Library design-facilitated high-throughput sequencing of synthetic peptide libraries

Alexander A. Vinogradov, Zachary P. Gates, Chi Zhang, Anthony J. Quartararo, Kathryn H. Halloran, Bradley L. Pentelute

Department of Chemistry, Massachusetts Institute of Technology, 18-596, 77 Massachusetts Avenue, Cambridge, Massachusetts, 02139, United States.

Supporting Information

Contents

1. General

Aza-1H-benzotriazole-1-yl)-1,1,3,3-tetramethyluronium hexafluorophosphate (HATU) and proteogenic N^{α}-Fmoc protected D-amino acids were purchased from Creosalus Inc. (KE). (1R,2R)-Fmoc-2-amino-1-cyclopentane carboxylic acid (Acp), (1R,2R)-Fmoc-2-amino-1-cyclohexane carboxylic acid (Ach), Fmoc-α-D-aminobutyric acid (Abu), Fmoc-β-alanine (β), Fmoc-δ-aminovaleric acid (Ava), Fmoc-D-cyclohexylalanine (Cya), Fmoc-D-4-fluorophenylalanine (Fph), Fmoc-D-4-aminohenylalanine (Aph), Fmoc-D-naphthylalanine (Nap), Fmoc-D-perfluorophenylalanine (Pfp), Fmoc-D-4-phenyl-phenylalanine (Phf), and Fmoc-D-3,4-dichlorophenylalanine (Cph) were from Chem-Impex International (Wood Dale, IL). $^{\alpha}$N-Boc-Glycyl ester of (4-hydroxymethyl)phenylacetic acid was purchased from PolyPeptide Group (Strasbourg, France). 30 μm monosized Tentagel S NH_2 resin was purchased from Rapp Polymere (Tuebingen, Germany).

N,N-Dimethylformamide (DMF), dichloromethane (DCM), diethyl ether, and HPLC-grade acetonitrile were from EMD Millipore. Triisoproyl silane (TIPS), and 1,2-Ethanedithiol (EDT) were from Alfa Aesar. Solvents for HPLC-MS were purchased from Fluka. All other reagents were purchased from Sigma-Aldrich.

All reagents were used as received.

Proteogenic amino acid residue encodings are reserved for corresponding D-amino acids throughout the manuscript. In other words, libraries were synthesized from D-amino acids where applicable.

2. Methods

2.1. Solid phase peptide synthesis

Individual peptides and peptide libraries were synthesized using established batch Fmoc SPPS techniques. Briefly, Fmoc-protected amino acids were dissolved in appropriate volume of 0.38 M HATU in DMF, and activated with 3 eq. of DIEA. Couplings were allowed to proceed for 10 to 30 minutes at room temperature with periodical gentle rocking of the resin suspension. $^{\alpha}$N-Fmoc protecting group removal was achieved by two 3 min treatments with 20% (v/v) piperidine in

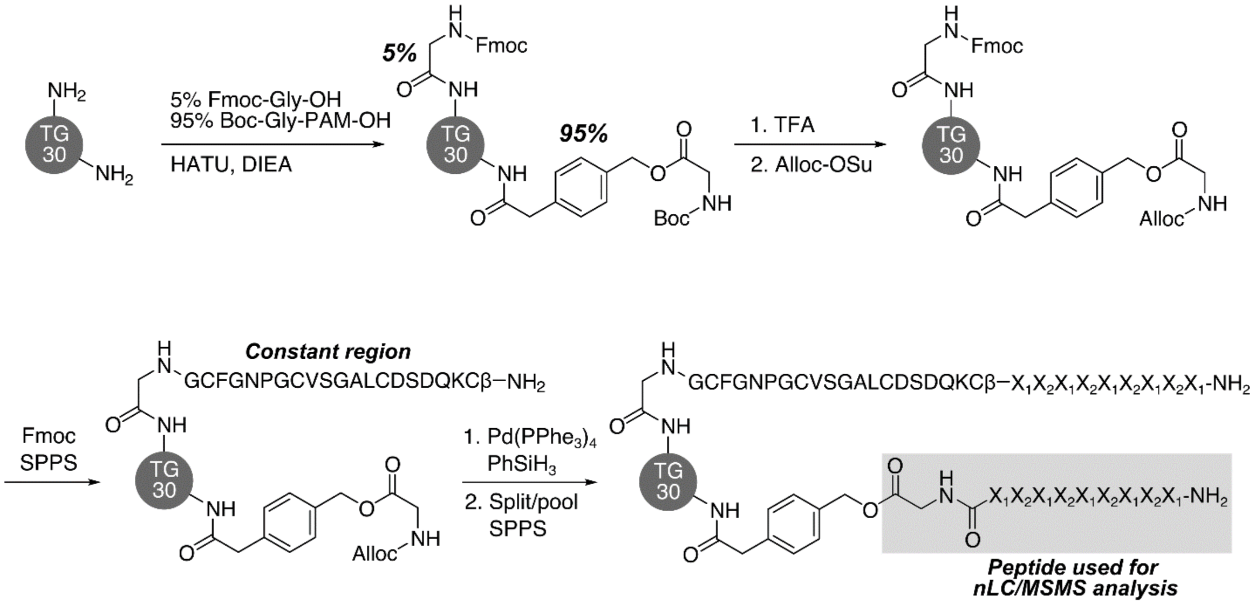
DMF. Side chain protection was as follows: Asn(Trt), Asp(OtBu), Cys(Trt), Gln(Trt), Glu(OtBu), His(Trt), Lys(Boc), Ser(tBu), Thr(tBu), Trp(Boc), Tyr(tBu).

2.2. Library synthesis

Library 1 was synthesized by manual split-pool Fmoc SPPS (section 2.1). Fully assembled library 1 contained peptide ss1-ss2-ss1-ss2-ss1-ss2-ss1-ss2-ss1-βCKQDSDCLAGSVCG-PNGFCG-CONH-Tentagel at 0.02 mmol/g loading, and ss1-ss2-ss1-ss2-ss1-ss2-ss1-ss2-ss1-Gly-PAM-CONH-Tentagel at 0.18 mmol/g. ss1 was any amino acid of the following set: Asp, Phe, His, Lys, Met, Pro, Trp, Leu. Analogously, ss2 was Ala, Glu, Gly, Gln, Ser, Thr, Val, Tyr.

Ile was excluded from the library design due to the fact that it is difficult to differentiate it from isomeric Leu without additional experimental manipulations. Cys was not used to avoid any potential complications associated with on-resin oxidation of displayed peptides. Asn was excluded due to the fact that it consistently underwent near quantitative deamidation to Asp during the PAM saponification step. Arg was not used because we found that peptides containing an internal Arg residue tend to yield CID fragmentation spectra of poor quality.

6 grams of resin (Tentagel S-NH2 30 μm resin from Rapp Polymere, 0.20 mmol/g amine loading) was first coupled to 4.5 mmol of Boc-Gly-PAM-OH and 0.5 mmol of Fmoc-Gly-OH to achieve dual functionalization of the resin (Scheme S1). Then Boc group was removed by treating with trifluoroacetic acid (TFA, twice, each with 40 mL for 2 minutes). The resin was washed with DMF (3 times, 50 mL each) and DCM (3 times, 50 mL each). 20 mL of 0.4 M Alloc-OSu in dry DCM and 3 mL of DIEA was added to the resin to functionalize the unmasked H_2N-Gly-PAM with Alloc protection group. After removal of the Fmoc group (two 3 minute treatments with 20% (v/v) piperidine in DMF), the constant region (βCKQDSDCLAGSVCGPNGFCG) was assembled following standard Fmoc protocols (section 2.1). Then, Alloc protection on Gly-PAM was removed with 400 mg of $Pd(PPh_3)_4$ and 8 mL of phenylsilane in 32 mL of dry DCM for 20 minutes at room temperature, and split-pool Fmoc SPPS ensued. Fully assembled library was deprotected with 2.5% (v/v) EDT, 2.5% (v/v) H_2O, and 1% (v/v) TIPS in TFA for 2 hours at room temperature. Deprotected library was washed with TFA, DCM, diethyl ether (five times each) and dried under reduced pressure.



Scheme S1. Synthesis of library 1. X_1: variable amino acids from ss_1 subset; X_2: variable amino acids from ss_2. TG30: Tentagel S-NH_2 30 µm beads.

Library 2 was synthesized on a spatially segregated Tentagel resin prepared using an unpublished functionalization protocol (Z. Gates, A. Vinogradov, B. Pentelute, manuscript in preparation). In this case, surface accessible area comprised 50% of the total bead volume. Interior of the resin bore H_2N-$(X)_9$-Gly-PAM-CONH-Tentagel peptide (X: D, K, F, Y, S, β, Ava, Abu, Acp, Ach, Cya, Fph, Aph, Nap, Pfp, Phf, Cph; expected frequency for D, K, F, Y, S and Abu was 10%, and for the other monomers it was 3.6%) at 0.20 mmol/g loading. Surface accessible part of the resin contained H_2N-$(X)_9$-CONH-Tentagel peptide at 0.02 mmol/g loading. Otherwise, synthesis of library 2 followed the procedure outlined above for library 1.

2.3. Synthesis of authentic peptides for sequencing validation

Peptides GCβWLSADEFPHG, GCβFLDEGYGPWG, GCβWLDEDTFMGG, GCβWLDTDPFPHG, GCβWLDTSEFPHG, GCβWLDPSLFPHG, GCβWADESAGPWG, GCβFLDEVEFPHG, and GCβFADASEFPHG were synthesized on Tentagel S-NH2 30 µm resin functionalized with Boc-Gly-PAM following procedures from section 2.1 and 2.2. Peptidyl resins were 2.5% (v/v) EDT, 2.5% (v/v) H2O, and 1% (v/v) TIPS in TFA for 2 hours at room temperature, washed with TFA, DCM, diethyl ether (five times each) and dried under reduced pressure. Analytical control over peptide quality was achieved by cleaving an aliquot of deprotected peptidyl resin with 10% (v/v) trifluoromethanesulfonic acid, 10% (v/v) p-cresol and 10% (v/v) thioanisole in TFA for 15 minutes on ice. Peptide carboxylates obtained in this way were analyzed on Agilent 6550 iFunnel Q-TOF LC-MS coupled to Agilent 1290 Infinity HPLC system equipped with Phenomenex Jupiter C4 column (150 x 1.0 mm ID, 5 μm 300Å silica). The analysis method was as follows. At 40 °C and a flow rate of 0.1 mL/min, the following gradient was used: 1% acetonitrile with 0.1% formic acid added (FA, solvent B) in water with 0.1% FA (solvent A) for 5 min, 1-51% B in A ramping linearly over 25 min, and then 51-70% B in A ramping linearly over 5 minutes. 10–20 ng/μL peptide solutions were subject to analysis. All chromatograms below are plots of total ion current (TIC) versus time.

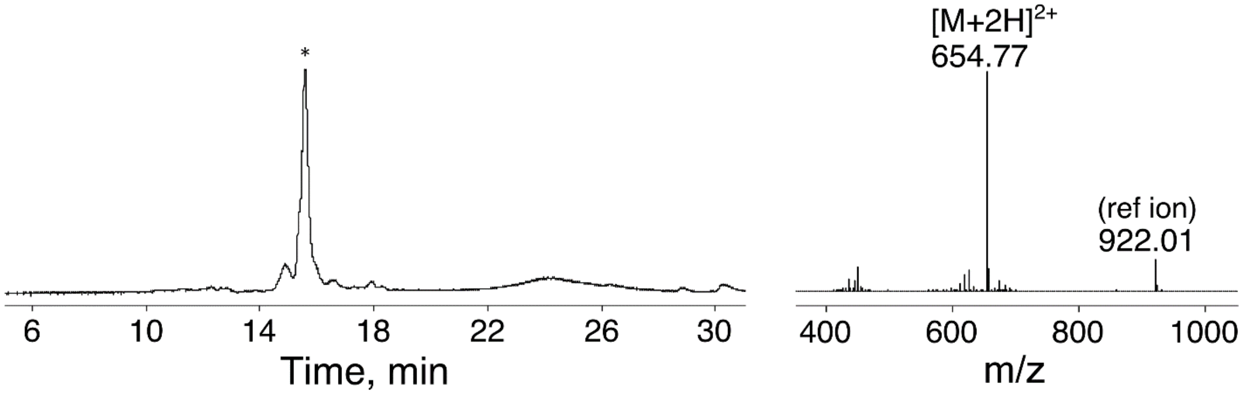


Figure S1. HPLC-MS (TIC) chromatogram for the crude H_2N- GCβFADASEFPHG-COOH on the left with a mass spectrum of major peak (labeled with an asterisk) on the right. Calc. monoisotopic mass = 1307.51 Da, Observed mass = 1307.53 Da.

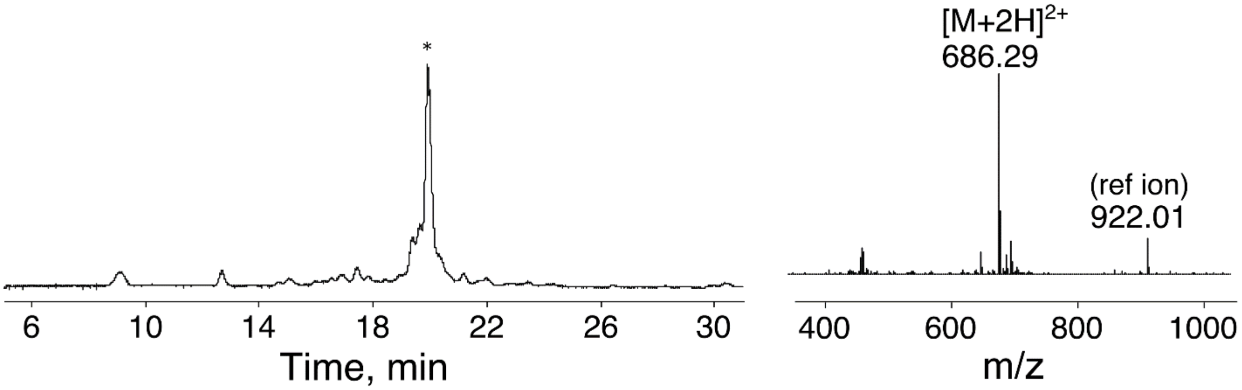


Figure S2. HPLC-MS (TIC) chromatogram for the crude H_2N- GCβFLDEGYGPWG-COOH on the left with a mass spectrum of major peak (labeled with an asterisk) on the right. Calc. monoisotopic mass = 1370.55 Da, Observed mass = 1370.57Da.

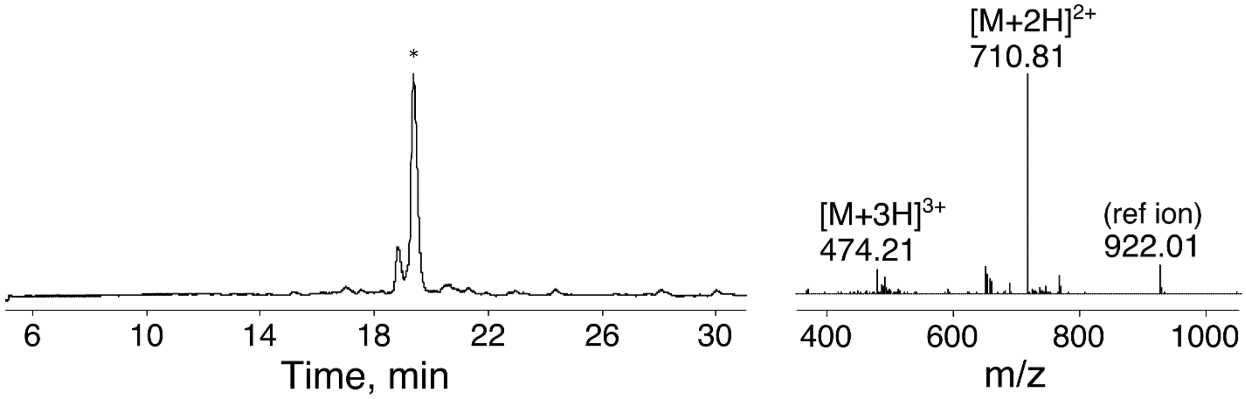


Figure S3. HPLC-MS (TIC) chromatogram for the crude H_2N- GCβFLDEVEFPHG-COOH on the left with a mass spectrum of major peak (labeled with an asterisk) on the right. Calc. monoisotopic mass = 1419.60 Da, Observed mass = 1419.61 Da.

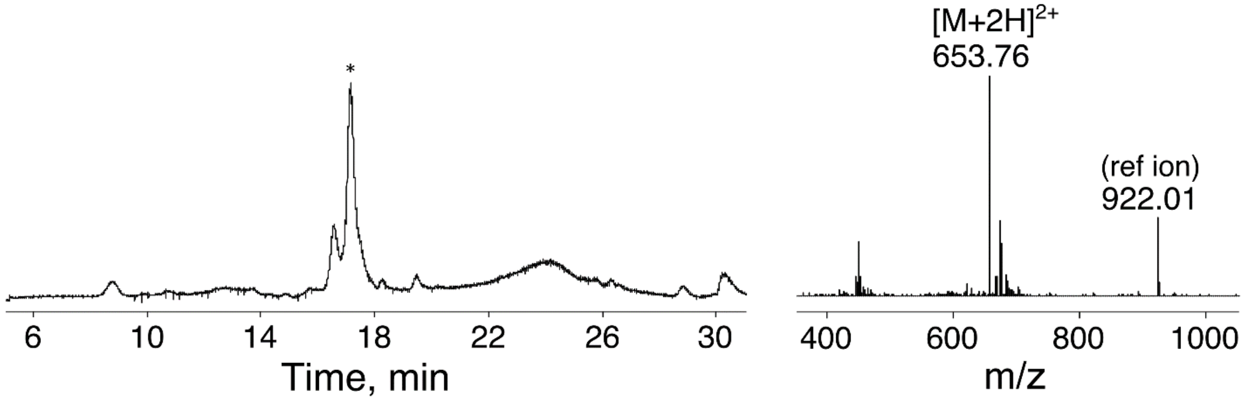


Figure S4. HPLC-MS (TIC) chromatogram for the crude H_2N- GCβWADESAGPWG-COOH on the left with a mass spectrum of major peak (labeled with an asterisk) on the right. Calc. monoisotopic mass = 1305.50 Da, Observed mass = 1305.51 Da.

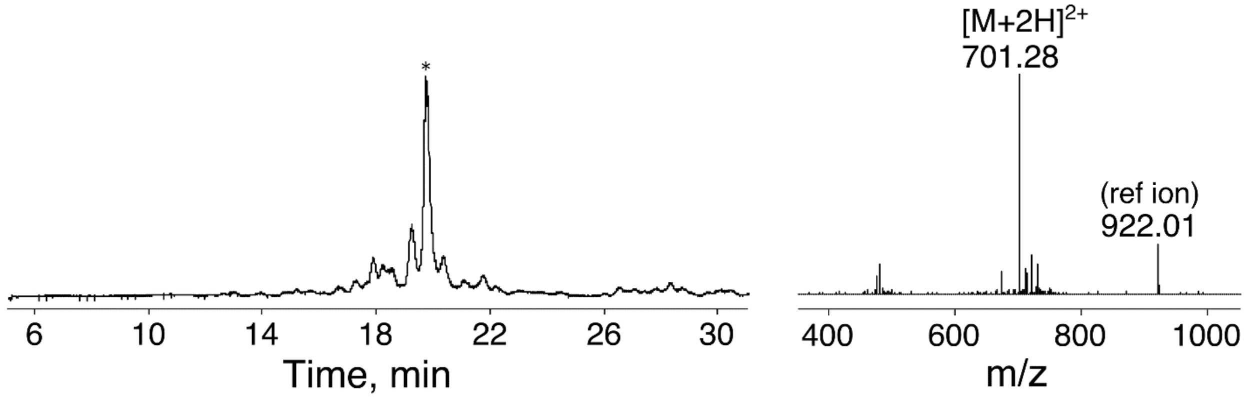


Figure S5. HPLC-MS (TIC) chromatogram for the crude H_2N- GCβWLDEDTFMGG-COOH on the left with a mass spectrum of major peak (labeled with an asterisk) on the right. Calc. monoisotopic mass = 1400.53 Da, Observed mass = 1400.54 Da.

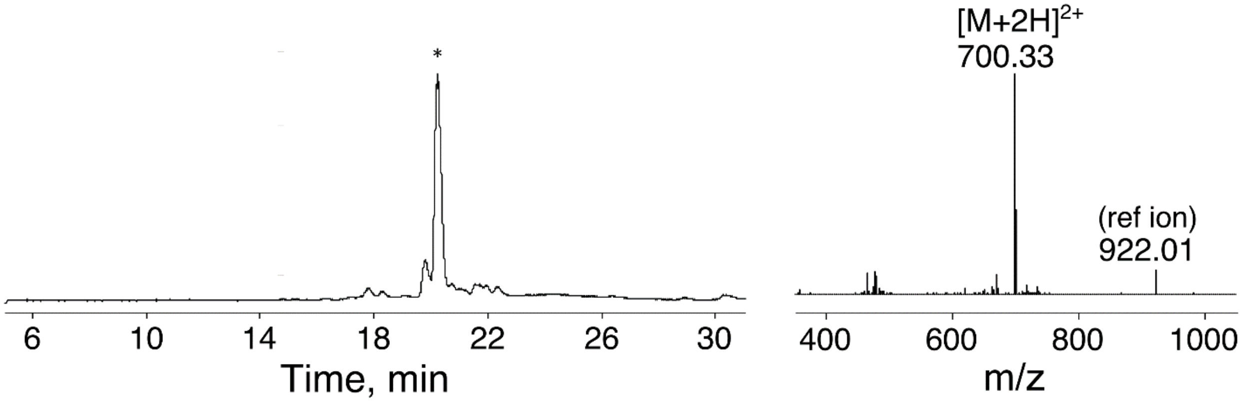


Figure S6. HPLC-MS (TIC) chromatogram for the crude H$_2$N- GCβWLDPSLFPHG-COOH on the left with a mass spectrum of major peak (labeled with an asterisk) on the right. Calc. monoisotopic mass = 1398.63 Da, Observed mass = 1398.64 Da.

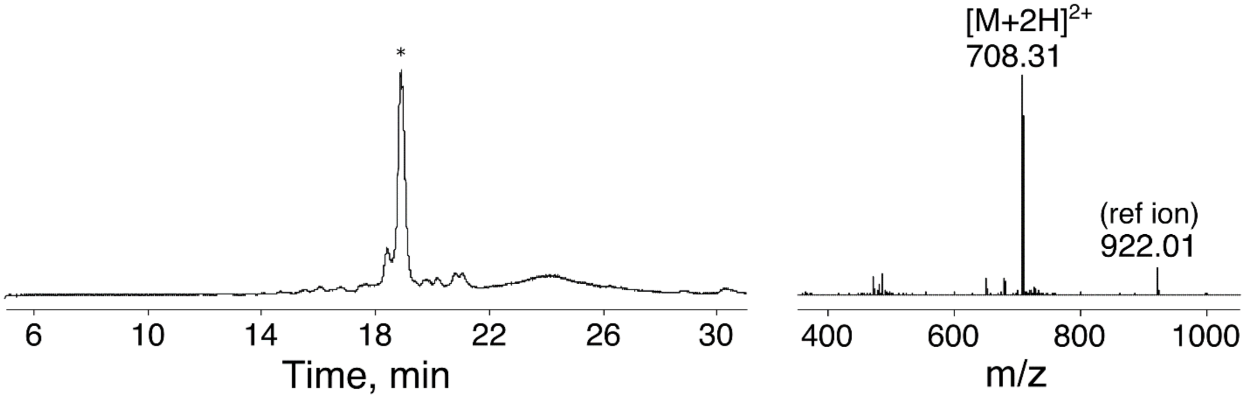


Figure S7. HPLC-MS (TIC) chromatogram for the crude H$_2$N- GCβWLDTDPFPHG-COOH on the left with a mass spectrum of major peak (labeled with an asterisk) on the right. Calc. monoisotopic mass = 1414.59 Da, Observed mass = 1414.61 Da.

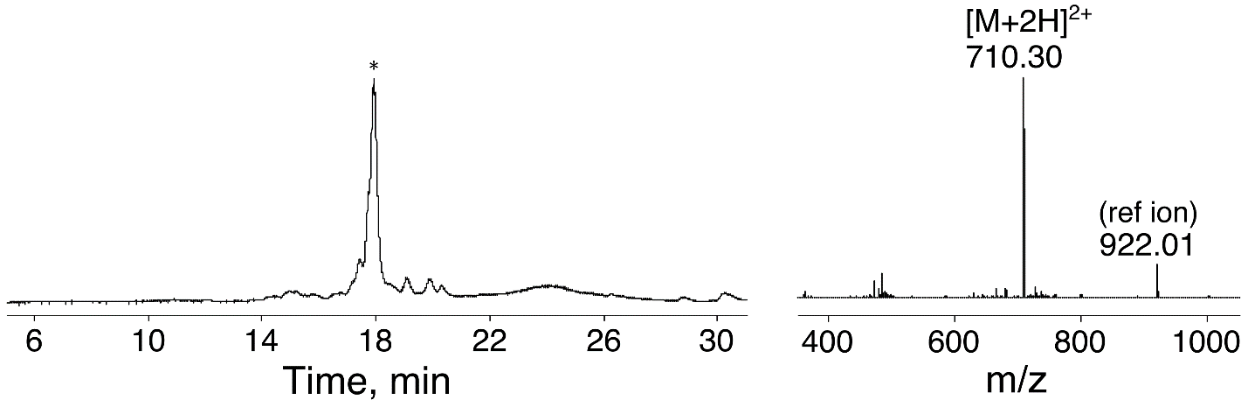


Figure S8. HPLC-MS (TIC) chromatogram for the crude H$_2$N- GCβWLDTSEFPHG -COOH on the left with a mass spectrum of major peak (labeled with an asterisk) on the right. Calc. monoisotopic mass = 1418.58 Da, Observed mass = 1418.59 Da.

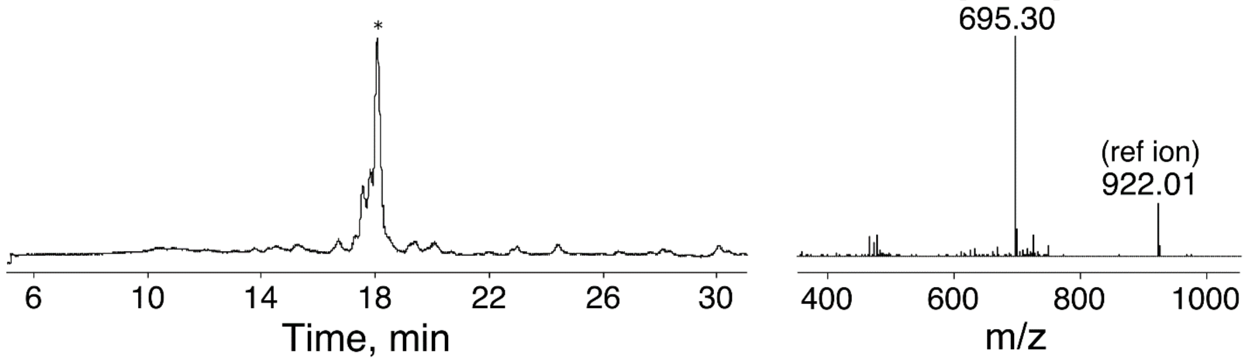


Figure S9. HPLC-MS (TIC) chromatogram for the crude H_2N- GCβWLSADEFPHG-COOH on the left with a mass spectrum of major peak (labeled with an asterisk) on the right. Calc. monoisotopic mass = 1388.57 Da, Observed mass = 1388.59 Da.

2.4. Library cleavage and nano-LC/MSMS analysis

2.4.1. PAM ester saponification

A deprotected, dried peptidyl resin bearing library peptides was suspended in water and sonicated until homogeneity. 2 µl aliquots containing 50-2000 beads were taken for analysis. The number of beads in each sample was counted manually under a bright-field microscope for samples containing less than 1000 beads or estimated for more complex suspensions. PAM ester saponification was carried out by adding 4 µl of 1M NaOH in water to the peptidyl resin suspensions. The cleavage reaction was allowed to proceed for 45 minutes at room temperature, after which it was quenched with 40 µl of 1% (v/v) TFA in water. The beads were spun down (1 min at 14000 rpm), and the supernatant was carried forward for nano-LC analysis.

2.4.2. nano-LC/MSMS analysis of library bead mixtures

Nano-LC/MSMS analysis was performed on Thermo Fisher Orbitrap Fusion Lumos Tribrid Mass Spectrometer coupled to Thermo Fisher EASY-nLC 1200 System equipped with Acclaim PepMap RSLC C18 column (250 mm x 75 µm ID, 2 µm 100Å silica). The standard nano-LC method was run at 40 °C and a flow rate of 300 nL/min with the following gradient: 1% of 80% acetonitrile in water with 0.1% formic acid added (solvent B') in water containing 2% methanol and 0.1% FA (solvent A') ramping linearly to 5% B' in A' over 2 minutes, followed by 5-61% B' in A' ramping linearly over 68 minutes, followed by 61-99% B' in A' ramping linearly over 5 minutes and finally 99% B' in A' for 5 minutes. MSMS acquisition over the course of the method duration was performed in a data-dependent style (Top N=15, z=2-10, intensity threshold = 10^5) with a dynamic precursor exclusion for 20 seconds after each scan. CID and HCD fragmentation spectra were acquired for every selected precursor ion. Orbitrap was used as a detection method for both primary (resolution=120000) and secondary (resolution=30000) mass spectra.

2.4.3. *De novo* peptide sequencing in PEAKS

De novo peptide sequencing was performed in PEAKS 7 or PEAKS 8 from Bioinformatics Solutions Inc. (ON, Canada). Sequencing data obtained as described in the section above was refined as follows. HCD and CID scans were merged within a 0.2 minute and 10 ppm window, mass precursor correction was performed, and primary mass filtration was performed as appropriate. De novo sequencing was performed allowing 15 ppm assignment errors and 0.05 Da individual fragment mass errors. For library 1 methionine oxide was selected as a variable PTM. For library 2, 2-aminobuitanoic acid was sequenced as a variable PTM on Gly, while Acp, Ach, Cha, Fph, Aph, Nap, Pfp, Phf and Cph were sequenced as fixed PTMs on unused Pro, Cys, Thr, Met, Leu, Asn, Glu, Trp and His, respectively. 15 candidate sequences were obtained for each preprocessed scan.

2.4.4. Post-*de novo* data analysis

After performing de novo sequencing as specified above, the list of all peptide candidates and a single top candidate peptide lists were exported as .csv files and further analyzed in Python 2.7.10. A number of open source libraries were used for parsing data and analyzing the outcomes: namely, Numpy (Stéfan van der Walt, S. Chris Colbert and Gaël Varoquaux, *Computing in Science & Engineering*, 13, 22-30, 2011), Pandas (Wes McKinney, *Proceedings of the 9th Python in Science Conference*, 51-56, 2010), Scipy (http://www.scipy.org/) and matplotlib (John D. Hunter, *Computing in Science & Engineering*, 9, 90-95, 2007).

First, working with a list of all peptide candidates, sequences not matching library design rules (sequence length, C-terminal Gly, correct monomers in every position) were eliminated from further consideration. Next, for scans with multiple remaining sequence candidates, a single peptide with highest ALC score per scan was retained, while the rest were excluded. After this, remaining sequences were labeled as "unique" and "non-unique" based on a number of criteria. Comparing peptides to each other, a number of attributes, including retention time difference, measured mass difference, and sequence distance (Hamming distance) were considered, and if peptides were found to be similar to each other, the one with lower ALC score was labeled as "non-unique". Finally, the list of unique sequences was refined further by a) identifying pairs of peptides with Hamming distance=1 and a Q/E mismatch, and eliminating sequences bearing “E” in the mismatched position; b) identifying pairs of H^+/Na^+ sequences and removing Na^+-derived ones; c) removing Met-oxide containing sequences if unoxidized ones were also present; d) identifying pairs of peptides with Hamming distance=1 and a Q/A or E/A mismatch, and eliminating sequences bearing “A” in the mismatched position (unidentified, fairly prominent side reaction). The list of remaining sequences was considered to be the end result of library decoding.

Technically, even for sparse libraries analyzed in this work, there is a non-zero probability that at least two beads in the sample will bear identical sequences: a fact that undermines the assumption that the number of sequences present in the sample equals to the number of beads. If this is the case, the workflow outlined above becomes less efficient, and would require additional modifications that were not explored. The probability that in a set of *n* randomly chosen beads from a greater pool that may contain as many as *d* sequences *at least two* beads will bear the same sequence can be estimated using the “birthday paradox” approximation. If $n \ll d$, the following formula is a good estimate for the resulting probability: $p(n,d) = 1 - e^{\frac{-n^2}{2d}}$. With $n = 660$ and $d = 1.34 \cdot 10^8$ (theoretical diversity of library 1) this probability is ~0.0016. We considered this value to be low enough to disregard the possibility of duplicate sequences in our samples.

3. Experimental data

3.1. Analysis of a library 1 sample containing 306 beads

A sample containing 306 beads from library 1 was analyzed in a manner described in section 2.4. Additional data analysis was performed following the procedure for a 660 bead sample outlined in the main text and is summarized in Figure S10. Results of this analysis corroborate those obtained for the 660 bead sample. The full sequence table containing identified peptides is provided in Appendix II.

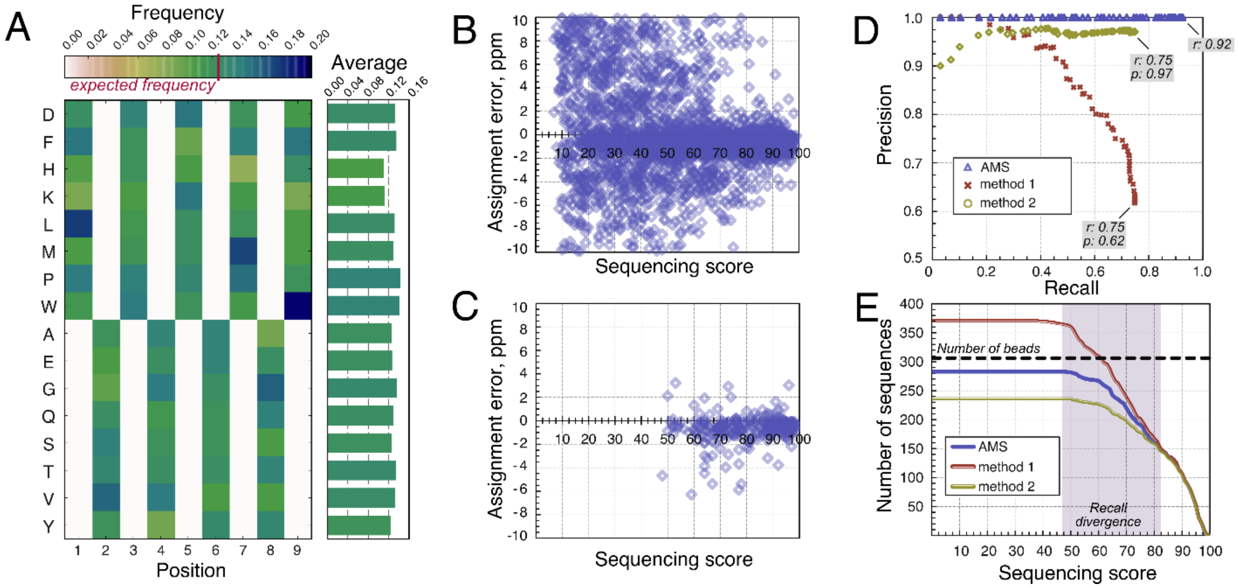


Figure S10. Evaluation of the role of AMS in increasing the confidence in sequencing results. All data are from the 306-bead sample (283 unique sequences identified). A) Color-coded positional amino acid frequency is shown on the left, and the mean amino acid frequencies are plotted on the right. Each non-zero cell in the matrix has the expected value of 0.125, and the observed values map close to it. B) Sequencing quality scatterplot for the unfiltered PEAKS output. C) Sequencing quality scatterplot for the final filtered data set. Most peptides with low sequencing score and/or large assignment errors are removed during post-processing. D) Precision-recall curves for different data filtration methods. Method 1 is inferior to AMS in both precision and recall. E) Total number of sequences recovered as a function of sequencing score for different data filtration methods. Results diverge in the region of medium (45-85) sequencing scores.

3.2. Matching fragmentation spectra from library and authentic peptides

For the experiments described below, a corresponding library was analyzed as described in section 2.4, except MSMS conditions differed in the following way. Agilent 6550 iFunnel Q-TOF LC-MS coupled to Agilent 1290 Infinity HPLC system equipped with Phenomenex Jupiter C4 column (150 x 1.0 mm ID, 5 µm 300Å silica) was used to perform the analysis. The HPLC was performed at 40°C and a flow rate of 0.1 mL/min with the following gradient: 1% acetonitrile with 0.1% formic acid added (FA, solvent B) in water with 0.1% FA (solvent A) for 5 min, 1-41% B in A ramping linearly over 65 min, and then 70% B in A for 7 minutes. The entirety of the sample was analyzed. MSMS acquisition over the course of the method duration was performed in a data-dependent style (Top N=10, z=2-10, intensity threshold = 7500) with a dynamic precursor exclusion for 30 seconds after each scan. CID fragmentation spectra at two different collision energies were acquired for every selected precursor ion. Authentic peptides were analyzed in an analogous fashion. Appropriate raw CID spectra were manually overlaid and are demonstrated in Fig. S11-17.

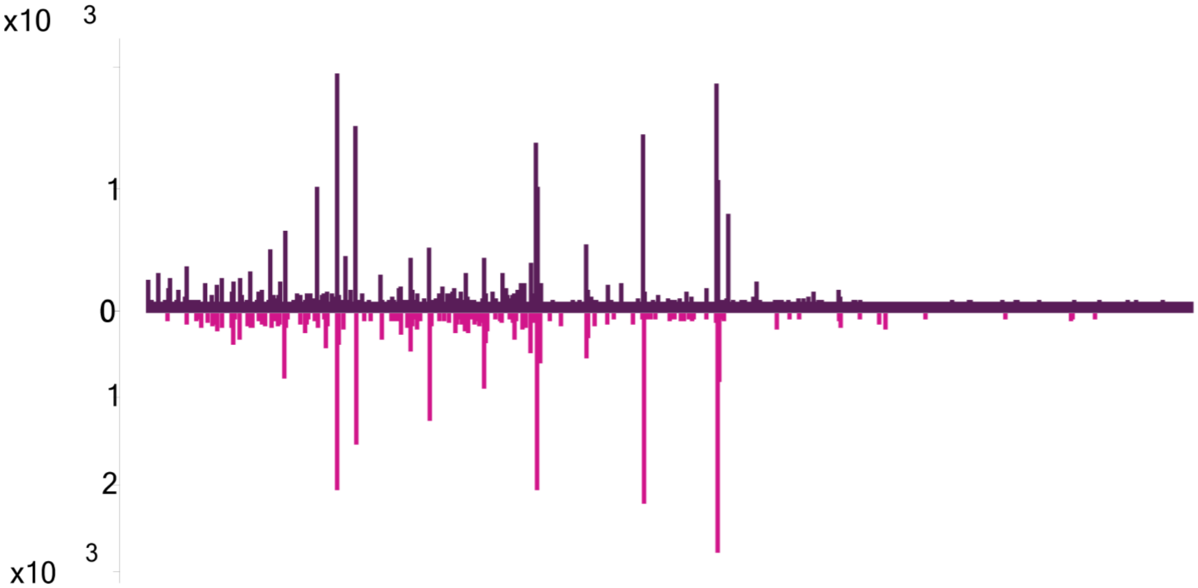


Figure S11. Overlaid raw CID fragmentation spectra (collision energy = 20.0 eV, precursor ion: 695.30 Da/e) for GCβWLSADEFPHG (β = β-alanine) peptide identified from a library sequencing analysis (purple color, top spectrum) and its authentic, separately re-synthesized counterpart (pink color, bottom spectrum).

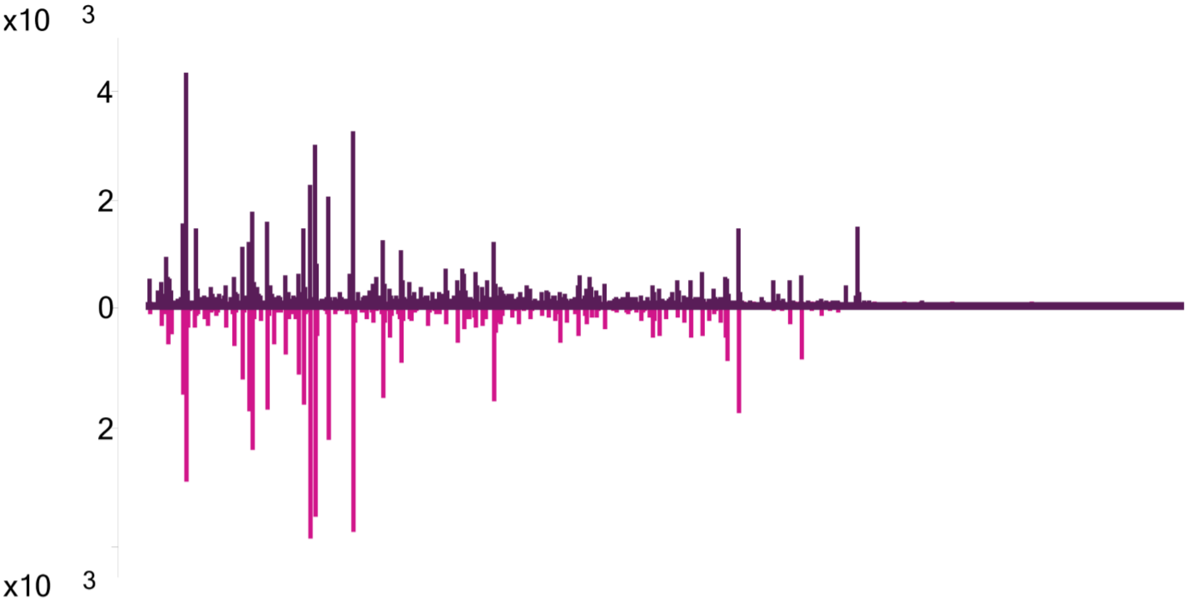


Figure S12. Overlaid raw CID fragmentation spectra (collision energy = 22.2 eV, precursor ion: 686.29 Da/e) for GCβFLDEGYGPWG (β = β-alanine) peptide identified from a library sequencing analysis (purple color, top spectrum) and its authentic, separately re-synthesized counterpart (pink color, bottom spectrum).

Figure S13. Overlaid raw CID fragmentation spectra (collision energy = 22.8 eV, precursor ion: 701.28 Da/e) for GCβWLDEDTFMGG (β = β-alanine) peptide identified from a library sequencing analysis (purple color, top spectrum) and its authentic, separately re-synthesized counterpart (pink color, bottom spectrum).

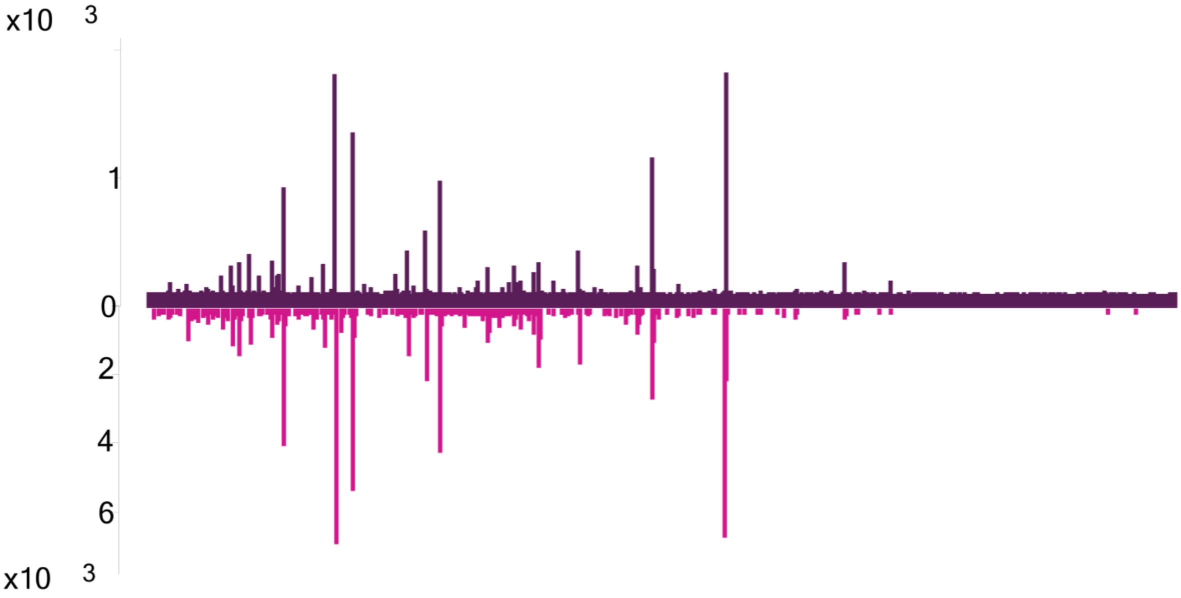


Figure S14. Overlaid raw CID fragmentation spectra (collision energy = 23.0 eV, precursor ion: 708.31 Da/e) for GCβWLDTDPFPHG (β = β-alanine) peptide identified from a library sequencing analysis (purple color, top spectrum) and its authentic, separately re-synthesized counterpart (pink color, bottom spectrum).

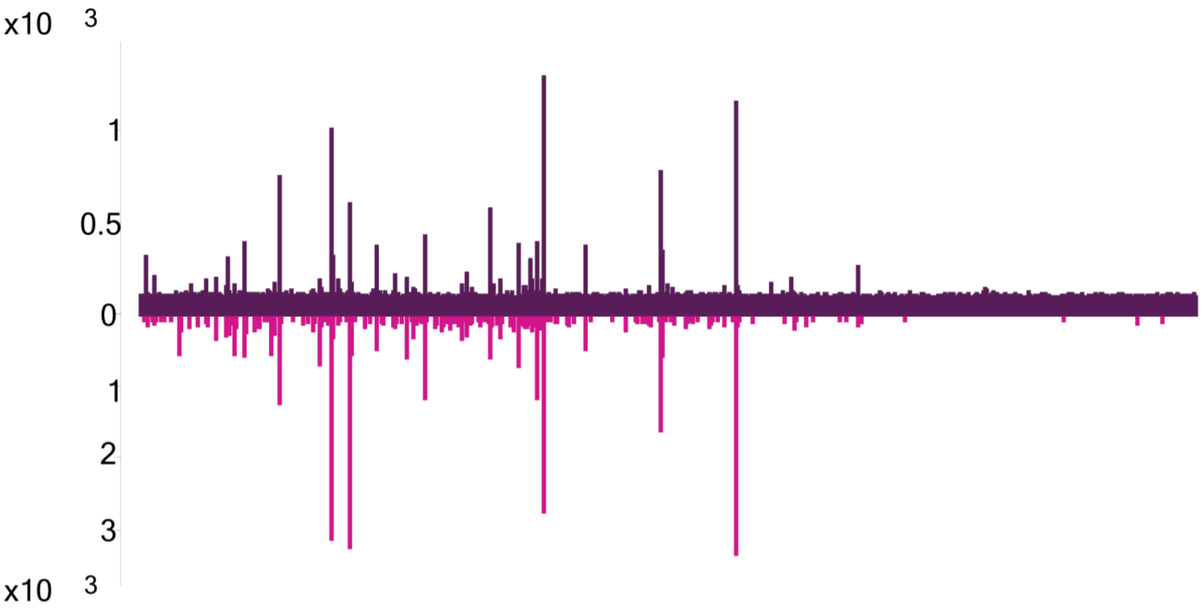


Figure S15. Overlaid raw CID fragmentation spectra (collision energy = 20.6 eV, precursor ion: 710.30 Da/e) for GCβWLDTSEFPHG (β = β-alanine) peptide identified from a library sequencing analysis (purple color, top spectrum) and its authentic, separately re-synthesized counterpart (pink color, bottom spectrum).

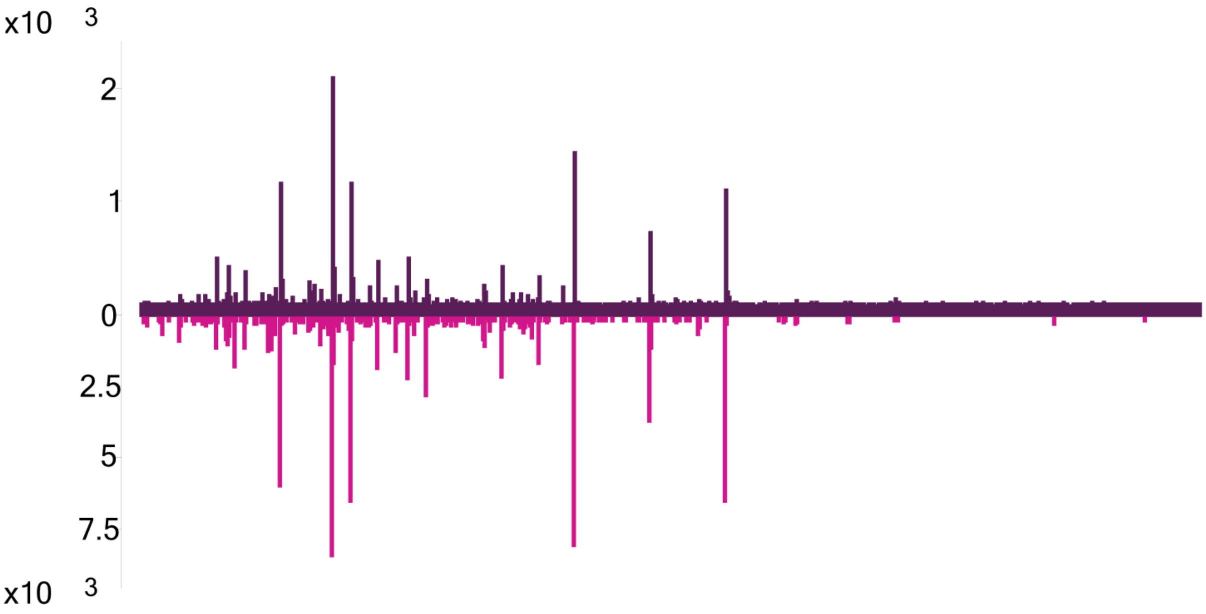


Figure S16. Overlaid raw CID fragmentation spectra (collision energy = 22.7 eV, precursor ion: 700.33 Da/e) for GCβWLDPSLFPHG (β = β-alanine) peptide identified from a library sequencing analysis (purple color, top spectrum) and its authentic, separately re-synthesized counterpart (pink color, bottom spectrum).

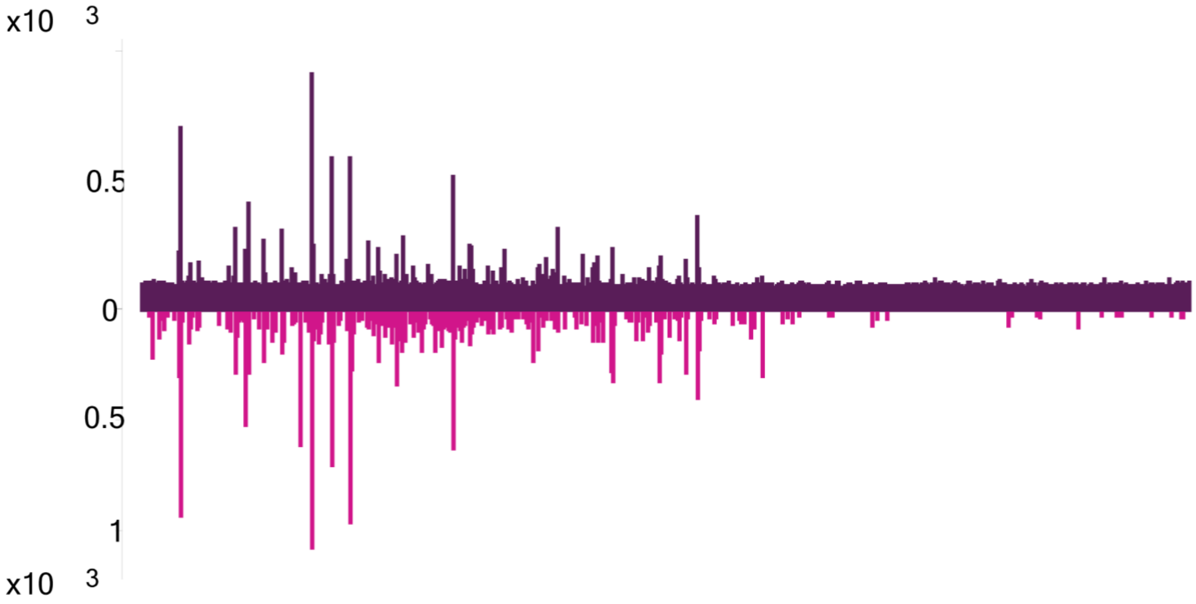


Figure S17. Overlaid raw CID fragmentation spectra (collision energy = 21.0 eV, precursor ion: 653.76 Da/e) for GCβWADESAGPWG (β = β-alanine) peptide identified from a library sequencing analysis (purple color, top spectrum) and its authentic, separately re-synthesized counterpart (pink color, bottom spectrum).

3.3. Construction of alternating monomer sets

Monomer subsets are constructed by dividing the total monomer pool into two subsets of equal size:

$$\mathcal{M}_1 \in \mathcal{M},\ \ \mathcal{M}_2 = \mathcal{M} \cap \mathcal{M}_1 \qquad (1)$$

such that

$$\forall\, p_1, p_2\ \in\ \mathcal{M}_1, \forall\, q_1, q_2\ \in\ \mathcal{M}_2 \colon \big| |m(p_1) - m(p_2)| - |m(q_1) - m(q_2)| \big| > \varepsilon, \qquad (2)$$

where *m(p)* is molecular weight of a monomer p in Da, and ε is a constant (in Da) determined by the accuracy of the mass spectrometer used for sequencing. We used $\varepsilon=0$ to construct our monomer subsets, but the values of up to 0.01 Da yield identical results for proteogenic amino acids.

Table S1 provides molecular weights for all possible ss_1-ss_2 dipeptide subsequences. As evident from the table, every dipeptide has unique mass, which eliminates ambiguous dipeptide assignments.

Table S1. Monoisotopic masses in Da of all dipeptides encodable with the alternating monomer set library design. ss$_1$: amino acid subset 1, ss$_2$: amino acid subset 2.

ss$_2$ ss$_1$	A	E	G	Q	S	T	V	Y
D	186.06	244.07	172.05	243.09	202.06	216.07	214.10	278.09
F	218.11	276.11	204.09	275.13	234.10	248.12	246.14	310.13
H	208.10	266.10	194.08	265.12	224.09	238.11	236.13	300.12
K	199.13	257.14	185.12	256.15	215.13	229.14	227.16	291.16
L	184.12	242.13	170.11	241.14	200.12	214.13	212.15	276.15
M	202.08	260.08	188.06	259.10	218.07	232.09	230.11	294.10
P	168.09	226.10	154.07	225.11	184.08	198.10	196.12	260.12
W	257.12	315.12	243.10	314.14	273.11	287.13	285.15	349.14

3.4. Amino acid frequency distribution χ^2-test for the sample of 660 library 1 beads

As Table S2 indicates, we found no evidence that there is statistically significant difference between assigned and designed amino acid frequencies (P-value=0.42) in the studied sample (n=587).

Table S2. χ^2-test statistic table for the amino acid distribution in the sample of 660 library 1 beads

	pos1	pos2	pos3	pos4	pos5	pos6	pos7	pos8	pos9	Sum	P-value
D	0.18		1.54		5.12		0.74		0.39	7.97	0.09
F	2.92		1.76		0.60		0.60		0.60	6.47	0.17
H	4.60		0.00		2.09		1.20		0.39	8.28	0.08
K	0.26		0.74		0.00		0.18		0.55	1.74	0.78
L	0.04		2.53		0.18		0.96		2.53	6.23	0.18
M	0.16		0.79		1.26		0.60		0.60	3.41	0.49
P	0.74		0.55		1.26		0.60		1.47	4.62	0.33
W	2.53		0.55		0.09		0.04		0.01	3.22	0.52
A		0.08		0.43		0.00		0.03		0.54	0.91
E		0.04		0.08		0.43		0.29		0.84	0.84
G		0.03		1.01		1.01		6.82		8.88	0.03
Q		0.60		0.08		0.55		0.96		2.18	0.53
S		0.08		2.09		0.04		0.39		2.59	0.46
T		0.26		0.03		0.03		1.84		2.15	0.54
V		2.53		0.04		0.60		0.01		3.17	0.37
Y		1.76		0.09		2.82		5.80		10.47	0.01
Sum	11.42	5.37	8.48	3.84	10.60	5.48	4.90	16.13	6.54	72.76	0.42
P-value	0.12	0.62	0.29	0.80	0.16	0.60	0.67	0.02	0.48	0.42	

3.5. Peptide separation on nano-LC

To illustrate the ability of nLC to separate mixtures containing hundreds of peptides we analyzed the 306 bead sample of library 1 peptides (section 3.1). To this end, we overlaid the chromatogram with the peptide identification timeline (the list of retention times for parsed sequences identified from the analysis) as shown in Fig. S18A. We found that that the chromatogram maintains individual features, and that peptides are identified throughout the duration of the nLC gradient. Additionally, we manually analyzed primary mass spectra obtained for this and other samples to ensure that individual ion signals do not consistently overlap, which becomes an important consideration during the isolation of individual precursor ions for further CID and HCD fragmentation. Two characteristic primary spectra observed throughout the course of the study are shown in Fig. S18B and S18C. Based on these observations we concluded that the use of nLC for the analysis of complex mixtures of synthetic peptides is fully adequate.

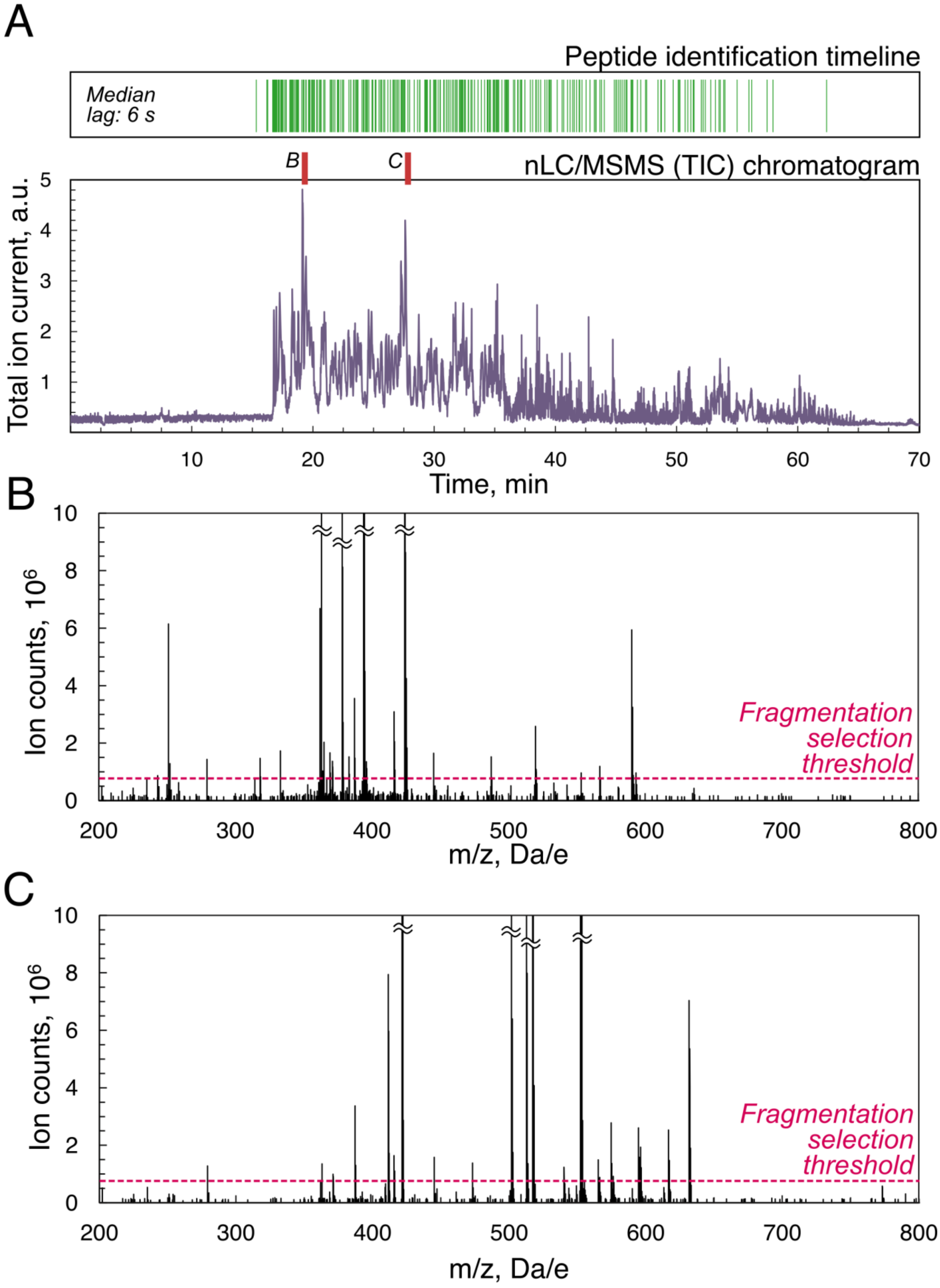

A
Peptide identification timeline
Median
lag: 6 s
B
C
nLC/MSMS (TIC) chromatogram
Total ion current, a.u.
5
4
3
2
1
10
20
30
40
50
60
70
Time, min
B
10
8
6
4
2
0
Ion counts, 10^6
Fragmentation
selection
threshold
200
300
400
500
600
700
800
m/z, Da/e
C
10
8
6
4
2
0
Ion counts, 10^6
Fragmentation
selection
threshold
200
300
400
500
600
700
800
m/z, Da/e

Figure S18. A) Overlay of a nLC/MSMS (TIC) chromatogram for the 306 bead sample (section 3.1) containing library 1 peptides with the peptide identification timeline (each vertical line represents an identified peptides; retention time values are taken from Appendix II). Peptides are identified throughout the gradient run time (median time between successive peptide identification events is 6 sec, mean value is 10 sec). B) Primary mass spectrum snapshot at 19.13 min of the LCMS run shown in A). Four most intense peaks are out of scale. The spectrum is clean with little to no m/z overlap between eluting peptides, which allows individual isolation of precursor ions for fragmentation. C) Analogously to B), primary mass spectrum snapshot at 27.61 min.

Appendix I. Sequences identified from the 660 bead sample

ALC	Area	Mass	Peptide	RT	Scan	m/z	ppm	z
70	3.96E+04	1021.4828	PGKVPSHEDG	7.97	1041	341.5004	-1.3	3
62	6.16E+04	1132.5049	HTPAHVHYDG	7.98	1044	378.5075	-1.4	3
83	6.49E+05	1164.604	HVLSHQPYKG	15.85	2076	389.2073	-1.2	3
51	7.56E+05	1132.6604	KVLGKQKEFG	15.88	2082	378.5596	-0.9	3
55	2.37E+05	1140.4736	HGDAFYHTHG	15.96	2094	381.1639	-1.2	3
88	1.52E+05	1146.5571	PYHVLSHTHG	16.06	2111	383.1917	-1.1	3
60	1.20E+05	1162.5806	KSKYLAHEMG	16.07	2114	388.5327	-1.5	3
80	5.77E+05	1124.5549	HAMAHQKVFG	16.23	2157	375.8578	-0.9	3
71	3.87E+05	1269.5527	HEFYHSHEKG	16.23	2159	424.1903	-0.6	3
51	1.34E+05	1195.5193	HEHSMAKYHG	16.24	2162	399.5124	-1.2	3
81	2.44E+06	1172.5186	MGKTHGWYHG	16.3	2181	391.8455	-1.1	3
89	2.59E+05	1155.5671	HTHSFEKTLG	16.31	2185	578.7894	-0.4	2
97	2.36E+06	1192.5989	LSHTKVHEWG	16.38	2209	597.3052	-0.3	2
79	2.28E+07	1123.5266	HVKEMGHVMG	16.38	2211	375.515	-0.9	3
91	2.31E+06	1068.6113	MALVKVKSHG	16.39	2213	357.21	-0.8	3
95	1.88E+07	1115.5513	HYLGHGFTKG	16.44	2236	372.8564	-1.2	3
75	4.59E+07	1094.7175	KVKVLQKVPG	16.45	2243	365.912	-0.8	3
78	1.11E+07	1094.5542	HTMTPQKVPG	16.46	2245	548.2831	-0.2	2
86	4.84E+06	1228.5261	DGHYHEWTKG	16.5	2266	410.5146	-1.3	3
85	3.76E+07	1213.6277	KVWVHTMEKG	16.55	2287	405.5483	-1.5	3
63	4.94E+06	1234.573	FQHQKTFQDG	16.55	2291	618.292	-0.7	2
83	4.49E+06	1135.5081	HELTHQMSPG	16.56	2295	568.7596	-0.7	2
86	2.89E+06	1247.5427	MEHQMYPQKG	16.56	2299	624.7768	-0.8	2
96	8.03E+06	1182.5208	FTHADYHVHG	16.58	2305	395.1796	-1.1	3
91	8.04E+06	1203.6145	MYMGKVKYKG	16.6	2316	402.2108	-1.0	3
88	2.52E+07	1255.6746	KYKVFQKQMG	16.61	2320	419.5643	-0.6	3
74	1.52E+07	1085.5154	HSWGLVHGHG	16.64	2337	362.8447	-0.8	3
95	1.05E+07	1110.5378	FVDSKAKEMG	16.65	2339	556.2748	-0.4	2
90	2.33E+06	1242.6396	FEKAKSKYWG	16.65	2343	415.2193	-0.8	3
92	1.92E+06	1103.54	FTKYPAPSHG	16.7	2368	552.776	-0.1	2
94	1.80E+07	1260.5522	DYKVDQHYHG	16.73	2385	421.1905	0.1	3
84	1.93E+07	1127.4641	MYHGPQMAHG	16.74	2391	376.8275	-0.9	3
60	9.07E+05	964.4977	KAPVDGPQPG	16.78	2406	483.2549	-0.4	2
96	1.25E+06	1244.5396	KYHEHTWGMG	16.79	2412	623.2758	0.1	2
84	1.76E+06	1055.54	PAKYLSPSHG	16.84	2433	352.8528	-1.0	3
56	5.27E+06	1162.5439	KQWAKEDAMG	16.89	2456	582.278	0.0	2
60	3.60E+06	1095.6223	KQHVKVMGLG	16.9	2460	548.8173	0.1	2
92	1.25E+07	1062.5093	PQLQHTPADG	16.9	2462	532.2607	-0.1	2

90	7.24E+05	1236.5234	WEMSKYPSHG	16.92	2474	619.2676	0.0	2
98	3.40E+06	1222.6345	KVHYKYLTDG	16.93	2480	612.3232	0.1	2
97	2.18E+06	1166.6006	PEKTLYMTKG	16.98	2500	584.3062	-0.2	2
93	2.53E+06	1157.5498	DTMQLTKQHG	16.98	2502	579.7808	-0.1	2
62	3.70E+05	998.5583	KAMVPAPTKG	17.01	2516	333.859	-1.0	3
95	1.32E+07	1136.5898	KYLAKTMEPG	17.11	2559	569.3013	0.6	2
94	1.79E+06	1149.5488	KEMTKSWSPG	17.12	2561	575.7808	0.6	2
87	6.71E+05	1198.6135	FYFTKTKAHG	17.18	2586	300.6595	-1.7	4
90	1.20E+06	1213.6455	FVKQHEKELG	17.23	2605	405.5544	-1.3	3
97	1.73E+06	1077.4912	LGKADYHSMG	17.24	2612	539.7518	0.3	2
94	5.29E+06	1104.5386	LQHAKSMSFG	17.26	2620	553.2756	0.5	2
91	1.90E+06	1177.5374	FQMQHTKAMG	17.3	2635	589.7747	0.0	2
87	2.91E+06	1153.5261	HSKAMYLTMG	17.33	2650	577.7689	-0.4	2
96	2.49E+07	1125.5488	HVLEPSMEKG	17.4	2675	563.7803	-0.2	2
96		1171.5774	FVDVKAHYHG	17.42	2686	586.7947	0.1	2
95	1.37E+06	1244.5574	WTHSWTKQDG	17.5	2719	623.2844	-0.4	2
94	3.48E+06	1190.572	PYHQFVDTKG	17.53	2736	596.2916	-0.7	2
77	1.16E+07	1109.5176	DTMTKGWSKG	17.64	2781	370.8453	-1.0	3
93	5.65E+06	1183.5508	FGKEKEDQFG	17.65	2785	592.7814	0.0	2
41	2.62E+05	1011.5025	DGLTFGFAKG	17.65	2789	506.755	-4.8	2
93	1.14E+06	1291.6211	HQWSHVKQWG	17.67	2797	646.8165	0.1	2
96	4.71E+06	1002.5345	DEKGLGKSLG	17.74	2825	502.2732	-0.6	2
97	6.59E+05	1110.5413	MSMELTKSKG	17.87	2883	556.2766	-0.2	2
87	2.50E+07	1077.4993	PQHGFGLEHG	17.89	2890	360.1725	-1.2	3
82	1.74E+07	1073.5505	KTDVKSWGPG	17.89	2892	537.7814	0.0	2
94	1.14E+07	1083.4656	LAMQHEDSPG	17.9	2894	542.7386	-0.5	2
89	2.91E+06	1061.5042	WAHTLSPGHG	17.9	2896	531.7581	-0.1	2
95	1.54E+06	1011.4985	DGLTDAKVHG	18.04	2957	506.7552	-0.5	2
95	2.29E+06	1071.5195	DVDSLTKTHG	18.12	2990	536.7659	0.1	2
88	4.66E+05	1225.5913	WSKQMSFQKG	18.14	2999	613.8013	-0.4	2
77	2.43E+06	1106.5508	WTPGPVKEHG	18.18	3014	554.2809	-1.0	2
94	1.02E+07	1015.4909	KVPGHSMGFG	18.2	3023	508.7513	-0.5	2
93	2.55E+07	1137.5276	FTHAPSMYKG	18.22	3030	380.1821	-0.5	3
94	2.45E+07	1038.4739	HAMAMTHALG	18.24	3040	520.243	-0.1	2
82	2.55E+06	1130.5508	WTHSKAFTPG	18.25	3046	566.2814	0.0	2
81	2.40E+06	1156.5586	MEKGKTFYPG	18.26	3050	579.2852	-0.2	2
93	5.99E+07	972.5029	LVPGHEPAPG	18.5	3156	487.2573	-0.8	2
94	2.94E+06	1024.4548	PGHGMSHVFG	18.52	3166	513.2332	-0.8	2
78	4.04E+07	1016.496	MALQKGDTPG	18.59	3198	509.2538	-0.8	2
94	1.55E+06	1200.5046	DEWVDEHSKG	18.64	3224	601.2576	-1.1	2
84	1.61E+07	1139.5547	MTPVWGKQHG	18.7	3246	380.8574	-1.7	3

96	3.56E+06	1126.6135	PYKQHTLALG	18.71	3252	564.3123	-1.0	2
87	4.63E+07	1182.5935	FGHVWQKQPG	18.75	3271	395.2038	-1.1	3
95	2.00E+07	1091.5037	PSFSKGFEHG	18.79	3288	364.8407	-1.0	3
96	2.69E+06	1130.572	FSHVDQLTKG	18.8	3290	566.2919	-0.2	2
94	2.29E+06	1234.5176	DEDYKYMSKG	18.88	3329	618.2643	-0.6	2
96	5.52E+06	1065.4993	LGDQHGHVFG	19.01	3384	533.7554	-0.6	2
86	3.86E+06	1187.5029	HQHSLYDTMG	19.02	3390	594.7557	-2.9	2
94	1.11E+07	1085.5505	LVFEHADAKG	19.09	3422	543.7814	0.0	2
57	5.00E+05	1193.6016	KYFGKVHQMG	19.13	3440	398.873	-1.6	3
57	3.86E+06	1122.5168	LGDQWAMVFG	19.17	3455	375.1793	1.6	3
83	1.92E+07	1225.5264	HAWQHQDTFG	19.24	3487	613.769	-0.1	2
89	5.20E+05	1137.5276	PTHGMTFYKG	19.25	3491	569.7694	-0.7	2
96	1.27E+06	1235.5723	HEHYFAKTFG	19.26	3493	618.7923	0.4	2
96	4.07E+06	1129.5767	PTLEKTFTHG	19.34	3561	565.7944	0.1	2
76	3.60E+06	1075.5483	KAKTPSWAMG	19.34	3531	538.7802	-0.2	2
87	2.42E+07	993.4702	MSPGPALQHG	19.54	3615	497.741	-0.5	2
56	1.28E+06	1006.3814	HADADAFGMG	19.55	3619	504.1964	-1.0	2
91	3.96E+07	1089.5608	FYLGHAPTKG	19.59	3634	364.1929	-1.3	3
81	1.53E+07	1071.5237	PYPEKAPVDG	19.59	3636	536.7677	-0.4	2
52	5.33E+05	1256.5938	WTPEHQFQKG	19.6	3642	629.3035	1.1	2
61	1.86E+07	1231.5444	HYWEKGMQPG	19.63	3653	616.7777	-0.7	2
95	1.25E+06	1151.5068	PYFSMGKEHG	19.69	3682	576.7589	-0.9	2
86	6.88E+06	1168.5256	KEKYPEMGMG	19.75	3708	585.2684	-0.6	2
80	6.59E+06	1078.4788	DTMQPAKTMG	19.78	3721	540.2451	-0.8	2
94	5.86E+06	1003.4822	DTPGLTDTKG	19.91	3778	502.7476	0.7	2
89	2.68E+06	1210.5442	MSHEFTFQKG	19.92	3782	404.521	-0.4	3
95	3.04E+07	1190.5391	HVDEKQMTFG	19.95	3795	596.2758	0.4	2
97	9.34E+06	1114.5593	LAWTKTHAMG	20.09	3858	558.2854	-0.6	2
98	2.64E+07	1080.491	FGMQKTPTDG	20.1	3862	541.2515	-0.1	2
82	1.46E+07	1163.5359	DQPVFVHEHG	20.11	3866	582.7734	-1.0	2
55	7.84E+06	1082.5508	KGHQFAPELG	20.35	3969	542.2814	-0.2	2
93	3.40E+06	1055.4519	DVDQDGHTLG	20.36	3979	528.7318	-0.5	2
96	3.60E+06	1147.5696	LTKEMGLYHG	20.44	4011	574.7905	-0.5	2
97	2.54E+07	1063.4836	HVLGWSDGHG	20.47	4025	532.7476	-0.6	2
91	6.41E+06	1132.5334	KTDQFAMVHG	20.54	4055	567.2726	-0.2	2
76	2.34E+06	1163.4224	DEDTMTHQMG	20.68	4119	582.7174	0.4	2
94	2.28E+07	1073.4236	PGMGHEFQDG	20.69	4124	537.7175	-0.7	2
98	2.52E+06	1149.5818	PAWEFSKTKG	20.7	4126	575.7965	-0.7	2
95	4.84E+07	1034.5298	HALGHYPALG	20.7	4128	518.2706	-0.9	2
91	6.72E+06	1108.4529	DQKSMSMEPG	20.83	4183	555.2321	-0.8	2
58	4.42E+06	1162.5659	FTDYKGKTFG	20.91	4220	388.528	-0.9	3

93	6.98E+06	926.3916	DGLGPGHSMG	20.93	4229	464.2019	-0.3	2
97	1.67E+07	1121.5327	HYMGPVFSKG	21.02	4269	561.7717	-1.2	2
83	6.91E+06	1240.5083	PEHQHGWYMG	21.03	4271	621.2595	-1.0	2
65	1.46E+06	1128.4395	DEMVHEDTPG	21.11	4305	565.2251	-1.2	2
94	4.61E+06	1225.5801	LTHYFEKTMG	21.23	4355	613.7955	-0.7	2
93	2.54E+06	1127.4785	WTFSHADAHG	21.24	4358	564.7449	-0.7	2
90	8.98E+06	990.444	DADGLGKQMG	21.38	4417	496.2278	-0.8	2
92	1.59E+06	1141.5703	WQHVLGMSKG	21.42	4432	571.7908	-0.7	2
81	9.31E+06	1191.5771	KSDTKEWELG	21.44	4441	596.7943	-0.4	2
90	2.42E+07	1136.4709	HSWYDGKGMG	21.61	4515	569.2415	-0.1	2
78	4.72E+06	1044.4148	DYHADVDGPG	21.62	4517	523.2134	-0.2	2
67	5.65E+05	1102.5559	LSHGKAWTFG	21.69	4571	552.2841	0.1	2
93	2.78E+06	1092.4758	DSKQMALEDG	21.64	4527	547.2437	-0.5	2
87	1.70E+06	1048.4824	KTFAPQDADG	21.67	4538	525.2471	-0.4	2
81	3.01E+07	936.4124	DVPGPAHGMG	21.7	4555	469.2122	-0.6	2
50	4.57E+06	1164.52	DEPVHEHVFG	21.73	4565	389.1793	-1.3	3
96	1.90E+07	1154.5906	HVWVMTKTPG	21.77	4584	578.3011	-0.4	2
95	1.71E+06	1256.5574	HEDAWQKTWG	21.78	4588	629.2844	-0.2	2
89	6.55E+06	1233.6506	WVFVKQDQKG	21.89	4641	617.8307	-0.8	2
54	1.17E+05	1048.5454	HALAHYPALG	21.91	4647	525.2786	-0.4	2
96	7.05E+06	1147.5662	FTFVKSPEHG	21.93	4658	574.7887	-0.7	2
94	5.55E+06	1116.5273	PVMGPTWEKG	21.96	4668	559.2692	-0.9	2
57	5.23E+06	1137.531	HSMAKYLTMG	21.98	4677	569.7715	-0.1	2
88	2.89E+07	1106.5356	LQLADEPQHG	21.99	4681	554.2736	-0.6	2
88	2.95E+07	1127.5513	WEPVHAPVHG	22.04	4704	376.8566	-0.6	3
96	1.07E+06	1189.5374	KSMVMQWSHG	22.06	4714	595.7741	-0.9	2
95	6.43E+06	1101.6545	PQLGKVKYLG	22.12	4740	551.8333	0.0	2
83	9.95E+06	1141.5801	MSHEKVLELG	22.16	4757	571.7961	0.0	2
95	3.10E+07	1210.6135	PTKQFGWYKG	22.16	4761	404.5438	-1.0	3
93	3.33E+07	1136.5171	PVFEKSMQDG	22.25	4799	569.2644	-0.3	2
89	9.99E+06	1096.5916	KYKGFTPSLG	22.32	4830	549.3018	0.0	2
76	4.98E+07	1099.5298	FVHQLSDTPG	22.37	4849	550.7711	0.3	2
95	3.05E+07	1142.4451	PGMQWEHSDG	22.37	4851	572.2283	-0.4	2
81	3.99E+07	1114.5017	HAMVFGHYPG	22.54	4926	558.2561	-1.4	2
94	1.12E+07	1164.52	KTHQDEFGFG	22.57	4941	583.2654	-1.0	2
95	6.87E+06	1192.5513	KQFSFVDEHG	22.58	4945	597.2813	-0.5	2
96	5.20E+07	1101.5608	FAKVPEHAFG	22.6	4954	368.1932	-0.4	3
95	8.63E+06	1254.5525	HTMTKTMYWG	22.6	4956	628.2821	-0.1	2
86	7.52E+06	1041.5464	MVHVKGMALG	22.64	4973	521.7791	-0.4	2
62	3.16E+05	1049.5142	LQLADEHAPG	22.69	4993	525.7632	0.0	2
72	3.92E+07	1049.4565	HAWADAPEPG	22.78	5031	525.7342	-0.4	2

79	6.23E+06	1150.4966	DTWEPTKAMG	22.79	5038	576.2535	-1.4	2
93	2.70E+07	1139.5134	PYDYDVPSKG	22.83	5053	570.7624	-0.6	2
78	1.77E+07	1013.5757	LAPVKTDTLG	22.84	5057	507.7937	-0.7	2
89	3.02E+06	1273.5649	FQKQDEMYLG	22.95	5109	637.788	-0.6	2
95	2.49E+06	1219.5444	WGMVDQKYHG	23.1	5172	610.7779	-0.4	2
94	6.35E+07	1087.5371	PAMVKEPYPG	23.1	5174	544.7745	-0.2	2
87	1.20E+06	1139.5798	WSKGFVMTKG	23.11	5176	380.8659	-1.2	3
93	2.56E+06	1247.6121	WVKEWGKQMG	23.11	5178	624.8118	-0.2	2
83	3.80E+06	1095.5825	LSWGKALQHG	23.14	5189	548.7972	-0.3	2
97	1.67E+07	1104.5308	PQMVMTKVDG	23.17	5200	553.2712	-0.4	2
86	2.02E+06	1238.5503	MTWELQHTHG	23.17	5204	413.856	-1.1	3
97	4.58E+06	986.4457	PTDGLGHSFG	23.24	5235	494.2289	-0.4	2
95	1.21E+07	1128.6292	HVFTKSLQLG	23.25	5241	565.3206	-0.1	2
62	9.91E+06	1046.4126	HEFGPSDAMG	23.28	5254	524.2125	0.1	2
89	1.52E+07	1094.4922	MQMSPVKSMG	23.39	5298	548.252	-0.3	2
91	2.63E+07	1014.477	DAPSKAPSWG	23.43	5317	508.2445	-0.3	2
76	3.70E+06	1160.4622	DYPSHEDELG	23.47	5337	581.2369	-0.3	2
86	3.95E+07	1126.4832	PGWYHADQPG	23.48	5342	564.2471	-0.9	2
94	1.14E+06	1224.5386	MYKSWGPYHG	23.49	5348	613.2745	-1.2	2
91	1.52E+05	1073.4778	LQDYDGLGHG	23.56	5401	537.7463	2.4	2
58	2.10E+07	1062.4077	MEHGDSPSFG	23.51	5353	532.2096	-0.7	2
97	3.60E+06	1158.5823	FVWSHGKELG	23.67	5424	580.2966	-0.9	2
82	6.53E+06	1187.645	KVKQPAFQWG	23.7	5436	594.8281	-0.6	2
93	2.18E+07	1227.5308	WTHYDVDVHG	23.71	5443	410.1829	-0.9	3
91	4.92E+07	1126.5691	MELEKQPVPG	23.76	5462	564.2903	-0.5	2
87	3.35E+06	1121.5327	FVKGWGMQPG	23.79	5478	561.7724	0.0	2
56	1.31E+07	1212.5928	KVHYPEWTPG	23.95	5546	607.3022	-0.2	2
96	1.50E+06	1183.6602	LQLYFTKSKG	24.02	5577	592.8356	-0.7	2
91	2.10E+06	1216.4529	MYMAHTDEFG	24.04	5585	609.2317	-1.1	2
79	1.26E+07	1171.5232	HYHGPVFQMG	24.06	5596	586.7672	-0.6	2
96	8.57E+06	1098.582	KQFGLELAHG	24.08	5606	550.2966	-0.8	2
80	5.94E+06	1189.5703	MAHYKGWQLG	24.21	5659	595.7906	-0.9	2
98	1.22E+07	1077.4993	DTHVLGHGWG	24.26	5678	539.7555	-0.4	2
90	4.23E+07	1115.561	HSLGKEFELG	24.26	5680	558.7863	-0.4	2
95	3.21E+07	1220.5825	LQKQPYWSDG	24.27	5684	611.2967	-0.8	2
93	7.90E+06	1205.511	HQMGHVFYMG	24.34	5718	603.7612	-0.4	2
95	5.41E+06	1121.6055	FVKGMVKAWG	24.48	5780	374.8744	-1.6	3
91	8.02E+06	1148.5979	KEHTWVPVPG	24.49	5787	575.3043	-1.1	2
90	3.64E+06	1294.6094	WEKVWEPQHG	24.5	5789	648.31	-0.8	2
73	4.69E+07	1009.5345	PGLAKGWQPG	24.56	5816	505.773	-0.7	2
84	4.84E+05	1079.5288	PGDAPYLYKG	24.56	5818	540.7704	-0.2	2

74	4.21E+06	1188.5022	MTPYPGWQHG	24.63	5848	595.2568	-0.4	2
93	8.41E+06	1073.46	WADALGHTMG	24.66	5863	537.7355	-1.0	2
92	1.01E+07	1163.5645	KEKGLEMSWG	24.67	5867	582.7878	-0.8	2
94	1.22E+07	1118.4087	DSDQMSHGWG	24.72	5886	560.21	-0.7	2
95	5.94E+07	1011.5389	KAPAPEPVFG	24.86	5947	506.7754	-0.5	2
93	6.40E+06	1069.4651	WVDTHAPGMG	24.91	5968	535.7384	-0.4	2
69	2.54E+06	1137.5818	WGDTKTFVKG	24.94	5984	380.2001	-0.8	3
98	2.71E+06	1159.6389	PVFYHVKTLG	24.95	5987	580.8253	-0.2	2
85	1.01E+07	1163.5532	LYPEPEMTKG	24.96	5991	582.7825	-0.2	2
93	1.26E+06	1226.5212	KTHSWSMYMG	24.96	5993	614.2657	-1.3	2
61	2.89E+07	1133.4812	MSHVFQDVDG	25.01	6014	567.7449	-3.0	2
95	2.31E+06	1204.6128	LSFYKSFEKG	25.1	6050	603.312	-0.7	2
89	3.03E+06	1236.5789	WQFQLQHGHG	25.16	6077	619.2949	-0.7	2
59	6.03E+05	1176.542	FQHAMVMQLG	25.19	6092	589.2762	-1.3	2
90	4.39E+06	1078.5481	MQPSLTFAKG	25.35	6157	540.2797	-0.9	2
84	1.96E+06	1154.4736	DQPEMGKYMG	25.37	6167	578.2424	-0.8	2
90	3.75E+06	1248.5444	DEMQKYLEHG	25.41	6184	625.2773	-1.3	2
91	1.14E+07	1234.4746	MEHTWQMTDG	25.41	6186	618.2424	-1.3	2
87	7.63E+06	1105.5557	HAFAKSLEFG	25.45	6203	553.7834	-0.9	2
96	4.35E+06	1110.5823	KTLGDVWVHG	25.46	6205	556.2963	-1.7	2
72	4.32E+06	1131.502	DYHQPVLGMG	25.48	6214	566.7563	-1.2	2
94	1.62E+07	1082.4524	DGKYPQMGMG	25.53	6237	542.2319	-0.8	2
85	2.89E+06	1276.5217	LQHTMEWEMG	25.54	6243	639.2663	-0.7	2
87	3.26E+06	1077.543	FAMVKAFAHG	25.56	6252	360.1868	-2.0	3
97	1.78E+06	1259.5723	PAKYWEWSHG	25.66	6296	630.7915	-0.8	2
84	2.09E+06	1213.5007	WQMEMAPQHG	25.71	6315	607.756	-0.5	2
96	2.00E+07	1167.4656	FQDVHGMYDG	25.74	6328	584.7381	-1.2	2
93	7.12E+05	1195.606	WADVKVMYKG	25.81	6359	598.8085	-0.7	2
95	4.69E+07	1191.5671	HVWEDVHTLG	25.87	6386	596.7892	-0.5	2
87	1.56E+07	1203.5496	HAHQMTFYLG	26.05	6462	602.78	-1.3	2
92	2.38E+07	1206.5679	MVMYHVWGKG	26.14	6498	403.195	-1.6	3
96	2.83E+07	1154.4736	MTDEMSWAKG	26.14	6500	578.2423	-0.9	2
95	1.82E+07	1245.5779	KVDYDQWVHG	26.15	6506	623.7944	-0.8	2
97	4.62E+06	1238.5906	WAHYMYKALG	26.18	6519	620.3003	-1.5	2
95	6.61E+06	1119.6077	FVLGWGKEKG	26.31	6573	560.8089	-1.7	2
73	3.61E+07	1180.4971	HQMEWAPEPG	26.36	6592	591.2535	-1.6	2
94	7.87E+06	1204.6028	WAHYKAPYLG	26.4	6611	603.3064	-1.6	2
66	2.54E+06	1138.5515	MQKYLGMVPG	26.46	6640	570.2809	-1.6	2
95	7.52E+06	1160.5801	MGHAKVWYLG	26.48	6648	581.2952	-1.4	2
94	5.70E+07	1108.446	FGDYLEHGDG	26.61	6707	555.2288	-0.6	2
97	5.30E+06	1266.614	MTKVKYFYMG	26.73	6758	634.3123	-1.0	2

92	2.66E+07	1247.5459	FQDYDTKQFG	26.79	6779	624.7781	-1.2	2
98	3.37E+06	1149.6182	LTFTLAHYKG	26.91	6833	575.8141	-1.8	2
80		1039.4974	PAKSDAFTFG	26.94	6846	520.7542	-1.2	2
87	1.12E+07	1225.613	FEKYHGLYLG	27.03	6886	613.8114	-1.7	2
85	1.44E+05	1273.6455	HQLTLYWEKG	27.1	6915	637.8273	-2.0	2
96	2.76E+07	1071.4509	DSDSPGKYFG	27.15	6937	536.7307	-1.6	2
97	2.37E+07	1105.5049	PAMQMTWGKG	27.2	6960	553.7578	-1.4	2
97	5.13E+06	1147.5042	PTFYMSMSKG	27.2	6962	574.7569	-2.1	2
92	6.67E+06	1210.5442	FTMAKQDQWG	27.21	6964	606.2768	-2.1	2
58	1.50E+07	1124.5073	WAHGLEPQMG	27.31	7011	563.2594	-0.5	2
88	1.84E+07	1094.5032	PTFSDTWGKG	27.32	7013	548.2575	-0.3	2
45	4.09E+05	1062.5281	HVPGMVHTLG	27.33	7019	532.2682	-3.7	2
81	4.26E+07	1143.5195	DQDTHVLYPG	27.36	7032	572.7654	-0.7	2
95	2.23E+07	1189.5801	HYKVLEDVMG	27.47	7080	595.7959	-0.2	2
92	5.62E+06	1022.4379	PVFTDGPSMG	27.55	7112	512.2247	-0.8	2
87	2.34E+07	1078.4753	KVDGMTWADG	27.59	7131	540.2438	0.1	2
92	2.67E+07	1139.5071	MTPSPEHVWG	27.7	7175	570.7593	-0.4	2
96	1.31E+07	1037.5029	DSLVFSKADG	27.71	7181	519.7573	-0.6	2
95	2.95E+07	1252.6353	HVLAWQWEKG	27.8	7219	627.3231	-0.7	2
71	3.49E+06	987.3934	PSDSWADGPG	27.8	7221	494.7026	-0.6	2
51	2.99E+05	1045.5444	KVFADAPELG	27.83	7233	523.7778	-1.1	2
86	1.83E+07	1094.5244	DAKQFTLTDG	27.87	7248	548.2679	-0.7	2
91	2.11E+07	1126.439	MEHTFSDGFG	28.01	7307	564.2253	-0.4	2
70	1.28E+06	1134.5015	WTDEPTKAMG	28.01	7311	568.2568	0.0	2
95	1.09E+06	1058.522	LEWGMAKAPG	28.11	7351	530.2667	-0.7	2
75	1.52E+06	1111.4678	FSPTMTPQMG	28.13	7361	556.7391	-1.6	2
96	1.37E+06	1278.5737	LEKQWEMQMG	28.2	7394	640.2921	-1.0	2
93	1.31E+07	1142.478	WTWGHTPSDG	28.21	7399	572.2448	-0.4	2
84	2.23E+06	1262.4949	KSDTWEMYMG	28.24	7413	632.2526	-1.2	2
95	4.25E+07	1028.4749	FGDVHVMAPG	28.26	7420	515.2433	-0.6	2
65	2.75E+07	1213.4929	WQMEMAMSKG	28.27	7424	607.7564	6.6	2
64	9.42E+06	1199.5876	KGHVWYWAPG	28.38	7471	600.7993	-0.9	2
97	6.89E+07	1107.5601	PGDVPYLYKG	28.58	7555	554.7855	-1.1	2
97	3.91E+07	942.4559	FGDGLGLAHG	28.58	7557	472.2334	-1.6	2
94	5.18E+06	1215.6035	KAHEFTLQWG	28.59	7563	608.8071	-1.0	2
83	4.09E+07	1232.5496	MELQDQHYLG	28.67	7595	617.2803	-0.6	2
96	2.82E+07	1060.4319	DGMTMVHVDG	28.72	7618	531.2218	-0.5	2
95	3.49E+07	1084.4824	DELAFEHAPG	28.74	7628	543.2471	-0.3	2
94	6.65E+06	1100.5039	DVFGFSHVHG	28.77	7639	551.2579	-0.3	2
93	7.30E+06	1292.5859	KEHEMYLTWG	28.79	7651	647.2987	-0.2	2
92	8.31E+06	1249.4709	MSWEDYPEHG	28.83	7666	625.7408	-0.9	2

90	5.01E+07	1235.5498	FSPYPYKYDG	28.87	7685	618.7805	-0.6	2
95	1.28E+07	1057.5015	PTLGMQFAHG	28.88	7687	529.7571	0.4	2
96	1.03E+07	1308.6501	WVKEFEKTWG	28.88	7689	655.3306	-0.4	2
93	2.93E+07	1145.4778	PEFGDTWTHG	28.88	7691	573.7449	0.0	2
96	5.34E+06	1213.5073	MSWSFEDQKG	28.88	7693	607.7593	-0.5	2
90	1.44E+06	1155.502	WSKQMAFSDG	28.89	7697	578.7568	-0.3	2
91	5.41E+06	1201.5591	KSMVFSFYHG	29.05	7767	601.7852	-0.5	2
97	2.50E+07	1148.5867	PTLSPYKTWG	29.06	7769	575.299	-0.7	2
59	3.67E+07	1138.5229	MEHQPALAWG	29.06	7773	570.2678	0.6	2
95	4.30E+07	1113.5818	WQLVDAKTPG	29.21	7835	557.7965	-0.8	2
62	2.30E+05	956.4716	FADGLGLAHG	29.25	7856	479.2403	-3.6	2
55	2.27E+05	1192.4463	MEHQMGMAWG	29.26	7860	597.2277	-2.4	2
96	3.11E+06	1195.5332	WSMADTKVWG	29.37	7905	598.7722	-0.7	2
44	5.73E+06	1028.4749	FGLAHEMAPG	29.73	8056	515.2419	-3.3	2
97	6.25E+06	1353.6541	MEWQKVWYKG	29.78	8075	677.8322	-0.9	2
93	9.48E+06	1092.5452	DQKTPTFSLG	29.8	8082	547.2783	-0.7	2
61	1.86E+06	1133.4778	HGPYFQDVDG	29.84	8103	567.7451	0.2	2
65	2.60E+06	1118.5278	MTDQLQPTLG	29.89	8122	560.2695	-0.9	2
58	1.17E+05	1222.6169	PSMQKVWYKG	29.89	8124	612.3124	-3.2	2
97	9.93E+06	1334.572	KGWYHYDYFG	29.99	8166	668.2911	-1.0	2
81	7.82E+05	1055.5037	HALTLSWGDG	30.06	8196	528.7576	-0.7	2
56	1.37E+07	1033.4209	PADQMVDAMG	30.25	8274	517.7159	-1.4	2
96	1.38E+06	1128.5386	WSLSLQHAMG	30.26	8282	565.2745	-1.5	2
59	3.68E+07	955.5524	KGLAPAMVLG	30.31	8299	478.782	-0.9	2
89	6.23E+05	1277.5386	KQDTFSWYMG	30.32	8307	639.7744	-1.3	2
89	3.14E+07	1268.5396	WAMQHQPEWG	30.36	8320	635.2755	-0.2	2
95	4.47E+06	1308.6138	WEFYLTKEHG	30.37	8326	655.3122	-0.8	2
43	7.22E+06	1062.4363	PEMTMSPVDG	30.46	8364	532.2242	-0.1	2
95	3.61E+07	1198.5295	FSDTPYHYLG	30.51	8389	600.2705	-0.4	2
72	4.96E+06	1143.4656	WQMQPGPEDG	30.52	8391	572.7384	-0.7	2
96	1.21E+07	1172.5979	DVLGWYHVKG	30.63	8439	587.3048	-0.2	2
95	2.29E+06	1193.554	LAWTMGKEWG	30.7	8469	597.7824	-0.9	2
98	2.97E+06	1152.5671	MVMTLTKAWG	30.72	8480	577.2889	-1.1	2
95	3.07E+07	1025.5181	FALADSKAFG	30.74	8488	513.7645	-1.4	2
98	4.99E+07	1176.5815	LYWEPAKVDG	30.77	8501	589.2961	-1.0	2
93	2.66E+05	978.5498	PGLTLTLAHG	30.8	8511	490.2802	-1.9	2
78	1.43E+06	1222.5229	FQPAHSWYMG	30.86	8536	612.2665	-1.5	2
82	7.49E+05	1129.4749	DGKYMEPSFG	30.87	8542	565.7429	-1.0	2
83	4.32E+07	1111.5701	LYPAFGPYKG	30.88	8545	556.7906	-0.8	2
71	2.74E+07	1122.5566	KQMYLGMVPG	30.88	8547	562.2838	-1.1	2
69	4.37E+07	1185.5454	WAHYPVDELG	31.01	8608	593.7782	-0.8	2

96	2.03E+07	1043.5076	FGFGPSKTFG	31.1	8642	522.7596	-0.5	2
86	1.53E+07	1081.4539	FYMQPGPADG	31.11	8646	541.7332	0.4	2
96	6.10E+06	1147.5371	MSFYFAKTPG	31.17	8674	574.7742	-0.7	2
61	4.27E+06	1198.533	FSDTWVMQLG	31.35	8749	600.2701	-3.8	2
87	2.95E+07	1103.5037	WTDTHGLAFG	31.49	8806	552.7576	-0.5	2
97	2.66E+07	1152.5273	FSWTKAMEPG	31.51	8817	577.2696	-0.2	2
95	2.63E+07	1129.5115	MTDGFEFVKG	31.52	8819	565.7614	-0.6	2
89	4.74E+07	1183.5549	KYFEFEPAPG	31.57	8844	592.7832	-0.4	2
92	7.48E+06	1291.635	LQKQWYPSWG	31.61	8859	646.8231	-0.5	2
92	1.50E+06	1370.6196	FYWYWGKQHG	31.62	8865	686.3147	-1.3	2
81	4.80E+06	1300.5183	DQFYHTWTMG	31.63	8867	651.2646	-0.5	2
97	2.62E+07	1156.5188	WTKAFGDEFG	31.7	8899	579.2654	0.1	2
68	4.60E+06	1055.5435	HSLGLQLTMG	31.71	8903	528.7775	-0.6	2
94	2.56E+07	1087.458	WGMGMEHALG	31.79	8938	544.7349	-0.3	2
95	1.76E+07	1111.4944	FAMQWGMGKG	31.97	9011	556.7529	-0.7	2
84	1.25E+07	1086.5862	WVPAPVKSFG	32	9024	544.2989	-0.5	2
97	2.81E+07	1271.5679	LYWEMQKSMG	32.07	9058	636.7894	-0.6	2
59	1.13E+07	1142.4814	HSDSWVPQMG	32.14	9087	572.246	-1.3	2
95	3.04E+07	1231.541	FVHTWGWQDG	32.22	9121	616.7757	-1.2	2
58	4.91E+05	1118.4153	DQDADEWSPG	32.23	9123	560.2129	-1.4	2
95	1.04E+07	1250.572	WVHQFSLYDG	32.25	9134	626.2913	-1.0	2
91	1.17E+06	1076.5688	KVPSLQMAFG	32.26	9136	539.29	-1.0	2
93	1.19E+07	1186.5659	FQPSDYKVFG	32.3	9153	594.2887	-0.4	2
90	1.42E+06	1339.635	WQKTPYWQFG	32.42	9207	670.8228	-0.7	2
96	3.34E+07	1134.5896	LAKAPVMYWG	32.43	9209	568.3005	-0.6	2
62	2.44E+06	1094.4712	MGHVMAMVFG	32.45	9216	548.2415	-0.3	2
96	5.77E+06	1284.604	KSWAHVWEWG	32.45	9218	643.3076	-0.5	2
79	1.47E+06	1012.3664	DSPGMSMTMG	32.59	9277	507.1887	-1.3	2
86	4.11E+07	1073.5757	KVFADVPELG	32.59	9279	537.7938	-0.3	2
96	9.84E+06	1131.4841	MSMAWVHVDG	32.64	9298	566.7474	-1.3	2
53	4.21E+07	1097.5505	DGHQPVLYLG	32.64	9300	549.7812	-0.3	2
60	1.37E+06	1049.4521	DGMQPVLSMG	32.65	9308	525.732	-0.4	2
97	2.31E+07	1091.4495	FGMGDSHVWG	32.68	9319	546.7307	-0.2	2
63	1.77E+06	1213.4675	HQDGFEFYDG	32.84	9386	607.7395	-0.3	2
84	1.68E+07	1002.4658	FALSDAPEPG	32.94	9429	502.2389	-0.3	2
71	6.67E+06	1270.5442	FQHYMQDVFG	32.97	9444	636.2778	-0.2	2
46	1.72E+06	1081.4175	MGPGDSPYWG	32.99	9454	541.7148	0.0	2
89	1.24E+07	1197.5667	KEDQFSFQLG	33.12	9506	599.7893	0.0	2
80	1.68E+05	1138.5771	KELGDVWVHG	33.24	9560	570.2944	-0.4	2
82	1.73E+06	1234.5442	MQHSFTWELG	33.26	9565	618.2778	-0.4	2
83	3.86E+06	1064.4695	LVDSLSMEDG	33.29	9578	533.2407	-0.3	2

52	6.80E+05	1113.5132	FADAFTWSLG	33.38	9618	557.7645	3.4	2
95	8.78E+06	1280.6553	KEKVWTWTFG	33.4	9625	641.3329	-0.9	2
97	1.15E+07	1090.5811	LGWAPYLSKG	33.43	9642	546.2963	-0.5	2
72	7.96E+06	1122.5742	KEMQFALSLG	33.48	9678	562.2906	-4.5	2
82	2.81E+06	1054.4277	MVDYLADGDG	33.45	9650	528.2197	-0.6	2
98	2.02E+06	989.5909	LGLAFTLAKG	33.47	9659	495.8013	-0.7	2
76	9.16E+06	1144.4495	FADQMQFSDG	33.55	9693	573.2299	-1.6	2
84	1.48E+05	1044.5393	LGFAPVHTFG	33.6	9716	523.2753	-1.0	2
70	1.08E+06	1127.4043	WGDEFSDTDG	33.64	9731	564.708	-0.3	2
98	3.44E+07	1049.5908	FAFVKAPTLG	33.68	9747	525.8015	0.0	2
62	3.81E+05	1171.5298	PTFEWEHGLG	33.71	9759	586.7709	0.0	2
95	2.27E+07	1379.6299	HEFEKVWYWG	33.73	9766	690.8203	-0.6	2
93	5.25E+05	1239.6321	LQKSWYMVLG	33.81	9801	620.8219	-0.1	2
97	3.33E+06	1120.5342	PTFYHGPVFG	33.83	9806	561.2726	-1.0	2
97	1.26E+06	1191.502	WVHAFTMEDG	33.84	9812	596.7565	-0.7	2
69	6.87E+06	1149.5012	PYDEMTPQLG	33.91	9842	575.756	-1.0	2
95	2.43E+06	1158.5708	LQFEFGFSKG	33.93	9850	580.2909	-0.9	2
93	2.98E+06	1015.5702	KVFALAPVDG	33.93	9852	508.7908	-0.8	2
93	1.53E+06	1235.5203	DYLYKEMSMG	33.94	9857	618.7656	-0.7	2
66	8.38E+05	1200.5928	KGPTLQWEWG	33.95	9861	601.3022	-0.3	2
95	1.35E+06	1207.6025	PVLYFQFTHG	33.97	9871	604.8069	-0.4	2
63	2.13E+06	1051.4314	MSLQDVDGMG	33.99	9877	526.7215	-0.6	2
77	3.67E+06	1177.5557	LAWTHSFYPG	34.03	9893	589.7842	0.6	2
94	1.02E+07	1202.5759	FYWTPSFAKG	34.06	9906	602.2936	-0.5	2
73	3.34E+07	1221.6182	KTPVWYFQPG	34.1	9924	611.8148	-0.3	2
87	1.89E+07	1105.4465	DGDSWGHYLG	34.17	9951	553.7292	-0.1	2
95	3.35E+06	1102.5447	LGFEPVHTFG	34.22	9974	552.2784	0.0	2
32	1.52E+06	1178.543	LAWTPQMYPG	34.27	9994	590.2753	-3.7	2
83	3.28E+05	1116.429	FVMAMEMADG	34.3	10005	559.2201	-0.8	2
92	1.17E+06	1275.5515	MYKEMEFELG	34.31	10009	638.7813	-0.5	2
78	1.61E+06	982.3702	DGDTFSMGPG	34.53	10097	492.191	-0.6	2
88	2.12E+07	1171.5947	KVMVFYDTLG	34.6	10121	586.803	-0.6	2
57	1.57E+06	1280.5649	WSHSWYLVMG	34.7	10164	641.2866	-2.7	2
82	2.92E+07	1256.5898	MEKYLAPYWG	34.83	10213	629.3001	-1.1	2
73	7.68E+05	1161.4946	MAPTMQWQPG	34.9	10246	581.7528	-0.9	2
92	2.83E+07	1178.5793	PGKVMEWYLG	34.91	10251	590.2955	-0.2	2
97	3.67E+07	1262.6084	PGWYLQKEWG	34.96	10269	632.3101	0.1	2
64	3.72E+05	1164.4216	HEDYPEMGMG	35.05	10310	583.22	5.4	2
86	1.17E+07	1175.532	KEPAMYFSFG	35.13	10340	588.7717	-0.4	2
97	8.36E+06	1149.5276	LSWVMSHSFG	35.21	10377	575.7693	-0.8	2
98	5.39E+06	1138.5845	LSWALAMYKG	35.22	10379	570.2979	-0.7	2

95	8.18E+06	1133.5505	DVPSWQKAFG	35.27	10398	567.7808	-0.9	2
61	1.43E+05	1191.5747	LAWTMAKEWG	35.34	10426	596.7928	-0.8	2
97	8.57E+05	1156.541	FTMSMAKVWG	35.37	10434	579.2761	-0.8	2
97	1.62E+07	1269.4939	DYDTWVHYDG	35.44	10458	635.7522	-1.0	2
86	7.43E+06	1121.5293	FGHTLAFSWG	35.56	10506	561.7703	-0.7	2
84	1.73E+07	1221.6182	WYPTKALTWG	35.63	10531	611.8147	-0.5	2
61	1.00E+07	996.524	DSHSLVLGLG	35.63	10533	499.2681	-0.1	2
66	8.29E+06	1161.4946	PSMTMQWQPG	35.65	10540	581.7527	-1.0	2
62	5.61E+05	1276.5256	PYPYMQMQFG	35.68	10556	639.2686	-0.1	2
72	2.71E+07	1225.5515	HQLVWGDEWG	35.69	10559	613.7806	-1.7	2
89	2.44E+07	1186.5771	LGLEHTWQFG	35.7	10562	594.2941	-0.8	2
96	1.63E+07	1180.6279	FYLAKTPVWG	35.76	10588	591.3196	-0.6	2
94	1.06E+06	1220.5688	FYKAWVFGMG	35.84	10620	611.2897	-1.1	2
76	4.40E+06	1022.4742	FVDSPTLGMG	36	10675	512.2424	-1.6	2
63	2.22E+05	1217.5427	FSPYPYKEMG	36.02	10686	609.7745	-4.6	2
95	1.22E+07	1269.5488	WTKEWGMEFG	36.11	10721	635.7798	-0.7	2
78	6.87E+05	968.3909	MSLAFGDGDG	36.14	10733	485.2013	-0.8	2
84	3.13E+06	1105.4961	LSLEMQDVDG	36.17	10742	553.7539	-0.4	2
96	1.69E+07	1178.5608	WELVFGKEDG	36.24	10772	590.2858	-0.9	2
63	3.10E+05	1185.5488	WEHTMVLVDG	36.42	10837	593.7781	-3.9	2
65	2.89E+05	1002.5021	PSPALYLADG	36.58	10890	502.2566	-1.3	2
95	3.52E+06	1248.5928	KAPEWQFTWG	36.7	10926	625.3009	-2.2	2
80	6.73E+06	1009.5233	WSPSPAPVLG	36.74	10941	505.7673	-0.9	2
92	8.05E+06	1229.5869	WQFYPAFSKG	36.87	10991	615.799	-0.6	2
94	1.17E+07	1182.5708	PGKYWEFSLG	36.88	10993	592.2913	-0.2	2
70	1.05E+07	1105.4751	DEPQPGLYMG	37	11035	553.7433	-0.5	2
97	3.80E+06	1315.551	LSFYDEHYWG	37.03	11047	658.7809	-0.7	2
89	2.62E+07	1162.5659	DEKVWGPYLG	37.31	11124	582.2886	-0.6	2
97	1.93E+07	1267.5332	LEMYFGHEWG	37.41	11159	634.7722	-0.4	2
89	2.15E+06	1169.4851	FEPAPGWYMG	37.43	11162	585.748	-1.0	2
61	3.32E+05	1113.5454	DGHVLQLEFG	37.54	11206	557.7786	-0.3	2
69	5.01E+06	1125.48	PQDAPYMTFG	37.6	11228	563.7457	-0.5	2
77	7.01E+06	1306.5361	KEMEFYMSWG	37.67	11250	654.2742	0.5	2
90	2.17E+07	1227.4985	FYWADEFGHG	37.68	11256	614.7547	-0.8	2
86	2.92E+06	1172.5503	KVWSFTDSFG	37.78	11285	587.2804	-1.3	2
78	1.58E+06	1003.6066	KGLVLSLAFG	37.79	11287	502.8086	-1.8	2
76	1.77E+06	1055.4229	DGFQMSLSDG	37.81	11292	528.7174	-0.3	2
95	6.74E+05	1393.6086	MYFYMYKYLG	37.99	11348	697.8099	-0.2	2
97	1.16E+07	1238.637	LTKEWVMYLG	38.11	11394	620.3245	0.1	2
62	3.93E+05	1064.623	LELTHVLALG	38.3	11455	533.3171	-1.0	2
63	7.37E+06	1158.498	FQPSFQDSFG	38.34	11467	580.2545	-0.9	2

97	1.11E+07	1163.5764	LAWGLYHTFG	38.37	11474	582.7933	-1.5	2
95	1.31E+07	1213.5955	WQLAKAFYMG	38.45	11498	607.8035	-0.2	2
82	6.15E+06	1152.4724	FSDEWGLQDG	38.48	11510	577.2422	0.1	2
85	1.32E+07	1208.5535	KEPSWEMVFG	38.52	11525	605.2826	-0.1	2
80	7.00E+05	1147.5662	KSWVDTWGLG	38.53	11530	574.789	-0.2	2
57	6.90E+05	1041.5352	PVMQPALVMG	38.62	11564	521.7734	-0.6	2
65	1.23E+07	1293.5488	KYDGMQWYFG	38.63	11567	647.78	-0.5	2
94	1.64E+07	1291.5808	MQWYLTHAWG	38.66	11578	646.7959	-0.6	2
54	7.37E+06	1158.5015	KEMAFQDSFG	38.69	11586	580.2549	-3.2	2
94	7.72E+06	1265.6082	FYLTHEWTLG	38.91	11659	633.8096	-0.6	2
91	2.88E+06	1138.5845	KVMTWGLTFG	39.01	11693	570.2977	-0.9	2
85	6.04E+06	1087.5007	MVPVPTWSDG	39.12	11721	544.756	-0.7	2
92	1.48E+06	1124.5291	FTFGFVDVHG	39.32	11788	563.2704	-0.2	2
85	9.01E+05	1193.6267	KVFVLSWQMG	39.44	11826	597.8188	-0.8	2
73	4.22E+06	1106.5032	LQDGPSFTWG	40.06	12001	554.2571	-1.0	2
91	1.34E+06	1179.5713	LGLYWSFTHG	40.12	12016	590.7914	-0.3	2
93	5.80E+05	1201.592	PTFYWVPVHG	40.2	12036	601.8019	-0.2	2
53	1.45E+06	1003.6066	LVKGLSLAFG	40.23	12046	502.8092	-0.5	2
94	1.15E+06	1139.6414	LVLAFVKYMG	40.65	12172	570.8265	-0.4	2
67	2.56E+06	1110.4626	FGMAWSMQPG	40.67	12179	556.2386	2.3	2
77	1.74E+06	1167.4939	MSLQPEMEFG	40.69	12186	584.7529	0.0	2
68	1.32E+07	1190.5244	LQPAWEDEFG	40.7	12191	596.268	-0.3	2
56	1.00E+06	1158.542	FVPYLYPGMG	40.78	12218	580.2766	-0.8	2
89	1.64E+06	1187.4958	WVPTFGMYDG	40.92	12255	594.7533	-1.0	2
79	1.58E+06	1046.5042	MGLGHVMVFG	40.96	12270	524.2579	-0.6	2
75	7.73E+06	1104.5161	PELEPYMGLG	40.99	12280	553.2637	-0.7	2
96	4.11E+03	1263.5781	MVWELYHVMG	41.02	12288	632.794	-1.5	2
64	4.77E+06	1136.5171	LGDQLQMEFG	41.02	12290	569.2641	-0.8	2
87	2.51E+06	1134.5347	LTFTDAPQWG	41.09	12319	568.2731	-0.5	2
55	6.50E+04	1284.585	WTLEWSMYLG	41.21	12356	643.3029	7.1	2
95	6.97E+06	1267.5696	WYLVHEFSMG	41.26	12368	634.79	-1.0	2
96	5.12E+06	1257.5454	WTFEFTHSFG	41.45	12414	629.7786	-0.1	2
71	1.27E+06	1077.459	WGMEFGPTPG	41.48	12425	539.7353	-0.5	2
62	4.09E+06	1129.5479	LTMTPEWVPG	41.6	12464	565.7795	-0.7	2
94	1.24E+06	1243.6025	FGLQHYLYFG	41.73	12502	622.8069	-0.5	2
82	1.24E+06	1218.6187	WAWSKSWVLG	41.81	12525	610.3143	-1.6	2
73	2.46E+05	1079.4924	PEFGLADQFG	41.83	12535	540.7513	-1.9	2
67	8.82E+06	1065.48	MADQLVDAFG	41.84	12537	533.7453	-1.5	2
50	5.15E+05	1169.5393	FQFTPEFTPG	41.93	12566	585.7753	-0.6	2
84	1.57E+06	1348.5876	PYWVFEHEWG	41.93	12568	675.2986	-1.5	2
73	4.24E+06	1148.4341	FSMYPEMGMG	41.94	12574	575.2225	-0.9	2

95	9.41E+05	1098.5134	DGWGKYFGLG	41.98	12586	550.2623	-0.8	2
93	2.45E+05	1117.6746	LTLVLVFEKG	41.98	12588	559.8427	-1.1	2
61	8.12E+05	1176.4934	DQWEDTLVDG	41.99	12594	589.2518	-1.5	2
86	1.43E+07	1274.5642	DEKYMYWALG	42.14	12633	638.288	0.1	2
53	5.34E+05	1095.4907	LSDTMSWSLG	42.25	12661	548.7513	-0.2	2
51	5.90E+05	1385.5862	FQMQWQPYWG	42.28	12672	693.7986	-0.4	2
96	1.54E+07	1317.5964	WVWEFQHVMG	42.35	12693	659.8043	0.3	2
66	5.51E+05	1150.4753	MSPTWGDVWG	42.48	12725	576.2435	-0.4	2
66	5.43E+05	1102.4641	DGMSFYLVDG	42.6	12759	552.2375	-1.0	2
81	1.68E+06	1067.4561	WTFGLSDADG	42.74	12797	534.7339	-0.3	2
74	8.89E+06	1176.5308	WVMQMSPELG	42.82	12820	589.2711	-0.5	2
83	1.33E+07	1234.5547	LYDYPTFYPG	43.13	12911	618.283	-0.4	2
81	8.32E+05	1311.5044	FQWEDEDTWG	43.28	12949	656.7582	0.3	2
93	3.32E+06	1191.5713	LVWEFTFGHG	43.29	12952	596.7916	0.0	2
65	1.54E+06	1095.4907	MTDSLSWSLG	43.56	13032	548.7515	0.2	2
62	1.12E+07	1099.491	WGPAMQWAPG	43.6	13046	550.7516	0.1	2
63	4.16E+06	1111.4468	FAMSWGPEMG	43.68	13062	556.7284	-1.9	2
89	2.75E+05	1286.5654	WQWGHVMTWG	43.8	13092	644.2873	-2.0	2
90	2.55E+07	1159.5549	DADVFYKVFG	43.84	13101	580.7828	-1.1	2
70	5.25E+05	1210.4963	MGLQWEDEFG	44.15	13192	606.2543	0.3	2
80	8.57E+05	1315.5178	FQFEMEWQDG	44.24	13214	658.7647	0.0	2
48	2.83E+05	1212.491	DYMGPQPYWG	44.26	13223	607.2504	-1.6	2
87	2.74E+06	1242.5378	WVMYPTFQDG	44.51	13273	622.2744	-0.8	2
91	6.80E+06	1155.4695	DYMGPAPYWG	44.64	13301	578.7402	-0.9	2
82	8.75E+06	1162.5447	LSPYWSPAWG	44.69	13315	582.2776	-1.3	2
97	4.35E+06	1269.6182	WEWYFALAKG	44.7	13318	635.815	0.1	2
96	1.27E+06	1281.5852	WEWEMVFAKG	44.72	13328	641.7981	-0.6	2
79	1.27E+06	1263.5923	HVLVFYDEWG	44.74	13334	632.8021	0.1	2
64	1.23E+06	1268.5767	WVFGHAWYFG	44.9	13375	635.2943	0.1	2
77	1.58E+06	1168.5288	PELELSDYFG	44.92	13380	585.2695	-1.6	2
71	1.57E+07	1110.5386	FALEPAFYPG	45.01	13402	556.2751	-0.5	2
84	9.77E+06	1251.5559	WTLSDQPYWG	45.14	13436	626.7834	-0.6	2
79	5.78E+06	1134.4805	MAPTWGDVWG	45.15	13440	568.2461	-0.3	2
55	1.18E+05	1100.4341	MAFVMEMADG	45.18	13445	551.2227	-0.8	2
77	1.71E+06	1199.5168	WYLTMTDVDG	45.24	13458	600.7645	0.2	2
96	9.59E+05	1305.603	DYFYKSLQWG	45.26	13462	653.8073	-0.2	2
88	4.11E+06	1042.4429	FELGMGDAFG	45.34	13483	522.227	-1.1	2
55	1.02E+06	1162.4675	PYMTMSFVDG	45.56	13541	582.2394	-0.7	2
79	7.29E+06	1233.5488	LEWSPQMTWG	45.71	13604	617.78	-0.5	2
73	3.42E+06	1187.5134	WSDYLGLYDG	45.9	13635	594.7621	-0.9	2
76	4.81E+05	1226.5454	DQLELQFYDG	46.15	13684	614.2785	-0.2	2

78	5.65E+05	1234.5869	LEWQFVLEDG	46.25	13706	618.2975	-3.0	2
57	2.74E+05	1236.5486	WQPEFELTMG	46.4	13741	619.2794	-1.3	2
52	2.03E+06	1210.4932	FQPGWEDEFG	46.75	13817	606.2537	2.0	2
72	5.71E+06	1086.5532	MGLSPQWVLG	46.81	13827	544.2805	-4.1	2
66	7.94E+05	1196.4443	WTDGMEDTWG	47.06	13873	599.2271	-1.8	2
78	4.85E+06	1191.5559	LQDELGFQWG	47.08	13877	596.7833	-1.0	2
74	2.83E+05	1162.4675	MEFTMSFVDG	47.11	13886	582.2393	-0.9	2
79	2.64E+06	1184.5503	WYLSFQDGLG	47.25	13923	593.2806	-0.9	2
86	2.35E+06	1180.5188	WTPVFSWSDG	47.67	14022	591.2649	-0.8	2
65	1.03E+06	1153.4651	DQFAMGWGWG	47.72	14014	577.738	-0.9	2
75	6.39E+06	1032.5645	FVLAFVPSPG	47.72	14016	517.2879	-0.9	2
58	4.23E+06	1191.4575	DQDSMVFYMG	47.75	14026	596.7342	-0.9	2
82	2.97E+05	1159.5762	LVLEWEDSLG	47.78	14036	580.795	1.7	2
80	9.83E+06	1038.5022	LADELAFGFG	47.83	14056	520.257	-0.5	2
84	3.98E+06	1190.5471	FYFVPAPYMG	48.31	14165	596.2776	-3.3	2
71	1.21E+05	1154.4492	FEDAMGWGWG	48.59	14223	578.2276	-5.2	2
91	2.24E+06	1285.5479	FYFSMQFYPG	48.84	14267	643.7775	-3.6	2
73	2.86E+06	1316.5283	WQDGMQFYWG	48.87	14273	659.2681	-2.9	2
86	6.13E+06	1226.543	LVMAWSDYWG	49.23	14362	614.2772	-0.4	2
61	9.36E+06	1216.6128	WVLQPEFELG	49.41	14420	609.3121	-0.4	2
77	6.53E+06	1176.5603	PSWAPYLTWG	49.61	14448	589.286	-0.2	2
68	3.68E+06	1135.5735	LAMSWYPVLG	49.66	14459	568.7906	-3.8	2
76	2.80E+06	1144.6279	FVPVWSLQLG	49.84	14494	573.318	-3.5	2
68	1.03E+06	1167.5635	WYLVDTMALG	49.91	14510	584.787	-1.2	2
78	9.33E+06	1183.5735	LAWAMYPYLG	49.94	14517	592.7926	-0.2	2
62	2.32E+06	1248.5564	WQPQDVFSWG	49.97	14530	625.2835	-0.9	2
66	5.15E+05	1349.5718	WEWYWTPEPG	50.07	14558	675.7911	-0.9	2
70	6.00E+06	1315.5696	MYPTWQFTWG	50.38	14631	658.7908	0.3	2
84	3.95E+05	1371.6135	LYLEWQDYWG	50.4	14635	686.8125	0.0	2
72	5.38E+05	1194.5378	WQMALVFEDG	50.67	14702	598.275	0.1	2
72	1.00E+06	1329.5852	PQLYMSWYWG	50.67	14704	665.7988	0.5	2
66	5.98E+04	1018.5555	LVLSMVMGLG	50.68	14707	510.2837	-0.4	2
75	3.94E+05	1197.5706	WSPYLSLEFG	50.79	14731	599.791	-0.5	2
68	1.96E+06	1281.5454	FSPEWTWSWG	50.82	14740	641.778	-0.9	2
58	4.21E+05	1191.4575	DAMQDVFYMG	50.96	14773	596.7347	-0.1	2
74	6.04E+05	1195.5405	PALYWEMVMG	51.04	14788	598.7762	0.0	2
72	4.34E+05	1263.4941	MSWEFEMTFG	51.28	14844	632.753	0.1	2
73	4.67E+06	1120.5342	LSWTWAFGPG	51.35	14862	561.2731	-0.1	2
71	9.00E+05	1188.5815	WVDTWVDVLG	51.41	14885	595.2965	-0.4	2
68	1.89E+05	1148.5325	MELGWGWTLG	51.57	14930	575.2716	-1.1	2
69	5.15E+05	1229.5427	MVDAWYFELG	51.78	14963	615.7762	-1.8	2

57	6.53E+05	1281.5454	WEPSFTWSWG	51.91	14990	641.7784	-0.3	2
65	7.67E+05	1239.4873	FYDGDYFAWG	51.94	14995	620.7493	-0.4	2
71	8.07E+06	1146.5498	FEWGWGPVLG	52.46	15102	574.2787	-3.8	2
89	3.76E+06	1171.4822	DEWYLGDAFG	52.91	15201	586.7449	-3.8	2
62	4.73E+06	1263.5713	WYWALEPGWG	53.31	15279	632.7886	-4.6	2
77	4.94E+05	1161.48	DQMAFAFEFG	53.34	15286	581.7454	-1.0	2
54	5.58E+05	1260.5308	MQWSFEMVFG	53.44	15313	631.2714	0.1	2
76	7.68E+06	1133.5791	DVMQLVPYLG	53.64	15355	567.7935	-3.6	2
85	4.51E+06	1174.5369	DVFVPYFTMG	54.27	15497	588.2734	-1.7	2
68	2.78E+05	1239.6174	LVDEWVLYFG	54.35	15509	620.8143	-0.5	2
77	6.37E+03	1167.5635	DQMVFVLYPG	54.42	15525	584.7877	0.0	2
69	9.16E+05	1093.5444	DGLVFSWTLG	55.32	15702	547.7782	-0.2	2
72	2.85E+06	1174.5811	WAPVFELAWG	55.45	15732	588.2953	-2.0	2
74	3.21E+05	1109.5029	DGWTLVFTDG	56.25	15883	555.757	-0.9	2
72	1.91E+05	1321.592	WAFYWAFQFG	59.25	16556	661.8015	-0.5	2
67	1.12E+05	1169.5757	DSWALYFVLG	60.13	16771	585.793	-1.4	2

Appendix II. Sequences identified from the 306 bead sample

ALC	Area	Mass	Peptide	RT	Scan	m/z	ppm	z
74	1.77E+06	1331.6621	KEHYWQKEKG	15.31	2005	333.922	-1.1	4
50	4.77E+05	1212.5312	WYHAKAHEDG	16.2	2120	405.1835	-0.9	3
75	1.07E+06	1250.6772	WQKTKTFQKG	16.26	2130	417.8986	-1.3	3
90	3.53E+06	1196.6553	LTKYWSKSKG	16.67	2194	399.8914	-1	3
71	9.12E+04	1082.5178	HVPTMAKQDG	16.7	2201	542.2653	-0.3	2
97	1.84E+06	1101.5356	KYLGHGHSFG	16.74	2214	551.774	-0.6	2
89	9.15E+05	1224.5061	DYHQHQFGHG	16.77	2224	409.1749	-1.3	3
62	2.34E+05	1150.4792	HSPQHSDTWG	16.8	2235	576.246	-0.2	2
82	1.20E+05	1133.5037	MSHSLQHTHG	16.86	2257	378.8408	-1.5	3
89	1.02E+05	1259.6221	MYKEKVKYDG	16.87	2260	420.8802	-1.3	3
81	8.50E+04	1166.5542	FGKYKEMAHG	16.91	2269	389.8575	-1.8	3
75	6.99E+05	1068.5715	FVPEKGKAHG	16.93	2282	357.1969	-1.2	3
98	6.79E+05	1231.5115	HEMEMAHYKG	16.99	2300	616.7618	-0.6	2
77	4.97E+05	1273.5991	HYKVHSFYHG	17.03	2318	425.5394	-0.9	3
64	3.93E+05	1103.4739	HSMSKEMTPG	17.14	2362	552.7435	-0.1	2
92	1.07E+06	1079.5149	KGHSPSPQWG	17.15	2366	540.7639	-0.2	2
93	1.07E+07	1115.4312	HQMTMGMSHG	17.17	2373	558.7216	-1	2
92	2.71E+06	1144.5513	KTLSDYHQPG	17.22	2396	573.2819	-0.4	2
94	1.10E+06	1027.5121	KGLTMSPTHG	17.22	2398	514.762	-1.3	2
97	5.65E+06	1088.5073	MQFVHGKADG	17.34	2450	545.2596	-1.1	2
97	2.67E+07	1194.5854	FGKYKEMVHG	17.35	2454	399.201	-2.2	3
90	1.26E+06	1142.4993	DEPQHEFGKG	17.39	2471	572.2557	-0.8	2
90	1.16E+06	1212.5789	PQWQHQPVHG	17.44	2496	607.2954	-0.8	2
78	8.30E+05	1138.5361	MTKEKVMTDG	17.45	2498	380.5183	-1.4	3
97	2.73E+06	1134.4763	PEHEHGLEMG	17.5	2522	568.2446	-0.1	2
73	1.96E+06	1093.5669	PAHGLQKTWG	17.63	2573	365.5286	-1.4	3
81	7.12E+06	1173.4695	HQPSHYMSMG	17.75	2623	587.7413	0	2
88	3.29E+07	1158.5093	LYPYHSDAHG	17.79	2637	387.1762	-0.8	3
87	8.24E+06	1000.4648	DTMGKAPQPG	18.09	2735	501.2386	-0.9	2
87	6.45E+05	1245.5349	FQHQMSFQHG	18.12	2746	623.7739	-0.1	2
58	6.56E+04	992.4828	PAHTLGFGHG	18.14	2755	331.8341	-1	3
95	4.11E+06	1030.5195	PVHVDTLGHG	18.22	2787	516.2661	-0.6	2
97	4.70E+06	1158.5049	KTDGKYMEMG	18.23	2789	580.2589	-0.2	2
92	1.49E+06	1172.437	WEDQHADTDG	18.24	2796	587.2252	0.3	2
86	6.95E+06	1142.5278	KTKTDEMSFG	18.31	2823	572.2698	-1.2	2
78	1.95E+05	1044.5352	PVHVDTLAHG	18.33	2829	349.1848	-1	3
91	6.64E+05	1231.5291	DQHVKEWSMG	18.34	2833	616.7709	-0.1	2
84	3.94E+06	1146.5571	HTHEHAFVLG	18.45	2904	574.2849	-0.3	2
95	1.14E+07	1068.4624	HSDVFVDGHG	18.57	2929	535.2375	-0.6	2
68	1.42E+05	1017.4702	HADGMVFGKG	18.64	2957	509.7411	-1.1	2
93	2.67E+06	1131.4954	MAWGKQMSHG	18.71	2984	566.754	-0.4	2

93	3.43E+07	966.4229	MADGPSPVHG	18.77	3008	484.2179	-0.4	2
70	5.54E+06	1104.4658	HSKSWSDAMG	18.8	3020	553.2391	-0.7	2
93	4.18E+06	1178.5542	FAHTKYPQMG	19.07	3124	590.2838	0.2	2
72	2.65E+05	980.4385	MADAPSPVHG	19.19	3172	491.2254	-1	2
77	2.61E+05	999.4808	LGMVHGKADG	19.26	3201	500.7451	-3.7	2
98	6.28E+06	1094.5508	PSLAHEKAWG	19.41	3259	548.2819	-0.2	2
88	9.66E+06	1246.6128	KVDQKQMQWG	19.43	3270	624.3128	-0.1	2
97	3.25E+07	1031.4858	HADAMVFGKG	19.63	3351	516.7491	-0.9	2
90	7.98E+06	1164.5564	FGWQKADEKG	19.68	3373	583.2842	-0.9	2
66	2.16E+07	1121.5032	MAKTMQMQPG	19.69	3377	561.7578	-0.6	2
71	2.29E+05	1050.5344	DAFADVKTKG	19.75	3403	351.1849	-0.1	3
90	1.91E+06	1052.3547	MGMGHEMGMG	19.88	3453	527.1837	-0.6	2
52	2.03E+05	1231.5444	HYWEKGMQPG	19.95	3485	616.7784	-0.5	2
93	2.75E+06	1196.5728	WSHAWTPQKG	19.96	3487	599.2925	-0.6	2
70	7.06E+06	1087.4392	PSMGPQHYDG	20.05	3524	544.726	-0.3	2
94	6.77E+06	1097.6233	KVWTPVPSKG	20.13	3556	549.818	-0.4	2
97	1.92E+06	1093.4927	PYDTLGDEKG	20.3	3617	547.7525	-0.7	2
60	2.30E+06	985.4716	KEDGDGPVLG	20.35	3637	493.742	-0.9	2
85	2.63E+06	1050.4651	DSLQDTKGMG	20.52	3684	526.2389	-0.5	2
95	4.42E+06	1146.4917	PTHAHYMSFG	20.61	3718	574.2516	-1.4	2
88	2.53E+06	1204.6353	HVKVHELTWG	20.67	3741	603.3238	-0.5	2
91	4.79E+06	1185.593	LQPTKYHGWG	20.89	3827	593.8028	-0.4	2
98	2.40E+07	1030.4177	PSMGPAHYDG	20.99	3866	516.2151	-0.6	2
64	1.38E+05	1172.5461	KELSDYHQPG	21.41	4001	587.2791	-0.8	2
92	1.92E+06	1050.4805	LTDGMAKGWG	21.55	4090	526.2448	-3.8	2
84	1.88E+06	1265.6306	HVHQKVFEWG	21.51	4036	633.821	-1.1	2
89	2.66E+06	1166.4373	PEMSMEHSFG	21.67	4101	584.2248	-0.6	2
94	3.55E+06	1233.5203	HYDAPQFYHG	21.81	4159	617.7664	-0.3	2
95	4.86E+06	1141.5767	KGLSDQKYFG	22.01	4231	571.7948	-0.1	2
51	2.59E+05	1007.478	PGMSKTLSMG	22.02	4235	504.7455	-0.1	2
95	1.68E+07	1168.5334	HSLYHVMEPG	22.08	4255	585.2729	-0.6	2
94	3.68E+07	1051.5007	LAKGMTDYPG	22.12	4270	526.7568	-0.3	2
91	4.02E+06	1281.6541	MYKTLQWQKG	22.3	4330	641.8336	0.2	2
71	3.28E+07	1053.5244	FTHGPQPTLG	22.45	4385	527.7685	-0.6	2
75	2.24E+06	1124.4419	HYMGPGPYMG	22.53	4415	563.2272	-0.5	2
90	1.27E+07	1032.491	DQLVMADGKG	22.96	4572	517.2517	-0.7	2
87	3.24E+07	1157.573	HQPGWQLVHG	23.11	4631	579.7927	-0.5	2
93	4.18E+07	1096.5188	PSPEKAPEWG	23.12	4636	549.2657	-0.5	2
94	3.13E+06	1107.5713	LTFTKGFTHG	23.34	4721	554.792	-0.4	2
97	2.24E+07	1021.4937	PGMSKTLTMG	23.38	4736	511.7533	-0.3	2
93	3.80E+07	1219.5774	HVWYHEPVPG	23.52	4789	610.7949	-0.5	2
92	6.74E+05	1152.5352	FEFQFGKGHG	23.58	4814	577.274	-0.2	2
89	4.07E+06	1142.5508	WEPYKGLGHG	23.65	4840	572.2818	-0.2	2
64	5.73E+04	1042.4541	PTFGHEMAPG	23.71	4864	522.2327	-1.9	2

88	3.63E+07	1106.5508	HTFAPELVHG	24.03	4976	554.2817	-0.4	2
72	2.60E+05	968.4086	DVDEPGPSPG	24.14	5021	485.2108	-0.4	2
70	1.50E+05	987.4872	LVKSDADSPG	24.21	5045	494.7495	-1.5	2
68	1.50E+05	1038.5862	LGFGLYKGKG	24.33	5088	347.2016	-1.9	3
64	2.82E+06	1158.5571	HQWGPELVHG	24.4	5112	580.284	-1.9	2
69	4.73E+05	1068.5239	LVDTPQWGPG	24.48	5138	535.2681	-0.8	2
95	8.22E+06	1166.6335	PEKGLYKYLG	24.49	5143	584.3231	-0.4	2
87	5.94E+05	1079.54	DGKTKAWAFG	24.61	5185	540.7765	-0.2	2
95	3.61E+06	1078.4753	FVHSLSMSDG	24.86	5285	540.2441	-0.3	2
83	5.42E+07	1016.5291	FQPGLGKVDG	24.89	5297	509.2711	-0.1	2
54	2.67E+06	1089.4106	MEMGPEDQPG	24.93	5310	545.7115	-0.6	2
61	1.36E+05	1050.3755	MGMAHEMGMG	25.13	5392	526.1942	-0.4	2
72	2.93E+06	1148.4443	HEPSMEDTFG	25.19	5412	575.2285	-0.4	2
95	1.30E+07	1119.5383	DVKEWAKGMG	25.45	5503	560.7754	-0.6	2
96	1.22E+06	1318.5806	FYHSMYWTKG	25.58	5551	660.2965	-0.3	2
95	1.69E+07	1023.5059	LTMSFGPSKG	25.66	5581	512.7593	-0.6	2
95	1.11E+07	1201.4612	DEHGMAHYWG	25.82	5638	601.7366	-0.8	2
88	4.01E+07	1116.5815	KELTPTFQPG	25.93	5674	559.2972	-0.3	2
97	4.60E+07	1120.5222	PVDEFQKAMG	26.17	5759	561.2672	-0.8	2
96	6.74E+06	1173.564	KSFGMAKYWG	26.39	5836	587.788	-0.8	2
87	2.66E+06	1096.5552	LVDTPVPYHG	26.6	5916	549.2844	0.4	2
68	7.42E+06	908.4426	PSPVMGPAPG	26.67	5942	455.2275	-1	2
56	1.76E+05	1048.5012	LTDAMAKGWG	26.77	5980	525.2568	-0.7	2
94	1.21E+07	1058.4304	DGDVHEPSFG	26.78	5983	530.2218	0	2
52	1.74E+05	1231.5774	KTHTWYPGWG	26.91	6036	616.7952	0.1	2
96	1.95E+06	1101.4912	MSFEHQLGPG	26.96	6055	551.7517	-0.8	2
97	4.28E+07	1024.4978	FGPVHTPVDG	27.09	6107	513.2552	-0.5	2
97	3.95E+07	1001.5579	LALVMSPSKG	27.26	6173	501.7856	-0.1	2
84	4.68E+06	944.4451	LTDAPSDGLG	27.32	6196	473.2287	-1	2
84	5.13E+05	1233.5964	KYHQMTWALG	27.39	6221	617.8039	-1.3	2
91	3.78E+07	1190.5278	WVPEMTDEKG	27.4	6228	596.2702	-0.4	2
95	2.42E+07	1032.5062	WGMTKSLGPG	27.5	6268	517.2593	-0.9	2
97	4.24E+07	1102.5923	HAFQFGLVKG	27.54	6283	552.3027	-0.1	2
81	4.72E+07	1147.4934	WAKADADEWG	27.57	6296	574.7531	-0.2	2
98	7.85E+06	1261.5913	MYHVDVKQWG	27.58	6302	631.8021	-0.1	2
98	3.30E+07	1155.5447	PYLSDTKEFG	27.83	6404	578.7786	-0.5	2
65	6.67E+05	1114.5627	LGMVMVKQHG	27.97	6489	558.2861	-3.2	2
90	1.98E+06	1258.6282	WQFVMVKQHG	28.34	6585	630.3201	-0.8	2
52	1.92E+05	1095.5601	LYFAKVDSPG	28.63	6682	548.7864	-0.4	2
98	4.95E+07	1153.5654	LYFEKVDSPG	28.79	6743	577.7888	-0.7	2
93	2.72E+06	1168.4683	MGMYHEPTFG	28.82	6754	585.2404	-0.5	2
69	6.89E+06	1153.4941	PSHAWADQWG	29.22	6886	577.7532	-0.6	2
62	2.93E+05	1014.4771	DAPGHTLTFG	29.26	6901	508.2448	-0.6	2
77	2.77E+06	1037.4487	LGDGPQMTFG	29.26	6903	519.7307	-0.5	2

86	1.52E+07	1183.5774	KSWAPQPQWG	29.27	6906	592.7952	-0.1	2
94	7.37E+06	1151.5974	PTFQKSLQFG	29.32	6925	576.8053	0.1	2
73	2.47E+05	1089.48	WSMEDVLGPG	29.38	6946	545.7465	-0.2	2
96	2.08E+07	1135.5662	FQKAWTLADG	29.44	6969	568.7891	-0.9	2
70	2.50E+06	1035.5349	DAHVLQLSPG	29.65	7054	518.7739	-0.4	2
94	1.03E+06	1156.5256	DTFVKQMTMG	29.68	7064	579.269	-0.6	2
82	3.93E+07	1094.6123	LVPVPAKEWG	29.68	7066	548.3128	0.2	2
54	1.53E+05	1178.5972	DVLQPYPYKG	29.94	7157	590.3048	-0.5	2
59	5.55E+04	1209.48	FADSMSWYFG	30.01	7182	605.7427	-6.3	2
94	2.32E+07	1072.4746	LVMSPEDEPG	30.08	7207	537.2437	-0.4	2
95	3.76E+06	1366.6094	WSHEKYFQWG	30.15	7237	684.3108	-0.4	2
93	2.77E+07	1226.6196	LQKQPQWGWG	30.33	7308	614.3163	0	2
76	3.36E+06	1166.5066	FVHVDAFEMG	30.48	7361	584.259	-1.3	2
88	3.31E+07	1177.6243	LTWVPQHQLG	30.5	7368	589.8178	-1.4	2
95	1.08E+06	1124.5901	MTKSLTFQLG	30.77	7457	563.3013	-0.6	2
70	2.69E+05	1009.5266	FALGKGMTLG	30.81	7471	505.7694	-1	2
96	1.23E+06	1277.5574	MTKQWAFYMG	31	7537	639.785	-0.2	2
88	3.33E+05	1203.5923	FQKEWAPELG	31.02	7542	602.8023	-0.5	2
88	1.74E+06	1188.6079	FVHVLAFYHG	31.16	7577	397.209	-1	3
95	3.90E+07	1042.5083	DVPGHTLTFG	31.3	7623	522.2604	-0.6	2
76	1.26E+05	1073.6121	LALALEKYPG	31.48	7687	537.8122	-0.8	2
97	1.78E+07	1162.5442	DQMQWALSKG	31.61	7729	582.2779	-1.2	2
98	5.35E+07	1139.5071	PVDAWVHEMG	31.76	7788	570.7596	-0.9	2
79	4.23E+07	1068.5603	DVPTKVPAWG	31.77	7793	535.2866	-0.2	2
95	1.22E+07	1023.5423	FALGKSMTLG	31.87	7832	512.7774	-0.7	2
74	3.31E+07	1201.5403	WSHVDYPELG	31.89	7835	601.776	-1.1	2
71	3.18E+06	1010.4015	PYDGLSDGMG	32.08	7902	506.2072	-0.4	2
69	2.48E+07	1120.5376	KSMVPGWYPG	32.11	7914	561.2747	-1.1	2
78	2.54E+07	998.492	LSPALTDEPG	32.14	7926	500.2527	0.1	2
84	2.96E+07	1112.5139	LAPQPEWTDG	32.22	7958	557.2637	0.3	2
98	5.82E+07	1131.6174	LALELEKYPG	32.27	7981	566.8151	-0.3	2
83	1.97E+07	1157.6233	WQPVFVPTKG	32.31	7998	579.8179	-0.4	2
79	2.81E+06	1147.4492	FAFQDTDTMG	32.38	8025	574.731	-0.2	2
52	7.23E+04	1049.5393	DAFVLSKVDG	32.51	8078	525.7756	-1.2	2
95	3.91E+06	1170.676	LVKQWSLQLG	32.52	8081	586.3439	-1	2
92	3.06E+07	1199.5547	FQWAPQHVMG	32.57	8099	600.7838	-0.1	2
96	2.98E+07	1227.5195	FQDEFTHTFG	32.81	8189	614.7659	-0.6	2
88	1.19E+07	986.4379	DVPVMGPTDG	32.82	8192	494.2251	-1	2
66	2.11E+07	1112.5535	LTPQLQMEPG	33.03	8272	557.2831	-0.4	2
90	6.06E+05	1201.5227	MSFTKGWSWG	33.12	8302	601.7673	-1	2
67	4.86E+05	1347.5229	WEHSFYMEFG	33.33	8380	674.7667	-1.8	2
95	2.76E+06	1169.5869	PTWVWEPAKG	33.62	8462	585.7994	-1	2
76	1.70E+06	1072.384	DSMGDTPYMG	33.88	8538	537.1987	0.1	2
94	4.13E+06	1248.5298	DYKTDEFQFG	34.16	8646	625.2711	-0.4	2

86	2.44E+05	1454.6409	HYWYWTWEKG	34.37	8720	728.3275	0.9	2
69	2.06E+07	1246.46	HEDYDYMAFG	34.41	8731	624.2361	-0.6	2
92	3.86E+06	1340.5647	PQPYHYMYWG	34.44	8744	671.2886	-0.3	2
71	5.09E+07	1231.6238	FQKEWVPELG	34.45	8747	616.818	-0.6	2
82	1.63E+07	1216.5037	FYDQPTDQFG	34.56	8820	609.258	-0.5	2
76	1.90E+05	1135.5662	LEFTKGFTHG	34.57	8789	568.7895	-0.2	2
93	3.04E+07	1212.5498	MALQWGHQWG	34.64	8816	607.2809	-0.8	2
83	2.35E+07	1062.5168	DVWGKGMTLG	34.87	8899	532.2653	0.6	2
93	1.99E+07	1305.5415	WTDEFTWQHG	34.94	8923	653.7769	-0.4	2
77	2.36E+06	1135.4392	HEFAMSWGDG	35.02	8951	568.7257	-0.8	2
94	1.36E+07	1190.478	WTDGFEWGHG	35.12	8987	596.2454	-0.3	2
98	1.77E+06	1314.6067	WSLYKQWTMG	35.12	8989	658.3096	-0.3	2
60	2.55E+05	1204.4937	WTDAFEWGHG	35.19	9011	603.2541	1.3	2
88	2.35E+07	1062.5232	LVPADTLYDG	35.21	9017	532.2673	-1.7	2
96	5.48E+06	1019.4382	LTDSPGMGWG	35.29	9051	510.7253	-0.8	2
93	9.11E+05	1228.624	LVWVDYHQLG	35.32	9062	615.3184	-0.2	2
70	1.88E+07	1111.4822	PSPEDVPEWG	35.58	9154	556.7477	0.1	2
94	1.31E+07	1171.6238	LQLELYHSLG	35.82	9232	586.819	1.1	2
90	2.98E+06	1294.6709	PQKQLYLYWG	35.9	9251	648.3419	0.	2
91	6.17E+04	1077.5706	DVFVLSKVDG	35.96	9268	539.7922	0.6	2
81	3.27E+05	1252.5513	FGKTDEWQWG	35.99	9280	627.2815	-1	2
96	5.98E+06	1175.5684	KYPSLYMAFG	36.04	9299	588.79	-1.2	2
95	1.27E+06	1268.6111	WEKEMTLYLG	36.13	9327	635.311	-1.5	2
86	2.29E+06	1207.5662	PTWYLSFTHG	36.53	9417	604.789	-0.9	2
90	4.30E+06	1306.5691	WSMEKYFYPG	36.64	9443	654.2908	-0.2	2
96	2.17E+06	1338.5305	FADYWEHEWG	36.89	9519	670.2706	-1.6	2
76	1.42E+06	1309.5405	HVMYMQMQWG	36.91	9527	655.7763	-0.6	2
95	2.53E+06	1193.5361	WSMYLVHAMG	37.09	9576	597.774	-1	2
78	1.24E+06	1090.4541	PAWSPSWGMG	37.18	9630	546.2332	-0.8	2
76	1.06E+06	1214.6157	FYMVKQFVPG	37.23	9616	608.3145	0.2	2
60	2.35E+06	1171.4458	DAPYDYWADG	37.48	9680	586.7294	-0.1	2
88	1.14E+07	1257.603	KQWTLYDTFG	37.94	9794	629.8082	0.3	2
92	9.09E+06	1082.4919	LVFTDYPGDG	38.13	9849	542.2521	-0.9	2
91	1.35E+07	1044.5239	DVLSFTHGLG	38.38	9914	523.2694	1.6	2
55	1.85E+06	1120.4683	MQWSDAPVMG	38.42	9928	561.2406	-0.1	2
92	2.51E+06	1097.4719	WSFGFGHGFG	38.43	9931	549.743	0.9	2
93	1.60E+05	1362.6245	WTKEWELEWG	38.59	9980	682.3182	-0.7	2
94	1.02E+07	1292.6377	WQWVKYPVMG	38.78	10043	647.3246	-1.1	2
80	8.23E+06	1095.4907	FQMVDTDALG	39.13	10138	548.7524	0.8	2
60	9.37E+05	1126.5559	LGHTWTWGLG	39.29	10183	564.2841	-0.8	2
73	5.24E+06	1079.4197	WSPADGFEDG	39.45	10232	540.718	2.9	2
95	3.72E+06	1125.6006	LAWVHVMTLG	39.48	10243	563.8063	-0.9	2
81	2.10E+07	1243.5549	KYFGFYDTFG	39.53	10269	622.7836	-0.6	2
84	1.68E+07	1294.5618	DTLYHQFEWG	39.49	10248	648.2874	0.1	2

64	1.07E+07	1209.5642	LTHGMVWYFG	39.52	10256	605.7877	-1.4	2
90	6.25E+06	1186.5811	KVFYWSFGPG	39.63	10290	594.2966	-0.8	2
50	1.20E+07	1171.6025	LVHVDTFVWG	39.65	10294	586.809	2.1	2
91	1.25E+06	1199.54	LYWGFSFSHG	40.15	10407	600.7758	-1.3	2
80	2.44E+06	1167.4292	MSDSDGWQWG	40.55	10501	584.7209	-0.3	2
67	6.24E+05	1219.551	LTFQPEDQWG	40.68	10538	610.7813	-1.1	2
89	4.67E+06	1224.5122	MYPQLSDEWG	41.01	10609	613.2629	0.5	2
90	1.26E+07	1156.5552	DVWAKSFTFG	41.21	10658	579.2837	-0.7	2
61	1.16E+05	1356.6501	KTFEWQLYWG	41.43	10722	679.3303	-1.7	2
76	5.53E+05	1106.5066	LSLSWAMQDG	41.55	10744	554.2593	-1	2
76	4.45E+05	1135.6311	KELYMVLALG	41.74	10782	568.822	-0.2	2
96	6.28E+05	1254.6438	KYPVPVWYFG	41.95	10825	628.3303	3	2
74	1.95E+05	1154.5066	LQWGFSMVDG	42.01	10847	578.261	2	2
71	8.85E+05	1316.5398	HSWEWAWQMG	42.19	10888	659.2758	-0.8	2
95	6.33E+05	1293.5488	DYFGMQKYWG	42.52	10948	647.7808	-0.1	2
66	1.45E+07	1203.5237	PYPAFYDQFG	42.85	11024	602.7686	0.5	2
81	5.23E+05	1057.5081	PALEWGLTDG	43.2	11104	529.7596	-1.8	2
64	3.00E+05	1154.4856	FSPAWAMSWG	43.31	11119	578.2467	-4.5	2
87	1.06E+06	1247.4475	MTWYDEMTDG	43.36	11128	624.7296	-1	2
72	7.16E+06	1184.5503	FQFYLAPQDG	43.67	11182	593.2814	-0.4	2
78	2.00E+06	1021.4657	FGPSFAWGPG	43.81	11210	511.7367	-5.4	2
81	7.73E+06	1131.5601	FVWEPTLSPG	44.04	11258	566.7855	-1.9	2
61	1.47E+07	1082.5073	PAFAFYPVDG	44.86	11444	542.2597	-1	2
67	1.40E+05	1039.4434	FGWAMSDGLG	45	11472	520.7255	-5.4	2
78	1.21E+07	1205.554	FEMQPQWALG	45.03	11481	603.783	-0.8	2
64	2.40E+05	1153.5325	MQLEDTLTFG	45.19	11508	577.7739	1.9	2
53	1.27E+04	1210.4963	DEFGLEMQWG	45.34	11541	606.2566	3.2	2
61	8.34E+05	990.5386	LSLSFAPSLG	45.5	11568	496.2754	-1.1	2
48	2.11E+05	1210.4998	MTDTLEMQWG	45.68	11600	606.2535	-4.7	2
67	2.79E+05	1149.488	WSPADQFGWG	45.82	11620	575.7488	-3	2
65	5.29E+05	1043.6016	FAPQLSLVLG	45.91	11638	522.8069	-0.9	2
65	2.41E+06	1293.5303	PEDQWYWVDG	46.23	11689	647.7706	-1.5	2
64	2.15E+05	1100.5391	FYLSLSLSDG	46.31	11700	551.2759	-0.3	2
81	2.56E+05	1004.5178	LALGDVDVFG	46.39	11714	503.2643	-2.4	2
88	1.59E+05	1188.554	MGWVWAFVHG	46.77	11767	595.2816	-3.2	2
73	2.06E+06	1182.4805	WGMAPTDYWG	47.03	11807	592.2463	-0.8	2
69	2.20E+05	1168.4683	WAWADTMTMG	47.43	11874	585.2402	-0.7	2
69	4.77E+06	1160.5688	PQWVMAPYLG	47.53	11893	581.2915	1	2
76	3.66E+05	1153.4751	MEFALEDGWG	48.46	12070	577.7441	0.1	2
71	2.55E+05	1178.5139	PYLTMGMYFG	48.69	12103	590.2628	-1.2	2
73	1.03E+05	1297.5403	WQWADYFEPG	48.75	12113	649.7765	-0.1	2
76	4.00E+06	1318.5505	DQWYPYLYDG	49.02	12164	660.2816	-0.2	2
64	1.84E+05	1208.5024	FEDAFTFEFG	49.71	12282	605.2559	-3	2
63	2.02E+05	1249.5146	FSMYWEMSLG	50.14	12344	625.7635	-0.4	2

63	4.69E+05	1159.4644	WGDTFAMEFG	50.19	12363	580.7386	-0.1	2
64	1.45E+05	1083.5422	PVMAKSFTFG	50.27	12388	542.7756	-3.9	2
72	2.95E+06	1091.5288	PGLTDYLAWG	50.71	12456	546.7688	-4	2
88	5.15E+04	1207.5662	LVWTFQDGWG	50.92	12498	604.7899	0.6	2
63	6.55E+05	1078.552	PVPYLVMGFG	51.16	12562	540.2819	-1.2	2
78	3.39E+05	1165.5479	LVFVDAMEWG	51.37	12609	583.78	-0.8	2
62	1.50E+05	1174.5403	LTDVFVMYMG	51.44	12624	588.277	0.6	2
65	1.84E+05	1264.5586	PEWTMVPYWG	52.03	12709	633.2855	-0.5	2
84	2.22E+06	1297.5479	FYWTPSMYFG	52.19	12733	649.7793	-1.6	2
81	4.47E+06	1224.5239	FEWEPAWGFG	52.36	12763	613.2675	-1.6	2
64	4.73E+06	1234.5559	WQPTWAFGWG	52.81	12857	618.2844	0	2
75	3.46E+05	1189.4717	FGWEDEFGFG	53.2	12952	595.7424	0	2
80	4.92E+05	1266.5413	MVWSLEMEWG	53.51	12999	634.2756	-2.3	2
69	3.91E+03	1183.5549	LEDALYWAFG	53.6	13019	592.7836	-0.6	2
77	4.52E+06	1214.4888	MYDVWGMAWG	53.89	13073	608.2473	-5.9	2
70	3.14E+05	1283.5798	MVWQWAPYFG	53.99	13088	642.7948	-2.4	2
73	5.00E+05	1206.5232	FSPEDYFVFG	54.98	13262	604.2664	-2.9	2
77	1.50E+06	1143.4873	DSLSFGFEWG	55.96	13418	572.7488	-2.5	2
69	1.84E+05	1341.5852	PEWQFYMVWG	56.2	13469	671.7985	-0.8	2
76	2.65E+05	1135.4609	DSWSFGFSFG	57.46	13658	568.7366	-0.8	2
70	4.45E+05	1415.5823	WYFEDEWVWG	57.94	13741	708.7972	-0.4	2
53	1.65E+05	1201.5479	DTMAWYFVLG	62.37	14486	601.7801	-0.5	2