

XiFDR File Description

Summary

Provides a summary on how the fdr estimation was performed.
It has several section:

Settings section:

Provides an overview of what settings where used to produce the result

xiFDR Version:	Version of XiFDR that produced the file		
Source:	Where the data where read from		
	Target FDRs:	Minimum supporting peptides	Directional
psm	FDR applied at PSMs		false
peptide pair	FDR applied at peptide pairs		false
protein group	FDR applied at protein groups	1	
Link	FDR applied at residue pairs	1	false
Protein Group Pair	FDR applied at protein group pairs	1	false
max next level fdr factor (report-factor):	deprecated		
minimum peptide length	Minimum length of peptide to be considered for FDR		
unique PSMs			
Accepted ambiguity:	do to ambiguity of peptide source a peptide pair can represent several links		
Links for one peptide pair	peptide pairs representing more unique links then this will be ignored		
Protein pairs for one peptide pair	peptide pairs representing more unique protein pairs then this will be ignored		
Length-Group:	PSMs and peptide pairs get split by the length of the shortest peptide		

Result Summary:

presents the number of unique matches that passed all FDRs. This including being filtered back to what passed higher level FDRs. Meaning if a PSM-level FDR of 5% was defined and also a peptide FDR of 5% then the PSM-numbers shown here are the ones that first passed the 5%PSM FDR and supported peptide pairs that passed the 5% Peptide Pair FDR. This is given ones for all and split into internal and between links and there into target-target, target-decoy and decoy matches.

class	all	Internal TT	Internal TD	Internal DD	Between TT	Between TD	Between DD	Linear T	Linear D
Input PSMs	all psms								
fdr PSMs	PSMS passed all FDRs	x	x	x	x	x	x	x	x
fdr Peptide Pairs	peptide pairs passed all FDRs	x	x	x	x	x	x	x	x
fdr Link	residue pairs passed all FDRs	x	x	x	x	x	x		
fdr Protein Group Pairs	protein pairs passed all FDRs	x	x	x	x	x	x		
fdr Protein Groups	protein groups passed all FDRs							x	x

Level Information

Then comes one section for each level of information:

It provides the information about what went into the calculation (e.g. what passed the lower level FDRs and prefilter)

Level detailed summary			
Group	Group 1	Group 2	...
Input	How many matches where considered in each group		
TT	How many target target entries where in the input		
TD	How many target decoy entries where in the input		
DD	How many decoy decoy entries where in the input		
passing fdr (0.05)	How many matches passed the FDR		
TT	How many target target matches passed the FDR		
TD	How many target decoy matches passed the FDR		
DD	How many decoy decoy matches passed the FDR		
last fdr < 0.05	What was the last fdr that did not exceed the target		

	FDR
higher fdr (> 0.05)	What would have been the next detectable FDR larger than the target FDR
lower fdr (<= 0.05)	What was the next detectable lower FDR below the “last FDR”
final	How many matches passed this FDR and higher level FDRs

PSM file

There are two PSM-files generated – one for linear PSMs (non-cross-linked) and one for cross-linked PSMs. Both share the same format but in the linear file all fields pertaining to peptide2 are empty.

Columns:

PSMID	A unique id assigned to a PSM either provided in the input or made up from scan run and peptide sequences
run	Run Name as provided in the input
exp charge	experimental spectrum information as provided from the input
exp m/z	
exp mass	
exp fractionalmass	the part of the “exp mass” that is behind the dot e.g. exp mass = 734.987 the fractional mass would be 0.987
match charge	the charge state matched
match mass	that mass of the peptides + cross-linker
match fractionalmass	as above for the match-mass
scan	Scan-number
Protein1	accession of protein1 (as in input)
Description1	description of protein 1 (as in input)
Decoy1	is the first protein a decoy protein
Protein2	accession of protein2 (as in input)
Description2	description of protein 2 (as in input)
Decoy2	is the second protein a decoy protein

PepSeq1	sequence of peptide1
PepSeq2	sequence of peptide 2
PepPos1	position of peptide 1 in protein1
PepPos2	position of peptide 2 in protein2
PeptideLength1	length of peptide1 in amino-acids
PeptideLength2	length of peptide2 in amino-acids
LinkPos1	Link-site in peptide1
LinkPos2	link-site in peptide 2
ProteinLinkPos1	link-site in protein 1
ProteinLinkPos2	link-site in protein 2
Charge	matched charge
Crosslinker	the name of the cross-linker involved with this match
Score	score of the PSM
isDecoy	is this a match involving a decoy peptide
isTT	is this a target target match
isTD	is this a target decoy match
isDD	is this a decoy decoy match
fdrGroup	under what group was this match considered
lowerFDR	next lower detectable FDR
fdr	FDR associated with the match score
higherFDR	next higher FDR

Peptide Pair

All cross-linked peptide pairs passing all FDRs

PeptidePairID	a numeric ID for the peptide pair
PSMIDs	all psms that support this peptide pair
Protein1	accession of protein1 (as in input)
Description1	description of protein 1 (as in input)

Decoy1	is the first protein a decoy protein
Protein2	accession of protein2 (as in input)
Description2	description of protein 2 (as in input)
Decoy2	is the second protein a decoy protein
Peptide1	sequence of peptide1
Peptide2	sequence of peptide 2
FromSite	Link-site in peptide1
ToSite	link-site in peptide 2
FromProteinSite	link-site in protein 1
ToProteinSite	link-site in protein 2
psmID	Legacy – to be deleted
Crosslinker	the cross-linker for this peptide pair
Score	the score as derived from PSMs
isDecoy	is this a match involving a decoy peptide
isTT	is this a target target match
isTD	is this a target decoy match
isDD	is this a decoy decoy match
fdrGroup	under what group was this match considered
fdr	FDR associated with the match score

Protein Group

Lists all protein groups that were identified in the sample

ProteinGroupID	a unique id assigned to the protein group
ProteinGroup	accession numbers of all proteins in this group
Descriptions	descriptions of all proteins in the group
Sequence	Amino acid sequences of all proteins in the group

Crosslinker	all cross-linker seen involved with the protein group
Score	a score for the protein group based on the peptide pairs supporting the group
isDecoy	is this a match involving a decoy peptide
isTT	is this a target target match
isTD	is this a target decoy match
isDD	is this a decoy decoy match
PSM IDs	list of all PSM-IDs supporting the Protein group
fdrGroup	under what group was this match considered
fdr	FDR associated with the match score
File Name1	Highest score of a psm supporting this protein group in the given run
File name 2	
...	

Link

All residue pairs that passed all FDRs

LinkID	A unique ID assign to each link
PeptidePairIDs	list of supporting peptide pair Ids
PSMIDs	list of supporting PSM Ids
Protein1	Protein 1 that is linked
Description1	description of protein1
Decoy1	is protein 1 a decoy?
Protein2	Protein 2 that is linked
Description2	description of protein2
Decoy2	is protein 2 a decoy?
fromSite	link site within protein 1
ToSite	link site within protein 2
Croslinkers	cross-linkers that this link was observed with this link

Score	score for the link based on all supporting peptide pairs
isDecoy	is this a match involving a decoy peptide
isTT	is this a target target match
isTD	is this a target decoy match
isDD	is this a decoy decoy match
count PSMs	how many PSMs support this link
count peptide pairs	how many unique peptide pairs support this link
fdrGroup	under what group was this match considered
fdr	FDR associated with the match score
File Name1	Highest score of a psm supporting this protein group in the given run
File name 2	
...	

PPI

List of all protein pairs that passed all FDRs

ProteinGroupPairID	A unique ID assigned to each protein pair
LinkIDs	list of supporting residue pair Ids
PeptidePairIDs	list of supporting peptide pair Ids
PSMIDs	list of supporting PSM Ids
Protein1	Protein 1 that is linked
Descriptions1	description of protein 1
isDecoy1	is protein 1 a decoy?
Protein2	Protein 2 that is linked
Description2	description of protein 2
isDecoy2	is protein 2 a decoy?
Crosslinker	cross-linkers that this link was observed linking these proteins
Score	score for the link based on all supporting residue pairs
isDecoy	is this a match involving a decoy peptide
isTT	is this a target target match
isTD	is this a target decoy match
isDD	is this a decoy decoy match

count PSMs	how many PSMs support this link
count peptide pairs	how many unique peptide pairs support this link
count links	how many unique residue pairs support this link
fdrGroup	under what group was this match considered
fdr	FDR associated with the match score