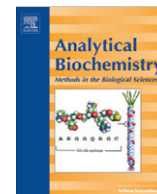


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Vapor conjugation of toluene diisocyanate to specific lysines of human albumin

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ABSTRACT

Exposure to toluene diisocyanate (TDI), an industrially important crosslinking agent used in the production of polyurethane products, can cause asthma in sensitive workers. Albumin has been identified as a major reaction target for TDI in vivo, and TDI–albumin reaction products have been proposed to serve as exposure biomarkers and to act as asthmagens, yet they remain incompletely characterized. In the current study, we used a multiplexed tandem mass spectrometry (MS/MS) approach to identify the sites of albumin conjugation by TDI vapors, modeling the air/liquid interface of the lung. Vapor phase TDI was found to react with human albumin in a dose-dependent manner, with up to 18 potential sites of conjugation, the most susceptible being Lys351 and the dilysine site Lys413–414. Sites of vapor TDI conjugation to albumin were quantitatively limited compared with those recently described for liquid phase TDI, especially in domains IIA and IIIB of albumin. We hypothesize that the orientation of albumin at the air/liquid interface plays an important role in vapor TDI conjugation and, thus, could influence biological responses to exposure and the development of in vitro assays for exposure and immune sensitivity.

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Diisocyanates are highly reactive electrophilic compounds that are industrially useful as crosslinking agents in polyurethane production for diverse products such as flexible and rigid foams, fibers, paints, and varnishes. Global diisocyanate production is dominated by two aromatic diisocyanates, toluene diisocyanate (TDI)¹ and methylene diphenyl diisocyanate (MDI), which together account for more than 90% of the diisocyanate market [1]. Exposure to TDI and other diisocyanates is associated with adverse health effects, including asthma, contact dermatitis, and hypersensitivity pneumonitis [2]. Worldwide, diisocyanates are the most commonly reported cause of occupational asthma, with an estimated 5% to 30% of exposed workers at risk for developing disease [2–5].

The mechanistic connections between diisocyanate exposure and health outcomes remain unclear, in large part due to uncertainty regarding diisocyanate reactivity in vivo. The self-protein albumin has been identified as a major reaction target for inhaled diisocyanate, and diisocyanate–albumin reaction products (e.g., conjugates), which accumulate in the circulating blood, may serve as biomarkers of exposure [6–9]. In some workers, diisocyanate–albumin-specific immunoglobulin E (IgE) can be measured in sera and may participate directly in asthma pathogenesis [10,11]. Thus,

a better understanding of diisocyanate–albumin reactivity is central to understanding exposure outcomes and to the development of assays for exposure monitoring and disease surveillance.

Human albumin possesses numerous functional groups that could potentially react with diisocyanate; however, diisocyanate–albumin conjugates that form in vivo in exposed workers remain largely uncharacterized due to technical limitations. Studies of diisocyanate–albumin reactivity to date have relied primarily on in vitro modeling and reveal a marked influence of exposure conditions on the conformation and antigenicity of the resulting diisocyanate–albumin reaction products [12,13]. For example, high concentrations of diisocyanate, relative to albumin, result in excessive amounts of diisocyanate conjugation, protein precipitation, and lack of specific antibody recognition [12–18]. Data to date suggest that under occupational exposure conditions (e.g., low diisocyanate concentrations), individual albumin molecules undergo limited conjugation.

The majority of in vitro studies on diisocyanate–albumin reactivity have been performed with liquid phase chemical; however, for volatile diisocyanates such as TDI, the airway microenvironment is exposed to vapor rather than liquid phase chemical [19]. TDI–albumin conjugates that form under such mixed (vapor/liquid) phase exposure conditions differ structurally and conformationally from those formed in liquid phase and have been hypothesized to more closely reflect those that form in vivo, based on immune recognition by IgE from diisocyanate asthma patients [16].

Tandem mass spectrometry (MS/MS) is well-suited to the structural analysis of modified peptides and proteins [20]. Accurate

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¹ Abbreviations used: TDI, toluene diisocyanate; MDI, methylene diphenyl diisocyanate; Ig, immunoglobulin; MS/MS, tandem mass spectrometry; PBS, phosphate-buffered saline; TDA, toluene diamine; mAb, monoclonal antibody; UPLC, ultra-performance liquid chromatography; qTOF, quadrupole time-of-flight; CID, collision-induced dissociation.

mass measurement of fragment ions can discriminate between iso-mass peptides produced by the enzymatic cleavage of large proteins [20,21]. The current study undertakes a comprehensive MS/MS approach [14,22,23] to unambiguously map the sites on human albumin conjugated by vapor phase TDI. A mixed (vapor/liquid) phase in vitro exposure system, in which vapor dose was titrated by varying the duration of exposure, was used to identify those sites on albumin most susceptible to vapor phase TDI conjugation. Preferential sites of vapor TDI conjugation were compared with those recently identified for liquid TDI and highlight the influence of exposure biophysics on TDI–albumin reactivity [14]. The data are discussed in the context of disease pathogenesis and the development of assays for exposure monitoring and disease surveillance.

Materials and methods

Preparation of vapor TDI–albumin conjugates

Vapor TDI–albumin conjugates were prepared by using a previously described isocyanate vapor phase exposure system [17]. In brief, TDI vapor concentrations in the range of 0.14 to 1.4 mg/m³ (~1–10 µmol/m³) were passively generated inside an exposure chamber monitored with an Autostep monitor (GMD, Pittsburgh, PA, USA). TDI was an 80:20 mixture of 2,4- and 2,6-TDI isomers obtained from Aldrich (St. Louis, MO, USA). Low endotoxin human albumin in phosphate-buffered saline (PBS, pH 7.2) at a concentration of 5 mg/ml (73 nmol/ml) was exposed in open 60-mm Petri dishes (Becton Dickinson, Franklin Lakes, NJ, USA) for 0 min (control), 20 min, 1 h, 4 h, and 24 h. The exposure unit was cleaned with 70% ethanol, and protein solutions were filtered (0.2 µm) before and after exposure.

Quantitation of dissolved TDI after vapor exposures

TDI from 0-min (control), 20-min, 1-h, 4-h, and 24-h exposures was trapped in open 60-mm Petri dishes containing 0.5% H₂SO₄. Reaction of TDI with dilute sulfuric acid results in rapid hydrolysis of TDI to toluene diamine (TDA), which is stable in solution. Aliquots (1 ml) of the TDA-containing trap solution were selected and buffered back to alkaline pH by adding 1 ml of saturated sodium borate. TDA was subsequently derivatized by adding 50 µl of 1 mg/ml fluorescamine (Fisher Scientific, Pittsburgh, PA, USA) in acetonitrile. Samples were quantified by fluorescence spectroscopy using an LS50B luminescence spectrometer (PerkinElmer, Waltham, MA, USA) controlled by FL WinLab software (version 4.00.02, PerkinElmer) using excitation at 410 nm and observing the emission at 510 nm. A calibration curve was generated using 2,4-TDA (Sigma–Aldrich, St. Louis, MO, USA).

Native gel and anti-TDI Western blot

TDI conjugation to human albumin was detected in native gels based on characteristic changes in electrophoretic mobility, as described previously [17,24]. For native protein analysis, samples were prepared in a 10% glycerol running buffer and then electrophoresed on 10% polyacrylamide gels and stained with Imperial protein stain (Pierce, Rockford, IL, USA). For Western blot analysis, samples were electrophoresed under reducing conditions (for optimal anti-TDI monoclonal antibody [mAb] binding) on precast 4% to 15% gradient gels and transferred to nitrocellulose using an aqueous trans-blot system (Bio-Rad, Hercules, CA, USA). Nitrocellulose membranes were blocked with 3% dry milk in PBS, probed with 1 µg/ml of the anti-TDI mAb 60G2 [25] followed by anti-mouse

IgG₁ (Pharmingen, San Diego, CA, USA), and developed with ECL reagent (Thermo Fisher Scientific, Rochester, NY, USA).

Trypsin digestion

Aliquots (100 µl) of each conjugate and control were taken for analysis. Disulfide bonds were reduced by reaction with tributylphosphine (5 mM) for 30 min at room temperature, followed by alkylation with iodoacetamide (15 mM) for 1 h at room temperature. Alkylation was quenched by further addition of tributylphosphine (5 mM) for 15 min at room temperature. Samples were twice dialyzed against 3 L of 25 mM NH₄HCO₃ using 3500-MWCO (molecular weight cutoff) mini dialysis units (Slide-A-Lyzer, Thermo Scientific, Waltham, MA, USA). Porcine trypsin was suspended in 25 mM NH₄HCO₃ and added to each aliquot at a 40:1 (protein/trypsin) ratio. Samples were incubated overnight at 37 °C with shaking (300 rpm). Samples were centrifuged at 14,100g in a microcentrifuge (MiniSpin, Eppendorf, Hamburg, Germany) to pellet any insoluble material.

Ultra-performance liquid chromatography

Enzymatic peptides were separated on a Waters (Milford, MA, USA) nanoACQUITY ultra-performance liquid chromatography (UPLC) system. Aliquots (1 µl) of the digest mixture were injected and trapped/desalted on a 5-µm Symmetry C₁₈ trapping column (180 µm × 20 mm) with 99.5:0.5 A/B (A: 0.1% formic acid; B: 0.1% formic acid in acetonitrile) at a flow rate of 15 µl/min for 1 min. Separation was performed on a 1.7-µm BEH130 C₁₈ analytical column (100 µm × 100 mm) using gradient elution at a flow rate of 400 nl/min and a gradient of 99:1 to 60:40 A/B over 60 min.

Tandem mass spectrometry

The eluent from the UPLC system was directed to the nanoelectrospray source of a Waters SYNAPT MS quadrupole time-of-flight (qTOF) mass spectrometer. Positive ion nanoelectrospray was performed using 10-µm PicoTip (Waters) emitters held at a potential of +3.5 kV. The cone voltage was held constant at +40 V for all experiments. Dry N₂ desolvation gas was supplied to the instrument via a nitrogen generator (NitroFlowLab, Parker Hannifin, Haverhill, MA, USA). [Glu1]-Fibrinopeptide B (100 fmol/µl in 75:25 A/B) was supplied to an orthogonal reference probe, and the [M+2H]²⁺ ion (*m/z* = 785.84265 u) was measured as an external calibrant at 30-s intervals. Collision-induced dissociation (CID) was performed using ultra-high-purity (UHP) argon as collision gas. Spectra were acquired in an “MS^{en}” fashion [22]. Briefly, alternating 1-s mass spectra are acquired. The first spectrum acquired at low (6 eV) collision energy allows high mass accuracy precursor ion mass measurement. The second spectrum acquired at high (15–30 eV ramp) collision energy allows high mass accuracy fragment ion mass measurement. The fragment ion spectra may be temporally correlated with precursor spectra postrun. This method of data acquisition allows all precursor ions to be fragmented and analyzed, as opposed to so-called “data-dependent acquisition” methods that require making real-time decisions on which ions to select for fragmentation, which may miss low-abundance precursor ions.

Data analysis

Data were analyzed with BioPharmaLynx (version 1.2, Waters), a software program for analysis of peptide mass maps and identification of sites of modification on known protein sequences. Default peptide mass map analysis criteria of 30 ppm mass error in both low and high collision energy mode were specified. Trypsin

was specified as the digestion enzyme, and two missed cleavages were allowed. The submitted protein sequence was taken from P02768, “serum albumin precursor, homo sapiens” (<http://www.uniprot.org/uniprot/P02768>), and the signal and propeptides (residues 1–24) were removed. Custom modifiers were created for two bound forms of TDI (see Fig. 1). The first (TDI*, $C_8H_8N_2O$, $m/z = 148.0637$ u) represents one isocyanate moiety bound to a peptide via a urea bond, whereas the second isocyanate moiety is hydrolyzed to the primary amine. The second (TDI, $C_9H_6N_2O_2$, $m/z = 174.0429$ u) represents TDI with both isocyanate moieties bound to a peptide via urea bonds. Identification of a potential TDI conjugation site proceeded via a rigorous procedure that involved the following steps. First, a potential peptide–TDI conjugation product with less than 30 ppm $m/\Delta m$ mass error in the analyte peptide mass map is observed. Second, comparison of analyte and control peptide mass map from unmodified human serum albumin shows that observed m/z and chromatographic retention time are unique to analyte. Third, MS/MS data contain b_n - and y_n -type ions consistent with the assigned sequence and modifier.

Results and discussion

Samples of human serum albumin were exposed to increasing doses of TDI vapors, for example, exposure for 0 min, 20 min, 1 h, 4 h, and 24 h. Quantification of TDI exposures by fluorescence spectrometry indicate that these vapor exposures result in diffusion of 0, 0.9, 4.6, 22.2, and 314.6 μg of TDI/ml into the liquid phases, respectively. These exposures correspond to approximate exposure (TDI/albumin) mol ratios of 0, 1:15, 1:3, 1.6:1, and 24:1, respectively. Exposed albumin samples display dose-dependent changes in electrophoretic mobility, consistent with TDI conjugation, as shown in Fig. 2A. The increased migration under native conditions reflects changes in charge and/or conformation of the protein and has been previously observed for diisocyanate-conjugated protein [17,24]. Dose-dependent conjugation of human

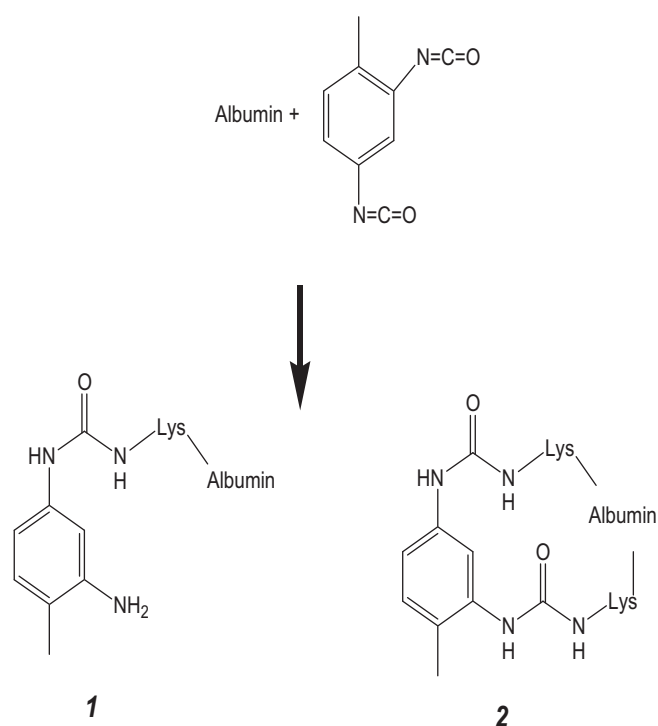


Fig. 1. Reaction of TDI with albumin. Hydrolysis of one isocyanate moiety to the amine results in adduct 1 (+148.0637 u) is shown. Reaction of both isocyanate moieties results in the intramolecular crosslinked adduct 2 (+174.0429 u).

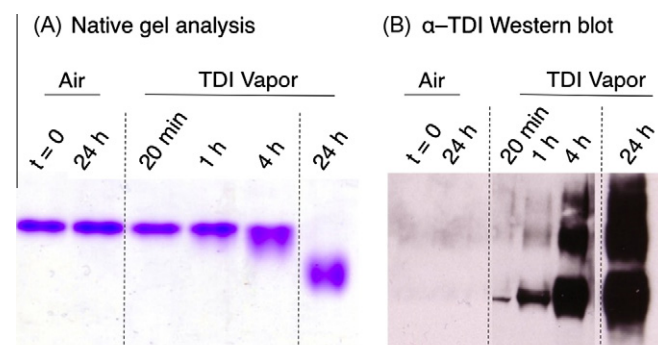


Fig. 2. (A) Native gel analysis of TDI–albumin conjugates. Albumin was exposed to TDI vapors or room air for varying time periods as labeled and was stained for protein. (B) Western blot parallel gels were blotted with anti-TDI mAb 60G2.

albumin by TDI vapor was further validated by Western blot with the anti-TDI mAb 60G2 (Fig. 2B).

A comprehensive map of TDI vapor conjugation sites on human albumin was obtained via UPLC–MS/MS analysis of trypsin-digested samples (presented in Fig. 3). The chemistry of vapor TDI conjugation to human serum albumin is similar to that described previously for liquid phase TDI and MDI (Fig. 1) [14,23,24]. TDI is observed to conjugate serum albumin in one of two forms. The first (TDI*, $C_8H_8N_2O$, $m/z = 148.0637$ u) results from hydrolysis of one isocyanate to a primary amine, whereas the second isocyanate moiety undergoes nucleophilic addition to the protein. The second (TDI, $C_9H_6N_2O_2$, $m/z = 174.0429$ u) is the result of both isocyanates undergoing nucleophilic addition to the protein, resulting in an intramolecular crosslinked species. This is often observed when two lysines are located in close proximity, such as is the case for the four dilysine motifs in human albumin. It should be noted that intermolecular crosslinking of two protein molecules via one TDI (e.g., $[2 M + TDI + H]^+$) is possible and is observed in limited amounts. In addition, polymerization of TDI on one protein site (e.g., $[M + \text{poly-TDI} + H]^+$) is also possible. Although we do not discount the possibility that crosslinked or poly-TDI species play a role in the human immune response to TDI in vivo, an in-depth analysis of the thousands of products theoretically formed by such conjugation is beyond the scope of this article.

The specific amino acids of human albumin that were conjugated by TDI vapor were identified through CID–MS/MS. Representative fragment ion spectra are presented for serum albumin tryptic fragments 411 to 428 (YTKKVPQVSTPTLVEVSR), 522 to 534 (QKKQTALVELVK), and 1 to 10 (DAHKSEVAHR) in Figs. 4A, 4B, and 4C, respectively. Peptide fragments are labeled according to a modified Roepstorff–Fohlman nomenclature [26] in which fragment ions containing TDI or the hydrolyzed amine are notated with an asterisk (e.g., b_n^* , y_n^*). Both Figs. 4A and 4B represent fragment ion spectra from species of the form $[M + TDI + H]^+$ or intramolecular crosslinked species. In both spectra, TDI reacts with ϵ -amines on the side chain of each of the dilysine motifs (Lys413–Lys414 and Lys524–Lys525). In Fig. 4A, b_n -type ions b_4^* , b_5^* , b_6^* , b_7^* , b_8^* , and b_{10}^* are observed, each increased in mass by 174.04 u over the theoretical unmodified b_n ion. Observation of a b_3 or b_3^* ion would require two bonds to be broken (the peptide bond between lysine residues and one of the urea bonds formed by TDI), a high energy fragmentation channel that is unlikely to be significantly populated (although a very small amount of the analogous b_3^* ion from fragment 522–524 is observed; see Fig. 4B). Unmodified y_1 to y_{10} ions indicate that TDI is not bound at the C-terminal end of the peptide. TDI can be unambiguously assigned to Lys524 and Lys525 based on the fragment ion

1 DAHKSEVAHR FKDLGEENFK ALVLIAFAQY LQQCPFEDHV KLVNEVTEFA
 51 KTCVADESAE NCDKSLHTLF GDKLCTVATL RETYGEMADC CAKQEPERNE
 101 CFLQHKDDNP NLPRLVRPEV DVMCTAFHDN EETFLKKYLY EIARRHPYFY
 151 APELLFFAKR YKAAFTECCQ AADKAACLLP KLDELRLDEGK ASSAKQRLKC
 201 ASLQKFGERA FKAWAVARLS QRFPAEFAE VSKLVTDLTk VHTECCHGDL
 251 LECADDRADL AKYICENQDS ISSKLKECCE KPLEKSHCI AEVENDEMPA
 301 DLPSLAADFV ESKDVCKNYA EAKDVFLGMF LYEYARRHPD YSVVLLRLA
 351 KTYETTLKCA CAADPHECY AKVDFEFKPL VEEPQNLIKQ NCELFEQLGE
 401 YKFQNALLVK YTKKKVPQVST PTLVEVSRNL GKVGSKCCKH PEAKRMPCAE
 451 DYLSVVLNQL CVLHEKTPVS DRVTKCCTES LVNRRPCFSA LEVDETYVPK
 501 EFNAETFTFH ADICTLSEKE RQIKKQTALV ELVKHKPKAT KEQLKAVMDD
 551 FAAFVEKCCK ADDKETCFAE EGKKLVAASQ AALGL

Fig. 3. Map of vapor/liquid TDI–albumin conjugation sites. All observed sites are underlined. Favored conjugation sites observed on 20 min of exposure are in bold. UPLC–qTOF MS^c analysis resulted in 100% sequence coverage of the protein.

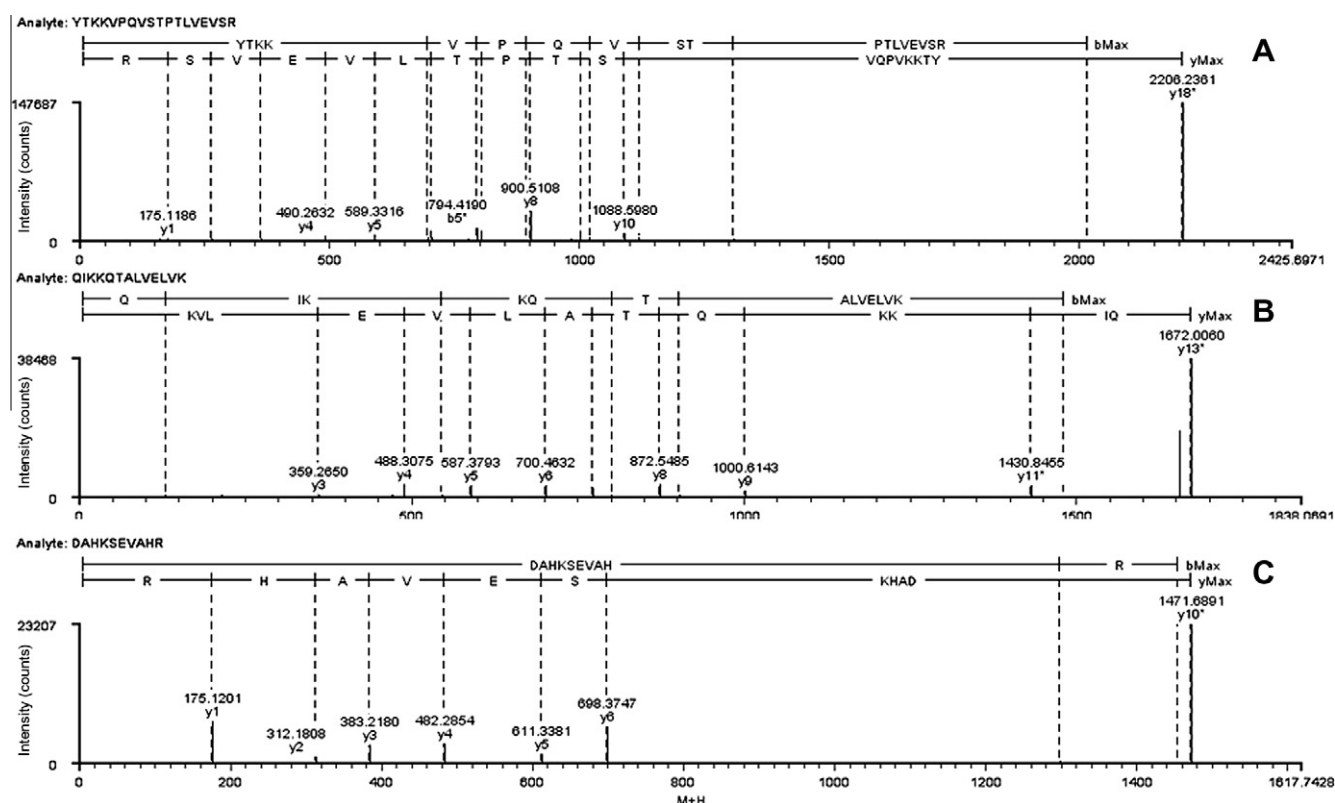


Fig. 4. MS/MS fragment ion spectra of human serum albumin fragment 411 to 428 (YTKKVPQVSTPTLVEVSR) [M+TDI+H]⁺ (A), human serum albumin fragment 522 to 534 (QIKKQTALVELVK) [M+TDI+H]⁺ (B), and human serum albumin fragment 1 to 10 (DAHKSEVAHR) [M+TDI*+TDI+H]⁺ (C) formed by vapor/liquid TDI exposure.

spectrum in Fig. 4B given observation of b_1 , b_3^* , b_5^* , and b_6^* ions. C-terminal ions confirm conjugation of TDI to Lys524 and Lys525 by observation of unmodified y_3 through y_9 and y_{11}^* , coupled with the absence of a y_{10} or y_{10}^* ion. Fig. 4C presents the fragment ion spectrum of the fragment 1 to 10 [M+TDI*+TDI+H]⁺ ion, which is formed by an intramolecular poly-TDI crosslink between the α -NH₂ of the N-terminal Asp1 and side chain ϵ -NH₂ of Lys4. The mass of this peptide is observed to be 322.10 u higher than that of the unmodified peptide. A series of unmodified y_1 to y_6 ions indicate that neither TDI nor TDI* is bound on the C-terminal residues SEVAHR. This Asp–TDI–TDI*–Lys linkage to the DAHK sequence results in a cyclic peptide; therefore, observation of y_7^* to y_9^* ions would require breaking two bonds. No confirmatory b_n -type ions are observed in this spectrum because of the higher proton affinity of the C-terminal arginine.

Table 1 presents the residues of human serum albumin observed to react with TDI as a function of exposure time. Conjugation proceeds in a dose-dependent manner, with more conjugation sites identified as TDI exposure time increases. Three TDI conjugation

sites (Lys351, Lys413, and Lys414) were observed for the shortest exposure (20 min) and, therefore, the lowest TDI dose (0.07:1 mol TDI/mol human serum albumin), suggesting that these sites are the favored loci of conjugation for TDI–albumin on vapor/liquid exposure. Lys413 and Lys414 make up one of four dilysine motifs in human serum albumin and have been previously identified as being particularly susceptible to nucleophilic addition with both TDI [14] and MDI [23,24] in liquid/liquid exposures. Interestingly, although Lys351 has been previously identified as a conjugation site for TDI and MDI, liquid/liquid titration of albumin demonstrated that conjugation to Lys351 was not observed until TDI/albumin molar ratios in excess of 10:1 were reached [14]. Similarly, Lys199 is a preferred conjugation site in liquid/liquid exposures (conjugate observed at 1:1 ratio), but this conjugate is not observed in vapor/liquid until a ratio of 24:1 is reached.

Sites of TDI–albumin conjugation observed for vapor/liquid exposures consist of a subset of those identified previously for liquid/liquid conjugations [14]. Liquid/liquid exposures resulted in conjugation at 37 sites on serum albumin, distributed approxi-

Table 1

Comparison of TDI–albumin conjugation sites for vapor/liquid and liquid/liquid exposures.

Residue	Vapor/liquid				Liquid/liquid ^a				Domain
	20 min(0.07:1)	1 h(0.35:1)	4 h(1.6:1)	24 h(24:1)	1:1	5:1	10:1	40:1	
Asp1			X	X	X	X	X	X	IA
Lys4			X	X	X	X	X	X	IA
Lys12			X	X			X	X	IA
Lys73			X	X				X	IA
Gln104								X	IA
Lys106				X				X	IA
Lys136								X	IB
Lys137			X	X			X	X	IB
Lys159			X	X				X	IB
Lys190				X			X	X	IB
Gln196							X	X	IIA
Lys199				X	X	X	X	X	IIA
Lys205							X	X	IIA
Lys212							X	X	IIA
Lys262								X	IIA
Lys274						X	X	X	IIA
Lys276							X	X	IIA
Lys281							X	X	IIA
Lys351	X	X	X	X			X	X	IIIB
Lys378				X		X	X	X	IIIB
Lys402								X	IIIA
Lys413	X	X	X	X	X	X	X	X	IIIA
Lys414	X	X	X	X	X	X	X	X	IIIA
Lys432				X		X	X	X	IIIA
Lys436				X			X	X	IIIA
Lys439							X	X	IIIA
Lys444				X	X	X	X	X	IIIA
Lys524		X	X	X	X	X	X	X	IIIB
Lys525		X	X	X	X	X	X	X	IIIB
Lys534						X	X	X	IIIB
Lys536						X	X	X	IIIB
Lys541						X	X	X	IIIB
Lys545						X	X	X	IIIB
Lys557							X	X	IIIB
Lys560							X	X	IIIB
Lys573					X	X	X	X	IIIB
Lys574					X	X	X	X	IIIB

^a TDI–albumin conjugation sites determined for liquid/liquid exposure are from Hettick and Siegel [14].

mately equally among all domains and subdomains. Vapor/liquid conjugations, however, result in conjugations primarily to domains I and IIIa, with only 3 reactive sites in domain II compared with 10 observed for liquid/liquid exposures. Similarly, only 2 of 10 liquid/liquid conjugation sites in domain IIIB are observed for vapor/liquid conjugation (see Fig. 5).

Although significant differences between vapor/liquid and liquid/liquid exposures are observed, it should be noted that differences in the experimental methodology exist between the studies. First, liquid/liquid TDI experiments were performed with 2,4- and 2,6-TDI independently, whereas this study used an 80:20 mixture of the two isomers, similar to that used in industrial applications. Although the liquid/liquid study noted no difference in the conjugation specificity of the two isomers, 2,4-TDI did result in ion abundances approximately 2-fold higher than those with 2,6-TDI. Second, the liquid/liquid exposure study used a measured volume of TDI introduced via pipette to a stirred bulk solution, whereas the current study relied on diffusion of the TDI vapors into a nonstirred albumin-containing solution. It can be reasonably suggested, therefore, that the liquid/liquid study results represent a complete list of the 37 sites on the serum albumin protein reactive to TDI at pH 7.4. Because the kinetics of the reaction of TDI with the serum albumin protein are fast relative to the rate of diffusion into the bulk solution, the current pH 7.4 vapor/liquid results suggest that those serum albumin protein molecules nearest the air/liquid interface are oriented in such a way as to present only a subset (18 of 37) of reactive sites. Ultimately, the bound location(s) of

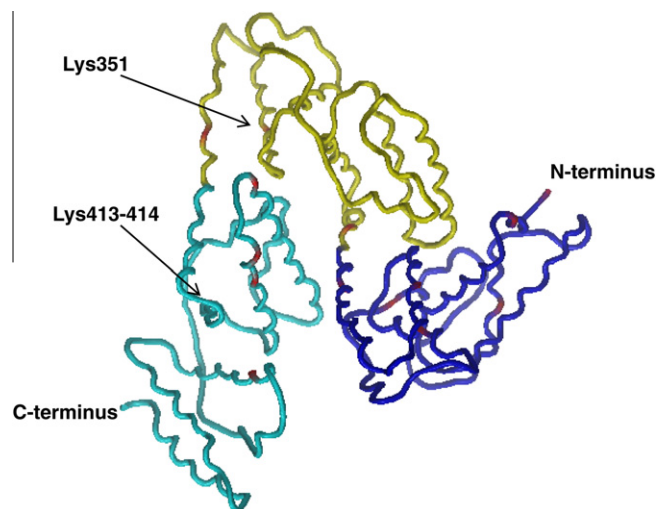


Fig. 5. Structure of human serum albumin. Domain I (blue), domain II (yellow), and domain III (cyan) are shown. TDI conjugation sites are identified in red. Chain starts at Lys4; therefore, Asp1 is not shown. (From He and Carter [30].)

TDI to albumin in vapor/liquid and liquid/liquid can be compared over a range of TDI/albumin ratios. Because TDI, once conjugated to albumin, results in a stable, covalently bonded species, TDI–albumin conjugates produced at the lowest exposures, whether from vapor/liquid or liquid/liquid exposures, can be compared.

The TDI conjugation sites identified for vapor/liquid exposures are presented on the ribbon model of human serum albumin in Fig. 5. Reactive lysine residues are generally located on α -helices, which in albumin have a hydrophobic and a hydrophilic side. These α -helices then self-orient on the basis of hydrophobic interactions into the overall three-dimensional arrangement of domains and subdomains. Orientation of proteins at air/liquid surfaces due to hydrophilic/phobic interactions can cause changes in orientation and conformation. Lin and coworkers [27] suggested that proteins spontaneously adsorb from aqueous solution to the air/water interface due to the energetically favorable dehydration of hydrophobic regions of the protein surface. Such behavior can be strongly influenced by the protein concentration, secondary structure of the protein, and solution chemistry. Furthermore, Kudryashova and coworkers determined that although a bulk solution of egg white ovalbumin was not aggregated in the bulk solution, the protein showed anisotropic motion at the surface, indicating a preferential orientation of the protein in at the interface [28]. We hypothesize that the observed differences in TDI conjugation sites between liquid/liquid and vapor/liquid models are due to a more ordered orientation of albumin at the surface than is present in bulk solution. Dockal and coworkers [29] studied the three-dimensional structure of the recombinant domains of human serum albumin and determined, on the basis of ultraviolet circular dichroism spectroscopy, that domain II is significantly more hydrophobic (37% α -helix content) than either domain I or III (46 or 53% α -helix content, respectively). We hypothesize that in this vapor/liquid model system, significant portions of serum albumin domains II and IIIb are blocked from TDI conjugation, most likely by protein aggregation/hydrophobic interactions.

In conclusion, we have used UPLC–MS/MS to determine the conjugation sites of TDI on albumin from vapor/liquid exposures. This exposure may more closely mimic the biophysics of exposure in the lung and shows increased propensity for TDI conjugation to domains I and IIIa of serum albumin than do previous studies using liquid/liquid exposures. Because the orientation of proteins at the air/water interface is strongly influenced by solution concentration and composition, experiments designed to more accurately model the airway, including components such as lung surfactant and glutathione, and ultimately in vivo exposures will be critical to identifying the ultimate bioactive form(s) of isocyanate/protein conjugates formed from airway exposures.

Acknowledgments

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Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at [doi:10.1016/j.ab.2011.12.013](https://doi.org/10.1016/j.ab.2011.12.013).

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Peptides Identified from Control Serum Albumin Digest

Peptide	Star t	En d	Modifiers	Mcalc	Mobs	z	Mer r	RT(min)	Intensity
DAHKSEVAHRFK	1	12		1423.7321	1423.6926	2	-27.7	27.9	11582
SEVAHRFK	5	12		972.5141	972.5174	1	3.4	27.5	52681
SEVAHRFK	5	12		972.5141	972.5593	1	46.5	40.9	7811
SEVAHRFKDLGEENFK	5	20		1904.938	1904.9167	2	-11.2	38	1336
FKDLGEENFK	11	20		1225.5979	1225.6145	2	13.5	26.4	3457913
FKDLGEENFK	11	20		1207.5873	1207.5765	3	-8.9	26.4	119837
FK	11	12		293.1739	293.174	1	0.3	26.4	13098
FKDLGEENF	11	19		1051.4974	1051.5118	2	13.7	26.4	9643
FKDLGEENFKALVLIAFAQYLQQCPFEDHVK	11	41	Carbamidomethyl C(1)	3696.865	3696.9148	4	13.5	44.1	28313
FK	11	12		275.1634	275.1649	1	5.5	26.4	9312
FK	11	12		293.1739	293.1689	1	-17.1	37.8	7215
FK	11	12		293.1739	293.1756	1	5.8	27.5	4765
FKDLGEENFKALVLIAFAQYLQQCPFEDHVK	11	41	Carbamidomethyl C(1)	3696.865	3696.8574	6	-2.1	27.7	4095
FKDLGEENFK	11	20		1225.5979	1225.604	2	5	30.4	3790
FKDLGEENFK	11	20		1225.5979	1225.6292	2	25.5	30.8	1508
FKDLGEENFK	11	20		1225.5979	1225.6321	2	27.9	24.7	1190
DLGEENFK	13	20		950.4345	950.446	1	12.1	26.5	661860
DL	13	14		228.111	228.1099	1	-4.8	26.5	36068
DLGEENFK	13	20		950.4345	950.4439	1	9.9	27.4	35884
DL	13	14		200.1161	200.1148	1	-6.5	26.5	35293
DLGEENFK	13	20		950.4345	950.4426	1	8.5	25	2424
DLGEENFKALVLIAFAQYLQQCPFEDHVK	13	41	Carbamidomethyl C(1)	3421.7017	3421.7527	3	14.9	46.6	44513
DLGEENFK	13	20		950.4345	950.4572	1	23.9	33	9692
LGEENFK	14	20		835.4076	835.422	2	17.2	26.5	10883
GEENFK	15	20		722.3235	722.3307	1	10	26.4	309583
GEENFK	15	20		704.3129	704.3184	1	7.8	26.4	35019
GEENFK	15	20		722.3235	722.3366	1	18.1	27	16747

EENFK	16	20		665.3021	665.2985	1	-5.4	26.4	112317
ALVLIAFAQYLQQCPFEDHVK	21	41	Carbamidomethyl C(1)	2489.2776	2489.3118	3	13.7	44.1	668421
ALVLIAFAQYLQQCPFEDHVKLVNEVTEFAK	21	51	Carbamidomethyl C(1)	3619.8748	3619.906	4	8.6	45.8	48177
ALVLIAFAQYLQQCPFEDHVK	21	41	Carbamidomethyl C(1)	2489.2776	2489.3096	3	12.9	45.3	9250
ALVLIAFAQYLQQCPFEDHVK	21	41	Carbamidomethyl C(1)	2472.2512	2472.2644	4	5.3	43.8	9052
ALVLIAFAQY	21	30		1089.6222	1089.6349	2	11.7	43.8	7751
ALVLI	21	25		509.3577	509.3621	1	8.6	43.8	5715
ALVLIAFAQYLQQCPFEDHVK	21	41	Carbamidomethyl C(1)	2489.2776	2489.3103	3	13.1	49	5328
ALVLIAFAQ	21	29		926.5589	926.5673	1	9.1	43.8	5288
ALVLIAFAQYL	21	31		1202.7063	1202.717	2	8.9	43.8	5041
ALVLIAF	21	27		727.4632	727.4699	1	9.2	43.8	4850
ALVLIAFAQYLQQCPFEDHVK	21	41	Carbamidomethyl C(1)	2489.2776	2489.3184	2	16.4	44.8	4701
ALVLIAFAQY	21	30		1089.6222	1089.6332	2	10.1	44.1	3681
ALVLIAFA	21	28		798.5003	798.5102	1	12.4	43.8	3446
ALVLIAFAQYL	21	31		1202.7063	1202.7139	2	6.3	44.1	2896
ALVLIAFAQYLQQCPFEDHVK	21	41	Carbamidomethyl C(1)	2489.2776	2489.314	3	14.6	42.8	1410
VLIAFAQYLQQCPFEDHVK	23	41	Carbamidomethyl C(1)	2305.1565	2305.1824	3	11.2	43.8	68163
VLIAFAQYLQQCPFEDHVK	23	41	Carbamidomethyl C(1)	2305.1565	2305.1741	3	7.6	44.1	14123
LIAFAQYLQQCPFEDHVK	24	41	Carbamidomethyl C(1)	2206.0881	2206.1055	3	7.9	44.1	3949
IAFAQYLQQCPFEDHVK	25	41	Carbamidomethyl C(1)	2093.0042	2093.0242	3	9.6	44.1	1959
AFAQYLQQCPFEDHVK	26	41	Carbamidomethyl C(1)	1979.92	1979.9396	3	9.9	43.8	26115
AFAQYLQQCPFEDHVK	26	41	Carbamidomethyl C(1)	1979.92	1979.9509	3	15.6	44.1	2723
FAQYLQQCPFEDHVK	27	41	Carbamidomethyl C(1)	1908.8829	1908.9202	2	19.5	43.8	10476
AQYLQQCPFEDHVK	28	41	Carbamidomethyl C(1)	1761.8145	1761.8451	2	17.4	44.5	7108
QYLQQCPFEDHVK	29	41	Carbamidomethyl C(1)	1690.7773	1690.8127	2	20.9	43.8	14224
QYLQQCPFEDHVK	29	41	Carbamidomethyl C(1)	1690.7773	1690.795	2	10.5	44.1	4270
YLQQCPFEDHVK	30	41	Carbamidomethyl C(1)	1562.7188	1562.7344	2	10	44.5	11400
YLQQCPFEDHVK	30	41	Carbamidomethyl C(1)	1562.7188	1562.7341	2	9.8	44.1	10404
LQQCPFEDHVK	31	41	Carbamidomethyl C(1)	1399.6554	1399.6666	2	8	44.1	11412
QQCPFEDHVK	32	41	Carbamidomethyl C(1)	1286.5714	1286.5859	2	11.3	43.8	25129
QQCPFEDHVK	32	41	Carbamidomethyl C(1)	1286.5714	1286.5847	2	10.3	44.1	6510

QCPFEDHVK	33	41	Carbamidomethyl C(1)	1158.5128	1158.5266	2	11.9	43.8	5293
CPFEDHVK	34	41	Carbamidomethyl C(1)	1030.4542	1030.4606	2	6.2	43.8	4430
CPFEDHVK	34	41	Carbamidomethyl C(1)	1030.4542	1030.4584	2	4.1	44.1	2308
LVNEVTEFAK	42	51		1148.6077	1148.6151	1	6.4	28.8	3993551
LV	42	43		212.1525	212.1513	1	-5.7	28.8	173626
LVNEV	42	46		554.3064	554.3095	1	5.6	28.8	98989
LV	42	43		184.1576	184.156	1	-8.7	28.8	69404
LVNE	42	45		455.238	455.234	1	-8.8	28.8	69268
LVN	42	44		326.1954	326.1947	1	-2.1	28.8	36038
LVNEVTEF	42	49		931.4651	931.4717	1	7.1	28.8	17501
LVNEVT	42	47		655.3541	655.3587	1	7	28.8	11300
LV	42	43		184.1576	184.1556	1	-10.9	28.2	8665
LVNEVTEFAK	42	51		1148.6077	1148.6196	2	10.4	30.4	5368
LVNE	42	45		438.2114	438.2149	1	8	28.8	4293
LVNEVTEFAKTCVADESAENCDK	42	64	Carbamidomethyl C(2)	2628.1685	2628.0928	2	-28.8	25.1	3294
LVNEVTEFAK	42	51		1148.6077	1148.6046	2	-2.7	36.4	2539
VNEVTEFAK	43	51		1035.5237	1035.5264	1	2.6	28.8	26132
NEVTEFAK	44	51		936.4553	936.4602	1	5.2	28.8	633200
VTEFAK	46	51		693.3698	693.3713	1	2.2	28.8	38891
TEFAK	47	51		594.3013	594.2836	1	-29.8	28.8	47988
AK	50	51		217.1426	217.1422	1	-1.8	28.8	14953
TCVADESAENCDK	52	64	Carbamidomethyl C(2)	1497.5713	1497.608	2	24.5	23.6	866862
TCVADESAENCDKSLHTLFGDK	52	73	Carbamidomethyl C(2)	2496.0898	2496.1636	4	29.6	25.4	56207
T	52	52		101.0477	101.0459	1	-17.8	25.5	15433
TCVADESAENCDKSLHTLFGDK	52	73	Carbamidomethyl C(2)	2496.0898	2496.0803	4	-3.8	29.2	3941
TCVADESAENCDK	52	64	Carbamidomethyl C(2)	1497.5713	1497.5829	1	7.7	25	1929
ENCDK	60	64	Carbamidomethyl C(1)	664.2487	664.2474	1	-2	23.6	4491
SLHTLFGDK	65	73		1016.5291	1016.5449	1	15.5	27.9	847583
SLHTLFGDKLCTVATLR	65	81	Carbamidomethyl C(1)	1931.0299	1931.0422	3	6.4	33.5	308322
SLHTLFGDKLCT	65	76	Carbamidomethyl C(1)	1372.6809	1372.6899	2	6.6	33.5	42762
SLHTL	65	69		533.2962	533.2997	1	6.6	27.9	27053

SLHTLFGDKLCT	65	76	Carbamidomethyl C(1)	1354.6704	1354.6949	2	18.1	33.5	15762
SLHTLFGDK	65	73		998.5185	998.5324	2	13.9	27.9	14396
SLHTLFGDKLCTV	65	77	Carbamidomethyl C(1)	1471.7494	1471.7671	2	12	33.5	13365
SLHTLFGDK	65	73		1016.5291	1016.5554	2	25.9	28.3	11795
SLH	65	67		337.175	337.1762	1	3.6	27.9	8515
SLHTLFGDKLC	65	75	Carbamidomethyl C(1)	1271.6333	1271.6506	2	13.6	33.5	7123
SLHTLFGDKLCTVATLR	65	81	Carbamidomethyl C(1)	1913.0193	1913.0205	4	0.6	33.5	7048
SLHTLFGDKLCTV	65	77	Carbamidomethyl C(1)	1443.7544	1443.7645	3	7	33.5	6254
SLHTLF	65	70		670.3802	670.3798	2	-0.6	27.9	4530
SLHTLFGDK	65	73		1016.5291	1016.5555	2	26	28.9	1624
LHTLFGDK	66	73		911.4865	911.4909	2	4.8	27.9	13487
HTLFGDK	67	73		798.4024	798.4065	2	5.1	27.9	9382
HTLFGDK	67	73		816.413	816.3931	1	-24.4	27.4	1945
TLFGDK	68	73		679.3541	679.3646	1	15.5	27.9	23419
LFGDK	69	73		578.3064	578.3207	1	24.7	27.9	6140
FGDK	70	73		465.2223	465.2294	1	15.3	27.9	59891
FGDKLCTVATLR	70	81	Carbamidomethyl C(1)	1379.7231	1379.7472	2	17.5	33.5	5613
GDKLCTVATLR	71	81	Carbamidomethyl C(1)	1232.6548	1232.6683	2	11	33.5	15044
LCTVATLR	74	81	Carbamidomethyl C(1)	932.5114	932.5209	1	10.2	26.3	634330
LCTVATLR	74	81	Carbamidomethyl C(1)	914.5008	914.502	2	1.3	26.3	97564
LC	74	75	Carbamidomethyl C(1)	273.1147	273.1156	1	3.3	26.3	58189
LCT	74	76	Carbamidomethyl C(1)	374.1624	374.164	1	4.3	26.3	18972
LC	74	75	Carbamidomethyl C(1)	245.1198	245.1189	1	-3.7	26.3	11014
LC	74	75	Carbamidomethyl C(1)	256.0882	256.0879	1	-1.2	26.3	8609
LCTVA	74	78	Carbamidomethyl C(1)	544.2679	544.2725	1	8.5	26.3	7298
LCTVATLR	74	81	Carbamidomethyl C(1)	932.5114	932.5132	2	1.9	27.1	6791
LCTV	74	77	Carbamidomethyl C(1)	473.2308	473.2313	1	1.1	26.3	6672
CTVATLR	75	81	Carbamidomethyl C(1)	819.4273	819.4231	1	-5.1	26.3	59634
TVATLR	76	81		659.3966	659.4135	1	25.6	26.3	218380
TVATLR	76	81		641.386	641.3846	2	-2.2	26.3	21676
VATLR	77	81		558.3489	558.3557	1	12.2	26.3	39123

ATLR	78	81		459.2805	459.2839	1	7.4	26.3	31683
ATLR	78	81		459.2805	459.2727	1	-17	33.5	20109
TLR	79	81		388.2434	388.2439	1	1.3	26.3	13517
TLR	79	81		388.2434	388.2363	1	-18.3	33.5	4251
ETYGEMADCCAK	82	93	Carbamidomethyl C(2)	1433.5262	1433.5615	2	24.6	25.1	381128
ETYGEMADCCAK	82	93	Carbamidomethyl C(2)	1433.5262	1433.5525	2	18.3	24.6	4205
ETYGEMADCCAK	82	93	Carbamidomethyl C(2)	1415.5156	1415.5508	2	24.9	25.1	3836
QEPERNECFLQHK	94	106	Carbamidomethyl C(1)	1713.7893	1713.8042	2	8.7	34.4	1047633
QEPERNECFLQHKDDNPNLPR	94	114	Carbamidomethyl C(1)	2635.2197	2635.2671	4	18	25.6	696657
QEPERNECFLQHK	94	106	Carbamidomethyl C(1)	1696.7628	1696.8022	2	23.2	25.7	566172
QEPERNECFLQHK	94	106	Carbamidomethyl C(1)	1713.7893	1713.8147	2	14.8	24.2	390695
QEPERNECFLQHK	94	106	Carbamidomethyl C(1)	1713.7893	1713.8059	2	9.7	33.8	122913
QEPERNECFLQHKDDNPNLPR	94	114	Carbamidomethyl C(1)	2617.2092	2617.2136	5	1.7	25.6	98054
QEPERNECFLQHKDDN	94	109	Carbamidomethyl C(1)	2039.8756	2039.9294	3	26.4	25.6	43218
QEPERNECFLQHKDDNPN	94	111	Carbamidomethyl C(1)	2233.9448	2233.9893	4	19.9	25.6	15983
QEPERNECFLQHKDDNPN	94	111	Carbamidomethyl C(1)	2250.9712	2251.0085	4	16.6	25.6	9708
QEPERNECFLQHK	94	106	Carbamidomethyl C(1)	1695.7788	1695.7628	3	-9.4	34.4	5300
QEPERNECFLQHK	94	106	Carbamidomethyl C(1)	1695.7788	1695.7932	3	8.5	24.2	63480
QEPERNECFLQHKDDNPNLPR	94	114	Carbamidomethyl C(1)	2635.2197	2635.2568	3	14.1	29.2	2281
QEPERNECFLQHK	94	106	Carbamidomethyl C(1)	1713.7893	1713.819	2	17.3	33.3	1807
QEPERNECFLQHKDDN	94	109	Carbamidomethyl C(1)	2022.849	2022.8733	4	12	25.6	1420
PERNECFLQHK	96	106	Carbamidomethyl C(1)	1456.6881	1456.7191	3	21.3	24.3	43058
PERNECFLQHKDDNPNLPR	96	114	Carbamidomethyl C(1)	2378.1187	2378.1736	4	23.1	25.6	61713
PERNECFLQHKDDNPNLPR	96	114	Carbamidomethyl C(1)	2361.092	2361.0911	5	-0.4	25.6	3867
NECFLQHKDDNPNLPR	99	114	Carbamidomethyl C(1)	1995.9221	1995.9659	3	21.9	26	547296
NECFLQHK	99	106	Carbamidomethyl C(1)	1074.4917	1074.5176	2	24.1	24.4	142491
NECFLQHKDDNPNLPRPRLVRPEV	99	120	Carbamidomethyl C(1)	2671.3289	2671.332	2	1.2	29.4	47957
NECFLQHKDDNPNLPR	99	114	Carbamidomethyl C(1)	1978.8956	1978.9146	4	9.6	26	41390
NECFLQHKDDNPN	99	111	Carbamidomethyl C(1)	1611.6736	1611.6953	2	13.5	26	21212
NECFLQHKDDN	99	109	Carbamidomethyl C(1)	1383.5514	1383.5881	2	26.5	26	12426
NECFLQHK	99	106	Carbamidomethyl C(1)	1057.4651	1057.5006	2	33.6	24.4	3184

NECFLQHKDDNPNLPR	99	136	Carbamidomethyl C(2)	4627.1685	4627.2412	3	15.7	26.4	20142
NECFLQHKDDNPNLPR	99	114	Carbamidomethyl C(1)	3991.8442	3991.9077	3	15.9	26	8036
NECFLQHKDDNPNLPR	99	114	Carbamidomethyl C(1)	1995.9221	1995.9595	3	18.7	27	5199
NECFLQHKDDNPNLPR	99	114	Carbamidomethyl C(1)	1995.9221	1995.9128	3	-4.7	35	2116
ECFLQHK	100	106	Carbamidomethyl C(1)	960.4488	960.4639	2	15.7	24	365853
ECFLQHKDDNPNLPR	100	114	Carbamidomethyl C(1)	1881.8792	1881.9203	3	21.8	26	11234
ECFLQHKDDNPNLPR	100	114	Carbamidomethyl C(1)	1864.8527	1864.9084	3	29.9	26	2815
CFLQHKDDNPNLPR	101	114	Carbamidomethyl C(1)	1752.8365	1752.8774	3	23.3	26	32485
FLQHK	102	106		671.3755	671.3935	1	26.8	24.5	11406
QHK	104	106		411.223	411.2132	1	-23.8	24.5	3683
DDNPNLPR	107	114		939.441	939.4466	1	6	24.5	405287
DDNPNL	107	112		668.2766	668.2853	1	13	24.5	35626
DDN	107	109		344.0968	344.0947	1	-6.1	24.5	31513
DD	107	108		230.0539	230.0515	1	-10.4	24.5	15167
DDN	107	109		326.0862	326.0817	1	-13.8	24.5	8921
DDNPN	107	111		555.1925	555.1967	1	7.6	24.5	6219
DDNPNLPR	107	114		939.441	939.4431	1	2.2	35.4	1518
PNLPR	110	114		595.3442	595.3466	1	4	24.5	207672
PNLPR	110	114		595.3442	595.3433	2	-1.5	26	26122
PNLPR	110	114		595.3442	595.3449	2	1.2	25.6	25828
LPR	112	114		384.2485	384.2504	1	4.9	25.6	10115
PR	113	114		271.1644	271.1639	1	-1.8	24.5	29140
PR	113	114		271.1644	271.1654	1	3.7	25.6	9989
PR	113	114		271.1644	271.1649	1	1.8	26	7761
RLVRPEVDVMCTAFHDNEETFLK	114	136	Carbamidomethyl C(1)	2805.3579	2805.2749	3	-29.6	35.4	2216
LVRPEVDVMCTAFHDNEETFLKK	115	137	Carbamidomethyl C(1)	2777.3516	2777.3872	3	12.8	33.4	721683
LVRPEVDVMCTAFHDNEETFLK	115	136	Carbamidomethyl C(1)	2649.2566	2649.3123	3	21	35	457693
LVRPEVDVMCTAFHDNEETFLKK	115	137	Carbamidomethyl C(1)	2759.3411	2759.3306	5	-3.8	33.4	58440
LVRPEVDVMCTAFHDNEETFLK	115	136	Carbamidomethyl C(1)	2631.2461	2631.2532	4	2.7	35	49268
LVRPEVDVMCTAFHDNEETFLKK	115	137	Carbamidomethyl C(1)	2777.3516	2777.3777	4	9.4	32.7	46932
LVRPEVDV	115	122		907.5127	907.5147	2	2.2	35	27811

LVRPEVDV	115	122		907.5127	907.5169	2	4.6	33.4	27670
LVRPEVDVM	115	123		1038.5532	1038.5598	2	6.4	35	25429
LVRPEVD	115	121		808.4443	808.435	2	-11.5	33.4	24949
LVRPEVDVMCTAFHDNEETFLKK	115	137	Carbamidomethyl C(1)	2777.3516	2777.3335	5	-6.5	32.5	10567
LVRPE	115	119		594.3489	594.3486	1	-0.5	33.4	9388
LVRPEVDVMCT	115	125	Carbamidomethyl C(1)	1299.6316	1299.6406	2	6.9	35	3610
LVRPEV	115	120		693.4174	693.419	2	2.3	33.4	9842
LVRPEVDVMCTAFHDNEETFLK	115	136	Carbamidomethyl C(1)	2649.2566	2649.2888	4	12.2	34.2	7991
LVRPEVDVM	115	123		1038.5532	1038.5626	2	9.1	33.4	5374
LVRPEVDVMCTAFHDNEETFLK	115	136	Carbamidomethyl C(1)	2649.2566	2649.2598	4	1.2	36	4537
LVRPEV	115	120		665.4224	665.4244	2	3	33.4	3454
LVRPEVDVMCTAFHDNEETFLKK	115	137	Carbamidomethyl C(1)	2777.3516	2777.3743	3	8.2	32.5	2656
LVRPEVDVMCTAFHDNEETFLK	115	136	Carbamidomethyl C(1)	2649.2566	2649.2517	3	-1.8	43.3	2040
LVRPEVDV	115	122		879.5178	879.5043	2	-15.3	33.4	1804
VRPEVDVMCTAFHDNEETFLKK	116	137	Carbamidomethyl C(1)	2664.2676	2664.3049	4	14	33.4	31158
RPEVDVMCTAFHDNEETFLKK	117	137	Carbamidomethyl C(1)	2565.1992	2565.2212	4	8.6	33.4	55067
RPEVDVMCTAFHDNEETFLK	117	136	Carbamidomethyl C(1)	2437.1042	2437.166	3	25.4	35	5244
PEVDVMCTAFHDNEETFLKK	118	137	Carbamidomethyl C(1)	2409.0981	2409.1316	4	13.9	33.4	1311
VDVMCTAFHDNEETFLKK	120	137	Carbamidomethyl C(1)	2183.0027	2183.0142	4	5.3	33.4	7658
DVMCTAFHDNEETFLKK	121	137	Carbamidomethyl C(1)	2083.9343	2083.9465	4	5.9	33.4	8650
DVMCTAFHDNEETFLK	121	136	Carbamidomethyl C(1)	1955.8394	1955.8633	3	12.2	35	8214
VMCTAFHDNEETFLKK	122	137	Carbamidomethyl C(1)	1968.9073	1968.9474	3	20.4	33.4	40718
VMCTAFHDNEETFLK	122	136	Carbamidomethyl C(1)	1840.8124	1840.8278	3	8.4	35	6383
MCTAFHDNEETFLKK	123	137	Carbamidomethyl C(1)	1869.839	1869.8596	3	11	33.4	68957
MCTAFHDNEETFLK	123	136	Carbamidomethyl C(1)	1741.744	1741.7544	2	6	35	50549
CTAFHDNEETFLKK	124	137	Carbamidomethyl C(1)	1738.7985	1738.8337	3	20.2	33.4	39320
CTAFHDNEETFLK	124	136	Carbamidomethyl C(1)	1610.7035	1610.7374	2	21	35	38701
CTAFHDNEETFLK	124	136	Carbamidomethyl C(1)	1610.7035	1610.7386	1	21.8	36.2	1262
TAFHDNEETFLK	125	136		1450.6729	1450.7021	2	20.1	35	12153
TAFHDNEETFLKK	125	137		1578.7678	1578.7814	3	8.6	33.4	5741
FHDNEETFLK	127	136		1278.588	1278.6053	2	13.5	35	13217

FHDNEETFLKK	127	137	1406.683	1406.712	2	20.6	33.4	3332
KYLYEIAR	137	144	1054.5811	1054.5885	2	7	27.2	103033
K	137	137	146.1055	146.1036	1	-13	28.8	29885
K	137	137	146.1055	146.1057	1	1.4	36.5	25579
KYL	137	139	404.2423	404.246	1	9.2	27.2	5928
K	137	137	146.1055	146.1027	1	-19.2	29.7	25552
K	137	137	146.1055	146.1038	1	-11.6	24.4	16931
K	137	137	146.1055	146.1037	1	-12.3	26.2	10309
K	137	137	146.1055	146.1029	1	-17.8	27.9	6674
KYLYEIAR	137	144	1054.5811	1054.5591	2	-20.9	34.1	2683
YLYEIAR	138	144	926.4861	926.4957	1	10.4	28	1612157
YL	138	139	276.1474	276.1488	1	5.1	28	104423
YL	138	139	248.1525	248.1504	1	-8.5	28	99027
YLY	138	140	439.2107	439.2105	1	-0.5	28	44455
Y	138	138	135.0684	135.0669	1	-11.1	28	40216
YLYEIAR	138	144	926.4861	926.4983	1	13.2	28.9	3604
YLYEIAR	138	144	908.4756	908.4689	2	-7.4	28	29231
YLYEIAR	138	144	926.4861	926.4932	1	7.7	28.7	2298
LYEIAR	139	144	763.4229	763.4301	1	9.4	28	128372
YEIAR	140	144	650.3387	650.3444	1	8.8	28	742927
YEIAR	140	144	650.3387	650.3426	1	6	27.5	9851
YEIAR	140	144	650.3387	650.3423	1	5.5	27.2	2995
EIAR	141	144	487.2754	487.2767	1	2.7	28	77920
IAR	142	144	358.2328	358.2297	1	-8.7	28	30587
IAR	142	144	358.2328	358.2239	1	-24.8	27.5	6510
AR	143	144	245.1488	245.1472	1	-6.5	28	17978
RHPYFYAPE	145	153	1160.5403	1160.5524	2	10.4	37.8	348336
RHPYFYA	145	151	934.4449	934.4477	2	3	37.8	264860
RHPYFYAPEL	145	154	1273.6244	1273.636	2	9.1	37.8	174790
RHPYFYAPELLFFAK	145	159	1897.9879	1898.0032	3	8.1	38.8	86179
RHPYFY	145	150	863.4078	863.4102	2	2.8	37.8	83258

RHPYFYAPELL	145	155	1386.7084	1386.7404	2	23.1	37.8	62967
R	145	145	174.1117	174.11	1	-9.8	28.4	28690
RHPYFYAPEL	145	154	1245.6294	1245.6451	2	12.6	37.8	23799
RHPYFYAPE	145	153	1132.5454	1132.5582	2	11.3	37.8	19334
R	145	145	174.1117	174.1107	1	-5.7	27.9	19255
RHPYFYAPEL	145	154	1255.6138	1255.6362	2	17.8	37.8	19005
RHPYFYAPELLFFAK	145	159	1897.9879	1898.0046	4	8.8	37.9	18727
RHPYFYAPELLFFAK	145	159	1879.9773	1880.0084	4	16.5	37.8	17904
RHPYF	145	149	700.3445	700.3469	2	3.4	37.8	15328
RHPYFYAP	145	152	1031.4977	1031.5171	2	18.8	37.8	13826
RHPYFY	145	150	835.413	835.4149	2	2.3	37.8	13422
RHPY	145	148	553.2761	553.2938	1	32	37.8	12190
RHPYFYAPE	145	153	1160.5403	1160.5441	2	3.3	38.8	9373
RHPYFYA	145	151	906.4501	906.4571	2	7.7	37.8	12349
RHPYFYAPELLFFA	145	158	1751.8823	1751.9163	2	19.4	37.8	11403
RHPYFYAPELLFFAKR	145	160	2054.0891	2054.0984	4	4.5	35.7	7500
RHPYFYAPELL	145	155	1368.6979	1368.7352	2	27.3	37.8	2340
RHPYFYAPELLFFAK	145	159	1897.9879	1897.999	3	5.8	40.3	2304
HPYFYAPELLFFAK	146	159	1741.8867	1741.9091	2	12.9	41	3248116
HPYFYA	146	151	778.3439	778.3615	1	22.6	41.6	3815
HPYFYAPELLFFAK	146	159	1741.8867	1741.9093	2	13	41.6	72464
PYFYAPELLFFAK	147	159	1604.8279	1604.8629	2	21.8	37.8	9706
YAPELLFFAK	150	159	1197.6433	1197.6561	2	10.7	37.8	10062
APELLFFAK	151	159	1034.5801	1034.593	2	12.5	37.8	25590
PELLFFAK	152	159	963.5429	963.5455	2	2.7	37.8	183178
PELLFFAK	152	159	945.5323	945.544	2	12.4	37.9	13207
PELLFFAK	152	159	963.5429	963.5506	2	8	41.6	5268
PELLFFAKR	152	160	1119.644	1119.6427	2	-1.2	37.8	2364
ELLFFAK	153	159	866.4902	866.5133	1	26.7	37.8	17073
ELLFFAK	153	159	866.4902	866.4983	1	9.3	42.8	4989
LLFFAK	154	159	737.4476	737.4686	1	28.5	37.8	62808

LFFAK	155	159		624.3635	624.3822	1	30	37.8	158281
FFAK	156	159		511.2794	511.2903	1	21.3	37.9	123751
YKAAFTECCQAADK	161	174	Carbamidomethyl C(2)	1661.7178	1661.7474	3	17.8	25	15116
YK	161	162		309.1689	309.1663	1	-8.4	33.9	3533
AAFTECCQAADK	163	174	Carbamidomethyl C(2)	1370.5596	1370.5913	2	23.1	24.4	1021257
AAFTECCQAADK	163	174	Carbamidomethyl C(2)	1370.5596	1370.578	2	13.4	25	28600
AAFTECCQAADKAAACLLPKLDEL	163	186	Carbamidomethyl C(3)	2750.3191	2750.3003	4	-6.8	26	9720
AAFTECCQAA	163	172	Carbamidomethyl C(2)	1109.4271	1109.4365	1	8.5	24.4	2012
AAFTECCQAADKAAACLLPK	163	181	Carbamidomethyl C(3)	2123.9802	2124.0281	2	22.6	39.3	2259
AAFTECCQAAD	163	173	Carbamidomethyl C(2)	1224.454	1224.4648	1	8.8	24.4	2165
FTECCQAADK	165	174	Carbamidomethyl C(2)	1228.4854	1228.5103	2	20.3	24.4	6465
TECCQAADK	166	174	Carbamidomethyl C(2)	1081.4169	1081.4552	1	35.4	24.4	2182
AACLL	175	179	Carbamidomethyl C(1)	528.273	528.2766	1	6.8	26.2	57594
AA	175	176		142.0742	142.0709	1	-23.2	26.2	18578
AAC	175	177	Carbamidomethyl C(1)	302.1049	302.1016	1	-10.9	26.2	16266
AACLLP	175	180	Carbamidomethyl C(1)	625.3258	625.3305	1	7.5	26.2	13289
AACLL	175	179	Carbamidomethyl C(1)	500.2781	500.2815	1	6.8	26.2	13016
AACLLPK	175	181	Carbamidomethyl C(1)	771.4313	771.4522	1	27.1	27.4	2790
AACLLPK	175	181	Carbamidomethyl C(1)	771.4313	771.4344	1	4	28.1	2525
AACLLPK	175	181	Carbamidomethyl C(1)	753.4208	753.428	2	9.6	26.2	2116
AACLLPK	175	181	Carbamidomethyl C(1)	771.4313	771.4363	1	6.5	26.2	757409
AACLLPKLDEL	175	190	Carbamidomethyl C(1)	1826.9561	1826.9421	2	-7.7	43.4	20084
AA	175	176		114.0793	114.0764	1	-25.4	26.2	11781
AACLLPKLDEL	175	190	Carbamidomethyl C(1)	1826.9561	1826.952	2	-2.2	42.7	6901
AACLLPKLDEL	175	190	Carbamidomethyl C(1)	1826.9561	1826.9393	2	-9.2	42.3	4577
AACLLPK	175	181	Carbamidomethyl C(1)	1542.8627	1542.8611	1	-1	26.2	2233
ACLLPK	176	181	Carbamidomethyl C(1)	700.3942	700.4032	1	12.8	26.2	283572
CLLPK	177	181	Carbamidomethyl C(1)	629.3571	629.345	1	-19.2	26.2	532162
CLLPK	177	181	Carbamidomethyl C(1)	611.3466	611.3466	2	0	26.2	4069
LLPK	178	181		469.3264	469.3332	1	14.5	26.2	51653
LPK	179	181		356.2423	356.2372	1	-14.3	26.2	20536

PK	180	181		243.1583	243.1566	1	-7	26.2	29247
PK	180	181		225.1477	225.1494	1	7.6	26.2	4355
LDELRDEGK	182	190		1073.5353	1073.5317	1	-3.4	24	1121117
LDELRDEGK	182	190		1073.5353	1073.5648	2	27.5	28	148190
LDELRDEGK	182	190		1073.5353	1073.548	2	11.8	27.8	79871
LDELR	182	186		598.3439	598.3438	1	-0.2	27.8	43150
LDELRDE	182	188		870.4083	870.411	1	3.1	24	14831
LD	182	183		228.111	228.1066	1	-19.3	24	8769
LDELRD	182	187		741.3657	741.366	1	0.4	24	7454
LDELRDEGK	182	190		1055.5247	1055.5259	3	1.1	24	6377
LDELRDEGK	182	190		1073.5353	1073.5425	2	6.7	25	8219
LD	182	183		200.1161	200.1128	1	-16.5	24	5852
DELRDEGK	183	190		942.4407	942.4418	2	1.2	24	44694
DELR	183	186		531.2653	531.2669	1	3	24.3	30419
ELRDEGK	184	190		845.4243	845.4192	2	-6	24	109632
ELRDEGK	184	190		827.4137	827.4079	2	-7	24	20614
ELR	184	186		416.2383	416.2305	1	-18.7	24.4	4083
DEGKASSAK	187	195		891.4297	891.4377	2	9	24.9	27574
DEGKASSAKQR	187	197		1175.5895	1175.588	2	-1.3	24.4	22320
DEGKASSAK	187	195		891.4297	891.438	1	9.3	25.6	9738
DEGKASSAKQR	187	197		1175.5895	1175.5787	2	-9.2	29.5	3139
DEGKASSAK	187	195		873.4192	873.4323	2	15	24.9	2877
EGK	188	190		332.1696	332.167	1	-7.8	24	19486
EGK	188	190		314.159	314.1559	1	-9.9	24	7585
GK	189	190		203.127	203.1244	1	-12.8	24	19190
ASSAK	191	195		462.2438	462.2443	1	1.1	27.8	3633
QRLKCASLQK	196	205	Carbamidomethyl C(1)	1230.6866	1230.691	2	3.6	40.7	1356
LK	198	199		259.1896	259.1952	1	21.6	30.5	108235
LKCASLQK	198	205	Carbamidomethyl C(1)	946.527	946.5284	2	1.5	23.7	3398
LK	198	199		259.1896	259.1946	1	19.3	36.5	11373
CASLQK	200	205	Carbamidomethyl C(1)	705.348	705.3557	1	10.9	23.7	6501

CASLQK	200	205	Carbamidomethyl C(1)	705.348	705.3558	2	11.1	24.7	2335
SLQK	202	205		474.2802	474.2782	1	-4.2	23.7	5490
FGERAFKAWAVAR	206	218		1507.8048	1507.7871	2	-11.7	43.6	23921
FGERAFKAWAVAR	206	218		1507.8048	1507.8463	2	27.5	39.3	11468
FGERAFKAWAVAR	206	218		1507.8048	1507.8346	2	19.8	42.5	5148
FGERAFK	206	212		853.4446	853.4428	1	-2.1	37.3	6136
FGERAFK	206	212		853.4446	853.4692	1	28.8	28.7	2300
AFK	210	212		364.2111	364.2099	1	-3.3	28.8	26542
AFK	210	212		364.2111	364.2202	1	25	39.1	4589
AFK	210	212		364.2111	364.2139	1	7.7	42.8	4415
AFK	210	212		364.2111	364.2105	1	-1.6	29.6	3325
AWAVAR	213	218		672.3707	672.3529	2	-26.5	37.8	1927
AWAVARLSQRFPK	213	225		1528.8627	1528.8359	3	-17.5	23.8	1516
LSQRFPK	219	225		874.5025	874.4858	1	-19.1	38.3	6194
LSQRFPKAEFAEVSK	219	233		1735.9257	1735.9729	2	27.2	30.7	3641
FPKAEFAEVSK	223	233		1251.6499	1251.6296	2	-16.2	24.7	7481
FPK	223	225		390.2267	390.2297	1	7.7	27.9	2535
FPKAEFAEVSK	223	233		1251.6499	1251.6406	3	-7.4	28.2	1562
FPKAEFAEVSK	223	233		1251.6499	1251.6501	2	0.2	27.5	1907
AEFAEVSK	226	233	Carbamidomethyl C(3)	879.4338	879.4413	1	8.5	24.8	1851485
AE	226	227		200.0797	200.0771	1	-13	24.8	117800
AEFAEVSK	226	233		861.4232	861.4185	2	-5.5	24.8	51777
AE	226	227		172.0848	172.0822	1	-15.1	24.8	44983
AEFAEV	226	231		646.2962	646.3076	1	17.6	24.8	35680
AEFAE	226	230		547.2278	547.2319	1	7.5	24.8	19843
AEFAEVS	226	232		733.3282	733.3338	1	7.6	24.8	17698
AEFA	226	229		418.1852	418.1851	1	-0.2	24.8	16814
AEFA	226	229		390.1903	390.1911	1	2.1	24.8	3742
AEFAEVSKLVTDLTQVHTECCHGDLLECADDR	226	257		3717.7073	3717.7302	2	6.2	25.8	13424
AEFAEVSK	226	233		879.4338	879.4381	1	4.9	42.6	2299
AEFAEVSK	226	233		879.4338	879.42	1	-15.7	36.3	1905

EFAEVSK	227	233		808.3967	808.403	1	7.8	24.8	135619
FAEVSK	228	233		679.3541	679.3637	1	14.1	24.8	1296284
FAEVSK	228	233		661.3435	661.3467	1	4.8	24.8	10828
AEVSK	229	233		532.2856	532.2839	1	-3.2	24.8	219033
VSK	231	233		332.206	332.2037	1	-6.9	24.8	28537
SK	232	233		233.1376	233.1366	1	-4.3	24.8	13863
LVTDLTK	234	240		788.4644	788.4721	1	9.8	25.8	1854591
LVTDLTK	234	240		770.4538	770.4346	2	-24.9	25.8	92077
LVTDLTK	234	240		1576.9287	1576.9105	1	-11.5	25.8	86609
LV	234	235		212.1525	212.1498	1	-12.7	25.8	81364
LV	234	235		184.1576	184.1528	1	-26.1	25.8	80796
LVTDLT	234	239		642.3588	642.368	1	14.3	25.8	13256
LVTDL	234	238		541.3112	541.3152	1	7.4	25.8	11870
LVTDLTKVHTECCHGDLLECADDR	234	257	Carbamidomethyl C(3)	2856.2842	2856.3196	5	12.4	26.5	9726
LVTD	234	237		428.2271	428.2329	1	13.5	25.9	8173
LVTDLTKVHTE	234	244		1208.6765	1208.6445	2	-26.5	26.1	8667
LVT	234	236		313.2002	313.1995	1	-2.2	25.8	8021
VTDLTK	235	240		675.3803	675.3885	1	12.1	25.8	744300
VTDLTK	235	240		657.3698	657.3745	1	7.1	25.8	28221
DLTK	237	240		475.2642	475.2647	1	1.1	25.8	57478
LTK	238	240		360.2373	360.2353	1	-5.6	25.8	17152
VHTECCHGDLLECADDRADLAK	241	262	Carbamidomethyl C(3)	2584.1106	2584.1499	2	15.2	26.7	1574845
VHTECCHGDL	241	250	Carbamidomethyl C(2)	1208.4703	1208.4958	2	21.1	26.7	949192
VHTECCHGDL	241	251	Carbamidomethyl C(2)	1321.5544	1321.5906	2	27.4	26.7	544378
VHTECCHGDL	241	251	Carbamidomethyl C(2)	1321.5544	1321.5477	2	-5.1	25.4	312537
VHTECCHGDLLE	241	252	Carbamidomethyl C(2)	1450.597	1450.6307	2	23.2	26.7	293351
VHTECCHGDLLECADDRADLAK	241	262	Carbamidomethyl C(3)	2584.1106	2584.1587	4	18.6	27.3	287178
VHTECCHGDLLE	241	252	Carbamidomethyl C(2)	1450.597	1450.6235	2	18.3	25.4	260195
VHTECCHGDLLECADDRADLAK	241	262	Carbamidomethyl C(3)	2584.1106	2584.1006	5	-3.9	26.7	250446
VHTECCHGDL	241	250	Carbamidomethyl C(2)	1208.4703	1208.4901	2	16.4	25.4	226291
VHTECCHGDLLECADDRADLAK	241	262	Carbamidomethyl C(3)	5168.2212	5168.1064	3	-22.2	26.7	215594

VHTECCHGDLLECADDR	241	257	Carbamidomethyl C(3)	4171.6606	4171.7173	3	13.6	25.4	171088
VHTECCHGDLLECADDRADLAK	241	262	Carbamidomethyl C(3)	2584.1106	2584.1802	3	26.9	26.1	136397
VHTECCHGDLLECADDRADLAK	241	262	Carbamidomethyl C(3)	2584.1106	2584.166	3	21.4	27.6	135111
VHTECCHGDDL	241	251	Carbamidomethyl C(2)	1293.5594	1293.587	2	21.3	26.7	123392
VHTECCHGD	241	249	Carbamidomethyl C(2)	1095.3862	1095.396	2	8.9	26.8	92928
VHTECCHGDLLECADDRADLAK	241	262	Carbamidomethyl C(3)	2566.0999	2566.1624	5	24.4	26.7	82977
VHTECCHGDLLEC	241	253	Carbamidomethyl C(3)	1610.6277	1610.6609	2	20.6	25.4	75630
VHTECCHGDLLEC	241	253	Carbamidomethyl C(3)	1610.6277	1610.6649	2	23.1	26.7	51386
VHTECCHGDL	241	250	Carbamidomethyl C(2)	1180.4755	1180.5007	2	21.3	26.7	43083
VHTECCHGDLLECADDR	241	257	Carbamidomethyl C(3)	2067.8198	2067.8354	4	7.5	25.4	20497
VHTECCHGDLLECA	241	254	Carbamidomethyl C(3)	1681.6648	1681.6899	3	14.9	25.4	20173
VHTECCHGDL	241	250	Carbamidomethyl C(2)	1208.4703	1208.4913	2	17.4	27.3	17815
VHTECCHGDLLECADDRADLAK	241	262	Carbamidomethyl C(3)	2584.1106	2584.1702	4	23.1	25.7	13075
VHTECCHGDL	241	250	Carbamidomethyl C(2)	1208.4703	1208.498	2	22.9	26.1	11789
VHTECCHGDLLECADDR	241	257	Carbamidomethyl C(3)	2085.8303	2085.9114	3	38.9	26	11368
VHTECCHGDDL	241	251	Carbamidomethyl C(2)	1303.5438	1303.575	2	23.9	25.5	10609
VHTECCHGDL	241	250	Carbamidomethyl C(2)	1208.4703	1208.4946	2	20.1	27.6	8291
VHTECCHGDLLE	241	252	Carbamidomethyl C(2)	1450.597	1450.6418	2	30.9	26.1	7317
VHTECCHGDLLECADDRAD	241	259	Carbamidomethyl C(3)	2253.8838	2253.9563	3	32.2	26.7	3345
VH	241	242		236.1273	236.1247	1	-11	26.8	15843
VHTECCHGDLLECADDR	241	257	Carbamidomethyl C(3)	2085.8303	2085.8845	3	26	24.7	2480
VHTECCHGDLLECADDRADLAKYICENQDSISSK	241	274	Carbamidomethyl C(4)	4008.7349	4008.7881	6	13.3	33.3	1659
LECADDRADLAK	251	262	Carbamidomethyl C(1)	1375.6401	1375.658	3	13	26.7	14363
LECADDRADLAK	251	262	Carbamidomethyl C(1)	1357.6296	1357.649	3	14.3	26.7	2409
ECADDRADLAK	252	262	Carbamidomethyl C(1)	1262.5562	1262.5798	2	18.7	26.7	704615
ECADDRADLAK	252	262	Carbamidomethyl C(1)	1244.5455	1244.5743	2	23.1	26.7	332480
ECADDRADLAK	252	262	Carbamidomethyl C(1)	1262.5562	1262.5721	2	12.6	27.7	34072
CADDRADLAK	253	262	Carbamidomethyl C(1)	1133.5135	1133.5549	2	36.5	26.7	756179
CADDRADLAK	253	262	Carbamidomethyl C(1)	1133.5135	1133.5547	2	36.3	27.2	229096
CADDRADLAK	253	262	Carbamidomethyl C(1)	1133.5135	1133.5339	2	18	26.1	16765
ADDRADLAK	254	262		973.4828	973.4943	2	11.8	26.7	196033

DDRADLAK	255	262		902.4457	902.448	2	2.5	26.7	89640
DRADLAK	256	262		787.4188	787.4225	2	4.7	26.7	35156
DRADLAK	256	262		787.4188	787.4234	2	5.8	27.7	6987
ADLAKYICENQDSISSK	258	274	Carbamidomethyl C(1)	1940.9149	1940.9023	4	-6.5	26.6	3239
ADLAKYICENQDSIS	258	272	Carbamidomethyl C(1)	1679.7825	1679.7714	2	-6.6	27.5	2743
ADLAKYICENQ	258	268	Carbamidomethyl C(1)	1277.6074	1277.5886	2	-14.7	26.6	1142
YICENQDSISSK	263	274	Carbamidomethyl C(1)	1442.6348	1442.6611	2	18.2	24.6	2365276
YICENQDSISSKLG	263	276	Carbamidomethyl C(1)	1683.8138	1683.7706	3	-25.7	23.7	197368
YICENQDSISSKL	263	275	Carbamidomethyl C(1)	1537.7083	1537.6831	3	-16.4	23.7	9362
YICENQDSISSK	263	274	Carbamidomethyl C(1)	1424.6243	1424.641	2	11.7	24.6	4625
YICENQDSISSK	263	274	Carbamidomethyl C(1)	1442.6348	1442.6376	2	1.9	25.4	23347
YICENQDSISSKLKECCEKPLLEK	263	286	Carbamidomethyl C(3)	2970.4138	2970.3921	5	-7.3	30.1	4460
YICENQDSI	263	271	Carbamidomethyl C(1)	1122.4652	1122.4716	1	5.7	24.6	2450
CENQDSISSK	265	274	Carbamidomethyl C(1)	1166.4874	1166.4951	1	6.6	24.6	2458
LKECCEKPLLEK	275	286	Carbamidomethyl C(2)	1545.7896	1545.8127	2	14.9	24.3	1172716
LKECCEKPL	275	283	Carbamidomethyl C(2)	1157.5574	1157.5737	2	14.1	24.3	61986
LKECCEKPLLEK	275	286	Carbamidomethyl C(2)	1545.7896	1545.8188	3	18.9	24.7	32475
LKECCEKPLLEK	275	286	Carbamidomethyl C(2)	1527.7789	1527.769	4	-6.5	24.3	22989
LKECCEKPLL	275	284	Carbamidomethyl C(2)	1270.6415	1270.6545	2	10.2	24.3	19480
LKECCEK	275	281	Carbamidomethyl C(2)	947.4205	947.4312	2	11.3	24.3	10235
LKECCEKPLLE	275	285	Carbamidomethyl C(2)	1399.684	1399.7075	2	16.8	24.3	7678
LKECCEKPLLEK	275	286	Carbamidomethyl C(2)	1545.7896	1545.8121	3	14.6	25.1	7334
LKECCEKPLL	275	284	Carbamidomethyl C(2)	1242.6465	1242.6813	3	28	24.3	6347
LK	275	276		241.179	241.1778	1	-5	24.3	5622
LKECCEK	275	281	Carbamidomethyl C(2)	930.394	930.4169	2	24.6	24.3	2402
LKECCEKPLLEKSHCIAEVENDEMPADLPSL	275	305	Carbamidomethyl C(3)	3635.698	3635.6775	5	-5.6	33.2	1514
KECCEKPLLEK	276	286	Carbamidomethyl C(2)	1432.7054	1432.7175	3	8.4	24.3	199499
KECCEKPLLEK	276	286	Carbamidomethyl C(2)	1415.679	1415.6886	3	6.8	24.3	57424
KECCEKPLLEK	276	286	Carbamidomethyl C(2)	1432.7054	1432.7238	3	12.8	25	2069
ECCEKPLLEK	277	286	Carbamidomethyl C(2)	1304.6105	1304.6234	2	9.9	24.4	342500
ECCEKPLLEK	277	286	Carbamidomethyl C(2)	1286.6	1286.6051	3	4	24.4	51387

ECCEKPLLEK	277	286	Carbamidomethyl C(2)	1304.6105	1304.6028	2	-5.9	31.3	11615
ECCEKPLLEKSHCIAEVENDEMPADLPSLAADFVESKDVC	277	317	Carbamidomethyl C(4)	4762.1582	4762.2134	7	11.6	29.2	24276
K	278	286	Carbamidomethyl C(2)	1175.5679	1175.5648	2	-2.6	31.3	8491
CCEKPLLEK	281	286		726.4639	726.4596	2	-5.9	24.4	10234
KPLLEK	281	313	Carbamidomethyl C(1)	3681.7905	3681.7786	2	-3.2	34	6518
KPLLEKSHCIAEVENDEMPADLPSLAADFVESK	283	286		501.3162	501.3158	1	-0.8	24.7	2606
LLEK	287	313	Carbamidomethyl C(1)	2973.3372	2973.3601	4	7.7	39.8	271796
SHCIAEVENDEMPADLPSLAADFVESK	287	313	Carbamidomethyl C(1)	2973.3372	2973.4014	3	21.6	36.2	49352
SHCIAEVENDEMPADLPSLAADFVESK	287	313	Carbamidomethyl C(1)	2955.3267	2955.3635	4	12.5	39.8	16560
SHCIAEVENDEMPADLPSLAADFVESK	287	313	Carbamidomethyl C(1)	2973.3372	2973.3948	3	19.4	38.7	3869
SHCIAEVENDEMPADLPSLAADFVESK	287	313	Carbamidomethyl C(1)	2973.3372	2973.384	2	15.7	24.4	15922
SHCIAEVENDEMPADLPSLA	287	306	Carbamidomethyl C(1)	2178.9561	2178.99	3	15.6	39.8	12723
SHCIAEVENDEMPADLPSLAADFV	287	310	Carbamidomethyl C(1)	2611.157	2611.1963	3	15.1	39.8	9836
SHCIAEVENDEM	287	298	Carbamidomethyl C(1)	1414.5493	1414.5767	2	19.4	39.8	8724
SHCIAEVENDEMPADLPSLAADFVESK	287	313	Carbamidomethyl C(1)	2973.3372	2973.3489	4	3.9	25.1	3054
SHCIAEVENDEMPADLPSL	287	305	Carbamidomethyl C(1)	2107.9189	2107.9507	3	15.1	39.8	2389
MPADLPSLAADFVESK	298	313		1689.8284	1689.8434	2	8.9	39.8	1874
PADLPSLAADFVESK	299	313		1558.7878	1558.8091	2	13.7	35.3	15197
PADLPSLAADFVESK	299	313		1558.7878	1558.8077	2	12.8	39.8	9690
LPSLAADFVESKDVC	302	317	Carbamidomethyl C(1)	1777.8921	1777.8527	3	-22.2	29.2	3584
PSLAADFVESK	303	313		1162.5869	1162.5984	2	9.9	39.8	3193
AADFVESK	306	313		865.4182	865.4111	2	-8.2	33.2	5160
AADFVESK	306	313		865.4182	865.4359	1	20.5	39.8	3870
ADFVESK	307	313		794.381	794.3727	1	-10.4	33.2	6356
DFVESK	308	313		723.3439	723.364	1	27.8	39.8	3857
FVESK	309	313		608.317	608.3137	1	-5.4	33.2	2744
DVCKNYAEAKDVFLGMFLYFYAR	314	336	Carbamidomethyl C(1)	2801.3193	2801.3728	4	19.1	40.5	34237
DVCKNYAEAKDVFLGMFLYFYAR	314	336	Carbamidomethyl C(1)	2801.3193	2801.3542	3	12.5	42	23643
DVCKNYAEAK	314	323	Carbamidomethyl C(1)	1196.5496	1196.5488	2	-0.7	23.6	5063
NYAEAKDVFLGMFLYFYAR	318	336		2299.0984	2299.1399	2	18.1	42.3	240713

NYAEAK	318	323	694.3286	694.3227	1	-8.5	33.4	315399
NYAEAKDVFLGMFLYFYAR	318	336	2299.0984	2299.0417	3	-24.7	38.8	9952
NYAEAKDVFLGMFLYFYARR	318	337	2455.1995	2455.2312	3	12.9	40.3	8570
NYAEAKDVFLGMFLYFY	318	334	2053.9495	2053.9902	2	19.8	42.3	4445
NYAEAKDVFLGMFLYFYA	318	335	2124.9866	2125.0308	2	20.8	42.3	4327
NYAEAKDVFLGMF	318	330	1485.6962	1485.7166	2	13.7	42.3	3879
NYAEAKDVFLGMFLYF	318	333	1890.8862	1890.9175	2	16.6	42.3	3809
NYAEAK	318	323	694.3286	694.3181	1	-15.1	34.9	1339
NYAEAKDVFLGMFLYFYAR	318	336	2281.0876	2281.1106	3	10.1	42.3	1081
DVFLGMFLYFYAR	324	336	1622.7803	1622.802	2	13.4	44.1	157562
DVFLGMFLYFYAR	324	336	1622.7803	1622.7966	2	10	49.1	71893
DVFLGMFLYFYAR	324	336	1622.7803	1622.8015	2	13.1	44.4	65795
DVFLGMFLYFYAR	324	336	1622.7803	1622.7988	2	11.4	45.3	38731
DVFLGMFLYFYAR	324	336	1622.7803	1622.7998	2	12	47.8	21379
DVFLGMFLYFYAR	324	336	1622.7803	1622.7469	1	-20.6	46.7	6785
DVFLGMFLYFYAR	324	336	1622.7803	1622.7974	2	10.5	47.2	6343
DVFLGMFLYFYAR	324	336	1622.7803	1622.7915	2	6.9	48	5293
DVFLGMFLYFYAR	324	336	1622.7803	1622.7465	1	-20.8	49.6	2253
DVFLGMFLYFYAR	324	336	1622.7803	1622.8081	2	17.1	43.2	1836
DVFLGMFLYFYARRHPDYSVVLLLR	324	348	3071.6055	3071.6348	3	9.5	41.2	18743
DVFLGMFLYFYARR	324	337	1778.8813	1778.9121	2	17.3	42.2	4782
DVFLGMFLYFYARR	324	337	1778.8813	1778.9088	2	15.5	41.9	3974
FLGMFLYFYAR	326	336	1408.6849	1408.701	2	11.4	49.1	6421
FLGMFLYFYAR	326	336	1408.6849	1408.7002	2	10.9	44.2	5859
FLGMFLYFYAR	326	336	1408.6849	1408.7024	2	12.4	47.2	4253
FLGMFLYFYAR	326	336	1408.6849	1408.7065	2	15.3	44.5	2294
FLYFYAR	330	336	960.4705	960.4553	2	-15.8	38.8	2230
YFYAR	332	336	700.3181	700.3218	1	5.3	49.1	6655
RHPDYSVVLLLR	337	348	1466.8358	1466.8656	2	20.3	30.7	535006
RHPDYSVVLLLR	337	348	1466.8358	1466.8446	2	6	30.3	251134
RHPDYSVVLLLR	337	348	1466.8358	1466.8602	2	16.6	32.7	66323

RHPDYSV	337	343	854.4035	854.3977	1	-6.8	30.2	41699
RHPDYSVVL	337	348	1466.8358	1466.8547	3	12.9	33.1	37162
RHPDYSVVL	337	348	1466.8358	1466.762	2	-50.3	25.1	30862
RHPDYSVVL	337	345	1066.5559	1066.5684	2	11.7	30.7	25788
RHPDYSV	337	344	953.4719	953.4733	2	1.5	30.7	24721
RHPDYSV	337	343	854.4035	854.3948	1	-10.2	30.7	21260
RHPDYSV	337	344	953.4719	953.4725	2	0.6	30.2	20500
RHPDYS	337	342	755.3351	755.3359	1	1.1	30.7	19566
RHPDYSV	337	343	836.3929	836.3971	2	5	30.7	15848
RHPDYS	337	342	737.3245	737.3244	1	-0.1	30.7	14800
RHPDYSVVL	337	348	1466.8358	1466.874	3	26	34.8	12228
RHPDYSVVL	337	345	1066.5559	1066.5677	2	11.1	30.2	11778
RHPDYSVVL	337	346	1179.64	1179.655	2	12.7	30.2	10605
RHPDYSVVL	337	348	1448.8252	1448.8361	3	7.5	30.7	8366
RHPDYSV	337	343	836.3929	836.3866	2	-7.5	30.2	6958
RHPDYSVVL	337	346	1179.64	1179.6501	2	8.6	30.7	6669
RHPDYSV	337	343	826.4086	826.4087	2	0.1	30.7	5651
RHPDYSVVL	337	348	1448.8252	1448.8406	3	10.6	30.2	5152
RHPDYSV	337	343	854.4035	854.3924	1	-13	32.7	4611
RHPDY	337	341	668.303	668.3067	1	5.5	30.7	4512
RHPDYS	337	342	737.3245	737.3206	2	-5.3	30.2	4344
RHPDYSVVL	337	348	1466.8358	1466.8506	2	10.1	40.5	3541
RHPDYSV	337	344	953.4719	953.4765	2	4.8	32.7	3172
RHPDYS	337	342	755.3351	755.3328	1	-3	32.7	2825
RHPDYSV	337	343	826.4086	826.4121	2	4.2	30.2	2513
RHPDYSV	337	344	925.477	925.4826	2	6.1	30.2	1482
RHPDYSVVL	337	348	1466.8358	1466.8402	3	3	33.6	13733
RHPDYSVVL	337	348	1466.8358	1466.8435	2	5.2	34	11113
RHPDYSVVLRLAK	337	351	1779.0519	1779.0598	4	4.4	34	4983
RHPDYSVVL	337	348	1466.8358	1466.8274	3	-5.7	36	4863
RHPDYSVVL	337	345	1066.5559	1066.564	2	7.6	32.7	2673

RHPDYSVV	337	344	953.4719	953.485	2	13.7	33.1	2150
RHPDYSVVLLLR	337	348	1466.8358	1466.8773	2	28.3	37.5	2148
RHPDYSV	337	343	854.4035	854.3922	1	-13.2	33.1	1938
RHPDYSV	337	343	836.3929	836.3956	2	3.2	32.7	1745
RHPDYS	337	342	737.3245	737.3211	1	-4.6	32.7	1620
RHPDYSVVLL	337	346	1179.64	1179.6561	2	13.6	32.7	1397
HPDYSVVLLLR	338	348	1310.7346	1310.7416	2	5.3	34.3	578423
HPDYSVVLLLR	338	348	1310.7346	1310.741	2	4.9	34.7	355477
HPDYSV	338	343	698.3024	698.3003	1	-3	34.4	135804
HPDYSVVLLLR	338	348	1310.7346	1310.7494	2	11.3	36.4	116460
HPDYSVV	338	344	797.3708	797.365	1	-7.3	34.3	60765
HPDYS	338	342	599.2339	599.2379	1	6.7	34.3	59745
HPDYS	338	342	581.2234	581.2188	1	-7.9	34.4	36122
HPDYSVVL	338	345	910.4548	910.4502	1	-5.1	34.7	17327
HPDYSV	338	343	680.2918	680.29	1	-2.6	34.4	12184
HPDYSVVLLLR	338	348	1293.7081	1293.6737	2	-26.6	36.4	11561
HPDYSVVLLLR	338	348	1310.7346	1310.7413	2	5.1	34.9	218008
HPDYSVVLLLR	338	348	1310.7346	1310.7429	2	6.3	35.4	28841
HPDYSVVLLLRRLAKTYETTLEK	338	359	2588.4214	2588.4548	3	12.9	40.6	7358
HPDY	338	341	512.202	512.1962	1	-11.3	34.4	6991
HPDYSVVLLLR	338	348	1310.7346	1310.7413	2	5.1	40.6	5253
HPDYSVVLLLR	338	348	1310.7346	1310.744	2	7.2	37.6	4486
HPDYSVVLLLR	338	348	1310.7346	1310.7507	2	12.3	36	3311
HPDYSVVLLLR	338	348	1310.7346	1310.748	2	10.2	36.9	1515
SVVLLLR	342	348	798.5327	798.5288	1	-4.9	30.2	5188
VVLLLR	343	348	711.5007	711.5007	1	0	30.2	8424
VVLLLR	343	348	711.5007	711.4975	1	-4.5	30.6	4432
VLLLR	344	348	612.4323	612.4265	1	-9.5	34.3	76263
VLLLR	344	348	612.4323	612.4258	1	-10.6	30.2	47800
VLLLR	344	348	612.4323	612.4275	1	-7.8	30.7	35986
VLLLR	344	348	612.4323	612.4252	1	-11.6	32.7	5774

VLLLR	344	348		612.4323	612.4309	1	-2.3	33.1	2949
LLLR	345	348		513.3638	513.3563	1	-14.6	34.3	93200
LLLR	345	348		513.3638	513.3588	1	-9.7	30.7	33437
LLLR	345	348		513.3638	513.3583	1	-10.7	31.1	24165
LLLR	345	348		513.3638	513.3557	1	-15.8	32.7	5884
LLLR	345	348		513.3638	513.359	1	-9.4	33.1	3535
LLR	346	348		400.2798	400.2714	1	-21	34.4	48882
LLR	346	348		400.2798	400.2724	1	-18.5	30.7	20533
LLR	346	348		400.2798	400.272	1	-19.5	30.2	19198
LLR	346	348		400.2798	400.2733	1	-16.2	32.7	3085
LR	347	348		287.1957	287.1907	1	-17.4	30.2	3805
LAKTY	349	353		576.3271	576.3257	1	-2.4	38	4444
LAK	349	351		330.2267	330.2297	1	9.1	26.8	5677
LAKTYETTL	349	357		1020.5491	1020.5772	2	27.5	42.6	2823
TYETTLEK	352	359		983.4811	983.4539	1	-27.7	24.6	1309492
TYETTLEK	352	359		983.4811	983.4971	1	16.3	29	655696
TYETTLEK	352	359		983.4811	983.4933	1	12.4	25	100258
TYETTLEK	352	359		965.4706	965.4797	2	9.4	24.5	72015
TY	352	353		264.111	264.1096	1	-5.3	24.5	65241
TY	352	353		236.1161	236.1142	1	-8	24.5	57836
TYE	352	354		393.1536	393.1524	1	-3.1	24.5	22175
TYETTLEK	352	359		983.4811	983.4767	1	-4.5	26	4567
TYETTLEK	352	359		983.4811	983.4949	1	14	26.4	1655
TYETTLEK	352	359		965.4706	965.4929	2	23.1	25	1644
YETTLEK	353	359		882.4335	882.4334	1	-0.1	24.6	25029
ETITLEK	354	359		719.3701	719.3753	1	7.2	24.5	458286
TTLEK	355	359		590.3275	590.3294	1	3.2	24.6	48115
CCAAADPHECYAK	360	372	Carbamidomethyl C(3)	1551.5906	1551.6265	2	23.1	23.6	614167
CCAAAD	360	365	Carbamidomethyl C(2)	648.1996	648.1982	1	-2.2	23.6	97887
CCAAADPHECYAK	360	372	Carbamidomethyl C(3)	1533.58	1533.5975	3	11.4	23.6	11840
CC	360	361	Carbamidomethyl C(2)	320.0614	320.0591	1	-7.2	23.6	4026

CCAAAD	360	365	Carbamidomethyl C(2)	630.1891	630.1866	1	-4	23.6	2027
PHECYAK	366	372	Carbamidomethyl C(1)	903.3909	903.4111	2	22.4	23.6	109306
VFDEFKPLVEEPQNLIK	373	389		2044.088	2044.1234	2	17.3	36.5	2696628
VFDEFKPLVEEPQNLI	373	388		1897.9825	1897.9974	2	7.9	37.8	985151
VFDEFKPLVEEPQNLIK	373	389		4088.176	4088.2344	3	14.3	36.5	373828
VFDEFKPLVEE	373	383		1332.6602	1332.6766	2	12.3	36.5	243663
VFDEFKPLVEEPQNLIK	373	389		2044.088	2044.0955	3	3.7	36	96847
VFDEFKPLVE	373	382		1203.6176	1203.6279	2	8.6	36.5	80677
VFDEFKPLVEEPQNLIK	373	389		2026.0775	2026.099	3	10.6	36.5	79322
VF	373	374		246.1368	246.1405	1	15	36.5	65894
VFDEF	373	377		637.2748	637.2899	1	23.7	36.5	32352
VFDEFKPLV	373	381		1074.575	1074.5841	2	8.5	36.5	26057
VFDEFKPLVEEPQNL	373	387		1784.8984	1784.9338	2	19.8	36.5	22115
VFDE	373	376		490.2064	490.2155	1	18.6	36.5	19078
VF	373	374		218.1419	218.1452	1	15.1	36.5	15359
VFDEFKPLVEEPQNLI	373	388		1897.9825	1898.0161	2	17.7	36.5	128257
VFDEFKPLVEEPQNLIK	373	389		2044.088	2044.1378	3	24.4	37.5	53211
VFDEFKPLVEEPQNLIK	373	389		2044.088	2044.0959	3	3.9	35.7	31380
VFDEFKPLVEEPQNLIK	373	389		2044.088	2044.0835	2	-2.2	33.4	13571
VFDEFKPLVEEPQNLIK	373	389		2044.088	2044.0986	4	5.2	36.5	7322
VFDEFKPLVEEPQNLIK	373	389		2044.088	2044.0905	3	1.2	40.2	7265
VFDEFKPLVEEPQNLIK	373	389		2044.088	2044.1108	2	11.2	40.6	5228
VFDEFKPLVEEPQNLIK	373	389		2044.088	2044.0902	2	1.1	38.7	3773
VFDEFKPLV	373	381		1046.5801	1046.5857	2	5.4	36.5	1951
VFDEFKPLVE	373	382		1185.6069	1185.636	2	24.5	36.5	1910
FDEFKPLVEEPQNLIK	374	389		1945.0197	1945.028	3	4.3	36.5	25585
DEFKPLVEEPQNLIK	375	389		1797.9512	1797.9917	2	22.5	36.5	238344
DEFKPLVEEPQNLIK	375	389		1797.9512	1797.9883	2	20.6	36	3251
EFKPLVEEPQNLIK	376	389		1682.9243	1682.9659	2	24.7	36.5	12590
FKPLVEEPQNLIK	377	389		1553.8817	1553.9128	2	20	36.5	11571
PLVEEPQNLIK	379	389		1278.7184	1278.7261	2	6	36.5	4949

EEPQNLIK	382	389		969.5131	969.5217	2	8.9	36.5	48074
EEPQNLIK	382	389		951.5025	951.5116	2	9.6	36.5	6099
EPQNLIK	383	389		840.4705	840.4732	2	3.2	36.5	11696
PQNLIK	384	389		711.4279	711.4303	2	3.4	36.5	40803
QNCELFEQLGEYK	390	402	Carbamidomethyl C(1)	1656.7454	1656.7767	2	18.9	34	3730412
QNCELFEQLGEYK	390	402	Carbamidomethyl C(1)	1656.7454	1656.7773	2	19.3	33.6	132603
QNCELFEQLGEYK	390	402	Carbamidomethyl C(1)	1639.7189	1639.7417	2	13.9	33.9	17970
QNCELFEQLGEYKFQNALLVR	390	410	Carbamidomethyl C(1)	2598.29	2598.2842	5	-2.2	28.2	10607
QNCELFEQLGEYK	390	402	Carbamidomethyl C(1)	1656.7454	1656.7668	2	12.9	34.9	102676
QNCELFEQLGEYKFQNALLVR	390	410	Carbamidomethyl C(1)	2598.29	2598.3335	3	16.7	38.9	12206
QNCELFEQLGEYK	390	402	Carbamidomethyl C(1)	1656.7454	1656.7886	2	26.1	36	7572
QNCELFEQLGEYKFQNALLVRYTK	390	413	Carbamidomethyl C(1)	2990.4961	2990.551	4	18.4	27.7	6491
QNCELFEQLGEYK	390	402	Carbamidomethyl C(1)	1656.7454	1656.7792	2	20.4	32.3	5231
QNCELFEQLGEYK	390	402	Carbamidomethyl C(1)	1656.7454	1656.7805	2	21.2	36.3	2928
QNCELFEQLGEYKFQNALLVRYTK	390	413	Carbamidomethyl C(1)	2990.4961	2990.4158	3	-26.9	32.3	2850
QNCELFEQLGEYK	390	402	Carbamidomethyl C(1)	1656.7454	1656.7705	2	15.2	32.7	1981
QNCELFEQLGEYKFQNALLVRYTK	390	413	Carbamidomethyl C(1)	2990.4961	2990.4724	5	-7.9	32.5	1235
LGEYK	398	402		608.317	608.3111	1	-9.7	33.9	18252
FQNALLVR	403	410		959.5552	959.5597	1	4.7	28.4	1073885
FQNALLVRYTK	403	413		1351.7612	1351.7468	2	-10.7	39.4	163903
FQNALLVR	403	410		942.5287	942.536	2	7.7	28.4	83958
FQ	403	404		275.127	275.1268	1	-0.7	28.7	68056
FQ	403	404		275.127	275.1273	1	1.1	28.4	66583
FQNALLVRYTK	403	413		1351.7612	1351.7474	2	-10.2	42.6	25303
FQNA	403	406		460.207	460.2103	1	7.2	28.4	24047
FQNALLV	403	409		785.4435	785.4473	1	4.8	28.4	20816
F	403	403		119.0735	119.0721	1	-11.8	28.4	19113
F	403	403		119.0735	119.0713	1	-18.5	29.3	17476
FQ	403	404		258.1004	258.1001	1	-1.2	28.4	16333
FQNALLVR	403	410		959.5552	959.539	1	-16.9	26.2	9011
FQNALLVRYTK	403	413		1351.7612	1351.7416	2	-14.5	41.4	6307

FQNALLVRYTK	403	413	1351.7612	1351.7444	2	-12.4	41.9	5803
FQNALLV	403	409	768.417	768.4251	1	10.5	28.4	5111
FQNALLVR	403	410	959.5552	959.5572	1	2.1	28.7	1027396
FQNALLVR	403	410	942.5287	942.5358	2	7.5	28.7	79527
FQNALLVRYTK	403	413	1351.7612	1351.7456	2	-11.5	40	56080
F	403	403	119.0735	119.0719	1	-13.4	28.7	17284
FQ	403	404	258.1004	258.1	1	-1.5	28.7	9844
FQNALLVR	403	410	959.5552	959.5569	2	1.8	29.8	7056
FQNALLVRYTKK	403	414	1479.8562	1479.8215	3	-23.4	27.9	6862
F	403	403	119.0735	119.0711	1	-20.2	27.9	4032
FQNA	403	406	443.1805	443.1842	1	8.3	28.4	3361
QNALLVR	404	410	812.4868	812.4877	2	1.1	28.4	30723
QNALLVR	404	410	794.4763	794.478	2	2.1	28.4	7767
QNALLVR	404	410	812.4868	812.4897	2	3.6	28.7	10981
NALLVR	405	410	684.4282	684.4342	1	8.8	28.4	247991
ALLVR	406	410	570.3853	570.382	1	-5.8	28.7	27997
ALLVR	406	410	570.3853	570.3893	1	7	28.4	19804
LLVR	407	410	499.3482	499.3475	1	-1.4	29.2	4746
LVR	408	410	386.2641	386.2633	1	-2.1	28.4	29426
LVR	408	410	386.2641	386.2628	1	-3.4	28.7	21662
VR	409	410	273.1801	273.1796	1	-1.8	28.4	14381
VR	409	410	273.1801	273.1783	1	-6.6	28.7	12496
KVPQVSTPTLVEVSR	414	428	1638.9304	1638.973	2	26	28.4	3185727
KVPQVSTPTLVEVSR	414	428	1638.9304	1638.9709	2	24.7	28.9	105229
KVPQVSTPTL	414	423	1050.6073	1050.6141	1	6.5	28.5	59459
KVPQVSTPTLVEVSR	414	428	1620.9199	1620.9438	3	14.7	28.9	20544
KVPQVSTPTLVEVSR	414	428	1638.9304	1638.9512	2	12.7	27.9	17090
KVPQ	414	417	452.2747	452.274	1	-1.5	28.4	8311
KVPQVSTPTLVEVSR	414	428	1638.9304	1638.9634	2	20.1	29.8	5846
KVPQVSTPTLVEVSR	414	428	1620.9199	1620.9199	3	0	27.9	2269
KVPQVSTPTLVEVSR	414	428	1638.9304	1638.9556	2	15.4	30.4	1765

VPQVSTPTLVEVSR	415	428		1510.8354	1510.8102	2	-16.7	30	854722
VPQVSTPTL	415	423		922.5124	922.506	1	-6.9	30	12081
VPQVSTPTLVEVS	415	427		1308.7289	1308.7412	2	9.4	30	11588
VPQVSTPT	415	422		809.4283	809.4183	1	-12.4	30	6348
VPQVSTPTLVEVSR	415	428		1510.8354	1510.8649	2	19.5	28.4	5355
VPQVSTPTL	415	423		904.5018	904.5108	2	10	30	5353
VPQVSTPTLVEVSR	415	428		1492.825	1492.8523	2	18.3	28.3	2357
VPQVSTPTLVEVS	415	427		1336.7238	1336.752	2	21.1	35.6	2012
VPQVSTPTL	415	423		905.4858	905.4858	1	0	30.1	2745
QVSTPTLVEVSR	417	428		1314.7144	1314.7109	1	-2.7	30	2494
PTLVEVSR	421	428		899.5076	899.5124	1	5.3	28.5	124243
PTLVEVSR	421	428		899.5076	899.4973	1	-11.5	30.9	76262
PTLVEVSR	421	428		899.5076	899.5119	2	4.8	30	7082
VEVSR	424	428		588.3231	588.3161	1	-11.9	30	18708
VEVSR	424	428		588.3231	588.3227	1	-0.7	29.1	12858
VSR	426	428		360.2121	360.209	1	-8.6	30.1	5031
NLGKVGs	429	435		655.3653	655.3708	1	8.4	27.9	7709
VGSKCCKHPEAK	433	444	Carbamidomethyl C(2)	1399.67	1399.6667	2	-2.4	44.5	16806
VGSKCCKHPEAK	433	444	Carbamidomethyl C(2)	1399.67	1399.6525	2	-12.5	32.8	8701
VGSKCCKHPEAK	433	444	Carbamidomethyl C(2)	1399.67	1399.6685	3	-1.1	25.5	1321
HPEAKR	440	445		736.398	736.3817	1	-22.1	24.8	29411
HPEAKR	440	445		736.398	736.3769	2	-28.7	33.9	2010
HPEAKRMPCAEDYLSVVLNQLCVLHEK	440	466	Carbamidomethyl C(2)	3235.594	3235.5164	3	-24	44.7	1209
RMPCAEDYLSVVLNQLCVLHEK	445	466	Carbamidomethyl C(2)	2673.3079	2673.355	3	17.6	42.6	862751
RMPCAEDYLSVVLNQLCVLHEK	445	466	Carbamidomethyl C(2)	2655.2971	2655.3225	4	9.6	42.6	27026
RMPCAEDYL	445	453	Carbamidomethyl C(1)	1135.4791	1135.4921	2	11.4	42.6	25641
RMPCAEDY	445	452	Carbamidomethyl C(1)	1022.395	1022.4059	2	10.7	42.6	19697
RMPCAEDYLSVVLNQLCVLHEK	445	466	Carbamidomethyl C(2)	2673.3079	2673.3604	3	19.6	41.8	17460
RMPCAEDYLS	445	454	Carbamidomethyl C(1)	1222.5111	1222.5254	2	11.7	42.6	13593
RMPCAEDYLSVVLNQLCVLHEK	445	466	Carbamidomethyl C(2)	2673.3079	2673.3	4	-3	29.1	4058
RMPCAEDYLSVVLNQLCVLHEKTPVSDR	445	472	Carbamidomethyl C(2)	3328.6367	3328.6772	4	12.2	41.9	6083

RMPCAEDYL	445	453	Carbamidomethyl C(1)	1117.4685	1117.4829	2	12.9	42.6	3588
RMPCAEDYL	445	453	Carbamidomethyl C(1)	1107.4841	1107.4948	2	9.7	42.6	2488
RMPCAEDY	445	452	Carbamidomethyl C(1)	994.4001	994.4121	2	12.1	42.6	2438
RMPCAE	445	450	Carbamidomethyl C(1)	744.3047	744.3071	2	3.2	42.6	2384
RMPCAEDYLSVVLNQLCVLHEK	445	466	Carbamidomethyl C(2)	2673.3079	2673.344	3	13.5	30	2010
MPCAEDYLSVVLNQLCVLHEK	446	466	Carbamidomethyl C(2)	2517.2065	2517.24	3	13.3	44.3	928220
MPCAEDYLSVVLNQLCVLHEK	446	466	Carbamidomethyl C(2)	2517.2065	2517.2029	5	-1.4	28.2	63293
MPCAEDYLSVVLNQLCVLHEK	446	466	Carbamidomethyl C(2)	5034.4131	5034.3457	3	-13.4	44.3	22627
MPCAEDYLSVVLNQLCVLHEK	446	466	Carbamidomethyl C(2)	2499.196	2499.2168	4	8.3	44.3	4663
MPCAEDYLSVVLNQLCVLHEK	446	466	Carbamidomethyl C(2)	2517.2065	2517.1697	2	-14.6	24.5	1713
MPCAEDY	446	452	Carbamidomethyl C(1)	866.2939	866.3084	1	16.7	44.3	3249
MPCAEDYLSVVLNQLCVLHEKTPVSDR	446	472	Carbamidomethyl C(2)	3172.5356	3172.5522	4	5.2	43.1	2812
MPCAEDYL	446	453	Carbamidomethyl C(1)	979.378	979.3858	2	8	44.3	1717
MPCAEDYLSVVLNQLCVLHEK	446	466	Carbamidomethyl C(2)	2499.196	2499.1807	5	-6.1	28.2	1667
EDYLSVVLNQLCVLHEK	450	466	Carbamidomethyl C(1)	2058.0457	2058.0784	2	15.9	42.6	5514
DYLSVVLNQLCVLHEK	451	466	Carbamidomethyl C(1)	1929.0031	1929.027	3	12.4	42.6	2154
YLSVVLNQLCVLHEK	452	466	Carbamidomethyl C(1)	1813.9761	1813.9979	2	12	42.6	16349
LSVVLNQLCVLHEK	453	466	Carbamidomethyl C(1)	1650.9127	1650.9368	2	14.6	42.6	21098
SVVLNQLCVLHEK	454	466	Carbamidomethyl C(1)	1537.8286	1537.8467	2	11.8	42.6	67213
VVLNQLCVLHEK	455	466	Carbamidomethyl C(1)	1450.7966	1450.8219	2	17.4	42.6	16551
VVLNQLCVLHEK	455	466	Carbamidomethyl C(1)	1450.7966	1450.8092	2	8.7	44.3	2373
VLNQLCVLHEK	456	466	Carbamidomethyl C(1)	1351.7283	1351.7424	2	10.4	44.3	10311
LNQLCVLHEK	457	466	Carbamidomethyl C(1)	1252.6598	1252.675	2	12.1	42.6	12924
LNQLCVLHEK	457	466	Carbamidomethyl C(1)	1252.6598	1252.6669	2	5.7	44.3	3064
TPVSDR	467	472		673.3395	673.3518	2	18.3	27.6	3227
TPVSDRVTKCCTESLVNR	467	484	Carbamidomethyl C(2)	2121.0308	2120.9851	2	-21.5	29.6	16208
VTKCCTESLVNR	473	484	Carbamidomethyl C(2)	1465.7018	1465.7556	2	36.7	38.3	2145
VTKCCTESLVNR	473	484	Carbamidomethyl C(2)	1465.7018	1465.6821	2	-13.4	36.9	3350
CCTESLVNR	476	484	Carbamidomethyl C(2)	1137.4907	1137.5087	2	15.8	24.5	1345376
CCTESLVNR	476	484	Carbamidomethyl C(2)	1137.4907	1137.5085	2	15.6	25	78695
CCTESLVNR	476	484	Carbamidomethyl C(2)	1119.4802	1119.4912	2	9.8	24.5	21294

CCTESLVNRRPCFSALEVDETYVPK	476	500	Carbamidomethyl C(3)	3029.4045	3029.3928	3	-3.9	27.4	2152
TESLVNR	478	484		817.4294	817.4248	1	-5.6	25	2299
RPCFSALEVDETYV	485	498	Carbamidomethyl C(1)	1666.7661	1666.7638	2	-1.4	30.7	910726
RPCFSALEVDETYVPK	485	500	Carbamidomethyl C(1)	1909.9244	1909.9336	3	4.8	31.3	528760
RPCFSALEVDETYV	485	498	Carbamidomethyl C(1)	1666.7661	1666.7944	2	17	31.3	451510
RPCFSALEV	485	493	Carbamidomethyl C(1)	1059.5172	1059.5239	2	6.3	30.7	160986
RPCFSALEVDETY	485	497	Carbamidomethyl C(1)	1567.6978	1567.7174	2	12.5	30.7	154483
RPCFSALEVDETYVPK	485	500	Carbamidomethyl C(1)	1891.9138	1891.9316	3	9.4	30.7	101703
RPCFSALE	485	492	Carbamidomethyl C(1)	960.4487	960.4546	2	6.1	30.7	85555
RPCFSALEVDET	485	496	Carbamidomethyl C(1)	1404.6344	1404.6511	2	11.9	30.7	81706
RPCFSALEVDETY	485	497	Carbamidomethyl C(1)	1567.6978	1567.7156	2	11.4	31.3	73280
RPCFSALEVDETYVPKEFNAETFTFHADICTLSEK	485	519	Carbamidomethyl C(2)	4150.9292	4150.9888	4	14.4	38.6	69828
RPCFSALEVDE	485	495	Carbamidomethyl C(1)	1303.5867	1303.6073	2	15.8	30.7	63987
RPCFSALEVD	485	494	Carbamidomethyl C(1)	1174.5441	1174.5759	2	27.1	30.7	41964
RPCFSALEVDET	485	496	Carbamidomethyl C(1)	1404.6344	1404.65	2	11.1	31.3	31220
RPCFSALEVDETY	485	497	Carbamidomethyl C(1)	1549.6871	1549.7073	2	13	30.7	28814
RPCFSALEVDETYVP	485	499	Carbamidomethyl C(1)	1763.8188	1763.8585	2	22.5	32.8	15353
RPCFSALEVDETYVP	485	499	Carbamidomethyl C(1)	1763.8188	1763.8497	2	17.5	30.7	10479
RPCFSALEVDETYVPK	485	500	Carbamidomethyl C(1)	1909.9244	1909.967	2	22.3	30.1	8132
RPCFSAL	485	491	Carbamidomethyl C(1)	831.4062	831.3951	1	-13.4	31.3	5449
RPCFSALEVDET	485	496	Carbamidomethyl C(1)	1386.6238	1386.6387	2	10.7	30.7	2306
RPCFSALEVDETYVPK	485	500	Carbamidomethyl C(1)	1891.9138	1891.9585	2	23.6	32.5	1468
RPCFSALEVDETYVPK	485	500	Carbamidomethyl C(1)	1909.9244	1909.8691	2	-29	30.7	3295712
RPCFSALEVDETYV	485	498	Carbamidomethyl C(1)	1648.7556	1648.7787	2	14	30.7	13417
RPCFSALEVDETYVPKEFNAETFTFHADICTLSEKER	485	521	Carbamidomethyl C(2)	4436.0728	4435.9883	7	-19	29	9414
RPCFSALEVDETYV	485	498	Carbamidomethyl C(1)	1648.7556	1648.8016	2	27.9	31.3	3223
RPCFSALEVDETYVPKEF	485	502	Carbamidomethyl C(1)	2168.0249	2168.062	3	17.1	27.3	2130
RPCFSALEV	485	493	Carbamidomethyl C(1)	1041.5066	1041.5148	2	7.9	30.7	2034
RPCFSALEV	485	493	Carbamidomethyl C(1)	1031.5222	1031.5354	2	12.8	30.7	1390
LEVDETYVPK	491	500		1191.6023	1191.6123	2	8.4	30.8	10845
LEVDETYVPK	491	500		1191.6023	1191.6151	2	10.7	31.4	5954

EVDETYVPK	492	500		1078.5182	1078.5078	1	-9.6	30.7	32069
VDETYVPK	493	500		949.4756	949.4636	1	-12.6	30.7	79888
VDETYVPK	493	500		949.4756	949.4636	1	-12.6	31.3	46067
VDETYVPK	493	500		932.4491	932.4627	2	14.6	30.7	3702
DETYVPK	494	500		850.4072	850.4001	1	-8.3	30.7	87490
DETYVPK	494	500		850.4072	850.4002	1	-8.2	31.3	70523
TYVPK	496	500		606.3377	606.3302	1	-12.4	30.7	39154
YVPK	497	500		505.29	505.2821	1	-15.6	31.7	5900
YVPK	497	500		505.29	505.2796	1	-20.6	30.7	31717
VPK	498	500		342.2267	342.2208	1	-17.2	31.3	51226
VPK	498	500		342.2267	342.2203	1	-18.7	30.7	31502
PK	499	500		243.1583	243.1542	1	-16.9	31.3	161051
EFNAETFTFHADICTLSEK	501	519	Carbamidomethyl C(1)	2259.0154	2259.0493	3	15	35.6	633538
EFNAETFTFHADICTLSEKER	501	521	Carbamidomethyl C(1)	2544.1592	2544.1765	3	6.8	33.8	321514
EFNAETFTFHADICTLSEK	501	519	Carbamidomethyl C(1)	2259.0154	2259.0771	3	27.3	36	180299
EFNAETFTFHADICTLSEKER	501	521	Carbamidomethyl C(1)	2544.1592	2544.1792	3	7.9	34.2	140609
EFNAETFTFHADICTLSEK	501	519	Carbamidomethyl C(1)	2259.0154	2259.0452	3	13.2	40.3	33784
EFNAETFTFHADICTLSEK	501	519	Carbamidomethyl C(1)	2241.0049	2241.0432	3	17.1	35.6	31500
EFNAETFTFHADICTLSEK	501	519	Carbamidomethyl C(1)	2259.0154	2259.0559	2	17.9	40.6	22266
EFNAETFTFHADICTLSEKER	501	521	Carbamidomethyl C(1)	2526.1484	2526.158	4	3.8	34.2	18491
EFNAETFTFHADICTLSEK	501	519	Carbamidomethyl C(1)	2259.0154	2259.0518	3	16.1	37.5	18464
EFNAETFTFHADICTLSEK	501	519	Carbamidomethyl C(1)	2259.0154	2259.0696	3	24	37	18101
EFNAETFTFHADICTLSEK	501	519	Carbamidomethyl C(1)	2259.0154	2259.05	3	15.3	38.5	7406
EFNAETFTFHADICTLSEK	501	519	Carbamidomethyl C(1)	2259.0154	2259.0605	3	20	39.7	7279
EFNAETFTFHADICTLSEK	501	519	Carbamidomethyl C(1)	2259.0154	2259.0454	3	13.3	42.1	6092
EFNAETFTFHADI	501	513		1494.6779	1494.6794	2	1	33.2	2928
EFNAETFTFHADICTLSEK	501	519	Carbamidomethyl C(1)	2241.0049	2241.0518	3	20.9	36.1	10953
EFNAETFTFHADICTLSEK	501	519	Carbamidomethyl C(1)	2259.0154	2259.0691	2	23.8	36.6	8761
EFNAETFTFHADICTLSEKERQIK	501	524	Carbamidomethyl C(1)	2913.3967	2913.3591	5	-12.9	30	7133
EFNAETFTFHADICTLSEK	501	519	Carbamidomethyl C(1)	2259.0154	2259.0464	3	13.7	38.9	5059
EFNAETFTFHADICTLSEK	501	519	Carbamidomethyl C(1)	2259.0154	2259.052	2	16.2	39.4	4226

EFNAETFTFHADICTLSEK	501	519	Carbamidomethyl C(1)	2259.0154	2259.0613	2	20.3	43.2	4017
EFNAETFTFHADICTLSEKER	501	521	Carbamidomethyl C(1)	2544.1592	2544.1819	4	8.9	36	2704
EFNAETFTFHADICTLSEK	501	519	Carbamidomethyl C(1)	2259.0154	2259.0669	2	22.8	49.6	2201
EFNAETFTFHADICTLSEK	501	519	Carbamidomethyl C(1)	2259.0154	2259.0408	3	11.2	47.8	1329
SEK	517	519		362.1801	362.1831	1	8.3	35.6	16144
ERQIKK	520	525		800.4868	800.4636	2	-29	26.1	19300
ERQIKK	520	525		800.4868	800.4746	1	-15.2	28.2	7261
ERQIK	520	524		672.3918	672.3959	2	6.1	26.8	2968
QIK	522	524		387.2482	387.244	1	-10.8	25.2	16739
IKK	523	525		387.2845	387.2904	1	15.2	28.2	5521
KQTALVELVK	525	534		1127.6914	1127.7089	2	15.5	27.8	593050
KQTALV	525	530		640.3908	640.3996	1	13.7	27.8	46501
KQTA	525	528		428.2383	428.2334	1	-11.4	27.8	32511
KQTALVE	525	531		769.4334	769.4515	1	23.5	27.8	23945
KQTAL	525	529		513.3275	513.3337	1	12.1	27.8	4015
QTALVELVK	526	534		999.5964	999.6002	1	3.8	29.7	1386419
QTALVELVK	526	534		981.5859	981.5886	2	2.8	29.7	320144
QTAL	526	529		413.2274	413.2266	1	-1.9	29.7	3885
QTALVELVK	526	534		999.5964	999.6119	1	15.5	27.8	3792
QTALVELVK	526	534		999.5964	999.6032	2	6.8	29.9	121560
QTALVELVK	526	534		999.5964	999.6054	2	9	30.4	3387
QTALVELVKHKPKATK	526	541		1790.0778	1790.1125	3	19.4	24.7	1634
ALVELVK	528	534		770.4902	770.4944	1	5.5	29.7	38224
LVELVK	529	534		699.4531	699.4521	1	-1.4	29.6	23560
LVELVK	529	534		699.4531	699.4509	1	-3.1	30	16697
VELVK	530	534		586.369	586.3684	1	-1	27.8	282497
VELVK	530	534		586.369	586.3622	1	-11.6	29.7	106998
ELVK	531	534		487.3006	487.2955	1	-10.5	29.7	117903
ELVK	531	534		469.29	469.294	1	8.5	27.8	15963
ELVK	531	534		487.3006	487.2905	1	-20.7	27.8	77396
LVK	532	534		358.258	358.2522	1	-16.2	27.8	13576

LVK	532	534		358.258	358.256	1	-5.6	29.7	8921
ATKEQLKAVMDDFAAFVEK	539	557		2140.0874	2140.0481	3	-18.4	33.7	2471
EQLKAVM	542	548		799.4262	799.4233	2	-3.6	25.7	6947
E	542	542		101.0477	101.0471	1	-5.9	26.7	35705
EQLKAVMDDFAAFVEK	542	557		1839.9076	1839.9496	3	22.8	33.8	2928
AVMDDFAAFVEK	546	557		1341.6274	1341.6805	2	39.6	37.4	796175
AVMDDF	546	551		678.2683	678.2997	1	46.3	37.4	8801
AVMDD	546	550		531.1999	531.2155	1	29.4	37.4	6557
AVMDDFAAFVEK	546	557		1341.6274	1341.655	2	20.6	37	4763
AVMDDFAAFVEK	546	557		1323.6169	1323.6306	2	10.4	37.4	4065
AVMDDFAAFVEK	546	557		1341.6274	1341.5989	2	-21.2	26	4106
MDDFAAFVEK	548	557		1171.522	1171.5267	2	4	37.4	35843
DDFAAFVEK	549	557		1040.4814	1040.5166	1	33.8	37.4	6863
AAFVEK	552	557		663.3591	663.3746	1	23.4	37.4	11722
AFVEK	553	557		592.322	592.3383	1	27.5	37.4	25033
FVEK	554	557		521.2849	521.299	1	27	37.4	16852
ADDKETCFAEEGKK	561	574	Carbamidomethyl C(1)	1626.7196	1626.7548	2	21.6	23.7	398253
ADDKETCFAEEGK	561	573	Carbamidomethyl C(1)	1498.6246	1498.6411	2	11	24.2	93725
ADDKETCFAEEGKK	561	574	Carbamidomethyl C(1)	1608.709	1608.7062	4	-1.7	23.7	3715
ADDKETCFAEEGKK	561	574	Carbamidomethyl C(1)	1626.7196	1626.7438	2	14.9	27.7	2549
ADDKETCF	561	568	Carbamidomethyl C(1)	966.3753	966.3819	1	6.8	23.7	1325
DKETCFAEEGKK	563	574	Carbamidomethyl C(1)	1440.6555	1440.6506	3	-3.4	23.7	54428
DKETCFAEEGK	563	573	Carbamidomethyl C(1)	1312.5605	1312.5947	2	26.1	24.2	4193
DKETCFAEEGKK	563	574	Carbamidomethyl C(1)	1423.6289	1423.6646	3	25.1	23.7	2030
ETCFAEEGK	565	573	Carbamidomethyl C(1)	1069.4386	1069.4441	1	5.1	24.2	2092
TCFAEEGKK	566	574	Carbamidomethyl C(1)	1068.491	1068.5134	2	21	23.7	2763
CFAEEGKK	567	574	Carbamidomethyl C(1)	967.4434	967.4512	2	8.1	23.7	6359
FAEEGKK	568	574		807.4127	807.4051	2	-9.4	23.7	8527
FAEEGKK	568	574		807.4127	807.4097	2	-3.7	24.4	6115
AEEGKK	569	574		660.3442	660.3435	1	-1.1	23.7	7609
EEGKK	570	574		589.3071	589.3078	1	1.2	23.7	5430

EGKK	571	574	460.2645	460.2615	1	-6.5	23.7	3064
KLVAASQAALGL	574	585	1140.6866	1140.7092	2	19.8	30.1	135888
KLVAASQAA	574	582	839.4865	839.4854	2	-1.3	30.1	1036
LVAASQAALGL	575	585	1012.5917	1012.5734	1	-18.1	34.7	539325
LVAASQAAL	575	583	824.4756	824.4718	1	-4.6	34.7	202274
LVAASQAA	575	582	711.3915	711.3855	1	-8.4	34	124926
LVAASQAALG	575	584	881.4971	881.4888	1	-9.4	34	96224
LVAASQAALGL	575	585	1012.5917	1012.5842	1	-7.4	35.4	81018
LVAASQA	575	581	640.3544	640.3488	1	-8.7	34.6	41838
LVAASQ	575	580	569.3173	569.3117	1	-9.8	34	34840
LVAASQAALGL	575	585	994.5811	994.5793	2	-1.8	34.1	33531
LVAASQAAL	575	583	824.4756	824.4817	1	7.4	35.4	28102
LVAASQAALGL	575	585	1012.5917	1012.6113	1	19.4	36.5	25235
LVAASQAAL	575	583	806.465	806.4581	1	-8.6	34	17847
LVAASQAA	575	582	693.381	693.3692	1	-17	34	10082
LV	575	576	212.1525	212.1486	1	-18.4	34.5	8437
LVAASQAALGL	575	585	1012.5917	1012.6234	1	31.3	37.5	7604
LVAASQAALGL	575	585	1012.5917	1012.6197	1	27.7	36.9	4999
LVAASQA	575	581	622.3439	622.3303	1	-21.9	34	4339
LVAASQAALGL	575	585	1012.5917	1012.5921	1	0.4	47.8	1555
LVAASQAA	575	582	711.3915	711.3853	1	-8.7	34.7	36182
LVAASQAALGL	575	585	994.5811	994.5833	2	2.2	34.6	24728
LVAASQAALG	575	584	881.4971	881.5046	1	8.5	35.4	8933
LVAASQA	575	581	640.3544	640.3534	1	-1.6	35.4	3195
LVAASQAALGL	575	585	1012.5917	1012.5981	2	6.3	36	2925
LVAASQA	575	581	640.3544	640.3665	1	18.9	36	2872
LVAASQAALGL	575	585	994.5811	994.5803	2	-0.8	35.4	2497
LVAASQAALG	575	584	881.4971	881.5061	2	10.2	36	2329
AASQAALGL	577	585	800.4392	800.4353	1	-4.9	34.7	27814
AASQAALGL	577	585	800.4392	800.4336	1	-7	35.4	2733
ASQAALGL	578	585	729.4021	729.4052	1	4.3	34	11034

ASQAALGL	578	585	729.4021	729.4164	1	19.6	34.7	9182
SQAALGL	579	585	658.365	658.3617	1	-5	34	26347
SQAALGL	579	585	658.365	658.3593	1	-8.7	34.6	13454
QAALGL	580	585	571.3329	571.325	1	-13.8	34.6	23961
AALGL	581	585	443.2744	443.2687	1	-12.9	34.1	21107
AALGL	581	585	443.2744	443.2686	1	-13.1	34.6	15064
ALGL	582	585	354.2267	354.2209	1	-16.4	34.1	7893
ALGL	582	585	372.2372	372.2326	1	-12.4	34	7364
LGL	583	585	301.2001	301.1956	1	-14.9	34.7	18184
GL	584	585	188.1161	188.1125	1	-19.1	34	38030

20 minute vapor conjugation

Peptide	Start	End	Modifiers	Mcalc	Mobs	z	Merr	RT(min)	Intensity
LAKTYETTLEK	349	359	TDI*(1)	1443.761	1443.778	2	12.0	27.7	49697
LAKTYETTLEK	349	359	TDI(1)	1469.7401	1469.773	2	22.2	38	1712
LAKTYETTLEK	349	359	TDI*(2)	1591.8247	1591.795	2	-18.7	24.2	6402
AKTYETTLEK	350	359	TDI*(1)	1330.6769	1330.656	2	-16.0	42.4	2841
FQNALLVRYTKK	403	414	TDI*(2)	1775.9835	1775.955	3	-15.8	23.8	45798
YTKKVPQVSTPTLVEVSR	411	428	TDI(1)	2205.1792	2205.227	2	21.7	36.1	29288
KVPQVSTPTLVEVSR	414	428	TDI*(1)	1786.9941	1787.038	2	24.6	30	11608
KVPQVSTPTLVEVSRNLGK	414	432	TDI*(2)	2347.3013	2347.276	4	-10.9	25.1	12820

1 hour vapor conjugation

Peptide	Start	End	Modifiers	Mcalc	Mobs	z	Merr	RT(min)	Intensity
LAKTY	349	353	TDI*(1)	724.3909	724.3893	2	-2.2	27.5	2537
LAKTYETTLEK	349	359	TDI*(1)	1443.761	1443.768	2	4.7	27.5	191847
LAKTYETTLEK	349	359	TDI(1)	1469.7401	1469.749	2	5.7	38.2	4115

LAKTYETTLKCCAAADPHECYAK	349	372	TDI(1),Carbamidomethyl C(3)	3003.3201	3003.395	3	25.0	30.6	23491
QNCELFEQLGEYKFQNALLVRYTK	390	413	TDI(1),Carbamidomethyl C(1)	3164.5388	3164.455	3	-26.5	40.4	10212
FQNALLVRYTK	403	413	TDI(1)	1525.8041	1525.828	2	15.8	36	9033
FQNALLVRYTKK	403	414	TDI(1)	1653.899	1653.915	3	9.8	32.6	4385
FQNALLVRYTKK	403	414	TDI*(2)	1775.9835	1775.949	3	-19.4	23	39088
FQNALLVRYTKK	403	414	TDI*(2)	1775.9835	1775.987	3	2.2	24.3	18292
YTKKVPQVSTPTLVEVS	411	427	TDI(1)	2031.0676	2031.044	3	-11.5	36	2938
YTKKVPQVSTPTLVEVSR	411	428	TDI(1)	2205.1792	2205.225	2	20.8	36	111020
YTKKVPQVSTPTLVEVSR	411	428	TDI(1)	2205.1792	2205.231	2	23.3	37	46916
YTKKVPQVSTPTLVEVSR	411	428	TDI(1),TDI*(1)	2353.2429	2353.265	3	9.3	24.1	1362
KVPQVSTPTLV	414	424	TDI*(1)	1297.7395	1297.743	2	2.5	29.6	2208
KVPQVSTPTLVEVSR	414	428	TDI*(1)	1768.9836	1769.016	3	18.1	31.2	3739
KVPQVSTPTLVEVSR	414	428	TDI*(1)	1786.9941	1787.037	2	23.8	29.6	46725
KVPQVSTPTLVEVSR	414	428	TDI(1)	1812.9734	1812.998	2	13.6	37.5	4938
ERQIKK	520	525	TDI(1),TDI*(1)	1122.5934	1122.601	2	6.9	28.4	2410
QIKK	522	525	TDI(1)	689.386	689.3953	1	13.5	31.2	3458
QIKKQTALVELVK	522	534	TDI(1)	1652.9613	1652.978	3	9.9	37.8	5160
QIKKQTALVELVK	522	534	TDI(1)	1670.9719	1671.008	2	21.5	37.8	91696
KQTA	525	528	TDI*(1)	576.3021	576.3069	1	8.3	29.6	5514
KQTALVELVK	525	534	TDI*(1)	1275.7551	1275.786	2	24.2	31.2	85573

4 hour vapor conjugation

Peptide	Start	End	Modifiers	Mcalc	Mobs	z	Merr	RT(min)	Intensity
DAHK	1	4	TDI(1)	643.2714	643.2893	1	27.8	28.3	15506
DAHKS	1	5	TDI(1)	712.2928	712.3054	1	17.7	25.5	4506
DAHKSE	1	6	TDI(1)	841.3354	841.3498	1	17.1	24.3	19227
DAHKSEV	1	7	TDI(1)	940.4039	940.4226	1	19.9	25.5	4649
DAHKSEVAHR	1	10	TDI*(1),TDI-N(1)	1470.6753	1470.694	2	12.4	28.4	192764
DAHKSEVAHRFK	1	12	TDI*(1)	1571.7958	1571.755	2	-26.0	33.5	25657

DAHKSEVAHRFK	1	12	TDI(1),TDI*(1)	1745.8386	1745.797	2	-24.1	35.1	3091
SEVAHRFK	5	12	TDI(1)	1146.557	1146.573	2	14.1	28.9	33132
SEVAHRFKDLGEENFK	5	20	TDI*(1)	2053.0017	2052.968	3	-16.5	26.2	169213
FKDLGEENFK	11	20	TDI*(1)	1373.6616	1373.677	2	10.9	29.6	44774
FKDLGEENFKALVLIAFAQYLQQCPFEDHVK	11	41	Carbamidomethyl C(1),TDI*(1)	3844.9287	3844.968	5	10.2	49.1	13306
TCVADESAENCDKSLHTLFGDKLCTVATLR	52	81	TDI(1),Carbamidomethyl C(3)	3584.6335	3584.693	3	16.7	42.1	377876
SLHTLFGDK	65	73	TDI*(1)	1146.5823	1146.593	2	9.7	38	1546
SLHTLFGDKLCTVATLR	65	81	Carbamidomethyl C(1),TDI*(1)	2079.0935	2079.126	3	15.6	38	156181
LVRPEVDVMCTAFHDNEETFLKK	115	137	Carbamidomethyl C(1),TDI*(1)	2908.3889	2908.418	5	9.9	35	1654
LVRPEVDVMCTAFHDNEETFLKK	115	137	Carbamidomethyl C(1),TDI*(1)	2925.4153	2925.467	4	17.6	35	34431
HPYFYAPELLFFAKR	146	160	TDI*(1)	2046.0516	2046.075	2	11.3	40.6	5241
LAKTY	349	353	TDI*(1)	696.3959	696.3973	2	2.0	28.2	5244
LAKTYETTLEK	349	359	TDI*(1)	1426.7344	1426.766	3	21.9	27.7	6351
LAKTYETTLEK	349	359	TDI*(1)	1443.761	1443.764	2	1.9	27.7	88617
LAKTYETTLEK	349	359	TDI(1)	1469.7401	1469.746	2	3.8	33.2	3451
CCAAADPHECYAKVFDEFKPLVEEPQNLIKQNCELF	360	395	TDI(1),Carbamidomethyl C(4),TDI*(2)	4821.1553	4821.221	5	13.6	38.8	1897
VFDEFKPLV	373	381	TDI*(1)	1222.6387	1222.633	2	-4.8	39.4	3110
VFDEFKPLVEEPQNLI	373	388	TDI*(1)	2046.0463	2046.091	2	21.7	39.4	1506
VFDEFKPLVEEPQNLIK	373	389	TDI*(1)	2192.1519	2192.173	3	9.4	38.8	41575
FQNALLVRYTKK	403	414	TDI(1)	1653.899	1653.948	2	29.6	41.8	2621
YTKKV	411	415	TDI(1)	793.4122	793.4175	1	6.7	35.2	2180
YTKKVPQV	411	418	TDI(1)	1117.592	1117.597	2	4.8	36.3	2193
YTKKVPQVST	411	420	TDI(1)	1305.6718	1305.683	2	8.3	36.3	2513
YTKKVPQVSTPTLVEVSR	411	428	TDI*(1)	2179.2002	2179.147	3	-24.6	39.2	1524
YTKKVPQVSTPTLVEVSR	411	428	TDI(1)	2205.1792	2205.21	2	13.8	35.2	319864
YTKKVPQVSTPTLVEVSR	411	428	TDI*(2)	2327.2639	2327.209	3	-23.6	42	8305
YTKKVPQVSTPTLVEVSR	411	428	TDI(1),TDI*(1)	2353.2429	2353.281	2	16.2	38.9	52714
KVPQVS	414	419	TDI*(1)	786.4388	786.4392	2	0.5	30.2	2514
KVPQVST	414	420	TDI*(1)	887.4865	887.485	1	-1.7	30.2	12349
KVPQVSTPTLV	414	424	TDI*(1)	1297.7395	1297.758	2	14.1	30.3	10938
KVPQVSTPTLVEV	414	426	TDI*(1)	1525.8505	1525.88	2	19.1	31.2	6978

KVPQVSTPTLVEVS	414	427	TDI*(1)	1612.8824	1612.904	2	13.3	30.2	6682
KVPQVSTPTLVEVSR	414	428	TDI*(1)	1786.9941	1787.024	2	16.5	30.3	279656
KVPQVSTPTLVEVSR	414	428	TDI(1)	1812.9734	1813.006	2	18.1	37.7	4978
EFNAETFTFHADICTLSEKERQIK	501	524	Carbamidomethyl C(1),TDI*(1)	3061.4604	3061.397	3	-20.6	30.9	6740
ERQIKK	520	525	TDI(1),TDI*(1)	1122.5934	1122.613	2	17.4	26.3	9667
QIKKQTAL	522	529	TDI(1)	1084.6029	1084.611	2	7.2	38	1250
QIKKQTALVELVK	522	534	TDI(1)	1670.9719	1670.993	2	12.8	38.1	170023
QIKKQTALVELVK	522	534	TDI*(2)	1793.0564	1793.064	3	4.1	34.5	1322
KQTALVELVK	525	534	TDI*(1)	1275.7551	1275.768	2	10.0	31	8145

24 hour vapor conjugation

Peptide	Start	End	Modifiers	Mcalc	Mobs	z	Merr	RT(min)	Intensity
DAHK	1	4	TDI(1)	643.2714	643.2869	1	24.1	28.6	8247
DAHKSE	1	6	TDI(1)	841.3354	841.3403	1	5.8	24.9	11921
DAHKSEV	1	7	TDI(1)	940.4039	940.4186	1	15.6	24.9	2432
DAHKSEVAHR	1	10	TDI*-N(1),TDI*(1)	1444.696	1444.728	3	22.1	24.2	1245
DAHKSEVAHR	1	10	TDI*(1),TDI-N(1)	1470.6753	1470.683	3	5.0	28.7	112705
DAHKSEVAHRFK	1	12	TDI*(1)	1571.7958	1571.765	2	-19.9	30.9	18029
SEVAHRFK	5	12	TDI(1)	1146.557	1146.569	2	10.0	29.2	22055
FKDLGEEN	11	18	TDI(1)	1106.4668	1106.439	2	-25.6	25.7	1880
FKDLGEENFK	11	20	TDI*(1)	1373.6616	1373.672	2	7.5	29.9	25159
SLHTLFGDKLCTVATLR	65	81	Carbamidomethyl C(1),TDI*(1)	2061.083	2061.109	4	12.8	38.3	3217
SLHTLFGDKLCTVATLR	65	81	Carbamidomethyl C(1),TDI*(1)	2079.0935	2079.127	3	16.0	38.3	78862
QEPERNECFLQHKDDNPNLPR	94	114	Carbamidomethyl C(1),TDI*(1)	2783.2834	2783.315	4	11.3	28.3	20914
QEPERNECFLQHKDDNPNLPR	94	114	TDI(1),Carbamidomethyl C(1)	2809.2627	2809.316	3	19.1	31.1	48733
NECFLQHKDDNPNLPR	99	114	Carbamidomethyl C(1),TDI*(1)	2143.9858	2144.024	3	18.0	29.7	15471
LVRPEVDMCTAFHDNEETFLKK	115	137	Carbamidomethyl C(1),TDI*(1)	2925.4153	2925.491	4	25.8	35.2	16282
LVRPEVDMCTAFHDNEETFLKKYLYEIAR	115	144	TDI(1),Carbamidomethyl C(1),TDI*(1)	4007.9338	4008.036	4	25.5	45	7880
KYLYEIAR	137	144	TDI*(1)	1202.6448	1202.646	2	0.7	30.2	4530

RHPYFYAPELLFFAK	145	159	TDI*(1)	2046.0516	2046.097	2	22.2	41.2	8030
RHPYFYAPELLFFAKR	145	160	TDI*(1)	2202.1526	2202.207	4	24.8	39.8	3985
RHPYFYAPELLFFAKR	145	160	TDI(1)	2228.1318	2228.107	2	-11.2	29.3	5541
HPYFYAPELLFFAK	146	159	TDI*(1)	1889.9504	1889.955	3	2.3	31.1	2650
HPYFYAPELLFFAKR	146	160	TDI*(1)	2046.0516	2046.097	3	22.0	42	13760
PELLFFAKR	152	160	TDI*(1)	1267.7078	1267.719	2	9.0	42	1288
LDELRDEGK	182	190	TDI*(1)	1221.599	1221.595	2	-3.0	28.5	1383
LDELRDEGKASSAK	182	195	TDI*(1)	1665.8323	1665.852	3	12.0	25.2	1252
ELRDEGK	184	190	TDI*(1)	993.488	993.4856	1	-2.4	29.3	5358
DEGKASSAKQR	187	197	TDI(1)	1349.6323	1349.634	2	1.4	24	1492
QRLKCASLQK	196	205	TDI(1),Carbamidomethyl C(1)	1404.7296	1404.69	2	-28.0	42.3	6396
LKCASLQK	198	205	Carbamidomethyl C(1),TDI*(1)	1094.5907	1094.592	2	1.2	25.2	11265
HPDYSVVLRLRLAKTYETTLEK	338	359	TDI*(1)	2736.4851	2736.531	4	16.7	40.7	2604
LAKTY	349	353	TDI*(1)	696.3959	696.3969	2	1.4	28.5	2669
LAKTYE	349	354	TDI*(1)	825.4385	825.4393	2	1.0	28.5	1522
LAKTYET	349	355	TDI*(1)	954.4811	954.4615	2	-20.5	28.5	2269
LAKTYETTLEK	349	359	TDI*(1)	1443.761	1443.765	2	2.8	27.6	37800
LAKTYETTLEK	349	359	TDI(1)	1469.7401	1469.74	2	-0.1	33.5	2787
LAKTYETTLEK	349	359	TDI(1),TDI*(1)	1617.8038	1617.797	3	-4.0	29.2	3679
LAKTYETTLEKCCAAADPHECYAK	349	372	TDI(1),Carbamidomethyl C(3)	3003.3201	3003.374	3	18.0	32.6	122567
KTYETTLEK	351	359	TDI*(1)	1259.6398	1259.641	2	1.1	28.5	3847
VFDEFKPLVEEPQNLIK	373	389	TDI*(1)	2192.1519	2192.201	3	22.5	39.5	44043
FQNALLVRYTK	403	413	TDI(1)	1525.8041	1525.83	2	17.1	36.6	3839
YTKK	411	414	TDI*(1)	686.3752	686.3826	1	10.8	26.6	7068
YTKK	411	414	TDI(1),TDI*(1)	860.4181	860.404	1	-16.4	37.8	1615
YTKKVPQV	411	418	TDI(1)	1117.592	1117.602	2	8.8	36.5	1946
YTKKVPQVS	411	419	TDI(1)	1204.624	1204.637	2	10.8	36.5	1350
YTKKVPQVST	411	420	TDI(1)	1305.6718	1305.694	2	16.8	36.5	2960
YTKKVPQVSTPTLV	411	424	TDI(1)	1715.9246	1715.967	2	24.9	36.5	1430
YTKKVPQVSTPTLVEVSR	411	428	TDI(1)	2187.1687	2187.218	3	22.4	36.5	15528
YTKKVPQVSTPTLVEVSR	411	428	TDI(1)	2205.1792	2205.23	2	23.0	36.5	303721

YTKKVPQVSTPTLVEVSR	411	428	TDI*(2)	2327.2639	2327.225	3	-16.7	42.2	3312
YTKKVPQVSTPTLVEVSR	411	428	TDI(1),TDI*(1)	2353.2429	2353.298	3	23.2	39.1	27650
KVPQVST	414	420	TDI*(1)	869.476	869.4829	2	7.9	30.9	4835
KVPQVST	414	420	TDI*(1)	887.4865	887.4887	1	2.5	30.9	6071
KVPQVSTPTLV	414	424	TDI*(1)	1297.7395	1297.748	2	6.5	30.9	5291
KVPQVSTPTLVEVS	414	427	TDI*(1)	1612.8824	1612.902	2	12.1	30.9	1585
KVPQVSTPTLVEVSR	414	428	TDI*(1)	1768.9836	1769.006	3	12.4	30.9	35631
KVPQVSTPTLVEVSR	414	428	TDI*(1)	1768.9836	1769.008	3	13.6	31.6	13656
KVPQVSTPTLVEVSR	414	428	TDI*(1)	1786.9941	1786.989	3	-2.8	30.4	2180
KVPQVSTPTLVEVSR	414	428	TDI*(1)	1786.9941	1787.015	2	11.9	30.9	135580
KVPQVSTPTLVEVSR	414	428	TDI*(1)	1786.9941	1787.018	2	13.2	31.6	52546
NLGKVGSKCCK	429	439	TDI(1),Carbamidomethyl C(2)	1423.67	1423.682	2	8.6	28.8	222273
NLGKVGSKCCK	429	439	TDI(1),Carbamidomethyl C(2),TDI*(1)	1571.7338	1571.743	2	5.9	34.2	10356
VGSKCCKHPEAK	433	444	TDI(1),Carbamidomethyl C(2)	1573.713	1573.729	3	10.2	24.4	1751
VGSKCCKHPEAK	433	444	TDI(1),Carbamidomethyl C(2),TDI*(1)	1721.7767	1721.818	3	23.9	26.5	1657
CCKHPEAK	437	444	Carbamidomethyl C(2),TDI*(1)	1176.517	1176.503	2	-12.2	24.9	3913
HPEAKR	440	445	TDI*(1)	884.4617	884.4427	1	-21.5	26.3	2067
HPEAKR	440	445	TDI(1)	910.4409	910.44	1	-1.0	30.7	1650
HPEAKRMPCAEDYLSVVLNQLCVLHEK	440	466	Carbamidomethyl C(2),TDI*(1)	3383.6577	3383.638	4	-5.9	38.7	5731
ERQIKK	520	525	TDI(1),TDI*(1)	1122.5934	1122.603	2	8.5	26.3	2440
QIKK	522	525	TDI(1)	689.386	689.3876	1	2.3	31.3	3857
QIKKQTALVELVK	522	534	TDI(1)	1652.9613	1652.988	3	16.3	38.4	13540
QIKKQTALVELVK	522	534	TDI(1)	1670.9719	1671.004	2	18.9	38.4	136192
QIKKQTALVELVK	522	534	TDI*(2)	1793.0564	1793.077	3	11.4	35	1301
KQTALVELVK	525	534	TDI*(1)	1275.7551	1275.764	2	6.8	31.3	48076