SearchGUI configuration file:

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"marshallableParameterType": "identification\_parameters",

"name": "search\_param\_2",

"description": "Fixed: Carbamidomethylation of C.\r\nVariable: Oxidation of M.\r\nFragment Tolerance: 0.05 Da.\r\nDB: UP000005640\_9606\_CrapConcatenated\_concatenated\_target\_decoy.fasta.\r\n",

"defaultDescription": true,

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"fragmentAccuracyType": "DA",

"precursorTolerance": 10.0,

"precursorToleranceDalton": 0.5,

"fragmentIonMZTolerance": 0.05,

"ptmSettings": {

"fixedModifications": [

"Carbamidomethylation of C"

],

"variableModifications": [

"Oxidation of M"

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"refinementVariableModifications": [],

"refinementFixedModifications": [

"Carbamidomethylation of C"

],

"colors": {

"Oxidation of M": {

"value": -16776961,

"falpha": 0.0

},

"Carbamidomethylation of C": {

"value": -4144960,

"falpha": 0.0

}

},

"backUp": {

"Oxidation of M": {

"type": 0,

"name": "Oxidation of M",

"shortName": "ox",

"mass": 15.99491461956,

"neutralLosses": [

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"composition": {

"atomChain": [

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"atomSymbol": "C",

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"atomSymbol": "H",

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"atomSymbol": "O",

"isotope": 0

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{

"atomSymbol": "S",

"isotope": 0

}

],

"mass1": -1.0

},

"name": "CH4OS",

"fixed": false

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],

"reporterIons": [],

"pattern": {

"length": 0,

"residueTargeted": {

"0": [

"M"

]

}

},

"atomChainAdded": {

"atomChain": [

{

"atomSymbol": "O",

"isotope": 0

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"mass1": 15.99491461956,

"stringValue1": "O"

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"cvTerm": {

"ontology": "UNIMOD",

"accession": "UNIMOD:35",

"name": "Oxidation"

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"Carbamidomethylation of C": {

"type": 0,

"name": "Carbamidomethylation of C",

"shortName": "cmm",

"mass": 57.02146372057,

"neutralLosses": [],

"reporterIons": [],

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"C"

]

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"atomSymbol": "N",

"isotope": 0

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"atomSymbol": "O",

"isotope": 0

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"mass1": 57.02146372057,

"stringValue1": "C(2)H(3)NO"

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"cvTerm": {

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"accession": "UNIMOD:4",

"name": "Carbamidomethyl"

}

}

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"nMissedCleavages": 2,

"digestionPreferences": {

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"enzymes": [

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"id": 0,

"name": "Trypsin",

"aminoAcidBefore": [],

"aminoAcidAfter": [],

"restrictionBefore": [],

"restrictionAfter": [],

"aminoAcidBeforeSet": [

"R",

"K"

],

"aminoAcidAfterSet": [],

"restrictionBeforeSet": [],

"restrictionAfterSet": [

"P"

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"isSemiSpecific": false,

"isWholeProtein": false,

"cvTerm": {

"ontology": "PSI-MS",

"accession": "MS:1001251",

"name": "Trypsin"

}

}

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"nMissedCleavages": {

"Trypsin": 2

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"specificity": {

"Trypsin": "specific"

}

},

"fastaFile": {

"path": "C:\\Users\\lenna\\Desktop\\genet\_data\\UP000005640\_9606\_CrapConcatenated\_concatenated\_target\_decoy.fasta"

},

"parametersFile": {},

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"rewindIons": [

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"minChargeSearched": {

"sign": 1,

"value": 2

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"maxChargeSearched": {

"sign": 1,

"value": 4

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"minIsotopicCorrection": 0,

"maxIsotopicCorrection": 1,

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"algorithmParameters": {

"1": {

"type": "com.compomics.util.experiment.identification.identification\_parameters.tool\_specific.OmssaParameters",

"data": {

"maxEValue": 100.0,

"hitListLength": 10,

"minimalChargeForMultipleChargedFragments": {

"sign": 1,

"value": 3

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"minPeptideLength": 8,

"maxPeptideLength": 30,

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"neutronThreshold": 1446.94,

"lowIntensityCutOff": 0.0,

"highIntensityCutOff": 0.2,

"intensityCutOffIncrement": 5.0E-4,

"singleChargeWindow": 27,

"doubleChargeWindow": 14,

"nPeaksInSingleChargeWindow": 2,

"nPeaksInDoubleChargeWindow": 2,

"maxHitsPerSpectrumPerCharge": 30,

"nAnnotatedMostIntensePeaks": 6,

"minAnnotatedPeaks": 2,

"minPeaks": 4,

"cleaveNtermMethionine": true,

"maxMzLadders": 128,

"maxFragmentCharge": 2,

"fractionOfPeaksForChargeEstimation": 0.95,

"determineChargePlusOneAlgorithmically": true,

"searchPositiveIons": true,

"minPrecPerSpectrum": 1,

"searchForwardFragmentFirst": false,

"searchRewindFragments": true,

"maxFragmentPerSeries": 100,

"useCorrelationCorrectionScore": true,

"consecutiveIonProbability": 0.5,

"iterativeSequenceEvalue": 0.0,

"iterativeReplaceEvalue": 0.0,

"iterativeSpectrumEvalue": 0.01,

"noProlineRuleSeries": [],

"ptmIndexes": {

"119": "Carbamidomethylation of C",

"120": "Oxidation of M"

}

}

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"2": {

"type": "com.compomics.util.experiment.identification.identification\_parameters.tool\_specific.XtandemParameters",

"data": {

"maxEValue": 0.01,

"outputResults": "all",

"dynamicRange": 100.0,

"nPeaks": 50,

"minPrecursorMass": 500.0,

"minFragmentMz": 200.0,

"minPeaksPerSpectrum": 5,

"proteinQuickAcetyl": true,

"quickPyrolidone": true,

"refine": true,

"refineSemi": false,

"refinePointMutations": false,

"refineSpectrumSynthesis": true,

"refineUnanticipatedCleavages": true,

"refineSnaps": true,

"maximumExpectationValueRefinement": 0.01,

"potentialModificationsForFullRefinment": false,

"skylinePath": "",

"outputProteins": true,

"outputSequences": false,

"outputSpectra": true,

"outputHistograms": false,

"stpBias": false,

"useNoiseSuppression": false,

"proteinPtmComplexity": 6.0

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"3": {

"type": "com.compomics.util.experiment.identification.identification\_parameters.tool\_specific.PepnovoParameters",

"data": {

"hitListLength": 10,

"estimateCharge": true,

"correctPrecursorMass": false,

"discardLowQualitySpectra": true,

"fragmentationModel": "CID\_IT\_TRYP",

"generateQuery": false

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"4": {

"type": "com.compomics.util.experiment.identification.identification\_parameters.tool\_specific.AndromedaParameters",

"data": {

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"maxCombinations": 250,

"topPeaks": 8,

"topPeaksWindow": 100,

"includeWater": true,

"includeAmmonia": true,

"dependentLosses": true,

"fragmentAll": false,

"empiricalCorrection": true,

"higherCharge": true,

"fragmentationMethod": "CID",

"maxNumberOfModifications": 5,

"minPeptideLengthNoEnzyme": 8,

"maxPeptideLengthNoEnzyme": 25,

"equalIL": false,

"numberOfCandidates": 10,

"ptmIndexes": {},

"decoyMode": "none"

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"5": {

"type": "com.compomics.util.experiment.identification.identification\_parameters.tool\_specific.MsAmandaParameters",

"data": {

"generateDecoy": false,

"instrumentID": "b, y",

"maxRank": 10,

"monoisotopic": true,

"lowMemoryMode": true

}

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"7": {

"type": "com.compomics.util.experiment.identification.identification\_parameters.tool\_specific.MsgfParameters",

"data": {

"searchDecoyDatabase": false,

"instrumentID": 3,

"fragmentationType": 3,

"protocol": 0,

"minPeptideLength": 8,

"maxPeptideLength": 30,

"numberOfSpectrumMarches": 10,

"additionalOutput": false,

"lowerIsotopeErrorRange": -1,

"upperIsotopeErrorRange": 2,

"numberTolerableTermini": 2,

"numberOfPtmsPerPeptide": 2

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"8": {

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"data": {

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"maxPeakCount": 100,

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"maxPrecursorAdjustment": 1.5,

"precursorAdjustmentStep": 0.1,

"numChargeStates": 3,

"outputSuffix": "",

"useChargeStateFromMS": true,

"duplicateSpectra": true,

"deisotopingMode": 0,

"isotopeMzTolerance": 0.25,

"complementMzTolerance": 0.1,

"tagLength": 4,

"maxDynamicMods": 2,

"maxTagCount": 10,

"intensityScoreWeight": 1.0,

"mzFidelityScoreWeight": 1.0,

"complementScoreWeight": 1.0,

"variablePtms": []

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"10": {

"type": "com.compomics.util.experiment.identification.identification\_parameters.tool\_specific.CometParameters",

"data": {

"numberOfSpectrumMatches": 10,

"maxVariableMods": 10,

"requireVariableMods": false,

"minPeaks": 10,

"minPeakIntensity": 0.0,

"removePrecursor": 0,

"removePrecursorTolerance": 1.5,

"lowerClearMzRange": 0.0,

"upperClearMzRange": 0.0,

"enzymeType": 2,

"isotopeCorrection": 1,

"minPrecursorMass": 600.0,

"maxPrecursorMass": 5000.0,

"maxFragmentCharge": 3,

"removeMethionine": false,

"batchSize": 0,

"theoreticalFragmentIonsSumOnly": false,

"fragmentBinOffset": 0.025,

"useSparseMatrix": true,

"selectedOutputFormat": "PepXML",

"printExpectScore": true

}

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"27": {

"type": "com.compomics.util.experiment.identification.identification\_parameters.tool\_specific.PNovoParameters",

"data": {

"numberOfPeptides": 10,

"lowerPrecursorMass": 300,

"upperPrecursorMass": 5000,

"acticationType": "HCD"

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"28": {

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"data": {

"fastIndexFolderName": "fasta-index",

"maxVariablePtmsPerTypePerPeptide": 2,

"minPeptideLength": 6,

"maxPeptideLength": 30,

"minPrecursorMass": 200.0,

"maxPrecursorMass": 7200.0,

"decoyFormat": "none",

"keepTerminalAminoAcids": "NC",

"decoySeed": 1,

"outputFolderName": "crux-output",

"printPeptides": false,

"verbosity": 30,

"monoisotopicPrecursor": true,

"clipNtermMethionine": false,

"digestionType": "full-digest",

"computeSpScore": false,

"numberOfSpectrumMatches": 10,

"computeExactPValues": false,

"minSpectrumMz": 0.0,

"minSpectrumPeaks": 20,

"spectrumCharges": "all",

"removePrecursor": false,

"removePrecursorTolerance": 1.5,

"printProgressIndicatorSize": 1000,

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"useNeutralLossPeaks": false,

"mzBinWidth": 0.02,

"mzBinOffset": 0.0,

"concatenateTargetDecoy": false,

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"sqtOutput": false,

"pepXmlOutput": false,

"mzidOutput": false,

"pinOutput": false,

"removeTempFolders": true

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"13": {

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"maxDynamicMods": 2,

"minTerminiCleavages": 2,

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"maxPrecursorMass": 5000.0,

"useSmartPlusThreeModel": true,

"computeXCorr": false,

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"classSizeMultiplier": 2,

"numberOfBatches": 50,

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"upperIsotopeCorrection": 2,

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"maxPeakCount": 300,

"outputFormat": "mzIdentML"

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"29": {

"type": "com.compomics.util.experiment.identification.identification\_parameters.tool\_specific.NovorParameters",

"data": {

"fragmentationMethod": "HCD",

"massAnalyzer": "FT"

}

}

}

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"annotationSettings": {

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"showAllPeaks": false,

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"intensityLimit": 0.75,

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"PRECURSOR\_ION": [

0

],

"RELATED\_ION": [

0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18 ],

"REPORTER\_ION": [],

"TAG\_FRAGMENT\_ION": [

1, 4

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"IMMONIUM\_ION": [

0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20 ]

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"neutralLossesList": [

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"atomSymbol": "H",

"isotope": 0

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"atomSymbol": "H",

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"isotope": 0

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],

"mass1": -1.0,

"stringValue1": "H(2)O"

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"name": "H2O",

"fixed": false,

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"D",

"E",

"S",

"T"

]

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{

"composition": {

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"isotope": 0

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"atomSymbol": "H",

"isotope": 0

}

],

"mass1": -1.0,

"stringValue1": "H(3)N"

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"name": "NH3",

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"N",

"Q",

"R"

]

},

{

"composition": {

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"atomSymbol": "C",

"isotope": 0

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"atomSymbol": "O",

"isotope": 0

},

{

"atomSymbol": "S",

"isotope": 0

}

],

"mass1": -1.0,

"stringValue1": "CH(4)OS"

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"name": "CH4OS",

"fixed": false

}

],

"neutralLossesAuto": true,

"reporterIons": true,

"relatedIons": true,

"fragmentIonAccuracy": 0.05,

"fragmentIonPpm": false,

"showForwardIonDeNovoTags": false,

"showRewindIonDeNovoTags": false,

"deNovoCharge": 1,

"highResolutionAnnotation": true,

"tiesResolution": "mostAccurateMz"

},

"sequenceMatchingPreferences": {

"sequenceMatchingType": "indistiguishableAminoAcids",

"limitX": 0.25,

"peptideMapperType": "fm\_index"

},

"peptideVariantsPreferences": {

"useSpecificCount": false,

"nVariants": 0,

"nAaDeletions": 0,

"nAaInsertions": 0,

"nAaSubstitutions": 0,

"nAaSwap": 0,

"aaSubstitutionMatrix": {

"name": "No Substitution",

"description": "No substitution",

"substitutions": {},

"reverseMap": {}

}

},

"genePreferences": {

"autoUpdate": true,

"useGeneMapping": true,

"selectedBackgroundSpecies": 9606

},

"psmScoringPreferences": {

"spectrumMatchingScores": {

"3": [

1

],

"8": [

1

],

"27": [

1

]

},

"defaultScores": [

-1

],

"minDecoysInBin": 10

},

"peptideAssumptionFilter": {

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"maxPepLength": 30,

"maxMassDeviation": 10.0,

"isPpm": true,

"unknownPtm": true,

"minIsotopes": 0,

"maxIsotopes": 1

},

"ptmScoringPreferences": {

"flr": 1.0,

"probabilitsticScoreCalculation": true,

"selectedProbabilisticScore": "PhosphoRS",

"estimateFlr": false,

"probabilisticScoreThreshold": 95.0,

"probabilisticScoreNeutralLosses": false,

"sequenceMatchingPreferences": {

"sequenceMatchingType": "aminoAcid",

"peptideMapperType": "fm\_index"

},

"alignNonConfidentPTMs": true

},

"proteinInferencePreferences": {

"proteinSequenceDatabase": {

"path": "D:\\db\\UP000005640\_9606\_CrapConcatenated\_concatenated\_target\_decoy.fasta"

},

"simplifyProteinGroups": true,

"simplifyGroupsScore": true,

"simplifyGroupsEvidence": true,

"simplifyGroupsEnzymaticity": true,

"simplifyGroupsUncharacterized": true

},

"idValidationPreferences": {

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"defaultPeptideFDR": 1.0,

"defaultPsmFDR": 1.0,

"separatePeptides": true,

"separatePsms": true,

"mergeSmallSubgroups": true,

"validationQCPreferences": {

"dbSize": false,

"firstDecoy": true,

"confidenceMargin": 1.0

} },

"fractionSettings": {

"proteinConfidenceMwPlots": 95.0,

"fractionMolecularWeightRanges": {}

}

}