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SUPPLEMENTARY INFORMATION
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Addendum: A cellular chemical probe targeting the chromodomains of Polycomb repressive complex 1

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Addendum to Supplementary Note

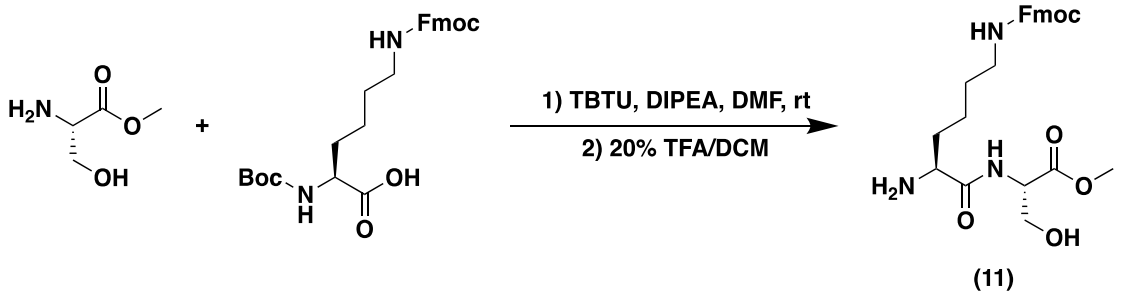
In 2016, we reported in *Nature Chemical Biology* the discovery of a chemical probe for the CBX domains of Polycomb repressive complex 1. In subsequent studies, we have seen that our original synthetic approach can sometimes lead to epimerization at the alanine position. Therefore, we now prefer the methods described below.

Synthesis of UNC3866, UNC4219, UNC4007 and UNC4195

(i) General procedures

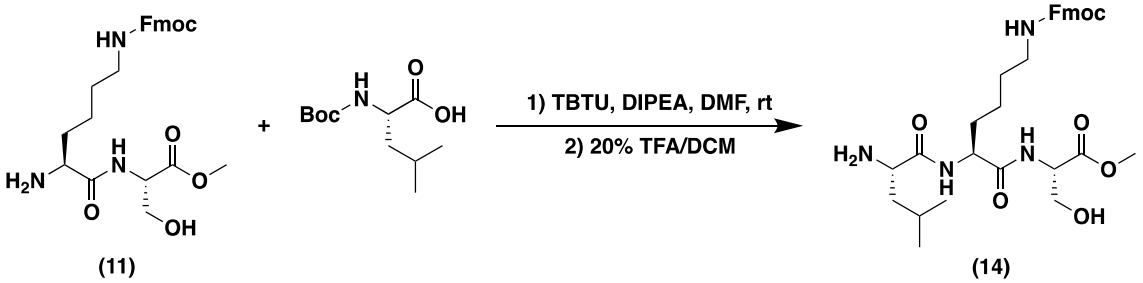
Analytical LCMS data for all compounds were acquired using an Agilent 6110 Series system with the UV detector set to 220 nm. Samples were injected (<10 µL) onto an Agilent Eclipse Plus 4.6 × 50 mm, 1.8 µm, C18 column at room temperature. Mobile phases A (H_2O + 0.1% acetic acid) and B (MeOH + 0.1% acetic acid) were used with a linear gradient from 10% to 100% B in 5.0 min, followed by a flush at 100% B for another 2 minutes with a flow rate of 1.0 mL/min. Mass spectra (MS) data were acquired in positive ion mode using an Agilent 6110 single quadrupole mass spectrometer with an electrospray ionization (ESI) source. Nuclear Magnetic Resonance (NMR) spectra were recorded on a Varian Mercury spectrometer at 400 MHz for proton (^{1}H NMR); chemical shifts are reported in ppm (δ) relative to residual protons in deuterated solvent peaks. *Due to intramolecular hydrogen-bonding, hydrogen-deuterium exchange between the amide protons of the molecule and the deuterated solvent is slow and requires overnight equilibration for complete exchange.* Normal phase column chromatography was performed with a Teledyne Isco CombiFlash®R_f using silica RediSep®R_f columns with the UV detector set to 220 nm and 254 nm. The mobile phases used are indicated for each compound. Reverse phase column chromatography was performed with a Teledyne Isco CombiFlash®R_f 200 using C18 RediSep®R_f Gold columns with the UV detector set to 220 nm and 254 nm. Mobile phases of A (H_2O + 0.1% TFA) and B (MeCN) were used with default column gradients. Preparative HPLC was performed using an Agilent Prep 1200 series with the UV detector set to 220 nm and 254 nm. Samples were injected onto a Phenomenex Luna 250 × 30 mm, 5 µm, C18 column at room temperature. Mobile phases of A (H_2O + 0.1% TFA) and B (MeOH or MeCN) were used with a flow rate of 40 mL/min. A general gradient of 0-15 minutes increasing from 10 to 100% B, followed by a 100% B flush for another 5 minutes was utilized. Small variations in this purification method were made as needed to achieve ideal separation for each compound. Analytical LCMS (at 220 nm) and NMR were used to establish the purity of targeted compounds. All compounds that were evaluated in biochemical and biophysical assays had >95% purity as determined by ^{1}H NMR and LC-MS.

(ii) Synthesis of UNC3866 (2) and Intermediates (11, 14-17)



Methyl N^6-(((9*H*-fluoren-9-yl)methoxy)carbonyl)-L-lysyl-L-serinate (11): N^6-(((*9H*-fluoren-9-yl)methoxy)carbonyl)-N^2-(*tert*-butoxycarbonyl)-L-lysine (5.00 g, 10.7mmol, 1.0 eq.), 1.40 g of methyl L-serinate hydrochloride (11.7 mmol, 1.1 eq.), and 4.11 g of TBTU (12.8 mmol, 1.2 eq.) were dissolved in 40 mL of a 7:1 mixture of EtOAc:DMF. DIPEA (5.6 mL, 32.0 mmol, 3.0 eq.) was added to the solution and the mixture was stirred at room temperature for 2 hrs. The reaction mixture was diluted with brine (100 mL) and extracted with EtOAc (150 mL). The organic extract was washed with brine (2X, 100 mL) and dried over Na_2SO_4. After filtration, the solvents were removed under reduced pressure. The residue was dissolved in 20 mL of a 20% solution of TFA/DCM. The solution was stirred for 30 minutes. Volatiles were removed under reduced pressure and the mixture was purified by reverse phase column chromatography ((H_20 + 0.1% TFA)/MeOH) to yield 4.63 g (74.4% over two steps) of the TFA salt of the title compound as a white solid.

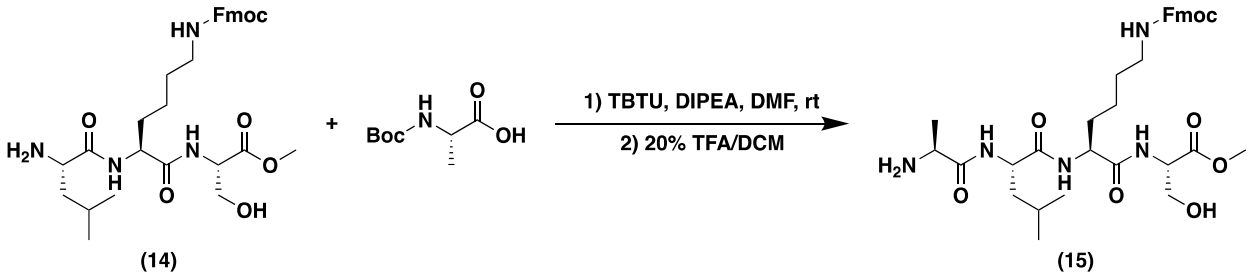
^{1}H NMR (400 MHz, Methanol-d_4) δ 7.79 (d, *J* = 7.6 Hz, 2H), 7.64 (d, *J* = 7.5 Hz, 2H), 7.39 (t, *J* = 7.4 Hz, 2H), 7.31 (t, *J* = 7.4 Hz, 2H), 4.58 (t, *J* = 4.4 Hz, 1H), 4.36 (d, *J* = 6.8 Hz, 2H), 4.19 (t, *J* = 6.7 Hz, 1H), 3.98 – 3.90 (m, 2H), 3.83 (dd, *J* = 11.2, 3.9 Hz, 1H), 3.71 (s, 3H), 3.14 (t, *J* = 6.6 Hz, 2H), 2.00 – 1.25 (m, 6H). MSI (ESI): 470 $[M+H]^+$. t_R = 4.65 min.



methyl N^6-(((9H-fluoren-9-yl)methoxy)carbonyl)-N^2-(L-leucyl)-L-lysyl-L-serinate (14): Compound **11** (4.63 g, 7.93 mmol, 1.0 eq.), 2.02 g of (*tert*-butoxycarbonyl)-L-leucine hydrate (8.73 mmol, 1.1 eq.), and 3.06 g of TBTU (9.52 mmol, 1.2 eq.) were dissolved in 40 mL of a 3:1 mixture of EtOAc:DMF. DIPEA (4.2

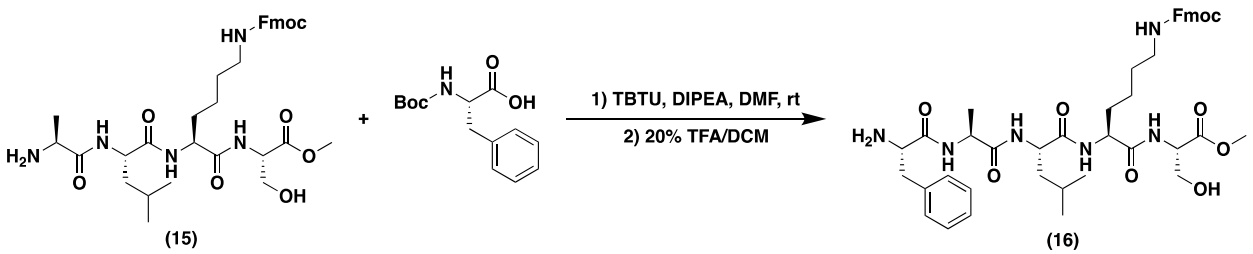
mL, 23.8 mmol, 3.0 eq.) was added to the solution and the mixture was stirred at room temperature for 2 hrs. The reaction mixture was diluted with brine (100 mL) and extracted with EtOAc (150 mL). The organic layer was washed with brine (2X, 100 mL) and dried over Na_2SO_4. After filtration, the solvents were removed under reduced pressure. The residue was dissolved in 20 mL of a 20% solution of TFA/DCM. The solution was stirred for 30 minutes. Volatiles were removed under reduced pressure and the mixture was purified by reverse phase column chromatography ((H_20 + 0.1% TFA)/MeOH) to yield 4.76 g (86% over two steps) of the TFA salt of the title compound as a white solid.

^{1}H NMR (400 MHz, Methanol-d_4) δ 7.79 (d, *J* = 7.5 Hz, 2H), 7.63 (d, *J* = 7.4 Hz, 2H), 7.38 (t, *J* = 7.4 Hz, 2H), 7.30 (t, *J* = 7.4 Hz, 2H), 4.54 – 4.42 (m, 2H), 4.34 (d, *J* = 6.8 Hz, 2H), 4.19 (t, *J* = 6.8 Hz, 1H), 3.95 – 3.88 (m, 2H), 3.78 (dd, *J* = 11.3, 4.0 Hz, 1H), 3.72 (s, 3H), 3.12 (t, *J* = 6.7 Hz, 2H), 1.93 – 1.24 (m, 9H), 0.99 (t, *J* = 6.2 Hz, 6H). MSI (ESI): 583 $[M+H]^+$. t_R = 4.83 min.



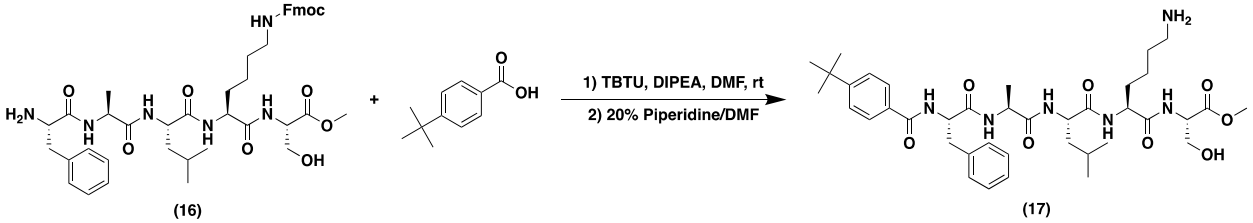
methyl N^6-(((9H-fluoren-9-yl)methoxy)carbonyl)-N^2-L-alanyl-L-leucyl-L-lysyl-L-serinate (15): Compound **14** (1.4 g, 2.0 mmol, 1.0 eq.), 420 mg of (*tert*-butoxycarbonyl)-L-alanine (2.2 mmol, 1.1 eq.), and 770 mg of TBTU (2.4 mmol, 1.2 eq.) were dissolved in 40 mL of a 3:1 mixture of EtOAc:DMF. DIPEA (1.1 mL, 6.0 mmol, 3.0 eq.) was added to the solution and the mixture was stirred at room temperature for 2 hrs. The reaction mixture was diluted with brine (100 mL) and extracted with EtOAc (150 mL). The organic layer was washed with brine (2X, 100 mL) and dried over Na_2SO_4. After filtration, the solvents were removed under reduced pressure. The residue was dissolved in 20 mL of a 20% solution of TFA/DCM. The solution was stirred for 30 minutes. Volatiles were removed under reduced pressure and the mixture was purified by reverse phase column chromatography ((H_20 + 0.1% TFA)/MeOH) to yield 1.26 g (84.1% over two steps) of the TFA salt of the title compound as a white solid.

^{1}H NMR (400 MHz, Methanol-d_4) δ 7.80 (d, *J* = 7.5 Hz, 2H), 7.64 (d, *J* = 7.5 Hz, 2H), 7.39 (t, *J* = 7.4 Hz, 2H), 7.31 (t, *J* = 7.3 Hz, 2H), 4.53 – 4.33 (m, 5H), 4.20 (t, *J* = 6.8 Hz, 1H), 3.97 – 3.87 (m, 2H), 3.79 (dd, *J* = 11.3, 4.0 Hz, 1H), 3.72 (s, 3H), 3.12 (t, *J* = 5.2 Hz, 2H), 1.92 – 1.55 (m, 6H), 1.50 (d, *J* = 7.0 Hz, 3H), 1.46 – 1.25 (m, 3H), 1.00 – 0.91 (m, 6H). MSI (ESI): 654 $[M+H]^+$. t_R = 4.79 min.



methyl N^6-(((9H-fluoren-9-yl)methoxy)carbonyl)-N^2-L-phenylalanyl-L-alanyl-L-leucyl-L-lysyl-L-serinate (16): Compound **15** (1.26 g, 1.64 mmol, 1.0 eq.), 479 mg of (*tert*-butoxycarbonyl)-L-phenylalanine (1.81 mmol, 1.1 eq.), and 632 mg of TBTU (1.97 mmol, 1.2 eq.) were dissolved in 40 mL of a 3:1 mixture of EtOAc:DMF. DIPEA (0.86 mL, 4.92 mmol, 3.0 eq.) was added to the solution and the mixture was stirred at room temperature for 2 hrs. The reaction mixture was diluted with brine (100 mL) and extracted with EtOAc (150 mL). The organic layer was washed with brine (2X, 100 mL) and dried over Na_2SO_4. After filtration, the solvents were removed under reduced pressure. The residue was dissolved in 20 mL of a 20% solution of TFA/DCM. The solution was stirred for 30 minutes. Volatiles were removed under reduced pressure and the mixture was purified by reverse phase column chromatography ((H_20 + 0.1% TFA)/MeOH) to yield 481 mg (32.1% over two steps) of the TFA salt of the title compound as a white solid.

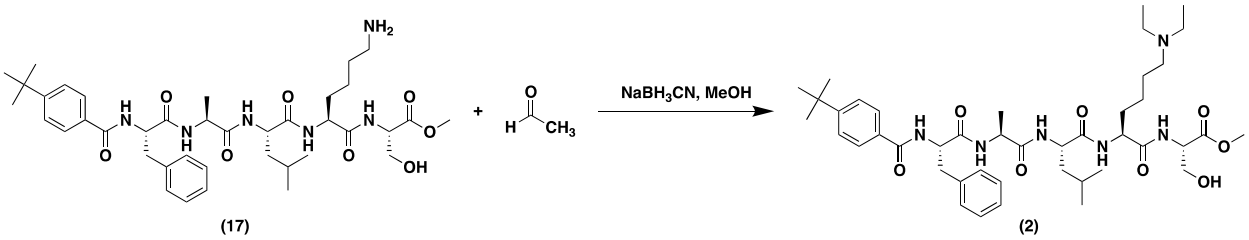
^{1}H NMR (400 MHz, Methanol-d_4) δ 7.78 (d, *J* = 7.6 Hz, 2H), 7.62 (d, *J* = 7.5 Hz, 2H), 7.41 – 7.23 (m, 9H), 4.52 – 4.38 (m, 4H), 4.32 (d, *J* = 6.9 Hz, 2H), 4.17 (t, *J* = 6.9 Hz, 1H), 4.10 (dd, *J* = 8.7, 5.2 Hz, 1H), 3.90 (dd, *J* = 11.3, 4.6 Hz, 1H), 3.78 (dd, *J* = 11.3, 4.0 Hz, 1H), 3.71 (s, 3H), 3.26 (dd, *J* = 5.1 Hz, 1H), 3.11 (t, *J* = 7.0 Hz, 2H), 2.98 (dd, *J* = 14.3, 8.8 Hz, 1H), 1.91 – 1.40 (m, 9H), 1.38 (d, *J* = 7.1 Hz, 3H), 1.00 – 0.91 (m, 6H). MSI (ESI): 801 $[M+H]^+$. t_R = 5.37 min.



methyl (4-(tert-butyl)benzoyl)-L-phenylalanyl-L-alanyl-L-leucyl-L-lysyl-L-serinate (17): Compound **16** (481 mg, 0.53 mmol, 1.0 eq.), 103 mg of 4-(tert-butyl)benzoic acid (0.58 mmol, 1.1 eq.), and 203 mg of TBTU (0.63 mmol, 1.2 eq.) were dissolved in 25 mL of a 3:1 mixture of EtOAc:DMF. DIPEA (0.28 mL, 1.58 mmol, 3.0 eq.) was added to the solution and the mixture was stirred at room temperature for 2 hrs.

The reaction mixture was diluted with brine (100 mL) and extracted with EtOAc (150 mL). The organic layer was washed with brine (2X, 100 mL) and dried over Na_2SO_4. After filtration, the solvents were removed under reduced pressure. The residue was taken up in 7 mL of a 20% solution of piperidine in DMF. The solution was stirred for 30 minutes. Volatiles were removed under reduced pressure and the mixture was purified by reverse phase column chromatography ((H_20 + 0.1% TFA)/MeOH) to yield 397 mg (82.5% over two steps) of the TFA salt of the title compound as a white solid.

^{1}H NMR (400 MHz, Methanol-d_4) δ 7.70 (d, *J* = 8.5 Hz, 2H), 7.48 (d, *J* = 8.5 Hz, 2H), 7.33 – 7.26 (m, 4H), 7.24 – 7.18 (m, 1H), 4.73 (dd, *J* = 9.3, 5.6 Hz, 1H), 4.58 (s, 1H), 4.52 – 4.27 (m, 4H), 3.91 (dd, *J* = 11.4, 4.6 Hz, 1H), 3.79 (dd, *J* = 11.3, 3.8 Hz, 1H), 3.74 (s, 3H), 3.26 (dd, *J* = 13.9, 5.6 Hz, 1H), 3.10 (dd, *J* = 13.9, 9.3 Hz, 1H), 2.92 (t, *J* = 7.5 Hz, 2H), 1.95 – 1.44 (m, 9H), 1.37 (d, *J* = 7.2 Hz, 3H), 1.33 (s, 9H), 0.95 – 0.89 (m, 6H). MSI (ESI): 739 $[M+H]^+$. t_R = 5.31 min.

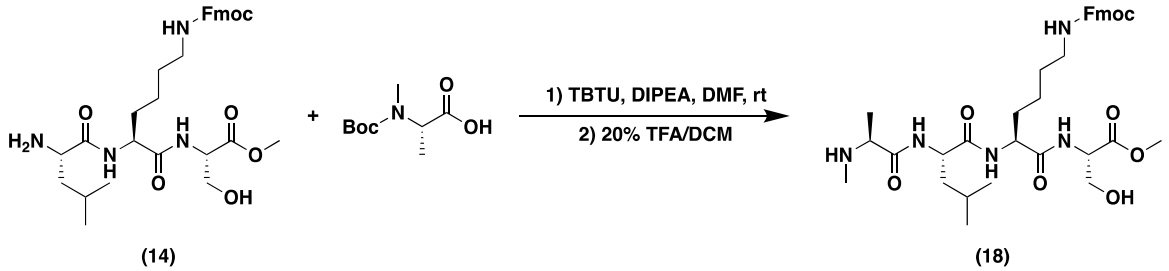


(17) (2)

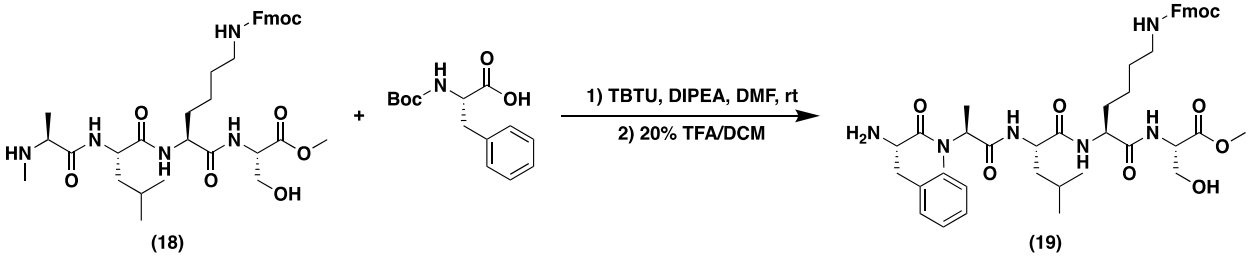
methyl N^2-(4-(tert-butyl)benzoyl)-L-phenylalanyl-L-alanyl-L-leucyl-N^6,N^6-diethyl-L-lysyl-L-serinate (2): Compound **17** (397 mg, 0.47 mmol, 1.0 eq.) was dissolved in 15 mL of MeOH. Acetaldehyde (130 μL, 2.33 mmol, 5.0 eq.) was added to the solution followed by 146 mg of sodium cyanoborohydride (2.33 mmol, 5.0 eq.) and the reaction mixture was stirred at room temperature for 1 hour. The volatiles were removed under reduced pressure and the crude mixture was purified by reverse phase column chromatography ((H_20 + 0.1% TFA)/MeOH) to yield 346 mg (80.4%) of the TFA salt of the title compound as a white solid.

^{1}H NMR (400 MHz, Methanol-d_4) δ 7.71 (d, *J* = 8.5 Hz, 2H), 7.48 (d, *J* = 8.6 Hz, 2H), 7.34 – 7.26 (m, 4H), 7.24 – 7.19 (m, 1H), 4.73 (dd, *J* = 9.3, 5.5 Hz, 1H), 4.52 – 4.28 (m, 4H), 3.91 (dd, *J* = 11.4, 4.6 Hz, 1H), 3.79 (dd, *J* = 11.4, 3.9 Hz, 1H), 3.74 (s, 3H), 3.30 – 3.04 (m, 8H), 2.00 – 1.42 (m, 9H), 1.38 (d, *J* = 7.2 Hz, 3H), 1.33 (s, 9H), 1.27 (t, *J* = 7.3 Hz, 6H), 0.92 (t, 6H). MSI (ESI): 795 $[M+H]^+$. t_R = 5.24 min.

(iii) Synthesis of UNC4219 (3) and Intermediates (18-20)



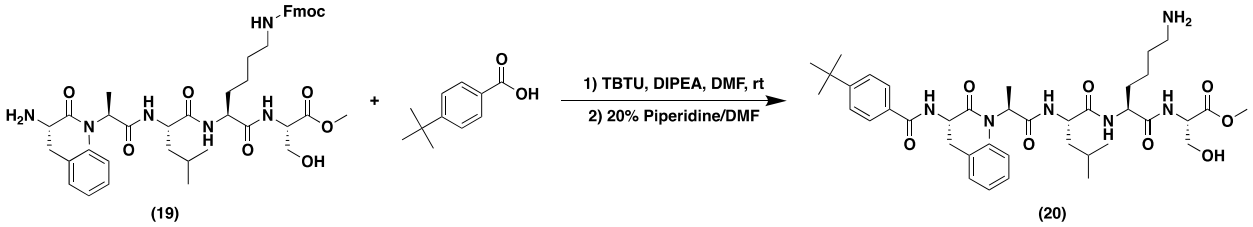
methyl N^6-(((9H-fluoren-9-yl)methoxy)carbonyl)-N^2-methyl-L-alanyl-L-leucyl-L-lysyl-L-serinate (18): Compound **14** (1.4 g, 2.0 mmol, 1.0 eq.), 0.45 g of N-(*tert*-butoxycarbonyl)-N-methyl-L-alanine (2.2 mmol, 1.1 eq.), and 0.77 g of TBTU (2.4 mmol, 1.2 eq.) were dissolved in 40 mL of a 3:1 mixture of EtOAc:DMF. DIPEA (1.1 mL, 6.0 mmol, 3.0 eq.) was added to the solution and the mixture was stirred at room temperature for 2 hrs. The reaction mixture was diluted with brine (100 mL) and extracted with EtOAc (150 mL). The organic layer was washed with brine (2X, 100 mL) and dried over Na_2SO_4. After filtration, the solvents were removed under reduced pressure. The residue was dissolved in 20 mL of a 20% solution of TFA/DCM. The solution was stirred for 30 minutes. Volatiles were removed under reduced pressure and the mixture was purified by reverse phase column chromatography ((H_20 + 0.1% TFA)/MeOH) to yield 1.35 g (84.1% over two steps) of the TFA salt of the title compound as a white solid. MSI (ESI): 668 $[M+H]^+$. t_R = 4.98 min.



methyl N^6-(((9H-fluoren-9-yl)methoxy)carbonyl)-N^2-N-(L-phenylalanyl)-N-methyl-L-alanyl-L-leucyl-L-lysyl-L-serinate (19): Compound **18** (1.35 g, 1.73 mmol, 1.0 eq.), 504 mg of (*tert*-butoxycarbonyl)-L-phenylalanine (1.90 mmol, 1.1 eq.), and 665 mg of TBTU (2.07 mmol, 1.2 eq.) were dissolved in 40 mL of a 3:1 mixture of EtOAc:DMF. DIPEA (0.90 mL, 5.18 mmol, 3.0 eq.) was added to the solution and the mixture was stirred at room temperature for 2 hrs. The reaction mixture was diluted with brine (100 mL) and extracted with EtOAc (150 mL). The organic layer was washed with brine (2X, 100 mL) and dried

over Na_2SO_4. After filtration, the solvents were removed under reduced pressure. The residue was dissolved in 20 mL of a 20% solution of TFA/DCM. The solution was stirred for 30 minutes. Volatiles were removed under reduced pressure and the mixture was purified by reverse phase column chromatography ((H_20 + 0.1% TFA)/MeOH) to yield 722 mg (45.1% over two steps) of the TFA salt of the title compound as a white solid.

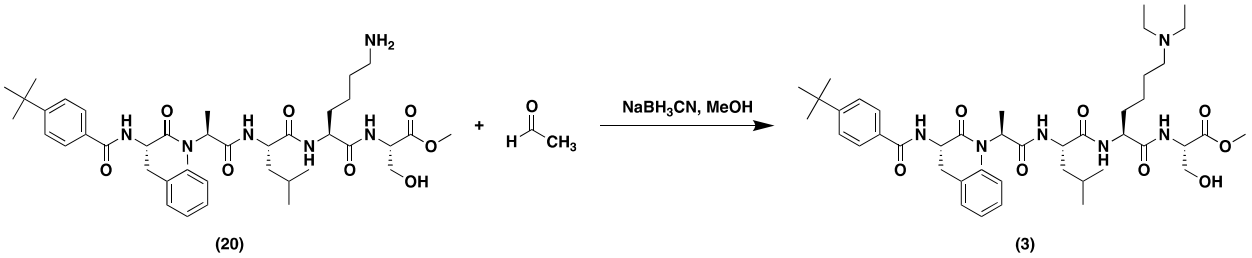
MSI (ESI): 815 $[M+H]^+$. t_R = 5.28 min.



(19) (20)

methyl N-((4-(tert-butyl)benzoyl)-L-phenylalanyl)-N-methyl-L-alanyl-L-leucyl-L-lysyl-L-serinate (20): Compound **19** (722 mg, 0.79 mmol, 1.0 eq.), 155 mg of 4-(tert-butyl)benzoic acid (0.87 mmol, 1.1 eq.), and 304 mg of TBTU (0.95 mmol, 1.2 eq.) were dissolved in 25 mL of a 3:1 mixture of EtOAc:DMF. DIPEA (0.41 mL, 2.37 mmol, 3.0 eq.) was added to the solution and the mixture was stirred at room temperature for 2 hrs. The reaction mixture was diluted with brine (100 mL) and extracted with EtOAc (150 mL). The organic layer was washed with brine (2X, 100 mL) and dried over Na_2SO_4. After filtration, the solvents were removed under reduced pressure. The residue was taken up in 7 mL of a 20% solution of piperidine in DMF. The solution was stirred for 30 minutes. Volatiles were removed under reduced pressure and the mixture was purified by reverse phase column chromatography ((H_20 + 0.1% TFA)/MeOH) to yield 580 mg (84.6% over two steps) of the TFA salt of the title compound as a white solid.

MSI (ESI): 753 $[M+H]^+$. t_R = 5.23 min.

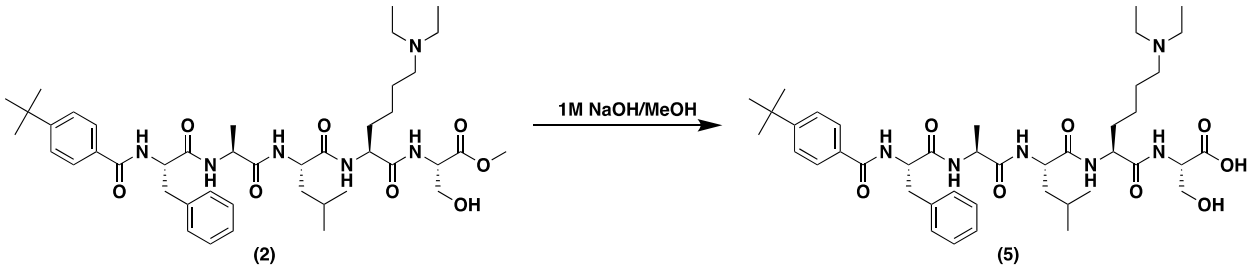


methyl N^2-N-((4-(tert-butyl)benzoyl)-L-phenylalanyl)-N-methyl-L-alanyl-L-leucyl-N^6,N^6-diethyl-L-lysyl-L-serinate (3): Compound **20** (580 mg, 0.68 mmol, 1.0 eq.) was dissolved in 15 mL of MeOH. Acetaldehyde (190 μL, 3.40 mmol, 5.0 eq.) was added to the solution followed by 214 mg of sodium cyanoborohydride (3.41 mmol, 5.0 eq.) and the reaction mixture was stirred at room temperature for 1 hour. The volatiles were removed under reduced pressure and the crude mixture was purified by reverse phase column chromatography ((H_20 + 0.1% TFA)/MeOH) to yield 505 mg (80.4%) of the TFA salt of the title compound as a white solid.

Note: Due to the N-methylation of the alanine residue, the final compound is present as a set of rotamers.

^{1}H NMR (400 MHz, Methanol-d_4) δ 7.90 – 7.64 (m, 3H), 7.54 – 7.47 (m, 3H), 7.38 – 7.21 (m, 8H), 5.31 (t, *J* = 8.0 Hz, 1H), 4.84 – 4.77 (m, 1H), 4.54 – 4.44 (m, 3H), 4.30 – 4.24 (m, 1H), 3.93 (dd, *J* = 11.3, 4.6 Hz, 1H), 3.81 (dd, *J* = 11.3, 3.8 Hz, 1H), 3.74 (s, 4H), 3.27 – 2.98 (m, 14H), 2.61 (s, 3H), 2.00 – 1.39 (m, 15H), 1.35 (d, *J* = 5.6 Hz, 16H), 1.29 (t, *J* = 7.4 Hz, 9H), 0.85 (t, *J* = 6.9 Hz, 9H), 0.44 (d, *J* = 6.8 Hz, 3H). MSI (ESI): 809 $[M+H]^+$. t_R = 5.17 min.

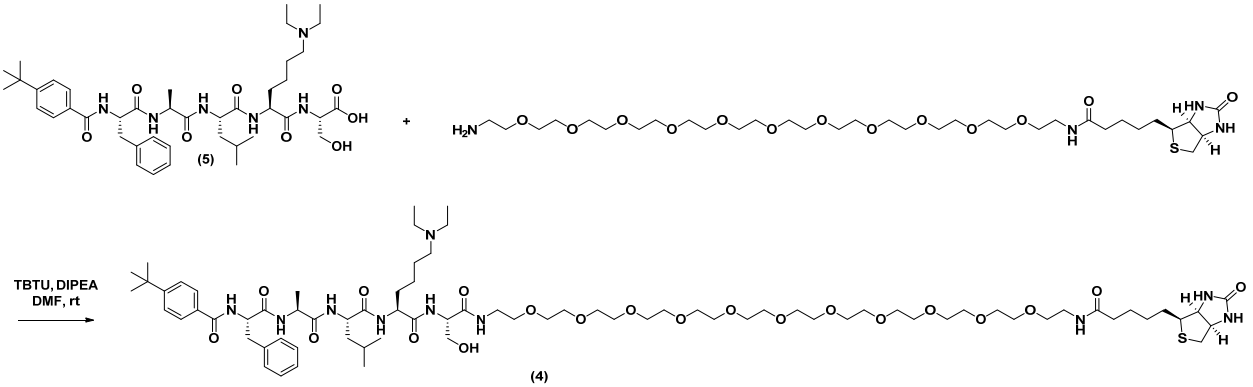
(iv) Synthesis of UNC4007 (5)



***N^2*-(4-(*tert*-butyl)benzoyl)-L-phenylalanyl-L-alanyl-L-leucyl-*N^6*,*N^6*-diethyl-L-lysyl-L-serine (5):** UNC3866 (**2**) (20 mg, 0.022 mmol, 1.0 eq.) was dissolved in 1 mL of a 1:1 mixture of MeOH:1M NaOH and stirred for 30 minutes at room temperature. The pH was neutralized to pH 7 with 37% HCl and the crude mixture was purified by preparative HPLC ((H_2O + 0.1% TFA)/MeCN) to yield 16.9 mg (81%) of the TFA salt of the title compound as a white solid.

^{1}H NMR (400 MHz, Methanol-d_4) δ 7.70 (d, *J* = 8.6 Hz, 2H), 7.48 (d, *J* = 8.7 Hz, 2H), 7.34 – 7.26 (m, 4H), 7.24 – 7.19 (m, 1H), 4.74 (dd, *J* = 9.3, 5.5 Hz, 1H), 4.50 – 4.27 (m, 4H), 3.93 (dd, *J* = 11.3, 4.6 Hz, 1H), 3.82 (dd, *J* = 11.3, 3.7 Hz, 1H), 3.29 – 3.04 (m, 8H), 2.01 – 1.42 (m, 9H), 1.37 (d, *J* = 7.2 Hz, 3H), 1.33 (s, 9H), 1.27 (t, *J* = 7.3 Hz, 6H), 0.92 (t, 6H). MSI (ESI): 781 $[M+H]^+$. t_R = 5.22 min.

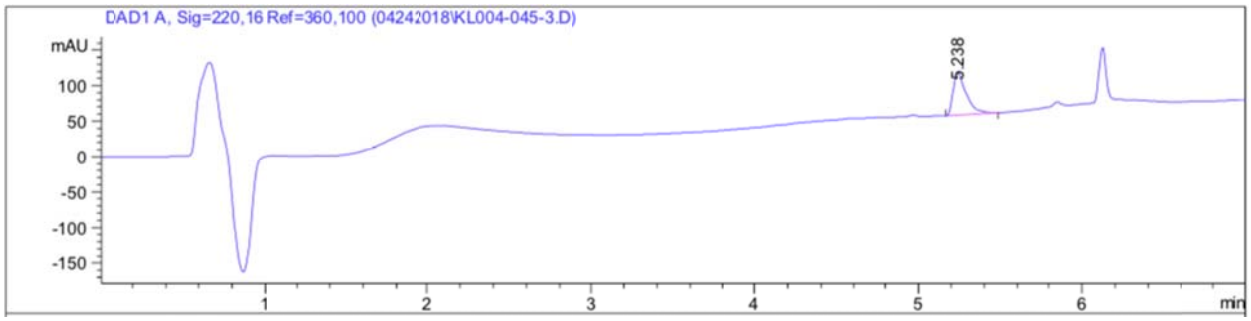
(v) Synthesis of UNC4195 (4)



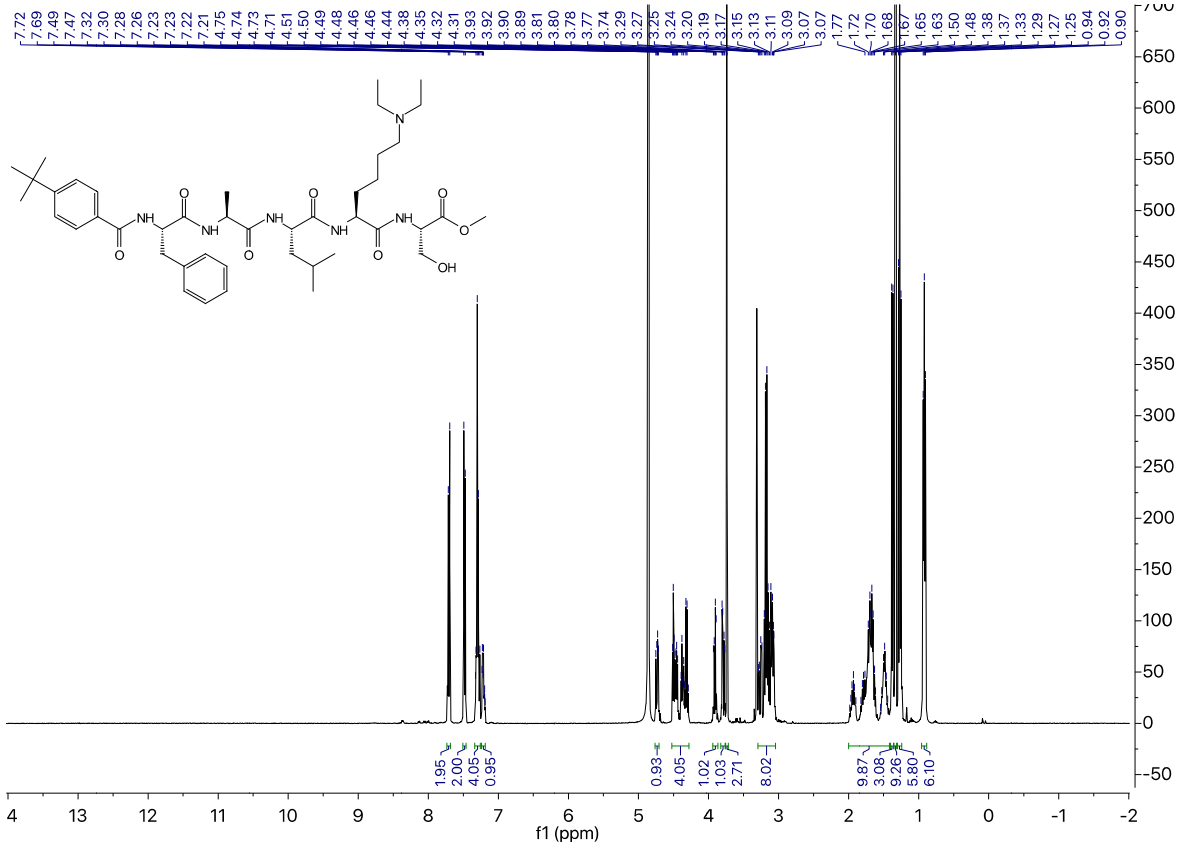
UNC4195 (4). UNC4007 (**5**) (10.0 mg, 0.012 mmol, 1.0 eq.), 10.9 mg of *N*-(35-amino-3,6,9,12,15,18,21,24,27,30,33-undecaoxapentatriacontyl)-5-(2-oxohexahydro-1*H*-thieno[3,4-*d*]imidazol-4-yl)pentanamide (0.014mmol, 1.1 eq.), and 5.34 mg of TBTU (0.017 mmol, 1.3 eq.) were dissolved in 1 mL of DMF. DIPEA (5 µL, 0.028 mmol, 2.2 eq.) was added to the solution and the mixture was stirred at room temperature for 1 hour. The mixture was diluted with methanol (0.5 mL) and purified by preparative HPLC ((H_2O + 0.1% TFA)/MeOH) to yield 9.3 mg (44%) of the TFA salt of the title compound as a clear oil. MSI (ESI): 767 $[M+2H]^{2+}$, 511 $[M+3H]^{3+}$. t_R = 4.67 min.

(vii) Spectral Data

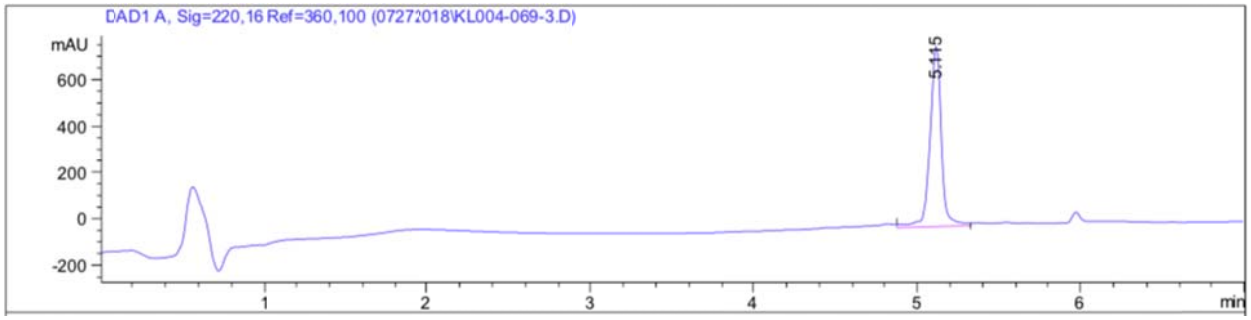
LCMS trace of UNC3866 (2) at 220 nm.



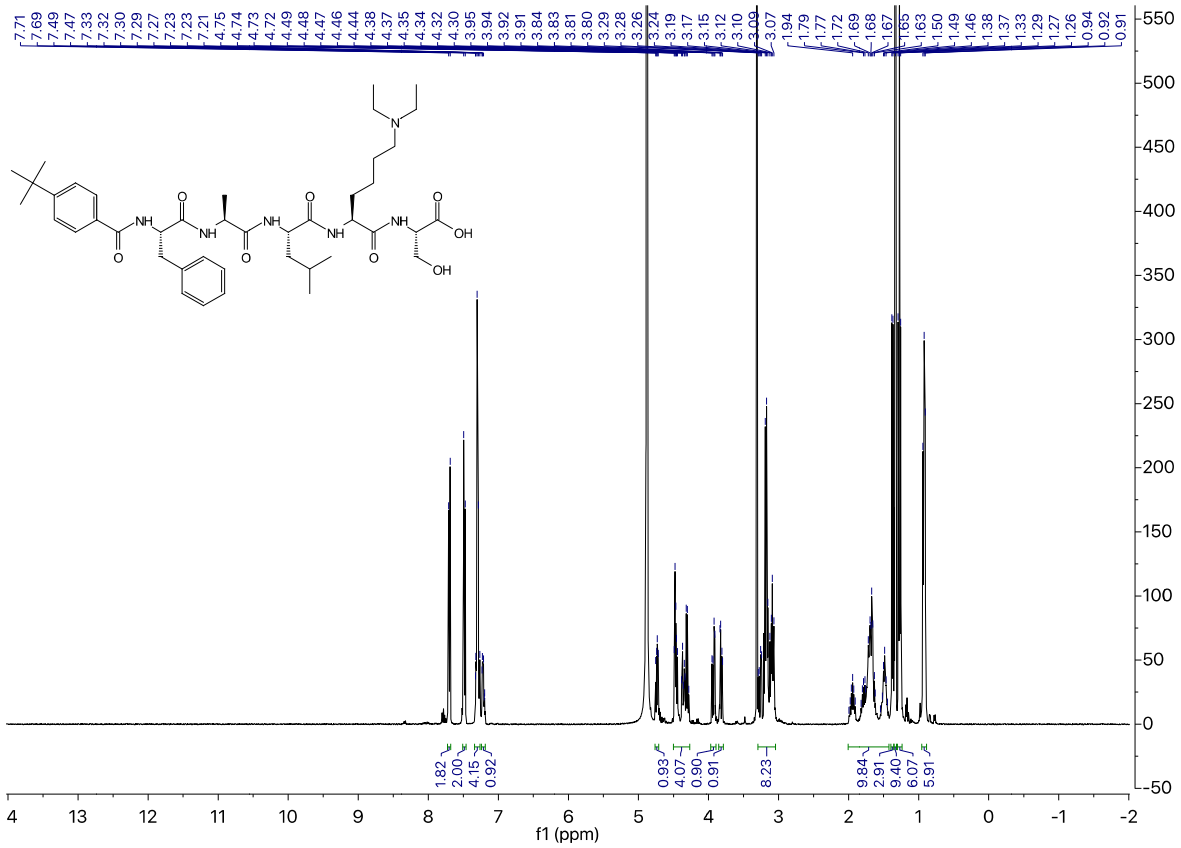
^{1}H NMR spectrum of UNC3866 (2) as a TFA salt.



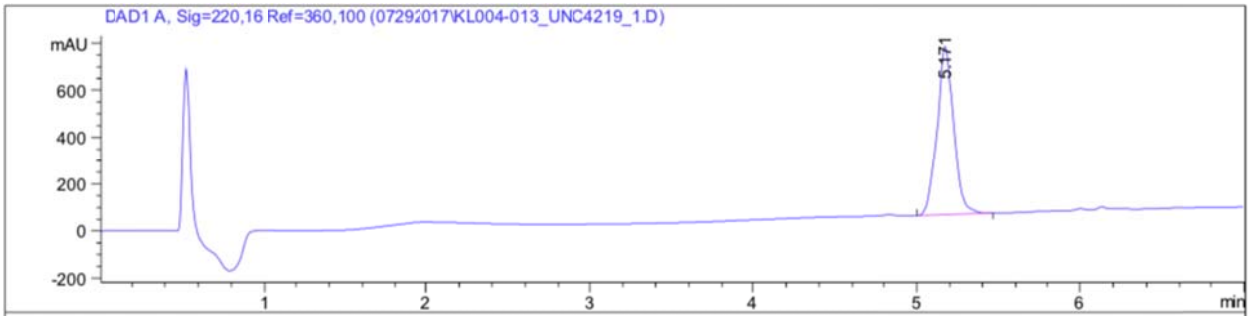
LCMS trace of UNC4007 (5) at 220 nm.



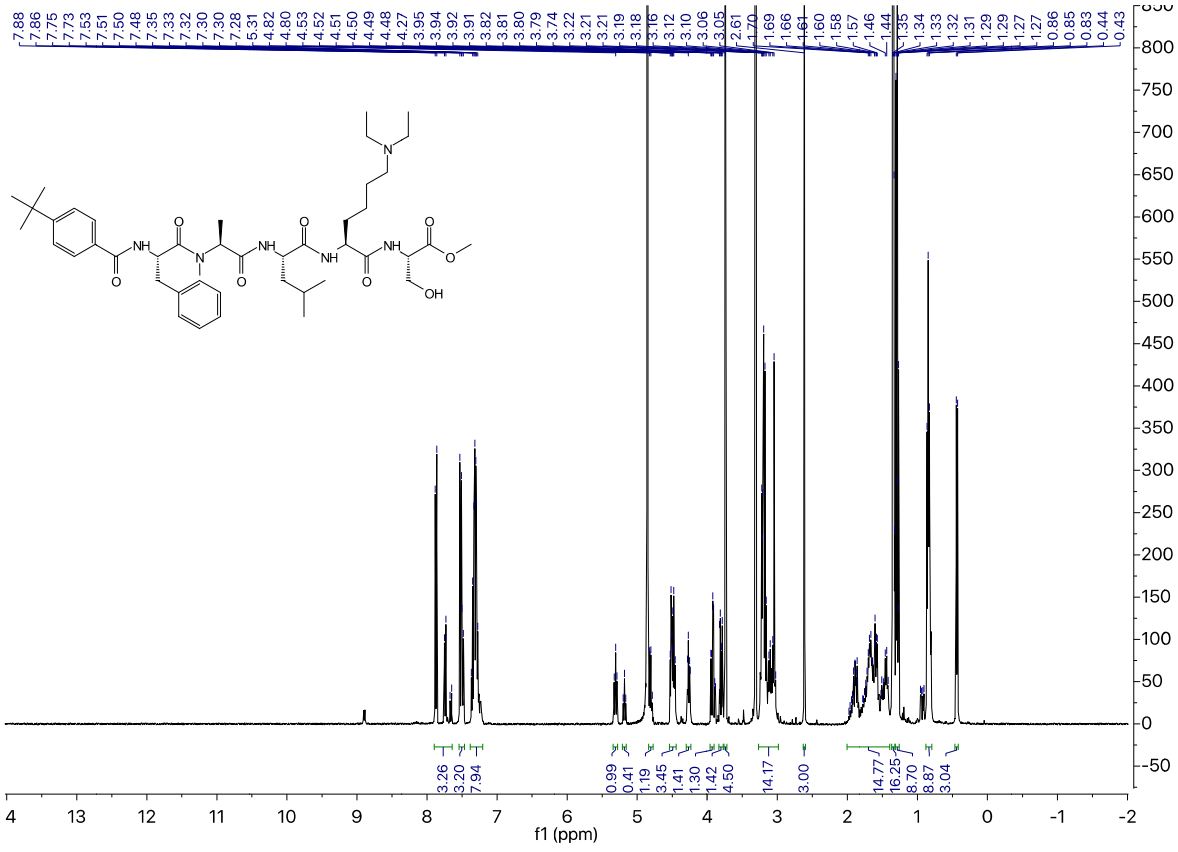
^{1}H NMR spectrum of UNC4007 (5) as a TFA salt.



LCMS trace of UNC4219 (3) at 220 nm.



^{1}H NMR spectrum of UNC4219 (3) as a TFA salt.



LCMS trace of UNC4195 (4) at 220 nm.