

XlinkViewer

1)
2)

Jan's XLink Viewer

File

Open...

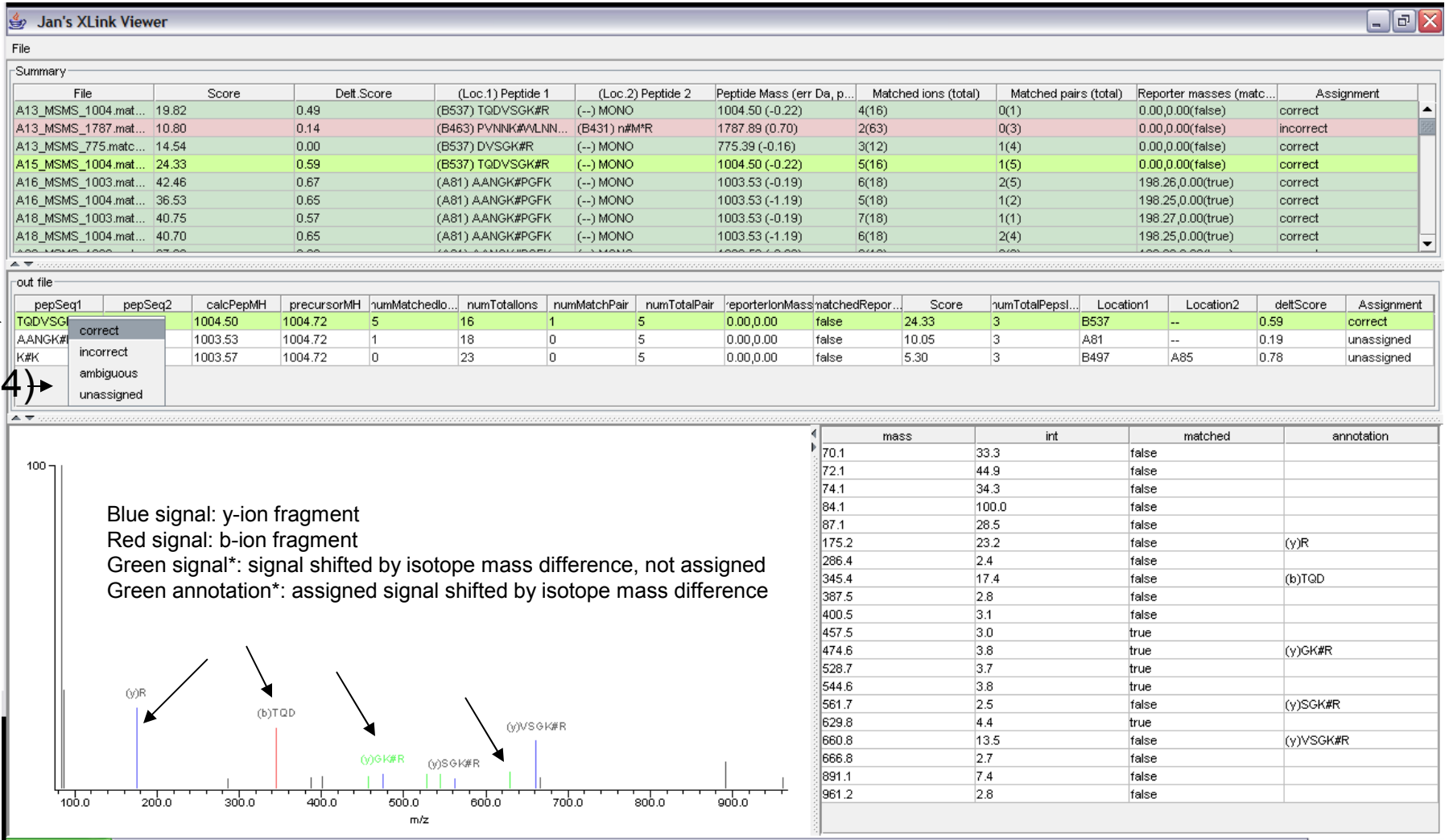
Simple report	Score	Delt. Score	(Loc.1) Peptide 1	(Loc.2) Peptide 2	Peptide Mass (err Da, p...)	Matched ions (total)	Matched pairs (total)	Reporter masses (matc...	Assignment
A13_MSMS_1004.mat...	19.82	0.49	(B537) TGDVSGK#R	(-) MONO	1004.50 (-0.22)	4(16)	0(1)	0.00,0.00(false)	correct
A13_MSMS_1787.mat...	10.80	0.14	(B463) PVNNGK#ALNN...	(B431) n#M#R	1787.89 (0.70)	2(63)	0(3)	0.00,0.00(false)	incorrect
A13_MSMS_775.matc...	14.54	0.00	(B537) DVSGK#R	(-) MONO	775.39 (-0.16)	3(12)	1(4)	0.00,0.00(false)	correct
A15_MSMS_1004.mat...	24.33	0.59	(B537) TGDVSGK#R	(-) MONO	1004.50 (-0.22)	5(16)	1(5)	0.00,0.00(false)	correct
A16_MSMS_1003.mat...	42.46	0.67	(A81) AANGK#PGFK	(-) MONO	1003.53 (-0.19)	6(18)	2(5)	198.26,0.00(true)	correct
A16_MSMS_1004.mat...	36.53	0.65	(A81) AANGK#PGFK	(-) MONO	1003.53 (-1.19)	5(18)	1(2)	198.25,0.00(true)	correct
A18_MSMS_1003.mat...	40.75	0.57	(A81) AANGK#PGFK	(-) MONO	1003.53 (-0.19)	7(18)	1(1)	198.27,0.00(true)	correct
A18_MSMS_1004.mat...	40.70	0.65	(A81) AANGK#PGFK	(-) MONO	1003.53 (-1.19)	6(18)	2(4)	198.25,0.00(true)	correct

out file

pepSeq1	pepSeq2	calcPepMH	precursorMH	numMatchedIo...	numTotalions	numMatchPair	numTotalPair	reporterIonMass	matchedRepor...	Score	numTotalPepI...	Location1	Location2	deltScore	Assignment
TGDVSGK#R	MONO	1004.50	1004.72	5	16	1	5	0.00,0.00	false	24.33	3	B537	--	0.59	correct
AANGK#PGFK	MONO	1003.53	1004.72	1	18	0	5	0.00,0.00	false	10.05	3	A81	--	0.19	unassigned
K#K	PGFK#QG	1003.57	1004.72	0	23	0	5	0.00,0.00	false	5.30	3	B497	A85	0.78	unassigned

mass	int	matched	annotation
70.1	33.3	false	
72.1	44.9	false	
74.1	34.3	false	
84.1	100.0	false	
87.1	28.5	false	
175.2	23.2	false	(y)R
286.4	2.4	false	
345.4	17.4	false	(b)TQD
387.5	2.8	false	
400.5	3.1	false	
457.5	3.0	true	
474.6	3.8	true	(y)GK#R
528.7	3.7	true	
544.6	3.8	true	
561.7	2.5	false	(y)SGK#R
629.8	4.4	true	
660.8	13.5	false	(y)VSGK#R
666.8	2.7	false	
891.1	7.4	false	
961.2	2.8	false	

- 1) Open *OUT*.html and wait for XlinkViewer to load data
- 2) Select individual MS/MS spectrum to be assigned



- 1) Select one or more assignment
 - 2) and label as either correct, incorrect, ambiguous, or leave unassigned
- * Green signals or annotations indicate peptide fragments that most possibly contain the isotope label of the cross-linking reagent, modified residues marked as e.g. K# or n# (N-terminus)

→ Every assigned entry labeled as either correct, ambiguous or incorrect is monitored in a file named xlink.res, see example below.

xlink.res	B13_MSMS_1349.match.txt.out	0	correct
	B3_MSMS_1045.match.txt.out	0	correct
	C18_MSMS_1002.match.txt.out	0	correct
	C18_MSMS_1046.match.txt.out	0	correct
	C24_MSMS_1202.match.txt.out	0	correct
	D11_MSMS_718.match.txt.out	0	correct
	D15_MSMS_1333.match.txt.out	0	correct
	D20_MSMS_1045.match.txt.out	0	correct
	D20_MSMS_870.match.txt.out	0	correct
	D22_MSMS_1045.match.txt.out	0	correct
	D22_MSMS_1046.match.txt.out	0	correct
	D22_MSMS_870.match.txt.out	0	correct
	D23_MSMS_1045.match.txt.out	0	correct
	D23_MSMS_1045.match.txt.out	1	ambiguous
	D24_MSMS_1046.match.txt.out	0	correct
	D5_MSMS_1012.match.txt.out	0	correct
	D5_MSMS_1046.match.txt.out	0	correct
	D7_MSMS_1012.match.txt.out	0	correct
	D7_MSMS_1046.match.txt.out	0	correct
	D7_MSMS_1047.match.txt.out	0	correct
	D9_MSMS_1012.match.txt.out	0	correct
	D9_MSMS_1046.match.txt.out	0	correct
	E17_MSMS_1362.match.txt.out	0	correct
	E21_MSMS_1016.match.txt.out	0	correct
	E22_MSMS_1877.match.txt.out	0	ambiguous
	E22_MSMS_1877.match.txt.out	1	ambiguous
	E23_MSMS_1016.match.txt.out	0	correct
	E2_MSMS_676.match.txt.out	0	correct
	E3_MSMS_1015.match.txt.out	0	correct
	E5_MSMS_1905.match.txt.out	1	correct
F3_MSMS_1571.match.txt.out	0	correct	
F5_MSMS_1571.match.txt.out	0	correct	
F9_MSMS_1571.match.txt.out	0	correct	
G11_MSMS_1894.match.txt.out	0	ambiguous	
G11_MSMS_1938.match.txt.out	0	correct	
G11_MSMS_1938.match.txt.out	1	ambiguous	
G11_MSMS_1970.match.txt.out	0	incorrect	
G9_MSMS_1938.match.txt.out	0	correct	

→ Therefore every change in XlinkViewer is kept in memory. The user can start working on a data set, stop and continue at any given time.

5)

Jan's XLink Viewer

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Simple report	Score	Delta Score	(Loc.1) Peptide 1	(Loc.2) Peptide 2	Peptide Mass (err Da, p...)	Matched ions (total)	Matched pairs (total)	Reporter masses (matc...	Assignment
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AANGK#PGFK	MONO	1003.53	1004.72	1	18	0	5	0.00,0.00	false	10.05	3	A81	--	0.19	unassigned
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629.8	4.4	true	
660.8	13.5	false	(y)VSGK#R
666.8	2.7	false	
891.1	7.4	false	
961.2	2.8	false	

5) After having manually selected all MS/MS spectra, export results to file "report.xls"