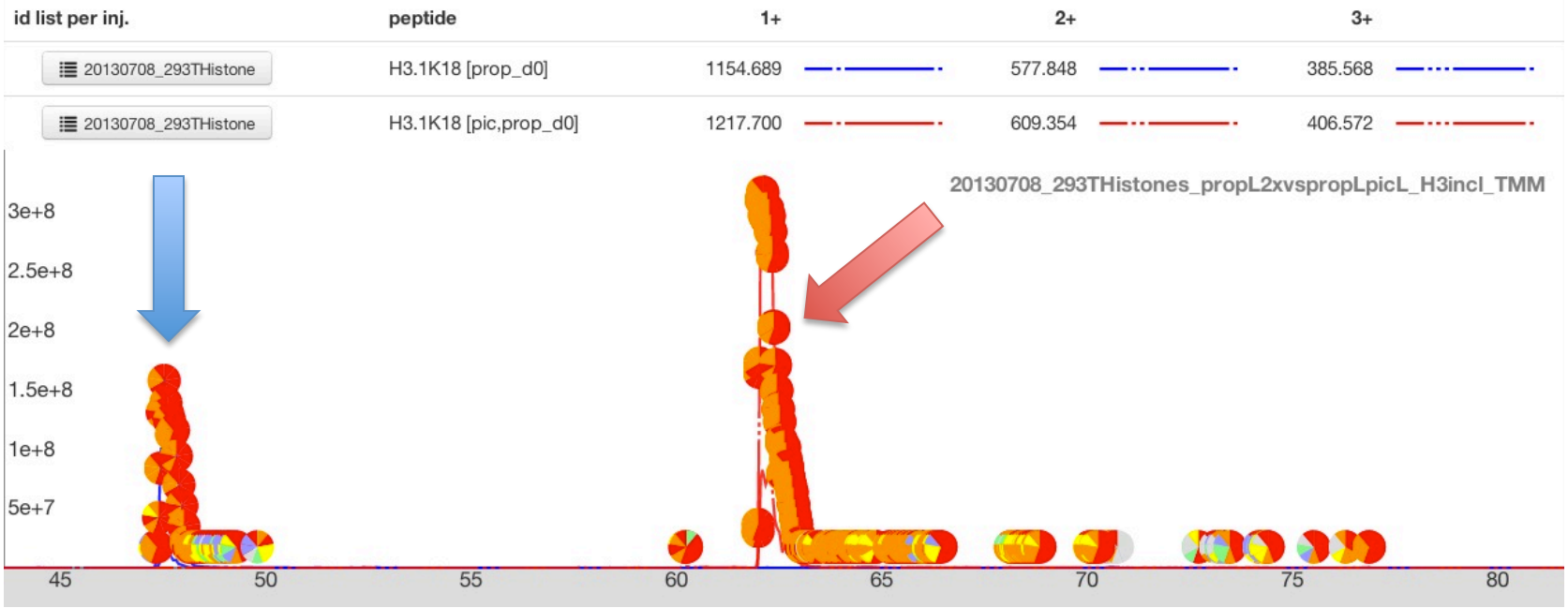
H3_K18-R26

KQLATKAAR

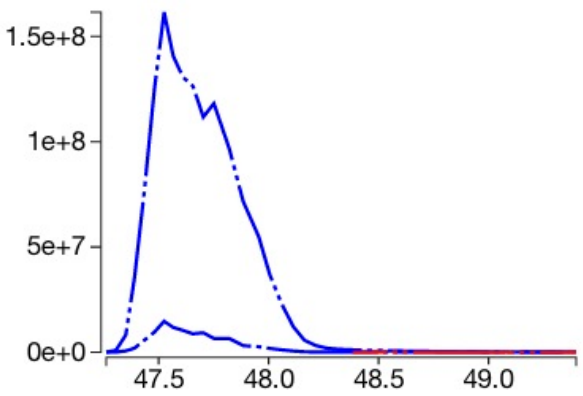
H3_K18-R26: KQLATKAAR



H3_K18-R26: KQLATKAAR

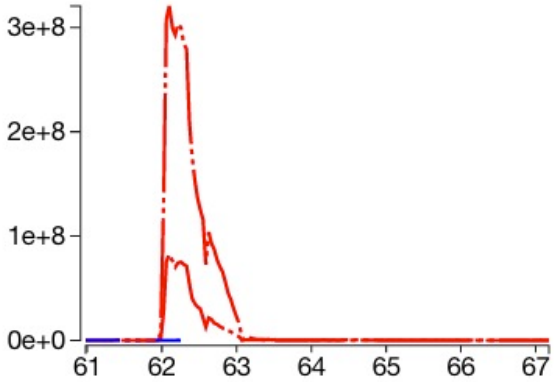
Quanti event: 47.1-49.4min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K18 [prop_d0]	1	1154.6892	2.8e+8
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K18 [pic,prop_d0]	1	1217.7001	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K18 [prop_d0]	2	577.8482	4.0e+9
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K18 [pic,prop_d0]	2	609.3537	6.6e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K18 [prop_d0]	3	385.5679	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K18 [pic,prop_d0]	3	406.5715	0.0e+0



Quanti event: 61.0-67.2min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K18 [prop_d0]	1	1154.6892	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K18 [pic,prop_d0]	1	1217.7001	2.3e+9
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K18 [prop_d0]	2	577.8482	2.1e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K18 [pic,prop_d0]	2	609.3537	9.7e+9
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K18 [prop_d0]	3	385.5679	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K18 [pic,prop_d0]	3	406.5715	0.0e+0



H3_K18-R26: Prop-KQLATKAAR MS/MS

Experimental spectrum

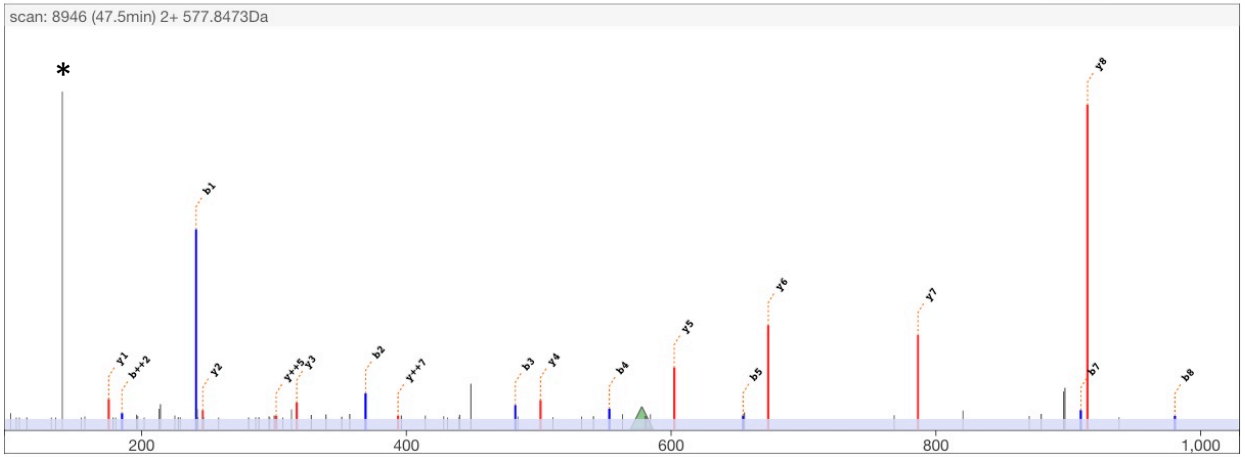
scan	8946
retention time	47.5min
precursor m/z	577.8473
precursor charge	2+

Theoretical

M H^{2+}	577.8482
MH Δ_{mass} Da	-0.0019
MH Δ_{mass} ppm	-1.6

edit peptide

{Propionyl}K{Propionyl}QLATK{Propionyl}AAR align



	b++	b		y	y++	
			Propionyl K	1098.66	549.84	9
1	121.08	241.15	Propionyl Q	914.54	457.77	8
2	185.11	369.21	L	786.48	393.75	7
3	241.65	482.30	A	673.40	337.20	6
4	277.17	553.33	T	602.36	301.68	5
5	327.69	654.38	K	501.31	251.16	4
6	419.76	838.50	Propionyl A	317.19	159.10	3
7	455.27	909.54	A	246.16	123.58	2
8	490.79	980.58	R	175.12	88.06	1
9	568.84	1136.68				

* = 140Da diagnostic ion

H3_K18-R26: PIC-KQLATKAAR MS/MS

Experimental spectrum

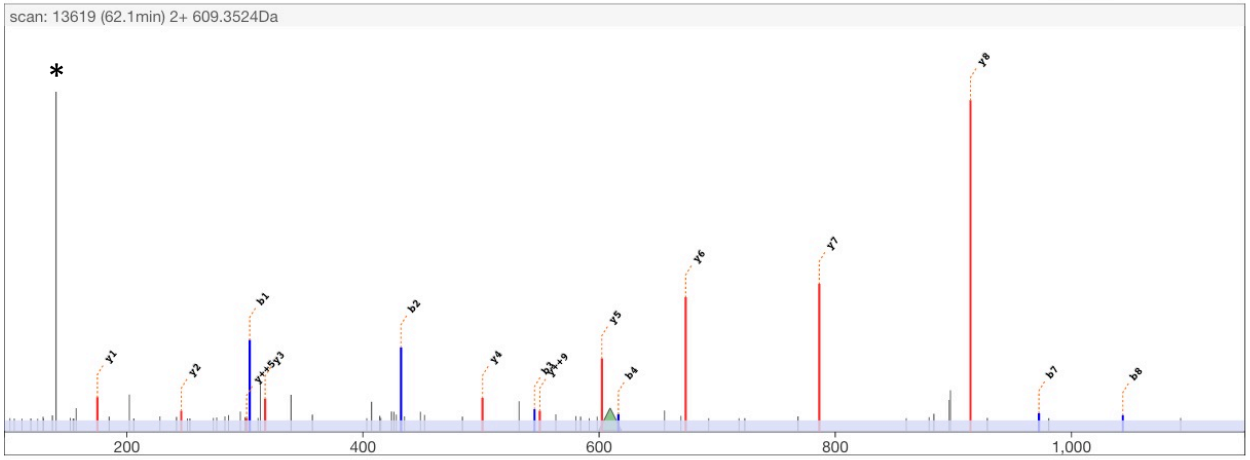
scan	13619
retention time	62.1min
precursor m/z	609.3524
precursor charge	2+

Theoretical

M H^{2+}	609.3537
MH Δ_{mass} Da	-0.0026
MH Δ_{mass} ppm	-2.2

edit peptide

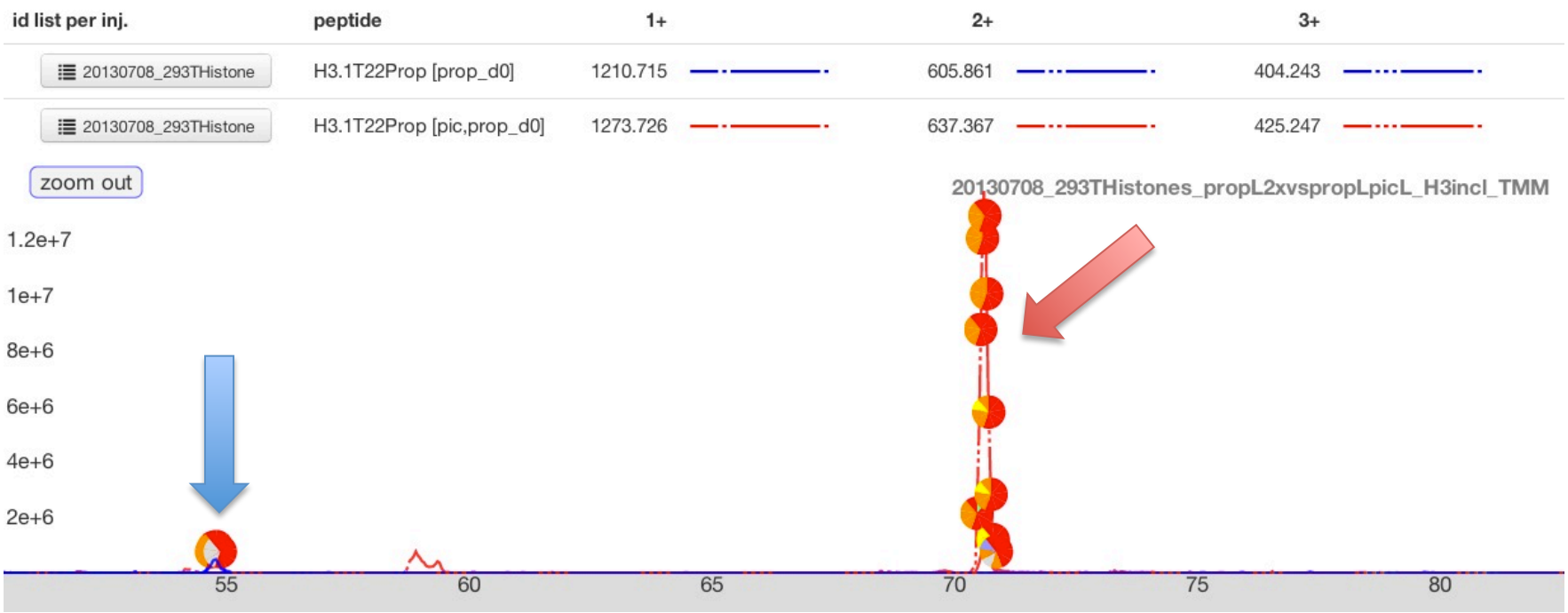
{PIC}K{Propionyl}QLATK{Propionyl}AAR align



	b++	b		y	y++	
	60.53	120.04	PIC K Propionyl	1098.66	549.84	9
1	152.59	304.17	Q	914.54	457.77	8
2	216.62	432.22	L	786.48	393.75	7
3	273.16	545.31	A	673.40	337.20	6
4	308.68	616.35	T	602.36	301.68	5
5	359.20	717.39	K Propionyl	501.31	251.16	4
6	451.26	901.51	A	317.19	159.10	3
7	486.78	972.55	A	246.16	123.58	2
8	522.30	1043.59	R	175.12	88.06	1
9	600.35	1199.69				

* = 140Da diagnostic ion

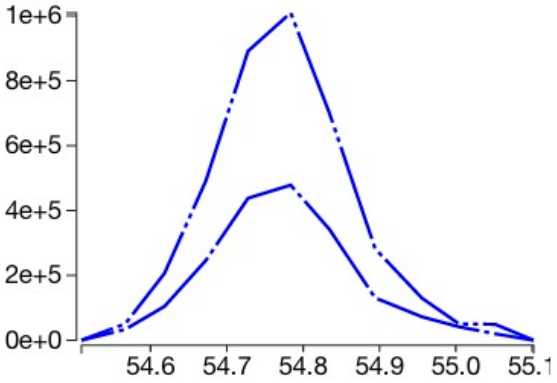
H3_K18-R26: KQLATPropKAAR



H3_K18-R26: KQLATPropKAAR

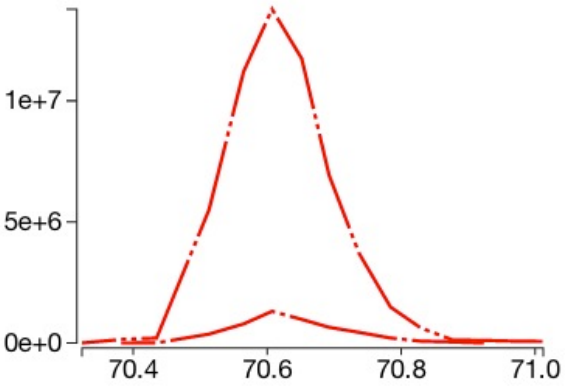
Quanti event: 54.5-55.3min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1T22Prop [prop_d0]	1	1210.7154	6.3e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1T22Prop [pic,prop_d0]	1	1273.7263	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1T22Prop [prop_d0]	2	605.8613	1.3e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1T22Prop [pic,prop_d0]	2	637.3668	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1T22Prop [prop_d0]	3	404.2433	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1T22Prop [pic,prop_d0]	3	425.2470	0.0e+0



Quanti event: 70.3-71.0min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1T22Prop [prop_d0]	1	1210.7154	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1T22Prop [pic,prop_d0]	1	1273.7263	1.3e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1T22Prop [prop_d0]	2	605.8613	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1T22Prop [pic,prop_d0]	2	637.3668	1.5e+8
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1T22Prop [prop_d0]	3	404.2433	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1T22Prop [pic,prop_d0]	3	425.2470	0.0e+0



H3_K18-R26: Prop-KQLATPropKAAR MS/MS

Experimental spectrum

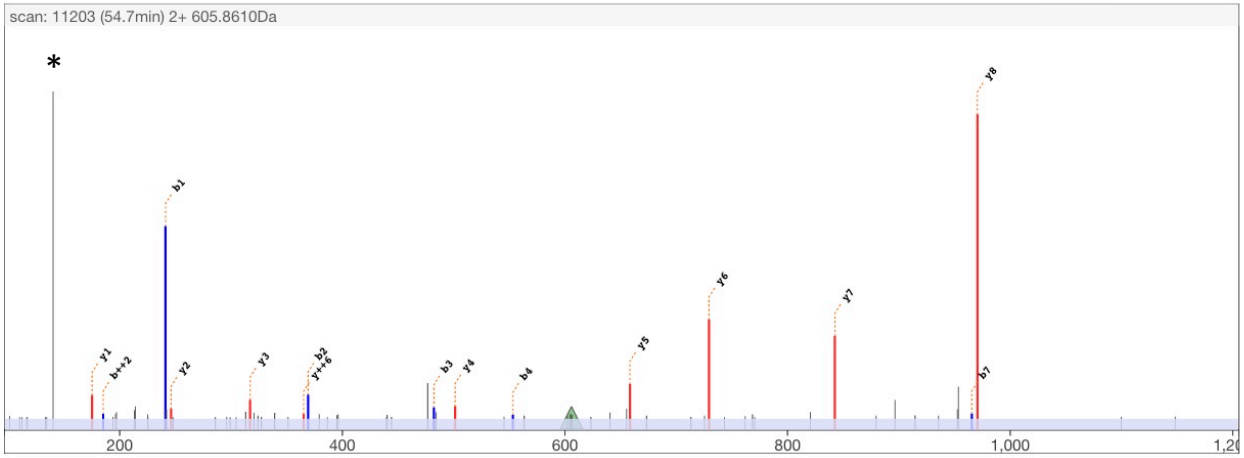
scan	11203
retention time	54.7min
precursor m/z	605.8610
precursor charge	2+

Theoretical

M H^{2+}	605.8613
MH Δ_{mass} Da	-0.0008
MH Δ_{mass} ppm	-0.6

edit peptide

{Propionyl}K{Propionyl}QLAT{Propionyl}K{Propionyl}AAR align



	b++	b		y	y++	
			Propionyl K	1154.69	577.85	9
1	121.08	241.15	Propionyl Q	970.57	485.79	8
2	185.11	369.21	L	842.51	421.76	7
3	241.65	482.30	A	729.43	365.22	6
4	277.17	553.33	T	658.39	329.70	5
5	355.71	710.41	Propionyl K	501.31	251.16	4
6	447.77	894.53	Propionyl A	317.19	159.10	3
7	483.29	965.57	A	246.16	123.58	2
8	518.81	1036.60	R	175.12	88.06	1
9	596.86	1192.70				

* = 140Da diagnostic ion

H3_K18-R26: PIC-KQLATPropKAAR MS/MS

Experimental spectrum

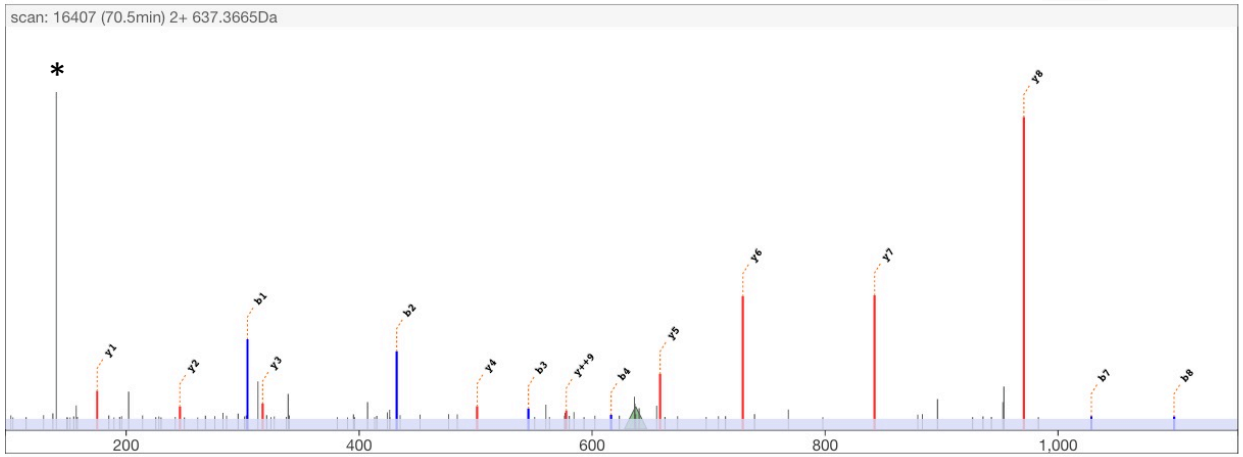
scan	16407
retention time	70.5min
precursor m/z	637.3665
precursor charge	2+

Theoretical

M H^{2+}	637.3668
MH Δ_{mass} Da	-0.0005
MH Δ_{mass} ppm	-0.4

edit peptide

{PIC}K{Propionyl}QLAT{Propionyl}K{Propionyl}AAR align

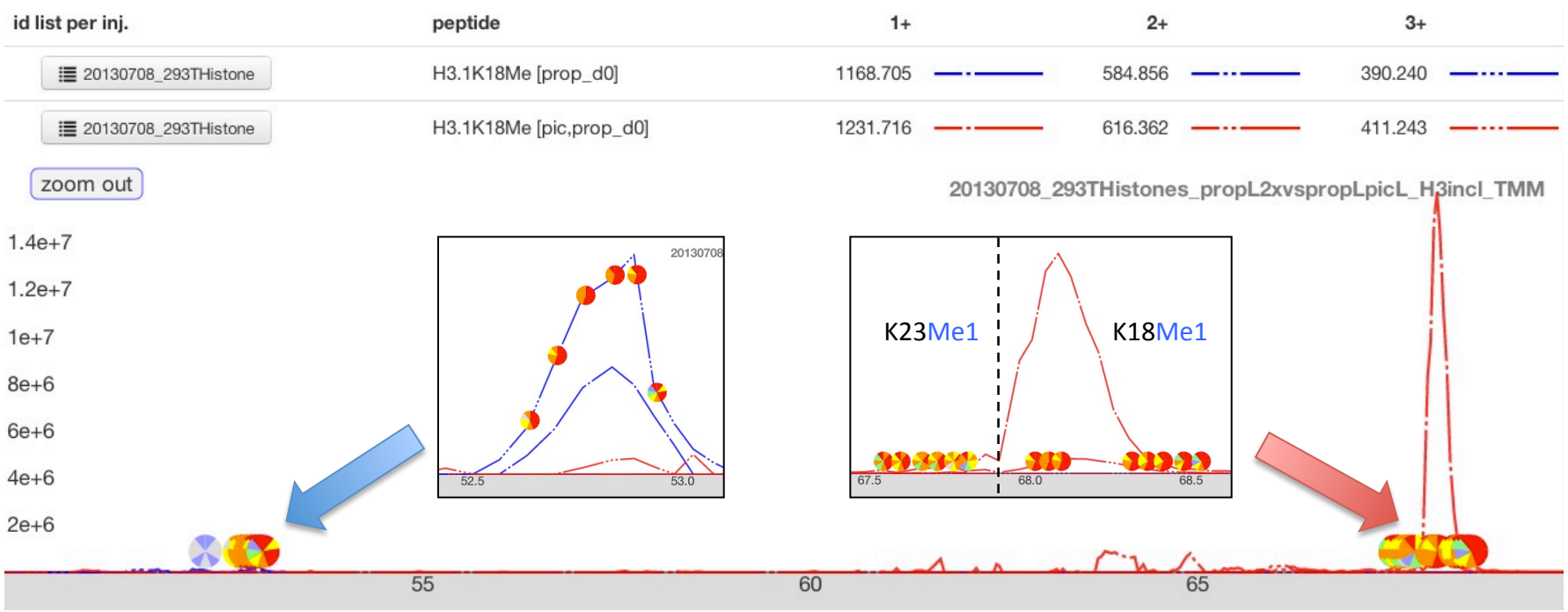


	b++	b		y	y++	
	60.53	120.04	PIC K Propionyl	1154.69	577.85	9
1	152.59	304.17	Q	970.57	485.79	8
2	216.62	432.22	L	842.51	421.76	7
3	273.16	545.31	A	729.43	365.22	6
4	308.68	616.35	T Propionyl	658.39	329.70	5
5	387.21	773.42	K Propionyl	501.31	251.16	4
6	479.27	957.54	A	317.19	159.10	3
7	514.79	1028.58	A	246.16	123.58	2
8	550.31	1099.61	R	175.12	88.06	1
9	628.36	1255.72				

* = 140Da diagnostic ion

H3_K18-R26: KMe1QLATKAAR

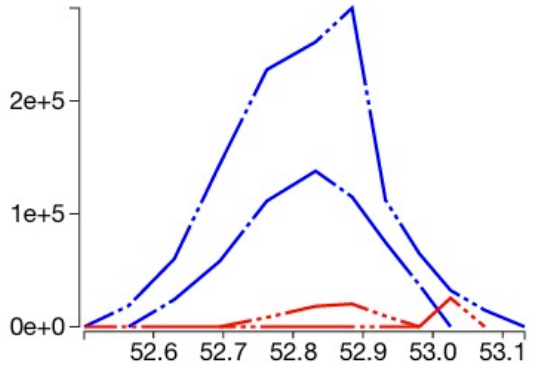
PIC-labeled peptides run as double-peak, Prop-labeled peptides. Earlier eluting peak is K23Me1, propionylated K23Me1 MS2s not detected (see page #xx).



H3_K18-R26: KMe1QLATKAAR

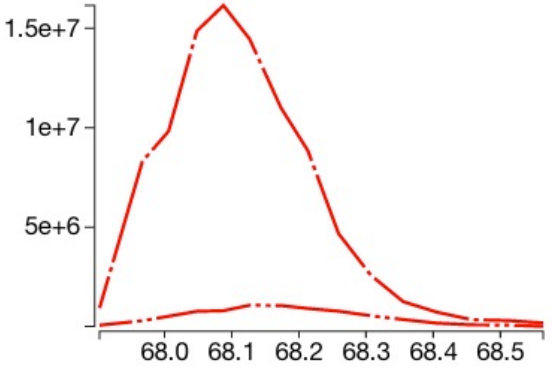
Quanti event: 52.5-53.1min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K18Me [prop_d0]	1	1168.7048	2.0e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K18Me [pic,prop_d0]	1	1231.7157	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K18Me [prop_d0]	2	584.8561	4.2e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K18Me [pic,prop_d0]	2	616.3615	7.2e+4
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K18Me [prop_d0]	3	390.2398	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K18Me [pic,prop_d0]	3	411.2434	1.9e+5



Quanti event: 67.9-68.6min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K18Me [prop_d0]	1	1168.7048	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K18Me [pic,prop_d0]	1	1231.7157	2.4e+8
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K18Me [prop_d0]	2	584.8561	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K18Me [pic,prop_d0]	2	616.3615	2.0e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K18Me [prop_d0]	3	390.2398	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K18Me [pic,prop_d0]	3	411.2434	0.0e+0



H3_K18-R26: Prop-KMe1QLATKAAR MS/MS

Experimental spectrum

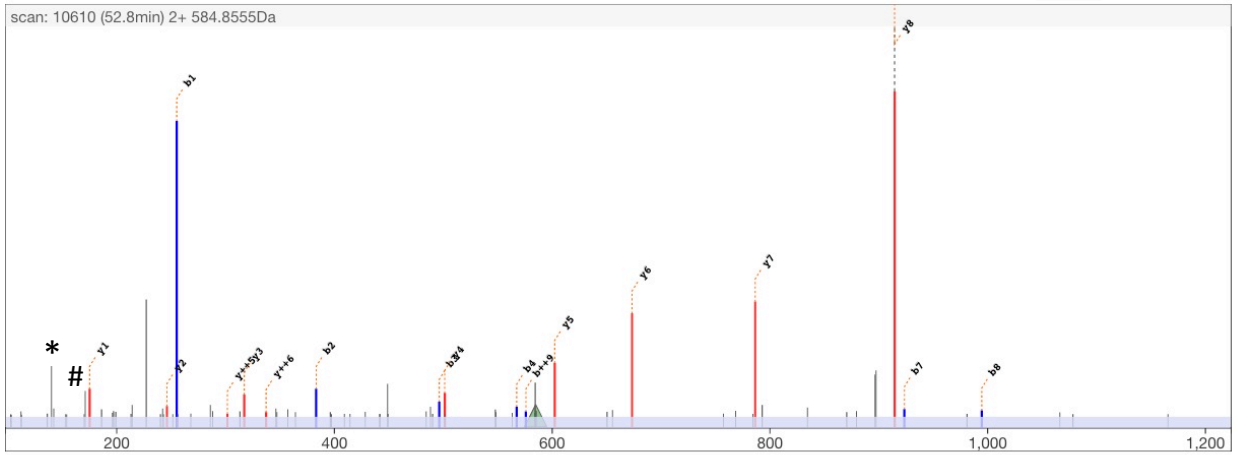
scan	10610
retention time	52.8min
precursor m/z	584.8555
precursor charge	2+

Theoretical

M H^{2+}	584.8561
MH Δ_{mass} Da	-0.0012
MH Δ_{mass} ppm	-1.0

edit peptide

{Propionyl}K{Methyl,Propionyl}QLATK{Propionyl}AAR align



	b++	b		y	y++	
			Propionyl K	1112.68	556.84	9
1	128.09	255.17	Methyl,Propionyl Q	914.54	457.77	8
2	192.12	383.23	L	786.48	393.75	7
3	248.66	496.31	A	673.40	337.20	6
4	284.18	567.35	T	602.36	301.68	5
5	334.70	668.40	K	501.31	251.16	4
6	426.76	852.52	Propionyl A	317.19	159.10	3
7	462.28	923.56	A	246.16	123.58	2
8	497.80	994.59	R	175.12	88.06	1
9	575.85	1150.69				

* = 140Da diagnostic ion
\# = 171Da diagnostic ion

H3_K18-R26: PIC-KMe1QLATKAAR MS/MS

Experimental spectrum

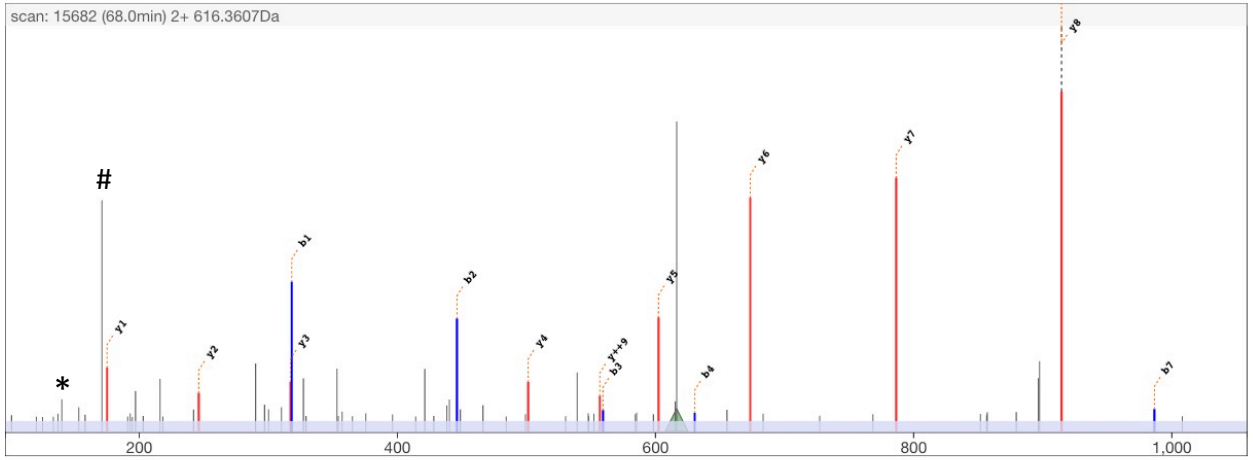
scan	15682
retention time	68.1min
precursor m/z	616.3607
precursor charge	2+

Theoretical

M H^{2+}	616.3615
MH Δ_{mass} Da	-0.0017
MH Δ_{mass} ppm	-1.4

edit peptide

{PIC}K{Methyl,Propionyl}QLATK{Propionyl}AAR align

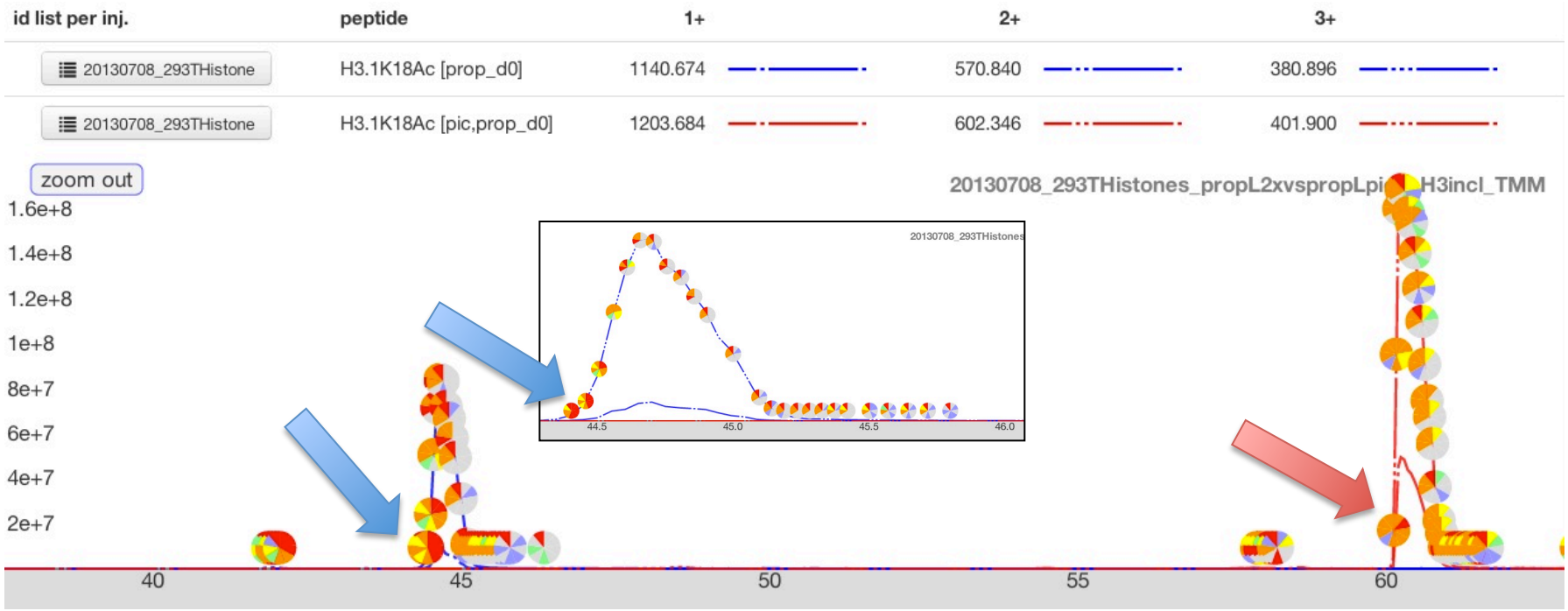


	b++	b		y	y++	
	60.53	120.04	PIC	1112.68	556.84	9
1	159.59	318.18	K Methyl,Propionyl	914.54	457.77	8
2	223.62	446.24	Q	786.48	393.75	7
3	280.17	559.32	L	673.40	337.20	6
4	315.68	630.36	A	602.36	301.68	5
5	366.21	731.41	T	501.31	251.16	4
6	458.27	915.53	K Propionyl	317.19	159.10	3
7	493.79	986.57	A	246.16	123.58	2
8	529.31	1057.60	A	175.12	88.06	1
9	607.36	1213.71	R			

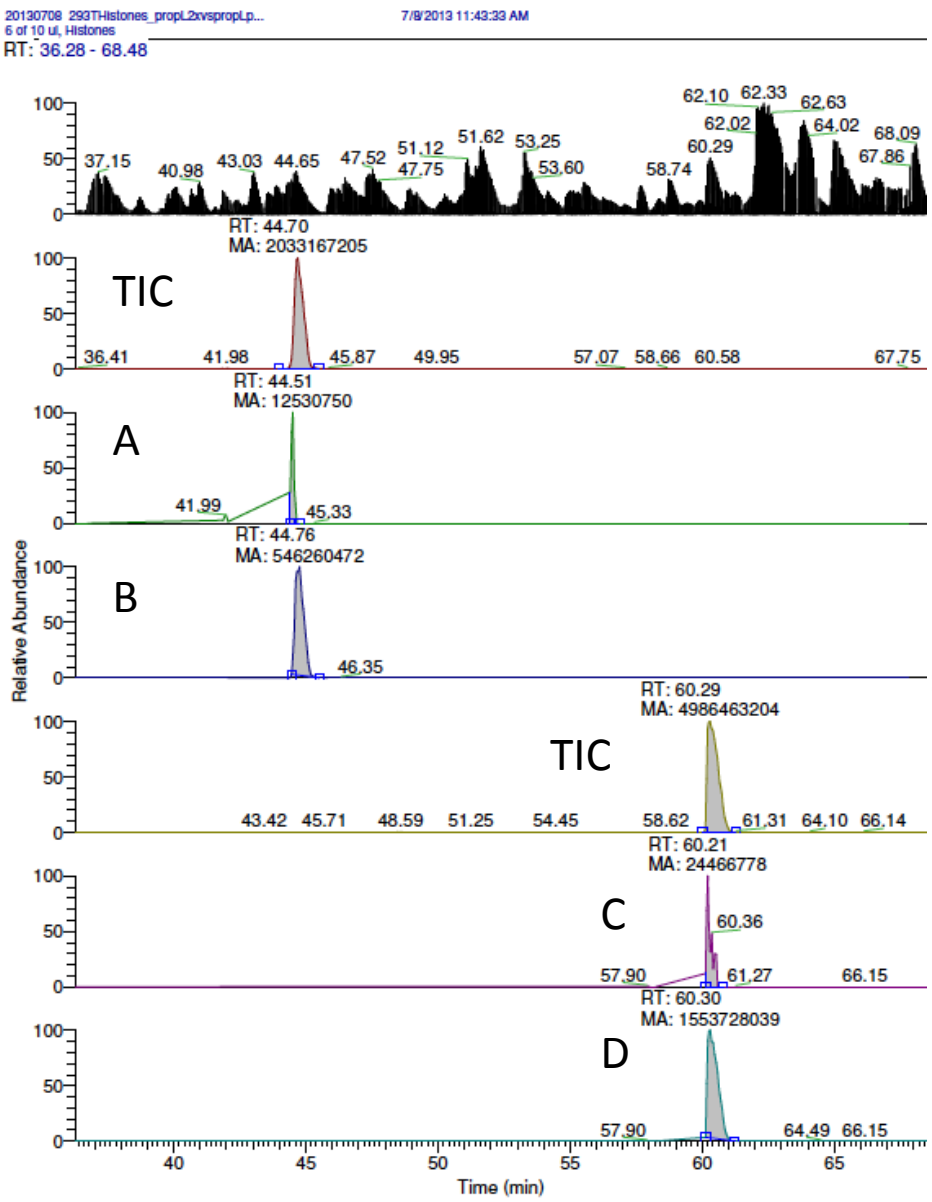
* = 140Da diagnostic ion
\# = 171Da diagnostic ion

H3_K18-R26: KAcQLATKAAR

Low abundance, peak overlaps with K23Ac. AUC determinated on MS2 level.
Only the first two MS2 from the Prop-Peak could be assigned as K18Ac, Rest is K23Ac!



H3_K18-R26: KAcQLATKAAR



AUC calculation on MS2 level:

<u>XIC-Prop 570.84 (2+)</u>
227.14, 355.20, 673.40, 786.48, 914.54

<u>XIC-PIC 602.35 (2+)</u>
290.15, 418.21, 673.40, 786.48, 914.54

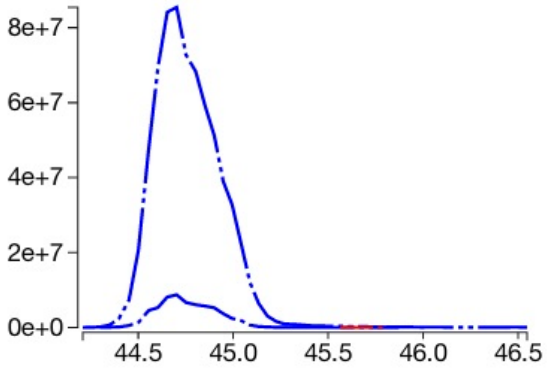
A = K18Ac-peak Prop
B = K23Ac-peak Prop
C = K18Ac-peak PIC
D = K23Ac-peak PIC

H3_K18-R26: KAcQLATKAAR and KQLATKAcAAR

AUC determinated on MS2 level (see page 159).

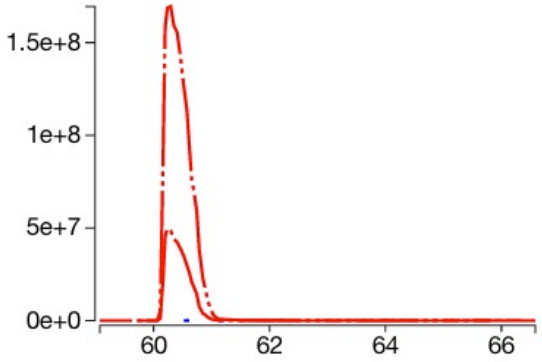
Quanti event: 44.1-46.6min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K23Ac [prop_d0]	1	1140.6735	1.8e+8
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K23Ac [pic,prop_d0]	1	1203.6844	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K23Ac [prop_d0]	2	570.8404	2.0e+9
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K23Ac [pic,prop_d0]	2	602.3459	8.3e+4
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K23Ac [prop_d0]	3	380.8960	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K23Ac [pic,prop_d0]	3	401.8997	0.0e+0



Quanti event: 59.0-66.6min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K23Ac [prop_d0]	1	1140.6735	7.6e+4
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K23Ac [pic,prop_d0]	1	1203.6844	1.4e+9
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K23Ac [prop_d0]	2	570.8404	6.4e+4
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K23Ac [pic,prop_d0]	2	602.3459	5.0e+9
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K23Ac [prop_d0]	3	380.8960	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K23Ac [pic,prop_d0]	3	401.8997	0.0e+0



H3_K18-R26: Prop-KAcQLATKAAR MS/MS

Experimental spectrum

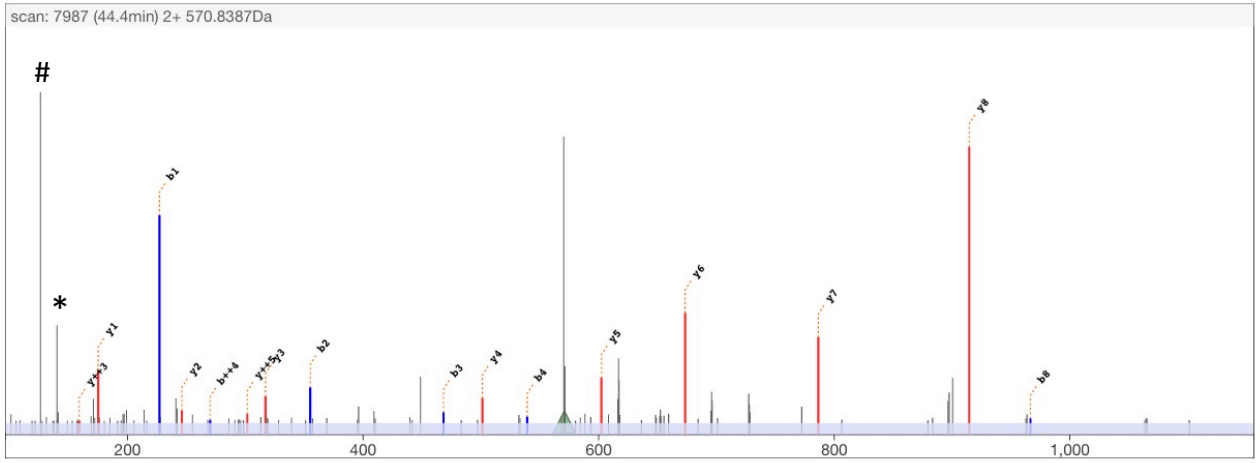
scan	7987
retention time	44.4min
precursor m/z	570.8387
precursor charge	2+

Theoretical

M H^{2+}	570.8404
MH Δ_{mass} Da	-0.0033
MH Δ_{mass} ppm	-2.9

edit peptide

{Propionyl}K{Acetyl}QLATK{Propionyl}AAR align



	b++	b		y	y++	
			Propionyl K	1084.65	542.83	9
1	114.07	227.14	Acetyl Q	914.54	457.77	8
2	178.10	355.20	L	786.48	393.75	7
3	234.64	468.28	A	673.40	337.20	6
4	270.16	539.32	T	602.36	301.68	5
5	320.69	640.37	K	501.31	251.16	4
6	412.75	824.49	Propionyl A	317.19	159.10	3
7	448.27	895.52	A	246.16	123.58	2
8	483.78	966.56	R	175.12	88.06	1
9	561.84	1122.66				

* = 140Da diagnostic ion
\# = 126Da diagnostic ion

H3_K18-R26: PIC-KAcQLATKAAR MS/MS

MS2 for PIC-K18Ac is mixed with PIC-K23Ac MS2 (y4-y8 denoted by arrows):

Experimental spectrum

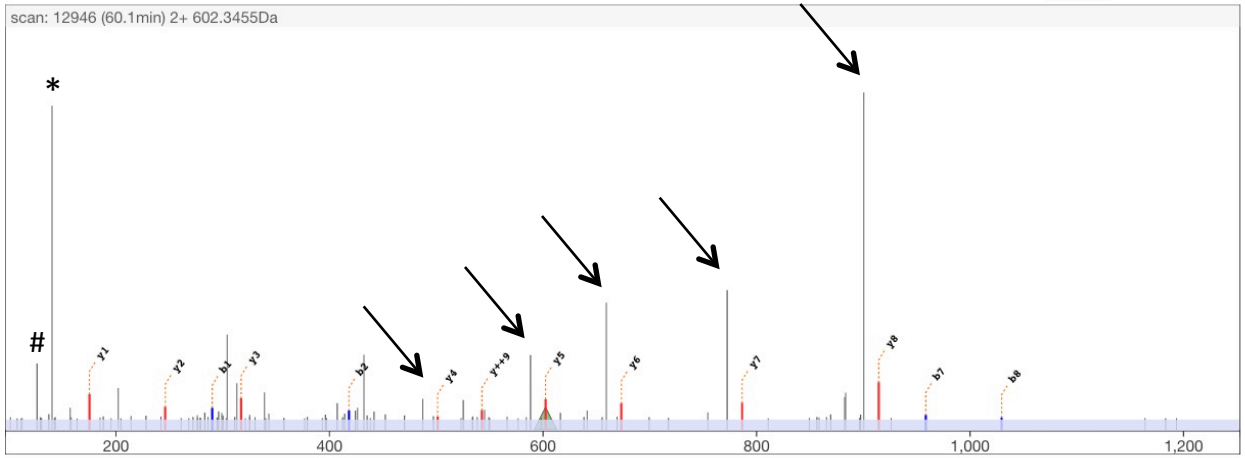
scan	12946
retention time	60.1min
precursor m/z	602.3455
precursor charge	2+

Theoretical

M H^{2+}	602.3459
MH Δ_{mass} Da	-0.0007
MH Δ_{mass} ppm	-0.6

edit peptide

{PIC}K{Acetyl}QLATK{Propionyl}AAR align

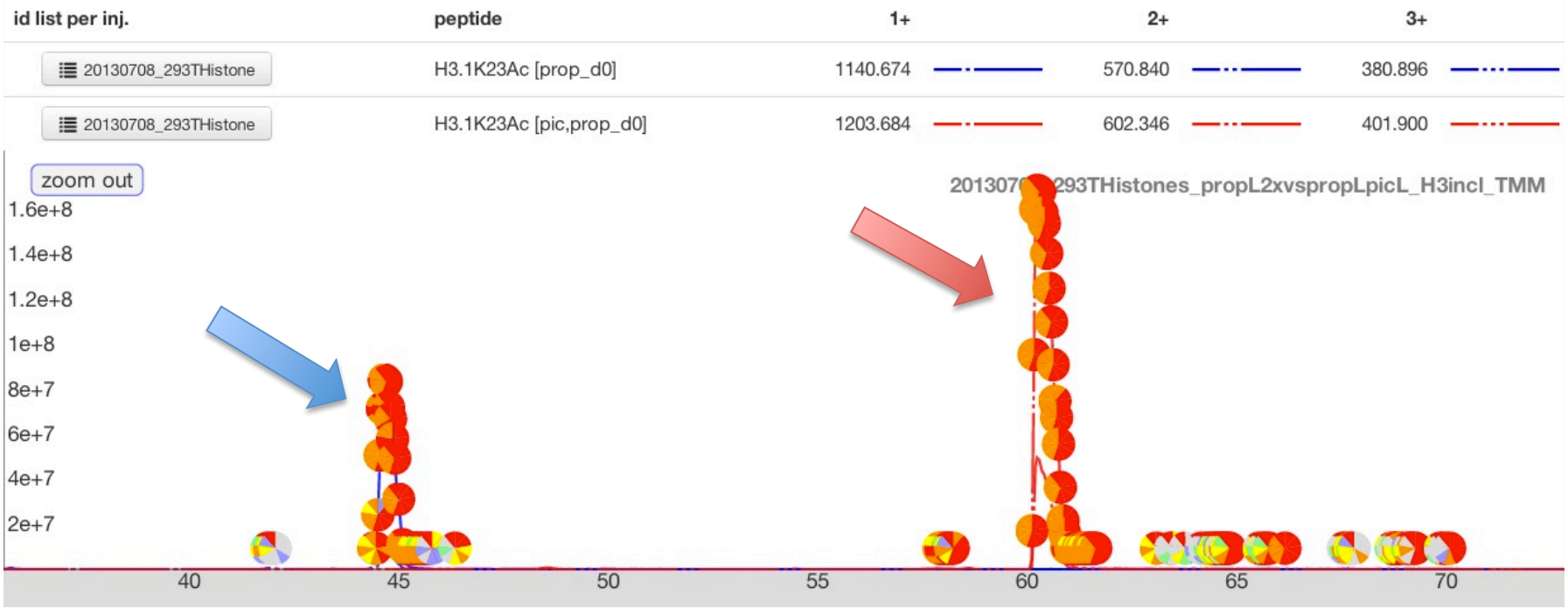


	b++	b		y	y++	
	60.53	120.04	PIC	1084.65	542.83	9
1	145.58	290.15	K Acetyl	914.54	457.77	8
2	209.61	418.21	Q	786.48	393.75	7
3	266.15	531.29	L	673.40	337.20	6
4	301.67	602.33	A	602.36	301.68	5
5	352.19	703.38	T	501.31	251.16	4
6	444.25	887.50	K Propionyl	317.19	159.10	3
7	479.77	958.54	A	246.16	123.58	2
8	515.29	1029.57	A	175.12	88.06	1
9	593.34	1185.67	R			

* = 140Da diagnostic ion
\# = 126Da diagnostic ion

H3_K18-R26: KQLATKAcAAR

Peak overlaps with K18Ac, more abundant mark. AUC determinated on MS2 level (see page 159).



H3_K18-R26: Prop-KQLATKAcAAR MS/MS

Experimental spectrum

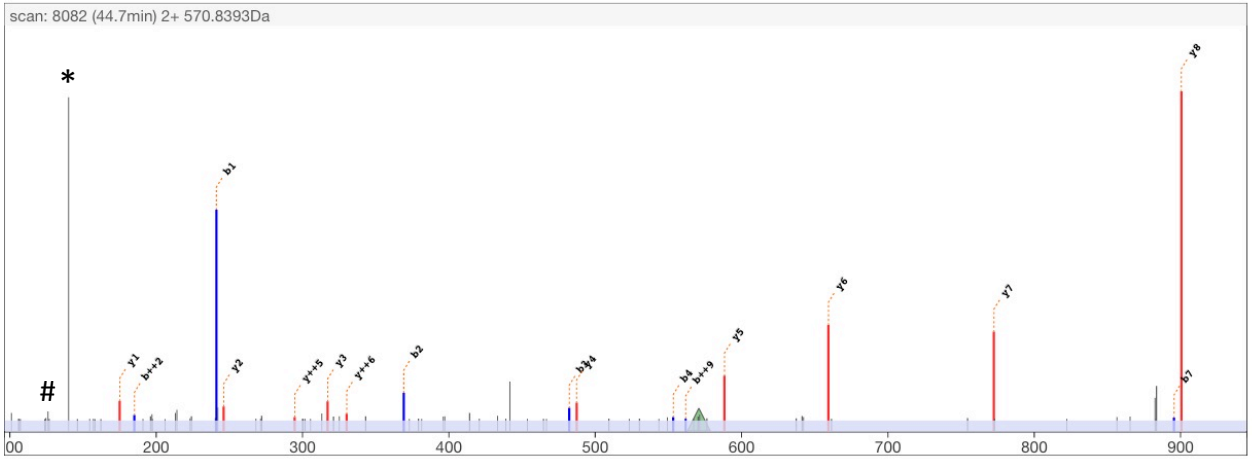
scan	8082
retention time	44.7min
precursor m/z	570.8393
precursor charge	2+

Theoretical

M H^{2+}	570.8404
MH Δ_{mass} Da	-0.0022
MH Δ_{mass} ppm	-1.9

edit peptide

{Propionyl}K{Propionyl}QLATK{Acetyl}AAR align



	b++	b		y	y++	
			Propionyl K	1084.65	542.83	9
1	121.08	241.15	Propionyl Q	900.53	450.77	8
2	185.11	369.21	L	772.47	386.74	7
3	241.65	482.30	A	659.38	330.20	6
4	277.17	553.33	T	588.35	294.68	5
5	327.69	654.38	K	487.30	244.15	4
6	412.75	824.49	Acetyl A	317.19	159.10	3
7	448.27	895.52	A	246.16	123.58	2
8	483.78	966.56	R	175.12	88.06	1
9	561.84	1122.66				

* = 140Da diagnostic ion
\# = 126Da diagnostic ion

H3_K18-R26: PIC-KQLATKAcAAR MS/MS

Experimental spectrum

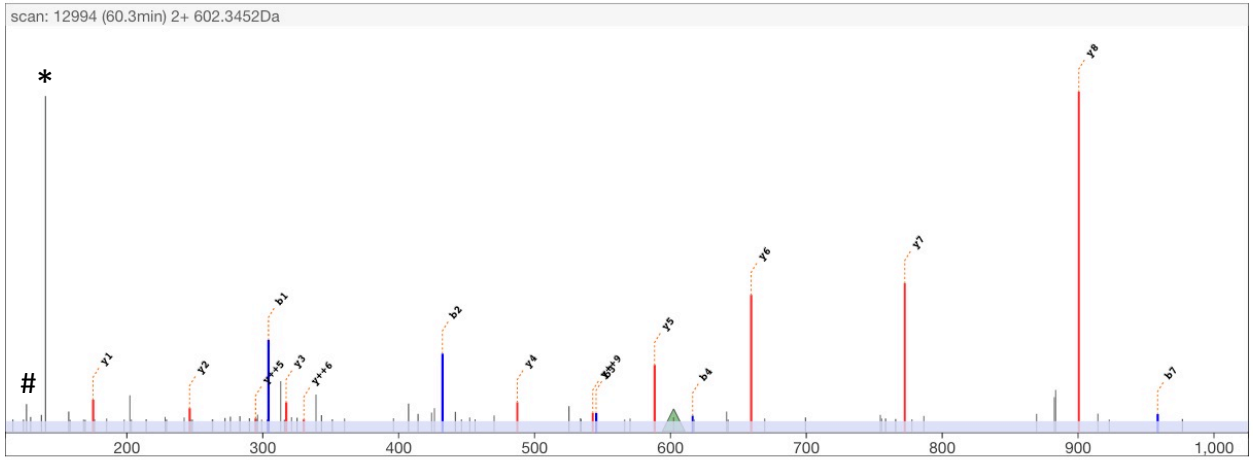
scan	12994
retention time	60.2min
precursor m/z	602.3452
precursor charge	2+

Theoretical

M H^{2+}	602.3459
MH Δ_{mass} Da	-0.0013
MH Δ_{mass} ppm	-1.1

edit peptide

{PIC}K{Propionyl}QLATK{Acetyl}AAR align

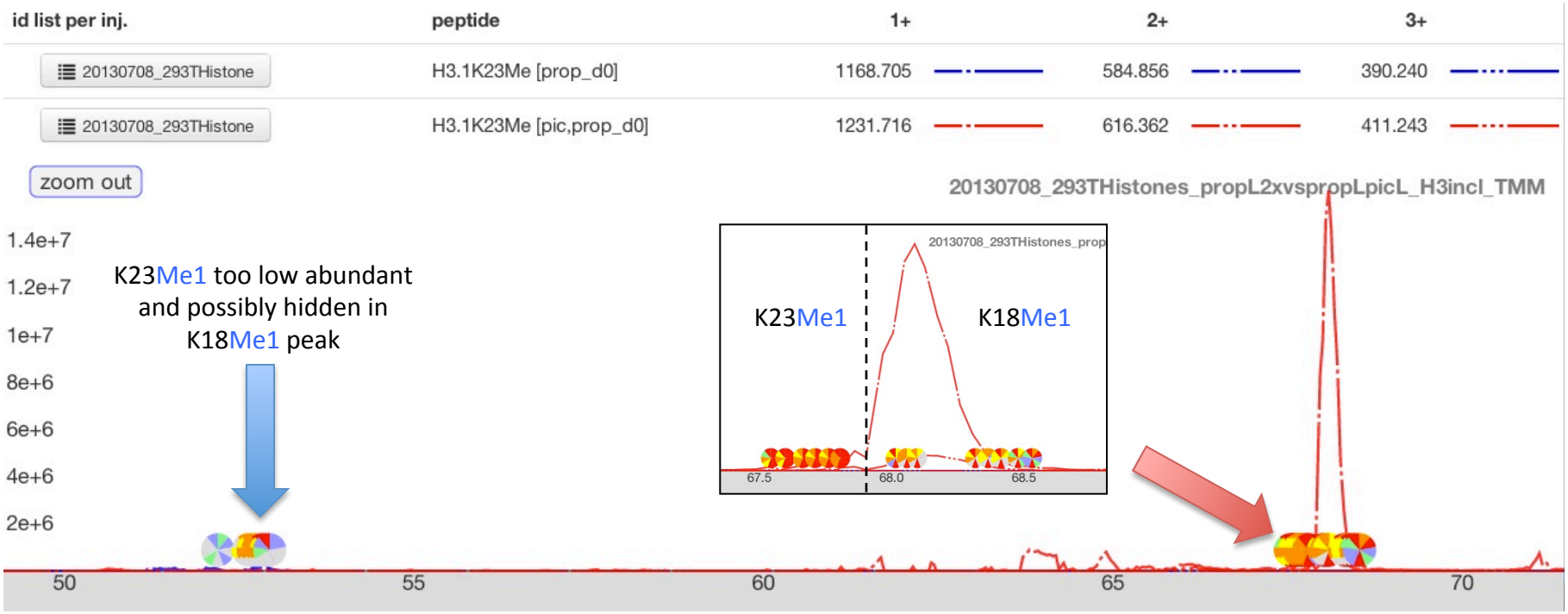


	b++	b		y	y++	
	60.53	120.04	PIC	1084.65	542.83	9
1	152.59	304.17	K Propionyl	900.53	450.77	8
2	216.62	432.22	Q	772.47	386.74	7
3	273.16	545.31	L	659.38	330.20	6
4	308.68	616.35	A	588.35	294.68	5
5	359.20	717.39	T	487.30	244.15	4
6	444.25	887.50	K Acetyl	317.19	159.10	3
7	479.77	958.54	A	246.16	123.58	2
8	515.29	1029.57	A	175.12	88.06	1
9	593.34	1185.67	R			

* = 140Da diagnostic ion
\# = 126Da diagnostic ion

H3_K18-R26: KQLATKMe1AAR

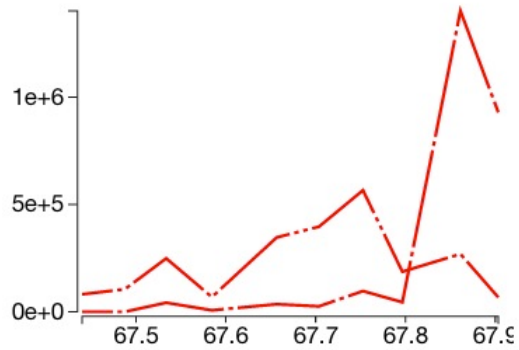
Double-peaks for PIC treatment (see K18Me1, slide #84): Earlier eluting peak is K23Me1!



H3_K18-R26: KQLATKMe1AAR

Quanti event: 67.4-67.9min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K23Me [prop_d0]	1	1168.7048	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K23Me [pic,prop_d0]	1	1231.7157	6.4e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K23Me [prop_d0]	2	584.8561	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K23Me [pic,prop_d0]	2	616.3615	6.9e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K23Me [prop_d0]	3	390.2398	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K23Me [pic,prop_d0]	3	411.2434	0.0e+0



Propionylation K23Me1 not found.

H3_K18-R26: PIC-KQLATKMe1AAR MS/MS

Experimental spectrum

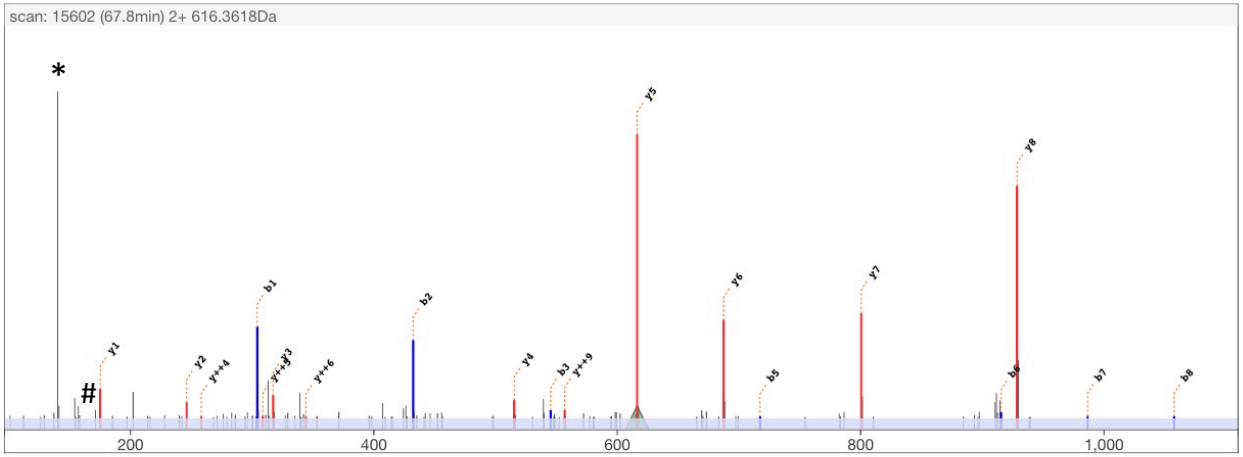
scan	15602
retention time	67.8min
precursor m/z	616.3618
precursor charge	2+

Theoretical

M H^{2+}	616.3615
MH Δ_{mass} Da	0.0006
MH Δ_{mass} ppm	0.5

edit peptide

{PIC}K{Propionyl}QLATK{Methyl,Propionyl}AAR align

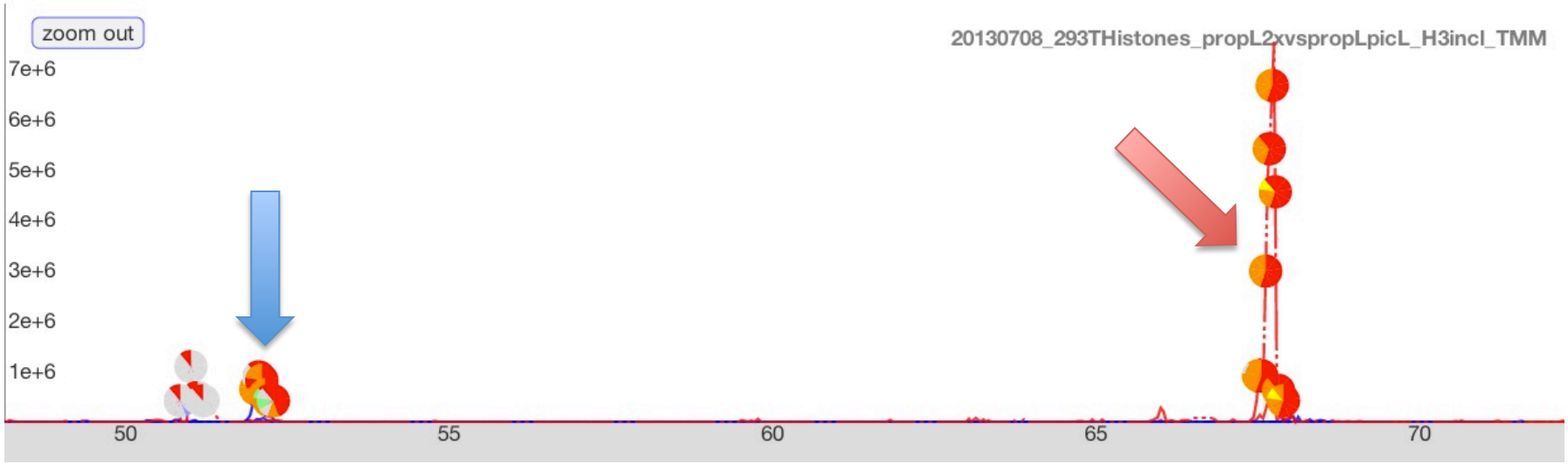


	b++	b		y	y++	
	60.53	120.04	PIC K Propionyl	1112.68	556.84	9
1	152.59	304.17	Q	928.56	464.78	8
2	216.62	432.22	L	800.50	400.75	7
3	273.16	545.31	A	687.41	344.21	6
4	308.68	616.35	T	616.38	308.69	5
5	359.20	717.39	K Methyl,Propionyl	515.33	258.17	4
6	458.27	915.53	A	317.19	159.10	3
7	493.79	986.57	A	246.16	123.58	2
8	529.31	1057.60	R	175.12	88.06	1
9	607.36	1213.71				

* = 140Da diagnostic ion
\# = 171Da diagnostic ion

H3_K18-R26: KQLATPropKAcAAR

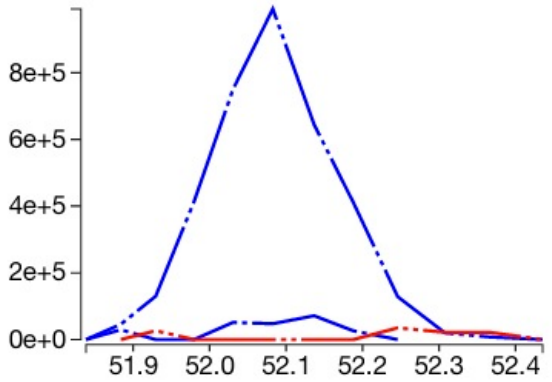
id list per inj.	peptide	1+	2+	3+
20130708_293THistone	H3.1T22PropK23Ac [prop_d0]	1196.700	598.854	399.571
20130708_293THistone	H3.1T22PropK23Ac [pic,prop_d0]	1259.711	630.359	420.575



H3_K18-R26: KQLATPropKAcAAR

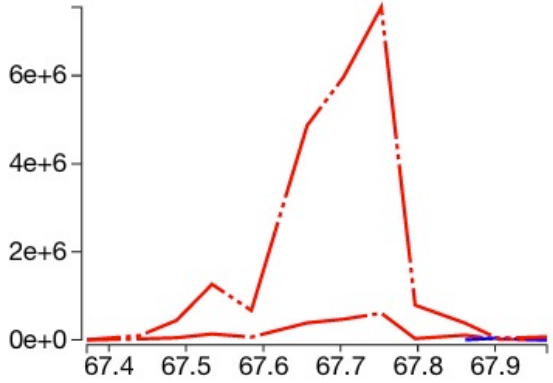
Quanti event: 51.8-52.5min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1T22PropK23Ac [prop_d0]	1	1196.6998	7.0e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1T22PropK23Ac [pic,prop_d0]	1	1259.7107	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1T22PropK23Ac [prop_d0]	2	598.8535	1.1e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1T22PropK23Ac [pic,prop_d0]	2	630.3590	3.6e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1T22PropK23Ac [prop_d0]	3	399.5714	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1T22PropK23Ac [pic,prop_d0]	3	420.5751	0.0e+0



Quanti event: 67.4-68.0min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1T22PropK23Ac [prop_d0]	1	1196.6998	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1T22PropK23Ac [pic,prop_d0]	1	1259.7107	5.7e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1T22PropK23Ac [prop_d0]	2	598.8535	1.3e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1T22PropK23Ac [pic,prop_d0]	2	630.3590	6.7e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1T22PropK23Ac [prop_d0]	3	399.5714	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1T22PropK23Ac [pic,prop_d0]	3	420.5751	0.0e+0



H3_K18-R26: Prop-KQLATPropKAcAAR MS/MS

Experimental spectrum

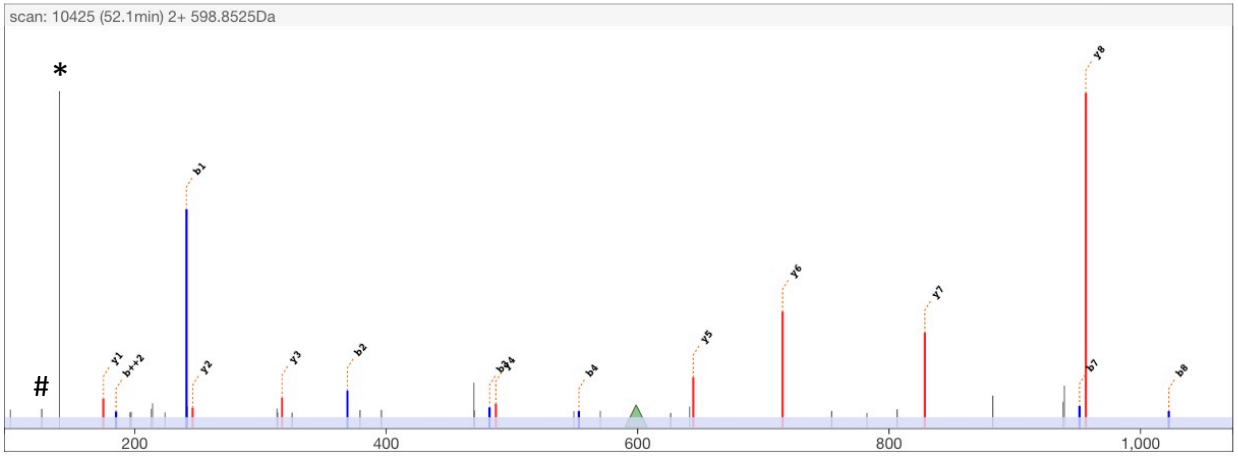
scan	10425
retention time	52.1min
precursor m/z	598.8525
precursor charge	2+

Theoretical

M H^{2+}	598.8535
MH Δ_{mass} Da	-0.0021
MH Δ_{mass} ppm	-1.7

edit peptide

{Propionyl}K{Propionyl}QLAT{Propionyl}K{Acetyl}AAR align



	b++	b		y	y++	
			Propionyl K	1140.67	570.84	9
1	121.08	241.15	Propionyl Q	956.55	478.78	8
2	185.11	369.21	L	828.49	414.75	7
3	241.65	482.30	A	715.41	358.21	6
4	277.17	553.33	T	644.37	322.69	5
5	355.71	710.41	Propionyl K	487.30	244.15	4
6	440.76	880.51	Acetyl A	317.19	159.10	3
7	476.28	951.55	A	246.16	123.58	2
8	511.80	1022.59	R	175.12	88.06	1
9	589.85	1178.69				

* = 140Da diagnostic ion
\# = 126Da diagnostic ion

H3_K18-R26: PIC-KQLATPropKAcAAR MS/MS

Experimental spectrum

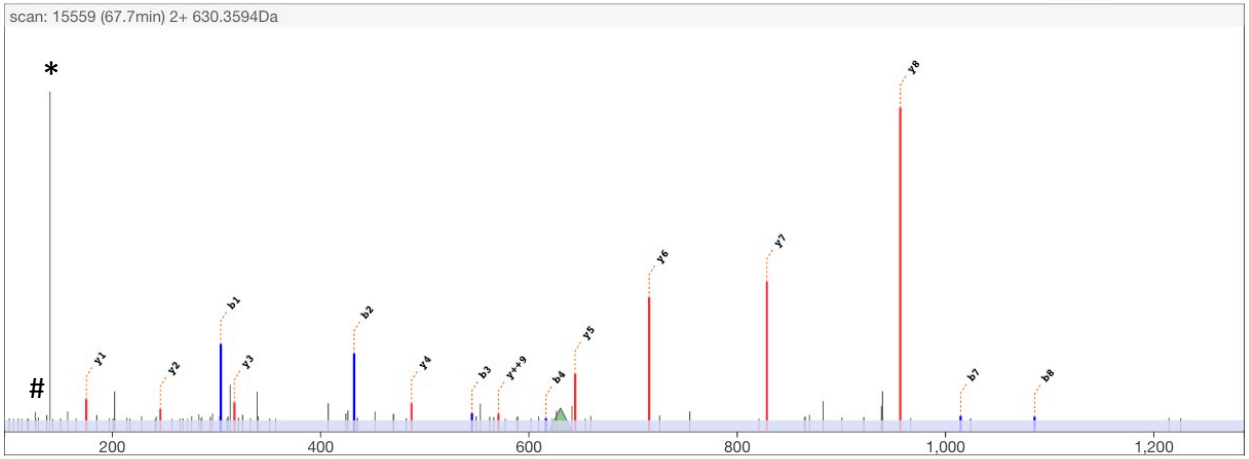
scan	15559
retention time	67.7min
precursor m/z	630.3594
precursor charge	2+

Theoretical

M H^{2+}	630.3590
MH Δ_{mass} Da	0.0008
MH Δ_{mass} ppm	0.7

edit peptide

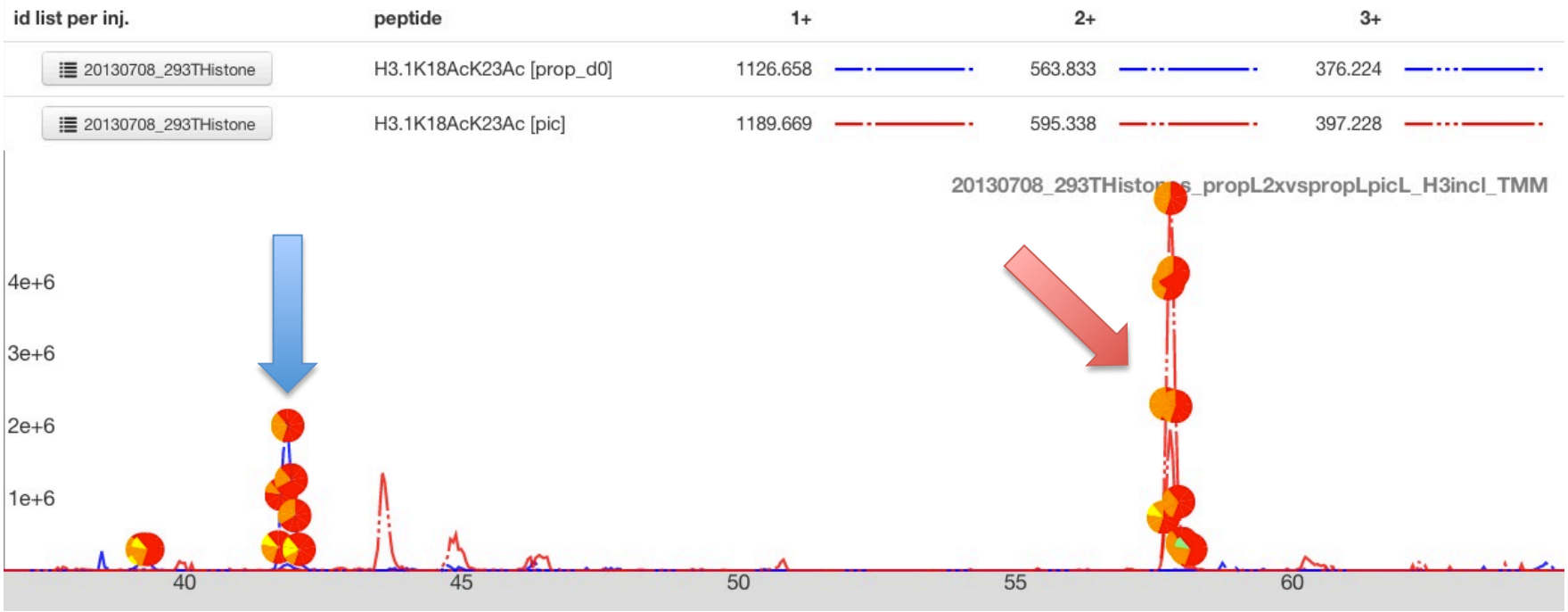
{PIC}K{Propionyl}QLAT{Propionyl}K{Acetyl}AAR align



	b++	b		y	y++	
	60.53	120.04	PIC	1140.67	570.84	9
1	152.59	304.17	K Propionyl	956.55	478.78	8
2	216.62	432.22	Q	828.49	414.75	7
3	273.16	545.31	L	715.41	358.21	6
4	308.68	616.35	A	644.37	322.69	5
5	387.21	773.42	T Propionyl	487.30	244.15	4
6	472.27	943.52	K Acetyl	317.19	159.10	3
7	507.78	1014.56	A	246.16	123.58	2
8	543.30	1085.60	A	175.12	88.06	1
9	621.35	1241.70	R			

* = 140Da diagnostic ion
\# = 126Da diagnostic ion

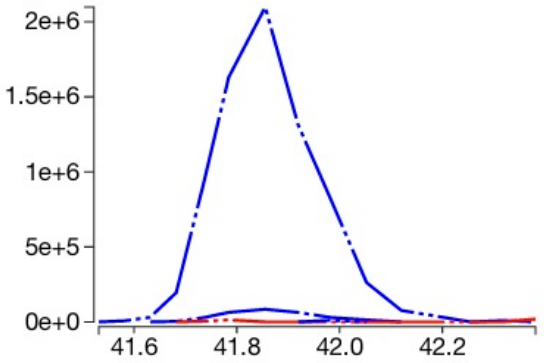
H3_K18-R26: KAcQLATKAcAAR



H3_K18-R26: KAcQLATKAcAAR

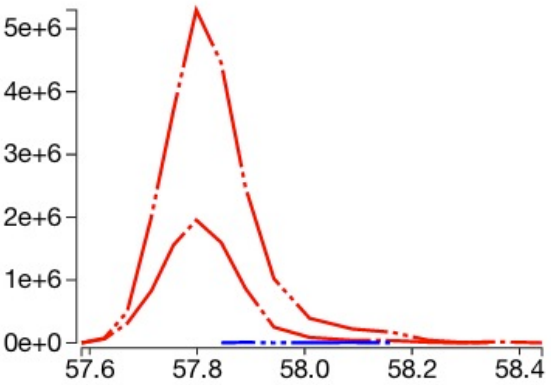
Quanti event: 41.4-42.4min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K18AcK23Ac [prop_d0]	1	1126.6579	1.1e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K18AcK23Ac [pic]	1	1189.6688	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K18AcK23Ac [prop_d0]	2	563.8326	2.8e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K18AcK23Ac [pic]	2	595.3380	1.0e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K18AcK23Ac [prop_d0]	3	376.2241	4.4e+4
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K18AcK23Ac [pic]	3	397.2278	0.0e+0



Quanti event: 57.3-58.5min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K18AcK23Ac [prop_d0]	1	1126.6579	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K18AcK23Ac [pic]	1	1189.6688	2.1e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K18AcK23Ac [prop_d0]	2	563.8326	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K18AcK23Ac [pic]	2	595.3380	5.7e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K18AcK23Ac [prop_d0]	3	376.2241	7.1e+4
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K18AcK23Ac [pic]	3	397.2278	0.0e+0



H3_K18-R26: Prop-KAcQLATKAcAAR MS/MS

Experimental spectrum

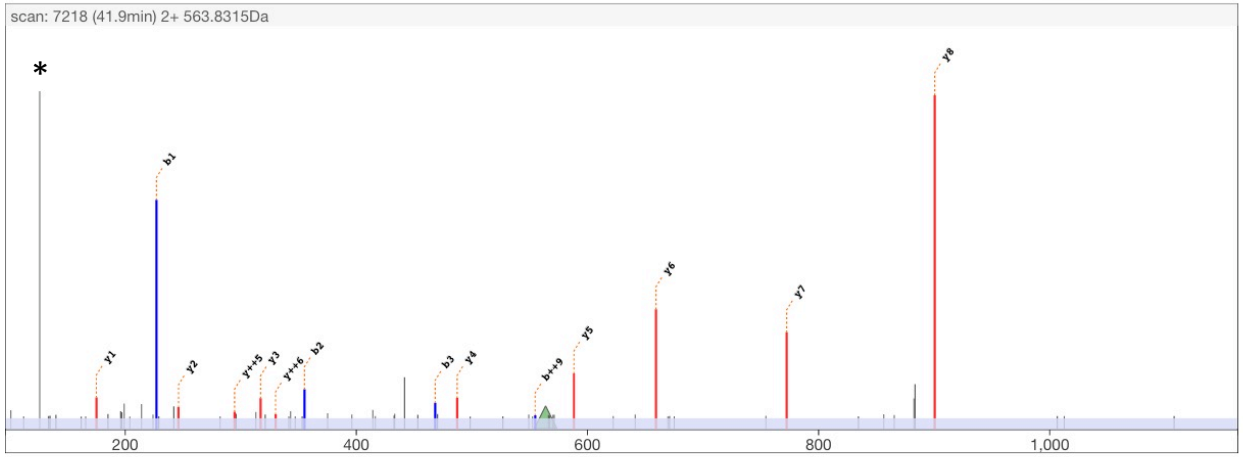
scan	7218
retention time	41.9min
precursor m/z	563.8315
precursor charge	2+

Theoretical

M H^{2+}	563.8326
MH Δ_{mass} Da	-0.0022
MH Δ_{mass} ppm	-1.9

edit peptide

{Propionyl}K{Acetyl}QLATK{Acetyl}AAR align



	b++	b		y	y++	
			Propionyl K	1070.63	535.82	9
1	114.07	227.14	Acetyl Q	900.53	450.77	8
2	178.10	355.20	L	772.47	386.74	7
3	234.64	468.28	A	659.38	330.20	6
4	270.16	539.32	T	588.35	294.68	5
5	320.69	640.37	K Acetyl	487.30	244.15	4
6	405.74	810.47	A	317.19	159.10	3
7	441.26	881.51	A	246.16	123.58	2
8	476.78	952.55	R	175.12	88.06	1
9	554.83	1108.65				

* = 126Da diagnostic ion

H3_K18-R26: PIC-KAcQLATKAcAAR MS/MS

Experimental spectrum

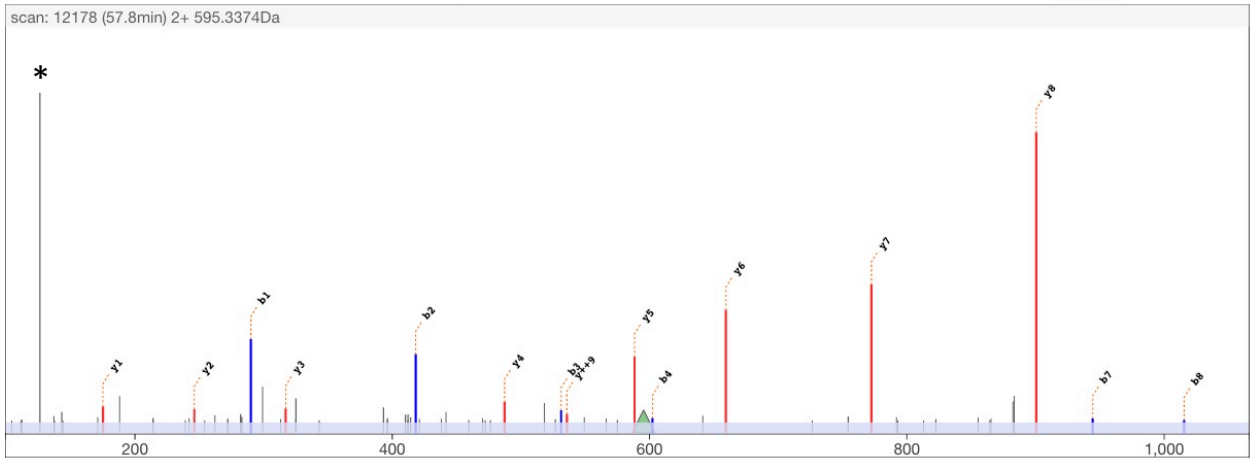
scan	12178
retention time	57.8min
precursor m/z	595.3374
precursor charge	2+

Theoretical

M H^{2+}	595.3380
MH Δ_{mass} Da	-0.0013
MH Δ_{mass} ppm	-1.1

edit peptide

{PIC}K{Acetyl}QLATK{Acetyl}AAR align



	b++	b		y	y++	
	60.53	120.04	PIC	1070.63	535.82	9
1	145.58	290.15	K Acetyl	900.53	450.77	8
2	209.61	418.21	Q	772.47	386.74	7
3	266.15	531.29	L	659.38	330.20	6
4	301.67	602.33	A	588.35	294.68	5
5	352.19	703.38	T	487.30	244.15	4
6	437.25	873.48	K Acetyl	317.19	159.10	3
7	472.76	944.52	A	246.16	123.58	2
8	508.28	1015.56	A	175.12	88.06	1
9	586.33	1171.66	R			

* = 126Da diagnostic ion