Supporting Information

Discovery of nucleic acid binding molecules from combinatorial biohybrid nucleobase peptide libraries

Sebastian Pomplun,[1] Zachary P. Gates,[1,†] Genwei Zhang,[1] Anthony J. Quartararo,[1] Bradley L. Pentelute[1-4*]

[1] Massachusetts Institute of Technology, Department of Chemistry, 77 Massachusetts Avenue, Cambridge, MA 02139, USA

[2] The Koch Institute for Integrative Cancer Research, Massachusetts Institute of Technology, 500 Main Street, Cambridge, MA 02142, USA

[3] Center for Environmental Health Sciences, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, MA 02139, USA

[4] Broad Institute of MIT and Harvard, 415 Main Street, Cambridge, MA 02142, USA

† Present address: Agency for Science, Technology and Research (A*STAR), p53Lab, 8A Biomedical Grove, Singapore 138648, Singapore

*Correspondence to: blp@mit.edu

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General materials and methods

Chemicals: Unless otherwise noted, all chemicals were obtained from commercial sources and used as received without further purification. Anhydrous tetrahydrofuran (THF) and *N*,*N*-diisopropylethylamine (DIEA) were obtained from a Seca Solvent Purification System by Pure Process Technology.

LC-MS analysis: LC-MS chromatograms and associated mass spectra were acquired using an Agilent 6550 ESI-QToF mass spectrometer or an Agilent 6520 ESI-QToF mass spectrometer. Mobile phases used for LC-MS analysis were solvent A (0.1% formic acid in water) and solvent B (0.1% formic acid in acetonitrile). The following LC-MS methods were used:

Method A: On 6550 MS; C_4 Phenomenex Jupiter column (1 x 150 mm, 5 µm); LC conditions: 1% B from 0–2 minutes, linear ramp from 5% to 61% B from 2–12 minutes, 0.1 mL/min flow rate.

Method B: On 6520 MS; Zorbax 300SB-C_3 column (2.1 x 150 mm, 5 µm); LC conditions: 1% B from 0–2 min, linear ramp from 5% to 61% B from 2–12 min, linear ramp from 61% to 90% 11-12 min, 0.8 mL/min flow rate.

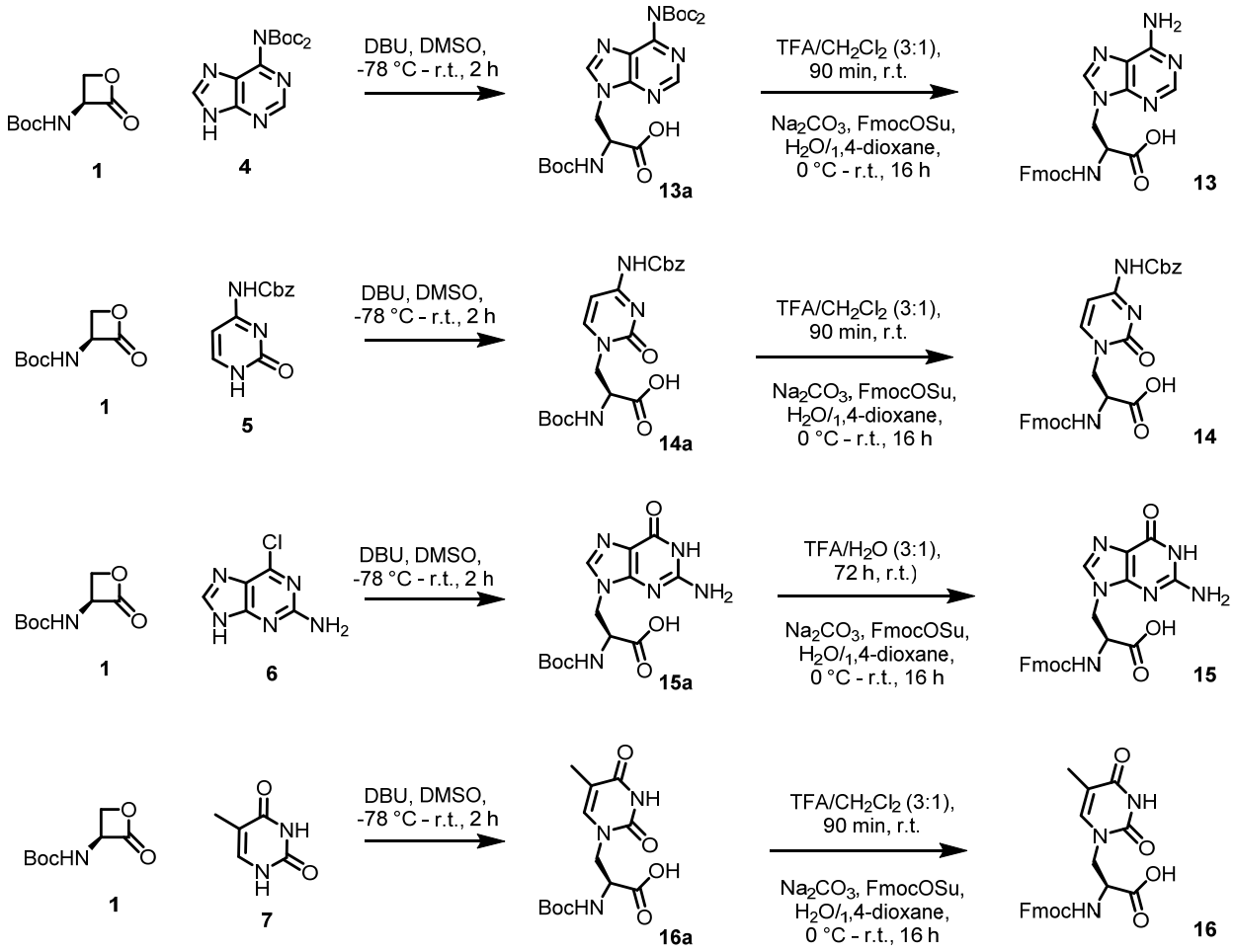
NMR analysis: NMR spectra were acquired on 400 or 500 MHz Bruker spectrometers at ambient temperature. Samples were prepared in chloroform-*d* (DMSO-d_6 or $CDCl_3$). ^{1}H NMR data are reported as chemical shifts with multiplicity, coupling constants (J) in Hz, and integrations. Proton chemical shifts are reported in ppm (δ) relative to tetramethylsilane (δ 0.00 ppm) and referenced to residual solvent ($CHCl_3$, δ 7.26 ppm or DMSO-d_6 , δ 2.50ppm (quintet, J_{HD}=1.9Hz)).[1] Multiplicity is reported as follows: singlet (s), broad singlet (bs), doublet (d), doublet of doublets (dd), triplet (t), quartet (q), multiplet (m), and overlapping multiplets (comp). ^{13}C NMR spectra were recorded on 500 (^{13}C 126) MHz Bruker spectrometers with proton decoupling at ambient temperature, unless otherwise noted. Carbon chemical shifts are reported in ppm (δ) and referenced to solvent ($CDCl_3$, δ 77.16 ppm).[1]

Nano-LC/MSMS analysis of peptide libraries: Nano-LC/MSMS analysis of library bead mixtures was performed on Thermo Fisher Orbitrap Fusion Lumos Tribrid Mass Spectrometer coupled to Thermo Fisher EASY-nLC 1200 System equipped with an Acclaim PepMap RSLC C18 column (150 mm x 75 µm ID, 2 µm particle size, 100 Å pore size) and a nanoViper C18 Trap Column (20 mm x 75 µm ID, 3 µm particle size, 100 Å pore size). 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 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 118 minutes, followed by 61-99% B' in A' ramping linearly over 5 minutes and finally 99% B' in A' for 5 minutes. MS^2 acquisition over the course of the method was performed in a data-dependent style (Top N=15, z=2-10, intensity threshold = 10^5) with a dynamic precursor exclusion for 30 seconds after each scan. CID and HCD fragmentation 9 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.

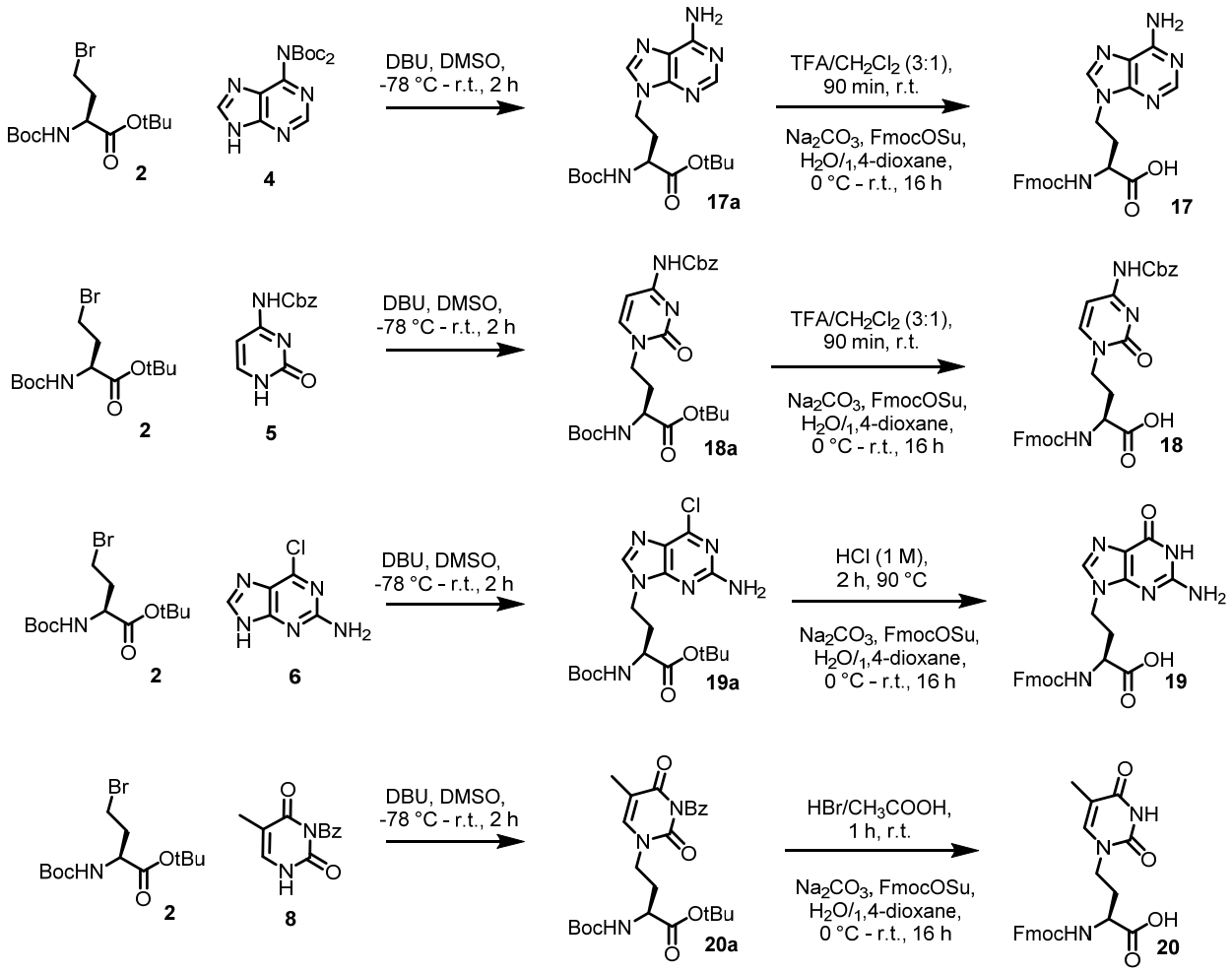
Purification: Normal-phase column chromatography was performed with a Biotage Selekt flash purification system, equipped with 25 g or 100 g Biotage Sfär Silica HC-D 20 µm columns, using an appropriate gradient of EtOAc/Hexanes. Reversed-phase column chromatography was performed with a Biotage Selekt flash purification system equipped with either 10 g Biotage SNAP Bio C18 20 µm columns or 25 g Biotage Sfär Bio C18 D 20 µm columns with an appropriate gradient of MeCN/H_2O (0.1% TFA). Reversed-phase preparative HPLC was performed using an Agilent mass directed purification system (1260 infinity LC and 6130 single quad MS), equipped with an Agilent Zorbax SB C3 column (9.4 x 250 mm, 5 µm), using an appropriate gradient of MeCN/H_2O (0.1% TFA).

Preparative organic synthesis of Fmoc protected nucleobase amino acid monomers

Schemes



SI Scheme 1. Synthesis of alanyl nucleobase monomers. Protecting group discussion: Attempts to use adenine without any N6 protecting group produced both **13a** and its regioisomer (7-adenilyl; data not shown). The bis-Boc protection on N6 directs the nucleophilic ring opening to the desired 9-adenilyl isomer. **13** could be used for SPPS without protecting on N6: no side reaction due to amide couplings on N6 were observed. Cytosine could be used without any N4 protecting groups: the monomer synthesis was successful and during SPPS no side reaction due to amide couplings on N4 were observed. After SPPS, however, we observed 20 - 30% elimination of the cytosine nucleobase from the nucleopeptides. N4-Cbz protection prevented this (not further investigated) side reaction.

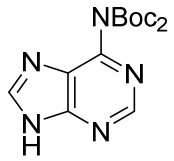


SI Scheme 2. Synthesis of homoalanyl nucleobase monomers. Protecting group discussion: Attempts to use adenine without any N6 protecting group produced both **17a** and its regioisomer (7-adenilyl; data not shown). The bis-Boc protection on N6 directs the nucleophilic substitution to the desired 9-adenilyl isomer. **17** could be used for SPPS without protecting on N6: no side reaction due to amide couplings on N6 were observed. While cytosine could be used without any N4 protecting group for the nucleophilic substitution step, during SPPS we observed side reaction due to amide couplings on N4. Prolonged acidic cleavages or permanence in aqueous conditions removed these secondary side chains, but to avoid inefficient SPPS, we used N4-Cbz protection. Unprotected thymidine afforded > 30% N3 regioisomer in the nucleophilic substitution. Benzoyl protection was used to generate pure **20a**.

Synthesis procedures

Synthesis of 6-N(Boc)$_2$-adenine (4)

According to Dey et al., J. Org. Chem. 2000, 65, 7697

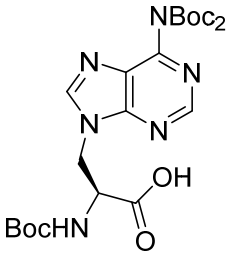


To a solution of adenine (2.70 g, 20.0 mmol) in THF (anhydrous, 100 mL) was added Boc anhydride (18.4 mL, 80 mmol) and 4-(Dimethylamino)pyridine (244 mg, 2.00 mmol). After 16 h stirring at room temperature the solvent was removed under reduced pressure and the mixture taken up in EtOAc (500 mL). The organic phase was washed with HCl (1 M, aq. sol., 100 mL) and NaCl (sat. aq. sol., 100 mL) and then dried under reduced pressure. The resulting slurry was redissolved in MeOH (200 mL), treated with $NaHCO_3$ (sat. aq. sol., 90 mL) and stirred for 1 h at 50 °C. The MeOH was then removed under reduced pressure, the solution diluted with H_2O and extracted with CH_2Cl_2 (3 x 100 mL). The organic phase was washed with HCl (1 M, aq. sol., 100 mL) and NaCl (sat. aq. sol., 100 mL) and then dried under reduced pressure affording the desired product as a colorless solid (4.00 g, 11.9 mmol, 60%).

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.81 (s, 1H), 8.64 (s, 1H), 1.37 (s, 18H).

TLC R_f (EtOAc) 0.59, visualized with UV light

Synthesis of Nα-Boc-β-(6-N(Boc)$_2$-9-adenilyl)alanine (13a)

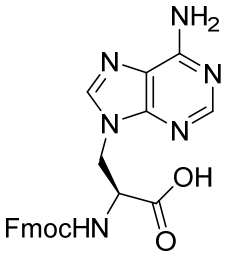


To a solution of **4** (3.00 g, 8.90 mmol) in DMSO (60 mL) was added DBU (1.23 g, 8 mmol) and stirred for 2 h at room temperature. The solution was then cooled to -78 °C and Boc-serinolactone (1.5 g, 8 mmol) dissolved in DMF (20 mL) was added dropwise. The reaction was allowed to warm up to room temperature and was stirred over-night. EtOAc (250 mL) was added to the solution and washed with aq. HCl (1 M, 3 x 50 mL). The organic layer was dried with Na_2SO_4 and solvent removed under reduced pressure. Column chromatography over SiO_2 (hexanes/EtOAc = 1:1) afforded the product as a colorless solid (1.75 g, 3.35 mmol, 38%).

^{1}H NMR (500 MHz, DMSO-*d*6) δ 13.09 (s, 1H), 8.85 (s, 1H), 8.49 (s, 1H), 7.39 – 7.30 (m, 1H), 4.71 (d, *J* = 9.0 Hz, 1H), 4.51 (t, *J* = 6.1 Hz, 2H), 1.37 (s, 27H).

^{13}C NMR (126 MHz, DMSO-d_6) δ 171.63, 162.77, 155.65, 153.70, 151.87, 150.45, 149.41, 147.52, 145.56, 128.12, 83.69, 83.59, 78.95, 53.12, 44.44, 36.25, 31.24, 28.47, 27.75.

Synthesis of Nα-Fmoc-β-(9-adeninyl)alanine (13)



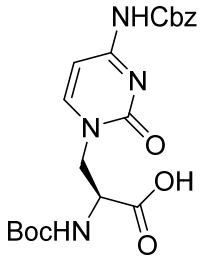
13a (1.75 g, 3.35 mmol) was dissolved in TFA/DCM (60 mL, 3:1) and stirred for 90 min at room temperature. The solvent was removed under reduced pressure and the mixture taken up in aq. Na_2CO_3 (10%, 50 mL) and 1,4-dioxane (20 mL) and cooled to 0 °C. FmocOSu (1.30 g, 4.02 mmol) was dissolved in 1,4-dioxane (30 mL) and added dropwise to the mixture. The reaction was allowed to reach room temperature and was stirred overnight. H_2O (100 mL) was added to the solution and washed with hexanes (3 x 50 mL). The aqueous phase was acidified with aq. HCl (6 M) until precipitation of a colorless solid was observed. The precipitate was filtered and washed with aq. HCl (1 M), affording the desired product as a colorless solid (800 mg, 1.80 mmol, 54% over two steps).

^{1}H NMR (400 MHz, DMSO-d_6) δ 13.25 (s, 1H), 8.46 (s, 2H), 8.35 (s, 1H), 8.25 (s, 1H), 7.90 (dd, *J* = 14.4, 7.8 Hz, 3H), 7.60 (dd, *J* = 12.6, 7.5 Hz, 2H), 7.41 (td, *J* = 7.5, 3.3 Hz, 2H), 7.36 – 7.27 (m, 2H), 4.69 – 4.62 (m, 1H), 4.57 – 4.44 (m, 2H), 4.29 – 4.12 (m, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 171.31, 156.30, 149.57, 144.14, 144.10, 143.56, 141.15, 128.12, 127.54, 125.60, 125.57, 120.59, 118.65, 66.25, 53.83, 46.95, 44.21.

HRMS (ESI-QToF) *m/z:* $[M+H]^+$ calcd 445.1546, found 445.1791.

Synthesis of Nα-Boc-(*N*4-Cbz-1-cytosinyl)alanine (14a)

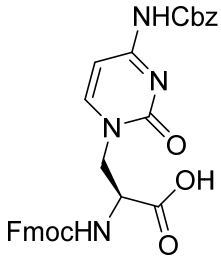


To a solution of Cbz-Cytosine (3.5 g, 14.3 mmol) in DMSO (30 mL) was added DBU (2.2 g, 14.3 mmol). The solution was stirred for 20 min at RT before adding dropwise a solution of Boc-serinolactone (3.2 g, 17.1 mmol) in DMSO (10 mL). After 3 h stirring, EtOAc (250 mL) was added to the solution and washed with aq. HCl (1 M, 3 x 50 mL). The organic layer was dried with Na_2SO_4 and solvent removed under reduced pressure. Column chromatography over SiO_2 (CH_2Cl_2 + 5% MeOH) afforded the product as a colorless solid (2.4 g, 5.6 mmol, 39%).

^{1}H NMR (500 MHz, DMSO-d_6) δ 7.85 (d, *J* = 7.4 Hz, 1H), 7.46 – 7.29 (m, 6H), 7.12 (d, *J* = 8.6 Hz, 1H), 6.97 (d, *J* = 7.6 Hz, 1H), 5.21 – 5.17 (m, 2H), 4.42 – 4.33 (m, 2H), 3.71 – 3.61 (m, 1H), 1.32 (d, *J* = 3.6 Hz, 9H).

HRMS (ESI-QToF) *m/z:* $[M+H]^+$ calcd 433.1723, found 433.1732.

Synthesis of Nα-Fmoc-(*N*4-Cbz-1-cytosinyl)alanine (14)



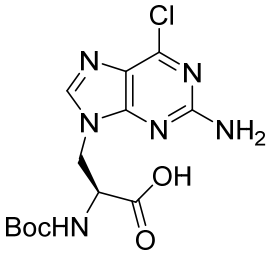
14a (2.4 g, 5.6 mmol) was dissolved in TFA/DCM (60 mL, 3:1) and stirred for 90 min at room temperature. The solvent was removed under reduced pressure and the mixture taken up in aq. Na_2CO_3 (10%, 50 mL) and 1,4-dioxane (20 mL) and cooled to 0 °C. FmocOSu (2.00 g, 5.9 mmol) was dissolved in 1,4-dioxane (30 mL) and added dropwise to the mixture. The reaction was allowed to reach room temperature and was stirred overnight. H_2O (100 mL) was added to the solution and washed with hexanes (3 x 50 mL). The aqueous phase was acidified with aq. HCl (6 M) until precipitation of a colorless solid was observed. The precipitate was filtered and washed with aq. HCl (1 M). The precipitate was the desired product (1.9 g, 3.4 mmol, 61%).

^{1}H NMR (400 MHz, DMSO-d_6) δ 10.81 (s, 1H), 7.94 – 7.75 (m, 4H), 7.63 (t, *J* = 7.5 Hz, 2H), 7.48 – 7.26 (m, 9H), 6.94 (d, *J* = 7.3 Hz, 1H), 5.24 – 5.14 (m, 2H), 4.49 – 4.36 (m, 2H), 4.35 – 4.17 (m, 3H), 3.84 – 3.70 (m, 1H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 171.66, 163.48, 156.44, 144.21, 144.13, 141.19, 136.43, 128.95, 128.64, 128.44, 128.40, 128.10, 127.51, 125.58, 120.58, 66.96, 66.17, 52.07, 47.02.

HRMS (ESI-QToF) *m/z:* $[M+H]^+$ calcd 555.1880, found 555.1880.

Synthesis of Nα-Boc-β-(2-amino-6-chloro-9-purinyl)alanine (15a)



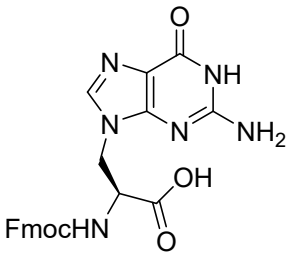
To a solution of 6-chloropurine (3.77 g, 22.3 mmol) in DMSO (40 mL) was added DBU (4.06 g, 26.6 mmol). The solution was stirred for 20 min at RT before adding dropwise a solution of Boc-serinolactone (5.0 g, 26.7 mmol) in DMSO (30 mL). After 2 h stirring, EtOAc (250 mL) was added to the solution and washed with aq. HCl (1 M, 3 x 50 mL). The organic layer was dried with Na_2SO_4 and solvent removed under reduced pressure. Column chromatography over SiO_2 (CH_2Cl_2 + 10% MeOH) afforded the product as a colorless solid (5.0 g, 14.0 mmol, 63%).

^{1}H NMR (400 MHz, DMSO-d_6) δ 13.10 (s, 1H), 7.94 (s, 1H), 7.29 (d, *J* = 8.6 Hz, 1H), 6.95 (s, 2H), 4.50 – 4.35 (m, 2H), 4.22 (dd, *J* = 13.5, 9.8 Hz, 1H), 1.29 (s, 9H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 171.70, 160.27, 155.70, 154.60, 149.75, 143.89, 123.71, 79.02, 52.88, 43.94, 40.90, 28.47, 27.97.

HRMS (SI-QToF) *m/z:* $[M+H]^+$ calcd 357.1078, found 357.1077.

Synthesis of Nα-Fmoc-β-((9-guaninyl)alanine (15)



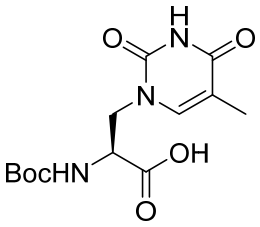
15a (5.0 g, 14.0 mmol) was dissolved in TFA/H_2O (80 mL, 3:1) and stirred for 72 h at room temperature. The solvent was removed under reduced pressure and the mixture taken up in aq. Na_2CO_3 (10%, 50 mL) and 1,4-dioxane (20 mL) and cooled to 0 °C. FmocOSu (5.7 g, 16.8 mmol) was dissolved in 1,4-dioxane (30 mL) and added dropwise to the mixture. The reaction was allowed to reach room temperature and was stirred overnight. H_2O (100 mL) was added to the solution and washed with hexanes (3 x 50 mL). The aqueous phase was acidified with aq. HCl (6 M) until precipitation of a colorless solid was observed. The precipitate was triturated with hexanes/CH_2Cl_2 (1:1), centrifuged and collected, affording the desired product (4.8 g, 10.4 mmol, 74%).

^{1}H NMR (400 MHz, DMSO-d_6) δ 13.19 (s, 1H), 10.84 (s, 1H), 7.89 (d, *J* = 7.7 Hz, 4H), 7.63 (dd, *J* = 15.6, 7.5 Hz, 2H), 7.45 – 7.39 (m, 2H), 7.37 – 7.27 (m, 2H), 6.70 (s, 2H), 4.49 – 4.37 (m, 2H), 4.34 – 4.14 (m, 4H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 171.70, 160.27, 155.70, 154.60, 149.75, 143.89, 123.71, 79.02, 52.88, 43.94, 40.90, 28.47, 27.97.

HRMS (SI-QToF) *m/z:* $[M+H]^+$ calcd 461.1573, found 461.1620.

Synthesis of Nα-Boc-β-(1-thyminyl)alanine (16a)



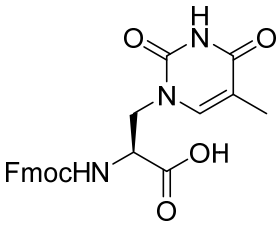
To a solution of Thymidine (2.81 g, 22.3 mmol) in DMSO (40 mL) was added DBU (4.06 g, 26.6 mmol). The solution was stirred for 20 min at RT before adding dropwise a solution of Boc-serinolactone (5.0 g, 26.7 mmol) in DMSO (30 mL). After 2 h stirring, EtOAc (250 mL) was added to the solution and washed with aq. HCl (1 M, 3 x 50 mL). The organic layer was dried with Na_2SO_4 and solvent removed under reduced pressure. Column chromatography over SiO_2 (CH_2Cl_2 + 5% MeOH) afforded the product as a colorless solid (2.0 g, 6.4.0 mmol, 29%).

^{1}H NMR (500 MHz, DMSO-d_6) δ 12.97 (s, 1H), 11.25 (s, 1H), 7.32 (s, 1H), 7.14 (d, *J* = 8.9 Hz, 1H), 4.37 – 4.28 (m, 1H), 4.21 (dd, *J* = 13.7, 4.8 Hz, 1H), 3.55 (dd, *J* = 13.7, 10.2 Hz, 1H), 1.73 (s, 3H), 1.33 (s, 9H).

^{13}C NMR (126 MHz, DMSO-d_6) δ 171.76, 164.76, 155.76, 151.33, 142.42, 138.18, 108.25, 78.93, 51.92, 49.03, 40.90, 28.55, 28.49, 28.19, 12.48, 12.27.

HRMS (SI-QToF) *m/z:* $[M+H]^+$ calcd. 314.1352, found 314.1339.

Synthesis of Nα-Fmoc-β-(1-thyminyl)alanine (16)



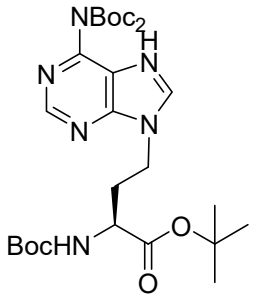
16a (2.0 g, 6.4 mmol) was dissolved in TFA/DCM (60 mL, 3:1) and stirred for 90 min at room temperature. The solvent was removed under reduced pressure and the mixture taken up in aq. Na_2CO_3 (10%, 50 mL) and 1,4-dioxane (20 mL) and cooled to 0 °C. FmocOSu (2.6 g, 7.7 mmol) was dissolved in 1,4-dioxane (30 mL) and added dropwise to the mixture. The reaction was allowed to reach room temperature and was stirred overnight. H_2O (100 mL) was added to the solution and washed with hexanes (3 x 50 mL). The aqueous phase was acidified with aq. HCl (6 M) until precipitation of a colorless solid was observed. The precipitate was filtered and washed with aq. HCl (1 M). The precipitate was the desired product (1.75 g, 4.0 mmol, 63%).

^{1}H NMR (500 MHz, DMSO-d_6) δ 13.09 (s, 1H), 11.29 (s, 1H), 7.89 (s, 2H), 7.78 (d, *J* = 8.9 Hz, 1H), 7.70 – 7.63 (m, 2H), 7.45 – 7.40 (m, 2H), 7.38 – 7.36 (m, 1H), 7.35 – 7.30 (m, 2H), 4.42 – 4.34 (m, 1H), 4.30 – 4.15 (m, 5H), 3.63 (dd, *J* = 13.8, 10.0 Hz, 1H), 1.61 (s, 3H).

^{13}C NMR (126 MHz, DMSO-d_6) δ 171.63, 164.74, 156.48, 151.33, 144.22, 144.08, 142.35, 141.18, 141.15, 128.14, 127.55, 127.53, 125.62, 120.62, 120.60, 108.42, 66.37, 52.56, 48.74, 47.00, 25.75, 12.38.

HRMS (SI-QToF) *m/z:* $[M+H]^+$ calcd. 436.1509, found 436.1545.

Synthesis of Nα-Boc-γ-(6-N(Boc)$_2$-9-adenilyl)alanine-O*t*Bu (17a)



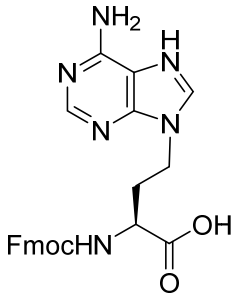
2 (1.5 g, 4.4 mmol), bisBoc-adenine (1.85 g, 5.5 mmol), K_2CO_3 (607 mg, 4.4 mmol), Cs_2CO_3 (1.4 g, 4.4 mmol) and tetrabuthylamonium iodide (162 mg, 0.44 mmol) were suspended in DMF (45 mL) and stirred at 50 °C for 16 h. EtOAc (300 mL) was added to the suspension and washed with aq. HCl (1 M, 2 x 100 mL) and NaCl (sat. aq. sol., 50 mL). Automated reversed phase column chromatography afforded the desired product as a colorless solid (1.5 g, 2.5 mmol, 58%).

^{1}H NMR (500 MHz, DMSO-d_6) δ 8.84 (s, 1H), 8.57 (s, 1H), 7.36 (d, *J* = 7.9 Hz, 1H), 4.46 – 4.28 (m, 2H), 3.77 – 3.68 (m, 1H), 2.42 – 2.33 (m, 1H), 2.17 – 2.07 (m, 1H), 1.43 – 1.34 (m, 27H).

^{13}C NMR (126 MHz, DMSO-d_6) δ 171.41, 155.94, 153.57, 151.86, 150.50, 149.50, 147.28, 128.24, 83.74, 81.16, 78.81, 52.17, 41.21, 30.76, 28.64, 28.35, 28.01, 27.76.

HRMS (SI-QToF) *m/z:* $[M+H]^+$ calcd. 593.3299, found 593.3199.

Synthesis of Nα-Fmoc-γ-(9-adenilyl)alanine (17)



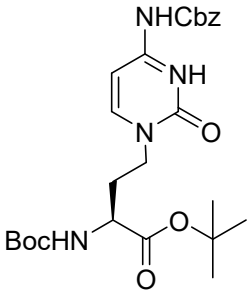
17a (1.59 g, 2.7 mmol) was dissolved in TFA/DCM (60 mL, 3:1) and stirred for 90 min at room temperature. The solvent was removed under reduced pressure and the mixture taken up in aq. Na_2CO_3 (10%, 50 mL) and 1,4-dioxane (20 mL) and cooled to 0 °C. FmocOSu (1.1 g, 3.24 mmol) was dissolved in 1,4-dioxane (30 mL) and added dropwise to the mixture. The reaction was allowed to reach room temperature and was stirred overnight. H_2O (100 mL) was added to the solution and washed with hexanes (3 x 50 mL). The aqueous phase was acidified with aq. HCl (6 M) until precipitation of a colorless solid was observed. The precipitate was filtered and washed with aq. HCl (1 M) affording the desired product (900 mg, 1.96 mmol, 73%) as a colorless solid.

^{1}H NMR (500 MHz, DMSO-d_6) δ 8.40 (d, *J* = 21.8 Hz, 2H), 7.95 – 7.72 (m, 5H), 7.47 – 7.33 (m, 4H), 4.41 – 4.22 (m, 5H), 3.97 – 3.86 (m, 1H), 2.47 – 2.33 (m, 1H), 2.24 – 2.11 (m, 1H).

^{13}C NMR (126 MHz, DMSO-d_6) δ 173.45, 156.61, 149.24, 144.29, 144.26, 143.74, 141.22, 128.14, 127.58, 125.77, 125.74, 120.63, 118.62, 66.17, 51.69, 47.13, 41.27, 31.06.

HRMS (SI-QToF) *m/z:* $[M+H]^+$ calcd. 459.1781, found 459.1855.

Synthesis of Nα-Boc-γ-(4-N(Cbz)-1-cytosinyl)alanine-O*t*Bu (18a)



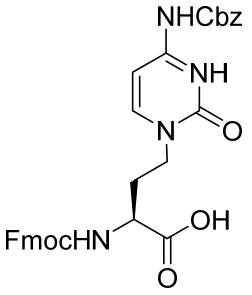
2 (1.0 g, 2.95 mmol), Cbz-cytosine (0.98 g, 2.95 mmol), K_2CO_3 (414 mg, 2.95 mmol), Cs_2CO_3 (828 mg, 2.95 mmol) and tetrabuthylamonium iodide (111 mg, 0. 2.95 mmol) were suspended in DMF (25 mL) and stirred at 50 °C for 16 h. EtOAc (300 mL) was added to the suspension and washed with aq. HCl (1M, 2 x 100 mL) and NaCl (sat. aq. sol., 50 mL). Automated reversed phase column chromatography afforded the desired product as a colorless solid (0.89 g, 1.77 mmol, 60%).

^{1}H NMR (400 MHz, DMSO-d_6) δ 10.75 (s, 0H), 7.97 (d, *J* = 7.3 Hz, 1H), 7.47 – 7.32 (m, 5H), 7.27 (d, *J* = 7.8 Hz, 1H), 6.98 (d, *J* = 7.3 Hz, 1H), 5.19 (s, 2H), 3.91 – 3.73 (m, 3H), 2.13 – 1.99 (m, 1H), 1.93 – 1.77 (m, 1H), 1.43 – 1.34 (m, 18H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 171.51, 163.25, 155.92, 155.29, 153.68, 150.37, 136.45, 128.94, 128.61, 128.38, 94.49, 81.11, 78.77, 66.91, 52.51, 47.37, 29.90, 28.63, 28.37, 28.04.

HRMS (SI-QToF) *m/z:* $[M+H]^+$ calcd. 503.2506, found 503.2769.

Synthesis of Nα-Fmoc-γ-(4-N(Cbz)-1-cytosinyl)alanine (18)



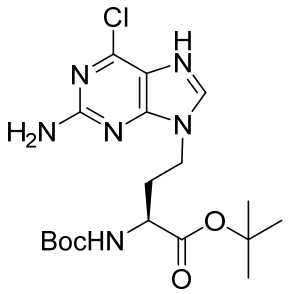
18a (1.26 g, 2.5 mmol) was dissolved in TFA/DCM (60 mL, 3:1) and stirred for 90 min at room temperature. The solvent was removed under reduced pressure and the mixture taken up in aq. Na_2CO_3 (10%, 50 mL) and 1,4-dioxane (20 mL) and cooled to 0 °C. FmocOSu (0.93 g, 2.75 mmol) was dissolved in 1,4-dioxane (30 mL) and added dropwise to the mixture. The reaction was allowed to reach room temperature and was stirred overnight. H_2O (100 mL) was added to the solution and washed with hexanes (3 x 50 mL). The aqueous phase was acidified with aq. HCl (6 M) until precipitation of a colorless solid was observed. The precipitate was filtered and washed with aq. HCl (1 M). The precipitate was the desired product (630 mg, 1.05 mmol, 42%).

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.99 – 7.85 (m, 4H), 7.77 – 7.69 (m, 3H), 7.48 – 7.32 (m, 10H), 6.98 (d, *J* = 7.2 Hz, 1H), 5.18 (s, 2H), 4.83 (d, *J* = 6.1 Hz, 1H), 4.45 – 4.19 (m, 3H), 4.00 – 3.91 (m, 1H), 3.91 – 3.78 (m, 2H), 2.24 – 2.11 (m, 1H), 2.01 – 1.89 (m, 1H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 173.62, 170.17, 163.22, 156.60, 155.27, 153.66, 151.58, 150.42, 144.28, 143.10, 141.30, 141.21, 136.42, 128.94, 128.61, 128.43, 128.40, 128.12, 127.77, 127.57, 127.55, 125.75, 125.69, 125.37, 120.77, 120.61, 120.58, 94.46, 72.34, 66.94, 66.13, 51.93, 47.54, 47.14, 46.43, 30.02, 25.75.

HRMS (SI-QToF) *m/z:* $[M+H]^+$ calcd. 596.2036, found 569.2147.

Synthesis of Nα-Boc-γ-(2-amino-6-chloro-9-purinyl)alanine-O*t*Bu (19a)



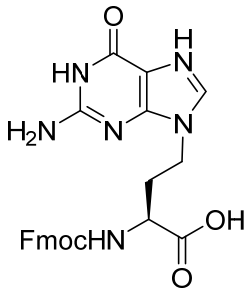
2 (1.5 g, 4.4 mmol), 6-chloropurine (935 mg, 5.5 mmol), K_2CO_3 (607 mg, 4.4 mmol), Cs_2CO_3 (1.4 g, 4.4 mmol) and tetrabuthylamonium iodide (162 mg, 0.44 mmol) were suspended in DMF (45 mL) and stirred at 50 °C for 16 h. EtOAc (300 mL) was added to the suspension and washed with aq. HCl (1 M, 2 x 100 mL) and NaCl (sat. aq. sol., 50 mL). Automated reversed phase column chromatography afforded the desired product as a colorless solid (1.32 g, 3.08 mmol, 70%).

^{1}H NMR (500 MHz, DMSO-d_6) δ 8.04 (s, 1H), 7.32 (d, *J* = 7.9 Hz, 1H), 6.95 (d, *J* = 7.6 Hz, 2H), 4.11 (t, *J* = 7.1 Hz, 2H), 3.80 – 3.69 (m, 1H), 2.34 – 2.21 (m, 1H), 2.09 – 1.97 (m, 1H), 1.38 (d, *J* = 20.0 Hz, 18H).

^{13}C NMR (126 MHz, DMSO-d_6) δ 171.45, 160.22, 155.96, 154.52, 149.78, 143.60, 123.79, 81.17, 78.84, 52.37, 40.76, 30.44, 28.63, 28.34, 28.02.

HRMS (SI-QToF) *m/z:* $[M+H]^+$ calcd. 427.1861, found 427.1785.

Synthesis of Nα-Fmoc-γ-(9-guaninyl)alanine (19)



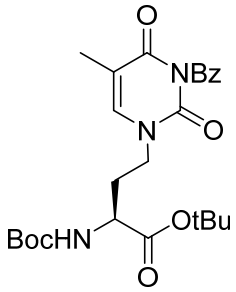
19a (1.3 g, 3.0 mmol) was dissolved in aq. HCl (1 M, 30 mL) and stirred for 2 h at 90 °C. The solvent was removed under reduced pressure and the mixture taken up in aq. Na_2CO_3 (10%, 50 mL) and 1,4-dioxane (20 mL) and cooled to 0 °C. FmocOSu (1.2 g, 3.6 mmol) was dissolved in 1,4-dioxane (30 mL) and added dropwise to the mixture. The reaction was allowed to reach room temperature and was stirred overnight. H_2O (100 mL) was added to the solution and washed with hexanes (3 x 50 mL). The aqueous phase was acidified with aq. HCl (6 M) until precipitation of a colorless solid was observed. The precipitate was triturated with hexanes/CH_2Cl_2 (1:1), centrifuged and collected, affording the desired product (600 mg, 1.26 mmol, 42%).

^{1}H NMR (500 MHz, DMSO-d_6) δ 12.82 (s, 1H), 11.40 (s, 1H), 8.55 (s, 1H), 7.91 (d, *J* = 7.5 Hz, 2H), 7.82 (d, *J* = 8.3 Hz, 1H), 7.74 (dd, *J* = 7.5, 2.9 Hz, 2H), 7.48 – 7.39 (m, 2H), 7.39 – 7.28 (m, 2H), 7.07 (s, 2H), 4.35 – 4.30 (m, 2H), 4.26 (t, *J* = 7.0 Hz, 1H), 4.16 – 4.10 (m, 2H), 4.01 – 3.95 (m, 1H), 2.41 – 2.31 (m, 1H), 2.17 – 2.06 (m, 1H).

^{13}C NMR (126 MHz, DMSO-d_6) δ 173.40, 156.61, 155.37, 150.73, 144.31, 144.22, 141.21, 137.63, 128.15, 127.58, 125.75, 120.63, 66.22, 51.73, 47.11, 41.74, 30.47.

HRMS (SI-QToF) *m/z:* $[M+H]^+$ calcd. 475.1730, found 475.1770.

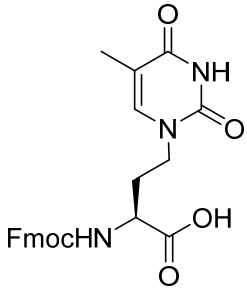
Synthesis of of Nα-Boc-γ-(3-(Bz)-1-thyminyl)alanine-O*t*Bu (20a)



2 (1.5 g, 4.4 mmol), benzoyl-thymidine (1.27 g, 5.5 mmol), K_2CO_3 (607 mg, 4.4 mmol), Cs_2CO_3 (1.4 g, 4.4 mmol) and tetrabuthylamonium iodide (162 mg, 0.44 mmol) were suspended in DMF (45 mL) and stirred at 50 °C for 16 h. EtOAc (300 mL) was added to the suspension and washed with aq. HCl (1M, 2 x 100 mL) and NaCl (sat. aq. sol., 50 mL). Automated reversed phase column chromatography afforded the desired product as a colorless solid (1.80 g, 3.52 mmol, 80%).

HRMS (SI-QToF) *m/z:* $[M+Na]^+$ calcd. 510.2216, found 510.1931.

Synthesis of Nα-Fmoc-γ-(1-thyminyl)alanine (20)



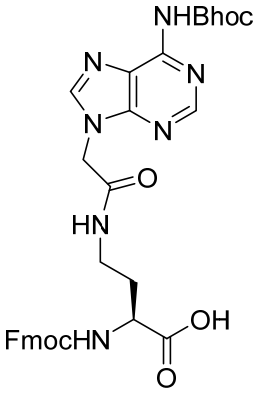
20a (1.66 g, 3.5 mmol) was dissolved in HBr (30% in AcOH, 25 mL) and stirred for 1 h, at room temperature. The solvent was removed under reduced pressure and the mixture taken up in aq. Na_2CO_3 (10%, 50 mL) and 1,4-dioxane (20 mL) and cooled to 0 °C. FmocOSu (1.4 g, 4.2 mmol) was dissolved in 1,4-dioxane (30 mL) and added dropwise to the mixture. The reaction was allowed to reach room temperature and was stirred overnight. H_2O (100 mL) was added to the solution and washed with hexanes (3 x 50 mL). The aqueous phase was acidified with aq. HCl (6 M) until precipitation of a colorless solid was observed. The precipitate was triturated with hexanes/CH_2Cl_2 (1:1), centrifuged and collected, affording the desired product (1.1 g, 2.4 mmol, 70%).

^{1}H NMR (500 MHz, DMSO-d_6) δ 12.74 (s, 1H), 11.24 (s, 1H), 7.91 (d, *J* = 7.5 Hz, 2H), 7.74 (dd, *J* = 8.3, 2.6 Hz, 2H), 7.48 – 7.39 (m, 3H), 7.35 (td, *J* = 7.4, 4.4 Hz, 2H), 4.37 – 4.23 (m, 3H), 3.97 (m, 1H), 3.76 – 3.64 (m, 2H), 2.09 (m, 1H), 1.96 – 1.85 (m, 1H), 1.73 (s, 3H).

^{13}C NMR (126 MHz, DMSO-d_6) δ 173.66, 164.75, 156.57, 151.31, 144.28, 141.84, 141.21, 128.14, 127.59, 125.76, 125.71, 120.63, 120.61, 108.93, 66.17, 51.88, 47.14, 45.14, 30.27, 12.43.

HRMS (SI-QToF) *m/z:* $[M+Na]^+$ calcd. 450.1665, found 450.1665.

Nα-Fmoc-Nγ-(6(Bhoc)-9-adenilylacetyl))-diaminobutyric acid (21)



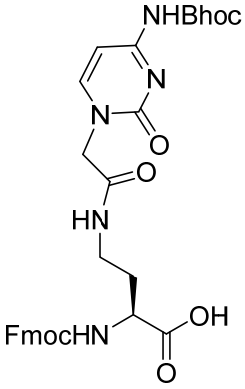
To a solution of Bhoc-Adenine-acetic acid (1.6 g, 4 mmol) in DMF (20 mL) were added TSTU (4 mmol, 1.2 g), and DIEA (16 mmol, 700 μL). The solution was stirred for 15 min at room temperature before adding Fmoc-Dap-OH (1.53 g, 4 mmol). After 2 h stirring at room temperature the solvent was removed under reduced pressure and reversed phase column chromatography (120 g C18, 35-100% MeCN in H_2O over 40 min) afforded the desired product as a colorless solid (800 mg, 1.1 mmol, 28 %).

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.68 (s, 1H), 10.90 (s, 1H), 8.59 (s, 1H), 8.40 (s, 1H), 7.89 (d, *J* = 7.5 Hz, 2H), 7.76 – 7.67 (m, 3H), 7.54 (d, *J* = 7.2 Hz, 4H), 7.43 – 7.28 (m, 14H), 6.83 (s, 1H), 4.32 – 4.18 (m, 3H), 3.23 – 3.14 (m, 2H), 1.99 – 1.88 (m, 1H), 1.85 – 1.71 (m, 1H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 174.12, 166.43, 156.62, 152.55, 151.86, 151.68, 149.49, 145.75, 144.29, 144.26, 141.31, 141.17, 129.29, 128.95, 128.51, 128.19, 128.10, 127.55, 127.15, 127.06, 126.96, 126.68, 125.77, 125.73, 122.61, 120.58, 77.80, 74.70, 66.13, 52.10, 47.09, 45.70, 36.49, 30.83.

HRMS (SI-QToF) *m/z:* $[M+H]^+$ calcd. 726.2676, found 726.2683.

Nα-Fmoc-Nγ-(4(Bhoc)-1-cytosinylacetyl))-diaminobutyric acid (22)



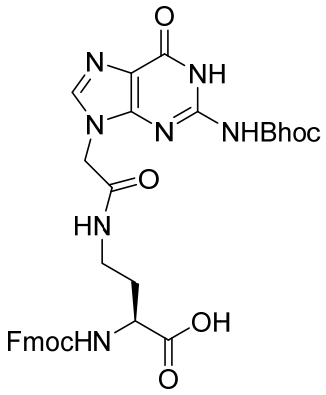
To a solution of Bhoc-C-acetic acid (1.5 g, 4 mmol) in DMF (20 mL) were added TSTU (4 mmol, 1.2 g), and DIEA (16 mmol, 700 μL). The solution was stirred for 15 min at room temperature before adding Fmoc-Dap-OH (1.53 g, 4 mmol). After 2 h stirring at room temperature the solvent was removed under reduced pressure and reversed phase column chromatography (120 g C18, 35-100% MeCN in H2O over 40 min) afforded the desired product as a colorless solid (610 mg, 0.87 mmol, 22%).

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.65 (s, 1H), 10.96 (s, 1H), 8.24 (t, *J* = 5.4 Hz, 1H), 7.95 (d, *J* = 7.3 Hz, 1H), 7.89 (d, *J* = 7.5 Hz, 2H), 7.77 – 7.65 (m, 3H), 7.50 – 7.29 (m, 16H), 6.93 (d, *J* = 7.3 Hz, 1H), 6.80 (s, 1H), 4.35 – 4.19 (m, 3H), 4.02 (dq, *J* = 9.4, 6.2, 4.7 Hz, 1H), 3.25 – 3.08 (m, 2H), 1.96 – 1.86 (m, 1H), 1.85 – 1.70 (m, 1H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 174.09, 167.05, 163.47, 156.60, 144.26, 141.17, 140.87, 129.06, 129.02, 128.31, 128.10, 127.56, 126.90, 125.74, 120.57, 94.07, 77.87, 66.15, 55.38, 52.18, 51.78, 47.09, 36.42, 31.16.

HRMS (SI-QToF) *m/z:* $[M+H]^+$ calcd. 702.2564, found 702.2492.

Nα-Fmoc-Nγ-(4(Bhoc)-9-guanidylacetyl))-diaminobutyric acid (23)



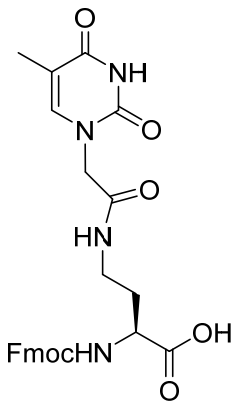
To a solution of Bhoc-G-acetic acid (1.7 g, 4 mmol) in DMF (20 mL) were added TSTU (4 mmol, 1.2 g), and DIEA (16 mmol, 700 μL). The solution was stirred for 15 min at room temperature before adding Fmoc-Dap-OH (1.53 g, 4 mmol). After 2 h stirring at room temperature the solvent was removed under reduced pressure and reversed phase column chromatography (120 g C18, 35-100% MeCN in H2O over 40 min) afforded the desired product as a colorless solid (750 mg, 1.0 mmol, 25%).

^{1}H NMR (400 MHz, DMSO-d_6) δ 11.23 (s, 1H), 8.36 – 8.27 (m, 1H), 7.96 (s, 1H), 7.93 – 7.87 (m, 3H), 7.76 – 7.67 (m, 3H), 7.49 – 7.29 (m, 14H), 6.86 (s, 1H), 4.32 – 4.19 (m, 3H), 4.08 – 3.99 (m, 1H), 3.63 – 3.53 (m, 1H), 3.24 – 3.05 (m, 3H), 2.01 – 1.88 (m, 1H), 1.83 – 1.71 (m, 1H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 174.13, 166.44, 156.70, 155.40, 154.16, 149.66, 147.61, 144.26, 141.18, 141.08, 140.47, 129.05, 128.51, 128.44, 128.12, 127.56, 127.14, 127.00, 126.90, 126.88, 126.68, 125.74, 120.59, 119.38, 78.51, 66.17, 52.07, 47.08, 45.72, 36.47, 30.81.

HRMS (SI-QToF) *m/z:* $[M+H]^+$ calcd. 742.2625, found 742.2654.

Nα-Fmoc-Nγ-(thymidylacetyl))-diaminobutyric acid (24)



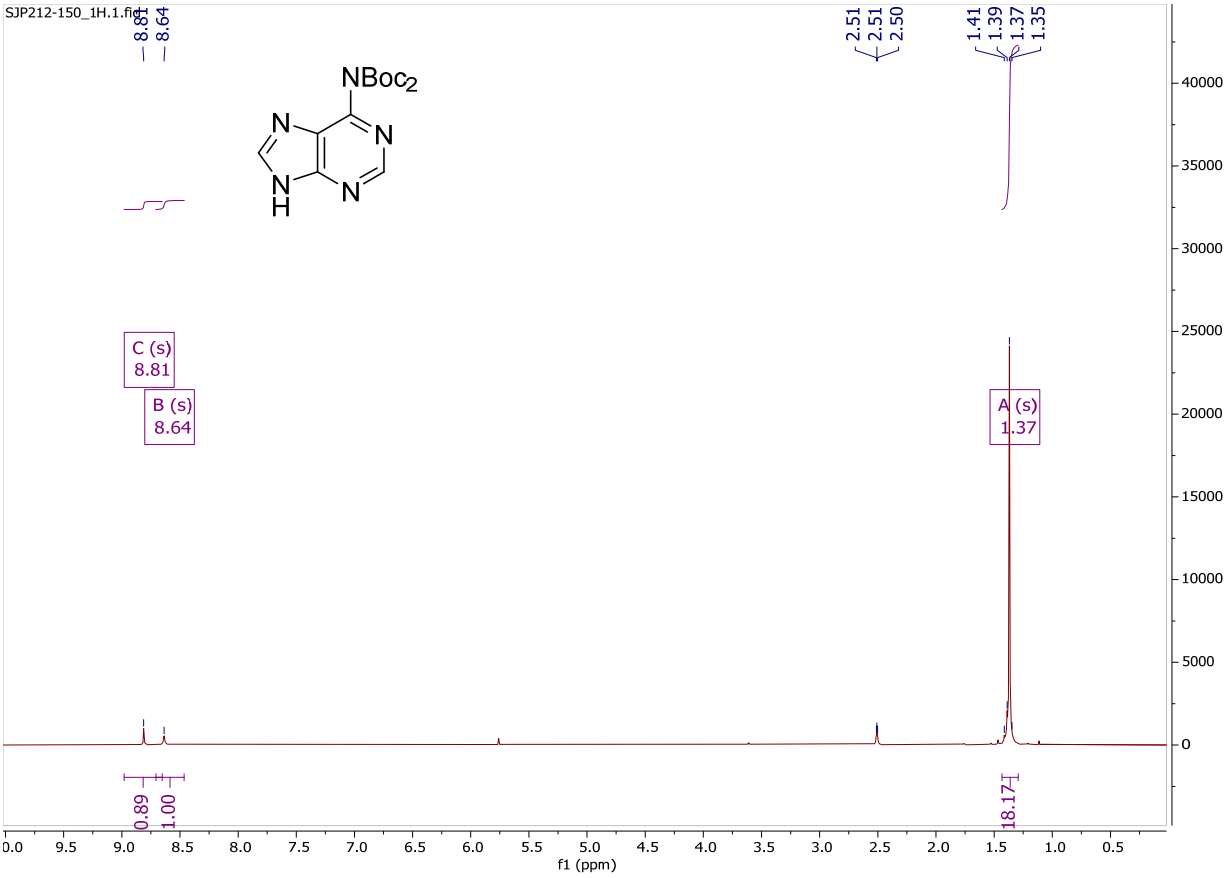
To a solution of T-acetic acid (736 mg, 4 mmol) in DMF (20 mL) were added TSTU (4 mmol, 1.2 g), and DIEA (16 mmol, 700 μL). The solution was stirred for 15 min at room temperature before adding Fmoc-Dap-OH (1.53 g, 4 mmol). After 2 h stirring at room temperature the solvent was removed under reduced pressure and reversed phase column chromatography (120 g C18, 35-100% MeCN in H2O over 40 min) afforded the desired product as a colorless solid (550 mg, 1.1 mmol, 28%).

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.68 (s, 1H), 11.26 (s, 1H), 8.18 (t, *J* = 5.5 Hz, 1H), 8.01 – 7.84 (m, 3H), 7.79 – 7.62 (m, 3H), 7.49 – 7.38 (m, 3H), 7.37 – 7.29 (m, 2H), 4.35 – 4.20 (m, 5H), 4.07 – 3.95 (m, 1H), 3.22 – 3.11 (m, 2H), 1.98 – 1.86 (m, 1H), 1.81 – 1.70 (m, 4H).

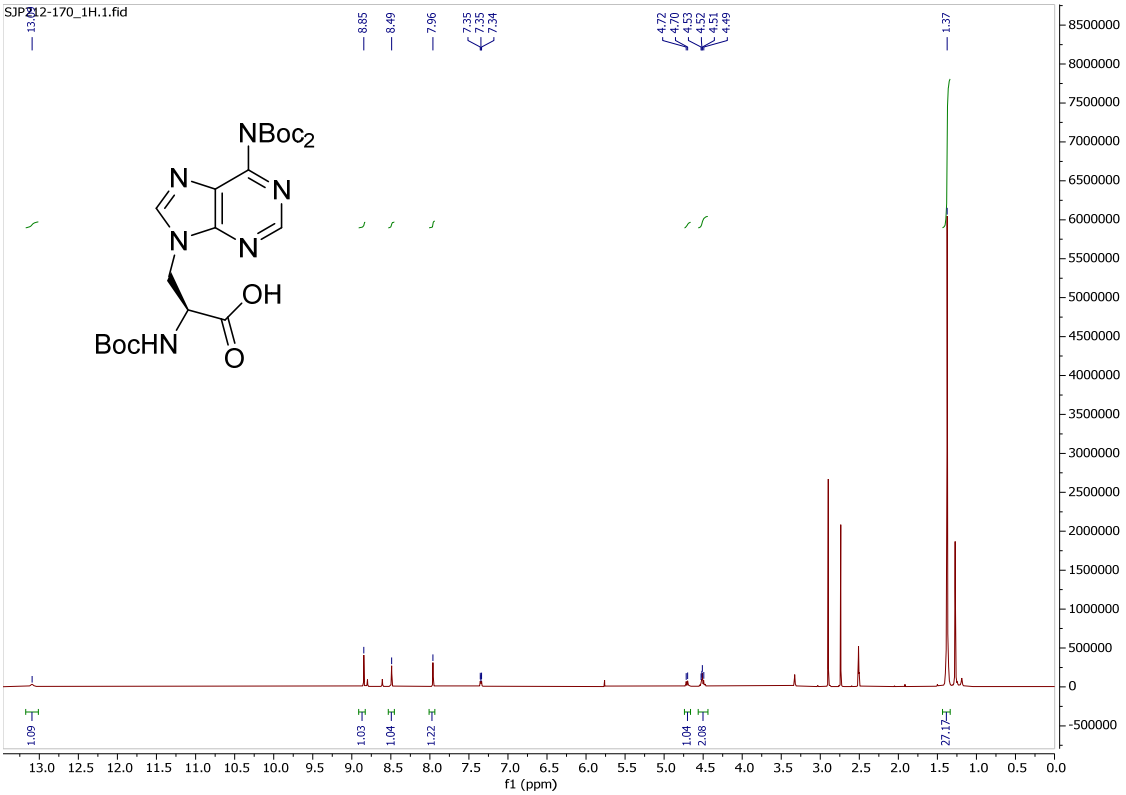
HRMS (SI-QToF) *m/z:* $[M+H]^+$ calcd. 507.1880, found 507.1875.

NMR spectra

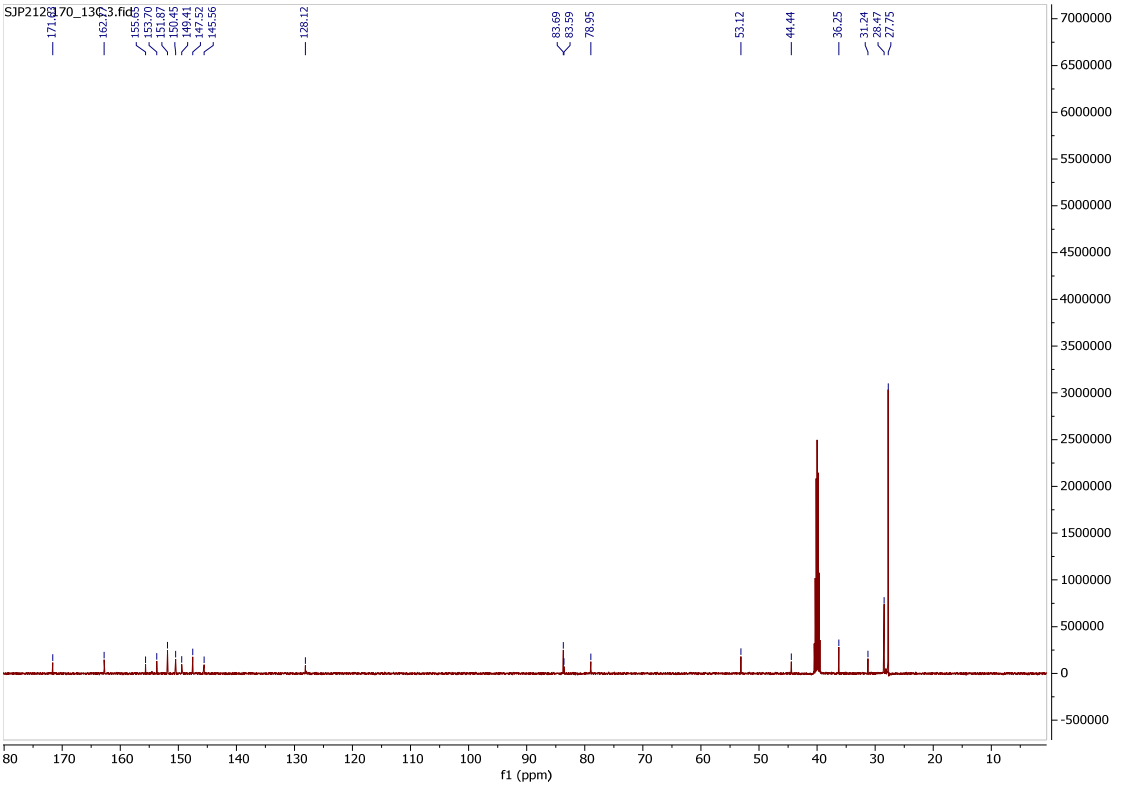
^{1}H NMR (4)



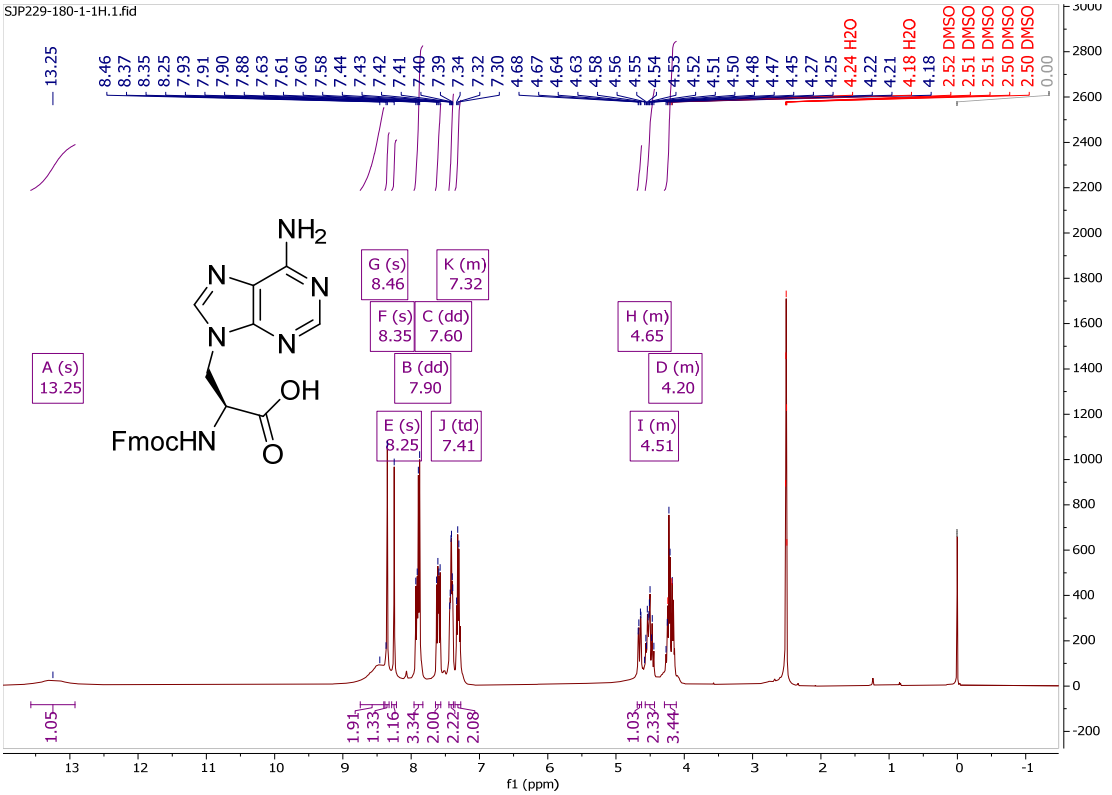
^{1}H NMR (13a)



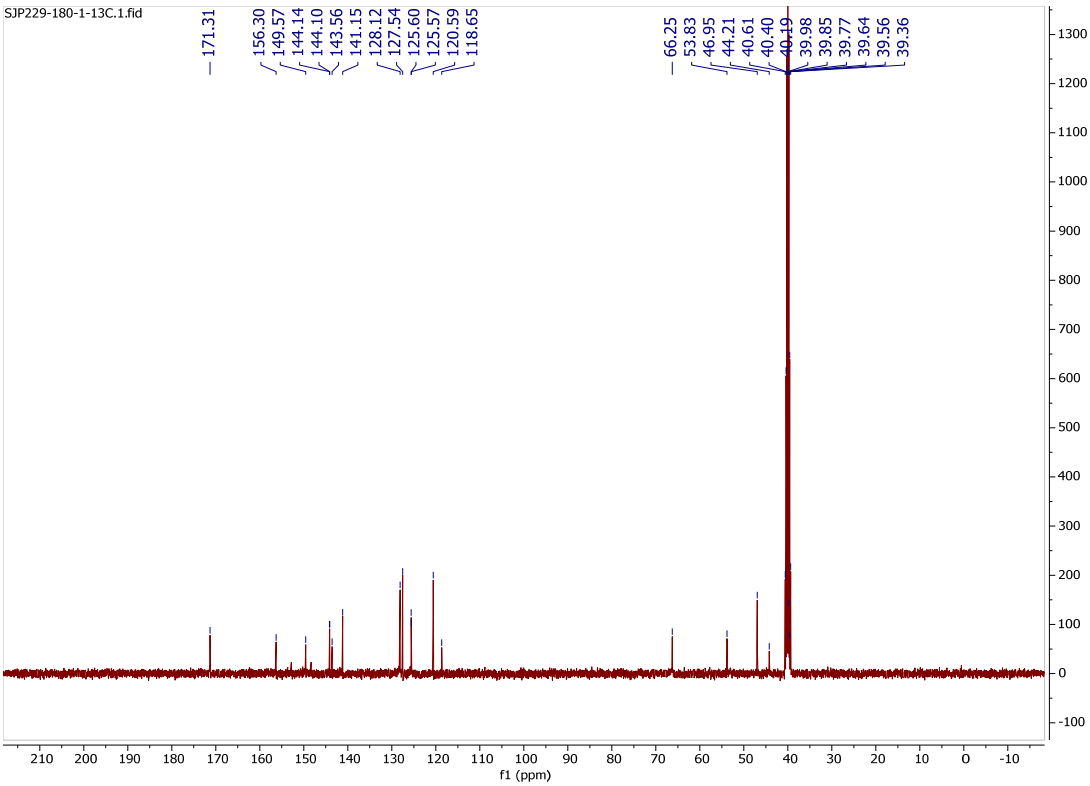
^{13}C NMR (13a)



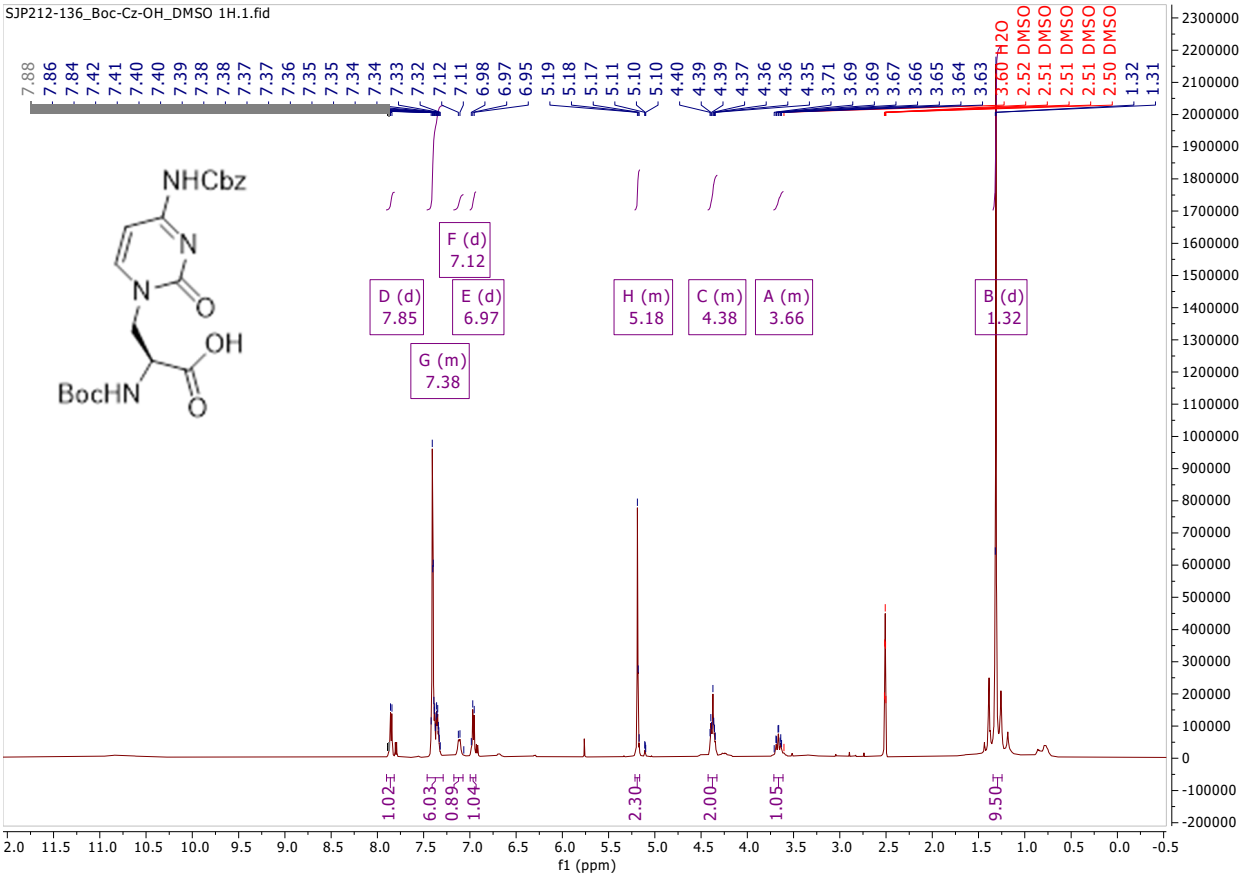
^{1}H NMR (13)



^{13}C NMR (13)



^{1}H NMR (14a)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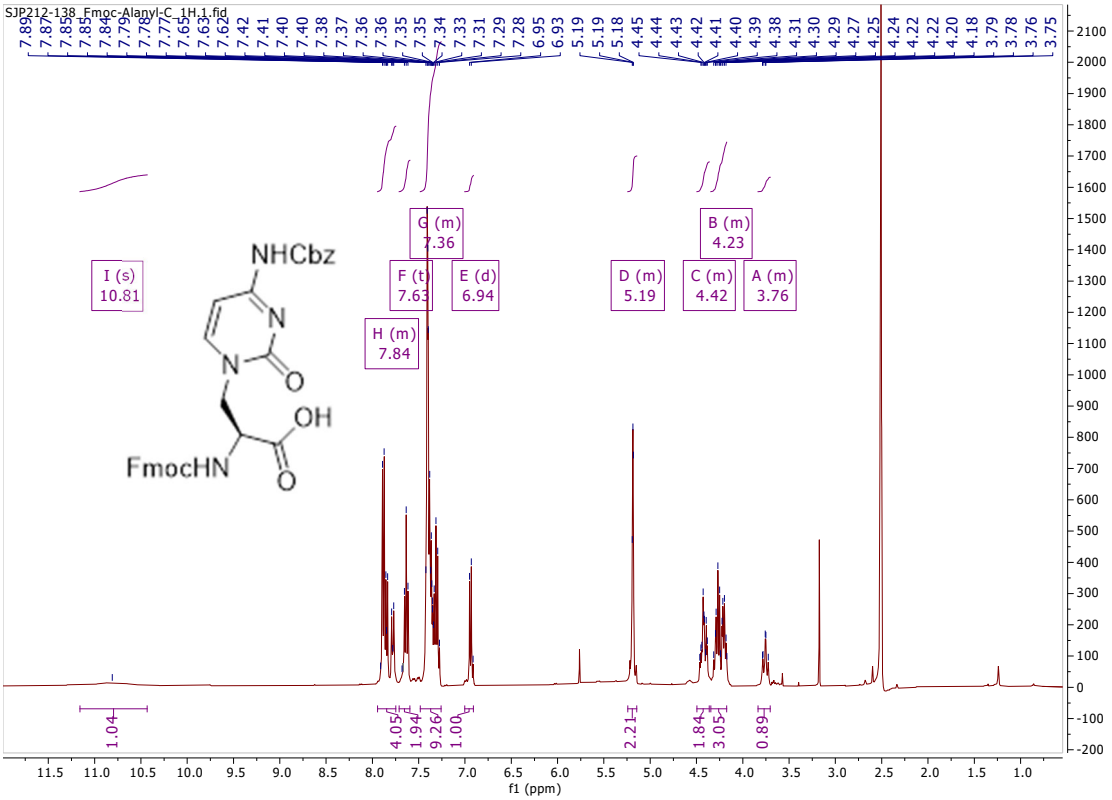
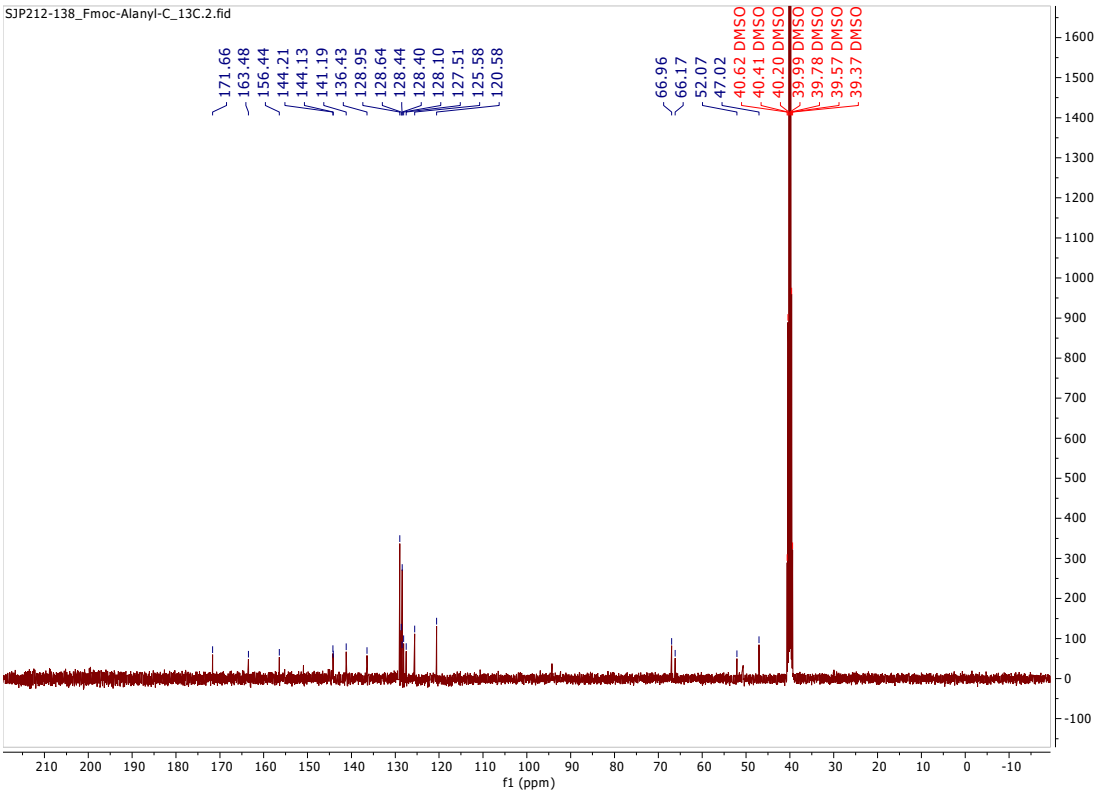
NHCbz
N
N
O
OH
BocHN
O
F (d) 7.12
D (d) 7.85
E (d) 6.97
H (m) 5.18
C (m) 4.38
A (m) 3.66
B (d) 1.32
G (m) 7.38
1.02
6.03
0.89
1.04
2.30
2.00
1.05
9.50
f1 (ppm)

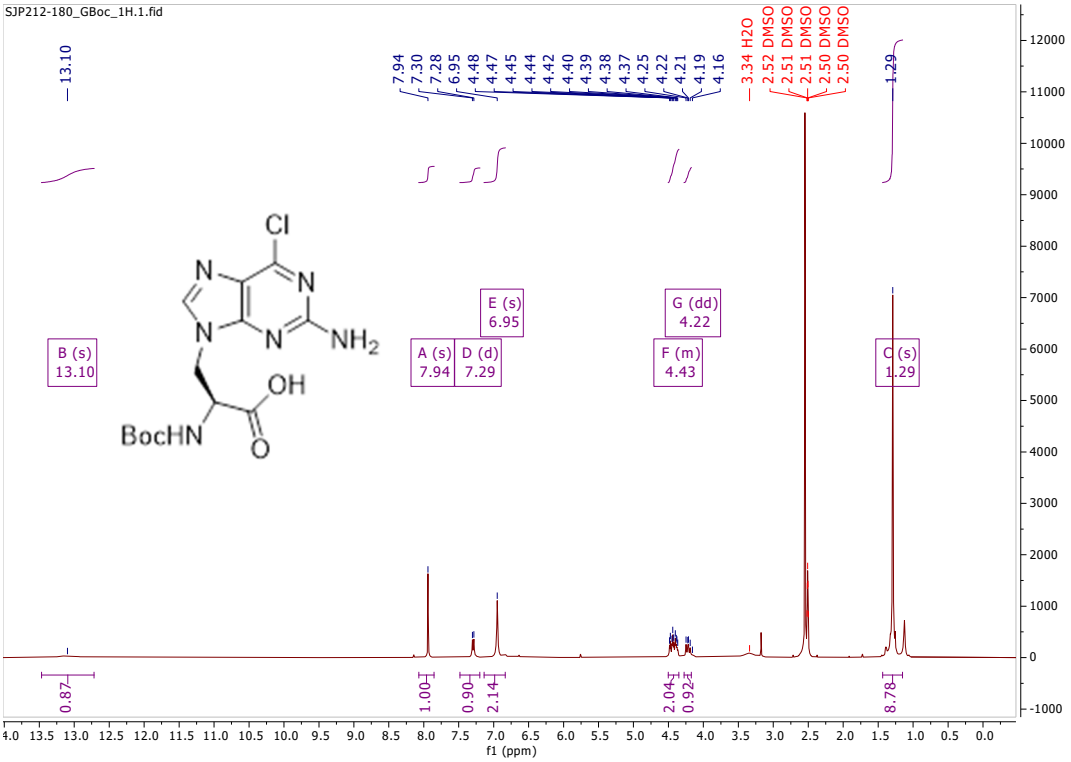
^{1}H NMR (14)



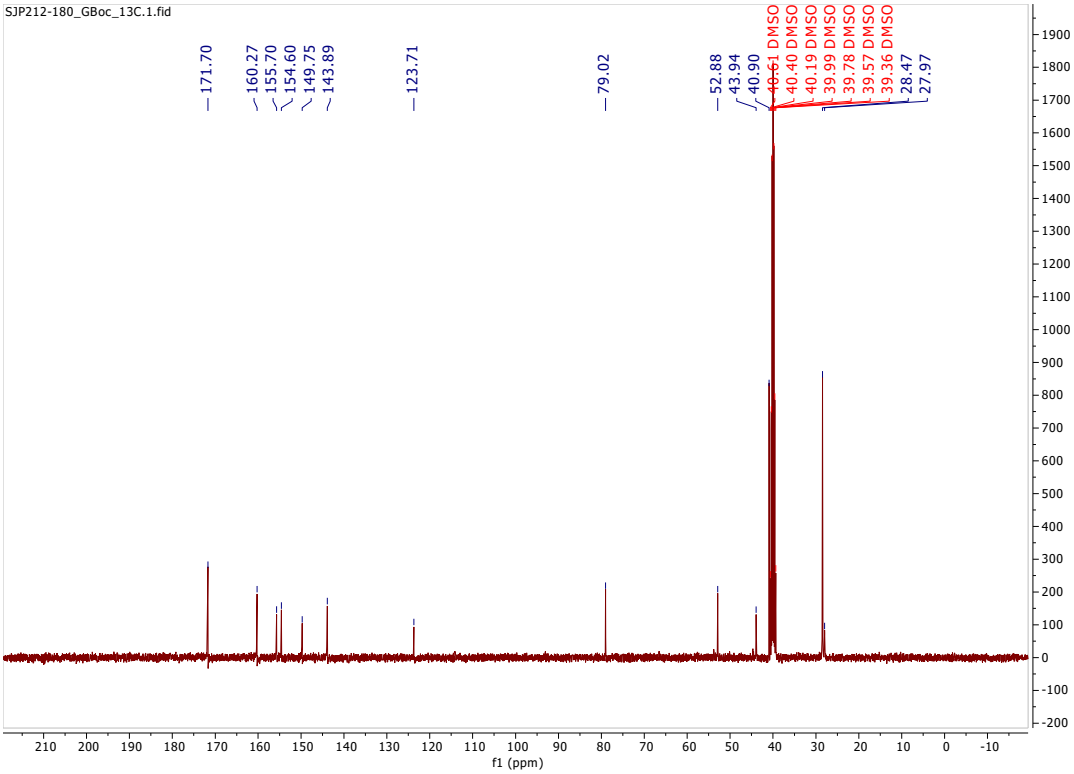
^{13}C NMR (14)



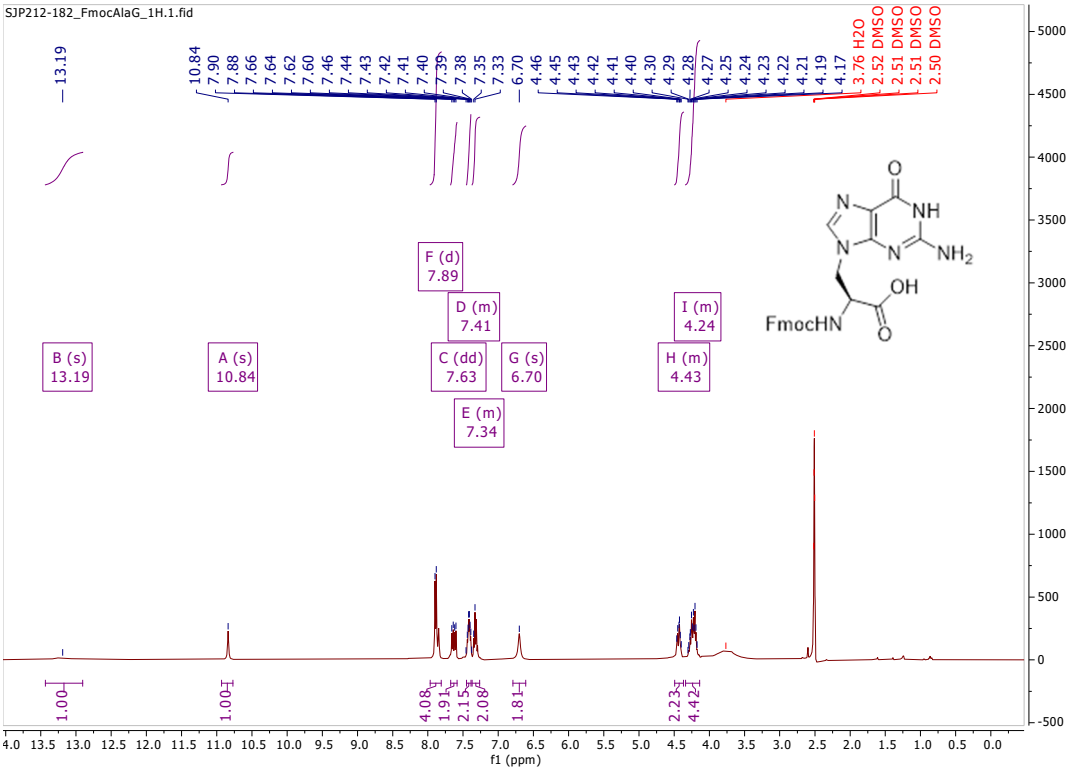
^{1}H NMR (15a)



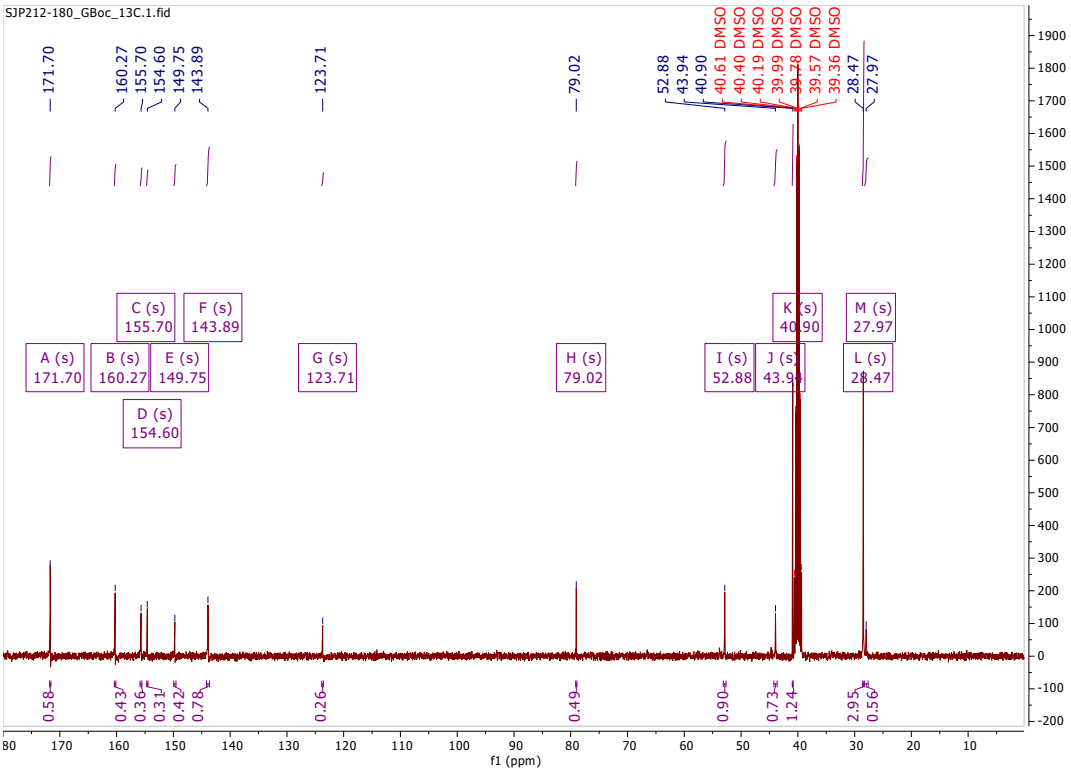
^{13}C NMR (15a)



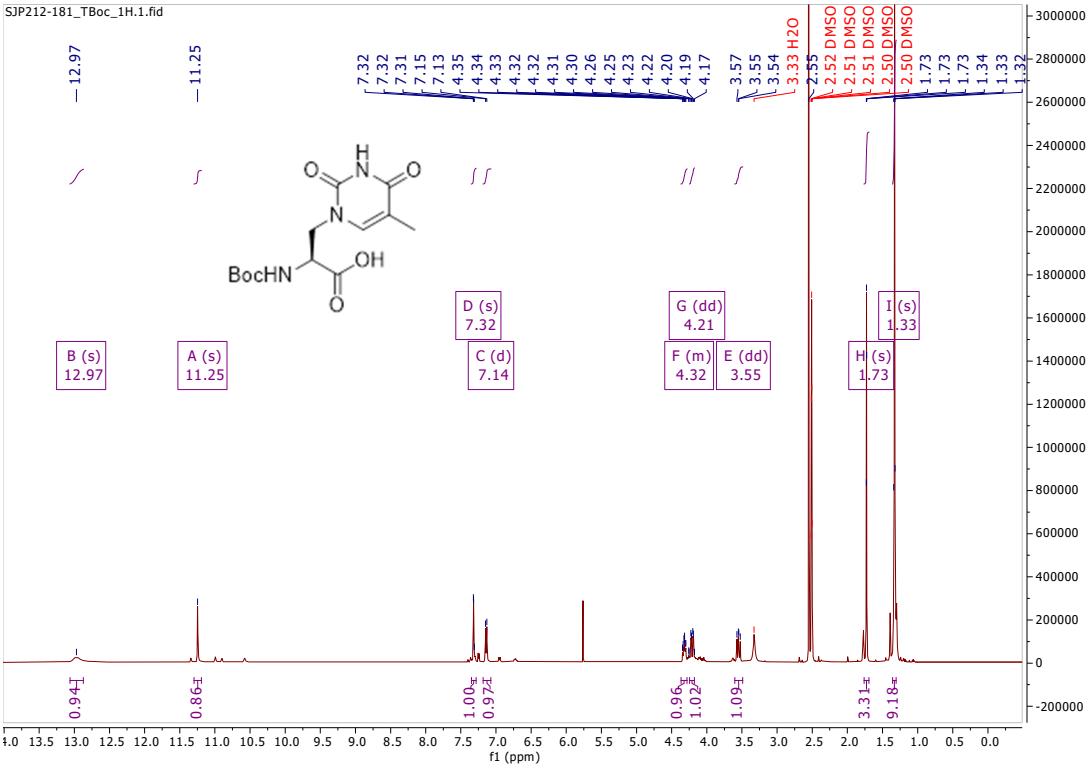
^{1}H NMR (15)



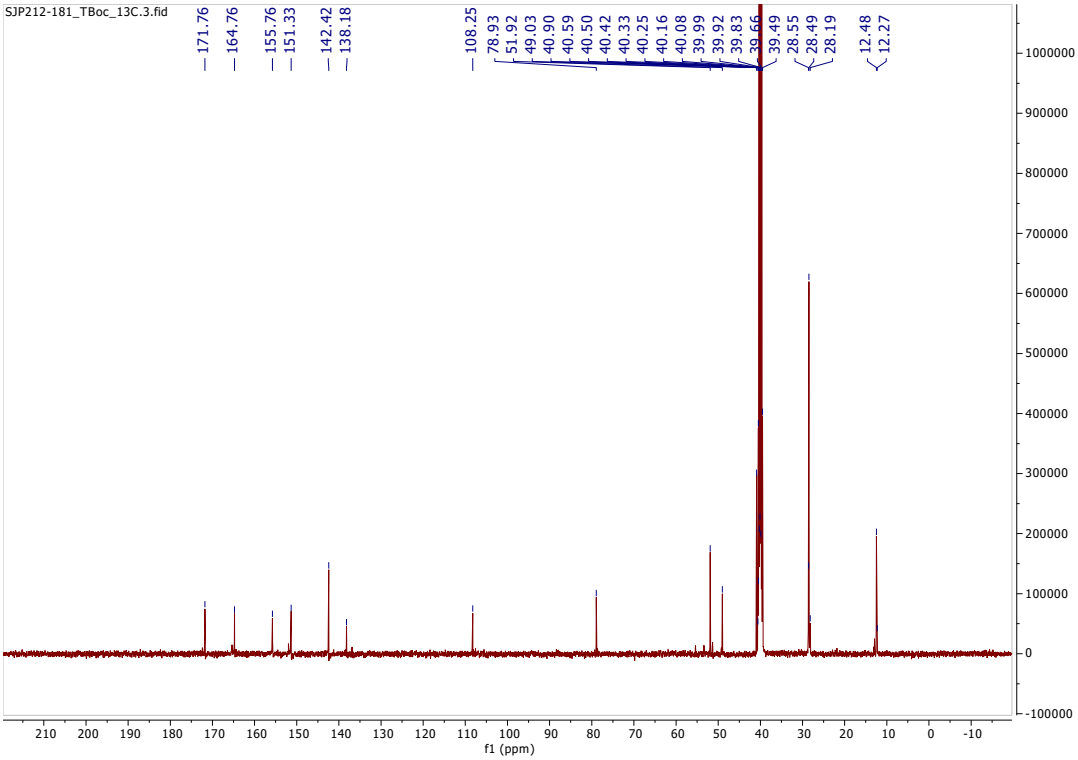
^{13}C NMR (15)



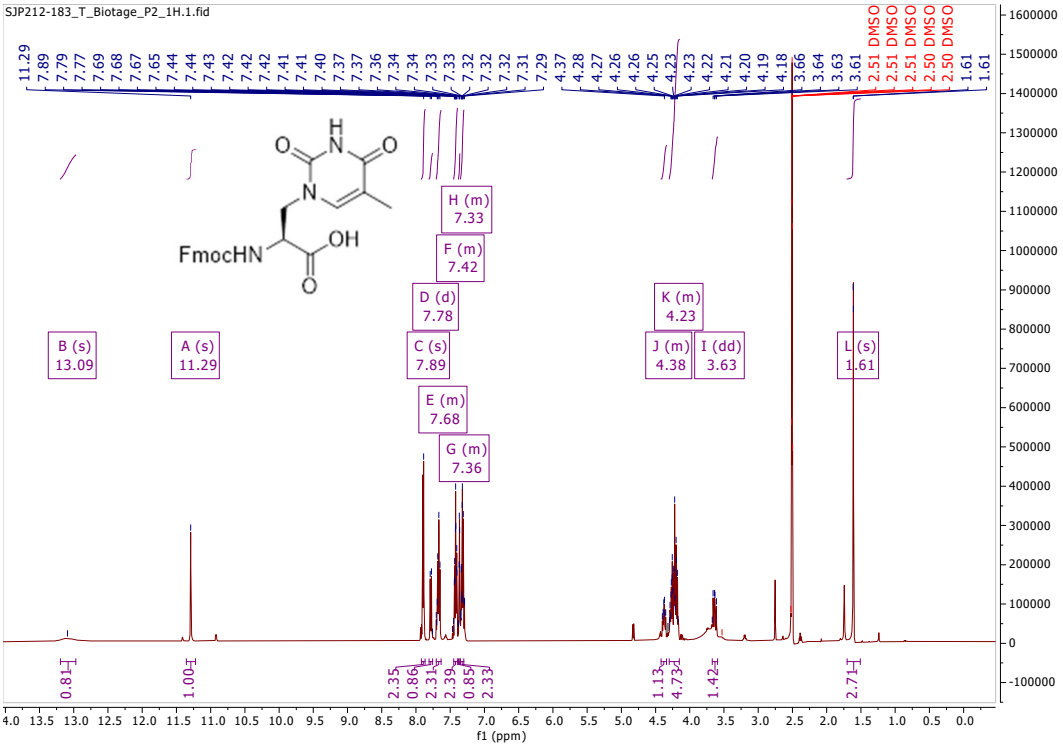
^{1}H NMR (16a)



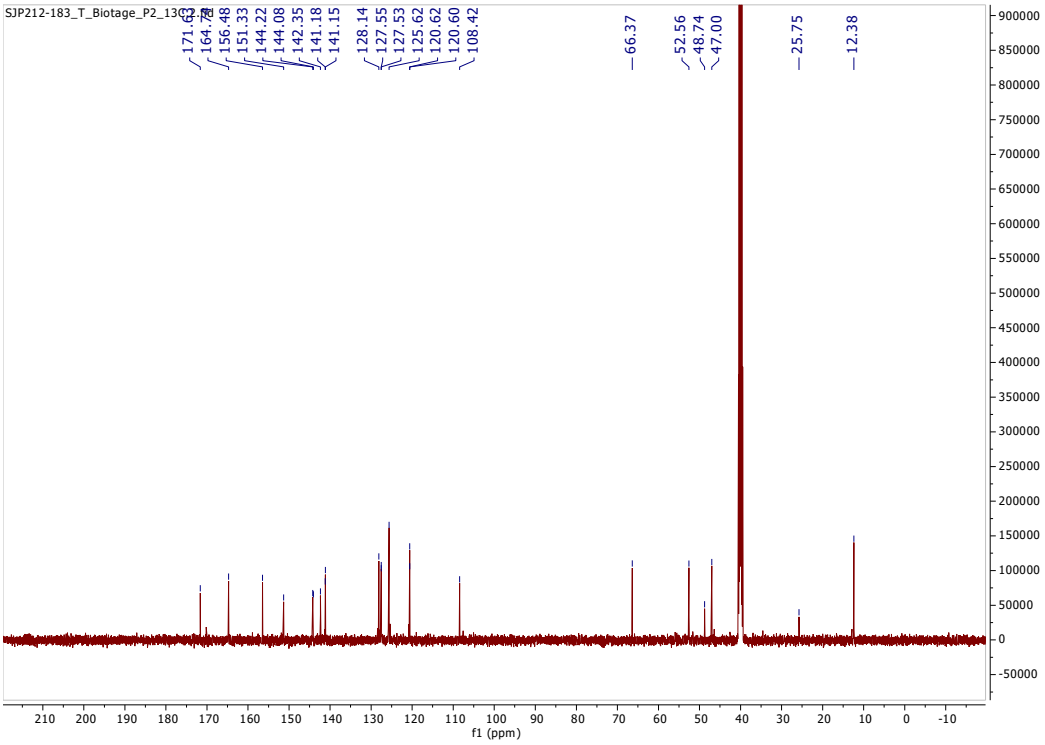
^{13}C NMR (16a)



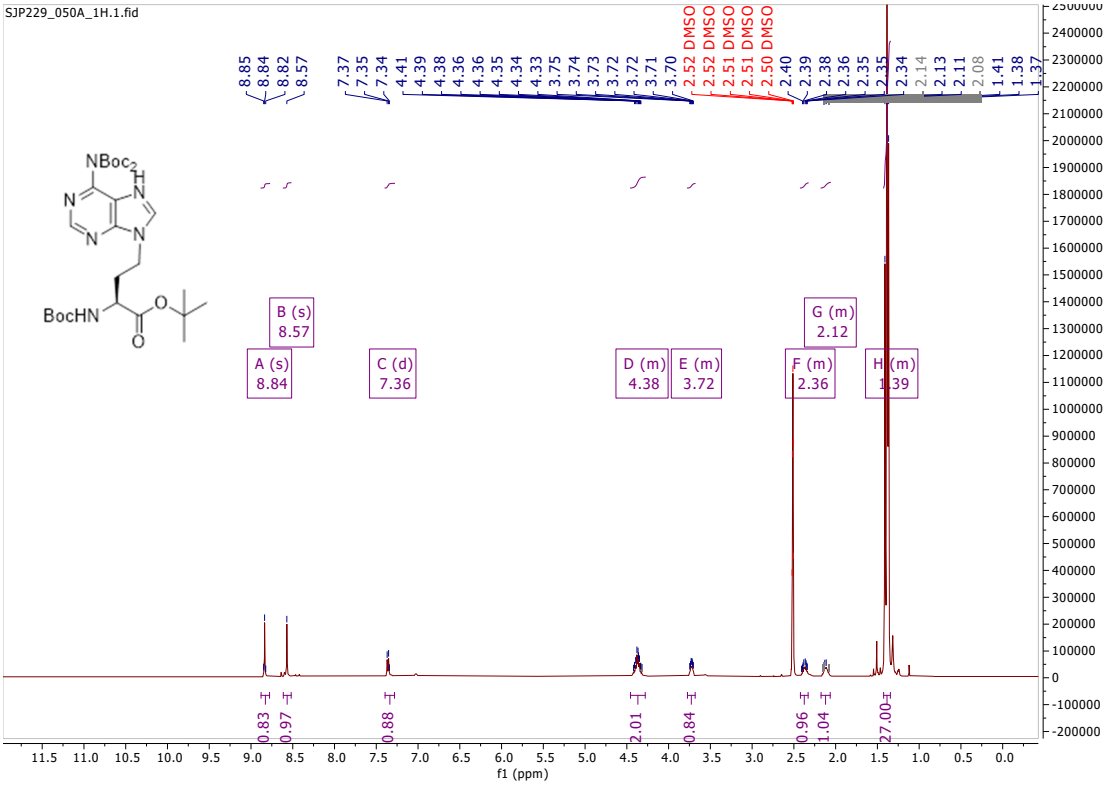
^{1}H NMR (16)



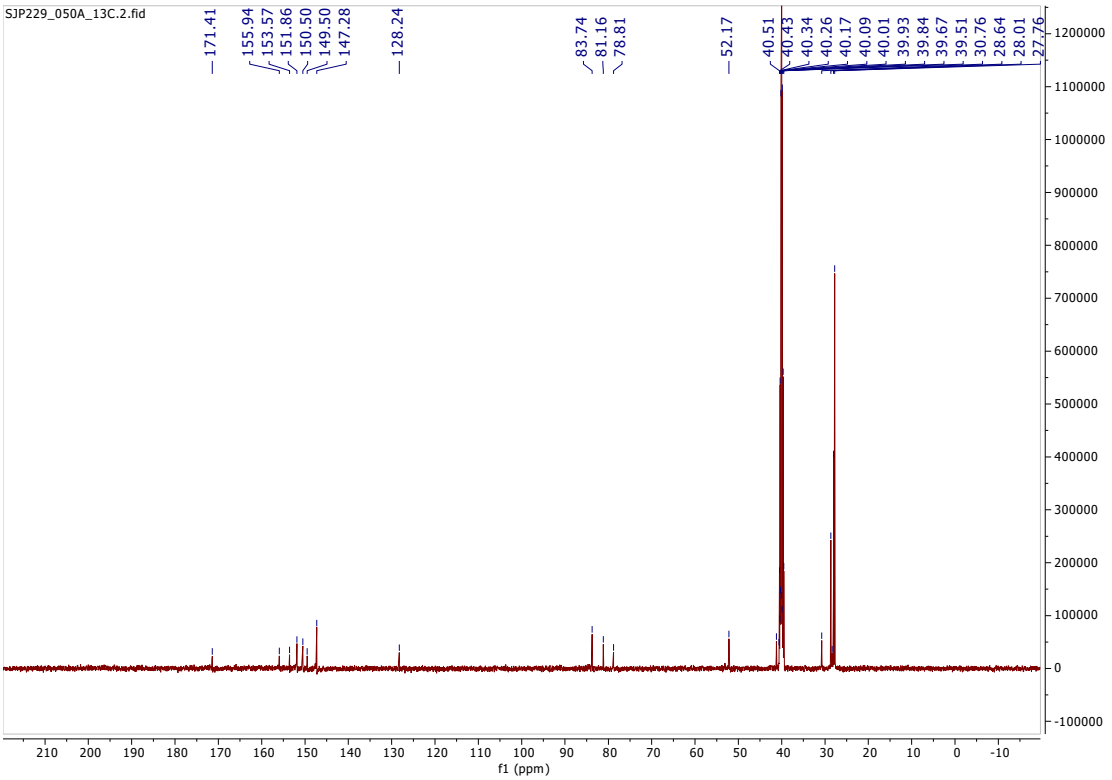
^{13}C NMR (16)



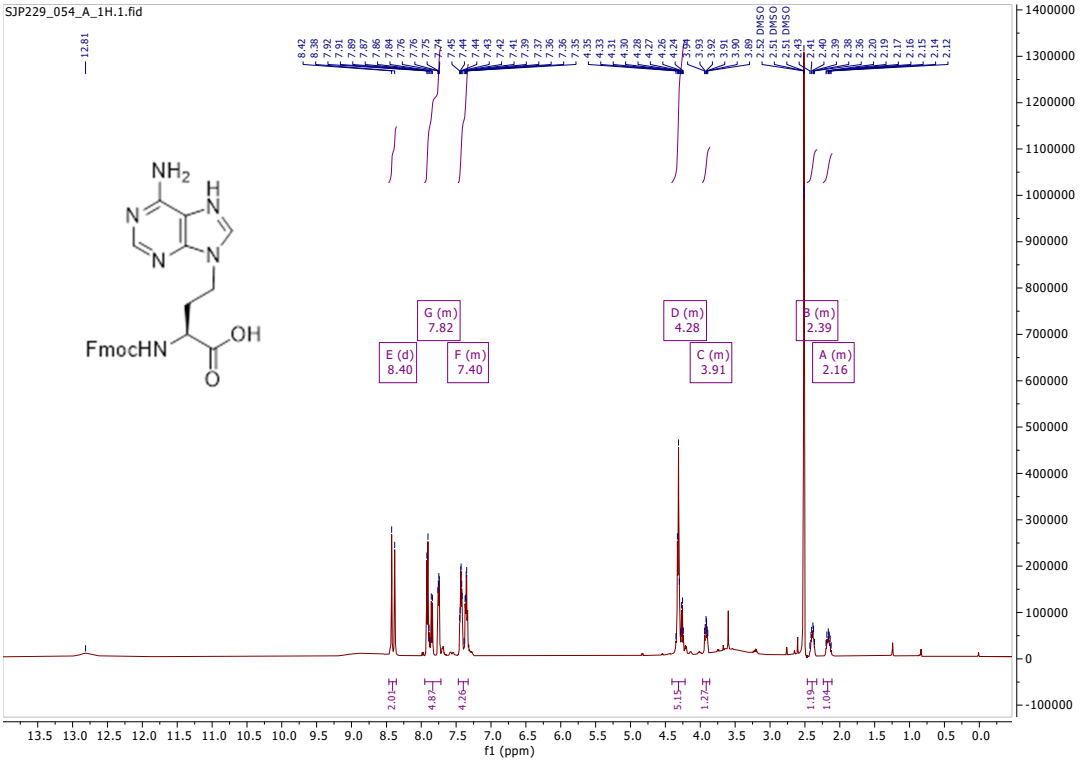
^{1}H NMR (17a)



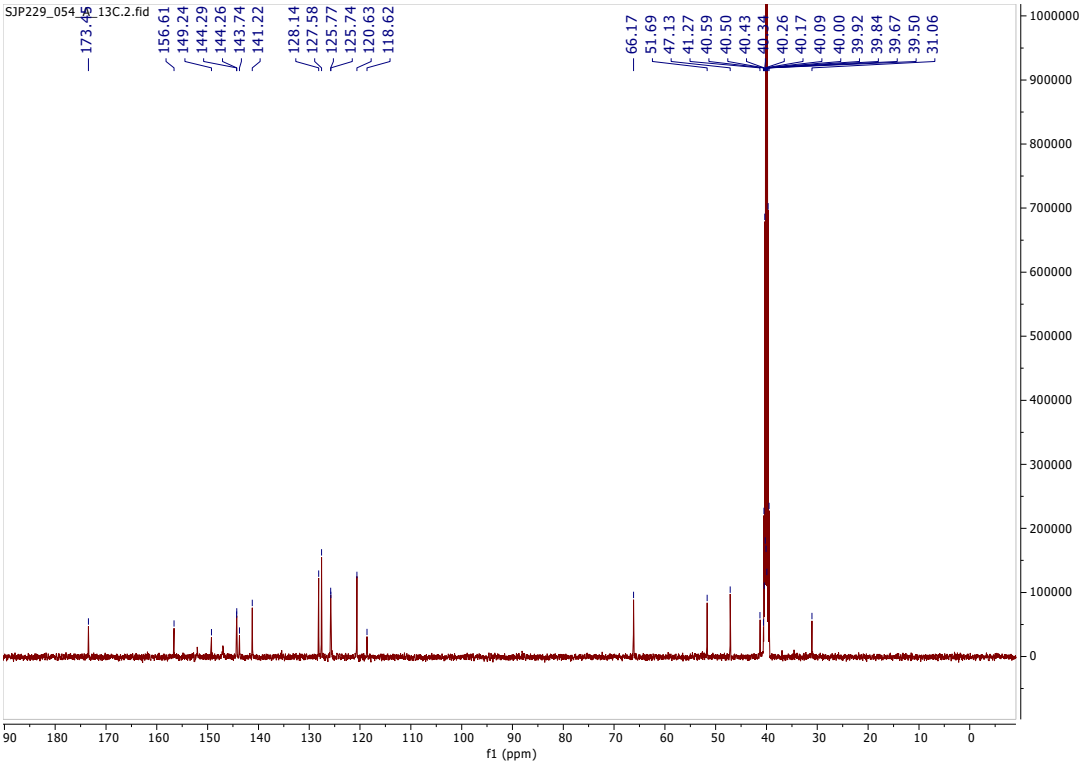
^{13}C NMR (17a)



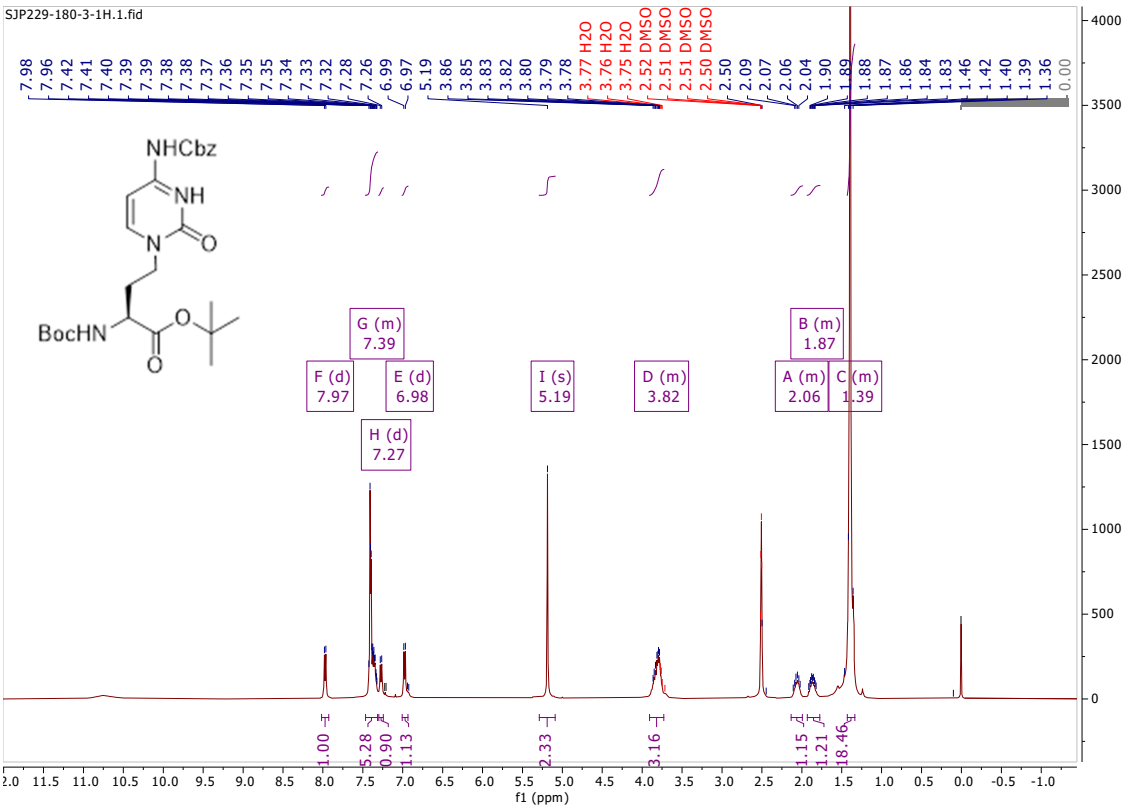
^{1}H NMR (17)



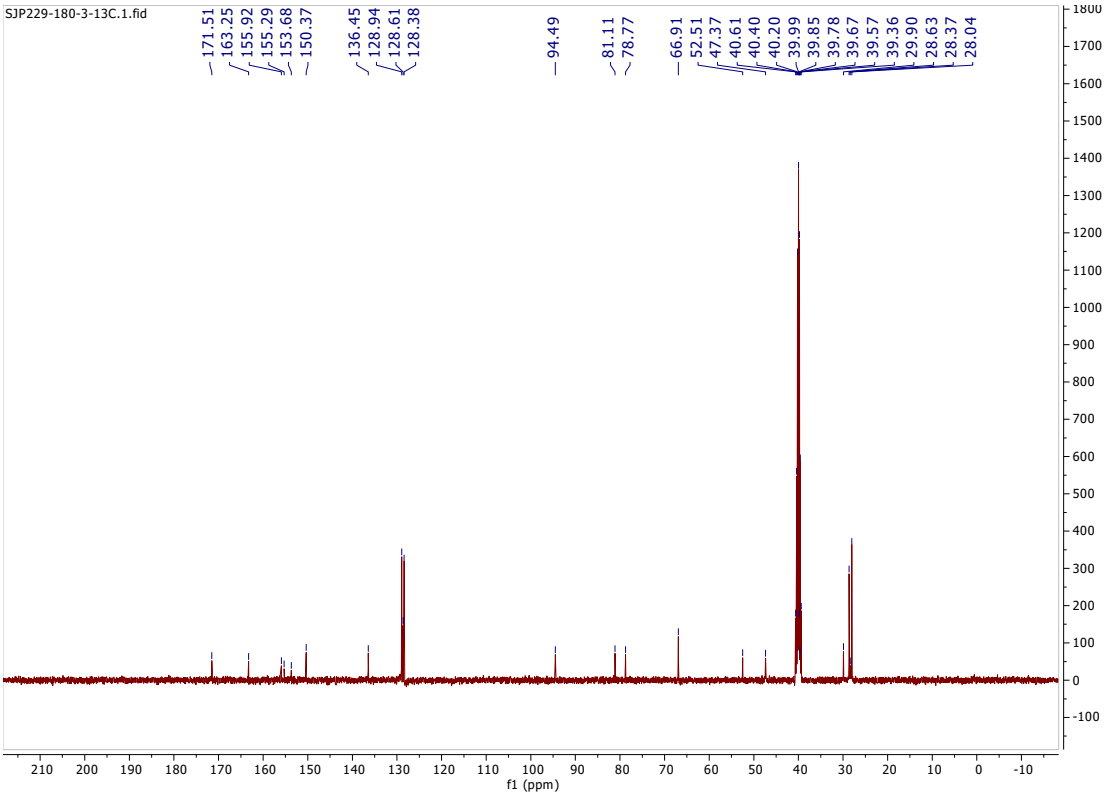
^{13}C NMR (17)



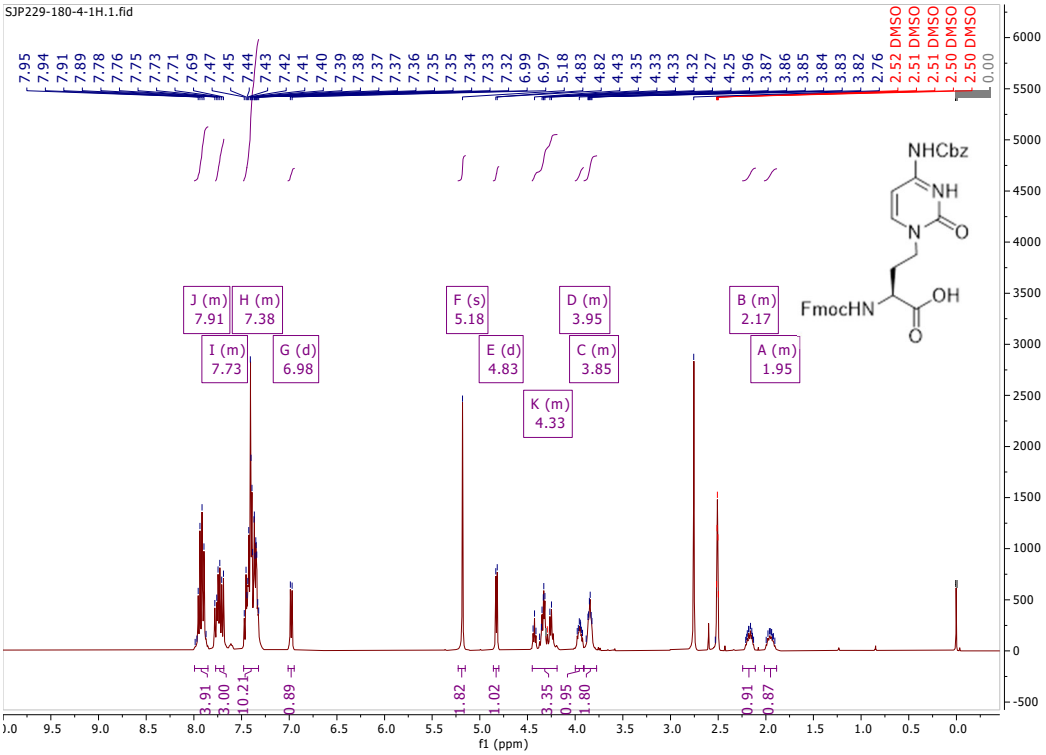
^{1}H NMR (18a)



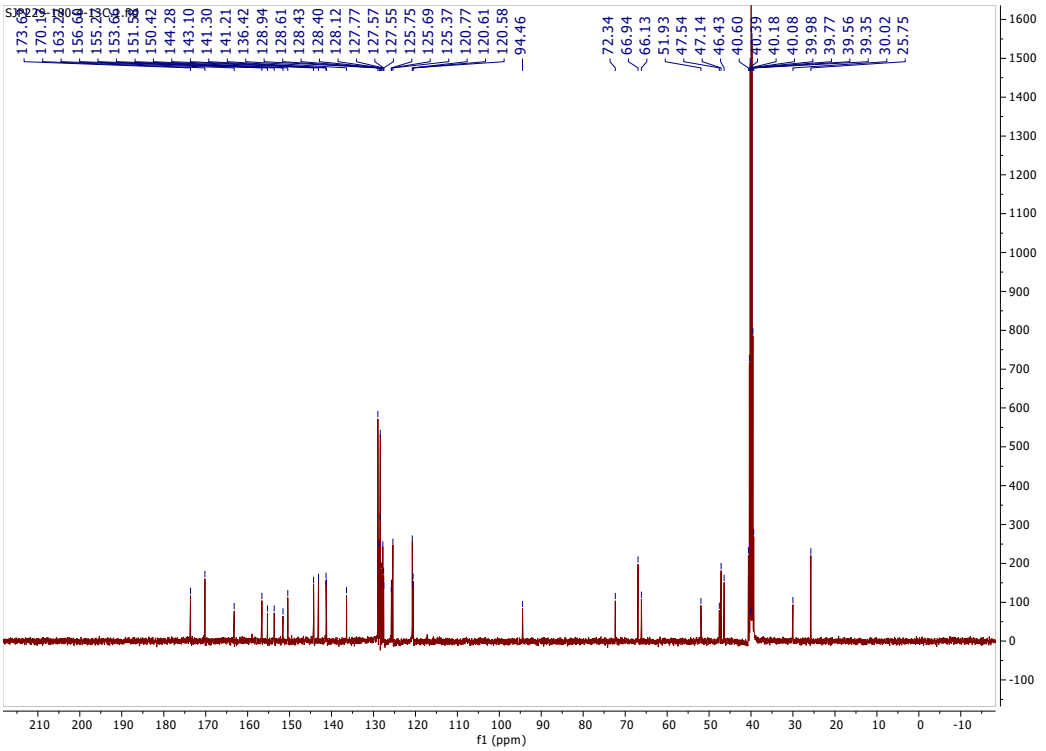
^{13}C NMR (18a)



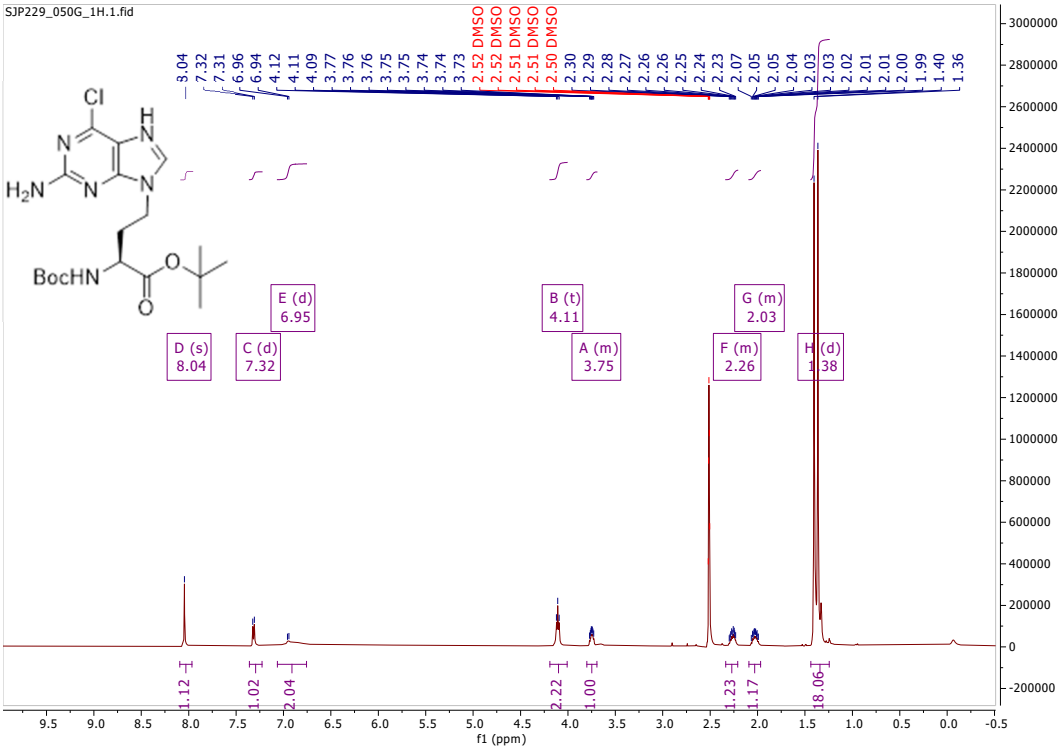
^{1}H NMR (18)



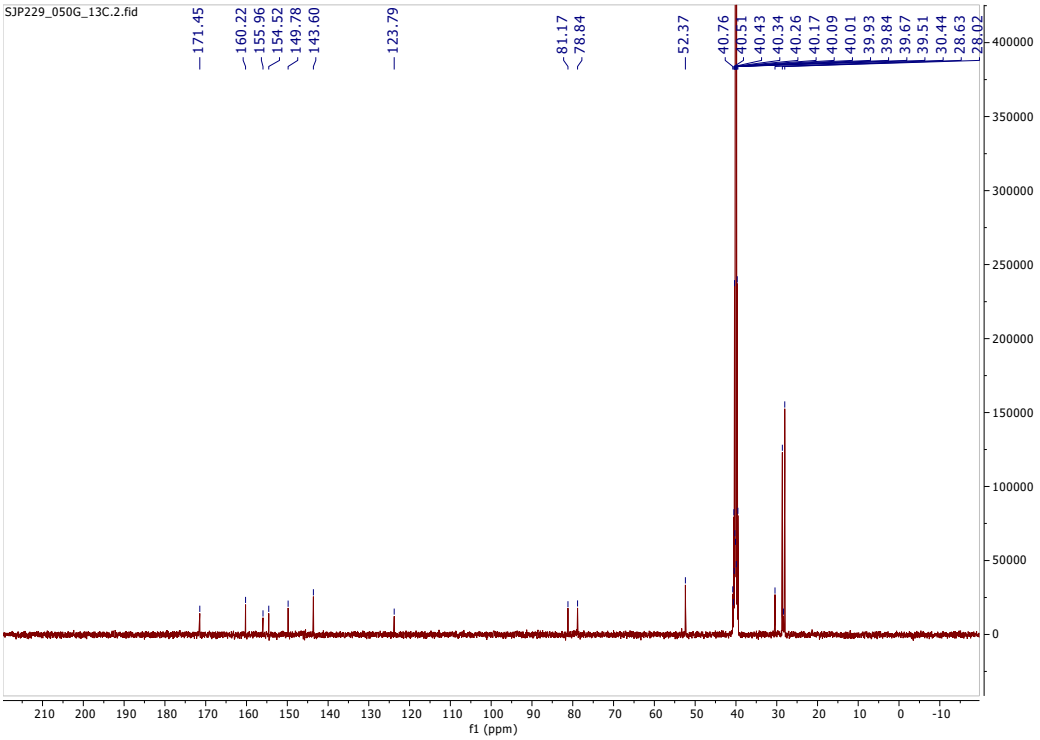
^{13}C NMR (18)



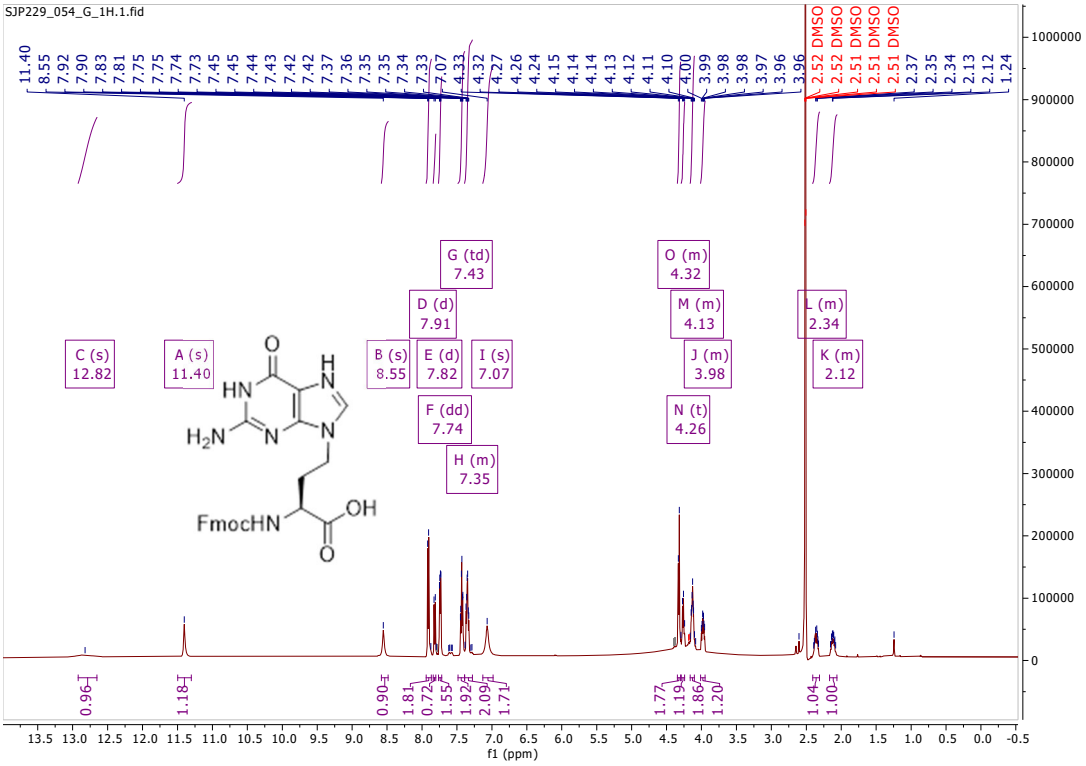
^{1}H NMR (19a)



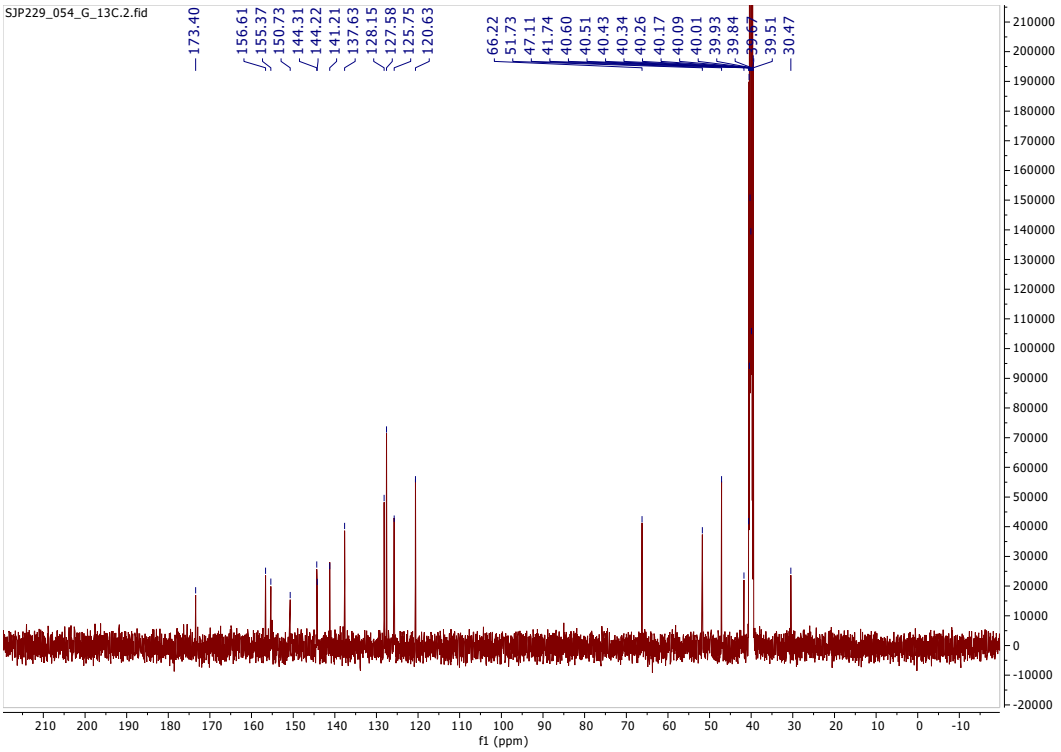
^{13}C NMR (19a)



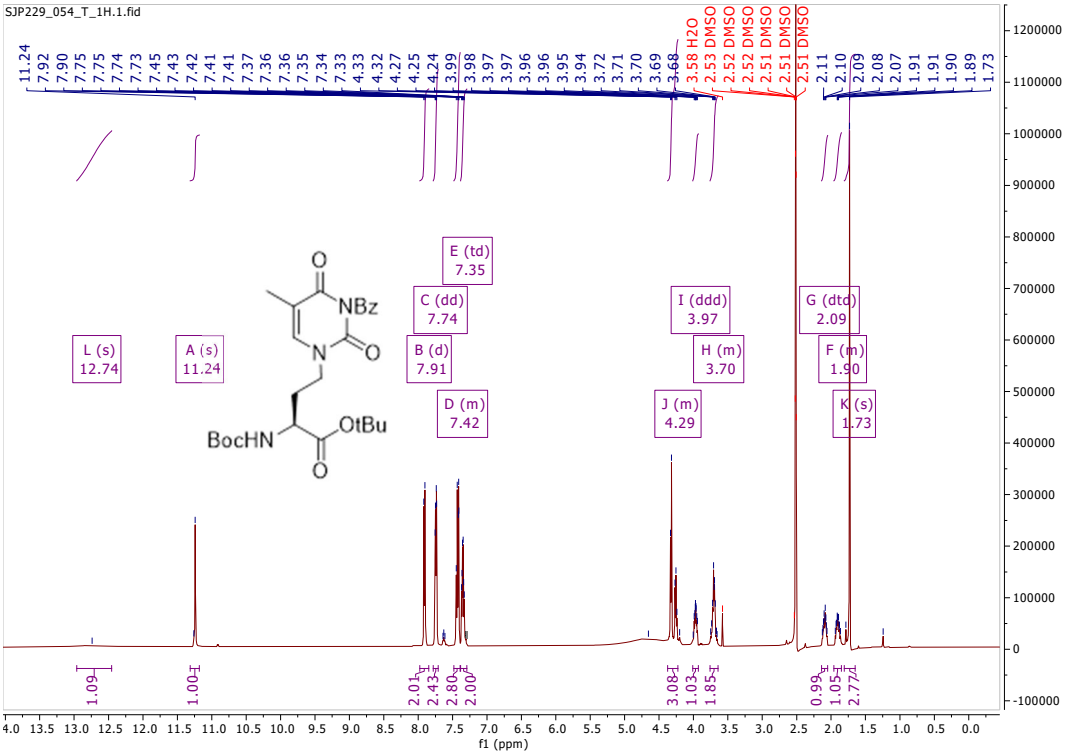
^{1}H NMR (19)



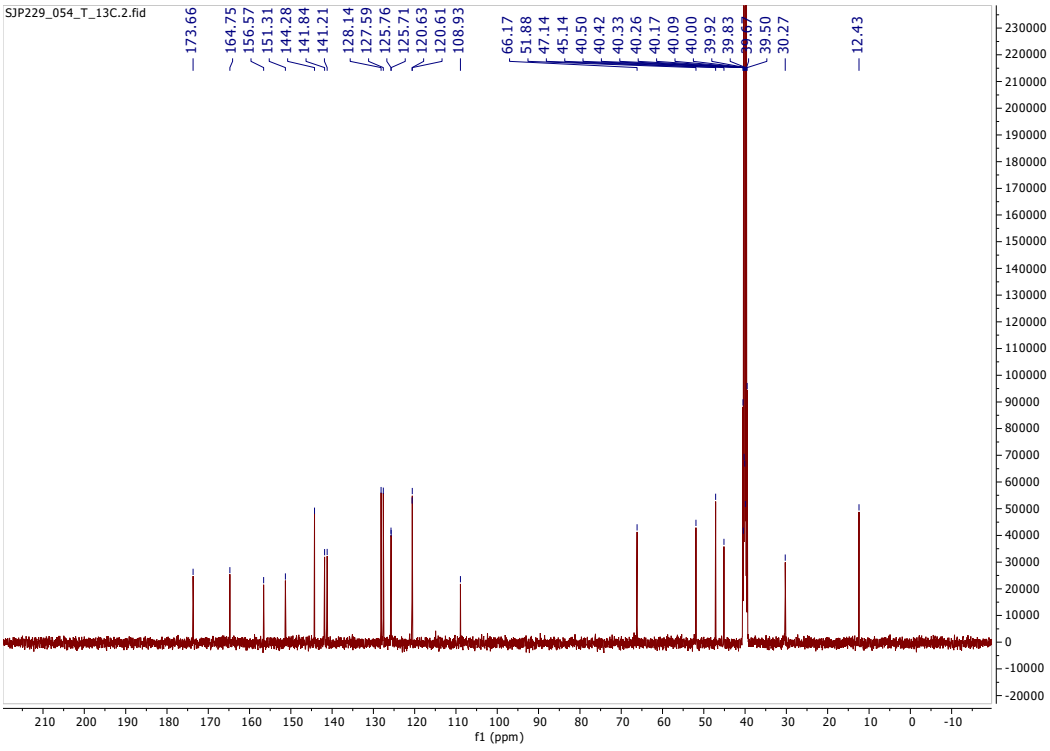
^{13}C NMR (19)



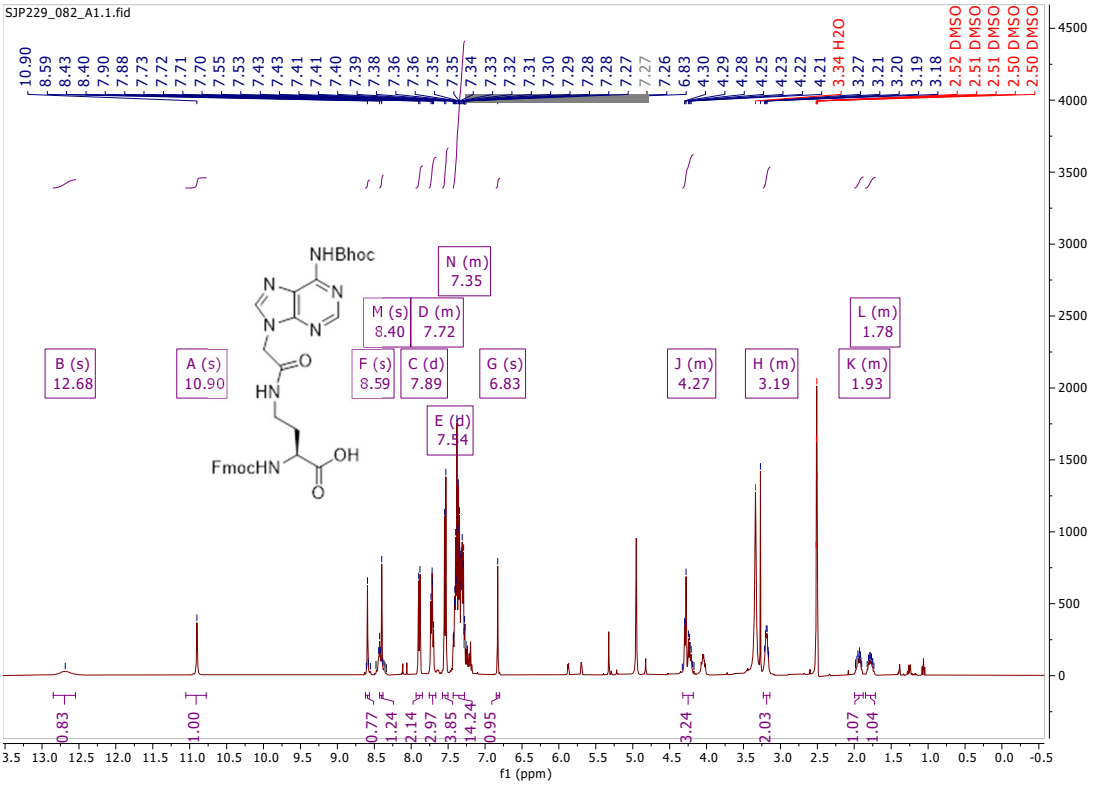
^{1}H NMR (20)



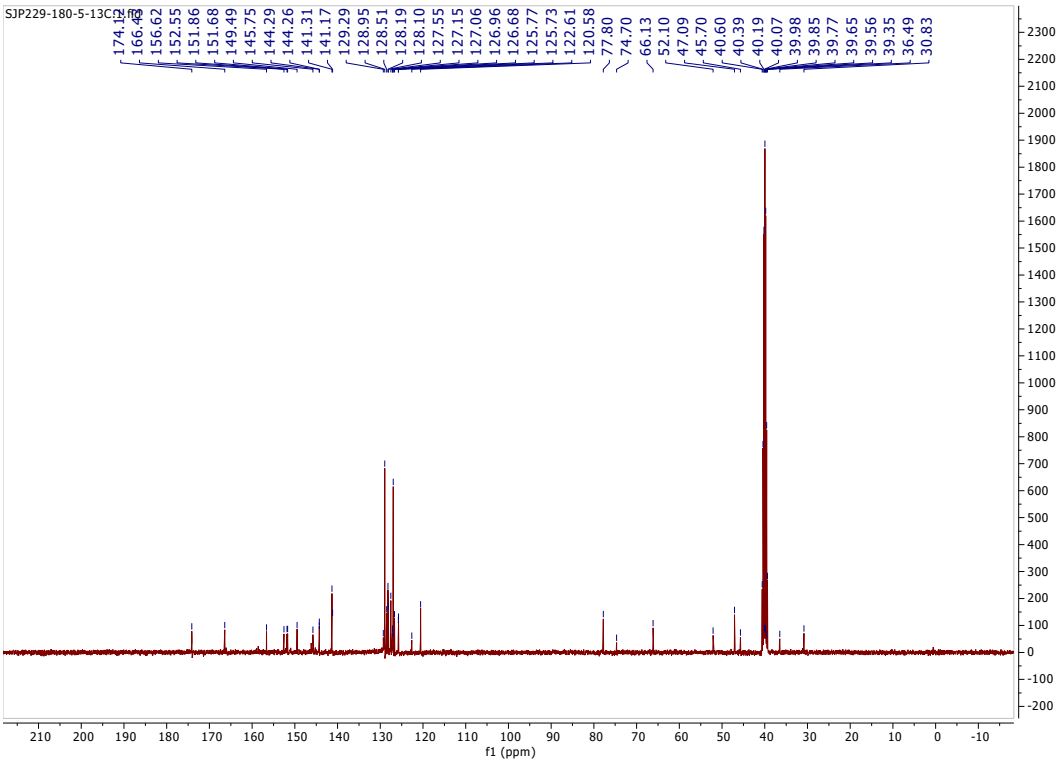
^{13}C NMR (20)



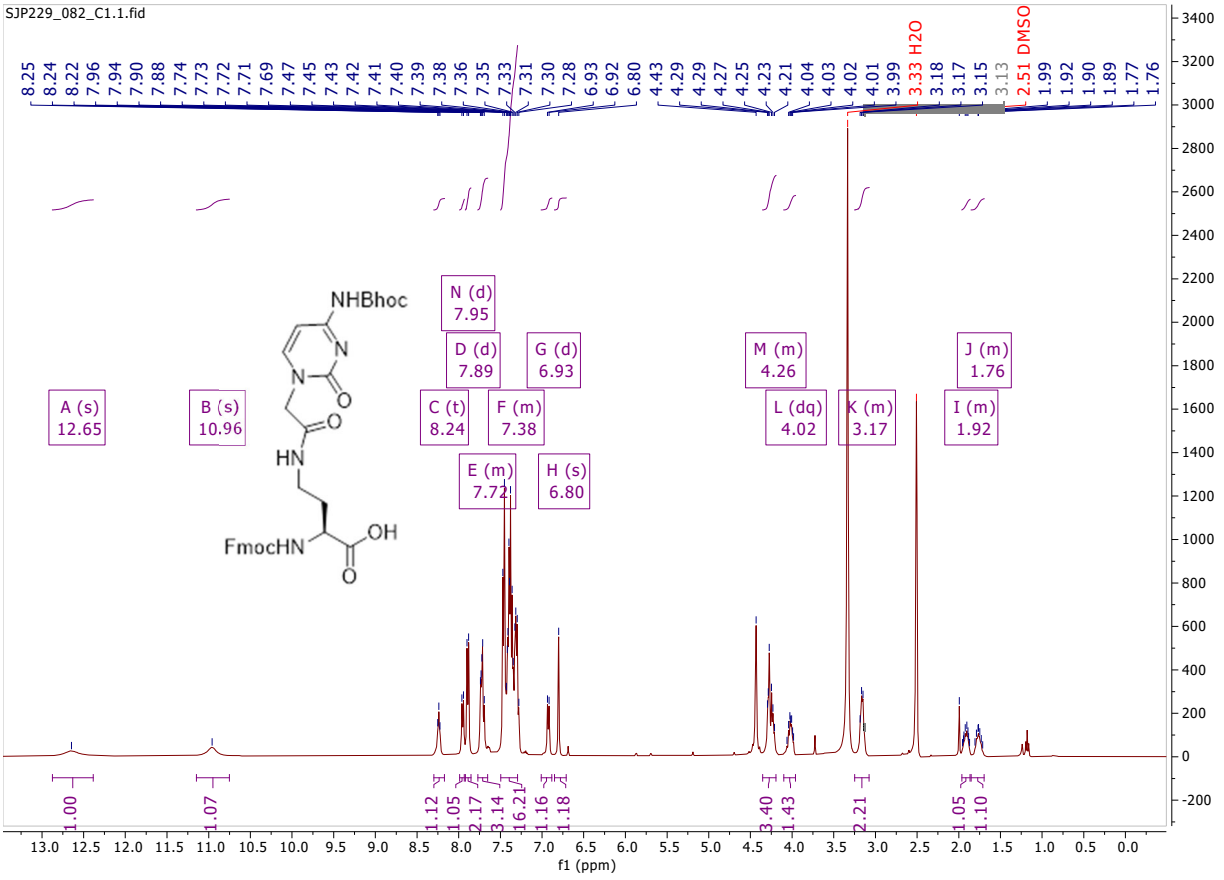
^{1}H NMR (21)



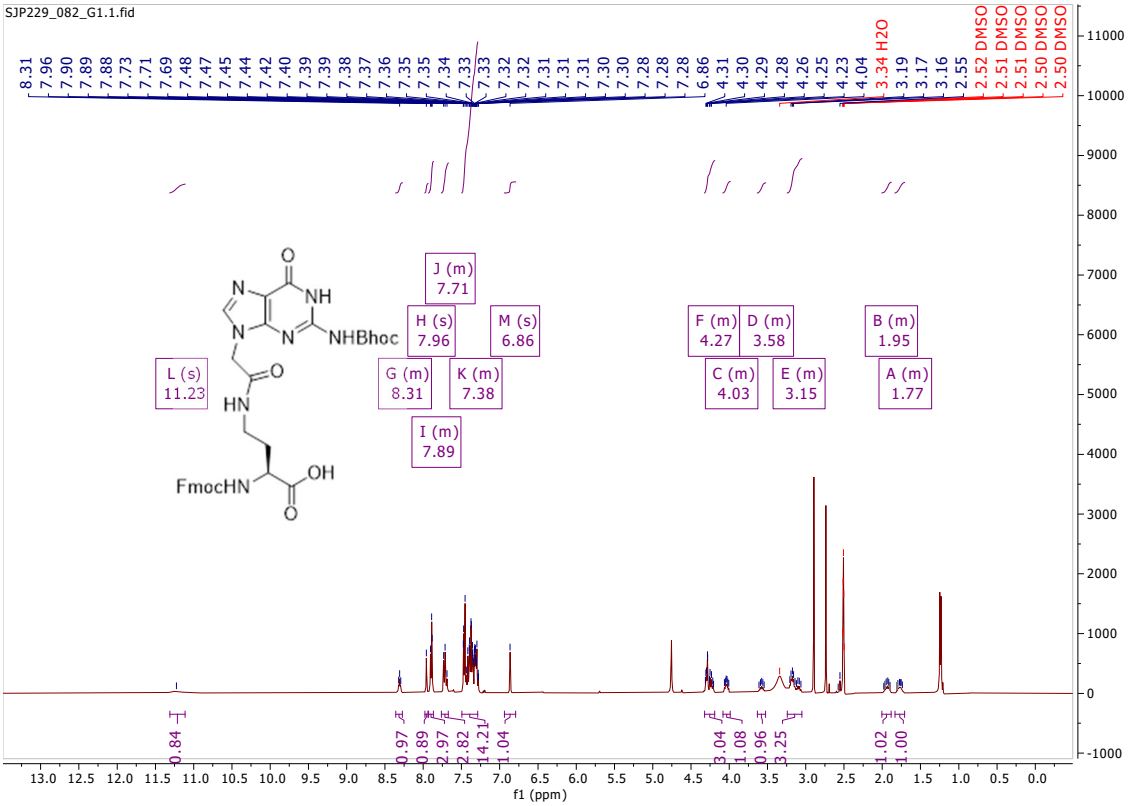
^{13}C NMR (21)



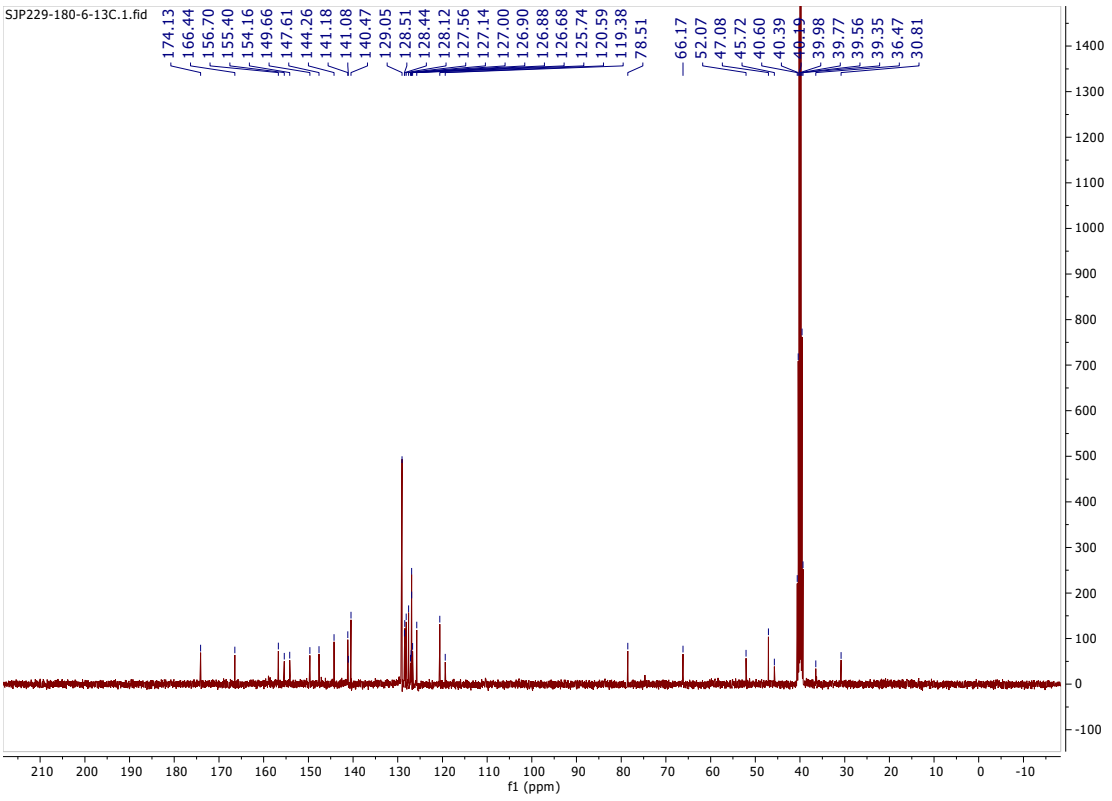
^{1}H NMR (22)


SJP229_082_C1.1.fid
NHBhoc
FmocHN
OH
A (s) 12.65
B (s) 10.96
C (t) 8.24
D (d) 7.89
E (m) 7.72
F (m) 7.38
G (d) 6.93
H (s) 6.80
I (m) 1.92
J (m) 1.76
K (m) 3.17
L (dq) 4.02
M (m) 4.26
N (d) 7.95
3.33 H2O
2.51 DMSO
f1 (ppm)

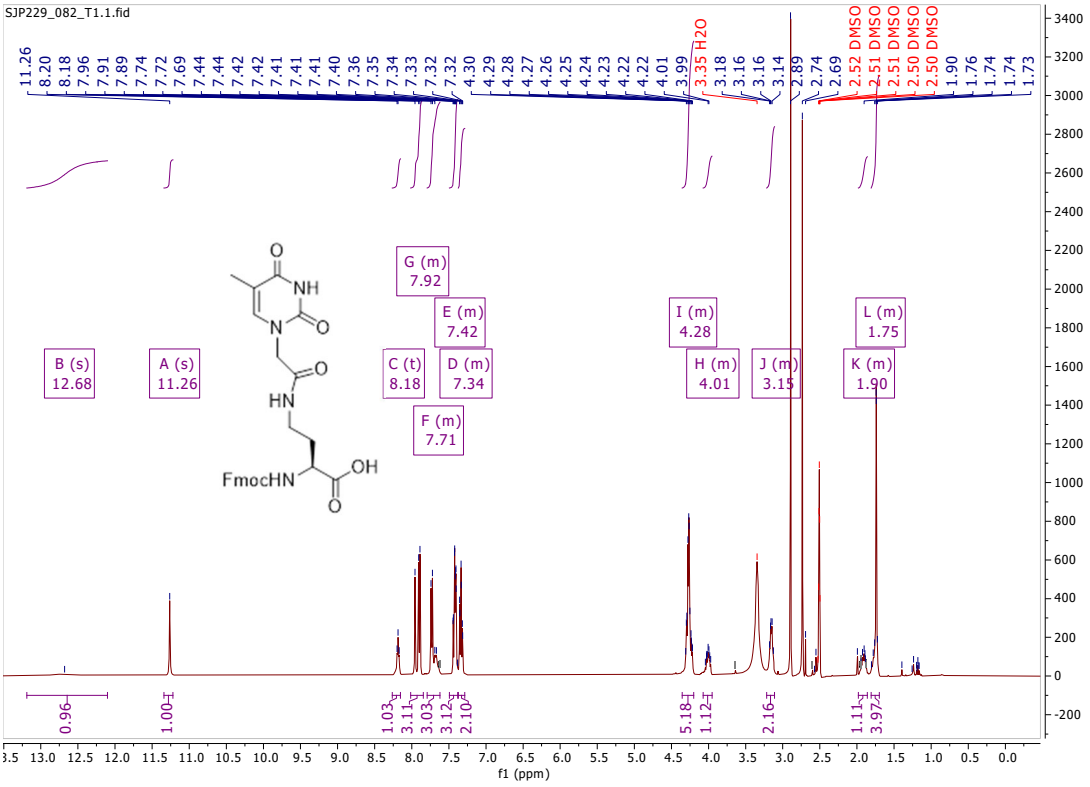
^{1}H NMR (23)



^{13}C NMR (23)



^{1}H NMR (24)


SJP229_082_T1.1.fid
B (s) 12.68
A (s) 11.26
G (m) 7.92
E (m) 7.42
C (t) 8.18
D (m) 7.34
F (m) 7.71
I (m) 4.28
H (m) 4.01
J (m) 3.15
L (m) 1.75
K (m) 1.90
FmocHN
OH
f1 (ppm)

Peptide synthesis procedures

General procedure for manual solid-phase peptide synthesis (SPPS). ChemMatrix® Rink amide resin (loading 0.49 mmol/g, typical scale: 200 mg, 0.1 mmol) was loaded into a fritted syringe (12 mL), swollen in DMF (5 mL) for 5 minutes and then drained. Each Nα-Fmoc protected amino acid (1.0 mmol, 10 equiv) was dissolved in DMF containing 0.39 M HATU (2.5 mL). Immediately before the coupling DIEA (500 µL, 30 equiv) was added to the mixture to activate the amino acid. This solution (after 15 seconds) was added to the resin and reacted for 10 min, with occasional stirring. After completion of the coupling step, the syringe was drained, and the resin was washed with DMF (3 x 10 mL). Fmoc deprotection was performed by addition of piperidine (20% in DMF, 5 mL), to the resin (1 x 1 min + 1 x 5 min), followed by draining and washing the resin with DMF (5 x 10 mL). Side chain protection was as follows: Asn(Trt), Asp(O^{t}Bu), Cys(Trt), Gln(Trt), Glu(O^{t}Bu), His(Trt), Lys(Boc), Ser(^{t}Bu), Thr(^{t}Bu), Trp(Boc), Tyr(^{t}Bu).

General procedure for the coupling of nucleobase monomers: for a 10 µmol scale coupling: nucleobase amino acid (50 µmol) and PyAOP (50 µmol) were dissolved in DMF (250 µL, 0.1 M reactant concentration). DIEA (150 µmol) was added and the solution incubated with the peptide resin for 20 min at room temperature with occasional stirring.

Procedure for nucleobase peptide cleavage. Upon completion of the peptide synthesis, the resin was treated with a cleavage cocktail containing (v/v) 63% TFA, 21% TMSOTf, 4% 1,2-ethanedithiol (EDT), 10% thioanisole and 2% cresol (v/v) at room temperature for 1 h. The TFA volume was then reduced under N_2 stream and cold diethyl ether (–78 °C) was added to precipitate the peptide. The resulting suspension was centrifugated at 4000 rpm for 3 min and the liquid was discarded. After repeating this step twice more, the pellet was dissolved in Milli-Q ultrapure water + 0.1% TFA and lyophilized.

Procedure for peptide cleavage. Upon completion of the peptide synthesis, the resin was treated with a cleavage cocktail containing 94% TFA, 2.5% water, 2.5% 1,2-ethanedithiol (EDT) and 1% triisopropylsilane (TIPS) (v/v) at room temperature for 2 h. The TFA volume was then reduced under N_2 stream and cold diethyl ether (–80 °C) was added to precipitate the peptide. The resulting suspension was centrifugated at 4000 rpm for 3 min and the liquid was discarded. After repeating this step twice more, the pellet was dissolved in Milli-Q ultrapure water + 0.1% TFA and lyophilized.

General procedure for solid-phase extraction (SPE) purification. Peptides were desalted using C18 SPE cartridges according to general procedures from Agilent Sample Prep Solutions Bond Elut.

Preparation of peptide solutions. Weight of lyophilized peptide was determined with analytical scale. The peptide's molecular weight plus n x 114 (n = number of K, R, H and N-term, 114 = mw TFA) was used to calculated number of moles. In case of the libraries the average mw of all used monomers was multiplied by the number of variable positions. The peptide was than dissolved in a volume according to the desired final concentration.

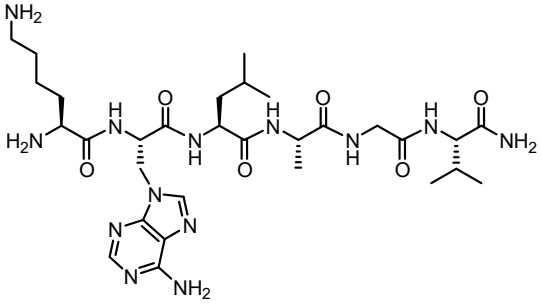
Determination of oligonucleotide concentration. The concentration of oligonulceotides was calculated using the Beer-Lambert law by measuring the absorbance of the oligo sample at 260 nm. The absorbance was measured by averaging at least two independent readings of the same sample on a BioTek Synergy HT plate reader outfitted with a BioTek Take 3 micro-volume plate.

Nucleobase peptide and peptide characterization

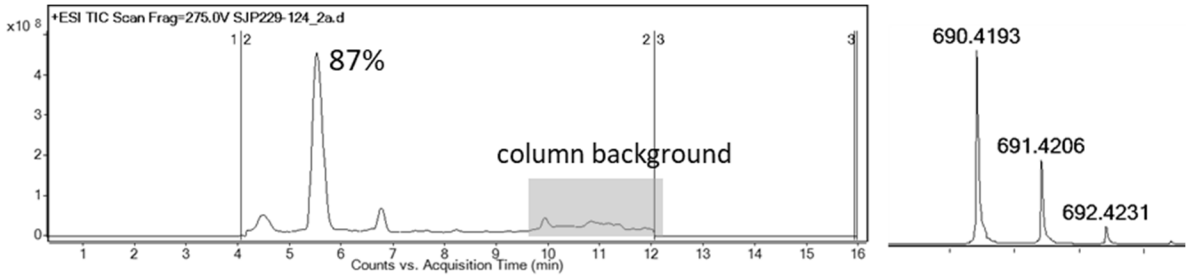
Test of nucleobase monomers incorporation into short peptide by SPPS

Individual purities were calculated by integration of relevant peaks in the LCMS TIC chromatograms

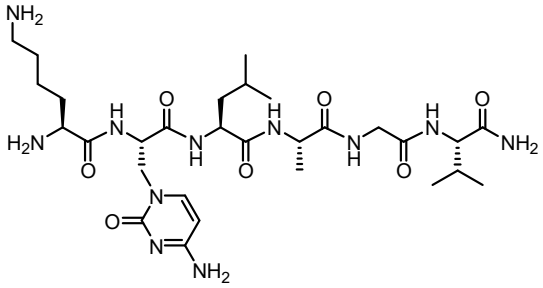
Nucleobase peptide 26



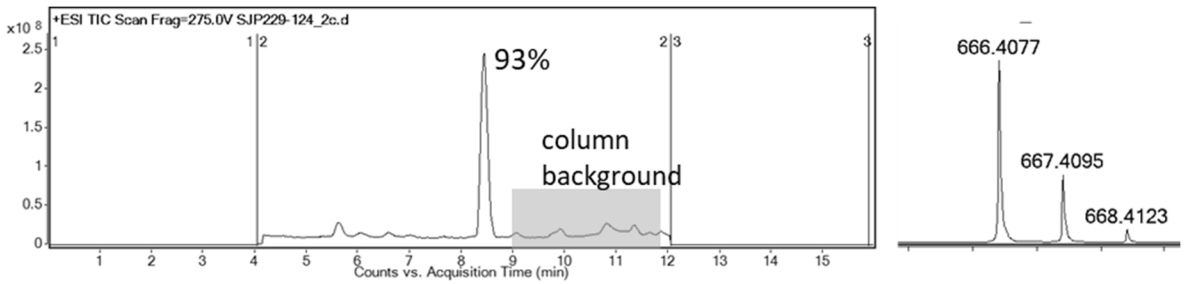
HRMS (SI-QToF) *m/z:* $[M+H]^+$ calcd. 690.416 found 690.419



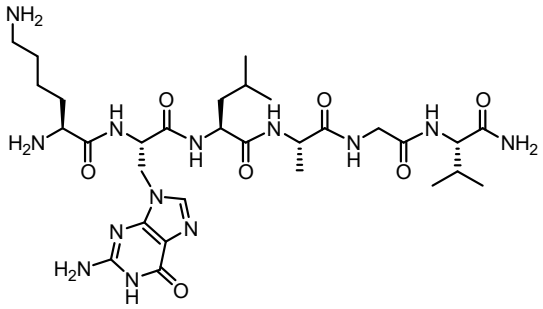
Nucleobase peptide 27



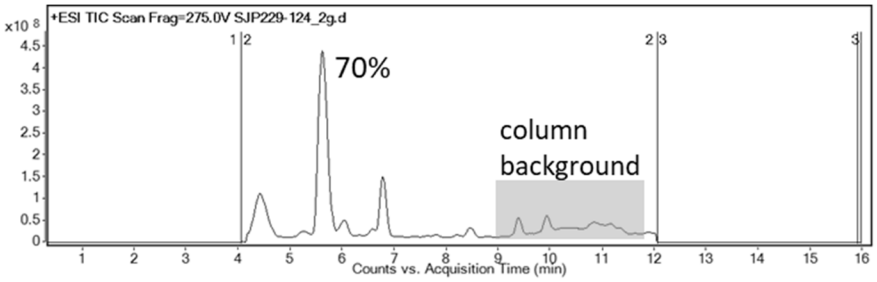
HRMS (SI-QToF) *m/z:* $[M+H]^+$ calcd. 666.405 found 666.408

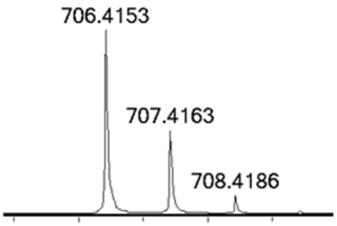

+ESI TIC Scan Frag=275.0V SJP229-124_2c.d
x10 8
93%
column
background
Counts vs. Acquisition Time (min)
666.4077
667.4095
668.4123

Nucleobase peptide 28

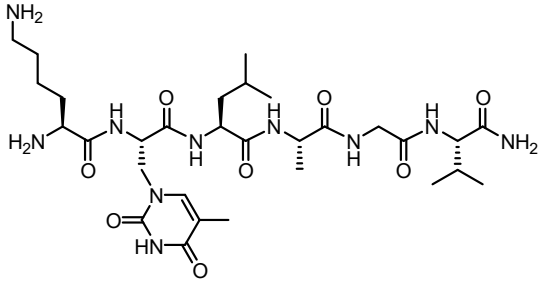


HRMS (SI-QToF) *m/z:* $[M+H]^+$ calcd. 706.411 found 706.415

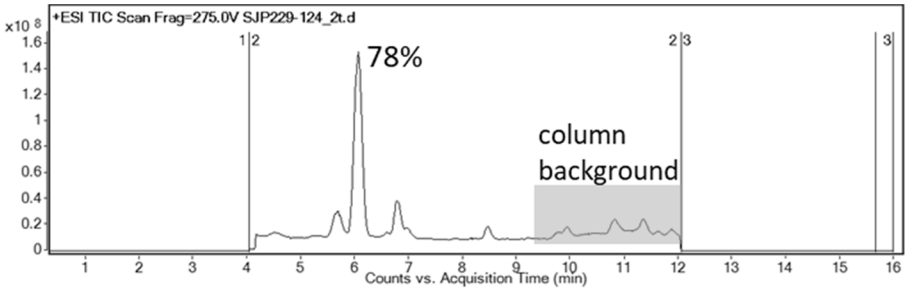


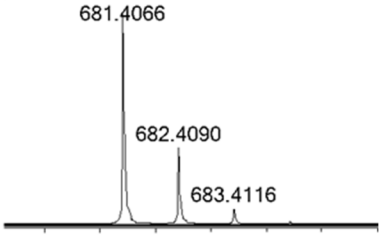


Nucleobase peptide 29

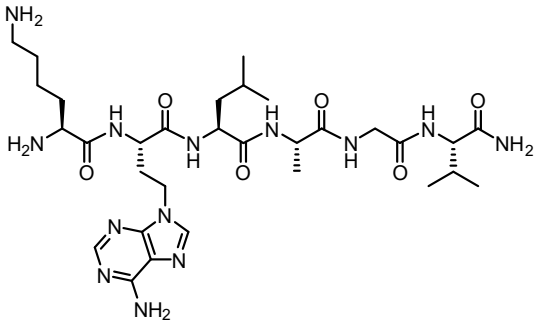


HRMS (SI-QToF) *m/z:* $[M+H]^+$ calcd. 681.402 found 681.407

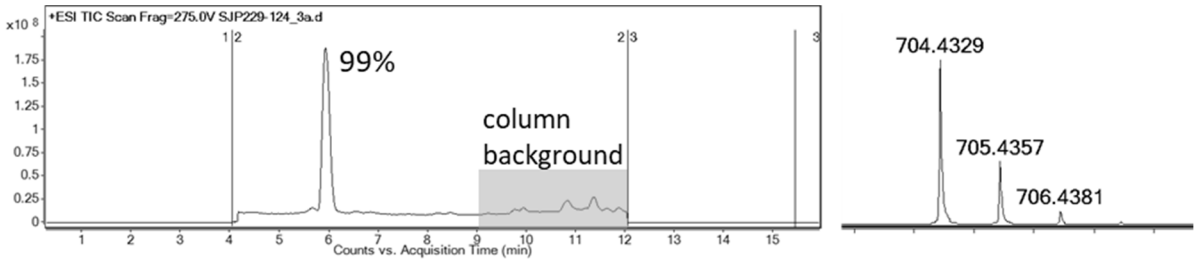




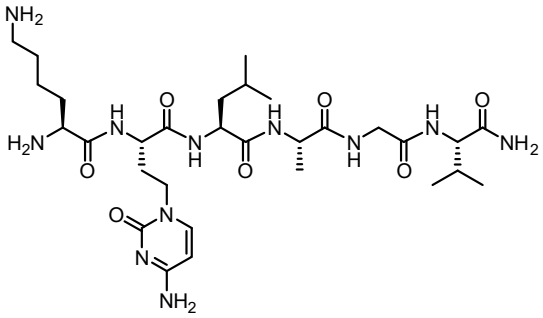
Nucleobase peptide 30



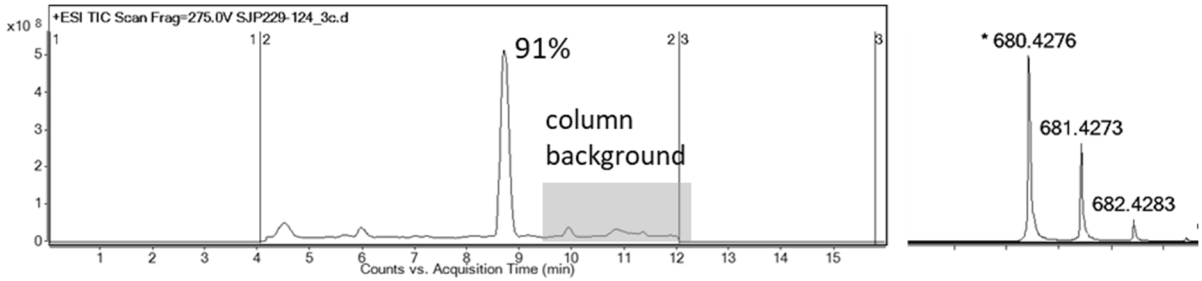
HRMS (SI-QToF) *m/z:* $[M+H]^+$ calcd. 704.432 found 704.433



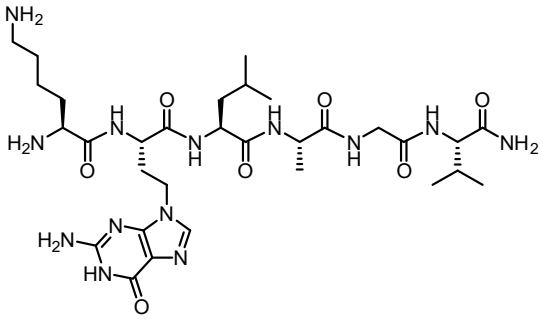
Nucleobase peptide 31



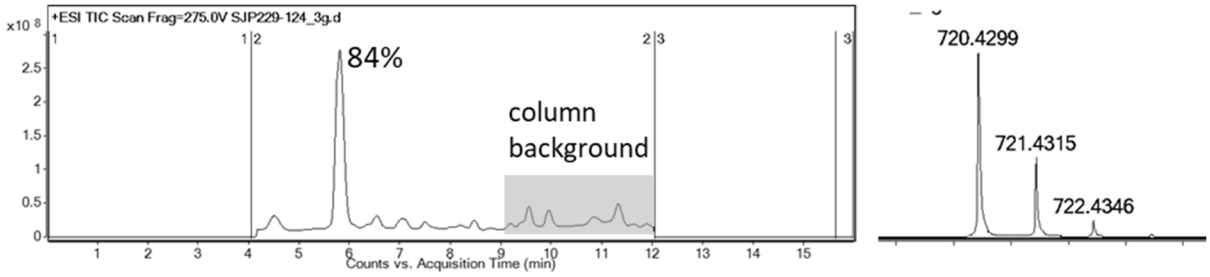
HRMS (SI-QToF) *m/z:* $[M+H]^+$ calcd. 680.421 found 680.428



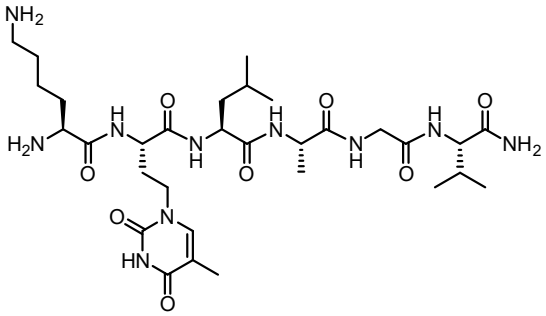
Nucleobase peptide 32



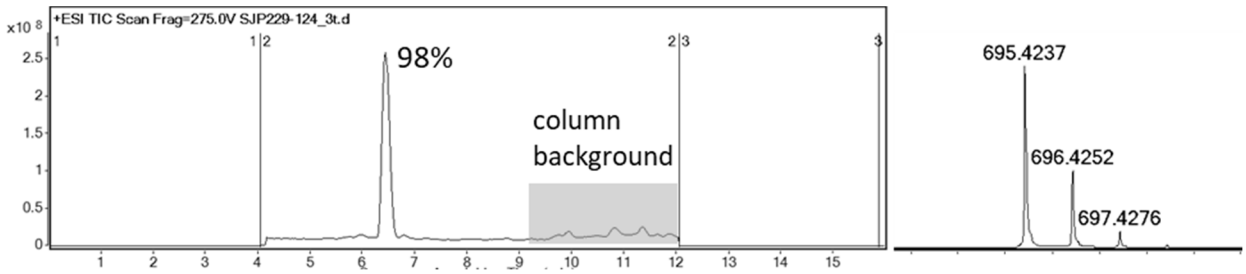
HRMS (SI-QToF) *m/z:* $[M+H]^+$ calcd. 720.427 found 720.430



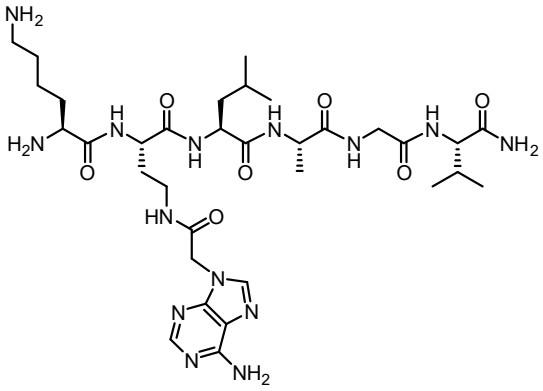
Nucleobase peptide 33



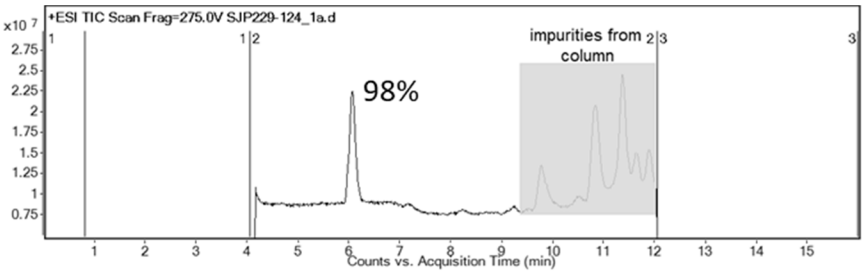
HRMS (SI-QToF) *m/z:* $[M+H]^+$ calcd. 695.420 found 695.424

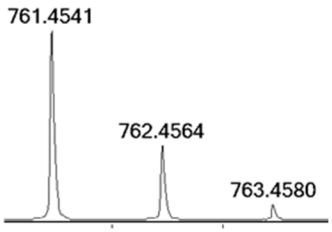


Nucleobase peptide 34

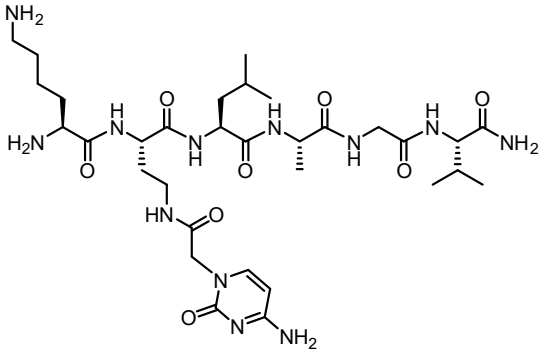


HRMS (SI-QToF) *m/z:* $[M+H]^+$ calcd. 761.454 found 761.454

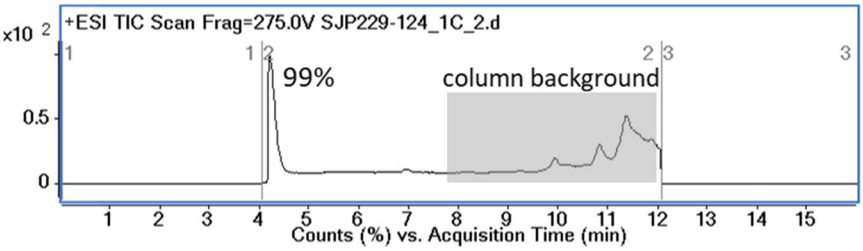


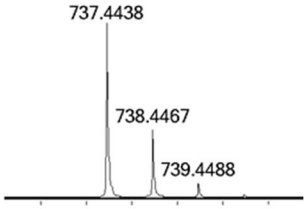


Nucleobase peptide 35

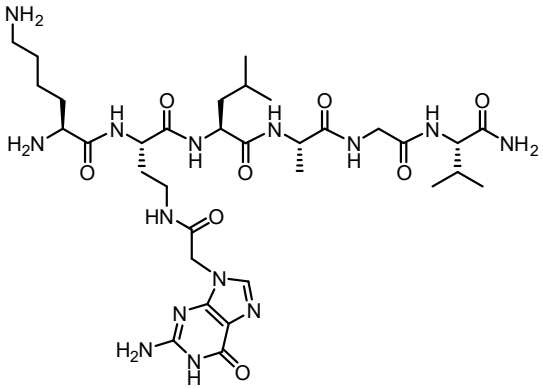


HRMS (SI-QToF) *m/z:* $[M+H]^+$ calcd. 737.442 found 737.444

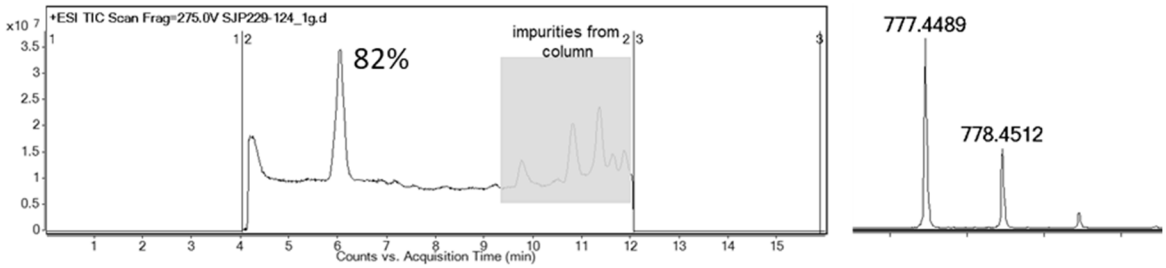




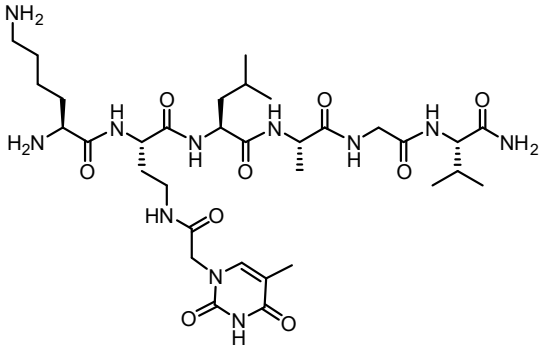
Nucleobase peptide 36



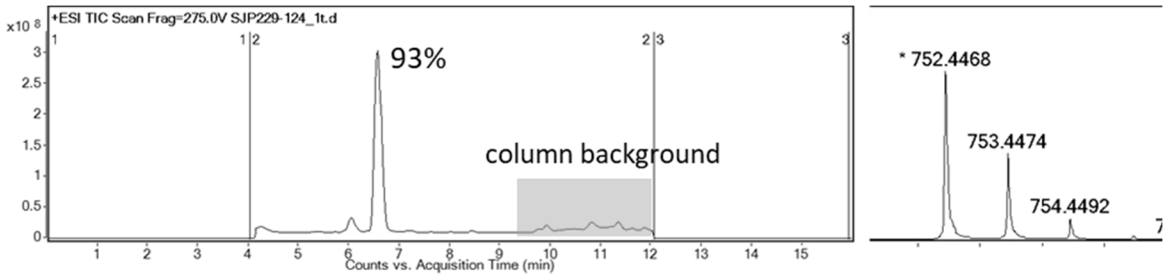
HRMS (SI-QToF) *m/z:* $[M+H]^+$ calcd. 777.448 found 777.449



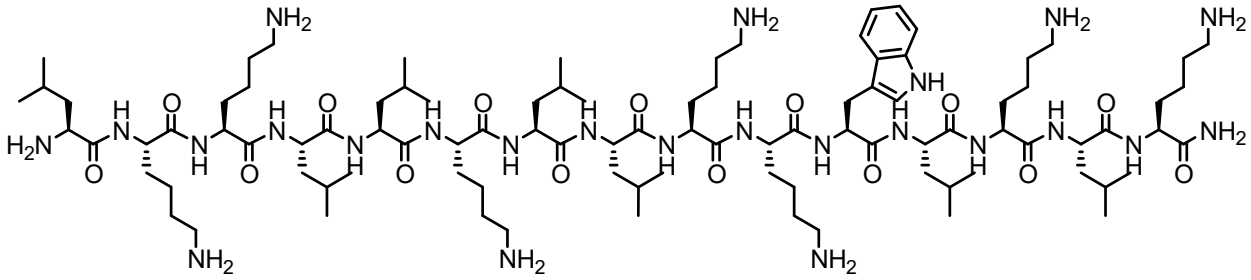
Nucleobase peptide 37



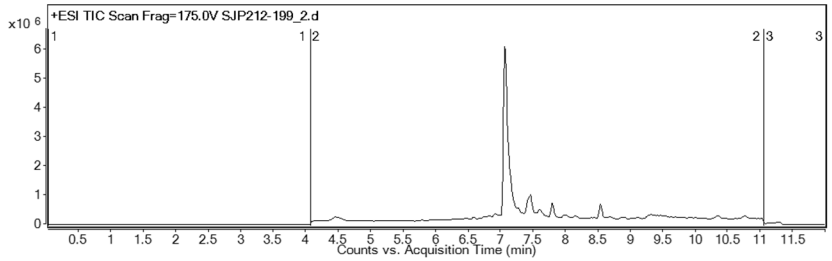
HRMS (SI-QToF) *m/z:* $[M+H]^+$ calcd. 752.442 found 752.447

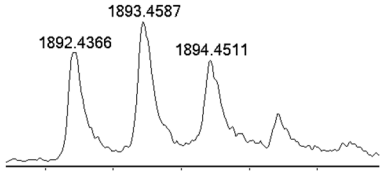


Peptide 38

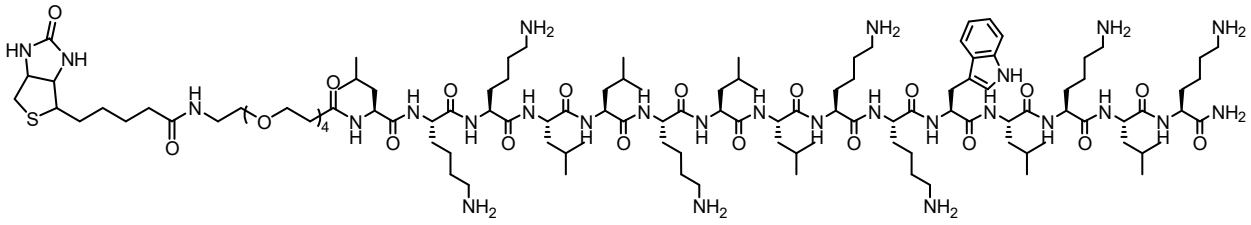


HRMS (SI-QToF) *m/z:* $[M+H]^+$ calcd. 1892.37 found 1892.44

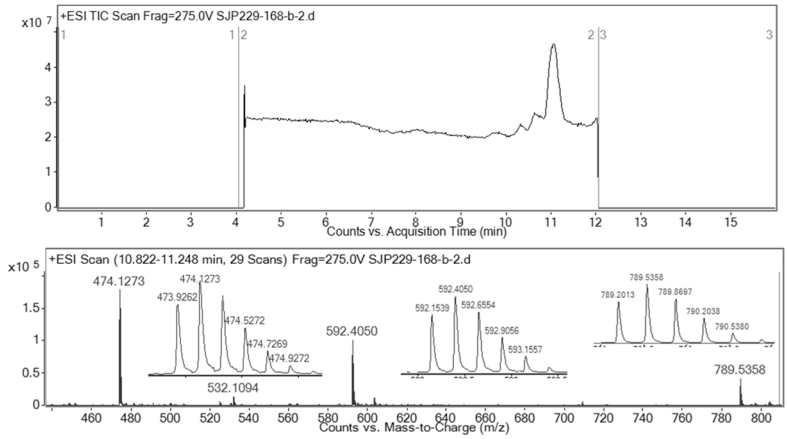




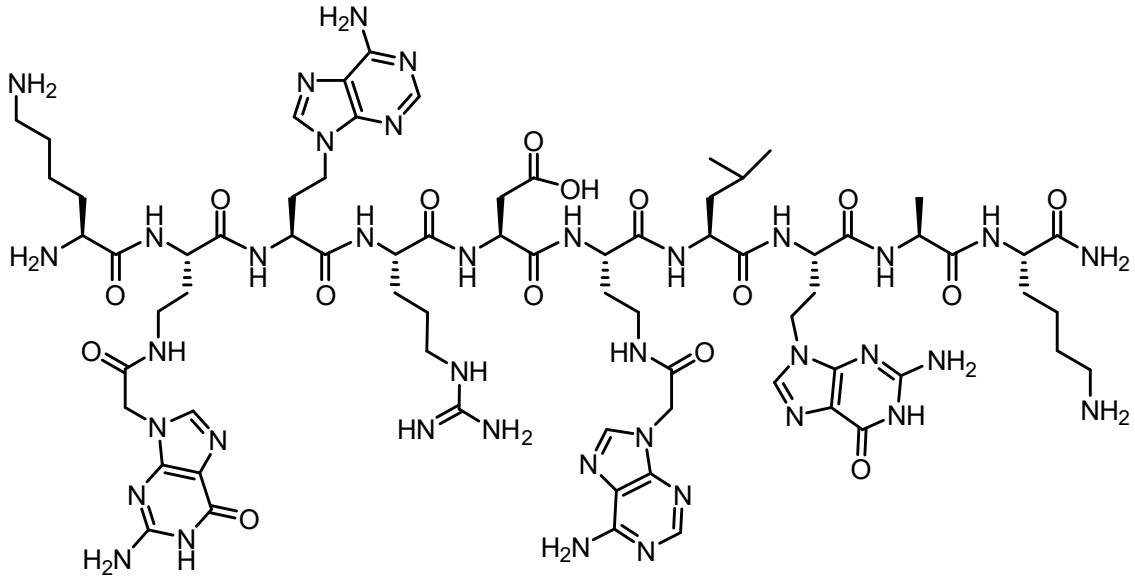
38 Biotin



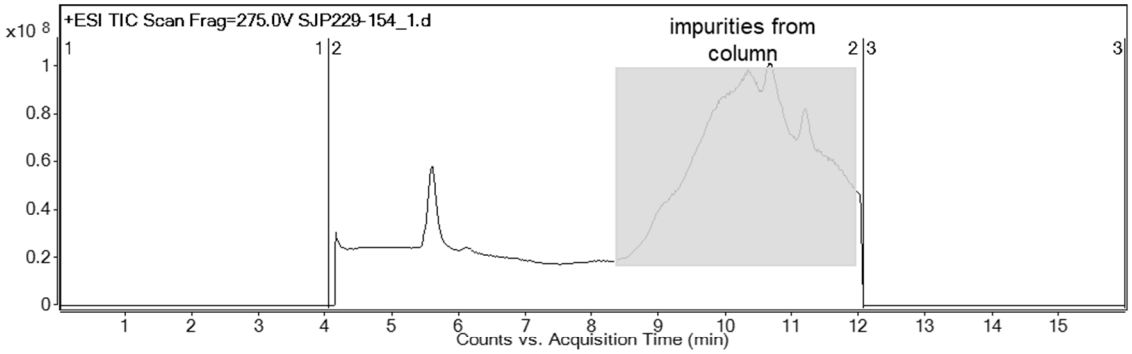
HRMS (SI-QToF) *m/z:* $[M+5H]^{5+}$ calcd. 473.924 found 473.926
$[M+4H]^{4+}$ calcd. 592.153 found 591.154
$[M+3H]^{3+}$ calcd. 789.201 found 780.201

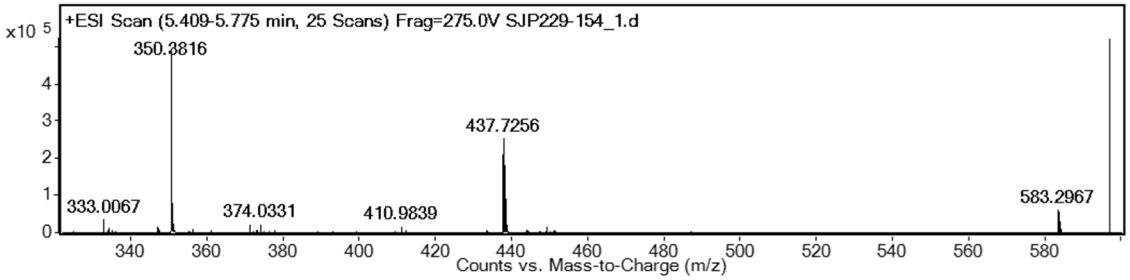


Nucleobase peptide 39

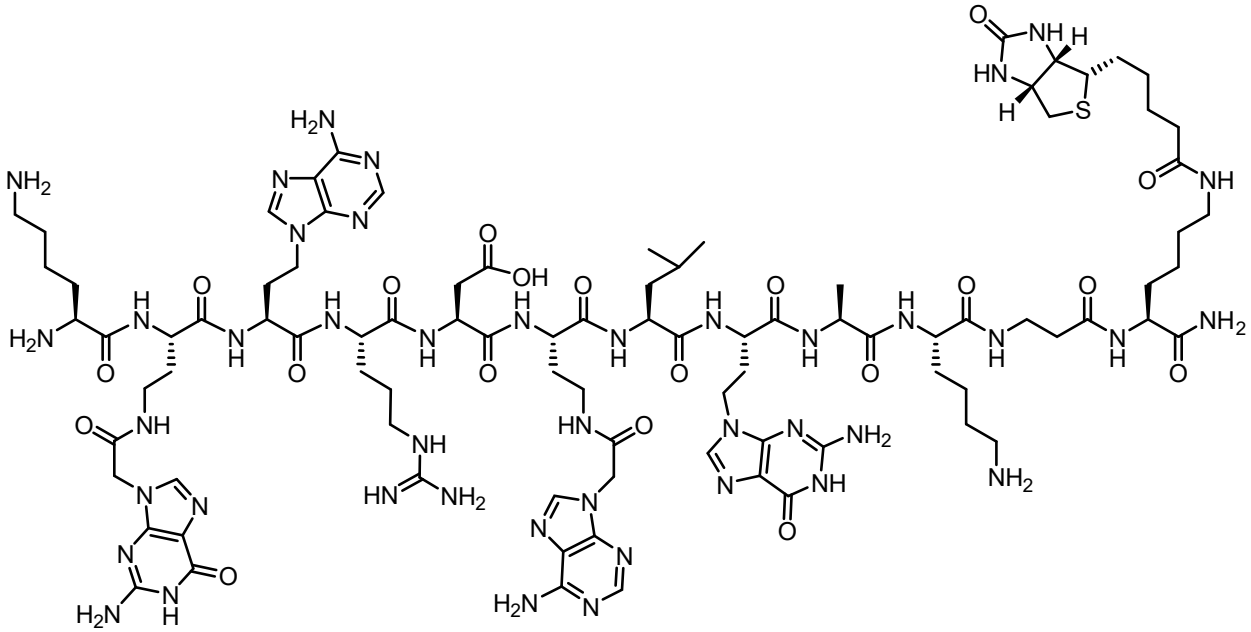


HRMS (SI-QToF) *m/z:* $[M+5H]^{4+}$ calcd. 350.381 found 350.382
$[M+4H]^{4+}$ calcd. 437.724 found 437.726
$[M+3H]^{3+}$ calcd. 583.296 found 583.297

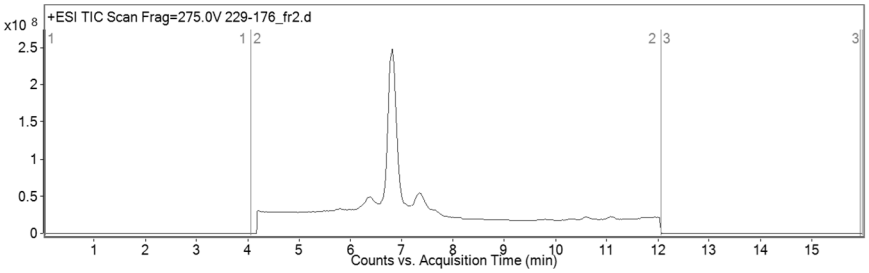


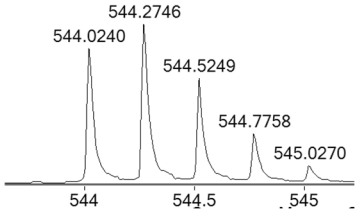


Nucleobase peptide 40



HRMS (SI-QToF) *m/z:* $[M+5H]^{5+}$ calcd. 435.423 found 435.421
$[M+4H]^{4+}$ calcd. 544.027 found 544.024
$[M+3H]^{3+}$ calcd. 725.0326 found 725.030
$[M+2H]^{2+}$ calcd. 1087.04 found 1087.04





Alanine scan

Original sequence: 39Biotin

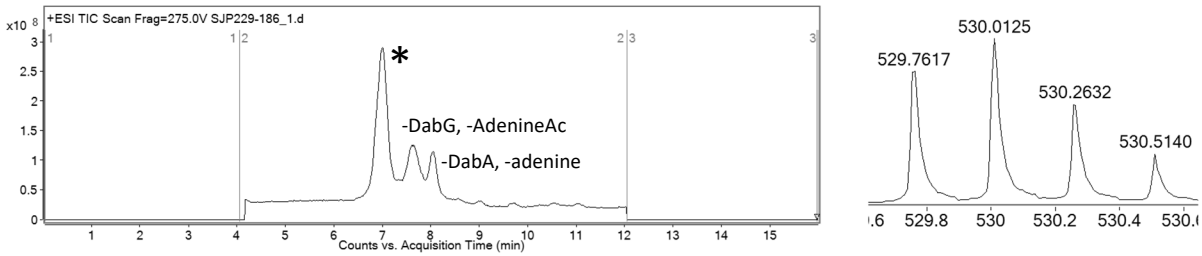
Lys – DabG – hAlaA – Arg – Asp -DabA – Leu -DabG – Ala – Lys – bAla – Lys(Biotin)-$CONH_2$

Nucleobase peptides were synthesized according to the general SPPS procedure, cleaved and used without further purification. Main product in each chromatogram is indicated with *.

AlaScan-1:

Ala – DabG – hAlaA – Arg – Asp -DabA – Leu -hAlaG – Ala – Lys – βAla – Lys(Biotin)-$CONH_2$

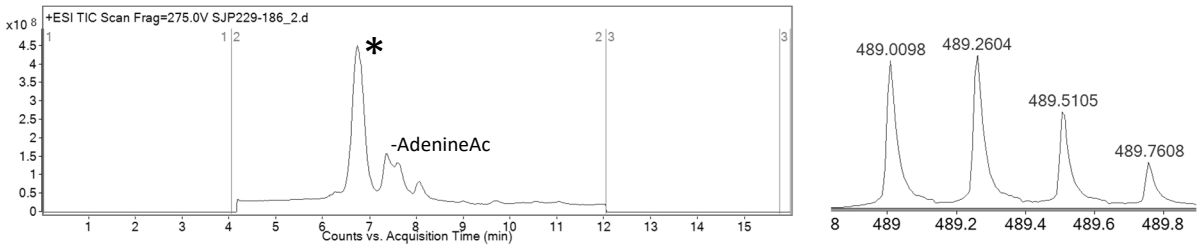
HRMS (SI-QToF) *m/z:* $[M+4H]^{4+}$ calcd. 529.762 found 529.762



AlaScan-2:

Lys – **Ala** – hAlaA – Arg – Asp -DabA – Leu - hAlaG – Ala – Lys – βAla – Lys(Biotin)-$CONH_2$

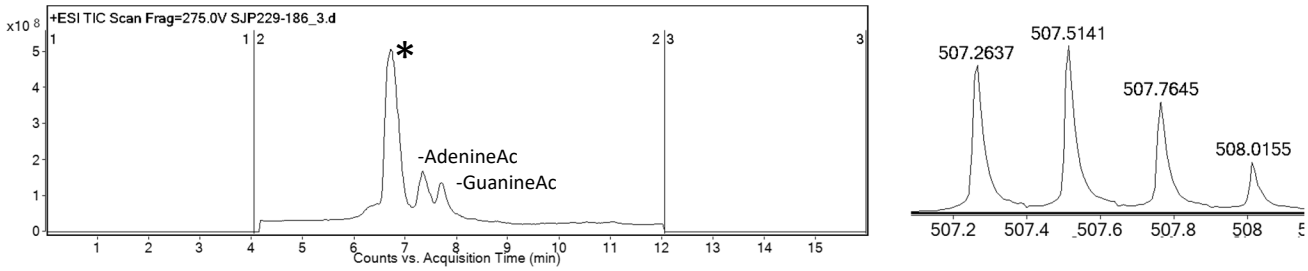
HRMS (SI-QToF) *m/z:* $[M+4H]^{4+}$ calcd. 489.009 found 489.010



AlaScan-3:

Lys – DabG – **Ala** – Arg – Asp -DabA – Leu - hAlaG – Ala – Lys – βAla – Lys(Biotin)-$CONH_2$

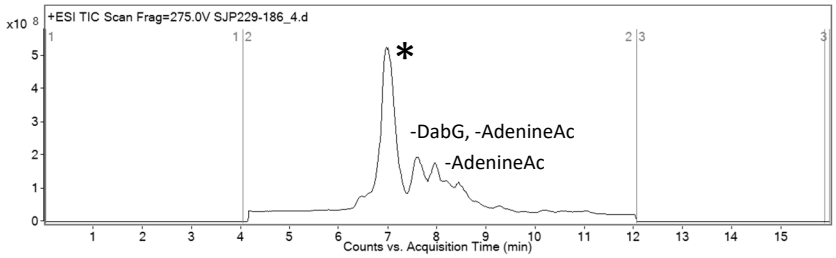
HRMS (SI-QToF) *m/z:* $[M+4H]^{4+}$ calcd. 507.263 found 507.264

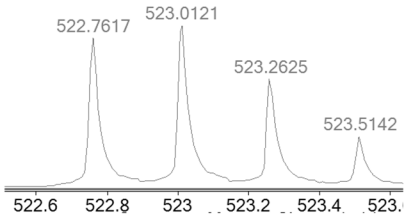


AlaScan-4:

Lys – DabG – hAlaA – **Ala**– Asp -DabA – Leu - hAlaG – Ala – Lys – βAla – Lys(Biotin)-$CONH_2$

HRMS (SI-QToF) *m/z:* $[M+4H]^{4+}$ calcd. 522.761 found 522.762

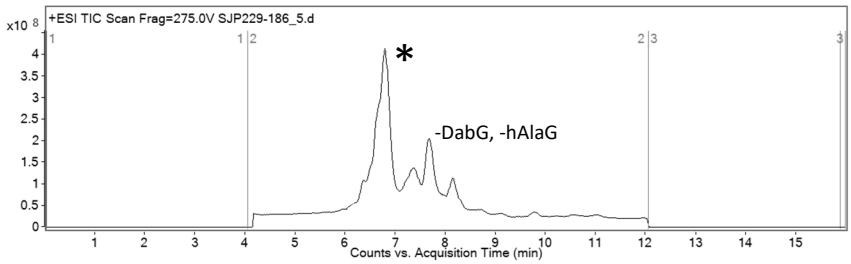


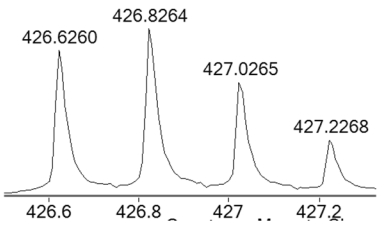


AlaScan-5:

Lys – DabG – hAlaA – Arg – **Ala** -DabA – Leu - hAlaG – Ala – Lys – βAla – Lys(Biotin)-$CONH_2$

HRMS (SI-QToF) *m/z:* $[M+5H]^{5+}$ calcd. 426.625 found 426.626

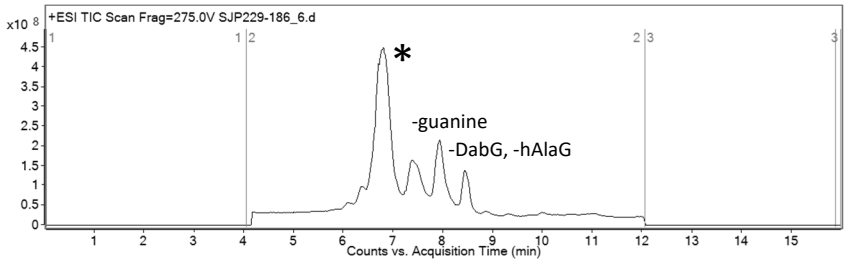


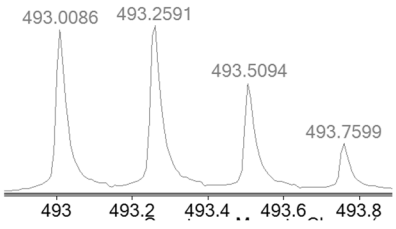


AlaScan-6:

Lys – DabG – hAlaA – Arg – Asp -**Ala** – Leu - hAlaG – Ala – Lys – βAla – Lys(Biotin)-$CONH_2$

HRMS (SI-QToF) *m/z:* $[M+4H]^{4+}$ calcd. 493.008 found 493.009

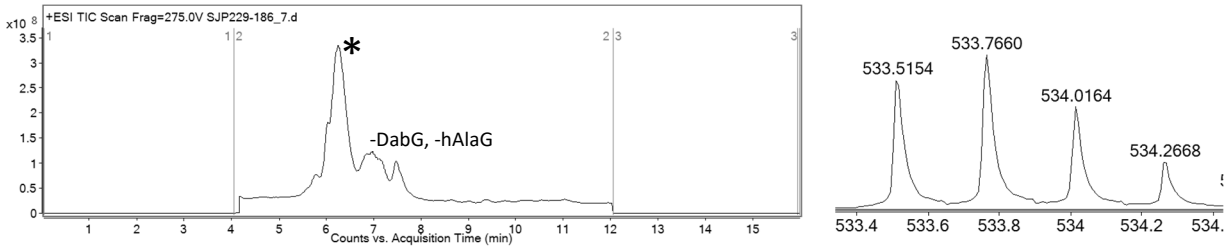




AlaScan-7:

Lys – DabG – hAlaA – Arg – Asp -DabA – **Ala** - hAlaG – Ala – Lys – βAla – Lys(Biotin)-$CONH_2$

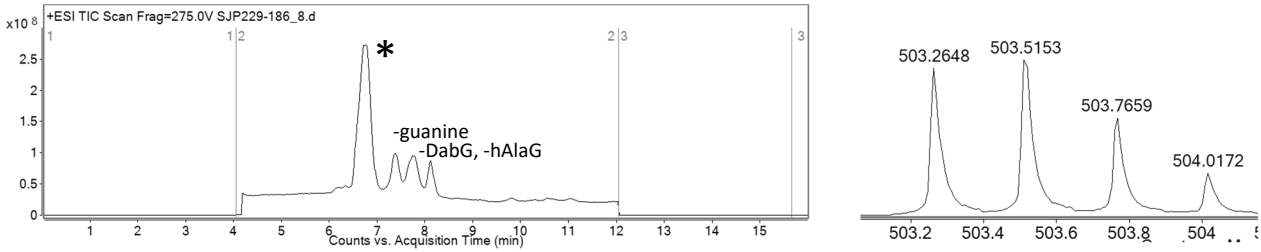
HRMS (SI-QToF) *m/z:* $[M+4H]^{4+}$ found 533.766



AlaScan-8:

Lys – DabG – hAlaA – Arg – Asp -DabA – Leu - **Ala** – Ala – Lys – βAla – Lys(Biotin)-$CONH_2$

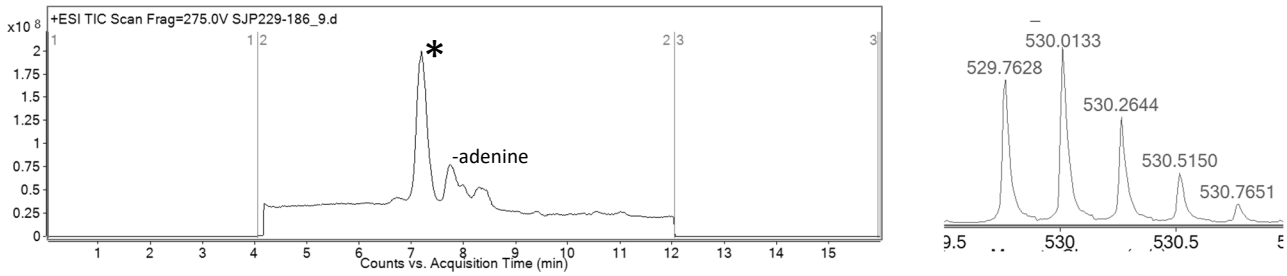
HRMS (SI-QToF) *m/z:* $[M+4H]^{4+}$ calcd. 503.264 found 503.265



AlaScan-9:

Lys – DabG – hAlaA – Arg – Asp -DabA – Leu - hAlaG – Ala – **Ala** – βAla – Lys(Biotin)-$CONH_2$

HRMS (SI-QToF) *m/z:* $[M+4H]^{4+}$ calcd. 526.762 found 526.763



Mutation of all 4 nucleobases

Original sequence: 39

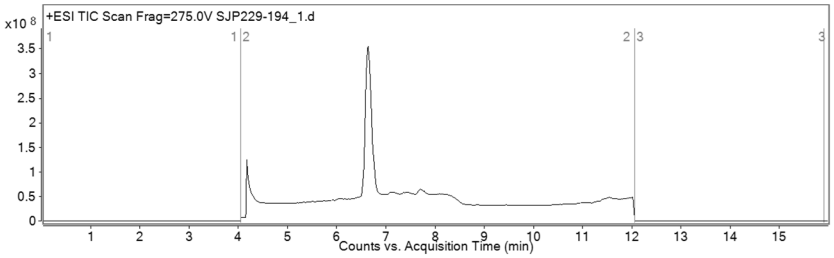
Lys – DabG – hAlaA – Arg – Asp -DabA – Leu -DabG – Ala – Lys – bAla – Lys(Biotin)-$CONH_2$

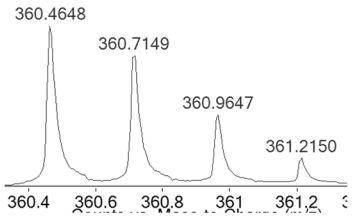
Peptides were synthesized according to the general SPPS procedure, cleaved and used without further purification

Tetra-Ala-mutant

Lys – **Ala** – **Ala** – Arg – Asp - **Ala** – Leu - **Ala** – Ala – Lys – bAla – Lys(Biotin)-$CONH_2$

HRMS (SI-QToF) *m/z:* $[M+4H]^{4+}$ calcd. 360.464 found 360.265

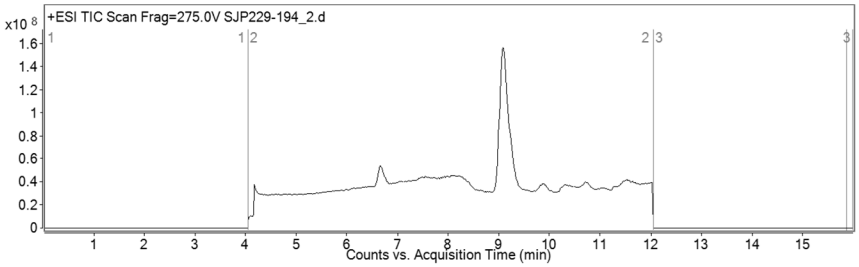


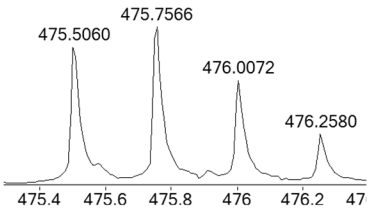


Tetra-Trp-mutant

Lys – **Trp** – **Trp** – Arg – Asp - **Trp** – Leu - **Trp** – Ala – Lys – bAla – Lys(Biotin)-$CONH_2$

HRMS (SI-QToF) *m/z:* $[M+4H]^{4+}$ calcd. 475.509 found 475.506

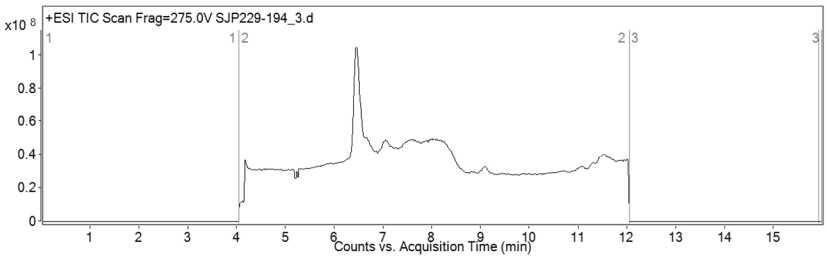


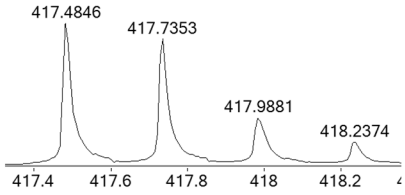


Tetra-Gln-mutant

Lys – **Gln** – **Gln** – Arg – Asp - **Gln** – Leu - **Gln** – Ala – Lys – bAla – Lys(Biotin)-$CONH_2$

HRMS (SI-QToF) *m/z:* $[M+4H]^{4+}$ calcd. 417.485 found 417.485





Synthesis and de novo sequencing of three nucleobase peptides test libraries

Procedure for split-and-pool synthesis of three nucleobase peptide test libraries (Alanyl library, homoalanyl library and Dab library): Coupling and Fmoc deprotection steps were performed according to the stoichiometries and procedures described above. Monosized Tentagel beads (90 µm diameter and loading 0.26 mmol/g, 100 mg for each library), were loaded into a peptide synthesis vessel, swollen in DMF and then coupled to Fmoc-Rink Amide linker. For variable positions the resin was suspended in DMF divided in equal aliquots in fritted syringes, coupled to the respective Fmoc amino acid and then pooled back into the peptide synthesis vessel before Fmoc deprotection. After completion of the synthesis the libraries were cleaved according to the general cleavage procedure described above and purified by solid phase extraction.

Sequencing of nucleobase peptide test libraries: Stock solutions of each of the three libraries were prepared (1 mM in 6 M guanidine·HCl, pH = 6.8). Prior to injection to the Orbitrap lumos for nanoLC-MS/MS analysis, the solutions were diluted to 12.8 µM solutions in guanidine·HCl (1 M, pH = 6.8). 1 µL, containing 12.8 pmol library, i.e. 50 fmol per individual member, was injected.

***De novo* sequencing with PEAKS and further filtering:** *De novo* peptide sequencing was performed in PEAKS 8.5 from Bioinformatics Solutions Inc. (ON, Canada). *De novo* sequencing was performed allowing 15 ppm assignment errors and 0.05 Da individual fragment mass errors. The nucleobase monomers were selected as variable PTMs (indicated as alanine + ΔMS). 15 candidate sequences were obtained for each preprocessed scan. The complete list of peptide candidates was exported as .csv file and then filtered using a Python script.[9] Briefly: sequences not matching library design rules (sequence length, correct monomers in every position) were eliminated from further consideration. Next, for scans with multiple remaining sequence candidates, a single peptide with highest ALC (average level of confidence) score per scan was retained, while the rest were excluded. After this, remaining sequences were labeled as “unique” and “non-unique” based on retention time, mass, and sequence similarity criteria. The resulting final list of unique sequences was used for analysis of the sequencing performance of nucleobase peptide libraries containing 0 – 4 nucleobase monomers.

Test libraries for sequencing validation

Library 1 design:

1	2	3	4	5	6	7	8	9
Ala	AlaC	Phe	AlaT	AlaG	Trp	AlaA	Tyr	Lys
Ser	His	Leu	Arg	Gln	Pro	Glu	Asn	

Full lists of unique sequences for the test library with alanyl nucleobase monomers

U = C-terminal amide, B = AlaA, J = AlaC, X = AlaG, Z = AlaT

Peptide	*ALC (%)*	*m/z*	*z*	*RT*	*Mass*	*ppm*
AHFRQPEYKU	99	392.2073	3	20.23	1173.604	-3.6
SHFRQWENKU	99	410.8744	3	20.24	1229.606	-3.4
AHFRQWENKU	99	405.5424	3	20.53	1213.61	-4.2
SJLRQWENKU	99	413.8813	3	21.03	1238.627	-3.6
AJLRQWENKU	99	408.5499	3	21.6	1222.632	-3.3
SJFRQWBNKU	99	450.2203	3	21.84	1347.645	-4.1
AHLZQPBYKU	99	418.8782	3	22.96	1253.617	-2.9
SJFRQWENKU	99	425.2093	3	23.39	1272.611	-3.9
AJFRQWENKU	99	419.8784	3	24.29	1256.616	-2.2
SHLRQWEYKU	99	415.8866	3	24.55	1244.641	-2.7
SHLZQWBNKU	99	437.5447	3	24.64	1309.618	-4.2
AHLZQWBNKU	99	432.2132	3	25.16	1293.623	-4
AHLRQWEYKU	99	410.5546	3	25.38	1228.647	-3.8
AHFZQPBYKU	99	430.2061	3	25.75	1287.601	-3.3
SHLZQWENKU	99	412.5336	3	26.64	1234.584	-4.2
SHFZQWBNKU	99	448.8734	3	26.87	1343.602	-2.7
AHLZQWENKU	99	407.2019	3	27.18	1218.589	-4.6
AJLRQWBYKU	99	449.9003	3	27.52	1346.686	-4.8
AHFZQWBNKU	99	443.5416	3	27.77	1327.607	-3.1
AHFZQPEYKU	99	405.195	3	27.94	1212.568	-3.6
SHFRQWEYKU	99	427.2143	3	28.51	1278.626	-3.7
SJLZQWBNKU	99	451.8797	3	28.74	1352.624	-4.7
SJLRQWEYKU	99	430.2217	3	29.22	1287.647	-3
SHFZQWENKU	99	423.8618	3	29.55	1268.569	-3.9
AHFRQWEYKU	99	421.8823	3	29.95	1262.631	-4.5
SJFRQWBYKU	99	466.5596	3	30.31	1396.665	-5.5
AJLRQWEYKU	99	424.8893	3	30.62	1271.652	-4.8
SJFZQWBNKU	99	463.208	3	31.38	1386.608	-4.1
SJLZQWENKU	99	639.7998	2	31.53	1277.59	-3.9
AJLRXWEYKU	99	455.5602	3	31.6	1363.665	-4.3
AJFRQWBYKU	99	461.228	3	31.81	1380.67	-5.7

AJFZQWBNKU	99	457.8764	3	32.49	1370.613	-3.9
SJFRQWEYKU	99	441.5495	3	33.54	1321.632	-3.8
SHLZQWBYKU	99	453.8848	3	34.86	1358.638	-3.9
SJFZQWENKU	99	656.7924	2	34.98	1311.575	-3.3
AJFRQWEYKU	99	436.2178	3	35.32	1305.637	-3.9
AHLZQWBYKU	99	448.5523	3	35.58	1342.643	-5.9
SHFZQWBYKU	99	465.2137	3	37.81	1392.622	-2.2
SHLZQWEYKU	99	428.8737	3	38.51	1283.605	-4.2
AHFZQWBYKU	99	459.8812	3	38.9	1376.627	-4.2
AHLZQWEYKU	99	423.5423	3	39.32	1267.61	-3.7
SJLZQWBYKU	99	468.2197	3	39.44	1401.644	-4.7
AJLZQWBYKU	99	462.8878	3	40.55	1385.649	-5.3
SHFZQWEYKU	99	440.2021	3	41.53	1317.589	-3.4
SJFZQWBYKU	99	479.5491	3	42.37	1435.628	-1.8
AHFZQWEYKU	99	434.8698	3	42.57	1301.594	-5.2
SJLZQWEYKU	99	664.3096	2	43.13	1326.611	-4.5
AJFZQWBYKU	99	474.2161	3	43.73	1419.633	-4.8
AHFZXWEYKU	99	465.5404	3	44.47	1393.606	-5
SJFZQWEYKU	99	681.303	2	46.21	1360.595	-2.5
SJFZXWEYKU	99	485.2071	3	48.21	1452.607	-5.3
AJFZXWEYKU	99	479.8765	3	49.81	1436.612	-3.2
AJLRQWBNKU	98	433.5605	3	20.41	1297.665	-4.2
SJFRQPEYKU	98	411.8741	3	21.48	1232.605	-3.5
SHFRXWENKU	98	441.545	3	21.5	1321.618	-3.3
SHLRQWBYKU	98	330.9247	4	23.36	1319.675	-3.8
SJFRXWENKU	98	455.8802	3	23.93	1364.623	-3.3
AHLRQWBYKU	98	326.9265	4	24.05	1303.68	-2.5
SHFRQWBYKU	98	339.421	4	26.36	1353.659	-3.2
AHLRXWEYKU	98	441.2252	3	27.42	1320.659	-3.7
AHLZXWENKU	98	437.8726	3	29.07	1310.602	-4.2
AHFZXWBNKU	98	474.2122	3	31.42	1419.619	-3.3
SJFZQPBNKU	97	433.5331	3	19.93	1297.581	-3.1
SJLRQWBNKU	97	438.8925	3	20	1313.66	-3.5
AHLRQWENKU	97	394.2144	3	20.25	1179.626	-4
SHLRQWENKU	97	399.5461	3	20.28	1195.621	-3.8
AHFRXWENKU	97	436.2132	3	21.84	1305.623	-3.9
AJFZQWENKU	97	432.8656	3	36.22	1295.58	-3.6
AJFRQPEYKU	96	406.5425	3	22.41	1216.61	-3.6
AJFRQWBNKU	96	333.9187	4	22.53	1331.65	-3
AHFZQWENKU	96	627.2914	2	30.32	1252.574	-4.4
SHFZXWBNKU	96	479.5428	3	30.83	1435.614	-5.3
SHLZQPBYKU	95	424.2096	3	22.31	1269.612	-3.7
SJLRXWBYKU	95	485.9024	3	30.22	1454.693	-5.1
AJFZXWBYKU	95	504.8872	3	47.35	1511.646	-3.8
SHFRQPEYKU	94	397.5391	3	19.44	1189.599	-3

AHFRQWBNKU	94	323.167	4	20.29	1288.644	-3.7
SJFRXWBYKU	94	497.2317	3	34.13	1488.677	-2.7
AJLZXWENKU	94	452.2083	3	34.24	1353.607	-3.3
SJLRQPEYKU	93	400.5462	3	19.27	1198.621	-3.2
AHFRQWBYKU	93	335.4222	4	27.91	1337.664	-3.1
AJFZQPEYKU	93	419.5298	3	31.28	1255.574	-4.7
AJLRQPBYKU	92	420.2255	3	19.68	1257.659	-3.5
SHFRQWBNKU	92	435.8854	3	20.15	1304.639	-3.2
SHFRXWEYKU	92	457.8847	3	30.65	1370.638	-4.2
SJLZQPBNKU	91	422.205	3	18.5	1263.597	-3
AHFRQPBYKU	91	417.2186	3	19.91	1248.638	-3.1
AJLRXWBYKU	91	480.5711	3	31.21	1438.698	-4.4
AJLZQWENKU	91	421.5368	3	32.63	1261.595	-5.2
AJLZXWBNKU	91	477.219	3	33.53	1428.641	-4
AJFZXWBNKU	91	488.5471	3	37.26	1462.625	-3.7
AHFZXWBYKU	91	490.5526	3	42.25	1468.64	-2.4
SJLRQWBYKU	90	455.2324	3	26.23	1362.681	-3.9
SHFRXWBYKU	89	362.4234	4	30.09	1445.671	-4.7
SJLZXWEYKU	89	473.8788	3	44.8	1418.623	-5.8
AJLZXWEYKU	89	468.5476	3	46.29	1402.628	-4.9
AHLZQPEYKU	88	393.8673	3	24.38	1178.583	-2.7
AJFRXWENKU	88	450.5482	3	24.77	1348.628	-4.1
SHFZXWENKU	88	454.5331	3	32.15	1360.581	-2.6
SHFZQPENKU	87	394.1866	3	18.3	1179.542	-3.7
SJFZQPENKU	87	612.2793	2	20.25	1222.548	-3.1
SHFRXWBNKU	87	350.1688	4	21.74	1396.651	-3.4
SJFZQPBYKU	87	449.8728	3	28.18	1346.602	-3.8
AHFZXWENKU	87	449.2008	3	32.61	1344.586	-4
AHLZXWEYKU	87	454.212	3	40.39	1359.622	-5.7
AJLZQPBYKU	86	433.2135	3	25.88	1296.622	-2.9
SJFRQPBYKU	85	436.885	3	20.75	1307.638	-4
AHFRXWEYKU	85	452.5527	3	32.04	1354.643	-5.1
AJFRXWBNKU	84	475.5592	3	24.76	1423.662	-4.2
SHLZXWBNKU	83	468.2159	3	28.33	1401.63	-3
SHLRXWEYKU	82	335.1698	4	26.89	1336.654	-2.7
SJLRXWEYKU	82	460.8914	3	30.43	1379.659	-5.1
AJLZQPBNKU	81	416.8732	3	18.83	1247.602	-3.4
SJFZXWENKU	81	468.8677	3	37.11	1403.587	-3.8
AHLRXWBYKU	80	349.9289	4	27.35	1395.692	-4.1
AHLZXWBYKU	80	479.2242	3	39.99	1434.655	-3.1
AHFZQPBNKU	79	413.8662	3	18.74	1238.581	-3
AHFZQPENKU	78	582.7794	2	18.6	1163.547	-2.4
SHFZQPEYKU	78	615.2871	2	26.94	1228.563	-2.3
SJLRQPBYKU	77	425.5573	3	19.31	1273.654	-3
SHFRQPBYKU	77	317.1642	4	19.49	1264.633	-3.7

SJLZXWBNKU	77	482.5512	3	32.75	1444.636	-2.7
AJFRXWBYKU	77	491.8991	3	35.27	1472.682	-4.4
AHFRXWBNKU	76	346.1701	4	22.11	1380.656	-3.5
AHFRXWBYKU	76	358.4248	4	30.92	1429.677	-4.6
AJLZQWEYKU	73	437.8772	3	44.23	1310.616	-4.6
AHLRXPEYKU	72	411.55	3	19.23	1231.632	-3.1
SHFZXWEYKU	72	470.8728	3	43.37	1409.601	-3.4
AHLZXWBNKU	71	462.8836	3	28.82	1385.635	-4.4
SJFZXWBYKU	71	510.219	3	45.95	1527.64	-3.5
SHLZQPEYKU	70	399.1988	3	23.75	1194.578	-3
SHLZXWEYKU	70	459.5446	3	40.68	1375.617	-3.7
SHLZXWBYKU	69	484.555	3	39.05	1450.65	-4.9
AJFZQWEYKU	69	449.205	3	47.58	1344.6	-5.1
AJFZQPBNKU	66	428.2007	3	20.5	1281.586	-4.8
AJFRQPBYKU	64	431.5538	3	21.17	1291.643	-3
AJLZQPENKU	63	587.2904	2	18.66	1172.569	-2
AJFZXWENKU	63	463.5359	3	38.39	1387.592	-4.4
SJFRXWEYKU	61	472.2193	3	35.13	1413.644	-5.5
SHFRQPENKU	59	571.2955	2	56.72	1140.579	-2.2
AJLRXWENKU	58	439.2203	3	21.98	1314.644	-3.8
SJLZQPENKU	53	595.2874	2	18.26	1188.564	-2.8

Library 2 design:

1	2	3	4	5	6	7	8	9
Ala	hAlaC	Phe	hAlaT	hAlaG	Trp	hAlaA	Tyr	Lys
Ser	His	Leu	Arg	Gln	Pro	Glu	Asn	

Full lists of unique sequences for the test library with homoalanyl nucleobase monomers

U = C-terminal amide, B = hAlaA, J = hAlaC, X = hAlaG, Z = hAlaT

Peptide	*ALC (%)*	*m/z*	*z*	*RT*	*Mass*	*ppm*
AHFZQPBNKU	99	423.2116	3	18.02	1266.605	6.7
SHFRQPEYKU	99	397.5396	3	18.21	1189.599	-1.9
SHFZQPENKU	99	398.8591	3	18.27	1193.555	0.5
SHFRQWENKU	99	410.8746	3	18.8	1229.606	-2.8
AHFRQPEYKU	99	392.2077	3	19.08	1173.604	-2.5
AHFRQWENKU	99	405.5429	3	19.13	1213.61	-2.9
AHLZXPENKU	99	417.5414	3	19.6	1249.604	-1.3
SJLRQWENKU	99	418.5536	3	20.31	1252.639	0
AHFRXWENKU	99	440.8849	3	21	1319.639	-4.5
AHLZQPBYKU	99	428.2235	3	22.78	1281.64	6.4
SHLZQPEYKU	99	403.8709	3	23.71	1208.591	0
SHFZQPBYKU	99	444.8817	3	23.9	1331.62	2.6
SHLRQWEYKU	99	415.886	3	24.11	1244.641	-4.1
AHFZQPBYKU	99	439.55	3	24.71	1315.625	2.6
AHLRQWEYKU	99	410.5535	3	25.12	1228.647	-6.4
AHLRXWEYKU	99	445.8977	3	26.57	1334.675	-2.9
SHLZXPEYKU	99	439.2134	3	27.02	1314.619	-0.7
AHFRQWBYKU	99	451.5661	3	27.13	1351.675	0.8
AHLZQWBNKU	99	441.556	3	27.53	1321.647	-0.4
SJLRQWEYKU	99	434.8938	3	27.62	1301.66	0
AHLZQWENKU	99	411.8748	3	27.72	1232.602	0.3
SHLZQWBNKU	99	446.8889	3	28.01	1337.642	2.3
AHLZXWBNKU	99	476.8998	3	28.05	1427.675	1.7
AHLZXPEYKU	99	433.8809	3	28.12	1298.625	-2.8
SHFRQWEYKU	99	427.2149	3	28.25	1278.626	-2.2
AHFZQPEYKU	99	409.8671	3	28.49	1226.58	-0.6
SHLZXWENKU	99	452.5478	3	29.44	1354.626	-2.9
AHLZXWENKU	99	447.2163	3	29.97	1338.631	-2.6
AHFRQWEYKU	99	421.8824	3	30.09	1262.631	-4.2
AHFZQWBNKU	99	452.886	3	31.04	1355.631	4
SHFZQWBNKU	99	458.2152	3	31.25	1371.626	-1.5
SHFZQWENKU	99	428.5341	3	31.39	1282.581	-0.7
AHFZQWENKU	99	423.2029	3	32.14	1266.586	0.5
SJFRQWEYKU	99	446.2207	3	32.47	1335.644	-2.9
AHFZXPEYKU	99	445.2097	3	32.79	1332.609	-1.2
SHFZXWENKU	99	463.8763	3	32.95	1388.61	-2

AHFZXWENKU	99	458.5442	3	33.78	1372.615	-3
SHLZQWBYKU	99	463.2287	3	36.6	1386.662	1.7
AHLZQWBYKU	99	457.8978	3	37.04	1370.667	3.4
AHLZXWBYKU	99	493.2404	3	38.47	1476.696	2.6
SHFZQWBYKU	99	474.5564	3	39.7	1420.646	0.9
AHFZQWBYKU	99	469.2244	3	40.58	1404.651	0
AHLZQWEYKU	99	428.2141	3	40.71	1281.623	-1.6
AHLZXWEYKU	99	463.5563	3	41.15	1387.651	-2.9
AHFZXWBYKU	99	378.6775	4	41.81	1510.68	0.6
SHFZQWEYKU	99	666.8074	2	43.82	1331.602	-1.1
SHFZXWEYKU	99	480.216	3	44.06	1437.63	-3
AHFZQWEYKU	99	439.5416	3	45.12	1315.607	-3
AHFZXWEYKU	99	474.8837	3	45.19	1421.636	-4.4
SJFZXWEYKU	99	499.2241	3	47.24	1494.648	1.3
SHFZQPBNKU	98	428.5418	3	17.65	1282.599	3.4
SJLRQPEYKU	98	405.2179	3	18.14	1212.633	-0.9
AHLRXWENKU	98	429.5605	3	18.71	1285.655	4
AHFZQPENKU	98	393.5273	3	18.77	1177.56	0.3
SJFRQPBYKU	98	446.2294	3	18.79	1335.662	3.3
SHLZXPENKU	98	422.873	3	18.95	1265.599	-1.4
AHFRQWBNKU	98	326.6713	4	20.15	1302.655	0.9
AHFZXPBNKU	98	458.5526	3	21.25	1372.633	2.1
SHLZQPBYKU	98	433.5542	3	22.25	1297.636	4.1
SJFRQWENKU	98	429.8812	3	22.58	1286.624	-1.4
SHLRQWBYKU	98	334.4287	4	23.49	1333.686	-0.3
AHLZQPEYKU	98	398.5392	3	24.58	1192.596	0
SHFZQPEYKU	98	415.1993	3	27.36	1242.575	0.8
SHFRXWEYKU	98	347.169	4	29.89	1384.654	-5.4
SJLZXPEYKU	98	458.219	3	30.29	1371.638	-1.8
SJFZQPEYKU	98	434.2049	3	31.06	1299.594	-0.4
SJLZXWENKU	98	471.5559	3	35.47	1411.644	1.4
SHLZXWBYKU	98	498.5714	3	38.05	1492.69	1.3
SJFZQWBNKU	98	477.224	3	38.21	1428.644	4.3
SJFZXWENKU	98	482.8838	3	38.43	1445.628	0.9
SJLZQWBYKU	98	482.2351	3	42.41	1443.68	2.2
SJFZQWBYKU	98	493.5644	3	44.44	1477.665	4.7
SHLRXWENKU	97	326.4186	4	18.45	1301.65	-3.3
AJFRQPBYKU	97	440.8978	3	18.83	1319.667	3.4
SJFZQPBNKU	97	447.5486	3	19.74	1339.617	5
SHFRQWBNKU	97	330.6698	4	19.98	1318.65	0.1
SJFZQPENKU	97	417.8656	3	20.98	1250.573	1.7
AJFZQPENKU	97	412.5341	3	21.12	1234.578	1.9
SHFZXPENKU	97	434.2004	3	21.89	1299.583	-3
SJFRQWBNKU	97	459.5647	3	23.4	1375.668	2.9
AHLRQWBYKU	97	330.4298	4	24.03	1317.691	-0.7

SJLZQPBYKU	97	452.56	3	24.75	1354.654	3.5
AHLRXWBYKU	97	356.9363	4	25.59	1423.72	-2.4
SHLRXWEYKU	97	338.6731	4	26.12	1350.67	-4.9
SJLZQPEYKU	97	422.8782	3	26.84	1265.609	2.9
SJFZQPBYKU	97	463.889	3	27.2	1388.638	5.2
SJFRQWBYKU	97	357.1793	4	30.5	1424.689	-0.3
AHFZXWBNKU	97	488.2277	3	31.78	1461.659	1.2
AJFRXWEYKU	97	476.2319	3	33.28	1425.678	-2.5
SJFZXPEYKU	97	469.5474	3	34.61	1405.622	-1
AJFZXWEYKU	97	493.8935	3	47.71	1478.654	3.4
SHLRQWBNKU	96	322.174	4	18.42	1284.666	0.9
AJLRXWENKU	96	448.5642	3	20.56	1342.673	-1.5
SJLZXPENKU	96	441.8802	3	21.46	1322.617	1.3
SJLRXWENKU	96	453.8947	3	21.66	1358.668	-4
SJLRQWBNKU	96	336.4283	4	21.69	1341.684	0.2
AHFRXPEYKU	96	427.5495	3	21.92	1279.633	-4.9
SHFRQWBYKU	96	342.9247	4	26.34	1367.67	-0.6
AJLZXWEYKU	96	482.5634	3	43.5	1444.669	-0.5
SJFZQWEYKU	96	463.8809	3	47.05	1388.62	0.6
SJLRQPBYKU	95	434.9009	3	17.82	1301.678	2.6
AJLZQPENKU	95	401.2056	3	18.3	1200.594	1.1
AHLRXPEYKU	95	416.2214	3	19.03	1245.648	-4.8
AHLZXPBNKU	95	447.2239	3	19.38	1338.649	0.8
AJFRQPEYKU	95	411.2141	3	20.85	1230.623	-1.7
AJLZQPEYKU	95	417.5464	3	27.03	1249.614	2.4
AHFRXWBYKU	95	365.4332	4	29.05	1457.704	-0.2
AJFZQPEYKU	95	428.8728	3	31.66	1283.598	-1.3
SJLZQWENKU	95	436.2126	3	34.22	1305.615	0.7
SJLZQWBNKU	95	465.896	3	36.91	1394.66	4.6
AHLRXWBNKU	94	344.6818	4	19.06	1374.699	-0.9
SJFRQPEYKU	94	416.5466	3	20.9	1246.617	0.5
AJFZXPENKU	94	447.8758	3	25.71	1340.607	-0.8
SJLZQPBNKU	93	436.2207	3	18.44	1305.633	5.4
AJLRQWENKU	93	413.222	3	18.94	1236.644	-0.1
SJFRXWENKU	93	465.2241	3	23.85	1392.652	-1.2
SHLRXWBYKU	93	360.9349	4	25.16	1439.715	-2.9
SJFZXPENKU	93	453.2068	3	25.4	1356.602	-2.1
AJLZXPEYKU	93	452.8888	3	30.75	1355.643	1.5
SJLZQWEYKU	93	452.5518	3	43.72	1354.636	-1.7
SHLRXPEYKU	92	316.4172	4	18.45	1261.643	-2.7
SHFZXPBNKU	92	348.1648	4	20.59	1388.628	1.5
AHFRXWBNKU	92	353.1781	4	21.49	1408.684	-0.3
AHLZXPBYKU	92	347.925	4	26.44	1387.669	1.5
SJFZXWBYKU	92	396.9316	4	44.83	1583.693	2.7
AJFZQPBNKU	91	442.217	3	19.84	1323.623	5

SJLRXWEYKU	91	470.2364	3	28.87	1407.688	-0.7
SHFZXWBNKU	91	493.5585	3	31.1	1477.655	-0.6
AJFZQWENKU	91	442.2094	3	36.82	1323.605	1.3
SHFZXWBYKU	91	382.6757	4	41.07	1526.675	-0.8
SHLRXWBNKU	90	348.6808	4	18.83	1390.694	-0.1
SHLZXPBNKU	90	339.6689	4	18.91	1354.644	2
SHFRXWENKU	90	334.9145	4	20.6	1335.634	-3.8
SJLZXPBNKU	90	471.5635	3	20.88	1411.662	4.9
AJFZQPBYKU	90	458.5573	3	27.44	1372.643	5.1
SJFZXPBYKU	90	374.6754	4	31.9	1494.667	4.1
AJLZXWENKU	90	466.2236	3	33.98	1395.649	0
AJLZQPBNKU	89	430.8893	3	18.4	1289.638	6.1
AJFRXWBNKU	89	489.5753	3	23.38	1465.702	1.7
SJFRXPEYKU	89	451.889	3	23.76	1352.646	-0.7
AJFRQWBYKU	89	353.1815	4	30.61	1408.694	2.4
SHLZXWEYKU	89	702.8286	2	40.95	1403.646	-2.5
SJLRXWBNKU	88	362.9362	4	21.82	1447.712	2.4
AJLZQWBNKU	88	460.5645	3	32.03	1378.665	5
AJFZXPEYKU	88	464.2175	3	35.31	1389.627	2.6
SJLZXWBNKU	88	501.239	3	35.4	1500.688	4.7
AJLZQWBYKU	88	476.9041	3	40.14	1427.685	3.7
SJLZXWBYKU	88	388.4347	4	42.6	1549.709	0.6
AJFZQWBYKU	88	488.2313	3	44.03	1461.67	1.7
SJLZXWEYKU	88	731.3401	2	44.24	1460.664	1.2
AJLRQWBNKU	87	332.4305	4	20.19	1325.689	3
SJFZXPBNKU	87	482.8906	3	23.21	1445.646	2.7
AJFZXPBNKU	87	477.5592	3	23.53	1429.651	3.3
AJLZQPBYKU	87	447.2281	3	24.98	1338.659	2.7
AJLRQWEYKU	87	429.5619	3	27.41	1285.665	-0.7
AJFZXWBNKU	87	507.2353	3	36.08	1518.678	4.2
AJFZXWBYKU	87	523.5753	3	44.77	1567.698	3.9
AJFRXPBYKU	86	476.2392	3	22.43	1425.696	0.1
AJFRQWBNKU	86	340.9267	4	22.83	1359.673	3.5
AJFRXPEYKU	86	446.5569	3	24.41	1336.651	-1.8
AHFRXWEYKU	86	343.1701	4	31.18	1368.659	-5.9
AJFRQWEYKU	86	440.8906	3	32.74	1319.649	0.6
AJLZQWEYKU	86	670.3287	2	43.33	1338.641	1.7
AJLZQWENKU	85	645.8191	2	31.9	1289.62	2.5
AJFZXWENKU	85	715.824	2	38.61	1429.633	0.2
SHLZQWENKU	84	625.3054	2	27.72	1248.597	-0.6
SHLRQPEYKU	83	386.2111	3	17.2	1155.615	-2.9
SHFRXPBYKU	83	347.1753	4	19.64	1384.672	-0.3
SHFRXPEYKU	83	324.9131	4	21.24	1295.628	-3.5
AJFZQWBNKU	83	707.3346	2	35.87	1412.649	3.9
SJLRQWBYKU	82	348.6842	4	27	1390.704	2.5

AJLZXPENKU	81	436.5486	3	21.74	1306.622	1.4
AJLRQPEYKU	80	399.886	3	18.25	1196.638	-1.7
AJLRXWBNKU	80	358.9366	4	20.71	1431.717	0
AJFRQWENKU	80	424.5495	3	22.07	1270.629	-1.5
AJLRQWBYKU	79	344.6858	4	26.63	1374.709	3.4
AJLRXPEYKU	78	435.2291	3	21.23	1302.667	-1
SJFZQWENKU	77	447.5406	3	37.2	1339.6	0.2
AJLZXWBYKU	77	512.246	3	41.17	1533.714	1.6
SJLRXPBYKU	76	470.2426	3	20.07	1407.706	-0.2
SHLZXWBNKU	76	361.925	4	27.83	1443.67	0.6
AJFZXPBYKU	76	493.8997	3	32.82	1478.672	3.9
AJLZXPBNKU	75	466.2315	3	21.24	1395.667	4.3
AJLZXPBYKU	75	362.1805	4	29.12	1444.687	3.9
SHFZXPBYKU	74	360.4199	4	28.52	1437.648	1.5
AJFZQWEYKU	74	458.5493	3	47.53	1372.625	0.8
AJLRXWEYKU	72	464.9033	3	28.15	1391.693	-3.8
AHFZXPBYKU	72	474.8919	3	29.71	1421.653	0.3
SHFZXPEYKU	72	450.5412	3	31.36	1348.604	-1.5
AJLZXWBNKU	71	495.9073	3	32.07	1484.693	4.4
SHLRXPBYKU	70	338.679	4	18.15	1350.688	-0.7
AJLRXWBYKU	70	494.5876	3	27.07	1480.738	2.1
AHLRQPBYKU	69	410.5625	3	17.25	1228.665	0.8
AHLRXPBYKU	69	334.6808	4	18.62	1334.693	0.6
SHLZXPBYKU	68	351.9233	4	25.77	1403.664	0.1
SJFRXPBYKU	67	361.4298	4	22.37	1441.69	-0.3
SHLZQWEYKU	64	433.5445	3	39.46	1297.617	-4.5
AJLRXPBYKU	61	348.9359	4	20.2	1391.711	2.5
AHFRXPBYKU	60	343.1765	4	20.42	1368.677	-0.4
SJFZXWBNKU	60	512.5652	3	37.3	1534.673	0.9
AHLRQPEYKU	57	380.8793	3	17.42	1139.62	-3.4
AHFRQPBYKU	57	421.8904	3	17.63	1262.649	0.5
SHLRQPBYKU	55	415.8936	3	26.05	1244.659	-0.3

Library 3 design:

1	2	3	4	5	6	7	8	9
Ala	DabC	Phe	DabT	DabG	Trp	DabA	Tyr	Lys
Ser	His	Leu	Arg	Gln	Pro	Glu	Asn	

Full lists of unique sequences for the test library with diaminobutanoic acid based nucleobase monomers

U = C-terminal amide, B = DabA, J = DabC, X = DabG, Z = DabT

Peptide	*ALC (%)*	*m/z*	*z*	*RT*	*Mass*	*ppm*
SHFZQPENKU	99	417.8659	3	15.62	1250.575	1
SHLZZPENKU	99	460.8875	3	15.84	1379.639	1.4
SHFRQPEYKU	99	397.5388	3	15.94	1189.599	-3.8
AHLRZPEYKU	99	435.2289	3	16.02	1302.669	-2.7
AHLZZPENKU	99	455.5548	3	16.63	1363.644	-1.1
AHFRQPEYKU	99	392.2072	3	16.66	1173.604	-3.8
SHFRQWENKU	99	410.8743	3	16.82	1229.606	-3.6
SHLRZWENKU	99	453.8949	3	16.92	1358.67	-5.1
AHFRQWENKU	99	405.5417	3	17.09	1213.61	-5.8
AHFRQWZNKU	99	454.2322	3	17.88	1359.675	-0.1
SHFZZPENKU	99	472.2149	3	18.01	1413.623	-0.4
AHFZZPENKU	99	466.8833	3	18.96	1397.628	-0.2
SHFRZWZNKU	99	513.9144	3	19.65	1538.719	1.8
SHFRZWENKU	99	465.2245	3	19.77	1392.654	-1.6
AHFRZWENKU	99	459.8923	3	20.19	1376.659	-2.9
AHFRZWZNKU	99	508.5823	3	20.2	1522.724	1
SHLRQWEYKU	99	415.8863	3	23.28	1244.641	-3.4
AHLRQWEYKU	99	410.5552	3	24.23	1228.647	-2.2
SHLZZPEYKU	99	477.228	3	24.42	1428.659	1.9
AHLZZPEYKU	99	471.8955	3	25.82	1412.665	0.2
AHLZQWENKU	99	430.882	3	26.7	1289.622	1.6
SHLRZWEYKU	99	470.2365	3	26.74	1407.69	-1.7
AHLRZWEYKU	99	464.9048	3	27.29	1391.695	-1.8
SHFRQWEYKU	99	427.2147	3	27.73	1278.626	-2.8
SHFZZPEYKU	99	488.5553	3	27.97	1462.644	0.2
AHFRQWZYKU	99	470.5727	3	28.01	1408.695	0.6
SHLZZWENKU	99	735.3419	2	28.37	1468.666	2.5
AZLRQWEYKU	99	448.5694	3	28.66	1342.685	1.1
AHLZZWENKU	99	485.2312	3	28.8	1452.671	0.7
AHFZZPEYKU	99	483.2245	3	29.2	1446.649	1.8
AHFRQWEYKU	99	421.8832	3	29.45	1262.631	-2.4
SHFZQWENKU	99	447.5413	3	29.56	1339.601	0.5
SHFRZWEYKU	99	481.5642	3	30.25	1441.674	-2.4

SHFZZWENKU	99	501.8901	3	30.84	1502.65	-0.9
AHFRZWEYKU	99	476.2326	3	31.31	1425.679	-2.4
AHFZZWENKU	99	496.5594	3	31.83	1486.655	0.9
SZFRQWEYKU	99	465.2292	3	32.46	1392.664	1.3
AZFRQWEYKU	99	459.8966	3	33.64	1376.669	-0.6
AZFRZWEYKU	99	514.246	3	35.56	1539.718	-0.9
SZFZZWENKU	99	539.905	3	36.48	1616.688	3.3
SHLZZWZYKU	99	555.5932	3	36.63	1663.751	4.4
SHLZQWEYKU	99	452.5528	3	38.13	1354.638	-0.7
AHLZQWEYKU	99	447.2216	3	39.36	1338.643	0.3
SHLZZWEYKU	99	506.9029	3	39.4	1517.686	0.6
AHLZZWEYKU	99	501.5717	3	40.32	1501.691	1.5
SHFZQWEYKU	99	463.8811	3	41.78	1388.622	-0.2
SHFZZWEYKU	99	518.2308	3	42.04	1551.67	0.1
AHFZQWEYKU	99	458.5499	3	42.97	1372.627	0.7
AHFZZWEYKU	99	512.8981	3	43.09	1535.675	-1.8
AHFZQPZNKU	98	461.2243	3	16.18	1380.645	4.7
AHFZQPENKU	98	412.5342	3	16.31	1234.58	0.8
SZLRQPEYKU	98	424.2242	3	16.41	1269.653	-1.9
AHLRZWZNKU	98	497.2532	3	17.44	1488.739	-1
AZLRZPEYKU	98	473.2437	3	19.77	1416.707	1.8
AZFRQPEYKU	98	430.2221	3	20.52	1287.643	1.5
SZFRQWZNKU	98	497.5778	3	21.15	1489.708	2.4
SZLRZWENKU	98	491.9105	3	22.33	1472.708	1.3
AZFRZPEYKU	98	484.5714	3	22.75	1450.691	0.9
SHLZQPEYKU	98	422.8777	3	22.78	1265.611	0.3
AHLZQWZNKU	98	479.5718	3	24.91	1435.687	4.9
SHLZQWENKU	98	436.2138	3	26.07	1305.617	2
AHFZQPZYKU	98	477.5636	3	26.38	1429.665	2.9
AHLRZWZYKU	98	385.4481	4	26.72	1537.76	2.4
AHLZZWZNKU	98	533.9205	3	27.17	1598.735	2.8
AZLZQPEYKU	98	455.5606	3	27.3	1363.654	4.4
SHFZQWZNKU	98	496.2311	3	27.42	1485.666	3.7
SZLRQWEYKU	98	453.9011	3	28.26	1358.68	1.4
SHFZZWZNKU	98	550.5815	3	28.7	1648.714	5.1
AHFZZWZNKU	98	545.2494	3	29.55	1632.72	4.2
SZLRZWZYKU	98	556.9402	3	30.33	1667.793	3.6
AHFZQWENKU	98	442.2093	3	30.41	1323.606	-0.4
SZLZZWZNKU	98	577.2672	3	31.17	1728.768	6.5
AZFZZPEYKU	98	521.2385	3	32.92	1560.687	4.3
SZFRZWEYKU	98	519.5786	3	35	1555.712	0.9
SHLZQWZYKU	98	501.2431	3	35.44	1500.702	3.8
AHLZQWZYKU	98	495.9115	3	36.47	1484.707	3.8
AHLZZWZYKU	98	412.9475	4	37.51	1647.756	3.2
SHFZQWZYKU	98	512.571	3	38.77	1534.686	3.2

SHFZZWZYKU	98	425.4424	4	39.33	1697.735	3.2
AZLZZWEYKU	98	539.5858	3	43.5	1615.729	3.9
SZLZZWEYKU	98	544.9175	3	43.7	1631.724	4
SZFZZWEYKU	98	556.2455	3	45.93	1665.709	3.7
SHLRZPEYKU	97	440.5604	3	15.48	1318.663	-3.1
AZLRQPEYKU	97	418.8932	3	16.76	1253.658	-0.4
SHLRZWZNKU	97	377.1904	4	16.88	1504.734	-1.2
SHFRQWZNKU	97	344.9242	4	17.03	1375.67	-1.6
AZLRQWENKU	97	432.2291	3	18.43	1293.664	0.8
SZFZQPENKU	97	455.8793	3	18.99	1364.613	2.3
AZFZQPENKU	97	450.5487	3	19.86	1348.618	4.5
SZFRQPEYKU	97	435.5536	3	19.94	1303.638	1.2
SZFRQWENKU	97	448.8889	3	21.8	1343.644	1.1
SZFRZWZNKU	97	551.9274	3	23.09	1652.757	2.3
SHLRZWZYKU	97	389.4463	4	26.21	1553.754	1
SHLZZWZNKU	97	539.2523	3	26.34	1614.73	3.1
AHFRZWZYKU	97	393.9439	4	29.84	1571.744	1.6
SZFZQPEYKU	97	472.2201	3	30.32	1413.633	3.6
AZLRZWEYKU	97	502.919	3	31.97	1505.733	1.4
SZFZZPEYKU	97	526.5698	3	32.14	1576.682	3.5
SZFZQWZNKU	97	534.2457	3	32.54	1599.704	6.9
SZFZQWZYKU	97	550.5857	3	42.38	1648.725	6.5
AHLRQPZYKU	96	429.5692	3	15.34	1285.685	0.9
SZLRZPEYKU	96	478.5745	3	19.04	1432.702	-0.1
AZLRZWZNKU	96	535.2693	3	21.26	1602.777	5.5
SHLZQPZYKU	96	471.5681	3	22.28	1411.675	5
AHLZQPZYKU	96	466.2354	3	23.22	1395.68	2.7
AZFRZWZNKU	96	546.597	3	23.31	1636.762	4.5
SHLRQWZYKU	96	348.6837	4	23.62	1390.706	-0.3
SHLZQWZNKU	96	484.9032	3	23.95	1451.682	4.3
SHFZQPZYKU	96	482.8956	3	25.27	1445.66	3.6
AHFZZPZYKU	96	531.9138	3	27.83	1592.713	3.8
AHFZQWZNKU	96	490.8983	3	28.18	1469.671	1.6
SZLZQWZNKU	96	522.9175	3	29.43	1565.72	7
AZFZQWENKU	96	480.2245	3	35.87	1437.645	4.9
SHFZQPZNKU	95	466.5559	3	15.47	1396.639	4.7
AHFRQPZYKU	95	440.8966	3	16.87	1319.669	-0.6
AZLZZPENKU	95	493.5691	3	20.38	1477.682	2.1
AHLZZPZYKU	95	520.5859	3	24.89	1558.729	4.4
SHFRQWZYKU	95	357.1795	4	27.18	1424.69	-0.8
AZLZZPZYKU	95	558.6006	3	28.33	1672.767	7.7
SZLZZPEYKU	95	515.2415	3	28.58	1542.698	3.4
SZFZQPZYKU	95	520.9103	3	28.73	1559.698	7.2
SZFZZPZYKU	95	575.2591	3	30.66	1722.747	5.2
SZFRQWZYKU	95	385.6908	4	31.3	1538.729	3.6

AZFZZPZYKU	95	569.9273	3	31.6	1706.752	5.1
AZLZQWENKU	95	468.8958	3	31.79	1403.66	3.7
AZLZZWZYKU	95	588.2761	3	40.95	1761.794	7.3
AZLZQPZNKU	94	487.9097	3	16.48	1460.698	6.2
AZLRQWZNKU	94	360.9406	4	18.17	1439.729	3.2
SZLRQWZNKU	94	364.9398	4	18.29	1455.724	4.4
SZFZQPZNKU	94	504.5701	3	18.39	1510.678	7.3
AZFRZWENKU	94	497.9069	3	24.6	1490.697	1
SHFRZWZYKU	94	397.9426	4	29.14	1587.739	1.6
SZLZQWZYKU	94	539.2581	3	39.83	1614.74	7.6
AHFZQWZYKU	94	380.6817	4	39.99	1518.691	4.2
AHFZZWZYKU	94	421.4441	4	40.29	1681.74	4.3
SZFZQWEYKU	94	501.8952	3	45.6	1502.66	2.5
AHFZZPZNKU	93	515.5734	3	18.02	1543.693	3.5
AZLRZWENKU	93	486.579	3	21.87	1456.713	1.6
SZFZZPENKU	93	510.2299	3	22.26	1527.662	4.1
SZLZQPZYKU	93	509.5818	3	25.74	1525.714	6.5
SZLZQPEYKU	93	460.8921	3	26.64	1379.649	3.8
SHFZZPZYKU	93	537.2458	3	26.93	1608.708	4.6
AZFZQPZYKU	93	515.5787	3	29.71	1543.703	7.2
AZLRZWZYKU	93	413.9581	4	30.65	1651.798	3.3
AZFZQPEYKU	93	466.8886	3	31.4	1397.638	4
AZFRQWZYKU	93	381.6922	4	32.53	1522.734	3.9
AZFZQWZNKU	93	528.9144	3	32.81	1583.709	7.7
SZFRZWZYKU	93	568.2689	3	33.38	1701.777	4.6
SZFZZWZNKU	93	588.5945	3	33.62	1762.753	5.2
AZFRZWZYKU	93	422.4547	4	33.82	1685.782	4.5
SZLRQPZYKU	92	472.914	3	16.86	1415.718	1.9
AZFZQPZNKU	92	499.2379	3	19.17	1494.683	6.1
AZFRQWZNKU	92	492.2476	3	21.69	1473.713	5.3
SZLRQWZYKU	92	502.5909	3	28.05	1504.744	4.6
AZLZQWZNKU	92	517.5864	3	29.21	1549.725	8
SZLZZWZYKU	92	593.6075	3	40.79	1777.789	6.9
AZFZZWZYKU	92	449.9548	4	43.36	1795.778	6.7
AHLZQPZNKU	91	449.8956	3	14.93	1346.66	3.6
SHLRQPEYKU	91	386.2108	3	14.96	1155.615	-3.7
AZLZQPENKU	91	439.219	3	16.42	1314.634	1.1
SHLRQWENKU	91	399.5454	3	16.84	1195.621	-5.6
SZFRQPZYKU	91	484.2436	3	19.87	1449.702	4.9
SHLZZPZYKU	91	525.9167	3	23.57	1574.724	2.8
AZLRQPZYKU	90	467.5824	3	17.39	1399.723	1.9
SZLRQWENKU	90	437.5607	3	18.7	1309.659	0.8
AZFZQWZYKU	90	545.2544	3	43	1632.73	7.3
AHLRQPEYKU	89	380.8794	3	15.25	1139.62	-3
AZLZQPZYKU	89	504.2508	3	26.68	1509.719	7.9

AZFZZWZNKU	89	583.2639	3	34.02	1746.758	6.8
AZFRZPENKU	88	468.231	3	14.85	1401.671	0.5
SHLRQPZYKU	87	434.901	3	14.94	1301.679	1.3
SZLRZWZNKU	87	405.7011	4	21.17	1618.772	1.9
AZLZZWZNKU	87	571.9355	3	31.19	1712.773	6.5
AZFZZWENKU	87	534.5741	3	36.59	1600.693	4.6
AZFZZWEYKU	87	550.9141	3	46.35	1649.714	4.1
AHLRZPZYKU	86	363.1913	4	16.46	1448.733	2.3
AHFRZPEYKU	86	335.1693	4	19.11	1336.653	-3.5
AHLRQWZYKU	86	344.6856	4	24.27	1374.711	1.8
SZFZZWZYKU	86	453.9525	4	42.87	1811.773	4.4
AZFZQWEYKU	86	496.5642	3	46.25	1486.665	3.8
AZLZQWZYKU	85	533.9264	3	40.01	1598.745	7.7
SZLZQWEYKU	85	490.5679	3	42.53	1468.676	4.3
SZFRZPZNKU	84	391.9414	4	14.84	1563.73	4.2
SHFZQPEYKU	84	650.8057	2	26.75	1299.595	1.3
AHFZQPEYKU	84	642.8075	2	27.99	1283.6	0.1
SZLZZWENKU	84	528.5765	3	34.53	1582.704	2.5
AZLZZPEYKU	83	509.9105	3	29.26	1526.703	4.6
AZLZQWEYKU	83	485.2364	3	42.67	1452.681	4.7
AZFRQWENKU	82	443.5575	3	22.43	1327.649	1.5
AZLZZWENKU	82	523.2454	3	33.87	1566.709	3.6
AZLRQWZYKU	81	373.1962	4	28.33	1488.749	4.3
AHLRZWENKU	79	448.5627	3	16.44	1342.675	-6.2
AZFZZPENKU	79	504.8978	3	22.77	1511.667	3.2
SZLRZPZYKU	78	527.2649	3	19.43	1578.766	4.3
AHLRQWENKU	77	394.2137	3	16.84	1179.626	-5.8
AZFRZPZYKU	77	533.2614	3	22.66	1596.756	4.1
SHLRZPZYKU	76	367.1899	4	16.07	1464.728	1.7
AHLZQPEYKU	76	625.8153	2	23.89	1249.616	0.1
SHFRZPZYKU	75	375.6859	4	18.41	1498.712	1.4
SZFRZWENKU	74	503.238	3	24.15	1506.692	0
AZFRQPZYKU	70	359.4358	4	20.54	1433.707	4.9
SHFRQPZYKU	67	334.9227	4	16.45	1335.664	-1.7
SZLRZWEYKU	67	381.4389	4	31.65	1521.728	-1.1
SZLZQPZNKU	66	493.2416	3	16.05	1476.693	6.6
AHFRZPZYKU	64	495.2473	3	19.42	1482.717	1.8
AZLRZPZYKU	64	391.7016	4	20.15	1562.771	3.8
SHFRZPEYKU	63	451.8883	3	18.05	1352.648	-3.3
SZFRZPEYKU	56	367.6793	4	22.23	1466.686	1.3

Synthesis and characterization of a 10^8-member nucleobase peptide library

Library design: $(X)_9K\text{-}CONH_2$ with X = 18 canonical amino acids (excluded Cys and Ile) & DabA, DabC, DabG, DabT, AlaA, AlaC, AlaG, AlaT, hAlaA, hAlaC, hAlaG, hAlaT.

Library synthesis: SPPS:

2.2 g of 30 µm TentaGel resin (0.26 mmol/g, 0.74 mmol, 1.0 x 10^8 beads) was transferred to a 25 mL peptide synthesis vessel, swollen in DMF, and then washed with DMF (3x). Fmoc-Rink amide linker (5 eq) was dissolved in HATU solution (0.38 M in DMF) activated with DIEA (1.86 mL, 10.7 mmol) immediately prior to coupling, and added to resin bed. Coupling was performed for 20 min; after this time, resin was washed with DMF (100 mL). Fmoc removal was carried out by treatment of resin with 20% piperidine in DMF (1 x 30 mL flow wash; 1 x 15 mL, 5 min batch treatments). Resin was then washed with DMF (150 mL). Coupling of Fmoc-Lys(Boc)-OH, subsequent Fmoc removal, and DMF washes were performed in the same manner.

At this stage, resin was suspended in DMF (10 mL), and divided in two parts (20% and 80%, respectively). The 20% part was divided evenly among 12 x 10 mL fritted plastic syringes and the 80% part was divided evenly among 18 x 10 mL fritted plastic syringes using a 5 mL Eppendorf pipette. Couplings were performed according to the procedure described in "Peptide synthesis procedures"**.** After coupling for 20 min, resins were washed with DMF (~10 mL ea.), poured back into a 25 mL synthesis vessel, and washed with DMF (100 mL). Fmoc removal was carried out by treatment of resin with 20% piperidine in DMF (1 x 30 mL flow wash; 1 x 15 mL, 5 min batch treatments). Resin was then washed with DMF (150 mL). Nine cycles of split-and-pool synthesis were performed using this procedure.

Cleavage and solid phase extraction were performed according to procedures described in section "Peptide synthesis procedures"**.**

450 mg lyophilized powder (~60% crude yield) were obtained.

The library was dissolved in 1x PBS pH = 7.2 + 5% DMF, aliquoted and stored at – 80 °C.

Library QC: A 1.0 mg aliquot of library resin (from **Section 6.1**) was suspended in 1.0 mL of Milli-Q water and sonicated to achieve a homogenous suspension (theory: 3 x 10^4 beads/mL). A 20 µL aliquot (theory: 650 beads; 4 pmol/peptide) was transferred to a plastic tube, spun down, and supernatant removed. Beads were then subjected to nucleobase peptide cleavage conditions. TFA was then evaporated under a stream of nitrogen, and cleaved peptide was resuspended in Milli-Q water (0.1% TFA). Sample was purified over a C18 ZipTip® (0.6 µL, MilliporeSigma, P/N ZTC18S096), eluted in 30/70 water/acetonitrile (0.1% TFA), and lyophilized. Powder was resuspended in 20 µL of Milli-Q water (0.1% FA), and 0.5 µL (~100 fmol/peptide) was submitted for nLC-MS/MS analysis.

Library QC sample 1

U = C-terminal amide, B = DabA, C = DabC, I = DabG, J = DabT, O = AlaA, U = AlaC, X = AlaG, Z = AlaT, b = hAlaA, c = hAlaC, i = hAlaG, j = hAlaT

Peptide	*ALC (%)*	*m/z*	*z*	*RT*	*Mass*	*ppm*
HJbADFFEDKU	99	497.8781	3	43.69	1490.635	-15
CVQMFCAFDKU	99	669.7984	2	46.54	1337.596	-10.4
LOASAWAJFKU	98	454.8922	3	32.48	1361.67	-10.9
VDCTYCFNbKU	98	486.546	3	33.38	1456.633	-11.2
DGSVLYAFCKU	98	551.2668	2	49.42	1100.533	-12.1
GMFGGEYCSKU	98	409.1783	3	51.16	1224.53	-13.5
GVVEPMFbVKU	98	408.2183	3	68.03	1221.64	-5.5
TCSSNAEBiKU	97	449.8585	3	24.64	1346.559	-4.2
DQGjDLXVKKU	97	444.2195	3	25.73	1329.651	-10.6
DSTCAYGAVKU	97	338.4905	3	27.2	1012.465	-15
DMSTCAKFIKU	97	440.8616	3	27.32	1319.585	-17
QAPELLjEGKU	97	398.2072	3	29.94	1191.622	-18.6
DDHDYGVOQKU	97	427.1839	3	33.26	1278.549	-14.8
YKYEGTjPCKU	97	482.2274	3	33.44	1443.682	-14.8
ITEGAKWTRKU	97	456.2318	3	35.03	1365.7	-19.8
CFYNDJTXGKU	97	527.5525	3	40.09	1579.657	-13.7
DMTCVVKFTKU	97	390.8661	3	41.13	1169.594	-14.8
TjHjJGEAYKU	97	496.8826	3	42.2	1487.644	-12
PMAEDEAYTKU	97	577.2566	2	47.46	1152.512	-11.8
YVNMLYTCAKU	97	402.1944	3	47.54	1203.578	-14
PAGVPMWWDKU	97	395.8594	3	49.31	1184.58	-20.1
AGQOGPBLcKU	97	671.8226	2	52.28	1341.657	-19.7
LEFALLARHKU	97	399.5758	3	53.32	1195.719	-11.2
MPVADGVJRKU	96	413.2117	3	23.55	1236.635	-17.7
TDZADRNAAKU	96	385.8484	3	27.4	1154.543	-16.6
jQcDYHWATKU	96	484.2166	3	36.32	1449.648	-13.5
IYGMDELQKKU	96	467.8851	3	40.52	1400.661	-19.8
LKGYSNADjKU	96	401.8675	3	40.55	1202.601	-17.2
TCDTWYTKXKU	96	455.5405	3	42.49	1363.609	-7
NMFLRCRYVKU	96	443.5684	3	46.21	1327.7	-12.9
PMAPMCPYTKU	96	569.259	2	47.35	1136.518	-12.8
EGSYTciTKKU	96	447.5533	3	49.56	1339.636	2
JSNjDALPDKU	96	667.2993	2	53.21	1332.598	-10.8
FTFQSMQMMKU	96	639.2849	2	69.43	1276.577	-16.8
VjFGEWEIVKU	96	498.2304	3	71.77	1491.697	-18.3
EMADYQSViKU	96	652.2917	2	80.55	1302.578	-7
PRJZRQGEJKU	95	532.9215	3	23.88	1595.758	-9.5

VECSLHWVYKU	95	470.9064	3	31.09	1409.716	-13
EMZASMDMDKU	95	417.8246	3	31.12	1250.473	-16.6
TNFCTJANjKU	95	458.1997	3	32.19	1371.592	-10.3
LOASAQEJFKU	95	454.8914	3	32.75	1361.654	-1.5
PYRFTCPPGKU	95	388.8654	3	32.84	1163.591	-14.2
DPMCCVSEVKU	95	419.8554	3	33.07	1256.559	-11.9
DDHYDGVZHKU	95	427.1839	3	33.1	1278.538	-6.2
QbEVJSEVEKU	95	477.5577	3	33.49	1429.661	-6.7
MNCFVALBRKU	95	452.5613	3	33.57	1354.68	-13.5
VGANDSjAMKU	95	550.7554	2	41.93	1099.505	-8.1
TjHjYCWAYKU	95	496.8824	3	42.27	1487.635	-6.1
FQLTBVAPVKU	95	319.9297	4	44.87	1275.714	-19.1
GMVQWQWKMKU	95	440.894	3	50.43	1319.663	-2.3
PLYDGETGEKU	95	554.2612	2	55.09	1106.524	-14.9
UDPYQNKQYKU	95	681.8253	2	63.95	1361.648	-8.5
NCSMAADcJKU	95	723.8056	2	64.19	1445.609	-8.8
TjFjJADAYKU	95	749.8266	2	65.95	1497.653	-9.8
ACGVQWWXLKU	95	437.2103	3	66.97	1308.63	-15.7
FDFLKZMSSKU	95	432.8791	3	70.11	1295.633	-13.8
TPSLVADTFKU	95	539.2932	2	73.29	1076.587	-13.7
FFAGYLVGXKU	95	610.8096	2	73.7	1219.625	-16.7
FFTMLTKIHKU	95	481.5804	3	77.39	1441.739	-13.7
SGMDTTUbRKU	94	431.5294	3	25.28	1291.591	-18.8
HEMJSMDMDKU	94	463.5095	3	27.34	1387.528	-15.2
EMDKSQPGEKU	94	383.1786	3	30.14	1146.534	-17.4
VECSLKNUYKU	94	470.9061	3	31.04	1409.712	-10.8
KVFQIWVGTKU	94	461.5847	3	31.35	1381.736	-2.6
LOVLVDQDQKU	94	420.898	3	32.46	1259.673	-1
GYFOWRTGDKU	94	444.8757	3	34.79	1331.627	-16.5
DYDTDQFYNKU	94	436.5208	3	40.49	1306.547	-4.7
ODTADYTKXKU	94	455.5395	3	42.77	1363.613	-11.8
CVGQEGYJMKU	94	476.5453	3	48.75	1426.632	-12.5
YZFCDFASEKU	94	652.2653	2	49.32	1302.534	-13.7
TPSLVJGTFKU	94	405.5487	3	56.89	1213.641	-13.9
DFILENDSEKU	94	462.8654	3	58.95	1385.595	-14.8
WLKLIMYIAKU	94	545.2761	3	61.12	1632.819	-7.8
GbDDYVLLQKU	94	423.216	3	65.06	1266.642	-12.8
SSGVQEGWLKU	94	545.2793	2	67.88	1088.562	-16.1
bCFLSVDYNKU	94	435.8759	3	73.92	1304.604	1.5
ZQTCMEQSDKU	93	632.2498	2	24.08	1262.502	-13.4
WbTFAVGGKKU	93	404.2153	3	25.73	1209.648	-19.3
XiHWAARAGKU	93	338.1688	4	26.07	1348.652	-4
LEGEQRTjKKU	93	432.8966	3	26.67	1295.692	-18.3
LNSPZDCVEKU	93	599.7719	2	27.85	1197.545	-13.2
KEYDYNVXEKU	93	352.4145	4	28.37	1405.638	-6.1

ADQSMSTVFKU	93	371.5124	3	29.27	1111.533	-16.1
DVGWJEIGVKU	93	482.5495	3	33.72	1444.654	-19.1
jTUGKbCRMKU	93	477.2228	3	35.64	1428.665	-13
ccFGVYMADKU	93	439.8673	3	36.1	1316.602	-16.6
TCCVLETjiKU	93	496.2341	3	38.51	1485.682	-1.3
POMPNANVjKU	93	428.2056	3	40.37	1281.612	-13.1
CTNDHFFTYKU	93	425.519	3	41.42	1273.555	-15.5
DGQXKTADOKU	93	429.1969	3	43.17	1284.582	-10
FADESVBLVKU	93	427.8877	3	62.19	1280.657	-12
cHEFPAPMRKU	93	435.8859	3	63.13	1304.653	-12.9
ijDATMPEGKU	93	645.7826	2	64.61	1289.555	-3.1
EGOLNAYADKU	93	395.1899	3	65.26	1182.553	-4.2
FDFLKYCFSKU	93	432.8796	3	68.89	1295.637	-15.7
CVEAVKAAjKU	93	425.5674	3	73.6	1273.681	-0.9
CPELWLDDAKU	93	594.7892	2	82.07	1187.565	-0.4
NLGEYXOGFKU	93	675.8098	2	83.05	1349.613	-5.5
EMDAYQSFiKU	93	676.2924	2	91.72	1350.578	-5.9
VPGVLVCQQKU	92	305.1761	4	25.04	1216.699	-19.8
VEIRVRjADKU	92	491.2498	3	28.32	1470.752	-16.3
bVVLVDGWQKU	92	420.8978	3	32.35	1259.684	-9.9
MGMjEOCLKKU	92	451.2036	3	34.35	1350.608	-13.9
XAPOVYMADKU	92	439.8667	3	36.13	1316.595	-12.4
XiGMEDLQKKU	92	467.8853	3	40.6	1400.648	-10.4
CVGAMSYbDKU	92	446.867	3	46.57	1337.596	-12.1
DFQLEQCTFKU	92	419.8625	3	61.34	1256.586	-16
UPHPYSKLEKU	92	426.5623	3	63.33	1276.668	-1.8
MMFLKYFCSKU	92	432.8787	3	70.27	1295.623	-6.6
VPLLVcADBKU	92	661.8654	2	92.72	1321.728	-8.5
TYQTFQPGVKU	91	389.8689	3	26.82	1166.608	-20.2
KYCTBGQJYKU	91	510.8956	3	26.96	1529.684	-12.7
KTHQDMiMWKU	91	479.8886	3	29.85	1436.656	-8.4
INEMIVSPSKU	91	491.552	3	32.28	1471.647	-8.7
VDTCYCFHZKU	91	486.546	3	33.47	1456.626	-6.8
AJcDYHAWTKU	91	484.2182	3	36.39	1449.646	-9.1
LYDISVMGRKU	91	340.4185	4	38.59	1357.667	-16
HHQDMjFGOKU	91	471.2018	3	41.86	1410.608	-17.4
PLYDZQTGEKU	91	415.5276	3	42.34	1243.583	-18
BNWQcYRGNKU	91	511.9114	3	43.18	1532.715	-1.9
MFAQPGMQFKU	91	592.2835	2	49.21	1182.568	-13
MGMjEXQKKKU	91	469.8891	3	50.01	1406.663	-12.3
FGSLbGSPEKU	91	569.7822	2	56.53	1137.564	-11.9
VcEQCTEVYKU	91	720.3445	2	60.76	1438.687	-8.8
LZSMLTZjLKU	91	468.5686	3	62.65	1402.7	-11.2
SDLAScZDSKU	91	605.7681	2	74.97	1209.534	-10.4
MEDAYQSWiKU	91	695.7971	2	91.38	1389.589	-6.6

ZPFLQNQAKKU	90	423.2333	3	24.6	1266.683	-4.1
PSGFCGYAGKU	90	493.2245	2	25.33	984.4487	-14.5
VYGNHLQHPKU	90	397.8793	3	27.03	1190.631	-12.5
PMIRVRjADKU	90	491.2498	3	28.33	1470.734	-4.2
YASPETAHFKU	90	383.8586	3	28.43	1148.562	-6.5
YTNCOQQWEKU	90	468.198	3	33.93	1401.6	-19.5
LLEDMLANLKU	90	290.4155	4	34.28	1157.648	-12.9
QBPXGYYDMKU	90	499.2083	3	38.9	1494.626	-15.5
GGEDGRLLVKU	90	348.2002	3	39.93	1041.593	-13.6
XiGMNNLQKKU	90	462.5545	3	40.4	1384.665	-16.8
MKVLTCNVMKU	90	389.2113	3	41.49	1164.618	-5.3
DYEDJGVNFKU	90	451.199	3	42.36	1350.58	-3.3
BDIGKAFDAKU	90	472.8883	3	49.75	1415.649	-3.9
KGMLFjjVDKU	90	452.2285	3	50.38	1353.68	-12.3
KTSLFjQUDKU	90	452.2279	3	50.52	1353.676	-10.4
KFXCLRIEFKU	90	527.5922	3	55.51	1579.768	-8.5
ZWAOVISYFKU	90	530.5729	3	58.13	1588.718	-13
MMQLEQTCFKU	90	419.8619	3	61.24	1256.572	-6.1
FBEFJADRFKU	90	400.6863	4	63.43	1598.739	-14.2
VFQZMDSZLKU	90	678.8128	2	69.63	1355.629	-13.3
YNETTYDTEKU	90	631.7781	2	71.2	1261.546	-3.5
NLEGYXFGOKU	90	675.8093	2	83.26	1349.613	-6.3
KiSLOHAiYKU	90	506.5835	3	88.87	1516.742	-8.7
PYFNRPcSSKU	89	322.9151	4	24.32	1287.644	-10
UBGVENEFHKU	89	471.8797	3	26.8	1412.639	-15.2
YVKGJCRENKU	89	378.1918	4	27.65	1508.751	-8.1
MCSTLENMCKU	89	436.1882	3	28.12	1305.558	-11.8
WDEDHAFVGKU	89	401.5187	3	28.19	1201.552	-14.4
KGRTUPMTNKU	89	404.5456	3	31.01	1210.635	-16.7
PKjETAEPGKU	89	388.8654	3	32.84	1163.591	-14
GVTPGAZFEKU	89	367.1838	3	36.14	1098.546	-14.8
WFKNMGNYDKU	89	434.5359	3	36.96	1300.602	-12.7
PTSCTSIFWKU	89	449.532	3	40.01	1345.598	-17.4
CVQMCYAFDKU	89	452.1984	3	46.64	1353.591	-13.1
WVBYDNFMGKU	89	478.5509	3	47.43	1432.64	-6.4
ETNMZIGFJKU	89	526.5522	3	48.54	1576.654	-12.1
HQDUGCFNFKU	89	637.7726	2	48.82	1273.541	-8.2
MYGFMTSTCKU	89	584.2464	2	50.43	1166.492	-12
DVTTGbWFGKU	89	409.867	3	50.91	1226.59	-8.9
HDBLEQCTFKU	89	465.5481	3	51.11	1393.625	-1.8
MVAFUVHTLKU	89	408.8902	3	52.5	1223.66	-8.9
EGQFDAESKKU	89	379.8546	3	54	1136.546	-3.6
FTFQMCQDFKU	89	647.2827	2	54.9	1292.568	-13.3
FSjDATDEWKU	89	653.778	2	56.12	1305.56	-14
WGDSDYTAQKU	89	585.259	2	58.28	1168.515	-9.7

DXbLENDSEKU	89	462.865	3	59.13	1385.577	-3.1
VFQZMDSALKU	89	616.8004	2	64.63	1231.602	-12.9
OGMYFjLOcKU	89	784.8489	2	66.93	1567.705	-14
PUETTYDTEKU	89	631.778	2	71.28	1261.557	-12.6
WMAYDEEMMKU	89	666.7696	2	83.19	1331.535	-7.7
KDHMPDWHDKU	88	436.5341	3	23.22	1306.588	-5.4
GVSHMPDiOKU	88	436.5341	3	23.27	1306.585	-3.8
EDVADRAOFKU	88	418.5429	3	23.65	1252.606	0.7
YNSLMNiMEKU	88	454.8643	3	26.89	1361.597	-19.4
GXSLMNiMEKU	88	454.864	3	26.98	1361.584	-9.8
LGYAETTSMKU	88	367.1816	3	28.75	1098.538	-13.5
STADAKWTRKU	88	388.209	3	30.09	1161.626	-17.6
PNLRCQMGTKU	88	382.8637	3	31.63	1145.58	-9.1
KARMMPANLKU	88	386.8847	3	33.91	1157.653	-17.5
bGSTLDWJEKU	88	473.5492	3	36.18	1417.64	-10
GVSFMPDiOKU	88	439.8704	3	37.84	1316.595	-4.3
KDEQXXYDMKU	88	499.2081	3	39.16	1494.617	-9.7
OSXMNNLQKKU	88	462.5541	3	40.67	1384.664	-17.3
AEEAPLAAAKU	88	485.2659	2	43.13	968.5291	-12.3
ALDMDYjMEKU	88	441.856	3	44.62	1322.561	-10.8
IGEjAVNJSKU	88	490.5491	3	44.65	1468.648	-15
PLYDOYGGEKU	88	415.5272	3	44.87	1243.573	-10.9
iPSZFDGVGKU	88	412.1923	3	46.33	1233.565	-7.7
jMMSGDZSLKU	88	424.5179	3	50.07	1270.541	-6.8
UNMSMYDDEKU	88	656.2488	2	54.17	1310.502	-14.4
ZWAFRBCYFKU	88	530.5732	3	57.89	1588.72	-13.9
VYADTYVNAKU	88	571.7902	2	58.46	1141.577	-9.5
DFIQNNMAEKU	88	693.7954	2	59.15	1385.589	-8.9
EZDMSEMENKU	88	653.7473	2	59.99	1305.497	-12.7
GLDNLVbOZKU	88	458.8907	3	62.15	1373.677	-19.4
EGFESVBLVKU	88	427.8863	3	62.31	1280.657	-15.2
VTLYZTAXEKU	88	669.825	2	73.88	1337.648	-9.1
DSVFLZMYTKU	88	649.3071	2	77.47	1296.617	-13.5
FMAWLGYDQKU	88	629.2974	2	90.75	1256.601	-16.6
GbTVQSMMTKU	87	400.5235	3	25.27	1198.565	-13.9
TDCTBKELYKU	87	458.8841	3	27.94	1373.645	-10.5
TGGANGWYiKU	87	396.1849	3	27.96	1185.544	-8.9
QRPANLLACKU	87	420.9104	3	27.98	1259.716	-5.4
HPCFQDPSWKU	87	348.6682	4	30.88	1390.648	-3.4
KARTEEANLKU	87	386.8847	3	34.13	1157.652	-16.7
GDQXKTGEOKU	87	429.198	3	39.87	1284.582	-7.4
MFEDYCRNFKU	87	676.2947	2	42.4	1350.585	-7.5
VBIbXNLGLKU	87	412.4495	4	42.66	1645.795	-15.8
EAFQMGFTQKU	87	593.2818	2	43.89	1184.565	-13.2
PLYDJGTGEKU	87	415.5267	3	44.52	1243.579	-16.6

LWPEOSKGKKU	87	319.6807	4	51.19	1274.7	-4.5
MFEDFBVNFKU	87	484.2203	3	51.71	1449.655	-11.2
EKYFADZNMKU	87	447.2	3	54.11	1338.603	-18.2
EKYFGEcDMKU	87	670.2972	2	54.15	1338.599	-14.5
EDLGYQADGKU	87	547.7515	2	54.4	1093.504	-14.2
GVUQLRIEFKU	87	482.9147	3	55.18	1445.738	-10.8
TCNDPFFTYKU	87	617.7737	2	55.96	1233.549	-13
GLBWEYQPFKU	87	361.1819	4	56.35	1440.699	-0.6
EMGEYAGSiKU	87	602.7598	2	66.55	1203.51	-4
WUSSYjAEFKU	87	703.3098	2	67.35	1404.618	-9.4
FMMLKYCFSKU	87	432.8794	3	68.98	1295.623	-4.9
PTHEFFWELKU	86	333.9173	4	23.94	1331.666	-19.6
LNSPADVCEKU	86	537.7586	2	24.48	1073.518	-13.9
GXSLMQMXEKU	86	454.8643	3	26.89	1361.583	-8.7
URQLFHYEFKU	86	362.4372	4	28.85	1445.732	-8.2
DMSOAKIMIKU	86	532.5631	3	29.05	1594.684	-10.1
FOESQDFFHKU	86	463.2067	3	30.86	1386.622	-16.9
FVKFTCPGNKU	86	570.2979	2	32.18	1138.596	-12.7
DRWCYEIGVKU	86	482.5495	3	33.73	1444.641	-9.8
VECTARZVYKU	86	470.9066	3	33.85	1409.712	-9.7
VCQVFSNPMKU	86	433.8851	3	35.4	1298.651	-13.1
DDPVVEDKLKU	86	386.2041	3	36.69	1155.614	-20
SGMDCVCFRKU	86	431.5307	3	38.32	1291.587	-12.6
PPMGGANVjKU	86	539.7701	2	38.57	1077.536	-9.4
PYNNWGECRKU	86	471.8884	3	38.83	1412.665	-15.3
DGQXQTWFGKU	86	429.1984	3	40.19	1284.575	-1.1
KDDRKjVDMKU	86	448.2313	3	40.74	1341.679	-5.4
VMGLTDXNLKU	86	605.3067	2	41.6	1208.608	-7.9
MFEDCYRNFKU	86	451.1982	3	47.03	1350.585	-8.9
WLIYSDSDKKU	86	477.889	3	47.6	1430.668	-16
TLKMNLKTGKU	86	378.229	3	48.04	1131.68	-12.9
FQLFOVAPVKU	86	417.9017	3	48.34	1250.704	-16.3
FMAMWEjRCKU	86	470.5421	3	60.94	1408.617	-9.1
FBEFYCWRFKU	86	400.6863	4	63.44	1598.729	-8.2
PWCWFNKYEKU	86	467.2177	3	64	1398.654	-16.5
FSjDATEDWKU	86	653.7798	2	64.83	1305.56	-11.1
TCNDFFFTYKU	86	642.7814	2	67.01	1283.565	-12.6
NAAGSDTHGKU	86	478.726	2	71.12	955.4471	-10.2
NEGOJGYDQKU	86	460.5227	3	76.87	1378.572	-18.6
ETGEWVHcIKU	86	735.3369	2	78.62	1468.667	-5.2
YDYDCVPTMKU	86	691.3022	2	92.36	1380.608	-13.4
jLVGQAPRIKU	85	342.6861	4	24.24	1366.729	-10.3
GPSIbVTVEKU	85	331.9164	4	28.5	1323.649	-9.6
KTHQXEMMWKU	85	479.8886	3	29.75	1436.655	-7.8
ZVGESDBFHKU	85	463.2068	3	30.95	1386.612	-9.5

DDHFADTOQKU	85	427.1839	3	33.27	1278.549	-14.8
CVLEPCWSAKU	85	641.8127	2	37	1281.624	-10.3
GVVKQWWOWKU	85	473.9196	3	37.11	1418.747	-7.2
VGANDSjSMKU	85	558.7521	2	42.01	1115.5	-9.2
CPFQSTFTQKU	85	593.2819	2	44.08	1184.565	-13.1
DKVILRAEDKU	85	455.2394	3	45.54	1362.711	-10.4
bWQMMPjDQKU	85	497.2162	3	47.24	1488.643	-10.8
FTbGSMQDFKU	85	426.5239	3	47.99	1276.573	-17.8
FQLRMYAPVKU	85	417.9019	3	48.42	1250.696	-9.6
PAFjYNUGEKU	85	438.5297	3	50.05	1312.592	-18.6
XUDETLEQjKU	85	490.8815	3	50.33	1469.637	-9.4
PDEGAGFTAKU	85	496.2384	2	50.96	990.477	-14.9
YDLVTSjFCKU	85	642.2972	2	54.6	1282.599	-14.6
UGVQLRIEFKU	85	482.9146	3	55.29	1445.738	-11.1
GLBWEYRLCKU	85	361.1818	4	56.25	1440.714	-10.9
EFFYBNNNEKU	85	493.5451	3	57.92	1477.643	-19.9
RWMGCRCLYKU	85	488.2416	3	63.94	1461.719	-10.8
XGSSIECFBKU	85	564.2339	3	65.84	1689.7	-12.1
MMEMSLSSSKU	85	565.2477	2	66.71	1128.498	-14.9
NAAGAZSSGKU	85	478.726	2	71.12	955.4471	-10.2
FOQAVKAAjKU	85	425.5672	3	73.77	1273.676	2.7
NBRTCLVFQKU	85	461.5719	3	77.73	1381.709	-10.9
EMADYQSYiKU	85	684.2884	2	79.55	1366.573	-7.9
NENDGYVLOKU	85	627.796	2	80.08	1253.59	-10
SPLVLNAcHKU	85	586.3288	2	83.36	1170.659	-13.6
NDGTRKCQTKU	84	383.8601	3	24.98	1148.572	-11.7
SYRGWYWORKU	84	376.9377	4	25.1	1503.738	-11.2
KSMUYVLMSKU	84	422.5512	3	25.13	1264.642	-8.1
ENSDCYGALKU	84	549.7458	2	25.85	1097.481	-3.7
ZYPVGEDBHKU	84	471.8783	3	26.94	1412.627	-10.2
MSVVAHNNEKU	84	376.5224	3	29.98	1126.555	-8.8
YVGPPGEDQKU	84	544.7659	2	37	1087.53	-11.6
cOYNDJTXGKU	84	527.5525	3	40.09	1579.645	-5.8
KDDPQFPNSKU	84	392.196	3	40.43	1173.578	-9.9
VGANADSjMKU	84	550.7546	2	42.25	1099.505	-9.5
OSEJAVNJSKU	84	735.3207	2	44.53	1468.647	-13.6
AOLTBVAPVKU	84	319.9303	4	44.98	1275.7	-6.1
LNDMSCZDRKU	84	425.8555	3	48.81	1274.55	-3.8
ICCFTLEQjKU	84	490.8817	3	50.16	1469.626	-1.5
GYDDFMPNSKU	84	586.7479	2	55.09	1171.497	-13.4
PXYQADYXAKU	84	697.804	2	56.32	1393.602	-6.4
PGYYQEGYAKU	84	587.7711	2	56.56	1173.545	-15.1
FUXENCREGKU	84	510.5565	3	56.75	1528.673	-16.6
LNRiLAASDKU	84	407.5594	3	58.71	1219.654	1.8
MYGFMTLNMKU	84	412.1919	3	63.15	1233.571	-13.7

ObEFJEGRFKU	84	533.9131	3	63.44	1598.726	-5.3
LTZFEGESKKU	84	411.5445	3	63.6	1231.62	-6.4
ijDATDEMSKU	84	669.7747	2	64.81	1337.54	-3.5
FFAGYLGXGKU	84	589.787	2	66.55	1177.578	-15.6
FFAGYLEXGKU	84	625.796	2	68.88	1249.599	-17.3
MWLBbCDFLKU	84	516.5708	3	69.43	1546.708	-11.4
VFQZMMAQUKU	84	678.8126	2	69.9	1355.623	-9
FBEMFJWVOKU	84	433.4458	4	71.33	1729.769	-8.9
TEEGWVHcIKU	84	735.3368	2	78.54	1468.667	-5.3
WMAYDQNMMKU	84	658.7725	2	83.05	1315.551	-15.9
FFAXLGENYKU	84	654.3129	2	85.41	1306.621	-7.1
OQWWGELNMKU	84	697.8178	2	86.7	1393.646	-18.1
KPRARENUEKU	83	436.236	3	24.45	1305.701	-11.8
VYGGGHLKiKU	83	397.8807	3	26.77	1190.643	-18.8
KTHEMWYMWKU	83	480.2219	3	29.68	1437.669	-17.3
DVAGDJDVNKU	83	399.8501	3	32.32	1196.538	-7.8
LGSPGAZFEKU	83	367.1843	3	35.89	1098.546	-13.4
YVGPPPSDNKU	83	536.7686	2	36.38	1071.535	-11.5
LYMBCVMGRKU	83	458.8859	3	38.76	1373.657	-15.6
LKXSNGEbjKU	83	474.5638	3	39.49	1420.675	-3.5
MGGTQYNODKU	83	608.7572	2	39.5	1215.52	-16.8
SUPDCNQLYKU	83	465.5512	3	42.29	1393.644	-8.9
MFEDKXGMFKU	83	451.1986	3	42.3	1350.596	-16.3
PQVPMWGEDKU	83	395.859	3	49	1184.565	-8
MYGFMTCSTKU	83	389.8316	3	50.54	1166.492	-16.5
KVKPRBFMGKU	83	455.5948	3	51.54	1363.771	-6.2
PDWSMQFTAKU	83	403.8556	3	53.26	1208.565	-16.3
cAYUbVKNQKU	83	481.2384	3	54.1	1440.716	-15.5
GYDDiCCCSKU	83	613.7068	2	55.23	1225.407	-6.4
GYDiCCCDSKU	83	613.7066	2	55.31	1225.407	-6.8
MMAMWEjRCKU	83	465.1995	3	55.85	1392.589	-9.1
GLBWEYLCRKU	83	481.2405	3	56.33	1440.714	-9.6
MFiTAGEMMKU	83	639.7773	2	58.66	1277.547	-5.8
UPHLFSAWLKU	83	426.5627	3	63.12	1276.683	-12.9
iGDDFVLLIKU	83	477.5699	3	73.55	1429.696	-5.8
SUXEEVQLYKU	83	697.825	2	73.65	1393.649	-9.6
FBEFFJWVOKU	83	437.4517	4	75.96	1745.797	-11.1
XbMSMEXjWKU	83	559.8909	3	91.15	1676.662	-6.8
EMEGYQSWiKU	83	695.7971	2	91.38	1389.589	-6.6
KPOARAWFLKU	82	330.6939	4	28.08	1318.752	-4.3
VECSLRAAYKU	82	429.566	3	28.88	1285.684	-6.4
QAPRQACSGKU	82	596.808	2	30.01	1191.617	-13.4
STWAKADTRKU	82	388.209	3	30.09	1161.626	-17.6
SDDCNPYVVKU	82	569.7559	2	31.7	1137.513	-13.4
LKQQUVHPGKU	82	405.2315	3	33.31	1212.684	-9.2

DDHFAECOQKU	82	432.5153	3	33.33	1294.526	-1.5
SCTFMSDDKKU	82	387.5017	3	35.48	1159.5	-14.5
CQFQCVGNNKU	82	479.2253	3	35.8	1434.677	-16
VPMGAQFNYKU	82	385.1988	3	37.6	1152.575	-0.4
MKVLTADNFKU	82	389.2113	3	41.6	1164.633	-17.6
LEMGVTCAGKU	82	336.5065	3	44.36	1006.494	3.8
LiPNGVLLBKU	82	454.5872	3	47.1	1360.753	-10.1
PMAGGNEiTKU	82	569.2595	2	47.4	1136.515	-9.4
TEZFYPEKLKU	82	674.8446	2	54.48	1347.682	-5.7
YSQMSYAMMKU	82	619.7672	2	57.47	1237.529	-7.6
CcPLMYVOEKU	82	382.6823	4	58.17	1526.723	-15.2
YYVNQUDOAKU	82	461.8786	3	58.61	1382.623	-6.3
YYVGGMLbXKU	82	456.5466	3	59.41	1366.642	-17.5
LAVLIMYIAKU	82	497.2543	3	63.4	1488.75	-6.2
QESFOSGEVKU	82	405.1929	3	71.5	1212.564	-5.4
UPFLFSKNQKU	82	644.3451	2	87.79	1286.688	-9.8
VPLLVZDOBKU	82	486.2563	3	92.78	1455.754	-4.5
DWPLLCPXIKU	82	741.3439	2	106.67	1480.689	-10.2
VSEAQjDMAKU	81	593.7718	2	24.02	1185.542	-10.7
SGMDTTCOVKU	81	431.5303	3	25.38	1291.579	-7.8
RCKYcCYNDKU	81	384.1783	4	25.74	1532.698	-8.6
KVTSCTiZDKU	81	437.2039	3	26.53	1308.6	-7.7
TGQGGGWYiKU	81	396.1846	3	28.09	1185.544	-9.6
EMDKSQAPDKU	81	383.1788	3	30.29	1146.534	-17
XDGVLKVGEKU	81	388.5445	3	35.9	1162.621	-7.6
LAAKQWWOWKU	81	473.9196	3	37.11	1418.747	-7.2
PPEODCSSGKU	81	561.7318	2	38.39	1121.467	-16.1
VTCLTDNiVKU	81	409.2038	3	41.51	1224.604	-11.8
KVIEMQLQVKU	81	464.9149	3	44.18	1391.745	-15.6
NMFLMKXVVKU	81	443.5692	3	46.34	1327.7	-11.1
CMLSZFDNVKU	81	417.5236	3	46.38	1249.558	-7.6
PTYAETTMSKU	81	564.2657	2	48.44	1126.533	-14.2
MAMWEjTSAKU	81	631.7783	2	48.83	1261.555	-10.7
PARPMEGWDKU	81	395.859	3	49	1184.576	-17.5
MYAQPMGQFKU	81	600.2808	2	49.34	1198.563	-13.2
AGQOGYjLcKU	81	671.8226	2	52.28	1341.638	-5.3
LBjPMMYYQKU	81	519.5757	3	60.82	1555.709	-2.3
FFAGYLAXGKU	81	596.795	2	68.5	1191.594	-15.3
MMFLKYYACKU	81	432.8793	3	69.05	1295.623	-5.3
NYETTYDMVKU	81	631.778	2	71.38	1261.565	-18.7
EGMEMSLOGKU	81	592.7656	2	78.17	1183.523	-5.1
KWWMSCPWWKU	81	479.5633	3	81.69	1435.668	-0.1
IRQQMGFVDKU	81	699.8371	2	84.59	1397.673	-9.3
PTHEFMiLPKU	80	333.9173	4	23.94	1331.656	-12
jKVMDGYQGKU	80	411.868	3	24.12	1232.594	-9.8

KQEKIVEAGKU	80	436.2352	3	24.57	1305.689	-4.1
FGQQLQEMMKU	80	413.5316	3	27.29	1237.595	-17.5
DMSOAGAFIKU	80	440.8618	3	27.38	1319.568	-3.4
XNGUPLMTHKU	80	432.871	3	28.59	1295.605	-10.9
VGANAYECYKU	80	558.7505	2	30.42	1115.507	-18.2
VLCFAAFSYKU	80	324.6733	4	31.65	1294.678	-10.3
DQYYDAHWKKU	80	451.5483	3	32.33	1351.631	-5.8
KMESAKEjOKU	80	341.4206	4	32.49	1361.659	-4.3
QOASDRRFGKU	80	423.219	3	32.49	1266.644	-7
VDOYCFNSMKU	80	365.1611	4	33.42	1456.637	-15
KALNPMMNLKU	80	290.415	4	34.2	1157.641	-9.1
GTQDASKGKKU	80	340.19	3	36.58	1017.557	-8.4
RWILPGSVMKU	80	455.2401	3	38.45	1362.708	-7.1
GGMPNVLLVKU	80	342.8689	3	39.79	1025.606	-20
ESCTWYTKXKU	80	455.5405	3	42.49	1363.609	-7
YASYMMASEKU	80	590.2526	2	46.58	1178.51	-16.5
PAGVDEZjDKU	80	411.8525	3	49.05	1232.539	-3
LNWPMDZVAKU	80	423.2083	3	52.36	1266.618	-11.8
MVAFMERTLKU	80	408.8887	3	52.67	1223.652	-6.1
DQYYWHNKKKU	80	470.2354	3	52.78	1407.705	-14.6
VcEQDSUVYKU	80	670.8118	2	54.74	1339.624	-10.9
VcETDYMVYKU	80	670.8118	2	54.74	1339.62	-8.1
PXYGAADYAKU	80	587.7712	2	56.47	1173.532	-3.1
EDQGEJVFQKU	80	672.8	2	61.72	1343.606	-15.4
XADDFVLLQKU	80	423.216	3	65.07	1266.647	-16.2
bMGMEHQjbKU	80	502.2166	3	65.16	1503.635	-4.8
ACGVQWIDLKU	80	437.2103	3	66.93	1308.614	-3.7
VCYVMZbEDKU	80	699.8027	2	71	1397.592	-1
NWYZDGGGFKU	80	413.1811	3	71.84	1236.531	-8
PYRYFQNSSKU	79	322.9151	4	24.33	1287.636	-3.7
LEHALLRAHKU	79	297.4313	4	24.39	1185.71	-11.2
EGbTFAVNKKU	79	404.2153	3	25.74	1209.632	-6.6
UFCDHAFVGKU	79	401.5199	3	28.31	1201.545	-6.2
KEXVNYDYEKU	79	469.5514	3	28.33	1405.638	-3.7
GAAPELLJEKU	79	398.2061	3	30.18	1191.62	-19.9
PIcPFNSYTKU	79	479.8911	3	34.54	1436.666	-9.8
MGMjEAbKMKU	79	451.2035	3	34.69	1350.603	-10.8
XFXiVRTGDKU	79	499.2296	3	35.3	1494.684	-11.6
MGLOcNSADKU	79	411.5202	3	37.39	1231.56	-16.8
NMPGGVLLVKU	79	342.869	3	39.69	1025.606	-19.6
PTFEFWEFLKU	79	448.2239	3	48.07	1341.676	-19.2
PAMjFVDADKU	79	401.1906	3	49.24	1200.557	-5.6
TLPKFNKTGKU	79	378.2296	3	49.27	1131.676	-8.1
LLKVAGYXbKU	79	443.5789	3	50.3	1327.733	-13.7
QKEFBEWEQKU	79	382.1794	4	50.55	1524.716	-18.4

LWUQQEQGKKU	79	441.8997	3	51.09	1322.684	-5.2
ZDDNABFMGKU	79	456.1907	3	51.61	1365.557	-5.3
EGMYQRcYYKU	79	477.5591	3	52.4	1429.653	1.8
ciFCVELAGKU	79	481.2392	3	53.88	1440.705	-6.4
EKYFCMFNMKU	79	447.2	3	54.11	1338.592	-10.6
SMHQUDFTYKU	79	445.8638	3	54.43	1334.583	-9.7
VcPCGCMVYKU	79	670.812	2	55.01	1339.62	-7.9
FKDTYKSSVKU	79	401.2174	3	58.4	1200.65	-16.4
SMEMSLSSSKU	79	543.2441	2	59.99	1084.489	-14.4
WCTLNAYGEKU	79	592.2823	2	65.24	1182.549	0.9
TVSWIZjVVKU	79	504.9136	3	68.4	1511.734	-10.1
ADASFXQEVKU	79	607.2866	2	71.58	1212.564	-4
YFKYACSbWKU	79	706.8279	2	72.82	1411.656	-10.6
bCFLSVMOGKU	79	435.8759	3	73.78	1304.609	-2
DSVFLYZMTKU	79	649.3088	2	77.61	1296.617	-10.8
TZFLSVYDNKU	79	640.8077	2	81.22	1279.62	-14.7
ZYPVGENOjKU	78	471.8781	3	26.54	1412.63	-12.7
KYbCSQQJYKU	78	510.8956	3	26.96	1529.686	-13.6
TDOQQFELYKU	78	458.884	3	27.86	1373.648	-12.5
TCKUQLMPSKU	78	454.9005	3	29.09	1361.694	-10.3
LETJFLDTNKU	78	449.2235	3	30.97	1344.663	-10.5
PNLBMSGGTKU	78	393.5258	3	31.49	1177.572	-13.5
YKYEGTiWHKU	78	361.9221	4	33.43	1443.68	-14.6
ZTVVHXWODKU	78	501.5598	3	33.43	1501.682	-16.5
YNCMVALBRKU	78	457.8925	3	33.66	1370.675	-14.3
KLNAPMMNLKU	78	290.415	4	34.09	1157.641	-9.1
STLDSPHMEKU	78	572.2679	2	35.11	1142.539	-15.5
KGbcLCFAGKU	78	346.4296	4	35.19	1381.71	-15.1
PPERCCDSGKU	78	545.7374	2	38.42	1089.47	-8.5
PDLGGANUQKU	78	539.77	2	38.82	1077.532	-5.6
KjNWRGbjMKU	78	389.4374	4	39.69	1553.743	-14.5
CGTTQYNODKU	78	616.7542	2	39.8	1231.515	-17.4
ASCTQYNODKU	78	616.7538	2	39.91	1231.515	-17.9
KQObFGYNQKU	78	478.5664	3	41.96	1432.693	-10.8
PAEDRWGEDKU	78	401.1896	3	43.22	1200.552	-4.4
EGGEXNMSGKU	78	564.2346	2	43.99	1126.457	-2.3
LNFBEQLQVKU	78	348.9379	4	44.29	1391.736	-9.9
CVQMCAFFDKU	78	669.7983	2	46.57	1337.596	-10.5
OXRPDDjDQKU	78	502.5481	3	47.39	1504.639	-10.7
GASEMICVFKU	78	470.5439	3	48.16	1408.636	-18.6
UNVLSRTIDKU	78	468.2346	3	48.56	1401.697	-10.4
jMMSGZSDLKU	78	424.5169	3	49.97	1270.541	-9.2
EGMYQYRcYKU	78	477.5594	3	52.3	1429.653	2.4
KAGESCiLGKU	78	563.2762	2	52.91	1124.552	-12.2
EjCPSLWOCKU	78	459.8679	3	53.18	1376.584	-1.4

KYYDDCMVYKU	78	492.2207	3	54.82	1473.666	-17.6
YNHLFSKNQKU	78	426.5627	3	63.12	1276.668	-1
EGRMXiLLYKU	78	488.2408	3	63.83	1461.717	-11
OGMYFcQCFKU	78	784.8489	2	66.93	1567.692	-5.8
OQADGELNMKU	78	604.7818	2	68.11	1207.552	-2
NNNFADESKKU	78	583.2761	2	69.46	1164.552	-12.5
WGUPCGFGQKU	78	579.7596	2	74.54	1157.519	-12.3
NDGTRVMMVKU	78	575.2874	2	75.08	1148.579	-16.6
AYNDASDLMKU	78	563.7549	2	75.16	1125.513	-15.2
iCSCTAYQVKU	78	618.2656	2	87.72	1234.534	-14.3
VPLLVcNEbKU	78	661.8631	2	92.96	1321.729	-13.1
ODSGSYXAGKU	78	604.2567	2	101.14	1206.503	-3.2
MCYRGJDRDKU	77	389.9282	4	25.48	1555.697	-8.6
GjQPKCVGNKU	77	569.7855	2	30.28	1137.568	-10.4
DPSXNYSEVKU	77	419.8554	3	33.07	1256.553	-7
STLDSHMPEKU	77	572.2678	2	34.95	1142.539	-15.7
STLDSUGQEKU	77	572.2681	2	35.02	1142.532	-8.7
MYEDCYRNFKU	77	456.5294	3	35.97	1366.58	-9.7
LNYMPDWHDKU	77	439.8701	3	37.97	1316.597	-6.5
FAPZJAGHZKU	77	461.5453	3	38.86	1381.623	-6.8
MPVSUGDPJKU	77	638.2935	2	39.16	1274.578	-4.5
PWZCSPKENKU	77	428.2019	3	42.87	1281.593	-6.7
NMFLMKLbSKU	77	443.5696	3	46.46	1327.696	-6.7
iFPMSYAMMKU	77	446.867	3	46.57	1337.584	-3.3
TNECOMCVFKU	77	475.8752	3	48.21	1424.614	-7.3
EDAGADJFQKU	77	623.2685	2	50.06	1244.538	-12.4
jMMSGYAFEKU	77	636.2743	2	50.1	1270.544	-8.2
FMVVBPIWOKU	77	419.699	4	50.67	1674.79	-13.6
OEGMYWAQWKU	77	467.8789	3	52.13	1400.62	-3.4
EjPCSLWCOKU	77	459.8667	3	53.27	1376.584	-3.9
HHLSZFDVNKU	77	430.8796	3	55.43	1289.627	-7.3
YDAYTQEMMKU	77	639.7772	2	58.76	1277.542	-1.6
VPLLVWATCKU	77	376.8858	3	61.42	1127.653	-15
CILTSTCPTKU	77	696.3297	2	64.59	1390.647	-1.3
AYECAcAFQKU	77	612.2767	2	66.97	1222.552	-10.7
MRADPESXJKU	77	473.5457	3	69.84	1417.623	-5
GGADYXOGFKU	77	413.1811	3	71.77	1236.528	-5.5
KCUPYSKLEKU	77	425.5551	3	75.06	1273.66	-13.1
ZSLGADEXcKU	77	664.2933	2	83.4	1326.578	-4.6
AUAYGEMMDKU	77	597.7453	2	88.62	1193.496	-16.6
ZSLGADEiUKU	77	664.2943	2	95.32	1326.582	-6.1
QNHALLKVHKU	76	297.4313	4	24.39	1185.71	-11.2
LNSPADCDLKU	76	537.7581	2	24.6	1073.518	-14.8
PSGSZGMAGKU	76	493.2245	2	25.33	984.4447	-10.4
QTMAGGQcUKU	76	597.2722	2	27.53	1192.549	-15.8

KPFQRAWFLKU	76	330.6942	4	27.99	1318.766	-14
KbKCRQYEFKU	76	362.4371	4	28.95	1445.742	-15.6
PNLAOQMGTKU	76	388.1942	3	31.43	1161.583	-18.8
TYVLEHMDQKU	76	421.5389	3	32.06	1261.613	-14.1
KGMRRDSiGKU	76	423.2188	3	32.38	1266.648	-10.9
NYGDPQQHNKU	76	600.2761	2	38.11	1198.548	-8.5
YjKCQjYDMKU	76	748.3107	2	39.11	1494.633	-17.2
MNTGAYNODKU	76	608.7574	2	39.65	1215.52	-16.5
DGQCPTWFGKU	76	429.1972	3	39.98	1284.595	-19.9
DGQcGPTWOKU	76	429.1983	3	40.09	1284.583	-7.5
PWZCSLQWGKU	76	433.5337	3	42.72	1297.603	-18
CUcMTWYTCKU	76	704.7883	2	44.46	1407.56	1.3
PLYDWHCSPKU	76	415.5272	3	44.88	1243.581	-16.9
LYCDKMFiNKU	76	771.8685	2	45.05	1541.727	-2.9
KIKNCVAPVKU	76	319.9301	4	45.09	1275.697	-4.7
CVAGMSiFDKU	76	669.7983	2	46.57	1337.601	-13.8
QbWMMPjDQKU	76	497.217	3	47.42	1488.643	-9.1
HQDGCUFNFKU	76	637.7719	2	48.9	1273.541	-9.2
MMAEANCEKKU	76	434.5371	3	49.5	1300.597	-5.8
LNJWQEWEQKU	76	509.2381	3	50.76	1524.707	-9.2
MMAMWEiYAKU	76	465.1995	3	55.85	1392.59	-9.2
YLGAFPDSSKU	76	542.2711	2	59.03	1082.54	-11.1
PEDbGINFMKU	76	482.5361	3	59.64	1444.611	-17.2
EDQADJVOAKU	76	672.8	2	61.67	1343.592	-5.1
SPLVLNAGEKU	76	513.7935	2	64.28	1025.587	-14.1
BMMMVLLGAKU	76	634.3214	2	65.09	1266.645	-13.4
MDEMSLSSSKU	76	557.2407	2	66.33	1112.484	-15.5
RVEONGGLFKU	76	611.8251	2	68.09	1221.648	-10.1
MMFLKMZSSKU	76	648.8163	2	69.15	1295.619	-0.6
NWYTCYGGFKU	76	413.1811	3	71.85	1236.539	-13.9
XSDDFVLLIKU	76	482.9008	3	73.81	1445.69	-6.7
MOPWLFEXDKU	76	496.8865	3	75.52	1487.663	-17
ZMMEMSLOGKU	76	662.7872	2	75.97	1323.564	-2.7
YcLDJEGGXKU	76	730.8116	2	79.52	1459.627	-12.1
NKHPSLKVHKU	75	297.4313	4	24.53	1185.71	-11.4
QTMANQWGMKU	75	597.2737	2	27.84	1192.548	-12.7
QPRANLLcQKU	75	315.9331	4	28.19	1259.718	-11.6
FYASMXNATKU	75	417.8536	3	29.11	1250.561	-17.7
HSKVCKJMVKU	75	491.5926	3	31.02	1471.774	-12.2
CEWFHCYNDKU	75	497.8743	3	31.87	1490.61	-6.1
MTLAERFAHKU	75	401.549	3	32.07	1201.639	-11.6
KSMLDNFELKU	75	408.5478	3	32.76	1222.638	-13.4
DPTVPSPMGKU	75	514.2587	2	33.67	1026.517	-13.7
AXPVOYMADKU	75	439.8676	3	36.37	1316.595	-10.4
VGYPTDNiVKU	75	409.2041	3	41.61	1224.601	-8.3

LTVGUBXNQKU	75	478.566	3	41.82	1432.687	-7.7
VQNAUGCAMKU	75	550.7548	2	42.14	1099.502	-5.8
FLFDCSYEOKU	75	452.1985	3	46.72	1353.592	-13.8
LNSAALEZNKU	75	385.1995	3	47.01	1152.589	-10.3
WSYTHGiTKKU	75	447.5536	3	49.77	1339.654	-11.3
NEMQNQFTAKU	75	403.8564	3	53.38	1208.561	-11.1
JScEGELPDKU	75	667.2971	2	53.54	1332.598	-13.9
YLTGPFSDGKU	75	542.2712	2	58.94	1082.54	-10.8
QWcWOQDFVKU	75	511.9091	3	62.53	1532.714	-5.5
MYGFMTTWAKU	75	412.1912	3	63.29	1233.567	-12.7
ZCMPYELKIKU	75	748.8423	2	63.96	1495.68	-7
GQKYNjOMFKU	75	476.5541	3	64.88	1426.665	-16.9
ijDATECETKU	75	669.7741	2	64.99	1337.54	-4.4
EEDOSGKbWKU	75	467.2103	3	65.5	1398.625	-11
KUOCCSQYYKU	75	469.1957	3	67.6	1404.593	-19.5
jTKYASCbWKU	75	706.8268	2	73	1411.649	-7.4
MWLSGbMMLKU	75	438.5442	3	74.3	1312.631	-15.6
ZCLPYSKLEKU	75	425.5552	3	74.88	1273.649	-4
YbPQSTFVDKU	75	651.3109	2	77.28	1300.627	-14.9
MAGELGYQDKU	75	555.7639	2	77.49	1109.518	-3.9
MAEGLGYNEKU	75	555.7655	2	77.69	1109.518	-1
XTLKOHAiYKU	75	506.5831	3	88.93	1516.742	-9.3
SKCDSVMFNKU	75	435.8761	3	91	1304.625	-13.9
DOSGSYGiGKU	75	604.2564	2	101.09	1206.503	-4.1
VSEAQjCDVKU	74	593.7697	2	24.17	1185.542	-14.3
KVTCTSiZDKU	74	437.2044	3	26.3	1308.6	-6.5
TITFAGPGVKU	74	584.2991	2	26.93	1166.594	-8.4
SSAAPPCQVKU	74	493.7525	2	27.27	985.5015	-11.2
TDZDQVNAAKU	74	385.8475	3	27.5	1154.532	-9.3
MSVVANANZKU	74	564.28	2	30.53	1126.555	-8.8
KGRZXLDTNKU	74	449.2242	3	31.19	1344.676	-18.6
KNKbFDTGGKU	74	404.5463	3	31.2	1210.627	-8.5
VEKSCAFWAKU	74	584.295	2	33.31	1166.591	-13
YTNCZHQWEKU	74	468.198	3	33.94	1401.588	-11.5
MLVENGPVGKU	74	348.1889	3	34.19	1041.564	-18.3
DDHFMSSWQKU	74	427.1833	3	34.65	1278.545	-13.3
KGDCCZLCcKU	74	469.2015	3	34.82	1404.606	-16.6
DASbLKVGEKU	74	388.5443	3	35.63	1162.616	-4.5
jTHVAEAJYKU	74	348.918	4	36.41	1391.651	-5.8
DDPVVEKMPKU	74	386.2041	3	36.68	1155.596	-4.6
CVLUDGSYAKU	74	641.8123	2	37.06	1281.617	-5.2
LKXSNWSMjKU	74	474.5637	3	39.4	1420.675	-4.2
DMOVVAGFTKU	74	390.8663	3	41.25	1169.576	0.6
HKACiJSSHKU	74	466.2148	3	44.55	1395.629	-4.6
FQLRDQFPVKU	74	426.2386	3	44.95	1275.709	-11.7

PWJSPKGEGKU	74	417.5389	3	45.44	1249.616	-16.9
YEUQWDMLSKU	74	460.209	3	46.25	1377.614	-6
TNEMIGcVFKU	74	470.5446	3	47.88	1408.638	-18.4
LNMFVRTGDKU	74	393.8748	3	48.33	1178.623	-17.3
FQFVLOAPVKU	74	417.9017	3	48.34	1250.704	-16.3
jMMSGYEAFKU	74	424.5179	3	50.07	1270.544	-9.9
VGAMCFAFDKU	74	544.2488	2	50.6	1086.499	-14.6
PMAMWEcHHKU	74	453.8703	3	51.71	1358.609	-14.8
YSADTKMPMKU	74	390.8578	3	52.63	1169.557	-4.8
MKSYKHSYFKU	74	439.8894	3	62.89	1316.67	-17.9
ijDATMDSPKU	74	653.7788	2	65.08	1305.55	-5
bMGMEHFHHKU	74	685.8054	2	65.21	1369.599	-1.9
ONDUGGFTYKU	74	642.7814	2	67.02	1283.554	-4.8
SSGVQQANXKU	74	569.2714	2	68	1136.544	-13.4
PCDFciLPVKU	74	498.5862	3	73.22	1492.736	0.5
ZKEESVMFNKU	74	435.8759	3	74.94	1304.618	-9.6
NDGTRQKCTKU	74	575.2874	2	75.08	1148.572	-10.2
DMCSAKEJFKU	74	491.2183	3	75.73	1470.658	-17
NEGODDHiQKU	74	460.5233	3	76.98	1378.563	-10.8
jDELWLDEGKU	74	656.8012	2	86.59	1311.606	-14.2
UPFLQHPLEKU	74	644.3453	2	87.73	1286.688	-9.4
KiLIHAFSYKU	74	506.5826	3	89.03	1516.755	-18.9
FMADALGWXKU	74	629.2974	2	90.76	1256.587	-5.6
VQCLLVcWBKU	74	486.2563	3	92.7	1455.758	-7.3
PTHEFMHcLKU	73	333.9179	4	24.23	1331.652	-7.3
KIHEENAKSKU	73	454.226	3	25.36	1359.675	-13.6
ELLTFCDMTKU	73	400.5243	3	25.41	1198.573	-18
ENSDPGCHLKU	73	549.747	2	25.63	1097.492	-11.8
LYMKYcJNDKU	73	384.1786	4	25.88	1532.712	-17.2
KYBCTGQJYKU	73	383.4232	4	26.93	1529.684	-13.4
GVLPEENiWKU	73	435.5531	3	29.82	1303.643	-4.2
EMDELTPGEKU	73	574.2639	2	30.4	1146.523	-8.3
TNFOYCANjKU	73	458.1994	3	32.39	1371.586	-7.1
DDHFWTCTQKU	73	427.1839	3	33.16	1278.545	-11.9
LNGMSiDYEKU	73	645.2869	2	36.36	1288.563	-2.5
NATGESKGKKU	73	340.1901	3	36.69	1017.557	-8.1
MXFMTSSCAKU	73	408.8392	3	37.85	1223.5	-3.2
KADBLEVGLKU	73	416.2349	3	37.87	1245.688	-4.4
MYOMTASCSKU	73	408.8387	3	38.04	1223.5	-4.4
GEFRTHQWMKU	73	440.2175	3	39.3	1317.64	-7.2
MNTQUTPCDKU	73	608.7569	2	39.74	1215.513	-10.9
MKVLTDGQFKU	73	389.2113	3	41.6	1164.633	-17.6
CVYCYZNZKKU	73	519.9015	3	49.1	1556.69	-4.4
ZOQLEQTCFKU	73	465.5481	3	51.12	1393.631	-6
XDDFMPGGSKU	73	586.7481	2	55.17	1171.483	-1.1

NYPMNNBWKKU	73	490.2327	3	55.53	1467.688	-8.2
DbMDAEjKMKU	73	465.1997	3	55.73	1392.595	-12.9
SYGAMSiFDKU	73	619.7672	2	57.47	1237.531	-8.6
DQDOUDTAQKU	73	435.192	3	58.27	1302.545	7
PXYAGDAYJKU	73	685.3001	2	59.87	1368.592	-4.3
PXYQADYZAKU	73	685.3001	2	59.88	1368.596	-7.5
AYQJCAFGAKU	73	612.2767	2	66.88	1222.551	-9.7
LZFDQEEIVKU	73	498.2304	3	71.78	1491.685	-10.1
WTbZNGWOFKU	73	518.9019	3	72.49	1553.688	-2.7
FQQJJTFEYKU	73	541.2451	3	74.43	1620.723	-6.1
jSFLSVMOGKU	73	640.8087	2	81.31	1279.621	-14.4
LAVDVZZMGKU	73	611.3015	2	84.37	1220.597	-7.1
YTSPNAWHjKU	73	656.3096	2	84.52	1310.613	-6.1
EZELPiDDSKU	73	680.7932	2	86.11	1359.581	-6.7
ZDYVLETjiKU	73	752.8436	2	102.66	1503.683	-6.9
TCbFQSTBTKU	73	704.3112	2	118.97	1406.627	-13.6
KHKYDGVBLKU	72	341.1898	4	23.12	1360.742	-8.6
KLKVACbGjKU	72	424.9002	3	23.95	1271.696	-13.3
CVGAVWNVEKU	72	417.8849	3	27.46	1250.647	-11.5
RjCCPLMTHKU	72	432.8709	3	28.74	1295.602	-8.6
GVSDVFRDMKU	72	384.8663	3	29.65	1151.576	1.3
PNLKMQACMKU	72	388.1951	3	31.34	1161.582	-15.9
KYSFRAFSYKU	72	324.6729	4	32.01	1294.682	-15
KARDLSDNLKU	72	386.8848	3	34.01	1157.652	-16.5
MLVQGDPVGKU	72	348.1889	3	34.04	1041.564	-18.4
YiVLNCAPAKU	72	453.9007	3	34.72	1358.691	-8.2
jTHVNFEFYKU	72	464.8886	3	36.4	1391.659	-10.9
jTHVMRCFYKU	72	464.8885	3	36.49	1391.656	-9
MYOMTSTCGKU	72	408.8388	3	37.95	1223.5	-4.3
KVTLNMiZDKU	72	459.5641	3	38.27	1375.679	-5.9
LYMBWMGVGKU	72	340.4185	4	38.84	1357.648	-2
VDGVQVUbCKU	72	415.5376	3	39.2	1243.595	-3.1
cTAYNANVjKU	72	428.2056	3	40.38	1281.615	-15.8
TVPDMQFCAKU	72	569.7644	2	41.03	1137.531	-14.7
TMPDGMCTYKU	72	573.2352	2	42.52	1144.471	-13.6
DTADYTKYGKU	72	580.7736	2	45.18	1159.551	-15.9
DRWJETEQRKU	72	378.9329	4	45.21	1511.719	-10.7
WQYEABFMGKU	72	478.5509	3	47.43	1432.64	-6.4
MGMjEPJLKKU	72	469.8905	3	50.08	1406.673	-16.2
ALTDFHQEMKU	72	406.8629	3	50.23	1217.586	-15.9
SYLETEQDAKU	72	591.7822	2	51.29	1181.556	-5.5
PDWbSSTTAKU	72	403.8566	3	53.19	1208.564	-13.4
VcEQcGTEYKU	72	670.8119	2	54.83	1339.62	-8.3
SMLSZMMVNKU	72	412.1926	3	55.44	1233.567	-8.9
DKJYXDAJDKU	72	535.891	3	55.89	1604.663	-7.3

WGDRYCDGAKU	72	585.2593	2	58.55	1168.508	-3.6
NMEMSLSSSKU	72	556.7492	2	60.48	1111.5	-14.7
KDMJZGYMDKU	72	483.1989	3	60.8	1446.598	-15.8
VMEMSLSSSKU	72	549.2618	2	63.43	1096.526	-15.1
YWMAVMVXHKU	72	461.8817	3	68.24	1382.649	-18.3
EDKcWMAGFKU	72	652.8066	2	68.51	1303.61	-8.5
LMEMSLSSSKU	72	556.2693	2	68.86	1110.541	-15.4
DZFFPAPMRKU	72	434.8784	3	71.87	1301.634	-15.6
cCCHFVLLIKU	72	482.9008	3	73.81	1445.688	-5.2
TEWADVHcIKU	72	490.5594	3	78.53	1468.667	-7.1
EMWYQCFFSKU	72	684.2886	2	79.64	1366.584	-15.4
NENGYDVLOKU	72	627.796	2	80.08	1253.59	-10
NENTGEFLOKU	72	627.7958	2	80.22	1253.59	-10.3
UXYETFJADKU	72	513.553	3	81.63	1537.64	-2
LcSEDTMjBKU	72	500.8893	3	81.89	1499.657	-7.1
LAVDVFWNCKU	72	597.3045	2	84.62	1192.606	-9.8
FFAGYSRMYKU	72	634.8077	2	85.42	1267.617	-12.8
XHDLGWEXcKU	72	506.5627	3	95.18	1516.654	8.3
XNMACMMTQKU	72	712.7953	2	106.45	1423.597	-14.9
NNVADRYCRKU	71	413.2107	3	23.76	1236.615	-3.5
GYVASQcUXKU	71	449.2079	3	26.35	1344.615	-9.7
TYQTSSTPRKU	71	389.8677	3	26.88	1166.604	-19.6
LPBYDDRQNKU	71	474.8966	3	27.59	1421.685	-12.2
KMPcMWTVEKU	71	336.4189	4	28.47	1341.665	-14
ZTVVHZMZOKU	71	501.5587	3	29.67	1501.675	-13.4
STADAKWEKKU	71	388.209	3	30.09	1161.614	-7.9
SDDEGAbTVKU	71	569.7559	2	31.71	1137.512	-12.8
WbSNRVGFGKU	71	423.2171	3	32.27	1266.644	-11.3
LBSAKCPZFKU	71	341.4206	4	32.49	1361.672	-13.4
TNFOYGQCjKU	71	458.1998	3	32.51	1371.586	-6.3
AMPALEGVLKU	71	343.2034	3	32.58	1026.59	-1.2
KGbPKDKDQKU	71	420.8979	3	32.6	1259.68	-6.5
VNEDDGVGTKU	71	516.7442	2	35.38	1031.488	-14
GKMNARQFLKU	71	397.8924	3	37.06	1190.671	-12.8
ZTVVXNEFDKU	71	455.8745	3	37.6	1364.622	-14.9
AFGAMGFTQKU	71	528.7612	2	37.94	1055.522	-13.7
KVTWDYKZDKU	71	459.5641	3	38.38	1375.689	-13.2
YAFPEQYDKKU	71	429.8785	3	39.67	1286.629	-12.1
DYTVPMPSGKU	71	547.264	2	42.62	1092.527	-12.8
NGSDEGIVVKU	71	597.7858	2	44.9	1193.553	3.7
ALDMDSUiMKU	71	662.2809	2	44.92	1322.561	-10.6
DNESYDbSEKU	71	652.2651	2	49.41	1302.518	-1.8
KFMDWAVKQKU	71	427.2307	3	49.6	1278.691	-16
MSVVAGGNEKU	71	495.7534	2	49.81	989.4964	-4.1
KVGXKMRWLKU	71	455.595	3	51.34	1363.777	-10.1

LNZWDPMVAKU	71	423.2083	3	52.47	1266.618	-11.8
YSWTKGGNMKU	71	390.8579	3	52.74	1169.565	-11.4
QQbjQSHJQKU	71	525.9037	3	52.89	1574.708	-11.9
YDYFYPKELKU	71	455.5613	3	54.64	1363.681	-13.9
TVSMYSVMNKU	71	579.7793	2	54.77	1157.557	-11.5
YNLDPMZJKKU	71	490.233	3	55.32	1467.689	-7.8
VKWQEGQcEKU	71	442.2246	3	59.88	1323.665	-9.9
EMEMSLSSSKU	71	564.2472	2	61.72	1126.5	-17.7
UPHLFARTEKU	71	426.5624	3	63.46	1276.679	-10.4
ACTKTSjSYKU	71	598.7842	2	67	1195.563	-7.2
CAGVQWWFWKU	71	655.313	2	67.12	1308.623	-8.4
KYUGCCAIYKU	71	469.1968	3	67.76	1404.592	-16.5
EDKSFGXQFKU	71	652.8059	2	68.79	1303.606	-6.5
KNCLSDOEVKU	71	462.8957	3	69.37	1385.687	-15.3
PUPDZSDMVKU	71	631.778	2	71.28	1261.551	-7.6
XDEGFVLLIKU	71	477.5696	3	73.73	1429.695	-5.7
GANWUBQBFKU	71	790.353	2	80.8	1578.708	-10.6
FMAWLYGNEKU	71	629.2978	2	91.2	1256.601	-16
ASCCWWVcIKU	71	489.5521	3	95.2	1465.62	9.6
XSDFQSTBTKU	71	704.3111	2	119.52	1406.613	-3.7

Library QC sample 2

U = C-terminal amide, B = DabA,C = DabC, I = DabG, J = DabT, O = AlaA, U = AlaC, X = AlaG, Z = AlaT, b = hAlaA, c = hAlaC, i = hAlaG, j = hAlaT

Peptide	*ALC (%)*	*m/z*	*z*	*RT*	*Mass*	*ppm*
LNbVPMTDJKU	99	467.5568	3	41.42	1399.669	-14.5
OGFDLSHTEKU	99	412.8596	3	55.79	1235.58	-18.3
PPMESMSAMKU	98	369.8318	3	27.29	1106.492	-16.9
ZDERQUSQMKU	98	465.8722	3	32.63	1394.611	-11.5
VGVPVLWGEKU	98	361.5452	3	37.22	1081.628	-13.5
jPQRCYEMMKU	98	465.2047	3	43.03	1392.607	-10.7
QELQDYYKGKU	98	424.2114	3	43.8	1269.635	-18.1
PYFJEYSYLKU	98	492.2309	3	48.59	1473.689	-12
AYPNFLMPHKU	98	406.2074	3	50.85	1215.622	-18.1
AYPNFPMVHKU	98	401.5353	3	52.22	1201.607	-18.9
DSATEVGWMKU	97	561.759	2	24.6	1121.518	-12.5
LVGVNRONYKU	97	317.1764	4	25.01	1264.69	-10.8
APVEAGWAFKU	97	358.8577	3	27.47	1073.566	-13.4
ASNLPEECJKU	97	628.2813	2	28.85	1254.562	-10.9
FCGSQWVEKKU	97	404.1996	3	28.92	1209.596	-16.1
GVNTVYDYYKU	97	407.5325	3	29.6	1219.587	-9.7
DHFNQQFDJKU	97	481.882	3	30.83	1442.628	-3
DXVQYQKWAKU	97	462.232	3	33.27	1383.679	-3.8
FHGVAYVFXKU	97	429.5515	3	38.6	1285.647	-11
FLNAGQSSSKU	97	519.2648	2	44.01	1036.53	-14.5
WNKLDTFPMKU	97	426.886	3	51.11	1277.659	-17.9
YDLSYNjSBKU	97	491.5511	3	51.93	1471.65	-12.9
DAFFNPDPcKU	97	415.2008	3	56.74	1242.575	4.5
TjOGGYLQVKU	97	639.3158	2	61.41	1276.639	-17.5
PVVGELDVQKU	97	541.8057	2	61.96	1081.613	-15
ZEYDTSFBFKU	97	502.5467	3	63.75	1504.642	-16
LYYRLSMPYKU	97	444.9071	3	64.64	1331.706	-4.9
KYAPFFDAYKU	97	416.8812	3	83.71	1247.634	-9.6
TKGSQQLDYKU	96	389.537	3	29.44	1165.609	-17.2
GVEMVPMEcKU	96	404.8606	3	35.57	1211.576	-13.2
GVEETVEEcKU	96	404.8596	3	35.67	1211.575	-14.7
QMEFYADLbKU	96	454.5433	3	36.98	1360.63	-16.1
KSHTYDQLSKU	96	402.5405	3	41.64	1204.62	-17.1
VNFDSKGEVKU	96	374.5294	3	46.93	1120.588	-18.9
LEEjVKPADKU	96	412.8874	3	55.12	1235.648	-6.2
INFYSZEFYKU	96	528.2289	3	61.94	1581.674	-5.9
EPPPCLVFYKU	96	596.3054	2	64.12	1190.616	-16.4
DSMSEFLYDKU	96	617.2769	2	86.66	1232.538	0.7
GLLJQDTYJKU	95	490.2335	3	22.63	1467.702	-15.8

VSTYBSWGYKU	95	455.5468	3	23.63	1363.636	-12.9
ADUEMQFDNKU	95	426.1833	3	24.45	1275.53	-1.6
FVDTGAWAJKU	95	420.5369	3	24.48	1258.605	-12.9
VUKNDSDcHKU	95	439.2052	3	27.21	1314.615	-15.8
APMPAGEKFKU	95	358.8579	3	27.74	1073.569	-15.9
YSGSQWNNKKU	95	404.1997	3	28.89	1209.589	-9.8
POMPNANVjKU	95	428.2049	3	39.48	1281.612	-14.9
jNSSMGDFLKU	95	603.7717	2	43.84	1205.547	-14.9
VFAPLERATKU	95	377.5577	3	43.93	1129.661	-8.4
EGLAEOELiKU	95	442.5533	3	44.32	1324.639	-0.7
jSDCEGTYiKU	95	498.2087	3	49.15	1491.617	-8.5
VOMPYGPKKKU	95	417.5677	3	50.2	1249.687	-4.2
ELLGDTYCMKU	95	586.2695	2	52.42	1170.541	-14.3
DAFFNPDYKKU	95	415.2003	3	57.09	1242.603	-19.4
YDLVDCPPVKU	95	574.2867	2	59.18	1146.574	-13.3
LYVXLAFPYKU	95	444.907	3	64.53	1331.714	-11
OGCDCLPQQKU	94	497.5651	3	25.27	1489.694	-13.9
EYVSRAVSQKU	94	389.212	3	29.13	1164.625	-9.2
FTXSDETNSKU	94	416.5114	3	29.32	1246.533	-16.3
VFAPLQTRAKU	94	377.2294	3	31.15	1128.677	-9.2
ACFFYEHRVKU	94	433.5463	3	31.93	1297.639	-16.8
VDTCYCFNbKU	94	486.5453	3	32.35	1456.633	-12.7
FKQUTKPLAKU	94	413.9104	3	33.29	1238.725	-12.4
FKLZTQPLAKU	94	413.9118	3	33.35	1238.714	0
GVVDFiAALKU	94	384.881	3	36.1	1151.621	0.6
LQVEMHCPMKU	94	405.5264	3	37.69	1213.577	-16.1
VFcLYCETSKU	94	428.2084	3	38.48	1281.614	-8.6
IQNMKLEQSKU	94	465.8959	3	39.22	1394.683	-12.2
XHZAMELPcKU	94	478.5568	3	39.93	1432.65	-0.8
VZBYRFLYQKU	94	529.2721	3	40.03	1584.8	-3.7
AFMASDSETKU	94	543.2437	2	41.17	1084.486	-12.1
QKMSCMFQMKU	94	420.8582	3	43.94	1259.565	-9.4
TGXLDILPQKU	94	461.2252	3	44.76	1380.675	-15.5
QPELGVTTjKU	94	394.2074	3	45.07	1179.622	-18.1
QELEDYYKGKU	94	424.5395	3	46.62	1270.619	-17.8
GFAVHNNJMKU	94	428.2041	3	48.46	1281.599	-6.9
QTYDEAELTKU	94	598.7834	2	51.04	1195.572	-16.6
jDbLPLRCYKU	94	478.5716	3	51.33	1432.707	-10.1
FYGVAYVOYKU	94	438.2183	3	54.75	1311.651	-13.7
LMIYCYFFDKU	94	760.3266	2	67.14	1518.653	-9.3
VYRAFYCGSKU	93	398.1991	3	27.2	1191.586	-8.7
PAVEAGAWFKU	93	358.8577	3	27.48	1073.566	-13.4
VQUBMPVPQKU	93	460.8977	3	27.5	1379.693	-16.1
DHFGGKBDJKU	93	481.882	3	28.3	1442.645	-14.2
GVVAQQCVLKU	93	397.8981	3	34.12	1190.684	-9.3

CPPMPMGVYKU	93	374.5125	3	36.41	1120.523	-6.6
LVGEFVBWKKU	93	345.6898	4	37.46	1378.756	-19.2
QLVEDHSEMKU	93	405.5264	3	37.62	1213.576	-15.4
IQNCRLEQSKU	93	465.8877	3	39.3	1394.658	-11.7
NMOPANiLLKU	93	446.5581	3	40.95	1336.669	-12.4
FMLCFNjSBKU	93	491.5519	3	42.63	1471.651	-11.9
QNDJMELYKKU	93	478.5569	3	43.67	1432.673	-16.5
GVjNDFOGLKU	93	421.2052	3	45.08	1260.608	-11.3
NNVcXGEPAKU	93	621.2866	2	52.43	1240.578	-15.3
LVFPGVIOFKU	93	467.5802	3	53.59	1399.737	-12.7
MMRMMTVGEKU	93	404.8588	3	54.1	1211.565	-8.3
SEMNEVZMLKU	93	637.7897	2	55.55	1273.58	-11.5
TjGFXLAGVKU	93	610.8073	2	59.31	1219.618	-14.6
LYYLAVOPYKU	93	666.8578	2	64.57	1331.714	-9.6
LMIYJGUIDKU	93	585.2448	3	66.79	1752.734	-12.1
MGFTCSLLFKU	93	382.5272	3	78.33	1144.577	-15.4
YUUYGCYFKKU	92	477.5469	3	24.92	1429.635	-11.2
KLTPFCbCSKU	92	415.2052	3	26.52	1242.607	-10.6
YQTCLLGVAKU	92	365.5367	3	26.53	1093.596	-6.5
jFjXGGKPSKU	92	453.2116	3	31.79	1356.638	-18.3
LGNCNLGLKKU	92	353.5387	3	37.17	1057.607	-11.8
DWDLNANVjKU	92	428.2051	3	39.38	1281.607	-10.7
SAXYYPTUAKU	92	433.8692	3	40.93	1298.59	-3.6
AFMACAMETKU	92	551.2404	2	41.31	1100.482	-14.1
NDcFKPMMYKU	92	456.209	3	42.71	1365.629	-17.3
FDBINDAYHKU	92	394.4185	4	43.27	1573.66	-9.8
VDVGPETFFKU	92	379.8652	3	45.76	1136.587	-11.3
UNSOEMWYFKU	92	496.5421	3	47.63	1486.631	-17.8
VEYFEbMYDKU	92	480.8782	3	47.82	1439.625	-8.4
jYVGGYLjiKU	92	725.8374	2	63.71	1449.685	-16.9
FTFQSMQMMKU	92	639.2847	2	67.93	1276.577	-17
IQNMQLEQSKU	91	465.8871	3	23.52	1394.647	-5.1
SLAMTCPZTKU	91	573.2679	2	23.56	1144.537	-13.6
EYTZNjRIGKU	91	521.2375	3	24.76	1560.689	0.9
KLNCKEUDSKU	91	415.2057	3	26.43	1242.614	-14.8
bAGVSKSjLKU	91	405.89	3	27.51	1214.656	-6.4
LNPGEPGJNKU	91	397.5318	3	28.93	1189.58	-5.1
NIDPYHRRFKU	91	508.2516	3	31.32	1521.744	-7.2
RUVPGCTFFKU	91	309.1585	4	32.66	1232.624	-15.1
FKLPUFPLAKU	91	310.6852	4	33.25	1238.729	-13.6
FUFIAPEGVKU	91	341.9186	4	34.54	1363.653	-5.3
MMNKQFDYCKU	91	436.1967	3	36.97	1305.567	1
EEAPPJOADKU	91	442.5327	3	39.83	1324.586	-7.6
KYLYEMUMYKU	91	483.2296	3	45.62	1446.679	-8.1
CHAEQcULcKU	91	515.2433	3	48.81	1542.719	-6.8

EGQDNOPbMKU	91	447.195	3	49.36	1338.57	-5.4
KYMPLELOYKU	91	463.2454	3	49.89	1386.723	-6.1
MPYYMMWOMKU	91	495.209	3	50.5	1482.618	-8.7
MYLCFNjSBKU	91	496.8815	3	52.09	1487.646	-15.9
VVSPYTPbAKU	91	393.5453	3	59.78	1177.631	-14.3
XANJMZEFYKU	91	528.2172	3	61.01	1581.649	-11.9
OSNMJZEFYKU	91	528.2169	3	61.13	1581.649	-12.6
INFYYCEYYKU	91	528.2153	3	61.36	1581.645	-13.2
TjGFGWFQVKU	91	639.3158	2	61.42	1276.632	-12
cYZAMQNYKKU	91	717.3338	2	71.17	1432.664	-7.5
DPTUMSSCLKU	90	436.8684	3	23.01	1307.599	-12.2
ADSMYAWJDKU	90	451.1884	3	24.19	1350.562	-13.7
DSEASKDSjKU	90	392.1765	3	24.3	1173.523	-13.1
ZKMGTFKLGKU	90	401.8868	3	24.81	1202.659	-17.2
EMEMAScPMKU	90	416.1761	3	28.04	1245.527	-16.5
KYXPECLVGKU	90	468.5761	3	30.84	1402.717	-7.6
LQNQLJZACKU	90	689.3266	2	33.32	1376.658	-13.7
MOVQYQKWAKU	90	462.2332	3	33.5	1383.698	-14.9
VMMRGLXSXKU	90	454.2179	3	33.82	1359.651	-14.2
VGXBDNYLVKU	90	467.8948	3	35.47	1400.675	-8.8
LZGMjTEYAKU	90	658.2991	2	35.91	1314.6	-12.3
GIIFMQPLZKU	90	532.913	3	39.06	1595.726	-5.5
SAXUDKTUAKU	90	433.8693	3	40.76	1298.598	-9
QNGGEDQDLKU	90	551.7497	2	41.45	1101.505	-18.4
LQWVFOSjAKU	90	464.2353	3	44.12	1389.702	-13.1
LVDKGHSbRKU	90	419.5656	3	45.96	1255.697	-17.1
bLGTCLAVHKU	90	386.8734	3	49.4	1157.62	-18.4
DYLSYNjBSKU	90	491.5524	3	51.79	1471.65	-10.1
SAFLJGOGGKU	90	603.288	2	52.84	1204.581	-15.8
TSGFXLAGVKU	90	549.7845	2	54.31	1097.573	-16.8
QNNKTYDjSKU	90	435.873	3	57.32	1304.608	-8.3
ELLGDTCFMKU	90	578.2717	2	78.04	1154.546	-15.1
VVPBVDAFFKU	90	432.5632	3	88.01	1294.688	-15.2
FKQTUKPLAKU	89	310.6847	4	26.67	1238.725	-12
LSCSTUAFIKU	89	442.867	3	27.3	1325.604	-18.5
SLAMTCPjSKU	89	382.5132	3	27.75	1144.534	-14.2
LPPGYLPMGKU	89	357.8697	3	27.99	1070.595	-7.1
MAAGSTFVXKU	89	377.5187	3	28.28	1129.545	-9.4
DHFNKGbDJKU	89	481.8811	3	28.55	1442.646	-17.1
GVYDLOPKKKU	89	417.5693	3	30.12	1249.704	-14.7
VODLYGPKKKU	89	417.5691	3	30.21	1249.704	-15.1
EFGQGSVMPKU	89	539.7638	2	34.68	1077.528	-13.5
TYKDDDCMEKU	89	465.5366	3	35.17	1393.588	-0.4
ZMGKAHFANKU	89	599.2935	2	36.46	1196.587	-12.6
VABYRYPYKKU	89	366.1998	4	36.92	1460.773	-1.9

AVHFSEAAJKU	89	408.8685	3	38.75	1223.6	-13.6
ESMNEVZMLKU	89	637.79	2	39.25	1273.58	-11.1
cYZCDELYKKU	89	483.8885	3	39.84	1448.648	-2.5
YLOYCRjEDKU	89	501.2234	3	40.26	1500.665	-11
cLGNUQMQVKU	89	430.883	3	40.35	1289.638	-8.4
AYPSSSLVHKU	89	363.1943	3	45.42	1086.582	-19.6
USDUGDMTVKU	89	404.5049	3	46.7	1210.515	-18.2
LQFAGBjSHKU	89	457.5558	3	47.85	1369.666	-15.1
KGYMQSVMXKU	89	430.8722	3	54.38	1289.612	-13.5
jDDDEXFFFKU	89	497.5324	3	58.04	1489.598	-15.3
KYLQDUUMYKU	89	483.2303	3	59.41	1446.683	-9.3
INFFCZEFYKU	89	528.2289	3	61.95	1581.656	5.4
GEYFFMZYKKU	89	469.5519	3	66.38	1405.649	-10.8
SDMSEFLMFKU	89	617.2755	2	86.76	1232.557	-16.6
LVjcSPMSNKU	88	426.5443	3	23.36	1276.628	-13.6
EGAERWKYEKU	88	432.2209	3	24.19	1293.647	-4.2
MDVGSUCPVKU	88	557.7529	2	25.15	1113.506	-13.1
GOCDiLNQQKU	88	497.5651	3	25.28	1489.674	-0.5
LPPGYGRQGKU	88	357.8711	3	25.93	1070.598	-6.6
GVLOCMjAHKU	88	473.5644	3	26.72	1417.682	-7.6
FMAHCNCTQKU	88	443.8612	3	28.52	1328.582	-15.2
TPKYMGEBHKU	88	455.5491	3	28.66	1363.651	-18.6
FCGSQWPMKKU	88	404.1996	3	28.92	1209.579	-1.4
ATMUNKEjbKU	88	476.5513	3	29.79	1426.656	-16.9
KYMGQNCLRKU	88	463.2448	3	30.81	1386.726	-9.4
FPTCYRQXJKU	88	509.9017	3	31.73	1526.69	-4.7
jFjYELGPSKU	88	453.2128	3	32.64	1356.64	-17.5
LVDWAPSWRKU	88	419.5656	3	34.6	1255.683	-6.2
LEFMKMCOQKU	88	454.2178	3	34.81	1359.636	-3.3
ZcMSQPNMYKU	88	462.8687	3	36.86	1385.594	-6.9
PcEYNPPFYKU	88	449.8809	3	37.71	1346.638	-12.3
DSEASRCAjKU	88	587.7615	2	38.82	1173.517	-7
ATMUEELjbKU	88	476.5501	3	39.64	1426.645	-11.6
LENKQFDCYKU	88	429.5464	3	42.63	1285.613	3.9
WNZSGTESDKU	88	609.253	2	45.13	1216.511	-16.1
jNSSSTELDKU	88	594.7668	2	46.14	1187.539	-16.6
EYGHMMMjAKU	88	435.8466	3	46.2	1304.544	-19.5
LNVLDTDCYKU	88	591.7916	2	47.41	1181.575	-5.3
ELLGDTFCMKU	88	578.2724	2	52.39	1154.546	-14
VEYFEjjLYKU	88	503.236	3	57.25	1506.709	-14.8
EGAMVFAQSKU	88	533.7623	2	59	1065.528	-16.4
YDLVDEGNPKU	88	574.7765	2	60.48	1147.551	-11
ENEVGYLjiKU	88	697.3271	2	61.59	1392.651	-8.2
FPVVQXGTQKU	88	611.8168	2	64.39	1221.637	-14.4
EPPEAKCKYKU	88	596.3071	2	64.41	1190.612	-10.3

VQSNVPFCcKU	87	405.534	3	24.52	1213.599	-15.9
MSVVCPHVEKU	87	376.5225	3	28.99	1126.563	-15.2
WLDYMSDRKKU	87	447.5555	3	29.54	1339.671	-19.4
VOLYDGPKKKU	87	417.5693	3	30.12	1249.704	-14.7
LZTSCTbZUKU	87	480.5421	3	30.57	1438.623	-12.8
MYVSYPGXRKU	87	440.5474	3	30.72	1318.635	-11.4
GHXGNQVMXKU	87	437.1948	3	31.28	1308.575	-9.9
DANPYGjiZKU	87	467.868	3	35.97	1400.595	-8.9
GcHFYAMPbKU	87	454.5433	3	36.98	1360.628	-14.7
VABYRFLPcKU	87	366.1991	4	37	1460.781	-9.3
EGGFDEiWAKU	87	424.5216	3	38.75	1270.549	-4.3
QDLQTFMjSKU	87	435.8716	3	41.52	1304.616	-17.3
EQVEAYjKFKU	87	450.5638	3	41.54	1348.675	-3.6
FUCESMMBQKU	87	535.8911	3	43.56	1604.673	-13.5
GVNTVYMFIKU	87	450.2173	3	46.37	1347.65	-14.6
PNYFJQXcLKU	87	794.8656	2	51.71	1587.737	-12.5
KXMQSVMYGKU	87	430.8709	3	54.24	1289.612	-16.5
ZAPAYPVMXKU	87	645.804	2	54.25	1289.609	-11.8
CbLYPVZDGKU	87	436.2035	3	54.4	1305.599	-8.1
CHLQYDYKGKU	87	627.3029	2	60.69	1252.602	-8.8
CHCPUjLLcKU	86	386.6838	4	24.28	1542.727	-13.2
GVCSSEMRKKU	86	375.1893	3	26.08	1122.564	-15.7
WQQQQMAQZKU	86	457.2176	3	26.32	1368.636	-3.5
DAHXDFRLGKU	86	426.5452	3	27.03	1276.617	-2.7
GTBZbCVMTKU	86	476.2077	3	28.18	1425.615	-9.6
FTXDCETNSKU	86	421.8428	3	29.38	1262.51	-2.6
IFGLECLGVKU	86	351.6835	4	30.75	1402.716	-7.9
KYLYCjYRCKU	86	483.2292	3	31.29	1446.687	-14.6
DHFELQEDJKU	86	475.8783	3	31.31	1424.628	-10.2
GEVPYNGDAKU	86	350.1753	3	31.64	1047.499	5.3
ZPVECGPKFKU	86	400.1996	3	34.43	1197.596	-16.2
LQNQLJCGjKU	86	689.3276	2	36.12	1376.655	-10.1
ZMGQANQLNKU	86	599.2942	2	36.52	1196.572	1.5
TYLVTETNNKU	86	394.5377	3	37.57	1180.609	-15
LMPNVGBLJKU	86	471.2402	3	38.34	1410.72	-15
WAVEAYjKFKU	86	338.1744	4	41.54	1348.69	-16
AYVSGDLVHKU	86	363.1941	3	45.12	1086.582	-20
SDUSLWNDXKU	86	455.1969	3	45.89	1362.581	-9.1
VEYTTCUSPKU	86	603.7745	2	47.94	1205.55	-12.7
FMLSYTMCDKU	86	462.5402	3	51.05	1384.622	-16.8
MSPNYLDVHKU	86	401.5354	3	52.3	1201.591	-5.8
QNLGDTYMCKU	86	586.2681	2	52.55	1170.516	4.8
jDLPLSATYKU	86	608.3137	2	53.32	1214.627	-11.3
VGAViEALFKU	86	583.8209	2	56.51	1165.636	-7.7
TEFYMNLPQKU	86	635.3097	2	68.97	1268.622	-13.8

YYLAFVbMCKU	86	452.215	3	71.66	1353.643	-14.8
OSDQPFFIWKU	86	516.8992	3	73.94	1547.691	-9.7
VRXGGKLSTKU	85	388.8875	3	21.44	1163.664	-19.7
ADUECRFDNKU	85	319.8891	4	24.46	1275.542	-11
DHFELQMMJKU	85	481.882	3	28.3	1442.639	-10.3
BDjDLYLGVKU	85	469.2306	3	29.02	1404.681	-7.9
QRMFYLTCHKU	85	332.165	4	29.18	1324.653	-16.8
VOEMFGPKKKU	85	422.9005	3	30.47	1265.681	-1.5
DNTFKGANDKU	85	370.1813	3	35.14	1107.531	-7.9
DAGGPYJiZKU	85	467.8682	3	35.83	1400.593	-7.5
GGXXEDGZFKU	85	448.5117	3	44.54	1342.53	-12.3
AGPQNRTYFKU	85	394.2075	3	44.99	1179.615	-12
GMSMYEjWNKU	85	451.8662	3	45.38	1352.561	11.5
cTLKMSiFFKU	85	357.9353	4	47.42	1427.722	-6.8
WGKTFVNRCKU	85	413.2216	3	50.04	1236.655	-9.9
WNKMPTFVEKU	85	426.8854	3	51.23	1277.659	-19.3
PMYFEjjLYKU	85	503.236	3	57.26	1506.691	-2.9
YLYFUQHTMKU	85	470.5575	3	58.41	1408.671	-14.4
LUSSCMVFEKU	85	408.1939	3	67.99	1221.564	-3
QVFPEQDNNKU	85	609.292	2	76.71	1216.584	-11.8
XAQNBLEQSKU	84	471.2177	3	23.45	1410.655	-17.1
EYTZNFbIGKU	84	521.2231	3	25.05	1560.667	-12.2
GVNXFVbZiKU	84	510.5723	3	25.16	1528.701	-3.7
AHWXSJNAJKU	84	522.2226	3	25.4	1563.674	-17.8
LWDJDDRKcKU	84	512.2471	3	27.31	1533.736	-10.8
EREQKVFGEKU	84	416.8868	3	28.96	1247.662	-18.8
RAPDAPGJNKU	84	595.7949	2	28.98	1189.591	-13.1
OCMQDFDCTKU	84	431.8369	3	29.24	1292.485	3
QOFYCGLKTKU	84	430.8835	3	29.51	1289.645	-12.6
ATMUELEjbKU	84	476.5513	3	29.8	1426.645	-9
KGjPARLjGKU	84	311.6777	4	30.15	1242.689	-5.7
LFSGIPSKAKU	84	408.8873	3	30.47	1223.651	-9.2
KYOPECLGVKU	84	463.2451	3	30.68	1386.722	-6.4
LZTSjTCOUKU	84	480.5419	3	30.69	1438.624	-14.1
KYLYCjQMYKU	84	483.2292	3	31.3	1446.676	-6.8
SDCPVTQCQKU	84	468.5563	3	34.27	1402.661	-9.7
SGGAMSQJYKU	84	398.5119	3	34.49	1192.525	-9.4
ZSCSPQYRWKU	84	450.2049	3	35.16	1347.614	-15.9
GVOIDNYLVKU	84	467.8941	3	35.38	1400.68	-14
DANPYEiHZKU	84	467.8685	3	35.89	1400.598	-10
XGGPDPGEAKU	84	523.7338	2	36.09	1045.469	-15.1
YiKSVVLTCKU	84	425.2308	3	36.21	1272.677	-4.8
TFTEQYKUQKU	84	676.3336	2	37.26	1350.668	-11.4
GVCQNLGLKKU	84	353.539	3	37.44	1057.607	-10.9
QLVEMHPCMKU	84	405.5264	3	37.62	1213.577	-16

XAOLLLGVAKU	84	403.2306	3	38.38	1206.685	-12.2
VCNLMTNDAKU	84	419.2039	3	44.46	1254.609	-15.2
LQFQbGjSHKU	84	457.5556	3	47.93	1369.668	-16.7
VTNTFWPCTKU	84	399.1954	3	48.05	1194.586	-17.9
TYLVMLCNNKU	84	599.3011	2	49.27	1196.605	-14.1
LVMXVLQOFKU	84	350.9372	4	53.46	1399.741	-15.1
cYUNQAMLAKU	84	437.8769	3	55.77	1310.627	-13.8
YDLPMDGPLKU	84	574.2868	2	59.26	1146.574	-13.2
TVYVUPPDYKU	84	420.8782	3	60.64	1259.63	-13.6
DMOPAQXLLKU	84	446.8837	3	61.4	1337.652	-17.3
TjGFGYQNVKU	84	611.2977	2	61.41	1220.591	-8.2
CTWLNVPLjKU	84	427.8901	3	72.24	1280.667	-14.4
TCGDMEXHBKU	83	472.1874	3	23.19	1413.547	-4.4
VGQGEXEPEKU	83	397.8483	3	24.28	1190.543	-16.6
MDVGSCPUVKU	83	372.1703	3	25.12	1113.506	-14.9
KPDONCDDLKU	83	417.5255	3	25.3	1249.562	-6.1
DAHXOLTLGKU	83	426.5457	3	27.07	1276.628	-10.4
DBjDLYLVGKU	83	469.2307	3	29.11	1404.681	-7.7
KCTJPSHSCKU	83	468.55	3	34.84	1402.643	-10.7
MSBTMPLPQKU	83	436.2147	3	34.85	1305.638	-11.7
NBMCQLNDYKU	83	468.1986	3	37.11	1401.597	-16.5
PDLGGANQUKU	83	539.7697	2	37.49	1077.532	-6.1
NNDjKPMMYKU	83	450.2054	3	39.4	1347.604	-6.7
FVSADiHTFKU	83	428.8743	3	39.98	1283.617	-12.1
FMMQADGHFKU	83	605.77	2	41.96	1209.542	-13.9
CSEMVOZMLKU	83	446.8657	3	42.23	1337.579	-2.8
LENKQFCMEKU	83	423.5421	3	43.15	1267.605	-0.6
EYDPEDMjAKU	83	435.8466	3	46.19	1304.531	-10.1
VZTPFcMTDKU	83	442.872	3	47	1325.616	-16.1
KYUVMPTUYKU	83	463.5639	3	48.22	1387.682	-8.7
VGAVCYPLFKU	83	548.301	2	53.84	1094.595	-6.7
ESMNNNYYLKU	83	637.7894	2	55.65	1273.576	-9.4
MFAYTQEMMKU	83	639.7762	2	57.06	1277.561	-18
LVFMPFHjWKU	83	471.5775	3	57.84	1411.72	-6.2
TjSOXLAGVKU	83	654.3214	2	58.36	1306.636	-6
TVYVULDEMKU	83	426.2104	3	61.08	1275.628	-14.6
jTGFGXLQVKU	83	639.3156	2	61.49	1276.639	-17.8
MVZMMNLPQKU	83	643.3063	2	69.06	1284.614	-12.6
TDMNEVMZLKU	83	637.7891	2	76.23	1273.58	-12.6
VGEMVPMEcKU	83	606.7864	2	77.41	1211.576	-14.5
WOLRGADALKU	83	411.5598	3	77.93	1231.669	-9.1
VSTYBSXSVKU	82	455.5468	3	23.63	1363.643	-18
TQAETYAAiKU	82	405.8662	3	24.79	1214.58	-2.5
UjMMTEjHHKU	82	504.2092	3	25.04	1509.63	-15.8
FiMDCLPQQKU	82	373.425	4	25.33	1489.696	-16.4

LPPOKTAGGKU	82	357.8711	3	25.83	1070.61	-17.1
EEDPGALKTKU	82	362.8613	3	26	1085.572	-8.6
GUQMHDNcVKU	82	434.5292	3	27.32	1300.581	-11.7
BMCRUSACVKU	82	500.5612	3	27.85	1498.679	-11.2
FAWQRQVGEKU	82	416.5578	3	28.64	1246.657	-4.4
MYHREYRPMKU	82	353.1761	4	29.8	1408.686	-7.2
ATMUHPHjbKU	82	476.5507	3	29.87	1426.646	-11.1
SGQMSQGjYKU	82	597.2659	2	34.84	1192.527	-7.9
XGYEQYVGWKU	82	450.2049	3	35.17	1347.611	-13.4
VVTNNXBIMKU	82	398.4318	4	35.66	1589.718	-12.3
KKYPFRYEOKU	82	487.9312	3	36.88	1460.779	-4.8
VZBYOVLYKKU	82	397.2059	4	39.83	1584.812	-10.8
DNLHSMHETKU	82	404.1899	3	41.47	1209.556	-6.8
PGTPcYAPWKU	82	403.8728	3	42.1	1208.606	-7.5
YSGWYDTFKKU	82	431.8745	3	43.7	1292.619	-13.4
YPVVQXGTQKU	82	619.8127	2	47.17	1237.632	-16.7
THLPLTADJKU	82	420.886	3	52.33	1259.658	-17.2
VDGLTTEFFKU	82	385.8696	3	55.43	1154.597	-8.8
YLYVFUSUMKU	82	705.3345	2	58.48	1408.671	-11.7
VVSPYUFGVKU	82	587.8175	2	59.94	1173.629	-7.6
ZQFSDMMZDKU	82	695.7707	2	60.36	1389.544	-12.5
KFAWGTCFFKU	82	411.8746	3	61.46	1232.617	-11.7
VUjYDNYLVKU	82	701.341	2	62.31	1400.681	-9.4
DSBTVELPQKU	82	430.8828	3	62.78	1289.642	-11.8
SVGEYXFRiKU	82	480.2266	3	63.18	1437.677	-13.1
KFUSQbSFFKU	82	472.5672	3	64.09	1414.696	-11.6
QQMCPNVFEKU	82	408.1933	3	67.73	1221.564	-4.4
TLQAGAjTKKU	81	375.8776	3	25.68	1124.627	-14.4
TFFNWGNACKU	81	396.1842	3	26.68	1185.539	-6.9
PBGYRJTGAKU	81	348.1712	4	26.73	1388.671	-10.8
QTGVbFNQbKU	81	339.92	4	27.93	1355.662	-8.2
QLVGACCPSKU	81	502.7474	2	28.04	1003.494	-14.1
VYNFQTMEJKU	81	356.9165	4	28.45	1423.651	-10.1
EYVWKVSAGKU	81	583.3152	2	29.26	1164.629	-11.4
cNYNQETYGKU	81	655.2895	2	31.25	1308.582	-13.1
DiSGGDQEGKU	81	563.2351	2	34.34	1124.46	-3.8
ETCDPYPMDKU	81	399.8294	3	34.79	1196.484	-14.9
TFTEGiKjVKU	81	451.2245	3	36.95	1350.677	-18.7
LQMGABjSHKU	81	452.2133	3	40.81	1353.638	-15.1
FMMQADFGHKU	81	605.7715	2	42.14	1209.542	-11.4
VFAPLPMKTKU	81	377.5577	3	43.93	1129.668	-15.1
VGODSKGEVKU	81	374.5293	3	47.11	1120.574	-6.8
TGDFCVFSDKU	81	422.5262	3	48.08	1264.579	-17.6
KYOPECLVGKU	81	463.2446	3	49.78	1386.722	-7.4
DYLSYTMCDKU	81	462.5402	3	51.05	1384.604	-3.4

QDNJMELPcKU	81	478.5551	3	52.12	1432.644	-0.4
QCSTTSFMEKU	81	580.7482	2	54.21	1159.5	-15.8
LVFEMRQOFKU	81	350.9362	4	55.15	1399.73	-10
QVFPQEDNNKU	81	609.2924	2	58.09	1216.584	-11.2
FLSYFUNHHKU	81	457.8909	3	60.73	1370.663	-8.9
GLJLQDTXjKU	80	490.2335	3	22.63	1467.689	-7.1
IQNMKNQQSKU	80	465.8866	3	23.42	1394.658	-14.2
LXFGVEGWIKU	80	482.5639	3	23.98	1444.685	-10.5
WAEWGKVYEKU	80	432.2221	3	24.09	1293.651	-4.7
cjEDYPbGHKU	80	489.2104	3	28.65	1464.629	-13.3
cUTAKXWEGKU	80	471.5538	3	29.14	1411.657	-12.4
TKGHLCFSFKU	80	583.8024	2	29.51	1165.607	-14.1
HSQOFETCSKU	80	423.8583	3	30.11	1268.547	5
FIGLECLVGKU	80	351.6836	4	30.82	1402.716	-7.6
MYVSMEUPRKU	80	330.6619	4	30.85	1318.627	-6.9
GPAELAWYFKU	80	394.2086	3	31.77	1179.608	-3.2
OEFEVSYCUKU	80	463.1979	3	32.12	1386.589	-12
NDSTDNCTRKU	80	434.2015	3	32.48	1299.587	-3.3
VQGGGGUGFKU	80	493.2484	2	33.23	984.489	-6.8
TYGWTECMEKU	80	465.5366	3	34.87	1393.604	-11.4
YALWKYEETKU	80	443.8924	3	35.32	1328.677	-16
DANUEVSJUKU	80	463.1985	3	35.49	1386.598	-17.5
KEcFHCMSTKU	80	435.2013	3	36.52	1302.593	-8.2
DANLDJYSZKU	80	462.5369	3	39.33	1384.596	-5.4
LCNVjDGSVKU	80	430.8811	3	40.51	1289.64	-14.3
FMARUDQcQKU	80	466.2195	3	42.83	1395.655	-12.7
FSCbCLTFKKU	80	324.1584	4	43.59	1292.623	-14
EQMFjMGZTKU	80	687.7896	2	44.66	1373.583	-13.3
OACLMBLPQKU	80	461.2234	3	44.97	1380.671	-16.2
EVAVYMBGXKU	80	464.2122	3	45.4	1389.641	-19.1
EFGGAGWFEKU	80	563.7639	2	45.55	1125.524	-10
UAFYADLSMKU	80	408.8594	3	45.67	1223.576	-15.7
LMVVQXGTQKU	80	611.8155	2	47.1	1221.64	-19.2
QAVGDVGIWKU	80	417.2061	3	47.74	1248.61	-11
MCENEVMZLKU	80	645.7866	2	55.59	1289.557	1.5
KMSQAMMPMKU	80	394.5243	3	55.94	1180.559	-6.5
ZQFDMCYYDKU	80	703.7675	2	56.03	1405.543	-16.2
VGAVGjPLbKU	80	583.8209	2	56.51	1165.639	-10.4
TECDPYNNDKU	80	599.2408	2	57.91	1196.477	-8.1
TGDYWBLPQKU	80	461.2246	3	58.09	1380.663	-7.8
AIDTVELPQKU	80	430.8828	3	62.58	1289.647	-15.5
LcEDVFFbUKU	80	496.9013	3	63.21	1487.709	-18.2
ZEYLCCFBFKU	80	507.8778	3	63.8	1520.638	-17.5
FPVVQNUPDKU	80	611.8168	2	64.44	1221.626	-5.2
KLTQMNUDSKU	80	622.306	2	66.18	1242.614	-13.3

DjLPLMPGHKU	80	608.3136	2	69	1214.62	-6.2
KFNCiTFFFKU	80	521.5892	3	76.56	1561.765	-12.2
KPCCYFNFLKU	80	631.3063	2	77.89	1260.615	-13.2
MGCYTALLFKU	80	382.5272	3	78.33	1144.577	-15.4
MGTCYALLFKU	80	573.2881	2	78.34	1144.577	-13.7
PISQMNVFEKU	80	457.2144	3	80.22	1368.635	-9.7
LEDTZTUDNKU	79	437.1952	3	22.23	1308.569	-4.2
DPUTSMSCLKU	79	436.8673	3	23.1	1307.599	-14.8
FDVQQRRLEKU	79	330.1889	4	23.62	1316.731	-3.6
VQRTFZMESKU	79	440.5538	3	24.4	1318.645	-4.3
PVNTLbLTHKU	79	310.678	4	26.18	1238.695	-9.9
jQTVGMjDNKU	79	655.2914	2	26.32	1308.582	-10.7
PBQTFLMUAKU	79	348.1712	4	26.86	1388.682	-19.3
DAHXbSLLGKU	79	320.16	4	27.17	1276.624	-10.3
TYNBTNUMTKU	79	476.2071	3	28.28	1425.626	-18.6
AGITEECMEKU	79	479.2046	3	33.39	1434.6	-5.9
KEGHFGUGMKU	79	390.5236	3	36.57	1168.556	-6
SLSMTCPZTKU	79	581.2649	2	36.6	1160.532	-14.2
LFSNHGSKAKU	79	363.2021	3	37.96	1086.594	-8.2
GLHFVQDZSKU	79	408.8685	3	38.75	1223.605	-17.2
WGFDEYAQEKU	79	424.5221	3	38.85	1270.562	-13.7
EPPFTGOWSKU	79	417.8665	3	39.36	1250.595	-13.5
LQMQQFDONKU	79	452.2137	3	40.89	1353.636	-12.2
LKUCCCCLLKU	79	451.8893	3	41.19	1352.658	-8.7
DOMDOPNDLKU	79	452.1966	3	42.07	1353.575	-4.9
YQVSGDANYKU	79	572.2668	2	43.35	1142.536	-14.4
QQNQYMYKGKU	79	429.5421	3	43.85	1285.624	-15
DWScVPGMVKU	79	404.5287	3	44.35	1210.588	-19.9
SMLSZMMVNKU	79	412.1911	3	44.95	1233.567	-12.5
YTZCGDMTVKU	79	404.5049	3	46.71	1210.511	-15.1
SESLYMGFGKU	79	559.2628	2	47.72	1116.527	-14.7
QKYJLTDNNKU	79	463.5639	3	48.33	1387.68	-7.2
UKRPTAZGEKU	79	420.882	3	52.2	1259.648	-19
AGCbASFMEKU	79	580.7482	2	54.21	1159.497	-13.1
GMFLDCPTSKU	79	415.8699	3	54.92	1244.593	-3.7
VDGVPTFZVKU	79	385.8697	3	55.3	1154.608	-18.3
QNLETFMjSKU	79	435.873	3	57.67	1304.616	-14.1
XGGXEXYMFKU	79	497.5334	3	57.94	1489.592	-9
YLYCFGHTMKU	79	470.558	3	58.33	1408.666	-10.1
VVAEMHYRGKU	79	594.8112	2	61.47	1187.623	-13
LNKiDPFDMKU	79	447.5488	3	64.46	1339.646	-15.9
YLiFUGHTMKU	79	470.5582	3	78.32	1408.658	-3.5
MZLAFVDXTKU	79	669.8237	2	91.88	1337.63	2.3
QQUXDAQGSKU	78	420.8516	3	23.42	1259.55	-13.8
VYRAFYCCSKU	78	347.4202	4	25.34	1385.662	-7.2

KGAWUPBTQKU	78	343.172	4	25.56	1368.685	-19.3
RSVNiJFFKKU	78	381.9513	4	25.81	1523.782	-4
YKjNZjjDFKU	78	409.6808	4	26.63	1634.714	-12.2
TjSYGCCHFKU	78	627.255	2	27.4	1252.509	-10.6
YSGDYWTFKKU	78	431.8748	3	27.54	1292.619	-12.5
SLAMTACTPKU	78	511.2563	2	30.13	1020.51	-11.4
TAMMLOPKKKU	78	417.5679	3	30.32	1249.69	-6.4
SPAFZGFZKKU	78	424.2121	3	30.58	1269.626	-8.6
EODPGNXbDKU	78	472.5247	3	34.4	1414.569	-11.6
UQJZDMVACKU	78	528.2291	3	34.44	1581.676	-6.9
CNSAWVVCVKU	78	419.2095	3	35.53	1254.625	-14.2
ZMGKAFAHNKU	78	599.2942	2	36.52	1196.587	-11.3
YFSHWGKKCKU	78	321.4155	4	36.86	1281.644	-8.8
VABVXFLYKKU	78	487.9301	3	36.99	1460.784	-10.7
UAHFiDVTMKU	78	341.159	4	37.08	1360.621	-10.5
HFLGGAGBNKU	78	587.7921	2	37.7	1173.585	-12.6
AFQHjLHCDKU	78	436.2046	3	38.33	1305.601	-6.8
CFTEQYKUEKU	78	452.2146	3	38.66	1353.614	6.3
FHGViVFGYKU	78	429.5506	3	38.72	1285.648	-13.7
DSEASKEZSKU	78	587.7628	2	39.12	1173.526	-12.8
UOGLYNDXOKU	78	379.9156	4	39.22	1515.648	-9.2
NTiCKPMMYKU	78	450.2057	3	39.33	1347.6	-3.9
FVSASjiGFKU	78	428.8743	3	40.63	1283.614	-9.6
KINDADPGCKU	78	347.162	4	40.77	1384.629	-7.2
LMPGiDQLSKU	78	407.8724	3	41.88	1220.609	-11.1
FMMQTCHSVKU	78	605.7711	2	42.05	1209.546	-14.9
LNKMiPMDMKU	78	335.9122	4	44.34	1339.632	-9.1
VGcNKCNHYKU	78	419.2037	3	44.37	1254.601	-9.2
TGYWDBLPQKU	78	461.2234	3	45.09	1380.663	-10.4
WVYQAENUGKU	78	637.3005	2	46.93	1272.6	-10.6
QPLTPbiFFKU	78	357.9355	4	47.37	1427.728	-10.8
KFMFSXKFFKU	78	357.9353	4	47.65	1427.728	-11.2
ZQLJCDFMEKU	78	491.872	3	47.76	1472.613	-13
AGRMATiMEKU	78	409.8604	3	48.13	1226.577	-14.1
bPGGYLAVHKU	78	386.8725	3	49.48	1157.616	-17.7
KbCSKKjAiKU	78	363.935	4	49.92	1451.736	-17.4
QTYDPVMMTKU	78	606.7816	2	51.18	1211.568	-15.8
cNYHGFMYGKU	78	655.2888	2	51.29	1308.579	-12.1
cPKDCPLObKU	78	472.5694	3	51.81	1414.682	2.9
TMTTYPVMXKU	78	645.8057	2	54.27	1289.601	-3.1
GJFSDMMZDKU	78	695.7704	2	55.89	1389.54	-9.8
NEBGDDYADKU	78	434.1786	3	56.52	1299.517	-2.1
ADUERCFDNKU	78	638.7727	2	57.31	1275.542	-8.3
bGCLMBLPQKU	78	461.2233	3	57.96	1380.666	-13.2
QKLYcCHSLKU	78	656.845	2	60.51	1311.684	-6.3

AEYMTbOAFKU	78	461.2068	3	61.18	1380.621	-16.4
ZEYMTbOAFKU	78	753.3185	2	63.72	1504.648	-17.2
QMNVDEGPLKU	78	565.2817	2	64.32	1128.56	-9.8
YALEGKDJBKU	78	488.5708	3	71.29	1462.696	-3.9
XADDFVLLIKU	78	477.5685	3	72.55	1429.695	-8.1
DSVFLYMZTKU	78	649.3076	2	76.64	1296.617	-12.7
VVAEFjbFGKU	78	661.8293	2	94.3	1321.66	-12.3
KBFDVLTRIKU	77	524.6091	3	23.17	1570.827	-14
GPYEcAXHYKU	77	459.8688	3	25.18	1376.609	-17.6
KSTAcSETSKU	77	377.856	3	26.06	1130.565	-16.4
XMHNSMFCjKU	77	475.8534	3	26.88	1424.562	-16.5
LFFNDSDcHKU	77	439.2045	3	27.34	1314.607	-11.7
NGbcCETNSKU	77	421.8418	3	29.58	1262.525	-16.8
IAFBLQQFQKU	77	525.5921	3	29.64	1573.77	-9.6
GOAFRNYCMKU	77	431.5324	3	30.34	1291.582	-4.8
LFSLMMREAKU	77	306.9167	4	30.7	1223.652	-11.4
LDViSAGMJKU	77	440.5422	3	31.38	1318.616	-8.6
DjNGADDEOKU	77	425.8338	3	33.49	1274.5	-15.7
LAOSMPTUYKU	77	431.8723	3	35.31	1292.62	-19
YLOYbGjEDKU	77	506.5547	3	40.44	1516.663	-13.9
QELQYMUAPKU	77	429.5439	3	43.91	1285.624	-10.7
KMQMSCFQMKU	77	420.8581	3	44.02	1259.565	-9.6
WLAEOQNPHKU	77	332.1662	4	44.43	1324.654	-13.5
KCPCYFNFLKU	77	631.3056	2	45.16	1260.615	-14.4
GVjNMMNFLKU	77	421.2053	3	45.44	1260.608	-11
KjZSYPYRCKU	77	483.2298	3	45.99	1446.68	-8.4
PQVOAcYWbKU	77	502.9087	3	46.16	1505.721	-11.3
AUEFEDTLSKU	77	609.7841	2	47.45	1217.568	-11.6
AUEGXNTLSKU	77	609.7842	2	47.78	1217.565	-9
bPGGYLGVHKU	77	382.2012	3	47.87	1143.601	-16.4
VTNTEAETOKU	77	399.1959	3	47.96	1194.574	-7.1
LNVLDTMECKU	77	582.7866	2	48.17	1163.568	-8
GVVDMNcALKU	77	380.5366	3	49.83	1138.588	-0.5
iPGGFPMVHKU	77	401.5353	3	52.22	1201.593	-7.7
LGGVFHHGKKU	77	539.8115	2	53.07	1077.62	-10.3
BVMGVWbVAKU	77	461.2382	3	53.1	1380.7	-4.9
TKGHLACYFKU	77	583.8041	2	53.33	1165.607	-11.1
NYcUQAMLAKU	77	437.8779	3	55.9	1310.627	-11.5
TjEAFSKDEKU	77	421.5318	3	56.85	1261.591	-13.6
FLSYUPVDSKU	77	617.8056	2	73.36	1233.614	-14.3
LFSYFHYMSKU	77	441.2142	3	74.72	1320.633	-9
QVFPQDENNKU	77	609.2919	2	76.49	1216.584	-12
LAVDVWESQKU	77	587.3084	2	83.4	1172.619	-14.2
MKKTSOTIFKU	76	366.9371	4	23	1463.731	-7.9
IXLDRANLVKU	76	480.2522	3	26.27	1437.744	-6.5

EFGGAGSMPKU	76	490.2314	2	27.06	978.4593	-11.2
YSTUQGQVOKU	76	431.875	3	27.78	1292.612	-7
QMPKTYDjSKU	76	435.8732	3	28.19	1304.616	-13.6
DHOGKQMMJKU	76	481.882	3	28.3	1442.637	-8.5
KjDDLCRVAKU	76	351.6885	4	28.74	1402.735	-7.3
TKGHFATMFKU	76	583.8024	2	29.52	1165.607	-14.1
LFSLHcCLAKU	76	408.8873	3	30.46	1223.657	-13.4
FDGPDDCTRKU	76	434.2005	3	32.41	1299.591	-8.5
AGCSTTiMEKU	76	580.7499	2	32.5	1159.487	-1.4
MQQYPRGVMKU	76	309.9088	4	33	1235.627	-16.8
LNjTZGUSTKU	76	435.2015	3	36.77	1302.604	-16
BNMRDGNDYKU	76	693.7996	2	37.02	1385.595	-7.3
DMVTCPNDLKU	76	378.8412	3	37.11	1133.521	-17.1
FEYODUVHQKU	76	483.5506	3	37.68	1447.649	-13.4
TWQVFVKARKU	76	421.256	3	38.87	1260.746	0.6
LFSLSLCcAKU	76	392.211	3	40.15	1173.63	-15.8
FEYTCNOZKKU	76	477.5477	3	40.36	1429.631	-6.8
LYOPcMjEDKU	76	376.1689	4	40.4	1500.662	-10.2
GCUcNYGPiKU	76	449.1917	3	41.24	1344.562	-6
GbPQTFMjSKU	76	441.2032	3	41.66	1320.607	-14.7
SLZFJAMLAKU	76	447.5585	3	43.35	1339.666	-9.4
FAFcCMTCWKU	76	443.8579	3	43.72	1328.558	-4.9
MCGMGGGPLKU	76	475.2174	2	43.73	948.4344	-14.8
LELMbTEEMKU	76	447.5469	3	44.22	1339.633	-10.8
ACFFYEVGVKU	76	387.8602	3	44.25	1160.569	-8.7
VGEjKXOZEKU	76	506.2243	3	47.21	1515.68	-18.8
VEYMSSUSPKU	76	603.7745	2	47.94	1205.55	-12.7
WQDNWEGFMKU	76	447.195	3	49.35	1338.582	-13.8
AYPNMTRVHKU	76	405.8789	3	49.61	1214.634	-16
NEKTFVNCRKU	76	413.221	3	50.15	1236.64	1.3
MYPZANjSBKU	76	496.8816	3	52.02	1487.639	-10.6
QNLGDTCFMKU	76	578.2724	2	52.39	1154.521	7.8
WiLGEGcFVKU	76	454.892	3	52.57	1361.671	-12.6
KAHRTYDjGKU	76	428.5546	3	53.15	1282.65	-6.3
CTGFDLSTJKU	76	412.8596	3	55.79	1235.556	0.7
cLGNQUMQVKU	76	645.8215	2	58.18	1289.638	-7.4
NiCCEXFFFKU	76	497.534	3	58.21	1489.589	-5.7
APPPLCVFYKU	76	567.3036	2	64.14	1132.61	-15.5
LMVVQGXTQKU	76	611.8168	2	64.39	1221.64	-17
AAFFPTCYLKU	76	580.2931	2	73.96	1158.59	-15.5
ELLGDTFMCKU	76	578.2717	2	78.36	1154.546	-15.2
MGFCSTLLFKU	76	573.287	2	78.44	1144.577	-15.6
KSCYViVOMKU	76	465.5564	3	90.87	1393.661	-10.1
DPTSUMSCLKU	75	436.8673	3	23.22	1307.599	-14.7
XFbUNCTVGKU	75	511.8987	3	23.65	1532.69	-10.4

FSGSSKSjLKU	75	383.5319	3	26.76	1147.596	-19
KSTYTjSOAKU	75	649.3109	2	28.12	1296.629	-17.1
GVEEQKVEOKU	75	416.8868	3	28.97	1247.637	1.3
SFSCMQDQSKU	75	580.2381	2	30.05	1158.48	-15.6
TFTEAGYKWKU	75	410.5434	3	31.39	1228.624	-12.8
DVAXMSDVNKU	75	399.8517	3	31.54	1196.536	-2
GHTLKSMiFKU	75	321.1694	4	34.35	1280.657	-6.3
EYVECGPKFKU	75	400.1996	3	34.44	1197.585	-6.8
TRRDMPNMBKU	75	474.8949	3	36.56	1421.682	-13.6
OANMCQFZYKU	75	468.1991	3	37.01	1401.582	-4.4
GVVDBCSMTKU	75	405.1868	3	37.05	1212.543	-3.8
PHGEjYVFYKU	75	337.662	4	37.31	1346.638	-13.9
PGHEYjVFYKU	75	449.8812	3	37.55	1346.638	-11.8
YNOPGKLVVKU	75	407.5657	3	38.19	1219.694	-15.1
EFAZHGHEGKU	75	603.2642	2	42.04	1204.537	-19.5
EGALDEXMTKU	75	606.7644	2	42.48	1211.535	-17.3
MMBQYNbMHKU	75	525.5563	3	43.26	1573.661	-8.8
DQDMALjDXKU	75	455.1975	3	45.98	1362.571	0.1
LCFDSXSLSKU	75	609.7846	2	47.62	1217.561	-5.2
AJPYPVZDGKU	75	436.2031	3	47.91	1305.606	-14
VYRMMGGNMKU	75	395.8564	3	50.71	1184.562	-12.2
PNYZbQCYLKU	75	530.245	3	51.6	1587.735	-13.8
jDMSLPLFIKU	75	483.9047	3	51.62	1448.695	-1.6
EPPFLHTYSKU	75	406.5425	3	52.13	1216.624	-15.1
RHTKAYDjGKU	75	428.5549	3	53.06	1282.65	-5.7
bCLYPVDZGKU	75	653.8029	2	54.4	1305.599	-6.1
KYFFCCQRTKU	75	490.9105	3	56.24	1469.73	-13.9
NGSCCcFYWKU	75	434.1772	3	56.42	1299.524	-11.2
jTEAFSbGPKU	75	421.5308	3	56.87	1261.588	-13.6
KEGLDTFPMKU	75	388.8732	3	57.7	1163.601	-2.6
QELQMFcPGKU	75	424.2124	3	59.3	1269.626	-8
TVYVGXLMMKU	75	420.8783	3	60.74	1259.627	-10.9
EGTSPPEEQKU	75	550.7649	2	60.8	1099.515	0.5
QEMFjTDMHKU	75	687.7889	2	63.03	1373.583	-14.1
KLTQQcCDSKU	75	622.3068	2	66.23	1242.611	-9.3
MVFYETQPQKU	75	635.3097	2	68.97	1268.622	-13.8
YYLAMVSJDKU	75	452.2151	3	71.82	1353.634	-8
AcMPXRETVKU	74	336.9172	4	22.74	1343.66	-14.9
jESBVGVDIKU	74	503.2223	3	22.86	1506.673	-18.4
EVGPHAPiNKU	74	394.5311	3	24.23	1180.585	-11.8
MKGNOPJEFKU	74	473.8901	3	24.24	1418.658	-6.9
DSEASSKDjKU	74	587.762	2	24.33	1173.523	-11.7
MZXQLKTTGKU	74	440.8882	3	27.73	1319.652	-6.8
MAAGSTVOYKU	74	377.5187	3	28.27	1129.545	-9.6
EFEVSDVECKU	74	395.1756	3	31.17	1182.523	-14.9

TFTEQcPjVKU	74	451.2234	3	37.06	1350.662	-9.9
TYLVHcGGNKU	74	394.5378	3	37.72	1180.607	-13
ZMGKPPTMNKU	74	399.8636	3	38.54	1196.579	-8.6
FHLGXVFGYKU	74	429.5511	3	38.86	1285.647	-11.8
OGULYNDXOKU	74	506.219	3	39.27	1515.648	-8.2
EGAVAQFAWKU	74	553.2941	2	40.68	1104.572	2
PASKYiPGEKU	74	403.8728	3	42.09	1208.606	-7.5
QELDEYSSDKU	74	606.7643	2	42.57	1211.531	-13.5
GiVGAMAXGKU	74	572.2663	2	43.17	1142.527	-7.7
YQVQDSGGYKU	74	572.2668	2	43.24	1142.536	-14.4
QNDJMELcPKU	74	478.5556	3	43.77	1432.644	0.6
MKKTjXSTEKU	74	460.8958	3	46.16	1379.67	-3.3
LMGNQAGFSKU	74	351.1795	3	46.84	1050.528	-10.9
KcGMPPYAGKU	74	571.2916	2	46.95	1140.583	-12.5
FPVVQGXTQKU	74	611.8151	2	47	1221.637	-17.2
AYPGGYRPHKU	74	382.2011	3	47.75	1143.594	-10.6
YjLAYGPPCKU	74	610.2899	2	48.69	1218.583	-14.2
DQKTFVNRCKU	74	413.2216	3	50.04	1236.64	2.6
CGAGGMWVUKU	74	618.2889	2	51.44	1234.573	-7.9
EPPFLTYHSKU	74	406.5436	3	51.85	1216.624	-12.3
iPNEDKTVSKU	74	417.547	3	52.38	1249.617	1.9
LELGDTYMCKU	74	586.2695	2	52.69	1170.541	-14.3
ASFLJSSSNKU	74	603.2892	2	53.04	1204.579	-12.9
NYCDYFYADKU	74	434.1783	3	56.35	1299.523	-7.7
MiPDVFFFCKU	74	505.5645	3	63.68	1513.7	-18.5
FPVVQNDUPKU	74	611.8165	2	64.54	1221.626	-5.8
DjLPLATSYKU	74	608.3129	2	67.43	1214.627	-12.5
ODALNVPLjKU	74	641.3326	2	72.22	1280.671	-15.7
FLiYFFANDKU	74	466.5576	3	80.84	1396.668	-12.3
KMQIcTOQMKU	73	396.441	4	22.84	1581.722	7.9
EVGVAbGbSKU	73	394.5322	3	24.07	1180.587	-10.5
HWSTTFKLGKU	73	401.8868	3	24.9	1202.656	-14.5
YUQMDEYFKKU	73	477.5469	3	24.93	1429.645	-18
VFSGTQiCPKU	73	449.8888	3	25.93	1346.655	-7.8
KHAHCMjAHKU	73	473.5646	3	26.78	1417.682	-7.1
YNTTSCYiLKU	73	491.8972	3	29.14	1472.687	-11.5
TVAMTCPATKU	73	511.2563	2	30.12	1020.51	-11.4
cNYGGUcYGKU	73	663.2864	2	31.3	1324.575	-12.3
LGPCNBTVGKU	73	388.1959	3	35.1	1161.577	-9.4
QYEGEWVFYKU	73	337.6625	4	37.45	1346.629	-6.2
HFLHGANZGKU	73	587.7925	2	37.79	1173.579	-7.3
DSBTVEPLQKU	73	430.8831	3	40.86	1289.642	-11.1
YLOYQMGBCKU	73	495.2187	3	41.37	1482.645	-7.3
DTCMVOMZLKU	73	669.796	2	42.19	1337.579	-1.2
ZTTLNUEESKU	73	432.5325	3	42.66	1294.59	-11.1

QELGAYFBGKU	73	429.5435	3	44.15	1285.626	-13.2
LVDKGTcOVKU	73	419.5649	3	45.84	1255.687	-10.9
YFEAUPPYSKU	73	427.5348	3	46.94	1279.599	-12.5
KATjDDVYQKU	73	425.8735	3	47.02	1274.623	-18.7
TYLVVMQCNKU	73	599.3011	2	49.27	1196.605	-14.1
GVjNDENFLKU	73	415.2019	3	52.11	1242.596	-10
WVYLTAZGEKU	73	420.882	3	52.2	1259.63	-4.4
KMFHQDFFFKU	73	344.1741	4	54.06	1372.675	-5.6
EcFSDMZMDKU	73	695.7695	2	56.23	1389.541	-11.9
MbYMYFAGIKU	73	506.8915	3	58.02	1517.65	1.5
AGVFPYjDEKU	73	617.2896	2	58.16	1232.58	-12.2
MGFQFELHFKU	73	428.2125	3	67.64	1281.633	-13.5
DjYMTAMIFKU	73	502.5476	3	68.18	1504.63	-6
FLSYPcAESKU	73	617.8055	2	73.68	1233.611	-11.6
KOAECjKFGKU	73	441.5538	3	94.61	1321.643	-2.8
GVSVCJPFKKU	72	345.1844	4	21.05	1376.722	-10.1
KDVKCXYFKKU	72	345.1845	4	21.06	1376.713	-3.3
EVGQWATTYKU	72	591.3046	2	23.9	1180.588	6
ASGGLPECJKU	72	563.7604	2	24.51	1125.519	-11.6
LTFFHNODLKU	72	335.1707	4	24.89	1336.679	-18.9
LDcGTiYTLKU	72	335.1711	4	25.07	1336.661	-4.1
PXQCRGKVEKU	72	421.8831	3	25.36	1262.641	-11
KHTPVULTHKU	72	310.678	4	26.18	1238.7	-13.6
LKTbYDGDSKU	72	415.2061	3	26.67	1242.606	-7.5
QTVGAFFJcKU	72	452.8913	3	27.93	1355.666	-10.2
KMGYTjSQFKU	72	433.2095	3	28.04	1296.626	-14.6
SKTYMJAGFKU	72	649.3109	2	28.12	1296.624	-12.9
OSEBXARbVKU	72	535.917	3	28.66	1604.744	-9
CHZPDYPBHKU	72	489.2116	3	28.82	1464.616	-1.9
cGXGGQVMXKU	72	655.2902	2	31.17	1308.572	-4.7
FOHZAANVHKU	72	331.1606	4	31.86	1320.634	-15.4
KTDJEQGMTKU	72	434.8699	3	32.96	1301.599	-8.6
FKKAFVEPFKU	72	310.6844	4	33.57	1238.718	-7.4
WGKNVFEKCKU	72	413.22	3	33.83	1236.644	-4.6
BQDKERTAIKU	72	385.9431	4	34.74	1539.745	-1
SPYCPSHEjKU	72	468.55	3	34.84	1402.63	-1.3
TYKMACIMEKU	72	465.5352	3	35	1393.605	-15
LEFEGCKOOKU	72	454.2169	3	35.76	1359.637	-5.5
LFSLAAHMAKU	72	363.2013	3	38.15	1086.601	-17.4
IQNMQNKQSKU	72	465.8959	3	39.23	1394.658	5.8
FNTHbNMOOKU	72	506.2189	3	39.37	1515.662	-17.9
EGTSPPEQEKU	72	550.7651	2	39.4	1099.515	1
YLOYXTYEDKU	72	506.555	3	40.33	1516.659	-10.8
FVSAjYAGFKU	72	399.8647	3	40.34	1196.595	-19.1
IACPAiNLLKU	72	339.1686	4	41.2	1352.663	-12.9

MXVGOVHLYKU	72	457.2256	3	42.25	1368.673	-13.4
SGDVNRMbEKU	72	418.197	3	45	1251.585	-12.2
EFAZCCTEGKU	72	665.2773	2	45.59	1328.552	-8.9
LLPCWCQSAKU	72	574.2831	2	47.3	1146.568	-14.2
DADXVFLYKKU	72	330.1691	4	47.38	1316.662	-11.5
UNSDDiWYFKU	72	496.5421	3	47.64	1486.613	-5.8
VTNTFPCTWKU	72	399.1954	3	48.05	1194.586	-17.9
DNMAUiSCLKU	72	481.5457	3	49.86	1441.634	-13.1
KMSAINKjFKU	72	484.9108	3	49.94	1451.717	-4.1
DNbUMSSCLKU	72	481.5463	3	50	1441.629	-8.2
TiLLTAGEZKU	72	420.8868	3	52.47	1259.638	0.7
FDTWMTVEGKU	72	404.8596	3	54.31	1211.565	-6.3
AAFFPCTYLKU	72	387.1967	3	55.06	1158.59	-18.4
KYICCNYHYKU	72	504.5459	3	55.44	1510.634	-11.9
YFEAFSATbKU	72	427.5357	3	55.63	1279.605	-15.6
KMDGODLGMKU	72	399.856	3	56.15	1196.554	-6.8
YFEAFMRGDKU	72	631.7956	2	57.01	1261.591	-11.6
LYGOAPFVHKU	72	412.2167	3	58.88	1233.652	-19.1
TjOGYLGAVKU	72	610.8073	2	59.31	1219.618	-14.6
TVYVUFGHMKU	72	420.8783	3	60.74	1259.623	-8.2
LNCRbPFDMKU	72	447.5488	3	64.46	1339.635	-7.4
VNFDVMRNVKU	72	407.5525	3	67.12	1219.65	-11.4
QKMEASFMEKU	72	409.8607	3	68.2	1226.579	-15.2
MVFYGWMPQKU	72	643.3063	2	69.06	1284.615	-12.9
AAFCAQQYLKU	72	571.2868	2	77.62	1140.575	-13.9
AAFQMNGYLKU	72	571.2888	2	77.76	1140.575	-10.5
VVAEUHWAOKU	72	441.5543	3	94.51	1321.654	-9.9
ADCPYEQJDKU	71	445.185	3	24.19	1332.536	-2.3
HPLYNCCHMKU	71	415.5172	3	24.82	1243.541	-9.2
SSAAPPAQMKU	71	493.7539	2	25.92	985.5015	-8.3
VGSYGVWiSKU	71	405.8722	3	25.96	1214.595	-0.3
SSAAPPCVQKU	71	493.7527	2	25.99	985.5015	-10.7
AXKVSAOPGKU	71	394.2042	3	28.18	1179.612	-18.1
GTBbCZVMTKU	71	476.2077	3	28.18	1425.615	-9.6
QMLNVYDjSKU	71	435.8732	3	28.2	1304.616	-13.6
UcTASATWBKU	71	471.5538	3	29.15	1411.651	-8.3
IFGLEPLFYKU	71	351.6836	4	30.83	1402.714	-5.9
cNYFGHMYGKU	71	655.2906	2	31.55	1308.579	-9.3
EPPEGEUVSKU	71	575.774	2	38.08	1149.542	-6.9
YQTCLLLNLKU	71	403.2306	3	38.38	1206.679	-7.9
FEYOANUEFKU	71	358.4121	4	40.31	1429.627	-5.7
SCBPAiNLLKU	71	339.1686	4	41.09	1352.658	-9.2
FAMASSDETKU	71	543.2419	2	41.35	1084.486	-15.3
AFMAPSCMTKU	71	543.2419	2	41.35	1084.487	-16.2
EFAACCTEGKU	71	603.2641	2	43.48	1204.525	-9.1

KIECQAYPAKU	71	443.21	3	43.6	1326.624	-12.2
KYFDLSQZTKU	71	441.89	3	44.18	1322.662	-10.4
ADSMYEibGKU	71	451.1892	3	45.66	1350.56	-10.3
RLWGcTFGVKU	71	419.5649	3	45.84	1255.69	-14
GNbDDDMTVKU	71	404.5054	3	46.61	1210.511	-13.4
LLZCGMFSAKU	71	582.28	2	47.47	1162.563	-14.8
LYMMVGOBSKU	71	469.5515	3	48.48	1405.655	-15.7
TYLVVNGCWKU	71	591.3021	2	49.57	1180.606	-14.1
EKLJRKLELKU	71	356.2147	4	49.68	1420.847	-12.1
QTYDPNCKTKU	71	598.7839	2	51.21	1195.566	-10.3
QGVLCPYVEKU	71	567.7949	2	51.77	1133.59	-13.3
FVRMANEBFKU	71	472.5692	3	51.88	1414.698	-8.7
GTFLJNSSSKU	71	603.2894	2	52.93	1204.579	-12.6
USGGQPFjLKU	71	407.8711	3	53.06	1220.602	-8.8
MMOETEcGjKU	71	477.8623	3	55.14	1430.587	-15.3
KPWQCIEWLKU	71	377.6854	4	57.73	1506.73	-11.3
VVSFVCPPOKU	71	393.5447	3	60.1	1177.618	-4.9
VUWWDXGLVKU	71	701.3401	2	62.42	1400.685	-13.8
CPGLDEXMTKU	71	606.7625	2	66.8	1211.518	-6
FTFQSMDbGKU	71	639.2849	2	68.08	1276.573	-13.6
YTLVVMEEAKU	71	591.3036	2	71.28	1180.616	-19.9
YYLAFGDCQKU	71	452.2148	3	71.75	1353.642	-14.3
INEPFFYQWKU	71	516.8998	3	74.12	1547.705	-17.5
AAFAQCQYLKU	71	571.2877	2	77.87	1140.575	-12.4
YLYVFSIPCKU	71	470.5573	3	78.51	1408.67	-14.2
LFiYVNEDHKU	71	466.5576	3	80.85	1396.664	-9.5
MXYVSVKWQKU	71	694.3459	2	93.63	1386.698	-14.7

ELISA

Buffer A (1x PBS, pH = 7.2 + 0.05% Tween 20)

Buffer B (FBS 10%, 0.05% Tween 20, 1x PBS, pH = 7.2)

An ELISA plate (96-well format) was washed with buffer A (3 x 200 µL per well). Nucleobase peptide library, peptide library or peptide **38** were added, each to three wells (each 100 µL, 100 µM in buffer A) and incubated for 1 h at room temperature. After this time, the supernatant was removed and the wells treated with blocking buffer (buffer B, 100 µL per well) and incubated overnight. A DNA library (Biotin-N_{20}, 50 µM in buffer A) was heated to 95 °C for 5 min and let cool down to room temperature over 15 minutes. DNA library (50 µM in buffer A, 100 µL per well) was added to all wells and incubated for 1 h at room temperature. The supernatant was removed, and the wells washed (2 x 200 µL buffer A per well). SA-HRP (1:2000 dilution) was added to each well and incubated 30 minutes. All wells were washed (2 x 200 µL buffer A per well). TMB ELISA substrate was added to the wells (50 µL) and after 5 minutes quenched with sulfuric acid (50 µL). The absorbance at 450 nm was determined for all treated wells.

Affinity selection

Buffer A: Tris 10 mM pH = 7.5; NaCl 150 mM; $MgCl_2$ 10 mM

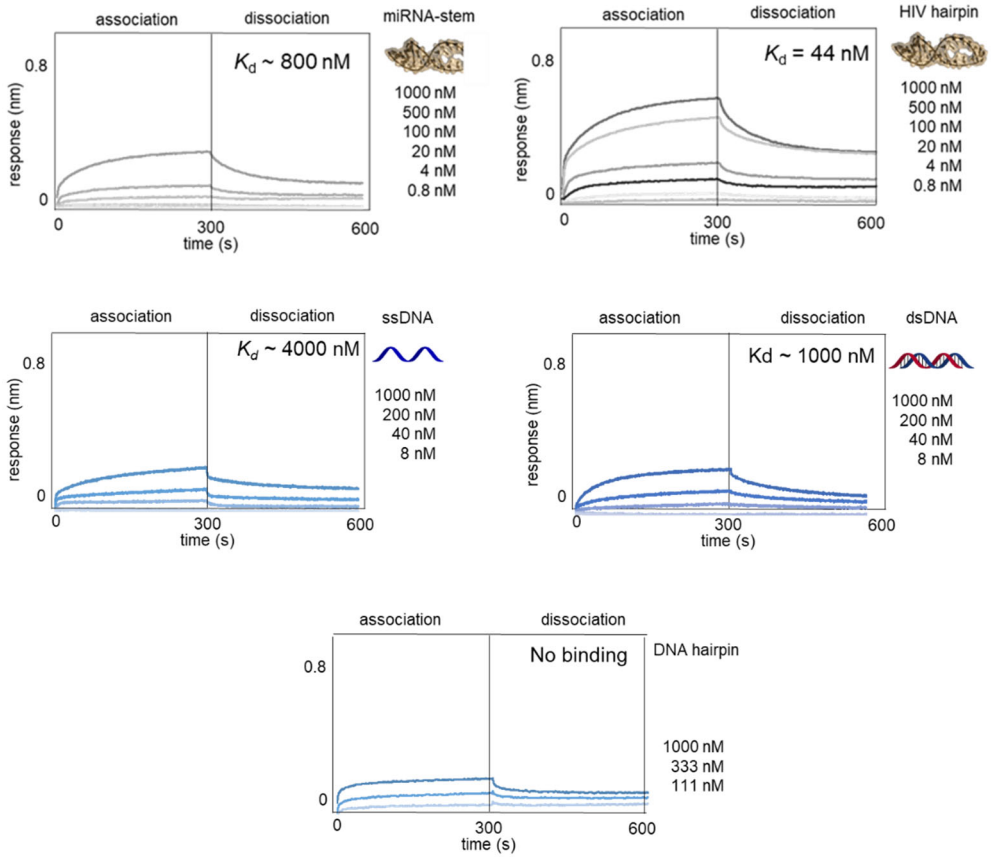
Buffer B: Tris 20mM pH = 7.5; NaCl 300 mM; $MgCl_2$ 20 mM; Tween 0.05 %; Yeast RNA 0.2 mg/mL; Biotin 2 mM

Buffer C: Guanidine-HCl 6 M, pH = 6.8; Phosphate 200 mM

Pre-miR-21 or pre-miR-155 (10 µM, 50 µL) was diluted to 500 µL with buffer A and heated to 95°C for 5 minutes and then left cooling down to room temperature for 15 minutes. 400 µL (4 mg) MyOne streptavidin beads were washed with buffer A (2 x 1 mL) and then incubated with biotin-pre-miRNA (21 or 155; 500 µL, 1 µM in Buffer A) at 4 °C for 30 minutes. The supernatant was removed, and the beads washed with buffer C (3 x 1 mL). The beads (for each miRNA) were divided in 4 parts and incubated with buffer B (800 µL) + library (200 µL, 6.25 mM in 1X PBS + 5 % DMF) for 120 minutes at 4 °C. After this time the supernatant removed and the beads washed with 2 x 500 µL Buffer A. To elute bound library members the beads were treated with 2 x 100 µL Buffer C. All samples were desalted with C18 ZipTips and lyophilized. The samples were taken up in water with 0.1% formic acid and analyzed by nanoLC-MS/MS. In parallel a control selection was performed on beads not loaded with miRNA, all other steps were identical.

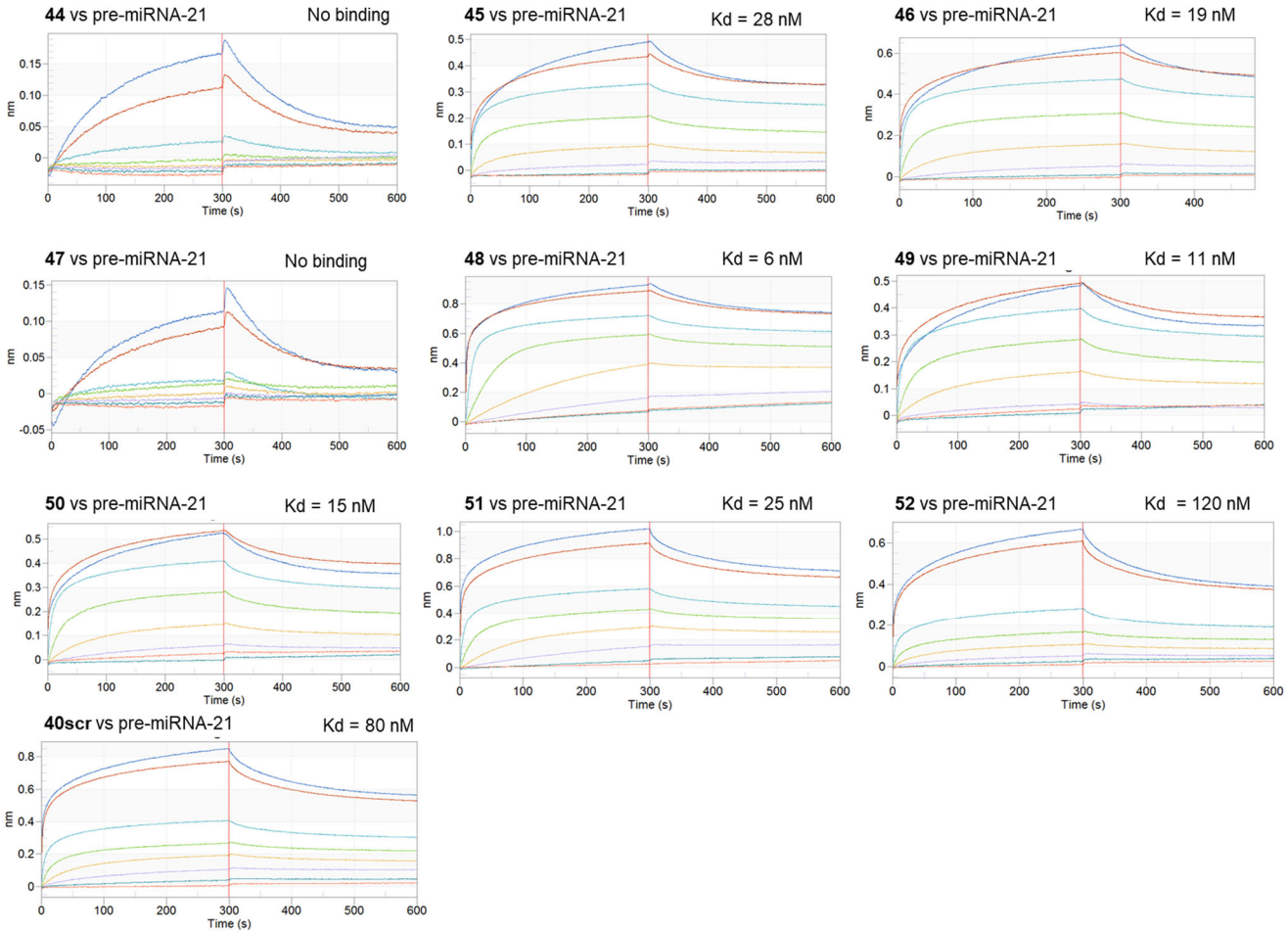
General procedure for biolayer interferometry (BLI)

Lyophilized peptides biotinylated on C-term lysine was dissolved to 1 mg/mL in 1x PBS and diluted 50-fold into 0.02% Tween-20, 1x PBS ('kinetic buffer') for immobilization onto streptavidin Octet biosensors (ForteBio; Menlo Park, CA). Biolayer interferometry (BLI) assays were performed in 96 well plates (GreinerBio-One; Kremsmünster, Austria; polypropylene, flat-bottom, chimney well) using an Octet Red96 System (ForteBio; Menlo Park, CA). Wells were filled with 200 µL of kinetic buffer, peptide solution, or RNA solution (prepared in kinetic buffer). Biotinylated peptide was immobilized onto the streptavidin tip for 120 s. Sensors were then dipped into kinetic buffer for 60 s, RNA solution (1 µM, 500 nM, 100 nM, 20 nM, 4 nM or 0.8 nM) for 300 s, and finally into kinetic buffer for 300 s. Measurements were carried out at 30 °C.

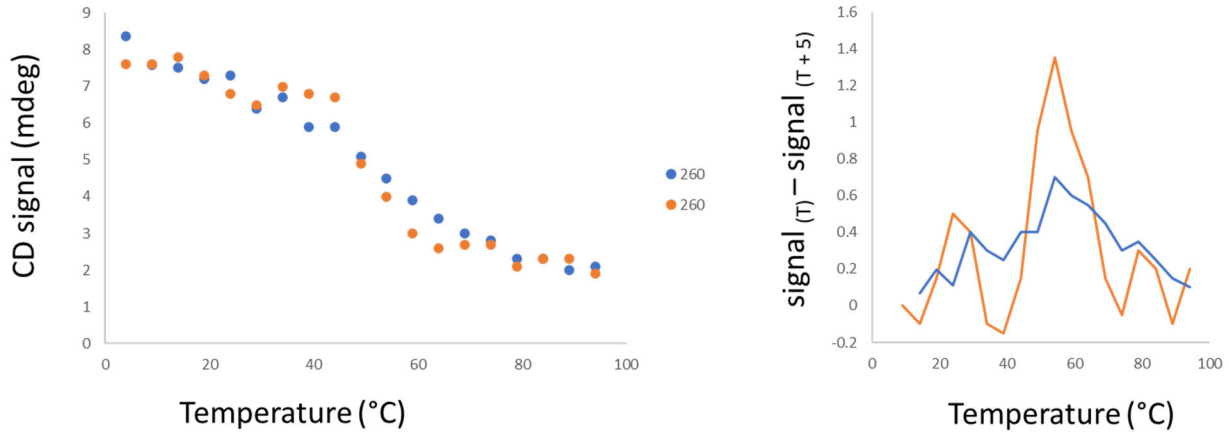


SI Figure 1. BLI curves ds-miRNA-stem, HIV hairpin, ssDNA, dsDNA and DNA hairpin. BLI tips with immobilized nucleobase peptide were dipped into solution containing RNA (association, 300 sec). RNA concentration range: 1000 nM, 500 nM, 100 nM, 20 nM, 4 nM, 0.8 nM. Dissociation was performed for 300 sec in kinetic buffer. miRNA-stem sequence: UAGCUUAUCAGACUGAUGUUG; CAACACCAGUCGAUGGGCUG. RNA harpin sequence: CGUGUCUUGGAGUGCUGAUCGGACACC. ssDNA and dsDNA sequence: CCGGCTGACACGTGGTATTAAT. DNA hairpin sequence: AGCTTATCAGACTGATGTTGACTGTTGAATCTCATGGCAACACC AGTCGATGGGCT. All oligonucleotides before usage were heated to 95°C for 5 minutes and let cool to room temperature over 15 minutes.

BLI curves alanine scan



SI Figure 2. Biolayer interferometry association and dissociation curves for alanine scan and scrambled hit. BLI tips with immobilized nucleobase peptide were dipped into solution containing pre-miRNA21 (association, 300 sec). RNA concentration range: 1000 nM, 500 nM, 100 nM, 20 nM, 4 nM, 0.8 nM. Dissociation was performed for 300 sec in kinetic buffer.



SI Figure 3. Melting curves of pre-miRNA-21 and pre-miRNA-21 + **39**, determined by circular dichroism (CD) at 260 nm. Samples were dissolved in 10 mM MES, 150 mM KCl, 1mM $MgCl_2$, 10% glycerol at 5 µM final concentration. Prior to measurement samples were heated to 95°C for 5 minutes and cooled down to room temperature over 15 minutes.