Figure 1

Fig. 1(A)

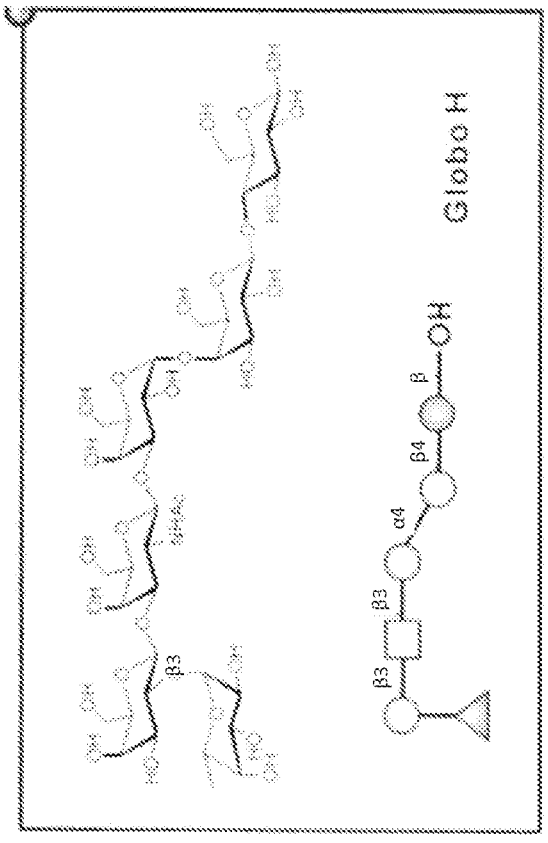


Fig. 1(B)



Figure 2

Fig. 2(A)

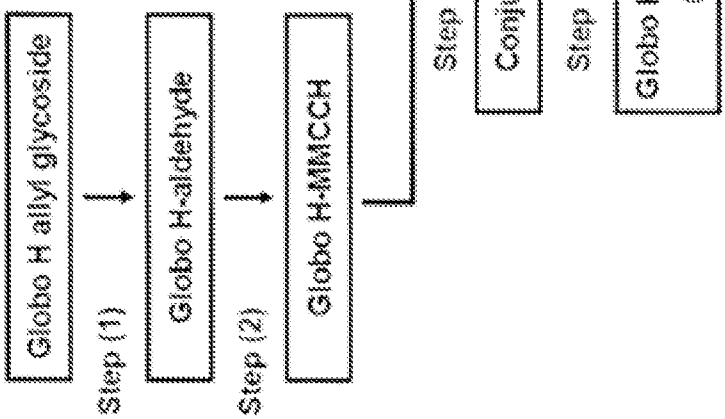


Fig. 2(B)

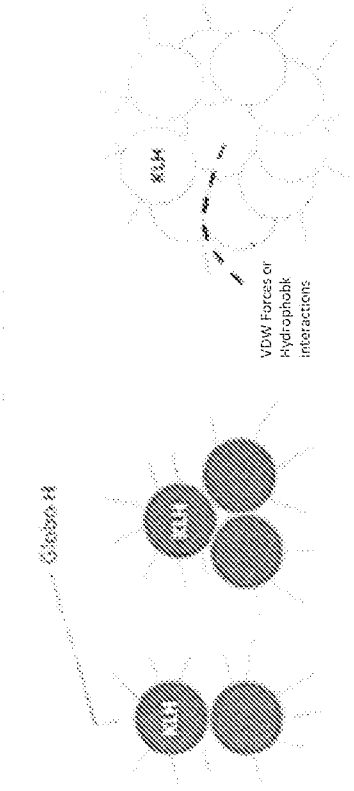


Figure 3

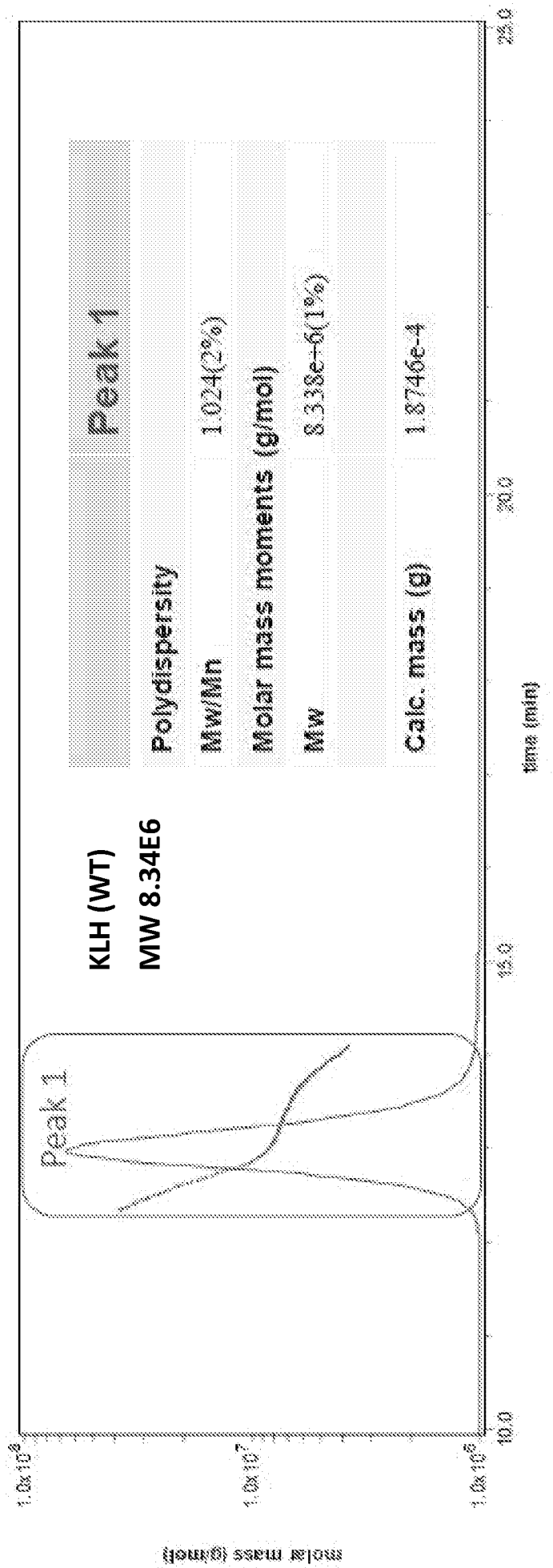

KLH (WT)
MW 8.34E6
Peak 1
Polydispersity
Mw/Mn 1.024(2%)
Molar mass moments (g/mol)
Mw 8.338e+6(1%)
Calc. mass (g) 1.8746e-4
Peak 1
1.0x10^8
1.0x10^7
1.0x10^6
molar mass (g/mol)
10.0
15.0
20.0
25.0
time (min)

Figure 4

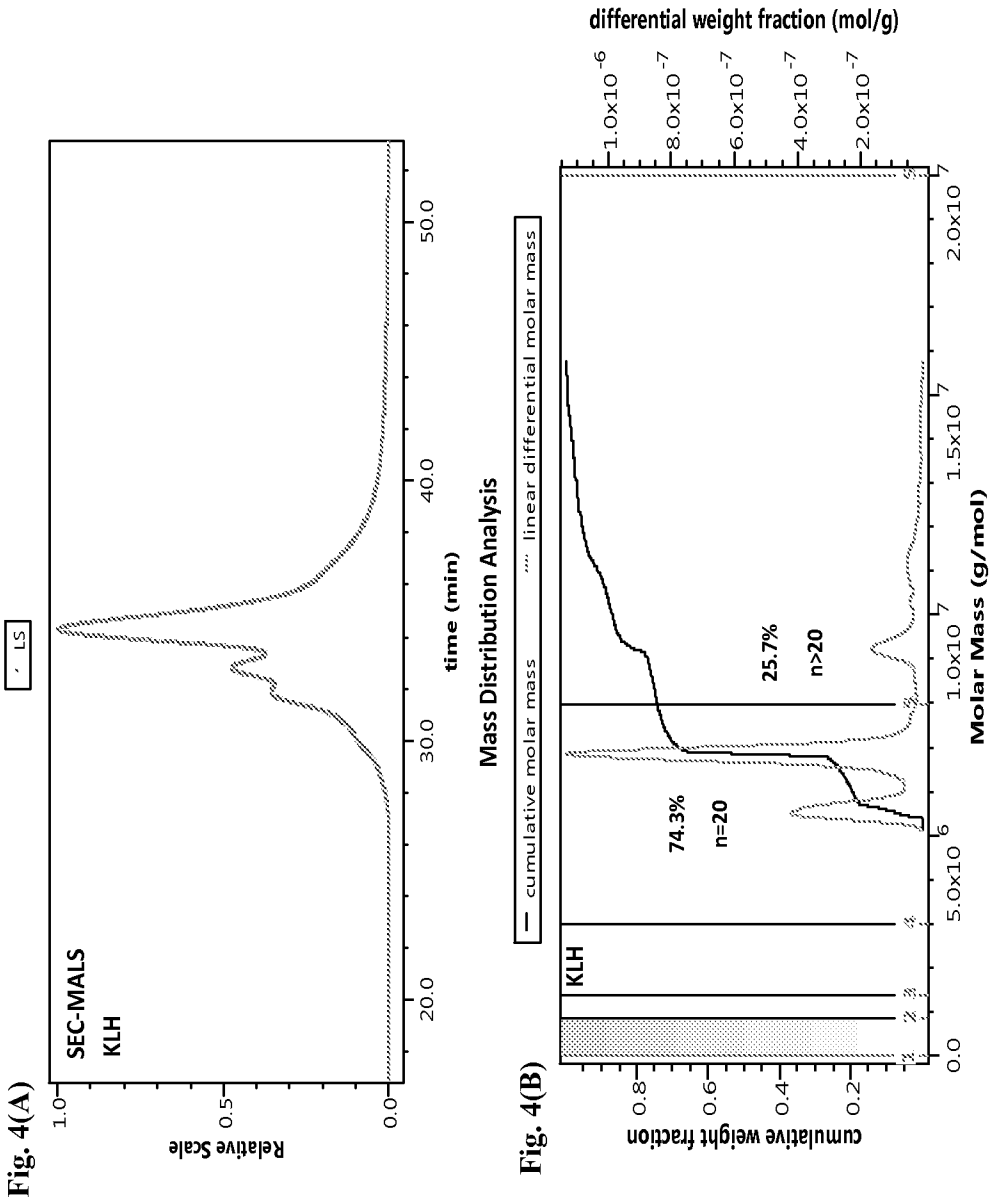

Fig. 4(A)
Size exclusion Chromatogram
LS
SEC-MALS
KLH
Relative Scale
1.0
0.5
0.0
20.0
30.0
40.0
50.0
time (min)
Fig. 4(B)
Mass Distribution Analysis
cumulative molar mass
linear differential molar mass
KLH
74.3%
n=20
25.7%
n>20
cumulative weight fraction
differential weight fraction (mol/g)
1.0x10-6
8.0x10-7
6.0x10-7
4.0x10-7
2.0x10-7
0.0
5.0x10
1.0x10
1.5x10
2.0x10
Molar Mass (g/mol)

Figure 4 (continued)

Fig. 4(C)

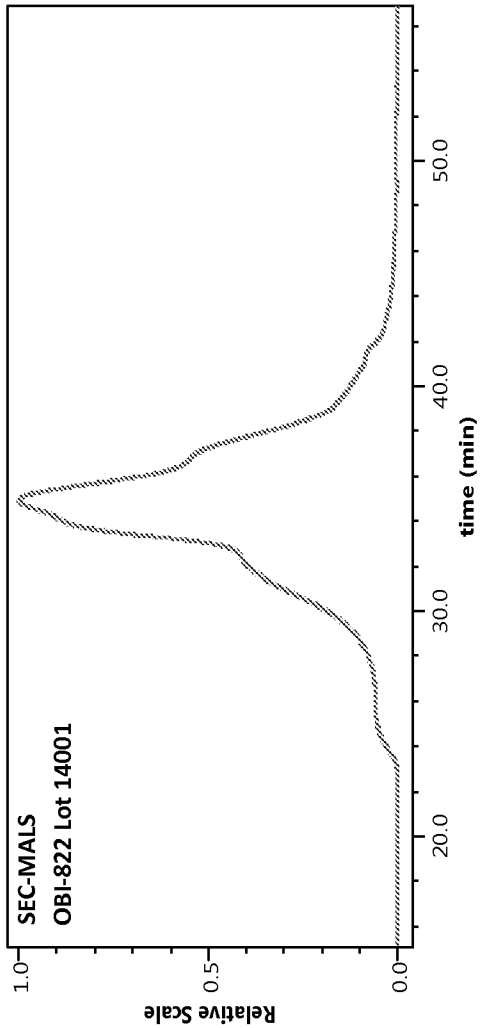


Fig. 4(D)

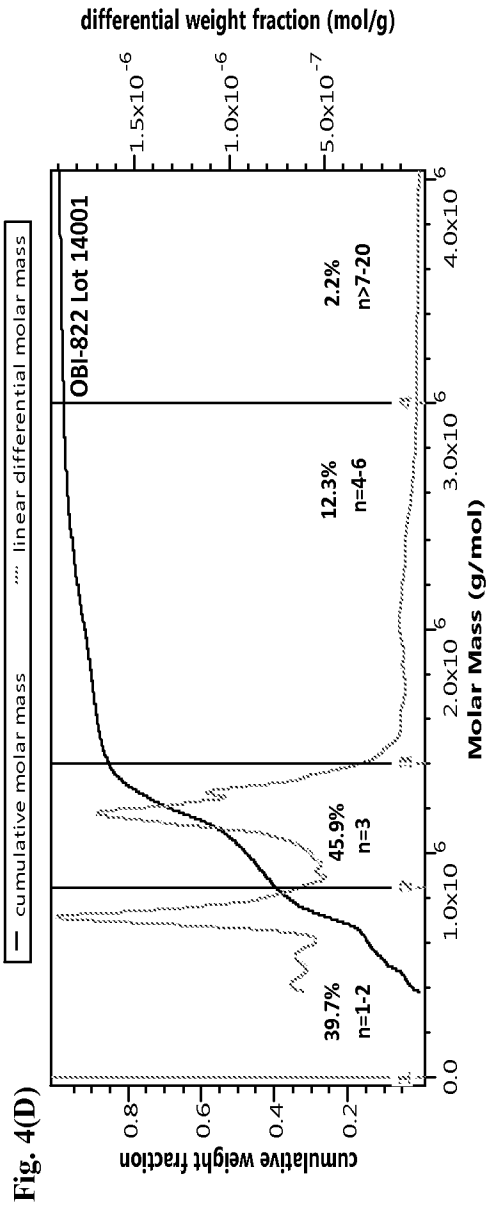


Figure 5

Fig. 5(A)

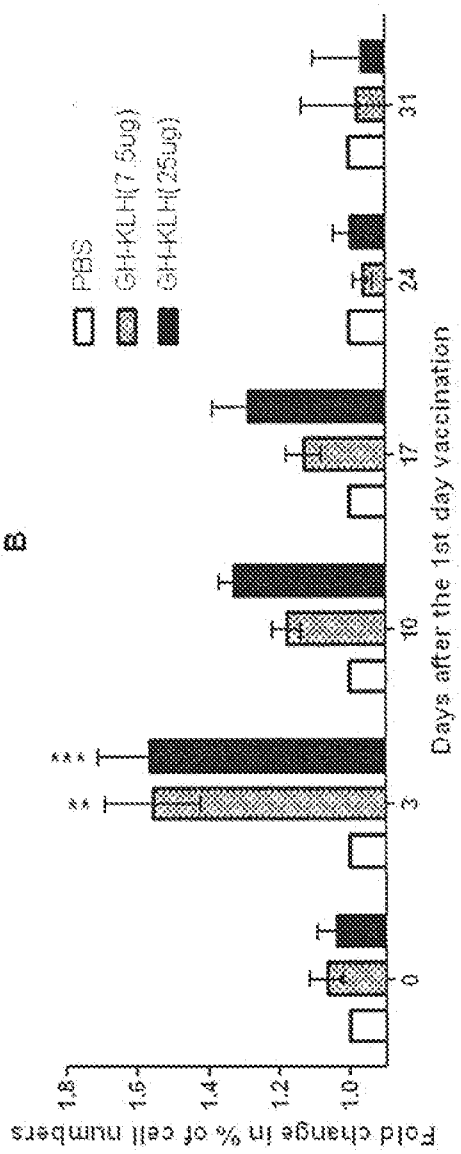


Figure 5 continued

Fig. 5(B)

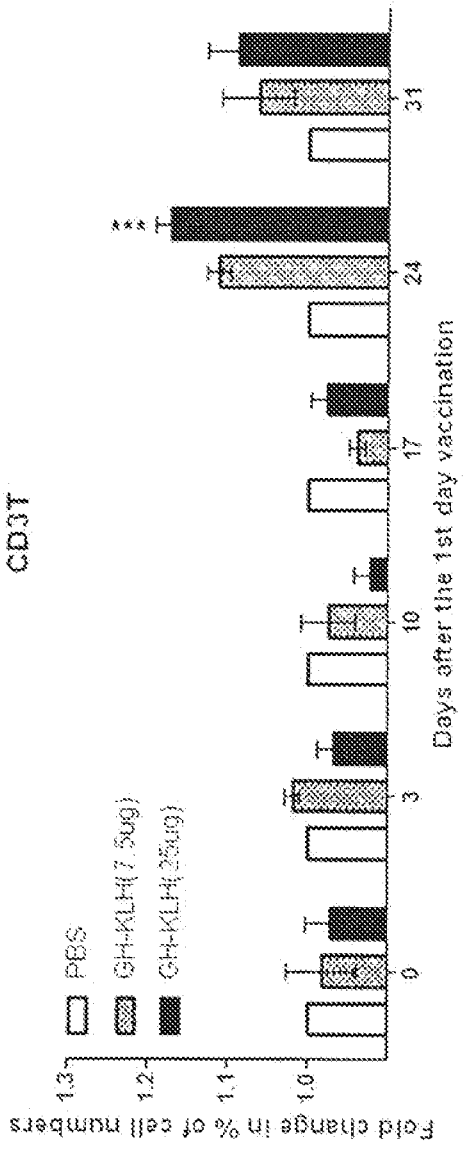


Figure 5 continued

Fig. 5(C)

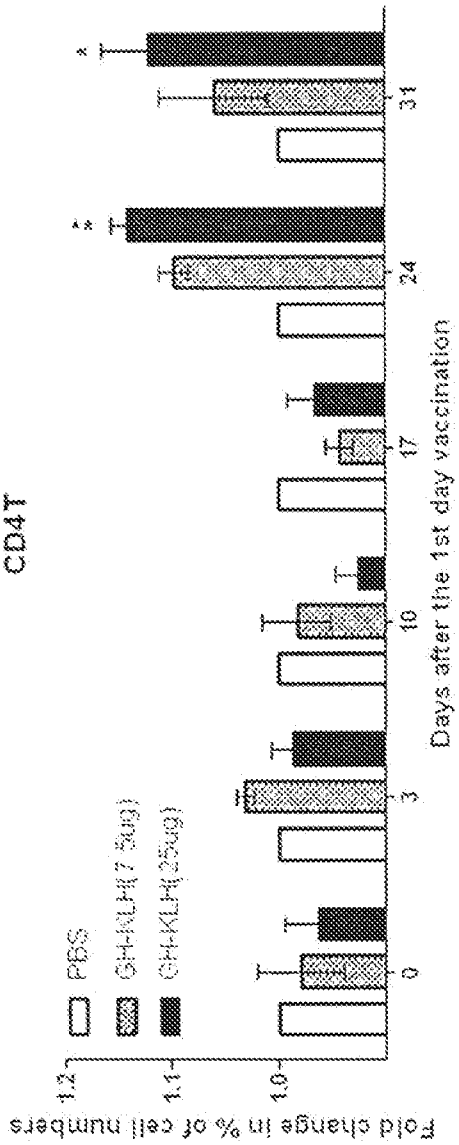


Figure 5 continued

Fig. 5(D)

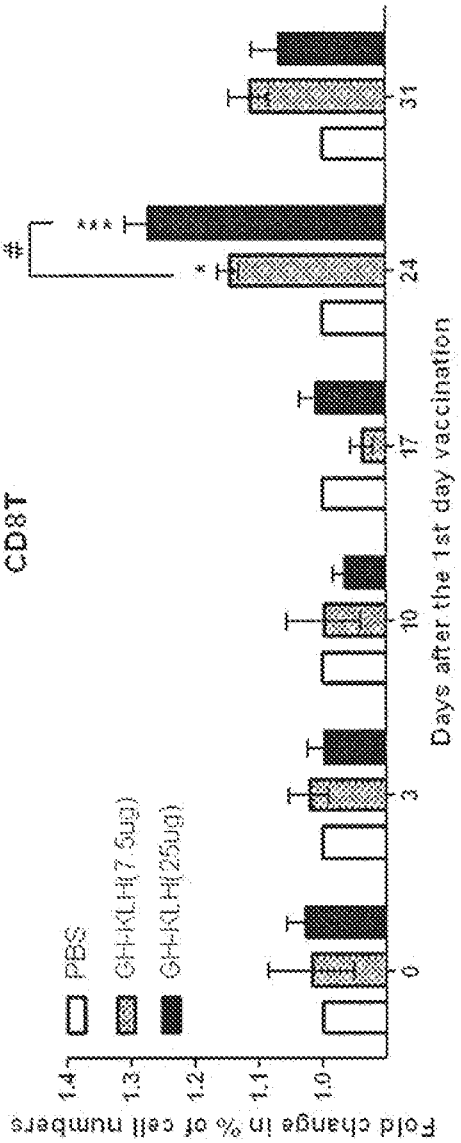


Figure 6

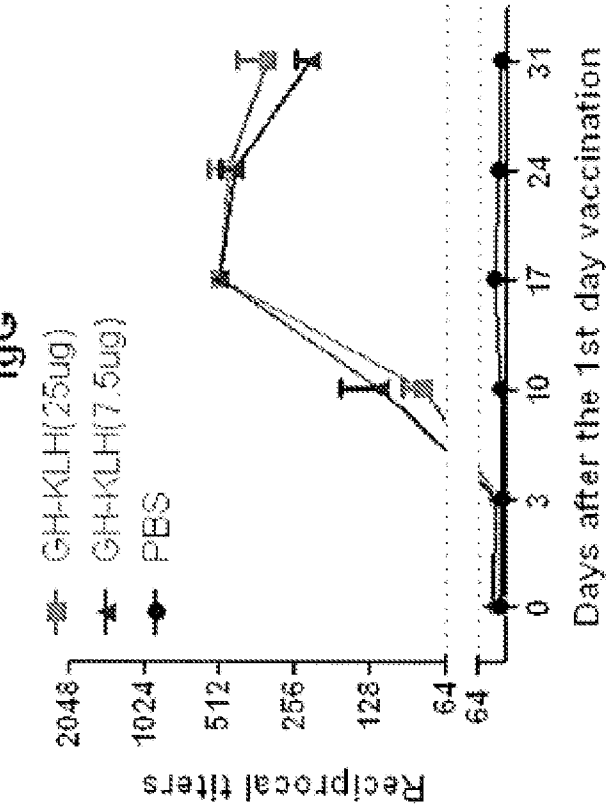


Figure 6B

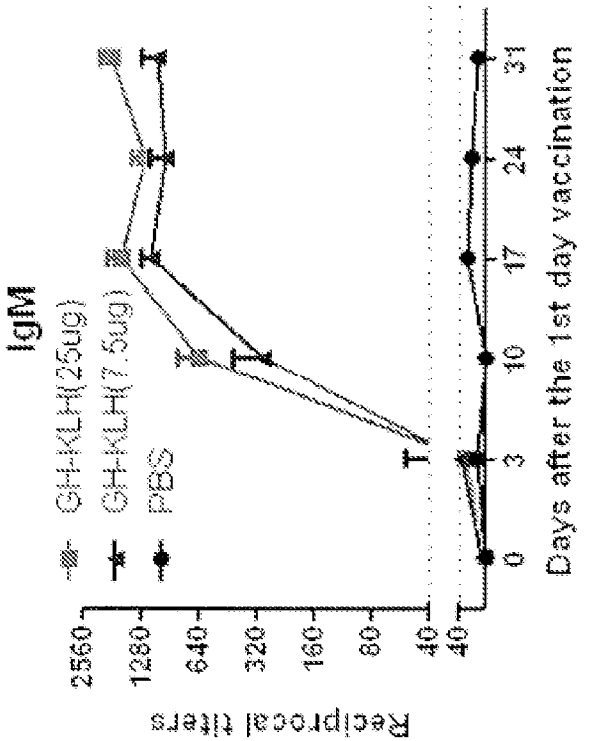


Figure 6A

Figure 7

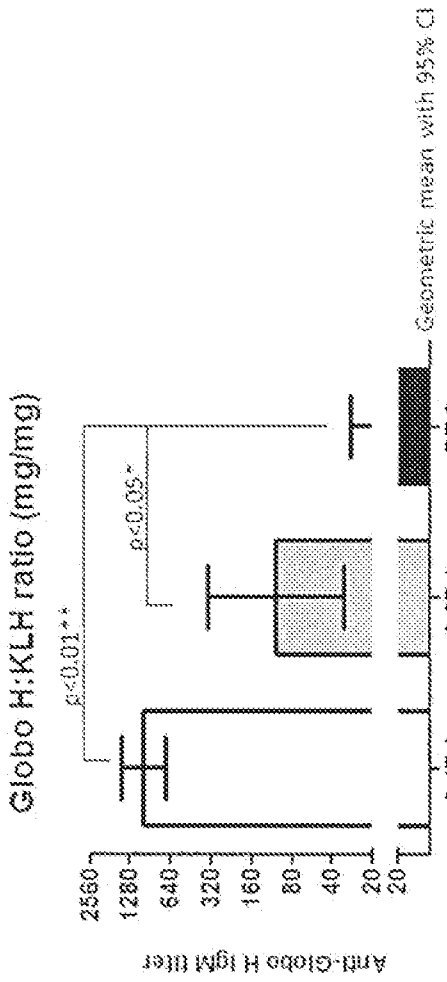

Globo H:KLH ratio (mg/mg)
p<0.01**
p<0.05*
Anti-Globo H IgM titer
2560
1280
640
320
160
80
40
20
20
0.17:1
0.07:1
PBS
Geometric mean with 95% CI

Figure 8

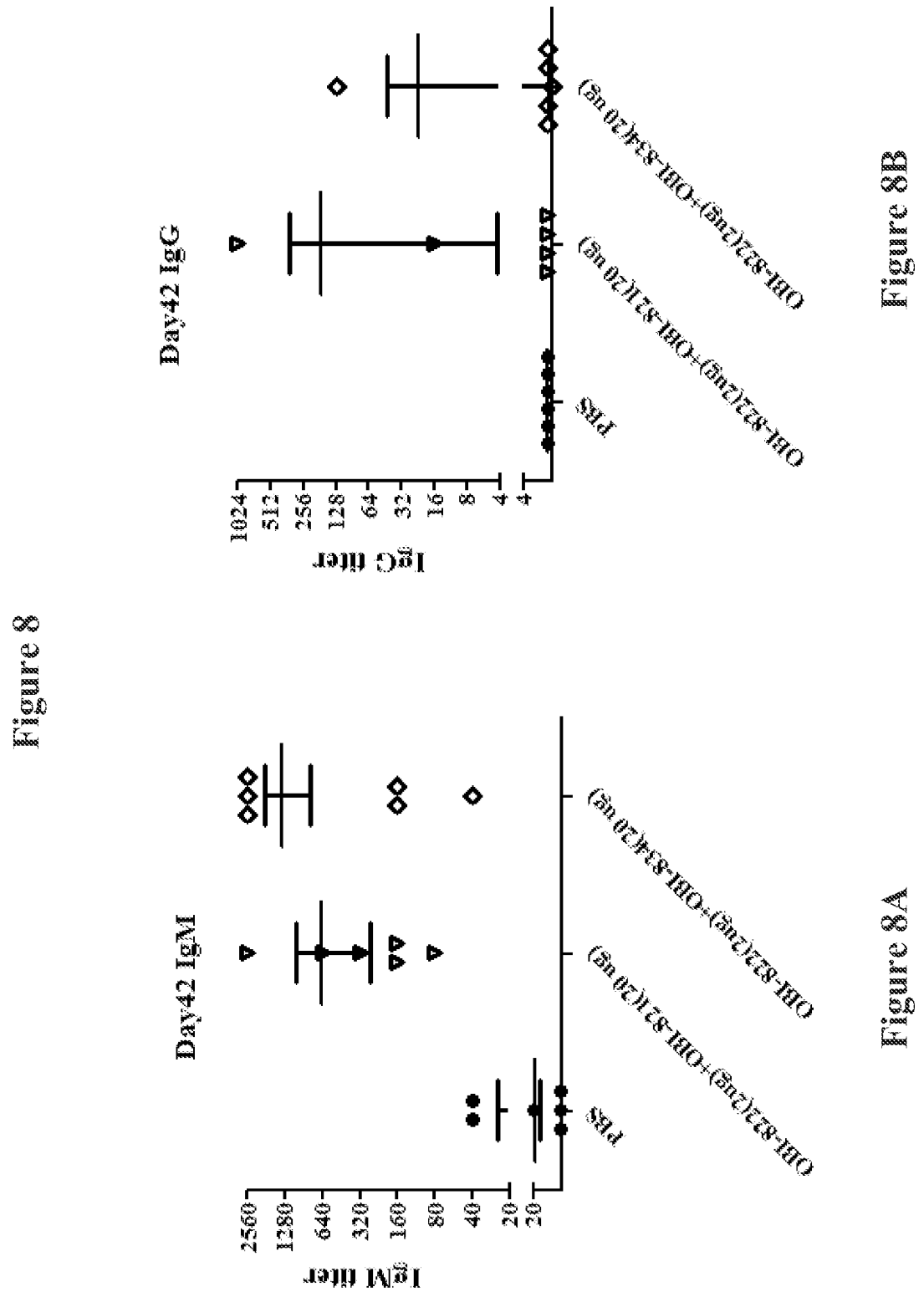


Figure 8A

Figure 8B

Figure 9

Fig. 9(A)

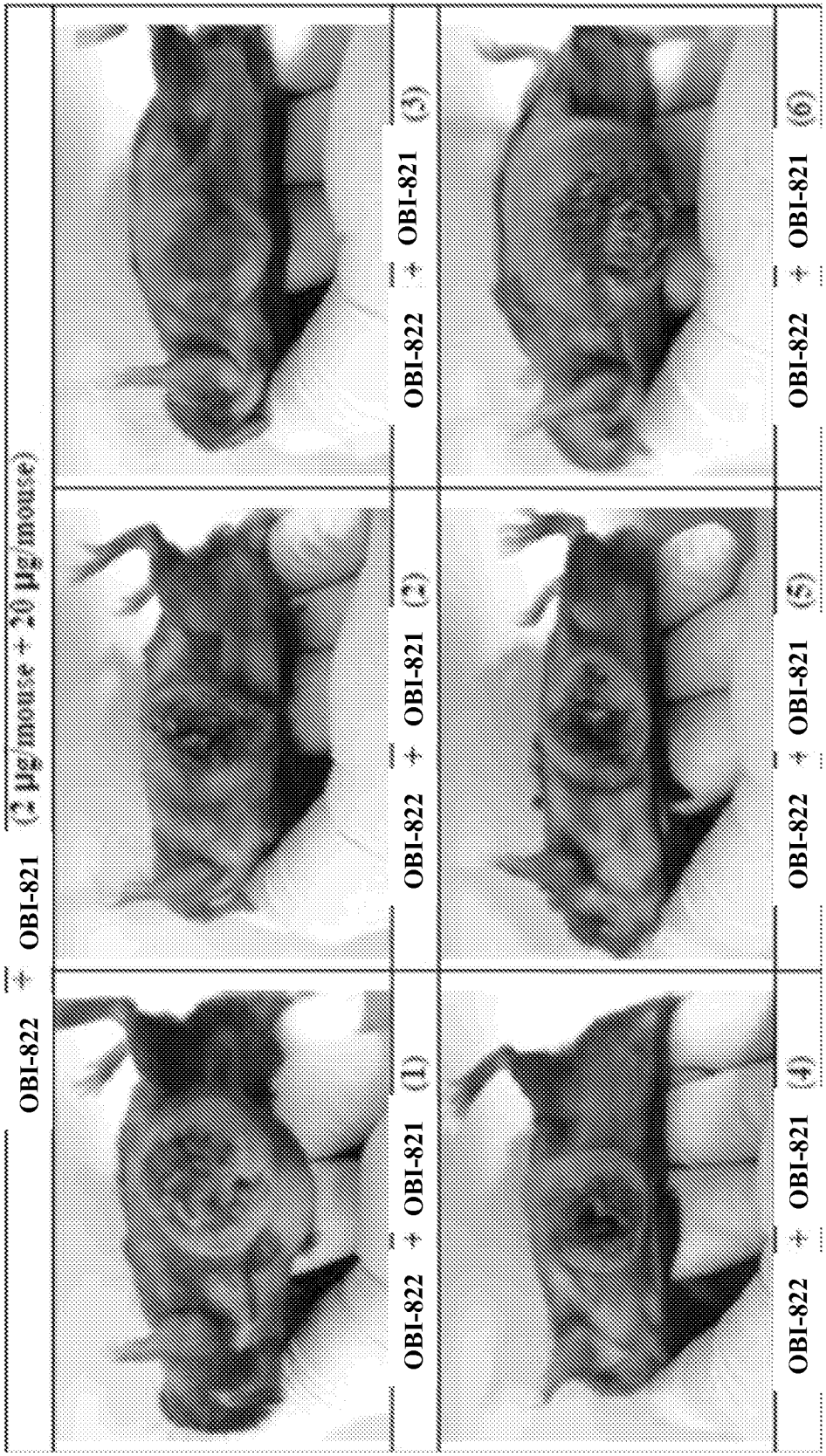


Figure 9 (continued)

Figure 9(B)

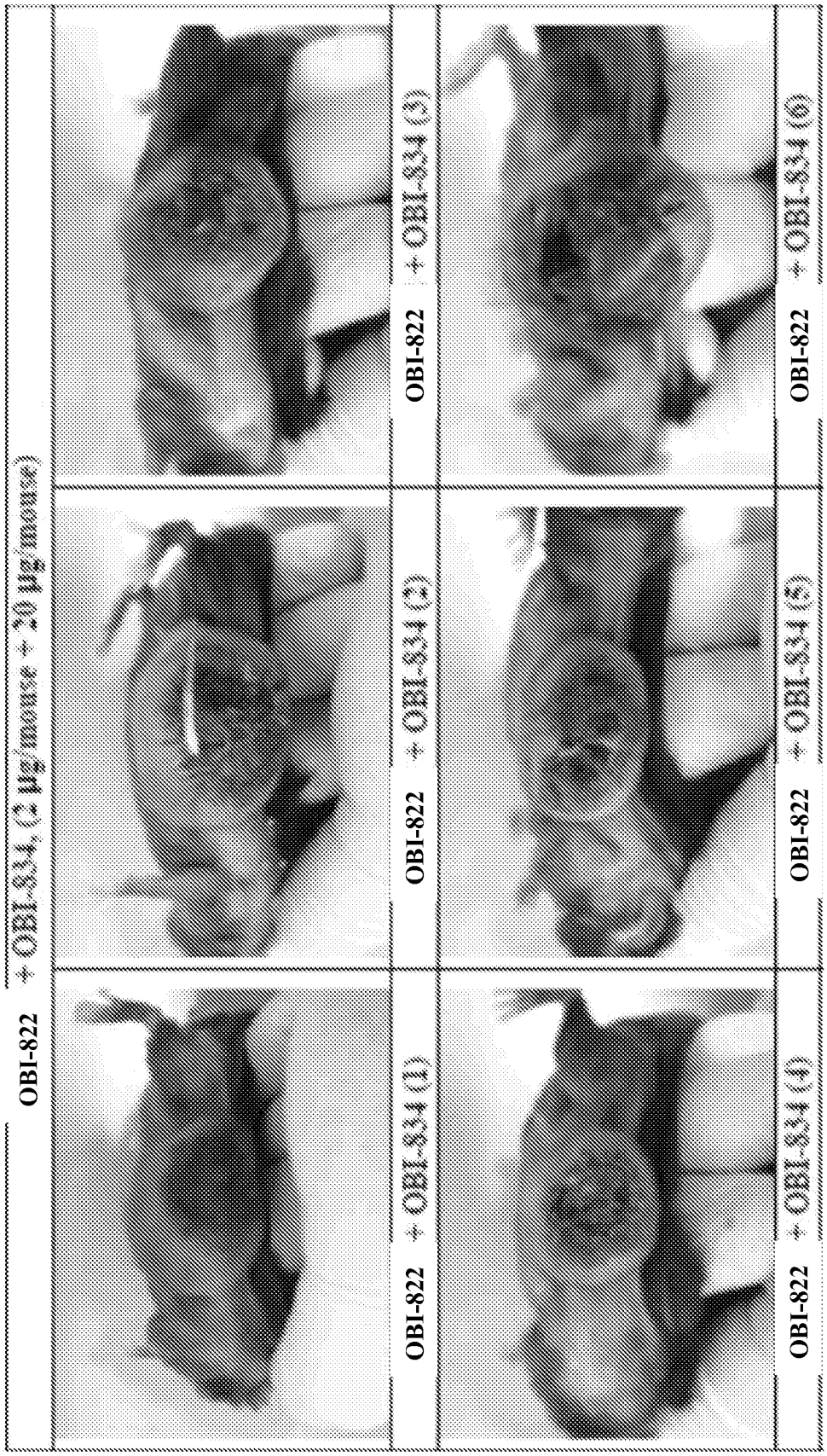


Figure 10

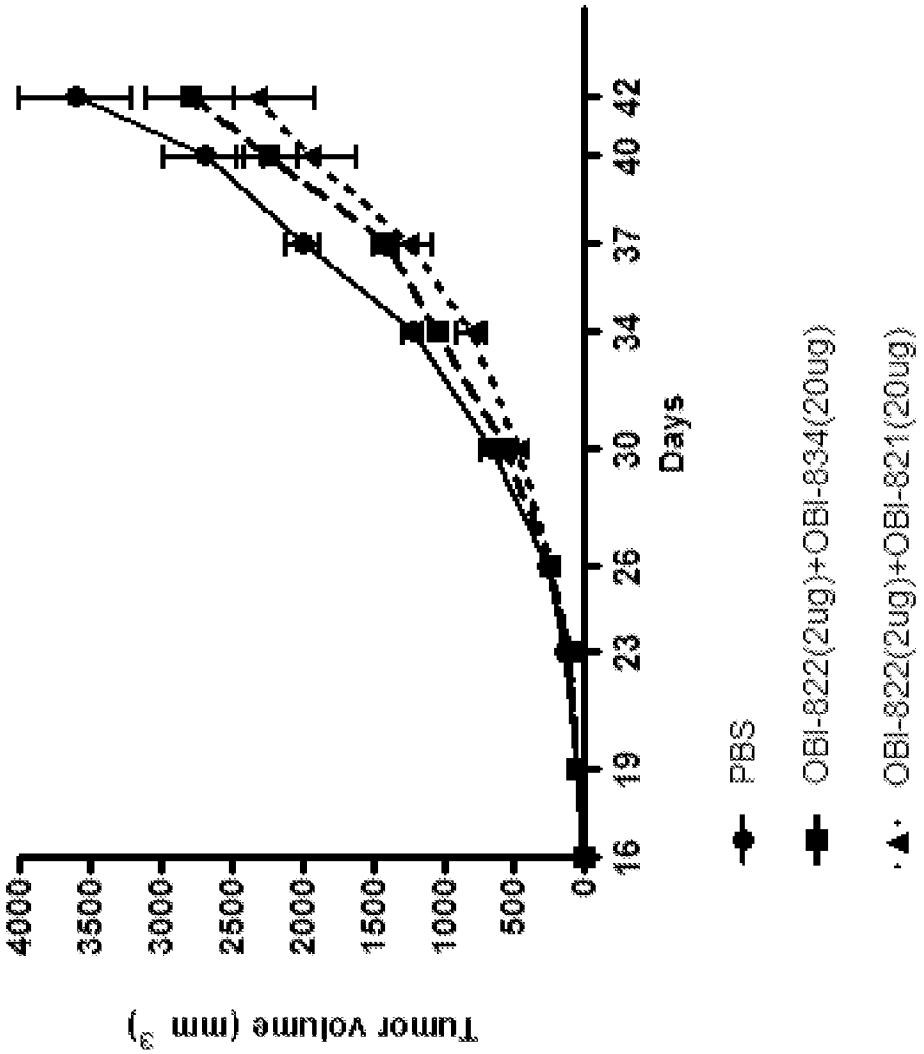
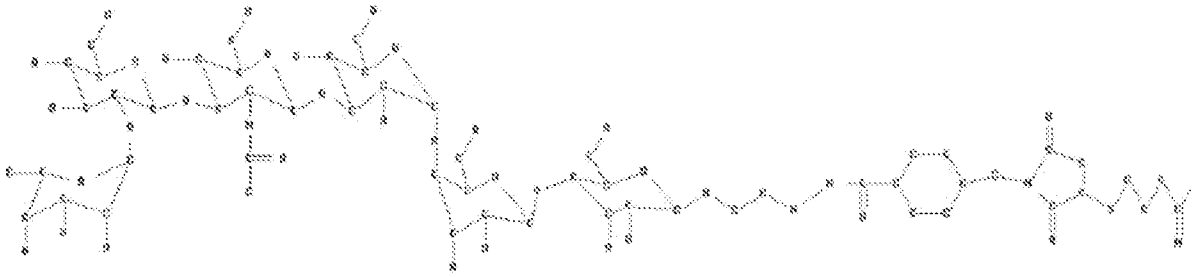

Tumor volume (mm 3)
4000
3500
3000
2500
2000
1500
1000
500
0
16
19
23
26
30
34
37
40
42
Days
PBS
OBI-822(2ug)+OBI-834(20ug)
OBI-822(2ug)+OBI-821(20ug)

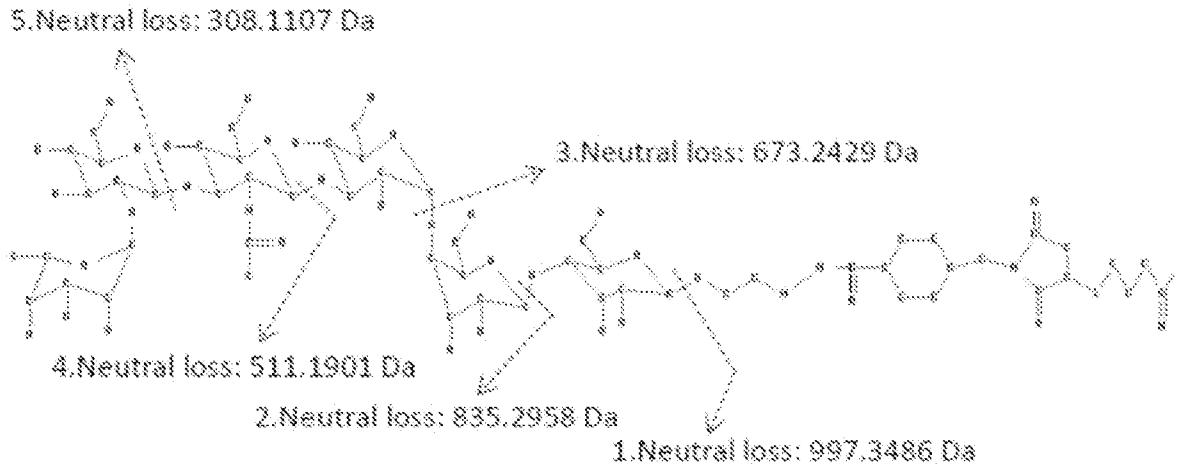
Figure 11

Figure 11A. Globo H derivative



Chemical formula: C(56) H(91) N(5) O(33) S(1)
Monoisotopic MW addition: 1393.5317 Da

Figure 11B. The neutral loss forms of Globo H derivative



1. Chemical formula: C(18) H(28) N(4) O(4) S(1)
   Monoisotopic MW addition: 396.1831 Da

2. Chemical formula: C(24) H(38) N(4) O(9) S(1)
   Monoisotopic MW addition: 558.2360 Da

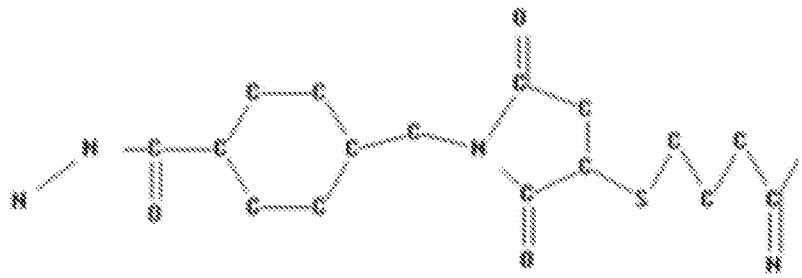
3. Chemical formula: C(30) H(48) N(4) O(14) S(1)
   Monoisotopic MW addition: 720.2888 Da

4. Chemical formula: C(36) H(58) N(4) O(19) S(1)
   Monoisotopic MW addition: 882.3416 Da

5. Chemical formula: C(44) H(71) N(5) O(24) S(1)
   Monoisotopic MW addition: 1085.4210 Da

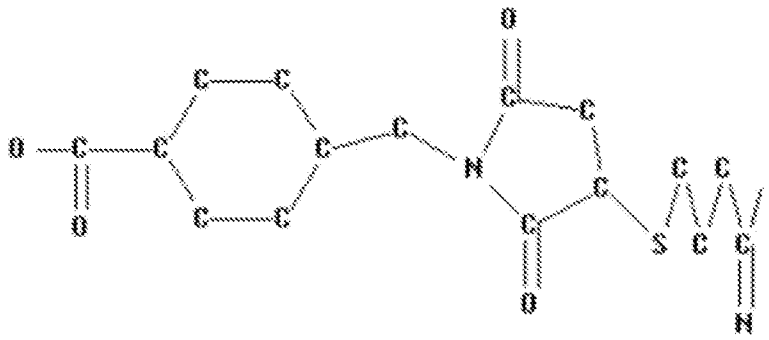
Figure 12

Figure 12A. MMCCH derivative



Chemical formula: C(16) H(24) N(4) O(3) S(1)
Monoisotopic MW addition: 352.1569 Da

Figure 12B. Deamidated MMCCH derivative



Chemical formula: C(16) H(22) N(2) O(4) S(1)
Monoisotopic MW addition: 338.1300 Da

Figure 13

Figure 13A. Globo H derivative analysis

Sample	1st LC-MS/MS	2nd LC-MS/MS
1	Figure 14	Figure 18
2	Figure 15	Figure 19
3	Figure 16	Figure 20
4	Figure 17	Figure 21

Figure 13B. MMCCH derivative analysis

Sample	1st LC-MS/MS	2nd LC-MS/MS
1	Figure 22	Figure 26
2	Figure 23	Figure 27
3	Figure 24	Figure 28
4	Figure 25	Figure 29

Figure 14. Identification details of Globo H-conjugated peptides for sample 1 (1st LC-MS/MS)

Table 14A. KLH 1

#	Start	End	Observed	Mr(expt)	Mr(calc)	ppm	Enzyme	MC	Score	E value	Peptide	Mod_site
1	142	149	847.4247	1692.8349	1692.8240	6.44	T	1	17	0.02	KNINDLTR +K_MMCCH_NL673 (K)	142
2	157	166	851.9063	1701.7981	1701.7933	2.82	T	1	14	0.039	EAFHKFQEDR +K_MMCCH_NL997 (K)	161
3	588	606	1132.8336	3395.4790	3395.4862	-2.09	T	1	16	0.022	EDKSAGGFQQLGAFHGEPK +Globo_H_MMCCH (K)	590
4	700	719	1015.1623	3042.4652	3042.4532	3.94	T	1	27	0.0019	SVQNKLFEQPEFGHYTSIAK +K_MMCCH_NL673 (K)	719
5	953	965	762.7177	2285.1311	2285.1249	2.71	T	1	52	6.30E-06	DLFKQPSVIHEPR +K_MMCCH_NL673 (K)	956
6	986	1000	1036.8300	3107.4681	3107.4578	3.31	T	1	20	0.011	KNIENLSLGELESLR +Globo_H_MMCCH (K)	986
7	1092	1114	806.3826	3221.5014	3221.5213	-6.18	T	1	24	0.0038	QHHYETNPFHHGKITHENEITTR +K_MMCCH_NL997 (K)	1104
8	1473	1489	905.7906	2714.3499	2714.3414	3.13	T	1	25	0.0034	KHGAVVGLPYWDWTLPR +K_MMCCH_NL673 (K)	1473
9	1923	1932	793.8990	1585.7834	1585.7745	5.68	T	1	17	0.02	NKVMPNPFAR +Deamidated (NQ); K_MMCCH_NL997 (K); Oxidation (M)	1924
10	2359	2367	846.4022	1690.7898	1690.7872	1.54	T	1	19	0.011	DKLFNDPER +K_MMCCH_NL835 (K)	2360
11	2851	2883	1027.9812	4107.8957	4107.8666	7.08	T	0	62	6.30E-07	VKPAHAGSCAGDIMHVPLHPFNYESVNNDDFTR +Deamidated (NQ); K_MMCCH_NL997 (K); Oxidation (M)	2852
12	2897	2919	814.6600	3254.6108	3254.5818	8.91	T	1	39	0.00012	FNYKYDNLNLHGHNIEELEEVLR +K_MMCCH_NL997 (K)	2900
13	3003	3021	953.1623	2856.4650	2856.4467	6.44	T	1	31	0.00072	KYDHTELDASVLPAPIIVR +K_MMCCH_NL673 (K)	3003
14	613	626	1151.5167	2301.0189	2301.0150	1.69	Th	5	13	0.05	ASKKFACCVHGMSV +K_MMCCH_NL673 (K)	616

Figure 14B. KLH 2

#	Start	End	Observed	Mr(expt)	Mr(calc)	ppm	Enzyme	MC	Score	E value	Peptide	Mod_site
1	26	41	1047.4908	3139.4507	3139.4364	4.55	T	1	27	0.002	KNVDSLSSDEVLALEK +Globo_H_MMCCH (K)	26
2	164	175	615.6599	1843.9579	1843.9516	3.42	T	1	37	0.00019	LFEKVQPGHHTR +K_MMCCH_NL997 (K)	167
3	249	271	1012.4535	3034.3386	3034.3371	0.49	T	1	26	0.0024	GKDPNSADCAHNLIHTPMEPFDR +Deamidated (NQ); K_MMCCH_NL997 (K); Oxidation (M)	250
4	281	293	630.2952	1887.8639	1887.8574	3.44	T	0	44	4.00E-05	EHAKPADSFDYGR +K_MMCCH_NL997 (K)	284
5	419	446	942.0073	3763.9999	3763.9720	7.44	T	1	28	0.0015	QPTLVHRPAKGHFDKPPVPVAQANLAVR +Deamidated (NQ); K_MMCCH_NL673 (K)	433
6	463	488	1131.8618	3392.5636	3392.5918	-8.28	T	2	73	5.20E-08	AMERFQNDKSVDGYQATVEFHALPAR +Deamidated (NQ); K_MMCCH_NL997 (K); Oxidation (M)	471
7	1097	1115	1008.4838	3022.4295	3022.4216	2.58	T	0	60	1.00E-06	KPLQPFGLDSVINPDDETR +K_MMCCH_NL511 (K)	1097
8	1123	1149	1157.0266	4624.0773	4624.0513	5.62	T	1	39	0.00013	VFDYKNNFDYEYESLAFNGLSIAQLDR +Globo_H_MMCCH (K)	1127
9	1355	1385	1217.5632	4866.2238	4866.1892	7.11	T	1	18	0.016	GSAVAVPYWDWTEKADSLPSLINDATYFNSR +Globo_H_MMCCH (K)	1368
10	1455	1480	853.1725	3408.6609	3408.6601	0.21	T	1	30	0.0009	AKYSLSSLDYTAFDPVFFLHHANVDR +K_MMCCH_NL997 (K)	1456
11	1508	1539	841.0049	4199.9883	4199.9680	4.83	T	1	30	0.0011	KPLQPFNNPELNSDSMTLKHNLPQDSFDYQNR +Deamidated (NQ); K_MMCCH_NL997 (K); Oxidation (M)	1526
12	1949	1963	574.7631	2295.0234	2295.0266	-1.44	T	0	51	8.30E-06	TQEFSKPEDTFDYHR +K_MMCCH_NL997 (K)	1954
13	1292	1303	908.4932	1814.9719	1814.9713	0.39	G	0	28	0.0015	SIRSAFLQIQKE +K_MMCCH_NL997 (K)	1302
14	1681	1691	839.9299	1677.8453	1677.8508	-3.28	G	0	15	0.032	GLSQHNLVRKE +2 Deamidated (NQ); K_MMCCH_NL997 (K)	1690
15	1589	1606	1136.1545	3405.4418	3405.4409	0.26	C	0	23	0.005	ICVEQGGEQNCKTKAGSF +Globo_H_MMCCH (K)	1602
16	1985	1995	586.6397	1756.8973	1756.8930	2.45	C	0	18	0.014	IKQQQEADRVF +K_MMCCH_NL997 (K)	1986
17	431	437	760.3697	1518.7248	1518.7164	5.60	Th	1	15	0.033	FDKPPVP +K_MMCCH_NL673 (K)	433
18	1496	1509	1047.4484	2092.8822	2092.9016	-9.27	Th	4	13	0.049	YNEADCAVNEMRKP +Deamidated (NQ); K_MMCCH_NL997 (K)	1508

"Start" and "End" indicates the number of residue of KLH1 or KLH2. "Observed" column implies the observed m/z value in the survey scan while "Mr(expt)", "Mr(calc)", "ppm" indicate the experimental molecular weight(MW), calculated MW, and the difference between observed MW and theoretical MW respectively. In the "Enzyme" column, T, C, G and Th stand for trypsin, chymotrypsin, Glu-C and thermolysin respectively. MC stands for missed cleavage. Scores are the peptide ion score directly reported from Mascot database search engine. E value denotes the expectation value for each identified peptide. The peptide sequences as well as its modifications are listed in "Peptide" column. "Mod_site" indicates the amino acid site of K in which identified as Globo_H_MMCCH, K_MMCCH_NL308, K_MMCCH_NL511, K_MMCCH_NL673, K_MMCCH_NL835, or K_MMCCH_NL997 modified for KLH1 or KLH2 sequence.

Figure 15. Identification details of Globo H-conjugated peptides for sample 2 (1st LC-MS/MS)

Figure 15A. KLH 1

#	Start	End	Observed	Mr(expt)	Mr(calc)	ppm	Enzyme	MC	Score	E value	Peptide	Mod_site
1	588	606	1132.8397	3395.4973	3395.4862	3.30	T	1	25	0.0035	EDKSAGGFQQLGAFHGEPK +Globo_H_MMCCH (K)	590
2	700	719	1069.1805	3204.5198	3204.5060	4.31	T	1	28	0.0016	SVQNKLFEQPEFGHYTSIAK +K_MMCCH_NL511 (K)	719
3	953	965	654.6852	1961.0337	1961.0193	7.34	T	1	42	6.00E-05	DLFKQPSVIHEPR +K_MMCCH_NL997 (K)	956
4	1092	1114	645.3080	3221.5038	3221.5213	-5.43	T	1	29	0.0013	QHHYETNPFHHGKITHENEITTR +K_MMCCH_NL997 (K)	1104
5	1923	1932	793.8966	1585.7787	1585.7745	2.65	T	1	14	0.04	NKVMPNPFAR +Deamidated (NQ); K_MMCCH_NL997 (K); Oxidation (M)	1924
6	2233	2251	721.5986	2882.3652	2882.3776	-4.30	T	2	60	9.30E-07	KEINTLTTAEVDNLKDAMR +Deamidated (NQ); K_MMCCH_NL673 (K)	2247
7	2851	2883	1027.9795	4107.8889	4107.8666	5.43	T	0	32	0.00058	VKPAHAGSCAGDIMHVPLHPFNYESVNNDDFTR +Deamidated (NQ); K_MMCCH_NL997 (K); Oxidation (M)	2852
8	158	169	733.6753	2198.0042	2197.9838	9.33	G	2	32	0.00064	AFHKFQEDRSVD +K_MMCCH_NL673 (K)	161
9	474	480	568.7975	1135.5804	1135.5808	-0.35	Th	1	16	0.024	VQHKAGT +K_MMCCH_NL997 (K)	477

Figure 15B. KLH 2

#	Start	End	Observed	Mr(expt)	Mr(calc)	ppm	Enzyme	MC	Score	E value	Peptide	Mod_site
1	26	41	1047.4899	3139.4478	3139.4364	3.63	T	1	29	0.0013	KNVDSLSSDEVLALEK +Globo_H_MMCCH (K)	26
2	164	175	615.6570	1843.9493	1843.9516	-1.25	T	1	36	0.00026	LFEKVQPGHHTR +K_MMCCH_NL997 (K)	167
3	249	280	1015.9750	4059.8708	4059.8513	4.80	T	2	26	0.0025	GKDPNSADCAHNLIHTPMEPFDRDTNPLDLTR +Deamidated (NQ); K_MMCCH_NL997 (K); Oxidation (M)	250
4	281	293	630.2964	1887.8673	1887.8574	5.30	T	0	50	1.10E-05	EHAKPADSFDYGR +K_MMCCH_NL997 (K)	284
5	467	488	1125.8617	3374.5632	3374.5500	3.91	T	1	69	1.10E-07	FQNDKSVDGYQATVEFHALPAR +K_MMCCH_NL511 (K)	471
6	1097	1115	847.0916	2538.2530	2538.2312	8.59	T	0	42	6.00E-05	KPLQPFGLDSVINPDDETR +2 Deamidated (NQ); K_MMCCH_NL997 (K)	1097
7	1123	1149	1157.0225	4624.0607	4624.0513	2.03	T	1	35	0.00033	VFDYKNNFDYEYESLAFNGLSIAQLDR +Globo_H_MMCCH (K)	1127
8	1455	1480	853.1709	3408.6545	3408.6601	-1.64	T	1	26	0.0026	AKYSLSSLDYTAFDPVFFLHHANVDR +K_MMCCH_NL997 (K)	1456
9	1508	1539	840.9999	4199.9633	4199.9680	-1.12	T	1	33	0.00054	KPLQPFNNPELNSDSMTLKHNLPQDSFDYQNR +Deamidated (NQ); K_MMCCH_NL997 (K); Oxidation (M)	1526
10	1949	1963	766.0179	2295.0318	2295.0266	2.27	T	0	29	0.0013	TQEFSKPEDTFDYHR +K_MMCCH_NL997 (K)	1954
11	1985	1995	586.6395	1756.8968	1756.8930	2.11	C	0	19	0.014	IKQQQEADRVF +K_MMCCH_NL997 (K)	1986
12	2463	2479	1104.1498	3309.4275	3309.4269	0.18	C	1	20	0.01	KAQSIHPEDVFDTDAPF +Globo_H_MMCCH (K)	2463

"Start" and "End" indicates the number of residue of KLH1 or KLH2. "Observed" column implies the observed m/z value in the survey scan while "Mr(expt)", "Mr(calc)", "ppm" indicate the experimental molecular weight(MW), calculated MW, and the difference between observed MW and theoretical MW respectively. In the "Enzyme" column, T, C, G and Th stand for trypsin, chymotrypsin, Glu-C and thermolysin respectively. MC stands for missed cleavage. Scores are the peptide ion score directly reported from Mascot database search engine. E value denotes the expectation value for each identified peptide. The peptide sequences as well as its modifications are listed in "Peptide" column. "Mod_site" indicates the amino acid site of K in which identified as Globo_H_MMCCH, K_MMCCH_NL308, K_MMCCH_NL511, K_MMCCH_NL673, K_MMCCH_NL835, or K_MMCCH_NL997 modified for KLH1 or KLH2 sequence.

Figure 16. Identification details of Globo H-conjugated peptides for sample 3 (1st LC-MS/MS)

Figure 16A. KLH 1

#	Start	End	Observed	Mr(expt)	Mr(calc)	ppm	Enzyme	MC	Score	E value	Peptide	Mod_site
1	377	402	852.1614	3404.6167	3404.6104	1.85	T	0	18	0.017	AHCAISLEHMHLKPFAFSSPLNNNEK +Deamidated (NQ); K_MMCCH_NL997 (K); Oxidation (M)	402
2	1092	1114	887.4109	3545.6145	3545.6270	-3.53	T	1	14	0.041	QHHYETNPFHHGKITHENEITTR +K_MMCCH_NL673 (K)	1104
3	1092	1114	806.3819	3221.4985	3221.5213	-7.08	T	1	27	0.002	QHHYETNPFHHGKITHENEITTR +K_MMCCH_NL997 (K)	1104
4	2233	2251	721.5988	2882.3662	2882.3776	-3.96	T	2	45	3.30E-05	KEINTLTTAEVDNLKDAMR +Deamidated (NQ); K_MMCCH_NL673 (K)	2247
5	2851	2883	1027.9769	4107.8786	4107.8666	2.92	T	0	46	2.60E-05	VKPAHAGSCAGDIMHVPLHPFNYESVNNDDFTR +Deamidated (NQ); K_MMCCH_NL997 (K); Oxidation (M)	2852

Figure 16B. KLH 2

#	Start	End	Observed	Mr(expt)	Mr(calc)	ppm	Enzyme	MC	Score	E value	Peptide	Mod_site
1	1097	1115	847.0920	2538.2543	2538.2312	9.10	T	0	34	0.00043	KPLQPFGLDSVINPDDETR +2 Deamidated (NQ); K_MMCCH_NL997 (K)	1097
2	1355	1385	1217.5588	4866.2063	4866.1892	3.49	T	1	23	0.0047	GSAVAVPYWDWTEKADSLPSLINDATYFNSR +Globo_H_MMCCH (K)	1368
3	1508	1539	841.0057	4199.9920	4199.9680	5.71	T	1	46	2.60E-05	KPLQPFNNPELNSDSMTLKHNLPQDSFDYQNR +Deamidated (NQ); K_MMCCH_NL997 (K); Oxidation (M)	1526
4	1949	1963	766.0202	2295.0388	2295.0266	5.27	T	0	37	0.0002	TQEFSKPEDTFDYHR +K_MMCCH_NL997 (K)	1954
5	2463	2479	1104.1526	3309.4359	3309.4269	2.72	C	1	17	0.019	KAQSIHPEDVFDTDAPF +Globo_H_MMCCH (K)	2463
6	2438	2447	1110.4959	2218.9771	2218.9749	0.99	Th	3	13	0.05	FILGGSKEMH +K_MMCCH_NL308 (K); Oxidation (M)	2444

"Start" and "End" indicates the number of residue of KLH1 or KLH2. "Observed" column implies the observed m/z value in the survey scan while "Mr(expt)", "Mr(calc)", "ppm" indicate the experimental molecular weight(MW), calculated MW, and the difference between observed MW and theoretical MW respectively. In the "Enzyme" column, T, C, G and Th stand for trypsin, chymotrypsin, Glu-C and thermolysin respectively. MC stands for missed cleavage. Scores are the peptide ion score directly reported from Mascot database search engine. E value denotes the expectation value for each identified peptide. The peptide sequences as well as its modifications are listed in "Peptide" column. "Mod_site" indicates the amino acid site of K in which identified as Globo_H_MMCCH, K_MMCCH_NL308, K_MMCCH_NL511, K_MMCCH_NL673, K_MMCCH_NL835, or K_MMCCH_NL997 modified for KLH1 or KLH2 sequence.

Figure 17. Identification details of Globo H-conjugated peptides for sample 4 (1st LC-MS/MS)

Figure 17A. KLH 1

#	Start	End	Observed	Mr(expt)	Mr(calc)	ppm	Enzyme	MC	Score	E value	Peptide	Mod_site
1	377	402	1135.8804	3404.6193	3404.6104	2.61	T	0	41	8.80E-05	AHCAISLEHMHLKPFAFSSPLNNNEK +Deamidated (NQ); K_MMCCH_NL997 (K); Oxidation (M)	402
2	953	965	654.6849	1961.0330	1961.0193	6.99	T	1	27	0.0021	DLFKQPSVIHEPR +K_MMCCH_NL997 (K)	956
3	1092	1114	806.3821	3221.4995	3221.5213	-6.80	T	1	18	0.015	QHHYETNPFHHGKITHENEITTR +K_MMCCH_NL997 (K)	1104
4	1923	1932	793.8979	1585.7812	1585.7745	4.29	T	1	17	0.021	NKVMPNPFAR +Deamidated (NQ); K_MMCCH_NL997 (K); Oxidation (M)	1924
5	2233	2251	721.5987	2882.3657	2882.3776	-4.16	T	2	41	7.90E-05	KEINTLTTAEVDNLKDAMR +Deamidated (NQ); K_MMCCH_NL673 (K)	2247
6	2359	2367	927.4296	1852.8447	1852.8400	2.54	T	1	21	0.0082	DKLFNDPER +K_MMCCH_NL673 (K)	2360
7	2851	2883	1027.9815	4107.8967	4107.8666	7.33	T	0	30	0.00094	VKPAHAGSCAGDIMHVPLHPFNYESVNNDDFTR +Deamidated (NQ); K_MMCCH_NL997 (K); Oxidation (M)	2852
8	506	512	850.4159	1698.8173	1698.8009	9.71	Th	2	14	0.037	LKDLDLT +K_MMCCH_NL511 (K)	507

Figure 17B. KLH 2

#	Start	End	Observed	Mr(expt)	Mr(calc)	ppm	Enzyme	MC	Score	E value	Peptide	Mod_site
1	164	175	615.6588	1843.9544	1843.9516	1.57	T	1	42	5.90E-05	LFEKVQPGHHTR +K_MMCCH_NL997 (K)	167
2	249	271	1012.4536	3034.3388	3034.3371	0.56	T	1	19	0.013	GKDPNSADCAHNLIHTPMEPFDR +Deamidated (NQ); K_MMCCH_NL997 (K); Oxidation (M)	250
3	281	293	630.2983	1887.8732	1887.8574	8.37	T	0	41	7.80E-05	EHAKPADSFDYGR +K_MMCCH_NL997 (K)	284
4	419	446	941.7554	3762.9925	3762.9879	1.20	T	1	26	0.0027	QPTLVHRPAKGHFDKPPVPVAQANLAVR +K_MMCCH_NL673 (K)	433
5	467	488	1071.8489	3212.5248	3212.4972	8.59	T	1	75	3.40E-08	FQNDKSVDGYQATVEFHALPAR +K_MMCCH_NL673 (K)	471
6	1097	1115	1178.8874	3533.6405	3533.6118	8.15	T	0	22	0.0069	KPLQPFGLDSVINPDDETR +Globo_H_MMCCH (K)	1097
7	1949	1963	766.0211	2295.0415	2295.0266	6.49	T	0	44	4.40E-05	TQEFSKPEDTFDYHR +K_MMCCH_NL997 (K)	1954
8	1985	1995	586.6405	1756.8997	1756.8930	3.81	C	0	22	0.0061	IKQQQEADRVF +K_MMCCH_NL997 (K)	1986
9	2463	2479	1104.1505	3309.4297	3309.4269	0.85	C	1	16	0.028	KAQSIHPEDVFDTDAPF +Globo_H_MMCCH (K)	2463
10	1525	1539	865.7426	2594.2060	2594.1959	3.89	Th	3	20	0.015	LKHNLPQDSFDYQNR +K_MMCCH_NL673 (K)	1526
11	1952	1963	646.6356	1936.8850	1936.8778	3.77	Th	2	55	3.00E-06	FSKPEDTFDYHR +K_MMCCH_NL997 (K)	1954

"Start" and "End" indicates the number of residue of KLH1 or KLH2. "Observed" column implies the observed m/z value in the survey scan while "Mr(expt)", "Mr(calc)", "ppm" indicate the experimental molecular weight(MW), calculated MW, and the difference between observed MW and theoretical MW respectively. In the "Enzyme" column, T, C, G and Th stand for trypsin, chymotrypsin, Glu-C and thermolysin respectively. MC stands for missed cleavage. Scores are the peptide ion score directly reported from Mascot database search engine. E value denotes the expectation value for each identified peptide. The peptide sequences as well as its modifications are listed in "Peptide" column. "Mod_site" indicates the amino acid site of K in which identified as Globo_H_MMCCH, K_MMCCH_NL308, K_MMCCH_NL511, K_MMCCH_NL673, K_MMCCH_NL835, or K_MMCCH_NL997 modified for KLH1 or KLH2 sequence.

Figure 18. Identification details of Globo H-conjugated peptides for sample 1 (2nd LC-MS/MS)

Figure 18A. KLH 1

#	Start	End	Observed	Mr(expt)	Mr(calc)	ppm	Enzyme	MC	Score	E value	Peptide	Mod_site
1	588	606	1132.8378	3395.4915	3395.4862	1.56	T	1	19	0.012	EDKSAGGFQQLGAFHGEPK +Globo_H_MMCCH (K)	590
2	700	719	1015.1627	3042.4663	3042.4532	4.31	T	1	30	0.00093	SVQNKLFEQPEFGHYTSIAK +K_MMCCH_NL673 (K)	719
3	953	965	762.7192	2285.1359	2285.1249	4.81	T	1	47	2.10E-05	DLFKQPSVIHEPR +K_MMCCH_NL673 (K)	956
4	1092	1114	1074.8417	3221.5032	3221.5213	-5.62	T	1	30	0.001	QHHYETNPFHHGKITHENEITTR +K_MMCCH_NL997 (K)	1104
5	1417	1445	980.2136	3916.8254	3916.8135	3.04	T	1	14	0.041	ADHSSDGFQAIASFHALPPLCPSPAASKR +K_MMCCH_NL511 (K)	1444
6	1473	1489	905.7894	2714.3463	2714.3414	1.81	T	1	17	0.022	KHGAVVGLPYWDWTLPR +K_MMCCH_NL673 (K)	1473
7	1923	1932	793.8984	1585.7822	1585.7745	4.86	T	1	15	0.034	NKVMPNPFAR +Deamidated (NQ); K_MMCCH_NL997 (K); Oxidation (M)	1924
8	2233	2251	721.5977	2882.3618	2882.3776	-5.48	T	2	23	0.0048	KEINTLTTAEVDNLKDAMR +Deamidated (NQ); K_MMCCH_NL673 (K)	2247
9	2359	2367	1008.4539	2014.8933	2014.8929	0.20	T	1	17	0.022	DKLFNDPER +K_MMCCH_NL511 (K)	2360
10	2851	2883	1027.9791	4107.8874	4107.8666	5.06	T	0	35	0.0003	VKPAHAGSCAGDIMHVPLHPFNYESVNNDDFTR +Deamidated (NQ); K_MMCCH_NL997 (K); Oxidation (M)	2852
11	2897	2919	814.6596	3254.6093	3254.5818	8.45	T	1	36	0.00024	FNYKYDNLNLHGHNIEELEEVLR +K_MMCCH_NL997 (K)	2900
12	3003	3021	953.1583	2856.4530	2856.4467	2.21	T	1	17	0.021	KYDHTELDASVLPAPIIVR +K_MMCCH_NL673 (K)	3003
13	158	169	733.6757	2198.0053	2197.9838	9.83	G	2	14	0.044	AFHKFQEDRSVD +K_MMCCH_NL673 (K)	161

Figure 18B. KLH 2

#	Start	End	Observed	Mr(expt)	Mr(calc)	ppm	Enzyme	MC	Score	E value	Peptide	Mod_site
1	26	41	1047.4894	3139.4463	3139.4364	3.15	T	1	17	0.021	KNVDSLSSDEVLALEK +Globo_H_MMCCH (K)	26
2	164	175	615.6602	1843.9587	1843.9516	3.85	T	1	38	0.00015	LFEKVQPGHHTR +K_MMCCH_NL997 (K)	167
3	281	293	630.2961	1887.8664	1887.8574	4.82	T	0	47	2.10E-05	EHAKPADSFDYGR +K_MMCCH_NL997 (K)	284
4	419	446	860.9789	3439.8867	3439.8663	5.93	T	1	25	0.0029	QPTLVHRPAKGHFDKPPVPVAQANLAVR +Deamidated (NQ); K_MMCCH_NL997 (K)	433
5	467	488	1125.8600	3374.5581	3374.5500	2.40	T	1	68	1.40E-07	FQNDKSVDGYQATVEFHALPAR +K_MMCCH_NL511 (K)	471
6	936	950	847.7374	2540.1903	2540.1682	8.70	T	1	15	0.029	KHGFTGGLPYWDWTR +K_MMCCH_NL673 (K)	936
7	1097	1115	1008.4823	3022.4251	3022.4216	1.12	T	0	54	3.80E-06	KPLQPFGLDSVINPDDETR +K_MMCCH_NL511 (K)	1097
8	1455	1480	853.1713	3408.6562	3408.6601	-1.14	T	1	27	0.0022	AKYSLSSLDYTAFDPVFFLHHANVDR +K_MMCCH_NL997 (K)	1456
9	1508	1539	841.0015	4199.9709	4199.9680	0.69	T	1	37	0.00018	KPLQPFNNPELNSDSMTLKHNLPQDSFDYQNR +Deamidated (NQ); K_MMCCH_NL997 (K); Oxidation (M)	1526
10	1949	1963	574.7651	2295.0315	2295.0266	2.09	T	0	55	3.30E-06	TQEFSKPEDTFDYHR +K_MMCCH_NL997 (K)	1954
11	2527	2541	691.3613	2071.0620	2071.0619	0.05	T	1	15	0.03	KDVTSLTASEIENLR +K_MMCCH_NL997 (K)	2527
12	3008	3025	845.4286	2533.2641	2533.2576	2.57	T	1	14	0.043	ALKEHGSHLGIPYWDWTK +K_MMCCH_NL997 (K)	3025
13	1292	1303	605.9988	1814.9745	1814.9713	1.82	G	0	16	0.023	SIRSAFLQIQKE +K_MMCCH_NL997 (K)	1302
14	2463	2479	1104.1495	3309.4268	3309.4269	-0.03	C	1	19	0.012	KAQSIHPEDVFDTDAPF +Globo_H_MMCCH (K)	2463
15	1554	1560	621.8187	1241.6229	1241.6326	-7.73	Th	1	14	0.036	IQKLDQT +Deamidated (NQ); K_MMCCH_NL997 (K)	1556

"Start" and "End" indicates the number of residue of KLH1 or KLH2. "Observed" column implies the observed m/z value in the survey scan while "Mr(expt)", "Mr(calc)", "ppm" indicate the experimental molecular weight(MW), calculated MW, and the difference between observed MW and theoretical MW respectively. In the "Enzyme" column, T, C, G and Th stand for trypsin, chymotrypsin, Glu-C and thermolysin respectively. MC stands for missed cleavage. Scores are the peptide ion score directly reported from Mascot database search engine. E value denotes the expectation value for each identified peptide. The peptide sequences as well as its modifications are listed in "Peptide" column. "Mod_site" indicates the amino acid site of K in which identified as Globo_H_MMCCH, K_MMCCH_NL308, K_MMCCH_NL511, K_MMCCH_NL673, K_MMCCH_NL835, or K_MMCCH_NL997 modified for KLH1 or KLH2 sequence.

Figure 19. Identification details of Globo H-conjugated peptides for sample 2 (2nd LC-MS/MS)

Figure 19A. KLH 1

#	Start	End	Observed	Mr(expt)	Mr(calc)	ppm	Enzyme	MC	Score	E value	Peptide	Mod_site
1	953	965	654.6824	1961.0253	1961.0193	3.06	T	1	46	2.60E-05	DLFKQPSVIHEPR +K_MMCCH_NL997 (K)	956
2	1092	1114	806.3803	3221.4919	3221.5213	-9.13	T	1	18	0.015	QHHYETNPFHHGKITHENEITTR +K_MMCCH_NL997 (K)	1104
3	1417	1445	1108.0071	4427.9992	4428.0036	-0.99	T	1	13	0.046	ADHSSDGFQAIASFHALPPLCPSPAASKR +Globo_H_MMCCH (K)	1444
4	2233	2251	721.5986	2882.3654	2882.3776	-4.23	T	2	37	0.0002	KEINTLTTAEVDNLKDAMR +Deamidated (NQ); K_MMCCH_NL673 (K)	2247
5	2359	2367	927.4279	1852.8413	1852.8400	0.65	T	1	17	0.02	DKLFNDPER +K_MMCCH_NL673 (K)	2360
6	2851	2883	1027.9758	4107.8742	4107.8666	1.85	T	0	37	0.00018	VKPAHAGSCAGDIMHVPLHPFNYESVNNDDFTR +Deamidated (NQ); K_MMCCH_NL997 (K); Oxidation (M)	2852
7	1649	1664	1104.1271	3309.3594	3309.3654	-1.81	C	2	14	0.038	NLNDHTHDFSKPEDTF +Globo_H_MMCCH (K)	1659

Figure 19B. KLH 2

#	Start	End	Observed	Mr(expt)	Mr(calc)	ppm	Enzyme	MC	Score	E value	Peptide	Mod_site
1	26	41	1047.4901	3139.4485	3139.4364	3.85	T	1	21	0.0089	KNVDSLSSDEVLALEK +Globo_H_MMCCH (K)	26
2	164	175	615.6576	1843.9509	1843.9516	-0.33	T	1	33	0.00046	LFEKVQPGHHTR +K_MMCCH_NL997 (K)	167
3	249	271	1012.4529	3034.3368	3034.3371	-0.10	T	1	16	0.025	GKDPNSADCAHNLIHTPMEPFDR +Deamidated (NQ); K_MMCCH_NL997 (K); Oxidation (M)	250
4	281	293	630.2961	1887.8666	1887.8574	4.87	T	0	49	1.10E-05	EHAKPADSFDYGR +K_MMCCH_NL997 (K)	284
5	419	446	942.0069	3763.9985	3763.9720	7.04	T	1	30	0.0011	QPTLVHRPAKGHFDKPPVPVAQANLAVR +Deamidated (NQ); K_MMCCH_NL673 (K)	433
6	467	488	1125.8563	3374.5471	3374.5500	-0.86	T	1	59	1.20E-06	FQNDKSVDGYQATVEFHALPAR +K_MMCCH_NL511 (K)	471
7	1097	1115	847.0906	2538.2501	2538.2312	7.45	T	0	26	0.0024	KPLQPFGLDSVINPDDETR +2 Deamidated (NQ); K_MMCCH_NL997 (K)	1097
8	1355	1385	1217.5574	4866.2004	4866.1892	2.28	T	1	15	0.029	GSAVAVPYWDWTEKADSLPSLINDATYFNSR +Globo_H_MMCCH (K)	1368
9	1508	1526	862.7620	2585.2642	2585.2505	5.30	T	0	15	0.03	KPLQPFNNPELNSDSMTLK +Deamidated (NQ); K_MMCCH_NL997 (K); Oxidation (M)	1526
10	1949	1963	928.0676	2781.1811	2781.1851	-1.44	T	0	49	1.20E-05	TQEFSKPEDTFDYHR +K_MMCCH_NL511 (K)	1954
11	2527	2541	691.3618	2071.0635	2071.0619	0.72	T	1	21	0.0083	KDVTSLTASEIENLR +K_MMCCH_NL997 (K)	2527
12	1292	1303	605.9978	1814.9716	1814.9713	0.17	G	0	16	0.026	SIRSAFLQIQKE +K_MMCCH_NL997 (K)	1302
13	1526	1540	1101.4783	3301.4130	3301.4232	-3.09	C	2	17	0.021	KHNLPQDSFDYQNRF +Globo_H_MMCCH (K)	1526
14	1985	1995	586.6373	1756.8902	1756.8930	-1.65	C	0	23	0.0049	IKQQQEADRVF +K_MMCCH_NL997 (K)	1986
15	2463	2479	1104.1492	3309.4257	3309.4269	-0.36	C	1	23	0.0045	KAQSIHPEDVFDTDAPF +Globo_H_MMCCH (K)	2463

"Start" and "End" indicates the number of residue of KLH1 or KLH2. "Observed" column implies the observed m/z value in the survey scan while "Mr(expt)", "Mr(calc)", "ppm" indicate the experimental molecular weight(MW), calculated MW, and the difference between observed MW and theoretical MW respectively. In the "Enzyme" column, T, C, G and Th stand for trypsin, chymotrypsin, Glu-C and thermolysin respectively. MC stands for missed cleavage. Scores are the peptide ion score directly reported from Mascot database search engine. E value denotes the expectation value for each identified peptide. The peptide sequences as well as its modifications are listed in "Peptide" column. "Mod_site" indicates the amino acid site of K in which identified as Globo_H_MMCCH, K_MMCCH_NL308, K_MMCCH_NL511, K_MMCCH_NL673, K_MMCCH_NL835, or K_MMCCH_NL997 modified for KLH1 or KLH2 sequence.

Figure 20. Identification details of Globo H-conjugated peptides for sample 3 (2nd LC-MS/MS)

Figure 20A. KLH 1

#	Start	End	Observed	Mr(expt)	Mr(calc)	ppm	Enzyme	MC	Score	E value	Peptide	Mod_site
1	377	402	852.1617	3404.6179	3404.6104	2.20	T	0	14	0.037	AHCAISLEHMHLKPFAFSSPLNNNEK +Deamidated (NQ); K_MMCCH_NL997 (K); Oxidation (M)	402
2	700	719	1069.1809	3204.5209	3204.5060	4.65	T	1	19	0.012	SVQNKLFEQPEFGHYTSIAK +K_MMCCH_NL511 (K)	719
3	1092	1114	806.3823	3221.4999	3221.5213	-6.64	T	1	17	0.019	QHHYETNPFHHGKITHENEITTR +K_MMCCH_NL997 (K)	1104
4	2233	2251	721.5977	2882.3618	2882.3776	-5.48	T	2	28	0.0016	KEINTLTTAEVDNLKDAMR +Deamidated (NQ); K_MMCCH_NL673 (K)	2247
5	2851	2883	1027.9711	4107.8552	4107.8666	-2.78	T	0	32	0.00067	VKPAHAGSCAGDIMHVPLHPFNYESVNNDDFTR +Deamidated (NQ); K_MMCCH_NL997 (K); Oxidation (M)	2852
6	158	169	733.6741	2198.0006	2197.9838	7.64	G	2	16	0.025	AFHKFQEDRSVD +K_MMCCH_NL673 (K)	161

Figure 20B. KLH 2

#	Start	End	Observed	Mr(expt)	Mr(calc)	ppm	Enzyme	MC	Score	E value	Peptide	Mod_site
1	419	446	941.7502	3762.9719	3762.9879	-4.28	T	1	16	0.028	QPTLVHRPAKGHFDKPPVPVAQANLAVR +K_MMCCH_NL673 (K)	433
2	1097	1115	847.0919	2538.2539	2538.2312	8.94	T	0	44	3.60E-05	KPLQPFGLDSVINPDDETR +2 Deamidated (NQ); K_MMCCH_NL997 (K)	1097
3	1355	1385	1217.5449	4866.1506	4866.1892	-7.95	T	1	23	0.0053	GSAVAVPYWDWTEKADSLPSLINDATYFNSR +Globo_H_MMCCH (K)	1368
4	1508	1539	841.0017	4199.9722	4199.9680	0.98	T	1	55	3.50E-06	KPLQPFNNPELNSDSMTLKHNLPQDSFDYQNR +Deamidated (NQ); K_MMCCH_NL997 (K); Oxidation (M)	1526
5	1224	1235	939.9670	1877.9195	1877.9022	9.21	Th	5	14	0.041	LHVGDNFFLKYE +Deamidated (NQ); K_MMCCH_NL997 (K)	1233

"Start" and "End" indicates the number of residue of KLH1 or KLH2. "Observed" column implies the observed m/z value in the survey scan while "Mr(expt)", "Mr(calc)", "ppm" indicate the experimental molecular weight(MW), calculated MW, and the difference between observed MW and theoretical MW respectively. In the "Enzyme" column, T, C, G and Th stand for trypsin, chymotrypsin, Glu-C and thermolysin respectively. MC stands for missed cleavage. Scores are the peptide ion score directly reported from Mascot database search engine. E value denotes the expectation value for each identified peptide. The peptide sequences as well as its modifications are listed in "Peptide" column. "Mod_site" indicates the amino acid site of K in which identified as Globo_H_MMCCH, K_MMCCH_NL308, K_MMCCH_NL511, K_MMCCH_NL673, K_MMCCH_NL835, or K_MMCCH_NL997 modified for KLH1 or KLH2 sequence

Figure 21. Identification details of Globo H-conjugated peptides for sample 4 (2nd LC-MS/MS)

Figure 21A. KLH 1

#	Start	End	Observed	Mr(expt)	Mr(calc)	ppm	Enzyme	MC	Score	E value	Peptide	Mod_site
1	778	789	986.5373	1971.0600	1971.0553	2.44	T	1	17	0.021	IWAIWQALQKYR +K_MMCCH_NL997 (K)	787
2	953	965	654.6835	1961.0288	1961.0193	4.84	T	1	32	0.00065	DLFKQPSVIHEPR +K_MMCCH_NL997 (K)	956
3	1092	1114	806.3824	3221.5007	3221.5213	-6.39	T	1	24	0.004	QHHYETNPFHHGKITHENEITTR +K_MMCCH_NL997 (K)	1104
4	1923	1932	793.8977	1585.7809	1585.7745	4.04	T	1	19	0.011	NKVMPNPFAR +Deamidated (NQ); K_MMCCH_NL997 (K); Oxidation (M)	1924
5	2233	2251	721.5991	2882.3671	2882.3776	-3.64	T	2	17	0.022	KEINTLTTAEVDNLKDAMR +Deamidated (NQ); K_MMCCH_NL673 (K)	2247
6	2851	2883	1027.9812	4107.8957	4107.8666	7.08	T	0	49	1.20E-05	VKPAHAGSCAGDIMHVPLHPFNYESVNNDDFTR +Deamidated (NQ); K_MMCCH_NL997 (K); Oxidation (M)	2852
7	1649	1664	1104.1299	3309.3678	3309.3654	0.73	C	2	14	0.042	NLNDHTHDFSKPEDTF +Globo_H_MMCCH (K)	1659
8	601	612	955.3971	2863.1694	2863.1715	-0.73	Th	1	26	0.0026	FHGEPKWCPSPE +Globo_H_MMCCH (K)	606
9	1580	1587	763.8522	1525.6899	1525.6858	2.69	Th	1	14	0.037	VGGKEPYG +K_MMCCH_NL673 (K)	1583

Figure 21B. KLH 2

#	Start	End	Observed	Mr(expt)	Mr(calc)	ppm	Enzyme	MC	Score	E value	Peptide	Mod_site
1	164	175	615.6603	1843.9592	1843.9516	4.12	T	1	40	0.00011	LFEKVQPGHHTR +K_MMCCH_NL997 (K)	167
2	281	293	630.2977	1887.8714	1887.8574	7.42	T	0	40	9.20E-05	EHAKPADSFDYGR +K_MMCCH_NL997 (K)	284
3	467	488	1071.8480	3212.5222	3212.4972	7.78	T	1	60	1.00E-06	FQNDKSVDGYQATVEFHALPAR +K_MMCCH_NL673 (K)	471
4	1097	1115	1178.8835	3533.6288	3533.6118	4.81	T	0	19	0.014	KPLQPFGLDSVINPDDETR +Globo_H_MMCCH (K)	1097
5	1949	1963	766.0208	2295.0406	2295.0266	6.10	T	0	34	0.00039	TQEFSKPEDTFDYHR +K_MMCCH_NL997 (K)	1954
6	2728	2739	986.5373	1971.0600	1971.0553	2.44	T	1	17	0.021	IWAIWQALQKYR +K_MMCCH_NL997 (K)	2737
7	1985	1995	586.6405	1756.8997	1756.8930	3.81	C	0	23	0.0046	IKQQQEADRVF +K_MMCCH_NL997 (K)	1986
8	2463	2479	1104.1527	3309.4363	3309.4269	2.84	C	1	14	0.037	KAQSIHPEDVFDTDAPF +Globo_H_MMCCH (K)	2463
9	893	904	955.3971	2863.1694	2863.1715	-0.73	Th	1	26	0.0026	FHGEPKWCPSPE +Globo_H_MMCCH (K)	898
10	1224	1233	1036.4961	2070.9776	2070.9707	3.33	Th	4	15	0.029	LHVGDNFFLK +K_MMCCH_NL511 (K)	1233
11	1952	1963	646.6351	1936.8834	1936.8778	2.89	Th	2	24	0.0041	FSKPEDTFDYHR +K_MMCCH_NL997 (K)	1954

"Start" and "End" indicates the number of residue of KLH1 or KLH2. "Observed" column implies the observed m/z value in the survey scan while "Mr(expt)", "Mr(calc)", "ppm" indicate the experimental molecular weight(MW), calculated MW, and the difference between observed MW and theoretical MW respectively. In the "Enzyme" column, T, C, G and Th stand for trypsin, chymotrypsin, Glu-C and thermolysin respectively. MC stands for missed cleavage. Scores are the peptide ion score directly reported from Mascot database search engine. E value denotes the expectation value for each identified peptide. The peptide sequences as well as its modifications are listed in "Peptide" column. "Mod_site" indicates the amino acid site of K in which identified as Globo_H_MMCCH, K_MMCCH_NL308, K_MMCCH_NL511, K_MMCCH_NL673, K_MMCCH_NL835, or K_MMCCH_NL997 modified for KLH1 or KLH2 sequence.

Figure 22. Identification details of MMCCH-conjugated peptides for sample 1 (1st LC-MS/MS)

Figure 22A. KLH 1

#	Start	End	Observed	Mr(expt)	Mr(calc)	ppm	Enzyme	MC	Score	E value	Peptide	Mod_site
1	124	141	785.4098	2353.2075	2353.2001	3.14	T	1	21	0.0086	GFTDPPVKHHQSANLLVR +dK_MMCCH-2 (K)	131
2	157	166	823.3666	1644.7187	1644.7242	-3.34	T	1	20	0.011	EAFHKFQEDR +Deamidated (NQ); dK_MMCCH-2 (K)	161
3	377	402	833.3975	3329.5607	3329.5784	-5.29	T	0	37	0.00019	AHCAISLEHMHLKPFAFSSPLNNNEK +dK_MMCCH-2 (K)	389
4	460	477	781.3958	2341.1654	2341.1624	1.28	T	1	19	0.014	TSANVDIFIKTTDSVQHK +dK_MMCCH-2 (K)	469
5	470	488	748.0436	2241.1091	2241.1100	-0.40	T	1	18	0.017	TTDSVQHKAGTFAVLGGSK +dK_MMCCH-2 (K)	477
6	489	496	718.8198	1435.6251	1435.6377	-8.78	T	1	15	0.029	EMKWGFDR +dK_MMCCH-1 (K); Oxidation (M)	491
7	553	560	663.8676	1325.7207	1325.7166	3.09	T	2	23	0.0051	VKFDKVPR +dK_MMCCH-2 (K)	554
8	566	570	485.2450	968.4754	968.4749	0.52	T	1	16	0.028	KNVDR +dK_MMCCH-2 (K)	566
9	581	587	547.8376	1093.6606	1093.6569	3.38	T	1	19	0.013	KALALLK +dK_MMCCH-2 (K)	581
10	588	606	781.0359	2340.0858	2340.0845	0.60	T	1	31	0.00076	EDKSAGGFQQLGAFHGEPK +dK_MMCCH-2 (K)	590
11	591	615	1004.4674	3010.3804	3010.3742	2.06	T	1	16	0.024	SAGGFQQLGAFHGEPKWCPSPEASK +dK_MMCCH-2 (K)	606
12	645	681	1158.5342	4630.1076	4630.1063	0.28	T	1	26	0.0025	HGYDGALPYWDWTSPLNHLPELADHEKYVDPEDGVEK +dK_MMCCH-2 (K)	671
13	682	699	1239.5814	2477.1483	2477.1434	1.98	T	1	18	0.016	HNPWFDGHIDTVDKTTTR +dK_MMCCH-2 (K)	695
14	700	719	887.7735	2660.2987	2660.2945	1.58	T	1	44	4.20E-05	SVQNKLFEQPEFGHYTSIAK +dK_MMCCH-2 (K)	704
15	778	789	957.9996	1913.9846	1913.9862	-0.84	T	1	32	0.00059	IWAIWQALQKYR +Deamidated (NQ); dK_MMCCH-2 (K)	787
16	790	804	669.3175	2004.9307	2004.9220	4.34	T	0	49	1.20E-05	GKPYNVANCAVTSMR +dK_MMCCH-2 (K)	791
17	858	863	520.3004	1038.5863	1038.5783	7.70	T	1	19	0.013	KLEAIK +dK_MMCCH-2 (K)	858
18	953	965	635.3312	1902.9717	1902.9662	2.89	T	1	47	1.90E-05	DLFKQPSVIHEPR +dK_MMCCH-2 (K)	956
19	986	1000	1027.0348	2052.0550	2052.0561	-0.54	T	1	84	4.40E-09	KNIENLSLGELESLR +dK_MMCCH-2 (K)	986
20	1048	1060	913.5302	1825.0459	1825.0423	1.97	T	1	26	0.0024	LYVVVVENALLKK +dK_MMCCH-2 (K)	1060
21	1092	1114	633.9023	3164.4753	3164.4523	7.30	T	1	33	0.00052	QHHYETNPFHHGKITHENEITTR +Deamidated (NQ); dK_MMCCH-2 (K)	1104
22	1118	1162	1131.7467	5653.6971	5653.6850	2.14	T	1	18	0.014	DSLFHSDYFYEQVLYALEQDNFCDFEIQLEILHNALHSLLGGKGK +dK_MMCCH-2 (K)	1162
23	1199	1203	353.1915	1056.5526	1056.5538	-1.23	T	1	17	0.019	KRPYR +dK_MMCCH-2 (K)	1199
24	1331	1338	620.3547	1238.6949	1238.6944	0.40	T	1	23	0.0054	LDITKALK +dK_MMCCH-2 (K)	1335

Figure 22A. KLH 1 (continued)

25	1395	1403	485.5956	1453.7651	1453.7599	3.58	T	2	25	0.0031	KDITQLDKR +dK_MMCCH-2 (K)	1395
26	1395	1403	598.3075	1791.9007	1791.8899	5.97	T	2	21	0.0084	KDITQLDKR +2 dK_MMCCH-2 (K)	1395, 1402
27	1417	1445	1125.2136	3372.6190	3372.6020	5.07	T	1	27	0.002	ADHSSDGFQAIASFHALPPLCPSPAASKR +dK_MMCCH-2 (K)	1444
28	1473	1489	778.4057	2332.1953	2332.1827	5.40	T	1	46	2.60E-05	KHGAVVGLPYWDWTLPR +dK_MMCCH-2 (K)	1473
29	1519	1530	898.9364	1795.8582	1795.8563	1.06	T	1	16	0.025	IEFEGENVHTKR +dK_MMCCH-2 (K)	1529
30	1721	1746	1092.8095	3275.4065	3275.3886	5.47	T	1	15	0.035	TAGDCEDAGYFTVLGGEKEMPWAFDR +dK_MMCCH-2 (K); Oxidation (M)	1738
31	1747	1758	613.9775	1838.9108	1838.9012	5.22	T	1	22	0.0067	LYKYDITETLDK +dK_MMCCH-2 (K)	1749
32	1923	1932	756.3798	1510.7451	1510.7425	1.72	T	1	29	0.0012	NKVMPNPFAR +dK_MMCCH-2 (K)	1924
33	2067	2076	746.8879	1491.7613	1491.7544	4.63	T	1	27	0.0021	KHAVPNDVFK +dK_MMCCH-2 (K)	2067
34	2068	2083	753.7155	2258.1247	2258.1194	2.35	T	1	16	0.025	HAVPNDVFKYELLGYR +dK_MMCCH-2 (K)	2076
35	2121	2149	890.4191	3557.6472	3557.6378	2.64	T	1	37	0.00021	TSADVQFQICKTSEDCHHGGQIFVLGGTK +dK_MMCCH-2 (K)	2131
36	2299	2314	715.0181	2142.0324	2142.0238	4.01	T	1	60	9.80E-07	LYTKQMEDALTAHGAR +dK_MMCCH-2 (K)	2302
37	2359	2367	736.3492	1470.6839	1470.6813	1.77	T	1	35	0.00034	DKLFNDPER +dK_MMCCH-2 (K)	2360
38	2461	2490	642.8196	3850.8742	3850.8638	2.70	T	0	16	0.026	RPLRPFSDPINHNAFTHSNAKPTDVFEYSR +dK_MMCCH-2 (K)	2481
39	2507	2514	682.3518	1362.6889	1362.6853	2.64	T	1	30	0.001	KLEHELEK +dK_MMCCH-2 (K)	2507
40	2515	2520	571.7622	1141.5099	1141.5074	2.19	T	1	19	0.012	QKEEDR +dK_MMCCH-2 (K)	2516
41	2595	2609	983.5271	1965.0396	1965.0493	-4.89	T	1	17	0.02	IIDTSGKQLPSDLIK +dK_MMCCH-2 (K)	2601
42	2621	2636	802.7155	2405.1245	2405.1083	6.74	T	1	51	8.60E-06	HHEKHHEDHHEDILVR +dK_MMCCH-2 (K)	2624
43	2637	2651	1069.5284	2137.0423	2137.0374	2.29	T	1	59	1.40E-06	KNIHSLSHHEAEELR +dK_MMCCH-2 (K)	2637
44	2652	2682	975.2011	3896.7753	3896.7563	4.90	T	1	14	0.041	DALYKLQNDESHGGYEHIAGFHGYPNLCPEK +dK_MMCCH-2 (K)	2656
45	2761	2814	1328.4260	6637.0938	6637.0821	1.76	T	1	20	0.0094	DVNEAIFQQTKFGEFSSIFYLALQALEEDNYCDFEVQYEILHNEVHALIGGAEK +4 Deamidated (NQ); dK_MMCCH-1 (K)	2771
46	2851	2883	1009.2216	4032.8574	4032.8346	5.65	T	0	69	1.20E-07	VKPAHAGSCAGDIMHVPLHPFNYESVNNDDFTR +dK_MMCCH-2 (K)	2852
47	2897	2919	1066.5184	3196.5335	3196.5287	1.47	T	1	55	3.20E-06	FNYKYDNLNLHGHNIEELEEVLR +dK_MMCCH-2 (K)	2900
48	2938	2947	730.4154	1458.8163	1458.8156	0.48	T	1	20	0.01	TTAVVKVYIK +dK_MMCCH-2 (K)	2943
49	3003	3021	825.7748	2474.3027	2474.2879	5.98	T	1	46	2.80E-05	KYDHTELDASVLPAPIIVR +dK_MMCCH-2 (K)	3003
50	3022	3044	966.5284	2896.5635	2896.5521	3.94	T	1	15	0.03	RPNNAVFDIIEIPIGKDVNLPPK +dK_MMCCH-2 (K)	3037

Figure 22A. KLH 1 (continued)

51	123	151	739.7915	3693.9211	3693.9049	4.39	G	2	31	0.00075	KGFTDPPVKHHQSANLLVRKNINDLTREE +dK_MMCCH-2 (K)	131
52	158	176	846.3878	2536.1415	2536.1329	3.39	G	3	25	0.0034	AFHKFQEDRSVDGYQATAE +dK_MMCCH-2 (K)	161
53	435	442	676.3259	1350.6373	1350.6312	4.52	G	1	15	0.03	NIEKMIHE +dK_MMCCH-2 (K)	438
54	526	544	777.7507	2330.2304	2330.2304	0.00	G	1	34	0.00038	VDGTKLASSLIPHASVIRE +dK_MMCCH-2 (K)	530
55	589	612	1102.8276	3305.4611	3305.4621	-0.30	G	1	13	0.048	DKSAGGFQQLGAFHGEPKWCPSPE +2 dK_MMCCH-2 (K)	590, 606
56	589	612	990.1173	2967.3301	2967.3320	-0.64	G	1	22	0.0057	DKSAGGFQQLGAFHGEPKWCPSPE +dK_MMCCH-2 (K)	606
57	711	726	1064.5625	2127.1104	2127.1074	1.41	G	0	16	0.025	FGHYTSIAKQVLLALE +dK_MMCCH-2 (K)	719
58	825	841	820.7039	2459.0898	2459.0780	4.76	G	1	26	0.0028	HSVPFNVFDYKTNFNYE +Deamidated (NQ); dK_MMCCH-2 (K)	835
59	847	860	643.6771	1928.0095	1928.0077	0.93	G	0	26	0.0024	FNGLSISQLNKKLE +dK_MMCCH-2 (K)	858
60	942	972	955.5030	3817.9829	3817.9614	5.63	G	3	17	0.019	VFDLKPASLGKDLFKQPSVIHEPRIGHHEGE +dK_MMCCH-2 (K)	946
61	942	970	727.3867	3631.8972	3631.8973	-0.03	G	2	32	0.0007	VFDLKPASLGKDLFKQPSVIHEPRIGHHE +dK_MMCCH-2 (K)	956
62	1055	1076	810.1674	3236.6403	3236.6402	0.03	G	1	32	0.00065	NALLKKGSSVAVPYWDWTKRIE +2 dK_MMCCH-2 (K)	1059, 1060
63	1055	1076	725.6326	2898.5012	2898.5102	-3.11	G	1	38	0.00018	NALLKKGSSVAVPYWDWTKRIE +dK_MMCCH-2 (K)	1060
64	1097	1108	878.4210	1754.8275	1754.8199	4.33	G	0	22	0.0064	TNPFHHGKITHE +dK_MMCCH-2 (K)	1104
65	1376	1396	864.3891	2590.1455	2590.1428	1.04	G	3	21	0.0072	AGTDSAHTDDGHTEPVMIRKD +dK_MMCCH-2 (K)	1395
66	1397	1413	774.4356	2320.2848	2320.2824	1.03	G	1	29	0.0012	ITQLDKRQQLSLVKALE +dK_MMCCH-2 (K)	1410
67	1506	1522	753.3769	2257.1088	2257.1089	-0.04	G	2	19	0.013	TGRDIPNPFIGSKIEFE +dK_MMCCH-2 (K)	1518
68	1755	1765	570.6054	1708.7944	1708.7913	1.81	G	2	26	0.0027	TLDKMNLRHDE +dK_MMCCH-2 (K)	1758
69	2059	2078	692.5998	2766.3703	2766.3588	4.16	G	1	15	0.032	INHNQFTKKHAVPNDVFKYE +dK_MMCCH-2 (K)	2076
70	2089	2100	854.4097	1706.8048	1706.8008	2.34	G	2	22	0.0065	IGGMNLHEIEKE +dK_MMCCH-2 (K)	2099
71	2647	2661	715.6793	2144.0161	2144.0095	3.08	G	4	24	0.0037	AEELRDALYKLQNDE +dK_MMCCH-2 (K)	2656
72	3090	3097	632.8041	1263.5937	1263.5879	4.59	G	0	13	0.048	LGKMYSVE +dK_MMCCH-2 (K)	3092
73	59	68	721.3473	1440.6800	1440.6781	1.32	C	1	37	0.0002	VLGGPSEMKW +dK_MMCCH-2 (K)	67
74	94	100	573.2999	1144.5853	1144.5838	1.31	C	1	15	0.031	TVKAELF +dK_MMCCH-2 (K)	96
75	429	450	990.8061	2969.3964	2969.3899	2.22	C	1	21	0.0078	GGISLENIEKMIHENQQEDRIY +dK_MMCCH-2 (K); Oxidation (M)	438
76	468	481	935.9773	1869.9400	1869.9295	5.62	C	0	19	0.014	IKTTDSVQHKAGTF +dK_MMCCH-2 (K)	469
77	584	595	787.4011	1572.7876	1572.7858	1.14	C	2	40	9.10E-05	ALLKEDKSAGGF +dK_MMCCH-2 (K)	590

Figure 22A. KLH 1 (continued)

78	715	722	599.3331	1196.6516	1196.6475	3.43	C	0	22	0.006	TSIAKQVL +dK_MMCCH-2 (K)	719
79	783	788	544.7778	1087.5410	1087.5372	3.49	C	1	26	0.0025	QALQKY +dK_MMCCH-2 (K)	787
80	830	838	743.3410	1484.6674	1484.6646	1.89	C	2	19	0.013	NVFDYKTNF +dK_MMCCH-2 (K)	835
81	1013	1018	516.7590	1031.5034	1031.4998	3.49	C	0	14	0.044	ESIAKF +dK_MMCCH-2 (K)	1017
82	1072	1087	744.7218	2231.1436	2231.1409	1.21	C	1	16	0.024	TKRIEHLPHLISDATY +dK_MMCCH-2 (K)	1073
83	1330	1337	620.3563	1238.6980	1238.6944	2.83	C	1	24	0.0036	KLDITKAL +dK_MMCCH-2 (K)	1335
84	1649	1664	752.3297	2253.9673	2253.9637	1.60	C	2	18	0.015	NLNDHTHDFSKPEDTF +dK_MMCCH-2 (K)	1659
85	1732	1742	792.8754	1583.7363	1583.7364	-0.06	C	1	17	0.02	TVLGGEKEMPW +dK_MMCCH-2 (K)	1738
86	1818	1827	753.3691	1504.7237	1504.7232	0.40	C	1	21	0.0074	SERDIGSLKY +dK_MMCCH-2 (K)	1826
87	2160	2184	1085.5110	3253.5111	3253.5179	-2.09	C	3	18	0.015	KYDITHALHDAHITPEDVFHPSEPF +dK_MMCCH-2 (K)	2160
88	2476	2488	923.9221	1845.8296	1845.8244	2.82	C	1	22	0.0062	THSNAKPTDVFEY +dK_MMCCH-2 (K)	2481
89	2656	2666	793.3529	1584.6913	1584.6879	2.15	C	1	29	0.0013	KLQNDESHGGY +dK_MMCCH-2 (K)	2656
90	2738	2749	856.3752	1710.7358	1710.7348	0.58	C	2	19	0.012	ADSGNNNPFFKY +dK_MMCCH-2 (K)	2748
91	2750	2779	1289.6239	3865.8499	3865.8621	-3.18	C	3	22	0.0058	HIRSINQDTVRDVNEAIFQQTKFGEFSSIF +2 Deamidated (NQ); dK_MMCCH-2 (K)	2771
92	2799	2815	744.3796	2230.1169	2230.1092	3.45	C	2	24	0.0042	EILHNEVHALIGGAEKY +dK_MMCCH-2 (K)	2814
93	2946	2960	965.4055	1928.7965	1928.7986	-1.09	C	1	26	0.0023	IKSGTDSDDEYAGSF +dK_MMCCH-2 (K)	2947
94	2961	2971	769.8917	1537.7689	1537.7673	1.04	C	1	17	0.019	VILGGAKEMPW +dK_MMCCH-2 (K)	2967
95	1	8	643.8054	1285.5963	1285.5934	2.26	Th	1	22	0.006	MTPEELKT +dK_MMCCH-2 (K)	7
96	38	56	861.6811	2582.0214	2582.0108	4.11	Th	2	14	0.041	VCIPDDNDRNDDHCEKAGD +dK_MMCCH-2 (K)	53
97	59	69	785.3774	1568.7402	1568.7367	2.23	Th	3	55	2.90E-06	VLGGPSEMKWQ +dK_MMCCH-2 (K)	67
98	78	84	569.2881	1136.5616	1136.5536	7.04	Th	1	47	2.10E-05	LSDTVHK +dK_MMCCH-2 (K)	84
99	117	124	620.8133	1239.6120	1239.6070	4.03	Th	1	23	0.0052	VVHHPEKG +dK_MMCCH-2 (K)	123
100	431	438	642.3345	1282.6545	1282.6479	5.15	Th	2	29	0.0013	ISLENIEK +dK_MMCCH-2 (K)	438
101	521	530	707.8455	1413.6764	1413.6698	4.67	Th	2	74	4.30E-08	VDITEVDGTK +dK_MMCCH-2 (K)	530
102	585	591	585.8113	1169.6080	1169.6002	6.67	Th	1	35	0.00032	LLKEDKS +dK_MMCCH-2 (K)	590
103	601	612	904.8973	1807.7801	1807.7698	5.70	Th	1	22	0.0058	FHGEPKWCPSPE +dK_MMCCH-2 (K)	606

Figure 22A. KLH 1 (continued)

104	666	672	607.2841	1212.5537	1212.5485	4.29	Th	2	24	0.0043	LADHEKY +dK_MMCCH-2 (K)	671
105	673	685	930.4190	1858.8235	1858.8196	2.10	Th	2	15	0.035	VDPEDGVEKHNPW +dK_MMCCH-2 (K)	681
106	821	828	617.8143	1233.6141	1233.6064	6.24	Th	1	14	0.036	VTKEHSVP +dK_MMCCH-2 (K)	823
107	831	837	612.7885	1223.5623	1223.5533	7.44	Th	2	18	0.016	VFDYKTN +dK_MMCCH-2 (K)	835
108	954	959	529.7656	1057.5167	1057.5154	1.23	Th	1	13	0.048	LFKQPS +Deamidated (NQ); dK_MMCCH-2 (K)	956
109	1100	1104	482.2296	962.4447	962.4433	1.45	Th	0	18	0.015	FHHGK +dK_MMCCH-2 (K)	1104
110	1219	1232	653.9534	1958.8383	1958.8316	3.42	Th	1	21	0.0077	FDKSDNNDEATKTH +dK_MMCCH-2 (K)	1230
111	1580	1587	572.7740	1143.5334	1143.5271	5.60	Th	1	15	0.029	VGGKEPYG +dK_MMCCH-2 (K)	1583
112	1657	1668	921.9191	1841.8236	1841.8182	2.93	Th	2	32	0.00063	FSKPEDTFDYQK +dK_MMCCH-2 (K)	1659
113	1657	1668	921.9192	1841.8238	1841.8182	3.04	Th	2	46	2.70E-05	FSKPEDTFDYQK +dK_MMCCH-2 (K)	1668
114	1733	1741	664.3235	1326.6325	1326.6312	1.06	Th	2	30	0.00096	VLGGEKEMP +dK_MMCCH-1 (K); Oxidation (M)	1738
115	1894	1904	850.4174	1698.8203	1698.8116	5.12	Th	5	40	9.40E-05	VAVPYWDWTKP +dK_MMCCH-2 (K)	1903
116	2064	2068	499.7604	997.5061	997.5055	0.60	Th	0	17	0.02	FTKKH +dK_MMCCH-2 (K)	2067
117	2094	2100	618.3057	1234.5969	1234.5903	5.35	Th	1	30	0.001	LHEIEKE +dK_MMCCH-2 (K)	2099
118	2129	2141	933.8789	1865.7433	1865.7495	-3.32	Th	0	19	0.012	ICKTSEDCHHGGQ +dK_MMCCH-2 (K)	2131
119	2238	2248	778.8803	1555.7459	1555.7440	1.29	Th	3	43	5.00E-05	LTTAEVDNLKD +dK_MMCCH-2 (K)	2247
120	2480	2487	622.7991	1243.5836	1243.5795	3.30	Th	2	13	0.046	AKPTDVFE +dK_MMCCH-2 (K)	2481
121	2512	2521	807.3992	1612.7838	1612.7766	4.40	Th	0	32	0.00068	LEKQKEEDRT +dK_MMCCH-2 (K)	2514
122	2595	2606	806.4045	1610.7945	1610.7862	5.15	Th	2	26	0.0026	IIDTSGKQLPSD +dK_MMCCH-2 (K)	2601
123	2607	2612	520.7803	1039.5461	1039.5446	1.44	Th	2	22	0.0057	LIKMPT +dK_MMCCH-2 (K)	2609
124	2766	2771	551.7865	1101.5584	1101.5529	5.08	Th	1	27	0.002	IFQQTK +dK_MMCCH-2 (K)	2771
125	2808	2816	638.3196	1274.6247	1274.6217	2.43	Th	3	21	0.0084	LIGGAEKYS +dK_MMCCH-2 (K)	2814
126	2946	2960	965.4089	1928.8032	1928.7986	2.38	Th	3	34	0.0004	IKSGTDSDDEYAGSF +dK_MMCCH-2 (K)	2947
127	2990	2996	583.2845	1164.5545	1164.5485	5.15	Th	1	38	0.00017	LTDDHVK +dK_MMCCH-2 (K)	2996

Figure 22B. KLH 2

#	Start	End	Observed	Mr(expt)	Mr(calc)	ppm	Enzyme	MC	Score	E value	Peptide	Mod_site
1	26	41	1043.0238	2084.0330	2084.0347	-0.82	T	1	70	9.50E-08	KNVDSLSSDEVLALEK +dK_MMCCH-2 (K)	26
2	147	155	694.3724	1386.7302	1386.7217	6.13	T	1	27	0.0018	ADITFLNKK +dK_MMCCH-2 (K)	155
3	164	175	596.3090	1785.9051	1785.8985	3.70	T	1	37	0.00018	LFEKVQPGHHTR +dK_MMCCH-2 (K)	167
4	249	271	987.4413	2959.3020	2959.3051	-1.05	T	1	32	0.00058	GKDPNSADCAHNLIHTPMEPFDR +dK_MMCCH-2 (K)	250
5	281	293	610.9457	1829.8152	1829.8043	5.96	T	0	54	3.90E-06	EHAKPADSFDYGR +dK_MMCCH-2 (K)	284
6	419	446	677.3701	3381.8139	3381.8132	0.21	T	1	45	3.20E-05	QPTLVHRPAKGHFDKPPVPVAQANLAVR +Deamidated (NQ); dK_MMCCH-2 (K)	428
7	429	446	752.0657	2253.1752	2253.1729	1.02	T	0	52	5.70E-06	GHFDKPPVPVAQANLAVR +dK_MMCCH-2 (K)	433
8	467	488	944.4583	2830.3529	2830.3385	5.12	T	1	71	8.30E-08	FQNDKSVDGYQATVEFHALPAR +dK_MMCCH-2 (K)	471
9	788	795	718.8198	1435.6251	1435.6377	-8.78	T	1	15	0.029	EMKWGFDR +dK_MMCCH-1 (K); Oxidation (M)	790
10	936	950	1080.0140	2158.0135	2158.0095	1.85	T	1	51	8.20E-06	KHGFTGGLPYWDWTR +dK_MMCCH-2 (K)	936
11	995	1052	1170.7135	7018.2375	7018.2306	0.98	T	1	15	0.032	DDLYQSPGFGHYTDIAKQVLLAFEQDDFCDFEVQFEIAHNFIHALVGGNEPYSMSSLR +dK_MMCCH-2 (K)	1011
12	1082	1096	996.4618	1990.9090	1990.9063	1.36	T	0	77	2.00E-08	GKPYNTANCAIASMR +dK_MMCCH-2 (K)	1083
13	1097	1115	827.0768	2478.2087	2478.2101	-0.56	T	0	84	3.90E-09	KPLQPFGLDSVINPDDETR +dK_MMCCH-2 (K)	1097
14	1123	1149	1190.5595	3568.6565	3568.6497	1.93	T	1	73	5.50E-08	VFDYKNNFDYEYESLAFNGLSIAQLDR +dK_MMCCH-2 (K)	1127
15	1295	1311	764.0672	2289.1798	2289.1715	3.63	T	1	17	0.021	SAFLQIQKEGIYENIAK +dK_MMCCH-2 (K)	1302
16	1355	1385	1271.2711	3810.7915	3810.7876	1.05	T	1	44	3.90E-05	GSAVAVPYWDWTEKADSLPSLINDATYFNSR +dK_MMCCH-2 (K)	1368
17	1409	1450	1097.7112	5483.5195	5483.5213	-0.33	T	1	33	0.00047	DPQPELWDNKDFYENVMLALEQDNFCDFEIQLELIHNALHSR +dK_MMCCH-2 (K)	1418
18	1455	1480	1117.8726	3350.5959	3350.6070	-3.34	T	1	63	5.50E-07	AKYSLSSLDYTAFDPVFFLHHANVDR +dK_MMCCH-2 (K)	1456
19	1493	1507	721.6653	2161.9742	2161.9594	6.80	T	1	59	1.20E-06	KKPYNEADCAVNEMR +dK_MMCCH-2 (K)	1493
20	1493	1507	721.6612	2161.9617	2161.9594	1.06	T	1	70	9.40E-08	KKPYNEADCAVNEMR +dK_MMCCH-2 (K)	1494
21	1508	1526	837.7524	2510.2353	2510.2185	6.69	T	0	20	0.01	KPLQPFNNPELNSDSMTLK +dK_MMCCH-2 (K)	1508
22	1508	1539	825.9995	4124.9612	4124.9360	6.08	T	1	23	0.0047	KPLQPFNNPELNSDSMTLKHNLPQDSFDYQNR +dK_MMCCH-2 (K)	1526
23	1542	1564	802.8925	3207.5407	3207.5448	-1.25	T	1	19	0.012	YQYDNLQFNHFSIQKLDQTIQAR +dK_MMCCH-2 (K)	1556
24	1622	1633	591.9809	1772.9209	1772.9171	2.14	T	1	18	0.015	LYKFDITSALHK +dK_MMCCH-2 (K)	1624

Figure 22B. KLH 2 (continued)

25	1690	1700	786.9194	1571.8243	1571.8116	8.08	T	1	13	0.049	KEVSSLTTLEK +dK_MMCCH-2 (K)	1690
26	1690	1704	532.2905	2125.1328	2125.1241	4.05	T	2	28	0.0015	KEVSSLTTLEKHFLR +dK_MMCCH-2 (K)	1700
27	1757	1768	612.9786	1835.9141	1835.9128	0.71	T	1	19	0.013	LYTVQFEDSLKR +dK_MMCCH-2 (K)	1767
28	1769	1803	1108.3084	4429.2045	4429.1882	3.70	T	0	28	0.0015	HGSIVGLPYWDWLKPQSALPDLVTQETYEHLFSHK +dK_MMCCH-2 (K)	1803
29	1804	1825	945.4654	2833.3743	2833.3633	3.92	T	1	23	0.0047	TFPNPFLKANIEFEGEGVTTER +dK_MMCCH-2 (K)	1811
30	1949	1963	560.2515	2236.9767	2236.9735	1.43	T	0	57	1.90E-06	TQEFSKPEDTFDYHR +dK_MMCCH-2 (K)	1954
31	2045	2052	660.3513	1318.6880	1318.6843	2.81	T	1	18	0.015	YDITKTLK +dK_MMCCH-2 (K)	2049
32	2116	2125	715.3626	1428.7107	1428.7105	0.14	T	1	15	0.029	DLASLKSAMR +dK_MMCCH-2 (K)	2121
33	2228	2239	870.4226	1738.8305	1738.8236	3.97	T	1	28	0.0017	GYIKSEDAYTVR +dK_MMCCH-2 (K)	2231
34	2453	2463	839.9324	1677.8502	1677.8436	3.93	T	1	17	0.021	NFKYDITQALK +dK_MMCCH-2 (K)	2455
35	2527	2541	1007.5171	2013.0196	2013.0088	5.37	T	1	86	2.60E-09	KDVTSLTASEIENLR +dK_MMCCH-2 (K)	2527
36	2728	2739	957.9996	1913.9846	1913.9862	-0.84	T	1	32	0.00059	IWAIWQALQKYR +Deamidated (NQ); dK_MMCCH-2 (K)	2737
37	2755	2764	764.3816	1526.7486	1526.7439	3.08	T	0	23	0.0053	QPLKPFSESR +Deamidated (NQ); dK_MMCCH-2 (K)	2758
38	3148	3155	629.3348	1256.6551	1256.6587	-2.86	T	1	15	0.032	KKPYNAAK +dK_MMCCH-2 (K)	3149
39	167	178	590.9649	1769.8729	1769.8705	1.30	G	0	44	4.00E-05	KVQPGHHTRLME +dK_MMCCH-2 (K)	167
40	318	322	456.7347	911.4549	911.4535	1.54	G	0	17	0.021	RAAKE +dK_MMCCH-2 (K)	321
41	433	456	975.8586	2924.5539	2924.5429	3.76	G	2	20	0.011	KPPVPVAQANLAVRKNINDLTAEE +dK_MMCCH-2 (K)	433
42	466	481	1098.4976	2194.9806	2194.9841	-1.59	G	2	29	0.0013	RFQNDKSVDGYQATVE +Deamidated (NQ); dK_MMCCH-2 (K)	471
43	1215	1235	721.6069	2882.3986	2882.3949	1.28	G	3	23	0.0054	ITQQLHDLDLHVGDNFFLKYE +dK_MMCCH-2 (K)	1233
44	1292	1303	879.4658	1756.9170	1756.9182	-0.68	G	0	49	1.20E-05	SIRSAFLQIQKE +dK_MMCCH-2 (K)	1302
45	1308	1320	904.9478	1807.8811	1807.8749	3.37	G	0	23	0.0051	NIAKFHGKPGLCE +dK_MMCCH-2 (K)	1311
46	1308	1320	603.6335	1807.8786	1807.8749	2.05	G	0	28	0.0014	NIAKFHGKPGLCE +dK_MMCCH-2 (K)	1315
47	1403	1422	921.4202	2761.2387	2761.2330	2.06	G	3	19	0.012	NAVTSRDPQPELWDNKDFYE +dK_MMCCH-2 (K)	1418
48	1952	1967	792.6824	2375.0255	2375.0205	2.11	G	3	35	0.00028	FSKPEDTFDYHRFGYE +dK_MMCCH-2 (K)	1954
49	1973	1990	811.7271	2432.1595	2432.1505	3.74	G	0	16	0.023	FVGMSVSSLHNYIKQQQE +dK_MMCCH-2 (K)	1986
50	2477	2484	644.8342	1287.6538	1287.6573	-2.72	G	0	25	0.0034	APFFIKVE +dK_MMCCH-2 (K)	2482
51	3386	3405	877.4154	2629.2244	2629.2271	-1.03	G	2	29	0.0013	LDHAYSLRDGHYYIAGPTKD +dK_MMCCH-2 (K)	3404
52	38	55	1181.0338	2360.0531	2360.0478	2.25	C	3	27	0.0019	ALEKALDDLQQDDSNQGY +dK_MMCCH-2 (K)	41

Figure 22B. KLH 2 (continued)

53	152	165	667.6938	2000.0595	2000.0513	4.10	C	2	14	0.041	LNKKTSRAVDDRLF +dK_MMCCH-2 (K)	154
54	166	176	547.2856	1638.8349	1638.8300	2.99	C	0	21	0.008	EKVQPGHHTRL +dK_MMCCH-2 (K)	167
55	277	296	883.7525	2648.2357	2648.2329	1.02	C	4	45	3.50E-05	DLTREHAKPADSFDYGRLGY +dK_MMCCH-2 (K)	284
56	364	373	735.3609	1468.7072	1468.7094	-1.50	C	2	22	0.0056	LLGGPTEMKW +dK_MMCCH-2 (K)	372
57	629	635	539.2520	1076.4895	1076.4848	4.27	C	0	26	0.0027	VGGSEKY +dK_MMCCH-2 (K)	634
58	1007	1015	669.8715	1337.7284	1337.7265	1.42	C	1	26	0.0024	TDIAKQVLL +dK_MMCCH-2 (K)	1011
59	1075	1080	544.7778	1087.5410	1087.5372	3.49	C	1	26	0.0025	QALQKY +dK_MMCCH-2 (K)	1079
60	1125	1139	1128.4790	2254.9434	2254.9405	1.33	C	5	18	0.016	DYKNNFDYEYESLAF +dK_MMCCH-2 (K)	1127
61	1298	1312	824.0845	2469.2316	2469.2324	-0.32	C	2	26	0.0023	LQIQKEGIYENIAKF +2 dK_MMCCH-2 (K)	1302, 1311
62	1298	1312	711.3758	2131.1055	2131.1023	1.50	C	2	27	0.0021	LQIQKEGIYENIAKF +dK_MMCCH-2 (K)	1311
63	1526	1534	712.3406	1422.6667	1422.6602	4.57	C	0	15	0.03	KHNLPQDSF +dK_MMCCH-2 (K)	1526
64	1589	1606	784.3575	2350.0506	2350.0392	4.85	C	0	13	0.05	ICVEQGGEQNCKTKAGSF +dK_MMCCH-2 (K)	1600
65	1589	1606	784.3556	2350.0451	2350.0392	2.51	C	0	32	0.00069	ICVEQGGEQNCKTKAGSF +dK_MMCCH-2 (K)	1602
66	1696	1702	607.3020	1212.5894	1212.5849	3.71	C	1	20	0.011	TTLEKHF +dK_MMCCH-2 (K)	1700
67	1708	1719	839.8415	1677.6685	1677.6651	2.09	C	0	17	0.019	KNMQADDSPDGY +dK_MMCCH-2 (K)	1708
68	1782	1796	1014.5055	2026.9964	2026.9921	2.12	C	1	31	0.00075	KPQSALPDLVTQETY +dK_MMCCH-2 (K)	1782
69	1801	1809	706.8381	1411.6617	1411.6595	1.56	C	0	16	0.024	SHKTFPNPF +dK_MMCCH-2 (K)	1803
70	1953	1964	627.2849	1878.8327	1878.8247	4.26	C	2	18	0.017	SKPEDTFDYHRF +dK_MMCCH-2 (K)	1954
71	1985	1995	850.4291	1698.8437	1698.8399	2.24	C	0	30	0.0011	IKQQQEADRVF +dK_MMCCH-2 (K)	1986
72	2001	2011	726.8453	1451.6761	1451.6755	0.41	C	1	21	0.008	KGFGQSASVSF +dK_MMCCH-2 (K)	2001
73	2455	2462	645.3257	1288.6369	1288.6373	-0.31	C	1	24	0.0038	KYDITQAL +dK_MMCCH-2 (K)	2455
74	2463	2479	1128.0194	2254.0243	2254.0253	-0.44	C	1	19	0.011	KAQSIHPEDVFDTDAPF +dK_MMCCH-2 (K)	2463
75	2506	2532	761.6026	3042.3813	3042.3738	2.47	C	0	24	0.0042	SAGEGHTDDHGSDHIAGSGVRKDVTSL +dK_MMCCH-2 (K)	2527
76	2754	2760	598.3314	1194.6483	1194.6471	1.00	C	1	17	0.022	KQPLKPF +dK_MMCCH-2 (K)	2754
77	2754	2760	598.3325	1194.6504	1194.6471	2.76	C	1	17	0.022	KQPLKPF +dK_MMCCH-2 (K)	2758
78	2865	2872	673.3662	1344.7179	1344.7112	4.98	C	1	22	0.0064	RYDITKVL +dK_MMCCH-2 (K)	2870
79	3235	3242	617.3142	1232.6139	1232.6111	2.27	C	0	30	0.0009	TSANVKIY +dK_MMCCH-2 (K)	3240
80	3398	3406	658.3369	1314.6593	1314.6530	4.79	C	1	15	0.029	YIAGPTKDL +dK_MMCCH-2 (K)	3404

Figure 22B. KLH 2 (continued)

81	69	75	604.2940	1206.5735	1206.5703	2.65	Th	0	13	0.045	VDKHEKN +dK_MMCCH-2 (K)	74
82	184	191	703.8044	1405.5942	1405.5894	3.41	Th	1	43	4.90E-05	LEQDEFCK +dK_MMCCH-2 (K)	191
83	247	260	631.6201	1891.8384	1891.8305	4.12	Th	2	21	0.0078	LRGKDPNSADCAHN +dK_MMCCH-2 (K)	250
84	283	293	782.8576	1563.7006	1563.7028	-1.34	Th	3	47	1.80E-05	AKPADSFDYGR +dK_MMCCH-2 (K)	284
85	364	374	763.8729	1525.7312	1525.7309	0.20	Th	3	33	0.00046	LLGGPTEMKWG +dK_MMCCH-2 (K)	372
86	629	636	582.7682	1163.5219	1163.5169	4.38	Th	1	20	0.01	VGGSEKYS +dK_MMCCH-2 (K)	634
87	893	904	904.8973	1807.7801	1807.7698	5.70	Th	1	22	0.0058	FHGEPKWCPSPE +dK_MMCCH-2 (K)	898
88	1362	1374	968.4312	1934.8479	1934.8397	4.24	Th	4	13	0.045	YWDWTEKADSLPS +dK_MMCCH-2 (K)	1368
89	1525	1539	738.3572	2212.0497	2212.0371	5.70	Th	3	36	0.00026	LKHNLPQDSFDYQNR +dK_MMCCH-2 (K)	1526
90	1589	1605	848.0453	2541.1142	2541.1008	5.27	Th	2	19	0.013	ICVEQGGEQNCKTKAGS +2 dK_MMCCH-2 (K)	1600, 1602
91	1589	1605	735.3340	2202.9801	2202.9708	4.22	Th	2	38	0.00015	ICVEQGGEQNCKTKAGS +dK_MMCCH-2 (K)	1602
92	1643	1648	537.7640	1073.5135	1073.5103	2.98	Th	2	14	0.037	FDIKVD +dK_MMCCH-2 (K)	1646
93	1800	1809	780.3752	1558.7359	1558.7279	5.13	Th	2	20	0.01	FSHKTFPNPF +dK_MMCCH-2 (K)	1803
94	1952	1963	627.2850	1878.8331	1878.8247	4.47	Th	2	55	3.40E-06	FSKPEDTFDYHR +dK_MMCCH-2 (K)	1954
95	1985	1993	727.3631	1452.7116	1452.7031	5.92	Th	1	21	0.0072	IKQQQEADR +dK_MMCCH-2 (K)	1986
96	2193	2199	667.3032	1332.5918	1332.5849	5.18	Th	2	24	0.0037	YWDWTKP +dK_MMCCH-2 (K)	2198
97	2200	2206	562.3082	1122.6018	1122.5995	2.05	Th	2	22	0.0062	ISKLPDL +dK_MMCCH-2 (K)	2202
98	2225	2229	462.2221	922.4297	922.4259	4.23	Th	2	21	0.0072	FAKGY +dK_MMCCH-2 (K)	2227
99	2359	2363	509.2315	1016.4485	1016.4460	2.46	Th	1	26	0.0028	FTKMH +dK_MMCCH-2 (K); Oxidation (M)	2361
100	2941	2950	720.8409	1439.6673	1439.6602	4.93	Th	3	45	3.00E-05	LDEANDLKNA +dK_MMCCH-2 (K)	2948
101	3009	3015	573.2771	1144.5396	1144.5335	5.33	Th	0	16	0.022	LKEHGSH +dK_MMCCH-2 (K)	3010
102	3399	3405	520.2615	1038.5084	1038.5056	2.70	Th	1	29	0.0011	IAGPTKD +dK_MMCCH-2 (K)	3404

"Start" and "End" indicates the number of residue of KLH1 or KLH2. "Observed" column implies the observed m/z value in the survey scan while "Mr(expt)", "Mr(calc)", "ppm" indicate the experimental molecular weight(MW), calculated MW, and the difference between observed MW and theoretical MW respectively. In the "Enzyme" column, T, C, G and Th stand for trypsin, chymotrypsin, Glu-C and thermolysin respectively. MC stands for missed cleavage. Scores are the peptide ion score directly reported from Mascot database search engine. E value denotes the expectation value for each identified peptide. The peptide sequences as well as its modifications are listed in "Peptide" column. "Mod_site" indicates the lysine conjugation site for KLH1 or KLH2.

Figure 23. Identification details of MMCCH-conjugated peptides for sample 2 (1st LC-MS/MS)

Figure 23A. KLH 1

#	Start	End	Observed	Mr(expt)	Mr(calc)	ppm	Enzyme	MC	Score	E value	Peptide	Mod_site
1	124	141	785.4092	2353.2059	2353.2001	2.46	T	1	25	0.0032	GFTDPPVKHHQSANLLVR +dK_MMCCH-2 (K)	131
2	142	149	656.3431	1310.6716	1310.6653	4.88	T	1	33	0.00048	KNINDLTR +dK_MMCCH-2 (K)	142
3	157	166	822.8833	1643.7520	1643.7402	7.18	T	1	18	0.014	EAFHKFQEDR +dK_MMCCH-2 (K)	161
4	184	192	726.8424	1451.6701	1451.6649	3.58	T	1	20	0.009	CPRPDAKDR +dK_MMCCH-2 (K)	190
5	553	560	663.8682	1325.7219	1325.7166	4.00	T	2	20	0.011	VKFDKVPR +dK_MMCCH-2 (K)	554
6	566	570	485.2449	968.4752	968.4749	0.31	T	1	16	0.025	KNVDR +dK_MMCCH-2 (K)	566
7	581	590	733.9201	1465.8256	1465.8214	2.93	T	2	24	0.0038	KALALLKEDK +dK_MMCCH-2 (K)	581
8	588	606	781.0359	2340.0858	2340.0845	0.60	T	1	26	0.0025	EDKSAGGFQQLGAFHGEPK +dK_MMCCH-2 (K)	590
9	645	681	1158.5337	4630.1057	4630.1063	-0.15	T	1	25	0.0032	HGYDGALPYWDWTSPLNHLPELADHEKYVDPEDGVEK +dK_MMCCH-2 (K)	671
10	682	699	620.2917	2477.1377	2477.1434	-2.34	T	1	18	0.015	HNPWFDGHIDTVDKTTTR +dK_MMCCH-2 (K)	695
11	700	719	887.7701	2660.2886	2660.2945	-2.22	T	1	48	1.60E-05	SVQNKLFEQPEFGHYTSIAK +dK_MMCCH-2 (K)	704
12	778	789	958.0007	1913.9869	1913.9862	0.37	T	1	22	0.0059	IWAIWQALQKYR +Deamidated (NQ); dK_MMCCH-2 (K)	787
13	790	804	1003.4695	2004.9244	2004.9220	1.20	T	0	56	2.60E-06	GKPYNVANCAVTSMR +dK_MMCCH-2 (K)	791
14	858	863	520.2990	1038.5835	1038.5783	4.91	T	1	16	0.024	KLEAIK +dK_MMCCH-2 (K)	858
15	953	965	635.3314	1902.9723	1902.9662	3.15	T	1	54	3.60E-06	DLFKQPSVIHEPR +dK_MMCCH-2 (K)	956
16	986	1000	1027.0338	2052.0531	2052.0561	-1.46	T	1	51	8.60E-06	KNIENLSLGELESLR +dK_MMCCH-2 (K)	986
17	1048	1060	913.5288	1825.0431	1825.0423	0.44	T	1	37	0.00021	LYVVVVENALLKK +dK_MMCCH-2 (K)	1060
18	1092	1114	791.8768	3163.4780	3163.4682	3.07	T	1	38	0.00017	QHHYETNPFHHGKITHENEITTR +dK_MMCCH-2 (K)	1104
19	1199	1203	353.1911	1056.5514	1056.5538	-2.37	T	1	17	0.019	KRPYR +dK_MMCCH-2 (K)	1199
20	1331	1338	620.3545	1238.6944	1238.6944	0.00	T	1	24	0.0039	LDITKALK +dK_MMCCH-2 (K)	1335
21	1395	1402	649.8365	1297.6585	1297.6588	-0.15	T	1	21	0.0078	KDITQLDK +dK_MMCCH-2 (K)	1395
22	1473	1489	778.4027	2332.1863	2332.1827	1.54	T	1	47	2.00E-05	KHGAVVGLPYWDWTLPR +dK_MMCCH-2 (K)	1473
23	1721	1746	1087.4764	3259.4075	3259.3937	4.23	T	1	13	0.047	TAGDCEDAGYFTVLGGEKEMPWAFDR +dK_MMCCH-2 (K)	1738
24	1747	1758	613.9770	1838.9091	1838.9012	4.35	T	1	21	0.0079	LYKYDITETLDK +dK_MMCCH-2 (K)	1749

Figure 23A. KLH 1 (continued)

25	1923	1932	756.3808	1510.7470	1510.7425	3.04	T	1	27	0.0019	NKVMPNPFAR +dK_MMCCH-2 (K)	1924
26	2100	2109	492.2468	1964.9580	1964.9601	-1.07	T	2	19	0.014	EIKDKQHHVR +2 dK_MMCCH-2 (K)	2102, 2104
27	2121	2149	1186.8922	3557.6548	3557.6378	4.78	T	1	46	2.80E-05	TSADVQFQICKTSEDCHHGGQIFVLGGTK +dK_MMCCH-2 (K)	2131
28	2359	2367	736.3499	1470.6853	1470.6813	2.72	T	1	35	0.00031	DKLFNDPER +dK_MMCCH-2 (K)	2360
29	2507	2514	682.3525	1362.6905	1362.6853	3.82	T	1	27	0.0019	KLEHELEK +dK_MMCCH-2 (K)	2507
30	2515	2520	571.7622	1141.5099	1141.5074	2.19	T	1	18	0.017	QKEEDR +dK_MMCCH-2 (K)	2516
31	2595	2609	983.5306	1965.0467	1965.0493	-1.27	T	1	21	0.0081	IIDTSGKQLPSDLIK +dK_MMCCH-2 (K)	2601
32	2621	2636	802.7113	2405.1121	2405.1083	1.54	T	1	55	3.00E-06	HHEKHHEDHHEDILVR +dK_MMCCH-2 (K)	2624
33	2637	2651	1069.5327	2137.0509	2137.0374	6.27	T	1	71	8.70E-08	KNIHSLSHHEAEELR +dK_MMCCH-2 (K)	2637
34	2761	2814	1324.8373	6619.1500	6619.1192	4.65	T	1	13	0.046	DVNEAIFQQTKFGEFSSIFYLALQALEEDNYCDFEVQYEILHNEVHALIGGAEK +dK_MMCCH-2 (K)	2771
35	2851	2883	1009.2160	4032.8349	4032.8346	0.07	T	0	30	0.001	VKPAHAGSCAGDIMHVPLHPFNYESVNNDDFTR +dK_MMCCH-2 (K)	2852
36	2897	2919	1066.5197	3196.5371	3196.5287	2.63	T	1	59	1.30E-06	FNYKYDNLNLHGHNIEELEEVLR +dK_MMCCH-2 (K)	2900
37	2999	3021	1106.2400	3315.6981	3315.6923	1.75	T	2	21	0.0071	FDLKKYDHTELDASVLPAPIIVR +2 dK_MMCCH-2 (K)	3002, 3003
38	3003	3021	825.7711	2474.2914	2474.2879	1.37	T	1	27	0.0022	KYDHTELDASVLPAPIIVR +dK_MMCCH-2 (K)	3003
39	123	151	616.6606	3693.9202	3693.9049	4.14	G	2	30	0.00099	KGFTDPPVKHHQSANLLVRKNINDLTREE +dK_MMCCH-2 (K)	123
40	123	151	616.6599	3693.9154	3693.9049	2.84	G	2	23	0.005	KGFTDPPVKHHQSANLLVRKNINDLTREE +dK_MMCCH-2 (K)	131
41	158	176	846.3828	2536.1266	2536.1329	-2.48	G	3	24	0.0038	AFHKFQEDRSVDGYQATAE +dK_MMCCH-2 (K)	161
42	435	442	676.3245	1350.6344	1350.6312	2.37	G	1	18	0.015	NIEKMIHE +dK_MMCCH-2 (K)	438
43	526	544	777.7501	2330.2285	2330.2304	-0.82	G	1	24	0.0044	VDGTKLASSLIPHASVIRE +dK_MMCCH-2 (K)	530
44	589	612	1102.8262	3305.4567	3305.4621	-1.63	G	1	34	0.00039	DKSAGGFQQLGAFHGEPKWCPSPE +2 dK_MMCCH-2 (K)	590, 606
45	589	612	990.1141	2967.3206	2967.3320	-3.84	G	1	23	0.0055	DKSAGGFQQLGAFHGEPKWCPSPE +dK_MMCCH-2 (K)	606
46	666	676	827.3729	1652.7313	1652.7392	-4.78	G	2	14	0.038	LADHEKYVDPE +dK_MMCCH-2 (K)	671
47	825	841	820.3713	2458.0922	2458.0940	-0.73	G	1	25	0.003	HSVPFNVFDYKTNFNYE +dK_MMCCH-2 (K)	835
48	847	860	643.6777	1928.0112	1928.0077	1.82	G	0	24	0.0043	FNGLSISQLNKKLE +dK_MMCCH-2 (K)	858
49	942	970	727.3804	3631.8658	3631.8973	-8.70	G	2	18	0.016	VFDLKPASLGKDLFKQPSVIHEPRIGHHE +dK_MMCCH-2 (K)	956
50	1055	1076	810.1655	3236.6328	3236.6402	-2.32	G	1	30	0.00092	NALLKKGSSVAVPYWDWTKRIE +2 dK_MMCCH-2 (K)	1059, 1060

Figure 23A. KLH 1 (continued)

51	1055	1076	725.6326	2898.5012	2898.5102	-3.11	G	1	37	0.0002	NALLKKGSSVAVPYWDWTKRIE +dK_MMCCH-2 (K)	1060
52	1097	1110	999.9615	1997.9085	1997.9054	1.60	G	1	22	0.0062	TNPFHHGKITHENE +dK_MMCCH-2 (K)	1104
53	1376	1396	864.3896	2590.1471	2590.1428	1.66	G	3	22	0.0067	AGTDSAHTDDGHTEPVMIRKD +dK_MMCCH-2 (K)	1395
54	1376	1413	915.2663	4571.2951	4571.2636	6.89	G	5	21	0.0079	AGTDSAHTDDGHTEPVMIRKDITQLDKRQQLSLVKALE +Deamidated (NQ); dK_MMCCH-2 (K); Oxidation (M)	1402
55	1397	1413	774.4324	2320.2753	2320.2824	-3.06	G	1	22	0.006	ITQLDKRQQLSLVKALE +dK_MMCCH-2 (K)	1410
56	1506	1522	753.3741	2257.1004	2257.1089	-3.77	G	2	21	0.0076	TGRDIPNPFIGSKIEFE +dK_MMCCH-2 (K)	1518
57	1755	1765	570.6044	1708.7915	1708.7913	0.12	G	2	27	0.0019	TLDKMNLRHDE +dK_MMCCH-2 (K)	1758
58	2089	2100	854.4117	1706.8088	1706.8008	4.75	G	2	41	7.40E-05	IGGMNLHEIEKE +dK_MMCCH-2 (K)	2099
59	2647	2661	715.6783	2144.0130	2144.0095	1.63	G	4	24	0.0043	AEELRDALYKLQNDE +dK_MMCCH-2 (K)	2656
60	3090	3097	632.8027	1263.5908	1263.5879	2.30	G	0	14	0.039	LGKMYSVE +dK_MMCCH-2 (K)	3092
61	59	68	721.3470	1440.6794	1440.6781	0.90	C	1	33	0.00045	VLGGPSEMKW +dK_MMCCH-2 (K)	67
62	160	171	909.9108	1817.8070	1817.8043	1.49	C	1	19	0.014	HKFQEDRSVDGY +dK_MMCCH-2 (K)	161
63	584	595	787.4013	1572.7879	1572.7858	1.40	C	2	36	0.00027	ALLKEDKSAGGF +dK_MMCCH-2 (K)	590
64	715	723	655.8733	1309.7320	1309.7316	0.38	C	1	15	0.032	TSIAKQVLL +dK_MMCCH-2 (K)	719
65	783	788	544.7770	1087.5394	1087.5372	2.02	C	1	18	0.017	QALQKY +dK_MMCCH-2 (K)	787
66	860	869	789.8865	1577.7584	1577.7548	2.28	C	1	13	0.045	EAIKSQDRFF +dK_MMCCH-2 (K)	863
67	944	955	821.4309	1640.8473	1640.8484	-0.67	C	3	15	0.035	DLKPASLGKDLF +dK_MMCCH-2 (K)	946
68	1013	1018	516.7577	1031.5009	1031.4998	1.16	C	0	22	0.0065	ESIAKF +dK_MMCCH-2 (K)	1017
69	1330	1337	620.3552	1238.6958	1238.6944	1.05	C	1	21	0.0071	KLDITKAL +dK_MMCCH-2 (K)	1335
70	1515	1521	566.2921	1130.5697	1130.5682	1.33	C	0	17	0.022	IGSKIEF +dK_MMCCH-2 (K)	1518
71	1649	1664	752.3290	2253.9651	2253.9637	0.62	C	2	15	0.034	NLNDHTHDFSKPEDTF +dK_MMCCH-2 (K)	1659
72	1818	1827	753.3682	1504.7218	1504.7232	-0.93	C	1	21	0.0077	SERDIGSLKY +dK_MMCCH-2 (K)	1826
73	2076	2082	612.3054	1222.5962	1222.5944	1.47	C	3	19	0.014	KYELLGY +dK_MMCCH-2 (K)	2076
74	2160	2184	1085.5089	3253.5049	3253.5179	-4.00	C	3	32	0.00064	KYDITHALHDAHITPEDVFHPSEPF +dK_MMCCH-2 (K)	2160
75	2476	2488	923.9213	1845.8280	1845.8244	1.95	C	1	26	0.0025	THSNAKPTDVFEY +dK_MMCCH-2 (K)	2481
76	2656	2672	747.3419	2239.0039	2239.0004	1.56	C	2	30	0.001	KLQNDESHGGYEHIAGF +dK_MMCCH-2 (K)	2656
77	2738	2749	856.3748	1710.7350	1710.7348	0.12	C	2	21	0.0074	ADSGNNNPFFKY +dK_MMCCH-2 (K)	2748

Figure 23A. KLH 1 (continued)

78	2946	2960	965.4052	1928.7957	1928.7986	-1.50	C	1	21	0.0072	IKSGTDSDDEYAGSF +dK_MMCCH-2 (K)	2947
79	2964	2971	607.2726	1212.5306	1212.5307	-0.08	C	0	17	0.02	GGAKEMPW +dK_MMCCH-2 (K)	2967
80	1	9	733.3323	1464.6500	1464.6516	-1.09	Th	2	19	0.014	MTPEELKTY +dK_MMCCH-2 (K); Oxidation (M)	7
81	38	56	861.6808	2582.0205	2582.0108	3.76	Th	2	17	0.019	VCIPDDNDRNDDHCEKAGD +dK_MMCCH-2 (K)	53
82	59	69	785.3759	1568.7371	1568.7367	0.25	Th	3	52	6.90E-06	VLGGPSEMKWQ +dK_MMCCH-2 (K)	67
83	78	84	569.2864	1136.5583	1136.5536	4.14	Th	1	34	0.00041	LSDTVHK +dK_MMCCH-2 (K)	84
84	117	124	620.8127	1239.6109	1239.6070	3.15	Th	1	24	0.0044	VVHHPEKG +dK_MMCCH-2 (K)	123
85	431	439	715.8506	1429.6866	1429.6833	2.38	Th	3	16	0.027	ISLENIEKM +dK_MMCCH-2 (K); Oxidation (M)	438
86	521	530	707.8433	1413.6720	1413.6698	1.56	Th	2	69	1.10E-07	VDITEVDGTK +dK_MMCCH-2 (K)	530
87	585	591	585.8104	1169.6062	1169.6002	5.13	Th	1	35	0.00033	LLKEDKS +dK_MMCCH-2 (K)	590
88	601	612	904.8962	1807.7779	1807.7698	4.48	Th	1	18	0.018	FHGEPKWCPSPE +dK_MMCCH-2 (K)	606
89	666	672	607.2816	1212.5486	1212.5485	0.08	Th	2	23	0.0045	LADHEKY +dK_MMCCH-2 (K)	671
90	821	828	617.8116	1233.6086	1233.6064	1.78	Th	1	23	0.005	VTKEHSVP +dK_MMCCH-2 (K)	823
91	831	837	612.7867	1223.5588	1223.5533	4.50	Th	2	22	0.007	VFDYKTN +dK_MMCCH-2 (K)	835
92	1100	1104	482.2287	962.4428	962.4433	-0.52	Th	0	20	0.0093	FHHGK +dK_MMCCH-2 (K)	1104
93	1111	1120	742.3818	1482.7491	1482.7388	6.95	Th	1	22	0.0066	ITTRDPKDSL +dK_MMCCH-2 (K)	1117
94	1156	1164	630.8400	1259.6654	1259.6584	5.56	Th	2	14	0.038	LLGGKGKYS +dK_MMCCH-2 (K)	1162
95	1219	1232	653.9541	1958.8405	1958.8316	4.54	Th	1	30	0.0011	FDKSDNNDEATKTH +dK_MMCCH-2 (K)	1221
96	1219	1232	980.4238	1958.8330	1958.8316	0.71	Th	1	37	0.0002	FDKSDNNDEATKTH +dK_MMCCH-2 (K)	1230
97	1580	1587	572.7732	1143.5319	1143.5271	4.28	Th	1	16	0.023	VGGKEPYG +dK_MMCCH-2 (K)	1583
98	1657	1668	921.9167	1841.8189	1841.8182	0.38	Th	2	49	1.30E-05	FSKPEDTFDYQK +dK_MMCCH-2 (K)	1659
99	1657	1668	921.9177	1841.8208	1841.8182	1.41	Th	2	56	2.20E-06	FSKPEDTFDYQK +dK_MMCCH-2 (K)	1668
100	1733	1741	664.3229	1326.6313	1326.6312	0.08	Th	2	17	0.02	VLGGEKEMP +dK_MMCCH-1 (K); Oxidation (M)	1738
101	1756	1760	479.7244	957.4342	957.4300	4.49	Th	1	16	0.024	LDKMN +dK_MMCCH-2 (K)	1758
102	1894	1904	850.4153	1698.8161	1698.8116	2.65	Th	5	42	5.60E-05	VAVPYWDWTKP +dK_MMCCH-2 (K)	1903
103	2064	2068	499.7591	997.5036	997.5055	-2.01	Th	0	18	0.014	FTKKH +dK_MMCCH-2 (K)	2067
104	2094	2100	618.3030	1234.5914	1234.5903	0.89	Th	1	27	0.0022	LHEIEKE +dK_MMCCH-2 (K)	2099

Figure 23A. KLH 1 (continued)

105	2129	2141	933.8804	1865.7462	1865.7495	-1.77	Th	0	25	0.0035	ICKTSEDCHHGGQ +dK_MMCCH-2 (K)	2131
106	2238	2248	778.8785	1555.7425	1555.7440	-0.90	Th	3	44	4.10E-05	LTTAEVDNLKD +dK_MMCCH-2 (K)	2247
107	2475	2487	915.9249	1829.8353	1829.8295	3.22	Th	3	17	0.018	FTHSNAKPTDVFE +dK_MMCCH-2 (K)	2481
108	2512	2521	807.3982	1612.7819	1612.7766	3.29	Th	0	35	0.00033	LEKQKEEDRT +dK_MMCCH-2 (K)	2514
109	2508	2521	708.0113	2121.0120	2121.0048	3.44	Th	1	14	0.042	LEHELEKQKEEDRT +dK_MMCCH-2 (K)	2516
110	2595	2606	806.4034	1610.7923	1610.7862	3.79	Th	2	35	0.00033	IIDTSGKQLPSD +dK_MMCCH-2 (K)	2601
111	2607	2612	520.7794	1039.5443	1039.5446	-0.29	Th	2	22	0.0058	LIKMPT +dK_MMCCH-2 (K)	2609
112	2766	2771	551.7853	1101.5561	1101.5529	3.00	Th	1	24	0.0043	IFQQTK +dK_MMCCH-2 (K)	2771
113	2808	2816	638.3184	1274.6223	1274.6217	0.47	Th	3	27	0.0018	LIGGAEKYS +dK_MMCCH-2 (K)	2814
114	2946	2960	965.4048	1928.7950	1928.7986	-1.87	Th	3	30	0.001	IKSGTDSDDEYAGSF +dK_MMCCH-2 (K)	2947
115	2990	2996	583.2842	1164.5538	1164.5485	4.55	Th	1	38	0.00016	LTDDHVK +dK_MMCCH-2 (K)	2996
116	3076	3084	724.3623	1446.7100	1446.7040	4.22	Th	2	13	0.046	FKCKVPPFS +dK_MMCCH-2 (K)	3079

Figure 23B. KLH 2

#	Start	End	Observed	Mr(expt)	Mr(calc)	ppm	Enzyme	MC	Score	E value	Peptide	Mod_site
1	26	41	1043.0241	2084.0335	2084.0347	-0.58	T	1	44	3.80E-05	KNVDSLSSDEVLALEK +dK_MMCCH-2 (K)	26
2	147	155	694.3694	1386.7242	1386.7217	1.80	T	1	22	0.006	ADITFLNKK +dK_MMCCH-2 (K)	155
3	164	175	596.3101	1785.9085	1785.8985	5.66	T	1	44	4.40E-05	LFEKVQPGHHTR +dK_MMCCH-2 (K)	167
4	249	271	987.4429	2959.3068	2959.3051	0.57	T	1	33	0.00051	GKDPNSADCAHNLIHTPMEPFDR +dK_MMCCH-2 (K)	250
5	281	293	610.9435	1829.8088	1829.8043	2.46	T	0	56	2.70E-06	EHAKPADSFDYGR +dK_MMCCH-2 (K)	284
6	419	446	846.4591	3381.8073	3381.8132	-1.74	T	1	24	0.0038	QPTLVHRPAKGHFDKPPVPVAQANLAVR +Deamidated (NQ); dK_MMCCH-2 (K)	428
7	429	446	752.0663	2253.1770	2253.1729	1.86	T	0	52	7.00E-06	GHFDKPPVPVAQANLAVR +dK_MMCCH-2 (K)	433
8	467	488	708.5934	2830.3444	2830.3385	2.08	T	1	65	2.90E-07	FQNDKSVDGYQATVEFHALPAR +dK_MMCCH-2 (K)	471
9	489	497	726.8424	1451.6701	1451.6649	3.58	T	1	20	0.009	CPRPDAKDR +dK_MMCCH-2 (K)	495
10	936	950	1080.0117	2158.0089	2158.0095	-0.28	T	1	46	2.60E-05	KHGFTGGLPYWDWTR +dK_MMCCH-2 (K)	936
11	1082	1096	996.4610	1990.9074	1990.9063	0.60	T	0	85	3.00E-09	GKPYNTANCAIASMR +dK_MMCCH-2 (K)	1083
12	1097	1115	827.0761	2478.2065	2478.2101	-1.45	T	0	56	2.60E-06	KPLQPFGLDSVINPDDETR +dK_MMCCH-2 (K)	1097
13	1123	1149	1190.5605	3568.6598	3568.6497	2.86	T	1	63	5.20E-07	VFDYKNNFDYEYESLAFNGLSIAQLDR +dK_MMCCH-2 (K)	1127
14	1355	1385	1271.2697	3810.7871	3810.7876	-0.10	T	1	27	0.0019	GSAVAVPYWDWTEKADSLPSLINDATYFNSR +dK_MMCCH-2 (K)	1368
15	1409	1450	1371.8883	5483.5241	5483.5213	0.51	T	1	54	4.10E-06	DPQPELWDNKDFYENVMLALEQDNFCDFEIQLELIHNALHSR +dK_MMCCH-2 (K)	1418
16	1455	1480	1117.8800	3350.6182	3350.6070	3.31	T	1	42	6.00E-05	AKYSLSSLDYTAFDPVFFLHHANVDR +dK_MMCCH-2 (K)	1456
17	1493	1507	721.6616	2161.9629	2161.9594	1.57	T	1	62	6.50E-07	KKPYNEADCAVNEMR +dK_MMCCH-2 (K)	1494
18	1542	1564	1070.1942	3207.5608	3207.5448	4.99	T	1	33	0.00048	YQYDNLQFNHFSIQKLDQTIQAR +dK_MMCCH-2 (K)	1556
19	1691	1704	999.5225	1997.0305	1997.0292	0.65	T	1	23	0.0055	EVSSLTTLEKHFLR +dK_MMCCH-2 (K)	1700
20	1757	1768	612.9788	1835.9146	1835.9128	1.03	T	1	16	0.025	LYTVQFEDSLKR +dK_MMCCH-2 (K)	1767
21	1804	1825	945.4641	2833.3705	2833.3633	2.54	T	1	39	0.00014	TFPNPFLKANIEFEGEGVTTER +dK_MMCCH-2 (K)	1811
22	1949	1963	1119.4961	2236.9776	2236.9735	1.83	T	0	45	3.30E-05	TQEFSKPEDTFDYHR +dK_MMCCH-2 (K)	1954
23	2228	2239	870.4186	1738.8227	1738.8236	-0.52	T	1	16	0.026	GYIKSEDAYTVR +dK_MMCCH-2 (K)	2231
24	2527	2541	1007.5152	2013.0158	2013.0088	3.48	T	1	79	1.40E-08	KDVTSLTASEIENLR +dK_MMCCH-2 (K)	2527

Figure 23B. KLH 2 (continued)

25	2728	2739	958.0007	1913.9869	1913.9862	0.37	T	1	22	0.0059	IWAIWQALQKYR +Deamidated (NQ); dK_MMCCH-2 (K)	2737
26	2755	2764	764.3814	1526.7483	1526.7439	2.88	T	0	33	0.00051	QPLKPFSESR +Deamidated (NQ); dK_MMCCH-2 (K)	2758
27	2866	2873	659.3627	1316.7108	1316.7050	4.40	T	1	21	0.0089	YDITKVLK +dK_MMCCH-2 (K)	2870
28	3148	3155	629.3356	1256.6567	1256.6587	-1.59	T	1	19	0.013	KKPYNAAK +dK_MMCCH-2 (K)	3149
29	167	178	590.9629	1769.8668	1769.8705	-2.09	G	0	38	0.00014	KVQPGHHTRLME +dK_MMCCH-2 (K)	167
30	433	456	975.8492	2924.5259	2924.5429	-5.81	G	2	16	0.025	KPPVPVAQANLAVRKNINDLTAEE +dK_MMCCH-2 (K)	433
31	466	481	732.3397	2193.9972	2194.0001	-1.32	G	2	25	0.0032	RFQNDKSVDGYQATVE +dK_MMCCH-2 (K)	471
32	1117	1135	1404.1260	2806.2374	2806.2373	0.04	G	3	16	0.024	HSVPFRVFDYKNNFDYEYE +dK_MMCCH-2 (K)	1127
33	1215	1235	721.6066	2882.3974	2882.3949	0.87	G	3	25	0.0031	ITQQLHDLDLHVGDNFFLKYE +dK_MMCCH-2 (K)	1233
34	1292	1303	879.4659	1756.9173	1756.9182	-0.46	G	0	42	5.80E-05	SIRSAFLQIQKE +dK_MMCCH-2 (K)	1302
35	1308	1320	904.9471	1807.8797	1807.8749	2.66	G	0	21	0.0082	NIAKFHGKPGLCE +dK_MMCCH-2 (K)	1311
36	1308	1320	603.6324	1807.8755	1807.8749	0.33	G	0	26	0.0026	NIAKFHGKPGLCE +dK_MMCCH-2 (K)	1315
37	1952	1967	792.6802	2375.0187	2375.0205	-0.76	G	3	34	0.00037	FSKPEDTFDYHRFGYE +dK_MMCCH-2 (K)	1954
38	1973	1990	811.7253	2432.1540	2432.1505	1.48	G	0	14	0.041	FVGMSVSSLHNYIKQQQE +dK_MMCCH-2 (K)	1986
39	2471	2484	990.9680	1979.9215	1979.9227	-0.61	G	3	22	0.0069	DVFDTDAPFFIKVE +dK_MMCCH-2 (K)	2482
40	3386	3405	658.3167	2629.2377	2629.2271	4.03	G	2	31	0.00087	LDHAYSLRDGHYYIAGPTKD +dK_MMCCH-2 (K)	3404
41	153	165	629.9987	1886.9742	1886.9673	3.66	C	1	15	0.031	NKKTSRAVDDRLF +dK_MMCCH-2 (K)	154
42	277	296	883.7534	2648.2384	2648.2329	2.08	C	4	41	8.10E-05	DLTREHAKPADSFDYGRLGY +dK_MMCCH-2 (K)	284
43	364	373	735.3599	1468.7052	1468.7094	-2.93	C	2	29	0.0012	LLGGPTEMKW +dK_MMCCH-2 (K)	372
44	432	443	793.9158	1585.8171	1585.8174	-0.19	C	0	16	0.027	DKPPVPVAQANL +dK_MMCCH-2 (K)	433
45	629	635	539.2513	1076.4881	1076.4848	3.07	C	0	16	0.024	VGGSEKY +dK_MMCCH-2 (K)	634
46	1075	1080	544.7770	1087.5394	1087.5372	2.02	C	1	18	0.017	QALQKY +dK_MMCCH-2 (K)	1079
47	1212	1230	875.0869	2622.2389	2622.2424	-1.33	C	4	17	0.02	KYEITQQLHDLDLHVGDNF +dK_MMCCH-2 (K)	1212
48	1298	1312	824.0828	2469.2266	2469.2324	-2.31	C	2	19	0.012	LQIQKEGIYENIAKF +2 dK_MMCCH-2 (K)	1302, 1311
49	1298	1312	711.3739	2131.0999	2131.1023	-1.17	C	2	36	0.00023	LQIQKEGIYENIAKF +dK_MMCCH-2 (K)	1311
50	1526	1536	851.3828	1700.7511	1700.7505	0.35	C	1	19	0.014	KHNLPQDSFDY +dK_MMCCH-2 (K)	1526
51	1589	1606	784.3549	2350.0428	2350.0392	1.53	C	0	23	0.0054	ICVEQGGEQNCKTKAGSF +dK_MMCCH-2 (K)	1602

Figure 23B. KLH 2 (continued)

52	1696	1702	607.3007	1212.5868	1212.5849	1.57	C	1	23	0.0045	TTLEKHF +dK_MMCCH-2 (K)	1700
53	1708	1719	839.8433	1677.6720	1677.6651	4.11	C	0	28	0.0015	KNMQADDSPDGY +dK_MMCCH-2 (K)	1708
54	1801	1809	706.8373	1411.6601	1411.6595	0.50	C	0	19	0.012	SHKTFPNPF +dK_MMCCH-2 (K)	1803
55	1985	1995	850.4278	1698.8410	1698.8399	0.65	C	0	32	0.00062	IKQQQEADRVF +dK_MMCCH-2 (K)	1986
56	2001	2011	726.8445	1451.6744	1451.6755	-0.76	C	1	22	0.0059	KGFGQSASVSF +dK_MMCCH-2 (K)	2001
57	2424	2438	1032.4364	2062.8582	2062.8621	-1.84	C	0	20	0.011	ICKTADDCHASGMIF +dK_MMCCH-2 (K)	2426
58	2455	2462	645.3273	1288.6401	1288.6373	2.17	C	1	19	0.013	KYDITQAL +dK_MMCCH-2 (K)	2455
59	2463	2479	752.3498	2254.0277	2254.0253	1.11	C	1	18	0.016	KAQSIHPEDVFDTDAPF +dK_MMCCH-2 (K)	2463
60	2506	2532	761.6044	3042.3884	3042.3738	4.80	C	0	19	0.012	SAGEGHTDDHGSDHIAGSGVRKDVTSL +dK_MMCCH-2 (K)	2527
61	2754	2760	598.3299	1194.6452	1194.6471	-1.51	C	1	18	0.017	KQPLKPF +dK_MMCCH-2 (K)	2754
62	2754	2760	598.3325	1194.6504	1194.6471	2.76	C	1	23	0.0046	KQPLKPF +dK_MMCCH-2 (K)	2758
63	2865	2872	673.3627	1344.7109	1344.7112	-0.15	C	1	15	0.032	RYDITKVL +dK_MMCCH-2 (K)	2870
64	3235	3242	617.3137	1232.6129	1232.6111	1.46	C	0	22	0.0057	TSANVKIY +dK_MMCCH-2 (K)	3240
65	3399	3406	576.8025	1151.5904	1151.5896	0.69	C	0	24	0.0036	IAGPTKDL +dK_MMCCH-2 (K)	3404
66	181	191	853.3754	1704.7363	1704.7375	-0.70	Th	3	58	1.50E-06	LDALEQDEFCK +dK_MMCCH-2 (K)	191
67	247	260	631.6194	1891.8363	1891.8305	3.07	Th	2	18	0.016	LRGKDPNSADCAHN +dK_MMCCH-2 (K)	250
68	283	293	782.8565	1563.6985	1563.7028	-2.75	Th	3	31	0.00076	AKPADSFDYGR +dK_MMCCH-2 (K)	284
69	365	374	715.3283	1428.6421	1428.6418	0.21	Th	2	41	7.20E-05	LGGPTEMKWG +dK_MMCCH-2 (K); Oxidation (M)	372
70	431	437	569.2861	1136.5576	1136.5576	0.00	Th	1	13	0.047	FDKPPVP +dK_MMCCH-2 (K)	433
71	467	472	538.7416	1075.4687	1075.4644	4.00	Th	0	13	0.045	FQNDKS +dK_MMCCH-2 (K)	471
72	629	636	582.7663	1163.5180	1163.5169	1.03	Th	1	24	0.0037	VGGSEKYS +dK_MMCCH-2 (K)	634
73	893	904	904.8962	1807.7779	1807.7698	4.48	Th	1	18	0.018	FHGEPKWCPSPE +dK_MMCCH-2 (K)	898
74	1414	1419	564.7561	1127.4976	1127.4957	1.69	Th	1	21	0.0075	LWDNKD +dK_MMCCH-2 (K)	1418
75	1525	1539	738.3547	2212.0424	2212.0371	2.40	Th	3	43	5.10E-05	LKHNLPQDSFDYQNR +dK_MMCCH-2 (K)	1526
76	1589	1605	735.3312	2202.9719	2202.9708	0.50	Th	2	29	0.0012	ICVEQGGEQNCKTKAGS +dK_MMCCH-2 (K)	1600
77	1589	1605	735.3312	2202.9717	2202.9708	0.41	Th	2	34	0.0004	ICVEQGGEQNCKTKAGS +dK_MMCCH-2 (K)	1602
78	1800	1809	780.3710	1558.7274	1558.7279	-0.32	Th	2	28	0.0017	FSHKTFPNPF +dK_MMCCH-2 (K)	1803

Figure 23B. KLH 2 (continued)

79	1952	1963	627.2840	1878.8302	1878.8247	2.93	Th	2	51	7.90E-06	FSKPEDTFDYHR +dK_MMCCH-2 (K)	1954
80	1985	1994	776.8959	1551.7772	1551.7715	3.67	Th	2	23	0.0045	IKQQQEADRV +dK_MMCCH-2 (K)	1986
81	2193	2199	667.3011	1332.5876	1332.5849	2.03	Th	2	27	0.0019	YWDWTKP +dK_MMCCH-2 (K)	2198
82	2200	2206	562.3088	1122.6031	1122.5995	3.30	Th	2	22	0.0061	ISKLPDL +dK_MMCCH-2 (K)	2202
83	2225	2229	462.2199	922.4251	922.4259	-0.76	Th	2	17	0.021	FAKGY +dK_MMCCH-2 (K)	2227
84	2359	2363	509.2324	1016.4503	1016.4460	4.33	Th	1	15	0.034	FTKMH +dK_MMCCH-2 (K); Oxidation (M)	2361
85	2941	2950	720.8391	1439.6635	1439.6602	2.29	Th	3	45	2.90E-05	LDEANDLKNA +dK_MMCCH-2 (K)	2948
86	3009	3015	573.2759	1144.5372	1144.5335	3.23	Th	0	15	0.033	LKEHGSH +dK_MMCCH-2 (K)	3010
87	3020	3026	662.2905	1322.5664	1322.5642	1.66	Th	2	20	0.0092	YWDWTKS +dK_MMCCH-2 (K)	3025
88	3399	3405	520.2601	1038.5057	1038.5056	0.10	Th	1	20	0.011	IAGPTKD +dK_MMCCH-2 (K)	3404

"Start" and "End" indicates the number of residue of KLH1 or KLH2. "Observed" column implies the observed m/z value in the survey scan while "Mr(expt)", "Mr(calc)", "ppm" indicate the experimental molecular weight(MW), calculated MW, and the difference between observed MW and theoretical MW respectively. In the "Enzyme" column, T, C, G and Th stand for trypsin, chymotrypsin, Glu-C and thermolysin respectively. MC stands for missed cleavage. Scores are the peptide ion score directly reported from Mascot database search engine. E value denotes the expectation value for each identified peptide. The peptide sequences as well as its modifications are listed in "Peptide" column. "Mod_site" indicates the lysine conjugation site for KLH1 or KLH2.

Figure 24. Identification details of MMCCH-conjugated peptides for sample 3 (1st LC-MS/MS)

Figure 24A. KLH 1

#	Start	End	Observed	Mr(expt)	Mr(calc)	ppm	Enzyme	MC	Score	E value	Peptide	Mod_site
1	124	141	589.3095	2353.2089	2353.2001	3.74	T	1	37	0.00018	GFTDPPVKHHQSANLLVR +dK_MMCCH-2 (K)	131
2	142	149	656.3412	1310.6678	1310.6653	1.98	T	1	35	0.00029	KNINDLTR +dK_MMCCH-2 (K)	142
3	157	166	822.8796	1643.7446	1643.7402	2.68	T	1	18	0.015	EAFHKFQEDR +dK_MMCCH-2 (K)	161
4	184	192	726.8427	1451.6707	1451.6649	4.00	T	1	22	0.0063	CPRPDAKDR +dK_MMCCH-2 (K)	190
5	377	402	833.4029	3329.5825	3329.5784	1.23	T	0	28	0.0016	AHCAISLEHMHLKPFAFSSPLNNNEK +dK_MMCCH-2 (K)	389
6	460	477	781.3949	2341.1629	2341.1624	0.21	T	1	22	0.0068	TSANVDIFIKTTDSVQHK +dK_MMCCH-2 (K)	469
7	470	488	748.0465	2241.1177	2241.1100	3.44	T	1	43	5.20E-05	TTDSVQHKAGTFAVLGGSK +dK_MMCCH-2 (K)	477
8	553	560	663.8680	1325.7214	1325.7166	3.62	T	2	21	0.0073	VKFDKVPR +dK_MMCCH-2 (K)	554
9	566	570	485.2456	968.4767	968.4749	1.86	T	1	17	0.018	KNVDR +dK_MMCCH-2 (K)	566
10	581	587	547.8373	1093.6601	1093.6569	2.93	T	1	22	0.006	KALALLK +dK_MMCCH-2 (K)	581
11	588	606	781.0351	2340.0835	2340.0845	-0.43	T	1	30	0.001	EDKSAGGFQQLGAFHGEPK +dK_MMCCH-2 (K)	590
12	591	615	753.6043	3010.3881	3010.3742	4.62	T	1	19	0.012	SAGGFQQLGAFHGEPKWCPSPEASK +dK_MMCCH-2 (K)	606
13	645	681	1158.5398	4630.1301	4630.1063	5.12	T	1	27	0.0018	HGYDGALPYWDWTSPLNHLPELADHEKYVDPEDGVEK +dK_MMCCH-2 (K)	671
14	682	699	620.2947	2477.1496	2477.1434	2.50	T	1	21	0.0082	HNPWFDGHIDTVDKTTTR +dK_MMCCH-2 (K)	695
15	700	719	887.7702	2660.2888	2660.2945	-2.14	T	1	39	0.00013	SVQNKLFEQPEFGHYTSIAK +dK_MMCCH-2 (K)	704
16	790	804	669.3174	2004.9305	2004.9220	4.24	T	0	38	0.00017	GKPYNVANCAVTSMR +dK_MMCCH-2 (K)	791
17	858	863	520.2993	1038.5840	1038.5783	5.39	T	1	23	0.0051	KLEAIK +dK_MMCCH-2 (K)	858
18	953	965	635.3319	1902.9737	1902.9662	3.94	T	1	53	4.80E-06	DLFKQPSVIHEPR +dK_MMCCH-2 (K)	956
19	986	1000	1027.0366	2052.0587	2052.0561	1.27	T	1	75	2.90E-08	KNIENLSLGELESLR +dK_MMCCH-2 (K)	986
20	1048	1060	609.3551	1825.0435	1825.0423	0.66	T	1	44	3.80E-05	LYVVVVENALLKK +dK_MMCCH-2 (K)	1060
21	1092	1114	791.8734	3163.4645	3163.4682	-1.17	T	1	28	0.0018	QHHYETNPFHHGKITHENEITTR +dK_MMCCH-2 (K)	1104
22	1199	1203	353.1914	1056.5522	1056.5538	-1.51	T	1	17	0.018	KRPYR +dK_MMCCH-2 (K)	1199
23	1331	1338	620.3551	1238.6956	1238.6944	0.97	T	1	17	0.018	LDITKALK +dK_MMCCH-2 (K)	1335
24	1395	1402	649.8379	1297.6612	1297.6588	1.85	T	1	26	0.0022	KDITQLDK +dK_MMCCH-2 (K)	1395

Figure 24A. KLH 1 (continued)

25	1395	1403	485.5953	1453.7639	1453.7599	2.75	T	2	16	0.025	KDITQLDKR +dK_MMCCH-2 (K)	1402
26	1417	1445	844.1611	3372.6154	3372.6020	4.00	T	1	19	0.012	ADHSSDGFQAIASFHALPPLCPSPAASKR +dK_MMCCH-2 (K)	1444
27	1473	1489	778.4021	2332.1845	2332.1827	0.77	T	1	47	1.90E-05	KHGAVVGLPYWDWTLPR +dK_MMCCH-2 (K)	1473
28	1721	1746	1092.8043	3275.3911	3275.3886	0.76	T	1	14	0.044	TAGDCEDAGYFTVLGGEKEMPWAFDR +dK_MMCCH-2 (K); Oxidation (M)	1738
29	1890	1922	879.8327	4394.1271	4394.1048	5.07	T	1	16	0.024	HGSSVAVPYWDWTKPIHNIPHLFTDKEYYDVWR +dK_MMCCH-2 (K)	1915
30	1923	1932	756.3803	1510.7461	1510.7425	2.38	T	1	26	0.0028	NKVMPNPFAR +dK_MMCCH-2 (K)	1924
31	2067	2076	746.8841	1491.7536	1491.7544	-0.54	T	1	28	0.0014	KHAVPNDVFK +dK_MMCCH-2 (K)	2067
32	2121	2149	890.4184	3557.6444	3557.6378	1.86	T	1	29	0.0013	TSADVQFQICKTSEDCHHGGQIFVLGGTK +dK_MMCCH-2 (K)	2131
33	2359	2367	736.8409	1471.6672	1471.6653	1.29	T	1	19	0.012	DKLFNDPER +Deamidated (NQ); dK_MMCCH-2 (K)	2360
34	2461	2490	642.8212	3850.8834	3850.8638	5.09	T	0	17	0.02	RPLRPFSDPINHNAFTHSNAKPTDVFEYSR +dK_MMCCH-2 (K)	2481
35	2507	2514	682.3522	1362.6898	1362.6853	3.30	T	1	40	9.90E-05	KLEHELEK +dK_MMCCH-2 (K)	2507
36	2515	2520	571.7623	1141.5100	1141.5074	2.28	T	1	19	0.013	QKEEDR +dK_MMCCH-2 (K)	2516
37	2595	2609	983.5305	1965.0465	1965.0493	-1.42	T	1	20	0.01	IIDTSGKQLPSDLIK +dK_MMCCH-2 (K)	2601
38	2621	2636	802.7087	2405.1044	2405.1083	-1.62	T	1	48	1.50E-05	HHEKHHEDHHEDILVR +dK_MMCCH-2 (K)	2624
39	2637	2651	1069.5308	2137.0470	2137.0374	4.45	T	1	61	8.10E-07	KNIHSLSHHEAEELR +dK_MMCCH-2 (K)	2637
40	2652	2682	975.1997	3896.7695	3896.7563	3.39	T	1	19	0.012	DALYKLQNDESHGGYEHIAGFHGYPNLCPEK +dK_MMCCH-2 (K)	2656
41	2657	2686	934.9150	3735.6311	3735.6358	-1.28	T	1	22	0.0068	LQNDESHGGYEHIAGFHGYPNLCPEKGDEK +dK_MMCCH-2 (K)	2682
42	2657	2686	1246.2205	3735.6396	3735.6358	0.99	T	1	24	0.0036	LQNDESHGGYEHIAGFHGYPNLCPEKGDEK +dK_MMCCH-2 (K)	2686
43	2714	2748	1087.7703	4347.0519	4347.0524	-0.12	T	1	32	0.00056	KHGSHLGIPYWDWTQTISSLPTFFADSGNNNPFFK +dK_MMCCH-2 (K)	2714
44	2851	2883	1009.2175	4032.8410	4032.8346	1.59	T	0	60	1.10E-06	VKPAHAGSCAGDIMHVPLHPFNYESVNNDDFTR +dK_MMCCH-2 (K)	2852
45	2897	2919	800.1419	3196.5385	3196.5287	3.07	T	1	66	2.30E-07	FNYKYDNLNLHGHNIEELEEVLR +dK_MMCCH-2 (K)	2900
46	2938	2947	730.4152	1458.8158	1458.8156	0.07	T	1	35	0.00028	TTAVVKVYIK +dK_MMCCH-2 (K)	2943
47	3003	3021	825.7698	2474.2877	2474.2879	-0.08	T	1	62	7.00E-07	KYDHTELDASVLPAPIIVR +dK_MMCCH-2 (K)	3003
48	3022	3044	966.5270	2896.5593	2896.5521	2.49	T	1	15	0.03	RPNNAVFDIIEIPIGKDVNLPPK +dK_MMCCH-2 (K)	3037
49	123	151	616.6582	3693.9058	3693.9049	0.24	G	2	27	0.0018	KGFTDPPVKHHQSANLLVRKNINDLTREE +dK_MMCCH-2 (K)	123
50	123	151	739.7917	3693.9221	3693.9049	4.63	G	2	22	0.006	KGFTDPPVKHHQSANLLVRKNINDLTREE +dK_MMCCH-2 (K)	131
51	158	176	846.3843	2536.1310	2536.1329	-0.75	G	3	20	0.011	AFHKFQEDRSVDGYQATAE +dK_MMCCH-2 (K)	161

Figure 24A. KLH 1 (continued)

52	526	544	777.7485	2330.2236	2330.2304	-2.92	G	1	22	0.0068	VDGTKLASSLIPHASVIRE +dK_MMCCH-2 (K)	530
53	589	612	1102.8267	3305.4582	3305.4621	-1.18	G	1	15	0.029	DKSAGGFQQLGAFHGEPKWCPSPE +2 dK_MMCCH-2 (K)	590, 606
54	825	841	820.3707	2458.0902	2458.0940	-1.55	G	1	24	0.004	HSVPFNVFDYKTNFNYE +dK_MMCCH-2 (K)	835
55	847	860	644.0053	1928.9941	1928.9917	1.24	G	0	17	0.019	FNGLSISQLNKKLE +Deamidated (NQ); dK_MMCCH-2 (K)	858
56	942	972	764.6007	3817.9672	3817.9614	1.52	G	3	17	0.021	VFDLKPASLGKDLFKQPSVIHEPRIGHHEGE +dK_MMCCH-2 (K)	946
57	942	970	908.9828	3631.9022	3631.8973	1.35	G	2	25	0.003	VFDLKPASLGKDLFKQPSVIHEPRIGHHE +dK_MMCCH-2 (K)	956
58	1397	1413	774.4363	2320.2872	2320.2824	2.07	G	1	16	0.024	ITQLDKRQQLSLVKALE +dK_MMCCH-2 (K)	1410
59	1495	1522	866.6916	3462.7373	3462.7381	-0.26	G	3	16	0.023	LLTVSTIHDPETGRDIPNPFIGSKIEFE +dK_MMCCH-2 (K)	1518
60	1755	1765	570.6053	1708.7940	1708.7913	1.64	G	2	18	0.016	TLDKMNLRHDE +dK_MMCCH-2 (K)	1758
61	2089	2100	854.4076	1706.8006	1706.8008	-0.06	G	2	21	0.0077	IGGMNLHEIEKE +dK_MMCCH-2 (K)	2099
62	2647	2661	715.6776	2144.0108	2144.0095	0.61	G	4	29	0.0013	AEELRDALYKLQNDE +dK_MMCCH-2 (K)	2656
63	3090	3097	632.8022	1263.5898	1263.5879	1.50	G	0	14	0.04	LGKMYSVE +dK_MMCCH-2 (K)	3092
64	59	68	729.3448	1456.6750	1456.6731	1.37	C	1	19	0.012	VLGGPSEMKW +dK_MMCCH-2 (K); Oxidation (M)	67
65	94	100	573.2989	1144.5833	1144.5838	-0.44	C	1	23	0.0048	TVKAELF +dK_MMCCH-2 (K)	96
66	140	159	692.6202	2766.4519	2766.4486	1.16	C	3	28	0.0018	VRKNINDLTREEVLNLREAF +dK_MMCCH-2 (K)	142
67	160	171	606.9435	1817.8086	1817.8043	2.37	C	1	19	0.012	HKFQEDRSVDGY +dK_MMCCH-2 (K)	161
68	429	450	990.8075	2969.4007	2969.3899	3.64	C	1	36	0.00024	GGISLENIEKMIHENQQEDRIY +dK_MMCCH-2 (K); Oxidation (M)	438
69	584	595	787.4017	1572.7888	1572.7858	1.91	C	2	42	6.40E-05	ALLKEDKSAGGF +dK_MMCCH-2 (K)	590
70	715	723	655.8735	1309.7325	1309.7316	0.76	C	1	26	0.0023	TSIAKQVLL +dK_MMCCH-2 (K)	719
71	783	788	544.7770	1087.5395	1087.5372	2.11	C	1	26	0.0024	QALQKY +dK_MMCCH-2 (K)	787
72	944	955	821.4324	1640.8503	1640.8484	1.16	C	3	25	0.0034	DLKPASLGKDLF +dK_MMCCH-2 (K)	946
73	1013	1018	516.7581	1031.5017	1031.4998	1.84	C	0	13	0.049	ESIAKF +dK_MMCCH-2 (K)	1017
74	1330	1337	620.3546	1238.6947	1238.6944	0.16	C	1	21	0.0089	KLDITKAL +dK_MMCCH-2 (K)	1335
75	1580	1586	544.2614	1086.5083	1086.5056	2.49	C	0	13	0.049	VGGKEPY +dK_MMCCH-2 (K)	1583
76	1649	1664	1127.9900	2253.9654	2253.9637	0.75	C	2	18	0.014	NLNDHTHDFSKPEDTF +dK_MMCCH-2 (K)	1659
77	1649	1669	979.4319	2935.2738	2935.2759	-0.72	C	4	24	0.0036	NLNDHTHDFSKPEDTFDYQKF +dK_MMCCH-2 (K)	1668
78	1732	1742	792.8744	1583.7342	1583.7364	-1.39	C	1	17	0.02	TVLGGEKEMPW +dK_MMCCH-2 (K)	1738

Figure 24A. KLH 1 (continued)

79	1818	1827	753.3699	1504.7253	1504.7232	1.40	C	1	18	0.018	SERDIGSLKY +dK_MMCCH-2 (K)	1826
80	2076	2082	612.3045	1222.5944	1222.5944	0.08	C	3	14	0.037	KYELLGY +dK_MMCCH-2 (K)	2076
81	2160	2184	1085.5143	3253.5210	3253.5179	0.95	C	3	21	0.0089	KYDITHALHDAHITPEDVFHPSEPF +dK_MMCCH-2 (K)	2160
82	2476	2488	923.9219	1845.8293	1845.8244	2.71	C	1	25	0.0029	THSNAKPTDVFEY +dK_MMCCH-2 (K)	2481
83	2656	2672	747.3428	2239.0067	2239.0004	2.81	C	2	30	0.00098	KLQNDESHGGYEHIAGF +dK_MMCCH-2 (K)	2656
84	2738	2749	856.3768	1710.7390	1710.7348	2.46	C	2	24	0.004	ADSGNNNPFFKY +dK_MMCCH-2 (K)	2748
85	2946	2960	965.4055	1928.7964	1928.7986	-1.14	C	1	40	9.10E-05	IKSGTDSDDEYAGSF +dK_MMCCH-2 (K)	2947
86	2961	2971	769.8918	1537.7691	1537.7673	1.24	C	1	21	0.0078	VILGGAKEMPW +dK_MMCCH-2 (K)	2967
87	1	9	733.3348	1464.6550	1464.6516	2.32	Th	2	17	0.021	MTPEELKTY +dK_MMCCH-2 (K); Oxidation (M)	7
88	38	56	861.6805	2582.0198	2582.0108	3.49	Th	2	15	0.033	VCIPDDNDRNDDHCEKAGD +dK_MMCCH-2 (K)	53
89	59	69	785.3774	1568.7402	1568.7367	2.23	Th	3	61	7.10E-07	VLGGPSEMKWQ +dK_MMCCH-2 (K)	67
90	78	84	569.2872	1136.5599	1136.5536	5.54	Th	1	49	1.10E-05	LSDTVHK +dK_MMCCH-2 (K)	84
91	116	124	670.3482	1338.6819	1338.6755	4.78	Th	2	27	0.002	VVVHHPEKG +dK_MMCCH-2 (K)	123
92	125	135	815.8878	1629.7611	1629.7610	0.06	Th	1	14	0.044	FTDPPVKHHQS +dK_MMCCH-2 (K)	131
93	431	439	707.8528	1413.6911	1413.6883	1.98	Th	3	39	0.00013	ISLENIEKM +dK_MMCCH-2 (K)	438
94	521	530	707.8450	1413.6754	1413.6698	3.96	Th	2	74	4.30E-08	VDITEVDGTK +dK_MMCCH-2 (K)	530
95	585	591	585.8101	1169.6057	1169.6002	4.70	Th	1	35	0.00034	LLKEDKS +dK_MMCCH-2 (K)	590
96	601	612	904.8956	1807.7767	1807.7698	3.82	Th	1	25	0.0035	FHGEPKWCPSPE +dK_MMCCH-2 (K)	606
97	666	672	607.2832	1212.5518	1212.5485	2.80	Th	2	23	0.0046	LADHEKY +dK_MMCCH-2 (K)	671
98	821	828	617.8120	1233.6095	1233.6064	2.51	Th	1	19	0.012	VTKEHSVP +dK_MMCCH-2 (K)	823
99	831	837	612.7877	1223.5608	1223.5533	6.13	Th	2	25	0.003	VFDYKTN +dK_MMCCH-2 (K)	835
100	1064	1074	586.9629	1757.8668	1757.8600	3.93	Th	5	15	0.032	VAVPYWDWTKR +dK_MMCCH-2 (K)	1073
101	1156	1164	630.8397	1259.6648	1259.6584	5.08	Th	2	22	0.0058	LLGGKGKYS +dK_MMCCH-2 (K)	1162
102	1219	1232	980.4239	1958.8332	1958.8316	0.82	Th	1	53	4.70E-06	FDKSDNNDEATKTH +dK_MMCCH-2 (K)	1230
103	1579	1587	665.8146	1329.6146	1329.6064	6.17	Th	2	19	0.012	WVGGKEPYG +dK_MMCCH-2 (K)	1583
104	1657	1668	921.9210	1841.8275	1841.8182	5.05	Th	2	42	6.10E-05	FSKPEDTFDYQK +dK_MMCCH-2 (K)	1659
105	1657	1668	921.9207	1841.8269	1841.8182	4.72	Th	2	50	9.90E-06	FSKPEDTFDYQK +dK_MMCCH-2 (K)	1668

Figure 24A. KLH 1 (continued)

106	1733	1741	664.3254	1326.6362	1326.6312	3.77	Th	2	17	0.022	VLGGEKEMP +dK_MMCCH-1 (K); Oxidation (M)	1738
107	1756	1760	479.7249	957.4353	957.4300	5.64	Th	1	13	0.049	LDKMN +dK_MMCCH-2 (K)	1758
108	1894	1904	850.4138	1698.8131	1698.8116	0.88	Th	5	29	0.0013	VAVPYWDWTKP +dK_MMCCH-2 (K)	1903
109	2094	2100	618.3031	1234.5916	1234.5903	1.05	Th	1	26	0.0024	LHEIEKE +dK_MMCCH-2 (K)	2099
110	2129	2141	933.8805	1865.7465	1865.7495	-1.61	Th	0	27	0.0019	ICKTSEDCHHGGQ +dK_MMCCH-2 (K)	2131
111	2238	2249	814.3991	1626.7837	1626.7811	1.60	Th	4	49	1.30E-05	LTTAEVDNLKDA +dK_MMCCH-2 (K)	2247
112	2475	2484	728.3341	1454.6535	1454.6500	2.41	Th	1	27	0.002	FTHSNAKPTD +dK_MMCCH-2 (K)	2481
113	2512	2521	538.6010	1612.7810	1612.7766	2.73	Th	0	33	0.00055	LEKQKEEDRT +dK_MMCCH-2 (K)	2514
114	2595	2607	862.9463	1723.8780	1723.8702	4.52	Th	3	30	0.0011	IIDTSGKQLPSDL +dK_MMCCH-2 (K)	2601
115	2607	2612	520.7814	1039.5483	1039.5446	3.56	Th	2	23	0.0056	LIKMPT +dK_MMCCH-2 (K)	2609
116	2766	2771	551.7883	1101.5621	1101.5529	8.35	Th	1	24	0.0041	IFQQTK +dK_MMCCH-2 (K)	2771
117	2808	2816	638.3212	1274.6279	1274.6217	4.94	Th	3	27	0.0019	LIGGAEKYS +dK_MMCCH-2 (K)	2814
118	2946	2960	965.4112	1928.8078	1928.7986	4.77	Th	3	54	3.80E-06	IKSGTDSDDEYAGSF +dK_MMCCH-2 (K)	2947
119	2961	2970	691.8644	1381.7142	1381.7098	3.18	Th	4	19	0.011	VILGGAKEMP +dK_MMCCH-1 (K); Oxidation (M)	2967
120	2990	2996	583.2855	1164.5565	1164.5485	6.87	Th	1	38	0.00015	LTDDHVK +dK_MMCCH-2 (K)	2996

Figure 24B. KLH 2

#	Start	End	Observed	Mr(expt)	Mr(calc)	ppm	Enzyme	MC	Score	E value	Peptide	Mod_site
1	26	41	1043.0231	2084.0316	2084.0347	-1.49	T	1	50	1.10E-05	KNVDSLSSDEVLALEK +dK_MMCCH-2 (K)	26
2	147	155	694.3697	1386.7249	1386.7217	2.31	T	1	47	2.20E-05	ADITFLNKK +dK_MMCCH-2 (K)	155
3	164	175	596.3073	1785.9001	1785.8985	0.90	T	1	36	0.00025	LFEKVQPGHHTR +dK_MMCCH-2 (K)	167
4	249	271	740.8343	2959.3081	2959.3051	0.98	T	1	25	0.0035	GKDPNSADCAHNLIHTPMEPFDR +dK_MMCCH-2 (K)	250
5	281	293	610.9426	1829.8061	1829.8043	0.98	T	0	50	1.00E-05	EHAKPADSFDYGR +dK_MMCCH-2 (K)	284
6	359	377	844.0674	2529.1803	2529.1861	-2.29	T	1	17	0.02	AGDFFLLGGPTEMKWGFYR +dK_MMCCH-2 (K)	372
7	419	446	677.3699	3381.8133	3381.8132	0.03	T	1	56	2.50E-06	QPTLVHRPAKGHFDKPPVPVAQANLAVR +Deamidated (NQ); dK_MMCCH-2 (K)	428
8	429	446	752.0684	2253.1833	2253.1729	4.62	T	0	56	2.50E-06	GHFDKPPVPVAQANLAVR +dK_MMCCH-2 (K)	433
9	467	488	944.4542	2830.3408	2830.3385	0.85	T	1	66	2.80E-07	FQNDKSVDGYQATVEFHALPAR +dK_MMCCH-2 (K)	471
10	489	497	726.8427	1451.6707	1451.6649	4.00	T	1	22	0.0063	CPRPDAKDR +dK_MMCCH-2 (K)	495
11	936	950	720.3431	2158.0074	2158.0095	-0.97	T	1	28	0.0016	KHGFTGGLPYWDWTR +dK_MMCCH-2 (K)	936
12	1082	1096	996.4633	1990.9120	1990.9063	2.86	T	0	22	0.006	GKPYNTANCAIASMR +dK_MMCCH-2 (K)	1083
13	1097	1115	827.0760	2478.2061	2478.2101	-1.57	T	0	78	1.60E-08	KPLQPFGLDSVINPDDETR +dK_MMCCH-2 (K)	1097
14	1123	1149	1190.5605	3568.6598	3568.6497	2.86	T	1	75	3.00E-08	VFDYKNNFDYEYESLAFNGLSIAQLDR +dK_MMCCH-2 (K)	1127
15	1295	1311	764.0679	2289.1818	2289.1715	4.50	T	1	17	0.018	SAFLQIQKEGIYENIAK +dK_MMCCH-2 (K)	1302
16	1355	1385	1271.2678	3810.7816	3810.7876	-1.55	T	1	52	6.40E-06	GSAVAVPYWDWTEKADSLPSLINDATYFNSR +dK_MMCCH-2 (K)	1368
17	1409	1450	1097.7150	5483.5388	5483.5213	3.19	T	1	18	0.016	DPQPELWDNKDFYENVMLALEQDNFCDFEIQLELIHNALHSR +dK_MMCCH-2 (K)	1418
18	1455	1480	838.6584	3350.6045	3350.6070	-0.78	T	1	56	2.70E-06	AKYSLSSLDYTAFDPVFFLHHANVDR +dK_MMCCH-2 (K)	1456
19	1493	1507	721.6590	2161.9552	2161.9594	-1.99	T	1	50	1.00E-05	KKPYNEADCAVNEMR +dK_MMCCH-2 (K)	1494
20	1508	1539	1032.2455	4124.9528	4124.9360	4.07	T	1	28	0.0014	KPLQPFNNPELNSDSMTLKHNLPQDSFDYQNR +dK_MMCCH-2 (K)	1526
21	1542	1564	1070.1910	3207.5513	3207.5448	2.03	T	1	47	1.80E-05	YQYDNLQFNHFSIQKLDQTIQAR +dK_MMCCH-2 (K)	1556
22	1757	1768	612.9789	1835.9148	1835.9128	1.09	T	1	22	0.0057	LYTVQFEDSLKR +dK_MMCCH-2 (K)	1767
23	1949	1963	560.2522	2236.9797	2236.9735	2.77	T	0	57	2.00E-06	TQEFSKPEDTFDYHR +dK_MMCCH-2 (K)	1954
24	2045	2052	660.3506	1318.6867	1318.6843	1.90	T	1	15	0.035	YDITKTLK +dK_MMCCH-2 (K)	2052

Figure 24B. KLH 2 (continued)

25	2058	2069	909.4624	1816.9102	1816.9070	1.82	T	1	24	0.0043	YDDTFTIKVHIK +dK_MMCCH-2 (K)	2065
26	2228	2239	870.4213	1738.8280	1738.8236	2.53	T	1	19	0.012	GYIKSEDAYTVR +dK_MMCCH-2 (K)	2231
27	2527	2541	1007.5135	2013.0124	2013.0088	1.79	T	1	50	9.00E-06	KDVTSLTASEIENLR +dK_MMCCH-2 (K)	2527
28	2755	2764	764.3831	1526.7517	1526.7439	5.11	T	0	19	0.013	QPLKPFSESR +Deamidated (NQ); dK_MMCCH-2 (K)	2758
29	2866	2873	659.3611	1316.7076	1316.7050	1.97	T	1	13	0.05	YDITKVLK +dK_MMCCH-2 (K)	2870
30	3148	3155	629.3355	1256.6565	1256.6587	-1.75	T	1	18	0.016	KKPYNAAK +dK_MMCCH-2 (K)	3149
31	433	456	975.8590	2924.5552	2924.5429	4.21	G	2	27	0.0019	KPPVPVAQANLAVRKNINDLTAEE +dK_MMCCH-2 (K)	433
32	466	481	1098.4963	2194.9781	2194.9841	-2.73	G	2	31	0.00082	RFQNDKSVDGYQATVE +Deamidated (NQ); dK_MMCCH-2 (K)	471
33	1215	1235	721.6063	2882.3959	2882.3949	0.35	G	3	28	0.0016	ITQQLHDLDLHVGDNFFLKYE +dK_MMCCH-2 (K)	1233
34	1292	1303	879.4652	1756.9159	1756.9182	-1.31	G	0	42	6.80E-05	SIRSAFLQIQKE +dK_MMCCH-2 (K)	1302
35	1308	1320	603.6326	1807.8761	1807.8749	0.61	G	0	20	0.01	NIAKFHGKPGLCE +dK_MMCCH-2 (K)	1315
36	1403	1422	921.4208	2761.2407	2761.2330	2.79	G	3	15	0.03	NAVTSRDPQPELWDNKDFYE +dK_MMCCH-2 (K)	1418
37	1952	1967	792.6837	2375.0293	2375.0205	3.71	G	3	19	0.014	FSKPEDTFDYHRFGYE +dK_MMCCH-2 (K)	1954
38	2477	2484	644.8373	1287.6600	1287.6573	2.10	G	0	22	0.0068	APFFIKVE +dK_MMCCH-2 (K)	2482
39	3386	3405	877.4165	2629.2277	2629.2271	0.23	G	2	21	0.0073	LDHAYSLRDGHYYIAGPTKD +dK_MMCCH-2 (K)	3404
40	38	55	1181.0392	2360.0638	2360.0478	6.78	C	3	14	0.036	ALEKALDDLQQDDSNQGY +dK_MMCCH-2 (K)	41
41	277	296	883.7539	2648.2399	2648.2329	2.64	C	4	39	0.00014	DLTREHAKPADSFDYGRLGY +dK_MMCCH-2 (K)	284
42	364	373	735.3606	1468.7066	1468.7094	-1.91	C	2	22	0.0067	LLGGPTEMKW +dK_MMCCH-2 (K)	372
43	432	443	793.9159	1585.8173	1585.8174	-0.06	C	0	26	0.0028	DKPPVPVAQANL +dK_MMCCH-2 (K)	433
44	629	635	539.2532	1076.4919	1076.4848	6.60	C	0	20	0.0095	VGGSEKY +dK_MMCCH-2 (K)	634
45	1007	1015	669.8709	1337.7271	1337.7265	0.52	C	1	16	0.025	TDIAKQVLL +dK_MMCCH-2 (K)	1011
46	1075	1080	544.7770	1087.5395	1087.5372	2.11	C	1	26	0.0024	QALQKY +dK_MMCCH-2 (K)	1079
47	1125	1134	854.8459	1707.6772	1707.6763	0.59	C	3	33	0.00052	DYKNNFDYEY +dK_MMCCH-2 (K)	1127
48	1162	1177	690.0399	2067.0979	2067.0863	5.61	C	4	18	0.015	AGFLLHEIGQSALVKF +dK_MMCCH-2 (K)	1176
49	1298	1306	715.3727	1428.7309	1428.7323	-0.91	C	1	20	0.01	LQIQKEGIY +dK_MMCCH-2 (K)	1302
50	1298	1312	824.0880	2469.2422	2469.2324	3.97	C	2	13	0.047	LQIQKEGIYENIAKF +2 dK_MMCCH-2 (K)	1302, 1311
51	1416	1426	863.3786	1724.7426	1724.7426	0.06	C	2	27	0.0022	DNKDFYENVML +dK_MMCCH-2 (K)	1418

Figure 24B. KLH 2 (continued)

52	1526	1540	749.6839	2246.0299	2246.0215	3.74	C	2	47	1.80E-05	KHNLPQDSFDYQNRF +dK_MMCCH-2 (K)	1526
53	1589	1606	784.3566	2350.0479	2350.0392	3.70	C	0	31	0.00076	ICVEQGGEQNCKTKAGSF +dK_MMCCH-2 (K)	1600
54	1589	1606	784.3541	2350.0404	2350.0392	0.51	C	0	30	0.001	ICVEQGGEQNCKTKAGSF +dK_MMCCH-2 (K)	1602
55	1696	1702	607.2995	1212.5844	1212.5849	-0.41	C	1	27	0.002	TTLEKHF +dK_MMCCH-2 (K)	1700
56	1708	1719	839.8421	1677.6696	1677.6651	2.74	C	0	38	0.00017	KNMQADDSPDGY +dK_MMCCH-2 (K)	1708
57	1801	1809	706.8386	1411.6627	1411.6595	2.27	C	0	24	0.0044	SHKTFPNPF +dK_MMCCH-2 (K)	1803
58	1985	1995	850.4311	1698.8476	1698.8399	4.53	C	0	39	0.00012	IKQQQEADRVF +dK_MMCCH-2 (K)	1986
59	2001	2011	726.8469	1451.6792	1451.6755	2.48	C	1	27	0.0021	KGFGQSASVSF +dK_MMCCH-2 (K)	2001
60	2194	2207	1042.5349	2083.0553	2083.0489	3.07	C	3	15	0.035	WDWTKPISKLPDLF +dK_MMCCH-2 (K)	2202
61	2230	2236	582.2687	1162.5228	1162.5216	1.03	C	0	14	0.042	IKSEDAY +dK_MMCCH-2 (K)	2231
62	2463	2479	1128.0164	2254.0182	2254.0253	-3.15	C	1	18	0.015	KAQSIHPEDVFDTDAPF +dK_MMCCH-2 (K)	2463
63	2506	2532	761.6029	3042.3825	3042.3738	2.89	C	0	17	0.021	SAGEGHTDDHGSDHIAGSGVRKDVTSL +dK_MMCCH-2 (K)	2527
64	2754	2760	598.3301	1194.6457	1194.6471	-1.17	C	1	15	0.029	KQPLKPF +dK_MMCCH-2 (K)	2754
65	2754	2760	598.3317	1194.6489	1194.6471	1.51	C	1	23	0.005	KQPLKPF +dK_MMCCH-2 (K)	2758
66	2865	2872	673.3643	1344.7141	1344.7112	2.16	C	1	13	0.046	RYDITKVL +dK_MMCCH-2 (K)	2870
67	3235	3242	617.3138	1232.6131	1232.6111	1.62	C	0	20	0.0099	TSANVKIY +dK_MMCCH-2 (K)	3240
68	3399	3406	576.8038	1151.5930	1151.5896	2.87	C	0	20	0.0093	IAGPTKDL +dK_MMCCH-2 (K)	3404
69	69	75	604.2924	1206.5703	1206.5703	0.00	Th	0	22	0.0069	VDKHEKN +dK_MMCCH-2 (K)	74
70	165	175	558.6142	1672.8208	1672.8144	3.83	Th	1	23	0.0053	FEKVQPGHHTR +dK_MMCCH-2 (K)	167
71	180	191	909.9193	1817.8241	1817.8216	1.38	Th	4	57	2.20E-06	ILDALEQDEFCK +dK_MMCCH-2 (K)	191
72	247	260	631.6202	1891.8389	1891.8305	4.44	Th	2	15	0.032	LRGKDPNSADCAHN +dK_MMCCH-2 (K)	250
73	283	293	782.8608	1563.7070	1563.7028	2.69	Th	3	39	0.00014	AKPADSFDYGR +dK_MMCCH-2 (K)	284
74	365	372	585.7805	1169.5465	1169.5461	0.34	Th	1	43	5.50E-05	LGGPTEMK +dK_MMCCH-2 (K)	372
75	431	437	569.2866	1136.5586	1136.5576	0.79	Th	1	13	0.046	FDKPPVP +dK_MMCCH-2 (K)	433
76	467	472	538.7430	1075.4714	1075.4644	6.51	Th	0	14	0.045	FQNDKS +dK_MMCCH-2 (K)	471
77	554	565	811.8927	1621.7708	1621.7658	3.14	Th	1	15	0.029	LDPVTGETKNNP +dK_MMCCH-2 (K)	562
78	629	636	582.7668	1163.5191	1163.5169	1.98	Th	1	22	0.006	VGGSEKYS +dK_MMCCH-2 (K)	634

Figure 24B. KLH 2 (continued)

79	893	904	904.8956	1807.7767	1807.7698	3.82	Th	1	25	0.0035	FHGEPKWCPSPE +dK_MMCCH-2 (K)	898
80	1362	1374	968.4326	1934.8507	1934.8397	5.69	Th	4	16	0.026	YWDWTEKADSLPS +dK_MMCCH-2 (K)	1368
81	1414	1419	564.7549	1127.4952	1127.4957	-0.44	Th	1	15	0.029	LWDNKD +dK_MMCCH-2 (K)	1418
82	1525	1539	738.3549	2212.0429	2212.0371	2.62	Th	3	48	1.50E-05	LKHNLPQDSFDYQNR +dK_MMCCH-2 (K)	1526
83	1589	1605	735.3308	2202.9706	2202.9708	-0.09	Th	2	18	0.017	ICVEQGGEQNCKTKAGS +dK_MMCCH-2 (K)	1600
84	1589	1605	735.3312	2202.9717	2202.9708	0.41	Th	2	39	0.00012	ICVEQGGEQNCKTKAGS +dK_MMCCH-2 (K)	1602
85	1800	1809	780.3749	1558.7353	1558.7279	4.75	Th	2	18	0.016	FSHKTFPNPF +dK_MMCCH-2 (K)	1803
86	1952	1963	940.4234	1878.8322	1878.8247	4.05	Th	2	28	0.0015	FSKPEDTFDYHR +dK_MMCCH-2 (K)	1954
87	1985	1994	776.8957	1551.7768	1551.7715	3.42	Th	2	22	0.0062	IKQQQEADRV +dK_MMCCH-2 (K)	1986
88	2193	2199	667.3019	1332.5892	1332.5849	3.23	Th	2	27	0.0021	YWDWTKP +dK_MMCCH-2 (K)	2198
89	2200	2206	562.3099	1122.6052	1122.5995	5.08	Th	2	24	0.004	ISKLPDL +dK_MMCCH-2 (K)	2202
90	2225	2229	462.2227	922.4309	922.4259	5.42	Th	2	17	0.022	FAKGY +dK_MMCCH-2 (K)	2227
91	2359	2363	509.2313	1016.4481	1016.4460	2.07	Th	1	14	0.04	FTKMH +dK_MMCCH-2 (K); Oxidation (M)	2361
92	2941	2950	720.8409	1439.6672	1439.6602	4.86	Th	3	42	5.90E-05	LDEANDLKNA +dK_MMCCH-2 (K)	2948
93	3009	3015	573.2752	1144.5359	1144.5335	2.01	Th	0	15	0.031	LKEHGSH +dK_MMCCH-2 (K)	3010
94	3020	3026	662.2903	1322.5661	1322.5642	1.51	Th	2	28	0.0017	YWDWTKS +dK_MMCCH-2 (K)	3025
95	3399	3405	520.2604	1038.5062	1038.5056	0.58	Th	1	27	0.002	IAGPTKD +dK_MMCCH-2 (K)	3404

"Start" and "End" indicates the number of residue of KLH1 or KLH2. "Observed" column implies the observed m/z value in the survey scan while "Mr(expt)", "Mr(calc)", "ppm" indicate the experimental molecular weight(MW), calculated MW, and the difference between observed MW and theoretical MW respectively. In the "Enzyme" column, T, C, G and Th stand for trypsin, chymotrypsin, Glu-C and thermolysin respectively. MC stands for missed cleavage. Scores are the peptide ion score directly reported from Mascot database search engine. E value denotes the expectation value for each identified peptide. The peptide sequences as well as its modifications are listed in "Peptide" column. "Mod_site" indicates the lysine conjugation site for KLH1 or KLH2.

Figure 25. Identification details of MMCCH-conjugated peptides for sample 4 (1st LC-MS/MS)

Figure 25A. KLH 1

#	Start	End	Observed	Mr(expt)	Mr(calc)	ppm	Enzyme	MC	Score	E value	Peptide	Mod_site
1	124	141	785.4103	2353.2092	2353.2001	3.87	T	1	19	0.011	GFTDPPVKHHQSANLLVR +dK_MMCCH-2 (K)	131
2	142	149	656.3425	1310.6705	1310.6653	4.04	T	1	35	0.00034	KNINDLTR +dK_MMCCH-2 (K)	142
3	157	166	822.8790	1643.7435	1643.7402	2.01	T	1	18	0.016	EAFHKFQEDR +dK_MMCCH-2 (K)	161
4	184	192	726.8442	1451.6738	1451.6649	6.13	T	1	22	0.0061	CPRPDAKDR +dK_MMCCH-2 (K)	190
5	470	488	748.0502	2241.1289	2241.1100	8.43	T	1	24	0.0039	TTDSVQHKAGTFAVLGGSK +dK_MMCCH-2 (K)	477
6	553	560	663.8695	1325.7245	1325.7166	5.96	T	2	22	0.0058	VKFDKVPR +dK_MMCCH-2 (K)	554
7	553	560	555.6243	1663.8510	1663.8466	2.64	T	2	15	0.029	VKFDKVPR +2 dK_MMCCH-2 (K)	554, 557
8	566	570	485.2455	968.4765	968.4749	1.65	T	1	17	0.022	KNVDR +dK_MMCCH-2 (K)	566
9	581	590	733.9194	1465.8242	1465.8214	1.91	T	2	40	0.00011	KALALLKEDK +dK_MMCCH-2 (K)	581
10	588	606	781.0386	2340.0941	2340.0845	4.10	T	1	21	0.008	EDKSAGGFQQLGAFHGEPK +dK_MMCCH-2 (K)	590
11	591	615	1004.4697	3010.3872	3010.3742	4.32	T	1	18	0.015	SAGGFQQLGAFHGEPKWCPSPEASK +dK_MMCCH-2 (K)	606
12	645	681	1158.5359	4630.1145	4630.1063	1.75	T	1	21	0.0072	HGYDGALPYWDWTSPLNHLPELADHEKYVDPEDGVEK +dK_MMCCH-2 (K)	671
13	682	699	620.2941	2477.1474	2477.1434	1.61	T	1	23	0.0045	HNPWFDGHIDTVDKTTTR +dK_MMCCH-2 (K)	695
14	700	719	887.7753	2660.3040	2660.2945	3.57	T	1	32	0.00064	SVQNKLFEQPEFGHYTSIAK +dK_MMCCH-2 (K)	704
15	790	804	1003.4777	2004.9409	2004.9220	9.43	T	0	63	5.00E-07	GKPYNVANCAVTSMR +dK_MMCCH-2 (K)	791
16	953	965	635.3326	1902.9761	1902.9662	5.20	T	1	46	2.40E-05	DLFKQPSVIHEPR +dK_MMCCH-2 (K)	956
17	986	1000	685.0287	2052.0642	2052.0561	4.00	T	1	68	1.80E-07	KNIENLSLGELESLR +dK_MMCCH-2 (K)	986
18	1048	1060	913.5324	1825.0503	1825.0423	4.38	T	1	19	0.013	LYVVVVENALLKK +dK_MMCCH-2 (K)	1060
19	1092	1114	633.7048	3163.4875	3163.4682	6.07	T	1	40	0.0001	QHHYETNPFHHGKITHENEITTR +dK_MMCCH-2 (K)	1104
20	1199	1203	353.1928	1056.5566	1056.5538	2.65	T	1	17	0.019	KRPYR +dK_MMCCH-2 (K)	1199
21	1395	1403	485.5976	1453.7709	1453.7599	7.57	T	2	29	0.0014	KDITQLDKR +dK_MMCCH-2 (K)	1395
22	1395	1403	598.3081	1791.9025	1791.8899	7.03	T	2	15	0.03	KDITQLDKR +2 dK_MMCCH-2 (K)	1395, 1402
23	1473	1489	778.4055	2332.1946	2332.1827	5.10	T	1	46	2.80E-05	KHGAVVGLPYWDWTLPR +dK_MMCCH-2 (K)	1473
24	1721	1746	1087.4788	3259.4145	3259.3937	6.38	T	1	15	0.031	TAGDCEDAGYFTVLGGEKEMPWAFDR +dK_MMCCH-2 (K)	1738

Figure 25A. KLH 1 (continued)

25	1747	1758	613.9782	1838.9128	1838.9012	6.31	T	1	27	0.0019	LYKYDITETLDK +dK_MMCCH-2 (K)	1749
26	1890	1922	1099.5339	4394.1067	4394.1048	0.43	T	1	13	0.048	HGSSVAVPYWDWTKPIHNIPHLFTDKEYYDVWR +dK_MMCCH-2 (K)	1915
27	1923	1932	756.3811	1510.7476	1510.7425	3.44	T	1	21	0.0077	NKVMPNPFAR +dK_MMCCH-2 (K)	1924
28	2100	2109	492.2501	1964.9713	1964.9601	5.70	T	2	21	0.0075	EIKDKQHHVR +2 dK_MMCCH-2 (K)	2102, 2104
29	2121	2149	890.4190	3557.6469	3557.6378	2.56	T	1	29	0.0012	TSADVQFQICKTSEDCHHGGQIFVLGGTK +dK_MMCCH-2 (K)	2131
30	2359	2367	736.3516	1470.6887	1470.6813	5.03	T	1	35	0.00032	DKLFNDPER +dK_MMCCH-2 (K)	2360
31	2507	2514	682.3550	1362.6955	1362.6853	7.49	T	1	22	0.0065	KLEHELEK +dK_MMCCH-2 (K)	2507
32	2515	2520	571.7631	1141.5117	1141.5074	3.77	T	1	19	0.013	QKEEDR +dK_MMCCH-2 (K)	2516
33	2621	2636	802.7125	2405.1157	2405.1083	3.08	T	1	47	2.10E-05	HHEKHHEDHHEDILVR +dK_MMCCH-2 (K)	2624
34	2637	2651	713.3571	2137.0495	2137.0374	5.66	T	1	69	1.40E-07	KNIHSLSHHEAEELR +dK_MMCCH-2 (K)	2637
35	2657	2686	1246.2233	3735.6480	3735.6358	3.24	T	1	17	0.019	LQNDESHGGYEHIAGFHGYPNLCPEKGDEK +dK_MMCCH-2 (K)	2686
36	2851	2883	807.5757	4032.8423	4032.8346	1.91	T	0	45	3.50E-05	VKPAHAGSCAGDIMHVPLHPFNYESVNNDDFTR +dK_MMCCH-2 (K)	2852
37	2897	2919	800.1410	3196.5351	3196.5287	2.00	T	1	53	5.10E-06	FNYKYDNLNLHGHNIEELEEVLR +dK_MMCCH-2 (K)	2900
38	3003	3021	825.7765	2474.3076	2474.2879	7.96	T	1	41	7.90E-05	KYDHTELDASVLPAPIIVR +dK_MMCCH-2 (K)	3003
39	123	151	807.4167	4032.0474	4032.0350	3.08	G	2	24	0.0036	KGFTDPPVKHHQSANLLVRKNINDLTREE +2 dK_MMCCH-2 (K)	123, 131
40	123	151	739.7923	3693.9251	3693.9049	5.47	G	2	33	0.00049	KGFTDPPVKHHQSANLLVRKNINDLTREE +dK_MMCCH-2 (K)	131
41	158	176	846.7141	2537.1203	2537.1169	1.34	G	3	23	0.0052	AFHKFQEDRSVDGYQATAE +Deamidated (NQ); dK_MMCCH-2 (K)	161
42	435	442	676.3256	1350.6366	1350.6312	4.00	G	1	14	0.038	NIEKMIHE +dK_MMCCH-2 (K)	438
43	526	544	777.7495	2330.2265	2330.2304	-1.67	G	1	29	0.0013	VDGTKLASSLIPHASVIRE +dK_MMCCH-2 (K)	530
44	589	612	1102.8308	3305.4706	3305.4621	2.60	G	1	14	0.037	DKSAGGFQQLGAFHGEPKWCPSPE +2 dK_MMCCH-2 (K)	590, 606
45	589	612	990.1188	2967.3345	2967.3320	0.84	G	1	28	0.0015	DKSAGGFQQLGAFHGEPKWCPSPE +dK_MMCCH-2 (K)	606
46	825	841	820.3754	2458.1045	2458.0940	4.27	G	1	25	0.003	HSVPFNVFDYKTNFNYE +dK_MMCCH-2 (K)	835
47	847	860	965.0179	1928.0212	1928.0077	7.00	G	0	17	0.018	FNGLSISQLNKKLE +dK_MMCCH-2 (K)	858
48	942	970	908.9860	3631.9147	3631.8973	4.79	G	2	20	0.01	VFDLKPASLGKDLFKQPSVIHEPRIGHHE +dK_MMCCH-2 (K)	956
49	1055	1076	810.1685	3236.6450	3236.6402	1.45	G	1	14	0.041	NALLKKGSSVAVPYWDWTKRIE +2 dK_MMCCH-2 (K)	1059, 1060
50	1055	1076	725.6360	2898.5149	2898.5102	1.62	G	1	18	0.018	NALLKKGSSVAVPYWDWTKRIE +dK_MMCCH-2 (K)	1073
51	1097	1110	999.9629	1997.9112	1997.9054	2.90	G	1	20	0.011	TNPFHHGKITHENE +dK_MMCCH-2 (K)	1104

Figure 25A. KLH 1 (continued)

52	1376	1396	864.3887	2590.1444	2590.1428	0.58	G	3	27	0.0021	AGTDSAHTDDGHTEPVMIRKD +dK_MMCCH-2 (K)	1395
53	1397	1413	774.4371	2320.2894	2320.2824	3.02	G	1	15	0.035	ITQLDKRQQLSLVKALE +dK_MMCCH-2 (K)	1402
54	1397	1413	774.4396	2320.2969	2320.2824	6.25	G	1	21	0.0089	ITQLDKRQQLSLVKALE +dK_MMCCH-2 (K)	1410
55	1506	1522	753.3802	2257.1187	2257.1089	4.34	G	2	27	0.0022	TGRDIPNPFIGSKIEFE +dK_MMCCH-2 (K)	1518
56	1755	1765	570.6056	1708.7949	1708.7913	2.17	G	2	31	0.00077	TLDKMNLRHDE +dK_MMCCH-2 (K)	1758
57	2059	2078	777.1311	3104.4953	3104.4888	2.09	G	1	18	0.018	INHNQFTKKHAVPNDVFKYE +2 dK_MMCCH-2 (K)	2067, 2076
58	2089	2100	854.4106	1706.8066	1706.8008	3.46	G	2	29	0.0012	IGGMNLHEIEKE +dK_MMCCH-2 (K)	2099
59	2647	2661	715.6794	2144.0163	2144.0095	3.17	G	4	29	0.0012	AEELRDALYKLQNDE +dK_MMCCH-2 (K)	2656
60	2765	2774	753.8675	1505.7204	1505.7225	-1.33	G	0	14	0.041	AIFQQTKFGE +dK_MMCCH-2 (K)	2771
61	3090	3097	632.8040	1263.5935	1263.5879	4.43	G	0	16	0.027	LGKMYSVE +dK_MMCCH-2 (K)	3092
62	94	100	573.2996	1144.5847	1144.5838	0.79	C	1	16	0.027	TVKAELF +dK_MMCCH-2 (K)	96
63	468	481	935.9766	1869.9387	1869.9295	4.92	C	0	22	0.0061	IKTTDSVQHKAGTF +dK_MMCCH-2 (K)	469
64	584	595	787.3998	1572.7851	1572.7858	-0.38	C	2	32	0.00063	ALLKEDKSAGGF +dK_MMCCH-2 (K)	590
65	715	723	655.8738	1309.7331	1309.7316	1.22	C	1	15	0.029	TSIAKQVLL +dK_MMCCH-2 (K)	719
66	783	788	544.7775	1087.5404	1087.5372	2.94	C	1	34	0.0004	QALQKY +dK_MMCCH-2 (K)	787
67	830	838	743.3415	1484.6684	1484.6646	2.56	C	2	16	0.025	NVFDYKTNF +dK_MMCCH-2 (K)	835
68	860	869	789.8851	1577.7556	1577.7548	0.51	C	1	13	0.047	EAIKSQDRFF +dK_MMCCH-2 (K)	863
69	956	974	638.3217	2549.2578	2549.2485	3.65	C	0	15	0.029	KQPSVIHEPRIGHHEGEVY +dK_MMCCH-2 (K)	956
70	1330	1337	620.3554	1238.6963	1238.6944	1.45	C	1	26	0.0028	KLDITKAL +dK_MMCCH-2 (K)	1335
71	1580	1586	544.2607	1086.5069	1086.5056	1.20	C	0	14	0.038	VGGKEPY +dK_MMCCH-2 (K)	1583
72	1649	1664	752.3309	2253.9708	2253.9637	3.15	C	2	17	0.02	NLNDHTHDFSKPEDTF +dK_MMCCH-2 (K)	1659
73	1818	1827	753.3695	1504.7245	1504.7232	0.86	C	1	25	0.0031	SERDIGSLKY +dK_MMCCH-2 (K)	1826
74	2076	2082	612.3039	1222.5932	1222.5944	-0.90	C	3	19	0.013	KYELLGY +dK_MMCCH-2 (K)	2076
75	2476	2488	923.9219	1845.8293	1845.8244	2.71	C	1	20	0.0097	THSNAKPTDVFEY +dK_MMCCH-2 (K)	2481
76	2656	2666	793.3512	1584.6878	1584.6879	0.00	C	1	22	0.0057	KLQNDESHGGY +dK_MMCCH-2 (K)	2656
77	2713	2723	787.9122	1573.8099	1573.8075	1.52	C	1	14	0.042	KKHGSHLGIPY +dK_MMCCH-2 (K)	2714
78	2809	2815	538.2603	1074.5059	1074.5056	0.37	C	0	19	0.014	IGGAEKY +dK_MMCCH-2 (K)	2814

Figure 25A. KLH 1 (continued)

79	2934	2945	816.4465	1630.8785	1630.8753	1.96	C	0	17	0.02	SGIRTTAVVKVY +dK_MMCCH-2 (K)	2943
80	2946	2960	965.4076	1928.8007	1928.7986	1.09	C	1	26	0.0027	IKSGTDSDDEYAGSF +dK_MMCCH-2 (K)	2947
81	2964	2971	607.2730	1212.5315	1212.5307	0.58	C	0	20	0.0092	GGAKEMPW +dK_MMCCH-2 (K)	2967
82	1	9	725.3406	1448.6667	1448.6567	6.90	Th	2	23	0.0054	MTPEELKTY +dK_MMCCH-2 (K)	7
83	38	56	861.6813	2582.0222	2582.0108	4.42	Th	2	13	0.047	VCIPDDNDRNDDHCEKAGD +dK_MMCCH-2 (K)	53
84	59	69	785.3785	1568.7424	1568.7367	3.63	Th	3	66	2.60E-07	VLGGPSEMKWQ +dK_MMCCH-2 (K)	67
85	78	84	569.2871	1136.5597	1136.5536	5.37	Th	1	49	1.20E-05	LSDTVHK +dK_MMCCH-2 (K)	84
86	116	124	447.2341	1338.6804	1338.6755	3.66	Th	2	31	0.00079	VVVHHPEKG +dK_MMCCH-2 (K)	123
87	125	135	815.8884	1629.7623	1629.7610	0.80	Th	1	16	0.023	FTDPPVKHHQS +dK_MMCCH-2 (K)	131
88	431	439	707.8542	1413.6938	1413.6883	3.89	Th	3	36	0.00025	ISLENIEKM +dK_MMCCH-2 (K)	438
89	519	530	807.9007	1613.7868	1613.7859	0.62	Th	3	60	9.80E-07	VTVDITEVDGTK +dK_MMCCH-2 (K)	530
90	585	591	585.8112	1169.6079	1169.6002	6.58	Th	1	26	0.0023	LLKEDKS +dK_MMCCH-2 (K)	590
91	601	612	904.8990	1807.7834	1807.7698	7.52	Th	1	25	0.0032	FHGEPKWCPSPE +dK_MMCCH-2 (K)	606
92	666	672	607.2826	1212.5507	1212.5485	1.90	Th	2	24	0.0039	LADHEKY +dK_MMCCH-2 (K)	671
93	829	837	743.3404	1484.6662	1484.6646	1.08	Th	3	21	0.0087	FNVFDYKTN +dK_MMCCH-2 (K)	835
94	1066	1074	530.2600	1587.7580	1587.7544	2.27	Th	3	14	0.043	VPYWDWTKR +dK_MMCCH-2 (K)	1073
95	1111	1120	742.3792	1482.7439	1482.7388	3.37	Th	1	16	0.025	ITTRDPKDSL +dK_MMCCH-2 (K)	1117
96	1219	1232	766.6617	2296.9634	2296.9617	0.74	Th	1	17	0.018	FDKSDNNDEATKTH +2 dK_MMCCH-2 (K)	1221, 1230
97	1219	1232	980.4233	1958.8321	1958.8316	0.26	Th	1	38	0.00014	FDKSDNNDEATKTH +dK_MMCCH-2 (K)	1230
98	1657	1668	921.9182	1841.8219	1841.8182	2.01	Th	2	56	2.60E-06	FSKPEDTFDYQK +dK_MMCCH-2 (K)	1659
99	1657	1668	921.9215	1841.8283	1841.8182	5.48	Th	2	57	2.20E-06	FSKPEDTFDYQK +dK_MMCCH-2 (K)	1668
100	1733	1741	664.3221	1326.6297	1326.6312	-1.13	Th	2	18	0.016	VLGGEKEMP +dK_MMCCH-1 (K); Oxidation (M)	1738
101	1894	1904	850.4122	1698.8098	1698.8116	-1.06	Th	5	37	0.00022	VAVPYWDWTKP +dK_MMCCH-2 (K)	1903
102	2064	2068	499.7597	997.5048	997.5055	-0.70	Th	0	21	0.008	FTKKH +dK_MMCCH-2 (K)	2067
103	2094	2100	618.3042	1234.5938	1234.5903	2.83	Th	1	27	0.0022	LHEIEKE +dK_MMCCH-2 (K)	2099
104	2238	2248	778.8801	1555.7457	1555.7440	1.09	Th	3	48	1.70E-05	LTTAEVDNLKD +dK_MMCCH-2 (K)	2247
105	2475	2490	746.3550	2236.0431	2236.0259	7.69	Th	4	22	0.006	FTHSNAKPTDVFEYSR +dK_MMCCH-2 (K)	2481

Figure 25A. KLH 1 (continued)

106	2512	2521	807.3973	1612.7801	1612.7766	2.17	Th	0	29	0.0013	LEKQKEEDRT +dK_MMCCH-2 (K)	2514
107	2508	2521	708.0122	2121.0148	2121.0048	4.71	Th	1	17	0.019	LEHELEKQKEEDRT +dK_MMCCH-2 (K)	2516
108	2595	2606	806.4047	1610.7949	1610.7862	5.40	Th	2	28	0.0016	IIDTSGKQLPSD +dK_MMCCH-2 (K)	2601
109	2607	2612	520.7805	1039.5465	1039.5446	1.83	Th	2	19	0.013	LIKMPT +dK_MMCCH-2 (K)	2609
110	2766	2771	551.7868	1101.5590	1101.5529	5.63	Th	1	29	0.0012	IFQQTK +dK_MMCCH-2 (K)	2771
111	2808	2816	638.3200	1274.6255	1274.6217	2.98	Th	3	27	0.0018	LIGGAEKYS +dK_MMCCH-2 (K)	2814
112	2946	2960	965.4102	1928.8059	1928.7986	3.78	Th	3	30	0.0011	IKSGTDSDDEYAGSF +dK_MMCCH-2 (K)	2947
113	2961	2970	691.8640	1381.7135	1381.7098	2.68	Th	4	18	0.016	VILGGAKEMP +dK_MMCCH-1 (K); Oxidation (M)	2967
114	2990	2996	583.2845	1164.5544	1164.5485	5.07	Th	1	38	0.00017	LTDDHVK +dK_MMCCH-2 (K)	2996

Figure 25B. KLH 2

#	Start	End	Observed	Mr(expt)	Mr(calc)	ppm	Enzyme	MC	Score	E value	Peptide	Mod_site
1	26	41	1043.0275	2084.0404	2084.0347	2.74	T	1	49	1.20E-05	KNVDSLSSDEVLALEK +dK_MMCCH-2 (K)	26
2	147	155	694.3721	1386.7297	1386.7217	5.77	T	1	35	0.00029	ADITFLNKK +dK_MMCCH-2 (K)	155
3	164	175	596.3124	1785.9155	1785.8985	9.52	T	1	42	6.60E-05	LFEKVQPGHHTR +dK_MMCCH-2 (K)	167
4	249	271	987.4443	2959.3110	2959.3051	1.99	T	1	36	0.00024	GKDPNSADCAHNLIHTPMEPFDR +dK_MMCCH-2 (K)	250
5	281	293	610.9466	1829.8179	1829.8043	7.49	T	0	54	4.30E-06	EHAKPADSFDYGR +dK_MMCCH-2 (K)	284
6	419	446	677.3707	3381.8173	3381.8132	1.21	T	1	27	0.0022	QPTLVHRPAKGHFDKPPVPVAQANLAVR +Deamidated (NQ); dK_MMCCH-2 (K)	428
7	429	446	752.0682	2253.1829	2253.1729	4.44	T	0	52	5.90E-06	GHFDKPPVPVAQANLAVR +dK_MMCCH-2 (K)	433
8	467	488	708.5943	2830.3481	2830.3385	3.39	T	1	69	1.30E-07	FQNDKSVDGYQATVEFHALPAR +dK_MMCCH-2 (K)	471
9	489	497	726.8442	1451.6738	1451.6649	6.13	T	1	22	0.0061	CPRPDAKDR +dK_MMCCH-2 (K)	495
10	936	950	720.3452	2158.0138	2158.0095	1.99	T	1	30	0.00097	KHGFTGGLPYWDWTR +dK_MMCCH-2 (K)	936
11	1082	1096	996.4687	1990.9228	1990.9063	8.29	T	0	46	2.70E-05	GKPYNTANCAIASMR +dK_MMCCH-2 (K)	1083
12	1097	1115	827.0787	2478.2142	2478.2101	1.65	T	0	66	2.30E-07	KPLQPFGLDSVINPDDETR +dK_MMCCH-2 (K)	1097
13	1123	1149	1190.5612	3568.6617	3568.6497	3.36	T	1	79	1.20E-08	VFDYKNNFDYEYESLAFNGLSIAQLDR +dK_MMCCH-2 (K)	1127
14	1355	1385	1271.2694	3810.7864	3810.7876	-0.31	T	1	38	0.00015	GSAVAVPYWDWTEKADSLPSLINDATYFNSR +dK_MMCCH-2 (K)	1368
15	1409	1450	1097.7141	5483.5342	5483.5213	2.35	T	1	40	9.60E-05	DPQPELWDNKDFYENVMLALEQDNFCDFEIQLELIHNALHSR +dK_MMCCH-2 (K)	1418
16	1455	1480	1117.8821	3350.6244	3350.6070	5.19	T	1	34	0.00044	AKYSLSSLDYTAFDPVFFLHHANVDR +dK_MMCCH-2 (K)	1456
17	1493	1507	721.6577	2161.9513	2161.9594	-3.75	T	1	66	2.40E-07	KKPYNEADCAVNEMR +dK_MMCCH-2 (K)	1494
18	1542	1564	802.8964	3207.5566	3207.5448	3.68	T	1	19	0.013	YQYDNLQFNHFSIQKLDQTIQAR +dK_MMCCH-2 (K)	1556
19	1622	1633	591.9822	1772.9247	1772.9171	4.29	T	1	30	0.00093	LYKFDITSALHK +dK_MMCCH-2 (K)	1624
20	1690	1704	532.2896	2125.1293	2125.1241	2.45	T	2	23	0.0046	KEVSSLTTLEKHFLR +dK_MMCCH-2 (K)	1700
21	1757	1768	612.9798	1835.9176	1835.9128	2.61	T	1	16	0.027	LYTVQFEDSLKR +dK_MMCCH-2 (K)	1767
22	1949	1963	560.2533	2236.9841	2236.9735	4.74	T	0	48	1.60E-05	TQEFSKPEDTFDYHR +dK_MMCCH-2 (K)	1954
23	2218	2231	937.4839	1872.9532	1872.9444	4.70	T	1	23	0.0049	DAVVNNPFAKGYIK +dK_MMCCH-2 (K)	2231

Figure 25B. KLH 2 (continued)

24	2400	2404	479.2450	956.4754	956.4749	0.52	T	1	16	0.025	KSQTR +dK_MMCCH-2 (K)	2400
25	2453	2463	839.9330	1677.8515	1677.8436	4.71	T	1	16	0.026	NFKYDITQALK +dK_MMCCH-2 (K)	2455
26	2527	2541	1007.5168	2013.0190	2013.0088	5.07	T	1	18	0.017	KDVTSLTASEIENLR +dK_MMCCH-2 (K)	2527
27	2755	2764	764.3846	1526.7546	1526.7439	7.01	T	0	37	0.00019	QPLKPFSESR +Deamidated (NQ); dK_MMCCH-2 (K)	2758
28	2810	2814	455.8921	1364.6544	1364.6468	5.50	T	2	15	0.031	KKEER +2 dK_MMCCH-2 (K)	2810, 2811
29	2866	2873	659.3627	1316.7108	1316.7050	4.40	T	1	16	0.023	YDITKVLK +dK_MMCCH-2 (K)	2870
30	3148	3155	629.3372	1256.6599	1256.6587	0.95	T	1	20	0.0093	KKPYNAAK +dK_MMCCH-2 (K)	3149
31	167	178	590.9643	1769.8710	1769.8705	0.28	G	0	22	0.0059	KVQPGHHTRLME +dK_MMCCH-2 (K)	167
32	311	322	567.6295	1699.8666	1699.8603	3.65	G	1	17	0.022	LNVYLGERAAKE +dK_MMCCH-2 (K)	321
33	433	456	975.8561	2924.5464	2924.5429	1.20	G	2	26	0.0023	KPPVPVAQANLAVRKNINDLTAEE +dK_MMCCH-2 (K)	433
34	466	481	1098.4999	2194.9852	2194.9841	0.50	G	2	32	0.00061	RFQNDKSVDGYQATVE +Deamidated (NQ); dK_MMCCH-2 (K)	471
35	1117	1133	1258.0826	2514.1507	2514.1314	7.68	G	2	17	0.021	HSVPFRVFDYKNNFDYE +dK_MMCCH-2 (K)	1127
36	1215	1235	961.8072	2882.3997	2882.3949	1.67	G	3	40	0.0001	ITQQLHDLDLHVGDNFFLKYE +dK_MMCCH-2 (K)	1233
37	1292	1303	879.4671	1756.9196	1756.9182	0.85	G	0	49	1.20E-05	SIRSAFLQIQKE +dK_MMCCH-2 (K)	1302
38	1308	1320	904.9448	1807.8751	1807.8749	0.06	G	0	28	0.0015	NIAKFHGKPGLCE +dK_MMCCH-2 (K)	1311
39	1308	1320	904.9462	1807.8778	1807.8749	1.55	G	0	35	0.00033	NIAKFHGKPGLCE +dK_MMCCH-2 (K)	1315
40	1403	1422	921.4190	2761.2350	2761.2330	0.72	G	3	23	0.0052	NAVTSRDPQPELWDNKDFYE +dK_MMCCH-2 (K)	1418
41	1952	1967	792.6818	2375.0236	2375.0205	1.31	G	3	31	0.00086	FSKPEDTFDYHRFGYE +dK_MMCCH-2 (K)	1954
42	1973	1990	817.0616	2448.1629	2448.1454	7.15	G	0	22	0.0063	FVGMSVSSLHNYIKQQQE +dK_MMCCH-2 (K); Oxidation (M)	1986
43	3386	3405	658.3166	2629.2375	2629.2271	3.96	G	2	24	0.0038	LDHAYSLRDGHYYIAGPTKD +dK_MMCCH-2 (K)	3404
44	277	296	883.7536	2648.2390	2648.2329	2.27	C	4	41	7.80E-05	DLTREHAKPADSFDYGRLGY +dK_MMCCH-2 (K)	284
45	629	635	539.2515	1076.4885	1076.4848	3.44	C	0	25	0.0034	VGGSEKY +dK_MMCCH-2 (K)	634
46	1075	1080	544.7775	1087.5404	1087.5372	2.94	C	1	34	0.0004	QALQKY +dK_MMCCH-2 (K)	1079
47	1212	1230	875.0881	2622.2424	2622.2424	-0.04	C	4	20	0.01	KYEITQQLHDLDLHVGDNF +dK_MMCCH-2 (K)	1212
48	1298	1306	715.3740	1428.7334	1428.7323	0.77	C	1	18	0.016	LQIQKEGIY +dK_MMCCH-2 (K)	1302
49	1416	1421	570.2391	1138.4637	1138.4641	-0.35	C	1	16	0.022	DNKDFY +dK_MMCCH-2 (K)	1418
50	1526	1540	749.6825	2246.0257	2246.0215	1.87	C	2	32	0.00061	KHNLPQDSFDYQNRF +dK_MMCCH-2 (K)	1526

Figure 25B. KLH 2 (continued)

51	1589	1606	784.3539	2350.0400	2350.0392	0.34	C	0	19	0.011	ICVEQGGEQNCKTKAGSF +dK_MMCCH-2 (K)	1602
52	1696	1702	607.3019	1212.5893	1212.5849	3.63	C	1	17	0.02	TTLEKHF +dK_MMCCH-2 (K)	1700
53	1801	1809	706.8394	1411.6643	1411.6595	3.40	C	0	14	0.043	SHKTFPNPF +dK_MMCCH-2 (K)	1803
54	1985	1995	850.4289	1698.8432	1698.8399	1.94	C	0	26	0.0023	IKQQQEADRVF +dK_MMCCH-2 (K)	1986
55	2455	2462	645.3275	1288.6405	1288.6373	2.48	C	1	22	0.0065	KYDITQAL +dK_MMCCH-2 (K)	2455
56	2463	2479	1128.0192	2254.0238	2254.0253	-0.67	C	1	16	0.027	KAQSIHPEDVFDTDAPF +dK_MMCCH-2 (K)	2463
57	2865	2872	673.3657	1344.7168	1344.7112	4.16	C	1	22	0.0067	RYDITKVL +dK_MMCCH-2 (K)	2870
58	3235	3242	617.3148	1232.6150	1232.6111	3.16	C	0	27	0.002	TSANVKIY +dK_MMCCH-2 (K)	3240
59	3399	3406	576.8029	1151.5912	1151.5896	1.30	C	0	39	0.00012	IAGPTKDL +dK_MMCCH-2 (K)	3404
60	165	175	558.6147	1672.8224	1672.8144	4.78	Th	1	22	0.0058	FEKVQPGHHTR +dK_MMCCH-2 (K)	167
61	180	191	909.9202	1817.8259	1817.8216	2.37	Th	4	65	3.30E-07	ILDALEQDEFCK +dK_MMCCH-2 (K)	191
62	247	260	631.6201	1891.8385	1891.8305	4.23	Th	2	13	0.046	LRGKDPNSADCAHN +dK_MMCCH-2 (K)	250
63	283	293	782.8600	1563.7054	1563.7028	1.73	Th	3	34	0.00039	AKPADSFDYGR +dK_MMCCH-2 (K)	284
64	364	372	642.3248	1282.6350	1282.6301	3.82	Th	2	41	7.30E-05	LLGGPTEMK +dK_MMCCH-2 (K)	372
65	431	437	569.2872	1136.5599	1136.5576	2.02	Th	1	13	0.045	FDKPPVP +dK_MMCCH-2 (K)	433
66	629	636	582.7666	1163.5186	1163.5169	1.55	Th	1	32	0.00069	VGGSEKYS +dK_MMCCH-2 (K)	634
67	893	904	904.8990	1807.7834	1807.7698	7.52	Th	1	25	0.0032	FHGEPKWCPSPE +dK_MMCCH-2 (K)	898
68	1123	1129	619.2855	1236.5564	1236.5485	6.39	Th	2	14	0.042	VFDYKNN +dK_MMCCH-2 (K)	1127
69	1414	1419	564.7574	1127.5003	1127.4957	4.08	Th	1	14	0.039	LWDNKD +dK_MMCCH-2 (K)	1418
70	1525	1539	738.3558	2212.0457	2212.0371	3.84	Th	3	48	1.50E-05	LKHNLPQDSFDYQNR +dK_MMCCH-2 (K)	1526
71	1589	1605	735.3320	2202.9741	2202.9708	1.50	Th	2	22	0.0068	ICVEQGGEQNCKTKAGS +dK_MMCCH-2 (K)	1600
72	1589	1605	735.3343	2202.9810	2202.9708	4.68	Th	2	38	0.00016	ICVEQGGEQNCKTKAGS +dK_MMCCH-2 (K)	1602
73	1800	1809	780.3723	1558.7301	1558.7279	1.41	Th	2	26	0.0025	FSHKTFPNPF +dK_MMCCH-2 (K)	1803
74	1952	1963	627.2842	1878.8309	1878.8247	3.30	Th	2	47	1.90E-05	FSKPEDTFDYHR +dK_MMCCH-2 (K)	1954
75	1985	1994	518.2667	1551.7783	1551.7715	4.38	Th	2	25	0.0034	IKQQQEADRV +dK_MMCCH-2 (K)	1986
76	2193	2199	667.3005	1332.5864	1332.5849	1.13	Th	2	22	0.0057	YWDWTKP +dK_MMCCH-2 (K)	2198
77	2200	2206	562.3085	1122.6025	1122.5995	2.67	Th	2	22	0.0057	ISKLPDL +dK_MMCCH-2 (K)	2202

Figure 25B. KLH 2 (continued)

78	2225	2229	462.2214	922.4282	922.4259	2.49	Th	2	14	0.036	FAKGY +dK_MMCCH-2 (K)	2227
79	2359	2363	509.2317	1016.4489	1016.4460	2.95	Th	1	17	0.019	FTKMH +dK_MMCCH-2 (K); Oxidation (M)	2361
80	2941	2950	720.8408	1439.6670	1439.6602	4.72	Th	3	45	2.80E-05	LDEANDLKNA +dK_MMCCH-2 (K)	2948
81	3009	3015	573.2736	1144.5327	1144.5335	-0.70	Th	0	14	0.041	LKEHGSH +dK_MMCCH-2 (K)	3010
82	3399	3405	520.2607	1038.5069	1038.5056	1.25	Th	1	25	0.0029	IAGPTKD +dK_MMCCH-2 (K)	3404

"Start" and "End" indicates the number of residue of KLH1 or KLH2. "Observed" column implies the observed m/z value in the survey scan while "Mr(expt)" "Mr(calc)", "ppm" indicate the experimental molecular weight(MW), calculated MW, and the difference between observed MW and theoretical MW respectively. In the "Enzyme" column, T, C, G and Th stand for trypsin, chymotrypsin, Glu-C and thermolysin respectively. MC stands for missed cleavage. Scores are the peptide ion score directly reported from Mascot database search engine. E value denotes the expectation value for each identified peptide. The peptide sequences as well as its modifications are listed in "Peptide" column. "Mod_site" indicates the lysine conjugation site for KLH1 or KLH2.

Figure 26. Identification details of MMCCH-conjugated peptides for sample 1 (2nd LC-MS/MS)

Figure 26A. KLH 1

#	Start	End	Observed	Mr(expt)	Mr(calc)	ppm	Enzyme	MC	Score	E value	Peptide	Mod_site
1	124	141	785.4114	2353.2125	2353.2001	5.27	T	1	14	0.037	GFTDPPVKHHQSANLLVR +dK_MMCCH-2 (K)	131
2	142	149	656.3405	1310.6665	1310.6653	0.92	T	1	25	0.003	KNINDLTR +dK_MMCCH-2 (K)	142
3	157	166	548.9218	1643.7436	1643.7402	2.07	T	1	20	0.011	EAFHKFQEDR +dK_MMCCH-2 (K)	161
4	460	477	781.3956	2341.1649	2341.1624	1.07	T	1	15	0.033	TSANVDIFIKTTDSVQHK +dK_MMCCH-2 (K)	469
5	470	488	748.0444	2241.1115	2241.1100	0.67	T	1	25	0.0034	TTDSVQHKAGTFAVLGGSK +dK_MMCCH-2 (K)	477
6	553	560	663.8681	1325.7216	1325.7166	3.85	T	2	24	0.0041	VKFDKVPR +dK_MMCCH-2 (K)	554
7	566	570	485.2447	968.4748	968.4749	-0.10	T	1	19	0.014	KNVDR +dK_MMCCH-2 (K)	566
8	581	587	547.8373	1093.6600	1093.6569	2.83	T	1	20	0.01	KALALLK +dK_MMCCH-2 (K)	581
9	588	606	781.0350	2340.0831	2340.0845	-0.60	T	1	29	0.0013	EDKSAGGFQQLGAFHGEPK +dK_MMCCH-2 (K)	590
10	645	681	1158.5393	4630.1281	4630.1063	4.71	T	1	18	0.014	HGYDGALPYWDWTSPLNHLPELADHEKYVDPEDGVEK +dK_MMCCH-2 (K)	671
11	682	699	1239.5804	2477.1463	2477.1434	1.17	T	1	16	0.025	HNPWFDGHIDTVDKTTTR +dK_MMCCH-2 (K)	695
12	700	719	887.7732	2660.2977	2660.2945	1.24	T	1	44	3.70E-05	SVQNKLFEQPEFGHYTSIAK +dK_MMCCH-2 (K)	704
13	778	789	958.0048	1913.9950	1913.9862	4.60	T	1	31	0.00074	IWAIWQALQKYR +Deamidated (NQ); dK_MMCCH-2 (K)	787
14	790	804	669.3164	2004.9274	2004.9220	2.69	T	0	37	0.00019	GKPYNVANCAVTSMR +dK_MMCCH-2 (K)	791
15	858	863	520.2980	1038.5814	1038.5783	2.98	T	1	17	0.019	KLEAIK +dK_MMCCH-2 (K)	858
16	953	965	635.3307	1902.9704	1902.9662	2.21	T	1	48	1.70E-05	DLFKQPSVIHEPR +dK_MMCCH-2 (K)	956
17	986	1000	685.0263	2052.0571	2052.0561	0.49	T	1	55	3.10E-06	KNIENLSLGELESLR +dK_MMCCH-2 (K)	986
18	1092	1114	791.8780	3163.4829	3163.4682	4.62	T	1	38	0.00015	QHHYETNPFHHGKITHENEITTR +dK_MMCCH-2 (K)	1104
19	1118	1162	1414.4275	5653.6810	5653.6850	-0.71	T	1	28	0.0015	DSLFHSDYFYEQVLYALEQDNFCDFEIQLEILHNALHSLLGGKGK +dK_MMCCH-2 (K)	1162
20	1199	1203	353.1912	1056.5517	1056.5538	-1.99	T	1	17	0.019	KRPYR +dK_MMCCH-2 (K)	1199
21	1395	1403	485.5965	1453.7677	1453.7599	5.37	T	2	33	0.00054	KDITQLDKR +dK_MMCCH-2 (K)	1395
22	1473	1489	778.4053	2332.1942	2332.1827	4.93	T	1	45	3.10E-05	KHGAVVGLPYWDWTLPR +dK_MMCCH-2 (K)	1473
23	1923	1932	756.3799	1510.7452	1510.7425	1.79	T	1	30	0.00099	NKVMPNPFAR +dK_MMCCH-2 (K)	1924

Figure 26A. KLH 1 (continued)

24	2067	2076	746.8890	1491.7635	1491.7544	6.10	T	1	19	0.011	KHAVPNDVFK +dK_MMCCH-2 (K)	2067
25	2068	2083	753.7155	2258.1247	2258.1194	2.35	T	1	13	0.047	HAVPNDVFKYELLGYR +dK_MMCCH-2 (K)	2076
26	2121	2149	890.4212	3557.6557	3557.6378	5.03	T	1	31	0.00073	TSADVQFQICKTSEDCHHGGQIFVLGGTK +dK_MMCCH-2 (K)	2131
27	2233	2251	834.0938	2499.2596	2499.2349	9.88	T	2	16	0.025	KEINTLTTAEVDNLKDAMR +dK_MMCCH-2 (K)	2247
28	2299	2314	715.0192	2142.0357	2142.0238	5.56	T	1	14	0.037	LYTKQMEDALTAHGAR +dK_MMCCH-2 (K)	2302
29	2359	2367	736.3490	1470.6834	1470.6813	1.43	T	1	34	0.00038	DKLFNDPER +dK_MMCCH-2 (K)	2360
30	2461	2490	642.8188	3850.8691	3850.8638	1.38	T	0	15	0.029	RPLRPFSDPINHNAFTHSNAKPTDVFEYSR +dK_MMCCH-2 (K)	2481
31	2507	2514	682.3505	1362.6865	1362.6853	0.88	T	1	33	0.00053	KLEHELEK +dK_MMCCH-2 (K)	2507
32	2515	2520	571.7624	1141.5103	1141.5074	2.63	T	1	22	0.0058	QKEEDR +dK_MMCCH-2 (K)	2516
33	2621	2636	802.7112	2405.1119	2405.1083	1.50	T	1	47	2.00E-05	HHEKHHEDHHEDILVR +dK_MMCCH-2 (K)	2624
34	2637	2651	1069.5295	2137.0445	2137.0374	3.32	T	1	59	1.40E-06	KNIHSLSHHEAEELR +dK_MMCCH-2 (K)	2637
35	2657	2686	934.9169	3735.6384	3735.6358	0.67	T	1	18	0.014	LQNDESHGGYEHIAGFHGYPNLCPEKGDEK +dK_MMCCH-2 (K)	2686
36	2761	2814	1328.4335	6637.1313	6637.0821	7.41	T	1	17	0.022	DVNEAIFQQTKFGEFSSIFYLALQALEEDNYCDFEVQYEILHNEVHALIGGAEK +4 Deamidated (NQ); dK_MMCCH-1 (K)	2771
37	2851	2883	807.5799	4032.8631	4032.8346	7.07	T	0	36	0.00023	VKPAHAGSCAGDIMHVPLHPFNYESVNNDDFTR +dK_MMCCH-2 (K)	2852
38	2897	2919	1066.5194	3196.5364	3196.5287	2.41	T	1	68	1.50E-07	FNYKYDNLNLHGHNIEELEEVLR +dK_MMCCH-2 (K)	2900
39	3003	3021	825.7721	2474.2944	2474.2879	2.63	T	1	39	0.00014	KYDHTELDASVLPAPIIVR +dK_MMCCH-2 (K)	3003
40	123	151	616.6594	3693.9130	3693.9049	2.19	G	2	19	0.013	KGFTDPPVKHHQSANLLVRKNINDLTREE +dK_MMCCH-2 (K)	123
41	123	151	739.7917	3693.9221	3693.9049	4.63	G	2	28	0.0015	KGFTDPPVKHHQSANLLVRKNINDLTREE +dK_MMCCH-2 (K)	131
42	158	176	846.3880	2536.1422	2536.1329	3.67	G	3	27	0.002	AFHKFQEDRSVDGYQATAE +dK_MMCCH-2 (K)	161
43	526	544	777.7497	2330.2272	2330.2304	-1.37	G	1	22	0.0064	VDGTKLASSLIPHASVIRE +dK_MMCCH-2 (K)	530
44	589	612	990.1168	2967.3286	2967.3320	-1.15	G	1	28	0.0015	DKSAGGFQQLGAFHGEPKWCPSPE +dK_MMCCH-2 (K)	606
45	825	841	820.7065	2459.0978	2459.0780	8.05	G	1	25	0.003	HSVPFNVFDYKTNFNYE +Deamidated (NQ); dK_MMCCH-2 (K)	835
46	942	972	764.6027	3817.9772	3817.9614	4.14	G	3	14	0.043	VFDLKPASLGKDLFKQPSVIHEPRIGHHEGE +dK_MMCCH-2 (K)	946
47	942	970	727.3896	3631.9116	3631.8973	3.91	G	2	16	0.024	VFDLKPASLGKDLFKQPSVIHEPRIGHHE +dK_MMCCH-2 (K)	956
48	1055	1076	810.1689	3236.6464	3236.6402	1.92	G	1	30	0.00099	NALLKKGSSVAVPYWDWTKRIE +2 dK_MMCCH-2 (K)	1059, 1060
49	1055	1076	725.6339	2898.5063	2898.5102	-1.35	G	1	41	7.10E-05	NALLKKGSSVAVPYWDWTKRIE +dK_MMCCH-2 (K)	1060

Figure 26A. KLH 1 (continued)

50	1055	1076	725.6342	2898.5076	2898.5102	-0.90	G	1	21	0.0085	NALLKKGSSVAVPYWDWTKRIE +dK_MMCCH-2 (K)	1073
51	1097	1110	999.9632	1997.9118	1997.9054	3.25	G	1	18	0.016	TNPFHHGKITHENE +dK_MMCCH-2 (K)	1104
52	1376	1396	648.5449	2590.1506	2590.1428	3.01	G	3	29	0.0012	AGTDSAHTDDGHTEPVMIRKD +dK_MMCCH-2 (K)	1395
53	1397	1413	774.4335	2320.2786	2320.2824	-1.64	G	1	25	0.0034	ITQLDKRQQLSLVKALE +dK_MMCCH-2 (K)	1410
54	1506	1522	753.3776	2257.1110	2257.1089	0.93	G	2	26	0.0028	TGRDIPNPFIGSKIEFE +dK_MMCCH-2 (K)	1518
55	1755	1765	570.6055	1708.7946	1708.7913	1.93	G	2	25	0.0031	TLDKMNLRHDE +dK_MMCCH-2 (K)	1758
56	2089	2100	854.4103	1706.8061	1706.8008	3.16	G	2	30	0.00094	IGGMNLHEIEKE +dK_MMCCH-2 (K)	2099
57	2647	2661	715.6783	2144.0130	2144.0095	1.63	G	4	18	0.016	AEELRDALYKLQNDE +dK_MMCCH-2 (K)	2656
58	3090	3097	632.8034	1263.5923	1263.5879	3.40	G	0	16	0.026	LGKMYSVE +dK_MMCCH-2 (K)	3092
59	59	68	721.3486	1440.6827	1440.6781	3.19	C	1	21	0.0084	VLGGPSEMKW +dK_MMCCH-2 (K)	67
60	94	100	573.2995	1144.5844	1144.5838	0.52	C	1	17	0.02	TVKAELF +dK_MMCCH-2 (K)	96
61	429	450	990.8052	2969.3937	2969.3899	1.31	C	1	14	0.036	GGISLENIEKMIHENQQEDRIY +dK_MMCCH-2 (K); Oxidation (M)	438
62	584	595	787.4013	1572.7879	1572.7858	1.40	C	2	46	2.60E-05	ALLKEDKSAGGF +dK_MMCCH-2 (K)	590
63	715	723	655.8741	1309.7336	1309.7316	1.60	C	1	15	0.032	TSIAKQVLL +dK_MMCCH-2 (K)	719
64	783	788	544.7768	1087.5390	1087.5372	1.66	C	1	23	0.0054	QALQKY +dK_MMCCH-2 (K)	787
65	830	838	743.3419	1484.6692	1484.6646	3.10	C	2	22	0.006	NVFDYKTNF +dK_MMCCH-2 (K)	835
66	944	955	821.4310	1640.8475	1640.8484	-0.55	C	3	18	0.016	DLKPASLGKDLF +dK_MMCCH-2 (K)	946
67	1330	1337	620.3562	1238.6978	1238.6944	2.74	C	1	22	0.0064	KLDITKAL +dK_MMCCH-2 (K)	1335
68	1580	1586	544.2618	1086.5091	1086.5056	3.22	C	0	23	0.0055	VGGKEPY +dK_MMCCH-2 (K)	1583
69	1818	1827	753.3697	1504.7249	1504.7232	1.20	C	1	18	0.015	SERDIGSLKY +dK_MMCCH-2 (K)	1826
70	2076	2082	612.3051	1222.5955	1222.5944	0.98	C	3	15	0.031	KYELLGY +dK_MMCCH-2 (K)	2076
71	2160	2184	814.3868	3253.5180	3253.5179	0.03	C	3	14	0.036	KYDITHALHDAHITPEDVFHPSEPF +dK_MMCCH-2 (K)	2160
72	2476	2488	923.9227	1845.8309	1845.8244	3.58	C	1	28	0.0017	THSNAKPTDVFEY +dK_MMCCH-2 (K)	2481
73	2656	2672	747.3438	2239.0094	2239.0004	4.02	C	2	26	0.0026	KLQNDESHGGYEHIAGF +dK_MMCCH-2 (K)	2656
74	2738	2749	856.3752	1710.7358	1710.7348	0.58	C	2	15	0.033	ADSGNNNPFFKY +dK_MMCCH-2 (K)	2748
75	2946	2960	965.4056	1928.7966	1928.7986	-1.04	C	1	24	0.0044	IKSGTDSDDEYAGSF +dK_MMCCH-2 (K)	2947
76	2961	2971	769.8948	1537.7751	1537.7673	5.07	C	1	16	0.024	VILGGAKEMPW +dK_MMCCH-2 (K)	2967

Figure 26A. KLH 1 (continued)

77	1	8	643.8057	1285.5968	1285.5934	2.64	Th	1	26	0.0026	MTPEELKT +dK_MMCCH-2 (K)	7
78	38	56	861.6823	2582.0251	2582.0108	5.54	Th	2	17	0.022	VCIPDDNDRNDDHCEKAGD +dK_MMCCH-2 (K)	53
79	59	69	785.3758	1568.7370	1568.7367	0.19	Th	3	59	1.40E-06	VLGGPSEMKWQ +dK_MMCCH-2 (K)	67
80	78	84	569.2868	1136.5590	1136.5536	4.75	Th	1	42	6.90E-05	LSDTVHK +dK_MMCCH-2 (K)	84
81	117	124	620.8154	1239.6162	1239.6070	7.34	Th	1	28	0.0016	VVHHPEKG +dK_MMCCH-2 (K)	123
82	269	282	660.0024	1976.9855	1976.9778	3.89	Th	4	27	0.0019	VIAFEENAPHTKRQ +dK_MMCCH-2 (K)	280
83	431	439	707.8527	1413.6908	1413.6883	1.70	Th	3	42	6.60E-05	ISLENIEKM +dK_MMCCH-2 (K)	438
84	521	530	707.8467	1413.6788	1413.6698	6.37	Th	2	74	4.30E-08	VDITEVDGTK +dK_MMCCH-2 (K)	530
85	585	591	585.8110	1169.6074	1169.6002	6.16	Th	1	35	0.00033	LLKEDKS +dK_MMCCH-2 (K)	590
86	601	612	904.8955	1807.7765	1807.7698	3.65	Th	1	21	0.0086	FHGEPKWCPSPE +dK_MMCCH-2 (K)	606
87	666	672	607.2842	1212.5539	1212.5485	4.45	Th	2	23	0.0046	LADHEKY +dK_MMCCH-2 (K)	671
88	831	837	612.7877	1223.5608	1223.5533	6.13	Th	2	17	0.019	VFDYKTN +dK_MMCCH-2 (K)	835
89	954	959	529.7660	1057.5175	1057.5154	1.99	Th	1	16	0.027	LFKQPS +Deamidated (NQ); dK_MMCCH-2 (K)	956
90	1100	1104	482.2290	962.4434	962.4433	0.10	Th	0	16	0.023	FHHGK +dK_MMCCH-2 (K)	1104
91	1111	1120	742.3796	1482.7446	1482.7388	3.91	Th	1	18	0.017	ITTRDPKDSL +dK_MMCCH-2 (K)	1117
92	1156	1164	630.8406	1259.6666	1259.6584	6.51	Th	2	17	0.019	LLGGKGKYS +dK_MMCCH-2 (K)	1162
93	1219	1232	980.4258	1958.8370	1958.8316	2.76	Th	1	58	1.60E-06	FDKSDNNDEATKTH +dK_MMCCH-2 (K)	1230
94	1580	1587	572.7747	1143.5348	1143.5271	6.73	Th	1	14	0.043	VGGKEPYG +dK_MMCCH-2 (K)	1583
95	1657	1668	921.9188	1841.8231	1841.8182	2.66	Th	2	34	0.00041	FSKPEDTFDYQK +dK_MMCCH-2 (K)	1659
96	1657	1668	921.9185	1841.8225	1841.8182	2.33	Th	2	39	0.00012	FSKPEDTFDYQK +dK_MMCCH-2 (K)	1668
97	1733	1741	664.3225	1326.6305	1326.6312	-0.53	Th	2	17	0.021	VLGGEKEMP +dK_MMCCH-1 (K); Oxidation (M)	1738
98	1898	1904	667.3018	1332.5891	1332.5849	3.15	Th	2	27	0.0021	YWDWTKP +dK_MMCCH-2 (K)	1903
99	2064	2068	499.7606	997.5067	997.5055	1.20	Th	0	22	0.007	FTKKH +dK_MMCCH-2 (K)	2067
100	2094	2100	618.3083	1234.6020	1234.5903	9.48	Th	1	26	0.0023	LHEIEKE +dK_MMCCH-2 (K)	2099
101	2129	2141	622.9256	1865.7550	1865.7495	2.95	Th	0	24	0.0041	ICKTSEDCHHGGQ +dK_MMCCH-2 (K)	2131
102	2238	2248	778.8793	1555.7440	1555.7440	0.00	Th	3	42	6.60E-05	LTTAEVDNLKD +dK_MMCCH-2 (K)	2247
103	2480	2487	622.7983	1243.5820	1243.5795	2.01	Th	2	20	0.0094	AKPTDVFE +dK_MMCCH-2 (K)	2481

Figure 26A. KLH 1 (continued)

104	2512	2521	807.3970	1612.7794	1612.7766	1.67	Th	0	32	0.00061	LEKQKEEDRT +dK_MMCCH-2 (K)	2514
105	2595	2606	806.4030	1610.7915	1610.7862	3.29	Th	2	34	0.00039	IIDTSGKQLPSD +dK_MMCCH-2 (K)	2601
106	2607	2612	520.7797	1039.5449	1039.5446	0.29	Th	2	19	0.014	LIKMPT +dK_MMCCH-2 (K)	2609
107	2766	2771	551.7854	1101.5562	1101.5529	3.09	Th	1	25	0.0029	IFQQTK +dK_MMCCH-2 (K)	2771
108	2808	2816	638.3187	1274.6229	1274.6217	1.02	Th	3	27	0.002	LIGGAEKYS +dK_MMCCH-2 (K)	2814
109	2946	2960	965.4091	1928.8037	1928.7986	2.64	Th	3	40	9.50E-05	IKSGTDSDDEYAGSF +dK_MMCCH-2 (K)	2947
110	2990	2996	583.2850	1164.5555	1164.5485	6.01	Th	1	38	0.00018	LTDDHVK +dK_MMCCH-2 (K)	2996
111	3076	3084	724.3611	1446.7077	1446.7040	2.63	Th	2	15	0.03	FKCKVPPFS +dK_MMCCH-2 (K)	3079

Figure 26B. KLH 2

#	Start	End	Observed	Mr(expt)	Mr(calc)	ppm	Enzyme	MC	Score	E value	Peptide	Mod_site
1	26	41	1043.0270	2084.0394	2084.0347	2.26	T	1	49	1.30E-05	KNVDSLSSDEVLALEK +dK_MMCCH-2 (K)	26
2	147	155	694.3710	1386.7275	1386.7217	4.18	T	1	19	0.014	ADITFLNKK +dK_MMCCH-2 (K)	155
3	164	175	596.3106	1785.9100	1785.8985	6.44	T	1	43	5.00E-05	LFEKVQPGHHTR +dK_MMCCH-2 (K)	167
4	249	271	987.4406	2959.3000	2959.3051	-1.72	T	1	30	0.001	GKDPNSADCAHNLIHTPMEPFDR +dK_MMCCH-2 (K)	250
5	281	293	610.9454	1829.8143	1829.8043	5.47	T	0	54	3.80E-06	EHAKPADSFDYGR +dK_MMCCH-2 (K)	284
6	419	446	846.4622	3381.8195	3381.8132	1.86	T	1	27	0.0021	QPTLVHRPAKGHFDKPPVPVAQANLAVR +Deamidated (NQ); dK_MMCCH-2 (K)	428
7	429	446	752.0668	2253.1785	2253.1729	2.49	T	0	41	7.30E-05	GHFDKPPVPVAQANLAVR +dK_MMCCH-2 (K)	433
8	462	466	486.7367	971.4589	971.4568	2.16	T	1	13	0.046	KAMER +dK_MMCCH-2 (K)	462
9	467	488	708.5958	2830.3539	2830.3385	5.48	T	1	69	1.10E-07	FQNDKSVDGYQATVEFHALPAR +dK_MMCCH-2 (K)	471
10	936	950	720.3436	2158.0089	2158.0095	-0.28	T	1	34	0.00037	KHGFTGGLPYWDWTR +dK_MMCCH-2 (K)	936
11	995	1052	1170.7141	7018.2410	7018.2306	1.48	T	1	13	0.047	DDLYQSPGFGHYTDIAKQVLLAFEQDDFCDFEVQFEIAHNFIHALVGGNEPYSMSSLR +dK_MMCCH-2 (K)	1011
12	1082	1096	996.4616	1990.9087	1990.9063	1.21	T	0	76	2.80E-08	GKPYNTANCAIASMR +dK_MMCCH-2 (K)	1083
13	1097	1115	827.0759	2478.2060	2478.2101	-1.65	T	0	68	1.50E-07	KPLQPFGLDSVINPDDETR +dK_MMCCH-2 (K)	1097
14	1123	1149	1190.5593	3568.6562	3568.6497	1.82	T	1	69	1.30E-07	VFDYKNNFDYEYESLAFNGLSIAQLDR +dK_MMCCH-2 (K)	1127
15	1355	1385	1271.2737	3810.7992	3810.7876	3.04	T	1	49	1.30E-05	GSAVAVPYWDWTEKADSLPSLINDATYFNSR +dK_MMCCH-2 (K)	1368
16	1409	1450	1371.8909	5483.5344	5483.5213	2.39	T	1	50	1.00E-05	DPQPELWDNKDFYENVMLALEQDNFCDFEIQLELIHNALHSR +dK_MMCCH-2 (K)	1418
17	1455	1480	1117.8749	3350.6028	3350.6070	-1.25	T	1	69	1.40E-07	AKYSLSSLDYTAFDPVFFLHHANVDR +dK_MMCCH-2 (K)	1456
18	1493	1507	721.6661	2161.9766	2161.9594	7.91	T	1	37	0.00021	KKPYNEADCAVNEMR +dK_MMCCH-2 (K)	1493
19	1493	1507	721.6617	2161.9634	2161.9594	1.85	T	1	49	1.30E-05	KKPYNEADCAVNEMR +dK_MMCCH-2 (K)	1494
20	1508	1526	837.7523	2510.2351	2510.2185	6.61	T	0	20	0.011	KPLQPFNNPELNSDSMTLK +dK_MMCCH-2 (K)	1508
21	1508	1539	825.9982	4124.9545	4124.9360	4.48	T	1	24	0.0041	KPLQPFNNPELNSDSMTLKHNLPQDSFDYQNR +dK_MMCCH-2 (K)	1526
22	1542	1564	1070.1957	3207.5652	3207.5448	6.39	T	1	23	0.0045	YQYDNLQFNHFSIQKLDQTIQAR +dK_MMCCH-2 (K)	1556
23	1690	1704	532.2902	2125.1318	2125.1241	3.58	T	2	17	0.022	KEVSSLTTLEKHFLR +dK_MMCCH-2 (K)	1700

Figure 26B. KLH 2 (continued)

24	1757	1768	612.9789	1835.9150	1835.9128	1.20	T	1	14	0.041	LYTVQFEDSLKR +dK_MMCCH-2 (K)	1767
25	1949	1963	746.6681	2236.9824	2236.9735	3.98	T	0	39	0.00013	TQEFSKPEDTFDYHR +dK_MMCCH-2 (K)	1954
26	2045	2052	660.3516	1318.6887	1318.6843	3.34	T	1	21	0.0084	YDITKTLK +dK_MMCCH-2 (K)	2049
27	2116	2125	715.3641	1428.7136	1428.7105	2.17	T	1	21	0.0083	DLASLKSAMR +dK_MMCCH-2 (K)	2121
28	2218	2231	937.4800	1872.9454	1872.9444	0.53	T	1	19	0.014	DAVVNNPFAKGYIK +dK_MMCCH-2 (K)	2227
29	2228	2239	870.4218	1738.8291	1738.8236	3.16	T	1	20	0.011	GYIKSEDAYTVR +dK_MMCCH-2 (K)	2231
30	2527	2541	1007.5172	2013.0197	2013.0088	5.41	T	1	26	0.0027	KDVTSLTASEIENLR +dK_MMCCH-2 (K)	2527
31	2728	2739	958.0048	1913.9950	1913.9862	4.60	T	1	31	0.00074	IWAIWQALQKYR +Deamidated (NQ); dK_MMCCH-2 (K)	2737
32	2755	2764	764.3823	1526.7500	1526.7439	4.00	T	0	33	0.00045	QPLKPFSESR +Deamidated (NQ); dK_MMCCH-2 (K)	2758
33	2866	2873	659.3626	1316.7107	1316.7050	4.33	T	1	15	0.029	YDITKVLK +dK_MMCCH-2 (K)	2870
34	3148	3155	629.3355	1256.6565	1256.6587	-1.75	T	1	19	0.013	KKPYNAAK +dK_MMCCH-2 (K)	3149
35	167	178	590.9645	1769.8716	1769.8705	0.62	G	0	36	0.00027	KVQPGHHTRLME +dK_MMCCH-2 (K)	167
36	433	456	975.8562	2924.5468	2924.5429	1.30	G	2	21	0.0088	KPPVPVAQANLAVRKNINDLTAEE +dK_MMCCH-2 (K)	433
37	466	481	1098.4998	2194.9850	2194.9841	0.41	G	2	35	0.00032	RFQNDKSVDGYQATVE +Deamidated (NQ); dK_MMCCH-2 (K)	471
38	1215	1235	721.6072	2882.3999	2882.3949	1.70	G	3	28	0.0017	ITQQLHDLDLHVGDNFFLKYE +dK_MMCCH-2 (K)	1233
39	1292	1303	879.4667	1756.9189	1756.9182	0.46	G	0	49	1.20E-05	SIRSAFLQIQKE +dK_MMCCH-2 (K)	1302
40	1308	1320	904.9512	1807.8878	1807.8749	7.08	G	0	17	0.018	NIAKFHGKPGLCE +dK_MMCCH-2 (K)	1311
41	1308	1320	904.9452	1807.8758	1807.8749	0.50	G	0	27	0.0022	NIAKFHGKPGLCE +dK_MMCCH-2 (K)	1315
42	1354	1378	1043.5070	3127.4991	3127.4961	0.96	G	3	17	0.019	RGSAVAVPYWDWTEKADSLPSLIND +dK_MMCCH-2 (K)	1368
43	1403	1422	921.4236	2761.2491	2761.2330	5.83	G	3	20	0.0092	NAVTSRDPQPELWDNKDFYE +dK_MMCCH-2 (K)	1418
44	1952	1967	792.6805	2375.0196	2375.0205	-0.38	G	3	37	0.00021	FSKPEDTFDYHRFGYE +dK_MMCCH-2 (K)	1954
45	1973	1990	817.0591	2448.1556	2448.1454	4.17	G	0	19	0.012	FVGMSVSSLHNYIKQQQE +dK_MMCCH-2 (K); Oxidation (M)	1986
46	2477	2484	644.8365	1287.6585	1287.6573	0.93	G	0	16	0.027	APFFIKVE +dK_MMCCH-2 (K)	2482
47	3386	3405	658.3146	2629.2292	2629.2271	0.80	G	2	25	0.0032	LDHAYSLRDGHYYIAGPTKD +dK_MMCCH-2 (K)	3404
48	152	165	667.6934	2000.0584	2000.0513	3.55	C	2	13	0.047	LNKKTSRAVDDRLF +dK_MMCCH-2 (K)	155
49	166	176	547.2858	1638.8355	1638.8300	3.30	C	0	24	0.0036	EKVQPGHHTRL +dK_MMCCH-2 (K)	167
50	277	296	883.7568	2648.2487	2648.2329	5.97	C	4	39	0.00014	DLTREHAKPADSFDYGRLGY +dK_MMCCH-2 (K)	284

Figure 26B. KLH 2 (continued)

51	364	373	743.3605	1484.7064	1484.7044	1.35	C	2	19	0.012	LLGGPTEMKW +dK_MMCCH-2 (K); Oxidation (M)	372
52	423	443	872.8013	2615.3820	2615.3795	0.96	C	1	13	0.05	VHRPAKGHFDKPPVPVAQANL +dK_MMCCH-2 (K)	428
53	629	635	539.2519	1076.4892	1076.4848	4.09	C	0	19	0.014	VGGSEKY +dK_MMCCH-2 (K)	634
54	1007	1015	669.8724	1337.7302	1337.7265	2.77	C	1	30	0.0011	TDIAKQVLL +dK_MMCCH-2 (K)	1011
55	1075	1080	544.7768	1087.5390	1087.5372	1.66	C	1	23	0.0054	QALQKY +dK_MMCCH-2 (K)	1079
56	1298	1306	715.3770	1428.7395	1428.7323	5.04	C	1	14	0.041	LQIQKEGIY +dK_MMCCH-2 (K)	1302
57	1526	1540	749.6843	2246.0312	2246.0215	4.32	C	2	36	0.00028	KHNLPQDSFDYQNRF +dK_MMCCH-2 (K)	1526
58	1589	1606	784.3560	2350.0461	2350.0392	2.94	C	0	24	0.0045	ICVEQGGEQNCKTKAGSF +dK_MMCCH-2 (K)	1602
59	1696	1702	607.3021	1212.5896	1212.5849	3.88	C	1	16	0.027	TTLEKHF +dK_MMCCH-2 (K)	1700
60	1708	1719	839.8457	1677.6768	1677.6651	7.03	C	0	16	0.023	KNMQADDSPDGY +dK_MMCCH-2 (K)	1708
61	1801	1809	706.8377	1411.6607	1411.6595	0.92	C	0	15	0.035	SHKTFPNPF +dK_MMCCH-2 (K)	1803
62	1985	1995	850.4290	1698.8435	1698.8399	2.12	C	0	42	6.20E-05	IKQQQEADRVF +dK_MMCCH-2 (K)	1986
63	1999	2003	458.2544	914.4942	914.4936	0.77	C	2	23	0.0046	LLKGF +dK_MMCCH-2 (K)	2001
64	2455	2462	645.3270	1288.6395	1288.6373	1.71	C	1	18	0.017	KYDITQAL +dK_MMCCH-2 (K)	2455
65	2463	2479	1128.0206	2254.0267	2254.0253	0.67	C	1	13	0.048	KAQSIHPEDVFDTDAPF +dK_MMCCH-2 (K)	2463
66	2754	2760	598.3320	1194.6494	1194.6471	1.93	C	1	22	0.0058	KQPLKPF +dK_MMCCH-2 (K)	2754
67	2754	2760	598.3337	1194.6529	1194.6471	4.85	C	1	24	0.0041	KQPLKPF +dK_MMCCH-2 (K)	2758
68	3235	3242	617.3142	1232.6139	1232.6111	2.27	C	0	27	0.002	TSANVKIY +dK_MMCCH-2 (K)	3240
69	165	175	558.6147	1672.8224	1672.8144	4.78	Th	1	16	0.025	FEKVQPGHHTR +dK_MMCCH-2 (K)	167
70	184	191	703.8036	1405.5927	1405.5894	2.42	Th	1	33	0.00052	LEQDEFCK +dK_MMCCH-2 (K)	191
71	247	260	631.6209	1891.8407	1891.8305	5.39	Th	2	17	0.021	LRGKDPNSADCAHN +dK_MMCCH-2 (K)	250
72	283	293	782.8585	1563.7025	1563.7028	-0.19	Th	3	47	2.00E-05	AKPADSFDYGR +dK_MMCCH-2 (K)	284
73	365	374	707.3312	1412.6478	1412.6469	0.71	Th	2	42	6.90E-05	LGGPTEMKWG +dK_MMCCH-2 (K)	372
74	467	472	538.7419	1075.4693	1075.4644	4.56	Th	0	13	0.048	FQNDKS +dK_MMCCH-2 (K)	471
75	554	565	811.8957	1621.7768	1621.7658	6.84	Th	1	18	0.016	LDPVTGETKNNP +dK_MMCCH-2 (K)	562
76	629	636	582.7667	1163.5189	1163.5169	1.72	Th	1	16	0.024	VGGSEKYS +dK_MMCCH-2 (K)	634
77	893	904	904.8955	1807.7765	1807.7698	3.65	Th	1	21	0.0086	FHGEPKWCPSPE +dK_MMCCH-2 (K)	898

Figure 26B. KLH 2 (continued)

78	1300	1308	716.3455	1430.6765	1430.6751	0.91	Th	2	23	0.0048	IQKEGIYEN +dK_MMCCH-2 (K)	1302
79	1414	1419	564.7546	1127.4947	1127.4957	-0.89	Th	1	14	0.04	LWDNKD +dK_MMCCH-2 (K)	1418
80	1525	1539	738.3547	2212.0422	2212.0371	2.31	Th	3	39	0.00012	LKHNLPQDSFDYQNR +dK_MMCCH-2 (K)	1526
81	1589	1605	735.3315	2202.9726	2202.9708	0.82	Th	2	18	0.017	ICVEQGGEQNCKTKAGS +dK_MMCCH-2 (K)	1600
82	1589	1605	735.3328	2202.9766	2202.9708	2.68	Th	2	21	0.0076	ICVEQGGEQNCKTKAGS +dK_MMCCH-2 (K)	1602
83	1800	1809	780.3729	1558.7313	1558.7279	2.18	Th	2	14	0.043	FSHKTFPNPF +dK_MMCCH-2 (K)	1803
84	1952	1963	627.2849	1878.8327	1878.8247	4.26	Th	2	48	1.70E-05	FSKPEDTFDYHR +dK_MMCCH-2 (K)	1954
85	1985	1994	776.8962	1551.7778	1551.7715	4.06	Th	2	28	0.0015	IKQQQEADRV +dK_MMCCH-2 (K)	1986
86	2193	2199	667.3018	1332.5891	1332.5849	3.15	Th	2	27	0.0021	YWDWTKP +dK_MMCCH-2 (K)	2198
87	2200	2206	562.3079	1122.6012	1122.5995	1.51	Th	2	19	0.013	ISKLPDL +dK_MMCCH-2 (K)	2202
88	2225	2229	462.2217	922.4289	922.4259	3.36	Th	2	22	0.0056	FAKGY +dK_MMCCH-2 (K)	2227
89	2230	2237	632.7946	1263.5747	1263.5693	4.27	Th	2	18	0.016	IKSEDAYT +dK_MMCCH-2 (K)	2231
90	2804	2815	937.4586	1872.9026	1872.9073	-2.51	Th	2	15	0.034	AMLQERKKEERT +Deamidated (NQ); dK_MMCCH-2 (K); Oxidation (M)	2811
91	2941	2950	720.8405	1439.6663	1439.6602	4.24	Th	3	49	1.30E-05	LDEANDLKNA +dK_MMCCH-2 (K)	2948
92	3009	3015	573.2770	1144.5395	1144.5335	5.24	Th	0	16	0.023	LKEHGSH +dK_MMCCH-2 (K)	3010
93	3399	3405	520.2615	1038.5085	1038.5056	2.79	Th	1	28	0.0015	IAGPTKD +dK_MMCCH-2 (K)	3404

"Start" and "End" indicates the number of residue of KLH1 or KLH2. "Observed" column implies the observed m/z value in the survey scan while "Mr(expt)", "Mr(calc)", "ppm" indicate the experimental molecular weight(MW), calculated MW, and the difference between observed MW and theoretical MW respectively. In the "Enzyme" column, T, C, G and Th stand for trypsin, chymotrypsin, Glu-C and thermolysin respectively. MC stands for missed cleavage. Scores are the peptide ion score directly reported from Mascot database search engine. E value denotes the expectation value for each identified peptide. The peptide sequences as well as its modifications are listed in "Peptide" column. "Mod_site" indicates the lysine conjugation site for KLH1 or KLH2.

Figure 27. Identification details of MMCCH-conjugated peptides for sample 2 (2nd LC-MS/MS)

Figure 27A. KLH 1

#	Start	End	Observed	Mr(expt)	Mr(calc)	ppm	Enzyme	MC	Score	E value	Peptide	Mod_site
1	124	141	785.4103	2353.2092	2353.2001	3.87	T	1	17	0.02	GFTDPPVKHHQSANLLVR +dK_MMCCH-2 (K)	131
2	142	149	656.3403	1310.6661	1310.6653	0.69	T	1	29	0.0013	KNINDLTR +dK_MMCCH-2 (K)	142
3	157	166	823.3675	1644.7204	1644.7242	-2.31	T	1	24	0.0038	EAFHKFQEDR +Deamidated (NQ); dK_MMCCH-2 (K)	161
4	184	192	726.8430	1451.6715	1451.6649	4.48	T	1	26	0.0026	CPRPDAKDR +dK_MMCCH-2 (K)	190
5	553	560	663.8685	1325.7224	1325.7166	4.37	T	2	26	0.0026	VKFDKVPR +dK_MMCCH-2 (K)	554
6	566	570	485.2447	968.4748	968.4749	-0.21	T	1	19	0.014	KNVDR +dK_MMCCH-2 (K)	566
7	581	587	547.8374	1093.6602	1093.6569	3.02	T	1	18	0.018	KALALLK +dK_MMCCH-2 (K)	581
8	588	606	781.0366	2340.0879	2340.0845	1.45	T	1	14	0.036	EDKSAGGFQQLGAFHGEPK +dK_MMCCH-2 (K)	590
9	645	681	1158.5381	4630.1233	4630.1063	3.65	T	1	18	0.015	HGYDGALPYWDWTSPLNHLPELADHEKYVDPEDGVEK +dK_MMCCH-2 (K)	671
10	682	699	620.2961	2477.1555	2477.1434	4.84	T	1	21	0.0075	HNPWFDGHIDTVDKTTTR +dK_MMCCH-2 (K)	695
11	700	719	887.7724	2660.2954	2660.2945	0.34	T	1	20	0.01	SVQNKLFEQPEFGHYTSIAK +dK_MMCCH-2 (K)	704
12	778	789	957.9997	1913.9848	1913.9862	-0.68	T	1	39	0.00012	IWAIWQALQKYR +Deamidated (NQ); dK_MMCCH-2 (K)	787
13	790	804	1003.4713	2004.9281	2004.9220	3.04	T	0	48	1.60E-05	GKPYNVANCAVTSMR +dK_MMCCH-2 (K)	791
14	858	863	520.2989	1038.5832	1038.5783	4.72	T	1	17	0.022	KLEAIK +dK_MMCCH-2 (K)	858
15	916	924	740.8735	1479.7324	1479.7319	0.27	T	1	16	0.025	VFKYDITEK +dK_MMCCH-2 (K)	918
16	953	965	635.3304	1902.9693	1902.9662	1.63	T	1	43	5.20E-05	DLFKQPSVIHEPR +dK_MMCCH-2 (K)	956
17	986	1000	1027.0363	2052.0579	2052.0561	0.93	T	1	66	2.50E-07	KNIENLSLGELESLR +dK_MMCCH-2 (K)	986
18	1092	1114	791.8748	3163.4699	3163.4682	0.54	T	1	41	8.30E-05	QHHYETNPFHHGKITHENEITTR +dK_MMCCH-2 (K)	1104
19	1118	1162	1414.4266	5653.6775	5653.6850	-1.34	T	1	23	0.0049	DSLFHSDYFYEQVLYALEQDNFCDFEIQLEILHNALHSLLGGKGK +dK_MMCCH-2 (K)	1162
20	1199	1203	353.1902	1056.5487	1056.5538	-4.83	T	1	17	0.02	KRPYR +dK_MMCCH-2 (K)	1199
21	1395	1403	727.8865	1453.7585	1453.7599	-0.96	T	2	30	0.00092	KDITQLDKR +dK_MMCCH-2 (K)	1395
22	1395	1403	598.3055	1791.8946	1791.8899	2.62	T	2	15	0.031	KDITQLDKR +2 dK_MMCCH-2 (K)	1395, 1402
23	1417	1445	1125.2129	3372.6168	3372.6020	4.42	T	1	16	0.024	ADHSSDGFQAIASFHALPPLCPSPAASKR +dK_MMCCH-2 (K)	1444

Figure 27A. KLH 1 (continued)

24	1473	1489	778.4003	2332.1790	2332.1827	-1.59	T	1	46	2.60E-05	KHGAVVGLPYWDWTLPR +dK_MMCCH-2 (K)	1473
25	1747	1758	613.9767	1838.9082	1838.9012	3.81	T	1	21	0.0084	LYKYDITETLDK +dK_MMCCH-2 (K)	1749
26	1923	1932	756.3794	1510.7442	1510.7425	1.19	T	1	28	0.0016	NKVMPNPFAR +dK_MMCCH-2 (K)	1924
27	2100	2109	492.2465	1964.9570	1964.9601	-1.58	T	2	20	0.0094	EIKDKQHHVR +2 dK_MMCCH-2 (K)	2102, 2104
28	2121	2149	890.4189	3557.6464	3557.6378	2.42	T	1	40	9.10E-05	TSADVQFQICKTSEDCHHGGQIFVLGGTK +dK_MMCCH-2 (K)	2131
29	2299	2314	715.0167	2142.0283	2142.0238	2.15	T	1	32	0.00069	LYTKQMEDALTAHGAR +dK_MMCCH-2 (K)	2302
30	2359	2367	736.3491	1470.6836	1470.6813	1.56	T	1	35	0.00031	DKLFNDPER +dK_MMCCH-2 (K)	2360
31	2507	2514	682.3539	1362.6932	1362.6853	5.80	T	1	40	0.0001	KLEHELEK +dK_MMCCH-2 (K)	2507
32	2515	2520	571.7606	1141.5066	1141.5074	-0.70	T	1	21	0.0086	QKEEDR +dK_MMCCH-2 (K)	2516
33	2595	2609	983.5358	1965.0571	1965.0493	4.02	T	1	15	0.035	IIDTSGKQLPSDLIK +dK_MMCCH-2 (K)	2601
34	2621	2636	802.7097	2405.1073	2405.1083	-0.42	T	1	51	8.60E-06	HHEKHHEDHHEDILVR +dK_MMCCH-2 (K)	2624
35	2637	2651	1069.5260	2137.0374	2137.0374	0.00	T	1	74	4.00E-08	KNIHSLSHHEAEELR +dK_MMCCH-2 (K)	2637
36	2761	2814	1324.8440	6619.1836	6619.1192	9.73	T	1	16	0.023	DVNEAIFQQTKFGEFSSIFYLALQALEEDNYCDFEVQYEILHNEVHALIGGAEK +dK_MMCCH-2 (K)	2771
37	2851	2883	1009.2193	4032.8481	4032.8346	3.35	T	0	51	7.20E-06	VKPAHAGSCAGDIMHVPLHPFNYESVNNDDFTR +dK_MMCCH-2 (K)	2852
38	2897	2919	1066.5216	3196.5430	3196.5287	4.47	T	1	75	3.50E-08	FNYKYDNLNLHGHNIEELEEVLR +dK_MMCCH-2 (K)	2900
39	2938	2947	730.4158	1458.8170	1458.8156	0.96	T	1	17	0.02	TTAVVKVYIK +dK_MMCCH-2 (K)	2943
40	3003	3021	825.7742	2474.3007	2474.2879	5.17	T	1	39	0.00013	KYDHTELDASVLPAPIIVR +dK_MMCCH-2 (K)	3003
41	123	151	616.6595	3693.9132	3693.9049	2.25	G	2	21	0.0073	KGFTDPPVKHHQSANLLVRKNINDLTREE +dK_MMCCH-2 (K)	123
42	123	151	673.0134	4032.0366	4032.0350	0.40	G	2	16	0.023	KGFTDPPVKHHQSANLLVRKNINDLTREE +2 dK_MMCCH-2 (K)	123, 142
43	123	151	739.7915	3693.9211	3693.9049	4.39	G	2	22	0.0063	KGFTDPPVKHHQSANLLVRKNINDLTREE +dK_MMCCH-2 (K)	131
44	158	176	846.3875	2536.1407	2536.1329	3.08	G	3	19	0.011	AFHKFQEDRSVDGYQATAE +dK_MMCCH-2 (K)	161
45	435	442	676.3240	1350.6335	1350.6312	1.78	G	1	26	0.0026	NIEKMIHE +dK_MMCCH-2 (K)	438
46	526	544	777.7499	2330.2280	2330.2304	-1.03	G	1	27	0.0021	VDGTKLASSLIPHASVIRE +dK_MMCCH-2 (K)	530
47	589	612	990.1188	2967.3345	2967.3320	0.84	G	1	16	0.024	DKSAGGFQQLGAFHGEPKWCPSPE +dK_MMCCH-2 (K)	606
48	825	841	820.3725	2458.0957	2458.0940	0.69	G	1	38	0.00015	HSVPFNVFDYKTNFNYE +dK_MMCCH-2 (K)	835
49	847	860	965.0152	1928.0158	1928.0077	4.20	G	0	23	0.005	FNGLSISQLNKKLE +dK_MMCCH-2 (K)	858

Figure 27A. KLH 1 (continued)

50	1055	1076	810.1688	3236.6462	3236.6402	1.82	G	1	24	0.0041	NALLKKGSSVAVPYWDWTKRIE +2 dK_MMCCH-2 (K)	1059, 1060
51	1055	1076	725.6330	2898.5029	2898.5102	-2.52	G	1	37	0.00021	NALLKKGSSVAVPYWDWTKRIE +dK_MMCCH-2 (K)	1060
52	1097	1110	999.9601	1997.9057	1997.9054	0.15	G	1	23	0.0052	TNPFHHGKITHENE +dK_MMCCH-2 (K)	1104
53	1376	1396	864.3901	2590.1484	2590.1428	2.16	G	3	20	0.011	AGTDSAHTDDGHTEPVMIRKD +dK_MMCCH-2 (K)	1395
54	1397	1413	665.6099	2658.4103	2658.4125	-0.79	G	1	13	0.046	ITQLDKRQQLSLVKALE +2 dK_MMCCH-2 (K)	1402, 1410
55	1397	1413	774.4366	2320.2879	2320.2824	2.37	G	1	22	0.0064	ITQLDKRQQLSLVKALE +dK_MMCCH-2 (K)	1410
56	1495	1522	866.6912	3462.7358	3462.7381	-0.66	G	3	21	0.0086	LLTVSTIHDPETGRDIPNPFIGSKIEFE +dK_MMCCH-2 (K)	1518
57	1755	1765	570.6042	1708.7909	1708.7913	-0.18	G	2	27	0.002	TLDKMNLRHDE +dK_MMCCH-2 (K)	1758
58	2089	2100	854.4125	1706.8104	1706.8008	5.68	G	2	20	0.011	IGGMNLHEIEKE +dK_MMCCH-2 (K)	2099
59	2647	2661	715.6751	2144.0035	2144.0095	-2.80	G	4	35	0.00035	AEELRDALYKLQNDE +dK_MMCCH-2 (K)	2656
60	3090	3097	632.8023	1263.5901	1263.5879	1.66	G	0	15	0.029	LGKMYSVE +dK_MMCCH-2 (K)	3092
61	59	68	729.3450	1456.6755	1456.6731	1.65	C	1	17	0.022	VLGGPSEMKW +dK_MMCCH-2 (K); Oxidation (M)	67
62	94	100	573.2991	1144.5836	1144.5838	-0.17	C	1	20	0.011	TVKAELF +dK_MMCCH-2 (K)	96
63	160	171	606.9445	1817.8116	1817.8043	4.02	C	1	17	0.021	HKFQEDRSVDGY +dK_MMCCH-2 (K)	161
64	587	595	638.7999	1275.5852	1275.5805	3.68	C	0	31	0.00081	KEDKSAGGF +dK_MMCCH-2 (K)	590
65	715	723	655.8767	1309.7387	1309.7316	5.50	C	1	20	0.0094	TSIAKQVLL +dK_MMCCH-2 (K)	719
66	783	788	544.7763	1087.5381	1087.5372	0.83	C	1	22	0.0067	QALQKY +dK_MMCCH-2 (K)	787
67	918	928	856.9330	1711.8515	1711.8491	1.40	C	2	14	0.038	KYDITEKLHDL +dK_MMCCH-2 (K)	924
68	1330	1337	620.3548	1238.6950	1238.6944	0.48	C	1	24	0.004	KLDITKAL +dK_MMCCH-2 (K)	1335
69	1431	1446	696.3564	2086.0473	2086.0492	-0.91	C	1	13	0.045	HALPPLCPSPAASKRF +dK_MMCCH-2 (K)	1444
70	1580	1586	544.2603	1086.5061	1086.5056	0.46	C	0	13	0.046	VGGKEPY +dK_MMCCH-2 (K)	1583
71	1649	1664	752.3298	2253.9675	2253.9637	1.69	C	2	14	0.044	NLNDHTHDFSKPEDTF +dK_MMCCH-2 (K)	1659
72	1818	1827	753.3687	1504.7227	1504.7232	-0.27	C	1	22	0.0061	SERDIGSLKY +dK_MMCCH-2 (K)	1826
73	2476	2488	923.9230	1845.8315	1845.8244	3.90	C	1	22	0.0061	THSNAKPTDVFEY +dK_MMCCH-2 (K)	2481
74	2656	2666	793.3514	1584.6882	1584.6879	0.25	C	1	32	0.00057	KLQNDESHGGY +dK_MMCCH-2 (K)	2656
75	2738	2749	856.3745	1710.7343	1710.7348	-0.29	C	2	19	0.013	ADSGNNNPFFKY +dK_MMCCH-2 (K)	2748
76	2946	2960	965.4053	1928.7960	1928.7986	-1.35	C	1	23	0.0053	IKSGTDSDDEYAGSF +dK_MMCCH-2 (K)	2947

Figure 27A. KLH 1 (continued)

77	2961	2971	769.8909	1537.7673	1537.7673	0.00	C	1	19	0.013	VILGGAKEMPW +dK_MMCCH-2 (K)	2967
78	1	9	725.3376	1448.6606	1448.6567	2.69	Th	2	25	0.0032	MTPEELKTY +dK_MMCCH-2 (K)	7
79	38	56	861.6801	2582.0183	2582.0108	2.90	Th	2	15	0.03	VCIPDDNDRNDDHCEKAGD +dK_MMCCH-2 (K)	53
80	59	69	785.3757	1568.7368	1568.7367	0.06	Th	3	58	1.70E-06	VLGGPSEMKWQ +dK_MMCCH-2 (K)	67
81	78	84	569.2871	1136.5595	1136.5536	5.19	Th	1	50	9.20E-06	LSDTVHK +dK_MMCCH-2 (K)	84
82	118	124	571.2781	1140.5417	1140.5386	2.72	Th	0	23	0.0046	VHHPEKG +dK_MMCCH-2 (K)	123
83	431	439	707.8519	1413.6893	1413.6883	0.71	Th	3	24	0.004	ISLENIEKM +dK_MMCCH-2 (K)	438
84	521	531	764.3844	1526.7542	1526.7538	0.26	Th	3	44	3.60E-05	VDITEVDGTKL +dK_MMCCH-2 (K)	530
85	585	591	585.8102	1169.6058	1169.6002	4.79	Th	1	35	0.00031	LLKEDKS +dK_MMCCH-2 (K)	590
86	601	612	904.8973	1807.7801	1807.7698	5.70	Th	1	18	0.018	FHGEPKWCPSPE +dK_MMCCH-2 (K)	606
87	666	672	607.2836	1212.5526	1212.5485	3.38	Th	2	23	0.0045	LADHEKY +dK_MMCCH-2 (K)	671
88	673	685	930.4165	1858.8184	1858.8196	-0.65	Th	2	14	0.044	VDPEDGVEKHNPW +dK_MMCCH-2 (K)	681
89	831	837	612.7872	1223.5598	1223.5533	5.31	Th	2	26	0.0023	VFDYKTN +dK_MMCCH-2 (K)	835
90	1156	1164	630.8394	1259.6642	1259.6584	4.60	Th	2	15	0.028	LLGGKGKYS +dK_MMCCH-2 (K)	1162
91	1219	1232	766.6633	2296.9682	2296.9617	2.83	Th	1	17	0.02	FDKSDNNDEATKTH +2 dK_MMCCH-2 (K)	1221, 1230
92	1219	1232	653.9531	1958.8376	1958.8316	3.01	Th	1	26	0.0024	FDKSDNNDEATKTH +dK_MMCCH-2 (K)	1230
93	1580	1587	572.7737	1143.5329	1143.5271	5.16	Th	1	18	0.016	VGGKEPYG +dK_MMCCH-2 (K)	1583
94	1657	1668	921.9181	1841.8216	1841.8182	1.85	Th	2	34	0.00042	FSKPEDTFDYQK +dK_MMCCH-2 (K)	1659
95	1657	1668	921.9170	1841.8194	1841.8182	0.65	Th	2	45	3.20E-05	FSKPEDTFDYQK +dK_MMCCH-2 (K)	1668
96	1733	1741	664.3219	1326.6292	1326.6312	-1.43	Th	2	17	0.019	VLGGEKEMP +dK_MMCCH-1 (K); Oxidation (M)	1738
97	1894	1904	850.4162	1698.8178	1698.8116	3.65	Th	5	36	0.00024	VAVPYWDWTKP +dK_MMCCH-2 (K)	1903
98	2064	2068	499.7590	997.5035	997.5055	-2.01	Th	0	20	0.0095	FTKKH +dK_MMCCH-2 (K)	2067
99	2094	2100	618.3051	1234.5957	1234.5903	4.29	Th	1	29	0.0013	LHEIEKE +dK_MMCCH-2 (K)	2099
100	2129	2141	622.9244	1865.7515	1865.7495	1.07	Th	0	26	0.0026	ICKTSEDCHHGGQ +dK_MMCCH-2 (K)	2131
101	2238	2249	814.3990	1626.7835	1626.7811	1.54	Th	4	45	3.40E-05	LTTAEVDNLKDA +dK_MMCCH-2 (K)	2247
102	2512	2521	807.3978	1612.7810	1612.7766	2.67	Th	0	25	0.0035	LEKQKEEDRT +dK_MMCCH-2 (K)	2514
103	2595	2606	806.4025	1610.7904	1610.7862	2.61	Th	2	31	0.00079	IIDTSGKQLPSD +dK_MMCCH-2 (K)	2601

Figure 27A. KLH 1 (continued)

104	2607	2612	520.7792	1039.5439	1039.5446	-0.67	Th	2	26	0.0027	LIKMPT +dK_MMCCH-2 (K)	2609
105	2766	2771	551.7890	1101.5634	1101.5529	9.62	Th	1	29	0.0013	IFQQTK +dK_MMCCH-2 (K)	2771
106	2808	2816	638.3207	1274.6268	1274.6217	4.08	Th	3	27	0.0018	LIGGAEKYS +dK_MMCCH-2 (K)	2814
107	2946	2960	965.4059	1928.7972	1928.7986	-0.73	Th	3	37	0.0002	IKSGTDSDDEYAGSF +dK_MMCCH-2 (K)	2947
108	2990	2996	583.2842	1164.5538	1164.5485	4.55	Th	1	38	0.00017	LTDDHVK +dK_MMCCH-2 (K)	2996

Figure 27B. KLH 2

#	Start	End	Observed	Mr(expt)	Mr(calc)	ppm	Enzyme	MC	Score	E value	Peptide	Mod_site
1	26	41	1043.0210	2084.0274	2084.0347	-3.50	T	1	32	0.00066	KNVDSLSSDEVLALEK +dK_MMCCH-2 (K)	26
2	147	155	694.3692	1386.7238	1386.7217	1.51	T	1	15	0.031	ADITFLNKK +dK_MMCCH-2 (K)	155
3	164	175	596.3080	1785.9023	1785.8985	2.13	T	1	33	0.00048	LFEKVQPGHHTR +dK_MMCCH-2 (K)	167
4	249	271	987.4402	2959.2989	2959.3051	-2.10	T	1	39	0.00012	GKDPNSADCAHNLIHTPMEPFDR +dK_MMCCH-2 (K)	250
5	281	293	610.9460	1829.8163	1829.8043	6.56	T	0	55	3.40E-06	EHAKPADSFDYGR +dK_MMCCH-2 (K)	284
6	359	377	849.4008	2545.1806	2545.1810	-0.16	T	1	14	0.041	AGDFFLLGGPTEMKWGFYR +dK_MMCCH-2 (K); Oxidation (M)	372
7	429	446	752.0674	2253.1805	2253.1729	3.37	T	0	52	6.60E-06	GHFDKPPVPVAQANLAVR +dK_MMCCH-2 (K)	433
8	467	488	708.5944	2830.3483	2830.3385	3.50	T	1	65	2.90E-07	FQNDKSVDGYQATVEFHALPAR +dK_MMCCH-2 (K)	471
9	489	497	726.8430	1451.6715	1451.6649	4.48	T	1	26	0.0026	CPRPDAKDR +dK_MMCCH-2 (K)	495
10	936	950	1080.0154	2158.0162	2158.0095	3.10	T	1	43	5.40E-05	KHGFTGGLPYWDWTR +dK_MMCCH-2 (K)	936
11	1082	1096	996.4625	1990.9104	1990.9063	2.06	T	0	38	0.00014	GKPYNTANCAIASMR +dK_MMCCH-2 (K)	1083
12	1097	1115	827.0796	2478.2169	2478.2101	2.78	T	0	65	3.10E-07	KPLQPFGLDSVINPDDETR +dK_MMCCH-2 (K)	1097
13	1123	1149	1190.5587	3568.6543	3568.6497	1.32	T	1	70	1.10E-07	VFDYKNNFDYEYESLAFNGLSIAQLDR +dK_MMCCH-2 (K)	1127
14	1355	1385	1271.2697	3810.7871	3810.7876	-0.10	T	1	27	0.0018	GSAVAVPYWDWTEKADSLPSLINDATYFNSR +dK_MMCCH-2 (K)	1368
15	1409	1450	1097.7139	5483.5330	5483.5213	2.13	T	1	37	0.00018	DPQPELWDNKDFYENVMLALEQDNFCDFEIQLELIHNALHSR +dK_MMCCH-2 (K)	1418
16	1455	1480	838.6586	3350.6054	3350.6070	-0.48	T	1	54	3.80E-06	AKYSLSSLDYTAFDPVFFLHHANVDR +dK_MMCCH-2 (K)	1456
17	1493	1507	721.6621	2161.9645	2161.9594	2.36	T	1	48	1.60E-05	KKPYNEADCAVNEMR +dK_MMCCH-2 (K)	1494
18	1542	1564	1070.1956	3207.5649	3207.5448	6.27	T	1	22	0.0058	YQYDNLQFNHFSIQKLDQTIQAR +dK_MMCCH-2 (K)	1556
19	1690	1704	709.3851	2125.1334	2125.1241	4.33	T	2	16	0.026	KEVSSLTTLEKHFLR +dK_MMCCH-2 (K)	1700
20	1757	1768	612.9798	1835.9176	1835.9128	2.61	T	1	14	0.043	LYTVQFEDSLKR +dK_MMCCH-2 (K)	1767
21	1804	1825	945.4659	2833.3760	2833.3633	4.48	T	1	14	0.044	TFPNPFLKANIEFEGEGVTTER +dK_MMCCH-2 (K)	1811
22	1949	1963	560.2521	2236.9795	2236.9735	2.64	T	0	55	2.90E-06	TQEFSKPEDTFDYHR +dK_MMCCH-2 (K)	1954
23	2045	2052	660.3509	1318.6872	1318.6843	2.27	T	1	15	0.034	YDITKTLK +dK_MMCCH-2 (K)	2049
24	2228	2239	870.4226	1738.8307	1738.8236	4.08	T	1	14	0.038	GYIKSEDAYTVR +dK_MMCCH-2 (K)	2231
25	2453	2463	839.9299	1677.8452	1677.8436	0.95	T	1	13	0.048	NFKYDITQALK +dK_MMCCH-2 (K)	2455

Figure 27B. KLH 2 (continued)

26	2527	2541	1007.5138	2013.0130	2013.0088	2.09	T	1	66	2.80E-07	KDVTSLTASEIENLR +dK_MMCCH-2 (K)	2527
27	2728	2739	957.9997	1913.9848	1913.9862	-0.68	T	1	39	0.00012	IWAIWQALQKYR +Deamidated (NQ); dK_MMCCH-2 (K)	2737
28	2755	2764	764.3805	1526.7464	1526.7439	1.64	T	0	33	0.00054	QPLKPFSESR +Deamidated (NQ); dK_MMCCH-2 (K)	2758
29	2866	2873	659.3614	1316.7083	1316.7050	2.51	T	1	18	0.016	YDITKVLK +dK_MMCCH-2 (K)	2870
30	3148	3155	629.3343	1256.6541	1256.6587	-3.58	T	1	16	0.028	KKPYNAAK +dK_MMCCH-2 (K)	3149
31	167	178	590.9642	1769.8707	1769.8705	0.11	G	0	27	0.0018	KVQPGHHTRLME +dK_MMCCH-2 (K)	167
32	466	481	1098.4980	2194.9815	2194.9841	-1.18	G	2	24	0.0036	RFQNDKSVDGYQATVE +Deamidated (NQ); dK_MMCCH-2 (K)	471
33	1215	1235	721.6050	2882.3908	2882.3949	-1.42	G	3	36	0.00026	ITQQLHDLDLHVGDNFFLKYE +dK_MMCCH-2 (K)	1233
34	1292	1303	879.4659	1756.9172	1756.9182	-0.57	G	0	36	0.00028	SIRSAFLQIQKE +dK_MMCCH-2 (K)	1302
35	1308	1320	904.9471	1807.8796	1807.8749	2.60	G	0	29	0.0014	NIAKFHGKPGLCE +dK_MMCCH-2 (K)	1315
36	1403	1422	921.4155	2761.2248	2761.2330	-2.97	G	3	23	0.0054	NAVTSRDPQPELWDNKDFYE +dK_MMCCH-2 (K)	1418
37	1952	1967	792.6802	2375.0189	2375.0205	-0.67	G	3	30	0.00092	FSKPEDTFDYHRFGYE +dK_MMCCH-2 (K)	1954
38	1973	1990	811.7284	2432.1635	2432.1505	5.39	G	0	21	0.008	FVGMSVSSLHNYIKQQQE +dK_MMCCH-2 (K)	1986
39	2477	2484	644.8361	1287.6576	1287.6573	0.16	G	0	25	0.003	APFFIKVE +dK_MMCCH-2 (K)	2482
40	3007	3011	477.7571	953.4996	953.5004	-0.84	G	0	13	0.045	RALKE +dK_MMCCH-2 (K)	3010
41	3386	3405	658.3147	2629.2297	2629.2271	0.99	G	2	30	0.00091	LDHAYSLRDGHYYIAGPTKD +dK_MMCCH-2 (K)	3404
42	277	296	883.7569	2648.2489	2648.2329	6.00	C	4	32	0.00056	DLTREHAKPADSFDYGRLGY +dK_MMCCH-2 (K)	284
43	364	373	743.3618	1484.7091	1484.7044	3.17	C	2	13	0.047	LLGGPTEMKW +dK_MMCCH-2 (K); Oxidation (M)	372
44	432	443	793.9156	1585.8166	1585.8174	-0.50	C	0	18	0.018	DKPPVPVAQANL +dK_MMCCH-2 (K)	433
45	629	635	539.2512	1076.4878	1076.4848	2.69	C	0	13	0.048	VGGSEKY +dK_MMCCH-2 (K)	634
46	1075	1080	544.7763	1087.5381	1087.5372	0.83	C	1	22	0.0067	QALQKY +dK_MMCCH-2 (K)	1079
47	1212	1230	875.0863	2622.2371	2622.2424	-2.06	C	4	14	0.04	KYEITQQLHDLDLHVGDNF +dK_MMCCH-2 (K)	1212
48	1416	1421	570.2397	1138.4648	1138.4641	0.61	C	1	17	0.018	DNKDFY +dK_MMCCH-2 (K)	1418
49	1589	1606	784.3536	2350.0391	2350.0392	-0.04	C	0	20	0.01	ICVEQGGEQNCKTKAGSF +dK_MMCCH-2 (K)	1602
50	1696	1702	607.3007	1212.5869	1212.5849	1.65	C	1	21	0.0086	TTLEKHF +dK_MMCCH-2 (K)	1700
51	1708	1719	839.8414	1677.6683	1677.6651	1.91	C	0	22	0.007	KNMQADDSPDGY +dK_MMCCH-2 (K)	1708
52	1782	1796	1014.5062	2026.9978	2026.9921	2.76	C	1	25	0.0029	KPQSALPDLVTQETY +dK_MMCCH-2 (K)	1782

Figure 27B. KLH 2 (continued)

53	1801	1809	706.8369	1411.6591	1411.6595	-0.21	C	0	28	0.0017	SHKTFPNPF +dK_MMCCH-2 (K)	1803
54	1982	1995	705.3458	2113.0155	2113.0051	4.92	C	1	25	0.0031	HNYIKQQQEADRVF +dK_MMCCH-2 (K)	1986
55	1999	2003	458.2542	914.4939	914.4936	0.44	C	2	26	0.0027	LLKGF +dK_MMCCH-2 (K)	2001
56	2455	2462	645.3264	1288.6381	1288.6373	0.62	C	1	18	0.017	KYDITQAL +dK_MMCCH-2 (K)	2455
57	2463	2479	1128.0186	2254.0225	2254.0253	-1.20	C	1	20	0.011	KAQSIHPEDVFDTDAPF +dK_MMCCH-2 (K)	2463
58	2754	2760	598.3323	1194.6501	1194.6471	2.51	C	1	23	0.0045	KQPLKPF +dK_MMCCH-2 (K)	2758
59	2865	2872	673.3627	1344.7108	1344.7112	-0.30	C	1	18	0.014	RYDITKVL +dK_MMCCH-2 (K)	2870
60	3235	3242	617.3138	1232.6130	1232.6111	1.54	C	0	19	0.012	TSANVKIY +dK_MMCCH-2 (K)	3240
61	3399	3406	576.8050	1151.5954	1151.5896	5.04	C	0	17	0.022	IAGPTKDL +dK_MMCCH-2 (K)	3404
62	184	191	703.8036	1405.5926	1405.5894	2.28	Th	1	41	8.60E-05	LEQDEFCK +dK_MMCCH-2 (K)	191
63	247	260	631.6191	1891.8356	1891.8305	2.70	Th	2	15	0.033	LRGKDPNSADCAHN +dK_MMCCH-2 (K)	250
64	283	293	782.8574	1563.7002	1563.7028	-1.66	Th	3	32	0.00071	AKPADSFDYGR +dK_MMCCH-2 (K)	284
65	365	372	585.7805	1169.5464	1169.5461	0.26	Th	1	40	9.60E-05	LGGPTEMK +dK_MMCCH-2 (K)	372
66	467	472	538.7411	1075.4677	1075.4644	3.07	Th	0	13	0.049	FQNDKS +dK_MMCCH-2 (K)	471
67	629	636	582.7668	1163.5191	1163.5169	1.98	Th	1	21	0.0074	VGGSEKYS +dK_MMCCH-2 (K)	634
68	893	904	904.8973	1807.7801	1807.7698	5.70	Th	1	18	0.018	FHGEPKWCPSPE +dK_MMCCH-2 (K)	898
69	1300	1308	716.3438	1430.6731	1430.6751	-1.47	Th	2	14	0.044	IQKEGIYEN +dK_MMCCH-2 (K)	1302
70	1414	1419	564.7560	1127.4975	1127.4957	1.60	Th	1	21	0.0077	LWDNKD +dK_MMCCH-2 (K)	1418
71	1525	1539	738.3560	2212.0461	2212.0371	4.02	Th	3	40	9.70E-05	LKHNLPQDSFDYQNR +dK_MMCCH-2 (K)	1526
72	1589	1605	735.3304	2202.9695	2202.9708	-0.59	Th	2	15	0.03	ICVEQGGEQNCKTKAGS +dK_MMCCH-2 (K)	1600
73	1589	1605	735.3321	2202.9744	2202.9708	1.68	Th	2	38	0.00016	ICVEQGGEQNCKTKAGS +dK_MMCCH-2 (K)	1602
74	1800	1809	780.3717	1558.7288	1558.7279	0.64	Th	2	16	0.026	FSHKTFPNPF +dK_MMCCH-2 (K)	1803
75	1952	1963	627.2838	1878.8294	1878.8247	2.50	Th	2	52	6.20E-06	FSKPEDTFDYHR +dK_MMCCH-2 (K)	1954
76	1985	1994	776.8953	1551.7760	1551.7715	2.90	Th	2	24	0.0038	IKQQQEADRV +dK_MMCCH-2 (K)	1986
77	2193	2199	667.3006	1332.5866	1332.5849	1.28	Th	2	27	0.002	YWDWTKP +dK_MMCCH-2 (K)	2198
78	2200	2206	562.3071	1122.5997	1122.5995	0.18	Th	2	19	0.014	ISKLPDL +dK_MMCCH-2 (K)	2202
79	2225	2229	462.2212	922.4278	922.4259	2.06	Th	2	22	0.0067	FAKGY +dK_MMCCH-2 (K)	2227

Figure 27B. KLH 2 (continued)

80	2230	2237	632.7943	1263.5739	1263.5693	3.72	Th	2	18	0.016	IKSEDAYT +dK_MMCCH-2 (K)	2231
81	2359	2363	509.2319	1016.4492	1016.4460	3.25	Th	1	21	0.0082	FTKMH +dK_MMCCH-2 (K); Oxidation (M)	2361
82	2941	2950	720.8395	1439.6645	1439.6602	2.99	Th	3	46	2.80E-05	LDEANDLKNA +dK_MMCCH-2 (K)	2948
83	3009	3015	573.2736	1144.5326	1144.5335	-0.87	Th	0	17	0.02	LKEHGSH +dK_MMCCH-2 (K)	3010
84	3399	3405	520.2613	1038.5080	1038.5056	2.31	Th	1	27	0.0022	IAGPTKD +dK_MMCCH-2 (K)	3404

"Start" and "End" indicates the number of residue of KLH1 or KLH2. "Observed" column implies the observed m/z value in the survey scan while "Mr(expt)", "Mr(calc)", "ppm" indicate the experimental molecular weight(MW), calculated MW, and the difference between observed MW and theoretical MW respectively. In the "Enzyme" column, T, C, G and Th stand for trypsin, chymotrypsin, Glu-C and thermolysin respectively. MC stands for missed cleavage. Scores are the peptide ion score directly reported from Mascot database search engine. E value denotes the expectation value for each identified peptide. The peptide sequences as well as its modifications are listed in "Peptide" column. "Mod_site" indicates the lysine conjugation site for KLH1 or KLH2.

Figure 28. Identification details of MMCCH-conjugated peptides for sample 3 (2nd LC-MS/MS)

Figure 28A. KLH 1

#	Start	End	Observed	Mr(expt)	Mr(calc)	ppm	Enzyme	MC	Score	E value	Peptide	Mod_site
1	124	141	589.3078	2353.2020	2353.2001	0.81	T	1	27	0.0018	GFTDPPVKHHQSANLLVR +dK_MMCCH-2 (K)	131
2	142	149	656.3417	1310.6689	1310.6653	2.82	T	1	26	0.0026	KNINDLTR +dK_MMCCH-2 (K)	142
3	157	166	822.8806	1643.7467	1643.7402	3.95	T	1	18	0.015	EAFHKFQEDR +dK_MMCCH-2 (K)	161
4	252	281	735.7524	3673.7255	3673.7008	6.72	T	1	20	0.011	TYVDSHGASHTNPFHSSVIAFEENAPHTKR +dK_MMCCH-2 (K)	280
5	460	477	781.3948	2341.1625	2341.1624	0.04	T	1	29	0.0012	TSANVDIFIKTTDSVQHK +dK_MMCCH-2 (K)	469
6	470	488	748.0457	2241.1153	2241.1100	2.36	T	1	41	7.70E-05	TTDSVQHKAGTFAVLGGSK +dK_MMCCH-2 (K)	477
7	553	560	663.8673	1325.7201	1325.7166	2.64	T	2	21	0.0076	VKFDKVPR +dK_MMCCH-2 (K)	554
8	553	560	442.9153	1325.7240	1325.7166	5.58	T	2	15	0.033	VKFDKVPR +dK_MMCCH-2 (K)	557
9	566	570	485.2460	968.4774	968.4749	2.48	T	1	15	0.029	KNVDR +dK_MMCCH-2 (K)	566
10	581	587	547.8371	1093.6596	1093.6569	2.47	T	1	29	0.0014	KALALLK +dK_MMCCH-2 (K)	581
11	588	606	781.0346	2340.0820	2340.0845	-1.07	T	1	29	0.0014	EDKSAGGFQQLGAFHGEPK +dK_MMCCH-2 (K)	590
12	591	615	1004.4717	3010.3934	3010.3742	6.38	T	1	18	0.017	SAGGFQQLGAFHGEPKWCPSPEASK +dK_MMCCH-2 (K)	606
13	645	681	1544.3801	4630.1186	4630.1063	2.63	T	1	27	0.0021	HGYDGALPYWDWTSPLNHLPELADHEKYVDPEDGVEK +dK_MMCCH-2 (K)	671
14	682	699	620.2958	2477.1540	2477.1434	4.28	T	1	26	0.0027	HNPWFDGHIDTVDKTTTR +dK_MMCCH-2 (K)	695
15	700	719	887.7726	2660.2959	2660.2945	0.53	T	1	51	8.60E-06	SVQNKLFEQPEFGHYTSIAK +dK_MMCCH-2 (K)	704
16	790	804	669.3168	2004.9287	2004.9220	3.34	T	0	35	0.0003	GKPYNVANCAVTSMR +dK_MMCCH-2 (K)	791
17	805	835	777.1814	3880.8706	3880.8771	-1.67	T	1	14	0.044	EPLQPFGLSANINTDHVTKEHSVPFNVFDYK +dK_MMCCH-2 (K)	823
18	858	863	520.2996	1038.5846	1038.5783	5.97	T	1	13	0.046	KLEAIK +dK_MMCCH-2 (K)	858
19	879	884	500.2816	998.5487	998.5470	1.60	T	1	14	0.042	KSSLVK +dK_MMCCH-2 (K)	879
20	953	965	635.3298	1902.9677	1902.9662	0.79	T	1	42	6.50E-05	DLFKQPSVIHEPR +dK_MMCCH-2 (K)	956
21	986	1000	1027.0387	2052.0628	2052.0561	3.31	T	1	77	2.20E-08	KNIENLSLGELESLR +dK_MMCCH-2 (K)	986
22	1048	1060	609.3545	1825.0416	1825.0423	-0.38	T	1	36	0.00025	LYVVVVENALLKK +dK_MMCCH-2 (K)	1060
23	1092	1114	791.8781	3163.4831	3163.4682	4.71	T	1	34	0.00041	QHHYETNPFHHGKITHENEITTR +dK_MMCCH-2 (K)	1104
24	1199	1203	353.1910	1056.5512	1056.5538	-2.46	T	1	17	0.019	KRPYR +dK_MMCCH-2 (K)	1199

Figure 28A. KLH 1 (continued)

25	1331	1338	620.3541	1238.6937	1238.6944	-0.57	T	1	18	0.014	LDITKALK +dK_MMCCH-2 (K)	1335
26	1395	1403	598.3055	1791.8948	1791.8899	2.73	T	2	17	0.021	KDITQLDKR +2 dK_MMCCH-2 (K)	1395, 1402
27	1395	1403	485.5956	1453.7648	1453.7599	3.37	T	2	17	0.019	KDITQLDKR +dK_MMCCH-2 (K)	1402
28	1417	1445	1125.2156	3372.6249	3372.6020	6.82	T	1	30	0.00092	ADHSSDGFQAIASFHALPPLCPSPAASKR +dK_MMCCH-2 (K)	1444
29	1473	1489	778.4014	2332.1823	2332.1827	-0.17	T	1	42	6.00E-05	KHGAVVGLPYWDWTLPR +dK_MMCCH-2 (K)	1473
30	1721	1746	1087.4750	3259.4031	3259.3937	2.88	T	1	34	0.00042	TAGDCEDAGYFTVLGGEKEMPWAFDR +dK_MMCCH-2 (K)	1738
31	1890	1922	879.8322	4394.1247	4394.1048	4.53	T	1	14	0.043	HGSSVAVPYWDWTKPIHNIPHLFTDKEYYDVWR +dK_MMCCH-2 (K)	1915
32	1923	1932	756.3802	1510.7458	1510.7425	2.25	T	1	25	0.0032	NKVMPNPFAR +dK_MMCCH-2 (K)	1924
33	2067	2076	746.8856	1491.7567	1491.7544	1.54	T	1	25	0.0032	KHAVPNDVFK +dK_MMCCH-2 (K)	2067
34	2068	2083	753.7166	2258.1280	2258.1194	3.81	T	1	14	0.041	HAVPNDVFKYELLGYR +dK_MMCCH-2 (K)	2076
35	2100	2109	492.2479	1964.9626	1964.9601	1.27	T	2	22	0.0068	EIKDKQHHVR +2 dK_MMCCH-2 (K)	2102, 2104
36	2121	2149	890.4148	3557.6301	3557.6378	-2.19	T	1	34	0.00036	TSADVQFQICKTSEDCHHGGQIFVLGGTK +dK_MMCCH-2 (K)	2131
37	2359	2367	736.3485	1470.6825	1470.6813	0.82	T	1	32	0.00068	DKLFNDPER +dK_MMCCH-2 (K)	2360
38	2461	2490	642.8189	3850.8694	3850.8638	1.45	T	0	16	0.024	RPLRPFSDPINHNAFTHSNAKPTDVFEYSR +dK_MMCCH-2 (K)	2481
39	2507	2514	682.3526	1362.6906	1362.6853	3.89	T	1	33	0.00049	KLEHELEK +dK_MMCCH-2 (K)	2507
40	2508	2516	746.3801	1490.7457	1490.7439	1.21	T	1	21	0.0082	LEHELEKQK +dK_MMCCH-2 (K)	2516
41	2595	2609	983.5291	1965.0437	1965.0493	-2.85	T	1	18	0.018	IIDTSGKQLPSDLIK +dK_MMCCH-2 (K)	2601
42	2621	2636	802.7109	2405.1110	2405.1083	1.12	T	1	48	1.80E-05	HHEKHHEDHHEDILVR +dK_MMCCH-2 (K)	2624
43	2637	2651	713.3541	2137.0406	2137.0374	1.45	T	1	61	7.40E-07	KNIHSLSHHEAEELR +dK_MMCCH-2 (K)	2637
44	2657	2686	1246.2177	3735.6311	3735.6358	-1.26	T	1	16	0.028	LQNDESHGGYEHIAGFHGYPNLCPEKGDEK +dK_MMCCH-2 (K)	2686
45	2714	2748	1087.7693	4347.0481	4347.0524	-1.01	T	1	47	1.80E-05	KHGSHLGIPYWDWTQTISSLPTFFADSGNNNPFFK +dK_MMCCH-2 (K)	2714
46	2851	2883	1009.2180	4032.8430	4032.8346	2.08	T	0	74	4.20E-08	VKPAHAGSCAGDIMHVPLHPFNYESVNNDDFTR +dK_MMCCH-2 (K)	2852
47	2897	2919	1066.5209	3196.5408	3196.5287	3.79	T	1	50	1.00E-05	FNYKYDNLNLHGHNIEELEEVLR +dK_MMCCH-2 (K)	2900
48	2938	2947	730.4150	1458.8154	1458.8156	-0.14	T	1	22	0.0064	TTAVVKVYIK +dK_MMCCH-2 (K)	2943
49	3003	3021	825.7742	2474.3007	2474.2879	5.17	T	1	54	3.90E-06	KYDHTELDASVLPAPIIVR +dK_MMCCH-2 (K)	3003
50	3022	3044	966.5219	2896.5439	2896.5521	-2.83	T	1	16	0.027	RPNNAVFDIIEIPIGKDVNLPPK +dK_MMCCH-2 (K)	3037
51	123	151	616.6577	3693.9026	3693.9049	-0.62	G	2	16	0.027	KGFTDPPVKHHQSANLLVRKNINDLTREE +dK_MMCCH-2 (K)	123

Figure 28A. KLH 1 (continued)

52	123	151	739.7898	3693.9126	3693.9049	2.06	G	2	20	0.01	KGFTDPPVKHHQSANLLVRKNINDLTREE +dK_MMCCH-2 (K)	131
53	158	176	846.3861	2536.1365	2536.1329	1.42	G	3	23	0.0055	AFHKFQEDRSVDGYQATAE +dK_MMCCH-2 (K)	161
54	526	544	777.7485	2330.2238	2330.2304	-2.83	G	1	15	0.032	VDGTKLASSLIPHASVIRE +dK_MMCCH-2 (K)	530
55	589	612	990.1155	2967.3248	2967.3320	-2.43	G	1	15	0.03	DKSAGGFQQLGAFHGEPKWCPSPE +dK_MMCCH-2 (K)	606
56	825	841	820.3744	2458.1013	2458.0940	2.97	G	1	22	0.0059	HSVPFNVFDYKTNFNYE +dK_MMCCH-2 (K)	835
57	942	972	955.4959	3817.9545	3817.9614	-1.81	G	3	20	0.011	VFDLKPASLGKDLFKQPSVIHEPRIGHHEGE +dK_MMCCH-2 (K)	946
58	942	970	727.3887	3631.9073	3631.8973	2.73	G	2	19	0.014	VFDLKPASLGKDLFKQPSVIHEPRIGHHE +dK_MMCCH-2 (K)	956
59	1055	1076	967.1804	2898.5194	2898.5102	3.17	G	1	24	0.0039	NALLKKGSSVAVPYWDWTKRIE +dK_MMCCH-2 (K)	1060
60	1397	1413	774.4367	2320.2883	2320.2824	2.54	G	1	21	0.0074	ITQLDKRQQLSLVKALE +dK_MMCCH-2 (K)	1410
61	1506	1522	753.3771	2257.1094	2257.1089	0.22	G	2	20	0.009	TGRDIPNPFIGSKIEFE +dK_MMCCH-2 (K)	1518
62	1755	1765	570.6043	1708.7911	1708.7913	-0.12	G	2	37	0.00022	TLDKMNLRHDE +dK_MMCCH-2 (K)	1758
63	2647	2661	715.6772	2144.0097	2144.0095	0.09	G	4	29	0.0012	AEELRDALYKLQNDE +dK_MMCCH-2 (K)	2656
64	59	68	729.3455	1456.6764	1456.6731	2.27	C	1	25	0.003	VLGGPSEMKW +dK_MMCCH-2 (K); Oxidation (M)	67
65	94	100	573.2996	1144.5846	1144.5838	0.61	C	1	23	0.0048	TVKAELF +dK_MMCCH-2 (K)	96
66	160	171	606.9457	1817.8152	1817.8043	6.00	C	1	15	0.035	HKFQEDRSVDGY +dK_MMCCH-2 (K)	161
67	429	450	990.8041	2969.3906	2969.3899	0.24	C	1	41	7.40E-05	GGISLENIEKMIHENQQEDRIY +dK_MMCCH-2 (K); Oxidation (M)	438
68	584	595	787.4019	1572.7892	1572.7858	2.16	C	2	37	0.0002	ALLKEDKSAGGF +dK_MMCCH-2 (K)	590
69	715	723	655.8740	1309.7334	1309.7316	1.37	C	1	20	0.0092	TSIAKQVLL +dK_MMCCH-2 (K)	719
70	783	788	544.7759	1087.5373	1087.5372	0.09	C	1	30	0.0011	QALQKY +dK_MMCCH-2 (K)	787
71	830	838	743.3391	1484.6635	1484.6646	-0.74	C	2	27	0.002	NVFDYKTNF +dK_MMCCH-2 (K)	835
72	918	928	856.9315	1711.8484	1711.8491	-0.41	C	2	42	7.10E-05	KYDITEKLHDL +dK_MMCCH-2 (K)	924
73	944	955	821.4331	1640.8517	1640.8484	2.01	C	3	24	0.0036	DLKPASLGKDLF +dK_MMCCH-2 (K)	946
74	1013	1018	516.7581	1031.5017	1031.4998	1.84	C	0	14	0.038	ESIAKF +dK_MMCCH-2 (K)	1017
75	1330	1337	620.3556	1238.6966	1238.6944	1.78	C	1	21	0.0073	KLDITKAL +dK_MMCCH-2 (K)	1335
76	1649	1664	1127.9868	2253.9591	2253.9637	-2.04	C	2	24	0.0037	NLNDHTHDFSKPEDTF +dK_MMCCH-2 (K)	1659
77	1649	1669	979.4308	2935.2705	2935.2759	-1.84	C	4	15	0.029	NLNDHTHDFSKPEDTFDYQKF +dK_MMCCH-2 (K)	1668
78	1732	1742	792.8743	1583.7340	1583.7364	-1.52	C	1	14	0.039	TVLGGEKEMPW +dK_MMCCH-2 (K)	1738

Figure 28A. KLH 1 (continued)

79	1818	1827	753.3699	1504.7253	1504.7232	1.40	C	1	22	0.0067	SERDIGSLKY +dK_MMCCH-2 (K)	1826
80	1913	1921	778.8339	1555.6532	1555.6541	-0.58	C	2	13	0.048	TDKEYYDVW +dK_MMCCH-2 (K)	1915
81	2476	2488	923.9222	1845.8299	1845.8244	3.03	C	1	25	0.0032	THSNAKPTDVFEY +dK_MMCCH-2 (K)	2481
82	2656	2666	793.3528	1584.6910	1584.6879	2.02	C	1	23	0.0052	KLQNDESHGGY +dK_MMCCH-2 (K)	2656
83	2713	2723	787.9119	1573.8093	1573.8075	1.14	C	1	17	0.021	KKHGSHLGIPY +dK_MMCCH-2 (K)	2714
84	2809	2815	538.2600	1074.5055	1074.5056	-0.09	C	0	31	0.00079	IGGAEKY +dK_MMCCH-2 (K)	2814
85	2946	2960	965.4038	1928.7931	1928.7986	-2.85	C	1	27	0.0021	IKSGTDSDDEYAGSF +dK_MMCCH-2 (K)	2947
86	2961	2971	769.8921	1537.7696	1537.7673	1.50	C	1	13	0.048	VILGGAKEMPW +dK_MMCCH-2 (K)	2967
87	1	9	733.3350	1464.6554	1464.6516	2.53	Th	2	25	0.003	MTPEELKTY +dK_MMCCH-2 (K); Oxidation (M)	7
88	38	56	861.6832	2582.0279	2582.0108	6.58	Th	2	25	0.0029	VCIPDDNDRNDDHCEKAGD +dK_MMCCH-2 (K)	53
89	59	69	785.3786	1568.7426	1568.7367	3.76	Th	3	54	4.20E-06	VLGGPSEMKWQ +dK_MMCCH-2 (K)	67
90	78	84	569.2875	1136.5604	1136.5536	5.98	Th	1	45	3.20E-05	LSDTVHK +dK_MMCCH-2 (K)	84
91	118	124	571.2790	1140.5435	1140.5386	4.30	Th	0	24	0.0042	VHHPEKG +dK_MMCCH-2 (K)	123
92	125	135	815.8901	1629.7656	1629.7610	2.82	Th	1	17	0.02	FTDPPVKHHQS +dK_MMCCH-2 (K)	131
93	272	282	848.3909	1694.7673	1694.7722	-2.89	Th	1	22	0.0065	FEENAPHTKRQ +Deamidated (NQ); dK_MMCCH-2 (K)	280
94	431	439	707.8525	1413.6904	1413.6883	1.49	Th	3	40	0.00011	ISLENIEKM +dK_MMCCH-2 (K)	438
95	521	530	707.8452	1413.6759	1413.6698	4.32	Th	2	69	1.20E-07	VDITEVDGTK +dK_MMCCH-2 (K)	530
96	585	591	585.8106	1169.6065	1169.6002	5.47	Th	1	35	0.00032	LLKEDKS +dK_MMCCH-2 (K)	590
97	601	612	904.8967	1807.7789	1807.7698	5.03	Th	1	22	0.0064	FHGEPKWCPSPE +dK_MMCCH-2 (K)	606
98	666	672	607.2830	1212.5514	1212.5485	2.39	Th	2	23	0.0047	LADHEKY +dK_MMCCH-2 (K)	671
99	821	828	617.8124	1233.6102	1233.6064	3.08	Th	1	22	0.0063	VTKEHSVP +dK_MMCCH-2 (K)	823
100	832	837	563.2518	1124.4891	1124.4848	3.82	Th	1	29	0.0014	FDYKTN +dK_MMCCH-2 (K)	835
101	954	959	529.7658	1057.5169	1057.5154	1.42	Th	1	14	0.042	LFKQPS +Deamidated (NQ); dK_MMCCH-2 (K)	956
102	1111	1120	742.3787	1482.7429	1482.7388	2.77	Th	1	18	0.017	ITTRDPKDSL +dK_MMCCH-2 (K)	1117
103	1156	1164	630.8383	1259.6621	1259.6584	2.94	Th	2	19	0.013	LLGGKGKYS +dK_MMCCH-2 (K)	1162
104	1219	1232	653.9537	1958.8392	1958.8316	3.88	Th	1	25	0.0032	FDKSDNNDEATKTH +dK_MMCCH-2 (K)	1230
105	1579	1587	665.8126	1329.6106	1329.6064	3.16	Th	2	20	0.011	WVGGKEPYG +dK_MMCCH-2 (K)	1583

Figure 28A. KLH 1 (continued)

106	1657	1668	921.9197	1841.8249	1841.8182	3.64	Th	2	32	0.00058	FSKPEDTFDYQK +dK_MMCCH-2 (K)	1659
107	1657	1668	921.9213	1841.8280	1841.8182	5.32	Th	2	44	4.20E-05	FSKPEDTFDYQK +dK_MMCCH-2 (K)	1668
108	1733	1741	664.3256	1326.6367	1326.6312	4.15	Th	2	14	0.04	VLGGEKEMP +dK_MMCCH-1 (K); Oxidation (M)	1738
109	1894	1904	850.4187	1698.8228	1698.8116	6.59	Th	5	34	0.00044	VAVPYWDWTKP +dK_MMCCH-2 (K)	1903
110	2064	2068	499.7599	997.5052	997.5055	-0.40	Th	0	19	0.014	FTKKH +dK_MMCCH-2 (K)	2067
111	2094	2100	618.3057	1234.5968	1234.5903	5.18	Th	1	26	0.0023	LHEIEKE +dK_MMCCH-2 (K)	2099
112	2129	2141	622.9242	1865.7507	1865.7495	0.64	Th	0	26	0.0026	ICKTSEDCHHGGQ +dK_MMCCH-2 (K)	2131
113	2238	2249	814.4017	1626.7888	1626.7811	4.73	Th	4	38	0.00015	LTTAEVDNLKDA +dK_MMCCH-2 (K)	2247
114	2480	2487	622.7999	1243.5852	1243.5795	4.58	Th	2	17	0.019	AKPTDVFE +dK_MMCCH-2 (K)	2481
115	2512	2521	538.6006	1612.7799	1612.7766	2.05	Th	0	41	8.60E-05	LEKQKEEDRT +dK_MMCCH-2 (K)	2514
116	2595	2606	806.4045	1610.7945	1610.7862	5.15	Th	2	26	0.0026	IIDTSGKQLPSD +dK_MMCCH-2 (K)	2601
117	2607	2612	520.7819	1039.5493	1039.5446	4.52	Th	2	25	0.0035	LIKMPT +dK_MMCCH-2 (K)	2609
118	2766	2771	551.7871	1101.5597	1101.5529	6.17	Th	1	25	0.0029	IFQQTK +dK_MMCCH-2 (K)	2771
119	2809	2816	581.7781	1161.5416	1161.5376	3.44	Th	2	13	0.045	IGGAEKYS +dK_MMCCH-2 (K)	2814
120	2946	2960	965.4075	1928.8004	1928.7986	0.93	Th	3	68	1.40E-07	IKSGTDSDDEYAGSF +dK_MMCCH-2 (K)	2947
121	2990	2996	583.2851	1164.5556	1164.5485	6.10	Th	1	33	0.00047	LTDDHVK +dK_MMCCH-2 (K)	2996

Figure 28B. KLH 2

#	Start	End	Observed	Mr(expt)	Mr(calc)	ppm	Enzyme	MC	Score	E value	Peptide	Mod_site
1	26	41	1043.0237	2084.0328	2084.0347	-0.91	T	1	54	4.20E-06	KNVDSLSSDEVLALEK +dK_MMCCH-2 (K)	26
2	147	155	694.3700	1386.7254	1386.7217	2.67	T	1	22	0.007	ADITFLNKK +dK_MMCCH-2 (K)	155
3	164	175	596.3071	1785.8996	1785.8985	0.62	T	1	36	0.00024	LFEKVQPGHHTR +dK_MMCCH-2 (K)	167
4	249	271	987.4432	2959.3077	2959.3051	0.88	T	1	28	0.0018	GKDPNSADCAHNLIHTPMEPFDR +dK_MMCCH-2 (K)	250
5	281	293	610.9432	1829.8079	1829.8043	1.97	T	0	55	3.30E-06	EHAKPADSFDYGR +dK_MMCCH-2 (K)	284
6	359	377	849.3962	2545.1669	2545.1810	-5.58	T	1	14	0.041	AGDFFLLGGPTEMKWGFYR +dK_MMCCH-2 (K); Oxidation (M)	372
7	419	446	677.3699	3381.8130	3381.8132	-0.06	T	1	45	3.20E-05	QPTLVHRPAKGHFDKPPVPVAQANLAVR +Deamidated (NQ); dK_MMCCH-2 (K)	428
8	429	446	752.0659	2253.1759	2253.1729	1.38	T	0	50	1.10E-05	GHFDKPPVPVAQANLAVR +dK_MMCCH-2 (K)	433
9	467	488	944.4543	2830.3410	2830.3385	0.88	T	1	70	9.50E-08	FQNDKSVDGYQATVEFHALPAR +dK_MMCCH-2 (K)	471
10	908	924	620.2817	2477.0979	2477.1166	-7.59	T	1	18	0.017	KFACCVHGMAVFPHWHR +dK_MMCCH-2 (K)	908
11	936	950	1080.0133	2158.0121	2158.0095	1.20	T	1	40	0.0001	KHGFTGGLPYWDWTR +dK_MMCCH-2 (K)	936
12	1082	1096	996.4623	1990.9100	1990.9063	1.86	T	0	14	0.041	GKPYNTANCAIASMR +dK_MMCCH-2 (K)	1083
13	1097	1115	827.0796	2478.2169	2478.2101	2.78	T	0	81	8.40E-09	KPLQPFGLDSVINPDDETR +dK_MMCCH-2 (K)	1097
14	1123	1149	1190.5598	3568.6576	3568.6497	2.21	T	1	67	1.80E-07	VFDYKNNFDYEYESLAFNGLSIAQLDR +dK_MMCCH-2 (K)	1127
15	1295	1311	764.0689	2289.1849	2289.1715	5.85	T	1	17	0.022	SAFLQIQKEGIYENIAK +dK_MMCCH-2 (K)	1302
16	1355	1385	953.7057	3810.7937	3810.7876	1.60	T	1	61	8.90E-07	GSAVAVPYWDWTEKADSLPSLINDATYFNSR +dK_MMCCH-2 (K)	1368
17	1409	1450	1371.8844	5483.5085	5483.5213	-2.33	T	1	33	0.00047	DPQPELWDNKDFYENVMLALEQDNFCDFEIQLELIHNALHSR +dK_MMCCH-2 (K)	1418
18	1455	1480	1117.8724	3350.5955	3350.6070	-3.43	T	1	58	1.50E-06	AKYSLSSLDYTAFDPVFFLHHANVDR +dK_MMCCH-2 (K)	1456
19	1493	1507	721.6637	2161.9693	2161.9594	4.53	T	1	58	1.50E-06	KKPYNEADCAVNEMR +dK_MMCCH-2 (K)	1494
20	1508	1539	825.9995	4124.9609	4124.9360	6.04	T	1	25	0.0033	KPLQPFNNPELNSDSMTLKHNLPQDSFDYQNR +dK_MMCCH-2 (K)	1526
21	1542	1564	1070.1924	3207.5553	3207.5448	3.30	T	1	18	0.018	YQYDNLQFNHFSIQKLDQTIQAR +dK_MMCCH-2 (K)	1556
22	1625	1646	906.8055	2717.3946	2717.3887	2.17	T	1	22	0.0062	FDITSALHKLGVPLDGHGFDIK +dK_MMCCH-2 (K)	1633
23	1757	1768	612.9796	1835.9168	1835.9128	2.23	T	1	18	0.015	LYTVQFEDSLKR +dK_MMCCH-2 (K)	1767
24	1949	1963	560.2521	2236.9792	2236.9735	2.55	T	0	52	6.90E-06	TQEFSKPEDTFDYHR +dK_MMCCH-2 (K)	1954

Figure 28B. KLH 2 (continued)

25	2045	2052	660.3497	1318.6848	1318.6843	0.38	T	1	21	0.0073	YDITKTLK +dK_MMCCH-2 (K)	2049
26	2058	2069	909.4633	1816.9121	1816.9070	2.81	T	1	14	0.036	YDDTFTIKVHIK +dK_MMCCH-2 (K)	2065
27	2228	2239	870.4176	1738.8206	1738.8236	-1.73	T	1	14	0.036	GYIKSEDAYTVR +dK_MMCCH-2 (K)	2231
28	2527	2541	1007.5128	2013.0110	2013.0088	1.04	T	1	56	2.30E-06	KDVTSLTASEIENLR +dK_MMCCH-2 (K)	2527
29	2755	2764	764.3820	1526.7494	1526.7439	3.60	T	0	19	0.012	QPLKPFSESR +Deamidated (NQ); dK_MMCCH-2 (K)	2758
30	2866	2873	659.3597	1316.7048	1316.7050	-0.15	T	1	13	0.046	YDITKVLK +dK_MMCCH-2 (K)	2870
31	3148	3155	629.3353	1256.6561	1256.6587	-2.07	T	1	17	0.02	KKPYNAAK +dK_MMCCH-2 (K)	3149
32	466	481	1098.4951	2194.9757	2194.9841	-3.83	G	2	25	0.0035	RFQNDKSVDGYQATVE +Deamidated (NQ); dK_MMCCH-2 (K)	471
33	1215	1235	962.1380	2883.3922	2883.3789	4.58	G	3	15	0.033	ITQQLHDLDLHVGDNFFLKYE +Deamidated (NQ); dK_MMCCH-2 (K)	1233
34	2477	2484	644.8370	1287.6594	1287.6573	1.63	G	0	15	0.031	APFFIKVE +dK_MMCCH-2 (K)	2482
35	1292	1303	586.6456	1756.9151	1756.9182	-1.76	G	0	21	0.008	SIRSAFLQIQKE +dK_MMCCH-2 (K)	1302
36	1292	1303	879.4651	1756.9156	1756.9182	-1.42	G	0	39	0.00011	SIRSAFLQIQKE +dK_MMCCH-2 (K)	1302
37	1292	1303	879.4658	1756.9170	1756.9182	-0.68	G	0	39	0.00012	SIRSAFLQIQKE +dK_MMCCH-2 (K)	1302
38	1292	1303	879.4702	1756.9259	1756.9182	4.38	G	0	26	0.0026	SIRSAFLQIQKE +dK_MMCCH-2 (K)	1302
39	1308	1320	603.6327	1807.8762	1807.8749	0.72	G	0	16	0.023	NIAKFHGKPGLCE +dK_MMCCH-2 (K)	1315
40	1290	1303	667.3554	1999.0444	1999.0448	-0.20	G	1	17	0.02	IESIRSAFLQIQKE +dK_MMCCH-2 (K)	1302
41	1290	1303	1000.5361	1999.0576	1999.0448	6.40	G	1	45	3.00E-05	IESIRSAFLQIQKE +dK_MMCCH-2 (K)	1302
42	466	481	732.3397	2193.9973	2194.0001	-1.28	G	2	15	0.032	RFQNDKSVDGYQATVE +dK_MMCCH-2 (K)	471
43	466	481	1098.0066	2193.9986	2194.0001	-0.68	G	2	16	0.026	RFQNDKSVDGYQATVE +dK_MMCCH-2 (K)	471
44	466	481	732.3409	2194.0008	2194.0001	0.32	G	2	16	0.026	RFQNDKSVDGYQATVE +dK_MMCCH-2 (K)	471
45	1952	1967	594.7626	2375.0212	2375.0205	0.29	G	3	18	0.017	FSKPEDTFDYHRFGYE +dK_MMCCH-2 (K)	1954
46	1952	1967	792.6822	2375.0247	2375.0205	1.77	G	3	21	0.0089	FSKPEDTFDYHRFGYE +dK_MMCCH-2 (K)	1954
47	3386	3405	877.4151	2629.2235	2629.2271	-1.37	G	2	15	0.031	LDHAYSLRDGHYYIAGPTKD +dK_MMCCH-2 (K)	3404
48	3386	3405	658.3136	2629.2253	2629.2271	-0.68	G	2	13	0.045	LDHAYSLRDGHYYIAGPTKD +dK_MMCCH-2 (K)	3404
49	1403	1422	921.4198	2761.2376	2761.2330	1.67	G	3	14	0.038	NAVTSRDPQPELWDNKDFYE +dK_MMCCH-2 (K)	1418
50	1215	1235	961.8065	2882.3976	2882.3949	0.90	G	3	32	0.00065	ITQQLHDLDLHVGDNFFLKYE +dK_MMCCH-2 (K)	1233
51	1215	1235	721.6078	2882.4021	2882.3949	2.46	G	3	18	0.018	ITQQLHDLDLHVGDNFFLKYE +dK_MMCCH-2 (K)	1233

Figure 28B. KLH 2 (continued)

52	1973	1990	817.0586	2448.1541	2448.1454	3.59	G	0	16	0.028	FVGMSVSSLHNYIKQQQE +dK_MMCCH-2 (K); Oxidation (M)	1986
53	277	296	883.7546	2648.2419	2648.2329	3.40	C	4	38	0.00017	DLTREHAKPADSFDYGRLGY +dK_MMCCH-2 (K)	284
54	315	325	808.4200	1614.8254	1614.8188	4.09	C	1	13	0.049	LGERAAKERTF +dK_MMCCH-2 (K)	321
55	629	635	539.2531	1076.4917	1076.4848	6.32	C	0	19	0.014	VGGSEKY +dK_MMCCH-2 (K)	634
56	1075	1080	544.7759	1087.5373	1087.5372	0.09	C	1	30	0.0011	QALQKY +dK_MMCCH-2 (K)	1079
57	1125	1134	854.8457	1707.6768	1707.6763	0.35	C	3	20	0.011	DYKNNFDYEY +dK_MMCCH-2 (K)	1127
58	1165	1177	896.9915	1791.9685	1791.9593	5.13	C	3	15	0.031	LLHEIGQSALVKF +dK_MMCCH-2 (K)	1176
59	1526	1540	749.6849	2246.0330	2246.0215	5.12	C	2	38	0.00015	KHNLPQDSFDYQNRF +dK_MMCCH-2 (K)	1526
60	1696	1702	607.3009	1212.5872	1212.5849	1.90	C	1	17	0.022	TTLEKHF +dK_MMCCH-2 (K)	1700
61	1708	1719	839.8434	1677.6723	1677.6651	4.35	C	0	28	0.0015	KNMQADDSPDGY +dK_MMCCH-2 (K)	1708
62	1801	1809	706.8389	1411.6632	1411.6595	2.62	C	0	16	0.026	SHKTFPNPF +dK_MMCCH-2 (K)	1803
63	1985	1995	850.4283	1698.8421	1698.8399	1.30	C	0	39	0.00014	IKQQQEADRVF +dK_MMCCH-2 (K)	1986
64	2001	2011	726.8464	1451.6783	1451.6755	1.93	C	1	28	0.0014	KGFGQSASVSF +dK_MMCCH-2 (K)	2001
65	2463	2479	1128.0177	2254.0208	2254.0253	-1.95	C	1	23	0.0055	KAQSIHPEDVFDTDAPF +dK_MMCCH-2 (K)	2463
66	2754	2760	598.3302	1194.6458	1194.6471	-1.00	C	1	25	0.0033	KQPLKPF +dK_MMCCH-2 (K)	2754
67	2754	2760	598.3341	1194.6537	1194.6471	5.52	C	1	14	0.041	KQPLKPF +dK_MMCCH-2 (K)	2758
68	2865	2872	673.3649	1344.7152	1344.7112	2.97	C	1	19	0.012	RYDITKVL +dK_MMCCH-2 (K)	2870
69	3235	3242	617.3129	1232.6112	1232.6111	0.08	C	0	34	0.00039	TSANVKIY +dK_MMCCH-2 (K)	3240
70	3399	3406	576.8040	1151.5934	1151.5896	3.21	C	0	23	0.005	IAGPTKDL +dK_MMCCH-2 (K)	3404
71	184	191	703.8063	1405.5980	1405.5894	6.12	Th	1	29	0.0013	LEQDEFCK +dK_MMCCH-2 (K)	191
72	247	257	785.8562	1569.6978	1569.6916	4.01	Th	1	20	0.0099	LRGKDPNSADC +dK_MMCCH-2 (K)	250
73	283	293	782.8611	1563.7077	1563.7028	3.20	Th	3	34	0.00038	AKPADSFDYGR +dK_MMCCH-2 (K)	284
74	365	372	585.7803	1169.5461	1169.5461	0.00	Th	1	31	0.00085	LGGPTEMK +dK_MMCCH-2 (K)	372
75	431	437	569.2877	1136.5609	1136.5576	2.90	Th	1	15	0.034	FDKPPVP +dK_MMCCH-2 (K)	433
76	629	636	582.7676	1163.5206	1163.5169	3.18	Th	1	22	0.0064	VGGSEKYS +dK_MMCCH-2 (K)	634
77	893	904	904.8967	1807.7789	1807.7698	5.03	Th	1	22	0.0064	FHGEPKWCPSPE +dK_MMCCH-2 (K)	898
78	1124	1129	569.7510	1137.4875	1137.4801	6.51	Th	1	13	0.049	FDYKNN +dK_MMCCH-2 (K)	1127

Figure 28B. KLH 2 (continued)

79	1525	1539	738.3566	2212.0481	2212.0371	4.93	Th	3	49	1.30E-05	LKHNLPQDSFDYQNR +dK_MMCCH-2 (K)	1526
80	1589	1605	735.3315	2202.9728	2202.9708	0.91	Th	2	18	0.015	ICVEQGGEQNCKTKAGS +dK_MMCCH-2 (K)	1600
81	1589	1605	735.3331	2202.9776	2202.9708	3.09	Th	2	34	0.00042	ICVEQGGEQNCKTKAGS +dK_MMCCH-2 (K)	1602
82	1800	1809	780.3743	1558.7340	1558.7279	3.91	Th	2	24	0.004	FSHKTFPNPF +dK_MMCCH-2 (K)	1803
83	1952	1963	627.2844	1878.8314	1878.8247	3.57	Th	2	47	2.00E-05	FSKPEDTFDYHR +dK_MMCCH-2 (K)	1954
84	1985	1994	776.8963	1551.7780	1551.7715	4.19	Th	2	20	0.0095	IKQQQEADRV +dK_MMCCH-2 (K)	1986
85	2193	2199	667.3038	1332.5931	1332.5849	6.15	Th	2	30	0.0011	YWDWTKP +dK_MMCCH-2 (K)	2198
86	2200	2206	562.3095	1122.6045	1122.5995	4.45	Th	2	21	0.0077	ISKLPDL +dK_MMCCH-2 (K)	2202
87	2225	2229	462.2224	922.4301	922.4259	4.66	Th	2	24	0.0039	FAKGY +dK_MMCCH-2 (K)	2227
88	2941	2950	720.8415	1439.6684	1439.6602	5.70	Th	3	46	2.60E-05	LDEANDLKNA +dK_MMCCH-2 (K)	2948
89	3009	3015	573.2734	1144.5322	1144.5335	-1.14	Th	0	16	0.025	LKEHGSH +dK_MMCCH-2 (K)	3010
90	3020	3026	662.2908	1322.5671	1322.5642	2.19	Th	2	19	0.011	YWDWTKS +dK_MMCCH-2 (K)	3025
91	3399	3405	520.2607	1038.5069	1038.5056	1.25	Th	1	27	0.002	IAGPTKD +dK_MMCCH-2 (K)	3404

"Start" and "End" indicates the number of residue of KLH1 or KLH2. "Observed" column implies the observed m/z value in the survey scan while "Mr(expt)", "Mr(calc)", "ppm" indicate the experimental molecular weight(MW), calculated MW, and the difference between observed MW and theoretical MW respectively. In the "Enzyme" column, T, C, G and Th stand for trypsin, chymotrypsin, Glu-C and thermolysin respectively. MC stands for missed cleavage. Scores are the peptide ion score directly reported from Mascot database search engine. E value denotes the expectation value for each identified peptide. The peptide sequences as well as its modifications are listed in "Peptide" column. "Mod_site" indicates the lysine conjugation site for KLH1 or KLH2.

Figure 29. Identification details of MMCCH-conjugated peptides for sample 4 (2nd LC-MS/MS)

Figure 29A. KLH 1

#	Start	End	Observed	Mr(expt)	Mr(calc)	ppm	Enzyme	MC	Score	E value	Peptide	Mod_site
1	124	141	785.4094	2353.2064	2353.2001	2.68	T	1	15	0.034	GFTDPPVKHHQSANLLVR +dK_MMCCH-2 (K)	131
2	142	149	656.3414	1310.6682	1310.6653	2.21	T	1	29	0.0012	KNINDLTR +dK_MMCCH-2 (K)	142
3	157	166	548.9227	1643.7464	1643.7402	3.71	T	1	21	0.008	EAFHKFQEDR +dK_MMCCH-2 (K)	161
4	184	192	484.8979	1451.6719	1451.6649	4.82	T	1	14	0.039	CPRPDAKDR +dK_MMCCH-2 (K)	190
5	553	560	663.8693	1325.7240	1325.7166	5.58	T	2	22	0.0068	VKFDKVPR +dK_MMCCH-2 (K)	554
6	566	570	485.2459	968.4772	968.4749	2.37	T	1	19	0.014	KNVDR +dK_MMCCH-2 (K)	566
7	581	590	733.9196	1465.8246	1465.8214	2.18	T	2	30	0.0011	KALALLKEDK +dK_MMCCH-2 (K)	581
8	588	606	781.0378	2340.0917	2340.0845	3.08	T	1	15	0.031	EDKSAGGFQQLGAFHGEPK +dK_MMCCH-2 (K)	590
9	591	615	1004.4722	3010.3949	3010.3742	6.88	T	1	16	0.027	SAGGFQQLGAFHGEPKWCPSPEASK +dK_MMCCH-2 (K)	606
10	682	699	620.2965	2477.1567	2477.1434	5.37	T	1	15	0.03	HNPWFDGHIDTVDKTTTR +dK_MMCCH-2 (K)	695
11	700	719	887.7751	2660.3034	2660.2945	3.38	T	1	20	0.0097	SVQNKLFEQPEFGHYTSIAK +dK_MMCCH-2 (K)	704
12	778	789	958.0043	1913.9941	1913.9862	4.13	T	1	15	0.03	IWAIWQALQKYR +Deamidated (NQ); dK_MMCCH-2 (K)	787
13	790	804	1003.4770	2004.9394	2004.9220	8.73	T	0	81	7.20E-09	GKPYNVANCAVTSMR +dK_MMCCH-2 (K)	791
14	858	863	520.3001	1038.5857	1038.5783	7.03	T	1	15	0.028	KLEAIK +dK_MMCCH-2 (K)	858
15	859	867	699.3604	1396.7061	1396.7020	2.94	T	1	15	0.034	LEAIKSQDR +dK_MMCCH-2 (K)	863
16	879	884	500.2828	998.5511	998.5470	4.11	T	1	14	0.04	KSSLVK +dK_MMCCH-2 (K)	879
17	953	965	635.3318	1902.9735	1902.9662	3.84	T	1	48	1.50E-05	DLFKQPSVIHEPR +dK_MMCCH-2 (K)	956
18	986	1000	685.0270	2052.0591	2052.0561	1.46	T	1	23	0.0047	KNIENLSLGELESLR +dK_MMCCH-2 (K)	986
19	1048	1060	913.5313	1825.0481	1825.0423	3.18	T	1	35	0.0003	LYVVVVENALLKK +dK_MMCCH-2 (K)	1060
20	1092	1114	791.8763	3163.4760	3163.4682	2.47	T	1	42	6.40E-05	QHHYETNPFHHGKITHENEITTR +dK_MMCCH-2 (K)	1104
21	1199	1203	353.1925	1056.5556	1056.5538	1.61	T	1	17	0.018	KRPYR +dK_MMCCH-2 (K)	1199
22	1395	1403	485.5970	1453.7692	1453.7599	6.40	T	2	31	0.00082	KDITQLDKR +dK_MMCCH-2 (K)	1395
23	1473	1489	778.4048	2332.1925	2332.1827	4.20	T	1	38	0.00015	KHGAVVGLPYWDWTLPR +dK_MMCCH-2 (K)	1473
24	1519	1530	599.6281	1795.8623	1795.8563	3.34	T	1	20	0.0096	IEFEGENVHTKR +dK_MMCCH-2 (K)	1529

Figure 29A. KLH 1 (continued)

25	1747	1758	613.9781	1838.9124	1838.9012	6.14	T	1	18	0.014	LYKYDITETLDK +dK_MMCCH-2 (K)	1749
26	1923	1932	756.3818	1510.7491	1510.7425	4.43	T	1	22	0.0064	NKVMPNPFAR +dK_MMCCH-2 (K)	1924
27	2100	2109	492.2497	1964.9698	1964.9601	4.94	T	2	16	0.027	EIKDKQHHVR +2 dK_MMCCH-2 (K)	2102, 2104
28	2121	2149	890.4196	3557.6494	3557.6378	3.26	T	1	23	0.0049	TSADVQFQICKTSEDCHHGGQIFVLGGTK +dK_MMCCH-2 (K)	2131
29	2299	2314	715.0188	2142.0346	2142.0238	5.04	T	1	37	0.00019	LYTKQMEDALTAHGAR +dK_MMCCH-2 (K)	2302
30	2359	2367	736.3524	1470.6903	1470.6813	6.12	T	1	32	0.00064	DKLFNDPER +dK_MMCCH-2 (K)	2360
31	2461	2490	642.8185	3850.8672	3850.8638	0.88	T	0	18	0.015	RPLRPFSDPINHNAFTHSNAKPTDVFEYSR +dK_MMCCH-2 (K)	2481
32	2507	2514	682.3542	1362.6938	1362.6853	6.24	T	1	33	0.00051	KLEHELEK +dK_MMCCH-2 (K)	2507
33	2515	2520	571.7616	1141.5086	1141.5074	1.14	T	1	17	0.018	QKEEDR +dK_MMCCH-2 (K)	2516
34	2621	2636	802.7122	2405.1147	2405.1083	2.62	T	1	51	8.10E-06	HHEKHHEDHHEDILVR +dK_MMCCH-2 (K)	2624
35	2637	2651	713.3541	2137.0404	2137.0374	1.36	T	1	59	1.20E-06	KNIHSLSHHEAEELR +dK_MMCCH-2 (K)	2637
36	2851	2883	807.5740	4032.8335	4032.8346	-0.27	T	0	42	6.80E-05	VKPAHAGSCAGDIMHVPLHPFNYESVNNDDFTR +dK_MMCCH-2 (K)	2852
37	2897	2919	800.1400	3196.5307	3196.5287	0.63	T	1	45	3.50E-05	FNYKYDNLNLHGHNIEELEEVLR +dK_MMCCH-2 (K)	2900
38	3003	3021	825.7752	2474.3036	2474.2879	6.35	T	1	17	0.018	KYDHTELDASVLPAPIIVR +dK_MMCCH-2 (K)	3003
39	123	151	673.0145	4032.0434	4032.0350	2.08	G	2	18	0.017	KGFTDPPVKHHQSANLLVRKNINDLTREE +2 dK_MMCCH-2 (K)	123, 131
40	123	151	739.7914	3693.9208	3693.9049	4.30	G	2	32	0.00068	KGFTDPPVKHHQSANLLVRKNINDLTREE +dK_MMCCH-2 (K)	131
41	158	169	606.2845	1815.8318	1815.8250	3.74	G	2	27	0.0019	AFHKFQEDRSVD +dK_MMCCH-2 (K)	161
42	435	442	676.3252	1350.6358	1350.6312	3.48	G	1	21	0.008	NIEKMIHE +dK_MMCCH-2 (K)	438
43	526	544	777.7501	2330.2285	2330.2304	-0.82	G	1	15	0.029	VDGTKLASSLIPHASVIRE +dK_MMCCH-2 (K)	530
44	589	612	990.1202	2967.3389	2967.3320	2.33	G	1	31	0.0008	DKSAGGFQQLGAFHGEPKWCPSPE +dK_MMCCH-2 (K)	606
45	825	841	820.3759	2458.1057	2458.0940	4.76	G	1	25	0.0031	HSVPFNVFDYKTNFNYE +dK_MMCCH-2 (K)	835
46	847	860	965.0205	1928.0265	1928.0077	9.75	G	0	19	0.013	FNGLSISQLNKKLE +dK_MMCCH-2 (K)	858
47	942	970	908.9841	3631.9074	3631.8973	2.78	G	2	15	0.035	VFDLKPASLGKDLFKQPSVIHEPRIGHHE +dK_MMCCH-2 (K)	956
48	1097	1110	999.9612	1997.9078	1997.9054	1.20	G	1	23	0.0049	TNPFHHGKITHENE +dK_MMCCH-2 (K)	1104
49	1376	1396	648.5447	2590.1496	2590.1428	2.63	G	3	22	0.0066	AGTDSAHTDDGHTEPVMIRKD +dK_MMCCH-2 (K)	1395
50	1397	1413	774.4365	2320.2876	2320.2824	2.20	G	1	14	0.044	ITQLDKRQQLSLVKALE +dK_MMCCH-2 (K)	1402
51	1397	1413	774.4338	2320.2797	2320.2824	-1.16	G	1	29	0.0011	ITQLDKRQQLSLVKALE +dK_MMCCH-2 (K)	1410

Figure 29A. KLH 1 (continued)

52	1495	1522	1155.5880	3463.7422	3463.7221	5.80	G	3	20	0.0096	LLTVSTIHDPETGRDIPNPFIGSKIEFE +Deamidated (NQ); dK_MMCCH-2 (K)	1518
53	1755	1765	570.6062	1708.7968	1708.7913	3.22	G	2	37	0.0002	TLDKMNLRHDE +dK_MMCCH-2 (K)	1758
54	2089	2100	854.4081	1706.8016	1706.8008	0.53	G	2	41	8.90E-05	IGGMNLHEIEKE +dK_MMCCH-2 (K)	2099
55	2624	2646	637.9164	3184.5458	3184.5373	2.67	G	4	14	0.036	KHHEDHHEDILVRKNIHSLSHHE +dK_MMCCH-2 (K)	2624
56	2647	2661	715.6800	2144.0181	2144.0095	4.01	G	4	22	0.0066	AEELRDALYKLQNDE +dK_MMCCH-2 (K)	2656
57	3090	3097	632.8043	1263.5940	1263.5879	4.75	G	0	16	0.027	LGKMYSVE +dK_MMCCH-2 (K)	3092
58	59	68	729.3447	1456.6749	1456.6731	1.24	C	1	30	0.00091	VLGGPSEMKW +dK_MMCCH-2 (K); Oxidation (M)	67
59	160	177	828.0412	2481.1018	2481.0907	4.47	C	2	14	0.043	HKFQEDRSVDGYQATAEY +dK_MMCCH-2 (K)	161
60	587	595	638.8013	1275.5880	1275.5805	5.88	C	0	33	0.00052	KEDKSAGGF +dK_MMCCH-2 (K)	590
61	715	723	655.8733	1309.7320	1309.7316	0.38	C	1	23	0.0056	TSIAKQVLL +dK_MMCCH-2 (K)	719
62	783	788	544.7773	1087.5400	1087.5372	2.57	C	1	30	0.0011	QALQKY +dK_MMCCH-2 (K)	787
63	830	838	743.3416	1484.6687	1484.6646	2.76	C	2	13	0.047	NVFDYKTNF +dK_MMCCH-2 (K)	835
64	860	868	716.3497	1430.6848	1430.6864	-1.12	C	0	14	0.038	EAIKSQDRF +dK_MMCCH-2 (K)	863
65	944	955	821.4307	1640.8469	1640.8484	-0.91	C	3	20	0.011	DLKPASLGKDLF +dK_MMCCH-2 (K)	946
66	1330	1337	620.3547	1238.6949	1238.6944	0.40	C	1	22	0.007	KLDITKAL +dK_MMCCH-2 (K)	1335
67	1431	1446	696.3586	2086.0541	2086.0492	2.35	C	1	16	0.026	HALPPLCPSPAASKRF +dK_MMCCH-2 (K)	1444
68	1580	1586	544.2616	1086.5086	1086.5056	2.85	C	0	17	0.02	VGGKEPY +dK_MMCCH-2 (K)	1583
69	1818	1827	753.3703	1504.7260	1504.7232	1.93	C	1	22	0.0062	SERDIGSLKY +dK_MMCCH-2 (K)	1826
70	2076	2082	612.3033	1222.5920	1222.5944	-1.96	C	3	14	0.037	KYELLGY +dK_MMCCH-2 (K)	2076
71	2476	2488	923.9218	1845.8291	1845.8244	2.55	C	1	17	0.02	THSNAKPTDVFEY +dK_MMCCH-2 (K)	2481
72	2656	2666	793.3524	1584.6902	1584.6879	1.45	C	1	24	0.0045	KLQNDESHGGY +dK_MMCCH-2 (K)	2656
73	2964	2971	607.2731	1212.5317	1212.5307	0.82	C	0	13	0.047	GGAKEMPW +dK_MMCCH-2 (K)	2967
74	1	9	725.3336	1448.6526	1448.6567	-2.90	Th	2	28	0.0015	MTPEELKTY +dK_MMCCH-2 (K)	7
75	38	56	861.6798	2582.0174	2582.0108	2.56	Th	2	19	0.013	VCIPDDNDRNDDHCEKAGD +dK_MMCCH-2 (K)	53
76	59	69	785.3771	1568.7397	1568.7367	1.91	Th	3	54	3.80E-06	VLGGPSEMKWQ +dK_MMCCH-2 (K)	67
77	78	84	569.2875	1136.5604	1136.5536	5.98	Th	1	52	6.40E-06	LSDTVHK +dK_MMCCH-2 (K)	84
78	118	124	571.2795	1140.5444	1140.5386	5.09	Th	0	24	0.0042	VHHPEKG +dK_MMCCH-2 (K)	123

Figure 29A. KLH 1 (continued)

79	431	439	707.8488	1413.6831	1413.6883	-3.75	Th	3	19	0.012	ISLENIEKM +dK_MMCCH-2 (K)	438
80	521	530	707.8455	1413.6765	1413.6698	4.74	Th	2	57	2.00E-06	VDITEVDGTK +dK_MMCCH-2 (K)	530
81	585	591	585.8103	1169.6060	1169.6002	5.04	Th	1	25	0.0029	LLKEDKS +dK_MMCCH-2 (K)	590
82	601	612	904.8980	1807.7813	1807.7698	6.36	Th	1	21	0.0084	FHGEPKWCPSPE +dK_MMCCH-2 (K)	606
83	666	672	607.2825	1212.5505	1212.5485	1.65	Th	2	25	0.0034	LADHEKY +dK_MMCCH-2 (K)	671
84	831	837	612.7867	1223.5589	1223.5533	4.66	Th	2	28	0.0017	VFDYKTN +dK_MMCCH-2 (K)	835
85	1219	1232	766.6623	2296.9650	2296.9617	1.48	Th	1	15	0.034	FDKSDNNDEATKTH +2 dK_MMCCH-2 (K)	1221, 1230
86	1580	1587	572.7716	1143.5287	1143.5271	1.40	Th	1	17	0.019	VGGKEPYG +dK_MMCCH-2 (K)	1583
87	1657	1668	921.9177	1841.8208	1841.8182	1.41	Th	2	35	0.00035	FSKPEDTFDYQK +dK_MMCCH-2 (K)	1659
88	1657	1668	921.9194	1841.8242	1841.8182	3.26	Th	2	30	0.00099	FSKPEDTFDYQK +dK_MMCCH-2 (K)	1668
89	1733	1741	664.3220	1326.6294	1326.6312	-1.36	Th	2	18	0.015	VLGGEKEMP +dK_MMCCH-1 (K); Oxidation (M)	1738
90	1894	1904	850.4149	1698.8152	1698.8116	2.12	Th	5	39	0.00012	VAVPYWDWTKP +dK_MMCCH-2 (K)	1903
91	2064	2068	499.7595	997.5045	997.5055	-1.00	Th	0	20	0.011	FTKKH +dK_MMCCH-2 (K)	2067
92	2094	2100	618.3040	1234.5934	1234.5903	2.43	Th	1	20	0.0093	LHEIEKE +dK_MMCCH-2 (K)	2099
93	2129	2141	622.9255	1865.7546	1865.7495	2.73	Th	0	19	0.014	ICKTSEDCHHGGQ +dK_MMCCH-2 (K)	2131
94	2238	2248	778.8811	1555.7476	1555.7440	2.38	Th	3	23	0.0051	LTTAEVDNLKD +dK_MMCCH-2 (K)	2247
95	2480	2490	825.8984	1649.7822	1649.7759	3.82	Th	3	26	0.0024	AKPTDVFEYSR +dK_MMCCH-2 (K)	2481
96	2512	2521	538.6002	1612.7787	1612.7766	1.24	Th	0	39	0.00013	LEKQKEEDRT +dK_MMCCH-2 (K)	2514
97	2512	2521	807.3967	1612.7788	1612.7766	1.30	Th	0	20	0.0096	LEKQKEEDRT +dK_MMCCH-2 (K)	2516
98	2595	2606	806.4067	1610.7988	1610.7862	7.82	Th	2	38	0.00017	IIDTSGKQLPSD +dK_MMCCH-2 (K)	2601
99	2607	2612	520.7801	1039.5456	1039.5446	0.96	Th	2	23	0.0052	LIKMPT +dK_MMCCH-2 (K)	2609
100	2766	2771	551.7874	1101.5603	1101.5529	6.72	Th	1	36	0.00025	IFQQTK +dK_MMCCH-2 (K)	2771
101	2808	2816	638.3197	1274.6248	1274.6217	2.51	Th	3	28	0.0017	LIGGAEKYS +dK_MMCCH-2 (K)	2814
102	2946	2960	965.4082	1928.8018	1928.7986	1.66	Th	3	34	0.00039	IKSGTDSDDEYAGSF +dK_MMCCH-2 (K)	2947
103	2990	2996	583.2842	1164.5539	1164.5485	4.64	Th	1	38	0.00014	LTDDHVK +dK_MMCCH-2 (K)	2996

Figure 29B. KLH 2

#	Start	End	Observed	Mr(expt)	Mr(calc)	ppm	Enzyme	MC	Score	E value	Peptide	Mod_site
1	26	41	1043.0233	2084.0321	2084.0347	-1.25	T	1	56	2.30E-06	KNVDSLSSDEVLALEK +dK_MMCCH-2 (K)	26
2	147	155	694.3710	1386.7274	1386.7217	4.11	T	1	32	0.00062	ADITFLNKK +dK_MMCCH-2 (K)	155
3	164	175	596.3118	1785.9135	1785.8985	8.40	T	1	41	8.70E-05	LFEKVQPGHHTR +dK_MMCCH-2 (K)	167
4	249	271	987.4451	2959.3136	2959.3051	2.84	T	1	25	0.003	GKDPNSADCAHNLIHTPMEPFDR +dK_MMCCH-2 (K)	250
5	281	293	610.9456	1829.8150	1829.8043	5.90	T	0	54	3.60E-06	EHAKPADSFDYGR +dK_MMCCH-2 (K)	284
6	419	446	846.4617	3381.8176	3381.8132	1.30	T	1	26	0.0025	QPTLVHRPAKGHFDKPPVPVAQANLAVR +Deamidated (NQ); dK_MMCCH-2 (K)	428
7	429	446	752.0691	2253.1854	2253.1729	5.59	T	0	50	9.70E-06	GHFDKPPVPVAQANLAVR +dK_MMCCH-2 (K)	433
8	467	488	944.4572	2830.3498	2830.3385	3.99	T	1	65	2.90E-07	FQNDKSVDGYQATVEFHALPAR +dK_MMCCH-2 (K)	471
9	489	497	484.8979	1451.6719	1451.6649	4.82	T	1	14	0.039	CPRPDAKDR +dK_MMCCH-2 (K)	495
10	936	950	720.3440	2158.0101	2158.0095	0.32	T	1	32	0.0007	KHGFTGGLPYWDWTR +dK_MMCCH-2 (K)	936
11	1082	1096	996.4645	1990.9144	1990.9063	4.07	T	0	77	1.80E-08	GKPYNTANCAIASMR +dK_MMCCH-2 (K)	1083
12	1097	1115	827.0785	2478.2138	2478.2101	1.49	T	0	66	2.50E-07	KPLQPFGLDSVINPDDETR +dK_MMCCH-2 (K)	1097
13	1123	1149	1190.5604	3568.6594	3568.6497	2.75	T	1	68	1.70E-07	VFDYKNNFDYEYESLAFNGLSIAQLDR +dK_MMCCH-2 (K)	1127
14	1295	1311	764.0680	2289.1821	2289.1715	4.67	T	1	13	0.05	SAFLQIQKEGIYENIAK +dK_MMCCH-2 (K)	1302
15	1355	1385	1271.2700	3810.7882	3810.7876	0.18	T	1	27	0.0022	GSAVAVPYWDWTEKADSLPSLINDATYFNSR +dK_MMCCH-2 (K)	1368
16	1409	1450	1371.8911	5483.5353	5483.5213	2.55	T	1	17	0.022	DPQPELWDNKDFYENVMLALEQDNFCDFEIQLELIHNALHSR +dK_MMCCH-2 (K)	1418
17	1455	1480	1117.8834	3350.6284	3350.6070	6.39	T	1	40	0.00011	AKYSLSSLDYTAFDPVFFLHHANVDR +dK_MMCCH-2 (K)	1456
18	1493	1507	721.6597	2161.9574	2161.9594	-0.97	T	1	55	3.20E-06	KKPYNEADCAVNEMR +dK_MMCCH-2 (K)	1494
19	1542	1564	802.8948	3207.5503	3207.5448	1.71	T	1	30	0.00094	YQYDNLQFNHFSIQKLDQTIQAR +dK_MMCCH-2 (K)	1556
20	1622	1633	591.9822	1772.9247	1772.9171	4.29	T	1	23	0.0047	LYKFDITSALHK +dK_MMCCH-2 (K)	1624
21	1690	1704	532.2889	2125.1267	2125.1241	1.18	T	2	21	0.0085	KEVSSLTTLEKHFLR +dK_MMCCH-2 (K)	1700
22	1949	1963	560.2532	2236.9836	2236.9735	4.47	T	0	46	2.30E-05	TQEFSKPEDTFDYHR +dK_MMCCH-2 (K)	1954
23	2400	2404	479.2446	956.4746	956.4749	-0.42	T	1	14	0.043	KSQTR +dK_MMCCH-2 (K)	2400
24	2527	2541	1007.5180	2013.0215	2013.0088	6.26	T	1	69	1.40E-07	KDVTSLTASEIENLR +dK_MMCCH-2 (K)	2527

Figure 29B. KLH 2 (continued)

25	2728	2739	958.0043	1913.9941	1913.9862	4.13	T	1	15	0.03	IWAIWQALQKYR +Deamidated (NQ); dK_MMCCH-2 (K)	2737
26	2755	2764	764.3857	1526.7569	1526.7439	8.51	T	0	34	0.00043	QPLKPFSESR +Deamidated (NQ); dK_MMCCH-2 (K)	2758
27	41	49	692.3309	1382.6472	1382.6388	6.08	G	2	20	0.01	KALDDLQQD +dK_MMCCH-2 (K)	41
28	167	178	590.9647	1769.8723	1769.8705	1.02	G	0	24	0.0036	KVQPGHHTRLME +dK_MMCCH-2 (K)	167
29	318	322	456.7346	911.4547	911.4535	1.43	G	0	18	0.018	RAAKE +dK_MMCCH-2 (K)	321
30	433	456	975.8574	2924.5504	2924.5429	2.56	G	2	21	0.0074	KPPVPVAQANLAVRKNINDLTAEE +dK_MMCCH-2 (K)	433
31	466	481	1098.5017	2194.9889	2194.9841	2.19	G	2	36	0.00023	RFQNDKSVDGYQATVE +Deamidated (NQ); dK_MMCCH-2 (K)	471
32	1117	1135	1404.1268	2806.2391	2806.2373	0.64	G	3	17	0.021	HSVPFRVFDYKNNFDYEYE +dK_MMCCH-2 (K)	1127
33	1215	1235	961.8077	2882.4014	2882.3949	2.26	G	3	40	9.80E-05	ITQQLHDLDLHVGDNFFLKYE +dK_MMCCH-2 (K)	1233
34	1292	1303	879.4660	1756.9174	1756.9182	-0.40	G	0	44	4.30E-05	SIRSAFLQIQKE +dK_MMCCH-2 (K)	1302
35	1308	1320	904.9468	1807.8791	1807.8749	2.32	G	0	22	0.0066	NIAKFHGKPGLCE +dK_MMCCH-2 (K)	1311
36	1308	1320	904.9480	1807.8814	1807.8749	3.60	G	0	34	0.00036	NIAKFHGKPGLCE +dK_MMCCH-2 (K)	1315
37	1354	1378	1043.5093	3127.5060	3127.4961	3.17	G	3	16	0.022	RGSAVAVPYWDWTEKADSLPSLIND +dK_MMCCH-2 (K)	1368
38	1403	1422	921.4252	2761.2537	2761.2330	7.50	G	3	17	0.018	NAVTSRDPQPELWDNKDFYE +dK_MMCCH-2 (K)	1418
39	1952	1967	792.6834	2375.0284	2375.0205	3.33	G	3	34	0.00036	FSKPEDTFDYHRFGYE +dK_MMCCH-2 (K)	1954
40	1973	1990	811.7261	2432.1566	2432.1505	2.51	G	0	24	0.0037	FVGMSVSSLHNYIKQQQE +dK_MMCCH-2 (K)	1986
41	2475	2484	752.8744	1503.7342	1503.7320	1.53	G	1	19	0.013	TDAPFFIKVE +dK_MMCCH-2 (K)	2482
42	3386	3405	658.3157	2629.2338	2629.2271	2.55	G	2	22	0.007	LDHAYSLRDGHYYIAGPTKD +dK_MMCCH-2 (K)	3404
43	277	296	883.7536	2648.2390	2648.2329	2.27	C	4	35	0.00034	DLTREHAKPADSFDYGRLGY +dK_MMCCH-2 (K)	284
44	629	635	539.2529	1076.4913	1076.4848	6.04	C	0	21	0.0076	VGGSEKY +dK_MMCCH-2 (K)	634
45	1007	1015	669.8713	1337.7280	1337.7265	1.12	C	1	27	0.0021	TDIAKQVLL +dK_MMCCH-2 (K)	1011
46	1075	1080	544.7773	1087.5400	1087.5372	2.57	C	1	30	0.0011	QALQKY +dK_MMCCH-2 (K)	1079
47	1298	1306	715.3745	1428.7343	1428.7323	1.47	C	1	14	0.045	LQIQKEGIY +dK_MMCCH-2 (K)	1302
48	1589	1606	784.3547	2350.0422	2350.0392	1.28	C	0	22	0.0068	ICVEQGGEQNCKTKAGSF +dK_MMCCH-2 (K)	1602
49	1696	1702	607.3019	1212.5892	1212.5849	3.55	C	1	23	0.0054	TTLEKHF +dK_MMCCH-2 (K)	1700
50	1782	1796	1014.5057	2026.9968	2026.9921	2.32	C	1	14	0.041	KPQSALPDLVTQETY +dK_MMCCH-2 (K)	1782
51	1801	1809	706.8389	1411.6632	1411.6595	2.62	C	0	15	0.033	SHKTFPNPF +dK_MMCCH-2 (K)	1803

Figure 29B. KLH 2 (continued)

52	1985	1995	850.4291	1698.8436	1698.8399	2.18	C	0	31	0.00089	IKQQQEADRVF +dK_MMCCH-2 (K)	1986
53	2001	2011	726.8444	1451.6743	1451.6755	-0.83	C	1	34	0.00042	KGFGQSASVSF +dK_MMCCH-2 (K)	2001
54	2455	2462	645.3267	1288.6388	1288.6373	1.16	C	1	21	0.0078	KYDITQAL +dK_MMCCH-2 (K)	2455
55	2463	2479	752.3476	2254.0210	2254.0253	-1.91	C	1	14	0.037	KAQSIHPEDVFDTDAPF +dK_MMCCH-2 (K)	2463
56	2754	2760	598.3323	1194.6501	1194.6471	2.51	C	1	14	0.04	KQPLKPF +dK_MMCCH-2 (K)	2758
57	2865	2872	673.3655	1344.7164	1344.7112	3.94	C	1	14	0.041	RYDITKVL +dK_MMCCH-2 (K)	2870
58	3235	3242	617.3137	1232.6129	1232.6111	1.46	C	0	29	0.0014	TSANVKIY +dK_MMCCH-2 (K)	3240
59	3399	3406	576.8031	1151.5916	1151.5896	1.74	C	0	19	0.014	IAGPTKDL +dK_MMCCH-2 (K)	3404
60	69	75	604.2934	1206.5722	1206.5703	1.66	Th	0	17	0.022	VDKHEKN +dK_MMCCH-2 (K)	74
61	165	175	558.6143	1672.8211	1672.8144	4.01	Th	1	13	0.048	FEKVQPGHHTR +dK_MMCCH-2 (K)	167
62	181	191	853.3782	1704.7419	1704.7375	2.58	Th	3	58	1.60E-06	LDALEQDEFCK +dK_MMCCH-2 (K)	191
63	247	257	785.8571	1569.6996	1569.6916	5.10	Th	1	13	0.046	LRGKDPNSADC +dK_MMCCH-2 (K)	250
64	278	293	734.3531	2200.0374	2200.0371	0.14	Th	4	26	0.0027	LTREHAKPADSFDYGR +dK_MMCCH-2 (K)	284
65	365	372	585.7806	1169.5466	1169.5461	0.43	Th	1	50	9.10E-06	LGGPTEMK +dK_MMCCH-2 (K)	372
66	431	437	569.2895	1136.5644	1136.5576	5.98	Th	1	16	0.025	FDKPPVP +dK_MMCCH-2 (K)	433
67	629	636	582.7663	1163.5180	1163.5169	1.03	Th	1	31	0.00077	VGGSEKYS +dK_MMCCH-2 (K)	634
68	893	904	904.8980	1807.7813	1807.7698	6.36	Th	1	21	0.0084	FHGEPKWCPSPE +dK_MMCCH-2 (K)	898
69	1123	1129	619.2853	1236.5560	1236.5485	6.07	Th	2	18	0.014	VFDYKNN +dK_MMCCH-2 (K)	1127
70	1414	1419	564.7562	1127.4979	1127.4957	1.95	Th	1	17	0.021	LWDNKD +dK_MMCCH-2 (K)	1418
71	1525	1539	738.3549	2212.0428	2212.0371	2.53	Th	3	36	0.00024	LKHNLPQDSFDYQNR +dK_MMCCH-2 (K)	1526
72	1589	1605	735.3313	2202.9721	2202.9708	0.59	Th	2	15	0.028	ICVEQGGEQNCKTKAGS +dK_MMCCH-2 (K)	1600
73	1589	1605	735.3325	2202.9757	2202.9708	2.27	Th	2	39	0.00013	ICVEQGGEQNCKTKAGS +dK_MMCCH-2 (K)	1602
74	1800	1809	780.3741	1558.7337	1558.7279	3.79	Th	2	18	0.016	FSHKTFPNPF +dK_MMCCH-2 (K)	1803
75	1952	1963	627.2840	1878.8302	1878.8247	2.93	Th	2	44	3.90E-05	FSKPEDTFDYHR +dK_MMCCH-2 (K)	1954
76	1985	1994	776.8959	1551.7772	1551.7715	3.67	Th	2	22	0.0064	IKQQQEADRV +dK_MMCCH-2 (K)	1986
77	2193	2199	667.3012	1332.5877	1332.5849	2.10	Th	2	25	0.0034	YWDWTKP +dK_MMCCH-2 (K)	2198
78	2200	2206	562.3086	1122.6026	1122.5995	2.85	Th	2	22	0.0062	ISKLPDL +dK_MMCCH-2 (K)	2202

Figure 29B. KLH 2 (continued)

79	2225	2229	462.2211	922.4277	922.4259	1.95	Th	2	23	0.0053	FAKGY +dK_MMCCH-2 (K)	2227
80	2230	2237	632.7936	1263.5726	1263.5693	2.61	Th	2	14	0.045	IKSEDAYT +dK_MMCCH-2 (K)	2231
81	2359	2363	509.2314	1016.4482	1016.4460	2.16	Th	1	26	0.0026	FTKMH +dK_MMCCH-2 (K); Oxidation (M)	2361
82	2941	2950	720.8408	1439.6670	1439.6602	4.72	Th	3	45	3.20E-05	LDEANDLKNA +dK_MMCCH-2 (K)	2948
83	3009	3015	573.2726	1144.5307	1144.5335	-2.45	Th	0	14	0.043	LKEHGSH +dK_MMCCH-2 (K)	3010
84	3399	3405	520.2607	1038.5069	1038.5056	1.25	Th	1	25	0.0029	IAGPTKD +dK_MMCCH-2 (K)	3404

"Start" and "End" indicates the number of residue of KLH1 or KLH2. "Observed" column implies the observed m/z value in the survey scan while "Mr(expt)", "Mr(calc)", "ppm" indicate the experimental molecular weight(MW), calculated MW, and the difference between observed MW and theoretical MW respectively. In the "Enzyme" column, T, C, G and Th stand for trypsin, chymotrypsin, Glu-C and thermolysin respectively. MC stands for missed cleavage. Scores are the peptide ion score directly reported from Mascot database search engine. E value denotes the expectation value for each identified peptide. The peptide sequences as well as its modifications are listed in "Peptide" column. "Mod_site" indicates the lysine conjugation site for KLH1 or KLH2.

Figure 30

Fig. 30(A) KLH 1 (1st LC-MS/MS)

#	K site	sample				#	K site	sample				#	K site	sample				#	K site	sample			
		1	2	3	4			1	2	3	4			1	2	3	4			1	2	3	4
1	K 7					51	K 879					101	K 2033					151	K 3044				
2	K 26					52	K 884					102	K 2066					152	K 3048				
3	K 53					53	K 918					103	K 2067					153	K 3052				
4	K 67					54	K 924					104	K 2076					154	K 3077				
5	K 84					55	K 929					105	K 2099					155	K 3079				
6	K 88					56	K 946					106	K 2102					156	K 3092				
7	K 96					57	K 952					107	K 2104						total	14	7	4	8
8	K 123					58	K 956	O	O		O	108	K 2131										
9	K 131					59	K 986	O				109	K 2149										
10	K 142	O				60	K 1017					110	K 2160										
11	K 161	O				61	K 1059					111	K 2187										
12	K 190					62	K 1060					112	K 2233										
13	K 251					63	K 1073					113	K 2247		O	O	O						
14	K 280					64	K 1104	O	O	O	O	114	K 2281										
15	K 289					65	K 1117					115	K 2302										
16	K 373					66	K 1160					116	K 2360	O			O						
17	K 389					67	K 1162					117	K 2460										
18	K 402			O	O	68	K 1199					118	K 2481										
19	K 411					69	K 1221					119	K 2506										
20	K 438					70	K 1230					120	K 2507										
21	K 469					71	K 1270					121	K 2514										
22	K 477					72	K 1303					122	K 2516										
23	K 488					73	K 1330					123	K 2531										
24	K 491					74	K 1335					124	K 2532										
25	K 499					75	K 1338					125	K 2579										
26	K 507				O	76	K 1339					126	K 2601										
27	K 530					77	K 1395					127	K 2609										
28	K 549					78	K 1402					128	K 2620										
29	K 554					79	K 1410					129	K 2624										
30	K 557					80	K 1416					130	K 2637										
31	K 566					81	K 1444					131	K 2656										
32	K 581					82	K 1473	O				132	K 2682										
33	K 587					83	K 1518					133	K 2686										
34	K 590	O	O			84	K 1529					134	K 2713										
35	K 606					85	K 1543					135	K 2714										
36	K 615					86	K 1583					136	K 2748										
37	K 616	O				87	K 1636					137	K 2771										
38	K 671					88	K 1640					138	K 2814										
39	K 681					89	K 1659					139	K 2838										
40	K 695					90	K 1668					140	K 2848										
41	K 704					91	K 1738					141	K 2852	O	O	O	O						
42	K 719	O	O			92	K 1749					142	K 2900	O									
43	K 787					93	K 1758					143	K 2924										
44	K 791					94	K 1809					144	K 2943										
45	K 823					95	K 1826					145	K 2947										
46	K 835					96	K 1853					146	K 2967										
47	K 857					97	K 1903					147	K 2996										
48	K 858					98	K 1915					148	K 3002										
49	K 863					99	K 1924	O	O		O	149	K 3003	O									
50	K 878					100	K 2022					150	K 3037										

Figure 30 (continued)

Fig. 30(B) KLH 2 (1st LC-MS/MS)

#	K site	sample				#	K site	sample				#	K site	sample			
		1	2	3	4			1	2	3	4			1	2	3	4
1	K 26	O	O			51	K 1127	O	O			101	K 2198				
2	K 41					52	K 1155					102	K 2202				
3	K 71					53	K 1176					103	K 2227				
4	K 74					54	K 1181					104	K 2231				
5	K 104					55	K 1212					105	K 2317				
6	K 105					56	K 1233					106	K 2327				
7	K 138					57	K 1280					107	K 2328				
8	K 154					58	K 1302	O				108	K 3330				
9	K 155					59	K 1311					109	K 2335				
10	K 167	O	O		O	60	K 1315					110	K 2345				
11	K 191					61	K 1368	O		O		111	K 2361				
12	K 250	O	O		O	62	K 1418					112	K 2400				
13	K 284	O	O		O	63	K 1456	O	O			113	K 2426				
14	K 321					64	K 1493					114	K 2444			O	
15	K 358					65	K 1494					115	K 2455				
16	K 372					66	K 1508	O				116	K 2463		O	O	O
17	K 401					67	K 1526	O	O	O	O	117	K 2482				
18	K 428					68	K 1556					118	K 2490				
19	K 433	O			O	69	K 1565					119	K 2527				
20	K 447					70	K 1600					120	K 2596				
21	K 462					71	K 1602	O				121	K 2737				
22	K 471	O	O		O	72	K 1624					122	K 2754				
23	K 495					73	K 1633					123	K 2758				
24	K 562					74	K 1646					124	K 2810				
25	K 585					75	K 1675					125	K 2811				
26	K 589					76	K 1690	O				126	K 2870				
27	K 634					77	K 1700					127	K 2873				
28	K 672					78	K 1705					128	K 2888				
29	K 675					79	K 1708					129	K 2903				
30	K 688					80	K 1767					130	K 2934				
31	K 701					81	K 1782					131	K 2948				
32	K 741					82	K 1803					132	K 2953				
33	K 774					83	K 1811					133	K 3010				
34	K 776					84	K 1835					134	K 3025				
35	K 787					85	K 1879					135	K 3045				
36	K 790					86	K 1921					136	K 3050				
37	K 798					87	K 1931					137	K 3145				
38	K 806					88	K 1935					138	K 3148				
39	K 848					89	K 1947					139	K 3149				
40	K 855					90	K 1954	O	O	O	O	140	K 3155				
41	K 858					91	K 1986	O	O		O	141	K 3184				
42	K 882					92	K 2001					142	K 3193				
43	K 898					93	K 2044					143	K 3240				
44	K 907					94	K 2049					144	K 3263				
45	K 908					95	K 2052					145	K 3274				
46	K 936					96	K 2055					146	K 3321				
47	K 1011					97	K 2065					147	K 3336				
48	K 1079					98	K 2069					148	K 3340				
49	K 1083					99	K 2092					149	K 3344				
50	K 1097	O	O	O	O	100	K 2121					150	K 3404				
													total	17	12	6	10

Figure 30 (continued)

Fig. 30(C) KLH 1 (2nd LC-MS/MS)

#	K site	sample				#	K site	sample				#	K site	sample				#	K site	sample			
		1	2	3	4			1	2	3	4			1	2	3	4			1	2	3	4
1	K 7					51	K 879					101	K 2033					151	K 3044				
2	K 26					52	K 884					102	K 2066					152	K 3048				
3	K 53					53	K 918					103	K 2067					153	K 3052				
4	K 67					54	K 924					104	K 2076					154	K 3077				
5	K 84					55	K 929					105	K 2099					155	K 3079				
6	K 88					56	K 946					106	K 2102					156	K 3092				
7	K 96					57	K 952					107	K 2104						total	13	7	6	9
8	K 123					58	K 956	O	O		O	108	K 2131										
9	K 131					59	K 986					109	K 2149										
10	K 142					60	K 1017					110	K 2160										
11	K 161	O		O		61	K 1059					111	K 2187										
12	K 190					62	K 1060					112	K 2233										
13	K 251					63	K 1073					113	K 2247	O	O	O	O						
14	K 280					64	K 1104	O	O	O	O	114	K 2281										
15	K 289					65	K 1117					115	K 2302										
16	K 373					66	K 1160					116	K 2360	O	O								
17	K 389					67	K 1162					117	K 2460										
18	K 402			O		68	K 1199					118	K 2481										
19	K 411					69	K 1221					119	K 2506										
20	K 438					70	K 1230					120	K 2507										
21	K 469					71	K 1270					121	K 2514										
22	K 477					72	K 1303					122	K 2516										
23	K 488					73	K 1330					123	K 2531										
24	K 491					74	K 1335					124	K 2532										
25	K 499					75	K 1338					125	K 2579										
26	K 507					76	K 1339					126	K 2601										
27	K 530					77	K 1395					127	K 2609										
28	K 549					78	K 1402					128	K 2620										
29	K 554					79	K 1410					129	K 2624										
30	K 557					80	K 1416					130	K 2637										
31	K 566					81	K 1444	O	O			131	K 2656										
32	K 581					82	K 1473	O				132	K 2682										
33	K 587					83	K 1518					133	K 2686										
34	K 590	O				84	K 1529					134	K 2713										
35	K 606				O	85	K 1543					135	K 2714										
36	K 615					86	K 1583				O	136	K 2748										
37	K 616					87	K 1636					137	K 2771										
38	K 671					88	K 1640					138	K 2814										
39	K 681					89	K 1659		O		O	139	K 2838										
40	K 695					90	K 1668					140	K 2848										
41	K 704					91	K 1738					141	K 2852	O	O	O	O						
42	K 719	O		O		92	K 1749					142	K 2900	O									
43	K 787				O	93	K 1758					143	K 2924										
44	K 791					94	K 1809					144	K 2943										
45	K 823					95	K 1826					145	K 2947										
46	K 835					96	K 1853					146	K 2967										
47	K 857					97	K 1903					147	K 2996										
48	K 858					98	K 1915					148	K 3002										
49	K 863					99	K 1924	O			O	149	K 3003	O									
50	K 878					100	K 2022					150	K 3037										

Figure 30 (continued)

Fig. 30(D) KLH 2 (2nd LC-MS/MS)

#	K site	sample				#	K site	sample				#	K site	sample			
		1	2	3	4			1	2	3	4			1	2	3	4
1	K 26	O	O			51	K 1127					101	K 2198				
2	K 41					52	K 1155					102	K 2202				
3	K 71					53	K 1176					103	K 2227				
4	K 74					54	K 1181					104	K 2231				
5	K 104					55	K 1212					105	K 2317				
6	K 105					56	K 1233			O	O	106	K 2327				
7	K 138					57	K 1280					107	K 2328				
8	K 154					58	K 1302	O	O			108	K 3330				
9	K 155					59	K 1311					109	K 2335				
10	K 167	O	O		O	60	K 1315					110	K 2345				
11	K 191					61	K 1368		O	O		111	K 2361				
12	K 250		O			62	K 1418					112	K 2400				
13	K 284	O	O		O	63	K 1456	O				113	K 2426				
14	K 321					64	K 1493					114	K 2444				
15	K 358					65	K 1494					115	K 2455				
16	K 372					66	K 1508					116	K 2463	O	O		O
17	K 401					67	K 1526	O	O	O		117	K 2482				
18	K 428					68	K 1556	O				118	K 2490				
19	K 433	O	O	O		69	K 1565					119	K 2527	O	O		
20	K 447					70	K 1600					120	K 2596				
21	K 462					71	K 1602					121	K 2737				O
22	K 471	O	O		O	72	K 1624					122	K 2754				
23	K 495					73	K 1633					123	K 2758				
24	K 562					74	K 1646					124	K 2810				
25	K 585					75	K 1675					125	K 2811				
26	K 589					76	K 1690					126	K 2870				
27	K 634					77	K 1700					127	K 2873				
28	K 672					78	K 1705					128	K 2888				
29	K 675					79	K 1708					129	K 2903				
30	K 688					80	K 1767					130	K 2934				
31	K 701					81	K 1782					131	K 2948				
32	K 741					82	K 1803					132	K 2953				
33	K 774					83	K 1811					133	K 3010				
34	K 776					84	K 1835					134	K 3025	O			
35	K 787					85	K 1879					135	K 3045				
36	K 790					86	K 1921					136	K 3050				
37	K 798					87	K 1931					137	K 3145				
38	K 806					88	K 1935					138	K 3148				
39	K 848					89	K 1947					139	K 3149				
40	K 855					90	K 1954	O	O		O	140	K 3155				
41	K 858					91	K 1986		O		O	141	K 3184				
42	K 882					92	K 2001					142	K 3193				
43	K 898				O	93	K 2044					143	K 3240				
44	K 907					94	K 2049					144	K 3263				
45	K 908					95	K 2052					145	K 3274				
46	K 936	O				96	K 2055					146	K 3321				
47	K 1011					97	K 2065					147	K 3336				
48	K 1079					98	K 2069					148	K 3340				
49	K 1083					99	K 2092					149	K 3344				
50	K 1097	O	O	O	O	100	K 2121					150	K 3404				
													total	15	14	5	10

Figure 31

Fig. 31(A) KLH 1 (1st LC-MS/MS)

#	K site	sample				#	K site	sample				#	K site	sample				#	K site	sample			
		1	2	3	4			1	2	3	4			1	2	3	4			1	2	3	4
1	K 7	O	O	O	O	51	K 879					101	K 2033					151	K 3044				
2	K 26					52	K 884					102	K 2066					152	K 3048				
3	K 53	O	O	O	O	53	K 918					103	K 2067	O	O	O	O	153	K 3052				
4	K 67	O	O	O	O	54	K 924					104	K 2076	O	O	O	O	154	K 3077				
5	K 84	O	O	O	O	55	K 929					105	K 2099	O	O	O	O	155	K 3079		O		
6	K 88					56	K 946	O	O	O		106	K 2102		O		O	156	K 3092	O	O	O	O
7	K 96	O		O	O	57	K 952					107	K 2104		O		O		**total**	**86**	**83**	**86**	**84**
8	K 123	O	O	O	O	58	K 956	O	O	O	O	108	K 2131	O	O	O	O						
9	K 131	O	O	O	O	59	K 986	O	O	O	O	109	K 2149										
10	K 142		O	O	O	60	K 1017	O	O	O		110	K 2160	O	O	O							
11	K 161	O	O	O	O	61	K 1059	O	O		O	111	K 2187										
12	K 190		O	O	O	62	K 1060	O	O	O	O	112	K 2233										
13	K 251					63	K 1073	O		O	O	113	K 2247	O	O	O	O						
14	K 280					64	K 1104	O	O	O	O	114	K 2281										
15	K 289					65	K 1117		O		O	115	K 2302	O									
16	K 373					66	K 1160					116	K 2360	O	O	O	O						
17	K 389	O		O		67	K 1162	O	O	O		117	K 2460										
18	K 402					68	K 1199	O	O	O	O	118	K 2481	O	O	O	O						
19	K 411					69	K 1221		O		O	119	K 2506										
20	K 438	O	O	O	O	70	K 1230	O	O	O	O	120	K 2507	O	O	O	O						
21	K 469	O		O	O	71	K 1270					121	K 2514	O	O	O	O						
22	K 477	O		O	O	72	K 1303					122	K 2516	O	O	O	O						
23	K 488					73	K 1330					123	K 2531										
24	K 491	O				74	K 1335	O	O	O	O	124	K 2532										
25	K 499					75	K 1338					125	K 2579										
26	K 507					76	K 1339					126	K 2601	O	O	O	O						
27	K 530	O	O	O	O	77	K 1395	O	O	O	O	127	K 2609	O	O	O	O						
28	K 549					78	K 1402	O	O	O	O	128	K 2620										
29	K 554	O	O	O	O	79	K 1410	O	O	O	O	129	K 2624	O	O	O	O						
30	K 557				O	80	K 1416					130	K 2637	O	O	O	O						
31	K 566	O	O	O	O	81	K 1444	O		O		131	K 2656	O	O	O	O						
32	K 581	O	O	O	O	82	K 1473	O	O	O	O	132	K 2682			O							
33	K 587					83	K 1518	O	O	O	O	133	K 2686			O	O						
34	K 590	O	O	O	O	84	K 1529	O				134	K 2713										
35	K 606	O	O	O	O	85	K 1543					135	K 2714			O	O						
36	K 615					86	K 1583	O	O	O	O	136	K 2748	O	O	O							
37	K 616					87	K 1636					137	K 2771	O	O	O	O						
38	K 671	O	O	O	O	88	K 1640					138	K 2814	O	O	O	O						
39	K 681	O				89	K 1659	O	O	O	O	139	K 2838										
40	K 695	O	O	O	O	90	K 1668	O	O	O	O	140	K 2848										
41	K 704	O	O	O	O	91	K 1738	O	O	O	O	141	K 2852	O	O	O	O						
42	K 719	O	O	O	O	92	K 1749	O	O		O	142	K 2900	O	O	O	O						
43	K 787	O	O	O	O	93	K 1758	O	O	O	O	143	K 2924										
44	K 791	O	O	O	O	94	K 1809					144	K 2943	O		O	O						
45	K 823	O	O	O		95	K 1826	O	O	O	O	145	K 2947	O	O	O	O						
46	K 835	O	O	O	O	96	K 1853					146	K 2967	O	O	O	O						
47	K 857					97	K 1903	O	O	O	O	147	K 2996	O	O	O	O						
48	K 858	O	O	O	O	98	K 1915			O	O	148	K 3002		O								
49	K 863		O		O	99	K 1924	O	O	O	O	149	K 3003	O	O	O	O						
50	K 878					100	K 2022					150	K 3037	O		O							

Figure 31 (continued)

Fig. 31(B) KLH 2 (1st LC-MS/MS)

#	K site	sample				#	K site	sample				#	K site	sample			
		1	2	3	4			1	2	3	4			1	2	3	4
1	K 26	O	O	O	O	51	K 1127	O	O	O	O	101	K 2198	O	O	O	O
2	K 41	O		O		52	K 1155					102	K 2202	O	O	O	O
3	K 71					53	K 1176			O		103	K 2227	O	O	O	O
4	K 74	O		O		54	K 1181					104	K 2231	O	O	O	O
5	K 104					55	K 1212		O		O	105	K 2317				
6	K 105					56	K 1233	O	O	O	O	106	K 2327				
7	K 138					57	K 1280					107	K 2328				
8	K 154	O	O			58	K 1302	O	O	O	O	108	K 3330				
9	K 155	O	O	O	O	59	K 1311	O	O	O	O	109	K 2335				
10	K 167	O	O	O	O	60	K 1315	O	O	O	O	110	K 2345				
11	K 191	O	O	O	O	61	K 1368	O	O	O	O	111	K 2361	O	O	O	O
12	K 250	O	O	O	O	62	K 1418	O	O	O	O	112	K 2400				O
13	K 284	O	O	O	O	63	K 1456	O	O	O	O	113	K 2426		O		
14	K 321	O			O	64	K 1493	O				114	K 2444				
15	K 358					65	K 1494	O	O	O	O	115	K 2455	O	O		O
16	K 372	O	O	O	O	66	K 1508	O				116	K 2463	O	O	O	O
17	K 401					67	K 1526	O	O	O	O	117	K 2482	O	O	O	
18	K 428	O	O	O	O	68	K 1556	O	O	O	O	118	K 2490				
19	K 433	O	O	O	O	69	K 1565					119	K 2527	O	O	O	O
20	K 447					70	K 1600	O	O	O	O	120	K 2596				
21	K 462					71	K 1602	O	O	O	O	121	K 2737	O	O		
22	K 471	O	O	O	O	72	K 1624	O			O	122	K 2754	O	O	O	
23	K 495		O	O	O	73	K 1633					123	K 2758	O	O	O	O
24	K 562			O		74	K 1646	O				124	K 2810				O
25	K 585					75	K 1675					125	K 2811				O
26	K 589					76	K 1690	O				126	K 2870	O	O	O	O
27	K 634	O	O	O	O	77	K 1700	O	O	O	O	127	K 2873				
28	K 672					78	K 1705					128	K 2888				
29	K 675					79	K 1708	O	O	O		129	K 2903				
30	K 688					80	K 1767	O	O	O	O	130	K 2934				
31	K 701					81	K 1782	O				131	K 2948	O	O	O	O
32	K 741					82	K 1803	O	O	O	O	132	K 2953				
33	K 774					83	K 1811	O	O			133	K 3010	O	O	O	O
34	K 776					84	K 1835					134	K 3025		O	O	
35	K 787					85	K 1879					135	K 3045				
36	K 790	O				86	K 1921					136	K 3050				
37	K 798					87	K 1931					137	K 3145				
38	K 806					88	K 1935					138	K 3148				
39	K 848					89	K 1947					139	K 3149	O	O	O	O
40	K 855					90	K 1954	O	O	O	O	140	K 3155				
41	K 858					91	K 1986	O	O	O	O	141	K 3184				
42	K 882					92	K 2001	O	O	O		142	K 3193				
43	K 898	O	O	O	O	93	K 2044					143	K 3240	O	O	O	O
44	K 907					94	K 2049	O				144	K 3263				
45	K 908					95	K 2052			O		145	K 3274				
46	K 936	O	O	O	O	96	K 2055					146	K 3321				
47	K 1011	O		O		97	K 2065			O		147	K 3336				
48	K 1079	O	O	O	O	98	K 2069					148	K 3340				
49	K 1083	O	O	O	O	99	K 2092					149	K 3344				
50	K 1097	O	O	O	O	100	K 2121	O				150	K 3404	O	O	O	O
													total	69	60	61	56

Figure 31 (continued)

Fig. 31(C) KLH 1 (2nd LC-MS/MS)

#	K site	sample				#	K site	sample				#	K site	sample				#	K site	sample			
		1	2	3	4			1	2	3	4			1	2	3	4			1	2	3	4
1	K 7	O	O	O	O	51	K 879			O	O	101	K 2033					151	K 3044				
2	K 26					52	K 884					102	K 2066					152	K 3048				
3	K 53	O	O	O	O	53	K 918		O			103	K 2067	O	O	O	O	153	K 3052				
4	K 67	O	O	O	O	54	K 924		O	O		104	K 2076	O		O	O	154	K 3077				
5	K 84	O	O	O	O	55	K 929					105	K 2099	O	O	O	O	155	K 3079	O			
6	K 88					56	K 946	O		O	O	106	K 2102		O	O	O	156	K 3092	O	O		O
7	K 96	O	O	O		57	K 952					107	K 2104		O	O	O		total	80	81	86	78
8	K 123	O	O	O	O	58	K 956	O	O	O	O	108	K 2131	O	O	O	O						
9	K 131	O	O	O	O	59	K 986	O	O	O	O	109	K 2149										
10	K 142	O	O	O	O	60	K 1017			O		110	K 2160	O									
11	K 161	O	O	O	O	61	K 1059	O	O			111	K 2187										
12	K 190		O		O	62	K 1060	O	O	O	O	112	K 2233										
13	K 251					63	K 1073	O				113	K 2247	O	O	O	O						
14	K 280	O		O		64	K 1104	O	O	O	O	114	K 2281										
15	K 289					65	K 1117	O		O		115	K 2302	O	O		O						
16	K 373					66	K 1160					116	K 2360	O	O	O	O						
17	K 389					67	K 1162	O	O	O		117	K 2460										
18	K 402					68	K 1199	O	O	O	O	118	K 2481	O	O	O	O						
19	K 411					69	K 1221		O		O	119	K 2506										
20	K 438	O	O	O	O	70	K 1230	O	O	O	O	120	K 2507	O	O	O	O						
21	K 469	O		O		71	K 1270					121	K 2514	O	O	O	O						
22	K 477	O		O		72	K 1303					122	K 2516	O	O	O	O						
23	K 488					73	K 1330					123	K 2531										
24	K 491					74	K 1335	O	O	O	O	124	K 2532										
25	K 499					75	K 1338					125	K 2579										
26	K 507					76	K 1339					126	K 2601	O	O	O	O						
27	K 530	O	O	O	O	77	K 1395	O	O	O	O	127	K 2609	O	O	O	O						
28	K 549					78	K 1402		O	O	O	128	K 2620										
29	K 554	O	O	O	O	79	K 1410	O	O	O	O	129	K 2624	O	O	O	O						
30	K 557			O		80	K 1416					130	K 2637	O	O	O	O						
31	K 566	O	O	O	O	81	K 1444		O	O	O	131	K 2656	O	O	O	O						
32	K 581	O	O	O	O	82	K 1473	O	O	O	O	132	K 2682										
33	K 587					83	K 1518	O	O	O	O	133	K 2686	O		O							
34	K 590	O	O	O	O	84	K 1529				O	134	K 2713										
35	K 606	O	O	O	O	85	K 1543					135	K 2714			O							
36	K 615					86	K 1583	O	O	O	O	136	K 2748	O	O								
37	K 616					87	K 1636					137	K 2771	O	O	O	O						
38	K 671	O	O	O	O	88	K 1640					138	K 2814	O	O	O	O						
39	K 681		O			89	K 1659	O	O	O	O	139	K 2838										
40	K 695	O	O	O	O	90	K 1668	O	O	O	O	140	K 2848										
41	K 704	O	O	O	O	91	K 1738	O	O	O	O	141	K 2852	O	O	O	O						
42	K 719	O	O	O	O	92	K 1749		O		O	142	K 2900	O	O	O	O						
43	K 787	O	O	O	O	93	K 1758	O	O	O	O	143	K 2924										
44	K 791	O	O	O	O	94	K 1809					144	K 2943		O	O							
45	K 823			O		95	K 1826	O	O	O	O	145	K 2947	O	O	O	O						
46	K 835	O	O	O	O	96	K 1853					146	K 2967	O	O	O	O						
47	K 857					97	K 1903	O	O	O	O	147	K 2996	O	O	O	O						
48	K 858	O	O	O	O	98	K 1915			O		148	K 3002										
49	K 863				O	99	K 1924	O	O	O	O	149	K 3003	O	O	O	O						
50	K 878					100	K 2022					150	K 3037			O							

Figure 31 (continued)

Fig. 31(D) KLH 2 (2nd LC-MS/MS)

#	K site	sample				#	K site	sample				#	K site	sample			
		1	2	3	4			1	2	3	4			1	2	3	4
1	K 26	O	O	O	O	51	K 1127	O	O	O	O	101	K 2198	O	O	O	O
2	K 41				O	52	K 1155					102	K 2202	O	O	O	O
3	K 71					53	K 1176			O		103	K 2227	O	O	O	O
4	K 74				O	54	K 1181					104	K 2231	O	O	O	O
5	K 104					55	K 1212		O			105	K 2317				
6	K 105					56	K 1233	O	O	O	O	106	K 2327				
7	K 138					57	K 1280					107	K 2328				
8	K 154					58	K 1302	O	O	O	O	108	K 3330				
9	K 155	O	O	O	O	59	K 1311	O			O	109	K 2335				
10	K 167	O	O	O	O	60	K 1315	O	O	O	O	110	K 2345				
11	K 191	O	O	O	O	61	K 1368	O	O	O	O	111	K 2361		O		O
12	K 250	O	O	O	O	62	K 1418	O	O	O	O	112	K 2400				O
13	K 284	O	O	O	O	63	K 1456	O	O	O	O	113	K 2426				
14	K 321			O	O	64	K 1493	O				114	K 2444				
15	K 358					65	K 1494	O	O	O	O	115	K 2455	O	O		O
16	K 372	O	O	O	O	66	K 1508	O				116	K 2463	O	O	O	O
17	K 401					67	K 1526	O	O	O	O	117	K 2482	O	O	O	O
18	K 428	O		O	O	68	K 1556	O	O	O	O	118	K 2490				
19	K 433	O	O	O	O	69	K 1565					119	K 2527	O	O	O	O
20	K 447					70	K 1600	O	O	O	O	120	K 2596				
21	K 462	O				71	K 1602	O	O	O	O	121	K 2737	O	O		O
22	K 471	O	O	O	O	72	K 1624				O	122	K 2754	O		O	
23	K 495		O		O	73	K 1633			O		123	K 2758	O	O	O	O
24	K 562	O				74	K 1646					124	K 2810				
25	K 585					75	K 1675					125	K 2811	O			
26	K 589					76	K 1690					126	K 2870	O	O	O	O
27	K 634	O	O	O	O	77	K 1700	O	O	O	O	127	K 2873				
28	K 672					78	K 1705					128	K 2888				
29	K 675					79	K 1708	O	O	O		129	K 2903				
30	K 688					80	K 1767	O	O	O		130	K 2934				
31	K 701					81	K 1782		O		O	131	K 2948	O	O	O	O
32	K 741					82	K 1803	O	O	O	O	132	K 2953				
33	K 774					83	K 1811		O			133	K 3010	O	O	O	O
34	K 776					84	K 1835					134	K 3025			O	
35	K 787					85	K 1879					135	K 3045				
36	K 790					86	K 1921					136	K 3050				
37	K 798					87	K 1931					137	K 3145				
38	K 806					88	K 1935					138	K 3148				
39	K 848					89	K 1947					139	K 3149	O	O	O	
40	K 855					90	K 1954	O	O	O	O	140	K 3155				
41	K 858					91	K 1986	O	O	O	O	141	K 3184				
42	K 882					92	K 2001	O	O	O	O	142	K 3193				
43	K 898	O	O	O	O	93	K 2044					143	K 3240	O	O	O	O
44	K 907					94	K 2049	O	O	O		144	K 3263				
45	K 908			O		95	K 2052					145	K 3274				
46	K 936	O	O	O	O	96	K 2055					146	K 3321				
47	K 1011	O			O	97	K 2065			O		147	K 3336				
48	K 1079	O	O	O	O	98	K 2069					148	K 3340				
49	K 1083	O	O	O	O	99	K 2092					149	K 3344				
50	K 1097	O	O	O	O	100	K 2121	O				150	K 3404	O	O	O	O
													total	61	56	57	58

Figure 32

Figure 32A. The summary of Globo-H conjugation analysis in the first LC-MS/MS run.

Sample	1			2			3			4		
KLH1/KLH2	KLH1	KLH2	total	KLH1	KLH2	total	KLH1	KLH2	total	KLH1	KLH2	total
Total K	156	150	306	156	150	306	156	150	306	156	150	306
Globo H-conjugated K	14	17	31	7	12	19	4	6	10	8	10	18
MMCCH-conjugated K	86	69	155	83	60	143	86	61	147	84	56	140

Figure 32B. The summary of Globo-H conjugation analysis in the second LC-MS/MS run.

Sample	1			2			3			4		
KLH1/KLH2	KLH1	KLH2	total	KLH1	KLH2	total	KLH1	KLH2	total	KLH1	KLH2	total
Total K	156	150	306	156	150	306	156	150	306	156	150	306
Globo H-conjugated K	13	15	28	7	14	21	6	5	11	9	10	19
MMCCH-conjugated K	80	61	141	81	56	137	86	57	143	78	58	136

The “Total K” indicates the numbers of lysine residues from KLH1 and KLH2 sequences. The “Globo H-conjugated K” indicates the numbers of identified Globo H conjugated lysines. The “MMCCH-conjugated K” indicates the numbers of identified MMCCH conjugated lysines.

Figure 33

Globo H and MMCCH derivative analysis on HNPQR residues

Sample	LC-MS/MS
1	Figure 34
2	Figure 35
3	Figure 36
4	Figure 37

Figure 34. Identification details of Globo H and MMCCH-conjugated peptides on HNPQR residues for sample 1

Figure 34A. KLH 1

#	Start	End	Observed	Mr(expt)	Mr(calc)	ppm	Enzyme	MC	Score	E value	Peptide	Mod_site
1	1036	1047	633.3067	1896.8983	1896.9028	-2.43	Th	3	42	7.20E-05	V**H**GMPTFPHWHR +GMd_NL997 (HKNPQR)	H1037
2	193	208	802.6955	2405.0647	2405.0479	6.99	T	0	18	0.017	YACCV**H**GMPIFPHWHR +Md_deamidated (HKNPQR)	H198
3	157	166	548.9234	1643.7484	1643.7402	4.99	T	1	19	0.012	EAF**H**KFQEDR +Md_deamidated (HKNPQR)	H160
4	1923	1932	756.3790	1510.7434	1510.7425	0.66	T	1	18	0.015	**N**KVMPNPFAR +Md_deamidated (HKNPQR)	N1923
5	1097	1110	999.9608	1997.9070	1997.9054	0.85	G	1	16	0.027	TNPF**H**HGKITHENE +Md_deamidated (HKNPQR)	H1101
6	686	692	578.7572	1155.4998	1155.5019	-1.82	Th	1	13	0.049	FDG**H**IDT +OBI822_Md (HKNPQR)	H689

Figure 34B. KLH 2

#	Start	End	Observed	Mr(expt)	Mr(calc)	ppm	Enzyme	MC	Score	E value	Peptide	Mod_site
1	2541	2556	856.3899	2566.1479	2566.1403	2.96	C	1	32	0.00058	RHALQSVMDDDG**PN**GF +Oxidation (M); 2 GMd_NL997 (HKNPQR)	P2553, N2554
2	3243	3256	657.3114	1968.9124	1968.9000	6.30	C	1	16	0.023	LVREGHDDE**N**VGSF +GMd_NL997 (HKNPQR)	N3252
3	1330	1341	633.3067	1896.8983	1896.9028	-2.43	Th	3	42	7.20E-05	V**H**GMPTFPHWHR +GMd_NL997 (HKNPQR)	H1331
4	281	293	915.9143	1829.8140	1829.8043	5.36	T	0	16	0.026	E**H**AKPADSFDYGR +Md_deamidated (HKNPQR)	H282
5	496	513	880.3888	2638.1446	2638.1239	7.85	T	1	33	0.00051	DRFACCV**H**GMATFPHWHR +Oxidation (M); Md_deamidated (HKNPQR)	H503
6	2755	2764	763.8912	1525.7678	1525.7599	5.24	T	0	33	0.00054	Q**P**LKPFSESR +Md_deamidated (HKNPQR)	P2756
7	466	481	1098.0108	2194.0070	2194.0001	3.19	G	2	18	0.036	RFQNDKSVDGY**Q**ATVE +Md_deamidated (HKNPQR)	Q477
8	277	289	608.9613	1823.8621	1823.8512	5.92	C	1	15	0.033	DLTREHAK**P**ADSF +Md_deamidated (HKNPQR)	P285
9	1383	1394	705.3279	2112.9619	2112.9510	5.16	C	1	20	0.023	NSRSQTFD**PN**PF +2 OBI822_Md (HKNPQR)	P1391, N1392
10	1383	1394	705.3276	2112.9610	2112.9510	4.73	C	1	19	0.028	NSRSQTFDP**NP**F +2 OBI822_Md (HKNPQR)	N1392, P1393
11	278	288	781.8885	1561.7624	1561.7559	4.23	Th	2	13	0.092	LTREHAK**P**ADS +Md_deamidated (HKNPQR)	P285
12	913	924	609.3028	1824.8866	1824.8817	2.69	Th	5	39	0.00038	V**H**GMAVFPHWHR +OBI822_Md (HKNPQR)	H914

"Start" and "End" indicate the number of residue of KLH1 or KLH2. "Observed" column implies the observed m/z value in the survey scan while "Mr(expt)", "Mr(calc)", "ppm" indicate the experimental molecular weight (MW), calculated MW, and the difference between observed MW and theoretical MW, respectively. In the "Enzyme" column, T, Th, G and C indicate trypsin, thermolysin, endoproteinase Glu-C and chymotrypsin, respectively. MC stands for missed cleavage. Scores are the peptide ion score directly reported from Mascot database search engine. E value denotes the expectation value for each identified peptide. The peptide sequences as well as its modifications are listed in "Peptide" column. "Mod_site" indicates the HNPQR conjugation site for KLH1 or KLH2 sequence.

Figure 35. Identification details of Globo H and MMCCH-conjugated peptides on HNPQR residues for sample 2

Figure 35A. KLH 1

#	Start	End	Observed	Mr(expt)	Mr(calc)	ppm	Enzyme	MC	Score	E value	Peptide	Mod_site
1	1187	1196	862.9495	1723.8844	1723.8868	-1.39	T	0	14	0.037	IWAIWQDLQ**R** +GMd_NL997 (HKNPQR)	R1196
2	1036	1047	633.3056	1896.8950	1896.9028	-4.16	Th	3	43	6.60E-05	V**H**GMPTFPHWHR +GMd_NL997 (HKNPQR)	H1037
3	157	166	548.9238	1643.7496	1643.7402	5.72	T	1	23	0.0053	EAF**H**KFQEDR +Md_deamidated (HKNPQR)	H160
4	193	208	802.6948	2405.0626	2405.0479	6.11	T	0	24	0.0039	YACCV**H**GMPIFPHWHR +Md_deamidated (HKNPQR)	H198
5	360	370	870.9418	1739.8690	1739.8527	9.37	T	0	17	0.02	LWAVWQALQM**R** +Deamidated (NQ); Md_deamidated (HKNPQR)	R370
6	1092	1114	1055.4976	3163.4710	3163.4682	0.85	T	1	21	0.0092	QHHYETNPF**H**HGKITHENEITTR +Md_deamidated (HKNPQR)	H1101
7	1092	1114	1055.4982	3163.4728	3163.4682	1.42	T	1	26	0.003	QHHYETNPFH**H**GKITHENEITTR +Md_deamidated (HKNPQR)	H1102
8	1923	1932	756.3809	1510.7472	1510.7425	3.18	T	1	25	0.0033	**N**KVMPNPFAR +Md_deamidated (HKNPQR)	N1923
9	2515	2520	571.7600	1141.5054	1141.5074	-1.66	T	1	15	0.03	**Q**KEEDR +Md_deamidated (HKNPQR)	Q2515
10	2647	2661	715.6796	2144.0170	2144.0095	3.45	G	4	25	0.0029	AEELRDALYKLQ**N**DE +Md_deamidated (HKNPQR)	N2659
11	1733	1741	664.3222	1326.6298	1326.6312	-0.98	Th	2	25	0.0029	VLGGEKEM**P** +Oxidation (M); OBI822_Md (HKNPQR)	P1741

Figure 35B. KLH 2

#	Start	End	Observed	Mr(expt)	Mr(calc)	ppm	Enzyme	MC	Score	E value	Peptide	Mod_site
1	1481	1490	862.9495	1723.8844	1723.8868	-1.39	T	0	14	0.037	IWAIWQDLQ**R** +GMd_NL997 (HKNPQR)	R1490
2	1948	1963	950.4320	2848.2742	2848.2949	-7.27	T	1	23	0.0046	**R**TQEFS**K**PEDTFDYHR +Deamidated (NQ); 2 GMd_NL997 (HKNPQR)	R1948
3	3243	3256	657.3103	1968.9091	1968.9000	4.62	C	1	18	0.015	LVREGHDDE**N**VGSF +GMd_NL997 (HKNPQR)	N3252
4	1330	1341	633.3056	1896.8950	1896.9028	-4.16	Th	3	43	6.60E-05	V**H**GMPTFPHWHR +GMd_NL997 (HKNPQR)	H1331
5	3243	3256	657.3101	1968.9085	1968.9000	4.32	Th	3	18	0.028	LVREGHDDE**N**VGSF +GMd_NL997 (HKNPQR)	N3252
6	159	175	781.7303	2342.1691	2342.1590	4.31	T	2	19	0.012	AVDD**R**LFEKVQPGHHTR +Md_deamidated (HKNPQR)	R163
7	281	293	915.9102	1829.8058	1829.8043	0.87	T	0	52	6.10E-06	E**H**AKPADSFDYGR +Md_deamidated (HKNPQR)	H282
8	496	513	880.3886	2638.1440	2638.1239	7.62	T	1	35	0.00033	DRFACCV**H**GMATFPHWHR +Oxidation (M); Md_deamidated (HKNPQR)	H503
9	2755	2764	763.8908	1525.7670	1525.7599	4.72	T	0	41	8.00E-05	Q**P**LKPFSESR +Md_deamidated (HKNPQR)	P2756
10	466	481	1098.0066	2193.9986	2194.0001	-0.64	G	2	17	0.049	RFQNDKSVDGY**Q**ATVE +Md_deamidated (HKNPQR)	Q477
11	913	924	609.3012	1824.8818	1824.8817	0.05	Th	5	20	0.031	V**H**GMAVFPHWHR +OBI822_Md (HKNPQR)	H914

"Start" and "End" indicate the number of residue of KLH1 or KLH2. "Observed" column implies the observed m/z value in the survey scan while "Mr(expt)", "Mr(calc)", "ppm" indicate the experimental molecular weight (MW), calculated MW, and the difference between observed MW and theoretical MW, respectively. In the "Enzyme" column, T, Th, G and C indicate trypsin, thermolysin, endoproteinase Glu-C and chymotrypsin, respectively. MC stands for missed cleavage. Scores are the peptide ion score directly reported from Mascot database search engine. E value denotes the expectation value for each identified peptide. The peptide sequences as well as its modifications are listed in "Peptide" column. "Mod_site" indicates the HNPQR conjugation site for KLH1 or KLH2 sequence.

Figure 36. Identification details of Globo H and MMCCH-conjugated peptides on HNPQR residues for sample 3

Figure 36A. KLH 1

#	Start	End	Observed	Mr(expt)	Mr(calc)	ppm	Enzyme	MC	Score	E value	Peptide	Mod_site
1	1036	1047	633.3054	1896.8944	1896.9028	-4.48	Th	3	43	6.80E-05	V**H**GMPTFPHWHR +GMd_NL997 (HKNPQR)	H1037
2	2754	2761	678.8257	1355.6368	1355.6503	-9.96	Th	1	22	0.0058	INQDTV**R**D +GMd_NL997 (HKNPQR)	R2760
3	157	166	548.9228	1643.7466	1643.7402	3.89	T	1	23	0.0047	EAF**H**KFQEDR +Md_deamidated (HKNPQR)	H160
4	193	208	802.6941	2405.0605	2405.0479	5.24	T	0	16	0.025	YACCV**H**GMPIFPHWHR +Md_deamidated (HKNPQR)	H198
5	2515	2520	571.7623	1141.5100	1141.5074	2.37	T	1	23	0.0045	**Q**KEEDR +Md_deamidated (HKNPQR)	Q2515
6	2625	2636	743.0091	2226.0055	2226.0099	-1.98	T	0	28	0.0017	**HH**EDHHEDILVR +OBI822_Md (HKNPQR); Md_deamidated (HKNPQR)	H2625, H2626
7	2647	2661	715.6772	2144.0098	2144.0095	0.09	G	4	32	0.00069	AEELRDALYKL**Q**NDE +Md_deamidated (HKNPQR)	Q2658
8	160	171	606.9428	1817.8066	1817.8043	1.27	C	1	20	0.0095	**H**KFQEDRSVDGY +Md_deamidated (HKNPQR)	H160
9	944	955	821.4324	1640.8502	1640.8484	1.16	C	3	35	0.00035	DLK**P**ASLGKDLF +Md_deamidated (HKNPQR)	P947
10	1649	1669	979.4319	2935.2739	2935.2759	-0.72	C	4	31	0.0025	NLNDHTHDFSKPEDTFDY**Q**KF +Md_deamidated (HKNPQR)	Q1667
11	2160	2184	1085.5138	3253.5196	3253.5179	0.52	C	3	21	0.01	KYDIT**H**ALHDAHITPEDVFHPSEPF +Md_deamidated (HKNPQR)	H2165
12	686	692	578.7544	1155.4942	1155.5019	-6.66	Th	1	14	0.04	FDG**H**IDT +OBI822_Md (HKNPQR)	H689
13	1733	1741	664.3258	1326.6370	1326.6312	4.45	Th	2	24	0.0036	VLGGEKEM**P** +Oxidation (M); OBI822_Md (HKNPQR)	P1741

Figure 36B. KLH 2

#	Start	End	Observed	Mr(expt)	Mr(calc)	ppm	Enzyme	MC	Score	E value	Peptide	Mod_site
1	3243	3256	657.3107	1968.9103	1968.9000	5.23	C	1	17	0.021	LVREGHDDE**N**VGSF +GMd_NL997 (HKNPQR)	N3252
2	1330	1341	633.3054	1896.8944	1896.9028	-4.48	Th	3	43	6.80E-05	V**H**GMPTFPHWHR +GMd_NL997 (HKNPQR)	H1331
3	3243	3256	657.3104	1968.9094	1968.9000	4.77	Th	3	25	0.0055	LVREGHDDE**N**VGSF +GMd_NL997 (HKNPQR)	N3252
4	159	175	781.7293	2342.1661	2342.1590	3.03	T	2	20	0.0096	AVDD**R**LFEKVQPGHHTR +Md_deamidated (HKNPQR)	R163
5	281	293	915.9102	1829.8058	1829.8043	0.87	T	0	44	4.50E-05	E**H**AKPADSFDYGR +Md_deamidated (HKNPQR)	H282
6	3275	3295	987.4552	2959.3438	2959.3494	-1.89	T	1	16	0.026	YDITEVANRL**N**MHHDDTFNFR +OBI822_Md (HKNPQR)	N3285
7	277	291	701.6560	2101.9462	2101.9415	2.24	C	2	15	0.048	DLTREHAK**P**ADSFDY +Md_deamidated (HKNPQR)	P285
8	1383	1394	705.3264	2112.9574	2112.9510	3.03	C	1	25	0.0079	NSRSQTFDP**NP**F +2 OBI822_Md (HKNPQR)	N1392, P1393
9	913	924	609.3025	1824.8857	1824.8817	2.19	Th	5	23	0.014	V**H**GMAVFPHWHR +OBI822_Md (HKNPQR)	H914

"Start" and "End" indicate the number of residue of KLH1 or KLH2. "Observed" column implies the observed m/z value in the survey scan while "Mr(expt)", "Mr(calc)", "ppm" indicate the experimental molecular weight (MW), calculated MW, and the difference between observed MW and theoretical MW, respectively. In the "Enzyme" column, T, Th, G and C indicate trypsin, thermolysin, endoproteinase Glu-C and chymotrypsin, respectively. MC stands for missed cleavage. Scores are the peptide ion score directly reported from Mascot database search engine. E value denotes the expectation value for each identified peptide. The peptide sequences as well as its modifications are listed in "Peptide" column. "Mod_site" indicates the HNPQR conjugation site for KLH1 or KLH2 sequence.

Figure 37. Identification details of Globo H and MMCCH-conjugated peptides on HNPQR residues for sample 4

Figure 37A. KLH 1

#	Start	End	Observed	Mr(expt)	Mr(calc)	ppm	Enzyme	MC	Score	E value	Peptide	Mod_site
1	1933	1944	597.6233	1789.8481	1789.8458	1.29	T	0	14	0.042	GYVPS**H**DTYTVR +GMd_NL997 (HKNPQR)	H1938
2	1036	1047	633.3073	1896.9001	1896.9028	-1.48	Th	3	39	0.00014	V**H**GMPTFPHWHR +GMd_NL997 (HKNPQR)	H1037
3	2754	2761	678.8262	1355.6378	1355.6503	-9.22	Th	1	32	0.00059	INQDTV**R**D +GMd_NL997 (HKNPQR)	R2760
4	157	166	548.9249	1643.7529	1643.7402	7.73	T	1	20	0.0093	EAF**H**KFQEDR +Md_deamidated (HKNPQR)	H160
6	2515	2520	571.7632	1141.5118	1141.5074	3.94	T	1	24	0.0043	**Q**KEEDR +Md_deamidated (HKNPQR)	Q2515
7	2647	2661	715.6789	2144.0149	2144.0095	2.47	G	4	30	0.00097	AEELRDALYKLQ**N**DE +Md_deamidated (HKNPQR)	N2659
8	1733	1741	664.3221	1326.6296	1326.6312	-1.13	Th	2	26	0.0024	VLGGEKEM**P** +Oxidation (M); OBI822_Md (HKNPQR)	P1741
9	1930	1934	483.2334	964.4522	964.4589	-6.84	Th	2	18	0.015	FA**R**GY +OBI822_Md (HKNPQR)	R1932

Figure 37B. KLH 2

#	Start	End	Observed	Mr(expt)	Mr(calc)	ppm	Enzyme	MC	Score	E value	Peptide	Mod_site
1	1948	1963	950.4304	2848.2694	2848.2949	-8.95	T	1	26	0.0023	**R**TQEFSKPEDTFDYHR +Deamidated (NQ); 2 GMd_NL997 (HKNPQR)	R1948
2	3243	3256	657.3107	1968.9103	1968.9000	5.23	C	1	19	0.011	LVREGHDDE**N**VGSF +GMd_NL997 (HKNPQR)	N3252
3	1330	1341	633.3073	1896.9001	1896.9028	-1.48	Th	3	39	0.00014	V**H**GMPTFPHWHR +GMd_NL997 (HKNPQR)	H1331
4	3243	3256	657.3099	1968.9079	1968.9000	4.01	Th	3	15	0.051	LVREGHDDE**N**VGSF +GMd_NL997 (HKNPQR)	N3252
5	281	293	915.9126	1829.8106	1829.8043	3.50	T	0	48	1.70E-05	E**H**AKPADSFDYGR +Md_deamidated (HKNPQR)	H282
6	1097	1115	827.0797	2478.2173	2478.2101	2.91	T	0	59	2.60E-06	KPL**Q**PFGLDSVINPDDETR +Md_deamidated (HKNPQR)	Q1100
7	2755	2764	764.3863	1526.7580	1526.7439	9.30	T	0	21	0.0075	Q**P**LKPFSESR +Deamidated (NQ); Md_deamidated (HKNPQR)	P2756
8	1383	1394	705.3266	2112.9580	2112.9510	3.31	C	1	20	0.024	NSRSQTFD**PN**PF +2 OBI822_Md (HKNPQR)	P1391, N1392
9	2360	2370	806.9017	1611.7888	1611.7789	6.14	C	1	16	0.026	TKM**H**AVPNTLF +Oxidation (M); Md_deamidated (HKNPQR)	H2363
10	913	924	609.3015	1824.8827	1824.8817	0.55	Th	5	20	0.031	V**H**GMAVFPHWHR +OBI822_Md (HKNPQR)	H914

"Start" and "End" indicate the number of residue of KLH1 or KLH2. "Observed" column implies the observed m/z value in the survey scan while "Mr(expt)", "Mr(calc)", "ppm" indicate the experimental molecular weight (MW), calculated MW, and the difference between observed MW and theoretical MW, respectively. In the "Enzyme" column, T, Th, G and C indicate trypsin, thermolysin, endoproteinase Glu-C and chymotrypsin, respectively. MC stands for missed cleavage. Scores are the peptide ion score directly reported from Mascot database search engine. E value denotes the expectation value for each identified peptide. The peptide sequences as well as its modifications are listed in "Peptide" column. "Mod_site" indicates the HNPQR conjugation site for KLH1 or KLH2 sequence.

Figure 38

Summary of Globo H and MMCCH derivative analysis on HNPQR residues

Sample	**1**			**2**			**3**			**4**		
KLH1/KLH2	KLH1	KLH2	Total	KLH1	KLH2	Total	KLH1	KLH2	Total	KLH1	KLH2	Total
Globo H-conjugated	1	4	5	2	4	6	2	2	4	3	3	6
MMCCH- conjugated	5	9	14	9	6	15	11	7	18	5	7	12