Supplementary Table 1. Number of peptides unmatched, mismatched and correctly matched at various significance levels by X!Tandem, OMSSA and Crux for precursor charge states +1, +2, and +3 when all ions in the query are available including neutral mass losses

Significance[a]	OMSSA			X!Tandem			Crux		
	+1 [e]	+2	+3	+1	+2	+3	+1	+2	+3
Unmatched[b]	1	1	1	69	67	63	0	0	0
Mismatch[c]	0	0	1	16	18	22	0	0	0
0	0	0	0	4	6	5	1	5	1
1	1	2	4	73	67	72	118	131	109
2	11	19	42	91	88	91	214	209	237
3	48	52	34	82	79	82	171	165	146
4	24	13	33	33	41	33	160	150	151
5	24	34	59	75	74	74	151	172	170
6	49	57	54	91	85	89	172	170	170
7	73	58	40	83	78	77	171	179	182
8	28	27	336	47	59	51	194	179	189
>=9	7591	7587	7246	7186	7188	7191	6498	6490	6495
Prop >6[d]	98.6%	98.5%	97.8%	94.4%	94.4%	94.4%	89.6%	89.4%	89.6%

[a] Significance threshold (t) for matched to be considered significant at *E*- or *p*-value $< 1 \times 10^{-t}$.

[b] Unmatched: the program does not provide a match with the program setting.

[c] Mismatched: the program provided an incorrect match.

[d] Percentage of the matches that have *E*- or *p*-value $< 1 \times 10^{-6}$.

[e] Peptide charge state.

Supplementary Table 2. Number of peptides unmatched, mismatched and correctly matched at various significance levels by X!Tandem, OMSSA and Crux for precursor charge states +1, +2, and +3 when all ions in the query are available excluding neutral mass losses

Significance[a]	OMSSA			X!Tandem			Crux		
	+1 [e]	+2	+3	+1	+2	+3	+1	+2	+3
Unmatched[b]	0	0	0	115	116	118	0	0	0
Mismatched[c]	0	0	0	11	13	17	0	0	0
0	0	0	0	2	4	3	1	5	2
1	0	1	1	73	70	72	129	153	124
2	1	0	2	93	90	93	236	228	233
3	2	5	6	80	81	80	226	193	171
4	10	30	78	30	32	33	178	175	140
5	75	52	6	69	71	67	170	163	151
6	4	7	4	95	90	94	172	186	159
7	5	3	63	74	76	74	213	190	198
8	63	68	79	13	17	13	200	245	207
>=9	7690	7684	7611	7195	7190	7186	6325	6312	6465
Prop >6[d]	98.9%	98.9%	98.8%	94.0%	93.9%	93.8%	88.0%	88.3%	89.5%

[a] Significance threshold (t) for matched to be considered significant at *E*- or *p*-value $< 1 \times 10^{-t}$.

[b] Unmatched: the program does not provide a match with the program setting.

[c] Mismatched: the program provided an incorrect match.

[d] Percentage of the matches that have *E*- or *p*-value $< 1 \times 10^{-6}$.

[e] Peptide charge state.

Supplementary Table 3. Number of peptides unmatched, mismatched and correctly matched at various significance levels by X!Tandem, OMSSA and Crux for precursor charge states +1, +2, and +3 when only *b*-ions in the query are available including neutral mass losses

Significance[a]	OMSSA			X!Tandem			Crux		
	+1 [e]	+2	+3	+1	+2	+3	+1	+2	+3
Unmatched[b]	0	0	0	79	76	75	0	0	0
Mismatched [c]	0	0	0	6	9	10	0	0	0
0	160	179	234	237	237	240	0	4	2
1	84	94	100	109	110	107	93	99	105
2	87	82	89	149	147	145	229	249	214
3	100	100	112	122	123	125	215	175	175
4	94	92	83	96	97	97	154	161	157
5	90	89	84	105	105	104	167	173	153
6	64	57	119	137	137	134	188	195	166
7	94	111	83	104	101	104	167	160	195
8	93	75	95	89	93	90	168	170	220
>=9	6984	6971	6851	6617	6615	6619	6469	6464	6463
Prop >6[d]	92.2%	91.9%	91.1%	88.5%	88.5%	88.5%	89.1%	89.0%	89.7%

[a] Significance threshold (t) for matched to be considered significant at *E*- or *p*-value $< 1 \times 10^{-t}$.

[b] Unmatched: the program does not provide a match with the program setting.

[c] Mismatched: the program provided an incorrect match.

[d] Percentage of the matches that have *E*- or *p*-value $< 1 \times 10^{-6}$.

[e] Peptide charge state.

Supplementary Table 4. Number of peptides unmatched, mismatched and correctly matched at various significance levels by X!Tandem, OMSSA and Crux for precursor charge states +1, +2, and +3 when only *y*-ions in the query are available including neutral mass losses

Significance[a]	OMSSA			X!Tandem			Crux		
	+1 [e]	+2	+3	+1	+2	+3	+1	+2	+3
Unmatched[b]	0	0	0	72	69	66	0	0	0
Mismatched[c]	0	0	1	15	17	20	0	0	0
0	48	55	95	138	135	138	2	8	7
1	62	76	96	113	109	112	131	140	135
2	86	86	104	156	161	155	196	190	186
3	99	99	95	113	112	116	155	171	161
4	88	86	98	98	94	99	169	149	171
5	89	91	74	109	108	106	140	158	167
6	77	79	90	139	143	138	173	157	193
7	73	70	96	105	109	106	196	185	228
8	90	99	110	103	103	104	226	226	257
>=9	7138	7109	6991	6689	6690	6690	6462	6466	6345
Prop >6[b]	94.0%	93.7%	92.8%	89.6%	89.7%	89.7%	89.9%	89.6%	89.5%

[a] Significance threshold (t) for matched to be considered significant at *E*- or *p*-value $< 1 \times 10^{-t}$.

[b] Unmatched: the program does not provide a match with the program setting.

[c] Mismatched: the program provided an incorrect match.

[d] Percentage of the matches that have *E*- or *p*-value $< 1 \times 10^{-6}$.

[e] Peptide charge state.

Supplementary Table 5. Number of peptides unmatched, mismatched and correctly matched at various significance levels by X!Tandem, OMSSA and Crux for precursor charge states +1, +2, and +3 when only random 50% of all ions in the query are available including neutral mass losses

Significance[a]	OMSSA			X!Tandem			Crux		
	+1 [e]	+2	+3	+1	+2	+3	+1	+2	+3
Unmatched[b]	1	0	0	73	75	66	0	0	0
Mismatched[c]	0	0	0	13	11	19	0	0	0
0	71	88	136	316	296	313	9	10	11
1	72	77	86	170	166	159	151	169	167
2	85	69	98	133	147	145	243	241	208
3	87	91	101	166	181	172	188	188	187
4	106	99	96	104	107	109	180	151	148
5	88	92	97	157	157	160	188	196	179
6	81	95	106	109	96	95	190	198	213
7	86	83	89	122	144	139	209	208	244
8	74	92	92	127	117	111	244	230	235
>=9	7099	7064	6949	6360	6353	6362	6248	6259	6258
Prop >6[d]	93.5%	93.4%	92.2%	85.6%	85.5%	85.4%	87.8%	87.8%	88.5%

[a] Significance threshold (t) for matched to be considered significant at *E*- or *p*-value $< 1 \times 10^{-t}$.

[b] Unmatched: the program does not provide a match with the program setting.

[c] Mismatched: the program provided an incorrect match.

[d] Percentage of the matches that have *E*- or *p*-value $< 1 \times 10^{-6}$.

[e] Peptide charge state.

Supplementary Table 6. Number of peptides unmatched, mismatched and correctly matched at various significance levels by X!Tandem, OMSSA and Crux for precursor charge states +1, +2, and +3 when only random 25% of all ions in the query are available including neutral mass losses

Significance[a]	OMSSA			X!Tandem			Crux		
	+1 [e]	+2	+3	+1	+2	+3	+1	+2	+3
Unmatched[b]	73	60	63	295	312	311	0	0	0
Mismatched[c]	4	0	1	10	10	13	0	0	0
0	492	512	506	1133	1113	1115	60	71	80
1	182	177	170	284	292	280	322	322	298
2	184	194	189	228	228	250	302	306	244
3	178	188	169	229	227	225	218	226	183
4	160	143	171	140	128	131	183	182	236
5	167	156	139	136	153	139	209	211	274
6	133	147	154	120	110	130	273	236	285
7	113	124	124	146	130	132	326	318	312
8	106	100	125	131	126	112	365	378	434
>=9	6058	6049	6039	4998	5021	5012	5592	5600	5504
Prop >6[d]	81.7%	81.8%	82.1%	68.7%	68.6%	68.6%	83.5%	83.2%	83.2%

[a] Significance threshold (t) for matched to be considered significant at *E*- or *p*-value $< 1 \times 10^{-t}$.

[b] Unmatched: the program does not provide a match with the program setting.

[c] Mismatched: the program provided an incorrect match.

[d] Percentage of the matches that have *E*- or *p*-value $< 1 \times 10^{-6}$.

[e] Peptide charge state.

Supplementary Table 7. Performance of OMSSA and X!Tandem in the identification of peptides with precursor charge states +1, +2, and +3 by match significance levels when the *b*-ion series is scored

Significance[a]	OMSSA			X!Tandem		
	+1[e]	+2	+3	+1	+2	+3
Unmatched[b]	415	396	373	75	75	71
Mismatched[c]	11	30	54	10	10	14
0	122	141	171	248	249	249
1	63	64	89	113	113	115
2	76	65	80	187	195	190
3	76	89	106	270	292	298
4	103	95	88	746	851	854
5	62	70	118	1902	1800	1788
6	102	118	110	1536	1471	1471
7	108	105	99	842	868	878
8	116	95	114	690	699	691
>=9	6596	6582	6448	1231	1227	1231
Prop >6[d]	88.2%	87.9%	86.3%	54.8%	54.3%	54.4%

[a] Significance threshold (t) for matched to be considered significant at *E*- or *p*-value $< 1 \times 10^{-t}$.

[b] Unmatched: the program does not provide a match with the program setting.

[c] Mismatched: the program provided an incorrect match.

[d] Percentage of the matches that have *E*- or *p*-value $< 1 \times 10^{-6}$.

[e] Peptide charge state.

Supplementary Table 8. Performance of OMSSA and X!Tandem in the identification of peptides with precursor charge states +1, +2, and +3 by match significance levels when the *y*-ion series is scored

Significance[a]	OMSSA			X!Tandem		
	+1[e]	+2	+3	+1	+2	+3
Unmatched[b]	365	361	355	74	70	70
Mismatched[c]	11	15	34	11	15	15
0	47	60	79	151	145	152
1	50	51	69	108	108	110
2	69	67	77	179	186	183
3	66	73	92	214	234	241
4	87	86	103	591	688	693
5	81	89	93	1785	1857	1853
6	90	84	113	1948	1794	1786
7	80	95	118	861	841	830
8	126	122	97	648	613	620
>=9	6778	6747	6620	1280	1299	1297
Prop >6[d]	90.1%	89.8%	88.5%	60.3%	57.9%	57.7%

[a] Significance threshold (t) for matched to be considered significant at *E*- or *p*-value $< 1 \times 10^{-t}$.

[b] Unmatched: the program does not provide a match with the program setting.

[c] Mismatched: the program provided an incorrect match.

[d] Percentage of the matches that have *E*- or *p*-value $< 1 \times 10^{-6}$.

[e] Peptide charge state.

Supplementary Table 9. Performance of OMSSA and X!Tandem in the identification of peptides with precursor charge states +1, +2, and +3, by ion series scored

Correctly matched[a]	Significance threshold[b]	*b*-ion series scored			*y*-ion series scored		
		+1[c]	+2	+3	+1	+2	+3
Both	Both	4003	3974	3980	4459	4288	4270
Both	OMSSA	2919	2926	2791	2615	2760	2678
Both	X!Tandem	0	0	3	0	0	1
Both	None	438	460	587	331	357	443
X!Tandem	X!Tandem	177	186	184	156	147	151
X!Tandem	None	228	219	220	204	213	222
OMSSA	None	64	64	64	69	69	69
None	None	21	21	21	16	16	16

[a] Both: OMSSA and X!Tandem both correctly identified the peptide; OMSSA: only OMSSA correctly identified the peptide; X!Tandem: only X!Tandem correctly identified the peptide; None: Neither OMSSA and X!Tandem correctly identified the peptide.

[b] Both: OMSSA and X!Tandem *E*-values were both $< 1 \times 10^{-6}$; OMSSA: only OMSSA *E*-value was $< 1 \times 10^{-6}$; X!Tandem: only X!Tandem *E*-value was $< 1 \times 10^{-6}$; None: Neither OMSSA and X!Tandem *E*-value was $< 1 \times 10^{-6}$.

[c] Peptide charge state.