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(54) Title: COMPOSITIONS OF A CARBOHYDRATE VACCINE FOR INDUCING IMMUNE RESPONSES AND USES THEREOF IN CANCER TREATMENT

Figure 1

Fig. 1(a)

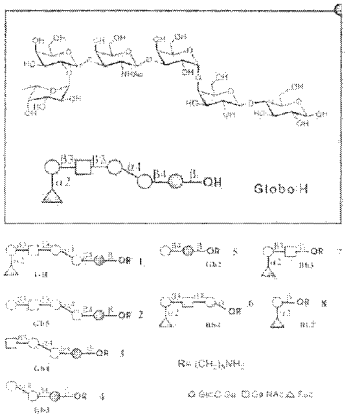
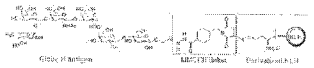


Fig. 1(b)



(57) Abstract: The invention encompasses therapeutic compositions including Globo H-KLH conjugates and/or therapeutic antibodies as well as methods of making and using the same to treat proliferative diseases such as cancer. The therapeutic conjugates include an antigen linked to a carrier. In particular the therapeutic conjugates include a Globo H moiety and a KLH moiety and/or a derivatized KLH moiety subunit optionally linked via a linker. The therapeutic compositions are in part envisaged to act as cancer vaccines for boosting the body's natural ability to protect itself, through the immune system from dangers posed by damaged or abnormal cells such as cancer cells. An effective immune response is one that reduces the severity of disease, including but not limited to, prevention of disease, delay in onset of disease, decreased severity of symptoms, decreased morbidity and delayed mortality.

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COMPOSITIONS OF A CARBOHYDRATE VACCINE FOR INDUCING IMMUNE RESPONSES AND USES THEREOF IN CANCER TREATMENT

FIELD OF THE INVENTION

[001] The invention encompasses compositions and methods for cancer immunotherapy in general and immunogenic glycoconjugates able to elicit anti-cancer immune responses in particular.

BACKGROUND OF THE INVENTION

[002] The use of synthetic carbohydrate conjugates to elicit antibodies was first demonstrated by Goebel and Avery in 1929. (Goebel, W. F., and Avery, O. T., J. Exp. Med., 1929, 50, 521; Avery, O. T., and Goebel, W. F., J. Exp. Med., 1929, 50, 533.) Carbohydrates were linked to carrier proteins via the benzenediazonium glycosides. Immunization of rabbits with the synthetic antigens generated polyclonal antibodies. Other workers (Allen, P. Z., and Goldstein, I. J., Biochemistry, 1967, 6, 3029; Rude, E., and Delius, M. M., Carbohydr. Res., 1968, 8, 219; Himmelspach, K., et al., Eur. J. Immunol., 1971, 1, 106; Fielder, R. J., et al., J. Immunol., 1970, 105, 265) developed similar techniques for conjugation of carbohydrates to protein carriers.

[003] Glycoconjugates may be used in active immunotherapy generated from vaccinations to specifically target known target agents on tumor cells. The response to carbohydrate antigens normally does not enlist the use of T-cells, which would aid in the body's rejection of the tumor. While the probability of complete tumor rejection as a result of vaccination with a conjugate is thought to be unlikely, such treatments will boost immune surveillance and recurrence of new tumor colonies can be reduced. (Dennis, J.,

Oxford Glycosystems Glyconews Second, 1992; Lloyd, K. O., in Specific Immunotherapy of Cancer with Vaccines, 1993, New York Academy of Sciences, 50-58). Toyokuni and Singhal have described a synthetic glycoconjugate (Toyokuni, T., et al., J. Am. Chem. Soc., 1994, 116, 395) that stimulated a measurable IgG titer, a result which is significant since an IgG response is generally associated with enlistment of helper T cells.

[004] The carbohydrate antigen Globo H (Fucα1→2 Galβ1→3 GalNAcβ1→3 Galα1→4 Galβ1→4 Glc) was first isolated as a ceramide-linked Glycolipid and identified in 1984 by Hakomori et al. from breast cancer MCF-7 cells. (Bremer E G, et al. (1984) J Biol Chem 259:14773-14777). Further studies with anti-Globo H monoclonal antibodies showed that Globo H was present on many other cancers, including prostate, gastric, pancreatic, lung, ovarian and colon cancers and only minimal expression on luminal surface of normal secretory tissue which is not readily accessible to immune system. (Ragupathi G, et al. (1997) Angew Chem Int Ed 36:125-128). In addition, it has been established that the serum of breast cancer patient contains high level of anti-Globo H antibody. (Gilewski T et al. (2001) Proc Natl Acad Sci USA 98:3270-3275; Huang C-Y, et al. (2006) Proc Natl Acad Sci USA 103:15-20; Wang C-C, et al. (2008) Proc Natl Acad Sci USA 105(33):11661-11666). Patients with Globo H-positive tumors showed a shorter survival in comparison to patients with Globo H-negative tumors. (Chang, Y-J, et al. (2007) Proc Natl Acad Sci USA 104(25):10299-10304). These findings render Globo H, a hexasaccharide epitope, an attractive tumor marker and a feasible target for cancer vaccine development.

[005] A synthetic Globo H vaccine in combination with an immunological adjuvant was shown to induce mainly IgM and to a lesser extent IgG antibodies in both prostate and metastatic breast cancer patients. In a phase I clinical trial, the vaccine also showed minimal toxicity with transient local skin reactions at the vaccination site. (Gilewski T et al. (2001) Proc Natl Acad Sci USA 98:3270-3275; Ragupathi G, et al. (1997) Angew Chem Int Ed 36:125-128; Slovin S F et al (1997) Proc Natl Acad Sci USA 96:5710-5715). Mild flu-like symptoms which have been observed in some of the patients were probably associated with the side effect of QS-21. A pentavalent vaccine containing five prostate and breast cancer associated carbohydrate antigens--Globo-H, GM2, STn, TF and Tn--conjugated to maleimide-modified carrier protein KLH has been reported to produce anti-Globo H sera with higher titers of IgG than IgM in ELISA assays. (Zhu J. et al. (2009) J. Am. Chem. Soc. 131(26):9298-9303).

[006] It is known that KLH contains glycosylated polypeptide subunits that assemble to form decameric (10-mer), didecameric (20-mer), and larger particles. These multimeric structures have been characterized by ultracentrifugation techniques that yield sedimentation coefficients of 11-19S for the dissociated subunits and 92-107S for the didecameric multimers. It is further known that a variety of factors may affect the size distribution of molluscam hemocyanins, including KLH. These factors include ionic strength, pH, temperature, pO_2, and the availability of certain divalent cations, notably calcium and magnesium. The current inventors have developed a composition with increased efficacy that is primarily comprised of dimers and trimers of KLH linked to a plurality of Globo H moieties.

[007] While vaccines have been developed to elicit antibody responses against Globo H, their anti-cancer efficacies are unsatisfactory due to low antigenicity of Globo H. There is a need for a new vaccine capable of eliciting high levels of immune responses targeting Globo H.

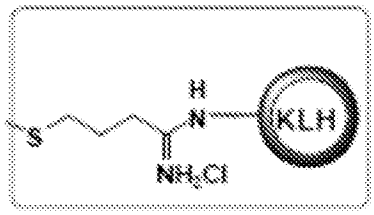
SUMMARY OF THE INVENTION

[008] The invention generally encompasses therapeutic and/or prophylactic compositions including Globo H, as well as, immunotherapeutics, vaccines, dosage forms, kits, and methods of manufacture, and treatment thereof.

[009] In one embodiment, the invention encompasses an isolated therapeutic conjugate comprising a Globo H moiety linked to a keyhole limpet hemocyanin (KLH) moiety subunit. In certain embodiments, the linkage is a covalent bond.

[010] In another embodiment, the invention encompasses an isolated therapeutic conjugate comprising a Globo H moiety covalently linked to a keyhole limpet hemocyanin (KLH) moiety subunit, wherein the KLH is a derivatized KLH. As used herein the term "covalently linked" when referring to Globo-H and KLH means: Globo-H is directly covalently linked to KLH, or Globo-H is covalently linked to derivatized KLH (as set forth herein), or Globo-H is covalently linked to KLH through a linker group (as set forth herein), or Globo-H is covalently linked to KLH through both a linker group and a derivatized KLH.

[011] In certain illustrative embodiments, the derivatized KLH of the invention has the following structure:



Derivatized KLH

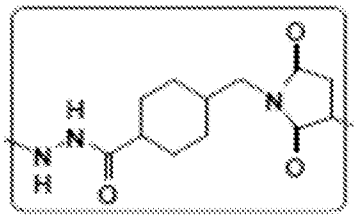
.

[012] In another embodiment, the invention encompasses an isolated therapeutic conjugate comprising a Globo H moiety covalently linked to a keyhole limpet hemocyanin (KLH) moiety subunit through a linker molecule.

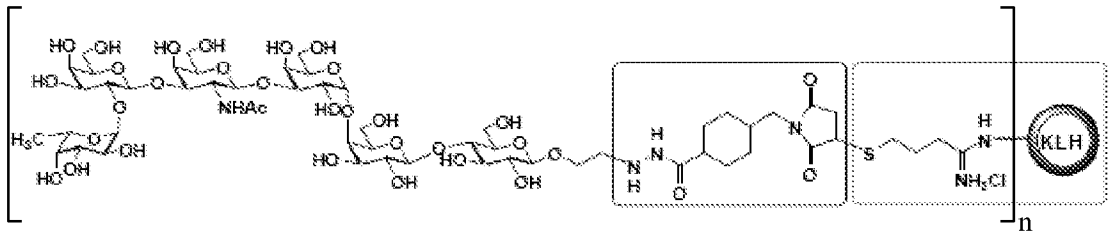
[013] In a preferred embodiment the Globo H moieties are bound to a lysine residue of a KLH moiety subunit.

[014] In one embodiment, there are total of exactly or about 145, 146, 147, 148, 149, 150, 151, 152, 153, 154, 155, 156, 157, 158, 159, 160 total lysine residues per KLH moiety subunit which are available for or actually directly or indirectly bind a Globo H moiety.

[015] In another embodiment, the invention encompasses an isolated therapeutic conjugate comprising a Globo H moiety covalently linked to a keyhole limpet hemocyanin (KLH) moiety subunit via a 4-(4-N-maleimidomethyl) cyclohexane-1-carboxyl hydrazide (MMCCH) linker group. The MMCCH linker of the invention has the following structure:



[016] In another illustrative embodiment, the invention encompasses an isolated therapeutic conjugate having the following general structure:



wherein n is an integer from about 1 to about 160. In certain embodiments, a monomeric KLH moiety can include from about 1 to about 160 Globo H moieties. One of ordinary skill in the art will recognize that the structures are illustrated as the iminium hydrochloride salts but can also exist or co-exist as the imine form. Accordingly, the invention encompasses both the imine as well as salts thereof including the iminium hydrochloride salt. In certain embodiments, a monomeric KLH moiety can include from about 1 to about 125 Globo H moieties. In certain embodiments, a monomeric KLH moiety can include from about 1 to about 100 Globo H moieties. In certain embodiments, a monomeric KLH moiety can include from about 1 to about 75 Globo H moieties. In certain embodiments, a monomeric KLH moiety can include from about 1 to about 50 Globo H moieties. In certain embodiments, a monomeric KLH moiety can

include from about 1 to about 25 Globo H moieties. In certain embodiments, a monomeric KLH moiety can include from about 1 to about 10 Globo H moieties.

[017] In certain embodiments, the Globo H moieties are conjugated to the KLH moieties covalently on basic amino acid residues. In certain embodiments, the basic amino acid residues are arginine, lysine, histidine, or a combination thereof.

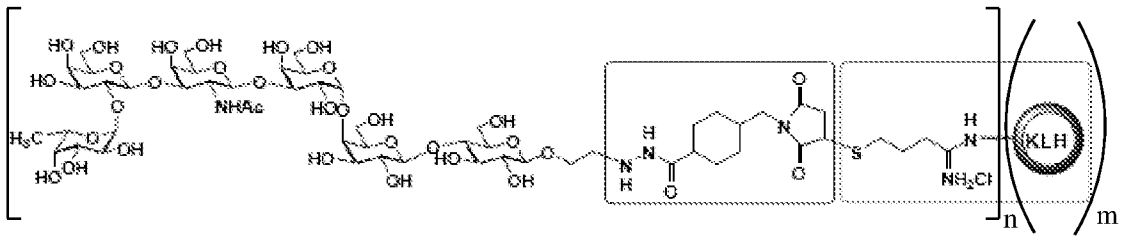
[018] In another embodiment the Globo H moieties are bound to lysine conjugation sites on a monomeric KLH moiety subunit.

[019] In another embodiment, there are exactly or about 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100, 101, 102, 103, 104, 105, 106, 107, 108, 109 or 110 lysine conjugation sites on each monomeric KLH moiety subunit available for binding to or actually bound to a Globo H moiety. In another embodiment, there are 62, 66, 67, 68, 70, 72, 76, 86, 87, 88, 90, 92, 93, 100 such lysine conjugation sites on each KLH moiety subunit.

[020] In certain therapeutic composition embodiments containing a mixture of moiety subunits (*e.g.,* KLH1 and KLH2 or variants thereof), total available lysine (for both subunits) as are counted together across the different subunit types the and may be or are exactly about 290, 291, 292, 293, 294, 295, 296, 297, 298, 299, 300, 301, 302, 303, 304, 305, 306, 307, 308, 309 or 310 in number. In such embodiments, there are or may be exactly or about 130, 131, 132, 133, 134, 135, 136, 137, 138, 139, 140, 141, 142, 143, 144, 145, 146, 147, 148, 149, 150, 151, 152, 153, 154, 155, 156, 157, 158, 159 or 160 lysine conjugation sites together across the different subunits (e.g., KLH1 and KLH2 or

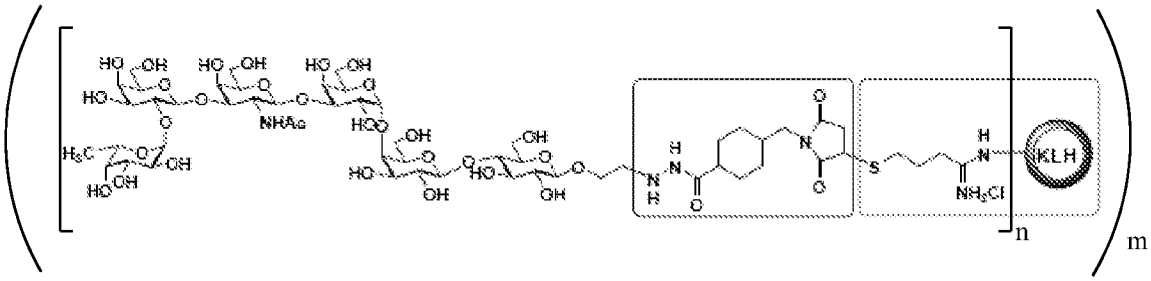
variants thereof). In other such embodiments, there are 136, 137, 141, 140, 143, 147 or 155 lysine conjugation sites.

[021] In another illustrative embodiment, the invention encompasses an isolated therapeutic conjugate having the following general structure:



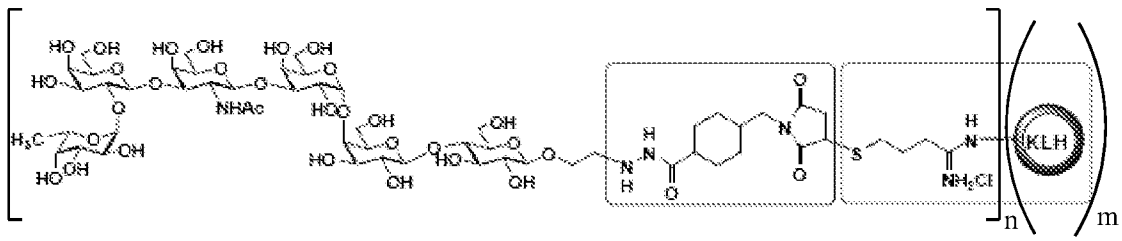
wherein n is independently an integer from about 1 to about 3000 and m is independently an integer from about 1 to about 20. In certain embodiments, when m is greater than 1, KLH moieties can aggregate to form multimeric structures. In certain embodiments, the aggregation is a covalent bond. In certain other embodiments, the aggregation is not a covalent bond (*e.g.,* the aggregation is formed by H-bonding or hydrophobic interactions). In certain embodiments, a monomeric KLH moiety (*i.e.,* where m = 1) can include from about 1 to about 160 Globo H moieties. In certain embodiments, a dimeric KLH moiety (*i.e.,* where m = 2) can include from about 1 to about 300 Globo H moieties. In certain embodiments, a trimeric KLH moiety (*i.e.,* where m = 3) can include from about 1 to about 450 Globo H moieties. In certain embodiments, a tetrameric KLH moiety (*i.e.,* where m = 4) can include from about 1 to about 600 Globo H moieties. In certain embodiments, a pentameric KLH moiety (*i.e.,* where m = 5) can include from about 1 to about 750 Globo H moieties.

[022] In another illustrative embodiment, the invention encompasses an isolated therapeutic conjugate having the following general structure:



wherein n is independently an integer from about 1 to about 150 and m is independently an integer from about 1 to about 20.

[023] In another embodiments, the invention encompasses an isolated therapeutic conjugate having the following general structure:



wherein n independently is an integer from about 1 to about 160, and wherein m is independently an integer from about 1 to about 20. In certain embodiments, m is an integer from about 1 to about 5. In certain embodiments, m is an integer from about 1 to about 3. In certain embodiments, m is 1. In certain embodiments, m is 2. In certain embodiments, m is 3. In certain embodiments, m is 4. In certain embodiments, m is 5. In certain embodiments, m is 6. In certain embodiments, m is 7. In certain embodiments, m is 8. In certain embodiments, m is 9. In certain embodiments, m is 10. In certain

embodiments, m is 11. In certain embodiments, m is 12. In certain embodiments, m is 13. In certain embodiments, m is 14. In certain embodiments, m is 15. In certain embodiments, m is 16. In certain embodiments, m is 17. In certain embodiments, m is 18. In certain embodiments, m is 19. In certain embodiments, m is 20. In certain embodiments, for any of the above embodiments, when m is 1 to 20, each n is 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100, 101, 102, 103, 104, 105, 106, 107, 108, 109, 110, 111, 112, 113, 114, 115, 116, 117, 118, 119, 120, 121, 122, 123, 124, 125, 126, 127, 128, 129, 130, 131, 132, 133, 134, 135, 136, 137, 138, 139, 140, 141, 142, 143, 144, 145, 146, 147, 148, 149, 150, 151, 152, 153, 154, 155, 156, 157, 158, 159, or 160, respectively.

[024] In certain embodiments, there is more than one Globo H moiety attached to each monomeric KLH moiety. In certain illustrative embodiments, the more than one Globo H moiety attached to each KLH moiety is attached via a linker. In other illustrative embodiments, the more than one Globo H moieties attached to each KLH moiety are attached via a linker and attached to a derivatized KLH moiety.

[025] In another embodiment, the ratio of Globo H moieties to KLH moiety subunits is at least 1. In another embodiment, the ratio of Globo H moieties to KLH moiety subunits is at least 10. In another embodiment, the ratio of Globo H moieties to KLH moiety is at least 25. In another embodiment, the ratio of Globo H moieties to KLH moiety subunits is at least 50. In a further embodiment, the ratio of Globo H moieties to KLH moiety

subunits is at least 100. In a further embodiment, the ratio of Globo H moieties to KLH moiety subunits is at least 150. In yet another embodiment, the ratio of Globo H moieties to KLH moiety subunits is at least 500. In yet a further embodiment, the ratio of Globo H moieties to KLH moiety subunits is at least 750. In still another embodiment, the ratio of Globo H moieties to KLH moiety subunits is at least 1000. In still another embodiment, the ratio of Globo H moieties to KLH moiety subunits is at least 1500. In still another embodiment, the ratio of Globo H moieties to KLH moiety subunits is at least 2000.

[026] In various embodiments, the invention encompasses a single monomer of KLH to multiple KLH subunits (*e.g.,* 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20) each having attached multiple Globo H moieties. In certain embodiments, the ratio of Globo H moieties to KLH moiety is the same. In other embodiments, the ratio of Globo H moieties to KLH moiety is different.

[027] Another embodiment of the invention encompasses a composition comprising at least two KLH moieties. For example, a derivatized KLH moiety in the form of a dimer. In another embodiment, the at least two KLH moieties are the same. In another embodiment, the at least two KLH moieties are different. In a further embodiment, the at least two KLH moieties have the same Globo H moiety to KLH moiety subunit ratio. In still a further embodiment, the at least two KLH moieties have a different Globo H moiety to KLH moiety subunit ratio.

[028] Another embodiment of the invention encompasses a therapeutic composition comprising at least three KLH moieties, for example, a derivatized KLH moiety in the form of a trimer. In certain embodiments, the at least three KLH moieties are the same.

In another embodiment, the at least three KLH moieties are not the same. In a further embodiment, the at least three KLH moieties have the same Globo H moiety to KLH moiety subunit ratio. In still a further embodiment, the at least three KLH moieties have a different Globo H moiety to KLH moiety subunit ratio.

[029] Another embodiment of the invention encompasses a therapeutic composition comprising at least four KLH moieties, for example, a derivatized KLH moiety in the form of a tetramer. In certain embodiments, the at least four KLH moieties are the same. In another embodiment, the at least four KLH moieties are not the same. In a further embodiment, the at least four KLH moieties have the same Globo H moiety to KLH moiety subunit ratio. In still a further embodiment, the at least four KLH moieties have a different Globo H moiety to KLH moiety subunit ratio.

[030] Another embodiment of the invention encompasses a therapeutic composition comprising at least five KLH moieties, for example, a derivatized KLH moiety in the form of a pentamer. In certain embodiments, the at least five KLH moieties are the same. In another embodiment, the at least five KLH moieties are not the same. In a further embodiment, the at least five KLH moieties have the same Globo H moiety to KLH moiety subunit ratio. In still a further embodiment, the at least five KLH moieties have a different Globo H moiety to KLH moiety subunit ratio.

[031] Another embodiment of the invention encompasses a therapeutic composition comprising at least six KLH moieties, for example, a derivatized KLH moiety in the form of a hexamer. In certain embodiments, the at least six KLH moieties are the same. In another embodiment, the at least six KLH moieties are not the same. In a further

embodiment, the at least six KLH moieties have the same Globo H moiety to KLH moiety subunit ratio. In still a further embodiment, the at least six KLH moieties have a different Globo H moiety to KLH moiety subunit ratio.

[032] In one embodiment, the Globo H moiety comprises (Fucα1→2 Galβ1→3 GalNAcβ1→3 Galα1→4 Galβ1→4 Glc). In a further embodiment, the KLH moiety subunit is a KLH-1 or KLH-2 moiety or a combination thereof. As used herein, the term "KLH" refers to KLH-1, KLH-2, and/or combinations thereof.

[033] In another embodiment, the KLH moiety subunit is at least 99% identical to a corresponding naturally occurring KLH moiety subunit.

[034] In another embodiment, the KLH moiety subunit is at least 95% identical to a corresponding naturally occurring KLH moiety subunit.

[035] In another embodiment, the KLH moiety subunit is at least 90% identical to a corresponding naturally occurring KLH moiety subunit.

[036] In another embodiment, the KLH moiety subunit is at least 80% identical to a corresponding naturally occurring KLH moiety subunit.

[037] In another embodiment, the KLH moiety subunit is at least 70% identical to a corresponding naturally occurring KLH moiety subunit.

[038] In another embodiment, the KLH moiety subunit is at least 60% identical to a corresponding naturally occurring KLH moiety subunit.

[039] In another embodiment, the Globo H moiety is covalently linked to a keyhole limpet hemocyanin (KLH) moiety subunit via a linker. In yet a further embodiment, the Globo H moiety is covalently linked to a keyhole limpet hemocyanin (KLH) moiety subunit by a 4-(4-N-maleimidomethyl) cyclohexane-1-carboxyl hydrazide (MMCCH) linkage. In another further embodiment, the Globo H moiety is covalently linked to a derivatized keyhole limpet hemocyanin (KLH) moiety subunit and is linked by a 4-(4-N-maleimidomethyl) cyclohexane-1-carboxyl hydrazide (MMCCH) linkage.

[040] In another embodiment, the isolated therapeutic conjugate has an epitope ratio based on a KLH monomer having molecular weight of about 350KDa to about 400KDa of at least or about 150. In another embodiment, the isolated therapeutic conjugate has an epitope ratio of at least or about 100. In a further embodiment, the isolated therapeutic conjugate has an epitope ratio of at least or about 75. In still a further embodiment, the isolated therapeutic conjugate has an epitope ratio of at least or about 50. In yet a further embodiment, the isolated therapeutic conjugate has an epitope ratio of at least or about 25. In still another embodiment, the isolated therapeutic conjugate has an epitope ratio of at least or about 15. In still another embodiment, the isolated therapeutic conjugate has an epitope ratio of at least or about 5. In still another embodiment, the isolated therapeutic conjugate has an epitope ratio of at least or about 1.

[041] Another embodiment of the invention encompasses a pharmaceutical composition comprising KLH moiety subunits, wherein each KLH moiety subunit comprises one or more Globo H moieties covalently linked to a keyhole limpet hemocyanin (KLH) moiety subunit. In certain embodiments, the pharmaceutical composition comprises dimers of at least two KLH moiety subunits, wherein each KLH moiety subunits comprises one or

more Globo H moieties covalently linked to a KLH moiety subunit. In certain embodiments, the pharmaceutical composition comprises trimers of at least three KLH moiety subunits, wherein each KLH moiety subunits comprises one or more Globo H moieties covalently linked to a KLH moiety subunit. In certain embodiments, the pharmaceutical composition comprises at least four KLH moiety subunits, wherein each KLH moiety subunit comprises one or more Globo H moieties covalently linked to a KLH moiety subunit. In certain embodiments, the pharmaceutical composition comprises a mixture of KLH moiety subunits (e.g., monomers, dimers, trimers, tetramers, pentamers etc.), wherein each KLH moiety subunits comprises multiple Globo H moieties covalently linked to a KLH moiety subunit.

[042] Another aspect of the invention relates to a pharmaceutical composition comprising monomers, dimers, trimers, tetramers, or pentamers or combinations thereof of KLH moieties, wherein each KLH comprises one or more Globo H moiety covalently linked to a keyhole limpet hemocyanin (KLH) moiety subunit.

[043] In one embodiment the invention, the epitope ratios of the therapeutic conjugates in the composition ranges from about 1 to 3000. In a further embodiment, the epitope ratios of the therapeutic conjugates in the composition range from about 75 to 2000. In still another embodiment, the epitope ratios of the therapeutic conjugates in the composition range from about 100 to 1000. In yet a further embodiment the average epitope ratio of the therapeutic conjugates in the composition ranges from about 150 to 500.

[044] In another embodiment, about 1% to 99% of the therapeutic conjugates in the composition are KLH monomers. In a further embodiment, about 0% to 99% of the therapeutic conjugates in the composition are KLH dimers. In still another embodiment, about 0% to 99% of the therapeutic conjugates in the composition are KLH trimers. In yet another embodiment, about 0% to 99% of the therapeutic conjugates in the composition are KLH tetramers. In a further embodiment, about 1% to 99% of the therapeutic conjugates in the composition are KLH pentamers. In yet another embodiment, about 0% to 99% of the therapeutic conjugates in the composition include 6 KLH subunits. In yet another embodiment, about 0% to 99% of the therapeutic conjugates in the composition include 7 KLH subunits. In yet another embodiment, about 0% to 99% of the therapeutic conjugates in the composition include 8 KLH subunits. In yet another embodiment, about 0% to 99% of the therapeutic conjugates in the composition include 9 KLH subunits. In yet another embodiment, about 0% to 99% of the therapeutic conjugates in the composition include 10 KLH subunits. In yet another embodiment, about 0% to 99% of the therapeutic conjugates in the composition include 11 KLH subunits. In yet another embodiment, about 0% to 99% of the therapeutic conjugates in the composition include 12 KLH subunits. In yet another embodiment, about 0% to 99% of the therapeutic conjugates in the composition include 13 KLH subunits. In yet another embodiment, about 0% to 99% of the therapeutic conjugates in the composition include 14 KLH subunits. In yet another embodiment, about 0% to 99% of the therapeutic conjugates in the composition include 15 KLH subunits. In yet another embodiment, about 0% to 99% of the therapeutic conjugates in the composition include 16 KLH subunits. In yet another embodiment, about 0% to 99% of the therapeutic

conjugates in the composition include 17 KLH subunits. In yet another embodiment, about 0% to 99% of the therapeutic conjugates in the composition include 18 KLH subunits. In yet another embodiment, about 0% to 99% of the therapeutic conjugates in the composition include 19 KLH subunits. In yet another embodiment, about 0% to 99% of the therapeutic conjugates in the composition include 20 KLH subunits. In still another embodiment, about 1% to 99% of the therapeutic conjugates in the composition are monomers, dimers, trimers, tetramers or combinations thereof. In still another embodiment, about 99% of the therapeutic conjugates in the composition are monomers, dimers, trimers, tetramers or combinations thereof.

[045] In another embodiment, the pharmaceutical composition comprises an adjuvant including, but not limited to, Freund's adjuvant, Toll-Like Receptor molecules, LPS, lipoproteins, lipopeptides, flagellin, double-stranded RNA, viral DNA, unmethylated CpG islands, levamisole, bacillus Calmette-Guerin, Isoprinosine, Zadaxin, PD-1 antagonists, PD-1 antibodies, CTLA antagonists, CTLA antibodies, interleukin, cytokines, GM-CSF, glycolipid, aluminum salt based, aluminum phosphate, alum, aluminum hydroxide, liposomes, TLR2 agonists, lipopeptide, nanoparticles, monophosphoryl lipid A, OPT-821 saponin, QS-21 saponin, oil in water nano-emulsions, and bacteria-like particle.

[046] In another embodiment, the pharmaceutical composition comprises a cytokine selected from the group consisting of IL-2, IL-12, IL-18, IL-2, IFN-γ, TNF, IL-4, IL-10, IL-13, IL-21, GM-CSF and TGF-β. In a further embodiment, the pharmaceutical composition comprises a chemokine.

[047] In a further embodiment, the therapeutic agent is administered as a pharmaceutical composition.

[048] In still another embodiment, the pharmaceutical composition comprises monoclonal antibodies, chemotherapeutics, hormonal therapeutic agents, retinoid receptor modulators, cytotoxic/cytostatic agents, antineoplastic agents, antiproliferative agents, anti-mTOR agents, anti-Her2 agents, anti-EGFR agents, prenyl-protein transferase inhibitors, HMG-CoA reductase inhibitors, nitrogen mustards, nitroso ureas, angiogenesis inhibitors, bevacizumab, inhibitors of cell proliferation and survival signaling pathway, apoptosis inducing agents, agents that interfere with cell cycle checkpoints, agents that interfere with receptor tyrosine kinases (RTKs), integrin blockers, NSAIDs, PPAR agonists, inhibitors of inherent multidrug resistance (MDR), anti-emetic agents, agents useful in the treatment of anemia, agents useful in the treatment of neutropenia, immunologic-enhancing drugs, biphosphonates, aromatase inhibitors, agents inducing terminal differentiation of neoplastic cells, γ-secretase inhibitors, cancer vaccines (*e.g.,* active immunotherapy), monoclonal antibody therapeutics (*e.g.,* passive immunotherapy), and any combination thereof.

[049] In another embodiment, the therapeutic compositions of the invention can further include PD-1/PD-L1 inhibitors (cytotoxic T cell lymphocyte (CTLs) immunotherapy), CTLA-4 immunotherapy, CDK4/6 inhibitors (target therapy), PI3K inhibitors (target therapy), mTOR inhibitors (target therapy), AKT inhibitors (target therapy), Pan-Her inhibitors (target therapy). These inhibitors can be modified to generate the respective monoclonal antibody as well. Such antibodies can be included in therapeutic compositions of the invention.

[050] In another embodiment, the pharmaceutical composition comprises a pharmaceutically acceptable carrier. In a further embodiment, the pharmaceutical composition is a cancer vaccine. In still another embodiment, the pharmaceutical composition is formulated for subcutaneous administration. In still another embodiment, the pharmaceutical composition is formulated for intramuscular administration. In still another embodiment, the pharmaceutical composition is formulated for intra-arterial administration. In still another embodiment, the pharmaceutical composition is formulated for intravenous administration.

[051] Another embodiment of the invention encompasses a method of treating a patient in need thereof comprising administering to the patient a therapeutically effective amount of the therapeutic composition comprising Globo H and KLH. In one embodiment, the patient has been diagnosed with or is suspected of having cancer. In another embodiment, the cancer is an epithelial cancer. In a further embodiment, the cancer is breast cancer. In still another embodiment, the therapeutically effective amount of a Globo-H moiety in the pharmaceutical/therapeutic composition may range from about 0.001μg/kg to about 250 mg/kg. In yet a further embodiment, the therapeutically effective amount Globo-H moiety in the pharmaceutical/therapeutic composition comprises about 10 μg/kg to about 50 μg/kg of one therapeutic conjugate per dose. In yet a further embodiment, the therapeutically effective amount Globo-H moiety in the pharmaceutical/therapeutic composition comprises about 0.10 μg/kg to about 0.75 μg/kg of one therapeutic conjugate per dose.

[052] In still another embodiment, the therapeutically effective amount of the Globo-H-KLH complex in the therapeutic composition may range from about 0.001μg/kg to about 250 mg/kg. In yet a further embodiment, the therapeutically effective amount of the Globo-H-KLH complex in the therapeutic composition comprises about 10 μg/kg to about 50 μg/kg of one therapeutic conjugate per dose. In yet a further embodiment, the therapeutically effective amount of the Globo-H-KLH complex in the therapeutic composition comprises about 0.60 μg/kg to about 4.50 μg/kg of one therapeutic conjugate per dose.

[053] In still another embodiment, the method is capable of extending progression free survival over a control placebo by about or at least 1 week. In still another embodiment, the method is capable of extending progression free survival over a control placebo by about or at least 2 weeks. In still another embodiment, the method is capable of extending progression free survival over a control placebo by about or at least 1 month. In still another embodiment, the method is capable of extending progression free survival over a control placebo by about or at least 3 months. In still another embodiment, the method is capable of extending progression free survival over a control placebo by about or at least 6 months. In yet another embodiment, the method is capable of extending or overall survival over a control placebo by about or at least 12 months.

BRIEF DESCRIPTION OF THE FIGURES

[054] A more complete understanding of the invention may be obtained by reference to the accompanying drawings, when considered in conjunction with the subsequent detailed description. The embodiments illustrated in the drawings are intended only to

exemplify the invention and should not be construed as limiting the invention to the illustrated embodiments.

[055] Figure 1A shows the chemical structure Globo H and as well as several exemplary Globo H analogs. Glc stands for glucose, Gal stands for galactose, GalNAc stands for N-acetylgalactosamine, and Fuc stands for fucose. Figure 1B shows an exemplary Globo H-KLH subunit conjugated by way of an MMCCH linker.

[056] Figure 2A shows an exemplary Globo H-KLH subunit conjugation synthesis pathway. Figure 2B shows Globo H-KLH dimers and trimers of the invention compared to Globo H conjugates disclosed in Slovin et al (1999), Proc Natl Acad Sci USA 96:5710-5 and Gilewski et al (2001), Proc Natl Acad Sci USA 98: 3270-5.

[057] Figure 3 shows the result of multi-angle laser scattering spectrometry (MALS) of native KLH (8.3 MDa).

[058] Figure 4 shows the result of size exclusion chromatography of native KLH (8.3 MDa).

[059] Figure 5 shows the chronological expansion of B/$CD3^+$T/$CD4^+$T/$CD8^+$T cell populations in Lewis rats immunized with a Globo H-KLH glycoconjugate according to the invention. Panels A-D represented B cell, CD3 T cell, CD4 T cell, and CD8 T cell populations, respectively. Data were presented as percentage of cell numbers in indicated group normalized to the percentage of cell numbers of PBS group. Multiple comparisons were analyzed using two-way ANOVA, followed by Bonferroni's post hoc tests. *, $p<0.05$, **, $p<0.01$, and ***, $p<0.001$ compared with PBS.

[060] Figure 6 shows the chronological changes in reciprocal titers of (A) IgM and (B) IgG antibodies in the blood from Lewis rats immunized with the glycoconjugate (Globo H-KLH) of the invention.

[061] Figure 7 shows the IgM antibody titers in mice in response to the glycoconjugate (Globo H-KLH) of the invention.

[062] Figure 8 illustrates the immunogenicity of C57BL/6 mice that were immunized with PBS, adjuvant only, or Globo H-KLH + adjuvant on day 0, 5, and 10. The sera were collected on day 14 for ELISA analysis to determine the anti-Globo H IgG and IgM production.

[063] Figure 9 illustrates the complement dependent cytotoxicity in which Globo H(+) or Globo H(-) TOV21G cells were plated in a 96-well plate. Anti-Globo H sera or control sera were added at a dilution of 1:50 or 1:100. The plate was then added with/without complement. The complement dependent cytotoxicity (CDC) was determined by LDH assay.

[064] Figure 10 illustrates the cytotoxicity of Globo H(+) or Globo H(-) TOV21G cells that were plated in a 96-well plate. Anti-Globo H sera or control sera were added at a dilution of 1:50 or 1:100. Human NK cells isolated from peripheral blood mononuclear cells (PBMCs) and activated with anti-CD3 antibody were used as effector cells. The effector cells were or were not then added for antibody-dependent cell-mediated cytotoxicity (ADCC) reaction at a ET ratio of 4:1, 2:1, or 1:1. The cytotoxicity was normalization with no mouse serum control of each cells in different ET ratio.

[065] Figure 11 illustrates irradiated NOD-SCID mice that were injected intraperitoneally with 1x 10 6 of Globo H-positive TOV21G cells on day 0. Anti-sera were separately collected from C57BL/6 mice after 3 vaccinations of 3 different treatments (PBS, adjuvant only, and Globo H-KLH/adjuvant). The NOD-SCID mice were given intraperitoneally 200 μl of aforementioned anti-sera for each mouse on day 0, 2, 4, 6, 9, 11, 13, and 16. The tumor images were traced by IVIS imaging system on day 3, 7, and 9.

[066] Figure 12 illustrates LLC1 (a lung cancer epithelial cancer cell line) tumor growth on Globo H KLH immunized C57BL/6 mice that were subcutaneously vaccinated with PBS, adjuvant only, or Globo H-KLH/adjuvant on day 0, 5, and 11. 1x105 LLC1 cells were subcutaneously injected into each mouse on day 16. The treatments were then subcutaneously administered on day 29 and 34. Tumor sizes were monitored on day 16, 21,25, 29, 32, 34, 37.

[067] Figure 13 shows a Table Summary of peptide identification.

[068] Figure 14 illustrates the identification details of Globo-H conjugated peptides for sample 1 (1^{st} LC-MS/MS) for KLH1 (a) and KLH2 (b).

[069] Figure 15 illustrates the identification details of Globo-H conjugated peptides for sample 2 (1^{st} LC-MS/MS) for KLH1 (a) and KLH2 (b).

[070] Figure 16 illustrates the identification details of Globo-H conjugated peptides for sample 3 (1^{st} LC-MS/MS) for KLH1 (a) and KLH2 (b).

[071] Figure 17 illustrates the identification details of Globo-H conjugated peptides for sample 4 (1st LC-MS/MS) for KLH1 (a) and KLH2 (b).

[072] Figure 18 illustrates the identification details of Globo-H conjugated peptides for sample 1 (2st LC-MS/MS) for KLH1 (a) and KLH2 (b).

[073] Figure 19 illustrates the identification details of Globo-H conjugated peptides for sample 2 (2st LC-MS/MS) for KLH1 (a) and KLH2 (b).

[074] Figure 20 illustrates the identification details of Globo-H conjugated peptides for sample 3 (2st LC-MS/MS) for KLH1 (a) and KLH2 (b).

[075] Figure 21 illustrates the identification details of Globo-H conjugated peptides for sample 4 (1st LC-MS/MS) for KLH1 (a) and KLH2 (b).

[076] Figure 22 Figure 14 illustrates the identification details of MMCCH-conjugated peptides for sample 1 (1st LC-MS/MS) for KLH1 (a) and KLH2 (b).

[077] Figure 23 illustrates the identification details of MMCCH-conjugated peptides for sample 2 (1st LC-MS/MS) for KLH1 (a) and KLH2 (b).

[078] Figure 24 illustrates the identification details of MMCCH-conjugated peptides for sample 3 (1st LC-MS/MS) for KLH1 (a) and KLH2 (b).

[079] Figure 25 illustrates the identification details of MMCCH-conjugated peptides for sample 4 (1st LC-MS/MS) for KLH1 (a) and KLH2 (b).

[080] Figure 26 illustrates the identification details of MMCCH-conjugated peptides for sample 1 (2st LC-MS/MS) for KLH1 (a) and KLH2 (b).

[081] Figure 27 illustrates the identification details of MMCCH-conjugated peptides for sample 2 (2^{st} LC-MS/MS) for KLH1 (a) and KLH2 (b).

[082] Figure 28 illustrates the identification details of MMCCH-conjugated peptides for sample 3 (2^{st} LC-MS/MS) for KLH1 (a) and KLH2 (b).

[083] Figure 29 illustrates the identification details of MMCCH-conjugated peptides for sample 4 (1^{st} LC-MS/MS) for KLH1 (a) and KLH2 (b).

[084] Figure 30 illustrates the summary of Globo-H conjugated lysine identification for (1^{st} LC-MS/MS) for KLH1 (a) and KLH2 (b) and (2^{nd} LC-MS/MS) for KLH1 (c) and KLH2 (d).

[085] Figure 31 illustrates the summary of MMCCH-conjugated lysine identification for (1^{st} LC-MS/MS) for KLH1 (a) and KLH2 (b) and (2^{nd} LC-MS/MS) for KLH1 (c) and KLH2 (d).

[086] Figure 32 illustrates a summary of the Globo-H conjugation analysis in the first (a) and second (b) LC-MS/MS runs.

[087] Figure 33(a) illustrates chemical formula: C(56) H(91) N(5) O(33) S(1), Monoisotopic MW addition: 1393.5317 Da. Figure 33(b) illustrates chemical formula: 1. 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.

[088] Figure 34(a) illustrates the chemical structure of MMCCH derivative. Chemical formula: C(16) H(24) N(4) O(3) S(1), Monoisotopic MW addition: 352.1569 Da. Figure 34(b) illustrates a deamidated MMCCH derivative, Chemical formula: C(16) H(22) N(2) O(4) S(1), Monoisotopic MW addition: 338.1300 Da.

DETAILED DESCRIPTION OF THE INVENTION

[089] The practice of the present invention will employ, unless otherwise indicated, conventional techniques of molecular biology, microbiology, and immunology, which are within the skill of the art. Such techniques are explained fully in the literature. See, for example, Molecular Cloning A Laboratory Manual, 2nd Ed., ed. by Sambrook, Fritsch and Maniatis (Cold Spring Harbor Laboratory Press, 1989); DNA Cloning, Volumes I and II (D. N. Glover ed., 1985); Culture Of Animal Cells (R. I. Freshney, Alan R. Liss, Inc., 1987); Immobilized Cells And Enzymes (IRL Press, 1986); B. Perbal, A Practical Guide To Molecular Cloning (1984); the treatise, Methods In Enzymology (Academic Press, Inc., N.Y.); Gene Transfer Vectors For Mammalian Cells (J. H. Miller and M. P. Calos eds., 1987, Cold Spring Harbor Laboratory); Methods In Enzymology, Vols. 154 and 155 (Wu et al. eds.), Immunochemical Methods In Cell And Molecular Biology (Mayer and Walker, eds., Academic Press, London, 1987); Antibodies: A Laboratory Manual, by Harlow and Lanes (Cold Spring Harbor Laboratory Press, 1988); and Handbook Of Experimental Immunology, Volumes I-IV (D. M. Weir and C. C. Blackwell, eds., 1986).

[090] The use of the word "a" or "an" when used in conjunction with the term "comprising" in the claims and/or the specification may mean "one," but it is also consistent with the meaning of "one or more," "at least one," and "one or more than one."

[091] Throughout this application, the term "about" is used to indicate that a value includes for example, the inherent variation of error for a measuring device, the method being employed to determine the value, or the variation that exists among the study subjects. Typically the term is meant to encompass approximately or less than 1%, 2%, 3%, 4%, 5%, 6%, 7%, 8%, 9%, 10%, 11%, 12%, 13%, 14%, 15%, 16%, 17%, 18%, 19% or 20% variability depending on the situation.

[092] As used herein, the term "alkyl" refers to a straight or branched monovalent hydrocarbon containing, unless otherwise stated, 1-20 carbon atoms, e.g., C_1-C_8 or C_1-C_4, which can be substituted or unsubstituted. Examples of alkyl include, but are not limited to, methyl, ethyl, *n*-propyl, *i*-propyl, *n*-butyl, *i*-butyl, and *t*-butyl.

[093] The use of the term "or" in the claims is used to mean "and/or" unless explicitly indicated to refer to alternatives only or the alternatives are mutually exclusive, although the disclosure supports a definition that refers to only alternatives and "and/or."

[094] As used in this specification and claim(s), the words "comprising" (and any form of comprising, such as "comprise" and "comprises"), "having" (and any form of having, such as "have" and "has"), "including" (and any form of including, such as "includes" and "include") or "containing" (and any form of containing, such as "contains" and "contain") are inclusive or open-ended and do not exclude additional, unrecited elements or method steps. It is contemplated that any embodiment discussed in this specification

can be implemented with respect to any method or composition of the invention, and vice versa. Furthermore, compositions of the invention can be used to achieve methods of the invention.

[095] "Treating" or "treating" is referred to herein as administration of a therapeutic composition to a subject with the purpose to cure, alleviate, relieve, remedy, prevent, or ameliorate a disorder, symptoms of the disorder, a disease state secondary to the disorder, or predisposition toward the disorder.

[096] An "effective amount" is an amount of a therapeutic composition that is capable of producing a medically desirable result as delineated herein in a treated subject. The medically desirable result may be objective (*i.e.,* measurable by some test or marker) or subjective (*i.e.,* subject gives an indication of or feels an effect).

[097] "Disease amenable to treatment with a therapeutic composition" as referred to herein means any procedures, conditions, disorders, ailments and/or illnesses which can be treated by the administration of the therapeutic compositions disclosed herein.

[098] A "proliferative disorder" is one in which too many of some type of cell are produced resulting in deterioration of health. A proliferative disorder can be benign or malignant. Proliferative disorders can include for example, cancer.

[099] A "cancer" that can be treated by the therapeutic compositions disclosed herein, is an abnormal growth of cells. Cancer cells have lost normal control mechanisms and thus are able to expand continuously, invade adjacent tissues, migrate to distant parts of the body, and promote the growth of new blood vessels from which the cells derive nutrients.

As used herein, a cancer can be malignant or benign. Cancer can develop from any tissue within the body. As cells grow and multiply, they form a mass of tissue, called a tumor. The term tumor refers to an abnormal growth or mass. Tumors can be cancerous (malignant) or noncancerous (benign). Cancerous tumors can invade neighboring tissues and spread throughout the body (metastasize). Benign tumors, however, generally do not invade neighboring tissues and do not spread throughout the body. Cancer can be divided into those of the blood and blood-forming tissues (leukemias and lymphomas) and "solid" tumors. "Solid" tumors can be carcinomas or sarcomas.

[0100] Cancers that may be treated by the therapeutic compositions of the invention include those classified by site include cancer of the oral cavity and pharynx (lip, tongue, salivary gland, floor of mouth, gum and other mouth, nasopharynx, tonsil, oropharynx, hypopharynx, other oral/pharynx); cancers of the digestive system (esophagus; stomach; small intestine; colon and rectum; anus, anal canal, and anorectum; liver; intrahepatic bile duct; gallbladder; other biliary; pancreas; retroperitoneum; peritoneum, omentum, and mesentery; other digestive); cancers of the respiratory system (nasal cavity, middle ear, and sinuses; larynx; lung and bronchus; pleura; trachea, mediastinum, and other respiratory); cancers of the mesothelioma; bones and joints; and soft tissue, including heart; skin cancers, including melanomas and other non-epithelial skin cancers; Kaposi's sarcoma and breast cancer; cancer of the female genital system (cervix uteri; corpus uteri; uterus, ovary; vagina; vulva; and other female genital); cancers of the male genital system (prostate gland; testis; penis; and other male genital); cancers of the urinary system (urinary bladder; kidney and renal pelvis; ureter; and other urinary); cancers of the eye and orbit; cancers of the brain and nervous system (brain; and other nervous system);

cancers of the endocrine system (thyroid gland and other endocrine, including thymus); lymphomas (Hodgkin's disease and non-Hodgkin's lymphoma), multiple myeloma, and leukemias (lymphocytic leukemia; myeloid leukemia; monocytic leukemia; and other leukemias).

[0101] Other cancers, classified by histological type, that may be suitable targets for the therapeutic compositions according to the present invention include, but are not limited to, neoplasm, malignant; Carcinoma, NOS; Carcinoma, undifferentiated, NOS; Giant and spindle cell carcinoma; Small cell carcinoma, NOS; Papillary carcinoma, NOS; Squamous cell carcinoma, NOS; Lymphoepithelial carcinoma; Basal cell carcinoma, NOS; Pilomatrix carcinoma; Transitional cell carcinoma, NOS; Papillary transitional cell carcinoma; Adenocarcinoma, NOS; Gastrinoma, malignant; Cholangiocarcinoma; Hepatocellular carcinoma, NOS; Combined hepatocellular carcinoma and cholangiocarcinoma; Trabecular adenocarcinoma; Adenoid cystic carcinoma; Adenocarcinoma in adenomatous polyp; Adenocarcinoma, familial polyposis coli; Solid carcinoma, NOS; Carcinoid tumor, malignant; Bronchioloalveolar adenocarcinoma; Papillary adenocarcinoma, NOS; Chromophobe carcinoma; Acidophil carcinoma; Oxyphilic adenocarcinoma; Basophil carcinoma; Clear cell adenocarcinoma, NOS; Granular cell carcinoma; Follicular adenocarcinoma, NOS; Papillary and follicular adenocarcinoma; Nonencapsulating sclerosing carcinoma; Adrenal cortical carcinoma; Endometroid carcinoma; Skin appendage carcinoma; Apocrine adenocarcinoma; Sebaceous adenocarcinoma; Ceruminous adenocarcinoma; Mucoepidermoid carcinoma; Cystadenocarcinoma, NOS; Papillary cystadenocarcinoma, NOS; Papillary serous cystadenocarcinoma; Mucinous cystadenocarcinoma, NOS; Mucinous adenocarcinoma;

Signet ring cell carcinoma; Infiltrating duct carcinoma; Medullary carcinoma, NOS; Lobular carcinoma; Inflammatory carcinoma; Paget's disease, mammary; Acinar cell carcinoma; Adenosquamous carcinoma; Adenocarcinoma w/ squamous metaplasia; Thymoma, malignant; Ovarian stromal tumor, malignant; Thecoma, malignant; Granulosa cell tumor, malignant; Androblastoma, malignant; Sertoli cell carcinoma; Leydig cell tumor, malignant; Lipid cell tumor, malignant; Paraganglioma, malignant; Extra-mammary paraganglioma, malignant; Pheochromocytoma; Glomangiosarcoma; Malignant melanoma, NOS; Amelanotic melanoma; Superficial spreading melanoma; Malig melanoma in giant pigmented nevus; Epithelioid cell melanoma; Blue nevus, malignant; Sarcoma, NOS; Fibrosarcoma, NOS; Fibrous histiocytoma, malignant; Myxosarcoma; Liposarcoma, NOS; Leiomyosarcoma, NOS; Rhabdomyosarcoma, NOS; Embryonal rhabdomyosarcoma; Alveolar rhabdomyosarcoma; Stromal sarcoma, NOS; Mixed tumor, malignant, NOS; Mullerian mixed tumor; Nephroblastoma; Hepatoblastoma; Carcinosarcoma, NOS; Mesenchymoma, malignant; Brenner tumor, malignant; Phyllodes tumor, malignant; Synovial sarcoma, NOS; Mesothelioma, malignant; Dysgerminoma; Embryonal carcinoma, NOS; Teratoma, malignant, NOS; Struma ovarii, malignant; Choriocarcinoma; Mesonephroma, malignant; Hemangiosarcoma; Hemangioendothelioma, malignant; Kaposi's sarcoma; Hemangiopericytoma, malignant; Lymphangiosarcoma; Osteosarcoma, NOS; Juxtacortical osteosarcoma; Chondrosarcoma, NOS; Chondroblastoma, malignant; Mesenchymal chondrosarcoma; Giant cell tumor of bone; Ewing's sarcoma; Odontogenic tumor, malignant; Ameloblastic odontosarcoma; Ameloblastoma, malignant; Ameloblastic fibrosarcoma; Pinealoma, malignant; Chordoma; Glioma, malignant;

Ependymoma, NOS; Astrocytoma, NOS; Protoplasmic astrocytoma; Fibrillary astrocytoma; Astroblastoma; Glioblastoma, NOS; Oligodendroglioma, NOS; Oligodendroblastoma; Primitive neuroectodermal; Cerebellar sarcoma, NOS; Ganglioneuroblastoma; Neuroblastoma, NOS; Retinoblastoma, NOS; Olfactory neurogenic tumor; Meningioma, malignant; Neurofibrosarcoma; Neurilemmoma, malignant; Granular cell tumor, malignant; Malignant lymphoma, NOS; Hodgkin's disease, NOS; Hodgkin's; paragranuloma, NOS; Malignant lymphoma, small lymphocytic; Malignant lymphoma, large cell, diffuse; Malignant lymphoma, follicular, NOS; Mycosis fungoides; Other specified non-Hodgkin's lymphomas; Malignant histiocytosis; Multiple myeloma; Mast cell sarcoma; Immunoproliferative small intestinal disease; Leukemia, NOS; Lymphoid leukemia, NOS; Plasma cell leukemia; Erythroleukemia; Lymphosarcoma cell leukemia; Myeloid leukemia, NOS; Basophilic leukemia; Eosinophilic leukemia; Monocytic leukemia, NOS; Mast cell leukemia; Megakaryoblastic leukemia; Myeloid sarcoma; and Hairy cell leukemia.

[0102] "Epithelial cancers" as defined herein refers to cancer(s) that develops from epithelium or related tissues in the skin, hollow viscera, and other organs. Epithelial cancers include but are not limited to breast cancer, lung cancer, liver cancer, buccal cancer, stomach cancer, colon cancer, nasopharyngeal cancer, dermal cancer, renal cancer, brain tumor, prostate cancer, ovarian cancer, cervical cancer, endometrial cancer, intestinal cancer, pancreatic cancer, and bladder cancer.

[0103] "Patient" or "Subject" as used herein refers to a mammalian subject diagnosed with or suspected of having or developing a proliferative disease such as cancer. Exemplary patients may be humans, apes, dogs, pigs, cattle, cats, horses, goats, sheep,

rodents and other mammalians that can benefit develop proliferative diseases such as cancer.

[0104] As used herein, "substantially purified" or "substantially isolated" refers to a molecule (e.g. a compound) in a state that it is separated from substantially all other molecules normally associated with it in its native state. Preferably, a substantially purified molecule is the predominant species present in a preparation. Particularly, a substantially purified molecule may be greater than 60% free, preferably 75% free, more preferably 90% free, and most preferably 95% free from the other molecules (exclusive of solvent) present in the natural mixture. The term "substantially purified" or "substantially isolated" is not intended to include molecules or substances present in their native state. In certain embodiments, the term "substantially purified" or "substantially isolated" includes purifying one KLH moiety from another KLH moiety (*e.g.,* substantially purifying or substantially isolating a KLH dimer moiety from a KLH trimer moiety). In another embodiment, the term "substantially purified" or "substantially isolated" does not include purifying one KLH moiety from another KLH moiety (e.g,, KLH dimers and KLH trimmers are included in a substantially purified or substantially isolated composition) but impurities are substantially removed.

[0105] "Administering" is referred to herein as providing a therapeutic composition of the invention to a patient. By way of example and not limitation, composition administration, e.g., injection, may be performed by intravenous (i.v.) injection, sub-cutaneous (s.c.) injection, intradermal (i.d.) injection, intraperitoneal (i.p.) injection, or intramuscular (i.m.) injection. One or more such routes may be employed. Parenteral administration can be, for example, by bolus injection or by gradual perfusion over time.

Alternatively, or concurrently, administration may be by the oral route. Additionally, administration may also be by surgical deposition of a bolus or positioning of a medical device.

[0106] "A patient in need thereof" is referred to herein as a patient diagnosed with or suspected of having a proliferative disorder. In one embodiment, the patient has or is likely to develop cancer.

[0107] As used herein, the term "antigen" is defined as any substance capable of eliciting an immune response, with or without the help of a protein carrier and/or an adjuvant. Preferably the antigen of the inventive compositions includes a carbohydrate and more preferably glycan-antigen and most preferably a Globo H moiety.

[0108] As used herein, the term "immunogenicity" refers to the ability of an immunogen, antigen, or vaccine to stimulate an immune response.

[0109] As used herein, the term "immunotherapy" refers to an array of treatment strategies based upon the concept of modulating the immune system to achieve a prophylactic and/or therapeutic goal.

[0110] As used herein, the term "epitope" is defined as the parts of an antigen molecule which contact the antigen binding site of an antibody or a T cell receptor.

[0111] The "therapeutic compositions" of the invention preferably include "therapeutic conjugates" and/or "therapeutic antibodies." The therapeutic conjugates include at least one antigen linked to a carrier. Preferably, the linkage of the therapeutic conjugate is covalent. In one embodiment of the therapeutic conjugate, the antigen is a glycan such as

Globo H moiety, and the carrier is a KLH moiety and/or a KLH moiety subunit. As such, the term therapeutic conjugate encompasses one or more KLH moiety subunits linked to one or more Globo H moieties. In one embodiment, the term therapeutic conjugate encompasses a one or more KLH moieties linked to about or at least 1, 10, 10^2 or 10^3 Globo H moieties. In another embodiment, the term therapeutic conjugate encompasses one or more KLH moieties linked to about 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100, 101, 102, 103, 104, 105, 106, 107, 108, 109, 110, 111, 112, 113, 114, 115, 116, 117, 118, 119, 120, 121, 122, 123, 124, 125, 126, 127, 128, 129, 130, 131, 132, 133, 134, 135, 136, 137, 138, 139, 140, 141, 142, 143, 144, 145, 146, 147, 148, 149, 150, 151, 152, 153, 154, 155, 156, 157, 158, 159, 160, or more Globo H moieties. Another embodiment encompasses isolated dimers, trimers, tetramers, pentamers or hexamers of such Globo H linked KLH moiety subunits, or combinations thereof.

[0112] In one embodiment, the therapeutic conjugate is: Fucα(1→2)Galβ(1→3)GalNAcβ(1→3)Galα(1→4)Galβ(1→4)Gluβ(1-O-ethylhydrazyl-1-carbonyl-cyclohexyl-4-(methyl-N-maleimido)-3-(thiobutyl-imidyl)-Keyhole Limpet Haemocyanin (KLH) also referred to as OPT-822.

[0113] "Therapeutic antibodies" are defined to be as antibodies (as further defined below) that specifically bind the inventive therapeutic conjugates and preferably the Globo H moiety portion of the therapeutic conjugates.

[0114] As used herein, the term "vaccine" refers to a therapeutic composition that contains a therapeutic conjugate that is used to confer immunity against a disease associated with the antigen. Cancer vaccines are designed to boost the body's natural ability to protect itself, through the immune system, from dangers posed by damaged or abnormal cells such as cancer cells. A protective immune response is one that reduces the severity of disease, including but not limited to, prevention of disease, delay in onset of disease, decreased severity of symptoms, decreased morbidity, and delayed mortality. Preferably, a vaccine is capable of activating both humoral immune response (e.g. stimulation of the production of antibodies by B lymphocytes) and cellular immune response (e.g. an immune response that is mediated by T-lymphocytes and/or other cells, such as NK cells and macrophages). Standard assays have been developed to determine the immune response such as enzyme-linked immunosorbent assay (ELISA), flow cytometry, cell proliferation assay, CTL assays, and ADCC/CDC assays.

[0115] As used herein, the term "glycan" refers to a polysaccharide, or oligosaccharide. Glycan is also used herein to refer to the carbohydrate portion of a glycoconjugate, such as a glycoprotein, glycolipid, glycopeptide, glycoproteome, peptidoglycan, lipopolysaccharide or a proteoglycan. Glycans usually consist solely of O-glycosidic linkages between monosaccharides. For example, cellulose is a glycan (or more specifically a glucan) composed of β-1,4-linked D-glucose, and chitin is a glycan composed of β-1,4-linked N-acetyl-D-glucosamine. Glycans can be homo or heteropolymers of monosaccharide residues, and can be linear or branched. Glycans can be found attached to proteins as in glycoproteins and proteoglycans. They are generally found on the exterior surface of cells. O- and N-linked glycans are very common in

eukaryotes but may also be found, although less commonly, in prokaryotes. N-Linked glycans are found attached to the R-group nitrogen (N) of asparagine in the sequon. The sequon is an Asn-X-Ser or Asn-X-Thr sequence, where X is any amino acid except praline. The preferred glycan is a Globo H moiety.

[0116] Globo H is a hexasaccharide, which is a member of a family of antigenic carbohydrates that are highly expressed on a various types of cancers, especially cancers of breast, prostate, pancreas, stomach, ovary, colon, and lung. In illustrative embodiments, certain patients exhibited no anti-Globo H antibody levels at time zero, and after immunization with the therapeutic composition of the invention high titers were detected. In other illustrative embodiments, certain patients exhibited anti-Globo H antibody levels at time zero, and after immunization with the therapeutic composition of the invention high titers were detected. In certain embodiments, the anti-Globo H antibody is expressed on the cancer cell surface as a glycolipid and possibly as a glycoprotein. In other embodiments, the serum of breast cancer patients contained high levels of antibodies against the Globo H epitope. In certain embodiments, this epitope is also targeted by the monoclonal antibodies Mbr1, VK9 and anti-SSEA-3 in immunohistochemistry studies. Although certain normal tissues also react with Mbr1, including normal breast, pancreas, small bowel, and prostate tissue, the antigen in these tissues is predominantly localized at the secretary borders where access to the immune system is restricted.

[0117] "Globo H moiety" is defined herein to be a glycan (i.e., a molecule containing a sugar moiety) that is Globo H or a fragment or analog thereof. Globo H is a glycan containing the hexasaccharide epitope (Fucα1→2 Galβ1→3 GalNAcβ1→3 Galα1→4

Galβ1→4 Glc), and optionally, a non-sugar moiety. Its fragment is a glycan containing a fragment of the hexasaccharide epitope and, if applicable, the non-sugar moiety. These oligosaccharides can be prepared by routine methods. (See Huang et al., Proc. Natl. Acad. Sci. USA 103:15-20 (2006)). If desired, they can be linked to a non-sugar moiety. U.S. patent application Ser. No. 12/485,546 relates to a method of producing antibody specific to Globo H or its fragment by administering to a non-human mammal (e.g., mouse, rabbit, goat, sheep, or horse) the immune composition described above and isolating from the mammalian antibody that binds to Globo H or its fragment.

[0118] Analogs of Globo H can be generated using glycan microarray and include those disclosed in Wang et al., Proc Natl Acad Sci U S A. 2008 August 19; 105(33): 11661–11666 and shown in Figure 1.

[0119] Globo H analogs preferably bind antibodies VK-9, Mbr1, and anti-SSEA-3. Preferably, the Globo H Analogs bind with a particular dissociation constant ($K_{D,surf}$). The Langmuir isotherm can be used for analyzing the binding curves to generate the dissociation constants on surface ($K_{D,surf}$). At the equilibrium conditions during incubation, the mean fluorescence of the replicate spots (F_{obs}) can be described by:

$$F_{obs} = F_{max}[P]/(K_{D,surf} + [P])$$

where F_{max} is the maximum fluorescence intensity, a measure of the amount of active carbohydrate on the surface, [P] is the total antibody concentration, and $K_{D,surf}$ is the equilibrium dissociation constant for surface carbohydrate and the antibody. As described in Wang et al. In some embodiments the preferred ($K_{D,surf}$) of Globo H analogs

is at least, about or exactly 0.4, 0.5., 0.6, 0.7, 0.8, 0.9, 1.0, 1.1, 1.2, 1.3, 1.4, 1.5 or 1.6 nM with respect to the VK-9, Mbr1, and anti-SSEA-3 antibodies described in Wang et al.

[0120] "Keyhole Limpet Hemocyanin" (KLH) is a large, multisubunit, oxygen-carrying, metalloprotein found in the hemolymph of the giant keyhole limpet, *Megathura crenulata*. KLH is heterogeneous glycosylated protein consisting of subunits with a molecular weight of about 350,000 to about 390,000 in aggregates with molecular weights of about 400 kDA (*e.g.*, a KLH monomer) to about 8000 kDA (*e.g.*, a KLH didecamer). Each domain of a KLH subunit contains two copper atoms that together bind a single oxygen molecule. When oxygen is bound to hemocyanin, the molecule takes on a distinctive transparent, opalescent blue color. In certain embodiments, the KLH protein is potently immunogenic yet safe in humans. In certain embodiments, KLH may be purified from the hemolymph of *Megathura crenulata* by a series of steps that typically includes ammonium sulfate precipitation and dialysis, and may involve chromatographic purification to obtain the highest purity. In certain embodiments, KLH purification may also include endotoxin removal, but this step may be unnecessary because the endotoxin can serve as an adjuvant when injected for antibody production. Preferably, a high quality KLH preparation with the clear opalescent blue color is the best indicator of KLH solubility. In certain embodiments, the KLH monomeric units assemble into a large multimer (decamer or didecamer) with a total molecular weight of about 4,000 kDa to 8,000 kDa. "Keyhole Limpet Hemocyanin moiety" or "KLH moiety" is defined herein to be a KLH1 (SEQ ID NO: 1) or KLH2 (SEQ ID NO. 2) protein or a protein substantially identical thereto or a mixture thereof. Substantially identical in this context means each KLH moiety has an amino sequence at least, about or exactly: 100,

99, 98, 97, 96, 95, 94, 93, 92, 91, 90, 89, 88, 87, 86, 85, 84, 83, 82, 81, 80, 79, 78, 77, 76 or 75 percent identical to that of native wild type KLH. In certain embodiments, the KLH of the invention has enhanced immunogenic activity, particularly enhanced anti-tumor activity. In certain embodiments, the KLH in the composition of the present invention comprises an intact, non-degraded subunit of approximately 400,000 in molecular weight. In other embodiments, the KLH of the invention comprises higher KLH multimers.

[0121] In certain embodiments, the higher KLH multimers have molecular weights of approximately 8-10 million with sedimentation coefficients of about 92-107S. The amount of higher KLH multimers present is based on sedimentation-equilibrium and/or sedimentation-velocity ultracentrifugation analyses. In other embodiments, the KLH of the invention demonstrates an enhanced immunogenic activity, particularly enhanced anti-tumor activity. The enhanced immunogenic activity is seen for example, but not limited, (a) with injection of KLH (without adjuvant), (b) with KLH used as an adjuvant, (c) with KLH used as a carrier immunogen for haptens or weakly immunogenic antigens, and (d) with KLH used as an anti-tumor agent. The KLH composition of the invention exhibits enhanced anti-tumor activity for many tumors, including, but not limited to, bladder, breast, ovarian tumors, etc. In certain embodiments, two KLH moieties can form a dimer via a covalent linkage between KLH monomers. Without being limited by theory, it is believed that the covalent linkage between KLH moieties is through a disulfide bond. In certain embodiments, two or more KLH moieties can form a dimer, trimer, tetramer, pentamer, etc. via a covalent linkage between KLH monomers, dimers,

trimers, etc. Without being limited by theory, it is believed that the covalent linkage between KLH moieties is through a disulfide bond.

[0122] There are a variety of methods for linking of a KLH moiety to an antigen, including direct conjugation and conjugation with a bifunctional linker group such as 4-(4-N-maleimidomethyl) cyclohexane-1-carboxyl hydrazide (MMCCH). Such linkage techniques are disclosed in U.S. Patent No. 6,544,952. In some embodiments, to prepare the therapeutic conjugates of the invention, for example, the Globo H allyl glycoside is converted to an aldehyde by ozonolysis and the aldehyde group is attached to the NH groups on the crosslinker MMCCH, giving Globo H-MMCCH; the carrier protein, KLH, is subjected to thiolation to produce KLH-SH; and the sulfhydryl groups on thiolated KLH are then attached to the maleimide group on the MMCCH, producing Globo H-KLH conjugates.

[0123] In one embodiment, Globo H allyl glycoside is prepared via chemical synthesis. A thiolating reagent, 2-iminothiolane and cGMP-grade KLH and 4-(4-*N*-maleimidomethyl)-cyclohexane-1-carboxyl hydrazide (MMCCH) linker are also used. In some embodiments the following steps are carried out: 1) Conversion of Globo H allyl glycoside to the Globo H-aldehyde; 2) Coupling of Globo H-aldehyde with MMCCH to Globo H-MMCCH, separately; 3) Chemical thiolation of KLH; 4) Conjugation of Globo H-MMCCH to the thiolated KLH; and 5) Purification of the Globo H-KLH conjugate (OPT-822). See for example Figure 2a.

[0124] In certain embodiments, during conjugation of a Globo H moiety protein to a KLH moiety, a KLH moiety protein in certain embodiments shows a reduction in

molecular weight compared to the intact molecule preferably due to Globo H moiety subunit dissociation. In other embodiments, the conjugation methods disclosed herein result in a KLH subunit dissociation not previously reported. While not wishing to be bound to any particular theory, it is envisaged that the high glycosylation level of the inventive Globo H moiety-KLH moiety subunit conjugates results in the formation hydrogen bonding between the Globo H moieties. As such, in certain embodiments, the Van Der Waals forces and hydrophobic interactions between the KLH moiety subunits are displaced by Globo H hydrogen bonding and this leads to KLH moiety subunit separation. Following conjugation, the KLH moiety subunits of a Globo H moiety-KLH moiety conjugate preferably aggregate to form novel monomers, dimers, trimers, tetramers, pentamers or hexamers or any combination thereof. The resulting therapeutic Globo H moiety-KLH moiety conjugates have an unexpectedly large epitope ratio resulting in unexpectedly superior immunogenic attributes. In certain embodiments, the Globo H moieties are conjugated to Lysines on KLH1 and KLH2. In other embodiments, the Globo H moieties are not conjugated to Lysines on KLH1 and KLH2. In certain embodiments, the Globo H-conjugated lysine sites are found conserved in the peptide mapping analysis suggesting the Globo H-KLH composition is unique in its structure.

[0125] In one embodiment, therapeutic compositions of the invention include one or more KLH moiety subunits wherein at least one such subunit is conjugated to at least, about or exactly 1, 10, 10^2 or 10^3 times: 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88,

89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100, 101, 102, 103, 104, 105, 106, 107, 108, 109, 110, 111, 112, 113, 114, 115, 116, 117, 118, 119, 120, 121, 122, 123, 124, 125, 126, 127, 128, 129, 130, 131, 132, 133, 134, 135, 136, 137, 138, 139, 140, 141, 142, 143, 144, 145, 146, 147, 148, 149, 150, 151, 152, 153, 154, 155, 156, 157, 158, 159 or 160 or more Globo H moieties.

[0126] The inventors found using mass spectrometric analysis that the Globo H moieties are conjugated to lysine residues of KLH. In certain embodiments, it is therefore preferred that the Globo H moieties are conjugated to lysine residues.

[0127] In one embodiment, there are total of exactly or about 145, 146, 147, 148, 149, 150, 151, 152, 153, 154, 155, 156, 157, 158, 159, 160 total lysine residues per KLH moiety subunit. In another embodiment there are exactly or about 150 or 156 lysine residues per KLH moiety subunit. In another embodiment, there are exactly or about 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100, 101, 102, 103, 104, 105, 106, 107, 108, 109 or 110 lysine conjugation sites on each KLH moiety subunit available for binding to or actually bound to a Globo H moiety. In another embodiment, there are 62, 66, 67, 68, 70, 72, 76, 86, 87, 88, 90, 92, 93, 100 such lysine conjugation sites on each KLH moiety subunit. Lysine conjugation sites are those lysine residues in the KLH moiety which are available for binding or actually bind to a Globo H moiety and/or a linker to a Globo H moiety such as for example an MMCCH linker.

[0128] In certain therapeutic embodiments containing a mixture of moiety subunits (e.g., KLH1 and KLH2 or variants thereof), total available lysine (for both subunits) as are

counted together across the different subunit types the and may be or are exactly about 290, 291, 292, 293, 294, 295, 296, 297, 298, 299, 300, 301, 302, 303, 304, 305, 306, 307, 308, 309 or 310 in number. In such embodiments, there are or may be exactly or about 130, 131, 132, 133, 134, 135, 136, 137, 138, 139, 140, 141, 142, 143, 144, 145, 146, 147, 148, 149, 150, 151, 152, 153, 154, 155, 156, 157, 158, 159 or 160 lysine conjugation sites together across the different subunits (e.g., KLH1 and KLH2 or variants thereof). In other such embodiments, there are 136, 137, 141, 140, 143, 147 or 155 lysine conjugation sites.

[0129] In a most preferred embodiment there are 136, 137, 140, 141, 143, 147 or 155 and lysine conjugation sites among the total 306 lysine residues in KLH1/KLH2.

[0130] In certain embodiments, the therapeutic compositions of the invention contain a mixture of KLH moiety subunit-Globo H moiety conjugates wherein such conjugates remain monomers or form dimers, trimers, tetramers, pentamers or hexamers or any combination thereof. In another embodiment, the therapeutic compositions of the invention include isolated KLH moiety subunit-Globo H moiety conjugate monomers, dimers, trimers or tetramers or combinations of thereof. In a further embodiment, the therapeutic compositions of the invention include only KLH moiety subunit-Globo H moiety conjugate dimers and trimers.

[0131] In another embodiment, the therapeutic compositions contain at least two KLH moiety subunits wherein each of the two KLH-moiety subunits is linked to different glycans. Other tumor-associated glycan antigens linkable to KLH moiety subunits can include but are not limited to GM2, GD2, GD3, fucosyl, GM1, sTn, sialyl-Lewis^x,

Lewis^{x}, sialyl Lewis^{a}, Lewis^{a}, sTn, TF, polysialic acid, Lewis^{y}, mucins, T antigen, and the like. In some embodiments only, at least or about 10, 20, 30, 40, 50, 60, 70, 80, 90 or 100 percent of the KLH moiety subunits in a therapeutic composition are linked to a Globo H moiety whereas the remaining KLH moiety subunits in the therapeutic composition are linked to other tumor-associated glycan antigens.

[0132] As used herein, "epitope ratio" relating to the therapeutic conjugates disclosed herein refers to for example, the relationship of antigen epitopes to carrier molecules in a therapeutic conjugate. Preferably, it refers to the relationship of Globo H moieties to KLH moieties. Most preferably the epitope ratio of a therapeutic conjugate is calculated using the following formula = (actual Globo H moiety weight/Globo H moiety molecular weight)/(actual KLH moiety weight/KLH moiety molecular weight). Epitope ratios are readily determinable by those of skill in the art. Preferably, the weights of Globo H are determined for example by high performance anion exchange chromatography with pulsed amperometric detection (HPAEC-PAD).

[0133] Preferably, the epitope ratios of the therapeutic conjugates of the invention are about, at least or exactly: 1, 10, 25, 50, 75, 100, 125, 150, 175, 200, 225, 250, 275, 300, 325, 350, 375, 400, 425, 450, 475, 500, 525, 575, 600, 625, 650, 675, 700, 725, 750, 775, 800, 825, 850, 875, 900, 925, 950, 975, 1000, 1025, 1050, 1075, 1100, 1125, 1150, 1175, 1200, 1225, 1250, 1275, 1300, 1325, 1350, 1375, 1400, 1425, 1450, 1475, 1500, 1525, 1550, 1575, 1600, 1625, 1650, 1675, 1700, 1725, 1750, 1775, 1800, 1825, 1850, 1875, 1900, 1925, 1950, 1975, 2000, 2025, 2050, 2075, 2100, 2125, 2150, 2175, 2200, 2225, 2250, 2275, 2300, 2325, 2350, 2375, 2400, 2425, 2450, 2475, 2500, 2525, 2550, 2575,

2600, 2625, 2650, 2675, 2700, 2725, 2750, 2775, 2800, 2825, 2850, 2875, 2900, 2925, 2950, 2975 or 3000.

[0134] In one embodiment, the therapeutic compositions of the invention include a mixture of therapeutic conjugates having a range of epitope ratios. In one embodiment, the range, the mean or the median epitope ratios of the therapeutic conjugates in the therapeutic composition is about 10 to about 3200, about 800 to about 2500, about 1000 to about 2000, about 1250 to about 1750 or about 1400 to about 1600. In another embodiment, the range, the mean or the median epitope ratios of the therapeutic conjugates in the therapeutic composition is about 10 to about 150, about 40 to about 125, about 50 to about 100, about 62 to about 87 or about 70 to about 80. In another embodiment, the range, the mean or the median epitope ratios of the therapeutic conjugates in the therapeutic composition is about 20 to about 300, about 80 to about 250, about 100 to about 200, about 125 to about 175 or about 140 to about 160. In another embodiment, the range, the mean or the median epitope ratios of the therapeutic conjugates in the therapeutic composition is about 30 to about 450, about 120 to about 375, about 150 to about 300, about 185 to about 260 or about 210 to about 240. In some the pharmaceutical compositions at least or about 30, 40, 50, 60, 70, 80, 90, 95, 98, 99, or 100% of the therapeutic conjugates exist as monomers, or as dimers, trimers, tetramers, pentamers, or combinations thereof.

ANTIBODIES TO THERAPEUTIC CONJUGATES

[0135] In certain illustrative embodiments, the invention also encompasses isolated therapeutic antibodies, which specifically bind the therapeutic conjugates disclosed

herein with affinity, as well as their use in the treatment and/or diagnosis of proliferative disease.

[0136] As used herein, the terms "antibody" and "antibodies" (immunoglobulins) encompass monoclonal antibodies (including full-length monoclonal antibodies), polyclonal antibodies, multispecific antibodies (e.g., bispecific antibodies) formed from at least two intact antibodies, human antibodies, humanized antibodies, camelised antibodies, chimeric antibodies, single-chain Fvs (scFv), single-chain antibodies, single domain antibodies, domain antibodies, Fab fragments, F(ab')2 fragments, antibody fragments that exhibit the desired biological activity, disulfide-linked Fvs (sdFv), and anti-idiotypic (anti-Id) antibodies (including, e.g., anti-Id antibodies to antibodies of the invention), intrabodies, and epitope-binding fragments of any of the above. In particular, antibodies include immunoglobulin molecules and immunologically active fragments of immunoglobulin molecules, i.e., molecules that contain an antigen-binding site Immunoglobulin molecules can be of any type (e.g., IgG, IgE, IgM, IgD, IgA and IgY), class (e.g., IgG1, IgG2, IgG3, IgG4, IgA1 and IgA2) or subclass.

[0137] "Affinity" of an antibody for an epitope, e.g., the Globo H moiety of a therapeutic conjugate, to be used in the treatment(s) described herein is a term well understood in the art and means the extent, or strength, of binding of antibody to epitope. Affinity may be measured and/or expressed in a number of ways known in the art, including, but not limited to, equilibrium dissociation constant (KD or Kd), apparent equilibrium dissociation constant (KD' or Kd'), and IC50 (amount needed to effect 50% inhibition in a competition assay). It is understood that, for purposes of this invention, an affinity is an average affinity for a given population of antibodies which bind to an epitope. Values of

KD' reported herein in terms of mg IgG per mL or mg/mL indicates mg Ig per mL of serum, although plasma can be used. When antibody affinity is used as a basis for administration of the treatment methods described herein, or selection for the treatment methods described herein, antibody affinity can be measured before and/or during treatment, and the values obtained can be used by a clinician in assessing whether a human patient is an appropriate candidate for treatment.

[0138] As used herein, the term "specifically binding," refers to the interaction between binding pairs (e.g., an antibody and an antigen). In various instances, specifically binding can be embodied by an affinity constant of at least or about 10-6 moles/liter, about 10-7 moles/liter, or about 10-8 moles/liter, or less.

BIOLOGICAL ASSAYS

[0139] In one embodiment, when administered to a patient, the therapeutic compositions containing therapeutic conjugates of the invention are able to induce anti-Globo H antibody titers at least or about 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 50, 100, 250, 500, 1000, 1500, 2000, 2500, 3000, 4000, or 5000 fold greater that the same anti-Globo H antibody titer prior to the administration (i.e., a pre-treatment baseline titer) in the same experiment. In certain embodiments the anti-Globo H antibodies are IgM antibodies. In another embodiment, the anti-Globo H antibodies are IgG antibodies.

[0140] The therapeutic compositions of the invention are capable of inducing both humoral and cellular responses in a subject. In certain embodiments, the vaccine composition of the invention induces production of Globo H moiety-specific IgG and

IgM antibodies and expansion of B cells and T cells (e.g. $CD3^+$T cells, $CD4^+$T cells and/or $CD8^+$T cells). Typically, these immune responses occur chronologically after administration. In a particular example, after administration, the B cell production appears at about day 3, 4, 5, 6, 7, 8, 9, 10, 20, 30, or 60 days, followed by production of IgG and IgM antibodies at about day 10, 20, 30, 60, or 90 and subsequent T cell production at about day 24, 30, 40, 50, 60, 90, 120, 150, or 180. The vaccine composition of the invention potentially provides a long term immunological protective effect which could prevent the growth of small quantities of cancer cells, thereby being ideal for minimal residual disease so as to achieve disease stabilization and survival improvement.

[0141] "Antibody-dependent cell-mediated cytotoxicity" and "ADCC" refer to a cell-mediated reaction in which non-specific cytotoxic cells (e.g., Natural Killer (NK) cells, neutrophils, and macrophages) recognize bound antibody on a target cell and subsequently cause lysis of the target cell. In one embodiment, such cells are human cells. While not wishing to be limited to any particular mechanism of action, these cytotoxic cells that mediate ADCC generally express Fc receptors (FcRs). The primary cells for mediating ADCC, NK cells, express FcγRIII, whereas monocytes express FcγRI, FcγRII, FcγRIII and/or FcγRIV. FcR expression on hematopoietic cells is summarized in Ravetch and Kinet, Annu. Rev. Immunol., 9:457-92 (1991). To assess ADCC activity of a molecule, an in vitro ADCC assay, such as that described in U.S. Pat. No. 5,500,362 or 5,821,337 may be performed. Useful effector cells for such assays include peripheral blood mononuclear cells (PBMC) and Natural Killer (NK) cells. Alternatively, or additionally, ADCC activity of the therapeutic conjugates of the invention may be

assessed *in vivo*, e.g., in an animal model such as that disclosed in Clynes et al., Proc. Natl. Acad. Sci. (USA), 95:652-656 (1998).

[0142] "Complement dependent cytotoxicity" or "CDC" refers to the ability of a therapeutic conjugate to initiate complement activation and lyse a target in the presence of complement. The complement activation pathway is initiated by the binding of the first component of the complement system (C1q) to a molecule (e.g., an antibody) complexed with a cognate antigen. To assess complement activation, a CDC assay, e.g., as described in Gazzano-Santaro et al., J. Immunol. Methods, 202:163 (1996), may be performed.

[0143] In another embodiment, when administered to a patient the therapeutic compositions containing therapeutic conjugates of the invention are able to induce the production in a patient/subject of anti-Globo H immune sera, which specifically binds to Globo H positive cancer cell lines, for example,MCF-7 cells.

COMBINATIONS

[0144] Therapeutic compositions can include other anti-cancer/anti-proliferative drugs as well as adjuvants and other immunomodulatory molecules such as cytokines or chemokines. These agents may all be delivered in a kit together in separate containers or a single container. The agents may be combined at the time of administration or at least or about 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23 or 24 minutes, hours or days prior to administration.

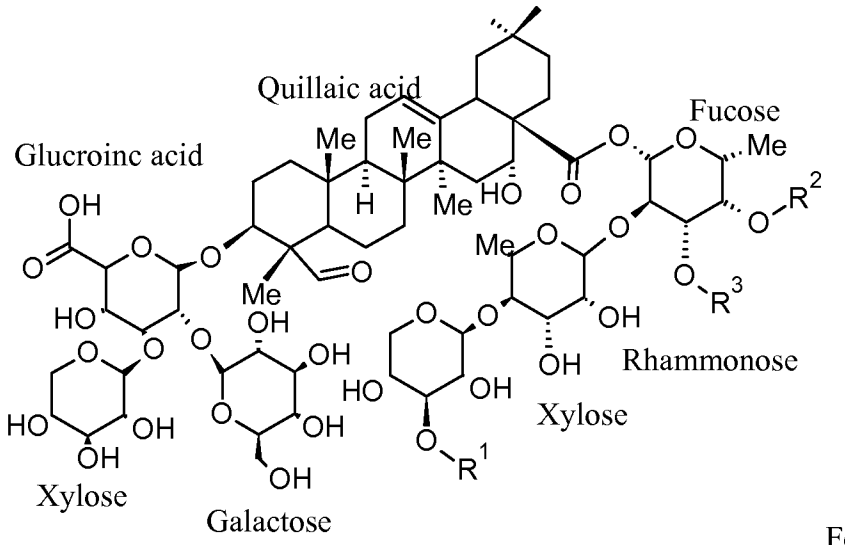
[0145] Adjuvants are pharmacological or immunological agents that modify the effects of other agents. They can be an inorganic or organic chemical, macromolecule or whole

cancer cells or portions thereof which enhance the immune response to given antigen. Adjuvants include complete and incomplete Freund's adjuvant, Toll-Like Receptor molecules and mimetics thereof, LPS, lipoproteins, lipopeptides, flagellin, double-stranded RNA, unmethylated CpG islands, levamisole, bacillus Calmette-Guerin, octreotide, isoprinosine and Zadaxin, various forms of DNA and RNA classically released by bacteria and viruses, PD-1 antagonists and CTLA antagonists. In one embodiment, the adjuvant is a saponin adjuvant.

[0146] In certain embodiment, the saponin adjuvant is OPT-821 saponin, which is substantially pure. In other embodiments, the OPT-821 saponin is a biologically active fragments thereof. The adjuvant may also encompass impure forms of OPT-821 saponins. The purified OPT-821 saponins exhibit enhanced adjuvant effect when administered with a vaccine described herein or admixed with other substantially pure saponin or non-saponin adjuvants.

[0147] OPT-821 saponins are naturally occurring glycosides, extracted in high purify from the bark of the *Quillaja saponaria* Molina tree, by high pressure liquid chromatography (HPLC), low pressure liquid silica chromatography, and hydrophilic interactive chromatography (HILIC) as described in, for example, U.S. Patent No. 5,057,540 and U.S. Patent No. 6,524,584, the content of which is incorporate by reference in its entirety. High-pressure liquid chromatography analysis shows that OPT-821 are a mixture of structurally related isomeric compounds. Different purified isomeric compounds of OPT-821 saponins have been identified and disclosed herein.

[0148] In certain embodiments, OPT-821 saponin comprise at least one isolated compound of formula I as follows:

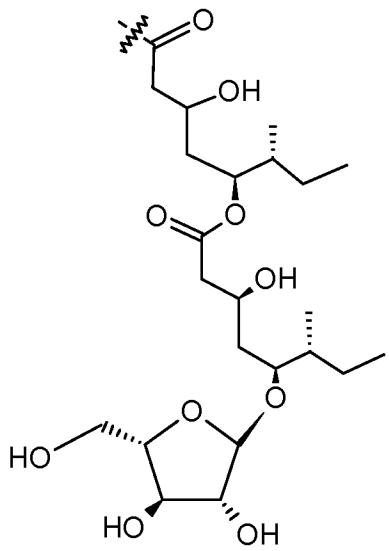


Formula (I)

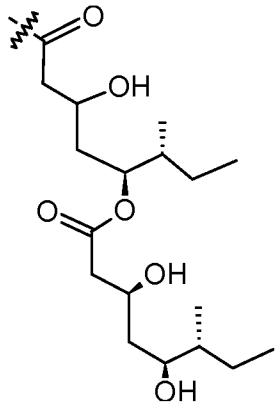
wherein

R^1 is β-D-Apiose or β-D-Xylose; and

R^2 and R^3 are independently H, alkyl,



(fatty acyl moiety for Compound 1989), or



(fatty acyl moiety for Compound 1857).

[0149] OPT-821 saponin can also comprise an isolated compound of formula I, wherein

(i) R^1 is β-D-Apiose, R^2 is the fatty acyl moiety for the 1989 compound depicted above, and R^3 is H (1989 compound V1A);

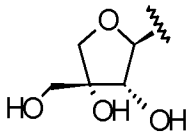
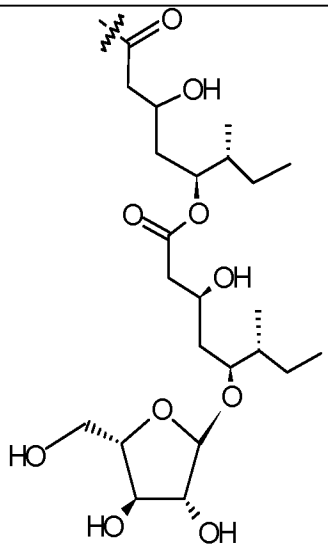
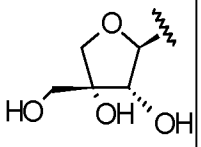
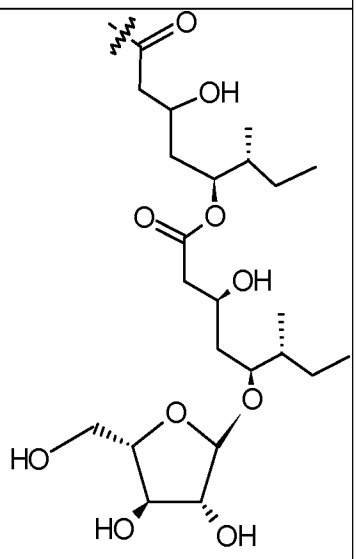
(ii) (ii) R^1 is β-D-Apiose, R^2 is H, and R^3 is the fatty acyl moiety fatty acyl moiety for the 1989 compound depicted above (1989 compound V1B);

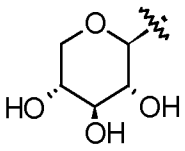
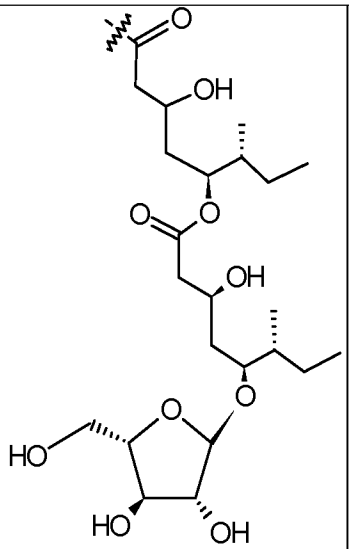
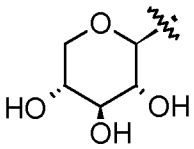
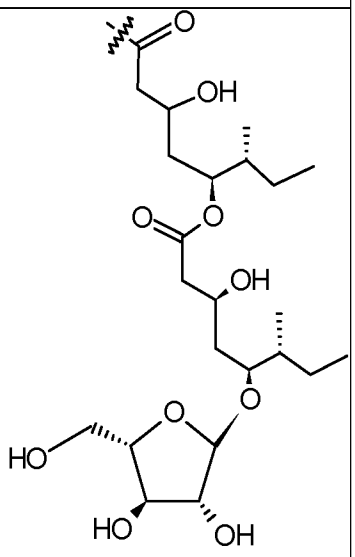
(iii) (iii) R^1 is β-D-Xylose, R^2 is the fatty acyl moiety fatty acyl moiety for the 1989 compound depicted above, and R^3 is H (1989 compound V2A); or

(iv) (iv) R^1 is β-D- Xylose, R^2 is H, and R^3 is the fatty acyl moiety fatty acyl moiety for the 1989 compound depicted above (1989 compound V2B). Collectively, 1989 compound V1A, 1989 compound V1B, 1989 compound V2A and 1989 compound V2B are called "1989 compounds mixture."

[0150] Table 1 summarizes the functional groups of 1989 compounds and the mole % of each 1857 compound in the 1857 compounds mixture.

Table 1

Mole %	R^1	R^2	R^3
1989 Compound V1A 64.5%	β-D-Apiose 		H
1989 Compound V1B 1.5%	β-D-Apiose 	H	

1989 Compound V2A 33.3%	β-D-Xylose 		H
1989 Compound V2B 0.7%	β-D-Xylose 	H	

[0151] OPT-821 saponin can comprise an isolated compound of formula I where:

(i) R^1 is β-D-Apiose, R^2 is the fatty acyl moiety for the 1857 compound depicted above, and R^3 is H (1857 compound V1A);

(ii) R^1 is β-D-Apiose, R^2 is H, and R^3 is the fatty acyl moiety for the 1857 compound depicted above (1857 compound V1B);

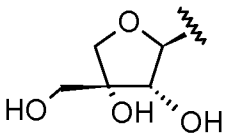
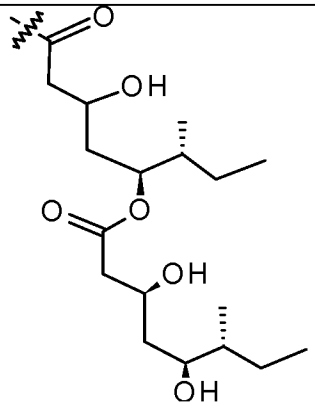
(iii) R^1 is β-D-Xylose, R^2 is the fatty acyl moiety for the 1857 compound depicted above, and R^3 is H (1857 compound V2A); or

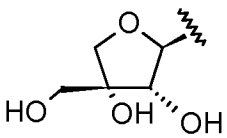
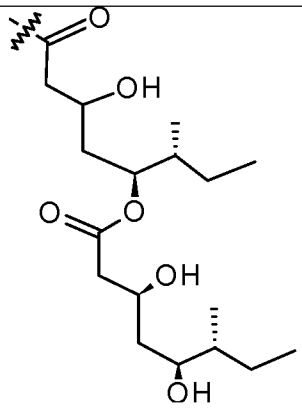
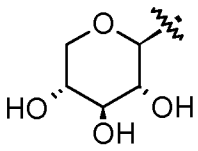
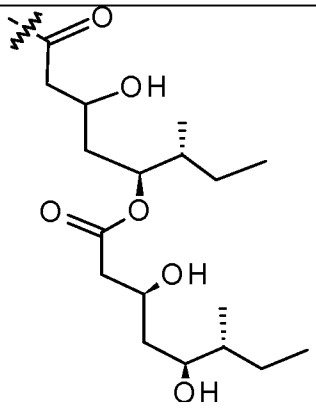
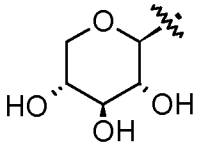
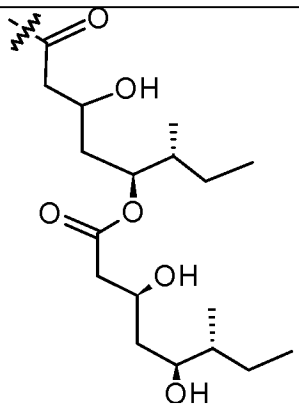
(iv) R^1 is β-D- Xylose, R^2 is H, and R^3 is the fatty acyl moiety for the 1857 compound depicted above (1857 compound V2B).

Collectively, 1857 compound V1A, 1857 compound V1B, 1857 compound V2A and 1857 compound V2B are called "1857 compounds mixture."

[0152] Table 2 summarizes the functional groups of 1857 compounds and the mole % of each 1857 compound in the 1857 compounds mixture. HPLC.

Table 2

Mole %	R^1	R^2	R^3
1857 Compound V1A 64.7%	β-D-Apiose 		H

1857 Compound V1B 1.3%	β-D-Apiose 	H	
1857 Compound V2A 33.4%	β-D-Xylose 		H
1857 Compound V2B 0.6%	β-D-Xylose 	H	

[0153] OPT-821 saponin comprises one or more of the following compounds:

(i) 1857 compound V1A; (ii) 1857 compound V1B;

(ii) 1857 compound V2A;

(iii) 1857 compound V2B;

(iv) 1989 compound V1A;

(v) 1989 compound V1B;

(vi) 1989 compound V2A; or

(vii) 1989 compound V2B.

[0154] The percentages of the 1857 compounds mixture and the 1989 compound mixture in OPT-821 saponin can range as follows:

(i) about 1 mole % to about 15 mole % of OPT-821 comprising an 1857 compounds mixture; and

(ii) about 85 mole % to about 99 mole % of OPT-821 comprising an 1989 compounds mixture.

[0155] All of the mole % can be varied by 0.1% increment (e.g. about 87% to about 90%, about 90.5% to about 97%, about 3.5% to about 11%, about 10% to about 14%).

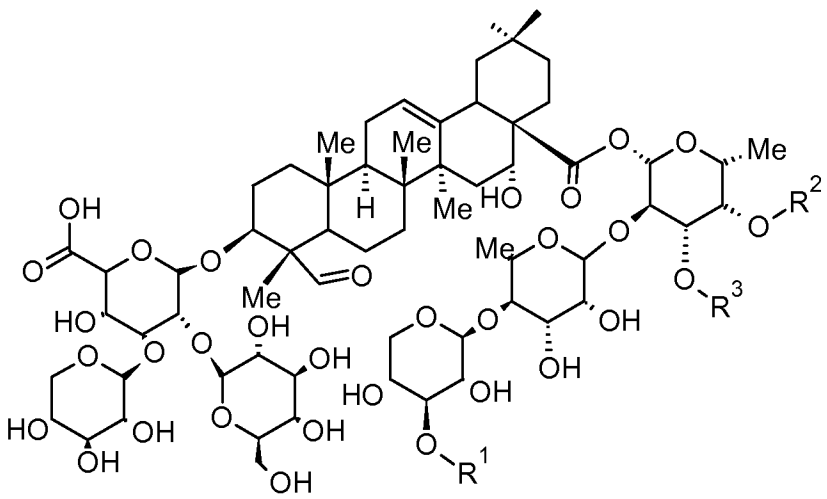
[0156] The 1989 compounds mixture may comprise about 60-70 mole % of 1989 compound V1A; about 1-5 mole % of 1989 compound V1B; about 30-40 mole % of 1989 compound V2A; and about 0.1-3 mole % of 1989 compound V2B. All of the mole % can be varied by 0.1 increment (e.g. 65%, 2.5%, 35.6%).

[0157] The 1857 compounds mixture may comprise about 60-70 mole % of 1857 compound V1A; about 1-5 mole % of 1857 compound V1B; about 30-40 mole % of

1857 compound V2A; and, about 0.1-3 mole % of 1857 compound V2B. All of the mole % can be varied by 0.1 increment (e.g., 65%, 2.5%, 35.6%).

[0158] In another embodiment, the substantially pure OPT-821 is purified from a crude Quillaja saponaria extract, wherein said OPT-821 is characterized by a single predominant peak which comprises 90% or more of the total area of all peaks of a chromatogram, excluding the solvent peak, when analyzed on reverse phase-HPLC on a Symmetry C18 column having 5 um particle size, 100 Å pore, 4.6mm IDx25cm L with a elution program comprising mobile phase of A:B 95%:5% to 75%:25% in 11 minutes , which mobile phase A is distilled water with 0.1% trifluoroacetic acid, and mobile phase B is acetonitrile with 0.1 % trifluoroacetic acid at a flow rate of 1ml/min.

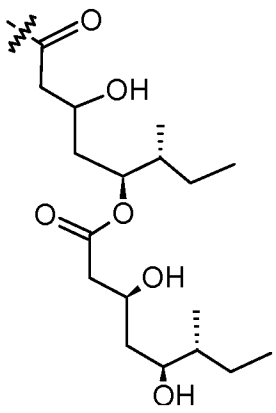
[0159] In one embodiment, the pharmaceutical composition comprises the compound of formula (I)



Formula (I)

wherein,

R^1 is β-D-Apiose or β-D-Xylose; and
R^2 and R^3 are independently H, alkyl, or



(Fatty acyl moiety for the 1857 Compound),

and a pharmaceutically acceptable carrier.

[0160] The vaccine can comprise a carbohydrate antigen or its immunogenic fragment and an OPT-821 saponin. In yet another embodiment, the vaccine comprises a carbohydrate antigen or its immunogenic fragment; a carrier protein and an OPT-821 saponin. In another embodiment, the vaccine comprises a carbohydrate antigen selected from Globo H, KLH, and an OPT-821 saponin. Non limiting examples of carrier protein include KLH.

[0161] As used herein, the term "cytokine" refers to any of numerous small, secreted proteins that regulate the intensity and duration of the immune response by affecting immune cells differentiation process usually involving changes in gene expression by which a precursor cell becomes a distinct specialized cell type. Cytokines have been variously named as lymphokines, interleukins, and chemokines, based on their presumed function, cell of secretion, or target of action. For example, some common interleukins include, but are not limited to, IL-2, IL-12, IL-18, IL-2, IFN-γ, TNF, IL-4, IL-10, IL-13, IL-21, GM-CSF, and TGF-β.

[0162] As used herein, the term "chemokine" refers to any of various small chemotactic cytokines released at the site of infection that provide a means for mobilization and

activation of lymphocytes. Chemokines attract leukocytes to infection sites. Chemokines have conserved cysteine residues that allow them to be assigned to four groups. The groups, with representative chemokines, are C-C chemokines (RANTES, MCP-1, MIP-1α, and MIP-1β), C-X-C chemokines (IL-8), C chemokines (Lymphotactin), and CXXXC chemokines (Fractalkine).

[0163] The therapeutic compositions of the invention can further include PD-1/PD-L1 inhibitors (cytotoxic T cell lymphocyte (CTLs) immunotherapy), CTLA-4 immunotherapy, CDK4/6 inhibitors (target therapy), PI3K inhibitors (target therapy), mTOR inhibitors (target therapy), AKT inhibitors (target therapy), Pan-Her inhibitors (target therapy). These inhibitors can be modified to generate the respective monoclonal antibody as well. Such antibodies can be included in therapeutic compositions of the invention.

[0164] The therapeutic compositions can include other anti-cancer/anti-proliferative or chemotherapeutic agents. In some embodiments, examples of such agents are found in Cancer Principles and Practice of Oncology by V.T. Devita and S. Hellman (editors), 6th edition (February 15, 2001), Lippincott Williams & Wilkins Publishers. Such anti-cancer agents include, but are not limited to, the following: hormonal therapeutic agents (e.g., selective estrogen receptor modulators, androgen receptor modulators), monoclonal antibody therapy, chemotherapy, retinoid receptor modulators, cytotoxic/cytostatic agents, antineoplastic agents, antiproliferative agents, prenyl-protein transferase inhibitors, HMG-CoA reductase inhibitors, nitrogen mustards, nitroso ureas, angiogenesis inhibitors (e.g., bevacizumab), inhibitors of cell proliferation and survival signaling pathway, apoptosis inducing agents, agents that interfere with cell cycle checkpoints,

agents that interfere with receptor tyrosine kinases (RTKs), mammalian target of rapamycin (mTOR) inhibitors, human epidermal growth factor receptor 2 (HER2) inhibitors, epidermal growth factor receptor (EGFR) inhibitors, integrin blockers, NSAIDs, PPAR agonists, inhibitors of inherent multidrug resistance (MDR), anti-emetic agents, agents useful in the treatment of anemia, agents useful in the treatment of neutropenia, immunologic-enhancing drugs, biphosphonates, aromatase inhibitors, agents inducing terminal differentiation of neoplastic cells, γ-secretase inhibitors, cancer vaccines, and any combination thereof.

FORMULATIONS OF THE INVENTION

[0165] The therapeutic compositions (also referred to herein as pharmaceutical compositions) generally include a pharmaceutically acceptable carrier. As used herein the language "pharmaceutically acceptable carrier" includes solvents, dispersion media, coatings, antibacterial and antifungal agents, isotonic and absorption delaying agents, and the like, compatible with pharmaceutical administration. Supplementary active compounds can also be incorporated into the compositions. A pharmaceutical composition is formulated to be compatible with its intended route of administration. Examples of routes of administration include parenteral, e.g., intravenous, intradermal, subcutaneous, intramuscular, intra-arterial, oral (e.g., inhalation), transdermal (topical), transmucosal, and rectal administration. Solutions or suspensions used for parenteral, intradermal, or subcutaneous application can include the following components: a sterile diluent such as water for injection, saline solution, phosphate buffered saline, tris-buffered saline, fixed oils, polyethylene glycols, glycerine, propylene glycol, or other synthetic solvents; antibacterial agents such as benzyl alcohol or methyl parabens;

antioxidants such as ascorbic acid or sodium bisulfite; chelating agents such as ethylenediaminetetraacetic acid; buffers such as acetates, citrates, or phosphates and agents for the adjustment of tonicity such as sodium chloride or dextrose. pH can be adjusted with acids or bases, such as hydrochloric acid or sodium hydroxide. The parenteral preparation can be enclosed in ampoules, disposable syringes, or multiple dose vials made of glass or plastic.

[0166] Pharmaceutical compositions suitable for an injectable use include sterile aqueous solutions (where water soluble) or dispersions and sterile powders for the extemporaneous preparation of sterile injectable solutions or dispersion. For intravenous administration, suitable carriers include physiological saline, bacteriostatic water, Cremophor EL® (BASF, Parsippany, N.J.), or phosphate buffered saline (PBS). In all cases, the composition should be sterile and should be fluid to the extent that easy syringability exists. It should be stable under the conditions of manufacture and storage and be preserved against the contaminating action of microorganisms such as bacteria and fungi. The carrier can be a solvent or dispersion medium containing, for example, water, ethanol, polyol (for example, glycerol, propylene glycol, and liquid polyethylene glycol, and the like), and suitable mixtures thereof. The proper fluidity can be maintained, for example, by the use of a coating such as lecithin, by the maintenance of the required particle size in the case of dispersion and by the use of surfactants. Prevention of the action of microorganisms can be achieved by various antibacterial and antifungal agents, for example, parabens, chlorobutanol, phenol, ascorbic acid, thimerosal, and the like. In many cases, it will be preferable to include isotonic agents, for example, sugars, polyalcohols such as manitol, sorbitol, or sodium chloride in the

composition. Prolonged absorption of the injectable compositions can be brought about by including in the composition an agent which delays absorption, for example, aluminum monostearate and gelatin.

[0167] Sterile injectable solutions can be prepared by incorporating the active compound in the required amount in an appropriate solvent with one or a combination of ingredients enumerated above, as required, followed by filtered sterilization. Generally, dispersions are prepared by incorporating the active compound into a sterile vehicle which contains a basic dispersion medium and the required other ingredients from those enumerated above. In the case of sterile powders for the preparation of sterile injectable solutions, methods of preparation include vacuum drying and freeze-drying, which yields a powder of the active ingredient plus any additional desired ingredient from a previously sterile-filtered solution thereof.

[0168] Oral compositions generally include an inert diluent or an edible carrier. For the purpose of oral therapeutic administration, the active compound can be incorporated with excipients and used in the form of tablets, troches, or capsules, e.g., gelatin capsules. Oral compositions can also be prepared using a fluid carrier for use as a mouthwash. Pharmaceutically compatible binding agents, or adjuvant materials can be included as part of the composition. The tablets, pills, capsules, troches and the like can contain any of the following ingredients, or compounds of a similar nature: a binder such as microcrystalline cellulose, gum tragacanth or gelatin; an excipient such as starch or lactose, a disintegrating agent such as alginic acid, Primogel, or corn starch; a lubricant such as magnesium stearate or sterotes; a glidant such as colloidal silicon dioxide; a

sweetening agent such as sucrose or saccharin; or a flavoring agent such as peppermint, methyl salicylate, or orange flavoring.

[0169] For administration by inhalation, the compounds are delivered in the form of an aerosol spray from pressured container or dispenser which contains a suitable propellant, e.g., a gas such as carbon dioxide, or a nebulizer.

[0170] Systemic administration can also be transmucosal or transdermal. For transmucosal or transdermal administration, penetrants appropriate to the barrier to be permeated are used in the formulation. Such penetrants are generally known in the art, and include, for example, for transmucosal administration, detergents, bile salts, and fusidic acid derivatives. Transmucosal administration may be accomplished through the use of nasal sprays or suppositories. For transdermal administration, the active compounds are formulated into ointments, salves, gels, or creams as generally known in the art. The compounds can also be prepared in the form of suppositories (e.g., with conventional suppository bases such as cocoa butter and other glycerides) or retention enemas for rectal delivery.

[0171] According to implementations, the active compounds are prepared with carriers that will protect the compound against rapid elimination from the body, such as a controlled release formulation, including implants and microencapsulated delivery systems. Biodegradable, biocompatible polymers can be used, such as ethylene vinyl acetate, polyanhydrides, polyglycolic acid, collagen, polyorthoesters, and polylactic acid. Methods for preparation of such formulations will be apparent to those skilled in the art. The materials can also be obtained commercially. Liposomal suspensions (including

liposomes targeted to infected cells with monoclonal antibodies to cell-specific antigens) can also be used as pharmaceutically acceptable carriers. These can be prepared according to methods known to those skilled in the art, for example, as described in U.S. Pat. No. 4,522,811, which is incorporated by reference herein.

[0172] It is advantageous to formulate oral or parenteral compositions in dosage unit form for ease of administration and uniformity of dosage. Dosage unit form as used herein refers to physically discrete units suited as unitary dosages for the subject to be treated; each unit containing a predetermined quantity of active compound calculated to produce the desired therapeutic effect in association with the required pharmaceutical carrier.

DOSAGE FORMS

[0173] Toxicity and therapeutic efficacy of such therapeutic compositions may be determined by standard pharmaceutical procedures in cell cultures or experimental animals, e.g., for determining the LD_{50} (the dose lethal to 50% of the population) and the ED_{50} (the dose therapeutically effective in 50% of the population). The dose ratio between toxic and therapeutic effects is the therapeutic index and it can be expressed as the ratio LD_{50}/ED_{50}. Therapeutic compositions which exhibit high therapeutic indices are preferred. While compounds that exhibit toxic side effects can be used, care should be taken to design a delivery system that targets such compounds to the site of affected location to minimize potential damage to uninfected cells and, thereby, reduce side effects.

[0174] Data obtained from cell culture assays and animal studies can be used in formulating a range of dosage for use in humans. The dosage of such compounds lies preferably within a range of circulating concentrations that include the ED_{50} with little or no toxicity. The dosage can vary within this range depending upon the dosage form employed and the route of administration utilized. For any compound used in the method of the disclosure, the therapeutically effective dose can be estimated initially from cell culture assays. A dose can be formulated in animal models to achieve a circulating plasma concentration range that includes the IC_{50} (i.e., the concentration of the test compound which achieves a half-maximal inhibition of symptoms) as determined in cell culture. Such information can be used to more accurately determine useful doses in humans. Levels in plasma may be measured, for example, by high performance liquid chromatography.

[0175] In some embodiments, a therapeutically effective amount of a therapeutic composition (i.e., an effective dosage) may range from about 0.001μg/kg to about 250 g/kg, 0.01 μg/kg to 10 g/kg, or 0.1 μg/kg to 1g/kg or about or at least: 0.001, 0.002, 0.003, 0.004, 0.005, 0.006, 0.007, 0.008, 0.009; 0.01, 0.02, 0.03, 0.04, 0.05, 0.06, 0.07, 0.08, 0.09;0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100, 125, 150, 175, 200, 225, or 250 grams or micrograms per kilogram of patient body weight, or other ranges that would be apparent and understood by artisans without undue experimentation. The skilled artisan

will appreciate that certain factors can influence the dosage and timing required to effectively treat a subject, including but not limited to the severity of the disease or disorder, previous treatments, the general health or age of the subject, and other diseases present.

[0176] In other embodiments, a therapeutically effective amount of Globo-H moiety in the therapeutic composition (*i.e.,* an effective dosage) may range from about 0.001μg/kg to about 250 g/kg, 0.01 μg/kg to 10 g/kg, or 0.1 μg/kg to 1g/kg or about or at least: 0.001, 0.002, 0.003, 0.004, 0.005, 0.006, 0.007, 0.008, 0.009; 0.01, 0.02, 0.03, 0.04, 0.05, 0.06, 0.07, 0.08, 0.09;0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100, 125, 150, 175, 200, 225, or 250 grams or micrograms per kilogram of patient body weight, or other ranges that would be apparent and understood by artisans without undue experimentation. The skilled artisan will appreciate that certain factors can influence the dosage and timing required to effectively treat a subject, including but not limited to the severity of the disease or disorder, previous treatments, the general health or age of the subject, and other diseases present.

[0177] In certain embodiments, the therapeutic compositions disclosed herein contain or are associated with, at least one therapeutic conjugate or therapeutic antibody whereby each at least one therapeutic conjugate or therapeutic antibody is present in single dose at

a concentration of about, at least or more than: 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98 or 99 each times 10^{-9}, 10^{-8}, $10^{-7}10^{-7}10^{-6}10^{-5}$ $10^{-4}10^{-3}10^{-2}10^{-1}$ molar per dose. Preferably, the therapeutic conjugate is present in single dose at a concentration between about: 1-100, 2-60, 3-50, 4-40, 5-30, 6-20, 7-15, 8-10, 2-18, 3-16, 4-14, 5-12, 6-10 or 7-8 μM.

[0178] In some embodiments, the therapeutic compositions disclosed herein contain or are associated with, at least one therapeutic conjugate or therapeutic antibody whereby each at least one therapeutic conjugate or therapeutic antibody is present in single dose at a concentration of about, at least or more than: 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98 or 99 each times 10^{-3}, 10^{-2}, 10^{-1}, or 10 micrograms. In certain embodiments about or at least 10, 20, 30, 40, 50, 60, 70, 80, 90, 100, 110, 120, 130, 140, 150 or more micrograms of one therapeutic conjugate or therapeutic antibody is included per dose.

[0179] In certain embodiments, the therapeutic compositions disclosed herein are administered in a dose about or at least or more than: 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23 or 24 times per day, week or month over a period

of about or at least or more than: 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23 or 24 days, weeks, months, or years.

KITS

[0180] According to another aspect, one or more kits of parts can be envisioned by the person skilled in the art, the kits of parts to perform at least one of the methods herein disclosed, the kit of parts comprising one or more therapeutic conjugates, anti-cancer/anti-proliferative agents, adjuvants, cytokines and/or chemokines. The therapeutic compositions comprising alone or in combination an effective amount of the therapeutic compositions disclosed herein according to the at least one of the above mentioned methods. The aforementioned agents may come in a single container or in different containers in the kit.

[0181] The kits possibly include also identifiers of a biological event, or other compounds identifiable by a person skilled upon reading of the present disclosure. The kit can also comprise at least one composition comprising an effective amount of the therapeutic compositions disclosed herein. The therapeutic compositions of the kits to perform the at least one method herein disclosed according to procedure identifiable by a person skilled in the art.

[0182] The disclosure also includes methods of treating proliferative diseases utilizing the therapeutic compositions disclosed herein. In one embodiment, the methods involve the treatment of cancer, e.g., breast cancer. The methods generally involve providing the therapeutic compositions disclosed herein to a patient in need thereof in an amount effective to treat the proliferative disorder.

[0183] In some embodiments, the therapeutic compositions of the invention are administered to a subject in need thereof (e.g., one having a cancer such as breast cancer) in a method that on average extends progression free survival or overall survival over a control placebo, e.g., a phosphate buffered saline placebo, by about or at least 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40 days, weeks, months, or years.

[0184] In some embodiments, the therapeutic compositions are given subcutaneously on week 0-2, 6, 14, and 26 in the absence of unacceptable toxicity or disease progression.

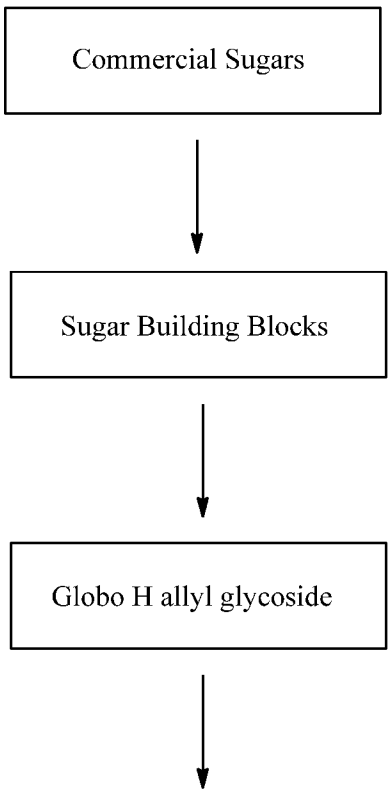
[0185] In some embodiments, the therapeutic compositions of the invention are administered to a subject in need thereof (e.g., one having a cancer such as breast cancer) in a method that on average shrinks the volume of a tumor in the patient relative to a control placebo, e.g., a phosphate buffered saline placebo, by about or at least 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 74 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 or more percent over the course of 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40 days, weeks, months, or years.

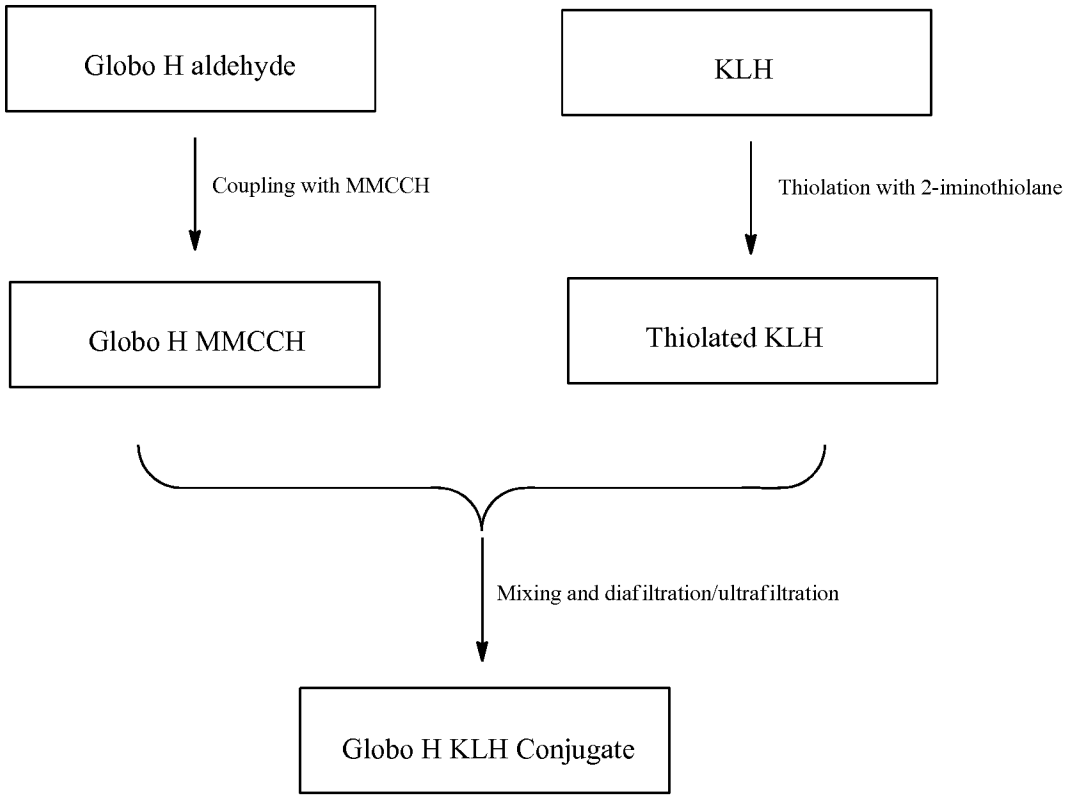
[0186] In some embodiments, tumors volumes may be accurately measured in at least one dimension (longest diameter in the plane of measurement is to be recorded) with a minimum size of 10mm by CT scan (CT scan slice thickness recommended to be in between 2.5 mm and 5 mm).

METHODS OF SYNTHESIZING THE COMPOSITIONS OF THE INVENTION

[0187] The Globo H hexasaccharide portion of the therapeutic compositions of the invention was chemically synthesized as the allyl glycoside and then prepared for conjugation with KLH.

[0188] In one illustrative embodiment, the chemical synthesis of Globo H involves the following general steps:





[0189] KLH was treated with 2-iminothiolane in an aqueous buffer. The thiolated KLH was then isolated from the unreacted 2-iminothiolane, via a size exclusion column of Sephadex G-15 column. The thiolated KLH was stored under inert gas (nitrogen or argon) atmosphere and used immediately for the conjugation with Globo HMMCCH.

EXAMPLES

[0190] Example 1: Preparation of Glycoconjugate of the Invention (Globo H-KLH)

[0191] Globo H allyl glycoside (commercially available) was converted to an aldehyde by ozonolysis. Globo H aldehyde was reacted with M_2C_2H (linker) and $NaCNBH_3$ to give Globo H-MMCCH. The mixture was purified with a column to receive Globo H-MMCCH. The fraction with Globo H-MMCCH positive was confirmed by high

performance liquid chromatography (HPLC) and then pooled together. KLH was dissolved in thiolation buffer and 2-iminothiolane was added into the reaction by portion. The reaction was incubated to completion and then KLH-SH was purified by a column. Globo H-MMCCH and KLH-SH were combined 2. The reaction was stirred to completion. Globo H-KLH was then purified to provide the final product. .

[0192] Example 2: Analysis of Weight Ratio of Globo H to KLH in the Glycoconjugate

[0193] The weight ratio of Globo H and KLH in the glycoconjugate as prepared was confirmed by high performance anion exchange chromatography with pulsed amperometric detection (HPAEC-PAD). The results are shown in Table 3.

[0194] Table 3: The Weight Ratio of Globo H and KLH in Glycoconjugate

Glycoconjugate preparations Epitope Ratio (KLH Didecamer MW:8,600,000 Da)	Epitope ratio (KLH monomer MW:400 kDa)	Globo H Weight to KLH moiety Weight (mg/mg)
3000	150	0.368
1950	97.5	0.239
1500	75	0.184
1050	52.5	0.129
300	15	0.037
100	5	0.012
20	1	0.002

[0195] Example 3: Analysis of Epitope Ratio of Globo H to KLH in the Glycoconjugate

[0196] The molecular weight of a KLH didecamer (the naturally aggregated form) is around 7.5 MDa ~ 8.6 MDa, as described in literatures, such as Micron 30 (1999) 597-623. The native KLH was confirmed by the size exclusion chromatography and multi-angle laser scattering spectrometry (MALS), having the molecular weight of around 8.6 M Da (see Figs. 3 and 4). The glycoconjugates of the invention (sample no. 5, the weight ratio of Globo H to KLH being 0.17: 1) were analyzed by the size exclusion chromatography. The results show that the glycoconjugate of the invention exhibited a reduced mass in molecular weight as compared with native aggregated KLH didecamers. See Fig. 4. The molecular ratios were then calculated as in Table 4.

Table 4: Calculation of Molecular Ratios of Globo H to KLH

Experimental Molecular Weight from Globo H-KLH (kDa)	**Mass of 75 Globo H per KLH subunit in Globo H-KLH: 75 (kDa)**	**Mass of KLH subunit: 359 kDa**	**Assumption of (Globo H) -(KLH multimer) from the experimental data**
1142	3*75=225	359*3= 1077	225+1077=1302 KLH forms a **trimer** after Globo H-KLH conjugation.
780	2*75=150	359*2=718	150+718=868 KLH forms a **dimer** after Globo H-KLH conjugation.
420	1*75=75	359*1=359	434

Experimental Molecular Weight from Globo H-KLH (kDa)	Mass of 75 Globo H per KLH subunit in Globo H-KLH: 75 (kDa)	Mass of KLH subunit: 359 kDa	Assumption of (Globo H) -(KLH multimer) from the experimental data
			KLH forms a **monomer** after Globo H-KLH conjugation.

* The above molecular ratio is calculated based on the formula as below:

$$\text{molecular ratio} = \frac{\text{Globo H Weight} / \text{Globo H M. W.}}{\frac{KLH\ Weight}{KLH\ Molecular\ Weight\ **}}$$

** The molecular weight of KLH depends on the forms of monomer, dimer or didecamer

[0197] Given the above, it was concluded that in the glycoconjugate of the invention, the KLH monomeric units form monomers, dimers and/or trimers after conjugation to Globo H.

[0198] Example 4: Preparation of Vaccine Compositions and Immunization in Rats

[0199] Different samples of the glycoconjugates (Globo H-KLH) as prepared in Example 1 were stored at 4 °C, and mixed with a saponin adjuvant under a laminar flow hood. The resultant vaccine compositions were placed on ice and transported to animal facility for subsequent immunization.

[0200] Three groups of Lewis rats were immunized with the various vaccine compositions as shown in Table 5.

Table 5: Groups of immunized rats

Groups	Vaccine compositions	Animal number	Route
I	GH-KLH* (25μg) + saponin adjuvant (25μg)	8	SC
II	GH-KLH* (7.5μg) + saponin adjuvant (25μg)	4	SC
III	PBS	4	SC

*GH: KLH = 0.17: 1 (w/w)

GH: Globo H

SC: Subcutaneous

PBS: phosphate buffered saline

[0201] The rats were immunized on day 0, 7, 14, and 21. Peripheral blood mononuclear cells (PBMC) and plasma were collected on day 0, 3, 10, 17, 24, and 31. Spleen, lymph node, and peritoneal wash were harvested on day 31.

[0202] Example 5: Assays for Induction of Humoral and Cellular Immune Responses in Rats

Example 5.1 Analysis of Immune Effector Cell Subpopulations by Flow Cytometry

[0203] The peripheral blood mononuclear cells (PBMCs) were isolated from the animals and then various immune effector cell subpopulations in the PBMC were identified by flow cytometry using specific antibodies against different cell markers The PBMCs, isolated from the immunized rats on day 0, 3, 10, 17, 24, and 31, were stained with different fluorescence (FITC)-conjugated antibodies and placed on ice for 30 minutes. After incubation, cells were washed with the washing buffer (1% bovine serum

albumin (Sigma) and 0.1% NaN_3 (Sigma) in phosphate buffered saline (UniRegion Biotech) and centrifuged at 350 g for 5 minutes. Cells were resuspended in washing buffer for determination of fluorescence by FACS Canto (BD Bioscience). The data were analyzed with BD FACSDiva (BD Bioscience) software. The results show that in the immunized rats by the glycoconjugate of the present invention, T cells, B cells, CD4+ T cells, and CD8+ T cells were significantly expanded when compared to the PBS control group. Specifically, the B cell population first appeared at day 3 and subsequent $CD3^+$ T, $CD4^+$ T and $CD8^+$ T cells appeared at day 24. See Fig. 5 (A)-(D).

Example 5.2 Globo H-specific antibody test by ELISA

[0204] The production of Globo H-specific antibodies in the plasma from the immunized rats was determined by ELISA assay. The results show the titers of Globo H-specific IgG began to rise at 10 days and peaked at 17 days after immunization. Similar patterns were observed in the production of Globo H-specific IgM antibody. See Fig. 5 (A)-(B). There was no response of Globo H-specific IgG and IgM antibody in rats treated with PBS, or KLH plus adjuvant only (data not shown).

[0205] In summary, in the immunized rats, B cell production appears at day 3, followed by production of IgM and IgG antibody against Globo H which appears at day 10 and subsequent $CD3^+$ T, $CD4^+$ T, and $CD8^+$ T cell which appears at day 24. The glycoconjugate (Globo H-KLH) of the invention is effective to induce both humoral and cellular responses.

[0206] Example 6: Immunization in mice and antibody test by ELISA

[0207] Different samples of the glycoconjugates (Globo H-KLH) were stored at 4 °C, and mixed with a saponin adjuvant under a laminar flow hood. The resultant vaccine compositions were placed on ice and transported to animal facility for subsequent immunization.

[0208] Balb/c mice of approximately eight weeks old were given Globo H-KLH with different carbohydrate-to-protein (Globo H: KLH) ratios once every week for four weeks (Day 0, 7, 14, and 21) via subcutaneous injection. Blood samples were collected through retro-orbital or facial vein without anticoagulant pre-immune or Day 0, and three days after each vaccination (Day 10, 17 and 24). Samples were then centrifuged to separate sera and red cells. Sera were collected and stored at -20°C, which were later analyzed by ELISA. Mann-Whitney t-test was used for statistical analysis.

[0209] As shown in Fig. 6, the glycoconjugate (Globo H-KLH), in combination with a saponin adjuvant, according to the invention, has been demonstrated to significantly induce the Globo H-specific IgM antibody responses in the animal model, as compared with the PBS control group. Specifically, the glycoconjugate with a weight ratio of 0.17: 1 (Globo H: KLH) induced a better antibody titer than the glycoconjugate with a weight ratio of 0.07: 1 (Globo H: KLH).

[0210] In summary, the glycoconjugate (Globo H-KLH), in combination with a proper adjuvant, according to the invention, has been demonstrated to induce unexpectedly superior humoral and cellular immune response in the animal model, particularly expansion of B cells and T cells including CTLs and IgM and IgG responses, which are important in cancer immunotherapy.

[0211] Example 7: Immunogenicity Study Of Globo H - KLH With Or Without Adjuvant Vaccine In Mice

[0212] The ability of Globo H composition of the invention, when paired with an adjuvant, to elicit an immune response in mice has been performed. The amount of Globo-H specific antibody induced by the immunotherapy was quantified by an ELISA and FACS.

[0213] Groups of 6-week-old female C57BL/6 mice were immunized subcutaneously with Globo H - KLH and adjuvant. Globo H - KLH dose levels are the equivalent of amount of Globo-H (in μg) in Globo H-KLH. Each injection contained a range of doses equivalent to 0.6 μg to 5.0 μg Globo-H in Globo H - KLH and 20 μg adjuvant. The immunizations occurred on Days 0, 8, and 14, and serum was collected on Day 0 (pre-injection) and Day 24 for comparative analysis by ELISA and FACS. Serological responses were measured by ELISA to determine the titer of antibodies against Globo H ceramide, and FACS to determine cell surface reactivity to Globo H positive MCF-7 cells.

[0214] Throughout the immunization, there was no obvious change in the behavior, appetite, general appearance, and grooming after vaccination. Ten days after the third immunization, sera were collected for determination of IgG and IgM anti-Globo H antibody titers by ELISA, using a titer ≥8 fold of the pre-treatment value as a criterion for positive response. As shown in Figure 2, there was no response in mice treated with Globo H alone, Globo H KLH conjugate, or adjuvant alone. In contrast, 14/15 mice treated with Globo H - KLH + adjuvant responded with significant IgG anti-Globo H

titers which did not appear to be dose dependent at an Globo H - KLH dosage of 0.6 to 5 μg. The average IgG titers for each dosage increased by 13 to 17.5 fold over the pre-treatment value. As to IgM anti-Globo H, one of the 15 mice showed an 8-fold increase in titer after immunization with adjuvant + Globo H - KLH. However, 5/15 had an IgM titer ≥4 fold of preimmune sera and a total of 6/15 had a titer ≥2 fold. The average IgM titers for each dosage increased by 2.5 fold over the pretreatment values.

[0215] The binding capacity of immune sera with Globo H-expressing breast cancer cell line, MCF-7 was determined by FACS analysis at 1:25 serum dilution. The post-treatment value of 30% above the pretreatment value (i.e. ≥1.3 fold increase) was considered as positive in this assay. As shown in Figure 3, immune sera from all of the adjuvant + Globo H - KLH treated groups contained IgM antibodies that reacted with MCF-7 cells, which ranged from 5~6 fold over pretreatment baseline. Moreover, immune sera from three-fifths of the mice treated with 0.6 μg or 2 μg Globo H - KLH + adjuvant, and two-fifths of those treated with 5 μg Globo H - KLH + adjuvant showed IgG antibodies that could bind to MCF-7 cells. The average binding capacities increased 1.3 to 2.0 fold over the pretreatment baseline.

[0216] Vaccination with Globo H - KLH and an adjuvant has demonstrated to elicit both IgG and IgM anti-Globo H responses in female C57BL/6 mice. The immune sera had the capacity of binding Globo H expressing breast cancer MCF-7 cells.

[0217] Example 8: LC-MS/MS Analysis of Globo-H Conjugation Sites on KLH

[0218] Globo H conjugation sites in four KLH samples using multiple enzyme digestion and LC-MS/MS were identified. The four Globo H-conjugated KLH samples were first digested with four different enzymes and then analyzed by LC-MS/MS and Mascot database search. Two types of derivatives were identified: Globo H derivative (Globo H + MMCCH) and the MMCCH derivative (MMCCH alone). The Globo H derivative and its neutral loss forms were taken into account for Globo H conjugation site identification. The MMCCH form and its deamidated form were taken into account for MMCCH conjugation site identification. Only those peptides with high quality MS/MS spectra and Mascot score were taken into account. For Globo H conjugation analysis, 31 and 28 conjugated lysines were observed from the two replicate LC-MS/MS analyses of OPT-822-13001-DP (sample 1); 19 and 21 conjugated lysines were observed from the two replicate LC-MS/MS analyses of OPT-822-13002-DP (sample 2); 10 and 11 conjugated lysines were observed from the two replicate LC-MS/MS analyses of OPT-822-13003-DP (sample 3); 18 and 19 conjugated lysines were observed from the two replicate LC-MS/MS analyses of OPT-822-13004-DS (sample 4). For MMCCH conjugation analysis, 155 and 141 conjugated lysines were found from the two replicate LC-MS/MS analyses of OPT-822-13001-DP (sample 1); 143 and 137 conjugated lysines were found from the two replicate LC-MS/MS analyses of OPT-822-13002-DP (sample 2); 147 and 143 conjugated lysines were found from the two replicate LC-MS/MS analyses of OPT-822-13003-DP (sample 3); 140 and 136 conjugated lysines were found from the two replicate LC-MS/MS analyses of OPT-822-13004-DS (sample 4).

[0219] Example 8 Materials and Methods:

[0220] Abbreviations in this section are as follows: K = Lysine; LC-MS/MS = Liquid Chromatography-Tandem Mass Spectrometry; DTT = Dithiolthreitol; IAM = Iodoacetamide; ACN = Acetonitrile; FA = Formic Acid; Glu-C = Endoproteinase Glu-C; ABC = Ammonium bicarbonate; RT = Room temperature; MW = Molecular weight.

[0221] The four KLH samples, sample 1-4, were first processed for buffer exchange into 50 mM ammonium bicarbonate buffer solution by 100 kDa cut-off Amicon Ultra Centrifugal Filters and denatured with 6 M urea. The samples were then reduced with 10 mM DTT at 37 °C for 1 hr, alkylated using 50 mM IAM for 30 mins in dark at RT and quenched with 50 mM DTT at RT for 5 mins. The resulting proteins were diluted until the urea concentration is 1 M and subjected to in-solution digestion with different enzymes as described in the following section.

[0222] In-solution digestion with different enzymes was performed with the following digestion conditions: (1) trypsin digestion at 37 °C for 24 hrs (protein: enzyme= 40:1) (2) Glu-C digestion at 37 °C for 24 hrs (protein: enzyme= 25:1); (3) chymotrypsin digestion at RT for 24 hrs (protein: enzyme= 25:1); (4) thermolysin digestion at 37 °C for 24 hrs (protein: enzyme= 25:1).

[0223] Digestion reactions were terminated by adding formic acid and all four digested samples were subjected to LC-MS/MS analysis.

[0224] Samples were analyzed with Q Exactive mass spectrometer (Thermo Scientific) coupled with Ultimate 3000 RSLC system (Dionex). The LC separation was performed using the C 18 column (Acclaim PepMap RSLC, 75 μm x 150 mm, 2 μm, 100 Å) with the gradient shown below:

Time (min)	A%	B%	Flow (µL/min)
0	99	1	0.25
5	99	1	0.25
35	90	10	0.25
67	65	35	0.25
77	15	85	0.25
82	99	1	0.25
90	99	1	0.25

Mobile phase A: 5% ACN/ 0.1% FA
Mobile phase B: 95% ACN/ 0.1% FA

[0225] In-source CID was set at 45 eV. Full MS scan was performed with the range of m/z 350-2000, and the ten most intense ions from MS scan were subjected to fragmentation for MS/MS spectra. Raw data were processed into peak lists by Proteome Discoverer 1.4 for Mascot database search.

[0226] Database search was performed with Mascot version 2.4.1 and Thermo Proteome Discoverer version 1.4 against the KLH1 and KLH2 [KLH1, EMBL accession # CAG28307.1; KLH2, EMBL accession # CAG28308.1. The parameters used were as follows: Enzyme: Trypsin, Glu-C, Chymotrypsin and Thermolysin according to the digestion method; Fixed modification: Carbamidomethyl (C).

[0227] Variable modifications for MMCCH derivatives (MMCCH alone): Deamidated (NQ), Oxidation (M), dK_MMCCH-1 (K), dK_MMCCH-2 (K).

[0228] Variable modifications for Globo H derivatives (Globo H + MMCCH): Deamidated (NQ), Oxidation (M), Globo_H_MMCCH (K), dK_MMCCH_NL997 (K),

dK_MMCCH_NL835 (K), dK_MMCCH_NL673 (K), dK_MMCCH_NL511 (K), dK_MMCCH_NL308 (K),Deamidated (NQ), Oxidation (M), Peptide Mass Tolerance: ± 10 ppm; Fragment Mass Tolerance: ± 0.05 Da; Max Missed Cleavages: 5; Instrument type: ESI-TRAP; Ion cut-off score: 13.

[0229] "dK_MMCCH-1" in the search parameters indicates the MMCCH-conjugated lysine with the MW addition of 352.1569 Da.

[0230] "dK_MMCCH-2" in the search parameters indicates the deamidated form of MMCCH-conjugated lysine with the MW addition of 338.1300 Da.

[0231] "Globo_H_MMCCH (K)" in the search parameters indicates the Globo H-conjugated lysine with the MW addition of 1393.5317 Da.

[0232] "dK_MMCCH_NL997" in the search parameters indicates the neutral loss form of Globo H-conjugated lysine with the MW addition of 396.1831 Da.

[0233] "dK_MMCCH_NL835" in the search parameters indicates the neutral loss form of Globo H-conjugated lysine with the MW addition of 558.2360 Da.

[0234] "dK_MMCCH_NL673" in the search parameters indicates the neutral loss form of Globo H-conjugated lysine with the MW addition of 720.2888 Da.

[0235] "dK_MMCCH_NL511" in the search parameters indicates the neutral loss form of Globo H-conjugated lysine with the MW addition of 882.3416 Da.

[0236] "dK_MMCCH_NL308" in the search parameters indicates the neutral loss form of Globo H-conjugated lysine with the MW addition of 1085.4210 Da.

[0237] The "MW addition" implies the molecular weight addition compared to intact lysine residue.

[0238] Example 8: Results

[0239] LC-MS/MS based techniques are tools for identification of protein and characterization of amino acid modification. Detailed information regarding peptide sequences and modification sites can be obtained by the assignment of fragment ions provided by MS/MS spectra. Mascot is a search engine and its probability based scoring algorithm has been well accepted. Mascot score was adopted in this study as a reference of confidence for protein sequencing and Globo H or MMCCH conjugation site identification. To extensively analyze the distribution of Globo H or MMCCH conjugation sites in sample 1-4, these samples were digested with multiple enzymes followed by LC-MS/MS analyses.

[0240] The expected chemical structure for Globo H derivative (Globo H + MMCCH) is shown in Figure 33A and the corresponding MW addition of 1393.53 Da on lysine-containing peptides can be observed among the results. Besides, the labile polysaccharides tend to fall off via neutral loss during the electrospray ionization in LC-MS analysis. Therefore, the molecular weight addition of 396.18 Da, 558.24 Da, 720.29 Da, 882.34 Da and 1085.42 Da resulted from neutral loss can also be observed for glycoconjugated peptides, as shown in Figure 33B. All the derivitization forms were considered for the identification of Globo H conjugation sites.

[0241] In addition, the MMCCH derivative is also observed (MMCCH alone) in these Globo H conjugated KLH samples. The expected chemical structure for MMCCH

derivative and its deamidated form are shown in Figure 34A and 34B and the corresponding MW addition of 352.16 Da and 338.13 Da respectively on lysine-containing peptides can be observed among the results. Both derivitization forms were considered for the identification of MMCCH conjugation sites. The conversion from Globo H derivative to MMCCH is not clear but it is supposed to happen during the sample treatment.

[0242] The mass accuracy of ± 10 ppm for precursor ion and ± 0.05 Da for fragment ion were used as the criteria for protein identification and spectra interpretation. The Globo H derivative as well as its neutral loss forms was chosen as variable modification for Globo H conjugation site identification, and MMCCH derivative as well as its deamidated form was chosen as variable modification for MMCCH conjugation site identification. Database search was performed against the sequence of KLH1 and KLH2 provided by sponsor. Only those peptides with high quality MS/MS spectra (ion score $\geq$ 13, $p < 0.05$) were listed in the report.

[0243] To demonstrate a repeatable result, the LC-MS/MS analysis was performed twice followed by individual Mascot database search for both Globo H conjugation site identification and MMCCH conjunction site identification, as summarized in Figure 17.

[0244] In Globo H conjugation site analysis, 31 and 28 lysines were found respectively in 1st LC-MS/MS and 2nd LC-MS/MS for sample 1; 19 and 21 lysines were found respectively in 1st LC-MS/MS and 2nd LC-MS/MS for sample 2; 10 and 11 lysines were found respectively in 1st LC-MS/MS and 2nd LC-MS/MS for sample 3; 18 and 19 lysines were found respectively in 1st LC-MS/MS and 2nd LC-MS/MS for sample 4. The

identification details are listed in Figures 14-21. In MMCCH conjugation analysis, 155 and 141 lysines were found respectively in 1st LC-MS/MS and 2nd LC-MS/MS for sample 1; 143 and 137 lysines were found respectively in 1st LC-MS/MS and 2nd LC-MS/MS for sample 2; 147 and 143 lysines were found respectively in 1st LC-MS/MS and 2nd LC-MS/MS for sample 3; 140 and 136 lysines were found respectively in 1st LC-MS/MS and 2nd LC-MS/MS for sample 4. The identification details are listed in Figures 22-29.

[0245] Globo H conjugation sites from multiple enzyme experiments are summarized in Figure 30 and MMCCH conjugation sites are summarized in Figure 31. The overall conjugation site analysis results for Globo H conjugated samples are summarized in Figure 32.

[0246] Example 8 Conclusion:

[0247] The mass spectrometric signals of Globo H derivative conjugated peptides are lower than those of MMCCH conjugated peptides due to the multiple neutral loss forms and lower ionization efficiency of polysaccharide, which makes the direct identification of Globo H conjugation more difficult. This is why the numbers of identified peptides are higher for MMCCH conjugation analysis. Therefore, the MMCCH results may be used to represent the Globo H conjugation.

[0248] The conjugation site analysis suggests that there are 155, 143, 147 and 140 lysine conjugation sites identified among the total 306 lysine residues in KLH1/KLH2 for sample 1-4, respectively. In the replicate analysis, 141, 137, 143 and 136 conjugation sites were identified for samples 1-4, respectively.

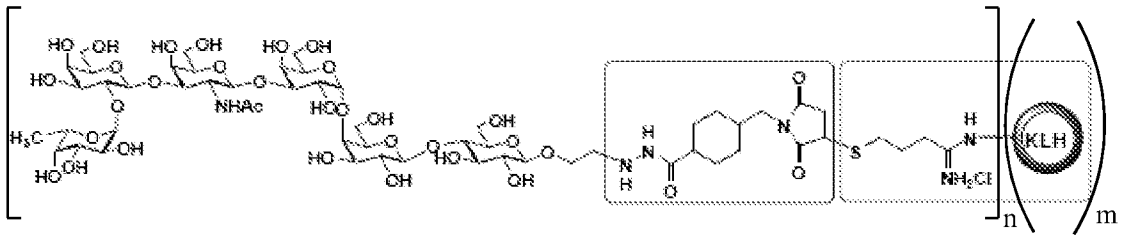
[0249] Unless defined otherwise, all technical and scientific terms and any acronyms used herein have the same meanings as commonly understood by one of ordinary skill in the art in the field of this invention. Although any compositions, methods, kits, and means for communicating information similar or equivalent to those described herein can be used to practice this invention, the preferred compositions, methods, kits, and means for communicating information are described herein.

[0250] All references cited herein are incorporated herein by reference to the full extent allowed by law. The discussion of those references is intended merely to summarize the assertions made by their authors. No admission is made that any reference (or a portion of any reference) is relevant prior art. Applicants reserve the right to challenge the accuracy and pertinence of any cited reference.

CLAIMS

What is claimed is:

1. A compound comprising the structure:



wherein

n independently is an integer from about 1 to about 800,

m is independently an integer from about 1 to about 5, and

wherein the Globo H moieties are covalently bound to the KLH moiety(ies) on basic amino acid residues.

2. The compound of claim 1, wherein m is 1 and n is from about 1 to about 150.

3. The compound of claim 1, wherein m is 2 and n is from about 1 to about 300

4. The compound of claim 1, wherein m is 3 and n is from about 1 to about 450.

5. The compound of claim 1, wherein m is 4 and n is from about 1 to about 600.

6. The compound of claim 1, wherein m is 5 and n is from about 1 to about 750.

7. The compound of claim 1, wherein n is from about 60 to about 100.

8. The compound of claim 1, wherein n is from about 70 to about 90.

9. The compound of claim 1, wherein n is from about 75 to about 80.

10. The compound of claim 1, wherein n is about 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100, 101, 102, 103, 104, 105, 106, 107, 108, 109, 110, 111, 112, 113, 114, 115, 116, 117, 118, 119, 120, 121, 122, 123, 124, 125, 126, 127, 128, 129, 130, 131, 132, 133, 134, 135, 136, 137, 138, 139, 140, 141, 142, 143, 144, 145, 146, 147, 148, 149, 150, 151, 152, 153, 154, 155, 156, 157, 158, 159, or 160.

11. A therapeutic composition comprising a plurality of Globo H moieties covalently linked to one or more keyhole limpet hemocyanin (KLH) moieties, wherein the ratio of the number of Globo H moieties to KLH moieties is from about 1:1 to about 150:1 expressed as the number of Globo H molecules to one monomeric KLH moiety.

12. A therapeutic composition comprising a plurality of Globo H moieties covalently linked to one keyhole limpet hemocyanin (KLH) moiety, wherein the number of Globo H moieties is from about 1 to about 150, expressed as the number of Globo H molecules to one monomeric KLH moiety.

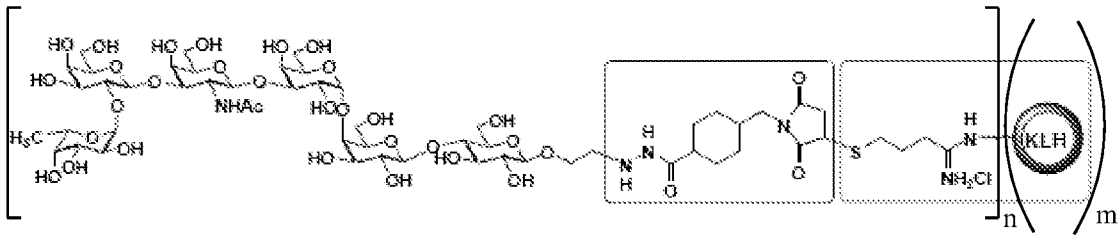
13. A therapeutic composition comprising a plurality of Globo H moieties covalently linked to two keyhole limpet hemocyanin (KLH) moieties, wherein the number of Globo H moieties is from about 1 to about 300, expressed as the number of Globo H molecules to a dimeric KLH moiety.

14. A therapeutic composition comprising a plurality of Globo H moieties covalently linked to three keyhole limpet hemocyanin (KLH) moieties, wherein the number of Globo H moieties is from about 1 to about 450, expressed as the number of Globo H molecules to a trimeric KLH moiety.

15. A therapeutic composition comprising a plurality of Globo H moieties covalently linked to four keyhole limpet hemocyanin (KLH) moieties, wherein the number of Globo H moieties is from about 1 to about 600, expressed as the number of Globo H molecules to a tetrameric KLH moiety.

16. A therapeutic composition comprising a plurality of Globo H moieties covalently linked to five keyhole limpet hemocyanin (KLH) moieties, wherein the number of Globo H moieties is from about 1 to about 750, expressed as the number of Globo H molecules to a pentameric KLH moiety.

17. A pharmaceutical composition comprising: a compound comprising the structure:



wherein n independently is an integer from about 1 to about 750, and wherein m is independently an integer from about 1 to about 5, and optionally a pharmaceutically acceptable carrier.

18. The composition of claim 17, wherein m is 1 and n is from about 1 to about 150.

19. The composition of claim 17, wherein m is 2 and n is from about 1 to about 300

20. The composition of claim 17, wherein m is 3 and n is from about 1 to about 50.

21. The composition of claim 17, wherein m is 4 and n is from about 1 to about 600.

22. The composition of claim 17, wherein m is 5 and n is from about 1 to about 750.

23. The compound of claim 17, wherein n is from about 60 to about 100.

24. The compound of claim 17, wherein n is from about 70 to about 90.

25. The compound of claim 17, wherein n is from about 75 to about 80.

26. The compound of claim 17, wherein n is about 62, 66, 67, 68, 70, 72, 76, 86, 87, 88, 90, 92, 93 or 100.

27. A pharmaceutical composition comprising a therapeutic conjugate comprising a plurality of Globo H moieties covalently linked to one or more keyhole limpet hemocyanin (KLH) moiety subunit, wherein the number of Globo H moieties to KLH moiety subunits is from about 1:1 to about 150:1.

28. A pharmaceutical composition comprising an therapeutic conjugate comprising a plurality of Globo H moieties covalently linked to one or more keyhole limpet hemocyanin (KLH) moiety subunit, wherein the KLH moieties exist as monomers, dimers, trimers, tetramers, and pentamers.

29. A pharmaceutical composition comprising an therapeutic conjugate comprising a plurality of Globo H moieties covalently linked to one or more keyhole limpet hemocyanin (KLH) moiety subunit, wherein the number of Globo H moieties to KLH moiety subunits is from about 1:1 to about 300:1, expressed as the number of Globo H molecules to a dimeric KLH moiety.

30. A pharmaceutical composition comprising an isolated therapeutic conjugate comprising a plurality of Globo H moieties covalently linked to one or more

keyhole limpet hemocyanin (KLH) moiety subunit, wherein the number of Globo H moieties to KLH moiety subunits is from about 1:1 to about 450:1, expressed as the number of Globo H molecules to one trimeric KLH moiety.

31. A pharmaceutical composition comprising an isolated therapeutic conjugate comprising a plurality of Globo H moieties covalently linked to one or more keyhole limpet hemocyanin (KLH) moiety subunit, wherein the number of Globo H moieties to KLH moiety subunits is from about 1:1 to about 600:1, expressed as the number of Globo H molecules to one tetrameric KLH moiety.

32. A pharmaceutical composition comprising an isolated therapeutic conjugate comprising a plurality of Globo H moieties covalently linked to one or more keyhole limpet hemocyanin (KLH) moiety subunit, wherein the number of Globo H moieties to KLH moiety subunits, expressed as the number of Globo H molecules versus one pentameric KLH is from about 10:1 to about 750:1, expressed as the number of Globo H molecules to one pentameric KLH moiety.

33. A pharmaceutical composition comprising monomers, dimers, trimers, tetramers or pentamers or combinations thereof of KLH moiety, wherein each KLH moiety comprises one or more Globo H moieties covalently linked to a KLH moiety.

34. The pharmaceutical composition of claim 33, wherein about 1% to about 99% of the therapeutic conjugates in the composition are monomers.

35. The pharmaceutical composition of claim 33, wherein about 1% to about 99% of the therapeutic conjugates in the composition are dimers.

36. The pharmaceutical composition of claim 33, wherein about 1% to about 99% of the therapeutic conjugates in the composition are trimers.

37. The pharmaceutical composition of claim 33, wherein about 1% to about 99% of the therapeutic conjugates in the composition are tetramers.

38. The pharmaceutical composition of claim 33, wherein about 1% to about 99% of the therapeutic conjugates in the composition are pentamers.

39. A pharmaceutical composition comprising a plurality of Globo H moieties covalently linked to one or more KLH moiety subunit, wherein about 1% to 99% of the KLH moieties in the composition are monomers, dimers, trimers, tetramers, pentamers, or combinations thereof.

40. The pharmaceutical composition of claim 33 further comprising an adjuvant, wherein the adjuvant is complete and incomplete Freund's adjuvant, Toll-Like Receptor molecules, LPS, lipoproteins, lipopeptides, flagellin, double-stranded RNA, viral DNA, unmethylated, CpG islands, levamisole, bacillus Calmette-Guerin, Isoprinosine, Zadaxin, PD-1 antagonists, PD-1 antibodies, CTLA antagonists, CTLA antibodies, interleukin, cytokines, GM-CSF, glycolipid, aluminum salt based, aluminum phosphate, alum, aluminum hydroxide, liposomes, TLR2 agonists, lipopeptide, nanoparticles, monophosphoryl lipid A, an OPT-821 saponin, oil in water nano-emulsions, and bacteria-like particle.

41. The pharmaceutical composition of claim 33 further comprising a cytokine selected from the group consisting of IL-2, IL-12, IL-18, IL-2, IFN-γ, TNF, IL-4, IL-10, IL-13, IL-21, GM-CSF and TGF-β.

42. The pharmaceutical composition of claim 33 further comprising a chemokine.

43. The pharmaceutical composition of claim 33 further comprising an agent selected from the group consisting of hormonal therapeutic agents (e.g., selective estrogen

receptor modulators, androgen receptor modulators), monoclonal antibody therapy, chemotherapy, retinoid receptor modulators, cytotoxic/cytostatic agents, antineoplastic agents, antiproliferative agents, prenyl-protein transferase inhibitors, HMG-CoA reductase inhibitors, nitrogen mustards, nitroso ureas, angiogenesis inhibitors (e.g., bevacizumab), inhibitors of cell proliferation and survival signaling pathway, apoptosis inducing agents, agents that interfere with cell cycle checkpoints, agents that interfere with receptor tyrosine kinases (RTKs), mammalian target of rapamycin (mTOR) inhibitors, human epidermal growth factor receptor 2 (HER2) inhibitors, epidermal growth factor receptor (EGFR) inhibitors, integrin blockers, NSAIDs, PPAR agonists, inhibitors of inherent multidrug resistance (MDR), anti-emetic agents, agents useful in the treatment of anemia, agents useful in the treatment of neutropenia, immunologic-enhancing drugs, biphosphonates, aromatase inhibitors, agents inducing terminal differentiation of neoplastic cells, γ-secretase inhibitors, cancer vaccines, PD-1/PD-L1 inhibitors (cytotoxic T cell lymphocyte (CTLs) immunotherapy), CTLA-4 immunotherapy, CDK4/6 inhibitors (target therapy), PI3K inhibitors (target therapy), mTOR inhibitors (target therapy), AKT inhibitors (target therapy), Pan-Her inhibitors (target therapy), and any combination thereof.

44. The pharmaceutical composition of claim 33 comprising a pharmaceutically acceptable carrier.

45. The pharmaceutical composition of claim 44, wherein the pharmaceutical composition is a cancer vaccine.

46. The pharmaceutical composition of claim 33 formulated for subcutaneous injection.

47. The pharmaceutical composition of claim 33 formulated for intravenous administration.

48. The pharmaceutical composition of claim 33 formulated for intra-muscular administration.

49. A method of treating cancer in a patient in need thereof comprising administering to the patient a therapeutically effective amount of the composition of claim 33.

50. The method of claim 49, wherein the cancer is ovarian cancer.

51. The method of claim 49, wherein the cancer is an epithelial cancer.

52. The method of claim 49, wherein the cancer is breast cancer.

53. The method of claim 49, wherein therapeutically effective amount of Globo-H moiety in the composition comprises from about 0.01 μg/kg to about 250 mg/kg.

54. The method of claim 49, wherein therapeutically effective amount of Globo-H moiety in the composition comprises from about 0.10 μg/kg to about 0.75 μg/kg.

55. The method of claim 49, wherein therapeutically effective amount of Globo-H-KLH complex in the composition comprises from about 0.01 μg/kg to about 250 mg/kg.

56. The method of claim 49, wherein therapeutically effective amount of Globo-H-KLH complex in the composition comprises from about 0.60 μg/kg to about 4.50 μg/kg.

57. A method of inducing antibodies in an animal or a human for the purpose of creating monoclonal antibodies for therapeutic or diagnostic uses comprising

administering to the animal or human an effective amount of the composition of claim 49.

Figure 1

Fig. 1(a)

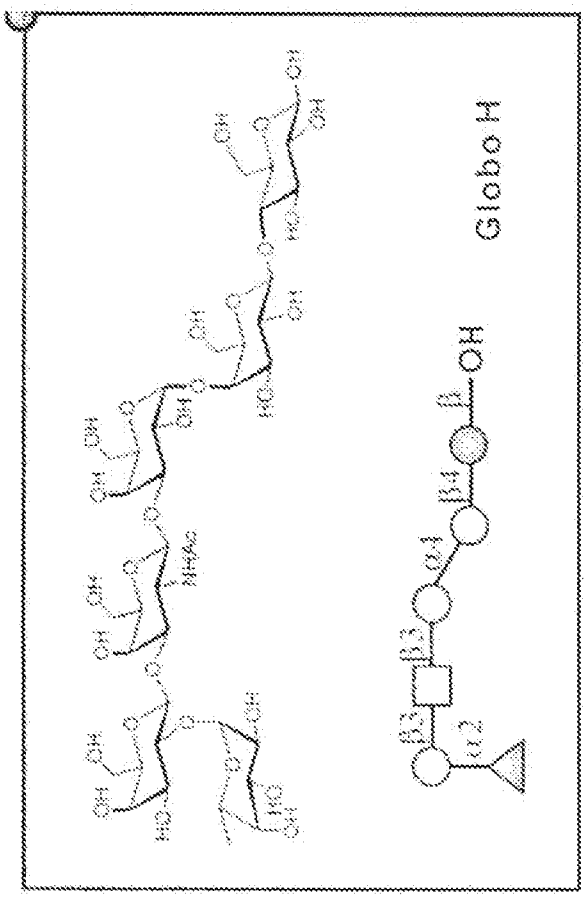


Fig. 1(b)

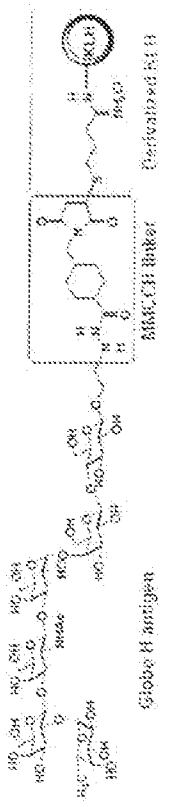


Figure 2

Fig. 2(a)

Fig. 2(b)

Figure 3

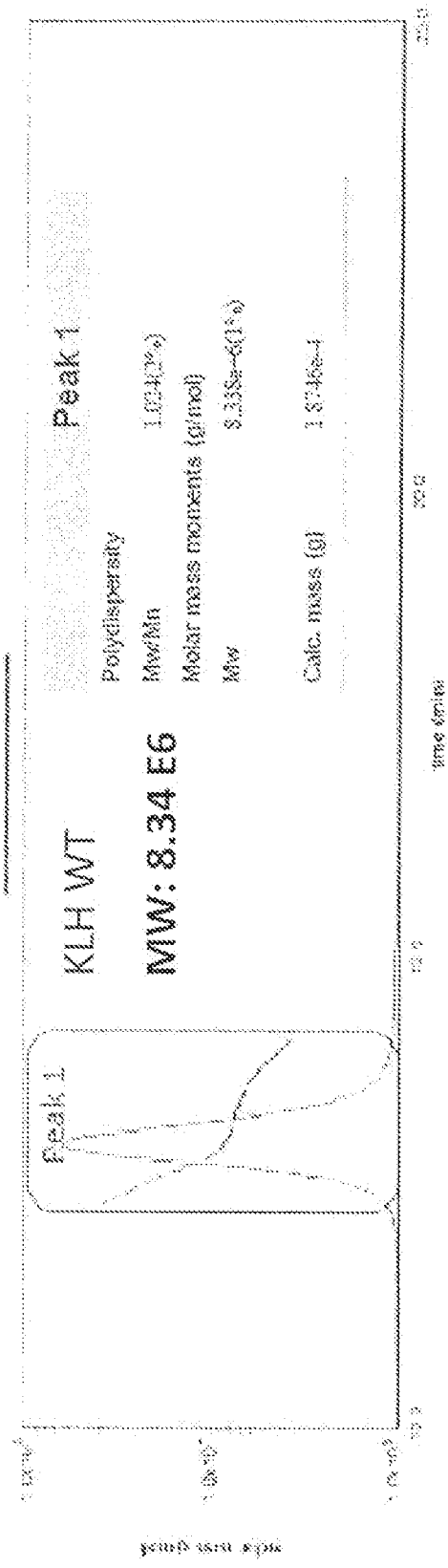

KLH WT
MW: 8.34 E6
Peak 1
Polydispersity
Mw/Mn
Molar mass moments (g/mol)
Mw
Calc. mass (g)
Peak 1
time (min)

Figure 4

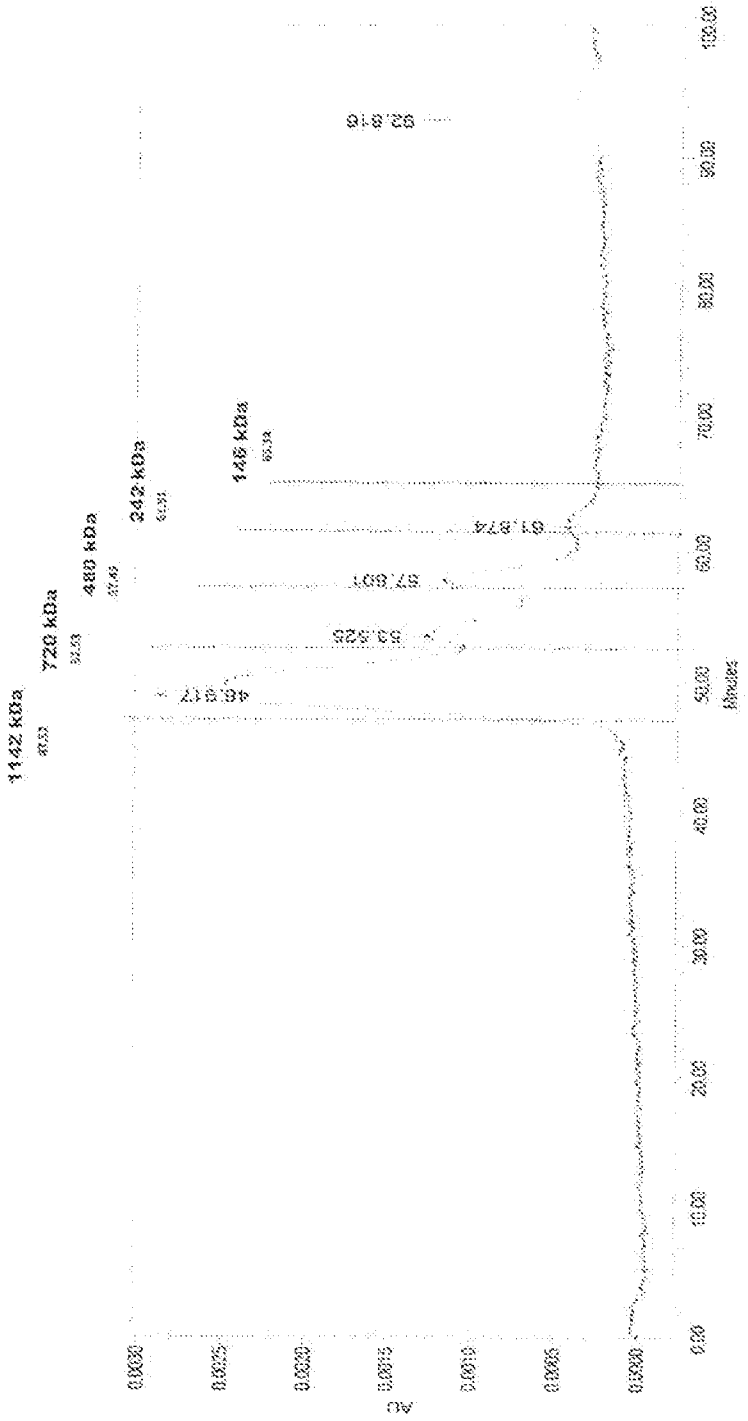

1142 kDa
720 kDa
480 kDa
242 kDa
146 kDa
92.816
67.874
57.607
53.425
46.917
AU
Minutes

Figure 5

Fig. 5(A)

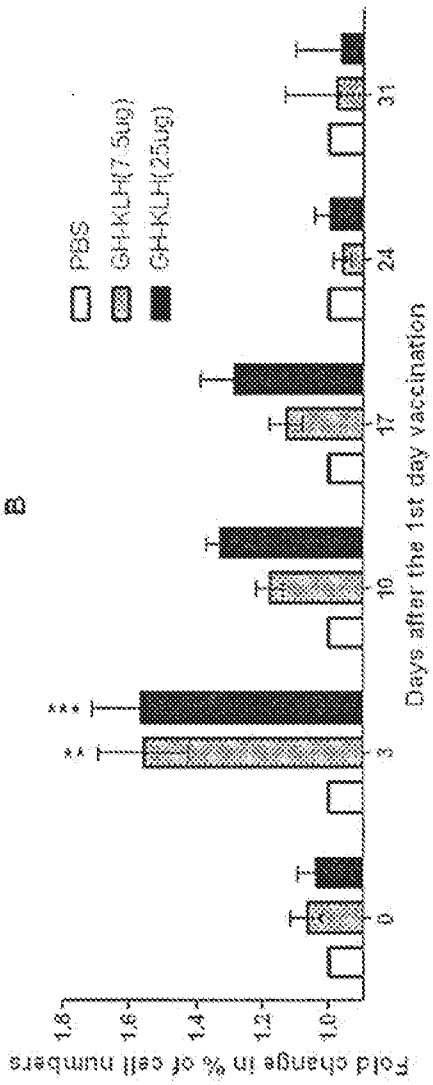


Figure 5 continued

Fig. 5(B)

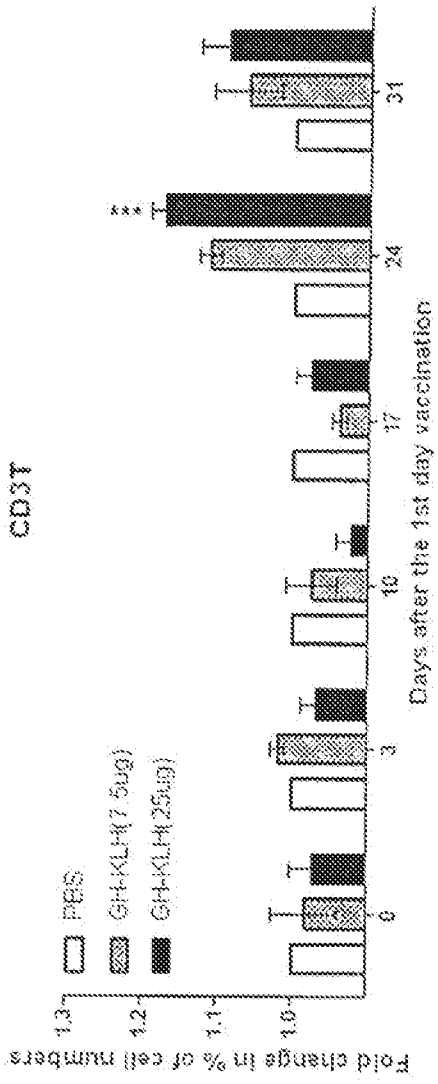


Figure 5 continued

Fig. 5(C)

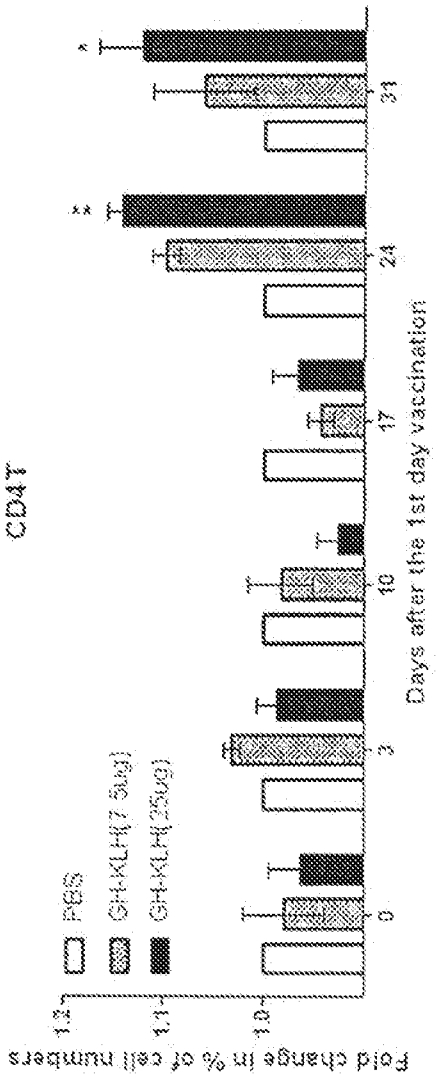


Figure 5 continued

Fig. 5(D)

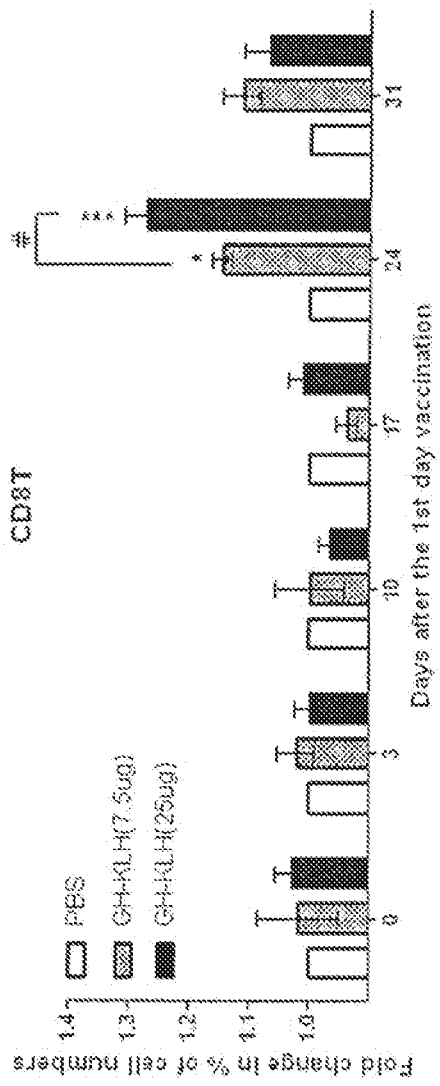


Figure 6

Fig. 6(A)

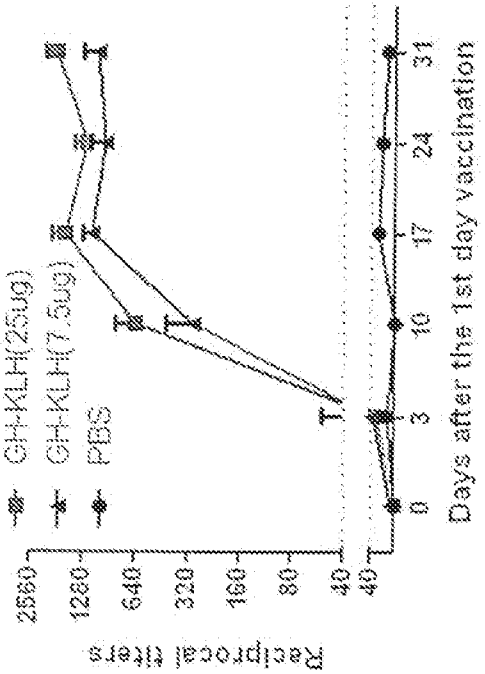


Figure 6 continued

Fig. 6(B)

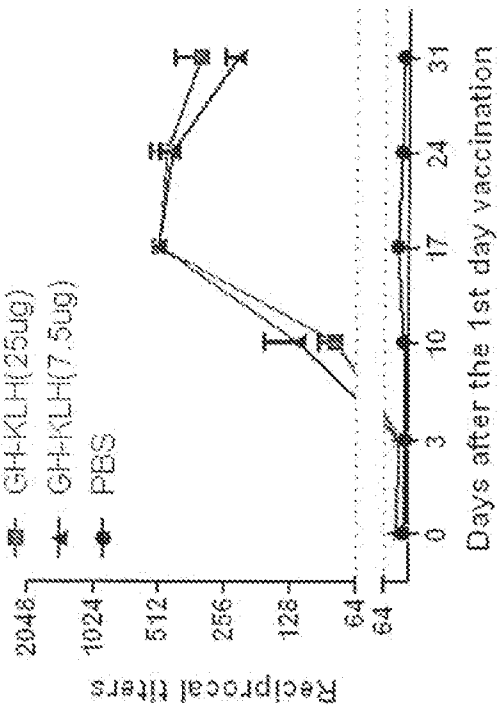


Figure 7

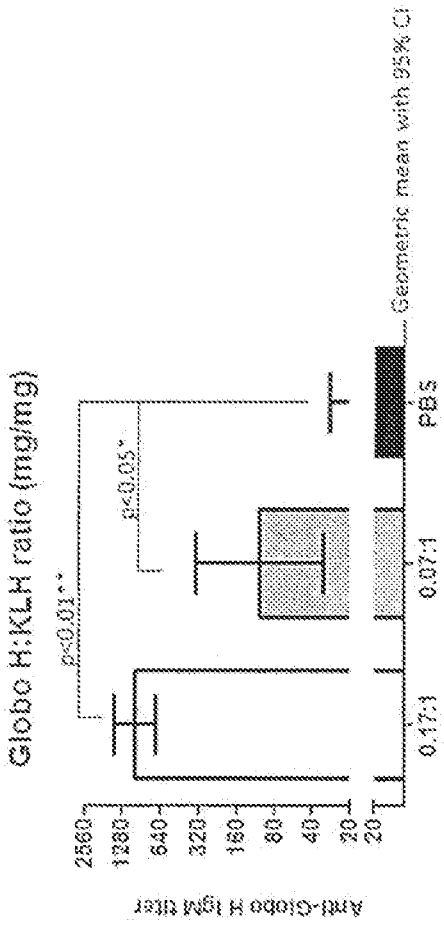

Globo H:KLH ratio (mg/mg)
p<0.01**
p<0.05*
Anti-Globo H IgM titer
2560
1280
640
320
160
80
40
20
20
0.17:1
0.07:1
PBS
Geometric mean with 95% CI

Figure 8

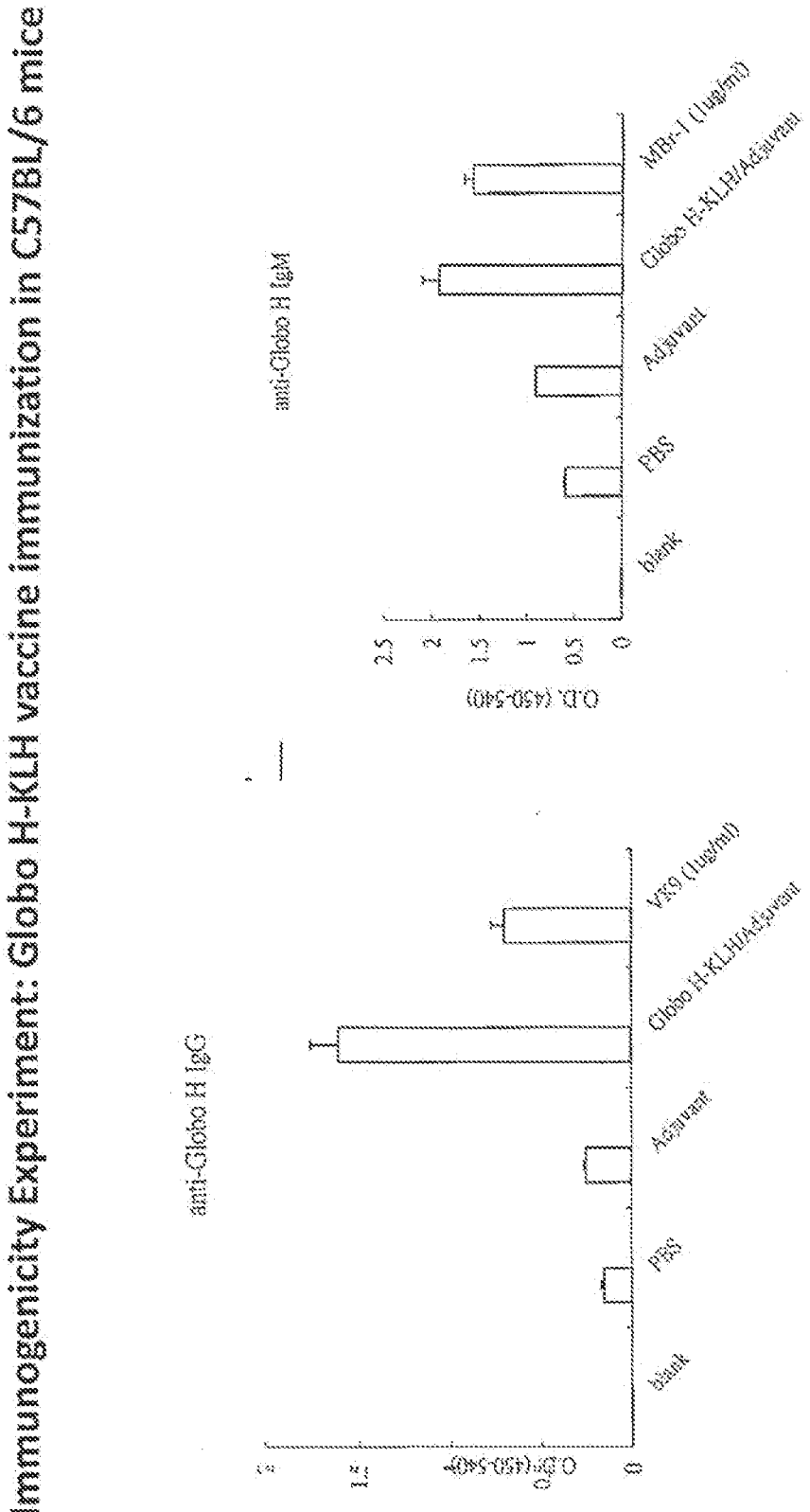


Fig 8(a)

Fig 8(b)

Figure 9

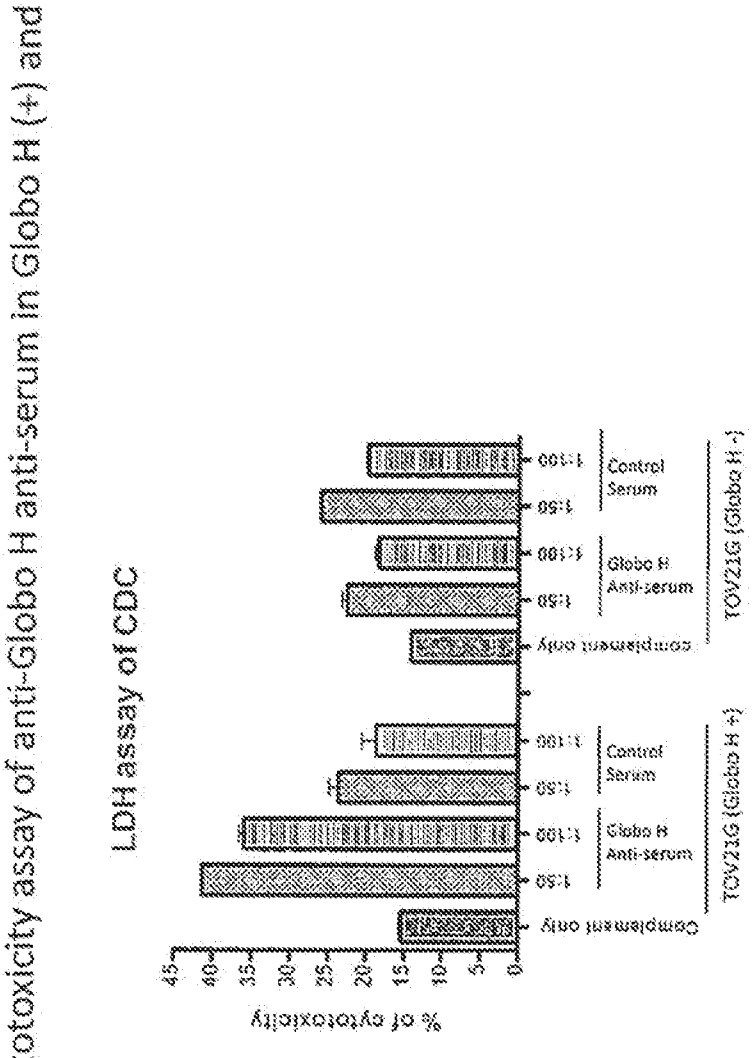

Complement dependent cytotoxicity assay of anti-Globo H anti-serum in Globo H (+) and Globo H(-) of TOV21G cells
LDH assay of CDC
% of cytotoxicity
45
40
35
30
25
20
15
10
5
0
Complement only
1:50
1:100
1:50
1:100
Globo H Anti-serum
Control Serum
TOV21G (Globo H +)
Complement only
1:50
1:100
1:50
1:100
Globo H Anti-serum
Control Serum
TOV21G (Globo H -)

Figure 10

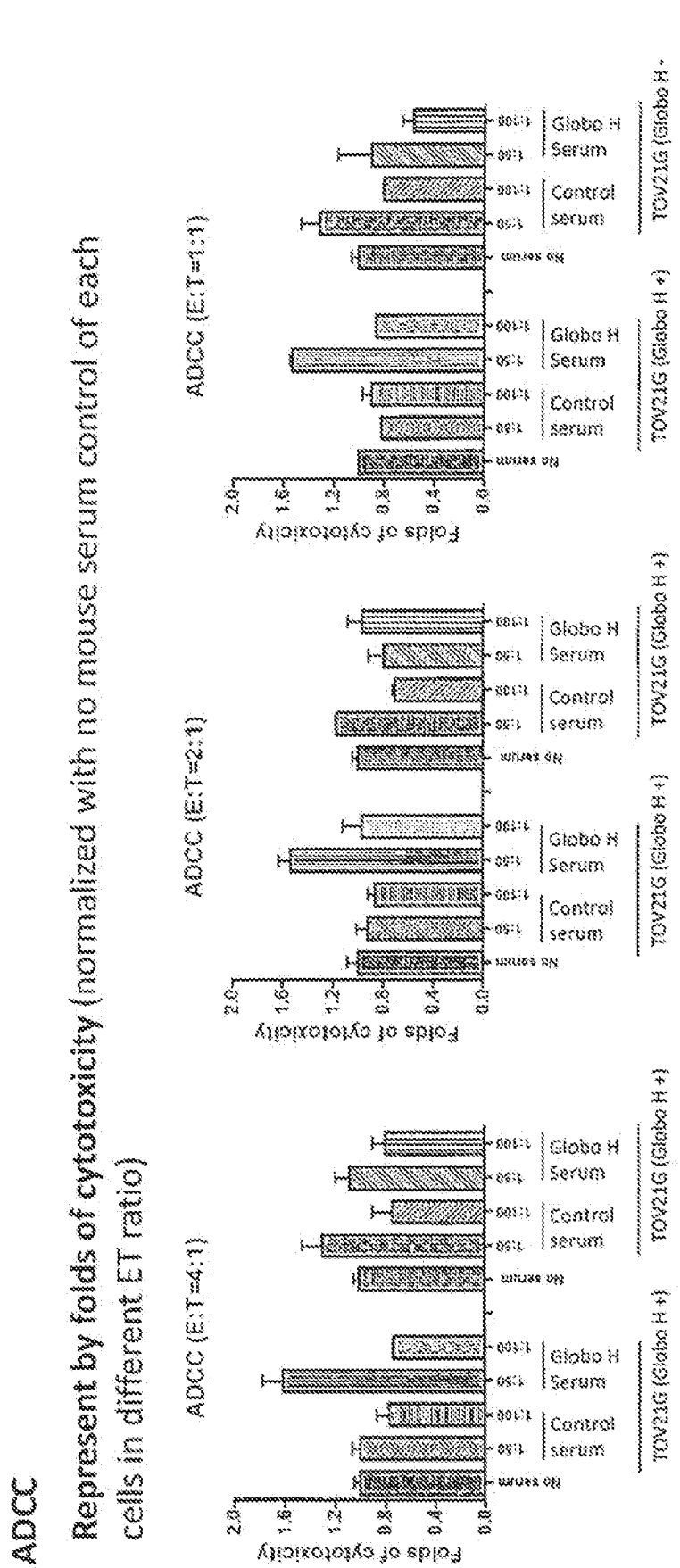


Fig 10(a) Fig 10(b) Fig 10(c)

Figure 11

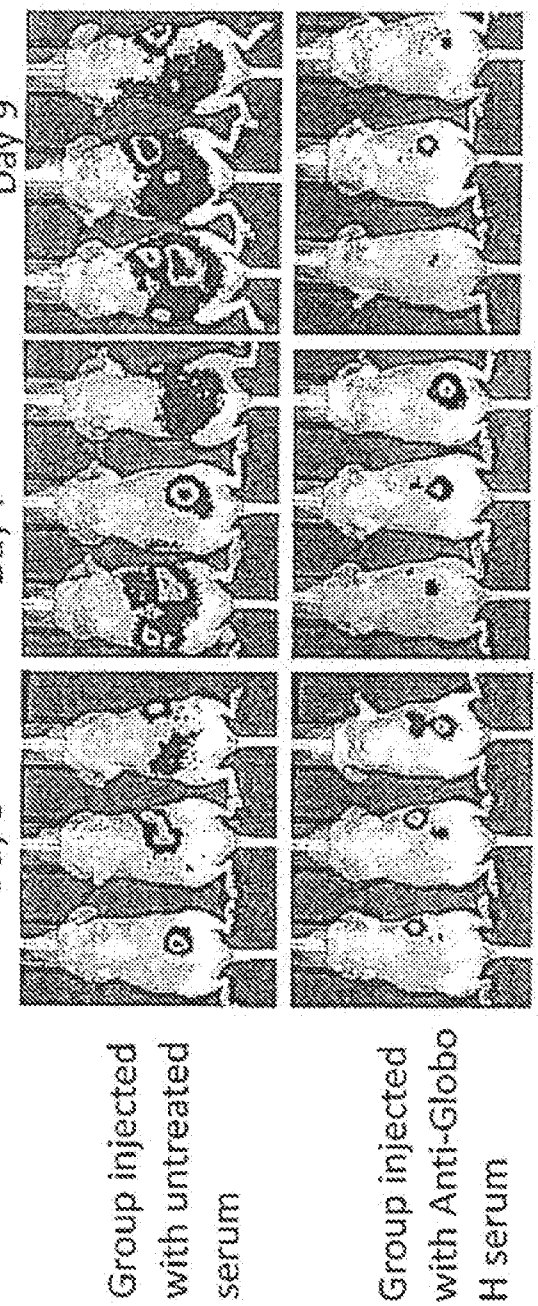

Day 3
Day 7
Day 9
Group injected with untreated serum
Group injected with Anti-Globo H serum

Figure 12

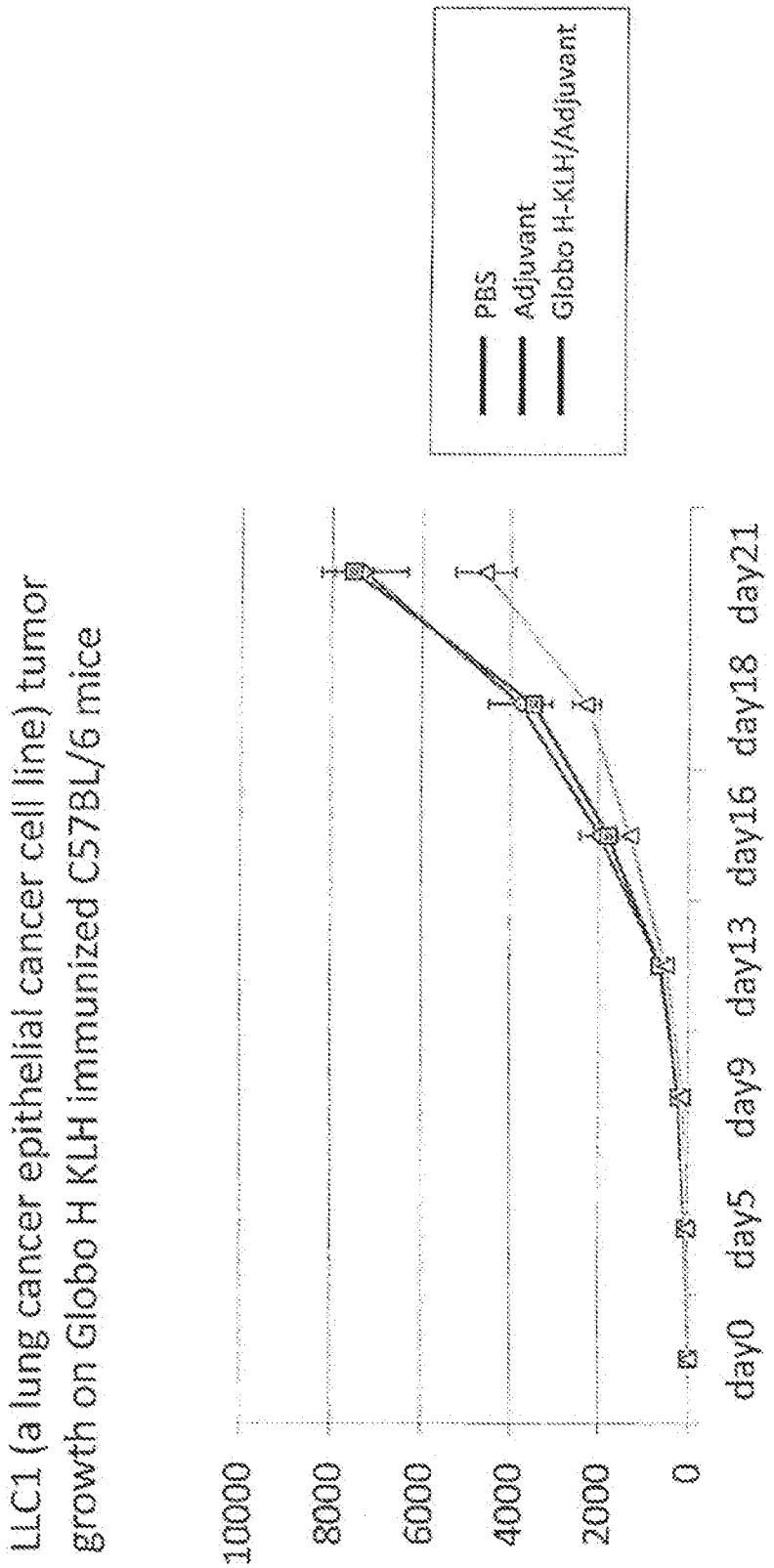

LLC1 (a lung cancer epithelial cancer cell line) tumor growth on Globo H KLH immunized C57BL/6 mice
PBS
Adjuvant
Globo H-KLH/Adjuvant
10000
8000
6000
4000
2000
0
day0
day5
day9
day13
day16
day18
day21

Figure 13

Sample	1st LC-MS/MS	2nd LC-MS/MS
1	Table 2.	Table 6.
2	Table 3.	Table 7.
3	Table 4.	Table 8.
4	Table 5.	Table 9.

Table 1B. MMCCH derivative analysis

Sample	1st LC-MS/MS	2nd LC-MS/MS
1	Table 10.	Table 14.
2	Table 11.	Table 15.
3	Table 12.	Table 16.
4	Table 13.	Table 17.

Figure 14

#	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	1701.7938	2.52	T	1	14	0.039	EAFHKFDEDR +K_MMCCH_NL997 (K)	161
3	588	606	1132.8246	3395.4720	3395.4862	-2.09	T	1	16	0.022	EPKSAGEFGQDLGAFHGEPK +Globo_H_MMCCH (K)	590
4	700	719	1015.1623	3042.4652	3042.4532	3.94	T	1	27	0.0019	SVQMKLFEQPEFGHYTSAK +K_MMCCH_NL673 (K)	719
5	953	965	762.7177	2285.1311	2285.1249	2.71	T	1	52	6.30E-06	DLFKQPSVHEPR +K_MMCCH_NL673 (K)	956
6	986	1000	1036.8300	3107.4681	3107.4578	3.31	T	1	20	0.011	KNERLSLGEESLR +Globo_H_MMCCH (K)	986
7	1092	1114	806.3825	3221.5034	3221.5213	-6.18	T	1	24	0.0038	QHHYETNPFHHHGKITHENEITR +K_MMCCH_NL997 (K)	1104
8	1473	1489	905.7906	2714.3499	2714.3414	3.13	T	1	25	0.0034	KHGAVVGLPYWGWTLPR +K_MMCCH_NL673 (K)	1473
9	1923	1932	703.8990	1585.7834	1585.7745	5.68	T	1	17	0.02	NKVMPKPFAR +Deamidated (NQ); K_MMCCH_NL997 (K); Oxidation (M)	1924
10	2358	2367	846.4022	1690.7836	1690.7872	1.54	T	1	19	0.011	DRLFNDPER +K_MMCCH_NL835 (K)	2360
11	2851	2883	1027.9812	4107.8957	4107.8666	7.08	T	0	62	6.30E-07	VKPAHAGSCAGDIMMVFLMPFNYESVNMDDFTR +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	FNYKYDNLMLHSHNEELEEVLR +K_MMCCH_NL997 (K)	2900
13	3003	3031	953.1823	2856.4650	2856.4467	6.44	T	1	31	0.00072	KYDHTELISASVLPAPIVR +K_MMCCH_NL673 (K)	3003
14	613	626	1151.5167	2301.0189	2301.0150	1.69	Tb	5	13	0.05	ASKKFACCVHGMSV +K_MMCCH_NL673 (K)	616

Figure 14 continued

#	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	179	615.6599	1843.9573	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	AMERFQNDKSVDGYGATVEFHALPAR +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	4866.1692	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	AKYSLSSLDYTAFDPVFFLNHANVDR +K_MMCCH_NL997 (K)	1456
11	1508	1539	841.0049	4199.9883	4199.9680	4.83	T	1	30	0.0011	KPLQPFNNPELNSDSMTLEHNLPQDSFDYQNR +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	IKQCQEADRVF +K_MMCCH_NL997 (K)	1986

Figure 14 continued

"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

#	Start	End	Observed	Mr(expt)	Mr(calc)	ppm	Enzyme	MC	Score	E value	Peptide	Mod_site
1	588	606	1133.6397	3395.4975	3395.4862	3.30	T	1	25	0.0035	EDKSAGGAGQQIGAFHGEPK +Gluto_H_MMCCH (K)	590
2	700	719	1069.1605	3204.5168	3204.5060	4.31	T	1	28	0.0016	SVQMKLFEQPEFGHYTSIAK +K_MMCCH_NL511 (K)	719
3	953	965	654.6852	1961.0337	1961.0193	7.34	T	1	42	6.00E-05	DLFKQPSVHHEPR +K_MMCCH_NL997 (K)	956
4	1092	1114	645.3080	3221.5038	3221.5213	-5.43	T	1	29	0.0013	QHHYETNPFHHGRITHENETTR +K_MMCCH_NL997 (K)	1104
5	1923	1932	793.9966	1585.7787	1585.7745	2.65	T	1	14	0.84	NKVMPWPTAR +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	KENTLTTARVDNLKDAMR +Deamidated (NQ); K_MMCCH_NL673 (K)	2247
7	2851	2883	1027.9795	4107.8889	4107.8666	5.43	T	0	32	0.00058	VRPAHAGSCAGSMMVFLHPFNYESVMMDDFTR +Deamidated (NQ); K_MMCCH_NL997 (K); Oxidation (M)	2852
8	158	169	733.6753	2198.0042	2197.9839	9.33	G	2	32	0.00064	APHRFQEDRSVD +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 15 continued

#	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	1843.9316	-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	283	630.3964	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)	1525
10	1949	1963	766.0179	2295.0316	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	KAQSIHPEDVPDTDAPF +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

Figure 15 continued

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

#	Start	End	Observed	Mr(expt)	Mr(calc)	ppm	Enzyme	MC	Score	E value	Peptide	Mod_site
1	377	402	652.1614	3404.8167	3404.8104	1.85	T	0	18	0.017	AHCASLEAMHLKPFAPSSPLMANEK +Deamidated (NQ); K_MMCCH_NL997 (K); Oxidation (M)	402
2	1092	1114	687.4109	3545.6345	3545.6270	-3.53	T	1	14	0.041	QHMYETMPFHHGKITHENEITR +K_MMCCH_NL673 (K)	1104
3	1092	1114	806.3819	3221.4985	3221.5213	-7.08	T	1	17	0.022	QHMYETMPFHHGKITHENEITR +K_MMCCH_NL997 (K)	1104
4	2233	2251	721.5998	2882.3662	2882.3776	-3.96	T	2	45	3.30E-05	KEINTLTTAEVDMLKDAMR +Deamidated (NQ); K_MMCCH_NL673 (K)	2247
5	2851	2883	1027.9769	4107.8786	4107.8966	2.92	T	0	46	2.60E-05	VKPAHAGSSAGDMMVPLHPPEMVESVAMDDFTR +Deamidated (NQ); K_MMCCH_NL997 (K); Oxidation (M)	2852

Figure 16 continued

#	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	4866.1692	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

#	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	AHCASLEHMHLKPFAPSPLMNKEK +Deamidated (NQ); K_MMCCH_N1997 (K); Oxidation (M)	402
2	953	965	654.6849	1961.0330	1961.0193	6.99	T	1	27	0.0021	DLFKGPSYHEPR +K_MMCCH_N1997 (K)	956
3	1092	1114	806.3821	3221.4995	3221.5213	-6.80	T	1	18	0.015	QHNYETMPFHNEKITHENEITTR +K_MMCCH_N1997 (K)	1104
4	1923	1932	793.8979	1585.7812	1585.7745	4.29	T	1	17	0.021	MKVARNPFAR +Deamidated (NQ); K_MMCCH_N1997 (K); Oxidation (M)	1924
5	2233	2251	721.9967	2882.3657	2882.3776	-4.16	T	2	41	7.90E-05	KENTLTTAGVDNLKQAMR +Deamidated (NQ); K_MMCCH_N1673 (K)	2247
6	2359	2367	927.4296	1852.8447	1852.8400	2.54	T	1	21	0.0052	DKLANDPER +K_MMCCH_N1673 (K)	2360
7	2851	2883	1027.9815	4107.8967	4107.8666	7.33	T	0	30	0.00034	VKPAHAGSCAGDIMGMFLHPFNYESVWNDDFTR +Deamidated (NQ); K_MMCCH_N1997 (K); Oxidation (M)	2852
8	506	512	850.4159	1698.8173	1698.8089	9.71	Th	2	34	0.037	LKDLDLT +K_MMCCH_N1511 (K)	507

Figure 17 continued

#	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	3762.9825	3762.9879	1.30	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	1119	1178.6874	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	IKQDQEADRVF +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)	2465
10	1525	1539	865.7426	2594.2060	2594.1959	3.89	Th	3	20	0.015	LKHNLPGDSFDYDNR +K_MMCCH_NL673 (K)	1526
11	1952	1963	646.6356	1936.8890	1936.8778	5.77	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

#	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	EDKSAGGFQQLGAFHGEPR +Globo_H_MMCCH (K)	590
2	702	719	1035.1627	3042.4663	3042.4532	4.31	T	1	36	0.00092	SVQAKLFEQPEFGHYTSIAK +K_MMCCH_NL673 (K)	719
3	953	965	762.7192	2285.1359	2285.1249	4.81	T	1	47	2.10E-05	DLFKQPSVMEPR +K_MMCCH_NL673 (K)	956
4	1092	1114	1074.8417	3221.5033	3221.5213	-5.62	T	1	30	0.001	QHHVETMPFHHGKITHENEITR +K_MMCCH_NL997 (K)	1104
5	1417	1445	980.2136	3916.8254	3916.8135	3.04	T	1	14	0.041	ADHSSDEFQAIASFHALPRLCPSPAASKR +K_MMCCH_NL511 (K)	1444
6	1473	1489	905.7894	2714.3463	2714.3414	1.81	T	1	17	0.022	KHGAVVSLPYWDWTLPR +K_MMCCH_NL673 (K)	1473
7	1923	1932	793.8984	1585.7822	1585.7745	4.86	T	1	15	0.034	KKVMPMPFAR +Deamidated (NQ); K_MMCCH_NL997 (K); Oxidation (M)	1924
8	2233	2251	721.3977	2882.3618	2882.3776	-5.48	T	2	23	0.0049	KENTLTTAEVDNLKDAMR +Deamidated (NQ); K_MMCCH_NL673 (K)	2247
9	2359	2367	1008.4539	2014.8933	2014.8923	0.20	T	1	17	0.022	DKLPMDPER +K_MMCCH_NL511 (K)	2360
10	2851	2869	1027.9791	4107.8674	4107.8665	5.06	T	0	35	0.0003	VKPAHASSCAGDMHYPLHPPNYESVMADDFTR +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	FNYKYDNLMLHGHREELEEVLR +K_MMCCH_NL997 (K)	2900
12	3003	3021	953.1583	2856.4530	2856.4467	2.21	T	1	17	0.021	KYDHTELDASVLPAPIVR +K_MMCCH_NL673 (K)	3003
13	158	169	733.6757	2198.0053	2197.9838	9.83	G	2	14	0.044	APHKPGEDKSVD +K_MMCCH_NL673 (K)	161

Figure 18 continued

#	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	3439.8667	3439.8663	5.93	T	1	35	0.0029	QFTLVHRPAKGHFDKPPVPVAQANLAVR +Deamidated (NQ); K_MMCCH_NL997 (K)	433
5	467	468	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	AKVSLSSLDYTAFDPVFFLHHANVDR +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	2.08	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	SIRSAFLQIQK6 +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

Figure 18 continued

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

#	Start	End	Observed	Mr(expt)	Mr(calc)	ppm	Enzyme	MC	Score	E value	Peptide	Mod_site
1	953	965	654.6624	1961.0253	1961.0193	3.06	T	1	46	2.60E-05	DLFKQPSVHEPR +K_MMCCH_M1997 (K)	956
2	1092	1114	906.3603	3221.4919	3221.5213	-9.13	T	1	18	0.015	QHHYETRPFHHGKITMEMEITR +K_MMCCH_M1997 (K)	1104
3	1417	1445	1108.0071	4427.9992	4428.0036	-0.99	T	1	13	0.046	ADHSSIGFQAIASFHALPPLCPSPAASKR +Globo_H_MMCCH (K)	1444
4	2233	2251	721.5986	2882.3654	2882.3776	-4.23	T	2	37	0.0002	KENTLTTAEVDNLKDAMR +Deamidated (NQ); K_MMCCH_M1673 (K)	2247
5	2359	2367	927.4279	1852.8413	1852.8400	0.65	T	1	17	0.02	DKLFMPPER +K_MMCCH_M1673 (K)	2360
6	2851	2883	1027.9758	4107.8742	4107.8666	1.85	T	0	37	0.00018	VKPAHASSCAGDMMYPLHPFNYESVNNEDFTR +Deamidated (NQ); K_MMCCH_M1997 (K); Oxidation (M)	2852
7	1649	1664	1104.1271	3309.3594	3309.3654	-1.81	C	2	14	0.038	NLNDHTHDPSKPEDTF +Globo_H_MMCCH (N)	1659

Figure 19 continued

#	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	1887.8665	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	FQNDKSVDGYQATVEPHALPAR +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	1101.4763	3301.4130	3301.4232	-3.09	C	2	17	0.021	KHNLPQDSFDYQNKF +Globo_H_MMCCH (K)	1526
14	1985	1995	586.6373	1756.8902	1756.8930	-1.65	C	0	23	0.0049	IKQQDEADRVF +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)",

Figure 19 continued

"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

#	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	AMCAISLEHKMHLKPFAFSSPLNMNEK +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	SVQNKLFEDPEFGHYTSIAK +K_MMCCH_NL511 (K)	719
3	1092	1114	806.3823	3221.4999	3221.5213	-6.64	T	1	17	0.019	QHHVETNPPHHGKITHENEITR +K_MMCCH_NL997 (K)	1104
4	2233	2251	721.5977	2882.3616	2882.3776	-5.48	T	2	28	0.0016	KENTLTTAEVDNLKDAMR +Deamidated (NQ); K_MMCCH_NL673 (K)	2247
5	2851	2883	1027.9711	4107.8552	4107.8666	-2.78	T	0	32	0.00067	VKPAHAGSCAGDIMNVFLHPTNVTESVNNDDFTR +Deamidated (NQ); K_MMCCH_NL997 (K); Oxidation (M)	2852
6	158	169	733.6741	2199.0006	2197.9838	7.64	G	2	16	0.025	AFHKQEDKSVD +K_MMCCH_NL673 (K)	161

Figure 20 continued

#	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	QFTLVHRPAKGHFDKPPVPVAQANLAVR +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)	1366
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

#	Start	End	Observed	Mr(expt)	Mr(calc)	ppm	Enzyme	MC	Score	E value	Peptide	Mod_site
1	778	789	996.5373	1971.0600	1971.0553	2.44	T	1	17	0.031	IWAIWQAIQKYR +K_MMCCH_NL997 (K)	787
2	953	965	654.6835	1961.0288	1961.0193	4.84	T	1	32	0.00065	DLFKGPSVIHEPR +K_MMCCH_NL997 (K)	956
3	1092	1114	808.3824	3221.5007	3221.5213	-6.39	T	1	24	0.004	QHHYETNPFHHGKITHENETTR +K_MMCCH_NL997 (K)	1104
4	1923	1932	793.8977	1585.7809	1585.7745	4.04	T	1	19	0.031	NKVAMPNPFAR +Deamidated (NQ); K_MMCCH_NL997 (K); Oxidation (M)	1924
5	2233	2251	721.5991	2882.3673	2882.3776	-3.64	T	2	17	0.022	KENTLTTAEVDNLKDAAR +Deamidated (NQ); K_MMCCH_NL673 (K)	2247
6	2851	2863	1027.9812	4107.8957	4107.8666	7.08	T	0	49	1.28E-05	VKPAHAGSCAGDMRVPLHPENYESVNNDDFTR +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	0.0036	FHGEPAWCPSPE +Globo_H_MMCCH (K)	606
9	1560	1587	763.8522	1525.6899	1525.6858	2.69	Th	1	14	0.037	VEGKEPYG +K_MMCCH_NL673 (K)	1563

Figure 21 continued

#	Start	End	Observed	Mr(expt)	Mr(calc)	ppm	Enzyme	MC	Score	E value	Peptide	Mod_site
1	164	175	615.6503	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	FQNDKSVDGYQATVEPHALPAR +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	766.0308	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

#	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	GFTDPPVKHHGSAMLVR +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	AHCAISLEMMHLKPFAPSPLMMMEK +dK_MMCCH-2 (K)	389
4	460	477	781.3958	2341.1654	2341.1824	1.28	T	1	19	0.014	TSAMVDIFKTTDSVGHK +dK_MMCCH-2 (K)	469
5	470	488	748.0436	2241.1091	2241.1100	-0.40	T	1	18	0.017	TTDSVGHKAGTFAVLGGSK +dK_MMCCH-2 (K)	477
6	489	496	719.8198	1436.6251	1435.6377	-8.78	T	1	15	0.029	EMKAKGFDR +dK_MMCCH-2 (K); Oxidation (M)	491
7	553	560	663.8676	1325.7207	1325.7166	3.09	T	2	23	0.0031	VKFDKVPR +dK_MMCCH-2 (K)	554
8	566	570	485.2459	968.4754	968.4749	0.52	T	1	16	0.038	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	EDNSAGGFQQLGAFHGEPR +dK_MMCCH-2 (K)	590
11	591	615	1004.4674	3010.3804	3010.3742	2.06	T	1	16	0.024	SAGGFQQLGAFHGEPRWCPSPEASK +dK_MMCCH-2 (K)	606
12	645	681	1158.5342	4630.1076	4630.1063	0.28	T	1	26	0.0025	HGYDGALPYWDNYTSPLNHLPELADHEKYVDPEDGVEK +dK_MMCCH-2 (K)	671
13	682	699	1239.5814	2477.1483	2477.1434	1.98	T	1	18	0.016	HNPWPDGHRDTVDKTTTR +dK_MMCCH-2 (K)	695
14	700	719	887.7735	2660.2987	2660.2945	1.58	T	1	44	4.20E-05	SVQNKLFEDPEFGHYTSIAK +dK_MMCCH-2 (K)	704
15	778	789	957.9996	1913.9846	1913.9862	-0.84	T	1	32	0.00059	IWAWDQAIQKYR +Deamidated (NQ); dK_MMCCH-2 (K)	787
16	790	804	669.3175	2004.9307	2004.9220	4.34	T	0	49	1.20E-05	GKPYWAWCAYTSMR +dK_MMCCH-2 (K)	791
17	858	863	520.3004	1038.5963	1038.5763	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

Figure 22 continued

19	986	1000	1027.0348	2052.0550	2052.0561	-0.54	T	1	64	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	QSLFHSDYFYEQVLYALEQDNFCDFEIQLEILHNALHSLLGGKGK +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	1238.6940	1238.6944	0.40	T	1	23	0.0054	LDITKALK +dK_MMCCH-2 (K)	1335
25	1395	1403	485.5956	1453.7651	1453.7589	3.58	T	2	25	0.0031	KDITQLDKR +dK_MMCCH-2 (K)	1395
26	1395	1403	598.3079	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	ADHSSDGFQAIASFHALPPLCFSPAASKR +dK_MMCCH-2 (K)	1444
28	1473	1489	778.4057	2332.1953	2332.1837	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	TAGDCEDAGYFTVLGGEKEMPWAFOR +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	NKVMPNPTAR +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	2258.1347	2258.1194	2.35	T	1	16	0.035	HAVPNDVFKYELLGYR +dK_MMCCH-2 (K)	2076
35	2131	2149	890.4191	3557.6472	3557.6378	2.64	T	1	37	0.00021	TSADVQFQICKTSEDCHHGGQIPVLGGTK +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	RPLRPFSDPINHNAFTHSNAKPTDVPEYSR +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

Figure 22 continued

41	2595	2609	983.5271	1965.0396	1965.0493	-4.89	T	1	17	0.02	IIDTSGKQLPSDUK +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	DVNEAIFQQTKFGEFSSIPYLALQALEEDNYCDFEVQYEILHNEVHALIGGAEK +4 Deamidated (NQ); dK_MMCCH-1 (K)	2771
46	2851	2883	1009.2216	4032.8574	4032.8346	5.65	T	0	69	1.30E-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
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	AFHKFQSDRSVDGYQATAE +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	VDGTKIASSLIPHASVIRE +dK_MMCCH-2 (K)	530
55	589	613	1102.6276	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	2459.0888	2459.0780	4.76	G	1	26	0.0028	HSVPFNVFDYKTNFNYE +Deamidated (NQ); dK_MMCCH-2 (K)	835
59	847	860	643.6771	1928.0085	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	VFDLKPASLGKDLFKQPSVIHEPRIGHIHE +dK_MMCCH-2 (K)	956
62	1059	1076	830.1674	3236.6403	3236.6402	0.03	G	1	32	0.00065	NALLKKGSSVAVPYWDWTKRIE +2 dK_MMCCH-2 (K)	1059, 1060

Figure 22 continued

63	1055	1076	725.6325	2898.5012	2898.5102	-3.11	G	1	38	0.00018	NALLKKGSSVAVPYWDWTKRIE +dK_MMCCH-2 (K)	1060
64	1087	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	2257.1069	-0.84	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	IGGMNLHSIEKE +dK_MMCCH-2 (K)	2099
71	2647	2661	715.6793	2144.0161	2144.0095	3.08	G	4	24	0.0037	AEELRQALYKLQNDE +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	VLSGPSEMKW +dK_MMCCH-2 (K)	67
74	94	100	573.3999	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	1869.9285	5.62	C	0	19	0.014	IKTTDSVQHKAGTF +dK_MMCCH-2 (K)	489
77	584	595	787.4011	1572.7876	1572.7858	1.14	C	2	40	9.10E-05	ALLKEDKSAGGF +dK_MMCCH-2 (K)	590
78	715	722	599.3331	1196.6515	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	0.0035	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

Figure 22 continued

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	923.9231	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	ERLHNEVHAUGGAEKY +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	55	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	0.0059	FHGEPKWCPSPE +dK_MMCCH-2 (K)	606
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

Figure 22 continued

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-1 (K)	1104
110	1219	1232	653.9534	1958.8383	1958.8316	3.42	Th	1	21	0.0077	FDRSDNNDEATKTH +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	VLGSEKEMP +dK_MMCCH-1 (K); Oxidation (M)	1738
115	1894	1904	850.4174	1698.8203	1698.8116	5.12	Th	3	40	9.40E-05	VAVPYWDWTKP +dK_MMCCH-2 (K)	1903
116	2064	2068	499.7804	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	622.7981	1243.5836	1243.5795	3.30	Th	3	13	0.046	AKPTDVFE +dK_MMCCH-2 (K)	2483
121	2512	2521	807.3982	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 22 continued

#	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-06	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)	157
4	249	271	987.4413	2959.3020	2959.3051	-1.05	T	1	32	0.00058	GKDPNSADCAHNLHTPMEPFDR +dK_MMCCH-2 (K)	250
5	281	293	610.9457	1829.8152	1829.8043	5.96	T	0	54	3.30E-06	EHAKPADSFDYGR +dK_MMCCH-2 (K)	284
6	419	446	677.3701	3381.6139	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	5.13	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	2158.0085	1.85	T	1	51	8.20E-06	KHGFTGGLPYWDWTR +dK_MMCCH-2 (K)	936
11	995	1052	1170.7133	7019.2375	7018.2306	0.98	T	1	15	0.032	DDLYQSPGFGHYTDIAKQVLLAFEQDDFCDFEVQFEIAHNFIHALVGGNEPYSMS SLR +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)	1093
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	VFDYKNMFDYEYESLAFNGLSIAQLDR +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	DPQPELWDNKDFYENVMLALEQDNFCDFEIQLEHHNALHSR +dK_MMCCH-2 (K)	1418

Figure 22 continued

38	1455	1480	1117.8726	3350.5959	3350.6070	-3.34	T	1	63	5.50E-07	AKYSLSSLDYTAFDPVFFLHHANVDR +dK_MMCCH-2 (K)	1456
39	1493	1507	721.6653	2161.9742	2161.9594	6.80	T	1	59	1.20E-06	KKPYNEADCAVNEMR +dK_MMCCH-2 (K)	1493
40	1493	1507	721.6612	2161.9617	2161.9594	1.06	T	1	70	9.40E-08	KKPYNEADCAVNEMR +dK_MMCCH-2 (K)	1494
41	1508	1525	837.7524	2510.2353	2510.2185	6.69	T	0	20	0.01	KPLQPFNNPELNSDSMTLK +dK_MMCCH-2 (K)	1508
42	1508	1539	825.9995	4124.9612	4124.9360	6.08	T	1	23	0.0047	KPLQPFNNPELNSDSMTLKHNLPQDSFDYQNR +dK_MMCCH-2 (K)	1526
43	1542	1564	802.8925	3207.5407	3207.5448	-1.25	T	1	19	0.012	YQYDNLQFNHFSIQKLDQTIQAR +dK_MMCCH-2 (K)	1556
44	1622	1633	591.9809	1772.9109	1772.9171	3.14	T	1	18	0.015	LYKPDITSALHK +dK_MMCCH-2 (K)	1624
45	1690	1700	786.9194	1571.8243	1571.8116	8.08	T	1	13	0.049	KEVSSLTTLEK +dK_MMCCH-2 (K)	1690
46	1690	1704	532.2905	2125.1328	2125.1241	4.05	T	2	28	0.0015	KEVSSLTTLEKHFLR +dK_MMCCH-2 (K)	1700
47	1757	1768	612.9786	1835.9141	1835.9128	0.71	T	1	19	0.013	LYTVQFEDSLKR +dK_MMCCH-2 (K)	1767
48	1769	1803	1108.3084	4429.2045	4429.1882	3.70	T	0	28	0.0015	HGSIVGLPYWDWLKPQSALPDLVTQETYEHLFSHK +dK_MMCCH-2 (K)	1803
49	1804	1825	945.4654	2833.3748	2833.3633	3.92	T	1	23	0.0047	TFPNPFLKANIEFEGEGVTTER +dK_MMCCH-2 (K)	1811
50	1949	1963	560.2515	2236.9767	2236.9735	1.43	T	0	57	1.80E-06	TQEFSKPEDTFDYHR +dK_MMCCH-2 (K)	1954
51	2045	2052	660.3513	1318.6880	1318.6843	2.81	T	1	18	0.015	YDITKTLK +dK_MMCCH-2 (K)	2049
52	2116	2125	715.3626	1428.7107	1428.7105	0.14	T	1	15	0.029	DLASLKSAMR +dK_MMCCH-2 (K)	2121
53	2228	2239	870.4226	1738.8305	1738.8236	3.97	T	1	28	0.0017	GYIKSEDAYTVR +dK_MMCCH-2 (K)	2231
54	2453	2463	839.9324	1677.8502	1677.8436	3.93	T	1	17	0.021	NFKYDITGALK +dK_MMCCH-2 (K)	2455
55	2527	2541	1007.5171	2013.0196	2013.0088	5.37	T	1	86	2.60E-09	KDVTSLTASEIENLR +dK_MMCCH-2 (K)	2527
56	2728	2739	957.9996	1913.9846	1913.9862	-0.84	T	1	32	0.00059	IWAIWQALQKYR +Deamidated (NQ); dK_MMCCH-2 (K)	2737
57	2755	2764	764.3818	1526.7486	1526.7459	3.08	T	0	23	0.0053	QPLKPFSESR +Deamidated (NQ); dK_MMCCH-2 (K)	2758
58	3148	3155	629.3348	1256.6551	1256.6587	-2.86	T	1	15	0.032	KKPYNAAK +dK_MMCCH-2 (K)	3149
59	167	178	590.9649	1769.8729	1769.8705	1.30	G	0	44	4.00E-05	KVQPGHHTRLME +dK_MMCCH-2 (K)	167
60	318	322	456.7347	911.4549	911.4535	1.54	G	0	17	0.021	RAAKE +dK_MMCCH-2 (K)	321

Figure 22 continued

41	433	456	975.8586	2924.5539	2924.5429	3.76	G	2	20	0.011	KPPVPVAQANLAVRKNINDLTAEE +dK_MMCCH-2 (K)	435
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	ITQQLHDLDLHVGDNFFLRYE +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	FSKPEDTFDYHRPGYE +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	2629.2171	-1.03	G	2	29	0.0013	LDHAYSLRDGHYYIAGFTKD +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
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	LLGGFTEMKW +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	19	0.03	KHNLPQDSF +dK_MMCCH-2 (K)	1526

Figure 22 continued

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	2.13	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	1878.8317	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	SAGEGHTDDHGSDHIAGSGVKKDVTSL +dK_MMCCH-2 (K)	2527
76	2754	2760	598.3314	1194.6483	1194.6471	1.00	C	1	17	0.023	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
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	1.60E-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

Figure 22 continued

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	738.9572	2212.0487	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	IKQCQEADR +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)	2188
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	462.2321	922.4297	922.4259	4.23	Th	2	21	0.0073	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

#	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	1310.6659	4.33	T	1	33	0.00048	KNIHDLTR +dK_MMCCH-2 (K)	142
3	157	166	822.9333	1643.7520	1643.7402	7.18	T	1	18	0.014	EAFRKPGEGR +dK_MMCCH-2 (K)	161
4	184	192	726.8424	1451.6701	1451.6649	3.58	T	1	20	0.009	CPAPDARGR +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	KNVDK +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	589	606	781.0359	2340.0858	2340.0845	0.60	T	1	25	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	2477.1277	2477.1434	-2.34	T	1	18	0.015	HNPWFDGHIDTVQKTTTR +dK_MMCCH-2 (K)	695
11	700	719	887.7701	2660.2885	2660.2945	-2.22	T	1	48	1.60E-05	SVQNKLFEGPEPEHYTSIAK +dK_MMCCH-2 (K)	704
12	778	789	956.0007	1913.9869	1913.9862	0.37	T	1	22	0.0059	IWAAWQALQKYR +Deamidated (NQ); dK_MMCCH-2 (K)	787
13	790	804	1003.4695	2004.9244	2004.9220	1.20	T	0	56	2.60E-05	GKPYNVANLAVTSMR +dK_MMCCH-2 (K)	791
14	858	863	520.2990	1038.5835	1038.5783	4.91	T	1	16	0.024	KLEAK +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	KNIENLSGFEGLR +dK_MMCCH-2 (K)	986
17	1048	1060	913.9288	1825.8431	1825.8423	0.44	T	1	37	0.00021	LYVVVENALKK +dK_MMCCH-2 (K)	1060
18	1092	1114	791.8768	3163.4730	3163.4682	3.07	T	1	39	0.00017	QHAYETNPFHHGKITHENETTR +dK_MMCCH-2 (K)	1104

Figure 23 continued

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	0.0076	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	TASDCEDAGYFFVLGGEKEMPWAFDR +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
25	1923	1932	756.3808	1510.7470	1510.7426	3.04	T	1	27	0.0019	NKVMPNPEAR +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	6619.1182	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	FNYKYDNLRLHGHNIEELEEVLR +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

Figure 23 continued

41	158	176	846.3828	2536.1266	2536.1329	-2.48	G	3	24	0.0038	AFHKFQEDRSVDGYQATAE +dK_MMCCH-2 (K)	161
42	436	442	676.3245	1350.6344	1350.6312	2.37	G	1	18	0.015	NIEKMIRE +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	DKSAGGFQQLGAPHGEPKWCPSPE +2 dK_MMCCH-2 (K)	590, 606
45	589	612	990.1141	2967.3206	2967.3320	-3.84	G	1	23	0.0055	DKSAGGFQQLGAPHGEPKWCPSPE +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	VFDLKPASLGKDLFKQPSVIHEPRIGHNE +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
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	AGTDSAHTDDGHTEPVMIRRD +dK_MMCCH-2 (K)	1395
54	1376	1413	915.2669	4571.2951	4571.2836	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	TGRDIPNFFIGSKIEFE +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

Figure 23 continued

63	584	595	787.4013	1572.7879	1572.7858	1.40	C	2	36	0.00027	ALLKEQRSAGGF +dK_MMCCH-2 (K)	590
64	715	723	655.8733	1309.7320	1308.7316	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	16	0.017	QALQKY +dK_MMCCH-2 (K)	787
66	860	869	789.8865	1577.7584	1577.7548	3.28	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	1130.5683	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	NLNDHTHDFSKPEDTP +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	KYELLGV +dK_MMCCH-2 (K)	2076
74	2150	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	3	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
78	2946	2960	965.4052	1928.7957	1928.7986	-1.50	C	1	21	0.0072	IRSGTDSDDEYAGSF +dK_MMCCH-2 (K)	2947
79	2964	2971	607.2726	1212.5305	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	VQPDDNDRNDDHCEKAGD +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

Figure 23 continued

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	VTKEHSVF +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
105	2129	2141	933.8804	1865.7462	1865.7495	-1.77	Th	0	25	0.0035	KCKTSEDCHHGGQ +dK_MMCCH-2 (K)	2131
106	2238	2248	778.8785	1555.7425	1555.7440	-0.90	Th	3	44	4.10E-05	ILTTAEVDNLKD +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

Figure 23 continued

109	2506	2571	708.0113	2121.0120	2111.0048	3.44	Th	1	14	0.042	LEHELEKGKEEDRT +dK_MMCCH-2 (K)	2516
110	2595	2606	806.4034	1610.7923	1610.7862	3.79	Th	2	35	0.00033	HDTSGKQLPSD +dK_MMCCH-2 (K)	2601
111	2607	2612	520.7794	1039.5443	1039.5446	-0.39	Th	2	22	0.0058	LRMPT +dK_MMCCH-2 (K)	2609
112	2766	2771	551.7853	1101.5561	1101.5529	3.00	Th	1	24	0.0043	IFCQTK +dK_MMCCH-2 (K)	2771
113	2809	2816	638.3184	1274.6223	1274.6217	0.47	Th	3	27	0.0019	LGSAAEKVS +dK_MMCCH-2 (K)	2814
114	2945	2960	965.4048	1928.7950	1928.7996	-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)	2995
116	3076	3084	724.3623	1446.7100	1446.7040	4.22	Th	2	13	0.046	FKCKVPPPS +dK_MMCCH-2 (K)	3079

Figure 23 continued

#	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	0.008	ADITFLNKK +dK_MMCCH-2 (K)	155
3	164	175	596.3101	1785.9085	1785.8985	5.66	T	1	44	4.40E-05	LFEKVQPGHNTR +dK_MMCCH-2 (K)	167
4	249	271	987.4429	2959.3068	2959.3051	0.57	T	1	33	0.00051	GKDPNSADCAHNLHTPMEPFDR +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	FQNDKSVDGYQATVEPHALPAR +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	KHGFTSGLPYWDWTR +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	1119	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	1271.3697	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	DPQPELWDNKDFYENVMLALEQDNFCDFEQLELIHNALHSR +dK_MMCCH-2 (K)	1418
16	1455	1480	1117.8600	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	2161.9584	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	YQYDNLQFNHPSIQKLDQTRQAR +dK_MMCCH-2 (K)	1556

Figure 23 continued

19	1681	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	GVIKSEDAYTVR +dK_MMCCH-2 (K)	2231
24	3527	2541	1007.5152	2013.0158	2013.0088	3.48	T	1	79	1.40E-08	KDVTSLTASEIERLR +dK_MMCCH-2 (K)	2527
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	580.9629	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	KPPVPVAQANLAVRKMINDLTAEE +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)	1137
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	SIRSAFLQIGKE +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	FVGMSVSSLHNYIKQGQCE +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	NRKTSRAVDDRLF +dK_MMCCH-2 (K)	154

Figure 23 continued

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	3	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
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	38	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	KGPGQSASVSF +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	645.3373	1288.6601	1288.6573	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

Figure 23 continued

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	631.6184	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	715.8283	1428.6421	1428.6418	0.21	Th	2	41	7.20E-05	LGGPTEMKWG +dK_MMCCH-2 (K); Oxidation (M)	372
70	431	437	569.3861	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	VGGSERYS +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	564.7961	1127.4976	1127.4957	1.69	Th	1	21	0.0075	LWDNKD +dK_MMCCH-2 (K)	1416
75	1525	1539	738.3547	2212.0424	2212.0371	2.40	Th	3	43	5.10E-05	LKHNLPGDSFDYQNR +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
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

Figure 23 continued

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

#	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	GFTDPPVRHHQSAMLVR +dK_MMCCH-2 (K)	131
2	142	149	656.3412	1310.6678	1310.6653	1.98	T	1	35	0.00029	KNMDITR +dK_MMCCH-2 (K)	142
3	157	166	822.8796	1643.7446	1643.7402	2.68	T	1	18	0.015	EAPHKFQEDR +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	AHCASLEHMHLKPFAFSSPLNNWEK +dK_MMCCH-2 (K)	389
6	460	477	781.3949	2341.1629	2341.1624	0.21	T	1	32	0.0068	TSAMVDIFKTTDSVQHK +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	VEFDKVPR +dK_MMCCH-2 (K)	554
9	566	570	485.2455	968.4757	968.4749	1.86	T	1	17	0.013	KNYDR +dK_MMCCH-2 (K)	566
10	583	587	547.8379	1093.6603	1093.6569	2.93	T	1	22	0.005	KALAIR +dK_MMCCH-2 (K)	581
11	588	606	781.0353	2340.0825	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	4630.1053	5.12	T	1	27	0.0018	HGYDGALPYWDWTSPLNHLPELADHEKYVDPEDGVPR +dK_MMCCH-2 (K)	671
14	682	699	620.2947	2477.1496	2477.1434	2.50	T	1	21	0.0082	HNPWFDGHHDTVQKTTTR +dK_MMCCH-2 (K)	695
15	700	719	887.7702	2660.2868	2660.2945	-2.14	T	1	39	0.00013	SVCDKLFEQPEPGHYTSIAK +dK_MMCCH-2 (K)	704
16	790	804	669.3174	2004.9305	2004.9220	4.24	T	0	38	0.00017	GKPVWAMCAVTSMR +dK_MMCCH-2 (K)	791
17	958	963	520.2993	1038.5840	1038.5763	5.39	T	1	23	0.0051	KLEAK +dK_MMCCH-2 (K)	858
18	953	965	635.3319	1902.9737	1902.9662	3.94	T	1	53	4.80E-06	ELFKGPSVHEPR +dK_MMCCH-2 (K)	956

Figure 24 continued

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	3163.4662	-1.17	T	1	28	0.0018	QHHYETNPFHHGKITHENEITTR +dK_MMCCH-2 (K)	1104
22	1189	1203	353.1914	1056.5522	1056.5538	-1.51	T	1	17	0.018	KRPYR +dK_MMCCH-2 (K)	1189
23	1331	1338	620.3551	1238.6956	1238.6944	0.97	T	1	17	0.018	LDITKALK +dK_MMCCH-2 (K)	1339
24	1395	1402	649.8379	1297.6612	1297.6588	1.85	T	1	26	0.0022	KDITQLDR +dK_MMCCH-2 (K)	1395
25	1395	1403	485.5953	1453.7639	1453.7599	2.75	T	2	16	0.035	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	776.4021	2332.1845	2332.1827	0.77	T	1	47	1.90E-05	KHGAVVGLPYWQWTLPR +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	KHAVPNDVPK +dK_MMCCH-2 (K)	2067
32	2121	2149	890.4184	3557.6444	3557.6378	1.86	T	1	29	0.0013	TSADVQFQICKTSEDCHHGGQIPVLGGTK +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	RPLRPFSQPINHNAFTHSNAKPTDVFEYSR +dK_MMCCH-2 (K)	2481
35	2507	2514	682.3522	1362.6898	1362.6853	3.30	T	1	40	9.90E-06	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	RDTSGKQLPSDLR +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

Figure 24 continued

42	3657	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	KHGSHLGIPYWDWTGTISSLPTFFADSGNNNPFFK +dK_MMCCH-2 (K)	2714
44	2851	2883	1009.2175	4032.8410	4032.8346	1.59	T	0	60	1.10E-06	VKPAHAGSCAGDIMHVPLHPFNYESVNNODFTR +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)	2949
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	RPNNAVFDIEIPIGKDVNLPPK +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
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	3305.4631	-1.48	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	1485	1522	866.6916	3462.7873	3462.7981	-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	692.8022	1263.5898	1263.5879	1.50	G	0	14	0.04	LGKMYSVE +dK_MMCCH-2 (K)	3092
64	59	68	729.3446	1456.6750	1456.6731	1.37	C	1	19	0.012	VLGGPSEMKW +dK_MMCCH-2 (K); Oxidation (M)	67

Figure 24 continued

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	26	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	GGISLENIEKMIHENQQEDGIY +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
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	KYELLISY +dK_MMCCH-2 (K)	2076
81	2160	2184	1085.5143	3253.5210	3253.5179	0.95	C	3	21	0.0069	KYDITHALHDAHITPEDVRHPSEPF +dK_MMCCH-2 (K)	2160
82	2476	2488	923.9319	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

Figure 24 continued

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	670.3483	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	707.8529	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	FDKSDNNDGATKTH +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	3	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
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	5.54	Th	1	13	0.049	LDKMN +dK_MMCCH-2 (K)	1758
108	1894	1904	650.4138	1698.8131	1698.8116	0.88	Th	5	39	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

Figure 24 continued

111	2238	2249	814.3991	1626.7937	1626.7811	1.60	Th	4	49	1.30E-05	LTTAEVDMLKDA +dK_MMCCH-2 (K)	2247
112	2475	2484	728.3341	1454.6535	1454.6500	2.41	Th	1	27	0.0002	FTHSNAKPTD +dK_MMCCH-2 (K)	2481
113	2512	2521	538.6010	1612.7810	1612.7766	2.73	Th	0	33	0.00035	LEKGKEEDRT +dK_MMCCH-2 (K)	2514
114	2595	2607	862.9463	1723.8780	1723.8702	4.52	Th	3	30	0.0011	HDTSEKQLPSDL +dK_MMCCH-2 (K)	2603
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	1101.5579	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	LIGGAEKY5 +dK_MMCCH-2 (K)	2814
118	2945	2960	965.4112	1928.8078	1928.7986	4.77	Th	3	54	3.80E-06	IKSGTDSDDEYAGSF +dK_MMCCH-2 (K)	2947
119	2953	2970	691.8644	1381.7142	1381.7098	3.18	Th	4	19	0.011	VILGGAKEMP +dK_MMCCH-2 (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 24 continued

#	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	GKDPNSADQAHNUHTPMEPFDR +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	944.0674	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	2830.3406	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	1271.2578	3810.7816	3810.7875	-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	DPQPELWDNKDFYENVMLALEQDNFCDFEIQLEUHNALHSR +dK_MMCCH-2 (K)	1418
18	1459	1480	838.6584	3350.6045	3350.6070	-0.78	T	1	56	2.70E-06	AKYSLSSLDYTAFDPVFFLHHANVDR +dK_MMCCH-2 (K)	1456

Figure 24 continued

19	1493	1507	721.6590	2161.9552	2161.9594	-1.99	T	1	50	1.00E-05	KKPYNEAGCAVNEMR +dK_MMCCH-2 (K)	1494
20	1508	1539	1031.2455	4124.9528	4124.9360	4.07	T	1	28	0.0014	KPLQPPNMPELNSDSMTLKHNLPQDSFDYQNR +dK_MMCCH-2 (K)	1535
21	1542	1564	1078.1910	3207.5513	3207.5448	2.03	T	1	47	1.80E-05	YQYDNLQPMHESQKLEQTIQAR +dK_MMCCH-2 (K)	1556
22	1757	1768	612.9789	1835.9148	1835.9128	1.09	T	1	23	0.0057	LYYVQFEDSLKR +dR_MMCCH-2 (K)	1767
23	1949	1963	560.2532	2236.9797	2236.9735	2.77	T	0	57	2.00E-06	TQESSMFEDTFDYHR +dK_MMCCH-2 (K)	1954
24	2045	2052	660.3586	1318.6867	1318.6843	1.90	T	1	15	0.035	YDITKTLK +dK_MMCCH-2 (K)	2052
25	2058	2063	909.4624	1816.9102	1816.9070	1.82	T	1	24	0.0049	YDDTFTIKVHHK +dK_MMCCH-2 (K)	2065
26	2228	2239	870.4213	1738.8280	1738.8236	2.53	T	1	19	0.012	GYKSEDAYTVR +dR_MMCCH-2 (K)	2231
27	2527	2541	1007.5135	2013.0124	2013.0088	1.79	T	1	50	9.00E-06	KDYTSITASEIEMR +dK_MMCCH-2 (K)	2527
28	2755	2764	764.3831	1526.7517	1526.7459	5.11	T	0	19	0.013	QPLKPFSEGR +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	2924.5439	4.21	G	2	27	0.0019	KPPVPVAQANLAVRKMMDLTAEE +dK_MMCCH-2 (K)	433
32	466	481	1098.4963	2194.9781	2194.9841	-2.73	G	2	31	0.00082	RFQNDKSVDGYCATVE +Deamidated (NQ); dK_MMCCH-2 (K)	471
33	1215	1235	721.6063	2882.3959	2882.3949	0.35	G	3	28	0.0016	ITTGQEHDLDLHVGDMFFLKYE +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	MAKEHGKPGLCE +dK_MMCCH-2 (K)	1315
36	1403	1422	921.4208	2761.2407	2761.2330	2.79	G	3	15	0.03	NAVTSKDPQPELWDNKDFYE +dK_MMCCH-2 (K)	1418
37	1952	1967	792.6837	2375.0293	2375.0205	3.71	G	3	19	0.014	FSKPEDTFDYHREGYE +dK_MMCCH-2 (K)	1954
38	2477	2484	644.8373	1287.6600	1287.6579	2.10	G	0	22	0.0068	APFFKVE +dK_MMCCH-2 (K)	2462
39	3386	3405	877.4165	2629.2277	2629.2171	0.73	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	0.035	ALERALDDLDQQDDSMQGY +dK_MMCCH-2 (K)	41
41	277	296	982.7539	2648.2399	2648.2329	2.64	C	4	39	0.00014	DLTREHAKPADSFDYGRLGY +dK_MMCCH-2 (K)	284

Figure 24 continued

42	364	373	735.3606	1468.7066	1468.7094	-1.91	C	2	22	0.0057	LLGGPTEMKW +dK_MMCCH-2 (K)	372
43	432	443	793.9159	1585.8173	1585.8174	-0.06	C	0	26	0.0028	DKPPVPVAGANL +dK_MMCCH-2 (K)	433
44	629	635	538.3532	1076.4919	1076.4848	6.60	C	0	20	0.0085	VGGSEKY +dK_MMCCH-2 (K)	634
45	1007	1015	669.8709	1337.7271	1337.7265	0.52	C	1	16	0.035	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	38	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
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	1042.5348	2083.0553	2083.0489	3.07	C	3	15	0.039	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	KDPLKPF +dK_MMCCH-2 (K)	2754

Figure 24 continued

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	3.67	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	VDKHEKR +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	1817.8316	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	473	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	582.7666	1163.5191	1163.5169	1.98	Th	1	22	0.006	VGGSEKYS +dK_MMCCH-2 (K)	634
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	26	0.0015	FSKPEDTFDYHR +dK_MMCCH-2 (K)	1954
87	1985	1994	776.8957	1551.7768	1551.7715	3.42	Th	3	22	0.0062	IKDQQEADRV +dK_MMCCH-2 (K)	1986

Figure 24 continued

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	LDEANDLRNA +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

#	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	GFTDPPVKHHQSAMLLVR +dK_MMCCH-2 (K)	131
2	142	149	656.3425	1310.6703	1310.6653	4.04	T	1	35	0.00024	KNMDLTR +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	1451.6739	1451.6649	6.13	T	1	22	0.0061	CPAPDAKDR +dK_MMCCH-2 (K)	190
5	470	488	748.0502	2241.1289	2241.1100	8.43	T	1	24	0.0039	TTDSWQHKAGTHAVLGGSK +dK_MMCCH-2 (K)	477
6	553	560	663.8695	1325.7245	1325.7165	5.96	T	2	22	0.0053	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
9	566	570	485.2455	968.4765	968.4749	1.65	T	1	17	0.022	KMVDK +dK_MMCCH-2 (K)	568
9	581	590	733.9194	1465.8242	1465.8214	1.91	T	2	40	0.00011	KALALLKEPK +dK_MMCCH-2 (K)	581
10	589	606	781.0386	2340.0941	2340.0845	4.10	T	1	21	0.008	EDKSAGGFQQLGAFHGEPK +dK_MMCCH-2 (K)	599
11	591	615	1004.4697	3010.3872	3010.3742	4.32	T	1	18	0.015	SAGGFQQLGAFHGEPKWCPSFEASK +dK_MMCCH-2 (K)	606
12	643	681	1158.5359	4630.1145	4630.1063	1.75	T	1	21	0.0072	HGYDGALPYWDWTSPLNHLPELADHEKYVEKFEDGVEK +dK_MMCCH-2 (K)	671
13	682	699	626.2941	2477.1474	2477.1434	1.61	T	1	23	0.0045	HAPWFDGHIDTVDKTTTR +dK_MMCCH-2 (K)	695
14	700	719	887.7753	2660.3040	2660.2945	3.57	T	1	32	0.00064	SVQSKLFEQPEFGHYTSIAK +dK_MMCCH-2 (K)	704
15	790	804	1003.4777	3004.9409	3004.9230	5.93	T	0	63	5.00E-07	EKPYWAMCAVTSMR +dK_MMCCH-2 (K)	791
16	953	965	635.3325	1902.9761	1902.9662	5.20	T	1	46	2.40E-05	DLFKGPSVIHEPR +dK_MMCCH-2 (K)	956
17	926	1000	685.0287	2052.0642	2052.0561	4.00	T	1	68	1.80E-07	KMENLSLEELEGLR +dK_MMCCH-2 (K)	936
18	1048	1060	913.5324	1825.0503	1825.0423	4.38	T	1	19	0.013	LVVVVEMALLKK +dK_MMCCH-2 (K)	1060

Figure 25 continued

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
25	1747	1758	613.9782	1838.9128	1838.9012	6.31	T	1	27	0.0019	LYRYDITETLDK +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	1510.7419	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	3557.6468	3557.6378	2.56	T	1	29	0.0012	TSADVQFQICKTSEDCHHGGQIPVLSGTK +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	HNEKHHEDHHEDILVR +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	1246.2333	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

Figure 25 continued

42	435	442	676.3355	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	FNGLSISCLNKKLE +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
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	INHNQFTKEHAVPNDVFKYE +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	2144.0085	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	573.2936	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

Figure 25 continued

65	715	723	655.6738	1309.7331	1309.7316	1.22	C	1	15	0.029	TSIAKQVLL +dK_MMCCH-2 (K)	719
66	783	788	544.7775	1087.5404	1087.5371	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	2549.2465	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	2253.9697	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	0.0097	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
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	30	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	VCIPDDNDRNDDHCERAGD +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	ILSDTVHK +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

Figure 25 continued

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	1613.7858	1613.7858	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	0.0089	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	VPYWDWTKB +dK_MMCCH-2 (K)	1073
95	1111	1120	742.8792	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	0.006	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	2249	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
106	2512	2521	807.3973	1612.7801	1612.7766	2.17	Th	0	39	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	HDTSGKQLPSD +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	1101.5539	5.63	Th	1	29	0.0012	IFDQTK +dK_MMCCH-2 (K)	2771

Figure 25 continued

111	2808	2816	638.3200	1274.6255	1274.6217	2.96	Th	3	27	0.0018	LGGAEKYS +dK_MMCCH-2 (K)	2814
112	2945	2960	965.4102	1928.8059	1928.7986	3.78	Th	3	30	0.0011	IKSSTDSSDDEVAGSF +dK_MMCCH-2 (K)	2947
113	2951	2970	691.8640	1381.7135	1381.7098	2.68	Th	4	18	0.016	VILGGAKEMP +dK_MMCCH-2 (K); Oxidation (M)	2967
114	2990	2996	583.2845	1164.5544	1164.5485	5.07	Th	1	38	0.00017	ITDDHVK +dK_MMCCH-2 (K)	2996

Figure 23 continued

#	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	ADTFLRKK +dK_MMCCH-2 (K)	155
3	164	175	596.3124	1785.9155	1785.8985	9.52	T	1	42	6.60E-05	LFEKVQPGHVTR +dK_MMCCH-2 (K)	167
4	249	271	987.4443	2959.3110	2959.3051	1.99	T	1	36	0.00024	GKDPNSADQAHWLHTPMEPPDR +dK_MMCCH-2 (K)	250
5	281	293	610.9466	1829.8179	1829.8043	7.49	T	0	53	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	QFTLVHSPAKGHFDKPPVPVAQAMLAVR +Deamidated (NQ); +dK_MMCCH-2 (K)	428
7	429	446	752.0662	2253.1839	2253.1729	4.44	T	0	52	5.90E-06	GHFDKPPVPVAQANLAVR +dK_MMCCH-2 (K)	433
8	467	488	708.3943	2830.3481	2830.3385	3.39	T	1	69	1.30E-07	FQNDKSVDGYQATVEPHAIPAR +dK_MMCCH-2 (K)	471
9	489	497	726.8442	1451.6738	1451.6649	6.13	T	1	22	0.0051	CPAPDAKDR +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	GKPYNTAMQAIASMR +dK_MMCCH-2 (K)	1083
12	1097	1115	827.0787	2478.2142	2478.2101	1.65	T	0	66	2.30E-07	KPLQPPGLDSVNPDDETR +dK_MMCCH-2 (K)	1097
13	1123	1148	1190.5612	3568.6617	3568.6497	3.36	T	1	79	1.20E-08	VFDYKMNFDYTYESLAFNGLSAQLDR +dK_MMCCH-2 (K)	1127
14	1355	1385	1272.2694	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	46	9.60E-05	DPQPELWDNKDFYEWVMLAIFQDNVCPPEQLELHNAALHSR +dK_MMCCH-2 (K)	1418
16	1455	1480	1117.8821	3350.6244	3350.6070	5.19	T	1	34	0.00044	AKYSLSSLDYTAFDPVFELHHAAVDR +dK_MMCCH-2 (K)	1456
17	1493	1507	721.6577	2161.9513	2161.9594	-3.75	T	1	66	2.40E-07	KGPYMEADCAVMEMR +dK_MMCCH-2 (K)	1494
18	1542	1564	802.8964	3207.5566	3207.5448	3.68	T	1	19	0.013	YDYDMLDFNHFSQKLDETDAR +dK_MMCCH-2 (K)	1556

Figure 25 continued

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	LYTVQFEQSLKR +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
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	2865	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	KPPVPVADANLAVRKNINDLTAEE +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	878.4671	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	FSKPEDTFDYHRPGYE +dK_MMCCH-2 (K)	1954

Figure 25 continued

42	1973	1990	817.0616	1443.1629	2448.1454	7.15	G	0	22	0.0063	FVGANSVSSLHWYIKQLQGE +dK_MMCCH-2 (K); Oxidation (M)	1986
43	3286	3405	658.3166	1628.2375	2639.2271	3.96	G	2	24	0.0038	LDHAYSLRDGHYYHAGPTKD +dK_MMCCH-2 (K)	3404
44	277	296	883.7536	2648.2390	2648.2329	2.27	C	4	41	7.30E-05	DETREHAKPADSFDYGRLGV +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	KYETTQQLHDLDLHYGDNF +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	570.2392	1138.4637	1138.4641	-0.35	C	1	16	0.022	DMKDFY +dK_MMCCH-2 (K)	1418
50	1526	1540	749.6825	2246.0257	2246.0215	1.87	C	2	32	0.00061	KNALPQDSFDYQNSF +dK_MMCCH-2 (K)	1526
51	1599	1606	784.3539	2350.0400	2350.0392	0.34	C	0	19	0.011	LVEQGGEQMCKTYAGSF +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	650.4289	1698.8432	1698.8399	1.94	C	0	26	0.0023	RKGGCEADRVF +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	1138.0192	2254.0238	2254.0253	-0.67	C	1	16	0.027	KAQSHPEDVFDTDAPF +dK_MMCCH-2 (K)	2463
57	2865	2872	673.3657	1344.7168	1344.7112	4.16	C	1	22	0.0067	KYDITKVL +dK_MMCCH-2 (K)	2870
58	3235	3242	617.3148	1232.6150	1232.6111	3.16	C	0	27	0.002	TSANVKNY +dK_MMCCH-2 (K)	3240
59	3399	3406	576.8029	1151.5912	1151.5896	1.30	C	0	39	0.00012	RAGPTKDL +dK_MMCCH-2 (K)	3404
60	165	175	559.6147	1672.8224	1672.8144	4.78	Th	1	22	0.0058	FEKVEPGHHTR +dK_MMCCH-2 (K)	167
61	180	191	909.9202	1817.8259	1817.8215	2.37	Th	4	65	3.30E-07	ILDALEQDEFGK +dK_MMCCH-2 (K)	191
62	247	260	631.6201	1891.8385	1891.8305	4.23	Th	2	13	0.046	LRGKDPMSADCAHN +dK_MMCCH-2 (K)	259
63	283	293	782.8600	1563.7054	1563.7028	1.73	Th	3	34	0.00035	AKPADSFDYGR +dK_MMCCH-2 (K)	284
64	364	372	642.3346	1282.6750	1282.6701	3.82	Th	2	41	7.30E-05	LLGGPTEMK +dK_MMCCH-2 (K)	372

Figure 25 continued

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	PHGEPKWCPSPE +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	735.3330	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	IKGQQEADRV +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
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.

Figure 25 continued

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

#	Start	End	Observed	Mr(expt)	Mr(calc)	ppm	Enzyme	MC	Score	E value	Peptide	Mod_site
1	124	141	785.4114	2352.2125	2353.2001	5.27	T	1	14	0.037	GFTDPPVKHHQSANLLVR +dK_MMCCH-2 (K)	131
2	142	149	556.3405	1110.6665	1110.6653	0.92	T	1	25	0.003	KNMDLTR +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	TSANVDFKTTDSVQHK +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	569	663.8681	1325.7216	1325.7166	3.85	T	2	24	0.0041	VKFDKVPR +dK_MMCCH-2 (K)	554
7	566	578	485.2447	968.4748	968.4749	-0.10	T	1	19	0.014	KWVDR +dK_MMCCH-2 (K)	565
8	581	597	547.8373	1093.6600	1093.6569	2.83	T	1	20	0.01	KALALLK +dK_MMCCH-2 (K)	583
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	HGYDGALPYWPDWTSPLNHLPELADHEKYVDPEDGVEK +dK_MMCCH-2 (K)	671
11	682	699	1239.5804	2477.1463	2477.1434	1.17	T	1	16	0.025	HMPWFDGHHDTVDKTTTR +dK_MMCCH-2 (K)	685
12	703	719	887.7732	2660.2977	2660.2945	1.24	T	1	44	3.75E-05	SVCMKLPEQPEGHYTSIAK +dK_MMCCH-2 (K)	704
13	778	789	958.8048	1913.9950	1913.9862	4.60	T	1	31	0.00074	IWAIWQALDKYR +Deamidated (NQ); dK_MMCCH-2 (K)	787
14	790	804	669.3164	2004.9274	2004.9220	2.69	T	0	37	0.00019	SKPYNWAWCAVTSMR +dK_MMCCH-2 (K)	791
15	658	668	520.2980	1038.5814	1038.5783	2.98	T	1	17	0.019	KLEAIK +dK_MMCCH-2 (K)	658
16	953	965	635.3307	1902.9704	1902.9662	2.21	T	1	48	1.70E-05	ELFKQPSVIHEPR +dK_MMCCH-2 (K)	956
17	986	1000	685.0263	2052.0571	2052.0561	0.49	T	1	55	3.10E-06	KMEMLSLGELESLR +dK_MMCCH-2 (K)	986
18	1092	1114	791.8780	3163.4839	3163.4832	4.62	T	1	38	0.00015	QHHYETNPPHHGKLTHENEITTR +dK_MMCCH-2 (K)	1104

Figure 26 continued

19	1118	1162	1414.4179	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	1385	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
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	2289	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	3850.8538	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	2405.1063	1.50	T	1	47	2.00E-05	HHEKHHEDHMEDILVR +dK_MMCCH-2 (K)	2624
34	2637	2651	1069.5295	2137.0449	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)	3771
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

Figure 26 continued

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	APHKPQEDRSVDGYQATAE +dK_MMCCH-2 (K)	161
43	526	544	777.7497	2330.2272	2330.2304	-1.37	G	1	22	0.0064	VDGTKLASSLPHASVIRE +dK_MMCCH-2 (K)	530
44	589	612	990.1168	2967.3286	2967.3320	-1.15	G	1	28	0.0015	DKSAGGFQQLGAPHGEPKWCPSPE +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	3817.9773	3817.9614	4.14	G	3	14	0.043	VFDLKPASLGKDLFKQPSVIHEPRIGHREGE +dK_MMCCH-2 (K)	946
47	942	970	727.3896	3631.9116	3631.8973	3.91	G	2	16	0.024	VFDLKPASLGKDLFKQPSVIHEPRIGHRE +dK_MMCCH-2 (K)	956
48	1055	1076	810.1589	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
50	1055	1076	725.6342	2898.5076	2898.5102	-0.90	G	1	21	0.0085	NALLKKGSSVAVPYWDWTKRIE +dK_MMCCH-2 (K)	1073
51	1087	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	3.15	G	2	30	0.00094	IGGMNLHEIEKE +dK_MMCCH-2 (K)	2099
57	2647	2661	715.6783	2144.0130	2144.0085	1.63	G	4	18	0.016	AEELRDALYRLQNDE +dK_MMCCH-2 (K)	2656
58	3090	3097	632.8034	1263.5923	1263.5879	3.40	G	0	15	0.026	LGKMYSVE +dK_MMCCH-2 (K)	3092
59	58	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	GGISLENIEKMIHENQQEDNIY +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

Figure 26 continued

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	814.3668	3253.5180	3253.5179	0.03	C	3	14	0.036	KYDITHALHDAHITPEDVRHPSEPP +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	1928.7965	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
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	VCIPDDNDRNGDHCEKAGD +dK_MMCCH-2 (K)	55
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	1136.5580	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

Figure 26 continued

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	1223.5609	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	1841.8235	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	618.3063	1234.6020	1234.5903	9.48	Th	1	26	0.0033	LHEIEKE +dK_MMCCH-2 (K)	2099
101	2139	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
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

Figure 26 continued

109	2946	2963	965.4091	1928.8037	1928.7986	2.64	Th	3	40	9.58E-05	KSGTDSDDEYAGSF +dK_MMCCH-2 (K)	2947
110	2998	2996	383.2650	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	FKCKVPPGS +dK_MMCCH-2 (K)	3079

Figure 26 continued

#	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	3381.8199	3381.8132	1.86	T	1	27	0.0021	QPTLVHSPAKGHFDKPPVPVAQANLAVR +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	708.5858	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	985	1052	1170.7141	7018.2410	7018.2306	1.48	T	1	13	0.047	DDLYQSPGFGHYTDIAKQVLLAFEQDQFCDFEVQFEIAHNFIHALVGGNEPYSMSSLR +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	66	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	GSAVAVPYWDWTEKADSLPSLNDATYFNSR +dK_MMCCH-2 (K)	1368
16	1409	1450	1371.8909	5483.5344	5483.5213	2.39	T	1	50	1.00E-05	DPQPELWDNKDFYENVVMLALEQDNFCDFEIQLELHHNALHSR +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

Figure 26 continued

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
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	746.6661	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)	2131
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	3159	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	2924.5466	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	RFQNDKSVDGYDATVE +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)	1313

Figure 26 continued

41	1308	1320	904.9452	1807.8758	1807.8749	0.50	G	0	27	0.0022	MAKFHSKPGLCE +dK_MMCCH-2 (K)	1315
42	1354	1378	1043.5070	3127.4981	3127.4981	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	NAVTSRDPQPELWDNKDFYC +dK_MMCCH-2 (K)	1418
44	1952	1967	792.6805	2375.0195	2375.0205	-0.38	G	3	37	0.00021	FSKPEDTFDYHRRGYC +dK_MMCCH-2 (K)	1954
45	1973	1990	817.0591	2448.1556	2448.1454	4.17	G	0	19	0.012	FVGMSVSSLHHYKQDDE +dK_MMCCH-2 (K); Oxidation (M)	1986
46	2477	2484	644.8365	1287.6585	1287.6573	0.93	G	0	15	0.037	APFFKVE +dK_MMCCH-2 (K)	2482
47	3386	3405	659.3146	2629.2232	2629.2271	0.80	G	2	25	0.0032	LEHAYSLRQGHYYIASFTKD +dK_MMCCH-2 (K)	3404
48	152	165	667.6934	2000.0584	2000.0513	3.55	C	2	13	0.047	LNKKTSKAVDDRLF +dK_MMCCH-2 (K)	155
49	166	176	547.2858	1638.8355	1638.8339	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
51	364	373	743.3505	1484.7084	1484.7044	1.35	C	2	19	0.012	LSGPTEMKQW +dK_MMCCH-2 (K); Oxidation (M)	372
52	423	442	872.8013	2615.3920	2615.3795	0.96	C	1	13	0.05	VHRPAKGHFDKPPVPVAQAKL +dK_MMCCH-2 (K)	428
53	629	635	539.2619	1076.4992	1076.4948	4.09	C	0	19	0.014	VEGSEKY +dK_MMCCH-2 (K)	634
54	1007	1015	669.8724	1337.7302	1337.7265	2.77	C	1	30	0.0031	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	1428.7385	1428.7323	5.04	C	1	14	0.041	LQIQKEGY +dK_MMCCH-2 (K)	1302
57	1535	1540	749.6943	2246.0813	2246.0715	4.32	C	2	36	0.00028	KMKLPQDSFDYQDKF +dK_MMCCH-2 (K)	1536
58	1589	1606	784.35680	2350.0461	2350.0392	2.94	C	0	24	0.0045	KVEQGGEQMKTKAGSF +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	839.3457	1677.6768	1677.6651	7.03	C	0	16	0.023	KNMQADDSPDGY +dK_MMCCH-2 (K)	1708
61	1801	1809	706.8377	2411.6607	3411.6598	0.92	C	0	15	0.035	SHKTFPAPF +dK_MMCCH-2 (K)	1803
62	1985	1995	850.4290	1698.8435	1698.8399	2.12	C	0	42	6.20E-05	IKCGDDEADKVF +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

Figure 26 continued

64	2455	2462	645.3370	1288.6395	1288.6373	1.71	C	1	18	0.017	KYDITQAL +dK_MMCCH-2 (K)	2455
65	3463	2479	1128.0306	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)	2756
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	LEQDEFOX +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	457	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
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	LWQNKD +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	34	0.043	FSHKTFPNPF +dK_MMCCH-2 (K)	1803
84	1952	1963	637.2849	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

Figure 26 continued

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	FARGY +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

#	Start	End	Observed	Mr(expt)	Mr(calc)	ppm	Enzyme	MC	Score	E value	Peptide	Mod_site
1	124	141	785.4103	2352.2092	2353.2021	3.87	T	1	17	0.02	GFTDAPVKHHGSANLVR +dK_MMCCH-2 (K)	131
2	142	149	656.3403	1310.6661	1310.6653	0.69	T	1	29	0.0013	KMNADLTR +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	726.3430	1451.6715	1451.6649	4.46	T	1	26	0.0026	CPRFDAKDR +dK_MMCCH-2 (K)	189
5	553	560	663.8685	1325.7224	1325.7166	4.37	T	2	25	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	EDKSASGFGGLGAPHGEPK +dK_MMCCH-2 (K)	590
9	645	661	1158.5381	4630.1233	4630.1063	3.65	T	1	18	0.013	HGYDGALPYWDWTSPLNHLPELADHEKYVDPEDGVEK +dK_MMCCH-2 (K)	671
10	682	699	620.2951	2477.1533	2477.1434	4.04	T	1	21	0.0075	HAPWFDSHIDTVDKTTTR +dK_MMCCH-2 (K)	695
11	700	719	887.7724	2660.2954	2660.2945	0.34	T	2	20	0.01	SVQNKLFEDPEFGHYTSIAK +dK_MMCCH-2 (K)	704
12	776	789	957.9997	1913.9846	1913.9862	-0.68	T	1	39	0.00012	IWAIWQALDKYR +Deamidated (NQ); dK_MMCCH-2 (K)	787
13	790	804	1003.4713	2004.9281	2004.9220	3.04	T	0	48	1.60E-05	GKFYNVANCAVTSMR +dK_MMCCH-2 (K)	791
14	858	863	520.2989	1038.5832	1038.5783	4.72	T	1	17	0.022	KLEAK +dK_MMCCH-2 (K)	858
15	916	924	740.9735	1479.7324	1479.7319	0.27	T	1	16	0.025	VFKYDTER +dK_MMCCH-2 (K)	918
16	953	965	635.3304	1902.9699	1902.9662	1.63	T	1	43	5.30E-05	DLFKQPSVIHEPR +dK_MMCCH-2 (K)	956
17	986	1000	1027.0363	2052.0579	2052.0561	0.93	T	1	66	2.50E-07	KMEMSLGGLESLR +dK_MMCCH-2 (K)	996
18	1092	1114	791.8748	3163.4699	3163.4682	0.54	T	1	41	8.30E-05	QHHYETNPHHHGKITHENEITTR +dK_MMCCH-2 (K)	1104

Figure 27 continued

19	1118	1162	1414.4266	5653.6775	5653.6850	-1.34	T	1	23	0.0049	DSLFHSDYFYEQVLYALEQDNFCDFEIQLEIUHNALHSLLGGKGK +dK_MMCCH-2 (K)	1162
20	1199	1203	353.1902	1056.5487	1056.5538	-4.83	T	1	17	0.02	K8PYR +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
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	1756	613.9767	1838.9082	1838.9012	3.81	T	1	21	0.0084	LVKYDITETLDK +dK_MMCCH-2 (K)	1749
26	1923	1932	756.3794	1510.7442	1510.7426	1.19	T	1	26	0.0016	NKVMPNPFAR +dK_MMCCH-2 (K)	1924
27	2100	2109	492.2465	1964.9570	1964.9601	-1.58	T	2	20	0.0084	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	TSADVQFQICKTSEDCHHGGQIPVLGGTK +dK_MMCCH-2 (K)	2131
29	2299	2314	715.0167	2142.0293	2142.0238	2.15	T	1	32	0.00069	LYTKQMEDALTAHGAR +dK_MMCCH-2 (K)	2302
30	2359	2367	736.3491	1470.6835	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	2405.1068	-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	ITAVVKVYIK +dK_MMCCH-2 (K)	2943

Figure 27 continued

40	3003	3021	625.7742	2474.3007	2474.2879	5.17	T	1	39	0.00013	KYDHTELDASKLPAPIWE +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	18	0.023	KGFTDPPVKHHQSANLLVRANINDLTREE +2 dK_MMCCH-2 (K)	123, 142
43	123	151	738.7915	3693.9211	3693.9049	4.39	G	2	22	0.0063	KGFTDPPVKHHQSANLLVRANINDLTREE +dK_MMCCH-2 (K)	131
44	158	176	846.3875	2536.1407	2536.1329	3.08	G	3	19	0.011	APHKRQSDRSVDGYQATAE +dK_MMCCH-2 (K)	151
45	435	442	676.3240	1350.6335	1350.6312	1.78	G	1	25	0.0026	NIEKAMHE +dK_MMCCH-2 (K)	438
46	526	544	777.7499	2330.2280	2330.2304	-1.03	G	1	27	0.0021	VDSTKLASSLPHASVIRE +dK_MMCCH-2 (K)	530
47	589	612	990.1188	2967.3343	2967.3320	0.84	G	1	16	0.024	DKSAGGFCQLEAPHGERKMCPSPE +dK_MMCCH-2 (K)	606
48	825	841	820.3725	2458.0957	2458.0940	0.69	G	1	32	0.00015	HSVPPAVPDYKTNFWYE +dK_MMCCH-2 (K)	835
49	847	860	965.0152	1928.0158	1928.0077	4.20	G	0	23	0.005	FNGLSISQLAKKLE +dK_MMCCH-2 (K)	858
50	1055	1076	810.1668	3236.6462	3236.6402	1.82	G	1	24	0.0041	MALLKKGSSVAVPYWDWTKRIE +2 dK_MMCCH-2 (K)	1059, 1060
51	1055	1076	725.6330	2898.5029	2898.5102	-2.52	G	1	37	0.00021	MALLKKGSSVAVPYWDWTKRIE +dK_MMCCH-2 (K)	1060
52	1097	1110	999.9801	1997.9057	1997.9054	0.15	G	1	23	0.0052	TNPFHHGKITHEME +dK_MMCCH-2 (K)	1104
53	1376	1396	864.3901	2590.1484	2590.1428	2.16	G	3	20	0.011	AGTDSAHTDDGHTEPVAMKKD +dK_MMCCH-2 (K)	1395
54	1397	1413	665.6099	2658.4103	2658.4125	-0.79	G	1	13	0.046	ITGLDMRQLSLVKALE +2 dK_MMCCH-2 (K)	1402, 1410
55	1397	1413	774.4366	2320.2879	2320.2824	2.37	G	1	22	0.0064	ITGLDMRQLSLVKALE +dK_MMCCH-2 (K)	1410
56	1485	1522	866.6912	3462.7358	3462.7381	-0.66	G	3	21	0.0086	LLTVSTHDPETGRDNPFFGSKREFE +dK_MMCCH-2 (K)	1518
57	1755	1765	570.6042	1708.7939	1708.7913	-0.18	G	2	27	0.002	TLDKMNLRHDE +dK_MMCCH-2 (K)	1758
58	2089	2100	854.4125	1706.8104	1706.8098	5.68	G	2	20	0.011	KGSMNLHEEKE +dK_MMCCH-2 (K)	2099
59	2647	2661	715.6753	2144.0035	2144.0095	-3.60	S	4	35	0.00035	AEELKDALYKLGMDE +dK_MMCCH-2 (K)	2656
60	3090	3097	632.8023	1263.5901	1263.5979	1.66	S	0	15	0.023	KGKMYSVE +dK_MMCCH-2 (K)	3092
61	59	68	729.3450	1456.6753	1456.6731	1.65	C	1	17	0.022	VLSGPSEMKW +dK_MMCCH-2 (K) Oxidation (M)	67
62	94	100	572.2991	1144.5838	1144.5838	-0.17	C	1	20	0.011	TVKAELF +dK_MMCCH-2 (K)	96

Figure 27 continued

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	KEDKSAGSF +dK_MMCCH-2 (K)	590
65	715	723	655.8767	1309.7387	1309.7338	3.50	C	1	20	0.0094	TSAKCVLL +dK_MMCCH-2 (K)	719
66	783	788	544.7769	1087.5391	1087.5372	0.83	C	1	22	0.0067	QALCKY +dK_MMCCH-2 (K)	787
67	918	928	856.9330	1711.8515	1711.8491	1.40	C	2	14	0.038	KYDTERLHDL +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	HALDPLCPSPAASKRF +dK_MMCCH-2 (K)	1444
70	1580	1586	544.2603	1086.5061	1086.5056	0.46	C	0	13	0.046	VSGKEPY +dK_MMCCH-2 (K)	1583
71	1649	1654	752.3298	2253.9675	2253.9637	1.69	C	2	14	0.044	MLNDHTHDPSKPEDTF +dK_MMCCH-2 (K)	1659
72	1818	1827	753.3687	1504.7227	1504.7232	-0.27	C	1	22	0.0061	SERDHSSLKY +dK_MMCCH-2 (K)	1826
73	2476	2488	923.9730	1845.9315	1845.9244	3.90	C	1	22	0.0061	THSNAKPTDVFEY +dK_MMCCH-2 (K)	2491
74	2656	2666	793.3514	1584.6882	1584.6879	0.25	C	1	32	0.00057	KLQNDEEHGGY +dK_MMCCH-2 (K)	2655
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
77	2961	2971	769.8909	1537.7673	1537.7673	0.00	C	1	19	0.013	VLGGAKEMPW +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	2581.0108	2.90	Th	2	15	0.03	VCPPDDNDRMDDDHCEKAGD +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	ISDTVHK +dK_MMCCH-2 (K)	84
82	118	124	571.2781	1140.5417	1140.5366	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	ISLEMEKM +dK_MMCCH-2 (K)	438
84	521	531	784.3844	1536.7542	1536.7538	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	LKEEDKS +dK_MMCCH-2 (K)	590

Figure 27 continued

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	1223.5583	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	786.6633	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	1612.7786	2.67	Th	0	25	0.0035	LEKQKEEDRT +dK_MMCCH-2 (K)	2514
103	2595	2606	806.4025	1610.7904	1610.7852	2.61	Th	2	31	0.00079	IIDTSGKQLPSD +dK_MMCCH-2 (K)	2601
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	LTEDHVK +dK_MMCCH-2 (K)	2996

Figure 27 continued

#	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	0.00033	KMVDSLSSDEVLALEK +dK_MMCCH-2 (K)	26
2	147	155	694.3692	1386.7238	1386.7217	1.51	T	1	15	0.031	AGTFLNKK +dK_MMCCH-2 (K)	155
3	164	175	596.3080	1785.9023	1785.8985	2.13	T	1	33	0.00048	LFRWQPGHWTR +dK_MMCCH-2 (K)	167
4	249	271	987.4402	2959.2989	2959.3051	-2.10	T	1	39	0.00012	GKDPNSADCAHWLHTPMEPFDR +dK_MMCCH-2 (K)	259
5	281	293	610.3460	1829.8163	1829.8043	6.56	T	0	55	3.40E-06	EHAKPADSFDYGR +dK_MMCCH-2 (K)	284
6	359	377	849.4008	2545.1805	2545.1810	-0.16	T	1	14	0.041	AGDFFLLGGFTEMKWGFYR +dK_MMCCH-2 (K); Oxidation (M)	372
7	429	446	752.0674	2253.1805	2253.1729	3.37	T	0	52	6.60E-06	GHFDKPPVPVAQAMLAVR +dK_MMCCH-2 (K)	433
8	467	489	709.5944	2830.3483	2830.3385	2.50	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	CPAPDAKDR +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	GKPYNTAMCAIASMR +dK_MMCCH-2 (K)	1083
12	1097	1115	827.0796	2478.2169	2478.2101	2.78	T	0	65	3.10E-07	KPLQPFGLDSVNPEDETR +dK_MMCCH-2 (K)	1097
13	1123	1149	1190.5587	3568.6543	3568.6497	1.32	T	1	70	1.10E-07	VFDYKNNFDYEYESLAFAGLSAAGLDR +dK_MMCCH-2 (K)	1127
14	1355	1385	1271.2897	3810.7871	3810.7876	-0.16	T	1	27	0.0018	GSAVAVPYWDWTERADSLPSLINDATYNSR +dK_MMCCH-2 (K)	1368
15	1409	1450	1097.7139	5483.5330	5483.5213	2.13	T	1	37	0.00018	DPQPELWDNKDPYENVMLALEDDMFCDFEDLELIHNALHSR +dK_MMCCH-2 (K)	1418
16	1455	1460	838.6586	3350.6054	3350.6070	-0.48	T	1	54	3.80E-06	AKYSLSSLDYTAFDPVFFLHHAWVDR +dK_MMCCH-2 (K)	1456
17	1493	1507	721.6621	2161.9645	2161.9594	2.36	T	1	48	1.60E-05	KKPYMEADCAVNEMR +dK_MMCCH-2 (K)	1494
18	1542	1564	1070.1956	3207.5649	3207.5448	6.27	T	1	22	0.0058	YQYDNLQPKHPSGKLDGTRQAR +dK_MMCCH-2 (K)	1556
19	1690	1704	709.3651	2125.1234	2125.1241	4.33	T	2	18	0.026	KEVSSLTTLEKHFLR +dK_MMCCH-2 (K)	1700

Figure 27 continued

20	1767	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	GVIKSEDAYTVR +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
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	QPLRPFSESR +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	KEPYNAAK +dK_MMCCH-2 (K)	3149
31	167	178	590.9642	1769.8707	1769.8705	0.11	G	0	27	0.0018	KVQPGHHTELME +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	NAVISRDPQPELWDNKDFYE +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	2432.1535	2432.1505	5.39	G	0	21	0.008	FVGMSVSSLHNYIKQQQQE +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

Figure 27 continued

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	-2.05	C	4	14	0.04	KYEITQQLHDLDLHVGDNF +dK_MMCCH-2 (K)	1212
48	1416	1421	570.2397	1138.4646	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
53	1801	1809	708.8369	1411.6591	1411.6595	-0.21	C	0	28	0.0017	SHKTPPNPF +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	KYDITKVL +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

Figure 27 continued

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	736.3560	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	19	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)	1805
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	IKQDGEADRV +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
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.

Figure 27 continued

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

#	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	GFTDPPVKHHDSANLLVR +dK_MMCCH-2 (K)	131
2	142	149	556.3417	1310.6669	1310.6653	2.82	T	1	26	0.0026	KNIMDLTR +dK_MMCCH-2 (K)	142
3	157	166	822.8806	1643.7457	1643.7402	3.35	T	1	18	0.015	EAFHKFQEDA +dK_MMCCH-2 (K)	161
4	252	281	735.7324	3673.7255	3673.7008	6.72	T	1	20	0.011	TYVDSHGASHTNPHHSVIAFEENAPHTKR +dK_MMCCH-2 (K)	280
5	460	477	781.3948	2341.1625	2341.1624	0.04	T	1	29	0.0012	TSANVDFIKTTDSVQHK +dK_MMCCH-2 (K)	469
6	470	488	748.0457	2241.1153	2241.1100	2.36	T	1	43	7.70E-05	TTDSVQHKAGTFAVLGGSK +dK_MMCCH-2 (K)	477
7	553	568	663.8673	1325.7201	1325.7166	2.64	T	2	21	0.0076	VKFDKVPR +dK_MMCCH-2 (K)	554
8	553	560	442.9193	1325.7240	1325.7166	5.59	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	KMVDR +dK_MMCCH-2 (K)	565
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	EDKSAGGFQDLGAFHGEPKWCPSPEASK +dK_MMCCH-2 (K)	590
12	591	615	1004.4717	3010.3934	3010.3742	6.38	T	1	18	0.017	SAGGFQDLGAFHGEPKWCPSPEASK +dK_MMCCH-2 (K)	606
13	645	681	1544.3801	4630.1186	4630.1063	2.63	T	1	27	0.0021	HGYDGALPYWDWTSPLAHHLPELADHEKYVDPEDGVEK +dK_MMCCH-2 (K)	671
14	682	699	620.2958	2477.1540	2477.1434	4.28	T	1	26	0.0027	HMPWFDDGHIDTVDKTTTR +dK_MMCCH-2 (K)	685
15	700	719	667.7736	2660.2959	2660.2945	0.53	T	1	51	6.60E-06	SVQMKLEEQPEEGHYTSIAK +dK_MMCCH-2 (K)	704
16	790	804	669.3168	2004.9237	2004.9220	3.34	T	0	35	0.0003	EKPPNVAMCAVTSMR +dK_MMCCH-2 (K)	791
17	805	835	777.1814	3880.8706	3880.8771	-1.67	T	1	14	0.044	EPLGPPEGLSANMTDHVTKEHSVPPNVFDYK +dK_MMCCH-2 (K)	823
18	858	863	520.2896	1038.5846	1038.5783	5.97	T	1	13	0.046	KLEAIK +dK_MMCCH-2 (K)	859

Figure 28 continued

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	1825.0433	-0.98	T	1	36	0.00025	LYVVVVENALLKK +dK_MMCCH-2 (K)	1060
23	1092	1114	791.8783	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
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	ADHSSDGFQAIASPHALPPLCPSPAASKR +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	TAGDCEDAGYFTVLGGEREMPWAFDR +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	1510.7435	2.25	T	1	25	0.0032	NKVMPNPEAR +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	TSADVQFQICKTSEDCHHGGQIPVLGGTK +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	RPLRPFSDPIWHNAFTHSNAKPTDVFEYSR +dK_MMCCH-2 (K)	2481
39	2507	2514	682.3526	1362.6906	1362.6853	3.89	T	1	33	0.00049	KLEHELER +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	RDTSGKQLFSDLIK +dK_MMCCH-2 (K)	2601

Figure 28 continued

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	KMIHSLSHHEAEELR +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	2746	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
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	AFHKFQEDRSVDGYGATAE +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	753.8771	2257.1094	2257.1089	0.22	G	2	20	0.009	TGRDIPNPFIGSKIEFE +dK_MMCCH-2 (K)	1518
62	1755	1765	570.6043	1708.7913	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

Figure 28 continued

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	806.9457	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	GGISLENIERMIHENQQEDRIY +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	1031.4988	1.84	C	0	14	0.038	ESIAKF +dK_MMCCH-2 (K)	1017
75	1330	1337	620.8556	1238.6965	1238.6944	1.78	C	1	21	0.0073	KLDITKAL +dK_MMCCH-2 (K)	1335
76	1649	1664	1127.9668	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
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	778.8939	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	793.3526	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	3946	2960	965.4038	1928.7931	1928.7986	-2.85	C	1	27	0.0021	IKSGTDSDDEYAGSF +dK_MMCCH-2 (K)	3947
86	2961	2971	769.8921	1537.7696	1537.7673	1.50	C	1	13	0.048	VLGGAKEMPW +dK_MMCCH-2 (K)	2967
87	1	9	733.3350	1464.6554	1464.6516	2.59	Th	2	25	0.003	MTPEELKTY +dK_MMCCH-2 (K); Oxidation (M)	7

Figure 28 continued

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	VHHPERG +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	FEENAPHTERQ +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	1482.7386	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	LLGGKSKYS +dK_MMCCH-2 (K)	1162
104	1219	1232	653.9537	1956.8392	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
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	997.5065	-0.40	Th	0	19	0.014	FTKKH +dK_MMCCH-2 (K)	2067

Figure 28 continued

111	2094	2100	618.3057	1234.5968	1234.5923	5.18	Th	1	26	0.0023	HEEEKE +dK_MMCCH-2 (K)	2099
112	2129	2141	622.9242	1865.7607	1865.7493	0.64	Th	0	26	0.0026	CKTSEDCHHGGQ +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	632.7999	1243.5852	1243.5795	4.58	Th	2	17	0.019	AKFTDVFE +dK_MMCCH-2 (K)	2483
115	2512	2521	536.6006	1612.7799	1612.7766	2.05	Th	0	43	8.60E-05	LEKDKEEDRT +dK_MMCCH-2 (K)	2514
116	2595	2606	806.4045	1610.7945	1610.7862	5.15	Th	2	26	0.0026	HDTSGKQLPSD +dK_MMCCH-2 (K)	2601
117	2607	2612	520.7819	1039.5493	1039.5448	4.52	Th	2	25	0.0035	LKKMPT +dK_MMCCH-2 (K)	2609
118	2766	2771	551.7871	1103.5597	1103.5529	6.17	Th	1	25	0.0029	FQQTK +dK_MMCCH-2 (K)	2771
119	2809	2816	581.7781	1161.5416	1161.5376	3.44	Th	2	13	0.045	EGAAEKYS +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	2930	2936	583.2851	1164.5556	1164.5485	6.10	Th	1	33	0.00047	LTDDHVK +dK_MMCCH-2 (K)	2936

Figure 28 continued

#	Start	End	Observed	Mr(expt)	Mr(calc)	ppm	Enzyme	MC	Score	E value	Peptide	Mod_site
1	25	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	1829.8048	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	3381.8330	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	2158.0131	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	3568.6575	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	SAFLQIDKEGIYENIAK +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	DPQPELWDNKDFYENVMLALEQDNFCDFEQLELIHNALHSR +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

Figure 28 continued

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
25	2049	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	4.56	G	3	15	0.083	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	1756.9153	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	NIARFHGKPGLCE +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

Figure 28 continued

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	1962	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
52	1973	1980	817.0586	2448.1541	2448.1454	3.59	G	0	16	0.026	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	628	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	QALDKY +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

Figure 28 continued

65	2463	2479	1128.0177	2254.0208	2254.0253	-1.99	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	KQFLKPF +dK_MMCCH-2 (K)	2754
67	2754	2760	598.3341	1194.6537	1194.6471	5.52	C	1	14	0.041	KQFLKPF +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	1563.7038	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	1163.5208	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
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)	1805
83	1952	1963	627.2844	1878.8314	1878.8247	3.57	Th	2	47	1.00E-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

Figure 28 continued

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

#	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	GFTGPPVKHQSANLLVR +dK_MMCCH-2 (K)	131
2	142	149	656.3414	1310.6682	1310.6653	2.21	T	1	29	0.0013	KNMEILTR +dK_MMCCH-2 (K)	142
3	157	166	548.9277	1643.7464	1643.7402	3.71	T	1	21	0.008	EAFHGFGEDR +dK_MMCCH-2 (K)	161
4	184	192	484.9979	1451.6719	1451.6649	4.82	T	1	14	0.039	EPRPDAKDR +dK_MMCCH-2 (K)	190
5	553	560	663.8693	1325.7240	1325.7166	5.58	T	2	22	0.0068	VKFDKVFR +dK_MMCCH-2 (K)	554
6	566	570	485.2459	968.4772	968.4749	2.37	T	1	19	0.014	KNVER +dK_MMCCH-2 (K)	566
7	581	590	733.9196	1465.8246	1465.8214	2.18	T	2	30	0.0011	KALALKEDK +dK_MMCCH-2 (K)	581
8	588	606	781.0378	2340.0917	2340.0845	3.08	T	1	15	0.031	EDKSAGGFGELGAFHGEPK +dK_MMCCH-2 (K)	590
9	591	615	1004.4722	3010.3949	3010.3742	6.88	T	1	16	0.027	SAGGFGQLGAFHGEPKWCPSPEASK +dK_MMCCH-2 (K)	606
10	682	699	620.2965	2477.1567	2477.1434	5.37	T	1	15	0.03	HAPWFEGHIDTVDKTTTR +dK_MMCCH-2 (K)	695
11	700	719	887.7751	2660.3034	2660.2945	3.38	T	1	20	0.0097	SVQNKLFEQFEFGHWTSAK +dK_MMCCH-2 (K)	704
12	776	789	958.0043	1913.9941	1913.9862	4.13	T	1	15	0.03	WAAWQAIQKYR +Deamidated (NQ); dK_MMCCH-2 (K)	787
13	790	804	1003.4770	2004.9394	2004.9270	6.73	T	0	81	7.20E-09	GKPYNVAMCAVTSNR +dK_MMCCH-2 (K)	791
14	858	863	520.3021	1038.5897	1038.5783	7.03	T	1	15	0.028	KLEAK +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	685.0370	2052.0991	2052.0861	1.45	T	1	23	0.0047	KNIENISLGELESLR +dK_MMCCH-2 (K)	986

Figure 29 continued

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
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	TSADVQFQICKTSEDCHHGGQIPVLGGTK +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	RPLSPFSDPINHNAFTHSNAKPTDVPEYSR +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	1.35	T	1	59	1.20E-06	KNIHSLSHHEAEELR +dK_MMCCH-2 (K)	2637
36	2851	2883	807.5740	4032.8335	4032.8546	-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	KYDHTELDASVLPAPHVR +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	739.7014	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

Figure 29 continued

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	DKSAGGFQQLGAPHGEPKWCPSPE +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	1087	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	AGTDSAHTDDGHTEPVMERKD +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
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	0.00093	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	1484.6648	2.75	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

Figure 29 continued

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	HALPPLCPSPAASKRP +dK_MMCCH-2 (K)	1444
68	1580	1586	544.2616	1086.5088	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	TRSNAKPTDVFEY +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	607.2791	1212.5317	1212.5307	0.82	C	0	13	0.047	GGAKEMPW +dK_MMCCH-2 (K)	2967
74	1	9	725.3536	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	68	765.3771	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
79	431	439	707.8498	1413.6831	1413.6883	-3.75	Th	3	19	0.012	ISLENEKM +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	6.35	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

Figure 29 continued

88	1657	1668	921.9194	1841.8242	1841.8182	3.36	Th	2	30	0.00089	FSKPEDTFDYQK +dK_MMCCH-2 (K)	1668
89	1733	1741	664.3220	1326.6294	1326.6312	-1.36	Th	2	18	0.015	VLGGEKEMIP +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	997.5035	-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	LHEEKE +dK_MMCCH-2 (K)	2099
93	2129	2141	622.9255	1865.7546	1865.7495	2.73	Th	0	19	0.014	KKTSEDCHHGGQ +dK_MMCCH-2 (K)	2131
94	2238	2248	778.3811	1555.7476	1555.7440	2.38	Th	3	23	0.0051	LTTAEVDMLKD +dK_MMCCH-2 (K)	2247
95	2480	2490	825.8984	1649.7822	1649.7759	3.82	Th	3	26	0.0024	AKPTDVFEYSK +dK_MMCCH-2 (K)	2481
96	2532	2521	938.6002	1612.7787	1612.7766	1.24	Th	0	33	0.00013	LEKQKEEDRT +dK_MMCCH-2 (K)	2514
97	2532	2511	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	3	38	0.00017	HDTSGKGLPSD +dK_MMCCH-2 (K)	2601
99	2607	2612	520.7801	1038.5456	1038.5446	0.96	Th	2	23	0.0052	LKMPT +dK_MMCCH-2 (K)	2609
100	2766	2771	551.7874	1101.5603	1101.5529	6.72	Th	1	36	0.00025	IPQQTK +dK_MMCCH-2 (K)	2771
101	2808	2816	638.3197	1274.6248	1274.6217	2.51	Th	3	28	0.0017	LGGAEKYS +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	1164.5538	1164.5485	4.64	Th	1	38	0.00014	LTDDHVK +dK_MMCCH-2 (K)	2996

Figure 29 continued

#	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	179	596.3118	1785.9135	1785.8985	8.40	T	1	41	8.70E-05	LFERVQPGHHTR +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	2253.1739	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	FQNDKSVDGYQATVERHALPAR +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	3.50E-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	3810.7676	0.16	T	1	27	0.0022	GSAVAVPYWDWTEKADSLFSLINDATYFNSR +dK_MMCCH-2 (K)	1368
16	1409	1450	1371.8911	5483.5353	5483.5213	2.55	T	1	17	0.022	DPQPELWDNKDFYENVMLALEQDNFCDFEQLEUHNALHSR +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	2161.9504	-0.97	T	1	55	3.20E-06	KKPYNEADCAVNEMR +dK_MMCCH-2 (K)	1494

Figure 29 continued

19	1542	1564	802.8948	3207.5503	3207.5448	1.71	T	1	30	0.00094	YQYDNLQFNHFSIQKLDQTIDAR +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	1680	1704	532.3688	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
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	KALDDLQGD +dK_MMCCH-2 (K)	41
28	167	178	590.9647	1769.8723	1769.8705	1.02	G	0	24	0.0036	KVQPSRHTRLME +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	ITQQLHDLDUHVGDNFFLKYE +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	1376	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	18	0.013	TDAPFFIKVE +dK_MMCCH-2 (K)	2482

Figure 29 continued

42	3386	3405	658.3157	2629.2338	2629.2271	2.55	G	2	22	0.007	LDHAVSLRDGHYYIAGPTKD +dK_MMCCH-2 (K)	3404
43	277	286	683.7536	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	1337.7269	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	2350.0412	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
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	KYQITQAL +dK_MMCCH-2 (K)	2455
55	2463	2479	752.3478	2254.0210	2254.0253	-1.91	C	1	14	0.037	KAQSIHPEDVFQTDAPF +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	1344.7113	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	FERVQPGHNTR +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	283	734.3531	2200.0374	2200.0371	0.14	Th	4	26	0.0027	LTREHAKPADSFDYGR +dK_MMCCH-2 (K)	284

Figure 29 continued

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	904.6980	1807.7613	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	1127.4857	1.85	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	739.3325	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
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	633.7936	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

Figure 29 continued

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

#	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 878					101	K 2033					151	K 3044				
2	K 16					52	K 884					102	K 2066					152	K 3048				
3	K 53					53	K 918					103	K 2067					153	K 3053				
4	K 67					54	K 924					104	K 2078					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 2235										
13	K 251					63	K 1078					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 1150					116	K 2360	O			O						
17	K 388					67	K 1162					117	K 2460										
18	K 402			O	O	68	K 1199					118	K 2491										
19	K 411					69	K 1221					119	K 2506										
20	K 428					70	K 1230					120	K 2507										
21	K 469					71	K 1270					121	K 2514										
22	K 477					72	K 1308					122	K 2518										
23	K 488					73	K 1330					123	K 2531										
24	K 491					74	K 1331					124	K 2532										
25	K 499					75	K 1338					125	K 2579										
26	K 507				O	76	K 1339					126	K 2601										
27	K 520					77	K 1366					127	K 2609										
28	K 549					78	K 1402					128	K 2630										
29	K 554					79	K 1410					129	K 2624										
30	K 557					80	K 1418					130	K 2687										
31	K 586					81	K 1446					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 1519					134	K 2713										
35	K 606					85	K 1543					135	K 2714										
36	K 615					86	K 1568					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 718	O	O			92	K 1743					142	K 2905	O									
43	K 757					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 2985										
48	K 858					98	K 1915					148	K 3002										
49	K 863					99	K 1924	O	O		O	149	K 3008	O									
50	K 878					100	K 2022					150	K 3037										

Figure 30 continued

#	K site	sample				#	K site	sample				#	K site	sample			
		1	2	3	4			1	2	3	4			1	2	3	4
1	K 25	O	O			51	K 1127	O	O			101	K 2198				
2	K 41					52	K 1155					102	K 2202				
3	K 73					53	K 1178					103	K 2227				
4	K 78					54	K 1181					104	K 2231				
5	K 104					55	K 1212					105	K 2317				
6	K 105					56	K 1239					106	K 2327				
7	K 138					57	K 1280					107	K 2328				
8	K 154					58	K 1302	O				108	K 2330				
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 2409				
13	K 289	O	O		O	63	K 1488	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 2486				
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 2813				
26	K 589					76	K 1680	O				126	K 2875				
27	K 594					77	K 1705					127	K 2878				
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 703					81	K 1782					131	K 2948				
32	K 741					82	K 1808					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 805					88	K 1935					138	K 3148				
39	K 848					89	K 1947					139	K 3349				
40	K 855					90	K 1954	O	O	O	O	140	K 3155				
41	K 856					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 3268				
45	K 909					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 2085					148	K 3340				
49	K 1088					99	K 2092					149	K 3344				
50	K 1097	O	O	O	O	100	K 2123					150	K 3404				
													total	17	12	6	10

Figure 30 continued

#	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 2078					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 2167										
12	K 180					62	K 1060					112	K 2238										
13	K 251					63	K 1073					113	K 2247	O	O	O	O						
14	K 260					64	K 1104	O	O	O	O	114	K 2281										
15	K 285					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 2551										
24	K 491					74	K 1335					124	K 2552										
25	K 499					75	K 1338					125	K 2579										
26	K 507					76	K 1339					126	K 2601										
27	K 536					77	K 1395					127	K 2605										
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 1475	O				132	K 2662										
33	K 587					83	K 1518					133	K 2666										
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 1699		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 718	O		O		92	K 1749					142	K 2860	O									
43	K 787				O	93	K 1758					143	K 2926										
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 1913					148	K 3002										
49	K 863					99	K 1924	O			O	149	K 3005	O									
50	K 878					100	K 2022					150	K 3037										

Figure 30 continued

#	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 61					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 1238			O	O	106	K 2327				
7	K 138					57	K 1280					107	K 2328				
8	K 154					58	K 1302	O	O			108	K 2330				
9	K 155					59	K 1331					109	K 2395				
10	K 167	O	O		O	60	K 1335					110	K 2348				
11	K 181					61	K 1368		O	O		111	K 2361				
12	K 250		O			62	K 1418					112	K 2406				
13	K 284	O	O		O	63	K 1458	O				113	K 2426				
14	K 324					64	K 1493					114	K 2448				
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 2550				
19	K 433	O	O	O		69	K 1568					119	K 2527	O	O		
20	K 447					70	K 1640					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 485					73	K 1635					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 2872				
27	K 634					77	K 1700					127	K 2873				
28	K 672					78	K 1705					128	K 2886				
29	K 675					79	K 1708					129	K 2903				
30	K 688					80	K 1767					130	K 2924				
31	K 703					81	K 1782					131	K 2948				
32	K 743					82	K 1803					132	K 2953				
33	K 774					83	K 1811					133	K 3015				
34	K 776					84	K 1835					134	K 3025	O			
35	K 787					85	K 1879					135	K 3045				
36	K 790					86	K 1923					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 2062					145	K 3278				
46	K 935	O				96	K 2065					146	K 3321				
47	K 1011					97	K 2065					147	K 3336				
48	K 1078					98	K 2089					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

#	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 3046				
2	K 26					52	K 884					102	K 2066					152	K 3048				
3	K 58	O	O	O	O	53	K 918					103	K 2067	O	O	O	O	153	K 3062				
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 2098	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 958	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 2148										
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 1075	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 285					65	K 1117		O		O	115	K 2302	O									
16	K 373					66	K 1160					116	K 2350	O	O	O	O						
17	K 385	O		O		67	K 1167	O	O	O		117	K 2458										
18	K 402					68	K 1195	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 1305					122	K 2536	O	O	O	O						
23	K 488					73	K 1330					123	K 2551										
24	K 491	O				74	K 1335	O	O	O	O	124	K 2562										
25	K 499					75	K 1336					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 1430	O	O	O	O	129	K 2628	O	O	O	O						
30	K 557				O	80	K 1436					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 1478	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 588	O	O	O	O	84	K 1529	O				134	K 2713										
35	K 606	O	O	O	O	85	K 1543					135	K 2719			O	O						
36	K 613					86	K 1583	O	O	O	O	136	K 2748	O	O	O							
37	K 616					87	K 1635					137	K 2771	O	O	O	O						
38	K 621	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 708	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 2880	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 1806					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 1868	O	O	O	O	147	K 2986	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

#	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 2186	O	O	O	O
2	K 41	O		O		52	K 1155					102	K 2202	O	O	O	O
3	K 71					53	K 1178			O		103	K 2217	O	O	O	O
4	K 79	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 1238	O	O	O	O	106	K 2507				
7	K 138					57	K 1280					107	K 2525				
8	K 154	O	O			58	K 1302	O	O	O	O	108	K 2530				
9	K 156	O	O	O	O	59	K 1311	O	O	O	O	109	K 2535				
10	K 167	O	O	O	O	60	K 1315	O	O	O	O	110	K 2545				
11	K 191	O	O	O	O	61	K 1368	O	O	O	O	111	K 2561	O	O	O	O
12	K 256	O	O	O	O	62	K 1418	O	O	O	O	112	K 2600				O
13	K 286	O	O	O	O	63	K 1456	O	O	O	O	113	K 2415		O		
14	K 321	O			O	64	K 1493	O				114	K 2446				
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 2465	O	O	O	O
17	K 403					67	K 1528	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 439	O	O	O	O	69	K 1565					119	K 2517	O	O	O	O
20	K 447					70	K 1600	O	O	O	O	120	K 2596				
21	K 482					71	K 1602	O	O	O	O	121	K 2737	O	O		
22	K 471	O	O	O	O	72	K 1634	O			O	122	K 2754	O	O	O	
23	K 485		O	O	O	73	K 1635					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 1760	O	O	O	O	127	K 2873				
28	K 672					78	K 1765					128	K 2888				
29	K 675					79	K 1798	O	O	O		129	K 2903				
30	K 868					80	K 1787	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 3023		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 3189	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 1078	O	O	O	O	98	K 2068					148	K 3340				
49	K 1088	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

#	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 2064					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 2078	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 2154		O	O	O		total	80	81	86	78
8	K 128	O	O	O	O	58	K 956	O	O	O	O	108	K 2161	O	O	O	O						
9	K 131	O	O	O	O	59	K 986	O	O	O	O	109	K 2168										
10	K 142	O	O	O	O	60	K 1017			O		110	K 2180	O									
11	K 161	O	O	O	O	61	K 1059	O	O			111	K 2187										
12	K 180		O		O	62	K 1060	O	O	O	O	112	K 2218										
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 388					67	K 1162	O	O	O		117	K 2460										
18	K 405					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 2532										
24	K 491					74	K 1335	O	O	O	O	124	K 2552										
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 548					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 1415					130	K 2627	O	O	O	O						
31	K 568	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 1472	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 2910	O	O	O	O						
43	K 787	O	O	O	O	93	K 1788	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 1833					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 3003										
49	K 868				O	99	K 1924	O	O	O	O	149	K 3008	O	O	O	O						
50	K 878					100	K 2022					150	K 3037			O							

Figure 31 continued

#	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 1153					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 1305	O	O	O	O	108	K 2330				
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 181	O	O	O	O	61	K 1368	O	O	O	O	111	K 2361		O		O
12	K 255	O	O	O	O	62	K 1418	O	O	O	O	112	K 2405				O
13	K 284	O	O	O	O	63	K 1456	O	O	O	O	113	K 2425				
14	K 321			O	O	64	K 1483	O				114	K 2444				
15	K 358					65	K 1484	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 2546				
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 1638			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 2878				
28	K 672					78	K 1705					128	K 2886				
29	K 675					79	K 1708	O	O	O		129	K 2905				
30	K 688					80	K 1767	O	O	O		130	K 2934				
31	K 701					81	K 1781		O		O	131	K 2948	O	O	O	O
32	K 741					82	K 1805	O	O	O	O	132	K 2959				
33	K 774					83	K 1811		O			133	K 3010	O	O	O	O
34	K 776					84	K 1836					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 856					90	K 1954	O	O	O	O	140	K 3155				
41	K 858					91	K 1988	O	O	O	O	141	K 3184				
42	K 882					92	K 2003	O	O	O	O	142	K 3189				
43	K 898	O	O	O	O	93	K 2044					143	K 3240	O	O	O	O
44	K 907					94	K 2046	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 2082					149	K 3348				
50	K 1097	O	O	O	O	100	K 2121	O				150	K 3406	O	O	O	O
													total	61	56	57	58

Figure 32

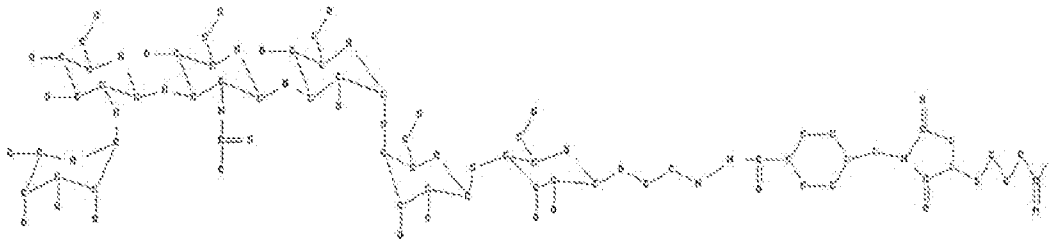
Sample	1			2			3			4		
KLH1/KLH2	KLH1	KLH2	total	KLH1	KLH2	total	KLH1	KLH2	total	KLH1	KLH2	total
Total K	156	150	306	156	150	306	156	150	306	156	150	306
Globo H-conjugated K	14	17	31	7	12	19	4	6	10	8	10	18
MMCCH-conjugated K	86	69	155	83	60	143	86	61	147	84	56	140

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.

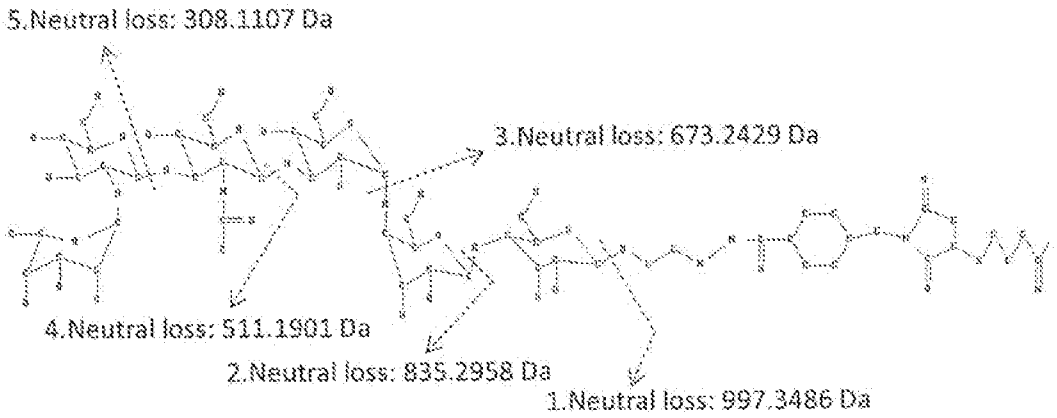
Figure 33

Globo H derivative



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

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

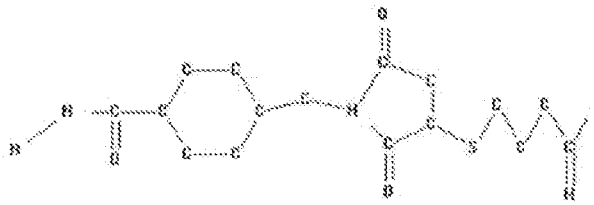
3. Chemical formula: C(30) H(48) N(4) O(14) S(1)
   Monoisotopic MW addition: 720.2888 Da

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

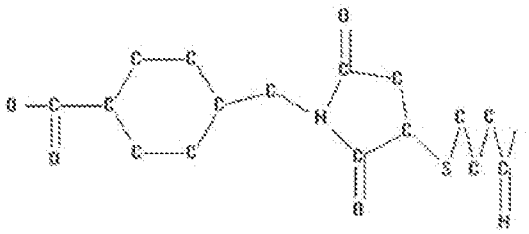
Figure 34

MMCCH derivative



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

deamidated MMCCH derivative



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