XiFDR Search Results File Description

The XiSearch output has several columns.
The columns fall into several categories:
- general match information
- per peptide information
- sub-scores
- final score

Following the columns are explained in these groups

General Match Information

Basic information pertaining the whole PSM.

Field	Description
Run	Name of the raw-file as passed out from the peak-list
Scan	scan number of the spectrum as passed out from the peak-list
ScanInputIndex	index of the spectrum in the peak-list
Source	name of the actual file containing the spectrum
ElutionStart	Start of the elution as passed out from the peak-list
ElutionEnd	end of the elution as passed out from the peak-list
PrecursorMass	The mass of the precursor as given by the peak-list
PrecoursorCharge	The charge of the precursor as given by the peak-list
PrecurserMZ	The m/z value of the precursor as given by the peak-list
CalcMass	the theoretical mass according to the matched peptides
CalcMZ	the theoretical m/z according to the matched peptides
validated	did it pass auto-validation (mainly the autovalidation score with some heuristics against some corner cases)
decoy	is this a decoy match
MatchRank	the rank of the match according to score (mostly)
Crosslinker	the name of the cross-linker (empty for linear matches)
CrosslinkerMass	the mass of the cross-linker
decoyCrosslinker	was the cross-linker found here defined as a decoy cross-linker

Per Peptide Information

Information about each peptide in the PSM. X is the number of the peptide.

Field	Description
ProteinX	accession number of the protein
FastaX	FASTA-header of the protein
ProteinXdecoy	is this protein a decoy protein
PeptideX	sequence of the peptide
BasePeptideX	sequence without any modification
PeptideLinkMapX	sequence of the peptide with associated linkage score (displaying a likelihood for a residue to be the linkage site)
PeptideMassX	Neutral Mass of the Peptide
StartX	start of the peptide in the protein
LengthPeptideX	length of the peptide
LinkX	linkage site in the peptide
Linked AminoAcid X	what amino-acid was linked
LinkWindowX	a +- 20 amino acid window around the detected protein linkage site
ProteinLinkX	where in the protein is the link
ProteinCountX	if the peptide was ambiguous in how many proteins was it found in total
PositionCountX	if the peptide was ambiguous in how often was it found in total
ModificationsX	list of modifications on this peptide
ModificationPositionsX	where in the peptides these modification are
ModificationMassesX	delta masses of the modifications
OpenModPositionX	Legacy column
OpenMassX	Legacy column
OpenModWindowX	Legacy column

Sub-Scores

XiSearch calculates a range of sub scores. Following is a description of all columns representing these sub-scores.

Candidate Sub-Scores

XiSearch does work in a multistage approach – first it generates a list of alpha candidates and from these a list of candidates peptide pairs that are then fully scored. The following scores pertain are derived from the candidate lists.

Field	Description
betaCount	for the given alpha peptide - how many beta peptides fit by mass
betaCountInverse	1/betaCount
mgcRank	rank of the alpha peptide among the list of alpha peptide candidates
mgxRank	rank of the peptide pair among the peptide pair candidates
mgcScore	candidate score of the alpha peptide
mgcDelta	difference to the second best alpha peptide candidate
mgcShiftedDelta	deprecated
mgcAlpha	=mgcScore
mgcBeta	the alpha candidate score for the beta peptide
mgxScore	the candidate score for the peptide pair
mgxDelta	difference to the second best peptide pair candidate score
delta	difference of the full score to the second best peptide pair (disregarding modifications)
deltaMod	difference of the full score to the second best peptide pair (considering modifications)
combinedDelta	average of delta and main score
match score	main score of the PSM (last entry per line)

Mass-Errors

Field	Description
Precoursor Error	ppm error of the precursor

Precoursor Absolute Error	absolute value of the precursor error
PrecoursorAbsoluteErrorRelative	the absolute error/max precursor error
1-ErrorRelative	1-PrecoursorAbsoluteErrorRelative
AverageMS2Error	The average error of all ms2 peak matches
MeanSquareError	MSE of the MS2 peak matches
MeanSquareRootError	MSRE of the MS2 peak matches
AverageRelativeMS2Error	mean of peak error/max error
Average1-RelativeMS2Error	mean of (1-peak error/max error)
AverageMS2ErrorPeptide1	Average error of all linear fragment matches for peptide1
AverageMS2ErrorPeptide2	Average error of all linear fragment matches for peptide2
AverageMS2ErrorCrossLinked	Average error of all cross-linked fragments

MS2 Fragment Charges

Field	Description
MaxCharge	maximal observed charge
AverageCharge	average observed charge
RelativeMaxCharge	MaxCharge/Precursor Charge
RelativeAverageCharge	AVerageCharge/Precursor Charge

Fragment occurrence

Score	Description	Name as Applied To		
		Whole match	for Peptide1	for Peptide2
total fragment matches	Number of fragment to peak matches	total fragment matches	peptide1 total fragment matches	peptide2 total fragment matches
lossy fragment matches	Number of neutral loss fragment to peak matches	lossy fragment matches	peptide1 lossy fragment matches	peptide2 lossy fragment matches
matched	Number of fragments matched (each unique b/y ion is only counted ones)	fragment matched	peptide1 matched	peptide2 matched
coverage	found fragmentation site/maximum fragmentation sites	fragment coverage	peptide1 coverage	peptide2 coverage
non lossy matched	Non neutral loss	fragment non	peptide1 non lossy	peptide2 non

	fragments matched	lossy matched	matched	lossy matched
non lossy coverage	Non neutral loss coverage	fragment non lossy coverage	peptide1 non lossy coverage	peptide2 non lossy coverage
lossy matched	Neutral loss fragments matched	fragment lossy matched	peptide1 lossy matched	peptide2 lossy matched
lossy coverage	Neutral loss fragment coverage	fragment lossy coverage	peptide1 lossy coverage	peptide2 lossy coverage
matched conservative	same as non-lossy coverage but if a fragment is observed in three distinct neutral loss states then it is a also counted as non-lossy	fragment matched conservative	peptide1 matched conservative	peptide2 matched conservative
conservative coverage	as fragment matched conservative but as coverage	fragment conservative coverage	peptide1 conservative coverage	peptide2 conservative coverage
unique matched	same as "matched" but for each peak only one fragment match is considered	fragment unique matched	peptide1 unique matched	peptide2 unique matched
unique matched non lossy	same as "matched non-lossy" but for each peak only one fragment match is considered	fragment unique matched non lossy	peptide1 unique matched non lossy	peptide2 unique matched non lossy
unique matched non lossy coverage	same as "matched non-lossy-coverage" but for each peak only one fragment match is considered	fragment unique matched non lossy coverage	peptide1 unique matched non lossy coverage	peptide2 unique matched non lossy coverage
unique matched lossy	same as "matched lossy" but for each peak only one fragment match is considered	fragment unique matched lossy	peptide1 unique matched lossy	peptide2 unique matched lossy
unique matched lossy coverage	same as "matched lossy coverage" but for each peak only one fragment match is considered	fragment unique matched lossy coverage	peptide1 unique matched lossy coverage	peptide2 unique matched lossy coverage
unique matched conservative	same as "matched conservative" but for each peak only one fragment match is considered	fragment unique matched conservative	peptide1 unique matched conservative	peptide2 unique matched conservative
unique matched conservative coverage	same as "matched coverage" but for each peak only one fragment match is considered	fragment unique matched conservative coverage	peptide1 unique matched conservative coverage	peptide2 unique matched conservative coverage
multimatched%	how many of the matched fragments are matched in more then one charge state	fragment multimatched%	peptide1 multimatched%	peptide2 multimatched%

sequencetag coverage%	how much of the peptides sequence is explained by consecutive fragments	fragment sequencetag coverage%	peptide1 sequencetag coverage%	peptide2 sequencetag coverage%

Search-Database derived Scores

Field	*Description*
FragmentLibraryScore	how specific are all peak taht are matched to the given peptide versus all other peptides
FragmentLibraryScoreLog	ln(FragmentLibraryScore)

Spectrum coverage

spectrum intensity coverage	how much of the total intensity of the spectrum is explained
spectra intensity nonlossy coverage	how much of the total intensity of the spectrum is explained by non-neutral loss fragments
spectra isotop%	how much of the spectrum intensity is contained in isotope clusters
spectra matched isotop%	how much of the spectrum isotope cluster are actually matched to something
spectra matched single%	how much of the single peaks are matched
spectra top10 matched%	how much of the top n peaks are explained
spectra top20 matched%	
spectra top40 matched%	
spectra top100 matched%	
spectrum peaks coverage	how much of the total number of peaks are matched
SpectraCoverageConservative	how much of the spectrum is explained either by fragments found as bassic (non-neutral loss) fragments + fragments that are not found as non-neutral loss but at least with three distinct neutral loss fragments

Preliminary Combinations of Sub-Scores

Pep1Score	some weighted combination of sub-scores pertaining to peptide1
Pep2Score	some weighted combination of sub-scores pertaining to peptide2
spectrum quality score	some weighted combination of sub-scores pertaining to the spectrum

Other Sub-Scores

Autovalidation	a ml model defining a match as being validated - this is the base of the "validated" column but is there filtered by additional criteria

Legacy Sub-Scores

Subscores that are still present but should no longer be considered

FragmentLibraryScoreExponential	
BS3ReporterIonScore	
Crosslinked	
Modified	
Containing	
J48ModeledManual001	
RandomTreeModeledManual	
AllScore	
AllScoreLib	
MatchScore	
NormScore	

Final Score

the sub-scores get normalized, weighted and averaged to calculated the final score for the match
This is the score in the last column of the CSV-file

match score	main score of the PSM