Figure 1

Fig. 1(A)

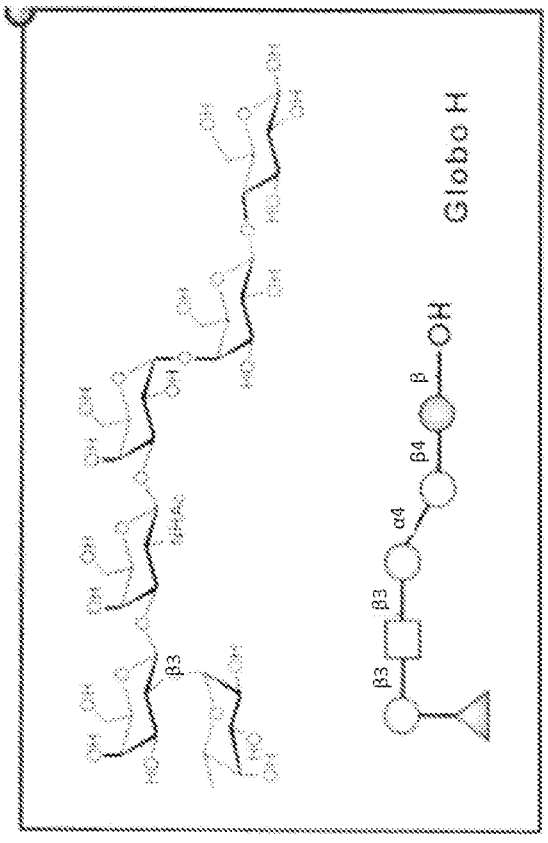



Fig. 1(B)



Figure 2

Fig. 2(A)

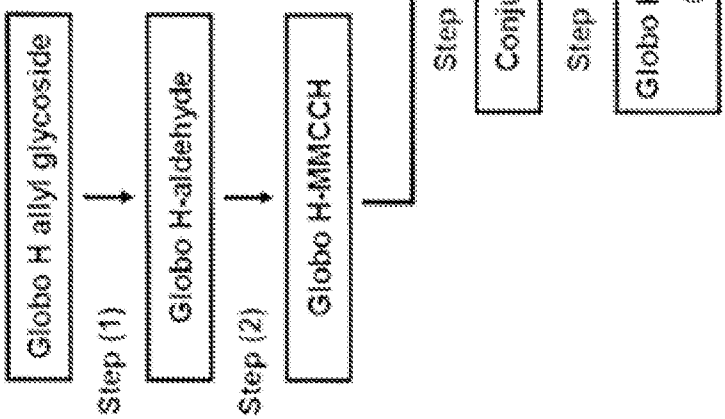



Fig. 2(B)

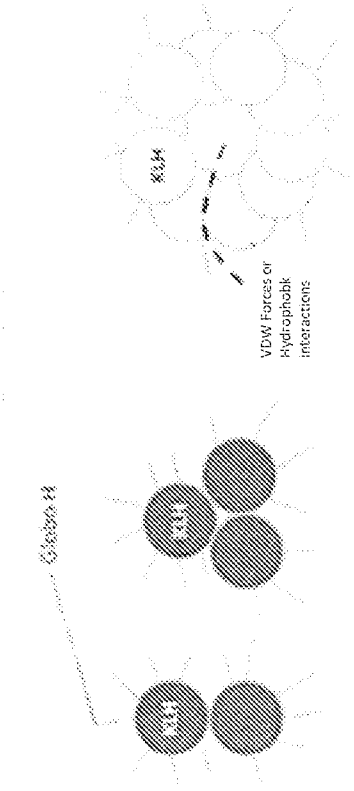


Figure 3

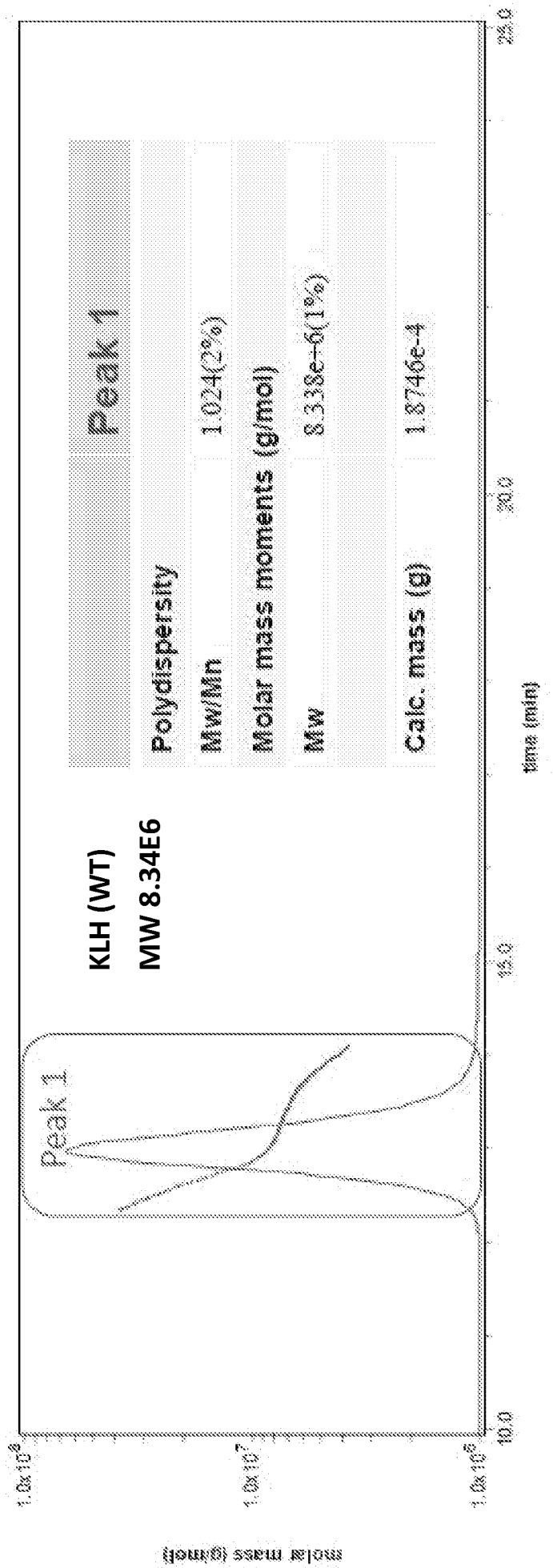

KLH (WT)
MW 8.34E6
Peak 1
Polydispersity
Mw/Mn 1.024(2%)
Molar mass moments (g/mol)
Mw 8.338e+6(1%)
Calc. mass (g) 1.8746e-4
Peak 1
1.0x10^8
1.0x10^7
1.0x10^6
molar mass (g/mol)
10.0
15.0
20.0
25.0
time (min)

**Figure 4**

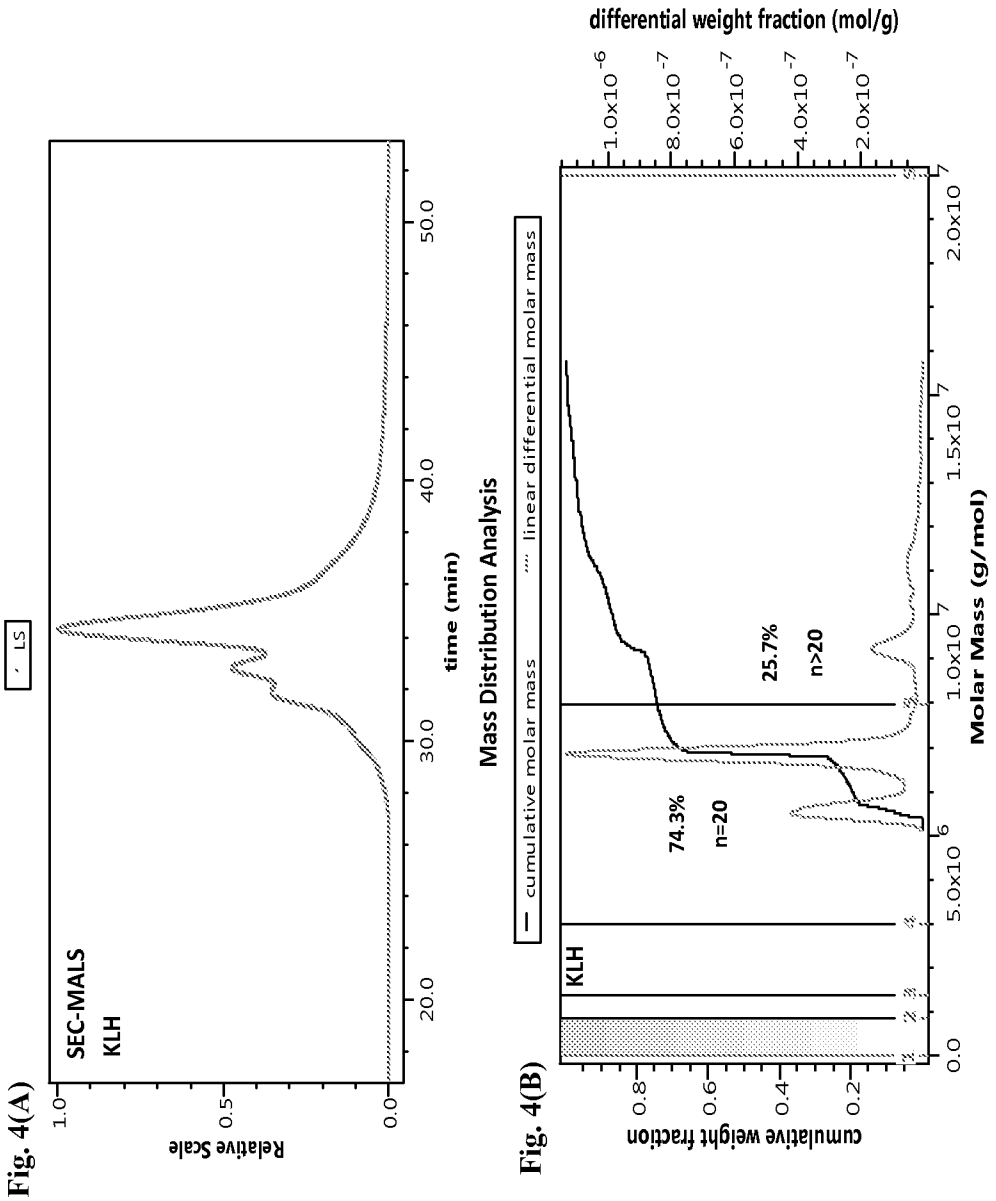

Fig. 4(A)
Size exclusion Chromatogram
LS
SEC-MALS
KLH
Relative Scale
1.0
0.5
0.0
20.0
30.0
40.0
50.0
time (min)
Fig. 4(B)
Mass Distribution Analysis
cumulative molar mass
linear differential molar mass
KLH
74.3%
n=20
25.7%
n>20
cumulative weight fraction
differential weight fraction (mol/g)
1.0x10-6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

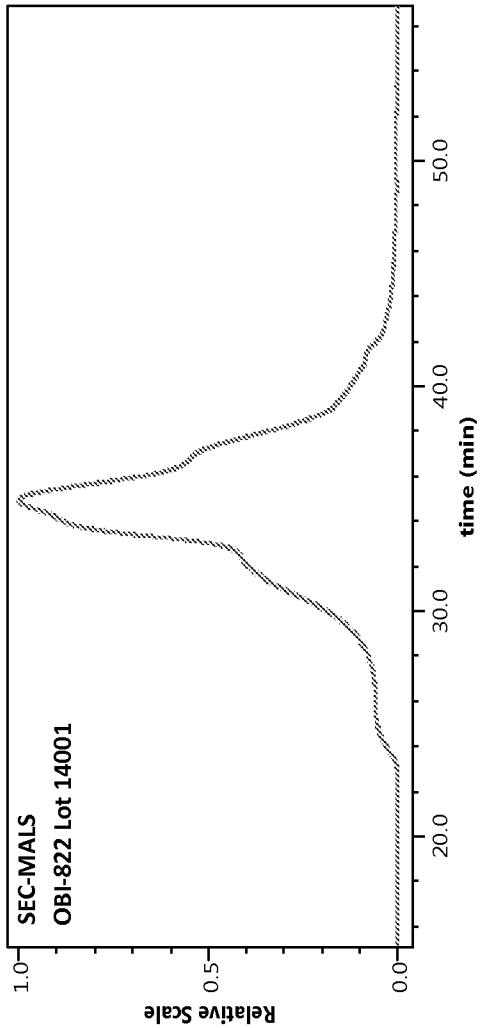



Fig. 4(D)

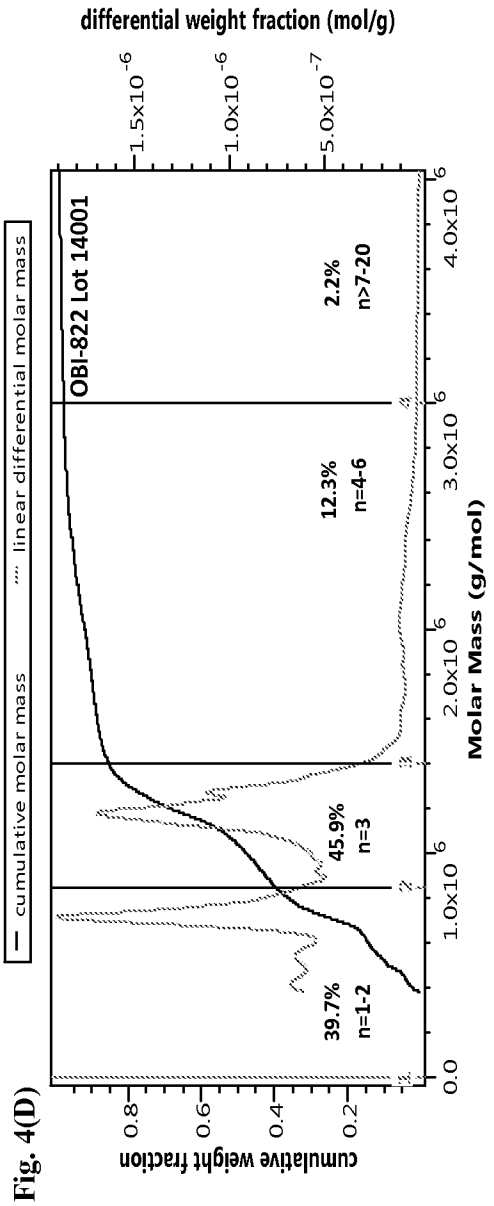


Figure 5

Fig. 5(A)

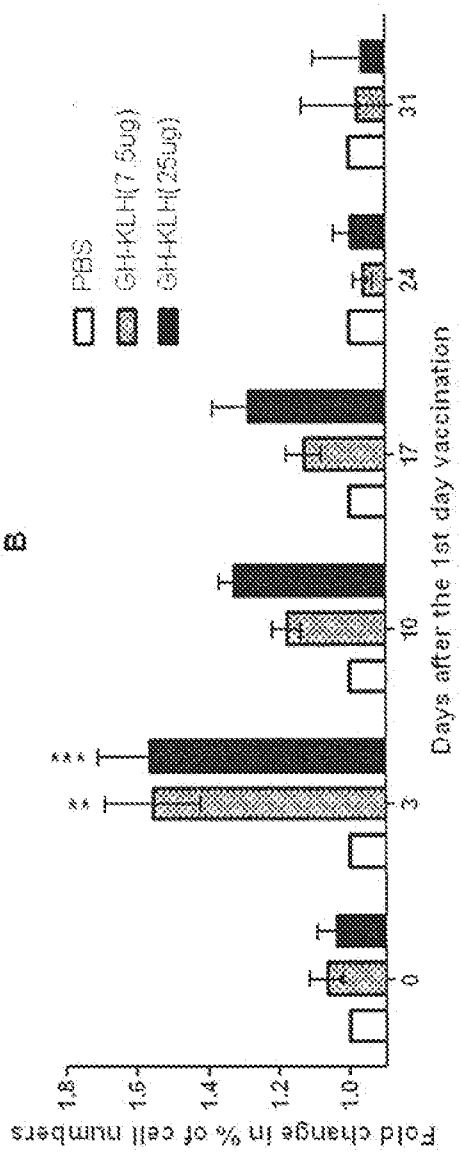


Figure 5 continued

Fig. 5(B)

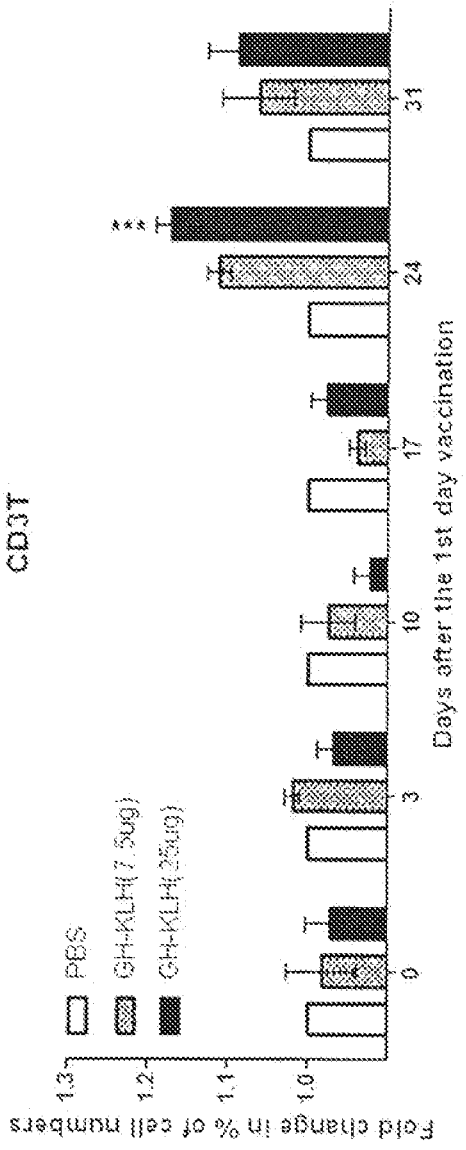


Figure 5 continued

Fig. 5(C)

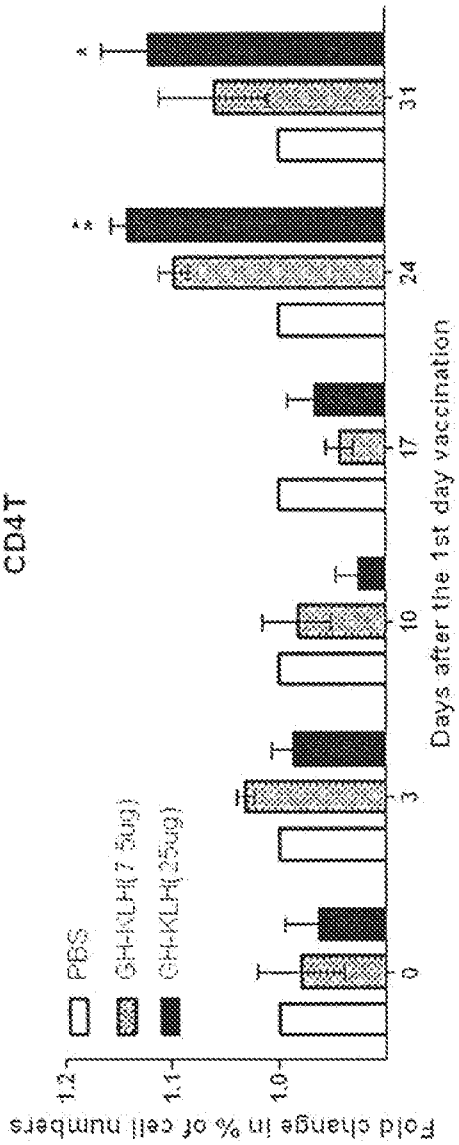


Figure 5 continued

Fig. 5(D)

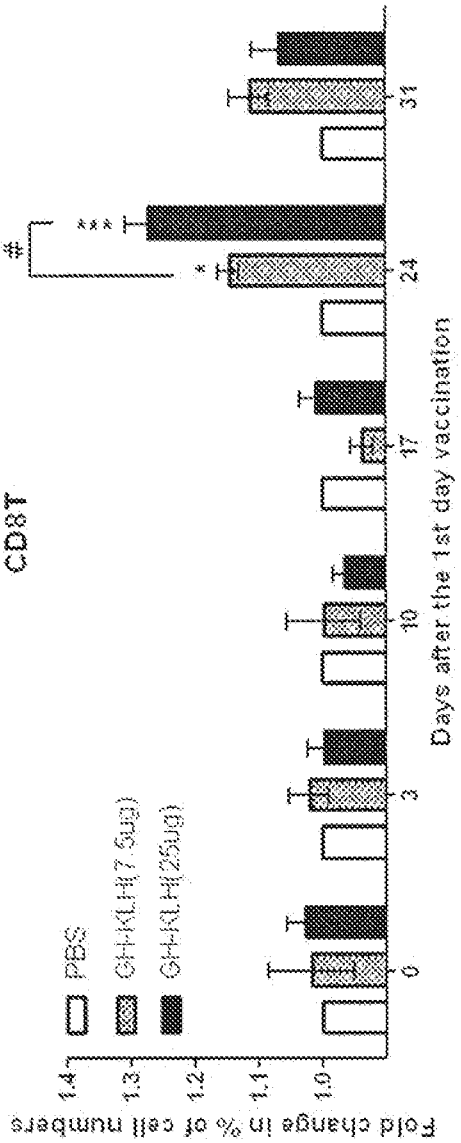


Figure 6

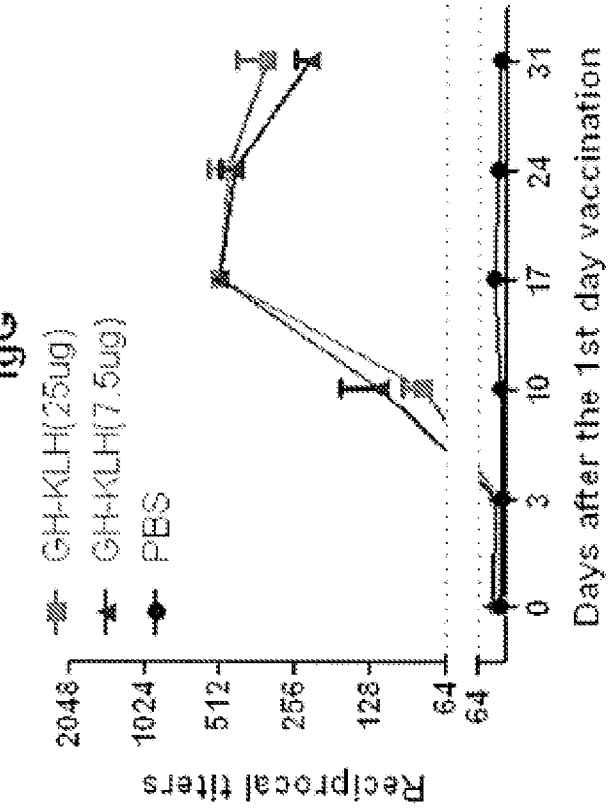



Figure 6B

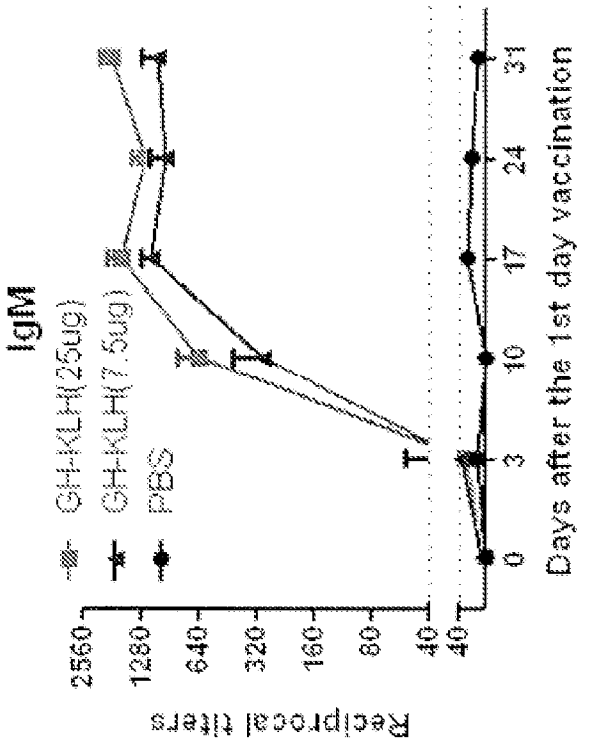



Figure 6A

Figure 7

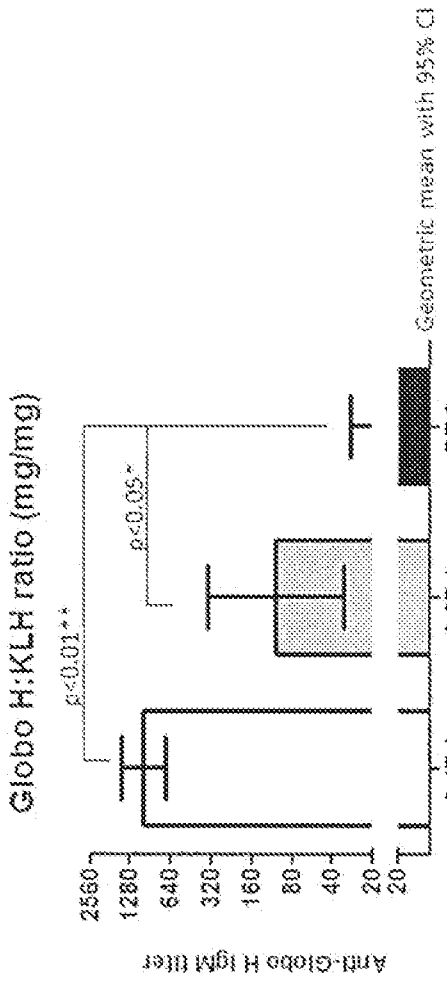

Globo H:KLH ratio (mg/mg)
p<0.01**
p<0.05*
Anti-Globo H IgM titer
2560
1280
640
320
160
80
40
20
20
0.17:1
0.07:1
PBS
Geometric mean with 95% CI

Figure 8

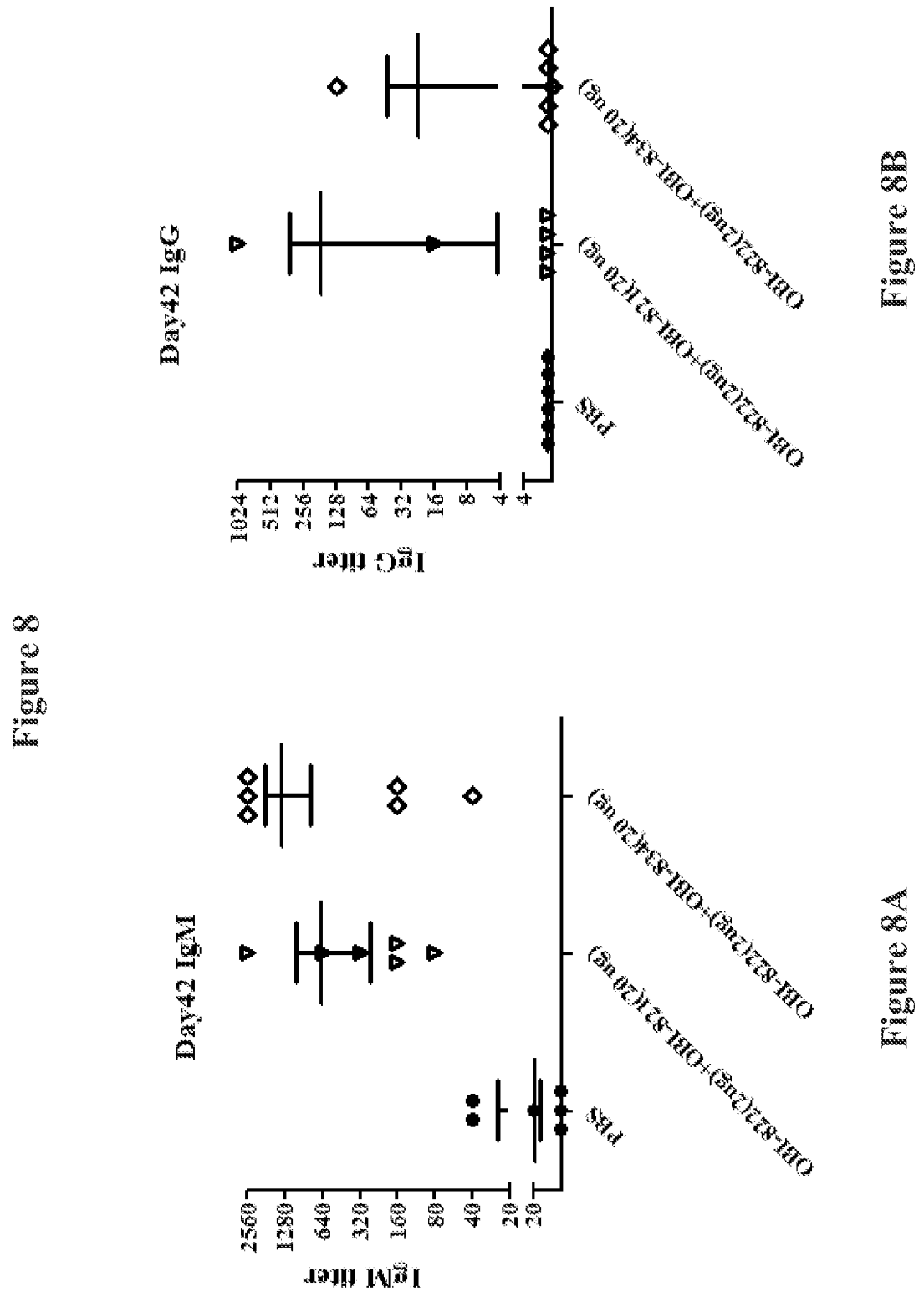



Figure 8A

Figure 8B

Figure 9

Fig. 9(A)

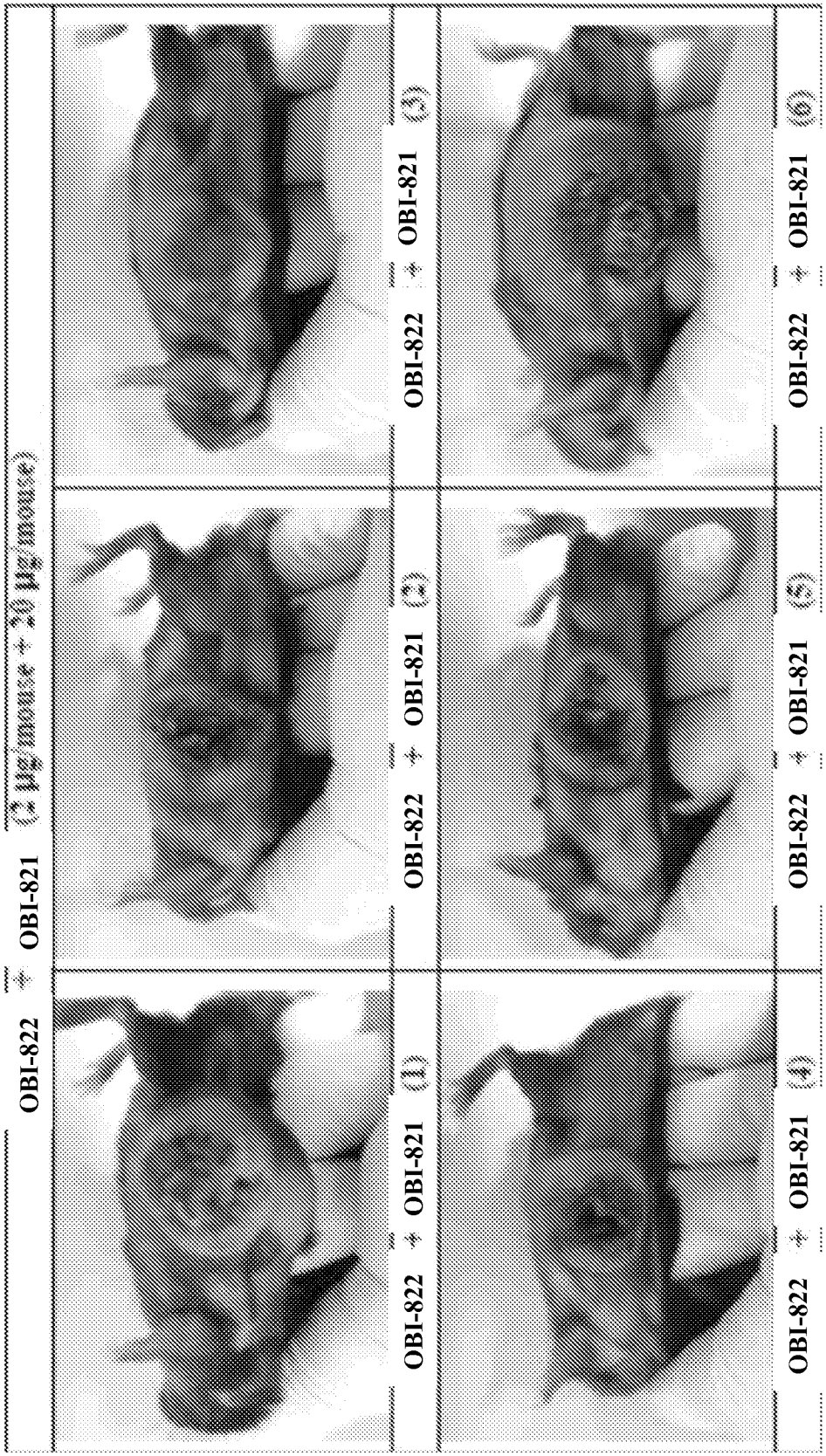


Figure 9 (continued)

Figure 9(B)

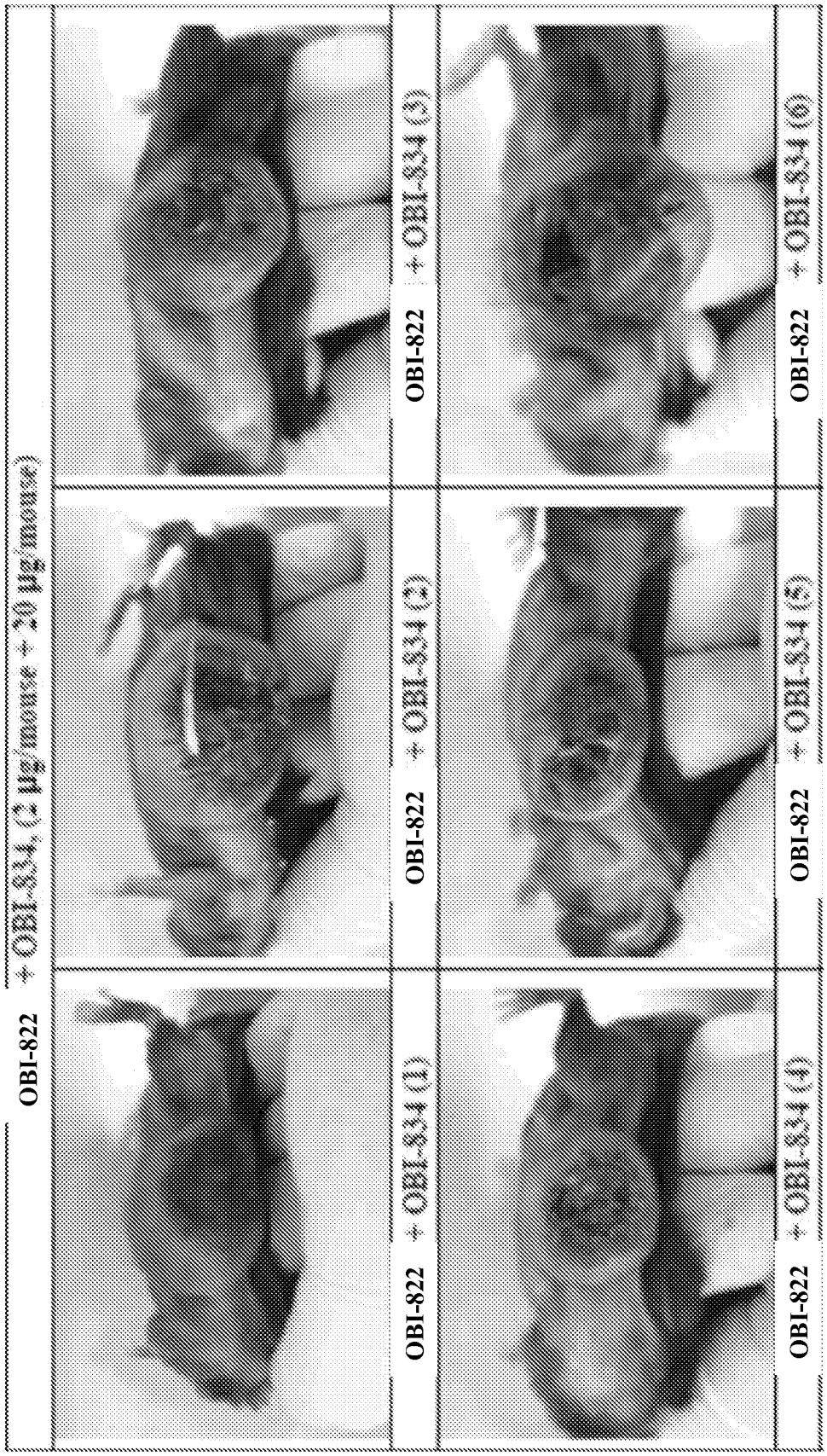
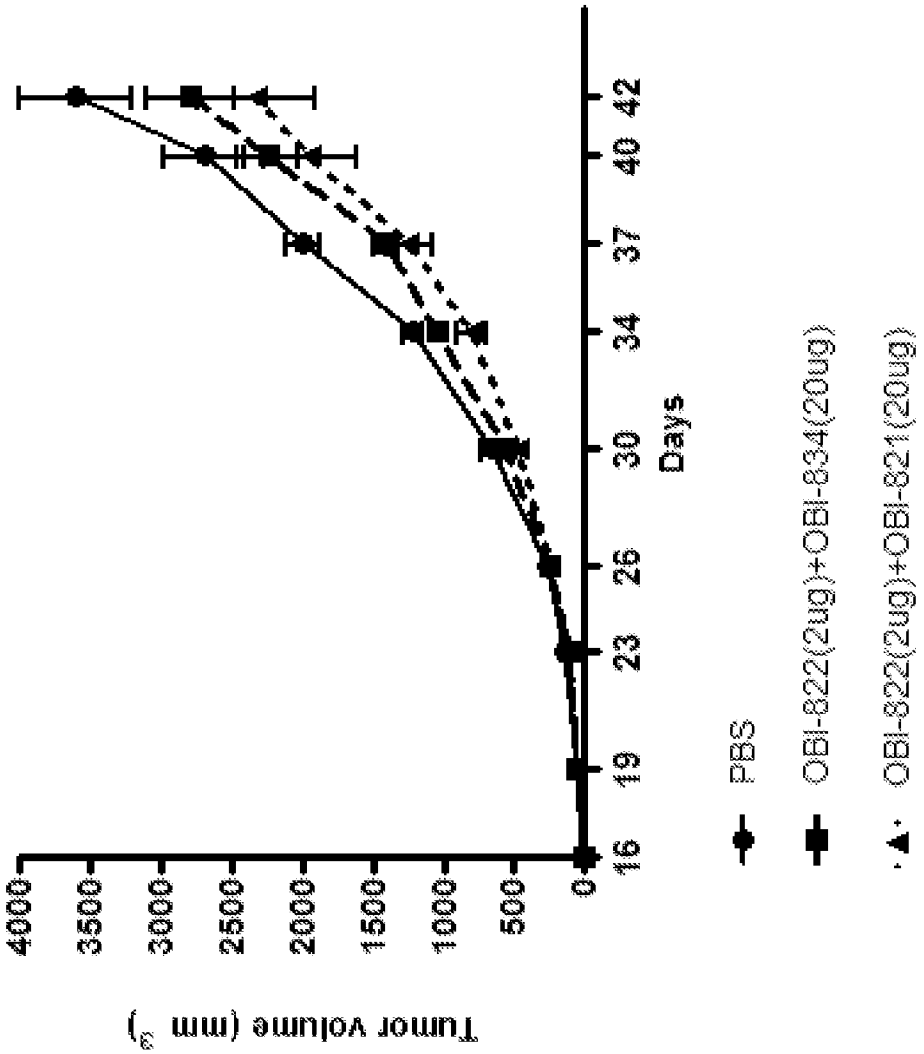
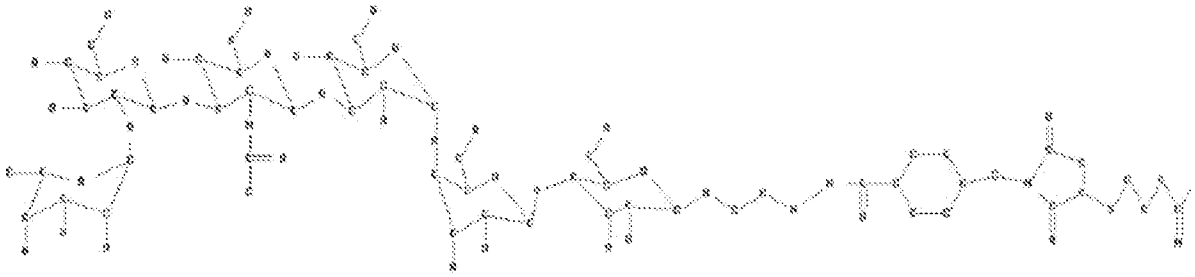


Figure 10


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)

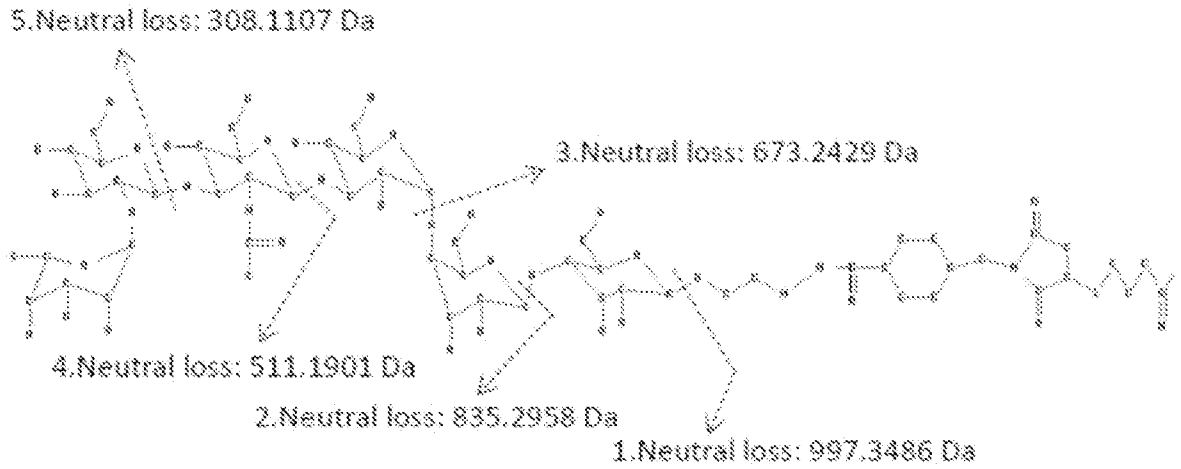
## Figure 11

### 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

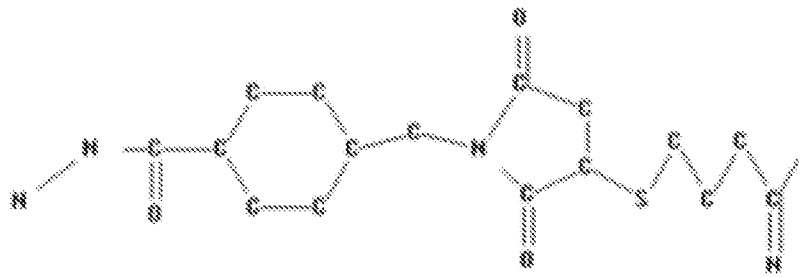
3. Chemical formula: C(30) H(48) N(4) O(14) S(1)
   Monoisotopic MW addition: 720.2888 Da

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

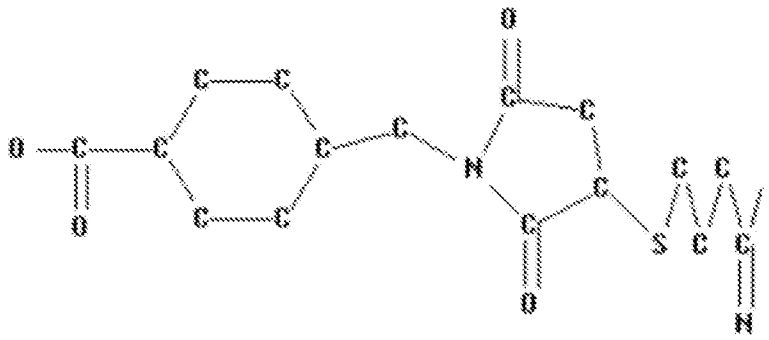
**Figure 12**

**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 |