
PrecursorIonSelector	PrecursorIonSelector
PrecursorMassCorrector	Corrects the precursor entries of MS/MS spectra, by using MS1 information.
PSMFeatureExtractor	Computes extra features for each input PSM.
SpectraFilterBernNorm	Applies thresholdfilter to peak spectra.
SpectraFilterMarkerMower	Applies thresholdfilter to peak spectra.
SpectraFilterNLargest	Applies thresholdfilter to peak spectra.
SpectraFilterNormalizer	Normalizes intensity of peak spectra.
SpectraFilterParentPeakMower	Applies thresholdfilter to peak spectra.
SpectraFilterScaler	Applies thresholdfilter to peak spectra.
SpectraFilterSqrtMower	Applies thresholdfilter to peak spectra.
SpectraFilterThresholdMower	Applies thresholdfilter to peak spectra.
SpectraFilterWindowMower	Applies thresholdfilter to peak spectra.
SpectraMerger	Merges spectra (each MS level separately), increasing S/N ratios.
TransformationEvaluation	Applies a transformation to a range of values

Protein inference

ConsensusID	Computes a consensus of peptide identifications of several identification engines.
FidoAdapter	Runs the protein inference engine Fido.
ProteinInference	Protein inference based on the number of identified peptides.
ProteinResolver	protein inference

Swath

OpenSwathAnalyzer	Picks peaks and finds features in an SWATH-MS or SRM experiment
OpenSwathAssayGenerator	Generates assays according to different models for a specific TraML
OpenSwathChromatogramExtractor	Extract chromatograms (XIC) from a MS2 map file.
OpenSwathConfidenceScoring	Compute confidence scores for OpenSwath results
OpenSwathDecoyGenerator	Generates decoys according to different models for a specific TraML
OpenSwathDIAPreScoring	Scoring spectra using the DIA scores.
OpenSwathFeatureXMLToTSV	Converts a featureXML to a mProphet tsv.
OpenSwathFileSplitter	Splits SWATH files into n files, each containing one window.
OpenSwathMzMLFileCacher	This tool caches the spectra and chromatogram data of an mzML to disk.
OpenSwathRewriteToFeatureXML	Combines featureXML and mProphet tsv to FDR filtered featureXML.
OpenSwathRTNormalizer	This tool will take a description of RT peptides and their normalized retention time to write out a
OpenSwathWorkflow	Complete workflow to run OpenSWATH
PyProphet export	Export tabular files, optional swath2stats export
PyProphet merge	Merge multiple osw files
PyProphet peptide	Peptide error-rate estimation
PyProphet protein	Protein error-rate estimation
PyProphet score	Error-rate estimation for MS1, MS2 and transition-level data
PyProphet subsample	Subsample OpenSWATH file
SvmTheoreticalSpectrumGeneratorTrainer	Trainer for SVM models as input for SvmTheoreticalSpectrumGenerator

PTMs

PTModel	Trains a model for the prediction of proteotypic peptides from a training set.
PTPredict	predicts the likelihood of peptides to be proteotypic via svm_model which is trained by PTModel

File formats and converters

MzTabExporter	Exports various XML formats to an mzTab file
FileConverter	Converts between different MS file formats.
FileFilter	Extracts or manipulates portions of data from peak, feature or consensus-feature files.
FileInfo	Shows basic information about the file, such as data ranges and file type.
FileMerger	Merges several MS files into one file.
FuzzyDiff	Compares two files, tolerating numeric differences.
MzMLSplitter	Splits an mzML file into multiple parts
QCMerger	Merges two qcml files together.
TargetedFileConverter	Converts different transition files for targeted proteomics / metabolomics analysis.
TextExporter	Exports various XML formats to a text file.
XMLValidator	Validates XML files against an XSD schema.

DIA

DIA_Umpire_SE	DIA signal extraction
diapysef library generation	generates spectral library for DIA analysis

Imaging

MSI classification	spatial classification of mass spectrometry imaging data
MSI combine	combine several mass spectrometry imaging datasets into one
MSI data exporter	exports imzML and Analyze7.5 to tabular files
MSI filtering	tool for filtering mass spectrometry imaging data
MSI mz images	mass spectrometry imaging m/z heatmaps
MSI plot spectra	mass spectrometry imaging mass spectra plots
MSI preprocessing	mass spectrometry imaging preprocessing
MSI Qualitycontrol	mass spectrometry imaging QC
MSI segmentation	mass spectrometry imaging spatial clustering

Database

Create Decoy Database (reverse)	Creates a decoy search database by adding reverse sequences to an existing database
CustomProDB	Generate protein FASTAs from exosome or transcriptome data
DatabaseFilter	Filters a protein database (FASTA format) based on identified proteins
DecoyDatabase	Create decoy protein DB from forward protein DB.
Digestor	Digests a protein database in-silico.

DigestorMotif	digests a protein database in-silico

De novo sequencing

CompNovo	Performs a de novo peptide identification using the CompNovo engine
CompNovoCID	Performs a de novo peptide identification using the CompNovo engine

Annotation and analysis

eggNOG Mapper	functional sequence annotation by orthology
idpEmbedder	Embed human/mouse gene metadata into IDPicker files
Pathway Matcher	PathwayMatcher is a software tool to search for pathways related to a list of proteins in Reactome
Unipept	retrieve taxonomy for peptides
InterProScan	Functional prediction of ORFs

In addition, there are multiple general annotation and analysis tools, including KEGG pathway analysis, GO enrichment analysis with g:profiler, etc.