

Experimental Metadata Specifications:

Proteomics Assay

Importance 1: Required, 2: Required if available, 3: Optional

LINCS Field Name	Definition	Importance
PROTEOMICS_Assay_Name	Type of LINCS assay	1
PROTEOMICS_Assay_Type	Type of peptide quantitation used	1
PROTEOMICS_SamplePrep_Digestion_Method	Type of digestion	1
PROTEOMICS_SamplePrep_Lysis_Buffer	Lysis buffer utilized for protein extraction method	1
PROTEOMICS_SamplePrep_Lysis_Protocol	Protocol information for cell lysis prior to analysis	1
PROTEOMICS_SamplePrep_Subcellular_Fractionation	Whether subcellular fraction was used	1
PROTEOMICS_SamplePrep_Subcellular_Fractionation_Target	Chemical or organelle class of subcellular fraction	1
PROTEOMICS_SamplePrep_Protein_Reduction_Agent	Method/chemical to force reduction of protein samples	2
PROTEOMICS_SamplePrep_Alkylation_Agent	Method/chemical to force alkylation of protein samples	2
PROTEOMICS_SamplePrep_Protein_Enrichment	Whether subset of protein(s) were enrich	1
PROTEOMICS_SamplePrep_Protein_Enrichment_Target	Define the target of enrichment	2
PROTEOMICS_SamplePrep_Protein_Fractionation	Whether protein samples were fractionated before digestion	1
PROTEOMICS_SamplePrep_Protein_Fractionation_mode	Method/mode of fractionation	2
PROTEOMICS_SamplePrep_Peptide_Enrichment	Whether peptides were enriched	1
PROTEOMICS_SamplePrep_Peptide_Enrichment_Target	Method/mode of enrichment	2
PROTEOMICS_SamplePrep_Peptide_Fractionation	Whether peptide were fractionated prior to LCMS	1
PROTEOMICS_SamplePrep_Peptide_Fractionation_mode	Method/mode of fractionation	2
PROTEOMICS_SamplePrep_Automation	Sample lysis and preparation was performed manually or though automation	1
PROTEOMICS_SamplePrep_Digestion_Enzyme	Define the protease used to generate peptides from the protein sample	1
PROTEOMICS_SamplePrep_Digestion_Standard	Whether a protein digestion standard was added to the sample prior to digestion	1
PROTEOMICS_SamplePrep_Digestion_ProteinStandard_AA_sequence	Provide AA sequence of protein(s) standard added to sample	2
PROTEOMICS_SamplePrep_PeptideStandard_AA_sequence	Provide AA sequence of peptide(s) standard added to sample	2
PROTEOMICS_SamplePrep_Sample_Clean_UP	Method for sample clean-up prior to LC-MS	2
PROTEOMICS_MS_Instrument	Instrument used to acquire data	1
PROTEOMICS_MS_Instrument_Software	Software utilized for data acquisition	1
PROTEOMICS_MS_Instrument_Software_Version	Version number of software used for data acquisition	1
PROTEOMICS_MS_Instrument_Sample_Interface	Type of sample-instrument interface	2
PROTEOMICS_MS_LC_Instrument	Instrument used for liquid chromatography	1
PROTEOMICS_MS_LC_Column	Column used with LC instrument	1
PROTEOMICS_MS_LC_Column_Flow_Rate	Flow rate through column	1
PROTEOMICS_Processing_Primary_Signal_Processing_Algorithm	Program to generate Level 1 data	1
PROTEOMICS_Processing_Primary_Signal_Processing_Version	Version number of search algorithm used	1
PROTEOMICS_Processing_Analyte_Detection_Mode	Source of spectra identification, e.g. fasta, spectral library	1
PROTEOMICS_Processing_Analyte_Database_Library_File	Provide the FASTA database or Spectral Library for the identification of analytes	1
PROTEOMICS_Processing_Static_Modification_AA	Specify static modifications (+/-amu) applied to the peptide identification search	1
PROTEOMICS_Processing_Differential_Modification_AA	Specify differential modifications (+/-amu) applied to the peptide identification search	1
PROTEOMICS_Processing_Statistical_Quantitation_Processing_Program	Statistical processing program	1
PROTEOMICS_Processing_Statistical_Processing	Link to data processing pipeline software	2
PROTEOMICS_Processing_Statistical_Processing_Version	Version of statistical processing program	1
PROTEOMICS_Processing_Database_Search_Engine	Specify database search engine	1
PROTEOMICS_Processing_Database_Search_Engine_Version	Version number of the used search engine	2
PROTEOMICS_Processing_Data_Filtering_for_Protein	Specify the protein filtering number and appropriate label, e.g. false discovery rate (FDR) or other method for protein identification	2
PROTEOMICS_Processing_Data_Filtering_for_Peptide	Specify the peptide number and appropriate label e.g. false discovery rate (FDR) or other method for protein identification	2
PROTEOMICS_Fragmentation_Type	Mode of peptide ion dissociation	2
PROTEOMICS_Fragmentation_Gas	Type of gas (if any) present in collision cell	2
PROTEOMICS_Fragmentation_Energy_Spread	Method of spreading collision energy over a range	2
PROTEOMICS_Mass_Analyzer_MS1	Type of mass analyzer used to read out parent ions	1
PROTEOMICS_Mass_Analyzer_MS2	Type of mass analyzer used to read out fragment ions	1
PROTEOMICS_Mass_Analyzer_Nominal_Resolution_At_MZ400_MS1	Approximate nominal resolution of mass analyzer at m/z=400 for fragment scans	2
PROTEOMICS_Mass_Analyzer_Nominal_Resolution_At_MZ400_MS2	Approximate nominal resolution of mass analyzer at m/z=400 for fragment scans	2