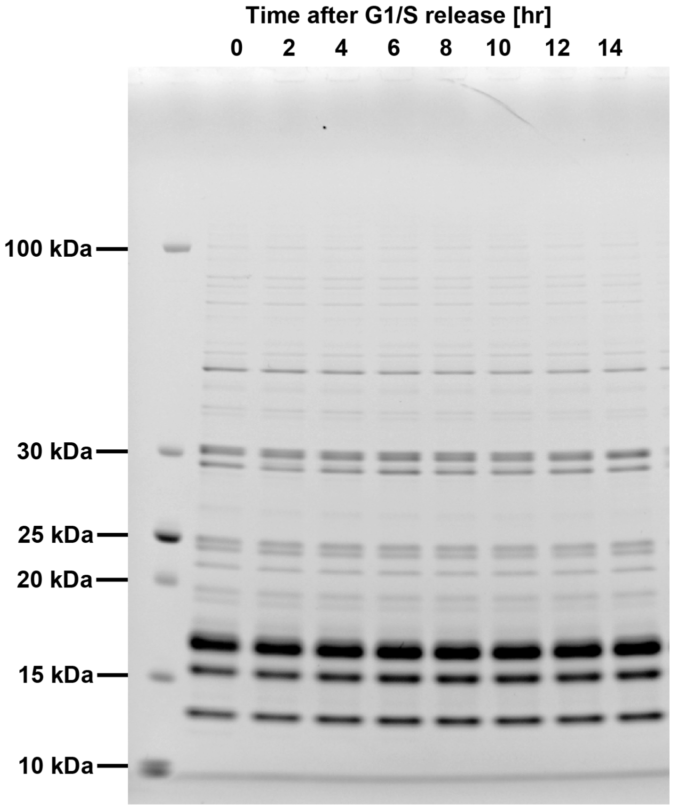
Mass Spectrom (Tokyo) 2015; 4(1): A0039; DOI: 10.5702/massspectrometry.A0039

Supporting Information



Histone extract 2.5 μg/lane, CBB stain.

Figure S1 Purity of histone extracts

Extracted histone samples were separated by gel electrophoresis, followed by Coomassie Brilliant Blue gel staining.

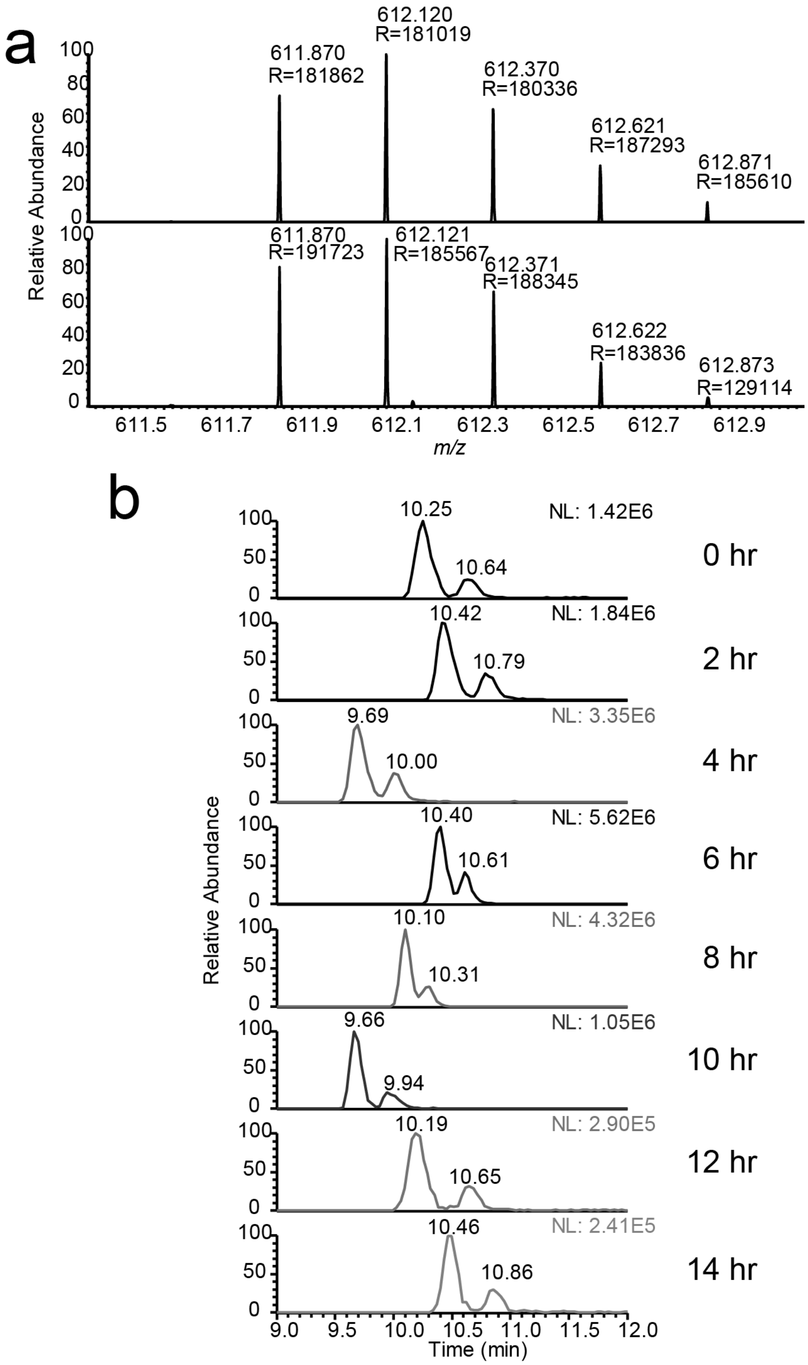


Figure S2 LC separation of H4 tail with Nac, K12 or K16 ac

(a) MS spectrum of m/z 611.870 (+4) ion with retention time of 10.25 min (upper panel) and of 10.64 min (lower panel) in data set 3 (0 hr). Expected *m/z* value is 611.870. Δppm is 0ppm. (b) Extracted ion chromatogram of m/z 611.870 for each time point sample in dataset 3, which corresponds to peak 9 & 10 in Fig. S3

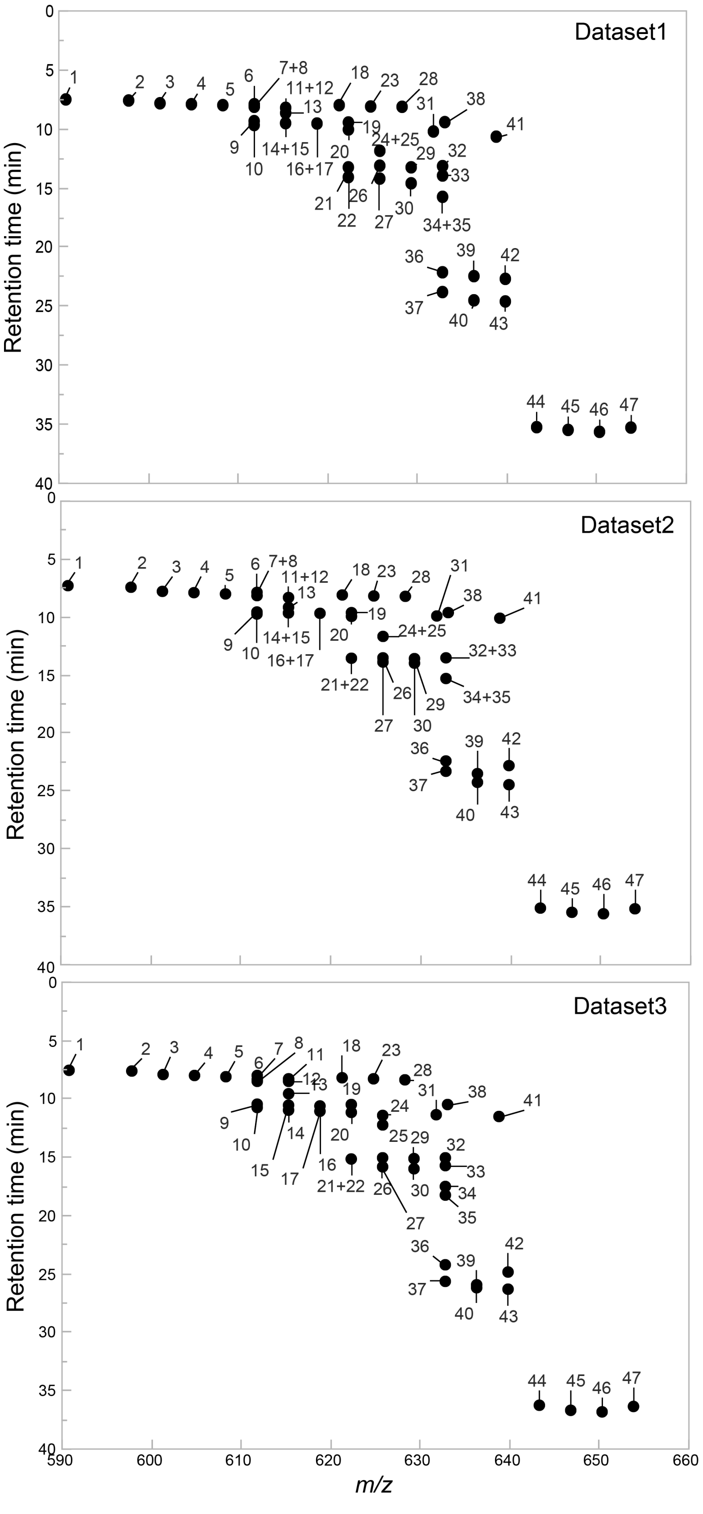


Figure S3 LC-MS maps for quadruply charged histone H4 tail peptide ions

Biological triplicates are separately shown.

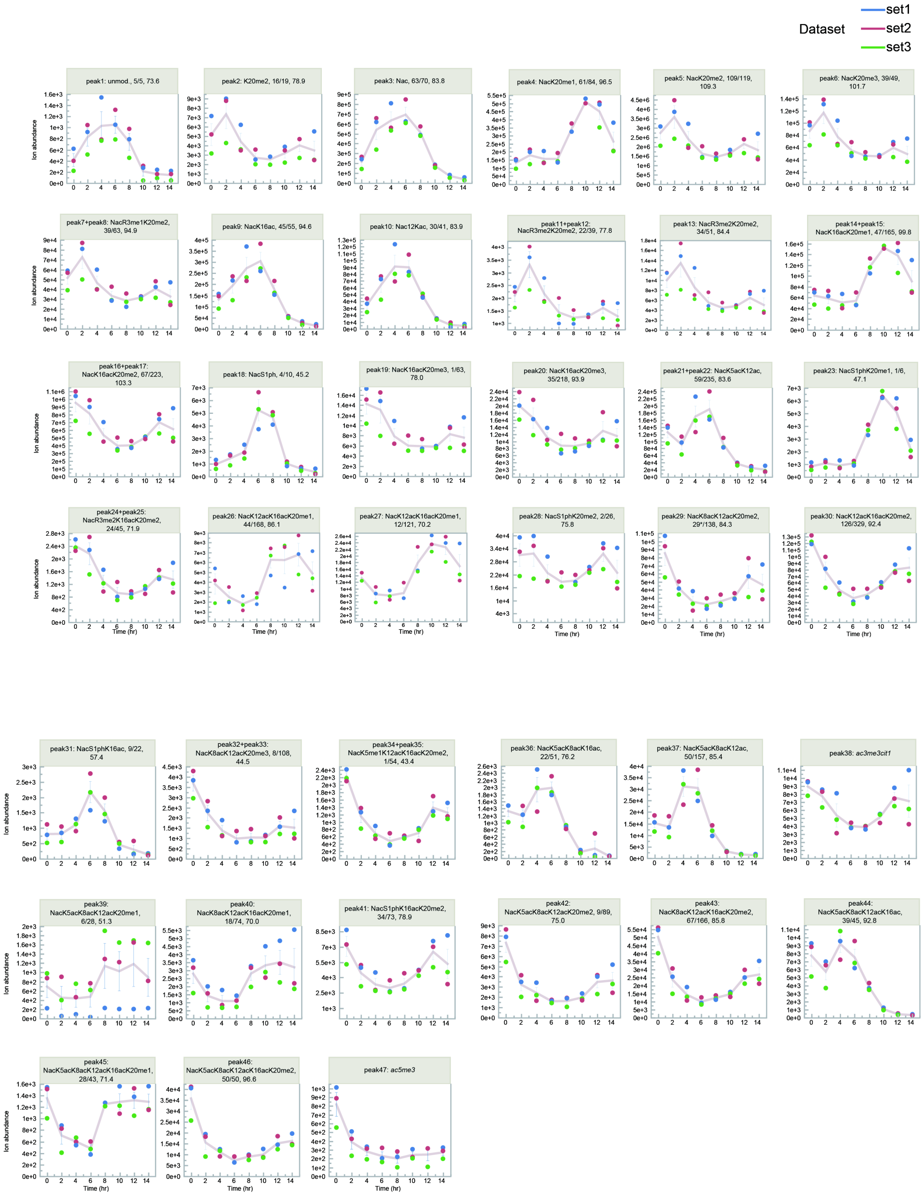


Figure S4 Complete quantitative data for each H4 tail peaks.

Temporal dynamics of each peak is shown. Peak No., PTM assignment, number of assigned MS/MS (number of assigned MS/MS spectra to the annotation / number of total MS/MS spectra acquired during the peak window, total of 3 datasets) and best MASCOT ion score are depicted on top of each graph. The peaks which were inseparable in some datasets such as peaks 11 and 12 were indicated as "peak X+Y" en bloc. Underspecified PTM assignment were written in *italics* to show total number of modifications. *: This includes top 4 assignment that was not listed in table S2.

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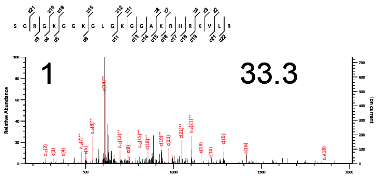
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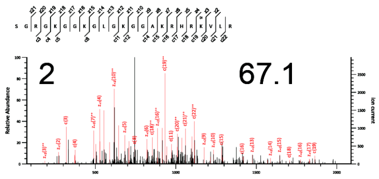
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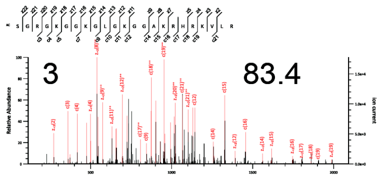
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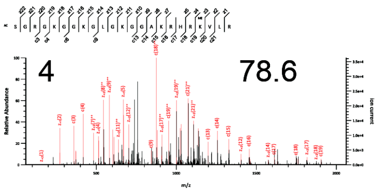
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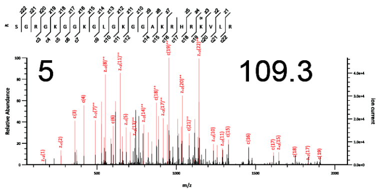
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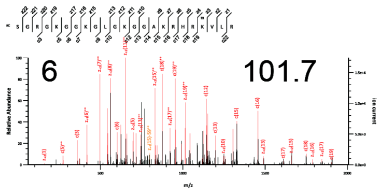
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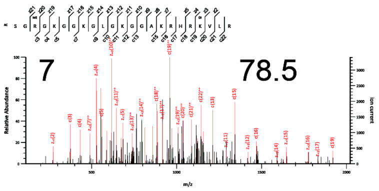
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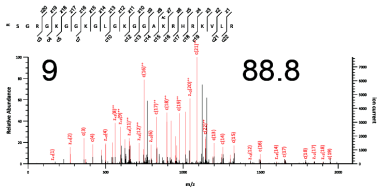
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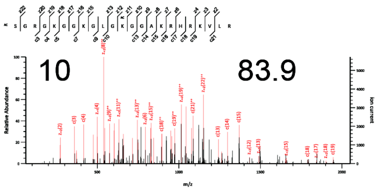
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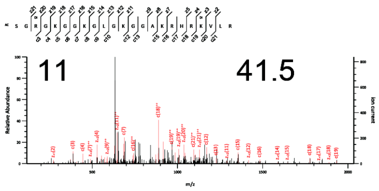
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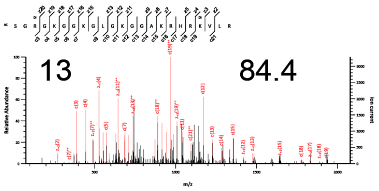
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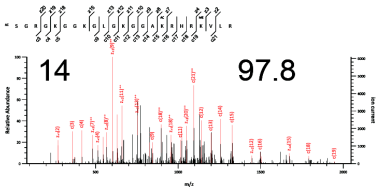
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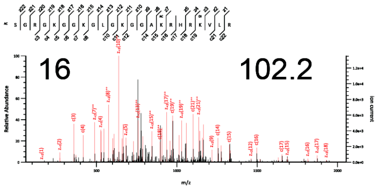
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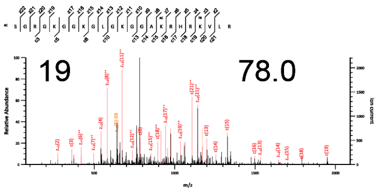
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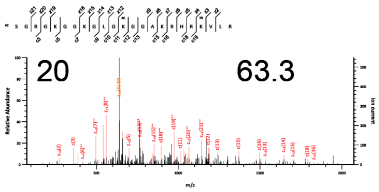
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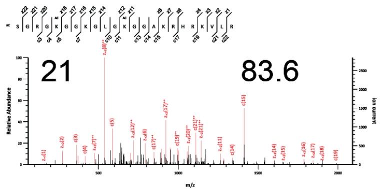
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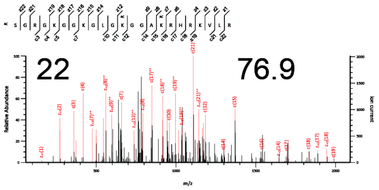
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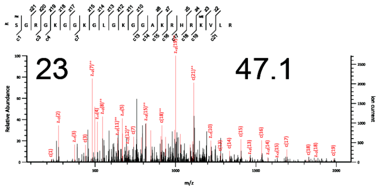
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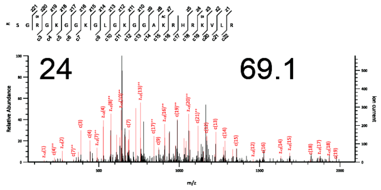
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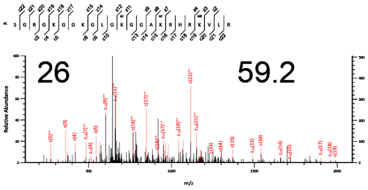
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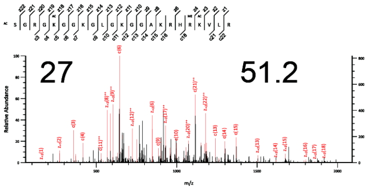
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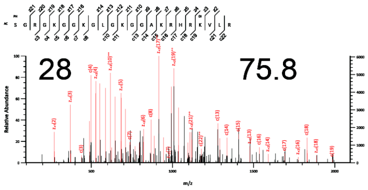
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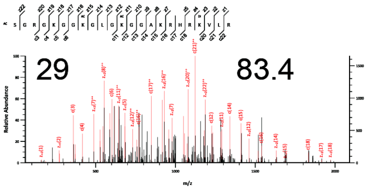
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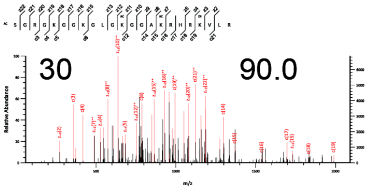
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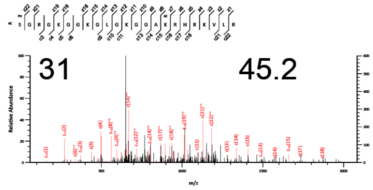
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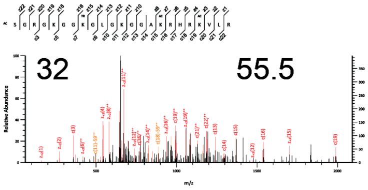
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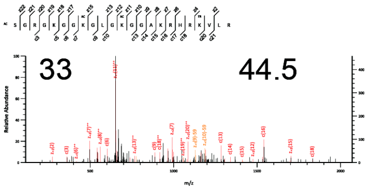
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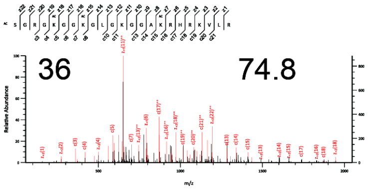
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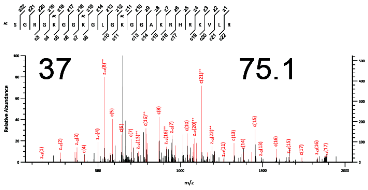
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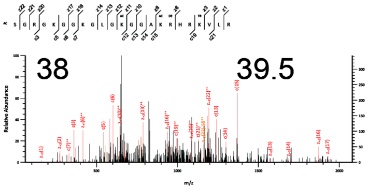
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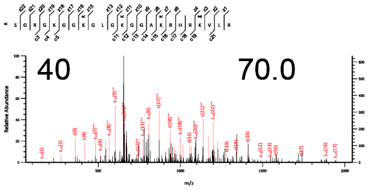
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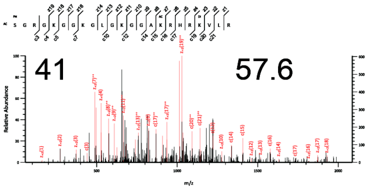
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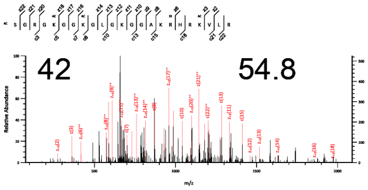
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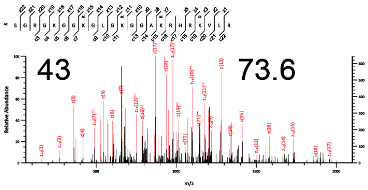
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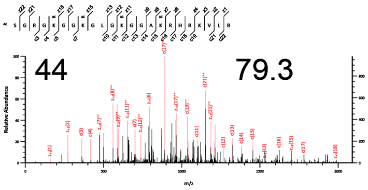
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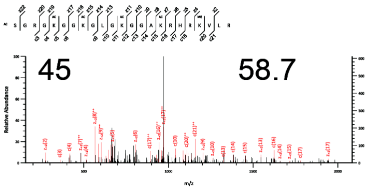
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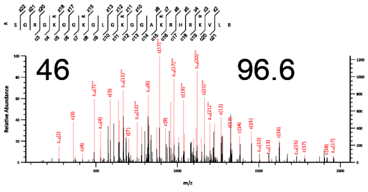
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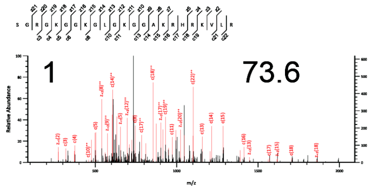
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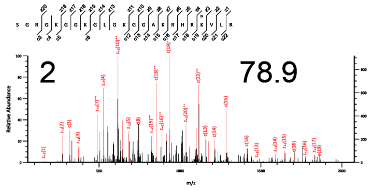
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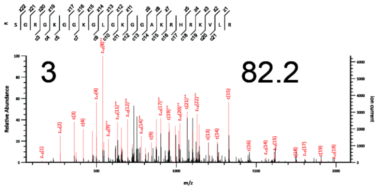
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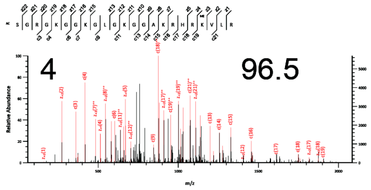
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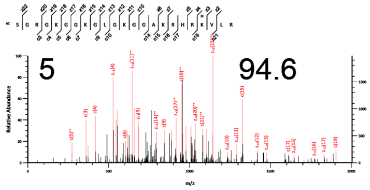
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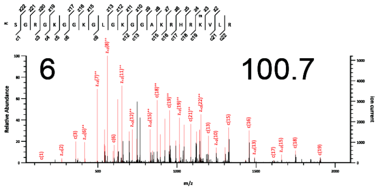
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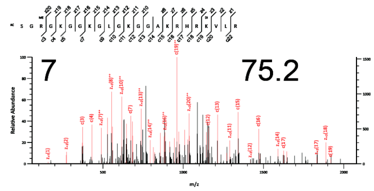
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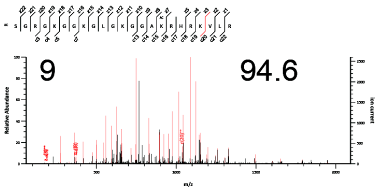
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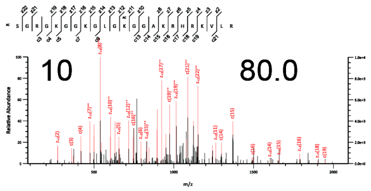
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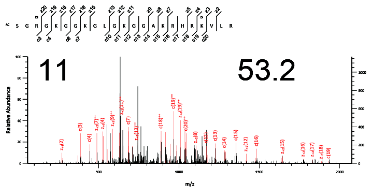
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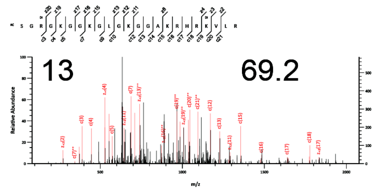
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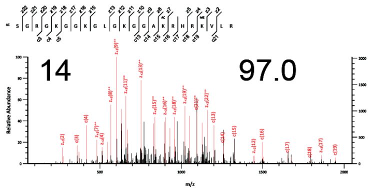
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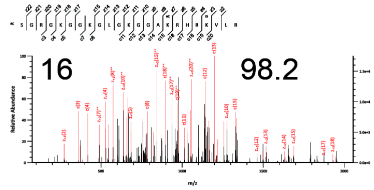
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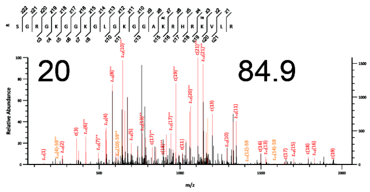
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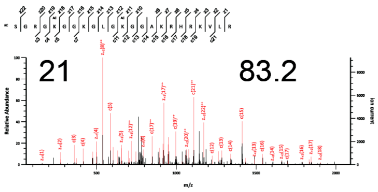
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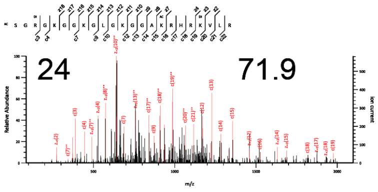
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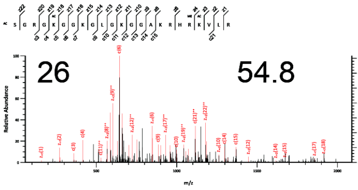

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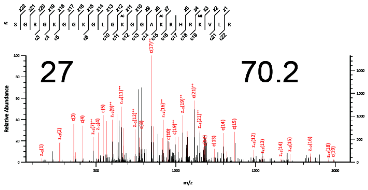

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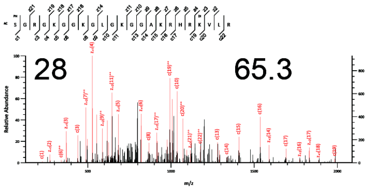

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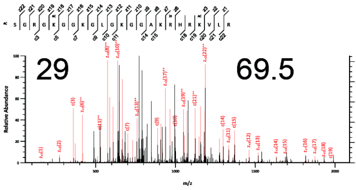

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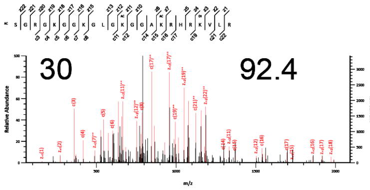

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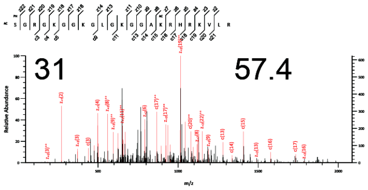

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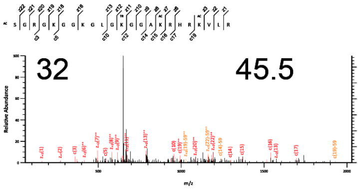

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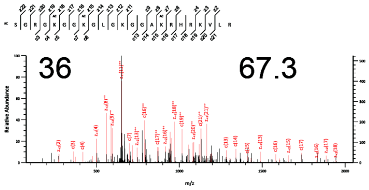

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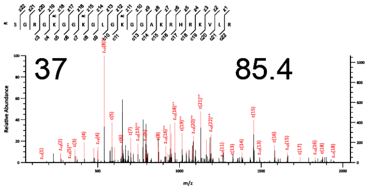

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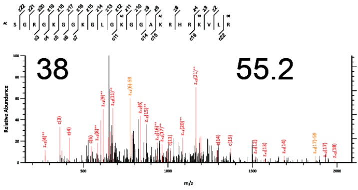

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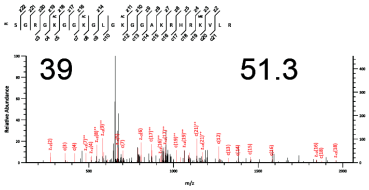

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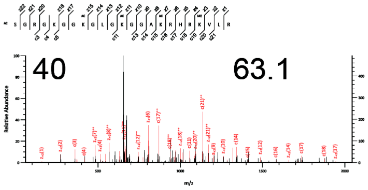

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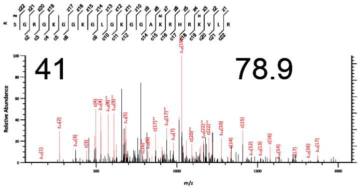

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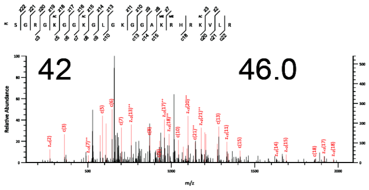

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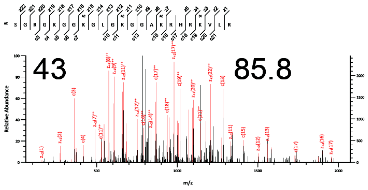

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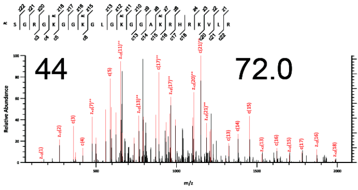

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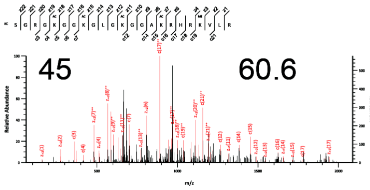

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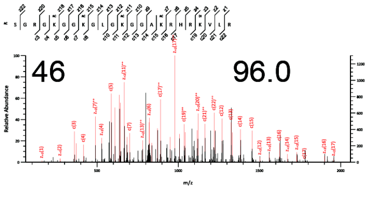

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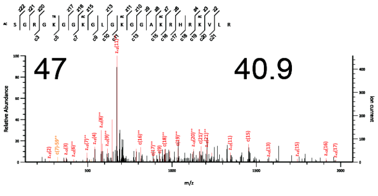

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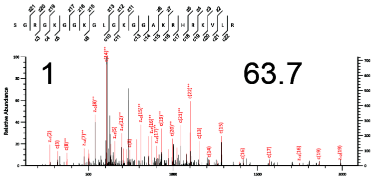
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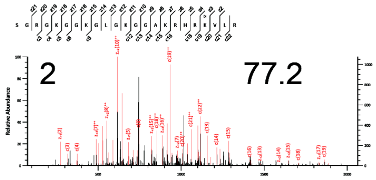
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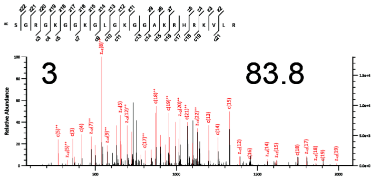
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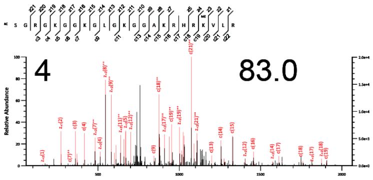
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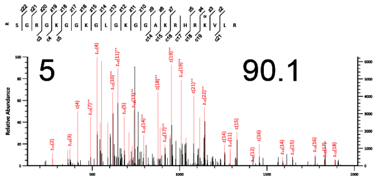
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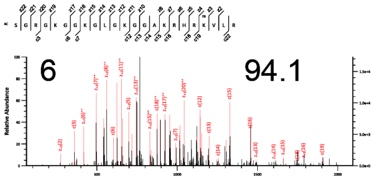
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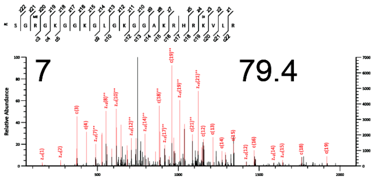
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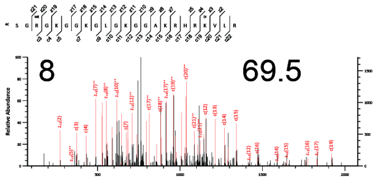
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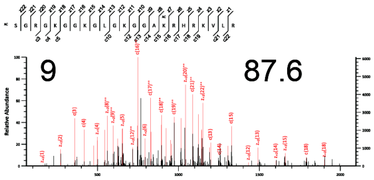
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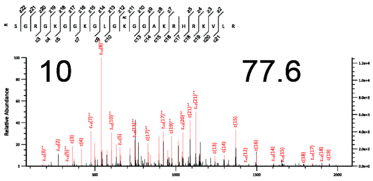
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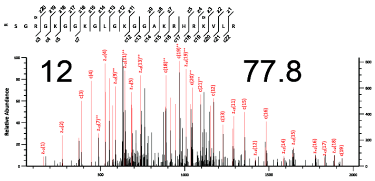
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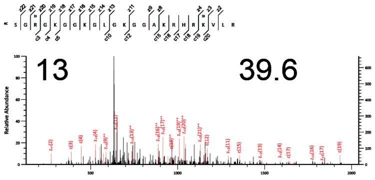
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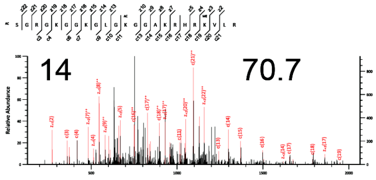
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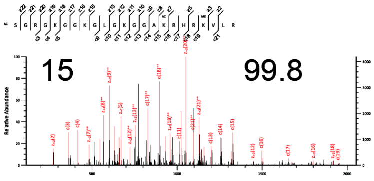
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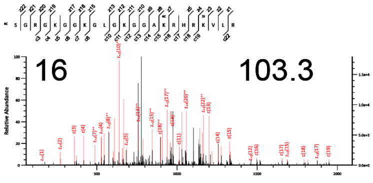
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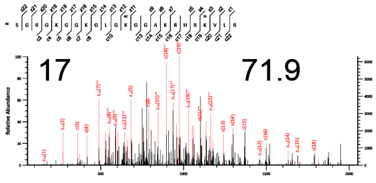
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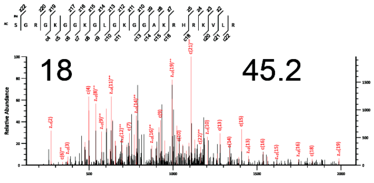
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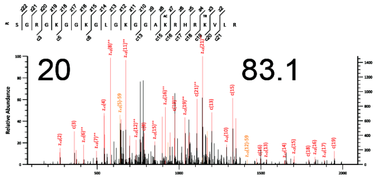
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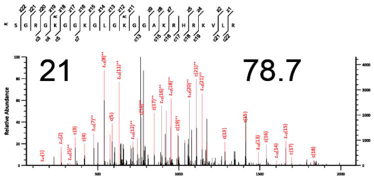
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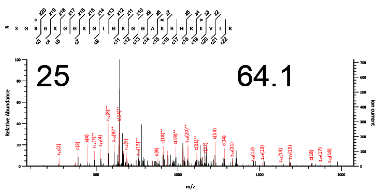
22 (-)

23 (-)

24 (-)

Set 3-2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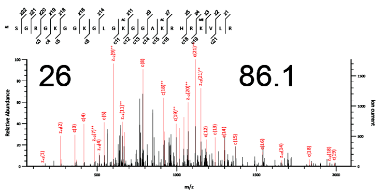
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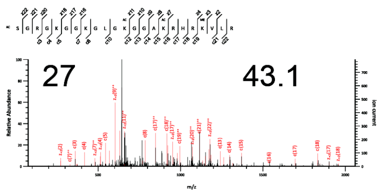
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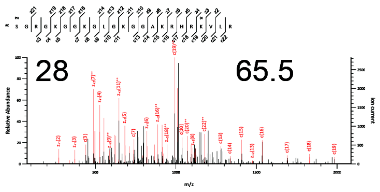
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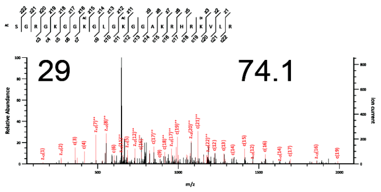
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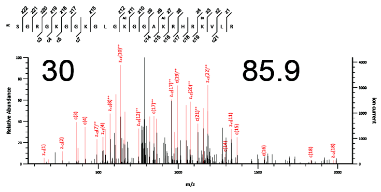
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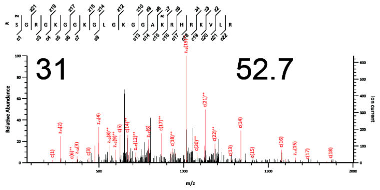
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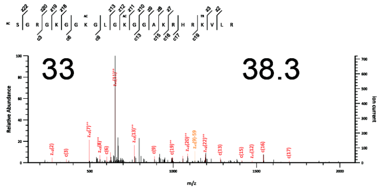
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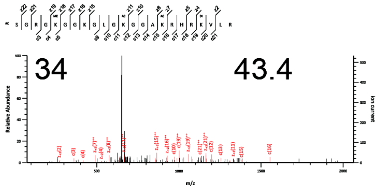
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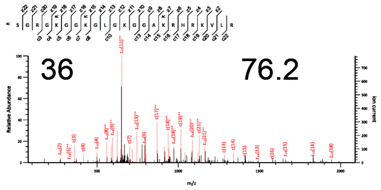
35 (-)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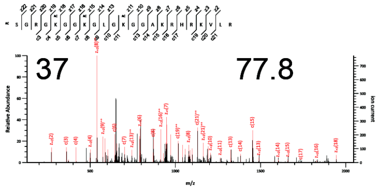
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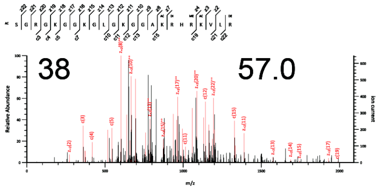
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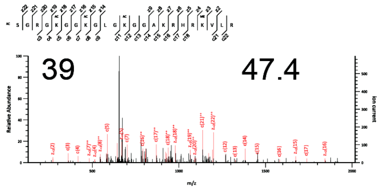
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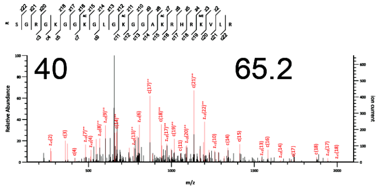
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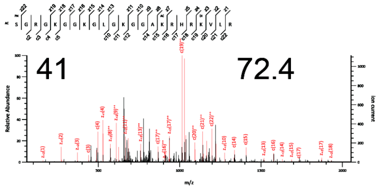
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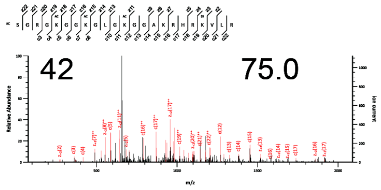
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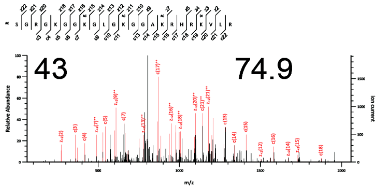
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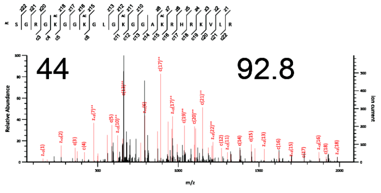
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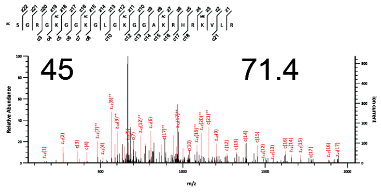
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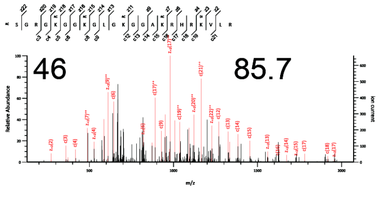

46 85.7

47 (-)

48 (-)

Figure S5 Best MS/MS spectra for each peaks.

MS/MS spectra whose MASCOT ion score are best among acquired MS/MS for each peak are shown together with the score.

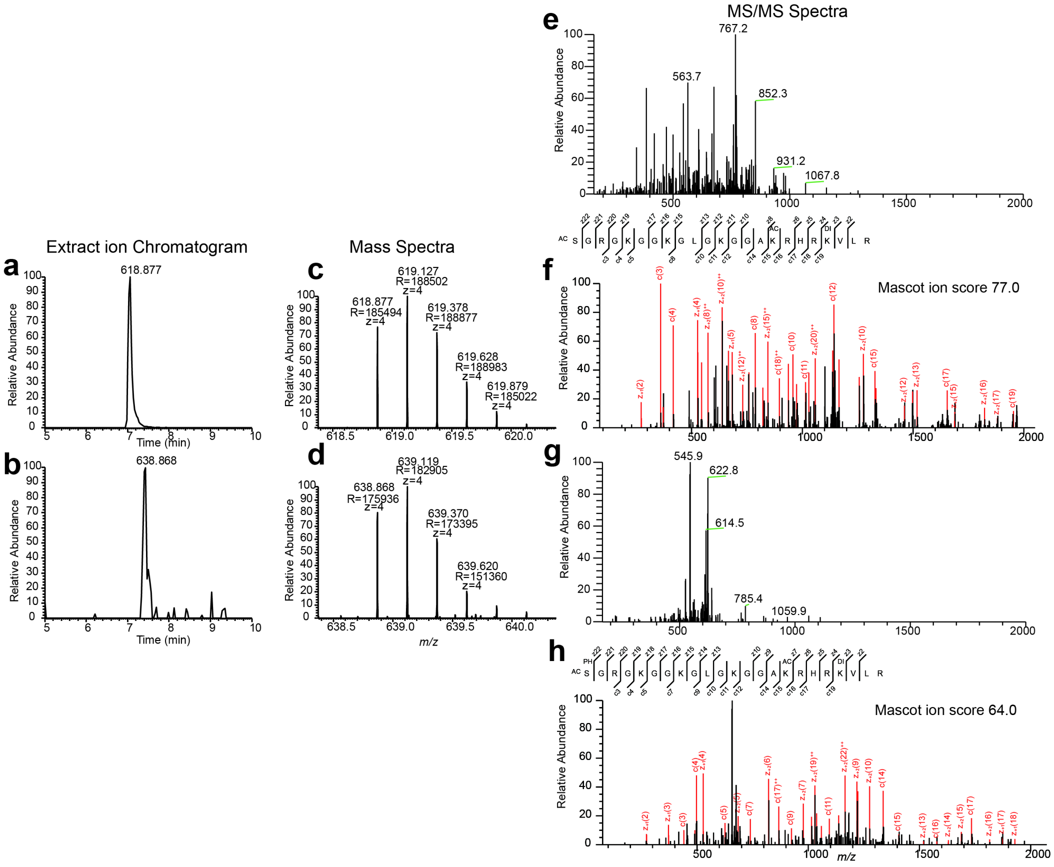


Figure S6 MS spectra of phosphorylated H4 tail peptides

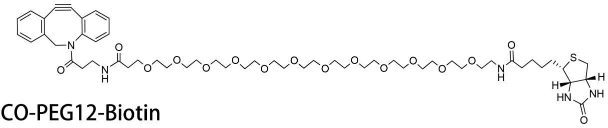
Histone-derived peptides were prepared from bovine histone. (a) Exact ion chromatogram for NacK16acK20me2. (b) Exact ion chromatogram for NacS1phK16acK20me2. (c) Mass spectra for NacK16acK20me2. Expected m/z value of is 618.878, Δppm is 1.6ppm. (d) Mass spectra for NacS1phK16acK20me2. Expected m/z value is 638.869, Δppm is 1.6ppm. (e) CID MS/MS spectra for NacK16acK20me2. (f) ETD MS/MS spectrum for NacK16acK20me2. (g) CID MS/MS spectra for NacS1phK16acK20me2. (h) ETD MS/MS spectrum for NacS1phK16acK20me2.

MASCOT peptide match result for the MS/MS spectra is shown for MS/MS spectrum above the threshold (MASCOT expect score < 0.05).

a

Probe 1: Dz-SGRGKGGKGLGKGGA-DLYDDDDK-G(F_{N_3})-amide
Probe 2: Dz-(pS)GRGKGGKGLGKGGA-DLYDDDDK-G(F_{N_3})-amide
Probe 3 (G7Bpa): Ac-SGRGKG(Bpa)KGLGKGGAK(F_{N_3})-amide
Probe 4 (G7Bpa): Ac-(pS)GRGKG(Bpa)KGLGKGGAK(F_{N_3})-amide
Probe 5 (G11Bpa): Ac-SGRGKGGKGL(Bpa)KGGAK(F_{N_3})-amide
Probe 6 (G11Bpa): Ac-(pS)GRGKGGKGL(Bpa)KGGAK(F_{N_3})-amide

b



DBCO-PEG12-Biotin

Figure S7 Design of peptide baits for pull-down experiments

(a) Full sequences of probes 1–6. Bpa: benzoylphenylalanine, F_{N_3}: azidophenylalanine. (b) Structure of dibenzylcyclooctyne–PEG12–Biotin (Jena Bioscience).

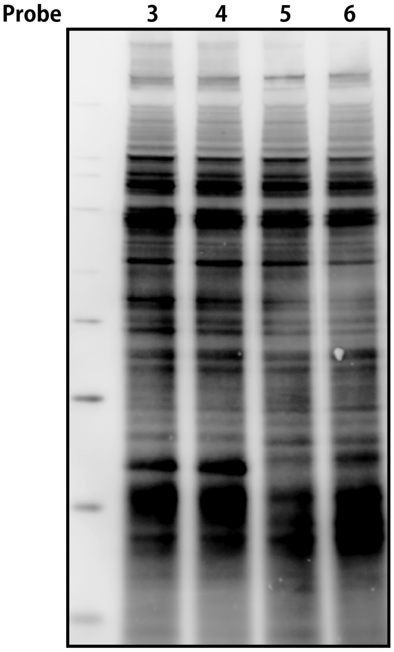


Figure S8 Landscape of pulled-down proteins by probes 3–6

Detection of crosslinked products by streptavidin–HRP.

Table S1 Complete lists of identified peptides

Lists generated by Progenesis QI software. MASCOT expect score < 0.05. Raw and normalized abundances of histone H4 and co-purified proteins are shown. Histone H4 C-terminal peptides DVVYALKRQGRTLYGFGG (+3 and +4) used for normalization are shown in bold blue font.

See Table S1.xlsx

Table S2 MS/MS spectrum assignment for each separated peak

Top 1 to 3 assignment and the number of MS/MS spectra assigned are listed for each peaks.

Set 1

PTM	m/z	Peak No	total MS/M	assigned MS/M	top hit	2nd hit	3d hit	unassign
–	590.864	1			unmod	–	–	
			1	1	1	–	–	0
me2	597.872	2			K20me2	R17me1K20me1		
			9	9	8	1	–	0
ac	601.368	3			Nac	–	–	
			23	22	22	–	–	1
ac1,me1	604.871	4			NacK20me1	–	–	
			27	21	21	–	–	6
ac1,me2	608.376	5			NacK20me2	NacR17me2	NacR19,K20me1	
			42	42	37	4	1	0
ac1,me3	611.877	6			NacK20me3	–	–	
			16	14	14	–	–	2
	611.878	7			NacR3me1K20me2	NacK20me3	NacR3me2K20me1 or NacK5me1K20me2	
		8	15	14	10	2	1	1
ac2	611.870	9			NacK16ac	NacK12ac	NacK8ac	
			17	17	15	1	1	0
	611.870	10			NacK12ac	NacK16ac	–	
			13	11	10	1	–	2
ac1me4	615.382	11			NacR3me2K20me2	–	–	
		12	10	3	3	–	–	7
	615.382	13			NacR3me2K20me2	–	–	
			20	16	16	–	–	4
ac2me1	615.374	14			NacK16acK20me1	NacK12acK20me1	–	
		15	53	30	16	14	–	23
ac2me2	618.878	16			NacK16acK20me2	NacK12acK20me2	NacK8acK20me2 or NacK16acR23me2	
		17	59	50	29	17	2	9
ac1p1	621.357	18			NacS1phos	–	–	
			3	0		–	–	3
ac2me3	622.380	19			NacK16acK20me3	–	–	
			18	1	1	–	–	17
	622.381	20			NacK12acK20me3	NacK16acK20me3	NacR3me1K16acK20me2	
			78	40	11	8	8	38
ac3	622.372	21			NacK5acK12ac	NacK5acK16ac	NacK5acK8ac	
			52	39	17	12	3	13
	622.372	22			Nack12acK16ac	NacK5acK12ac	NacK8acK16ac	
			34	17	14	2	1	17
ac1me1p1	624.862	23			NacS1phosK20me1	–	–	
			2	2	1	–	–	0
ac2me4	625.885	24			NacR3me2K16acK20me2	–	–	
		25	20	10	10	–	–	10
ac3me1	625.876	26			NacK12acK16acK20me1	NacK8K12acK20me1	NacK5K8K20me1	
			71	34	20	9	4	37
	625.876	27			NacK5acR19meK20ac	NacK12acK16acK20me1	–	
			26	3	2	1	–	23
ac1me2p1	628.366	28			NacS1phosK20me2	–	–	
			4	4	4	–	–	0
ac3me2	629.380	29			NacK8acK12acK20me2	NacK5acK8acK20me2	NacK12acK16acK20me2	
			48	38	11	9	6	10
	629.380	30			NacK12acK16acK20me2	NacK8acK12acK20me2	NacK12acK16acR19me2	
			88	57	46	7	2	31
ac2p1	631.861	31			NacS1phosK16ac	–	–	
			6	3	3	–	–	3
ac3me3	632.884	32			NacK8me3K16acK20ac	NacR3meK5me2K16acK20ac	–	
			8	2	1	1	–	6
	632.884	33			NacK8acK12acK20me3	NacK12me3K16acK20ac	NacK12acK16acK20me3 or NacK12,16acR17me2R19me1	
			28	7	3	2	1	21
	632.884	34			–	–	–	
		35	18	0	–	–	–	18
ac4	632.874	36			NacK5acK8acK16ac	–	–	
			13	10	10	–	–	3
	632.875	37			NacK5acK8acK12ac	NacK5acK12acK16ac	NacK8acK12acK16ac	
			60	45	17	11	11	15
ac3me3cit1	633.132	38			NacK12,16acR17citK20me3	NacK12me3K16,20acR19cit	NacK12,16acR17me1R19citK20me2	
			33	3	1	1	1	30
ac4me1	636.378	39			–	–	–	
			2	0	–	–	–	2
	636.379	40			NacK8acK12acK16acK20me1	NacK5acK8acK12acK20me1	NacK5,8,12acR17me1	
			33	13	8	4	1	20
ac2me2p1	638.869	41			NacS1phosK16acK20me2	–	–	
			27	10	10	–	–	17
ac4me2	639.882	42			NacK5acK8acK16me1R17me1K20ac	NacK5acK8acR17me2K20ac	NacK5acK8acK16me1R19me1K20ac	
			35	9	3	3	1	26
	639.883	43			NacK8acK12acK16acK20me2	NacK5acK8acK12acK20me2	NacK5acK8acK12acR17me2	
			59	45	24	18	1	14
ac5	643.377	44			NacK5acK8acK12acK16ac	–	–	
			16	13	13	–	–	3
ac5me1	646.881	45			NacK5acK8acK12acK16acK20me1	–	–	
			12	10	10	–	–	2
ac5me2	650.385	46			NacK5acK8acK12acK16acK20me2	–	–	
			15	15	15	–	–	0
ac5me3	653.889	47			–	–	–	
			4	0	–	–	–	4

Set 2

PTM	m/z	Peak N	total MS/M	assigned MS/M	top hit	2nd hit	3d hit	unassign
–	590.864	1			unmod	–	–	
			2	2	2	–	–	0
me2	597.872	2			K20me2	R19me2	–	
			4	4	3	1	–	0
ac	601.368	3			Nac	–	–	
			22	20	20	–	–	2
ac1,me1	604.871	4			NacK20me1	NacR19me1	–	
			29	21	20	1	–	8
ac1,me2	608.376	5			NacK20me2	NacR17me2 or NacR19me1K20me1 or NacR23me2	–	
			38	38	35	1	–	0
ac1,me3	611.877	6			NacK20me3	–	–	
			17	10	10	–	–	7
	611.878	7			NacR3me1K20me2	NacK20me3	NacR3me2K20me1	
		8	21	20	13	6	1	1
ac2	611.870	9			NacK16ac	NacK12ac	NacK20ac	
			18	18	15	2	1	0
	611.870	10			NacK12ac	NacK8ac	–	
			9	7	6	1	–	2
ac1me4	615.382	11			NacR3me2K20me2	–	–	
		12	10	6	6	–	–	4
	615.382	13			NacR3me2K20me2	–	–	
			19	15	15	–	–	4
ac2me1	615.374	14			NacK16acK20me1	NacK12acK20me1	NacK16acR19me1	
		15	53	25	15	9	1	28
ac2me2	618.878	16			NacK16acK20me2	NacK12acK20me2	NacK8acK20me2	
		17	88	48	24	17	3	40
ac1p1	621.357	18			–	–	–	
			3	0	0	–	–	3
ac2me3	622.380	19			–	–	–	
			23	0	–	–	–	23
	622.381	20			NacK16acK20me3	NacR3meK16acK20me2	NacK12acK20me3	
			66	39	12	12	5	27
ac3	622.372	21			NacK5acK12ac	NacK5acK16ac	NacK12acK16ac	
		22	66	48	17	13	12	18
ac1me1p1	624.862	23			NacS1phosK20me1	–	–	
			4	0	0	–	–	4
ac2me4	625.885	24			NacR3me2K16acK20me2	–	–	
		25	12	7	7	–	–	5
ac3me1	625.876	26			NacK5acR19me1K20ac	NacK8acK12acK20me1	NacK5acR17me1K20ac	
			24	10	5	2	2	14
	625.876	27			NacK12acK16acK20me1	NacK8acK12acK20me1	NacK5acK8acK20me1	
			62	19	10	6	2	43
ac1me2p1	628.366	28			NacS1phosK20me2	–	–	
			2	2	2	–	–	0
ac3me2	629.380	29			NacK5acR17me2K20ac	NacK12K16acK20me2	NacK5acK8acK20me2	
			39	26	9	5	4	13
	629.380	30			NacK12acK16acK20me2	NacK8acK12acK20me2	NacK5acK8acK20me2	
			126	48	37	7	3	78
ac2p1	631.861	31			NacS1phosK16ac	–	–	
			5	3	3	–	–	2
ac3me3	632.884	32			NacK12me3K16acK20ac	NacK8acK12acK20me3	–	
		33	28	9	3	2	–	19
	632.884	34			–	–	–	
		35	19	0	–	–	–	19
ac4	632.874	36			NacK5acK8acK16ac	–	–	
			19	5	5	–	–	14
	632.875	37			NacK5acK8acK12ac	NacK8acK12acK16ac	NacK5acK12acK16ac	
			54	47	19	10	10	7
ac3me3cit1	633.132	38			NacK12K16acK20me3R23cit	NacK16acR17me2R19me1K20acR23cit	–	
			31	6	2	2	–	25
ac4me1	636.378	39			NacK5acK8acK12acK20me1	NacK5acK8acK12acR17me1	–	
			14	5	4	1	–	9
	636.379	40			NacK8acK12acK16acK20me1	–	–	
			28	5	5	–	–	23
ac2me2p1	638.869	41			NacS1phosK16acK20me2	–	–	
			23	14	14	–	–	9
ac4me2	639.882	42			NacK5acK8acK16me1R17me1K20ac	NacK5acK8acK12acK20me2	NacK5acK8acR17me2K20ac	
			31	15	8	6	1	16
	639.883	43			NacK8acK12acK16acK20me2	NacK5acK8acK12acK20me2	–	
			67	43	27	13	–	24
ac5	643.377	44			NacK5acK8acK12acK16ac	–	–	
			13	12	12	–	–	1
ac5me1	646.881	45			NacK5acK8acK12acK16acK20me1	NacK5acK8acK12acK16acR19me1	–	
			18	10	9	1	–	8
ac5me2	650.385	46			NacK5acK8acK12acK16acK20me2	–	–	
			17	17	17	–	–	0
ac5me3	653.889	47			NacK5me3K8acK12acK16acK20ac	NacK5acK8me3K12acK16acK20ac	–	
			3	2	1	1	–	1

Set 3

PTM	m/z	Peak N	total MS/M	assigned MS/M	top hit	2nd hit	3d hit	unassign
–	590.864	1			unmod	–	–	
			2	2	2	–	–	0
me2	597.872	2			K20me2	R17me1R19me1	–	
			6	6	5	1	–	0
ac	601.368	3			Nac	–	–	
			25	21	21	–	–	4
ac1,me1	604.871	4			NacK20me1	NacR3me1	–	
			28	20	20	1	–	8
ac1,me2	608.376	5			NacK20me2	NacR17me2 or NacR19me1K20me1	–	
			39	39	37	1	–	0
ac1,me3	611.877	6			NacK20me3	–	–	
			16	15	15	–	–	1
	611.878	7			NacR3me1K20me2	–	–	
			10	10	10	–	–	0
	611.878	8			NacR3me1K20me2	–	–	
			17	6	6	–	–	11
ac2	611.870	9			NacK16ac	NacK20ac	–	
			20	16	15	1	–	4
	611.870	10			NacK12ac	–	–	
			19	14	14	–	–	5
ac1me4	615.382	11			–	–	–	
			0	0	–	–	–	0
	615.382	12			NacR3me2K20me2	–	–	
			19	13	13	–	–	6
	615.382	13			NacR3me2K20me2	NacR3me2R19me1K20me1	–	
			12	4	3	1	–	8
ac2me1	615.374	14			NacK12acK20me1	NacK8acK20me1	NacK12acR19me1 or NacK16acK20me1 or NacR17me1K20ac	
			34	16	9	4	1	18
	615.374	15			NacK16acK20me1	–	–	
			25	16	16	–	–	9
ac2me2	618.878	16			NacK16acK20me2	NacK8acK20me2	NacR17me1R19me1K20ac or NacK16acR18me1K20me1	
			34	18	14	2	1	16
	618.878	17			NacK12acK20me2	NacK8acK20me2	NacK16acK20me2	
			42	26	14	6	6	16
ac1p1	621.357	18			NacS1phos	–	–	
			4	3	3	–	–	1
ac2me3	622.380	19			–	–	–	
			22	0	–	–	–	22
	622.380	20			NacK16acK20me3	NacR3meK16acK20me2	NacK12acK20me3	
			74	40	15	11	7	34
ac3	622.372	21			NacK5acK12ac	NacK12acK16ac	NacK5acK16ac	
		22	83	61	25	16	9	22
ac1me1p1	624.862	23			–	–	–	
			0	0	–	–	–	0
ac2me4	625.885	24			–	–	–	
			0	0	–	–	–	0
	625.885	25			NacR3me2K16acK20me2	NacR3me2K16acR19me1K20me1	–	
			13	8	7	1	–	5
ac3me1	625.876	26			NacK12acK16acK20me1	NacK8acK12acK20me1	NacK5acK8acK20me1	
			73	38	24	9	4	35
	625.876	27			NacK12acK16acK20me1	NacK5acR17meK20ac	–	
			33	3	2	1	–	30
ac1me2p1	628.366	28			NacS1phosK20me2	–	–	
			2	2	2	–	–	0
ac3me2	629.380	29			NacK8acK12acK20me2	NacK5acR17me2K20ac	NacK5acK8acK20me2	
			51	43	14	9	8	8
	629.380	30			NacK12acK16acK20me2	NacK8acK12acK20me2	NacK12acK16acR19me1K20me1	
			115	49	43	5	1	66
ac2p1	631.861	31			NacS1phosK16ac	–	–	
			11	3	3	–	–	8
ac3me3	632.884	32			–	–	–	
			13	0	–	–	–	13
	632.884	33			NacK8acK12acK20me3	NacK5acK12me3K20ac	NacK8me3K16acK20ac	
			31	8	3	2	2	23
	632.884	34			NacK5me1K12acK16acK20me2	–	–	
			14	1	1	–	–	13
	632.884	35			–	–	–	
			3	0	–	–	–	3
ac4	632.874	36			NacK5acK8acK16ac	NacK5acK12acK16ac	NacK5acK8acK20ac	
			19	10	7	2	1	9
	632.875	37			NacK5acK8acK12ac	NacK8acK12acK16ac	NacK5acK12acK16ac	
			43	28	14	7	6	15
ac3me3cit1	633.132	38			NacK16acR17me2R19me1K20acR23cit	NacK12K16acK20me3R23cit	–	
			43	4	3	1	–	39
ac4me1	636.378	39			NacK5acK8acK12acK20me1	–	–	
			12	2	2	–	–	10
	636.379	40			NacK8acK12acK16acK20me1	NacK8acK12acK16acR19me1	–	
			13	6	5	1	–	7
ac2me2p1	638.869	41			NacS1phosK16acK20me2	NacS1phosK16acR17me1K20me1	–	
			23	11	10	1	–	12
ac4me2	639.882	42			NacK5acK8acK12acK20me2	NacK5acK8acK16me1R17me1K20ac	–	
			23	5	3	2	–	18
	639.883	43			NacK8acK12acK16acK20me2	NacK5acK8acK12acK20me2	NacK5acK8acR17me2K20ac	
			40	32	16	15	1	8
ac5	643.377	44			NacK5acK8acK12acK16ac	–	–	
			16	14	14	–	–	2
ac5me1	646.881	45			NacK5acK8acK12acK16acK20me1	–	–	
			13	9	9	–	–	4
ac5me2	650.385	46			NacK5acK8acK12acK16acK20me2	–	–	
			18	18	18	–	–	0
ac5me3	653.889	47			–	–	–	
			1	0	–	–	–	1

Table S3 Combinatorial acetylation

From the MASCOT results obtained for all datasets, combinatorial acetylation (K5/K8/K12/K16) was counted and best ion scores were indicated. This list was limited on common PTMs showed in Fig. 1b. This list includes chromatographically overlapped co-eluting species. Pep_score, pep_expect and pep_var_pos_conf were all derived from MASCOT search results, each of which stands for MASCOT ion score, MASCOT peptide expect and MASCOT delta score. MASCOT peptide expect are mirrors of the MASCOT ion scores which are adjusted with length and uniqueness of the peptide to show statistical relevances of the peptide match searching for each peptide. MASCOT delta scores are derived from the difference between rank 1 ion score and rank 2 ion score, which indicate probabilities of a precise PTM localization for a single modification. When multiple rank 1 identification for one MS/MS spectrum existed, its assignment was represented with the top one on the Mascot list.

Spectral counts

		S1ph	–				+			–	
		R3	me0				me0			me1	me2
		K20	me0	me1	me2	me3	me0	me1	me2	me2	me2
acetylation	0	none	11		36						
	1	N	615	203	1133	90	6	2	8	69	96
	2	N+K16	160	105	176	47	10		63	62	23
		N+K12	95	75	113	34				4	
		N+K8	4	12	22						
	3	N+K12+K16	93	83	201	10					
		N+K8+K12	13	31	74	7					
		N+K5+K8	6	10	32						
		N+K5+K12	138								
		N+K5+K16	73								
		N+K8+K16	20								
	4	N+K8+K12+K16	58	62	137						
		N+K5+K8+K12	114	23	98						
		N+K5+K8+K16	63								
		N+K5+K12+K16	54								
	5	N+K5+K8+K12+K16	85	29	77						

pep_score

		S1ph	−				+			−	
		R3	me0				me0			me1	me2
		K20	me0	me1	me2	me3	me0	me1	me2	me2	me2
acetylation	0	none	73.59		81.89						
	1	N	113.37	103.84	109.33	101.69	53.25	47.11	75.83	79.37	84.43
	2	N+K16	101.56	99.77	123.16	93.91	57.42		78.92	79.16	71.85
		N+K12	109.75	106.51	105.43	84.85				43.1	
		N+K8	63.77	69.09	71.88						
	3	N+K12+K16	91.17	91.14	92.39	61.31					
		N+K8+K12	56.63	63.73	83.38	50.55					
		N+K5+K8	58.76	66.56	71.6						
		N+K5+K12	99.2								
		N+K5+K16	75.09								
		N+K8+K16	79.03								
	4	N+K8+K12+K16	81.21	71	85.75						
		N+K5+K8+K12	85.44	53.99	96.27						
		N+K5+K8+K16	76.16								
		N+K5+K12+K16	85.58								
	5	N+K5+K8+K12+K16	92.78	71.37	96.59						

pep_expect

		S1ph	−				+			−	
		R3	me0				me0			me1	me2
		K20	me0	me1	me2	me3	me0	me1	me2	me2	me2
acetylation	0	none	4.5.E-07		7.3.E-07						
	1	N	8.3.E-10	6.8.E-09	1.7.E-09	9.0.E-09	1.7.E-03	6.7.E-03	8.4.E-06	1.5.E-06	4.1.E-07
	2	N+K16	1.6.E-08	2.2.E-08	9.6.E-11	7.2.E-08	6.9.E-04		4.5.E-06	2.3.E-06	1.0.E-05
		N+K12	2.3.E-09	4.8.E-09	5.4.E-09	5.9.E-07				8.5.E-03	
		N+K8	9.0.E-05	2.5.E-05	1.2.E-05						
	3	N+K12+K16	1.8.E-07	1.7.E-07	1.2.E-07	1.5.E-04					
		N+K8+K12	2.3.E-04	9.3.E-05	9.2.E-07	1.8.E-03					
		N+K5+K8	3.1.E-04	4.8.E-05	1.4.E-05						
		N+K5+K12	3.0.E-08								
		N+K5+K16	7.4.E-06								
		N+K8+K16	3.1.E-06								
	4	N+K8+K12+K16	2.1.E-06	2.1.E-05	6.7.E-07						
		N+K5+K8+K12	4.3.E-07	2.1.E-04	6.2.E-08						
		N+K5+K8+K16	6.7.E-06								
		N+K5+K12+K16	7.8.E-07								
	5	N+K5+K8+K12+K16	1.7.E-07	7.1.E-06	6.6.E-08						

pep_var_pos_conf

		S1ph	−				+			−	
		R3	me0				me0			me1	me2
		K20	me0	me1	me2	me3	me0	me1	me2	me2	me2
acetylation	0	none			0.9391						
	1	N	0.9998	0.9809	0.9575	0.9927	0.9946	0.859	0.8807	0.5927	0.838
	2	N+K16	0.9983	0.9346	0.918	0.6448	0.9385		0.918	0.1328	0.5549
		N+K12	0.9993	0.8859	0.8843	0.5895				0.031	
		N+K8	0.6548	0.6388	0.5887						
	3	N+K12+K16	0.9977	0.8755	0.9369	0.4555					
		N+K8+K12	0.6044	0.7657	0.8208	0.2398					
		N+K5+K8	0.7925	0.8761	0.6642						
		N+K5+K12	0.9994								
		N+K5+K16	0.9942								
		N+K8+K16	0.9770								
	4	N+K8+K12+K16	0.9916	0.795	0.8443						
		N+K5+K8+K12	0.9996	0.9341	0.9656						
		N+K5+K8+K16	0.9980								
		N+K5+K12+K16	0.9954								
	5	N+K5+K8+K12+K16	0.9998	0.9037	0.9658						

Table S4 Identified 14-3-3 derived peptides list

All the peptides assigned as 14-3-3 protein in the in-gel digestion experiment (Fig. 5) are shown.

1433E_HUMAN 170/255 amino acids (67% coverage)

Sequence	Peptide Probability	Mascot Ion score	Modifications	Observed	Actual Mass	Charge	Delta Da	Delta PPM	Retention Time (sec)	Start	Stop	Other Proteins
(-)mDDREDLVYQAK(L)	100%	38.6	Oxidation (+16), Acetyl (+42)	770.852	1539.690	2	0.002	1.5	643	1	12	
(-)mDDREDLVYQAK(L)	100%	36.4	Oxidation (+16), Acetyl (+42)	770.852	1539.690	2	0.002	1.4	641	1	12	
(K)LAEQAERYDEmVESmKK(V)	100%	48.6	Oxidation (+16), Oxidation (+16)	696.991	2087.952	3	0.001	0.5	529	13	29	
(K)LAEQAERYDEmVESmKK(V)	99%	26.3	Oxidation (+16), Oxidation (+16)	696.991	2087.952	3	0.001	0.5	531	13	29	
(R)YDEmVESmKK(V)	97%	26.5	Oxidation (+16), Oxidation (+16)	646.281	1290.548	2	0.001	0.5	387	20	29	
(R)YDEmVESmKK(V)	97%	26.1	Oxidation (+16), Oxidation (+16)	646.281	1290.548	2	0.001	0.6	386	20	29	
(K)KVAGmDVELTVEER(N)	100%	34.1	Oxidation (+16)	531.271	1590.792	3	0.000	−0.1	620	29	42	
(K)VAGmDVELTVEER(N)	100%	93.5	Oxidation (+16)	732.357	1462.699	2	0.001	0.9	681	30	42	
(K)VAGmDVELTVEER(N)	100%	89.7	Oxidation (+16)	732.357	1462.699	2	0.001	0.8	683	30	42	
(R)NLLSVAYK(N)	99%	54.4		454.266	906.518	2	0.000	0.1	770	43	50	1433Z_HUMAN,1433G_HUMAN,1433S_HUMAN,1433F_HUMAN
(R)NLLSVAYK(N)	99%	53.0		454.266	906.518	2	0.000	0.2	769	43	50	1433Z_HUMAN,1433G_HUMAN,1433S_HUMAN,1433F_HUMAN
(R)IISSIEQK(E)	99%	62.5		459.269	916.523	2	0.000	−0.2	541	62	69	
(R)IISSIEQK(E)	99%	40.8		459.269	916.523	2	0.000	−0.2	543	62	69	
(R)IISSIEQKEENKGGEDKLK(M)	100%	45.5		715.719	2144.135	3	0.002	0.8	492	62	80	
(R)IISSIEQKEENKGGEDKLK(M)	100%	36.9		715.719	2144.135	3	0.002	1.1	490	62	80	
(K)EENKGGEDKLK(M)	100%	50.8		623.818	1245.621	2	0.000	0.3	331	70	80	
(R)QmVETELK(L)	99%	56.0	Oxidation (+16)	497.250	992.485	2	0.000	−0.5	513	87	94	
(R)QmVETELK(L)	99%	55.8	Oxidation (+16)	497.250	992.485	2	0.000	−0.2	514	87	94	
(K)LIccDILDVLDK(H)	100%	57.2	Carbamidomethyl (+57), Carbamidomethyl (+57)	738.876	1475.738	2	0.001	0.7	1043	95	106	
(K)HLIPAANTGESK(V)	100%	69.0		619.331	1236.647	2	0.001	0.6	485	107	118	
(K)HLIPAANTGESK(V)	100%	58.9		619.331	1236.647	2	0.001	0.7	487	107	118	
(R)YLAEFATGNDR(K)	100%	64.4		628.799	1255.584	2	0.001	0.7	719	131	141	
(R)YLAEFATGNDR(K)	100%	61.9		628.799	1255.584	2	0.001	0.6	717	131	141	
(R)YLAEFATGNDRK(E)	100%	45.4		462.233	1383.678	3	0.000	−0.2	633	131	142	
(R)YLAEFATGNDRK(E)	100%	40.3		462.233	1383.678	3	0.000	−0.1	634	131	142	
(K)EAAENSLVAYK(A)	100%	61.9		597.804	1193.594	2	0.001	0.7	631	143	153	
(K)EAAENSLVAYK(A)	100%	59.7		597.804	1193.593	2	0.001	0.5	634	143	153	
(K)AASDIAmTELPPTHPIR(L)	100%	63.4	Oxidation (+16)	612.649	1834.926	3	0.001	0.6	647	154	170	
(K)AASDIAmTELPPTHPIR(L)	100%	62.8	Oxidation (+16)	612.649	1834.926	3	0.001	0.6	645	154	170	
(K)AASDIAmTELPPTHPIR(L)	100%	60.8	Oxidation (+16)	612.649	1834.926	3	0.001	0.4	715	154	170	
(K)AAFDDAIAELDTLSEESYK(D)	100%	114.1		1044.489	2086.963	2	0.004	1.9	1104	197	215	
(K)AAFDDAIAELDTLSEESYK(D)	100%	67.9		696.661	2086.960	3	0.002	0.9	1104	197	215	
(K)AAFDDAIAELDTLSEESYK(D)	100%	85.8		1044.488	2086.961	2	0.003	1.4	1102	197	215	
(K)AAFDDAIAELDTLSEESYK(D)	100%	63.6		696.661	2086.960	3	0.001	0.6	1102	197	215	
(K)DSTLImQLLR(D)	100%	70.5	Oxidation (+16)	603.332	1204.649	2	0.000	0.2	1023	216	225	1433Z_HUMAN,1433G_HUMAN,1433S_HUMAN,1433F_HUMAN
(K)DSTLImQLLR(D)	100%	56.1	Oxidation (+16)	603.332	1204.649	2	0.000	0.1	1028	216	225	1433Z_HUMAN,1433G_HUMAN,1433S_HUMAN,1433F_HUMAN

1433F_HUMAN 78/246 amino acids (32% coverage)

Sequence	Peptide Probability	Mascot Ion score	Modifications	Observed	Actual Mass	Charge	Delta Da	Delta PPM	Retention Time (sec)	Start	Stop	Other Proteins
(M)gDREQLLQR(A)	100%	32.9	Acetyl (+42)	578.807	1155.600	2	0.000	0.1	605	2	10	
(R)YDDmASAmK(A)	100%	48.3	Oxidation (+16), Oxidation (+16)	532.207	1062.400	2	0.000	−0.4	368	20	28	
(K)AVTELNEPLSNEDR(N)	100%	87.9		793.888	1585.761	2	0.003	1.7	662	29	42	
(K)AVTELNEPLSNEDR(N)	100%	81.7		793.888	1585.761	2	0.002	1.4	665	29	42	
(R)NLLSVAYK(N)	99%	54.5		454.266	906.518	2	0.000	0.0	768	43	50	1433Z_HUMAN,1433G_HUMAN,1433S_HUMAN,1433E_HUMAN
(R)NLLSVAYK(N)	99%	52.0		454.266	906.518	2	0.000	0.0	769	43	50	1433Z_HUMAN,1433G_HUMAN,1433S_HUMAN,1433E_HUMAN
(R)VISSIEQK(T)	99%	56.1		452.261	902.507	2	0.000	−0.2	505	62	69	1433G_HUMAN,1433S_HUMAN
(R)VISSIEQK(T)	99%	55.3		452.261	902.507	2	0.000	−0.2	503	62	69	1433G_HUMAN,1433S_HUMAN
(R)YLAEVASGEK(K)	100%	70.3		533.774	1065.534	2	0.000	−0.3	579	133	142	
(R)YLAEVASGEK(K)	100%	47.4		533.775	1065.534	2	0.000	0.1	581	133	142	
(K)EQmQPTHPIR(L)	95%	26.2	Oxidation (+16)	626.809	1251.603	2	0.000	0.1	390	163	172	
(K)DSTLImQLLR(D)	100%	70.7	Oxidation (+16)	603.332	1204.649	2	0.000	0.1	1038	218	227	1433Z_HUMAN,1433G_HUMAN,1433S_HUMAN,1433E_HUMAN
(K)DSTLImQLLR(D)	100%	66.3	Oxidation (+16)	603.332	1204.649	2	0.000	0.1	1026	218	227	1433Z_HUMAN,1433G_HUMAN,1433S_HUMAN,1433E_HUMAN
(K)DSTLImQLLR(D)	100%	60.9	Oxidation (+16)	603.332	1204.649	2	0.000	0.1	1024	218	227	1433Z_HUMAN,1433G_HUMAN,1433S_HUMAN,1433E_HUMAN
(K)DSTLImQLLR(D)	100%	56.1	Oxidation (+16)	603.332	1204.649	2	0.000	0.0	1037	218	227	1433Z_HUMAN,1433G_HUMAN,1433S_HUMAN,1433E_HUMAN

1433G_HUMAN 98/247 amino acids (40% coverage)

Sequence	Peptide Probability	Mascot Ion score	Modifications	Observed	Actual Mass	Charge	Delta Da	Delta PPM	Retention Time (sec)	Start	Stop	Other Proteins
(M)vDREQLVQK(A)	100%	43.8	Acetyl (+42)	578.820	1155.625	2	0.000	0.4	589	2	10	
(M)vDREQLVQK(A)	99%	30.7	Acetyl (+42)	578.820	1155.625	2	0.000	0.1	595	2	10	
(R)YDDmAAAmK(N)	100%	51.1	Oxidation (+16), Oxidation (+16)	524.209	1046.404	2	−0.001	−0.7	383	20	28	
(R)YDDmAAAmK(N)	100%	51.0	Oxidation (+16), Oxidation (+16)	524.209	1046.404	2	−0.001	−0.8	384	20	28	
(K)NVTELNEPLSNEER(N)	100%	93.2		822.399	1642.783	2	0.003	1.6	673	29	42	
(K)NVTELNEPLSNEER(N)	100%	92.1		822.398	1642.782	2	0.002	1.3	671	29	42	
(R)NLLSVAYK(N)	99%	54.5		454.266	906.518	2	0.000	0.0	768	43	50	1433Z_HUMAN,1433S_HUMAN,1433E_HUMAN,1433F_HUMAN
(R)NLLSVAYK(N)	99%	52.0		454.266	906.518	2	0.000	0.0	769	43	50	1433Z_HUMAN,1433S_HUMAN,1433E_HUMAN,1433F_HUMAN
(R)VISSIEQK(T)	99%	56.1		452.261	902.507	2	0.000	−0.2	505	62	69	1433S_HUMAN,1433F_HUMAN
(R)VISSIEQK(T)	99%	55.3		452.261	902.507	2	0.000	−0.2	503	62	69	1433S_HUMAN,1433F_HUMAN
(R)YLAEVATGEK(R)	100%	74.5		540.782	1079.550	2	0.000	−0.3	596	133	142	
(R)YLAEVATGEK(R)	100%	69.6		540.782	1079.550	2	0.000	−0.4	599	133	142	
(K)RATVVESSEK(A)	100%	38.6		553.296	1104.577	2	0.000	−0.3	365	143	152	
(K)RATVVESSEK(A)	97%	27.3		553.296	1104.577	2	0.000	−0.1	368	143	152	
(R)ATVVESSEK(A)	100%	65.0		475.245	948.476	2	0.000	−0.3	401	144	152	
(R)ATVVESSEK(A)	100%	61.2		475.245	948.476	2	0.000	−0.3	399	144	152	
(K)AYSEAHEISK(E)	100%	66.8		567.775	1133.535	2	0.000	0.0	426	153	162	
(K)AYSEAHEISK(E)	100%	59.9		567.775	1133.535	2	0.000	−0.1	429	153	162	
(K)EHmQPTHPIR(L)	100%	32.1	Oxidation (+16)	631.309	1260.604	2	0.000	0.3	351	163	172	
(K)DSTLImQLLR(D)	100%	70.7	Oxidation (+16)	603.332	1204.649	2	0.000	0.1	1038	218	227	1433Z_HUMAN,1433S_HUMAN,1433E_HUMAN,1433F_HUMAN
(K)DSTLImQLLR(D)	100%	66.3	Oxidation (+16)	603.332	1204.649	2	0.000	0.1	1026	218	227	1433Z_HUMAN,1433S_HUMAN,1433E_HUMAN,1433F_HUMAN
(K)DSTLImQLLR(D)	100%	60.9	Oxidation (+16)	603.332	1204.649	2	0.000	0.1	1024	218	227	1433Z_HUMAN,1433S_HUMAN,1433E_HUMAN,1433F_HUMAN
(K)DSTLImQLLR(D)	100%	56.1	Oxidation (+16)	603.332	1204.649	2	0.000	0.0	1037	218	227	1433Z_HUMAN,1433S_HUMAN,1433E_HUMAN,1433F_HUMAN

1433S_HUMAN 122/248 amino acids (49% coverage)

Sequence	Peptide Probability	Mascot Delta Ion Score	Modifications	Observed	Actual Mass	Charge	Delta Da	Inten sity	Retention Time (sec)	Start	Stop	Other Proteins
(K)LAEQAERYEDmAAFmK(G)	100%	43.8	Oxidation (+16), Oxidation (+16)	645.626	1933.857	3	0.001	0.7	622	12	27	
(R)YEDmAAFmK(G)	100%	54.1	Oxidation (+16), Oxidation (+16)	569.233	1136.451	2	−0.001	−1.0	547	19	27	
(K)GAVEKGEELScEER(N)	100%	48.3	Carbamidomethyl (+57)	531.579	1591.715	3	0.000	−0.2	503	28	41	
(K)GAVEKGEELScEER(N)	100%	57.2	Carbamidomethyl (+57)	796.866	1591.717	2	0.002	1.1	503	28	41	
(K)GAVEKGEELScEER(N)	100%	28.8	Carbamidomethyl (+57)	531.579	1591.715	3	0.000	−0.2	505	28	41	
(R)NLLSVAYK(N)	99%	54.4		454.266	906.518	2	0.000	0.1	770	42	49	1433Z_HUMAN,1433G_HUMAN,1433E_HUMAN,1433F_HUMAN
(R)NLLSVAYK(N)	99%	53.0		454.266	906.518	2	0.000	0.2	769	42	49	1433Z_HUMAN,1433G_HUMAN,1433E_HUMAN,1433F_HUMAN
(R)VLSSIEQK(S)	99%	61.9		452.261	902.507	2	0.000	−0.2	524	61	68	1433G_HUMAN,1433F_HUMAN
(R)VLSSIEQK(S)	99%	56.9		452.261	902.507	2	0.000	−0.1	522	61	68	1433G_HUMAN,1433F_HUMAN
(R)VLSSIEQK(S)	99%	48.4		452.261	902.507	2	0.000	−0.2	505	61	68	1433G_HUMAN,1433F_HUMAN
(R)VLSSIEQK(S)	99%	42.3		452.261	902.507	2	0.000	−0.3	507	61	68	1433G_HUMAN,1433F_HUMAN
(K)SNEEGSEEKGPEVR(E)	100%	61.7		516.237	1545.691	3	0.000	−0.2	403	69	82	
(K)SNEEGSEEKGPEVR(E)	100%	77.1		773.854	1545.693	2	0.002	1.6	406	69	82	
(K)SNEEGSEEKGPEVR(E)	100%	47.3		516.237	1545.690	3	0.000	−0.3	401	69	82	
(K)SNEEGSEEKGPEVR(E)	100%	58.6		773.854	1545.693	2	0.002	1.2	404	69	82	
(R)YLAEVATGDDK(K)	100%	87.2		591.288	1180.562	2	0.000	0.2	601	130	140	
(R)YLAEVATGDDK(K)	100%	79.1		591.288	1180.562	2	0.000	0.3	599	130	140	
(R)YLAEVATGDDKKR(I)	100%	59.5		489.260	1464.757	3	−0.001	−0.4	485	130	142	
(R)YLAEVATGDDKKR(I)	100%	49.2		489.260	1464.757	3	−0.001	−0.4	487	130	142	
(R)SAYQEAmDISK(K)	100%	56.9	Oxidation (+16)	629.785	1257.555	2	0.000	−0.1	595	149	159	
(K)EmPPTNPIR(L)	100%	34.9	Oxidation (+16)	535.768	1069.522	2	−0.001	−0.7	527	161	169	
(K)EmPPTNPIR(L)	99%	32.5	Oxidation (+16)	535.768	1069.522	2	−0.001	−0.7	529	161	169	
(K)TTFDEAmADLHTLSEDSYK(D)	100%	38.5	Oxidation (+16)	730.657	2188.949	3	0.002	0.8	852	196	214	
(K)DSTLImQLLR(D)	100%	70.5	Oxidation (+16)	603.332	1204.649	2	0.000	0.2	1023	215	224	1433Z_HUMAN,1433G_HUMAN,1433E_HUMAN,1433F_HUMAN
(K)DSTLImQLLR(D)	100%	56.1	Oxidation (+16)	603.332	1204.649	2	0.000	0.1	1028	215	224	1433Z_HUMAN,1433G_HUMAN,1433E_HUMAN,1433F_HUMAN

1433Z_HUMAN 102/245 amino acids (42% coverage)

Sequence	Peptide Probability	Mascot Ion score	Modifications	Observed	Actual Mass	Charge	Delta Da	Delta PPM	Retention Time (sec)	Start	Stop	Other Proteins
(-)mDKNELVQK(A)	100%	50.5	Oxidation (+16), Acetyl (+42)	581.793	1161.571	2	0.000	0.3	486	1	9	
(-)mDKNELVQK(A)	100%	44.0	Oxidation (+16), Acetyl (+42)	581.793	1161.571	2	0.000	0.3	489	1	9	
(R)YDDmAAcmK(S)	100%	50.1	Oxidation (+16), Carbamidomethyl (+57), Oxidation (+16)	568.707	1135.399	2	0.000	0.0	392	19	27	
(R)YDDmAAcmK(S)	100%	47.0	Oxidation (+16), Carbamidomethyl (+57), Oxidation (+16)	568.706	1135.398	2	0.000	−0.3	390	19	27	
(K)SVTEQGAELSNEER(N)	100%	107.2		774.861	1547.708	2	0.001	0.9	542	28	41	
(K)SVTEQGAELSNEER(N)	100%	103.3		774.861	1547.708	2	0.001	0.7	544	28	41	
(K)SVTEQGAELSNEER(N)	100%	65.6		516.909	1547.706	3	0.000	0.0	542	28	41	
(R)NLLSVAYK(N)	99%	54.5		454.266	906.518	2	0.000	0.0	768	42	49	1433G_HUMAN,1433S_HUMAN,1433E_HUMAN,1433F_HUMAN
(R)NLLSVAYK(N)	99%	52.0		454.266	906.518	2	0.000	0.0	769	42	49	1433G_HUMAN,1433S_HUMAN,1433E_HUMAN,1433F_HUMAN
(K)FLIPNASQAESK(V)	100%	66.2		652.846	1303.678	2	0.001	0.7	742	104	115	
(K)FLIPNASQAESK(V)	100%	55.7		652.846	1303.678	2	0.001	0.6	739	104	115	
(R)YLAEVAAGDDK(K)	100%	58.8		576.283	1150.551	2	0.000	0.1	601	128	138	
(R)YLAEVAAGDDKK(G)	100%	59.8		427.223	1278.646	3	0.000	0.2	525	128	139	
(R)YLAEVAAGDDKK(G)	100%	56.5		427.223	1278.646	3	0.001	0.4	527	128	139	
(R)YLAEVAAGDDKK(G)	100%	60.6		640.330	1278.646	2	0.000	0.3	525	128	139	
(R)YLAEVAAGDDKK(G)	100%	56.6		640.330	1278.646	2	0.000	0.2	527	128	139	
(K)GIVDQSQQAYQEAFEISK(K)	100%	129.2		1020.999	2039.983	2	0.003	1.6	886	140	157	
(K)GIVDQSQQAYQEAFEISK(K)	100%	112.6		1020.999	2039.983	2	0.003	1.5	884	140	157	
(K)GIVDQSQQAYQEAFEISK(K)	100%	78.1		681.001	2039.982	3	0.002	1.1	886	140	157	
(K)GIVDQSQQAYQEAFEISK(K)	100%	52.0		681.001	2039.982	3	0.002	0.8	889	140	157	
(K)KEmQPTHPIR(L)	99%	30.4	Oxidation (+16)	626.827	1251.640	2	0.000	0.2	353	158	167	
(K)EmQPTHPIR(L)	100%	53.3	Oxidation (+16)	562.779	1123.544	2	0.000	−0.3	387	159	167	
(K)EmQPTHPIR(L)	100%	52.5	Oxidation (+16)	562.779	1123.544	2	0.000	−0.3	389	159	167	
(K)DSTLImQLLR(D)	100%	70.7	Oxidation (+16)	603.332	1204.649	2	0.000	0.1	1038	213	222	1433G_HUMAN,1433S_HUMAN,1433E_HUMAN,1433F_HUMAN
(K)DSTLImQLLR(D)	100%	66.3	Oxidation (+16)	603.332	1204.649	2	0.000	0.1	1026	213	222	1433G_HUMAN,1433S_HUMAN,1433E_HUMAN,1433F_HUMAN
(K)DSTLImQLLR(D)	100%	60.9	Oxidation (+16)	603.332	1204.649	2	0.000	0.1	1024	213	222	1433G_HUMAN,1433S_HUMAN,1433E_HUMAN,1433F_HUMAN
(K)DSTLImQLLR(D)	100%	56.1	Oxidation (+16)	603.332	1204.649	2	0.000	0.0	1037	213	222	1433G_HUMAN,1433S_HUMAN,1433E_HUMAN,1433F_HUMAN