1. **Normalisation routine**

**Parameters:**

inputFile:

outputFile:

processingLevel: Normalisation level

“peptide” or “feature”

quantLayerType: Quant layer type

Ex. “AssayQuantLayer”

inputDataTypeAccession: Input feature datatype CV accession

Ex. "MS:1001840"

outDataTypeAccession: Output normalised peptide datatype

accession

Ex. "MS:1001891"

decoyTag: Decoy protein tag (prefix or suffix)

Ex. “XXX\_”

**Execution example in the command line:**

Java -jar PeptideAbundanceNormalisation-1.0-SNAPSHOT-jar-with-dependencies.jar "ex1.mzq" "ex1\_normalised.mzq" “AssayQuantLayer” "MS:1001840" "MS:1001891" "peptide" "XXX\_"

**2. Protein inference routine**

**Parameters**

in\_file: input file name with path

out\_file: output file name with path

quantLT: quant layer type

Ex. “AssayQuantLayer”

inputDataTypeAccession: peptide datatype CV accession

for inference in terms of normalised data

Ex. "MS:1001891"

inputRaw DataTypeAccession: raw peptide datatype CV accession

for inference in terms of raw data

Ex. "MS:1001893"

outputProteinGroupDTAccession: output protein group data type

accession

Ex. "MS:1001890"

outputProteinGroupDTName: output protein group data type name

"Progenesis: protein normalised abundance"

outputRawProteinGroupDTAccession: output raw protein group

data type accession

Ex. "MS:1001892"

outputRawProteinGroupDTName: output protein group data type

name

"Progenesis: protein raw abundance"

abundanceOperation: abundance calculation operator

Ex. “sum”

**Execution example in the command line:**

Java -jar ProteinAbundanceInference-1.0-SNAPSHOT-jar-with-dependencies.jar "ex2.mzq" "ex2\_inference.mzq" “AssayQuantLayer” "MS:1001891" "MS:1001893" "MS:1001890" "Progenesis: protein normalised abundance" "MS:1001892" "Progenesis: protein raw abundance" "sum"