Supplementary Figure

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In-Source Fragmentation and the Sources of Partially Tryptic Peptides in Shotgun Proteomics

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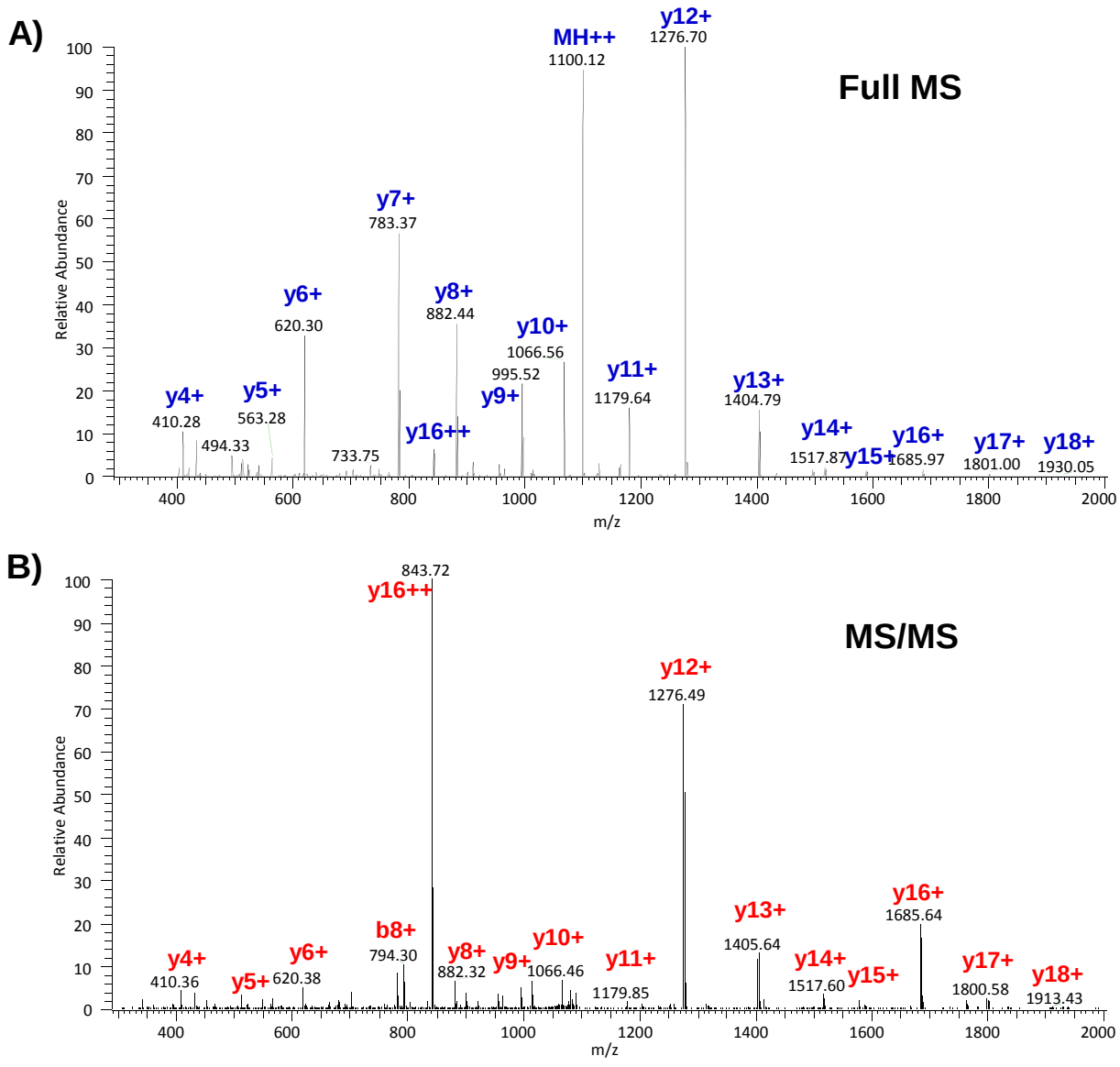
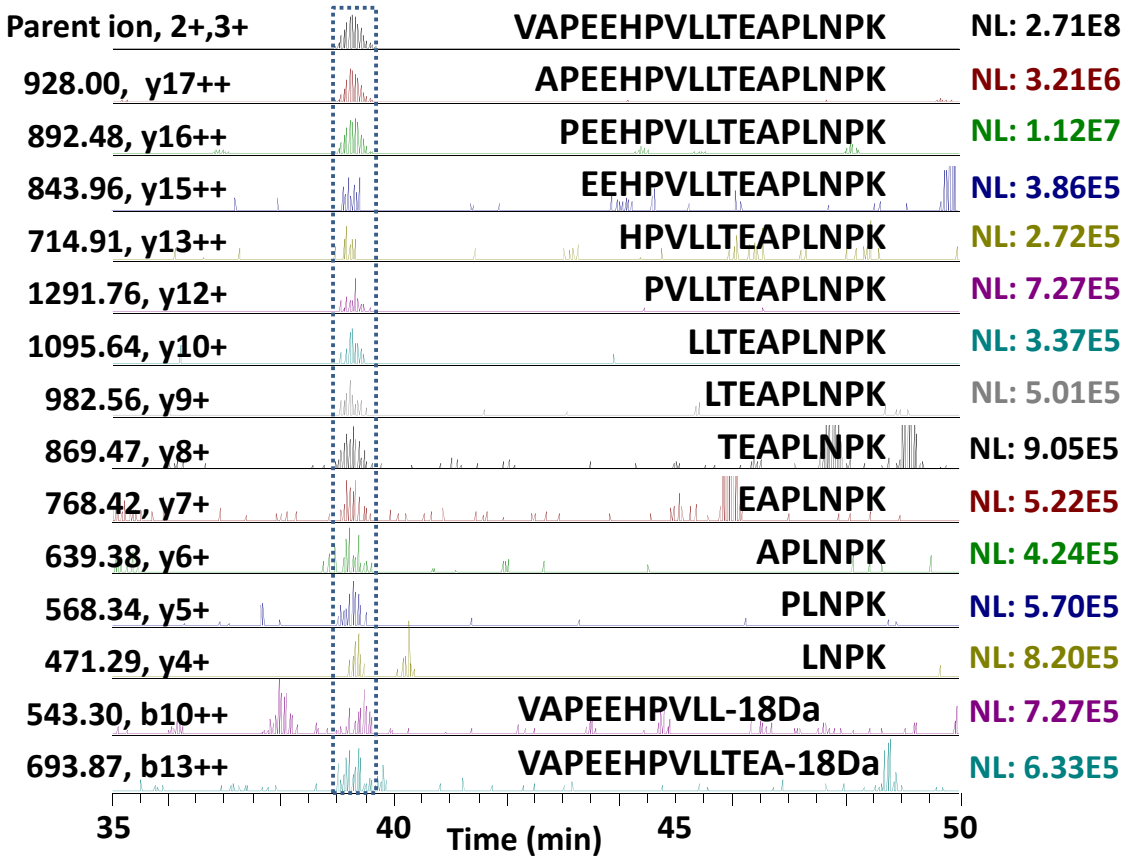
Supplementary Figure 1. Summed full MS scan of AVVQDPALKPLALVYGEATSR in Figure 1A showing its most detectable y-ions (A). MS/MS spectrum of the same peptide for comparison (B). Extracted ion chromatograms of VAPEEHPVLLTEAPLNPK from actin, cytoplasmic 1 in mouse brain lysate as another example showing a series of in-source fragments; only y17 and y16 ions were identified by the data base search (C).



C)

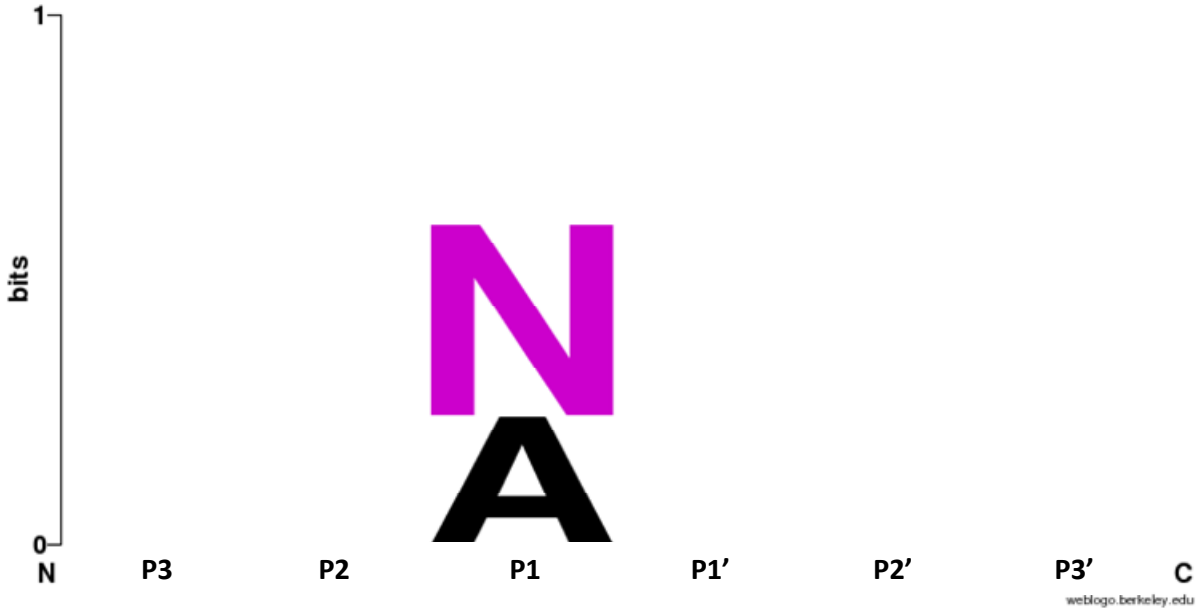

Parent ion, 2+,3+
VAPEEHPVLLTEAPLNPK
NL: 2.71E8
928.00, y17++
APEEHPVLLTEAPLNPK
NL: 3.21E6
892.48, y16++
PEEHPVLLTEAPLNPK
NL: 1.12E7
843.96, y15++
EEHPVLLTEAPLNPK
NL: 3.86E5
714.91, y13++
HPVLLTEAPLNPK
NL: 2.72E5
1291.76, y12+
PVLLTEAPLNPK
NL: 7.27E5
1095.64, y10+
LLTEAPLNPK
NL: 3.37E5
982.56, y9+
LTEAPLNPK
NL: 5.01E5
869.47, y8+
TEAPLNPK
NL: 9.05E5
768.42, y7+
EAPLNPK
NL: 5.22E5
639.38, y6+
APLNPK
NL: 4.24E5
568.34, y5+
PLNPK
NL: 5.70E5
471.29, y4+
LNPK
NL: 8.20E5
543.30, b10++
VAPEEHPVLL-18Da
NL: 7.27E5
693.87, b13++
VAPEEHPVLLTEA-18Da
NL: 6.33E5
35
40
Time (min)
45
50

Supplementary Figure 2. B-ion type semitryptic peptides of trypsin itself (A) and their sequence motif from the peptides with more than two spectral counts (B).

A)

Peptide	Reference	MH	MSGF_Min	Xcorr_Max	Spectral Count
K.SSYPGQITGN.M	TRYP_PIG	1023.474	8.503E-12	1.418	4
K.IITHPNFNGN.T	TRYP_PIG	1126.564	1.182E-11	2.215	2
K.IITHPNFNGNTLD.N	TRYP_PIG	1455.723	2.635E-12	3.321	1
R.LGEHNIDVLEGNEQFIN.A	TRYP_PIG	1940.935	1.637E-17	4.998	8
R.LGEHNIDVLEGNEQFINA.A	TRYP_PIG	2011.972	7.438E-14	4.826	3
R.LGEHNIDVLEGNEQFINAA.K	TRYP_PIG	2083.009	1.800E-13	5.281	7

B)



Supplementary Figure 3. Sequence motifs of [KR].P-cleaved semitryptic peptides (A) and [KR]P-containing, non-cleaved peptides (B).