

SUPPORTING INFORMATION

Impact of charges on the hybridization kinetics and thermal duplex stability of PNA

Miguel López-Tena^a and Nicolas Winssinger^{*a}

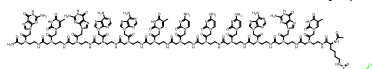
nicolas.winssinger@unige.ch

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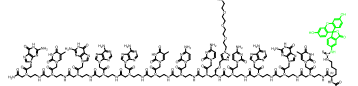
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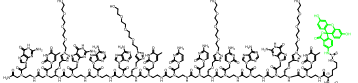
PNA1-ach-F: C-Ter: GTG AAT CCC AGT-Lys(FITC)-Ac



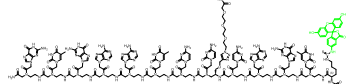
PNA1-H1-F: C-Ter: GTG AAT CC^HC AGT-Lys(FITC)-Ac



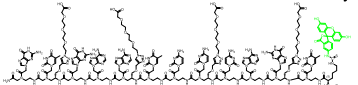
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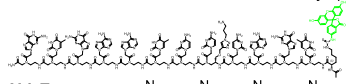
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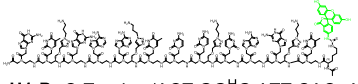
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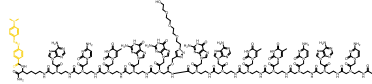
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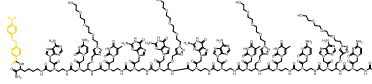
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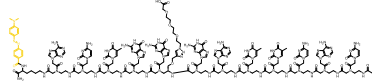
PNA1-H1-D: C-Ter: Lys(ACT GG^HG ATT CAC -Ac)-DabcyI



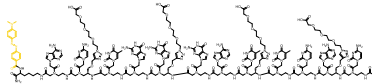
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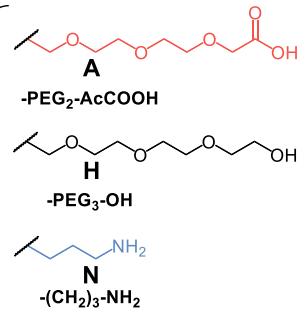
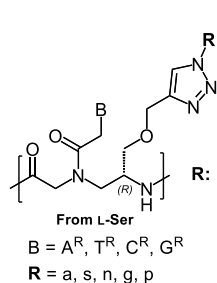
PNA1-A4-D: C-Ter: Lys(AC^AT GG^AG AT^AT CA^AC -Ac)-DabcyI



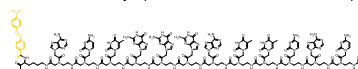
DNA1-D: 5'- CACTTAGGGTCA- 3' 3'-DabcyI modification

DNA3-D: 5'- CACTTAGAGTCA- 3' 3'-DabcyI modification / A:C mismatch

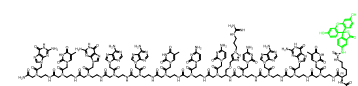
DNA5-D: 5'- CACTTAGCGTCA- 3' 3'-DabcyI modification / C:C mismatch



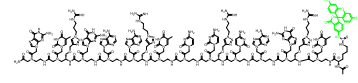
PNA1-ach-D: C-Ter: Lys(ACT GGG ATT CAC -Ac)-DabcyI



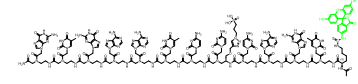
PNA1-G1-F: C-Ter: GTG AAT CC^GC AGT-Lys(FITC)-Ac



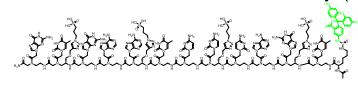
PNA1-G4-F: C-Ter: GT^GG AA^GT CC^GC AG^GT-Lys(FITC)-Ac



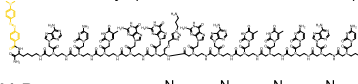
PNA-P1-F: C-Ter: GTG AAT CC^PC AGT-Lys(FITC)-Ac



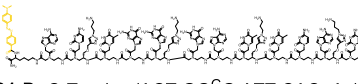
PNA1-P4-F: C-Ter: GT^PG AA^PT CC^PC AG^PT-Lys(FITC)-Ac



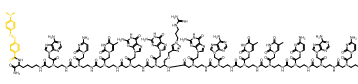
PNA1-N1-D: C-Ter: Lys(ACT GG^NG ATT CAC -Ac)-DabcyI



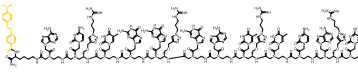
PNA1-N4-D: C-Ter: Lys(AC^NT GG^NG AT^NT CA^NC -Ac)-DabcyI



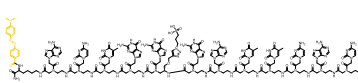
PNA1-G1-D: C-Ter: Lys(ACT GG^GG ATT CAC -Ac)-DabcyI



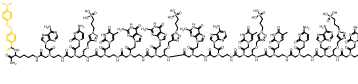
PNA1-G4-D: C-Ter: Lys(AC^GT GG^GG AT^GT CA^GC -Ac)-DabcyI



PNA1-P1-D: C-Ter: Lys(ACT GG^PG ATT CAC -Ac)-DabcyI



PNA1-P4-D: C-Ter: Lys(AC^PT GG^PG AT^PT CA^PC -Ac)-DabcyI



DNA2-F: 5'- TGACCCTAAGTG -3' 5'-FITC modification

DNA4-D: 5'- CACTTAGTGTCA- 3' 3'-DabcyI modification / T:C mismatch

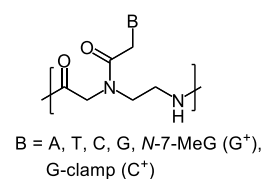
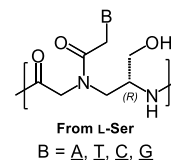
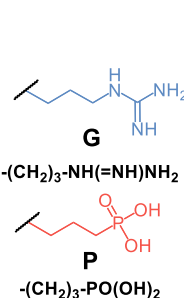
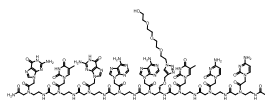
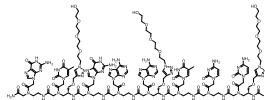


Figure S1. Detailed structures of all PNA/DNA oligomers used in this work for FRET T_m and K_D measurements.

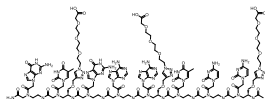
PNA2-H1: C-Ter: GTG AA^HT CC -Ac



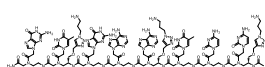
PNA2-H3: C-Ter: GT^HG AA^HT CC^H -Ac



PNA2-A3: C-Ter: GT^AG AA^AT CC^A -Ac

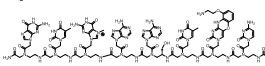


PNA2-N3: C-Ter: GT^NG AA^NT CC^N -Ac

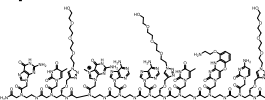


DNA6-Bt: 5'- CAC TTA GG- 3' 5'-Biotin modification

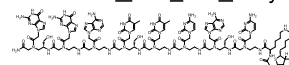
PNA2-pc-ach: C-Ter: GTG⁺ AAT C⁺C -Ac



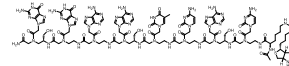
PNA2-pc-H3: C-Ter: GT^HG⁺ AA^HT C⁺C^H -Ac



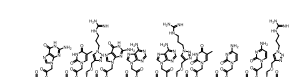
PNA3-Bt: C-Ter: GG ATT CAC-Lys(Bt)-Ac



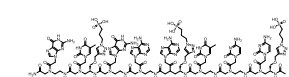
PNA3-AAmm-Bt: C-Ter: GG AAT CAC-Lys(Bt)-Ac
A:A mismatch



PNA2-G3: C-Ter: GT^GG AA^GT CC^G -Ac



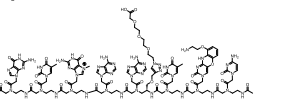
PNA2-P3: C-Ter: GT^PG AA^PT CC^P -Ac



DNA7-Bt: 5'- CAC TAA GG- 3' 5'-Biotin modification /
A:A mismatch

DNA-8: 5'- CC TAA GTG- 3'

PNA2-pc-A1: C-Ter: GTG⁺ AA^AT C⁺C -Ac



PNA2-pc-A3: C-Ter: GT^AG⁺ AA^AT C⁺C^A -Ac

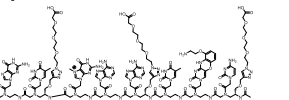


Figure S1 continued. Detailed structures of all PNA/DNA oligomers used in this work for FRET T_m and K_D measurements.

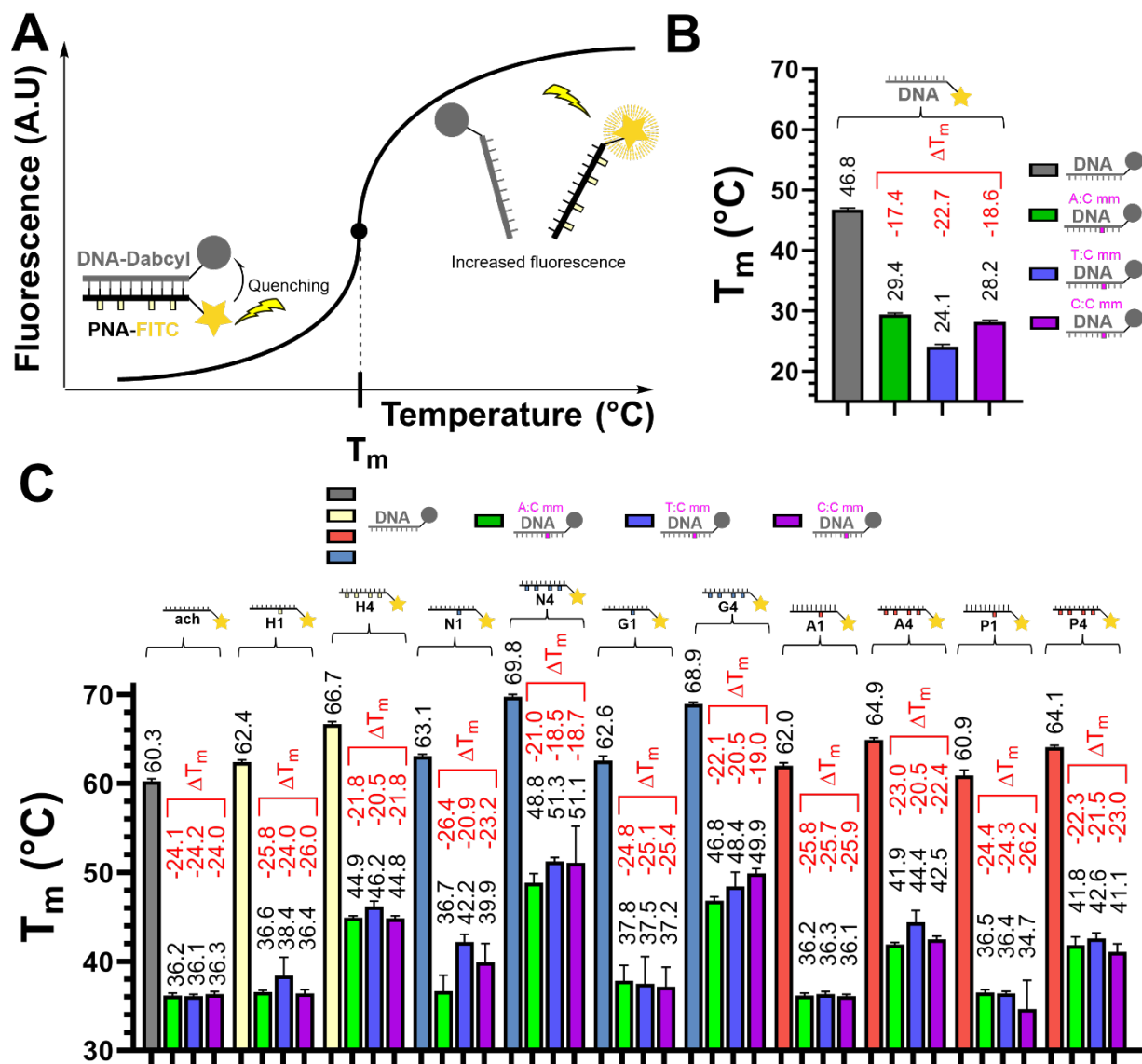
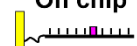


Figure S2. A) Scheme of the FRET melting temperature analysis curves for DNA labelled with Dabcyl quencher and PNA with FITC. B) Melting temperatures for DNA-DNA duplexes, perfect matched sequence versus A:Cmm, T:Cmm and C:Cmm. C) Melting temperatures for PNA-DNA duplexes, perfect matched sequence versus A:Cmm, T:Cmm and C:Cmm.

On chip



PNA3-AAmm-Bt A:A mm	$k_{on} \times 10^4$ ($M^{-1}s^{-1}$)	$k_{off} \times 10^{-3}$ (s^{-1})	K_D (nM)		$k_{on} \times 10^4$ ($M^{-1}s^{-1}$)	$k_{off} \times 10^{-3}$ (s^{-1})	K_D (nM)
PNA2-ach	3.0	2.1	71	DNA8	4.9	258.2	5225
PNA2-H1	1.4	2.0	147	PNA2-H3	1.8	1.2	65
PNA2-N3	1.4	1.2	80	PNA2-A3	1.1	1.1	98
PNA2-G3	2.6	1.2	44	PNA2-P3	2.8	2.3	155

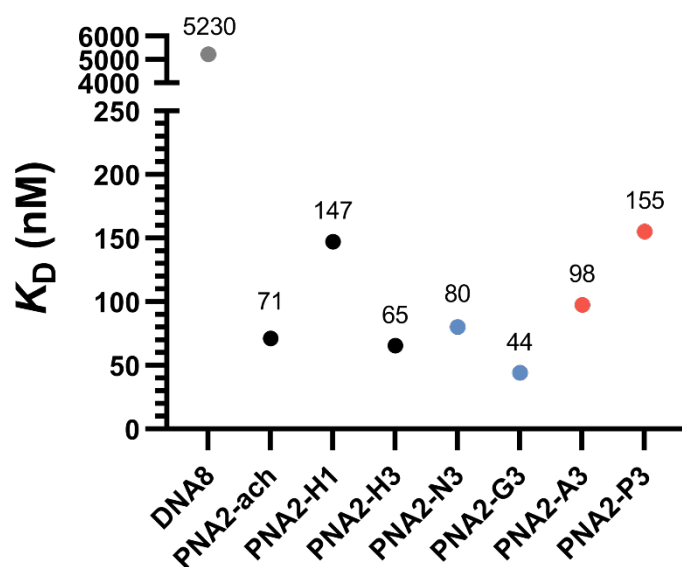


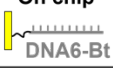
Figure S3. SPR dissociation equilibrium constants (K_D), association rates (k_{on}) and dissociation rates (k_{off}) for PNAs for PNA3-AAmm-Bt immobilized on the chip.

DNA6-Bt: 5'-CAC TTA GG-3' 5'-Bt
DNA-8: 5'-CC TAA GTG-3'
PNA2-ach: C-Ter: GTG AAT CC-Ac

PNA2-pc-ach: C-Ter: GTG⁺ AAT CC⁺-Ac
PNA2-pc-A1: C-Ter: GTG⁺ AA^AT CC⁺-Ac
PNA2-pc-A3: C-Ter: GT^AG⁺ AA^AT C^AC⁺-Ac
PNA2-pc-H3: C-Ter: GT^HG⁺ AA^HT C^HC⁺-Ac

N-7-MeG (G⁺),
 G-clamp (C⁺)

On chip



	$k_{on} \times 10^4$ (M ⁻¹ s ⁻¹)	$k_{off} \times 10^{-3}$ (s ⁻¹)	K_D (nM)		$k_{on} \times 10^4$ (M ⁻¹ s ⁻¹)	$k_{off} \times 10^{-3}$ (s ⁻¹)	K_D (nM)
DNA8	39 ± 2	329 ± 6	8600 ± 2000	PNA2-pc-H3	7.9 ± 0.5	2.79 ± 0.06	35 ± 2
PNA2-ach	8.88 ± 0.01	113 ± 7	1280 ± 80	PNA2-pc-A1	4.5 ± 0.2	5.99 ± 0.01	135 ± 6
PNA2-pc-ach	38.8 ± 0.3	18.68 ± 0.08	48.1 ± 0.6	PNA2-pc-A3	2.12 ± 0.09	2.55 ± 0.06	121 ± 5

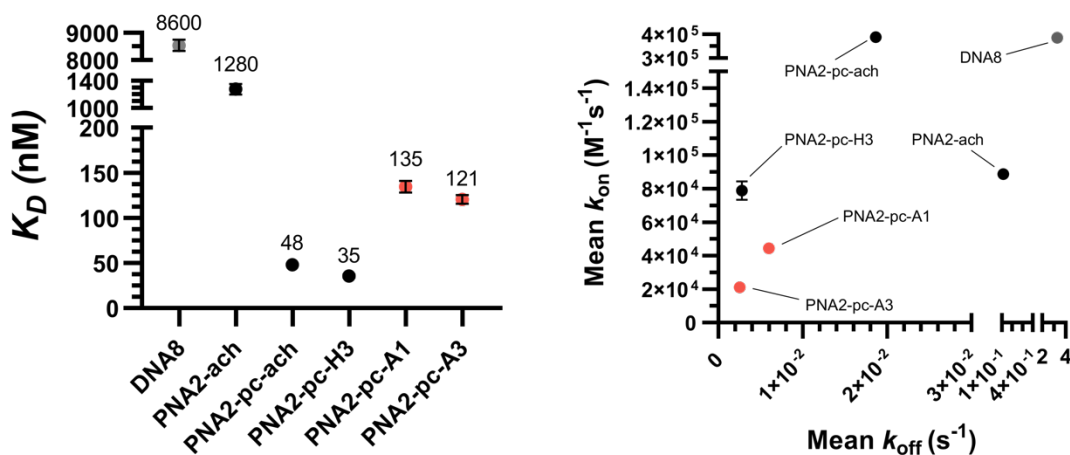


Figure S4. SPR dissociation equilibrium constants (K_D), association rates (k_{on}) and dissociation rates (k_{off}) for pc-PNAs for **DNA6-Bt** immobilized on the chip. Data presented as the average of duplicate measurements ($n = 2$) and reported as the mean ± 95% CI ($z = 1.96$). Plotted error bars represent the standard deviation (SD).

Abbreviations

AcN	Acetonitrile
Boc	Tert-butyloxycarbonyl
DCM	Dichloromethane
DHB	2,5-Dihydroxybenzoic acid
DIPEA	N,N-Diisopropylethylamine
DMF	Dimethylformamide
DMSO	Dimethyl sulfoxide
ESI	Electrospray ionization
EtOAc	Ethyl acetate
FITC	Fluorescein isothiocyanate
Fmoc	Fluorenylmethoxycarbonyl
HATU	Hexafluorophosphate Azabenzotriazole Tetramethyl Uronium
HPLC	High performance liquid chromatography
LC-MS	Liquid chromatography-mass spectrometry
MALDI	Matrix-assisted laser desorption/ionization
MS	Mass spectrometry
PEG	Polyethylene glycol
PNA	Peptide Nucleic Acid
TEA	Triethyl amine
TFA	Trifluoroacetic acid
THF	Tetrahydrofuran
THPTA	Tris(3-hydroxypropyltriazolylmethyl)amine

Synthesis of PNA oligomers

Synthesis of the reported PNA oligomers was performed starting from 5.0 mg of Fmoc-Rink-Amide PEG AM resin (0.33mmol/g, IrisBiotech) by iterative cycles of solid phase peptide synthesis following our previous reports.^{1,2}

Protocols for the synthesis of compounds Az-A/H/N/G/P

2-[2-[2-(2-Azidoethoxy)ethoxy]ethoxy]ethanol (Az-H)

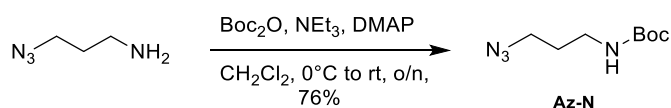
Azido alcohol (Az-H) was synthesized according to the previous reported protocols.³

¹H NMR (400 MHz, CDCl₃): δ 3.87 (s, 1H), 3.70 – 3.66 (m, 2H), 3.64 – 3.60 (m, 12H), 3.60 – 3.53 (m, 2H), 3.35 (t, *J* = 5.1, 5.1 Hz, 2H).

2-[2-[2-(2-Azidoethoxy)ethoxy]ethoxy]acetic acid (Az-A)

Azido acetic acid (Az-A) was synthesized according to previous reported protocols.³

¹H NMR (400 MHz, CDCl₃): δ 9.69 (br. s, 1H), 4.15 (s, 2H), 3.73 – 3.61 (m, 10H), 3.35 (t, *J* = 5.2, 5.2 Hz, 2H).



Tert-butyl (3-azidopropyl)carbamate (Az-N)

To a stirred solution of 3-azidopropan-1-amine (400mg, 4 mmol, 1 eq) in CH₂Cl₂ (5 mL) at 0°C, triethylamine (556 μL, 4 mmol, 1 eq) and 4-dimethylaminopyridine (24mg, 0.2 mmol, 0.05eq) were added. Then, di-tert-butyl dicarbonate (872 mg, 4 mmol, 1 eq) was added in one portion and the reaction mixture was left to warm to room temperature overnight. The reaction mixture was partitioned between Et₂O (60 mL) and NH₄Cl (sat.) (20 mL). The organic layer was separated, washed again with NH₄Cl (sat.) (2 x 20 mL), brine, dried over anhydrous Na₂SO₄, filtered, and concentrated in vacuo. The resulting crude residue was purified by column chromatography (10-30% EtOAc/pentane) to give Az-N.

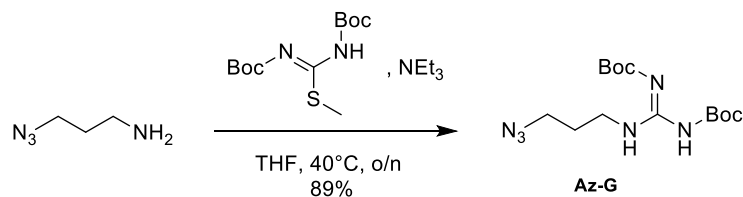
Yield: 611mg (76%). Isolated as a pale yellow oil. Spectroscopic data in accordance with previous reports.⁴

R_f: 0.70 in 1/3 EtOAc/Pentane. UV inactive and stains yellow with KMnO₄ stain.

HR-MS/TOF-MS-ES+: *m/z* expected for [M+Na]⁺: 223.1171, *m/z* found: 223.1181

¹H NMR (300 MHz, CDCl₃): δ 4.66 (br. s, 1H), 3.35 (t, *J* = 6.7 Hz, 2H), 3.26 – 3.15 (m, 2H), 1.76 (p, *J* = 6.7 Hz, 2H), 1.44 (s, 9H).

¹³C NMR (75 MHz, CDCl₃): δ 156.1, 79.6, 49.3, 38.2, 29.4, 28.5.



N², N³-Bis(tert-butoxycarbonyl)-N¹-(3-azidopropyl)guanidine (Az-G)

To a stirred solution of N,N'-Di-Boc-S-methylisothiourea (300 mg, 1.03 mmol, 1 eq) in THF (3.2 mL) at room temperature, a solution of 3-azidopropan-1-amine (258 mg, 2.58 mmol, 2.5 eq) and triethylamine (430 μ L, 3.09 mmol, 3 eq) in THF (2 mL) were added. The reaction mixture was left to stir at 40°C overnight. Then, concentrated in vacuo and the resulting crude residue was purified by column chromatography (10% EtOAc/pentane) to give **Az-G**.

Yield: 272mg (89%). Isolated as a white solid.

R_f: 0.30 in 10% EtOAc/Pentane. UV inactive and stains yellow with KMnO₄ stain.

HR-MS/TOF-MS-ES⁺: *m/z* expected for [M+Na]⁺: 365.1913, *m/z* found: 365.1920

¹H NMR (300 MHz, CDCl₃): δ 11.48 (br. s, 1H), 8.42 (br. s, 1H), 3.51 (m, 2H), 3.38 (t, *J* = 6.8 Hz, 2H), 1.86 (p, *J* = 6.8 Hz, 2H), 1.49 (m, 18H).

¹³C NMR (75 MHz, CDCl₃): δ 163.7, 156.4, 153.4, 83.4, 79.5, 49.3, 38.3, 28.6, 28.4, 28.2.



Dibenzyl (3-azidopropyl)phosphonate (Az-P)

To a stirred solution of diethyl (3-azidopropyl)phosphonate (300 mg, 1.4 mmol, 1 eq) in CH₂Cl₂ (1 mL) at room temperature, TMS-Br (648 μ L, 4.8 mmol, 3.5 eq) were added and stirred under N₂ atmosphere for 4h. Then, excess of TMS-Br removed by CH₂Cl₂ co-evaporations (2 x 5 mL). The residual yellow oil was redissolved CH₂Cl₂ (1.5 mL) with 2 drops of DMF. Cooled to 0°C and (COCl)₂ (908 μ L, 10.1 mmol, 7.4 eq) added dropwise under inert atmosphere (strong bubbling). The mixture was left to warm to room temperature for 2h before removing the excess (COCl)₂ by CH₂Cl₂ co-evaporations (2 x 5 mL). The residual orange oil was redissolved in CH₂Cl₂ (1 mL) and cooled to 0°, then a solution of benzyl alcohol (560 μ L, 5.4 mmol, 4 eq), 4-dimethylaminopyridine (17 mg, 0.1 mmol, 0.1 eq) and triethylamine (1.14 mL, 8.2 mmol, 6 eq) in CH₂Cl₂ (1.5 mL) was dropwise added under inert atmosphere (strong exotherm). The reaction mixture was left to warm to room temperature for 30min, partitioned between Et₂O (60 mL) and NH₄Cl (sat.) (20 mL). The organic layer was separated, washed again with NH₄Cl (sat.) (2 x 20 mL), water (1 x 20 mL), 1M NaOH (3 x 20 mL), brine, dried over anhydrous Na₂SO₄, filtered, and concentrated in vacuo. The resulting crude residue was purified by column chromatography (10-30% acetone/pentane) to give **Az-p**.

Yield: 121mg (24%). Isolated as a pale yellow oil.

R_f: 0.60 in 30% acetone/pentane. UV active and stains yellow with KMnO₄ stain.

HR-MS/TOF-MS-ES⁺: *m/z* expected for [M+Na]⁺: 368.1140, *m/z* found: 368.1147

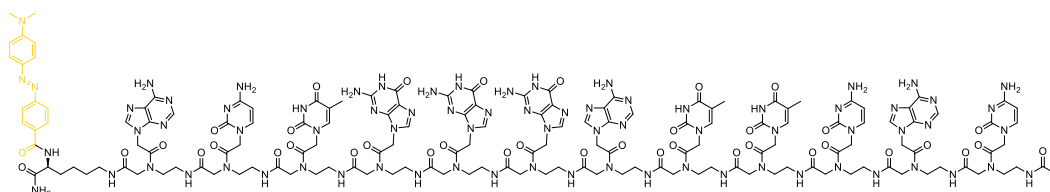
¹H NMR (400 MHz, CDCl₃): δ 7.42 – 7.29 (m, 10H), 5.10 – 4.92 (m, 4H), 3.43 – 3.19 (m, 2H), 2.24 – 1.67 (m, 4H).

¹³C NMR (101 MHz, CDCl₃): δ 136.4, 136.4, 128.8, 128.7, 128.1, 67.5, 67.4, 51.6, 51.4, 33.7, 33.5, 26.0, 25.9, 25.7, 24.3, 24.2, 22.7, 22.5, 22.4.

³¹P NMR (121 MHz, CDCl₃): δ 34.8, 32.0 (major), 31.7.

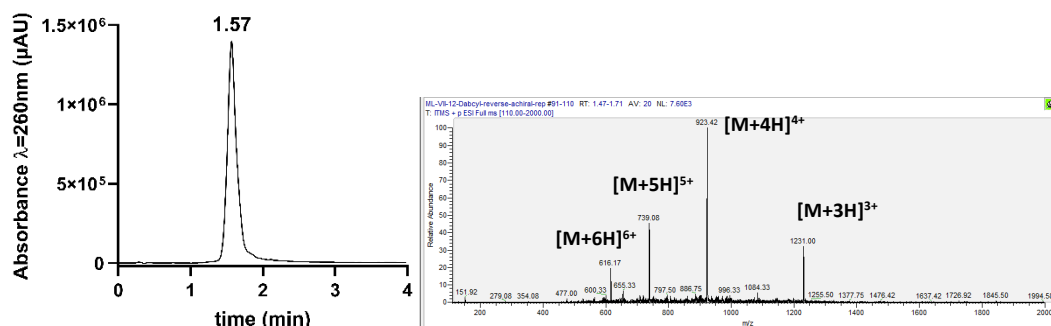
Characterisation of PNA oligomers

PNA1- ach-D: C-Ter: Lys(ACT GGG ATT CAC -Ac)-Dabcyl

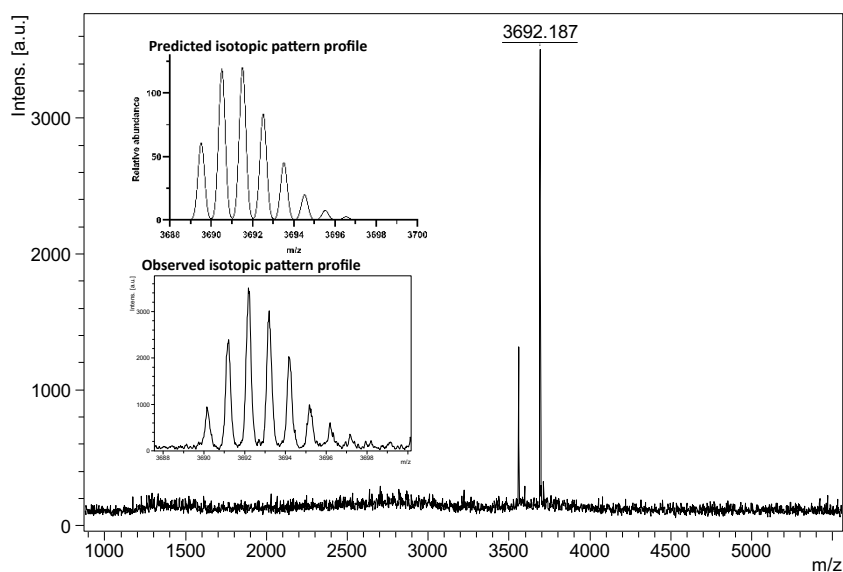


Chemical Formula: C₁₅₂H₁₈₉N₇₅O₃₉ **Exact Mass:** 3688.511 **Molecular Weight:** 3690.670

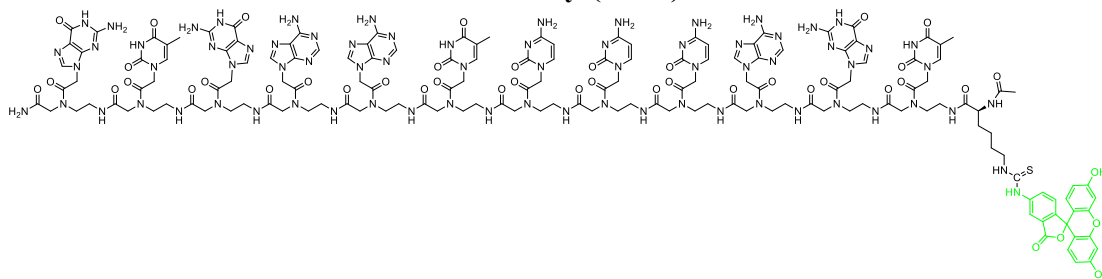
LC-MS-ESI+: m/z expected for $[M+6H]^{6+}$: 616.1, m/z found: 616.2; m/z expected for $[M+5H]^{5+}$: 739.1, m/z found: 739.1; m/z expected for $[M+4H]^{4+}$: 923.6, m/z found: 923.4; m/z expected for $[M+3H]^{3+}$: 1231.2, m/z found: 1231.0.



MALDI-TOF-MS: m/z expected for $[M+H]^+$: 3691.511, m/z found: 3692.187. In all PNAs containing Dabcyl quencher have a secondary peak with a -132 m/z corresponding to a fragmentation of the quencher.

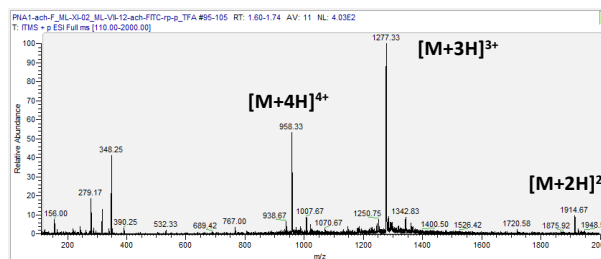
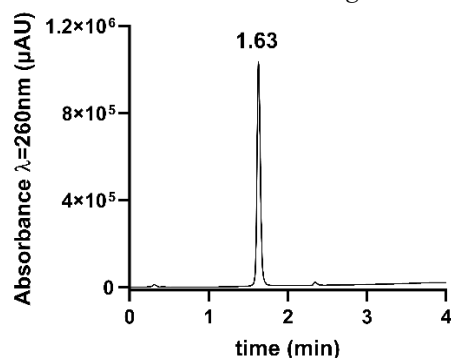


PNA1-ach-F: C-Ter: GTG AAT CCC AGT-Lys(FITC)-Ac

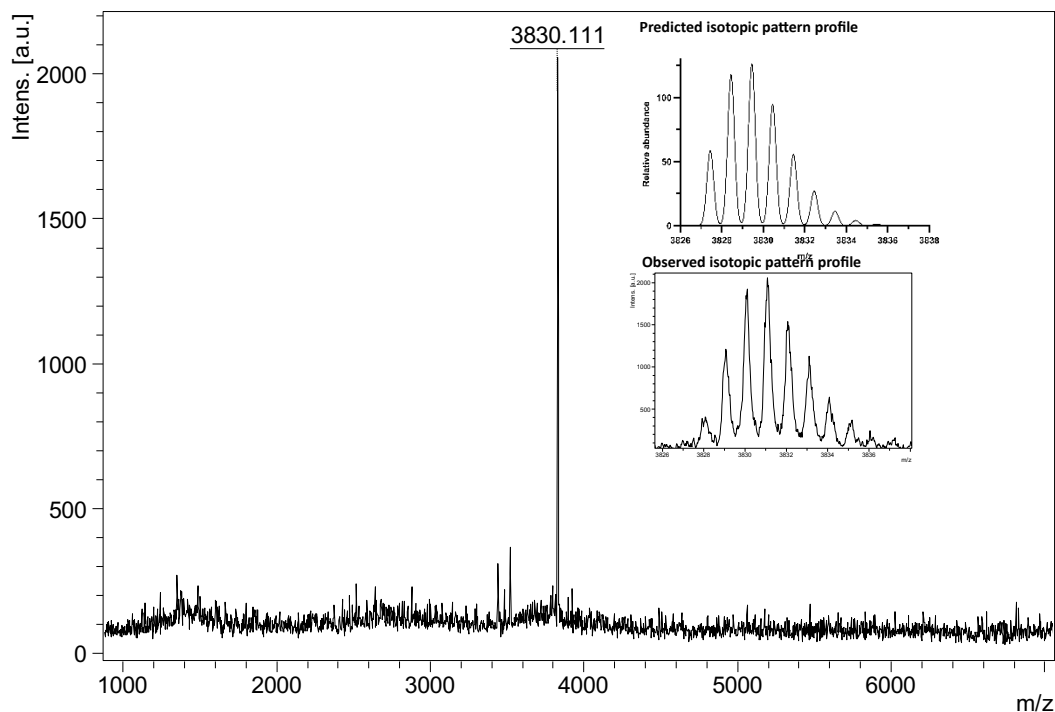


Chemical Formula: C₁₅₈H₁₈₇N₇₃O₄₃S **Exact Mass:** 3826.441 **Molecular Weight:** 3828.762

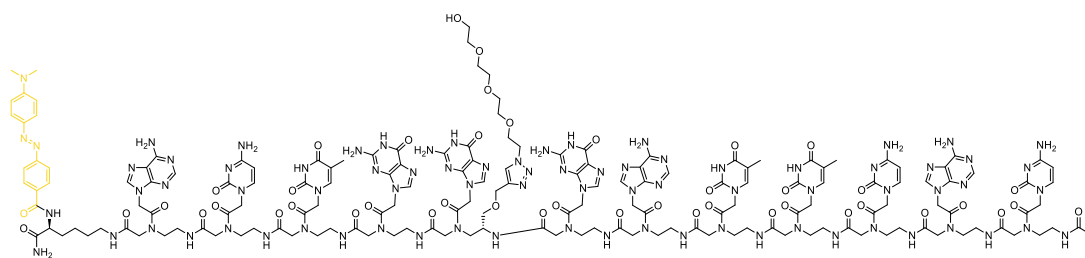
LC-MS-ESI+: *m/z* expected for [M+4H]⁴⁺: 958.1, *m/z* found: 958.3; *m/z* expected for [M+3H]³⁺: 1277.2, *m/z* found: 1277.3; *m/z* expected for [M+2H]²⁺: 1915.2, *m/z* found: 1914.7. (0.1% aqueous TFA solution and 0.1% TFA in HPLC grade acetonitrile used as eluents.)



MALDI-TOF-MS: *m/z* expected for [M+H]⁺: 3829.438, *m/z* found: 3830.111

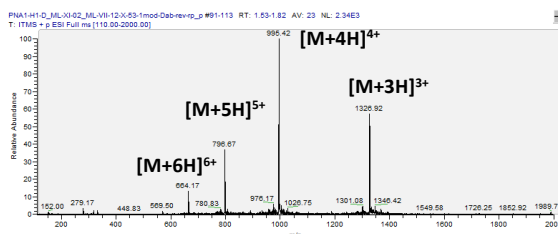
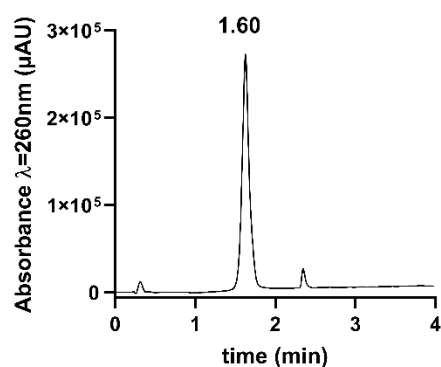


PNA1-H1-D: C-Ter: Lys(ACT GG^HG ATT CAC -Ac)-Dabcyl

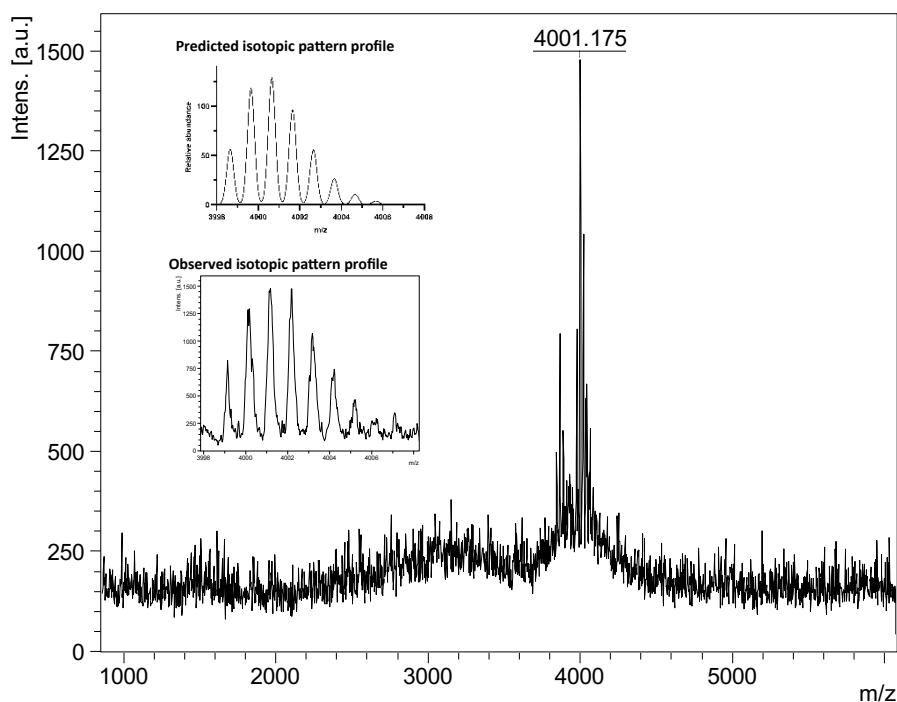


Chemical Formula: C₁₆₄H₂₁₀N₇₈O₄₄ **Exact Mass:** 3975.659 **Molecular Weight:** 3977.986

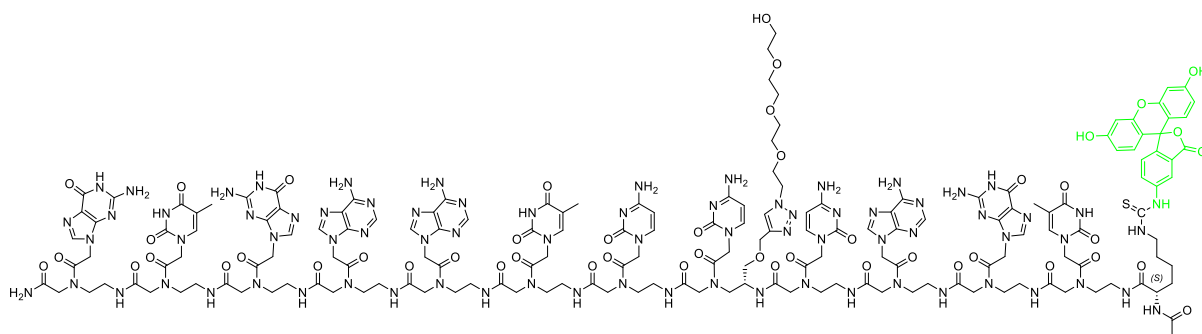
LC-MS-ESI+: m/z expected for $[M+6H]^{6+}$: 664.0, m/z found: 664.2; m/z expected for $[M+5H]^{5+}$: 796.5, m/z found: 796.7; m/z expected for $[M+4H]^{4+}$: 995.4, m/z found: 995.4; m/z expected for $[M+3H]^{3+}$: 1326.9, m/z found: 1326.9.



MALDI-TOF-MS: m/z expected for $[M+Na]^+$: 4000.656 m/z found: 4001.175. In all PNAs containing Dabcyl quencher have a secondary peak with a -132 m/z corresponding to a fragmentation of the quencher.

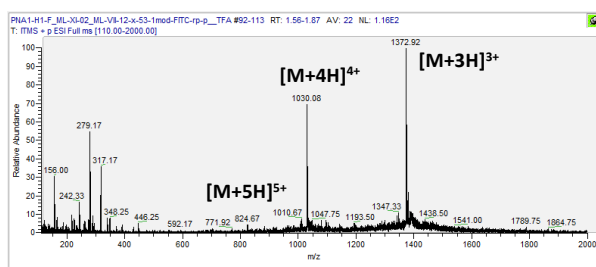
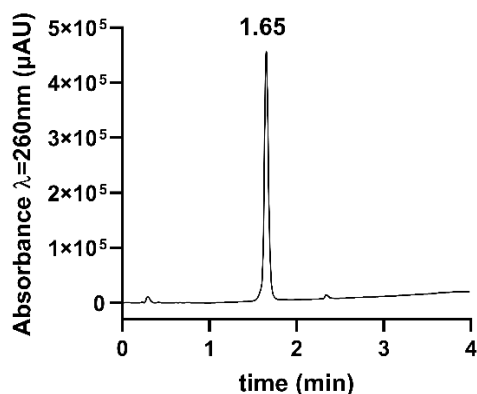


PNA1-H1-F: C-Ter: GTG AAT CC^HC AGT-Lys(FITC)-Ac

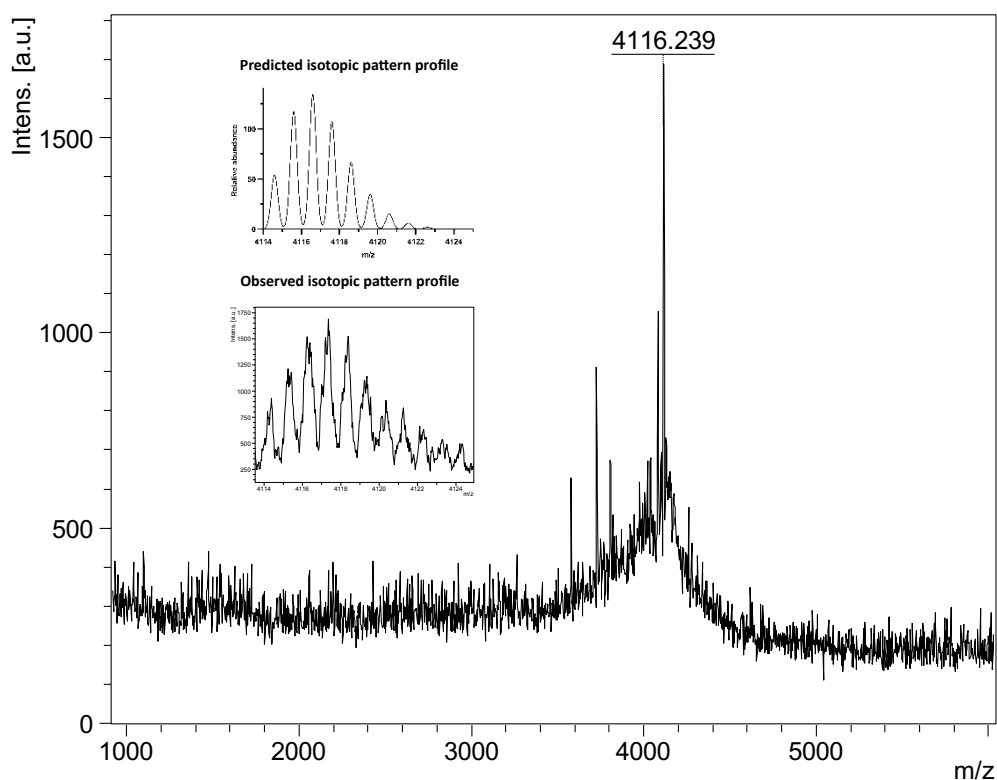


Chemical Formula: C₁₇₀H₂₀₈N₇₆O₄₈S **Exact Mass:** 4113.589 **Molecular Weight:** 4116.078

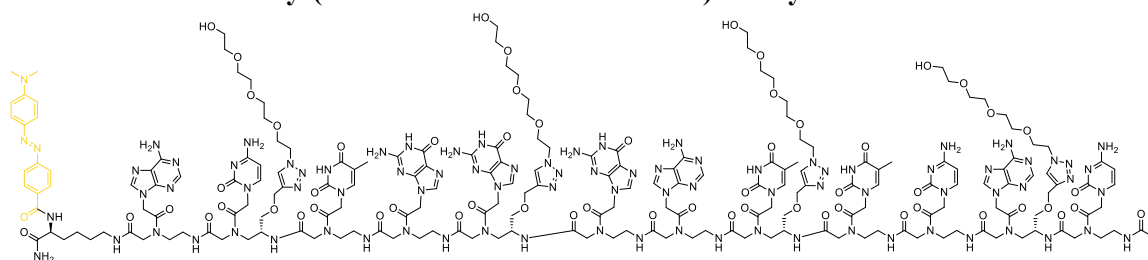
LC-MS-ESI+: m/z expected for $[M+5H]^{5+}$: 824.1, m/z found: 824.7; m/z expected for $[M+4H]^{4+}$: 1029.9, m/z found: 1030.1; m/z expected for $[M+3H]^{3+}$: 1372.9, m/z found: 1372.9. (0.1% aqueous TFA solution and 0.1% TFA in HPLC grade acetonitrile used as eluents.)



MALDI-TOF-MS: m/z expected for $[M+H]^+$: 4116.604, m/z found: 4116.239

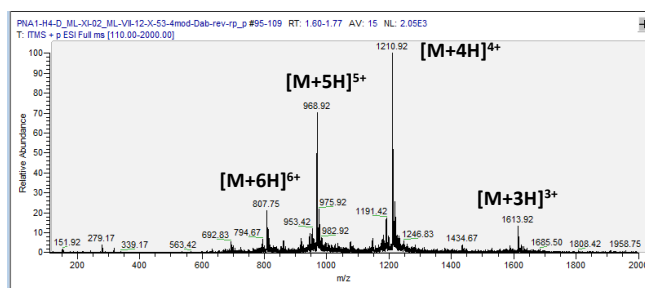
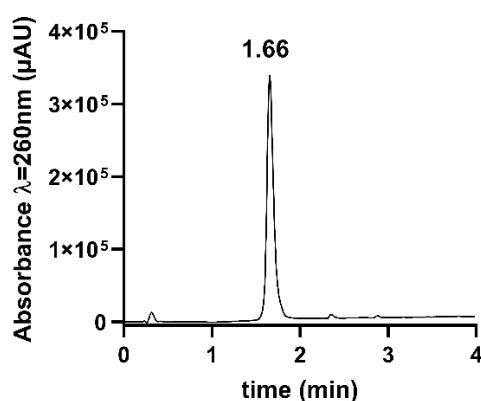


PNA1-H4-D: C-Ter: Lys(AC^HT GG^HG AT^HT CA^HC -Ac)-Dabcyl

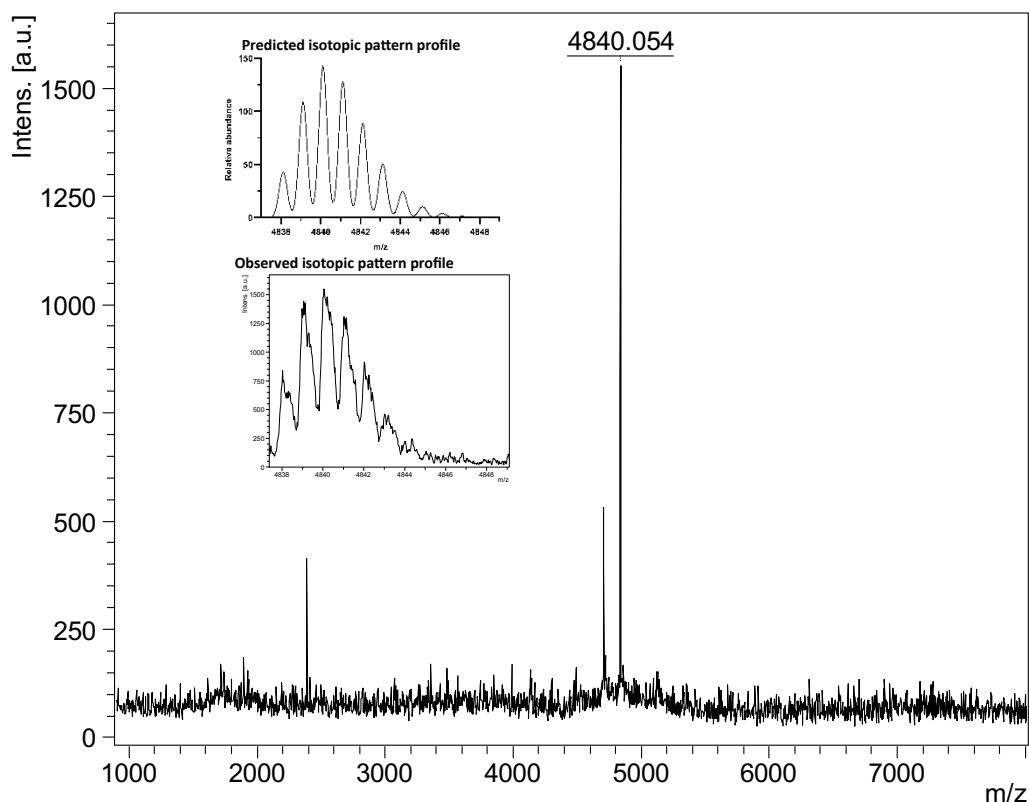


Chemical Formula: C₂₀₀H₂₇₃N₈₇O₅₉ **Exact Mass:** 4837.104 **Molecular Weight:** 4839.934

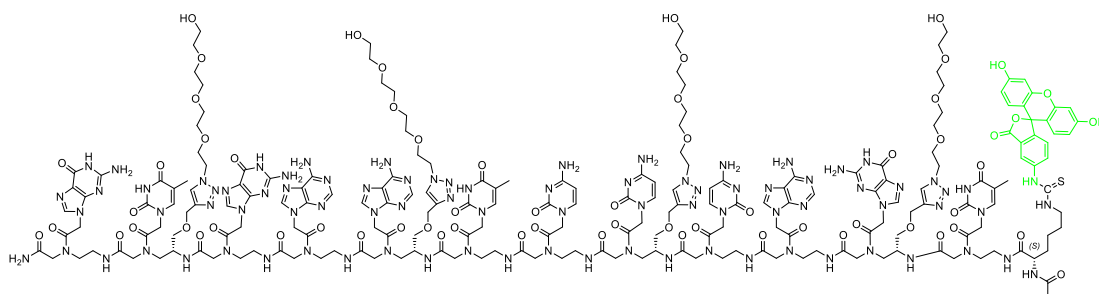
LC-MS-ESI+: m/z expected for $[M+6H]^{6+}$: 807.5, m/z found: 807.8 m/z expected for $[M+5H]^{5+}$: 968.8, m/z found: 968.9; m/z expected for $[M+4H]^{4+}$: 1210.8, m/z found: 1210.9; m/z expected for $[M+3H]^{3+}$: 1614.0, m/z found: 1613.9.



MALDI-TOF-MS: m/z expected for $[M+H]^+$: 4840.114, m/z found: 4840.054. In all PNAs containing Dabcyl quencher have a secondary peak with a -132 m/z corresponding to a fragmentation of the quencher.

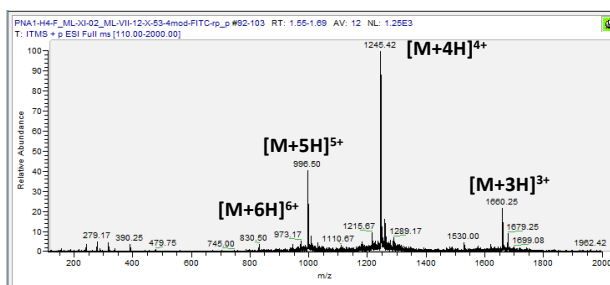
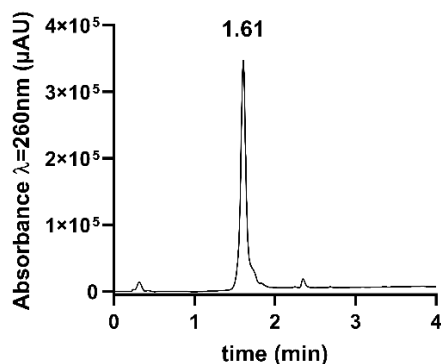


PNA1-H4-F: C-Ter: GT^HG AA^HT CC^HC AG^HT-Lys(FITC)-Ac

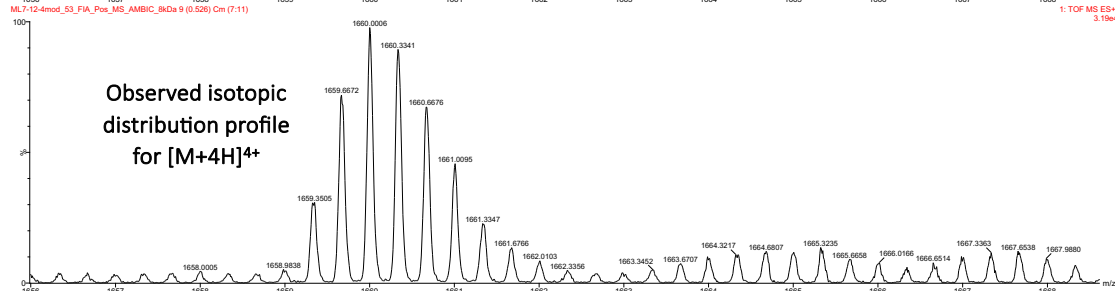
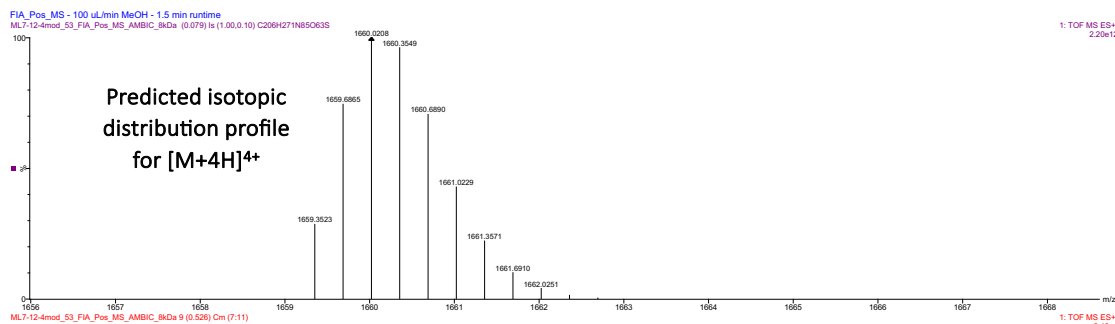
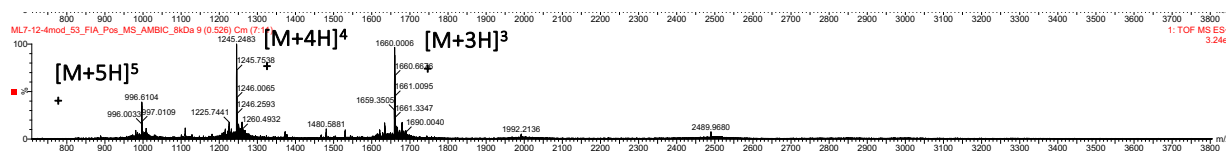


Chemical Formula: C₂₀₆H₂₇₁N₈₅O₆₃S **Exact Mass:** 4975.034 **Molecular Weight:** 4978.026

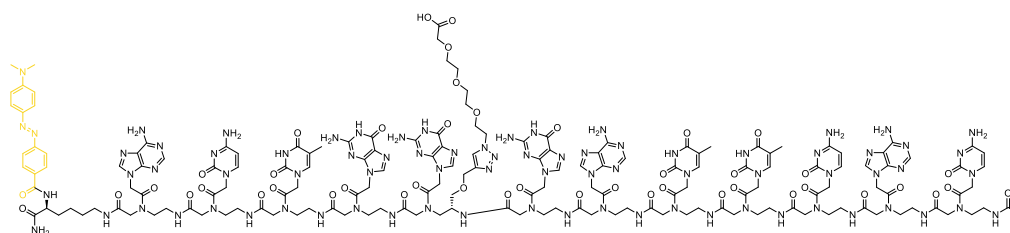
LC-MS-ESI+: *m/z* expected for [M+6H]⁶⁺: 830.5, *m/z* found: 830.5; *m/z* expected for [M+5H]⁵⁺: 996.4, *m/z* found: 996.5; *m/z* expected for [M+4H]⁴⁺: 1245.3, *m/z* found: 1245.4; *m/z* expected for [M+3H]³⁺: 1660.0, *m/z* found: 1660.3.



HR-MS/TOF-MS-ES+: *m/z* expected for [M+3H]³⁺: 1660.0208, *m/z* found: 1660.0006; *m/z* expected for [M+4H]⁴⁺: 1245.2675, *m/z* found: 1245.2483; *m/z* expected for [M+5H]⁵⁺: 996.4156, *m/z* found: 996.6104

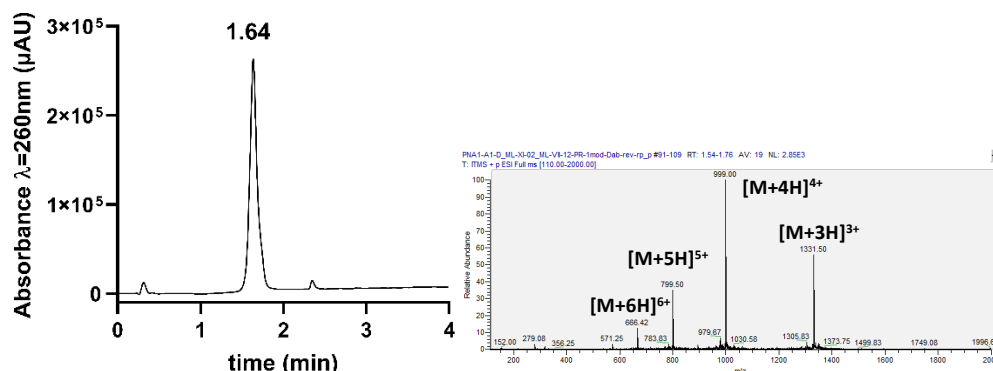


PNA1-A1-D: C-Ter: Lys(ACT GG^AG ATT CAC -Ac)-Dabcyl

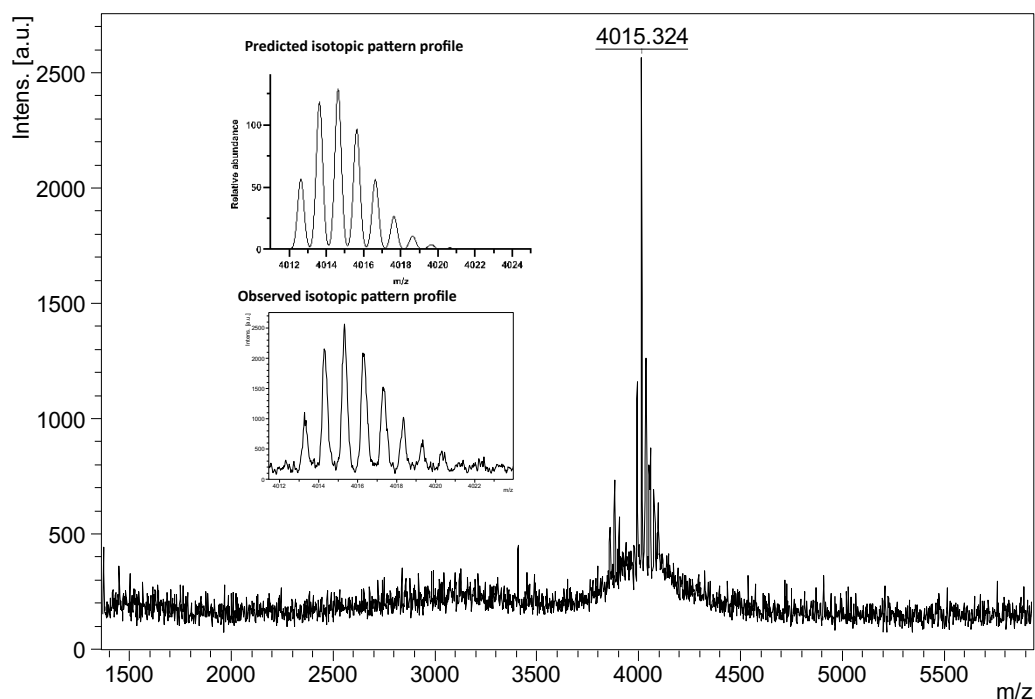


Chemical Formula: C₁₆₄H₂₀₈N₇₈O₄₅ **Exact Mass:** 3989.639 **Molecular Weight:** 3991.969

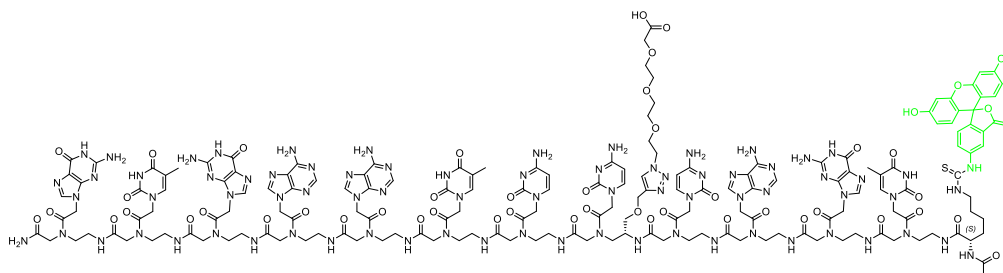
LC-MS-ESI+: m/z expected for $[M+6H]^{6+}$: 666.3, m/z found: 666.4; m/z expected for $[M+5H]^{5+}$: 799.3, m/z found: 799.5; m/z expected for $[M+4H]^{4+}$: 998.9, m/z found: 990.0; m/z expected for $[M+3H]^{3+}$: 1331.6, m/z found: 1331.5.



MALDI-TOF-MS: m/z expected for $[M+\text{Na}]^+$: 4014.641, m/z found: 4015.324. *In all PNAs containing Dabcyl quencher have a secondary peak with a -132 m/z corresponding to a fragmentation of the quencher.*

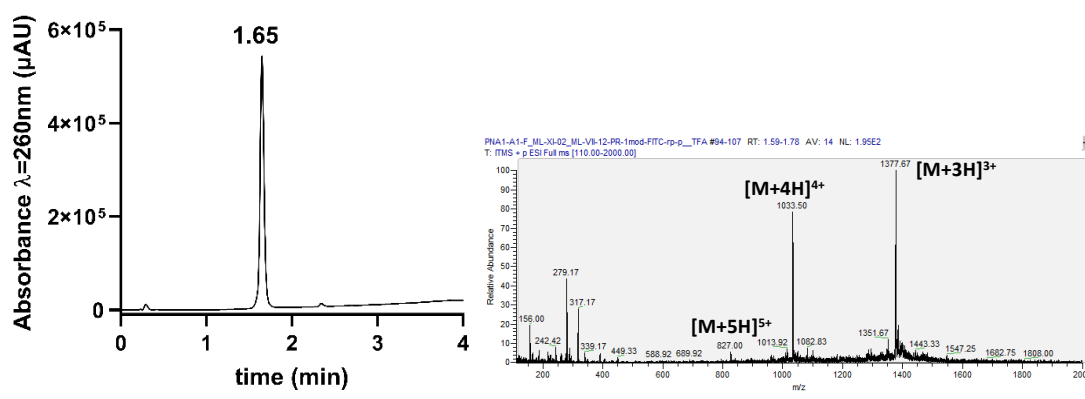


PNA1-A1-F: C-Ter: GTG AAT CC^A AGT-Lys(FITC)-Ac

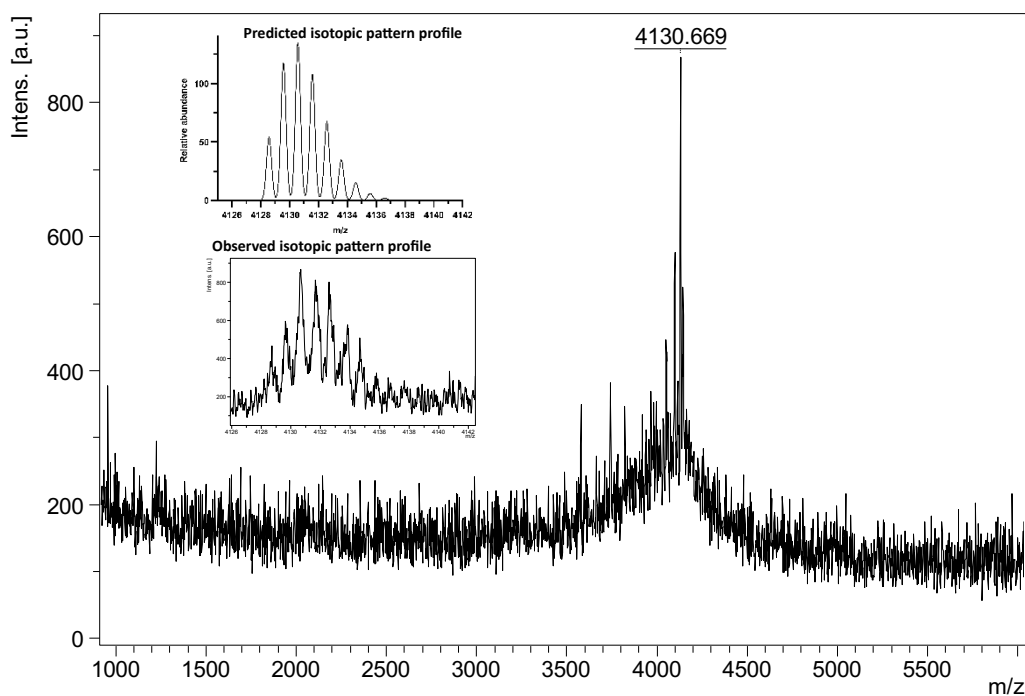


Chemical Formula: C₁₇₀H₂₀₆N₇₆O₄₉S **Exact Mass:** 4127.568 **Molecular Weight:** 4130.061

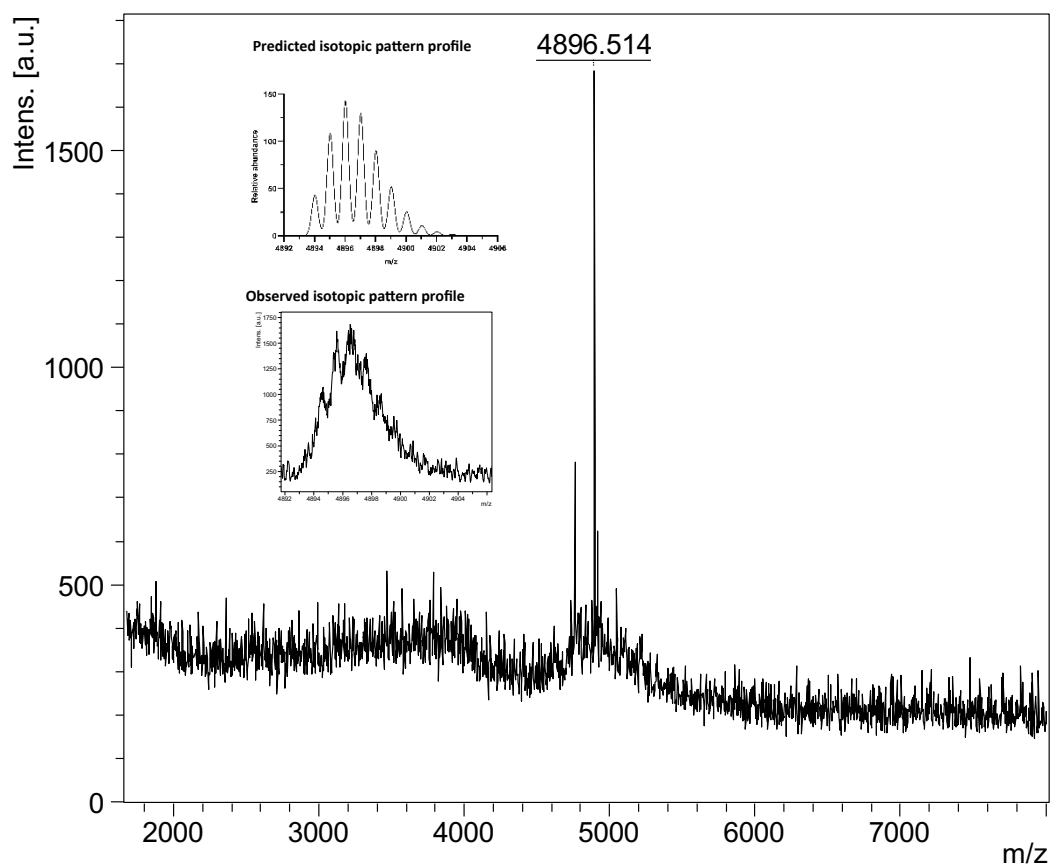
LC-MS-ESI+: m/z expected for $[M+5H]^{5+}$: 826.9, m/z found: 827.0; m/z expected for $[M+4H]^{4+}$: 1033.4, m/z found: 1033.5; m/z expected for $[M+3H]^{3+}$: 1377.5, m/z found: 1377.7. (0.1% aqueous TFA solution and 0.1% TFA in HPLC grade acetonitrile used as eluents.)



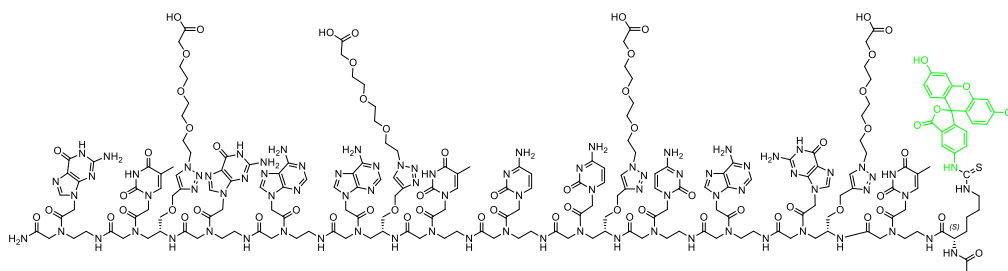
MALDI-TOF-MS: m/z expected for $[M+H]^+$: 4130.594, m/z found: 4130.669.



MALDI-TOF-MS: m/z expected for $[M+H]^+$: 4896.017, m/z found: 4896.514. In all PNAs containing Dabcyl quencher have a secondary peak with a $-132 m/z$ corresponding to a fragmentation of the quencher.

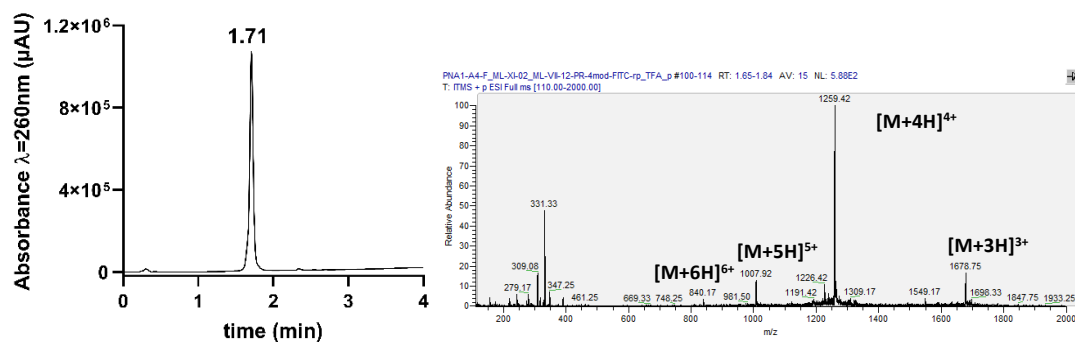


PNA1-A4-F: C-Ter: GT^AG AA^AT CC^AC AG^AT-Lys(FITC)-Ac

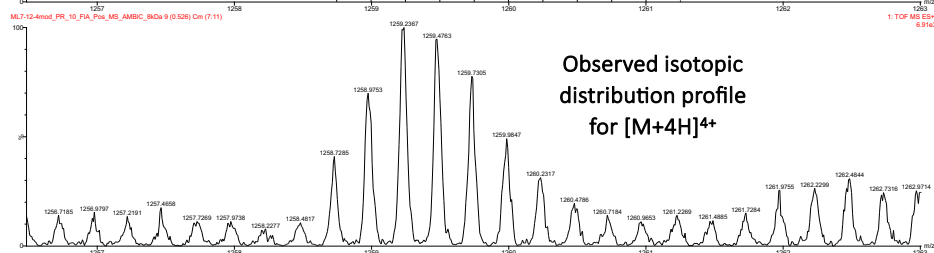
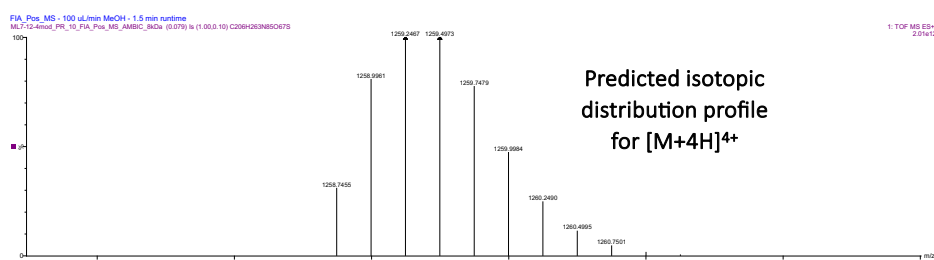
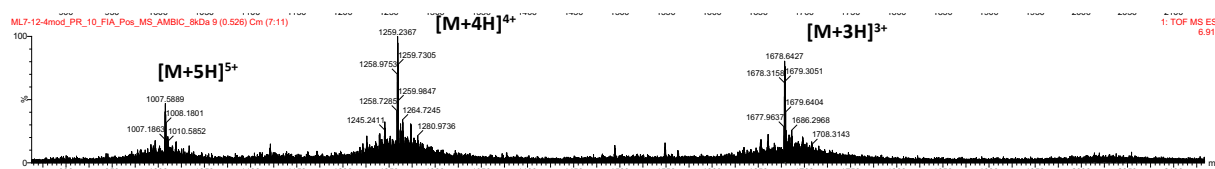


Chemical Formula: C₂₀₆H₂₆₃N₈₅O₆₇S **Exact Mass:** 5030.951 **Molecular Weight:** 5033.958

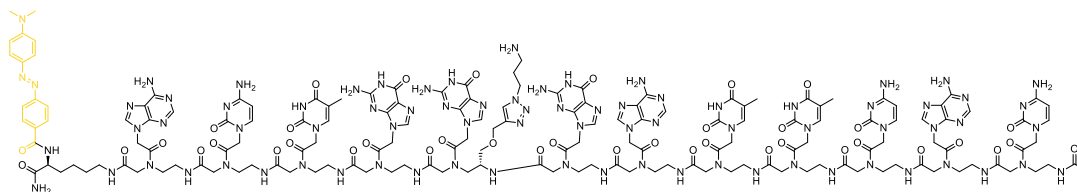
LC-MS-ESI+: m/z expected for $[M+6H]^{6+}$: 839.8, m/z found: 840.0 m/z expected for $[M+5H]^{5+}$: 1007.6, m/z found: 1007.7; m/z expected for $[M+4H]^{4+}$: 1259.2, m/z found: 1259.3; m/z expected for $[M+3H]^{3+}$: 1678.7, m/z found: 1678.8. (0.1% aqueous TFA solution and 0.1% TFA in HPLC grade acetonitrile used as eluents.)



HR-MS/TOF-MS-ES+: m/z expected for $[M+3H]^{3+}$: 1678.6598, m/z found: 1678.6427; m/z expected for $[M+4H]^{4+}$: 1259.2467, m/z found: 1259.2367; m/z expected for $[M+5H]^{5+}$: 1007.5990, m/z found: 1007.5889

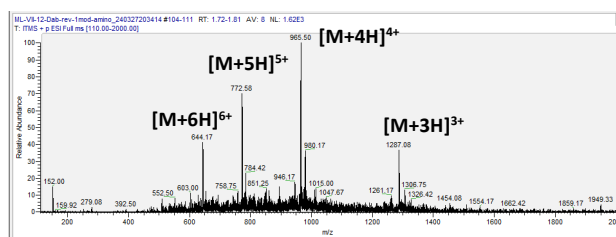
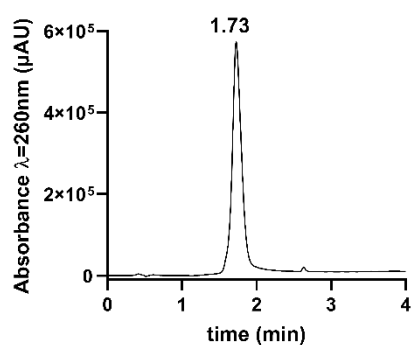


PNA1-N1-D: C-Ter: Lys(ACT GG^NG ATT CAC -Ac)-Dabcyl

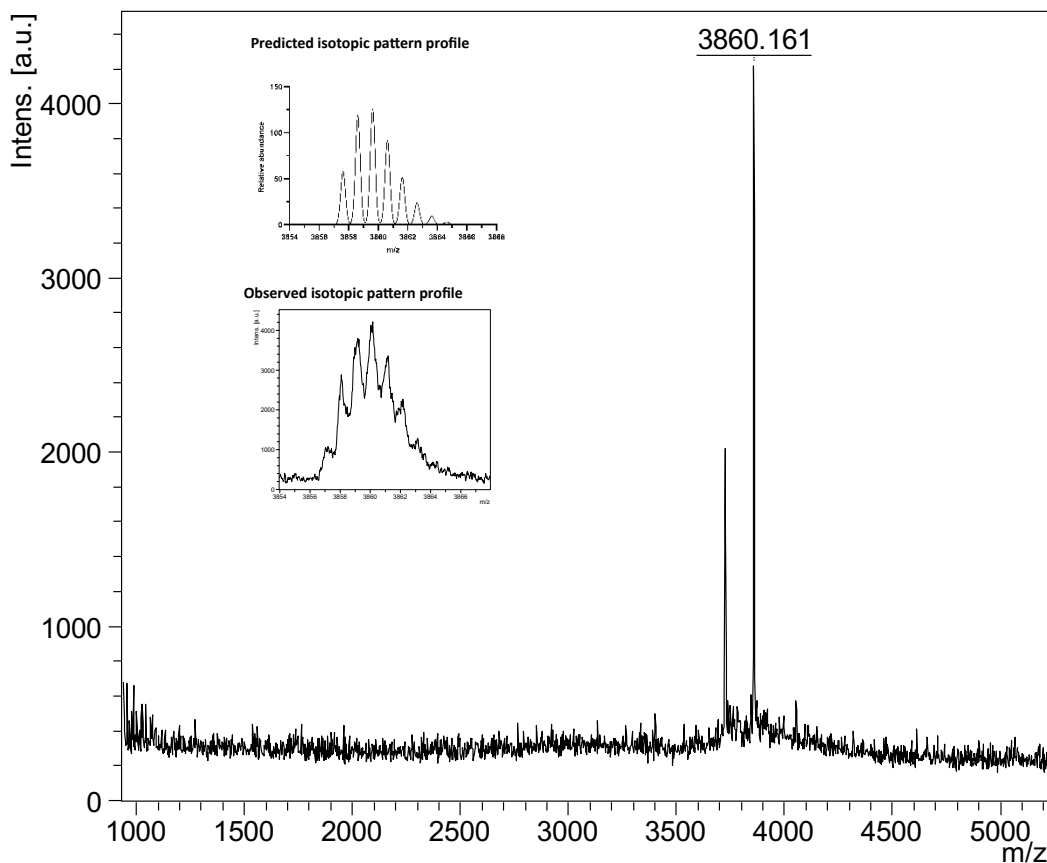


Chemical Formula: C₁₅₉H₂₀₁N₇₉O₄₀ **Exact Mass:** 3856.612 **Molecular Weight:** 3858.870

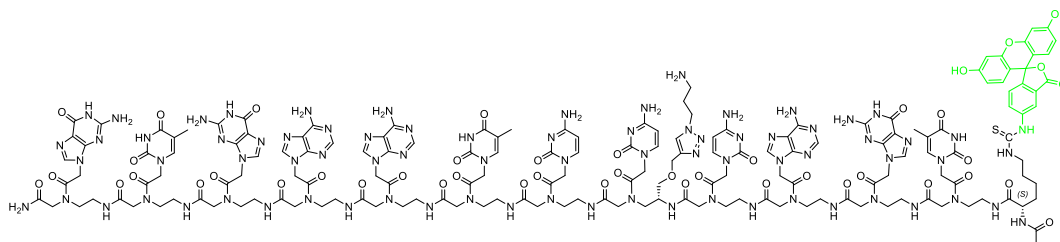
LC-MS-ESI+: m/z expected for $[M+6H]^{6+}$: 644.1, m/z found: 644.2; m/z expected for $[M+5H]^{5+}$: 772.7, m/z found: 772.6; m/z expected for $[M+4H]^{4+}$: 965.7, m/z found: 965.5; m/z expected for $[M+3H]^{3+}$: 1287.1, m/z found: 1267.1.



MALDI-TOF-MS: m/z expected for $[M+H]^+$: 3859.633, m/z found: 3860.161. In all PNAs containing Dabcyl quencher have a secondary peak with a -132 m/z corresponding to a fragmentation of the quencher.

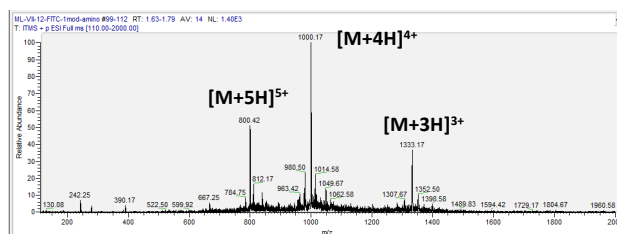
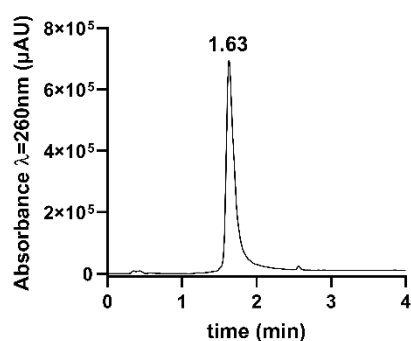


PNA1-N1-F: C-Ter: GTG AAT CC^NC AGT-Lys(FITC)-Ac

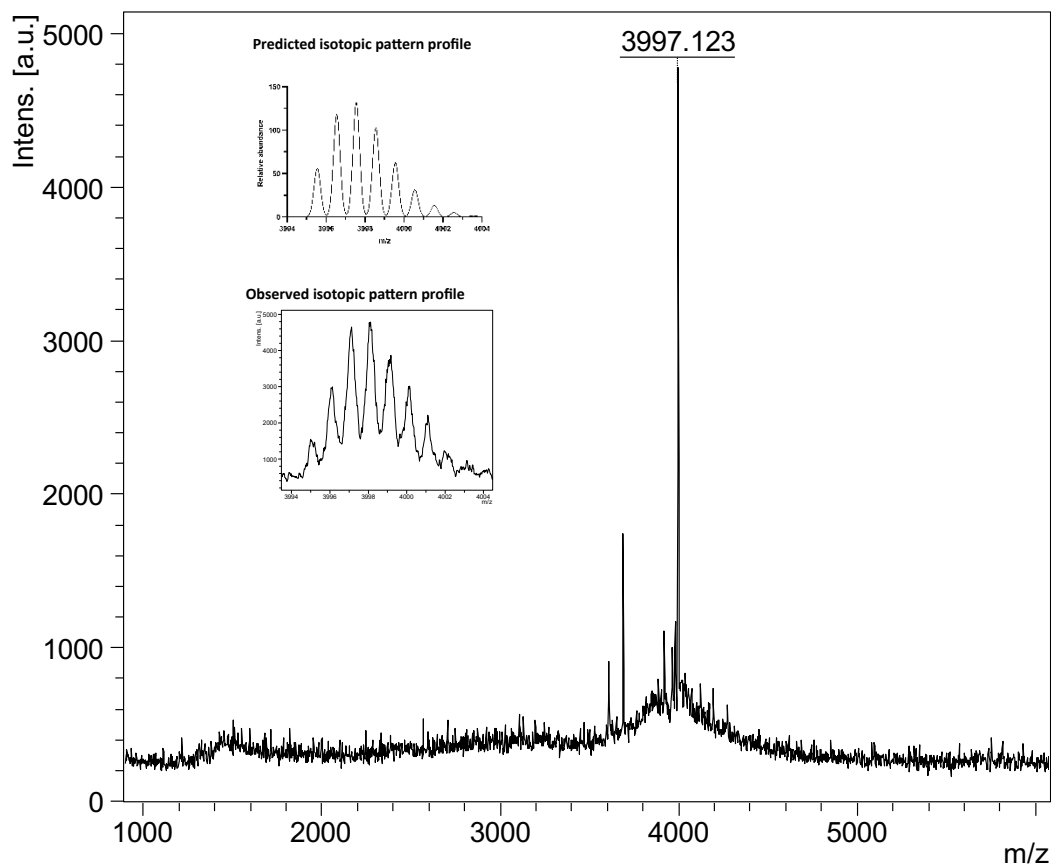


Chemical Formula: C₁₆₅H₁₉₉N₇₇O₄₄S **Exact Mass:** 3994.542 **Molecular Weight:** 3996.962

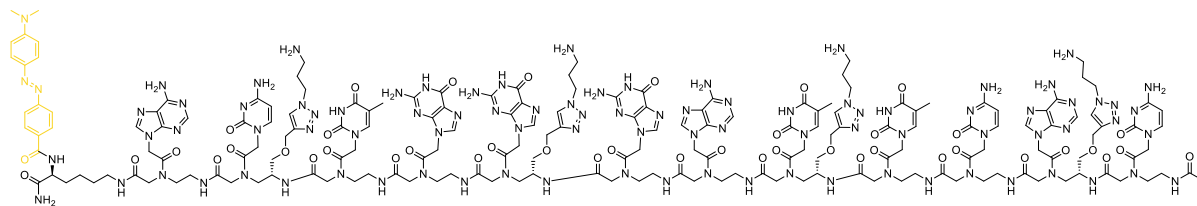
LC-MS-ESI+: *m/z* expected for [M+5H]⁵⁺: 800.3, *m/z* found: 800.4; *m/z* expected for [M+4H]⁴⁺: 1000.1, *m/z* found: 1000.2; *m/z* expected for [M+3H]³⁺: 1333.2, *m/z* found: 1333.2.



MALDI-TOF-MS: *m/z* expected for [M+H]⁺: 3997.550, *m/z* found: 3997.123.

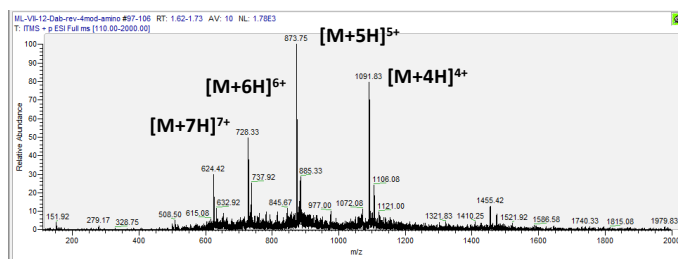
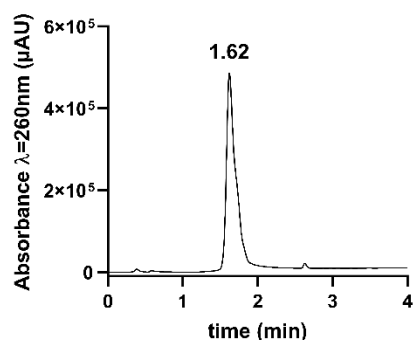


PNA1-N4-D: C-Ter: Lys(AC^NT GG^NG AT^NT CA^NC -Ac)-Dabcyl

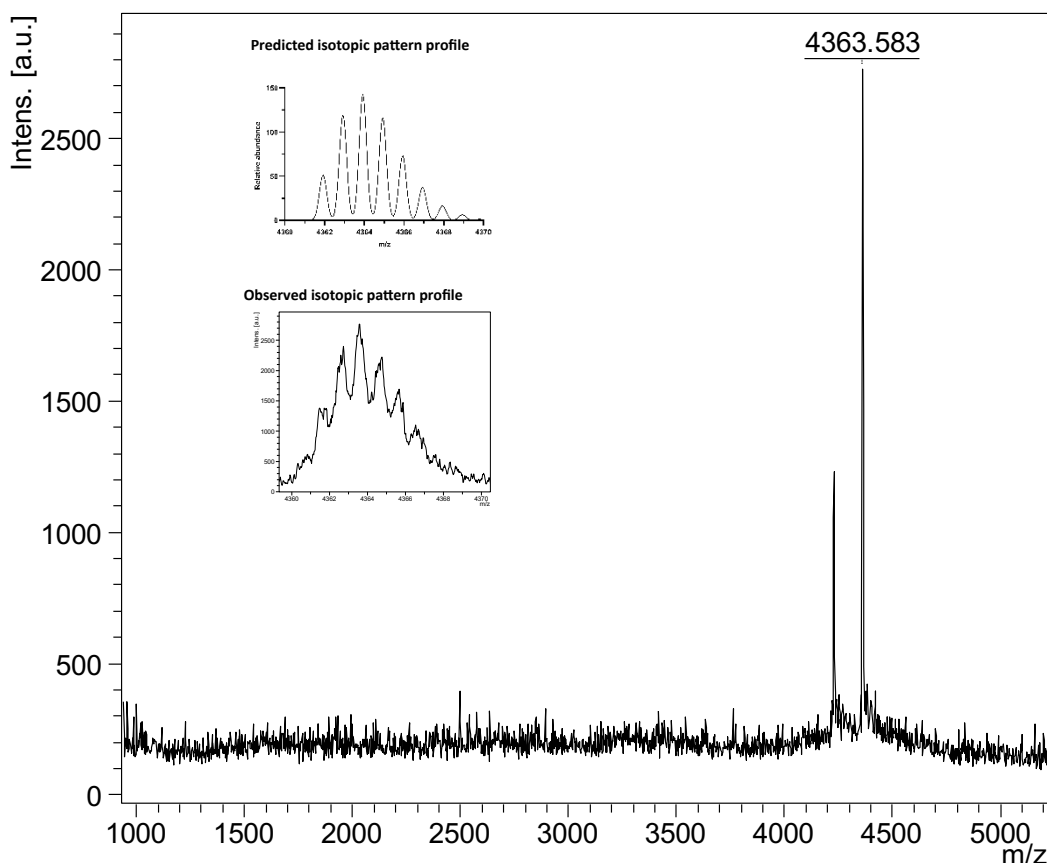


Chemical Formula: C₁₈₀H₂₃₇N₉₁O₄₃ **Exact Mass:** 4360.916 **Molecular Weight:** 4363.470

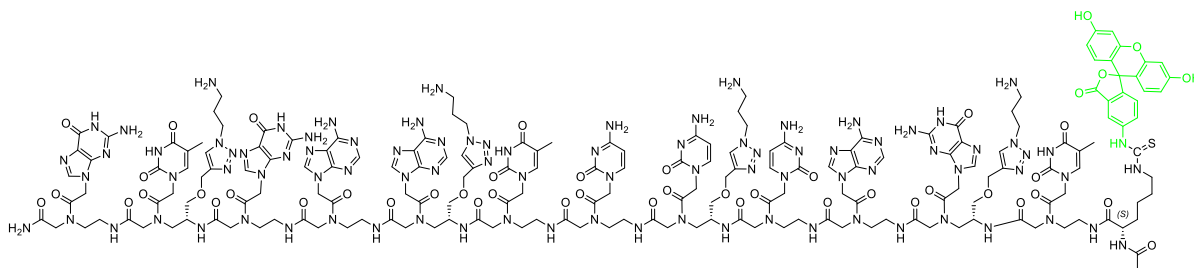
LC-MS-ESI+: m/z expected for $[M+7H]^{7+}$: 624.3, m/z found: 624.4; m/z expected for $[M+6H]^{6+}$: 728.2, m/z found: 728.3; m/z expected for $[M+5H]^{5+}$: 873.6, m/z found: 873.8; m/z expected for $[M+4H]^{4+}$: 1091.7, m/z found: 1091.8.



MALDI-TOF-MS: m/z expected for $[M+H]^+$: 4363.937, m/z found: 4363.583. *In all PNAs containing Dabcyl quencher have a secondary peak with a -132 m/z corresponding to a fragmentation of the quencher.*

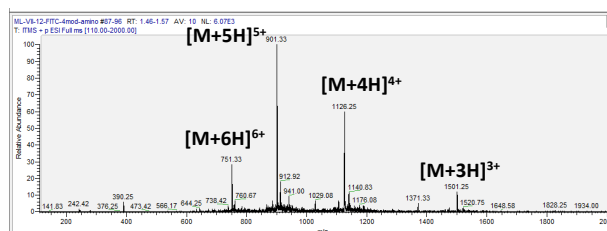
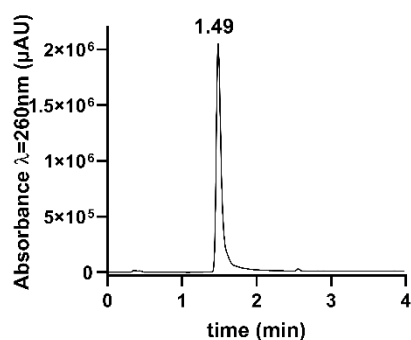


PNA1-N4-F: C-Ter: GT^NG AA^NT CC^NC AG^NT-Lys(FITC)-Ac

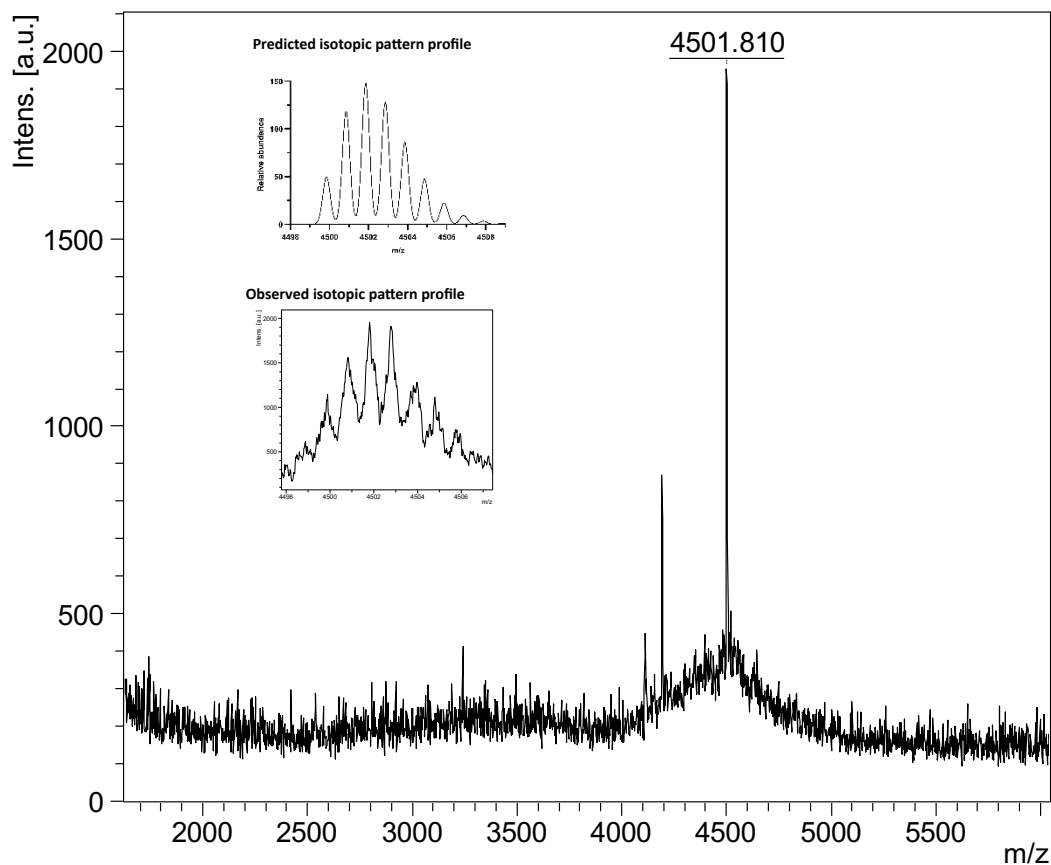


Chemical Formula: C₁₈₆H₂₃₅N₈₉O₄₇S **Exact Mass:** 4498.846 **Molecular Weight:** 4501.562

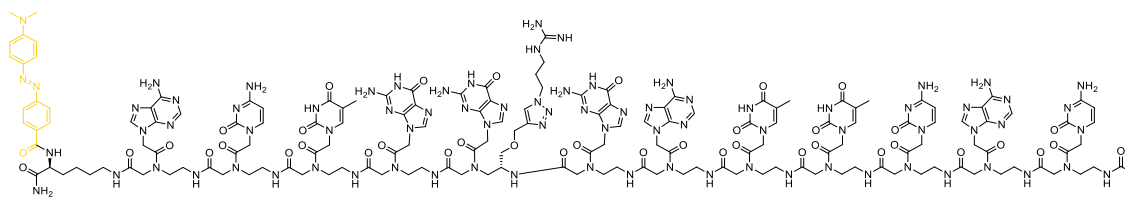
LC-MS-ESI+: m/z expected for $[M+6H]^{6+}$: 751.1, m/z found: 751.3; m/z expected for $[M+5H]^{5+}$: 901.2, m/z found: 901.3; m/z expected for $[M+4H]^{4+}$: 1126.2, m/z found: 1126.3; m/z expected for $[M+3H]^{3+}$: 1501.3, m/z found: 1501.3.



MALDI-TOF-MS: m/z expected for $[M+H]^+$: 4501.872, m/z found: 4501.810.

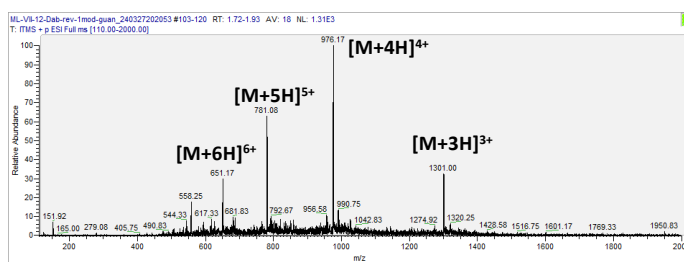
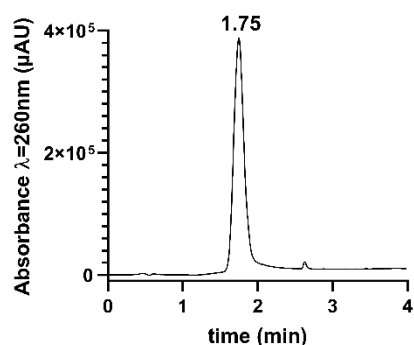


PNA1-G1-D: C-Ter: Lys(ACT GG^G ATT CAC -Ac)-Dabcyl

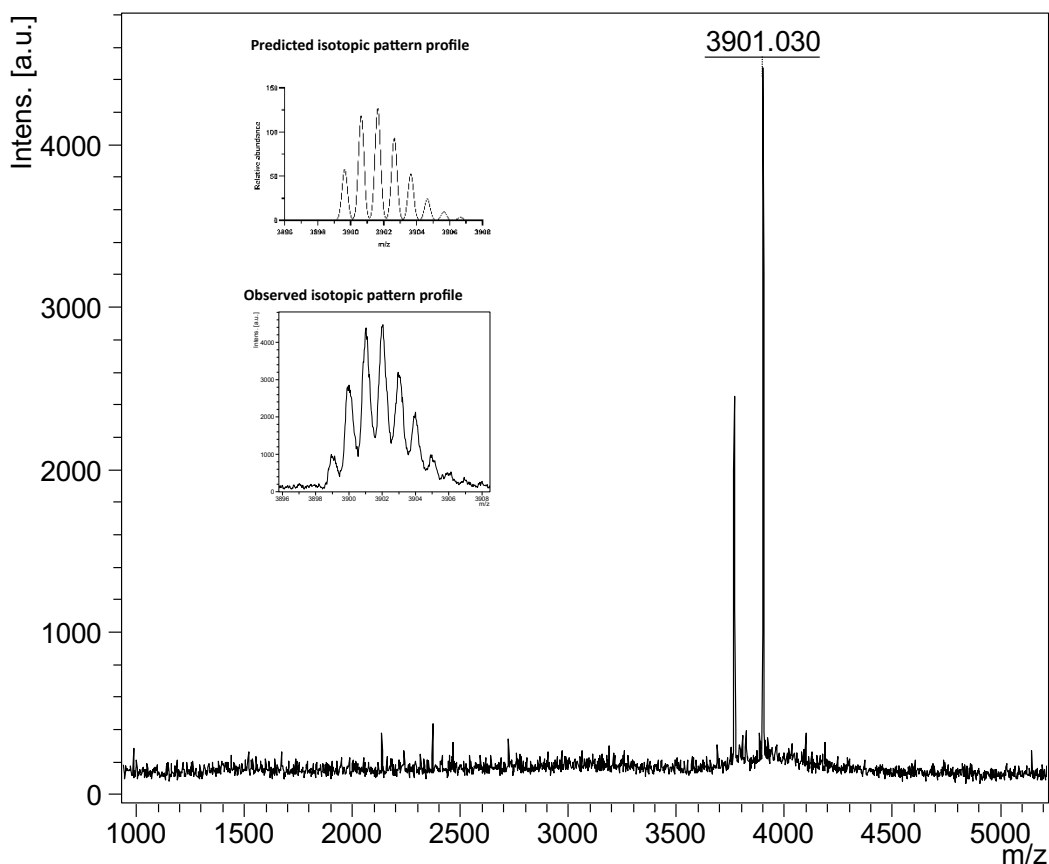


Chemical Formula: C₁₆₀H₂₀₃N₈₁O₄₀ **Exact Mass:** 3898.634 **Molecular Weight:** 3900.911

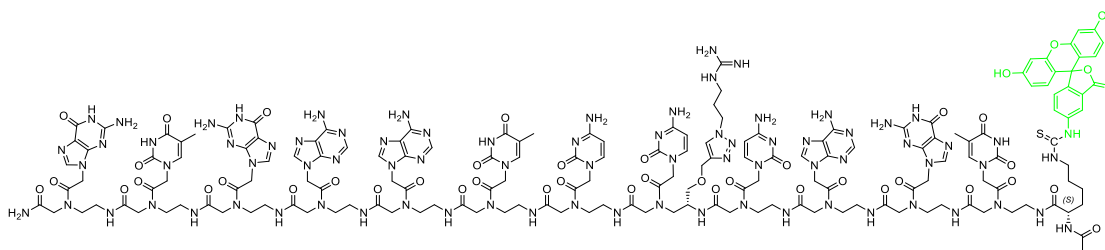
LC-MS-ESI+: m/z expected for $[M+6H]^{6+}$: 651.1, m/z found: 651.2; m/z expected for $[M+5H]^{5+}$: 781.1, m/z found: 781.1; m/z expected for $[M+4H]^{4+}$: 976.2, m/z found: 976.2; m/z expected for $[M+3H]^{3+}$: 1031.2, m/z found: 1031.0.



MALDI-TOF-MS: m/z expected for $[M+H]^+$: 3901.648, m/z found: 3901.030. In all PNAs containing Dabcyl quencher have a secondary peak with a -132 m/z corresponding to a fragmentation of the quencher.

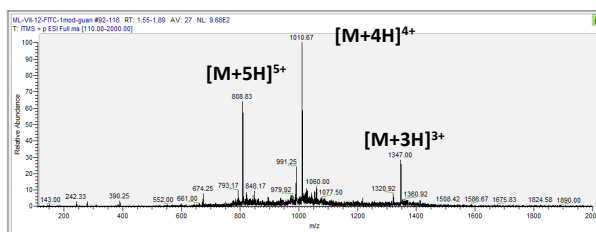
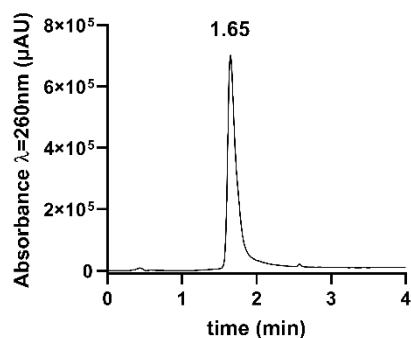


PNA1-G1-F: C-Ter: GTG AAT CC^GC AGT-Lys(FITC)-Ac

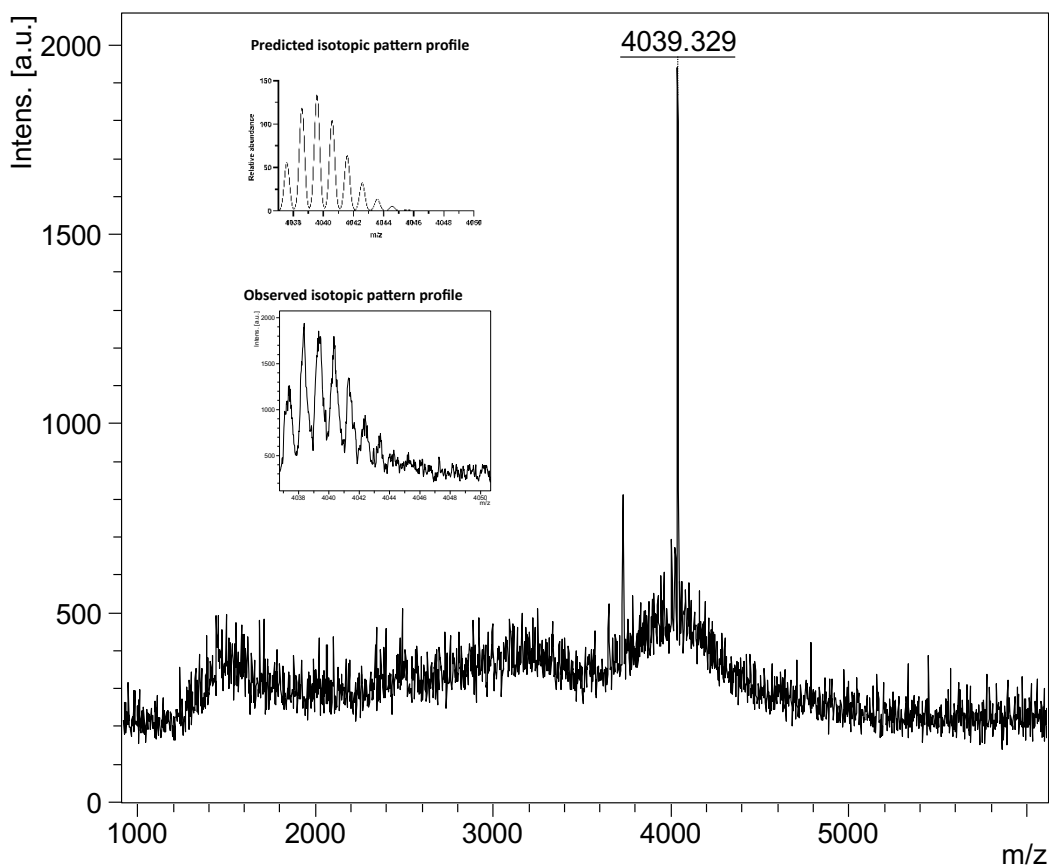


Chemical Formula: C₁₆₆H₂₀₁N₇₉O₄₄S **Exact Mass:** 4036.564 **Molecular Weight:** 4039.003

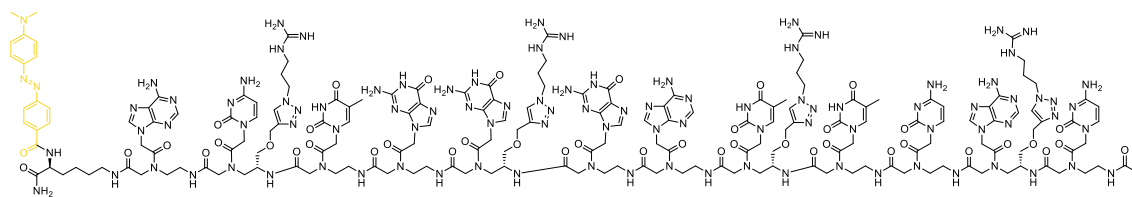
LC-MS-ESI+: *m/z* expected for [M+5H]⁵⁺: 808.7, *m/z* found: 808.8; *m/z* expected for [M+4H]⁴⁺: 1010.6, *m/z* found: 1010.7; *m/z* expected for [M+3H]³⁺: 1347.0, *m/z* found: 1347.0.



MALDI-TOF-MS: *m/z* expected for [M+H]⁺: 4039.563, *m/z* found: 4039.329.

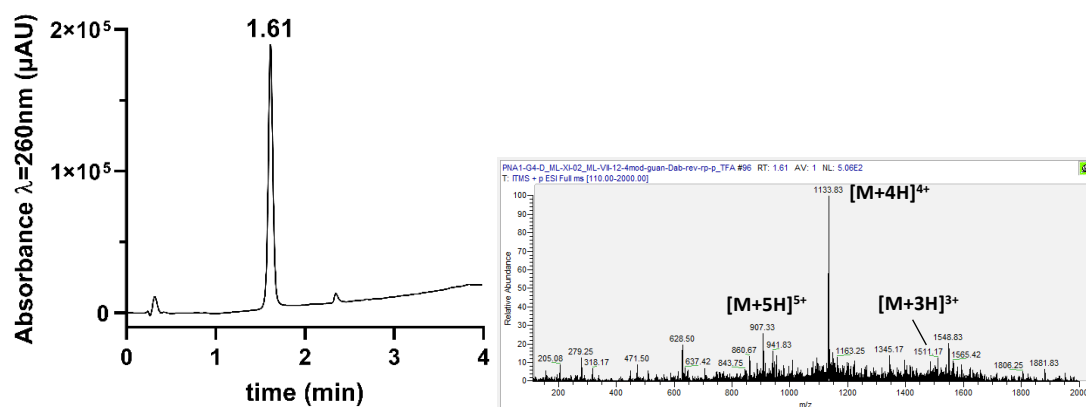


PNA1-G4-D: C-Ter: Lys(AC^GT GG^GG AT^GT CA^CC -Ac)-Dabcyl

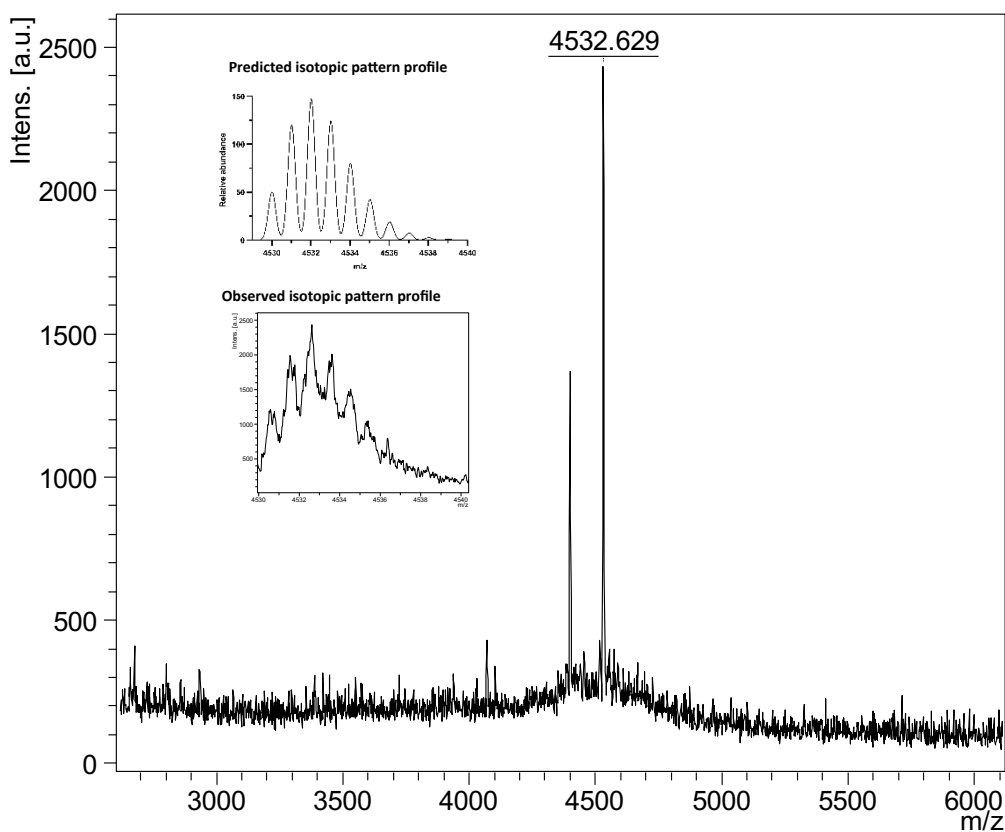


Chemical Formula: C₁₈₄H₂₄₅N₉₉O₄₃ **Exact Mass:** 4529.003 **Molecular Weight:** 4531.634

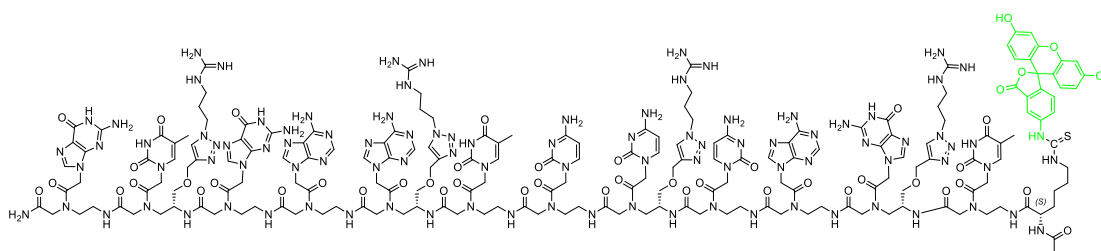
LC-MS-ESI+: m/z expected for $[M+5H]^{5+}$: 907.2, m/z found: 907.3; m/z expected for $[M+4H]^{4+}$: 1133.8, m/z found: 1133.9; m/z expected for $[M+3H]^{3+}$: 1511.3, m/z found: 1511.2. (0.1% aqueous TFA solution and 0.1% TFA in HPLC grade acetonitrile used as eluents.)



MALDI-TOF-MS: m/z expected for $[M+H]^+$: 4532.004, m/z found: 4532.629. In all PNAs containing Dabcyl quencher have a secondary peak with a -132 m/z corresponding to a fragmentation of the quencher.

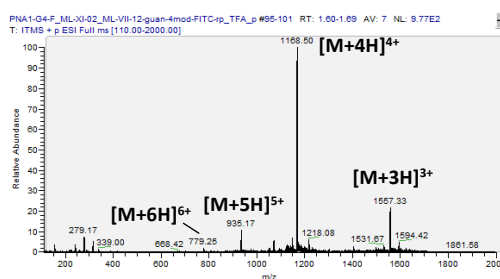
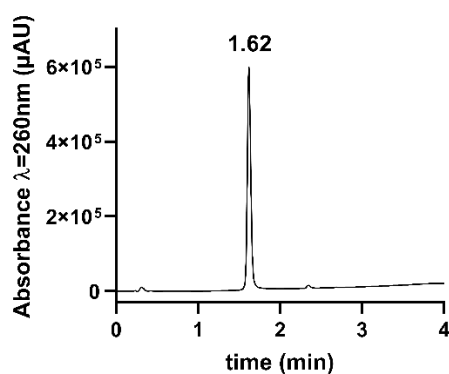


PNA1-G4-F: C-Ter: GT^G AA^GT CC^GC AG^GT-Lys(FITC)-Ac

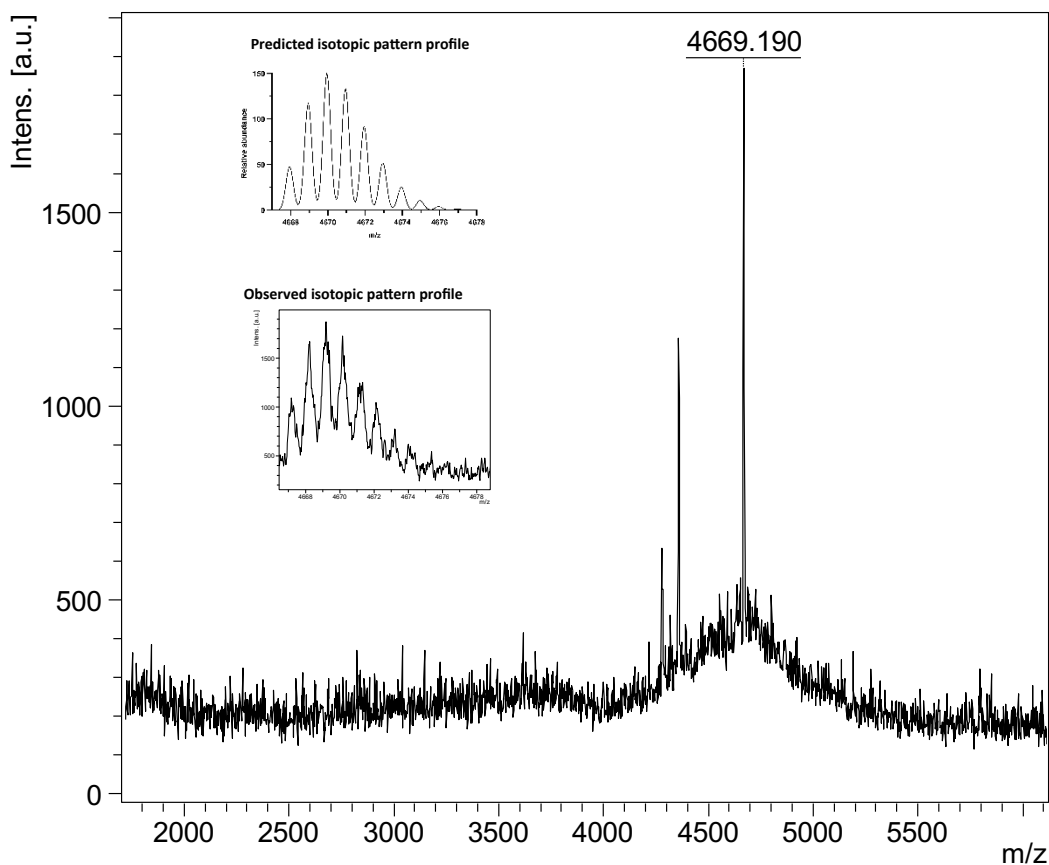


Chemical Formula: C₁₉₀H₂₄₃N₉₇O₄₇S **Exact Mass:** 4666.933 **Molecular Weight:** 4669.726

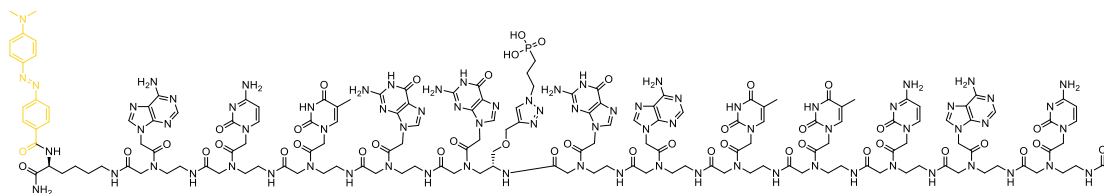
LC-MS-ESI+: m/z expected for $[M+6H]^{6+}$: 779.2, m/z found: 779.3; m/z expected for $[M+5H]^{5+}$: 934.8, m/z found: 935.2; m/z expected for $[M+4H]^{4+}$: 1168.2, m/z found: 1168.5; m/z expected for $[M+3H]^{3+}$: 1557.3, m/z found: 1557.3. (0.1% aqueous TFA solution and 0.1% TFA in HPLC grade acetonitrile used as eluents.)



MALDI-TOF-MS: m/z expected for $[M+H]^+$: 4669.931, m/z found: 4669.190.

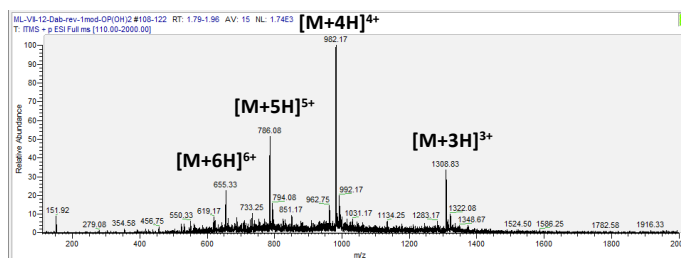
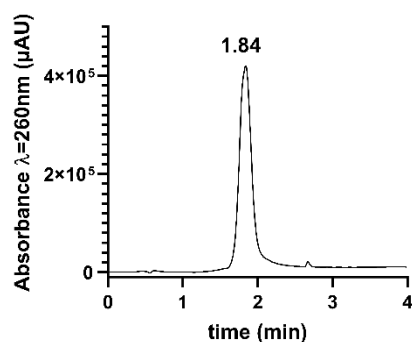


PNA1-P1-D: C-Ter: Lys(ACT GG^PG ATT CAC -Ac)-Dabcyl

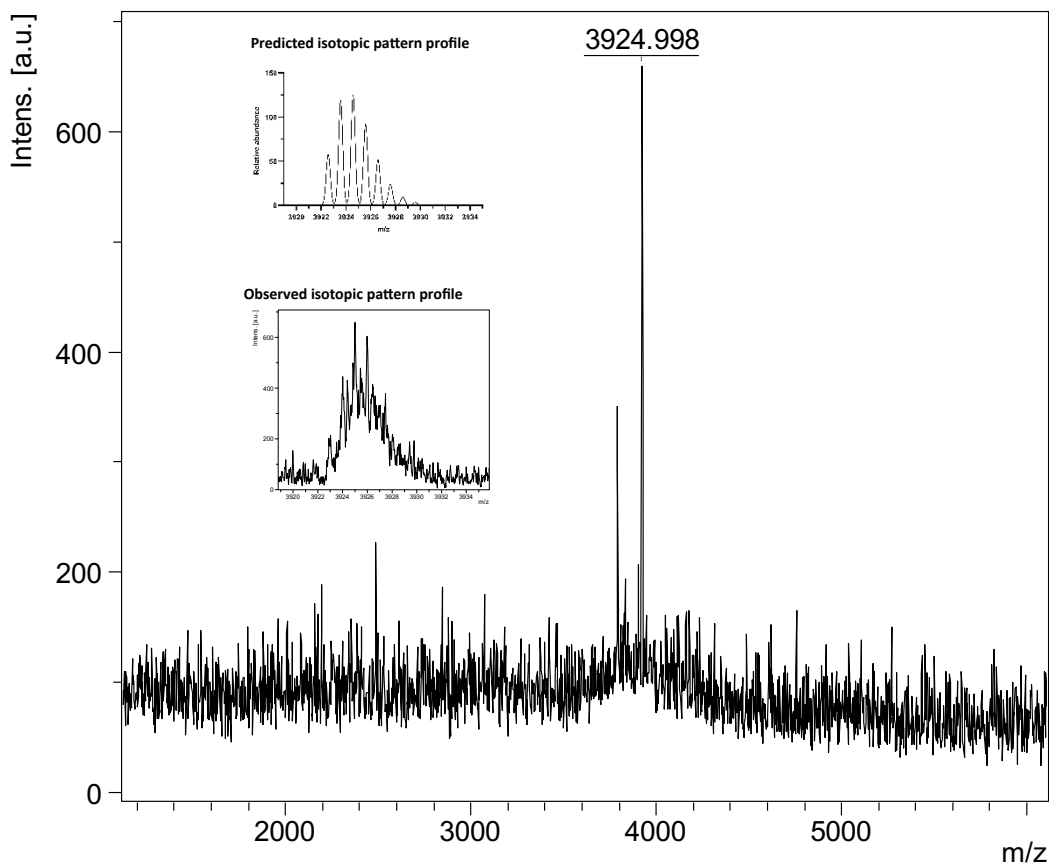


Chemical Formula: C₁₅₉H₂₀₁N₇₈O₄₃P **Exact Mass:** 3921.568 **Molecular Weight:** 3923.834

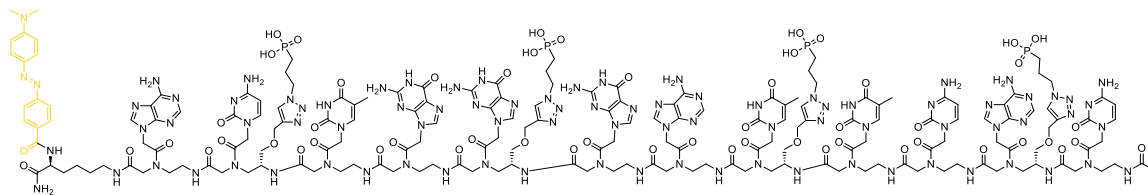
LC-MS-ESI+: m/z expected for $[M+6H]^{6+}$: 654.9, m/z found: 655.3; m/z expected for $[M+5H]^{5+}$: 785.7, m/z found: 786.1; m/z expected for $[M+4H]^{4+}$: 981.9, m/z found: 982.2; m/z expected for $[M+3H]^{3+}$: 1308.8, m/z found: 1308.8.



MALDI-TOF-MS: m/z expected for $[M+H]^+$: 3924.575, m/z found: 3924.998. In all PNAs containing Dabcyl quencher have a secondary peak with a -132 m/z corresponding to a fragmentation of the quencher.

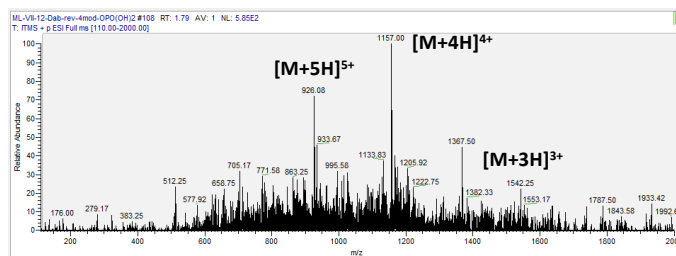
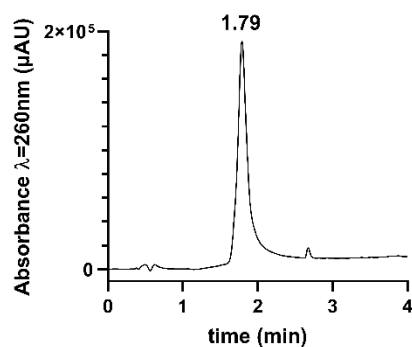


PNA1-P4-D: C-Ter: Lys(AC^PT GG^PG AT^PT CA^PC -Ac)-DabcyI

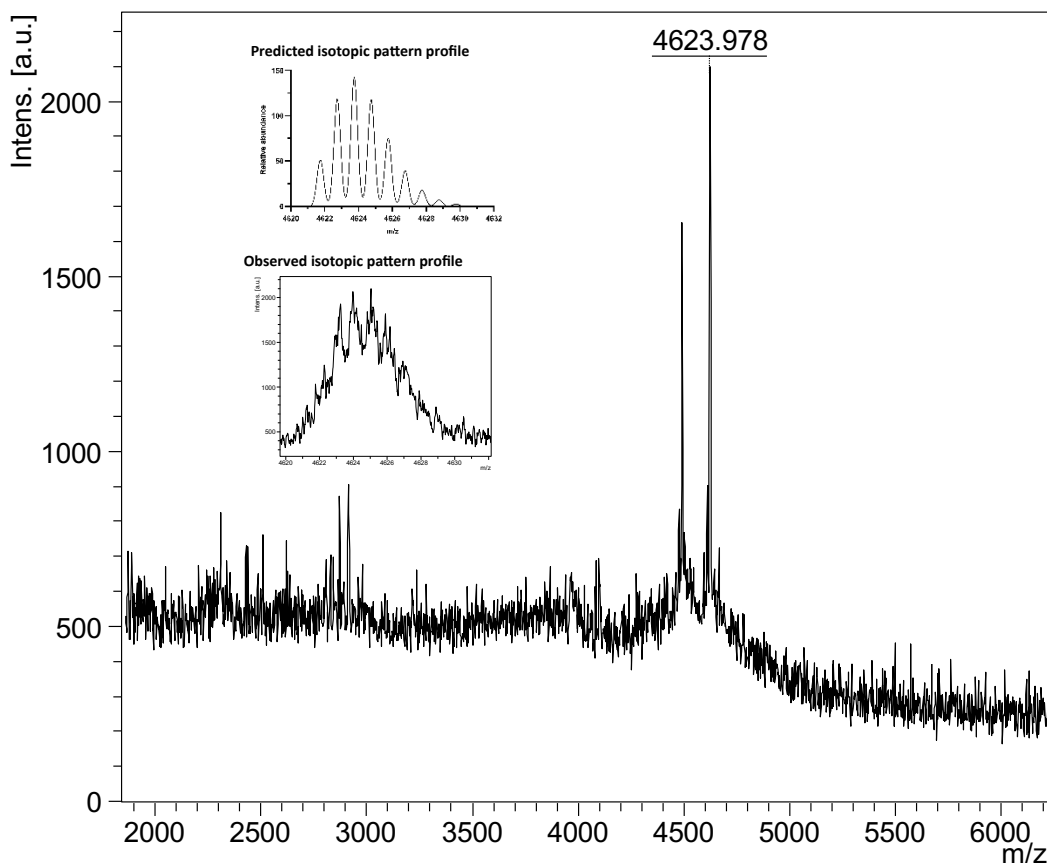


Chemical Formula: C₁₈₀H₂₃₇N₈₇O₅₅P₄ **Exact Mass:** 4620.737 **Molecular Weight:** 4623.325

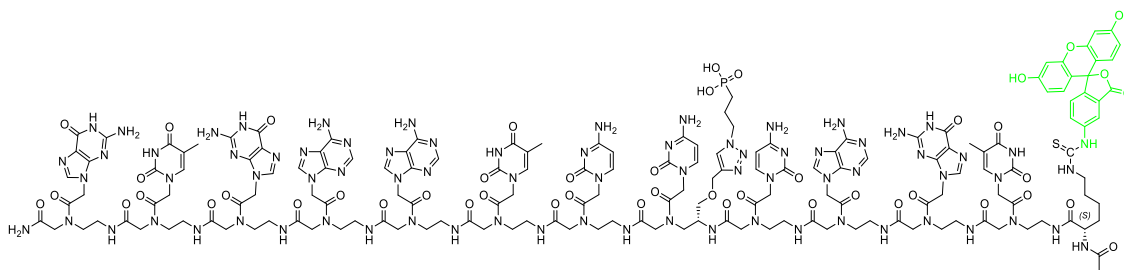
LC-MS-ESI+: m/z expected for $[M+5H]^{5+}$: 925.6, m/z found: 926.1; m/z expected for $[M+4H]^{4+}$: 1156.9, m/z found: 1157.0; m/z expected for $[M+3H]^{3+}$: 1541.9, m/z found: 1542.3.



MALDI-TOF-MS: m/z expected for $[M+H]^+$: 4624.752, m/z found: 4623.978. In all PNAs containing DabcyI quencher have a secondary peak with a -132 m/z corresponding to a fragmentation of the quencher.

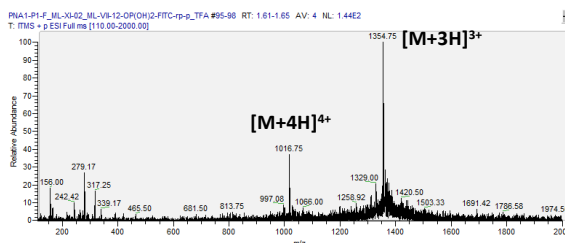
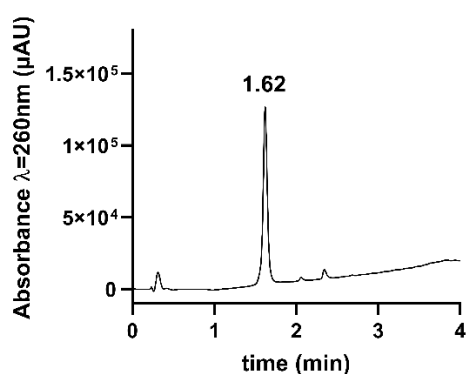


PNA1-P1-F: C-Ter: GTG AAT CC^PC AGT-Lys(FITC)-Ac

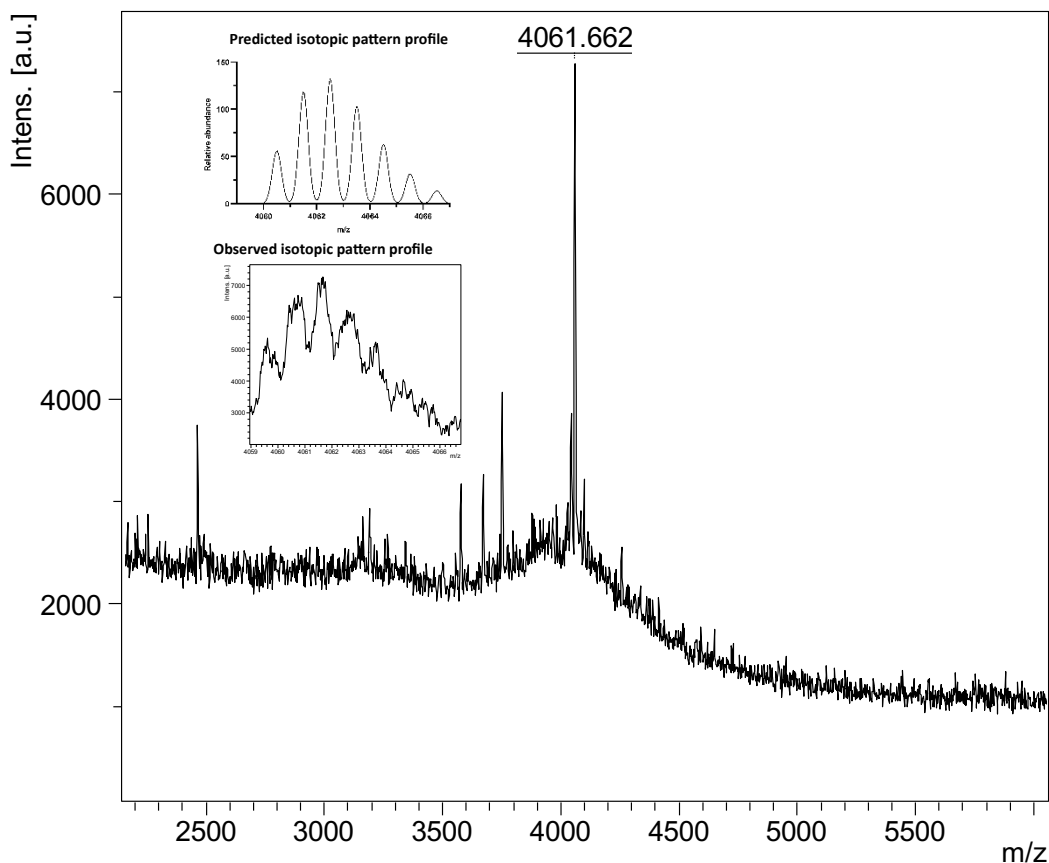


Chemical Formula: C₁₆₅H₁₉₉N₇₆O₄₇PS **Exact Mass:** 4059.498 **Molecular Weight:** 4061.926

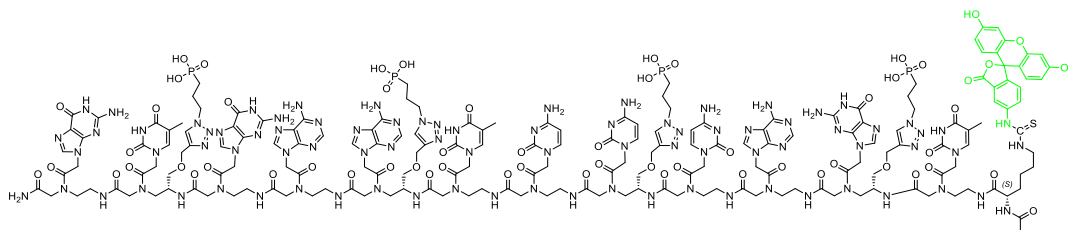
LC-MS-ESI+: m/z expected for $[M+4H]^{4+}$: 1016.4, m/z found: 1016.8; m/z expected for $[M+3H]^{3+}$: 1354.8, m/z found: 1354.8. (0.1% aqueous TFA solution and 0.1% TFA in HPLC grade acetonitrile used as eluents.)



MALDI-TOF-MS: m/z expected for $[M+H]^+$: 4062.514, m/z found: 4061.662.

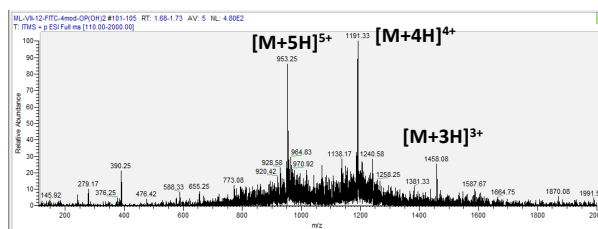
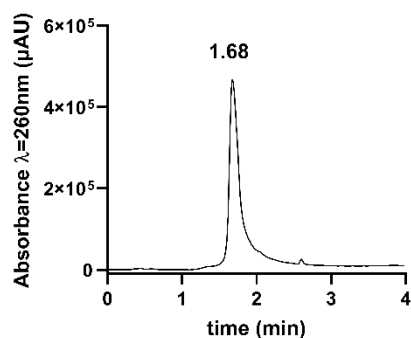


PNA1-P4-F: C-Ter: GT^PGAA^{PT}CC^PCAG^{PT}-Lys(FITC)-Ac

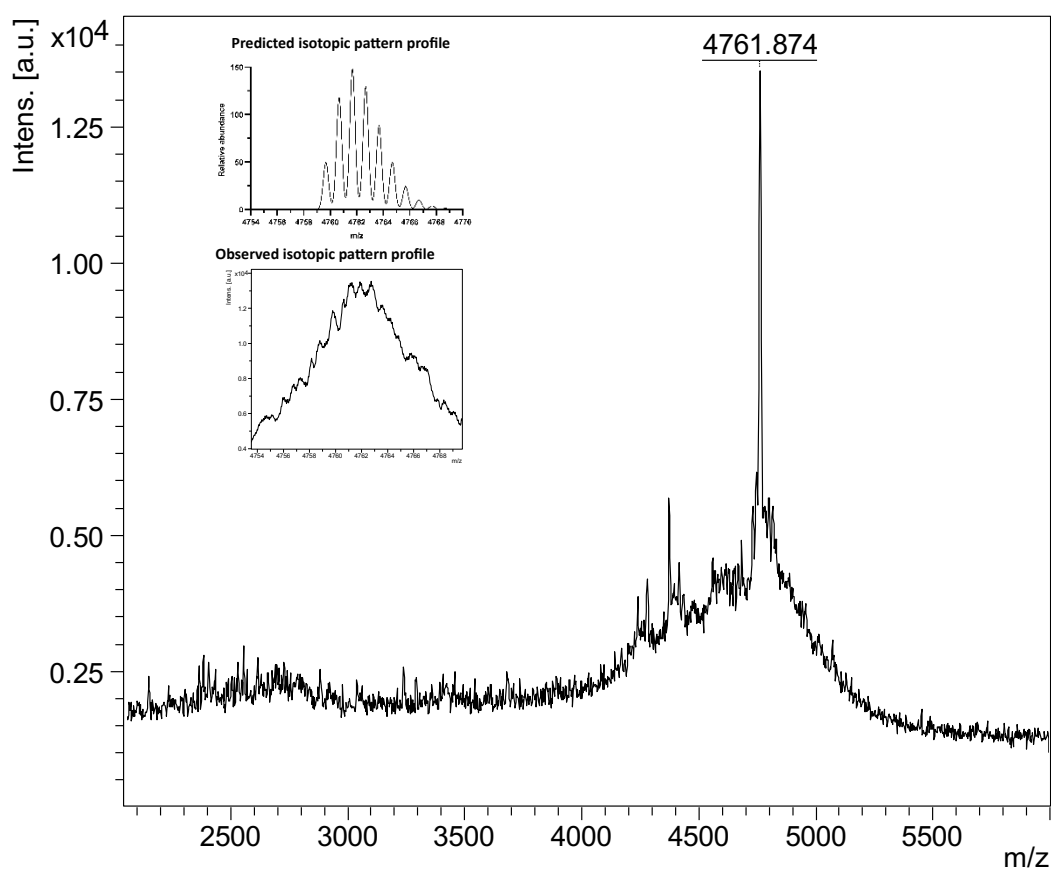


Chemical Formula: C₁₈₆H₂₃₅N₈₅O₅₉P₄S **Exact Mass:** 4758.667 **Molecular Weight:** 4761.417

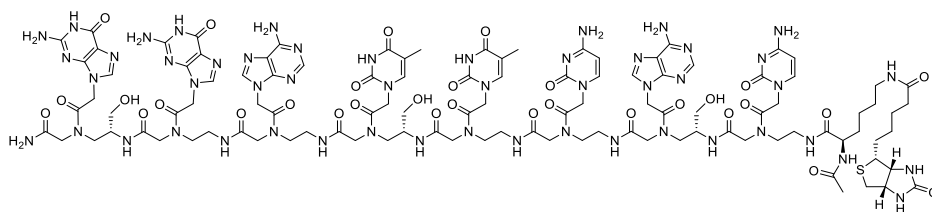
LC-MS-ESI+: m/z expected for $[M+5H]^{5+}$: 953.1, m/z found: 953.3; m/z expected for $[M+4H]^{4+}$: 1191.2, m/z found: 1191.3; m/z expected for $[M+3H]^{3+}$: 1587.9, m/z found: 1587.7.



MALDI-TOF-MS: m/z expected for $[M+H]^+$: 4761.677, m/z found: 4761.874.

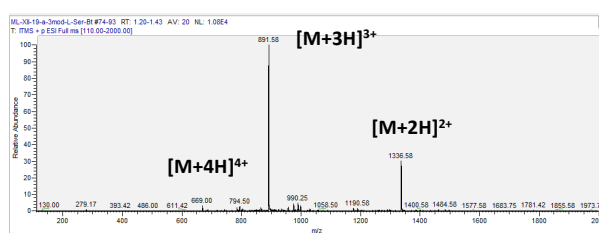
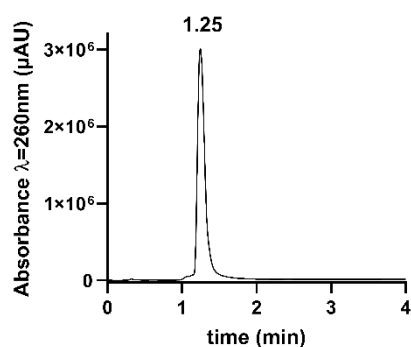


PNA3-Bt: C-Ter: GGATT CAC-Lys(Bt)-Ac

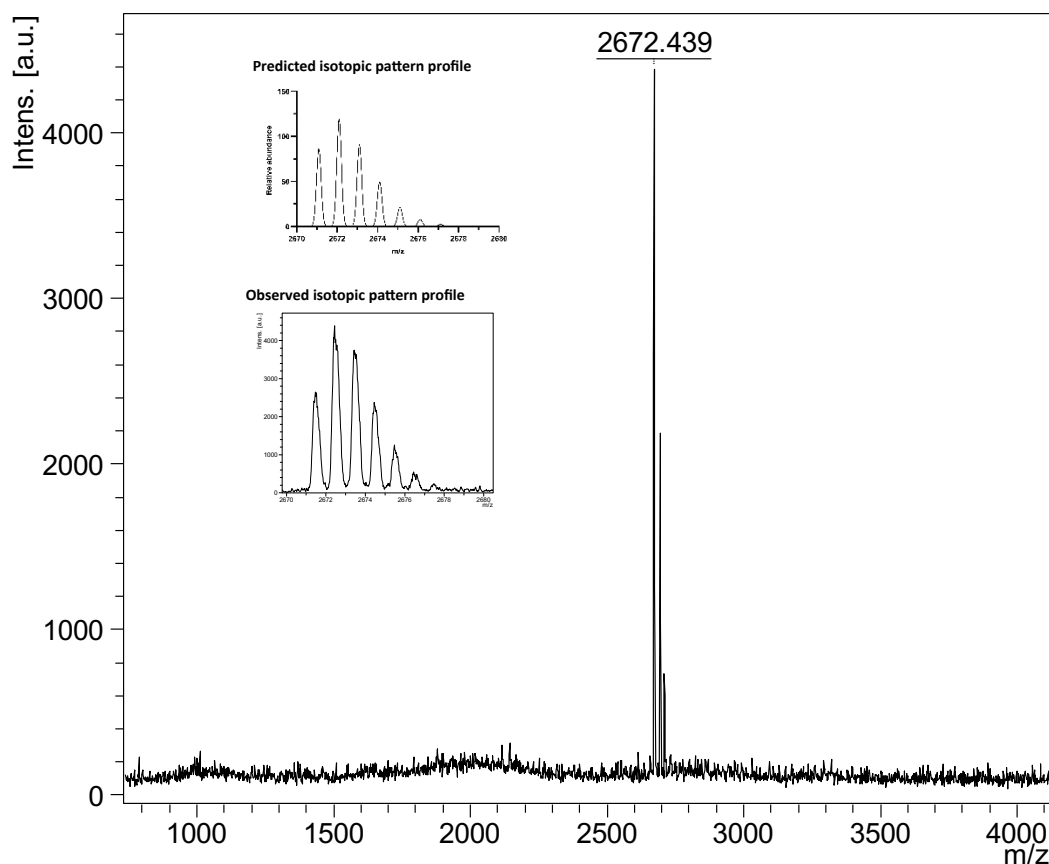


Chemical Formula: C₁₀₇H₁₄₃N₅₁O₃₁S **Exact Mass:** 2670.090 **Molecular Weight:** 2671.707

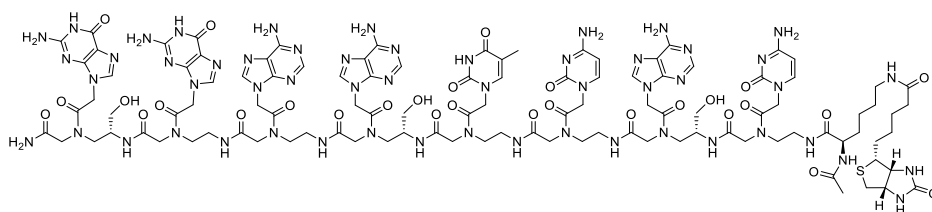
LC-MS-ESI+: m/z expected for $[M+4H]^{4+}$: 668.8, m/z found: 669.0; m/z expected for $[M+3H]^{3+}$: 891.1, m/z found: 891.6; m/z expected for $[M+2H]^{2+}$: 1336.6, m/z found: 1336.6.



MALDI-TOF-MS: m/z expected for $[M+H]^+$: 2672.104, m/z found: 2672.439.

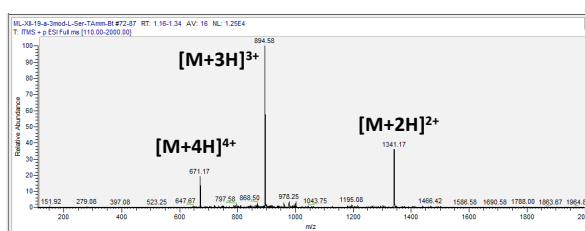
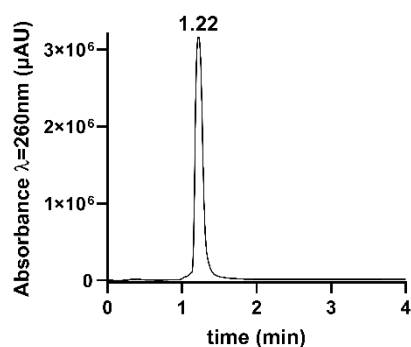


PNA3-AAmBt: C-Ter: GG AT CAC-Lys(Bt)-Ac

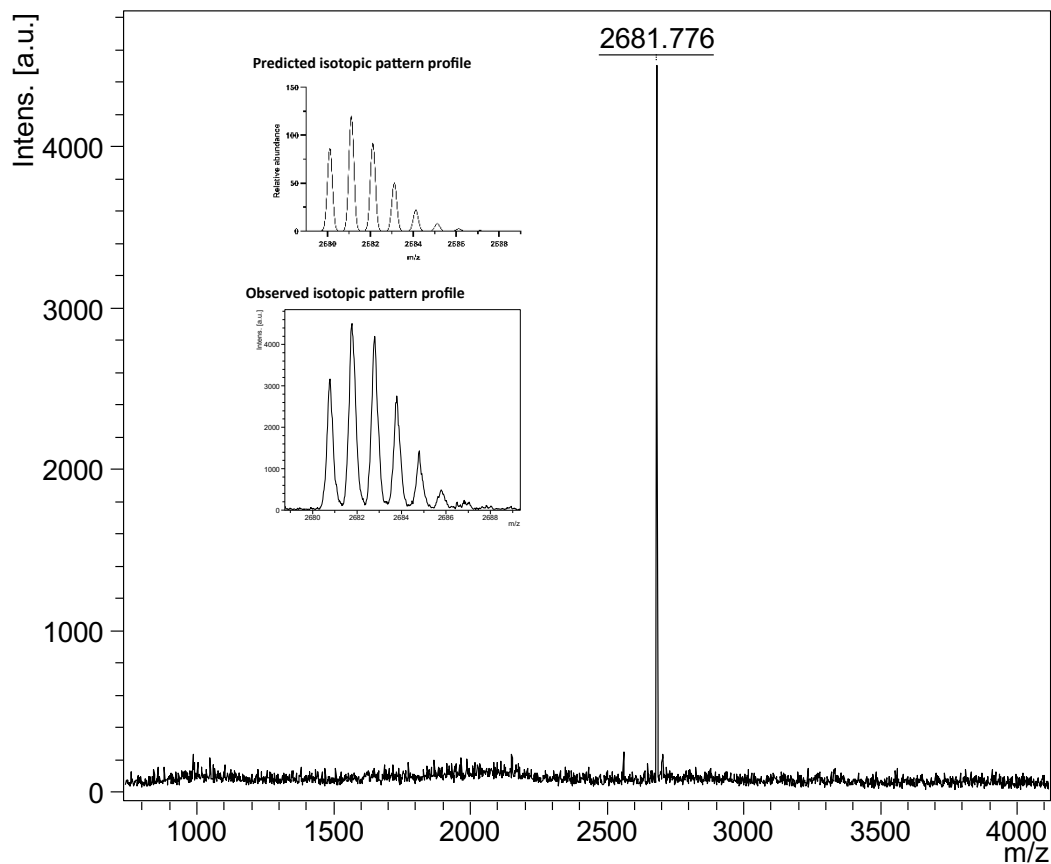


Chemical Formula: C₁₀₇H₁₄₂N₅₄O₂₉S **Exact Mass:** 2679.102 **Molecular Weight:** 2680.722

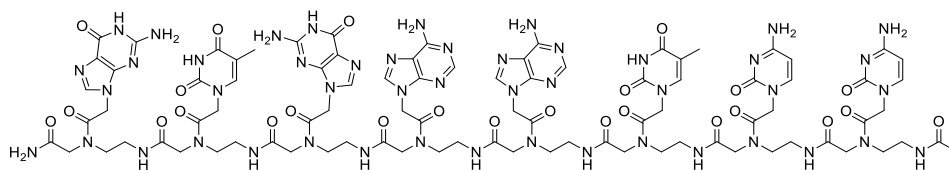
LC-MS-ESI+: m/z expected for $[M+4H]^{4+}$: 671.0, m/z found: 671.2; m/z expected for $[M+3H]^{3+}$: 894.4, m/z found: 894.6; m/z expected for $[M+2H]^{2+}$: 1341.1, m/z found: 1341.2.



MALDI-TOF-MS: m/z expected for $[M+H]^+$: 2681.121, m/z found: 2681.776.

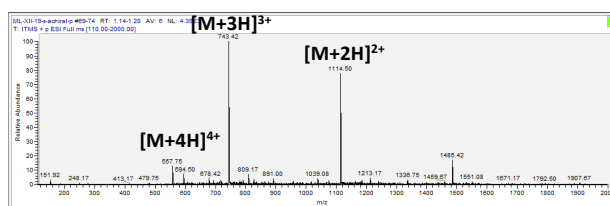
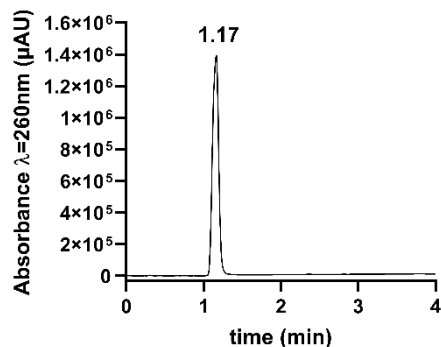


PNA2-ach: C-Ter: GTG AAT CC -Ac

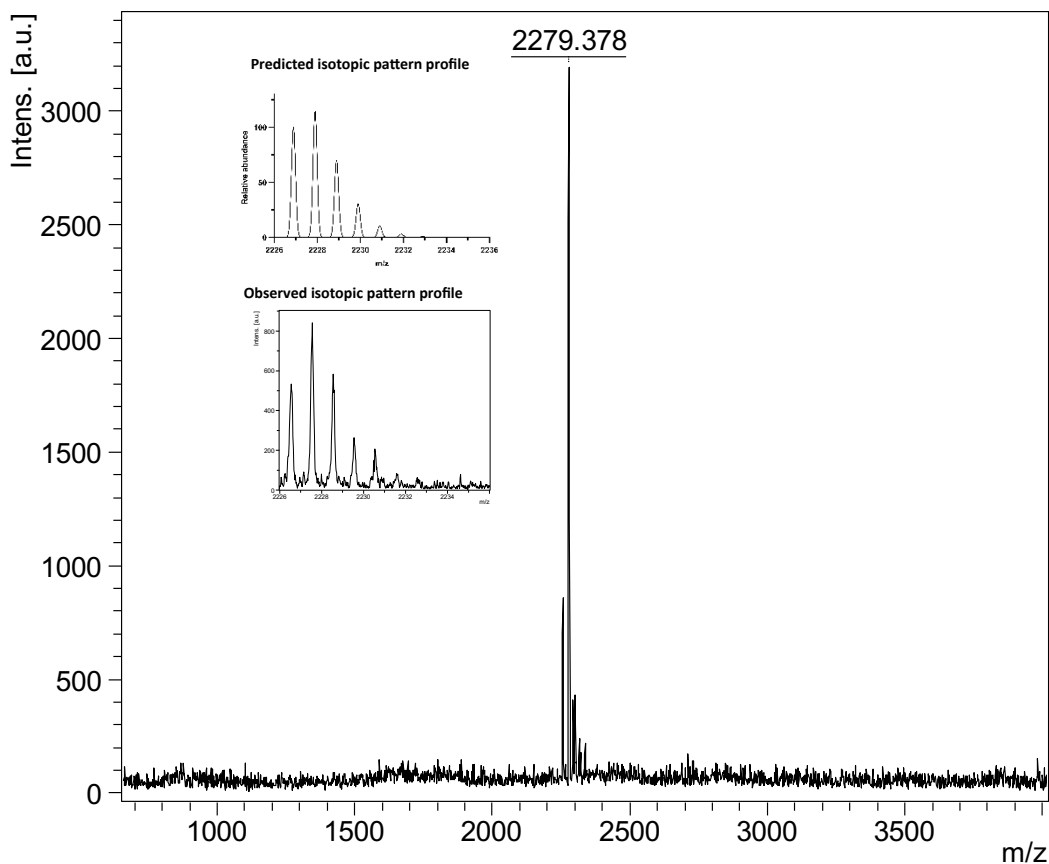


Chemical Formula: C₈₈H₁₁₁N₄₇O₂₅ **Exact Mass:** 2225.886 **Molecular Weight:** 2227.160

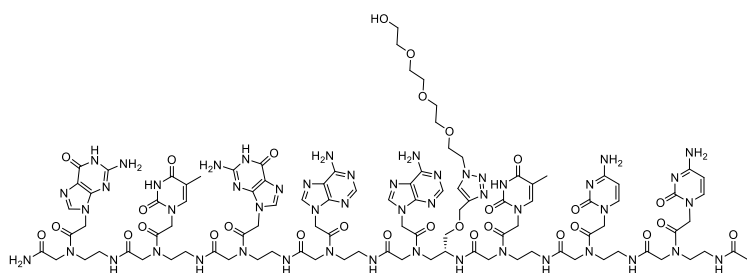
LC-MS-ESI+: m/z expected for $[M+4H]^{4+}$: 557.7, m/z found: 557.8; m/z expected for $[M+3H]^{3+}$: 743.3, m/z found: 743.4; m/z expected for $[M+2H]^{2+}$: 1114.5, m/z found: 1114.5.



MALDI-TOF-MS: m/z expected for $[M+Na]^+$: 2227.901, m/z found: 2227.556.

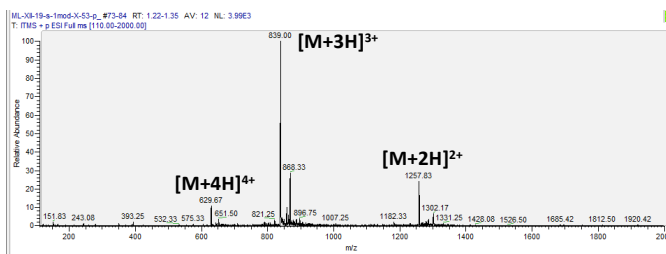
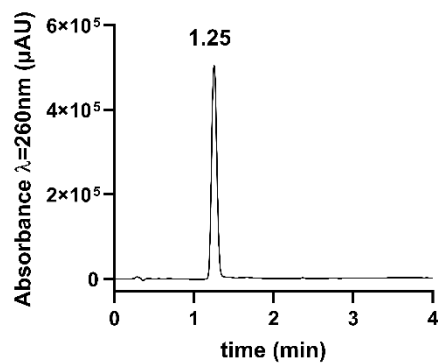


PNA2-H1: C-Ter: GTG AA^HT CC -Ac

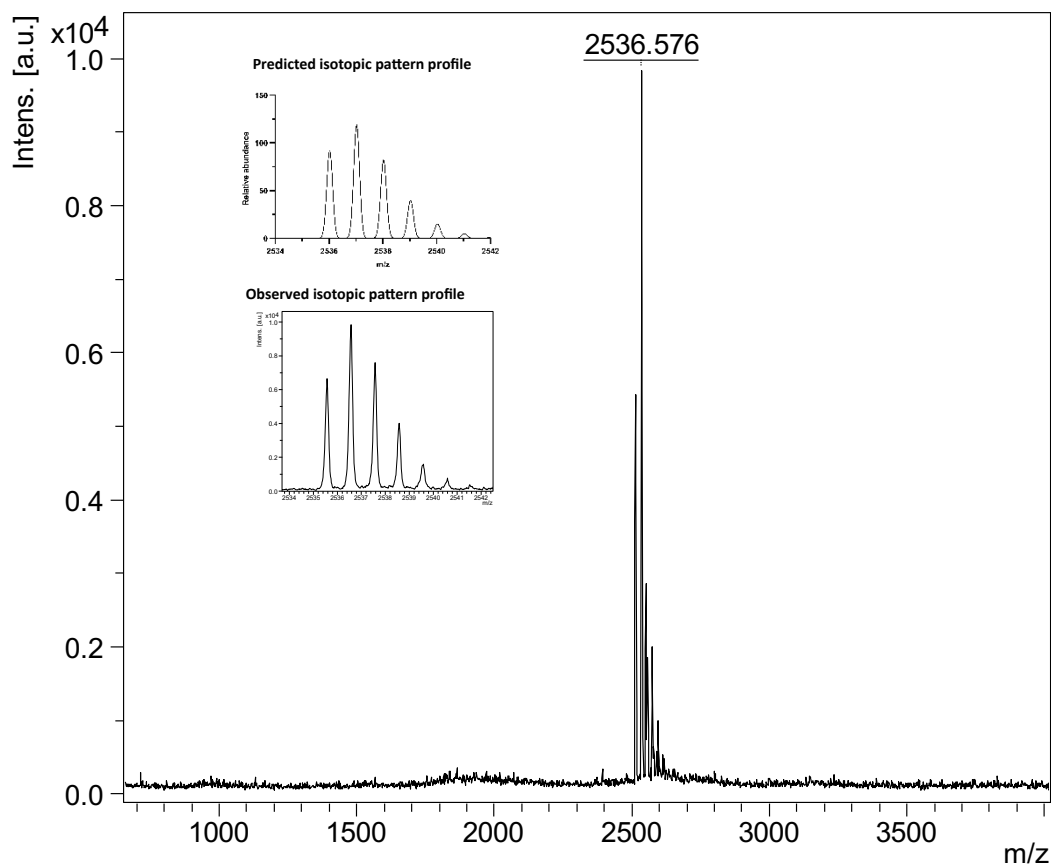


Chemical Formula: C₁₀₀H₁₃₂N₅₀O₃₀ **Exact Mass:** 2513.034 **Molecular Weight:** 2514.476

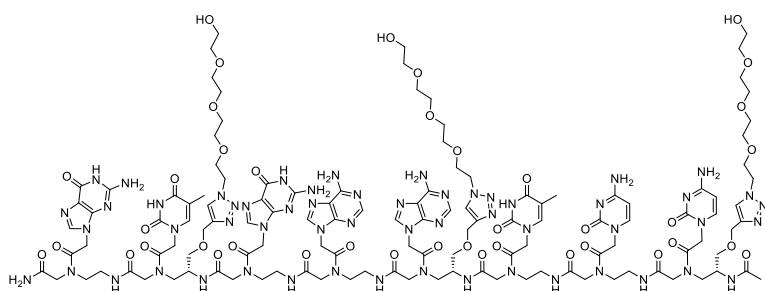
LC-MS-ESI+: m/z expected for $[M+4H]^{4+}$: 629.5, m/z found: 629.7; m/z expected for $[M+3H]^{3+}$: 839.0, m/z found: 839.0; m/z expected for $[M+2H]^{2+}$: 1258.0, m/z found: 1257.8.



MALDI-TOF-MS: m/z expected for $[M+Na]^+$: 2537.030, m/z found: 2536.576.

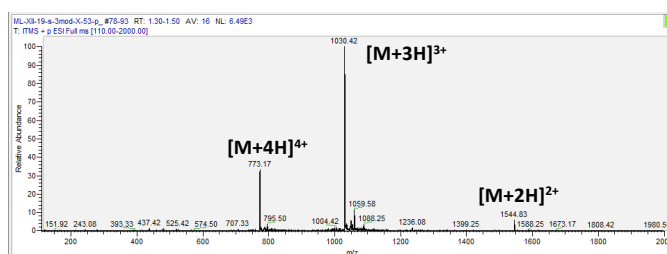
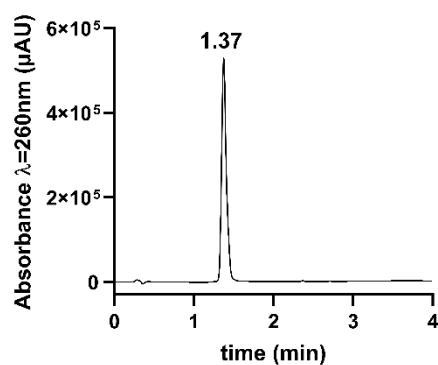


PNA2-H3: C-Ter: GT^HG AA^HT CC^H-Ac

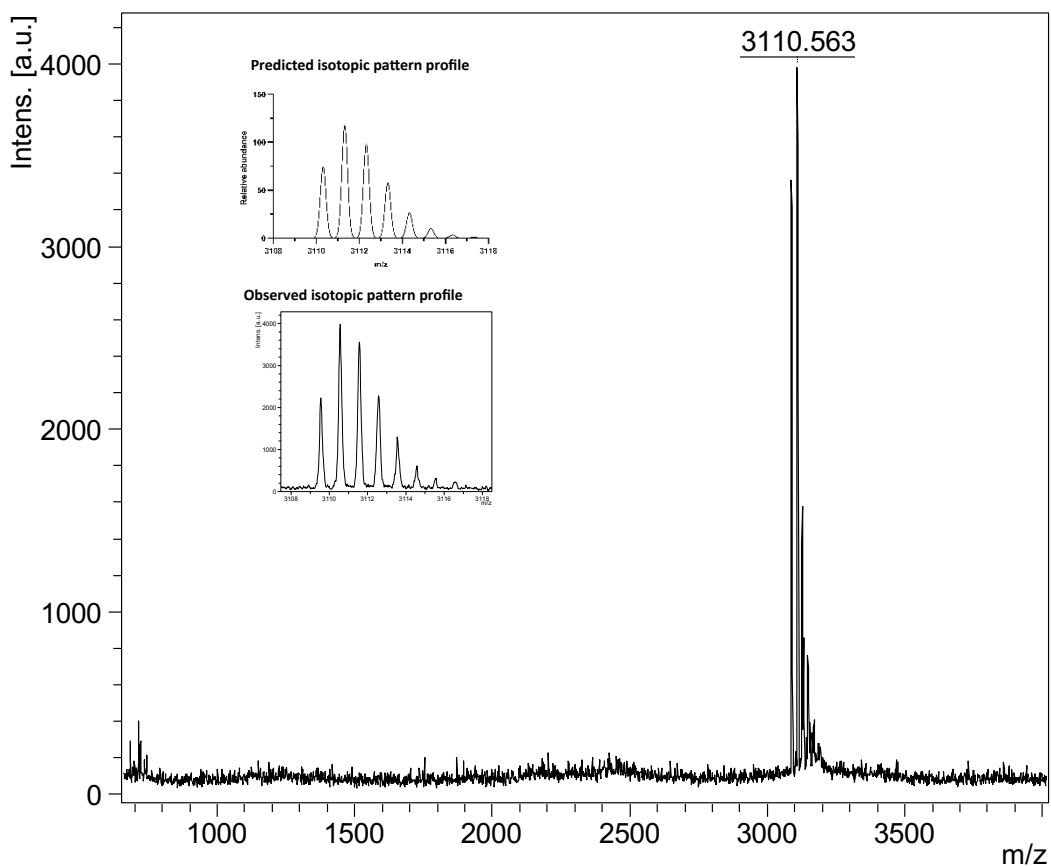


Chemical Formula: C₁₂₄H₁₇₄N₅₆O₄₀ **Exact Mass:** 3087.330 **Molecular Weight:** 3089.108

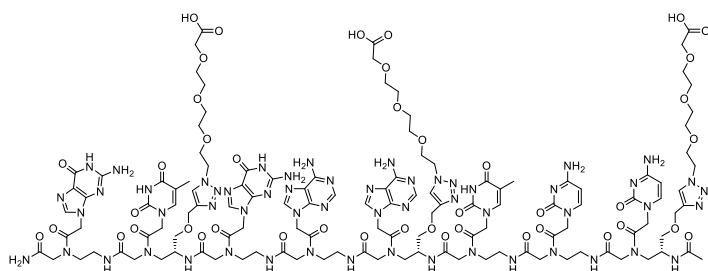
LC-MS-ESI+: m/z expected for [M+4H]⁴⁺: 773.3, m/z found: 773.2; m/z expected for [M+3H]³⁺: 1030.4, m/z found: 1030.4; m/z expected for [M+2H]²⁺: 1545.2, m/z found: 1544.8.



MALDI-TOF-MS: m/z expected for [M+Na]⁺: 3111.313, m/z found: 3110.563.

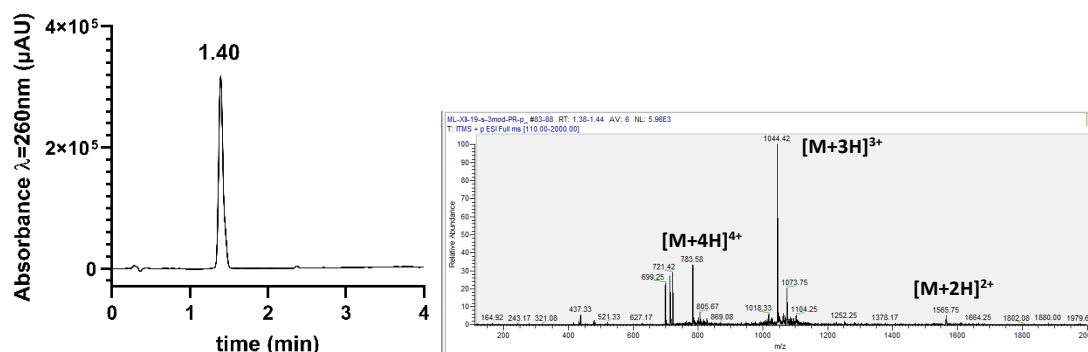


PNA2-A3: C-Ter: GT^AG AA^AT CC^A -Ac

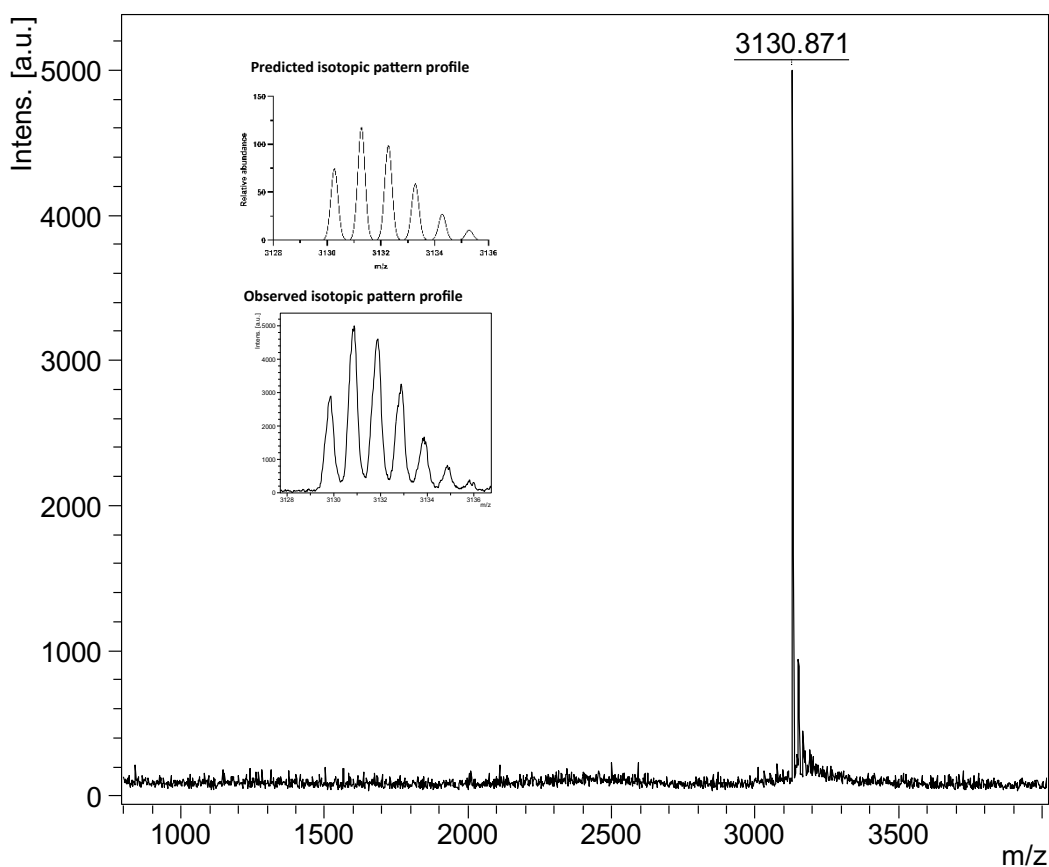


Chemical Formula: C₁₂₄H₁₆₈N₅₆O₄₃ **Exact Mass:** 3129.268 **Molecular Weight:** 3131.057

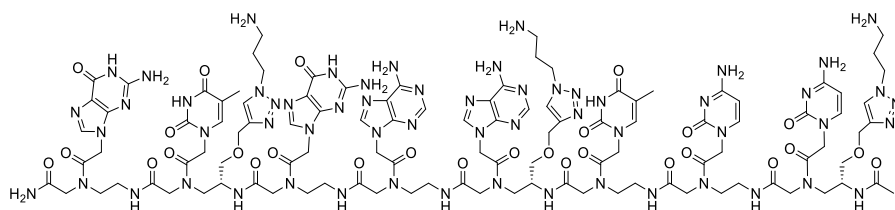
LC-MS-ESI+: m/z expected for $[M+4H]^{4+}$: 783.6, m/z found: 783.6; m/z expected for $[M+3H]^{3+}$: 1044.4, m/z found: 1044.4; m/z expected for $[M+2H]^{2+}$: 1566.1, m/z found: 1565.8.



MALDI-TOF-MS: m/z expected for $[M+H]^+$: 3131.282, m/z found: 3130.871.

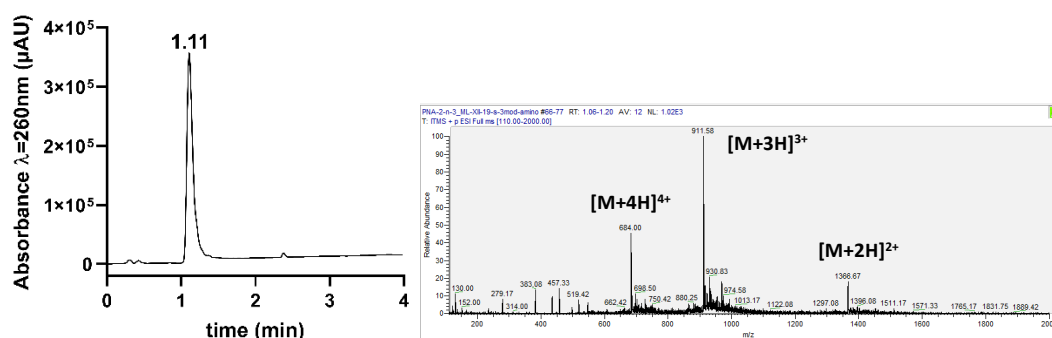


PNA2-N3: C-Ter: GT^NG AA^NT CC^N-Ac

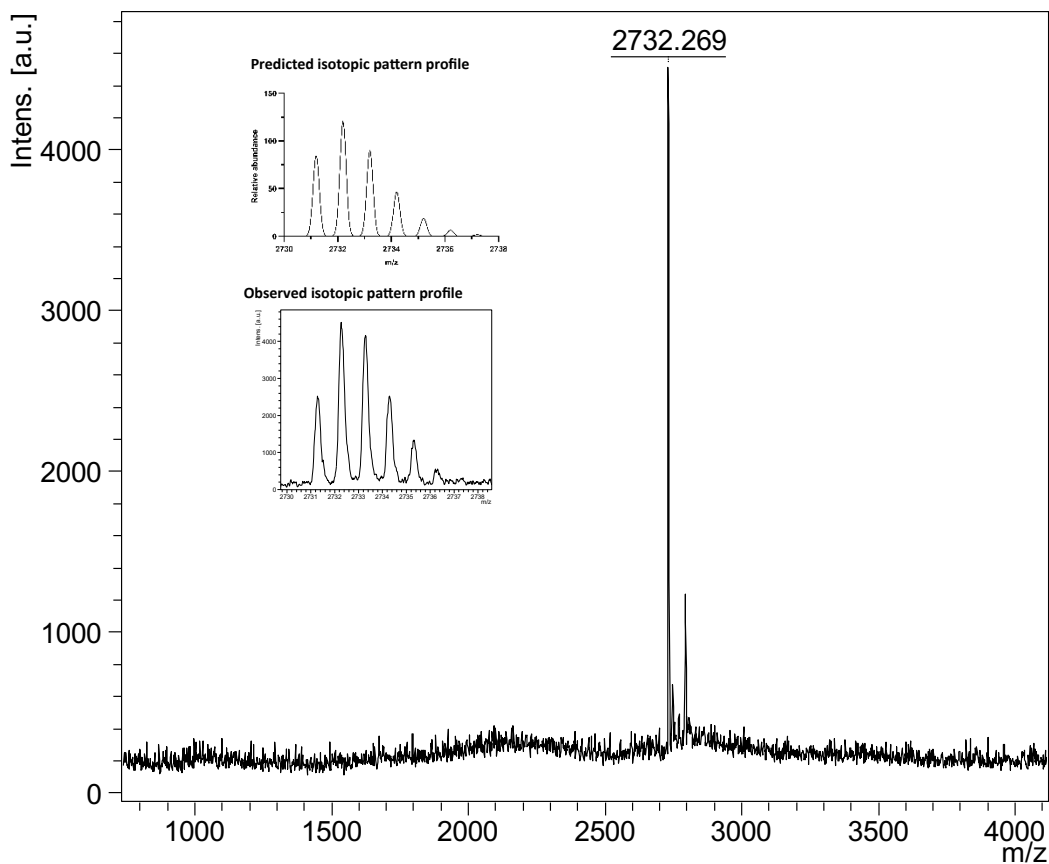


Chemical Formula: C₁₀₉H₁₄₇N₅₉O₂₈ **Exact Mass:** 2730.189 **Molecular Weight:** 2731.760

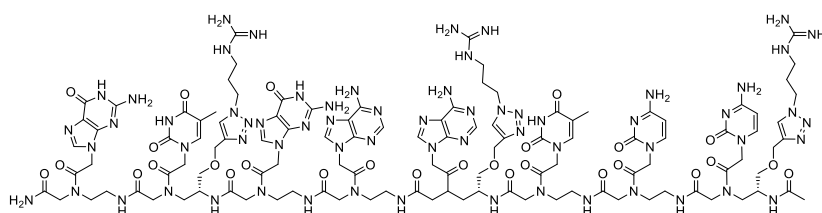
LC-MS-ESI+: *m/z* expected for [M+4H]⁴⁺: 683.8, *m/z* found: 684.0; *m/z* expected for [M+3H]³⁺: 911.4, *m/z* found: 911.6; *m/z* expected for [M+2H]²⁺: 1366.6, *m/z* found: 1366.7 .



MALDI-TOF-MS: *m/z* expected for [M+H]⁺: 2732.194, *m/z* found: 2732.269.

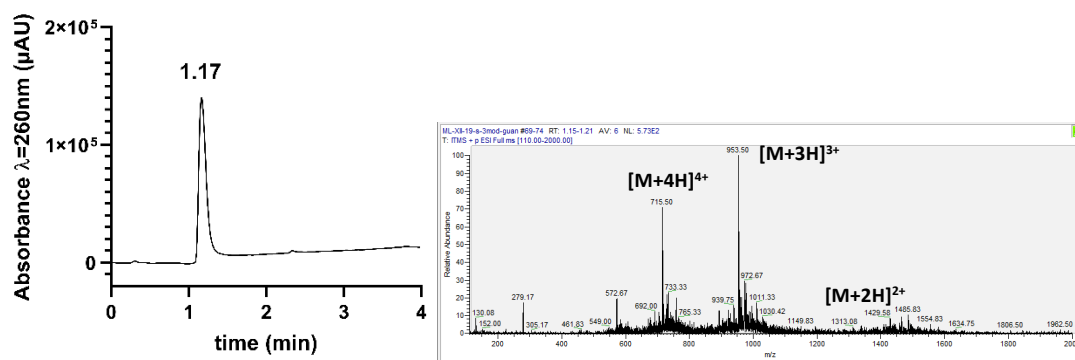


PNA2-G3: C-Ter: GT^GG AA^GT CC^G-Ac

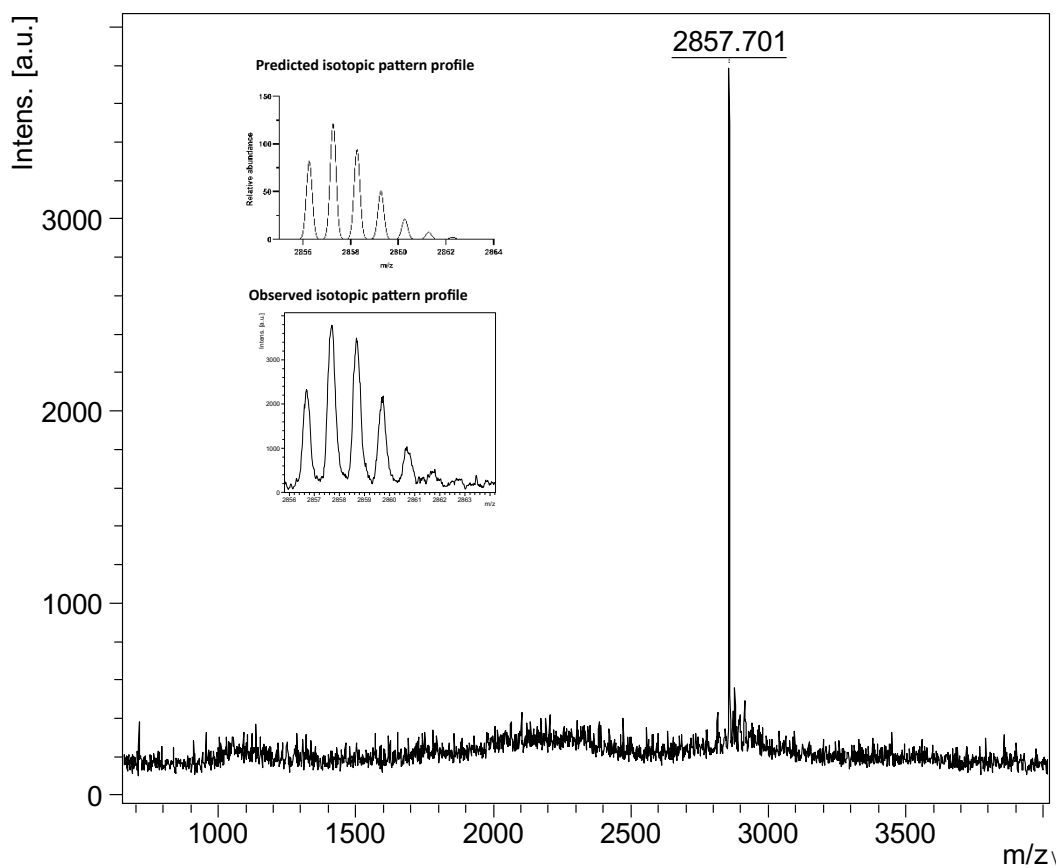


Chemical Formula: C₁₁₃H₁₅₄N₆₄O₂₈ **Exact Mass:** 2855.259 **Molecular Weight:** 2856.895

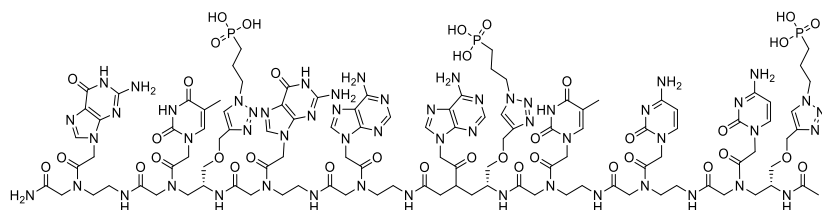
LC-MS-ESI+: m/z expected for $[M+4H]^{4+}$: 715.1, m/z found: 715.5; m/z expected for $[M+3H]^{3+}$: 953.1, m/z found: 953.5; m/z expected for $[M+2H]^{2+}$: 1429.1, m/z found: 1429.6.



MALDI-TOF-MS: m/z expected for $[M+H]^+$: 2857.269, m/z found: 2857.701.

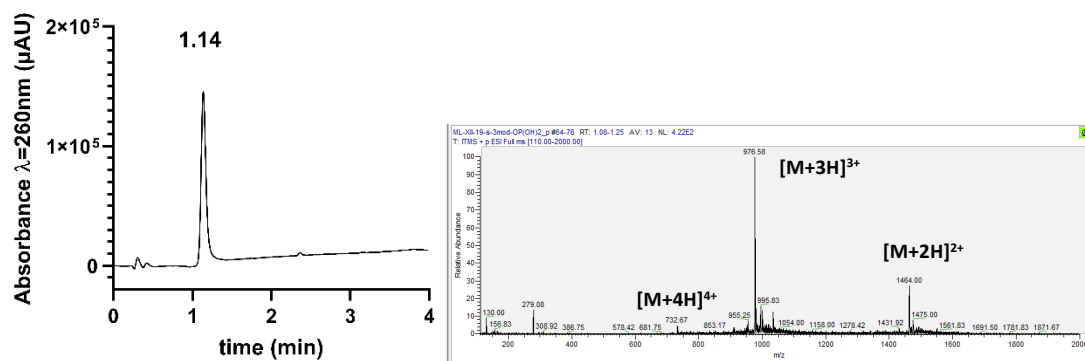


PNA2-P3: C-Ter: GT^PG AA^{PT}CC^P-Ac

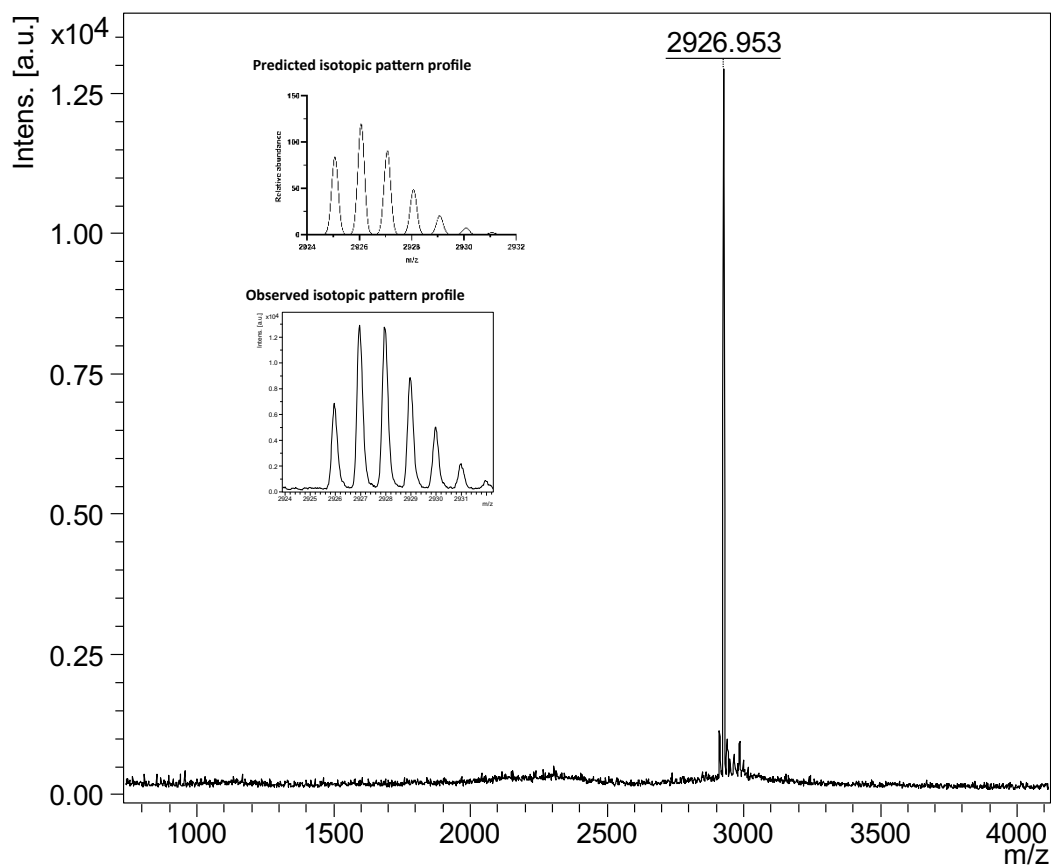


Chemical Formula: C₁₁₀H₁₄₈N₅₅O₃₇P₃ **Exact Mass:** 2924.060 **Molecular Weight:** 2925.663

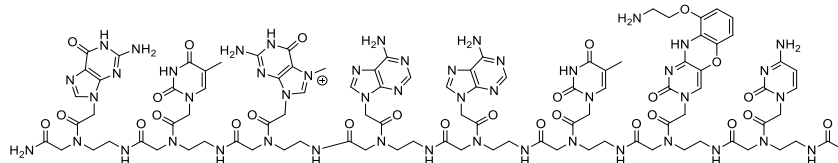
LC-MS-ESI+: m/z expected for $[M+4H]^{4+}$: 732.3, m/z found: 732.7; m/z expected for $[M+3H]^{3+}$: 976.0, m/z found: 976.6; m/z expected for $[M+2H]^{2+}$: 1463.5, m/z found: 1464.0.



MALDI-TOF-MS: m/z expected for $[M+H]^+$: 2926.089, m/z found: 2926.953.

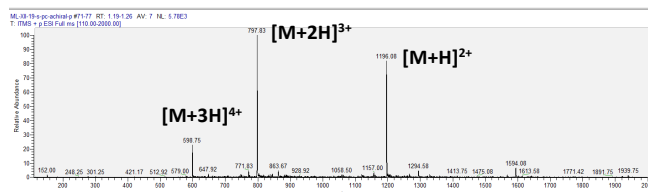
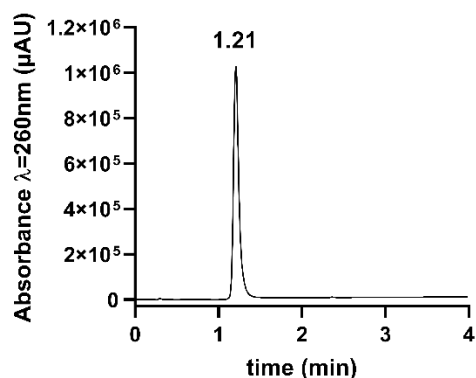


PNA2-pc-ach: C-Ter: GTG⁺ AAT C⁺C -Ac

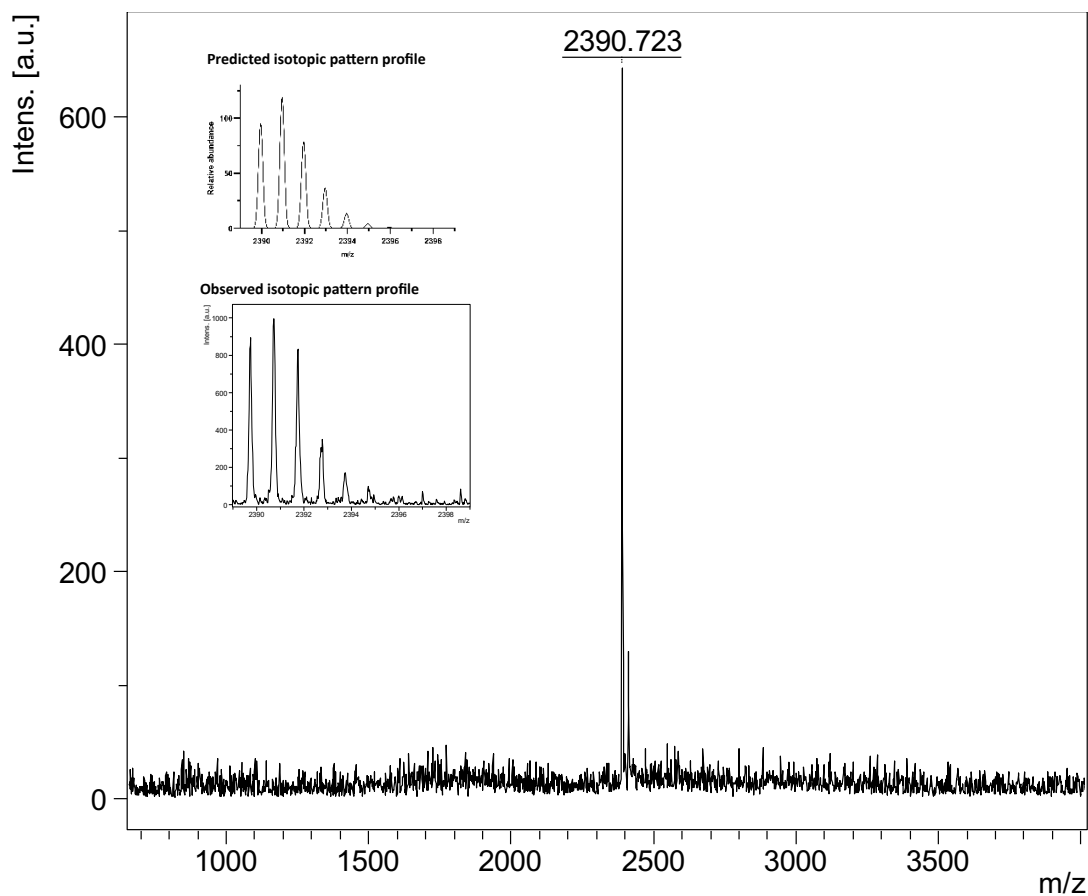


Chemical Formula: C₉₇H₁₂₁N₄₈O₂₇⁺ **Exact Mass:** 2389.957 **Molecular Weight:** 2391.343

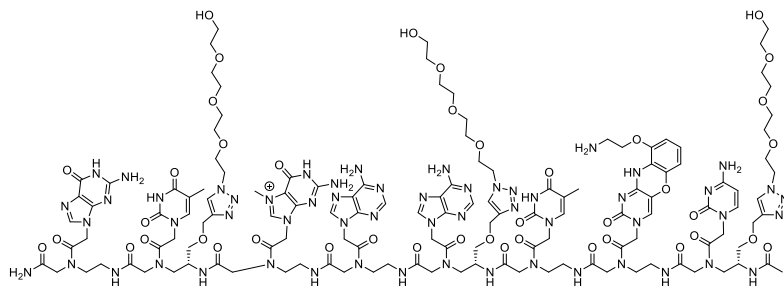
LC-MS-ESI+: *m/z* expected for [M+3H]⁴⁺: 598.5, *m/z* found: 598.8; *m/z* expected for [M+2H]³⁺: 797.7, *m/z* found: 797.8; *m/z* expected for [M+H]²⁺: 1196.0, *m/z* found: 1196.1.



MALDI-TOF-MS: *m/z* expected for [M+H]⁺: 2390.968, *m/z* found: 2390.723.

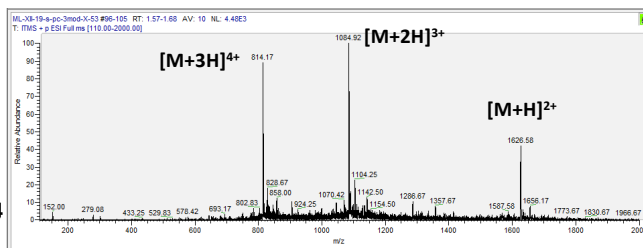
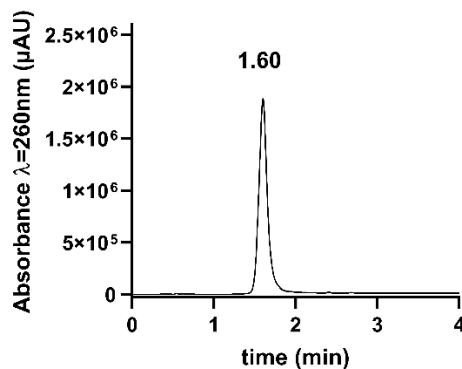


PNA2-pc-H3: C-Ter: GT^HG⁺ AA^HT C⁺C^H -Ac

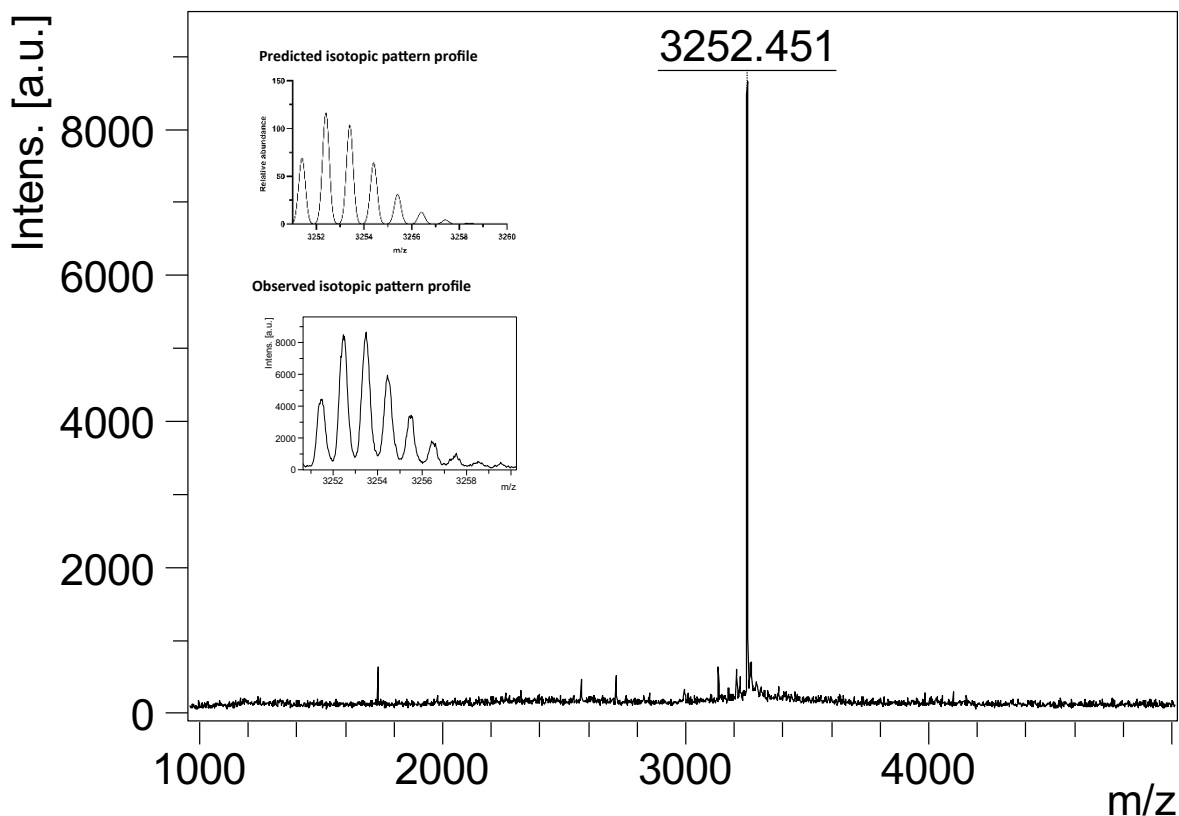


Chemical Formula: C₁₃₃H₁₈₄N₅₇O₄₂⁺ **Exact Mass:** 3251.401 **Molecular Weight:** 3253.291

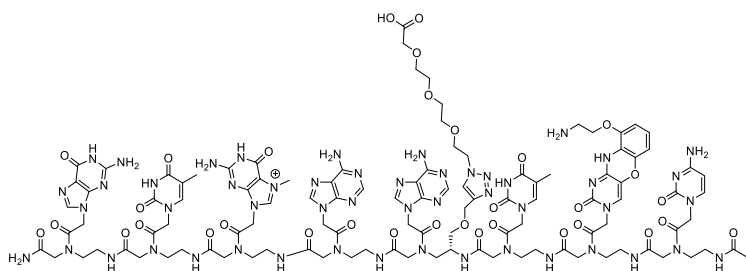
LC-MS-ESI+: *m/z* expected for [M+3H]⁴⁺: 813.9, *m/z* found: 814.2; *m/z* expected for [M+2H]³⁺: 1084.8, *m/z* found: 1084.9; *m/z* expected for [M+H]²⁺: 1626.7, *m/z* found: 1626.6.



MALDI-TOF-MS: *m/z* expected for [M+H]⁺: 3252.420, *m/z* found: 3252.451.

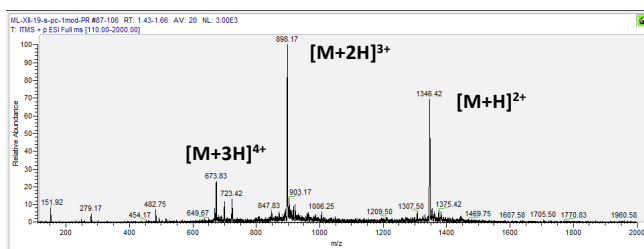
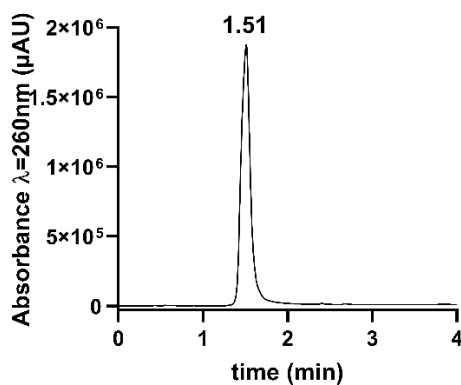


PNA2-pc-A1: C-Ter: GTG⁺ AA^AT C⁺C -Ac

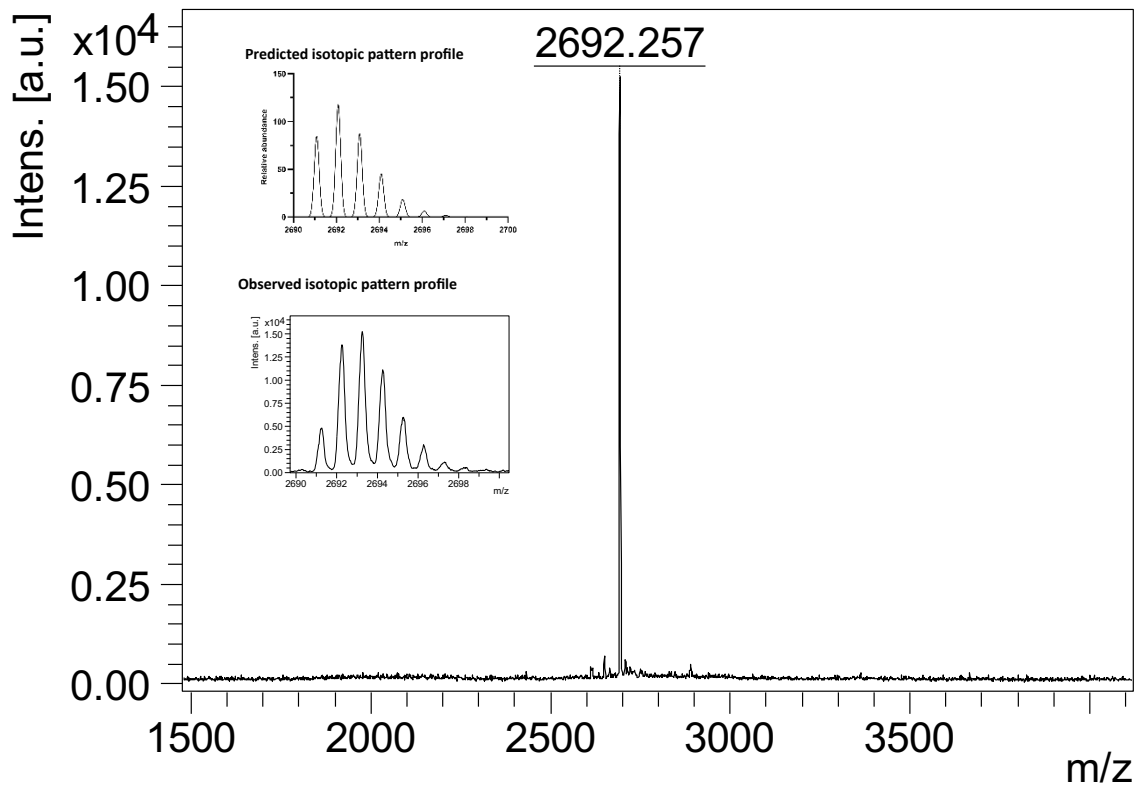


Chemical Formula: C₁₀₉H₁₄₀N₅₁O₃₃⁺ **Exact Mass:** 2691.084 **Molecular Weight:** 2692.642

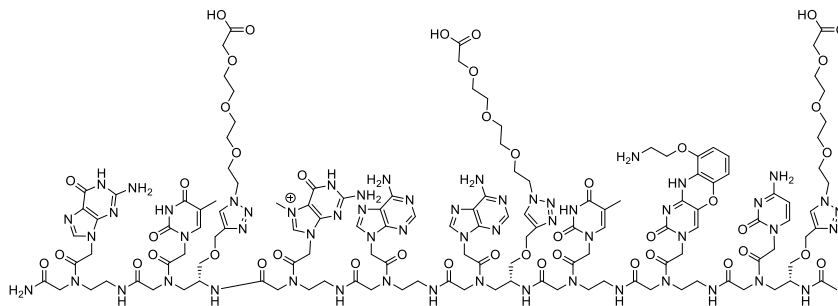
LC-MS-ESI+: *m/z* expected for [M+3H]⁴⁺: 673.8, *m/z* found: 673.8; *m/z* expected for [M+2H]³⁺: 898.0, *m/z* found: 898.2; *m/z* expected for [M+H]²⁺: 1346.5, *m/z* found: 1346.4.



MALDI-TOF-MS: *m/z* expected for [M+H]⁺: 2692.079, *m/z* found: 2692.257.

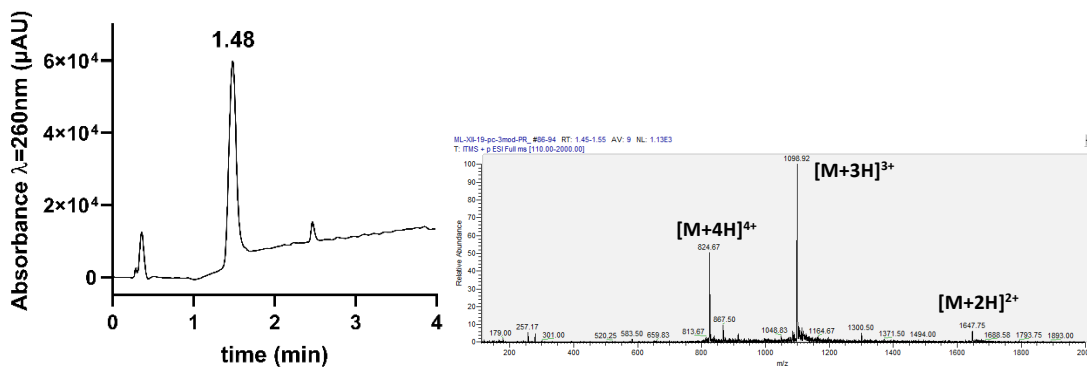


PNA2-pc-A3: C-Ter: GT^AG⁺ AA^AT C⁺C^A -Ac

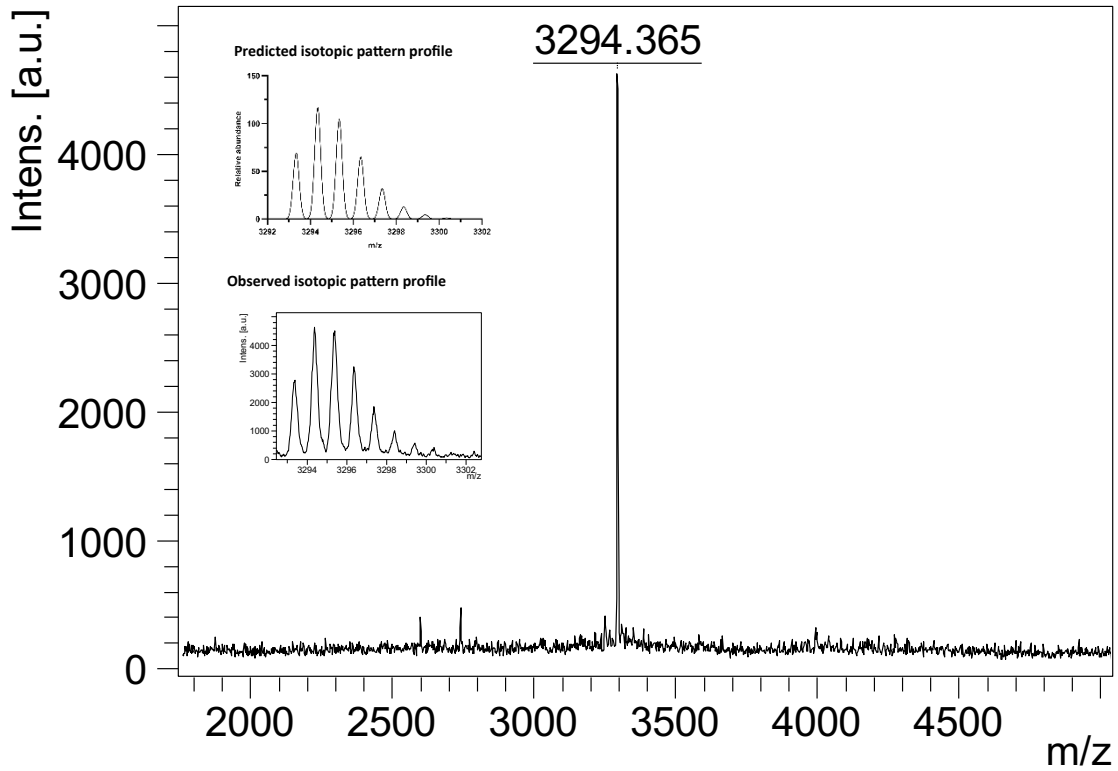


Chemical Formula: C₁₃₃H₁₇₈N₅₇O₄₅⁺ **Exact Mass:** 3293.339 **Molecular Weight:** 3295.240

LC-MS-ESI+: m/z expected for [M+3H]⁴⁺: 824.3, m/z found: 827.7; m/z expected for [M+2H]³⁺: 1098.8, m/z found: 1098.9; m/z expected for [M+H]²⁺: 1647.7, m/z found: 1647.8.



MALDI-TOF-MS: m/z expected for [M+H]⁺: 3294.351, m/z found: 3294.365.

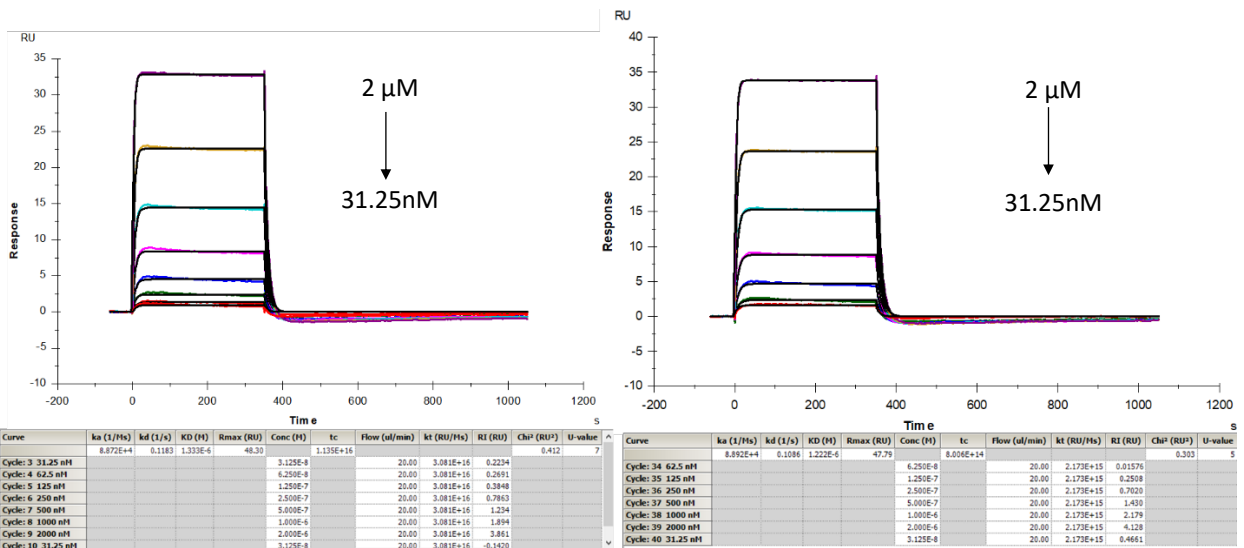


Copies of the SPR response curves and the 1:1 binding model fitting curves.

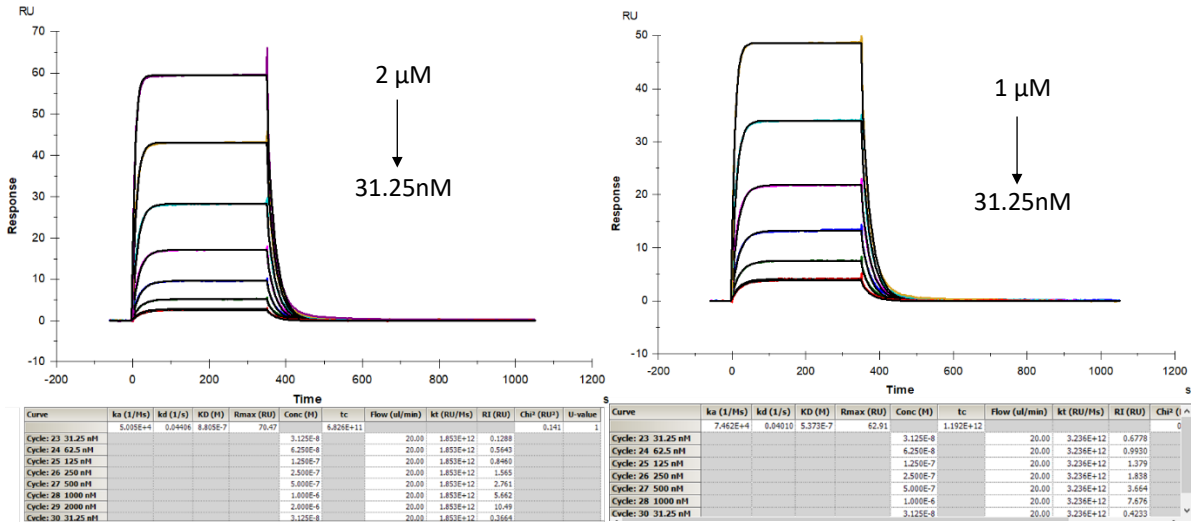
DNA6-Bt on chip



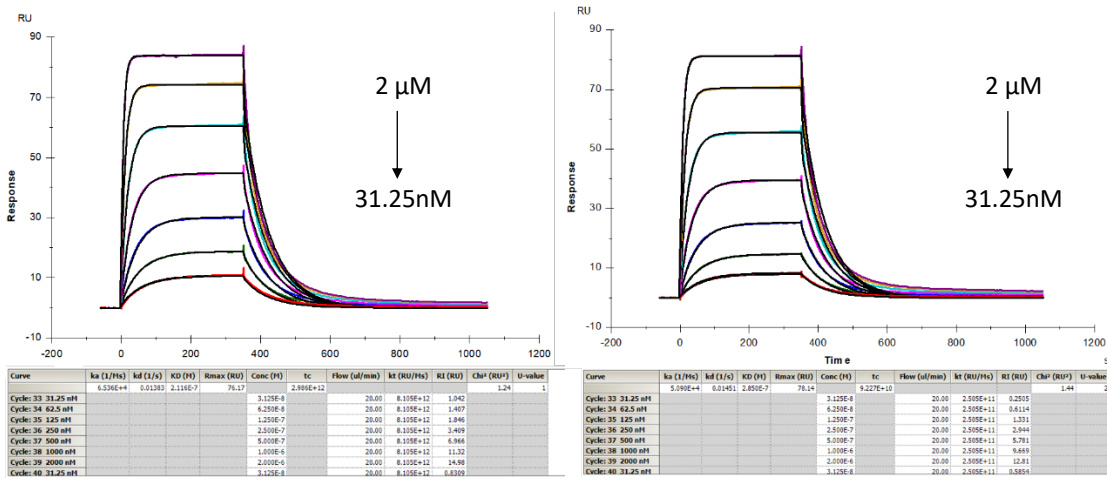
PNA2-ach



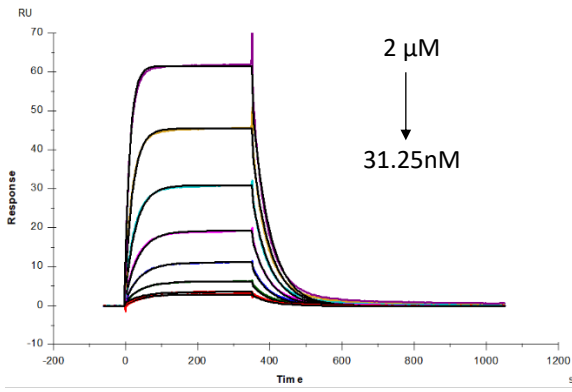
PNA2-H1



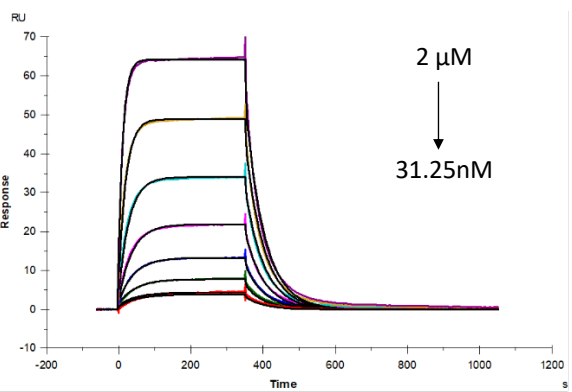
PNA2-H3



PNA2-A3

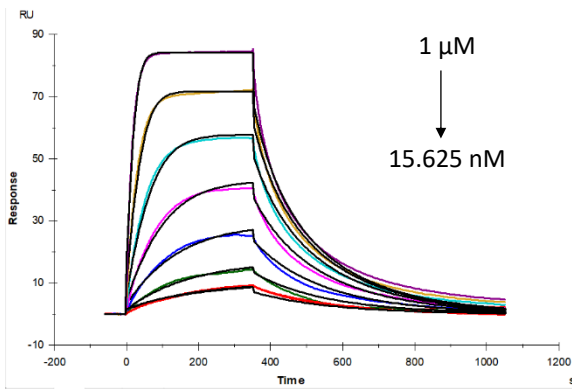


Curve	ka (1/Hz)	kd (1/s)	KD (M)	Rmax (RU)	Conc (M)	tc	Flow (ul/min)	kt (RU/Hz)	RI (RU)	Chi² (RU²)	U-value
Cycle: 53 31.25 nM	2.537E+4	0.02045	8.052E-7	73.08	3.125E-8	2.876E+8	20.00	7.802E+8	6.2314	0.435	2
Cycle: 54 62.5 nM				6.250E-8	20.00	7.802E+8	20.00	7.802E+8	6.9803		
Cycle: 55 125 nM				1.250E-7	20.00	7.802E+8	20.00	7.802E+8	1.526		
Cycle: 56 250 nM				2.500E-7	20.00	7.802E+8	20.00	7.802E+8	1.896		
Cycle: 57 500 nM				5.000E-7	20.00	7.802E+8	20.00	7.802E+8	2.941		
Cycle: 58 1000 nM				1.000E-6	20.00	7.802E+8	20.00	7.802E+8	5.314		
Cycle: 59 2000 nM				2.000E-6	20.00	7.802E+8	20.00	7.802E+8	9.468		
Cycle: 60 31.25 nM				3.125E-8	20.00	7.802E+8	20.00	7.802E+8	6.8246		

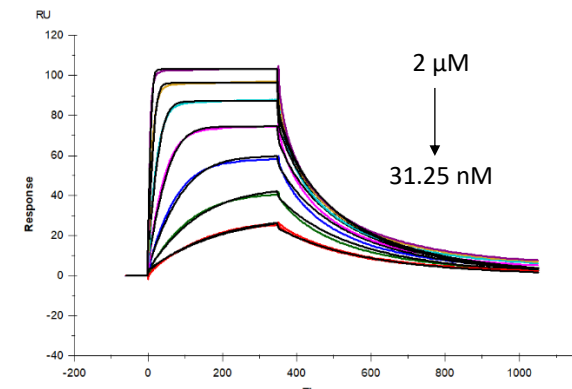


Curve	ka (1/Hz)	kd (1/s)	KD (M)	Rmax (RU)	Conc (M)	tc	Flow (ul/min)	kt (RU/Hz)	RI (RU)	Chi² (RU²)	U-value
Cycle: 53 31.25 nM	3.021E+4	0.01941	6.429E-7	71.68	3.125E-8	1.248E+8	20.00	3.389E+8	1.688	0.411	1
Cycle: 54 62.5 nM				6.250E-8	20.00	3.389E+8	20.00	3.389E+8	1.502		
Cycle: 55 125 nM				1.250E-7	20.00	3.389E+8	20.00	3.389E+8	1.271		
Cycle: 56 250 nM				2.500E-7	20.00	3.389E+8	20.00	3.389E+8	1.984		
Cycle: 57 500 nM				5.000E-7	20.00	3.389E+8	20.00	3.389E+8	2.963		
Cycle: 58 1000 nM				1.000E-6	20.00	3.389E+8	20.00	3.389E+8	5.678		
Cycle: 59 2000 nM				2.000E-6	20.00	3.389E+8	20.00	3.389E+8	10.55		
Cycle: 60 31.25 nM				3.125E-8	20.00	3.389E+8	20.00	3.389E+8	6.6645		

PNA2-N3

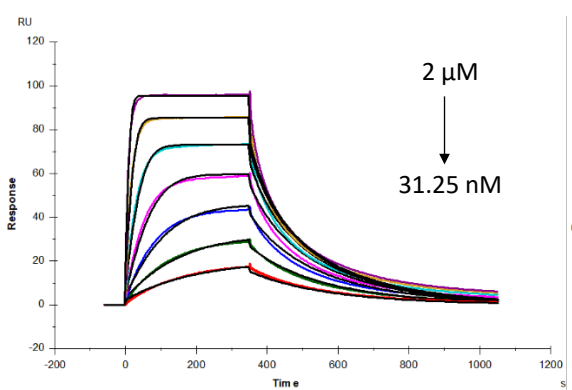


Curve	ka (1/Hz)	kd (1/s)	KD (M)	Rmax (RU)	Conc (M)	tc	Flow (ul/min)	kt (RU/Hz)	RI (RU)	Chi² (RU²)	U-value
Cycle: 13 15.625 nM	8.237E+4	0.01039	1.251E-7	77.48	1.562E-8	1.765E+8	20.00	4.792E+8	1.486	1.41	2
Cycle: 14 31.25 nM				3.125E-8	20.00	4.792E+8	20.00	4.792E+8	1.603		
Cycle: 15 62.5 nM				6.250E-8	20.00	4.792E+8	20.00	4.792E+8	3.215		
Cycle: 16 125 nM				1.250E-7	20.00	4.792E+8	20.00	4.792E+8	6.487		
Cycle: 17 250 nM				2.500E-7	20.00	4.792E+8	20.00	4.792E+8	6.251		
Cycle: 18 500 nM				5.000E-7	20.00	4.792E+8	20.00	4.792E+8	9.801		
Cycle: 19 1000 nM				1.000E-6	20.00	4.792E+8	20.00	4.792E+8	15.33		

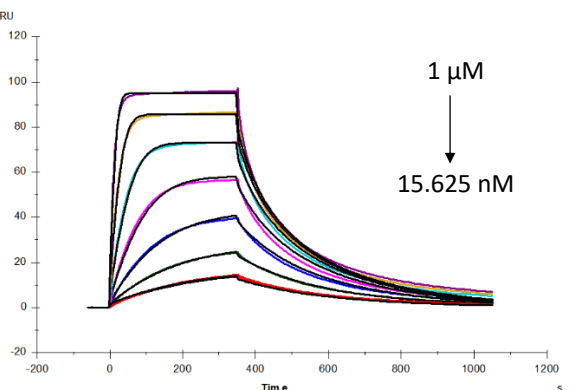


Curve	ka (1/Hz)	kd (1/s)	KD (M)	Rmax (RU)	Conc (M)	tc	Flow (ul/min)	kt (RU/Hz)	RI (RU)	Chi² (RU²)	U-value
Cycle: 33 31.25 nM	1.563E+5	0.01045	6.685E-8	84.73	3.125E-8	2.464E+8	20.00	6.689E+8	2.403	2.23	2
Cycle: 34 62.5 nM				6.250E-8	20.00	6.689E+8	20.00	6.689E+8	3.104		
Cycle: 35 125 nM				1.250E-7	20.00	6.689E+8	20.00	6.689E+8	4.536		
Cycle: 36 250 nM				2.500E-7	20.00	6.689E+8	20.00	6.689E+8	7.566		
Cycle: 37 500 nM				5.000E-7	20.00	6.689E+8	20.00	6.689E+8	12.23		
Cycle: 38 1000 nM				1.000E-6	20.00	6.689E+8	20.00	6.689E+8	16.71		
Cycle: 39 2000 nM				2.000E-6	20.00	6.689E+8	20.00	6.689E+8	26.82		

PNA2-G3

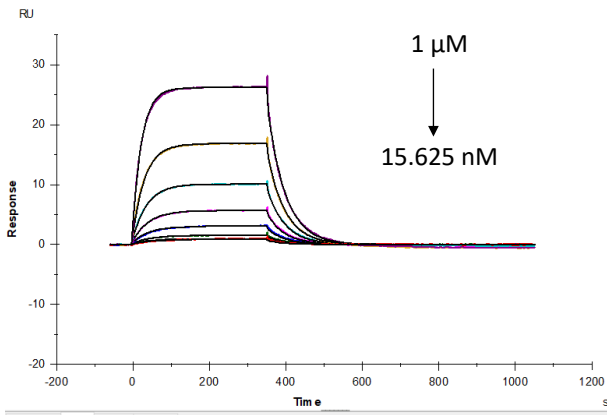


Curve	ka (1/Hz)	kd (1/s)	KD (M)	Rmax (RU)	Conc (M)	tc	Flow (ul/min)	kt (RU/Hz)	RI (RU)	Chi² (RU²)	U-value
Cycle: 13 31.25 nM	8.530E+4	0.01093	1.280E-7	78.83	3.125E-8	1.577E+8	20.00	4.552E+8	2.358	2.04	2
Cycle: 14 62.5 nM				6.250E-8	20.00	4.552E+8	20.00	4.552E+8	3.193		
Cycle: 15 125 nM				1.250E-7	20.00	4.552E+8	20.00	4.552E+8	3.879		
Cycle: 16 250 nM				2.500E-7	20.00	4.552E+8	20.00	4.552E+8	4.807		
Cycle: 17 500 nM				5.000E-7	20.00	4.552E+8	20.00	4.552E+8	8.339		
Cycle: 18 1000 nM				1.000E-6	20.00	4.552E+8	20.00	4.552E+8	14.17		
Cycle: 19 2000 nM				2.000E-6	20.00	4.552E+8	20.00	4.552E+8	20.72		
Cycle: 20 31.25 nM				3.125E-8	20.00	4.552E+8	20.00	4.552E+8	2.323		

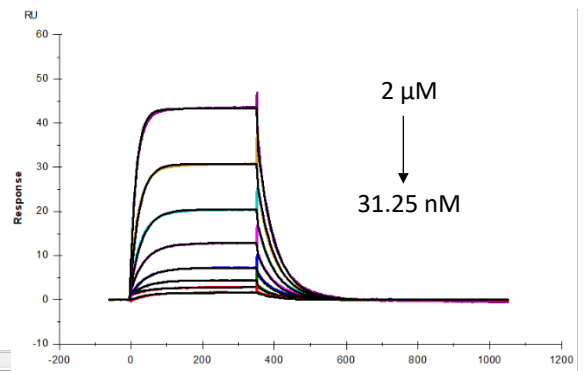


Curve	ka (1/Hz)	kd (1/s)	KD (M)	Rmax (RU)	Conc (M)	tc	Flow (ul/min)	kt (RU/Hz)	RI (RU)	Chi² (RU²)	U-value
Cycle: 33 15.625 nM	1.521E+5	0.01050	6.906E-8	84.40	1.562E-8	2.448E+8	20.00	6.624E+8	1.250	1.41	2
Cycle: 34 31.25 nM				3.125E-8	20.00	6.624E+8	20.00	6.624E+8	1.894		
Cycle: 35 62.5 nM				6.250E-8	20.00	6.624E+8	20.00	6.624E+8	2.941		
Cycle: 36 125 nM				1.250E-7	20.00	6.624E+8	20.00	6.624E+8	3.861		
Cycle: 37 250 nM				2.500E-7	20.00	6.624E+8	20.00	6.624E+8	6.955		
Cycle: 38 500 nM				5.000E-7	20.00	6.624E+8	20.00	6.624E+8	11.45		
Cycle: 39 1000 nM				1.000E-6	20.00	6.624E+8	20.00	6.624E+8	16.14		

PNA2-P3

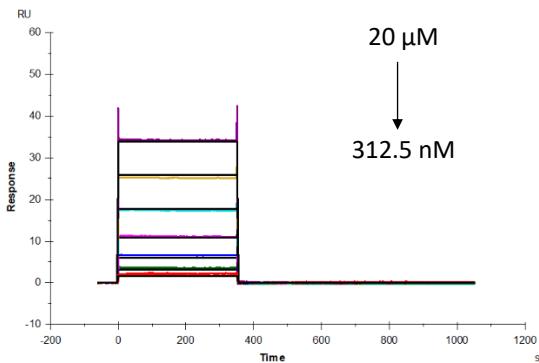


Curve	ka (1/Ms)	kd (1/s)	KD (M)	Rmax (RU)	Conc (M)	tc	Flow (ul/min)	kt (RU/Hz)	RI (RU)	Chi² (RU²)	U-value
Cycle: 53 15.625 nM	2.003E+4	0.02141	1.069E-6	49.07	1.563E-8	4.167E+8	20.00	1.131E+9	0.2328	0.0379	1
Cycle: 54 31.25 nM					3.125E-8		20.00	1.131E+9	0.1563		
Cycle: 55 62.5 nM					6.250E-8		20.00	1.131E+9	0.3705		
Cycle: 56 125 nM					1.250E-7		20.00	1.131E+9	0.5474		
Cycle: 57 250 nM					2.500E-7		20.00	1.131E+9	0.8215		
Cycle: 58 500 nM					5.000E-7		20.00	1.131E+9	1.192		
Cycle: 59 1000 nM					1.000E-6		20.00	1.131E+9	2.464		
Cycle: 60 15.625 nM					1.563E-8		20.00	1.131E+9	0.1382		

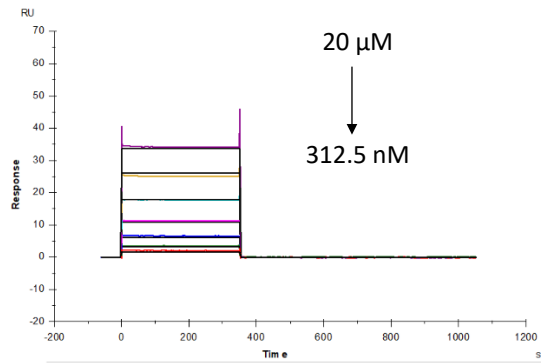


Curve	ka (1/Ms)	kd (1/s)	KD (M)	Rmax (RU)	Conc (M)	tc	Flow (ul/min)	kt (RU/Hz)	RI (RU)	Chi² (RU²)	U-value
Cycle: 53 31.25 nM	1.960E+4	0.02050	1.046E-6	56.18	3.125E-8	1.087E+10	20.00	2.890E+10	1.180	0.159	1
Cycle: 54 62.5 nM					6.250E-8		20.00	2.890E+10	1.279		
Cycle: 55 125 nM					1.250E-7		20.00	2.890E+10	1.241		
Cycle: 56 250 nM					2.500E-7		20.00	2.890E+10	1.992		
Cycle: 57 500 nM					5.000E-7		20.00	2.890E+10	2.391		
Cycle: 58 1000 nM					1.000E-6		20.00	2.890E+10	3.320		
Cycle: 59 2000 nM					2.000E-6		20.00	2.890E+10	6.399		
Cycle: 60 31.25 nM					3.125E-8		20.00	2.890E+10	0.1544		

DNA8

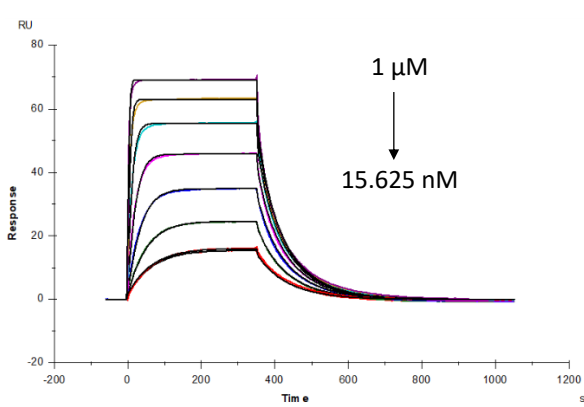


Curve	ka (1/Ms)	kd (1/s)	KD (M)	Rmax (RU)	Conc (M)	Chi² (RU²)	U-value
Cycle: 23 312.5 nM	3.739E+5	3.250	8.692E-6	48.53	3.125E-7	0.777	N/A
Cycle: 24 625 nM					6.250E-7		
Cycle: 25 1250 nM					1.250E-6		
Cycle: 26 2500 nM					2.500E-6		
Cycle: 27 5000 nM					5.000E-6		
Cycle: 28 10000 nM					1.000E-5		
Cycle: 29 20000 nM					2.000E-5		
Cycle: 30 312.5 nM					3.125E-7		

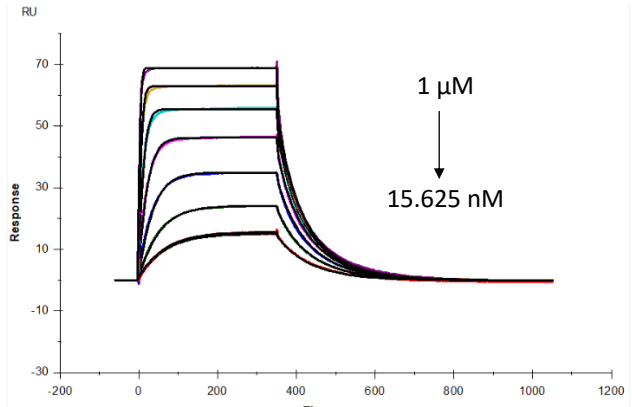


Curve	ka (1/Ms)	kd (1/s)	KD (M)	Rmax (RU)	Conc (M)	Chi² (RU²)	U-value
Cycle: 53 312.5 nM	3.970E+5	3.335	8.400E-6	47.96	3.125E-7	0.805	N/A
Cycle: 54 625 nM					6.250E-7		
Cycle: 55 1250 nM					1.250E-6		
Cycle: 56 2500 nM					2.500E-6		
Cycle: 57 5000 nM					5.000E-6		
Cycle: 58 10000 nM					1.000E-5		
Cycle: 59 20000 nM					2.000E-5		
Cycle: 60 312.5 nM					3.125E-7		

PNA2-pc-ach

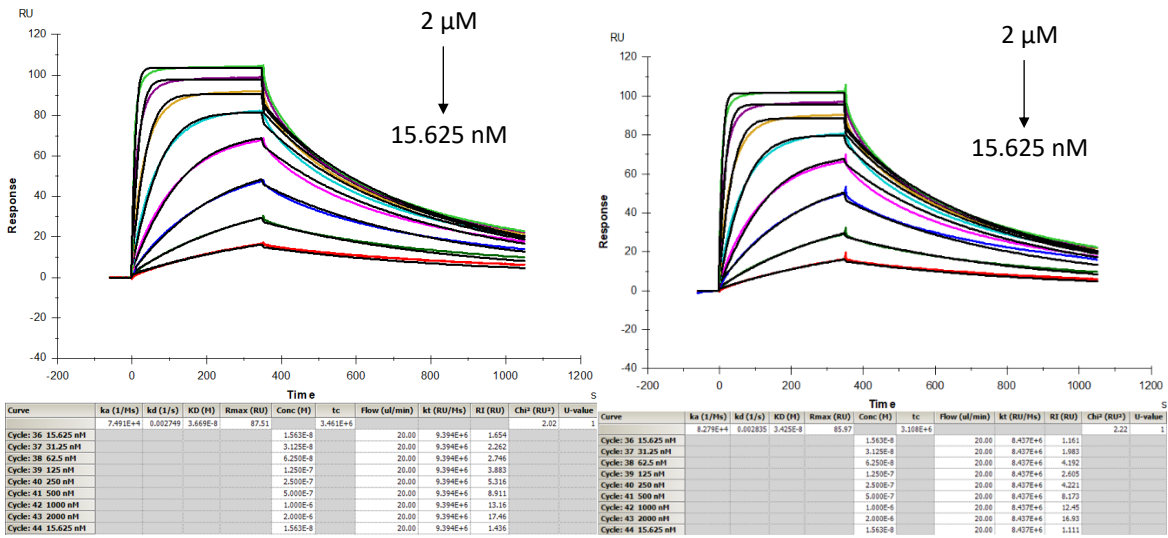


Curve	ka (1/Ms)	kd (1/s)	KD (M)	Rmax (RU)	Conc (M)	tc	Flow (ul/min)	kt (RU/Hz)	RI (RU)	Chi² (RU²)	U-value
Cycle: 13 15.625 nM	3.860E+5	0.01873	4.854E-8	58.76	1.563E-8	1.247E+7	20.00	3.394E+7	1.212	0.287	1
Cycle: 14 31.25 nM					3.125E-8		20.00	3.394E+7	1.607		
Cycle: 15 62.5 nM					6.250E-8		20.00	3.394E+7	1.825		
Cycle: 16 125 nM					1.250E-7		20.00	3.394E+7	3.467		
Cycle: 17 250 nM					2.500E-7		20.00	3.394E+7	6.189		
Cycle: 18 500 nM					5.000E-7		20.00	3.394E+7	9.595		
Cycle: 19 1000 nM					1.000E-6		20.00	3.394E+7	13.13		
Cycle: 20 15.625 nM					1.563E-8		20.00	3.394E+7	1.732		

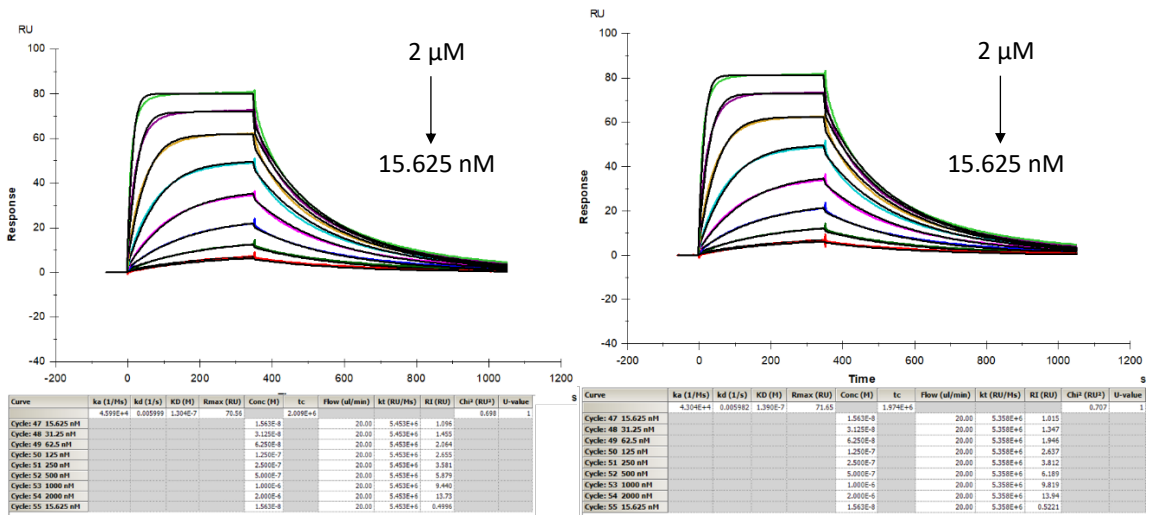


Curve	ka (1/Ms)	kd (1/s)	KD (M)	Rmax (RU)	Conc (M)	tc	Flow (ul/min)	kt (RU/Hz)	RI (RU)	Chi² (RU²)	U-value
Cycle: 43 15.625 nM	3.902E+5	0.01862	4.771E-8	58.50	1.563E-8	1.168E+7	20.00	3.171E+7	0.6966	0.246	1
Cycle: 44 31.25 nM					3.125E-8		20.00	3.171E+7	1.098		
Cycle: 45 62.5 nM					6.250E-8		20.00	3.171E+7	1.733		
Cycle: 46 125 nM					1.250E-7		20.00	3.171E+7	3.874		
Cycle: 47 250 nM					2.500E-7		20.00	3.171E+7	6.363		
Cycle: 48 500 nM					5.000E-7		20.00	3.171E+7	9.526		
Cycle: 49 1000 nM					1.000E-6		20.00	3.171E+7	12.93		
Cycle: 50 15.625 nM					1.563E-8		20.00	3.171E+7	1.198		

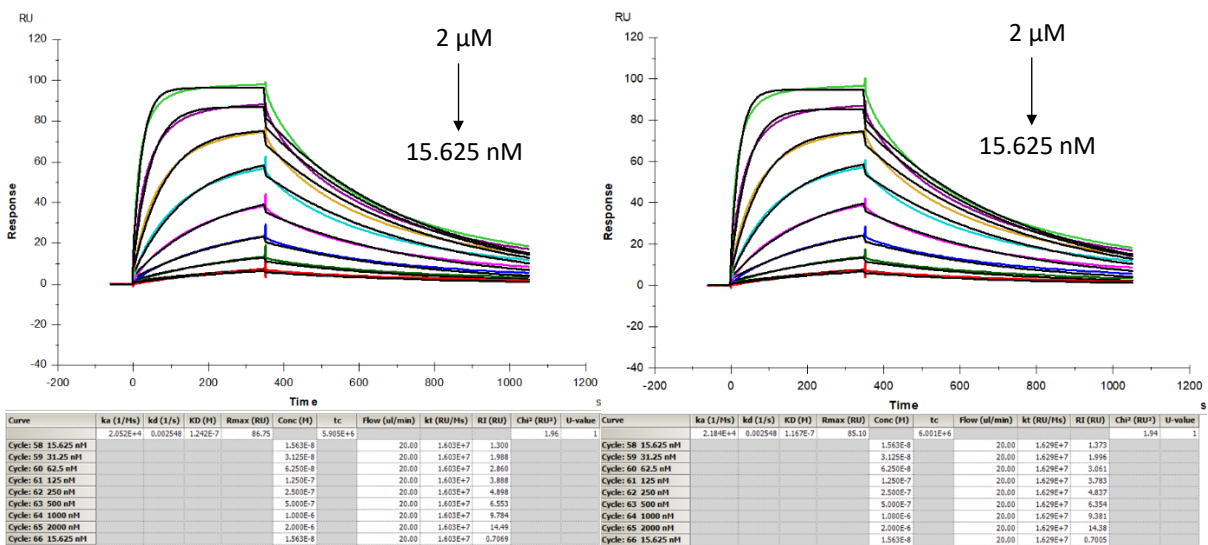
PNA2-pc-H3



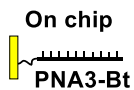
PNA2-pc-A1



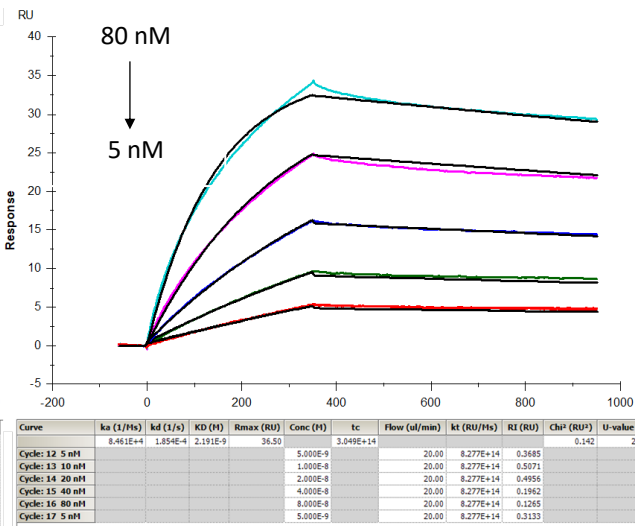
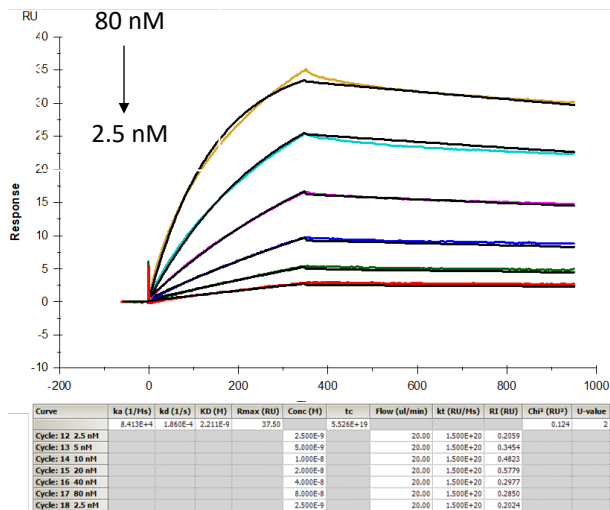
PNA2-pc-A3



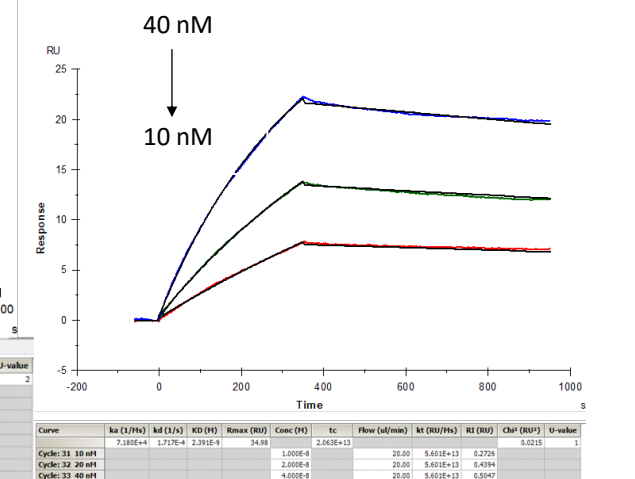
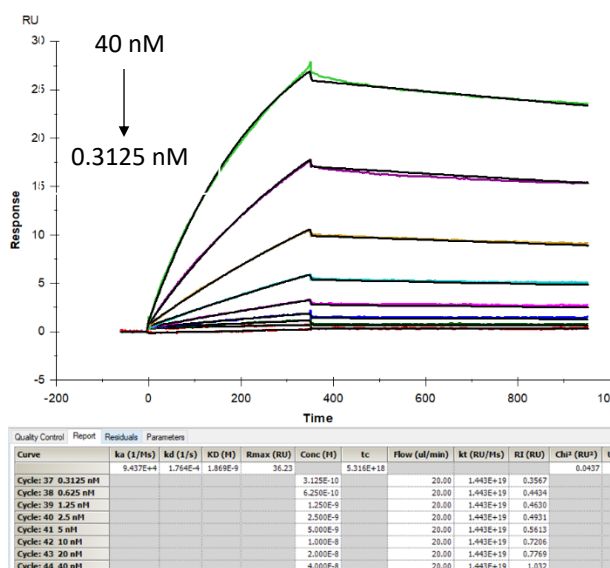
PNA3-Bt on chip



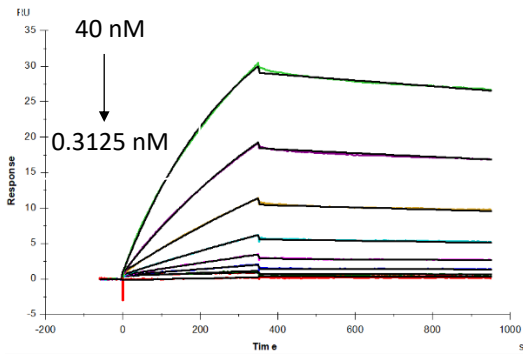
PNA2-ach



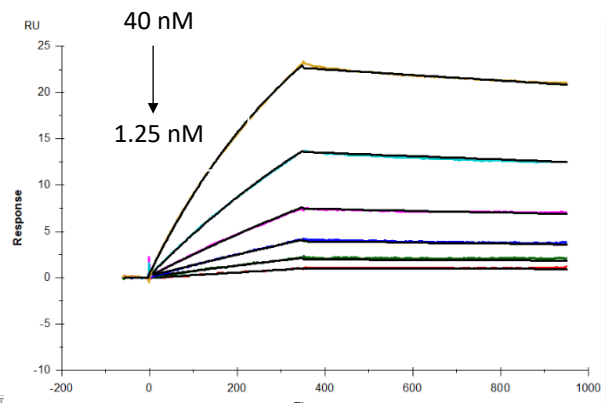
PNA2-H1



PNA2-H3

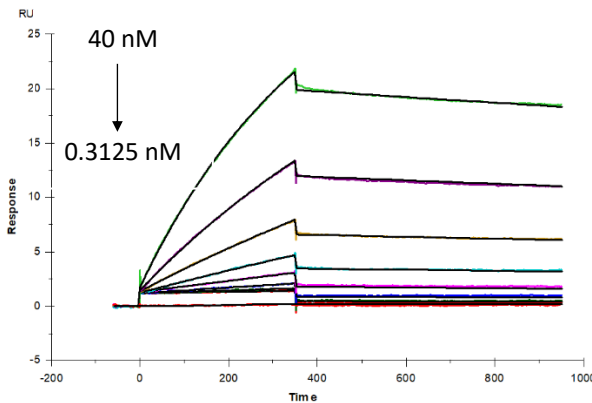


Curve	ka (1/Hz)	kd (1/s)	KD (M)	Rmax (RU)	Conc (M)	tc	Flow (ul/min)	kt (RU/Hz)	RI (RU)	Chi² (RU²)	U-value
Cycle: 48 0.3125 nM	7.968E+4	1.49E+4	1.875E-9	44.11	3.125E-10	2.512E+17	20.00	6.818E+17	0.5395	0.0668	3
Cycle: 49 0.625 nM					6.250E-10		20.00	6.818E+17	0.4462		
Cycle: 50 1.25 nM					1.250E-9		20.00	6.818E+17	0.5566		
Cycle: 51 2.5 nM					2.500E-9		20.00	6.818E+17	0.5892		
Cycle: 52 5 nM					5.000E-9		20.00	6.818E+17	0.6423		
Cycle: 53 10 nM					1.000E-8		20.00	6.818E+17	0.6734		
Cycle: 54 20 nM					2.000E-8		20.00	6.818E+17	0.6853		
Cycle: 55 40 nM					4.000E-8		20.00	6.818E+17	1.012		

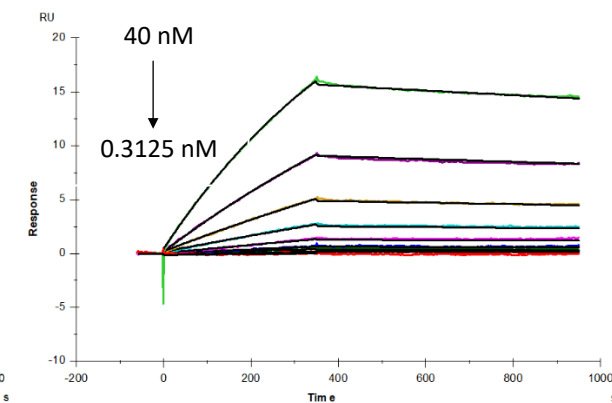


Curve	ka (1/Hz)	kd (1/s)	KD (M)	Rmax (RU)	Conc (M)	tc	Flow (ul/min)	kt (RU/Hz)	RI (RU)	Chi² (RU²)	U-value
Cycle: 39 1.25 nM	5.849E+4	1.381E+4	2.361E-9	41.31	1.250E-9	1.609E+17	20.00	4.367E+17	-0.01018	0.0142	2
Cycle: 40 2.5 nM					2.500E-9		20.00	4.367E+17	0.1462		
Cycle: 41 5 nM					5.000E-9		20.00	4.367E+17	0.1882		
Cycle: 42 10 nM					1.000E-8		20.00	4.367E+17	0.1793		
Cycle: 43 20 nM					2.000E-8		20.00	4.367E+17	0.1857		
Cycle: 44 40 nM					4.000E-8		20.00	4.367E+17	0.3908		

PNA2-A3

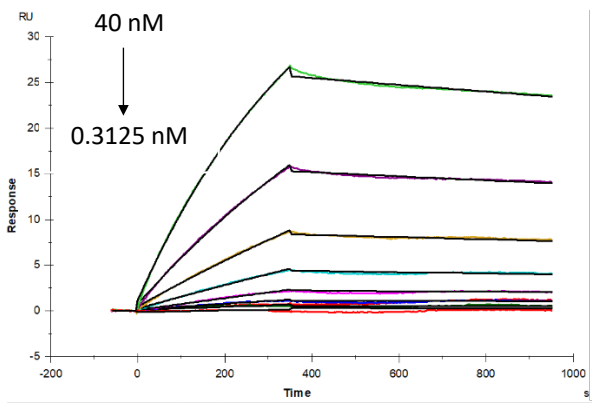


Curve	ka (1/Hz)	kd (1/s)	KD (M)	Rmax (RU)	Conc (M)	tc	Flow (ul/min)	kt (RU/Hz)	RI (RU)	Chi² (RU²)	U-value
Cycle: 70 0.3125 nM	5.472E+4	1.350E+4	2.286E-9	35.77	3.125E-10	5.136E+12	20.00	1.394E+13	1.194	0.187	9
Cycle: 71 0.625 nM					6.250E-10		20.00	1.394E+13	1.194		
Cycle: 72 1.25 nM					1.250E-9		20.00	1.394E+13	1.203		
Cycle: 73 2.5 nM					2.500E-9		20.00	1.394E+13	1.307		
Cycle: 74 5 nM					5.000E-9		20.00	1.394E+13	1.254		
Cycle: 75 10 nM					1.000E-8		20.00	1.394E+13	1.374		
Cycle: 76 20 nM					2.000E-8		20.00	1.394E+13	1.463		
Cycle: 77 40 nM					4.000E-8		20.00	1.394E+13	1.751		

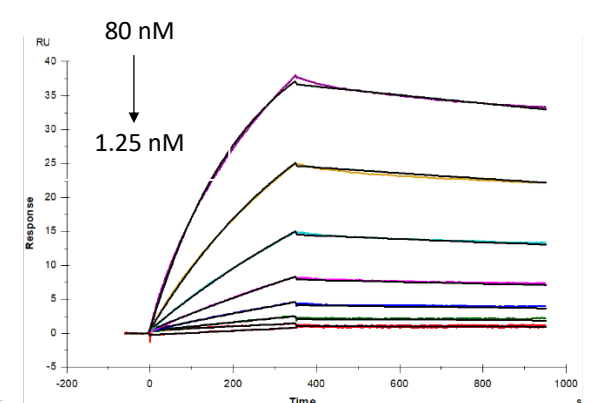


Curve	ka (1/Hz)	kd (1/s)	KD (M)	Rmax (RU)	Conc (M)	tc	Flow (ul/min)	kt (RU/Hz)	RI (RU)	Chi² (RU²)	U-value
Cycle: 59 0.3125 nM	4.562E+4	1.403E+4	3.141E-9	33.91	3.125E-10	6.488E+14	20.00	2.575E+15	3.942E-4	0.0126	3
Cycle: 60 0.625 nM					6.250E-10		20.00	2.575E+15	0.68497		
Cycle: 61 1.25 nM					1.250E-9		20.00	2.575E+15	0.009189		
Cycle: 62 2.5 nM					2.500E-9		20.00	2.575E+15	0.04633		
Cycle: 63 5 nM					5.000E-9		20.00	2.575E+15	0.1697		
Cycle: 64 10 nM					1.000E-8		20.00	2.575E+15	0.2155		
Cycle: 65 20 nM					2.000E-8		20.00	2.575E+15	0.1516		
Cycle: 66 40 nM					4.000E-8		20.00	2.575E+15	0.4059		

PNA2-N3



Curve	ka (1/Hz)	kd (1/s)	KD (M)	Rmax (RU)	Conc (M)	tc	Flow (ul/min)	kt (RU/Hz)	RI (RU)	Chi² (RU²)	U-value
Cycle: 15 0.3125 nM	5.603E+4	1.513E+4	2.672E-9	48.16	3.125E-10	8.894E+7	20.00	2.403E+8	0.3342	0.0586	4
Cycle: 16 0.625 nM					6.250E-10		20.00	2.403E+8	0.1136		
Cycle: 17 1.25 nM					1.250E-9		20.00	2.403E+8	0.1103		
Cycle: 18 2.5 nM					2.500E-9		20.00	2.403E+8	0.08813		
Cycle: 19 5 nM					5.000E-9		20.00	2.403E+8	0.2414		
Cycle: 20 10 nM					1.000E-8		20.00	2.403E+8	0.4646		
Cycle: 21 20 nM					2.000E-8		20.00	2.403E+8	0.7589		
Cycle: 22 40 nM					4.000E-8		20.00	2.403E+8	1.126		

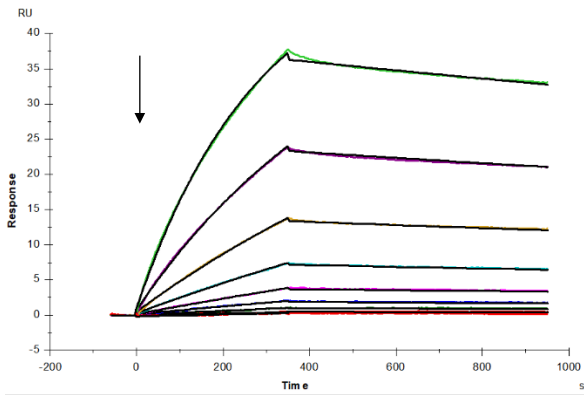


Curve	ka (1/Hz)	kd (1/s)	KD (M)	Rmax (RU)	Conc (M)	tc	Flow (ul/min)	kt (RU/Hz)	RI (RU)	Chi² (RU²)	U-value
Cycle: 14 1.25 nM	5.266E+4	1.766E+4	3.357E-9	48.87	1.250E-9	1.164E+16	20.00	3.159E+16	0.4195	0.0407	2
Cycle: 15 2.5 nM					2.500E-9		20.00	3.159E+16	0.4000		
Cycle: 16 5 nM					5.000E-9		20.00	3.159E+16	0.4920		
Cycle: 17 10 nM					1.000E-8		20.00	3.159E+16	0.4726		
Cycle: 18 20 nM					2.000E-8		20.00	3.159E+16	0.5161		
Cycle: 19 40 nM					4.000E-8		20.00	3.159E+16	0.5127		
Cycle: 20 80 nM					8.000E-8		20.00	3.159E+16	0.5382		
Cycle: 21 1.25 nM					1.250E-9		20.00	3.159E+16	-0.2310		

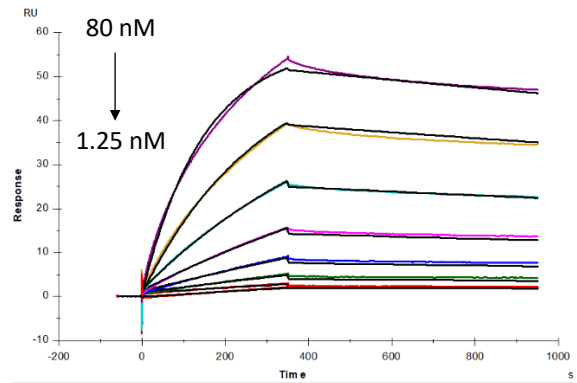
PNA2-G3

40 nM

0.3125 nM

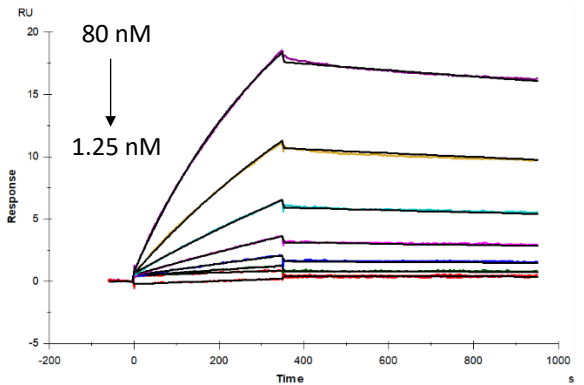


Curve	ka (1/Hz)	kd (1/s)	KD (M)	Rmax (RU)	Conc (M)	tc	Flow (ul/min)	kt (RU/Hz)	RI (RU)	Chi² (RU²)	U-value
Cycle: 37 0.3125 nM	6.49E+4	1.70E+1	2.01E-9	53.40	3.125E-10	1.922E+17	20.00	5.21E+17	-0.803214	0.0193	1
Cycle: 38 0.625 nM					6.25E-10		20.00	5.21E+17	0.88495		
Cycle: 39 1.25 nM					1.25E-9		20.00	5.21E+17	0.1522		
Cycle: 40 2.5 nM					2.5E-9		20.00	5.21E+17	0.1803		
Cycle: 41 5 nM					5.00E-9		20.00	5.21E+17	0.2688		
Cycle: 42 10 nM					1.00E-8		20.00	5.21E+17	0.5563		
Cycle: 43 20 nM					2.00E-8		20.00	5.21E+17	0.7709		
Cycle: 44 40 nM					4.00E-8		20.00	5.21E+17	1.621		

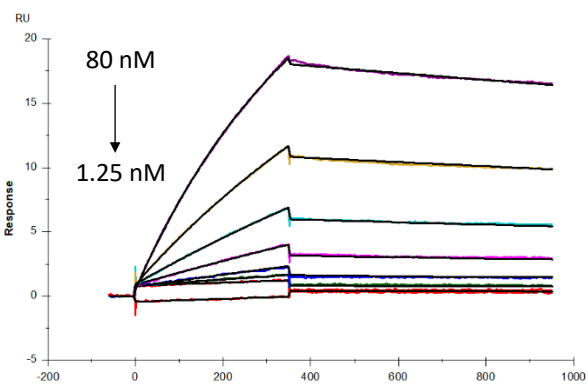


Curve	ka (1/Hz)	kd (1/s)	KD (M)	Rmax (RU)	Conc (M)	tc	Flow (ul/min)	kt (RU/Hz)	RI (RU)	Chi² (RU²)	U-value
Cycle: 34 1.25 nM	6.28E+4	1.80E+1	2.17E-9	58.31	1.25E-9	2.216E+17	20.00	6.01E+17	0.8208	6.32E-4	3
Cycle: 35 2.5 nM					2.50E-9		20.00	6.01E+17	0.8559		
Cycle: 36 5 nM					5.00E-9		20.00	6.01E+17	1.199		
Cycle: 37 10 nM					1.00E-8		20.00	6.01E+17	1.377		
Cycle: 38 20 nM					2.00E-8		20.00	6.01E+17	1.474		
Cycle: 39 40 nM					4.00E-8		20.00	6.01E+17	0.6323		
Cycle: 40 80 nM					8.00E-8		20.00	6.01E+17	0.4646		
Cycle: 41 1.25 nM					1.25E-9		20.00	6.01E+17	-0.66564		

PNA2-P3

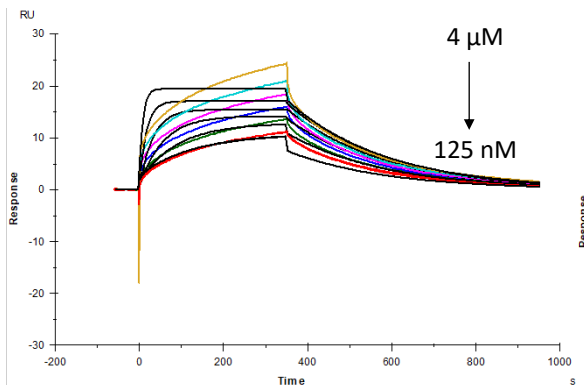


Curve	ka (1/Hz)	kd (1/s)	KD (M)	Rmax (RU)	Conc (M)	tc	Flow (ul/min)	kt (RU/Hz)	RI (RU)	Chi² (RU²)	U-value
Cycle: 24 1.25 nM	3.143E+4	1.519E+1	4.833E-9	30.71	1.25E-9	9.792E+14	20.00	2.65E+15	0.4590	0.0284	3
Cycle: 25 2.5 nM					2.50E-9		20.00	2.65E+15	0.4422		
Cycle: 26 5 nM					5.00E-9		20.00	2.65E+15	0.4740		
Cycle: 27 10 nM					1.00E-8		20.00	2.65E+15	0.5241		
Cycle: 28 20 nM					2.00E-8		20.00	2.65E+15	0.5343		
Cycle: 29 40 nM					4.00E-8		20.00	2.65E+15	0.6417		
Cycle: 30 80 nM					8.00E-8		20.00	2.65E+15	0.8215		
Cycle: 31 1.25 nM					1.25E-9		20.00	2.65E+15	-0.2055		

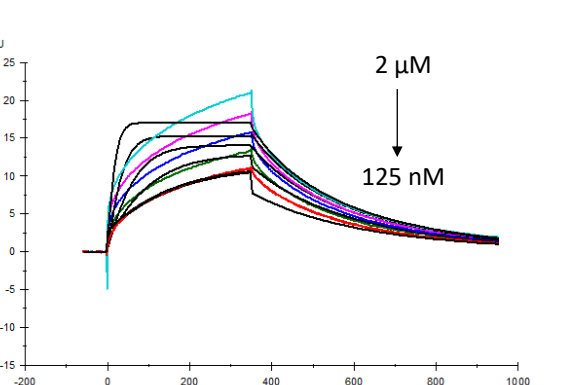


Curve	ka (1/Hz)	kd (1/s)	KD (M)	Rmax (RU)	Conc (M)	tc	Flow (ul/min)	kt (RU/Hz)	RI (RU)	Chi² (RU²)	U-value
Cycle: 54 1.25 nM	2.64E+4	1.542E+1	5.311E-9	32.85	1.25E-9	4.28E+15	20.00	1.163E+16	0.8124	0.0639	5
Cycle: 55 2.5 nM					2.50E-9		20.00	1.163E+16	0.8241		
Cycle: 56 5 nM					5.00E-9		20.00	1.163E+16	0.7278		
Cycle: 57 10 nM					1.00E-8		20.00	1.163E+16	0.8819		
Cycle: 58 20 nM					2.00E-8		20.00	1.163E+16	0.9424		
Cycle: 59 40 nM					4.00E-8		20.00	1.163E+16	0.8953		
Cycle: 60 80 nM					8.00E-8		20.00	1.163E+16	0.5166		
Cycle: 61 1.25 nM					1.25E-9		20.00	1.163E+16	-0.4483		

DNA8



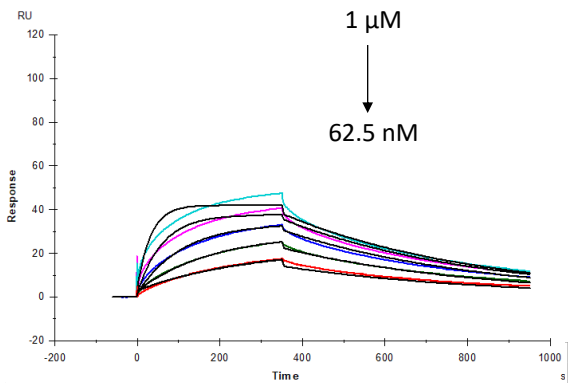
Curve	ka (1/Hz)	kd (1/s)	KD (M)	Rmax (RU)	Conc (M)	tc	Flow (ul/min)	kt (RU/Hz)	RI (RU)	Chi² (RU²)	U-value
Cycle: 4 1.25 nM	2.778E+4	0.004234	1.524E-7	17.95	1.25E-7	1.877E+8	20.00	5.095E+8	2.713	1.54	4
Cycle: 5 250 nM					2.50E-7		20.00	5.095E+8	1.657		
Cycle: 6 500 nM					5.00E-7		20.00	5.095E+8	0.4654		
Cycle: 7 1000 nM					1.00E-6		20.00	5.095E+8	-0.05186		
Cycle: 8 2000 nM					2.00E-6		20.00	5.095E+8	0.4380		
Cycle: 9 4000 nM					4.00E-6		20.00	5.095E+8	2.183		
Cycle: 10 1.25 nM					1.25E-7		20.00	5.095E+8	2.786		



Curve	ka (1/Hz)	kd (1/s)	KD (M)	Rmax (RU)	Conc (M)	tc	Flow (ul/min)	kt (RU/Hz)	RI (RU)	Chi² (RU²)	U-value
Cycle: 4 1.25 nM	4.10E+4	0.005440	1.326E-7	17.36	1.25E-7	3.52E+5	20.00	9.580E+5	2.643	0.944	4
Cycle: 5 250 nM					2.50E-7		20.00	9.580E+5	1.458		
Cycle: 6 500 nM					5.00E-7		20.00	9.580E+5	0.2073		
Cycle: 7 1000 nM					1.00E-6		20.00	9.580E+5	-0.1707		
Cycle: 8 2000 nM					2.00E-6		20.00	9.580E+5	0.6028		
Cycle: 9 1.25 nM					1.25E-7		20.00	9.580E+5	2.838		

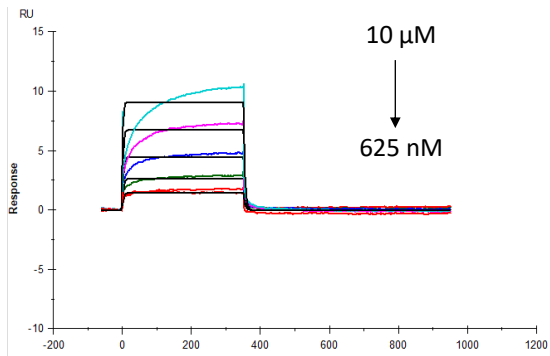
PNA3-AAm-Bt on chip A:A mismatch

PNA2-ach



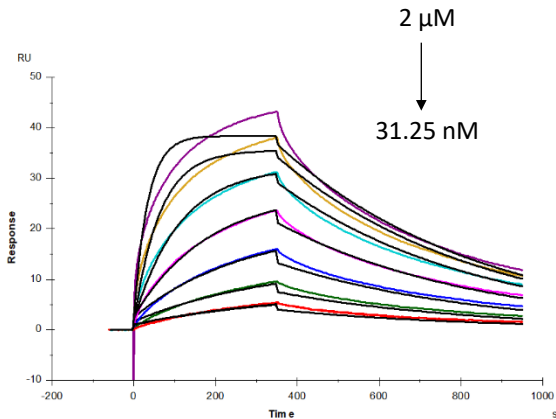
Curve	ka (1/Hz)	kd (1/s)	KD (M)	Rmax (RU)	Conc (M)	tc	Flow (ul/min)	kt (RU/Hz)	RI (RU)	Chi² (RU²)	U-value
Cycle: 12 62.5 nM	2.96E+4	0.002106	7.101E-8	40.91	6.250E-8	1.013E+7	20.00	2.749E+7	2.947	2.10	2
Cycle: 13 125 nM					1.250E-7		20.00	2.749E+7	2.937		
Cycle: 14 250 nM					2.500E-7		20.00	2.749E+7	1.822		
Cycle: 15 500 nM					5.000E-7		20.00	2.749E+7	1.875		
Cycle: 16 1000 nM					1.000E-6		20.00	2.749E+7	3.856		
Cycle: 17 62.5 nM					6.250E-8		20.00	2.749E+7	3.038		

DNA8



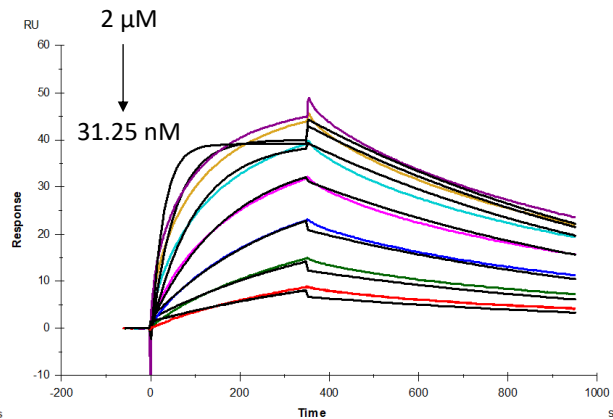
Curve	ka (1/Hz)	kd (1/s)	KD (M)	Rmax (RU)	Conc (M)	Chi² (RU²)	U-value
Cycle: 4 625 nM	4.941E+4	0.2582	5.225E-6	13.76	6.250E-7	0.320	N/A
Cycle: 5 1250 nM					1.250E-6		
Cycle: 6 2500 nM					2.500E-6		
Cycle: 7 5000 nM					5.000E-6		
Cycle: 8 10000 nM					1.000E-5		
Cycle: 9 625 nM					6.250E-7		

PNA2-H1



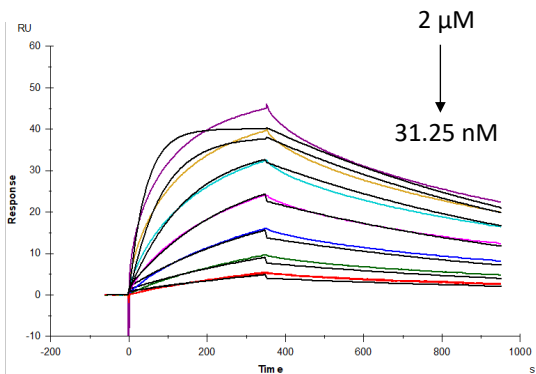
Curve	ka (1/Hz)	kd (1/s)	KD (M)	Rmax (RU)	Conc (M)	tc	Flow (ul/min)	kt (RU/Hz)	RI (RU)	Chi² (RU²)	U-value
Cycle: 34 31.25 nM	1.382E+4	0.002035	1.473E-7	39.49	3.125E-8	1.887E+13	20.00	5.122E+13	1.812	1.10	1
Cycle: 35 62.5 nM					6.250E-8		20.00	5.122E+13	1.482		
Cycle: 36 125 nM					1.250E-7		20.00	5.122E+13	2.445		
Cycle: 37 250 nM					2.500E-7		20.00	5.122E+13	2.559		
Cycle: 38 500 nM					5.000E-7		20.00	5.122E+13	1.762		
Cycle: 39 1000 nM					1.000E-6		20.00	5.122E+13	1.143		
Cycle: 40 2000 nM					2.000E-6		20.00	5.122E+13	1.638		
Cycle: 41 31.25 nM					3.125E-8		20.00	5.122E+13	1.108		

PNA-H3



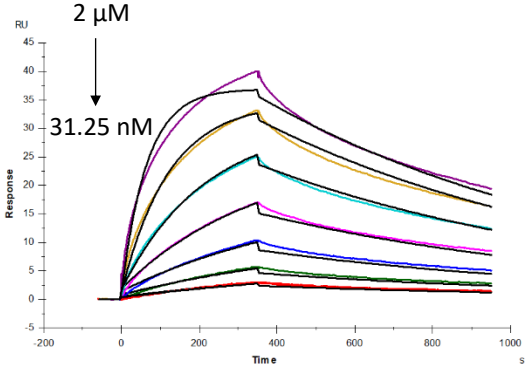
Curve	ka (1/Hz)	kd (1/s)	KD (M)	Rmax (RU)	Conc (M)	tc	Flow (ul/min)	kt (RU/Hz)	RI (RU)	Chi² (RU²)	U-value
Cycle: 44 31.25 nM	1.768E+4	0.001156	6.535E-8	45.90	3.125E-8	3.412E+14	20.00	9.262E+14	1.393	2.08	2
Cycle: 45 62.5 nM					6.250E-8		20.00	9.262E+14	1.938		
Cycle: 46 125 nM					1.250E-7		20.00	9.262E+14	2.007		
Cycle: 47 250 nM					2.500E-7		20.00	9.262E+14	0.9595		
Cycle: 48 500 nM					5.000E-7		20.00	9.262E+14	-1.182		
Cycle: 49 1000 nM					1.000E-6		20.00	9.262E+14	-3.058		
Cycle: 50 2000 nM					2.000E-6		20.00	9.262E+14	-5.325		
Cycle: 51 31.25 nM					3.125E-8		20.00	9.262E+14	-1.427		

PNA2-A3



Curve	ka (1/Hz)	kd (1/s)	KD (M)	Rmax (RU)	Conc (M)	tc	Flow (ul/min)	kt (RU/Hz)	RI (RU)	Chi² (RU²)	U-value
Cycle: 64 31.25 nM	1.112E+4	0.001085	9.761E-8	42.42	3.125E-8	1.978E+14	20.00	5.376E+14	0.9517	1.42	2
Cycle: 65 62.5 nM					6.250E-8		20.00	5.376E+14	1.430		
Cycle: 66 125 nM					1.250E-7		20.00	5.376E+14	1.895		
Cycle: 67 250 nM					2.500E-7		20.00	5.376E+14	1.841		
Cycle: 68 500 nM					5.000E-7		20.00	5.376E+14	0.7315		
Cycle: 69 1000 nM					1.000E-6		20.00	5.376E+14	-0.4545		
Cycle: 70 2000 nM					2.000E-6		20.00	5.376E+14	-0.3459		
Flush: 71 31.25 nM					3.125E-8		20.00	5.376E+14	0.8644		

PNA-P3



Curve	ka (1/Hz)	kd (1/s)	KD (M)	Rmax (RU)	Conc (M)	tc	Flow (ul/min)	kt (RU/Hz)	RI (RU)	Chi² (RU²)	U-value
Cycle: 54 31.25 nM	7115	0.001104	1.552E-7	38.41	3.125E-8	7.363E+13	20.00	1.999E+14	0.4922	0.489	1
Cycle: 55 62.5 nM					6.250E-8		20.00	1.999E+14	0.8493		
Cycle: 56 125 nM					1.250E-7		20.00	1.999E+14	1.441		
Cycle: 57 250 nM					2.500E-7		20.00	1.999E+14	1.958		
Cycle: 58 500 nM					5.000E-7		20.00	1.999E+14	1.718		
Cycle: 59 1000 nM					1.000E-6		20.00	1.999E+14	1.187		
Cycle: 60 2000 nM					2.000E-6		20.00	1.999E+14	1.115		
Cycle: 61 31.25 nM					3.125E-8		20.00	1.999E+14	0.3318		

PNA2-N3

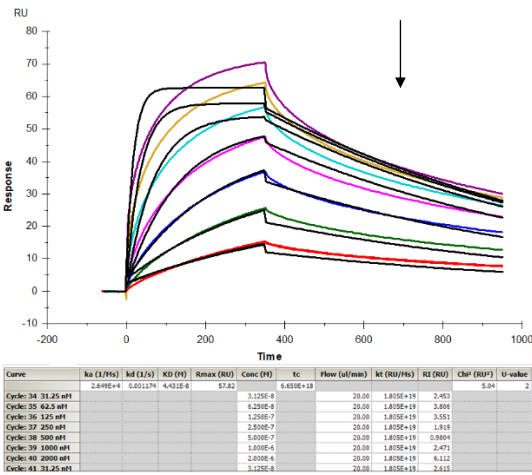
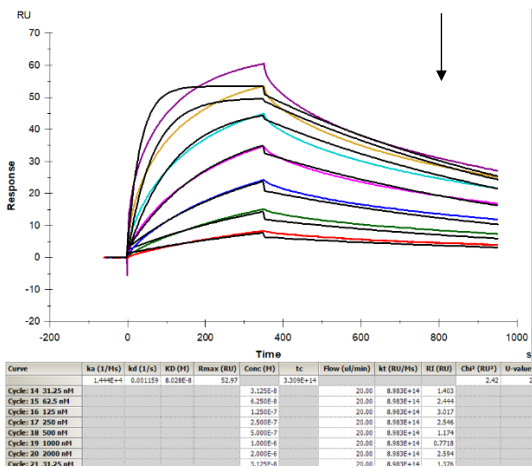
2 µM

31.25 nM

PNA-G3

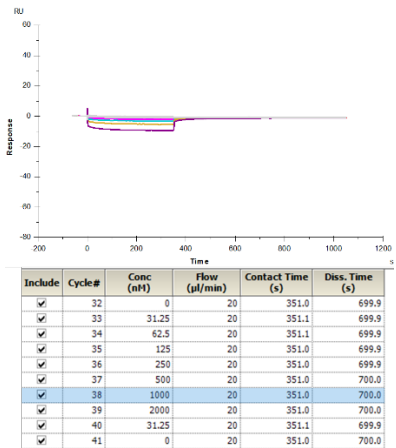
2 µM

31.25 nM

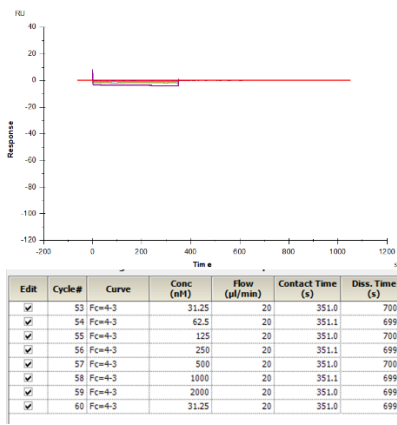


DNA7-Bt on chip A: A mismatch (No binding observed at the concentrations tested)

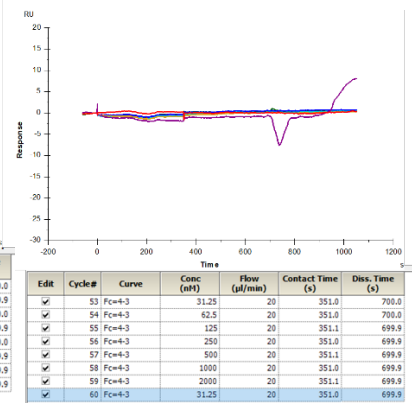
PNA2-H3



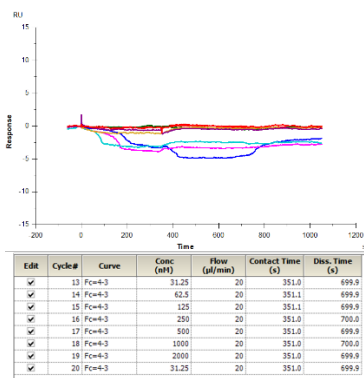
PNA2-A3



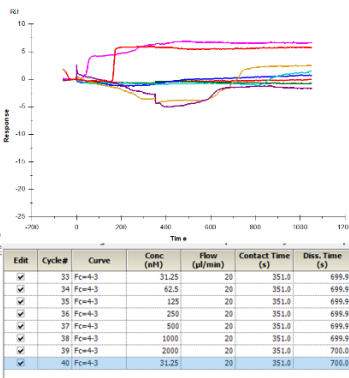
PNA2-P3



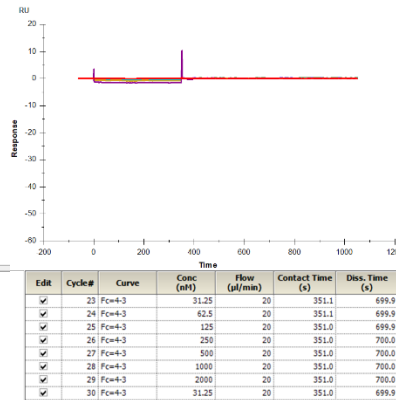
PNA2-N3



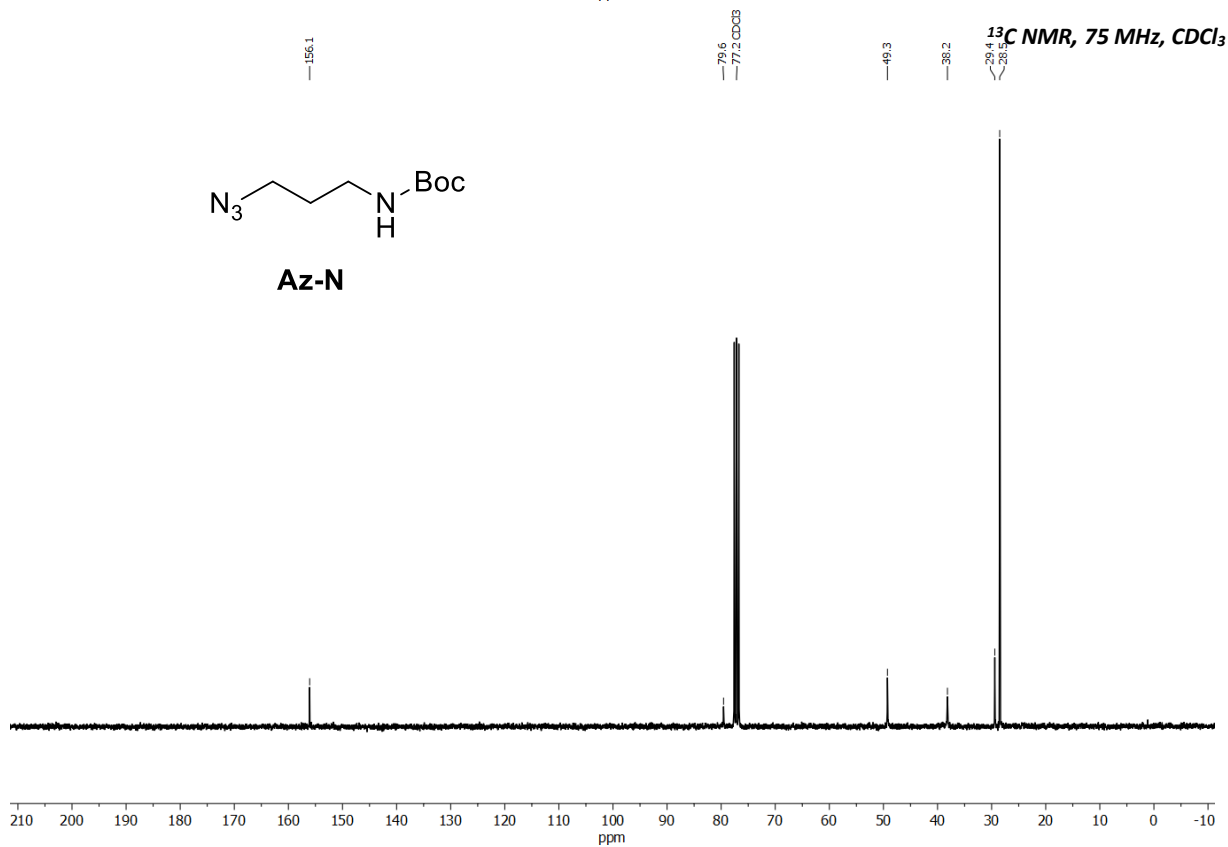
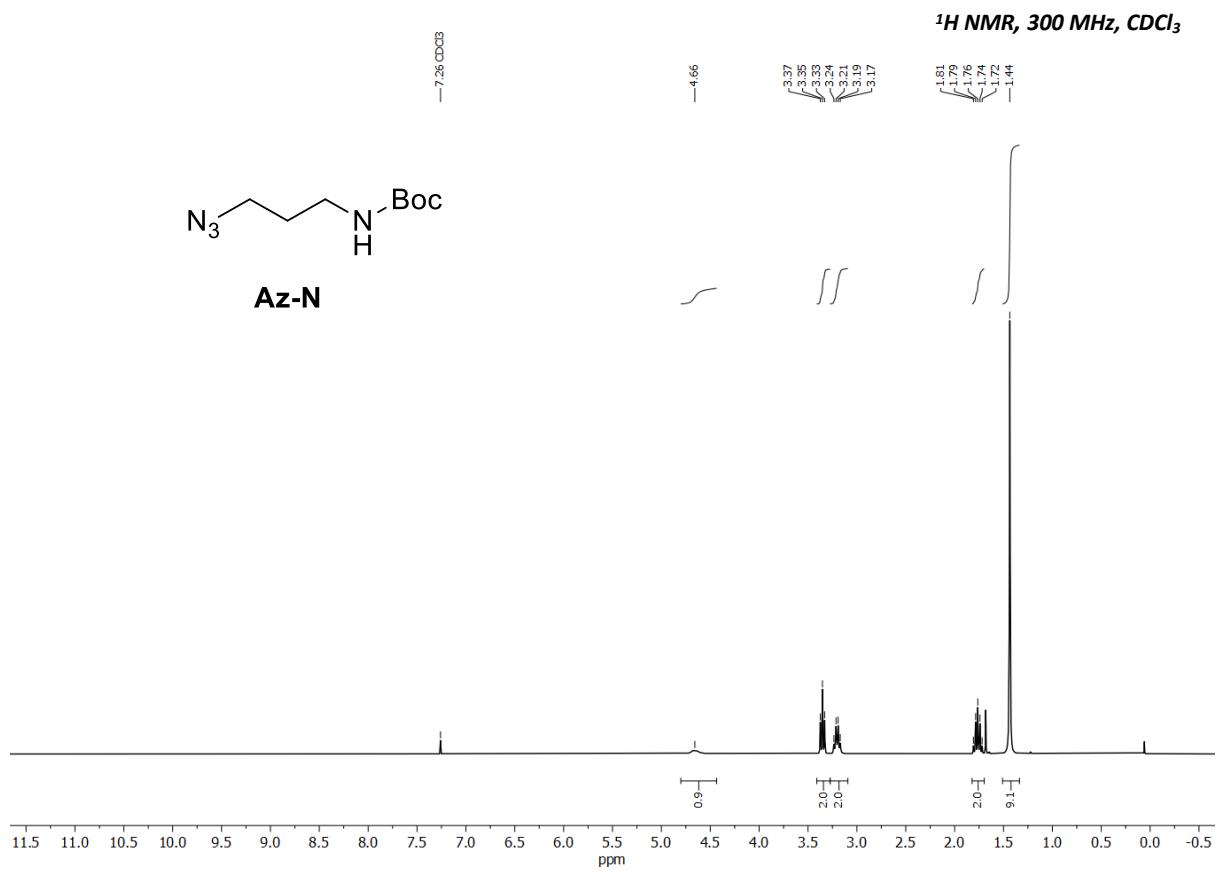
PNA2-G3

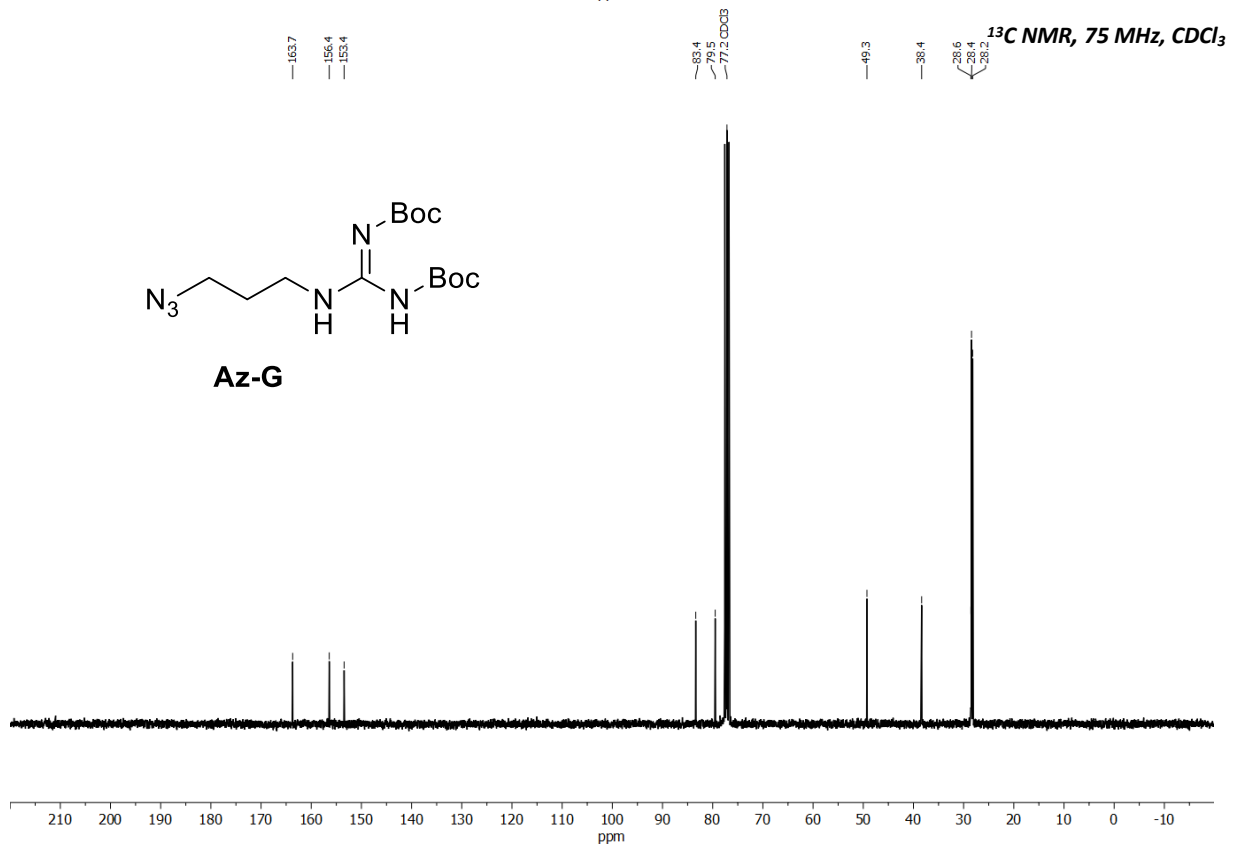
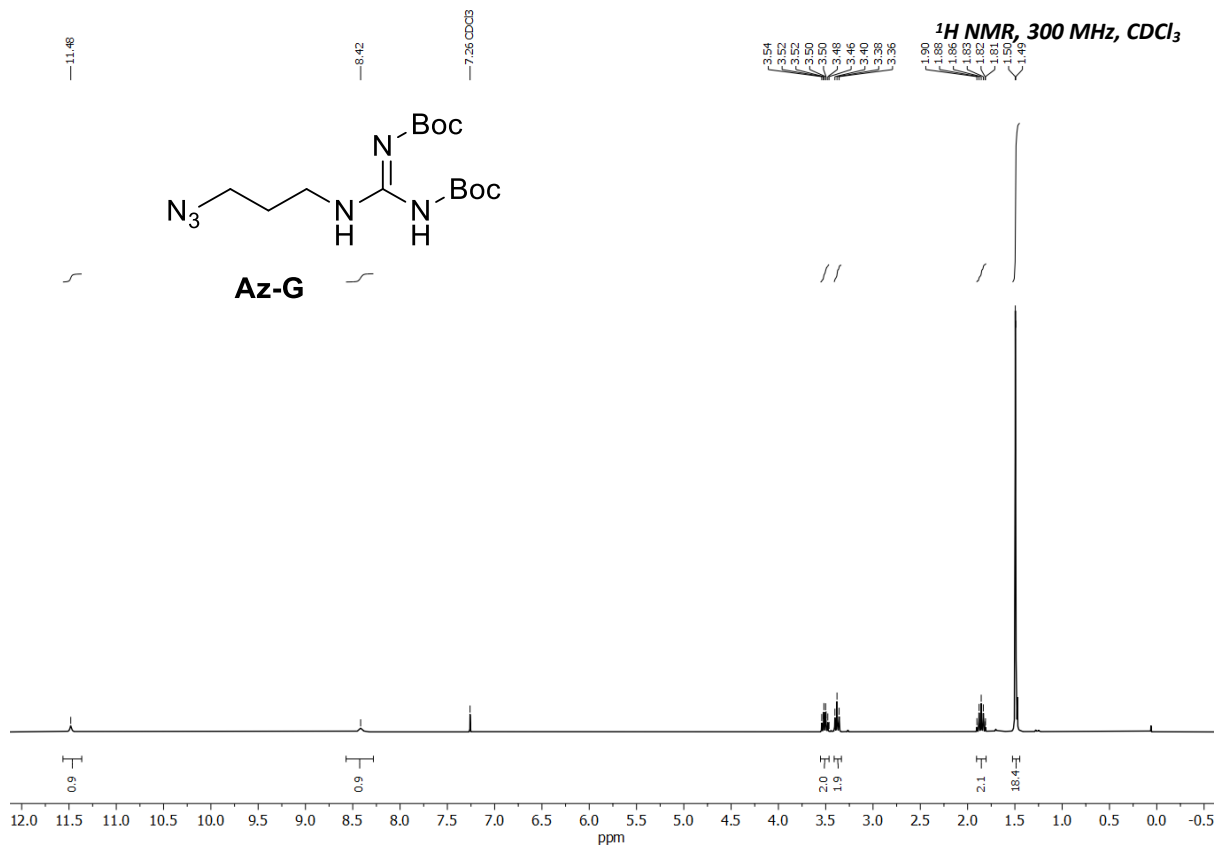


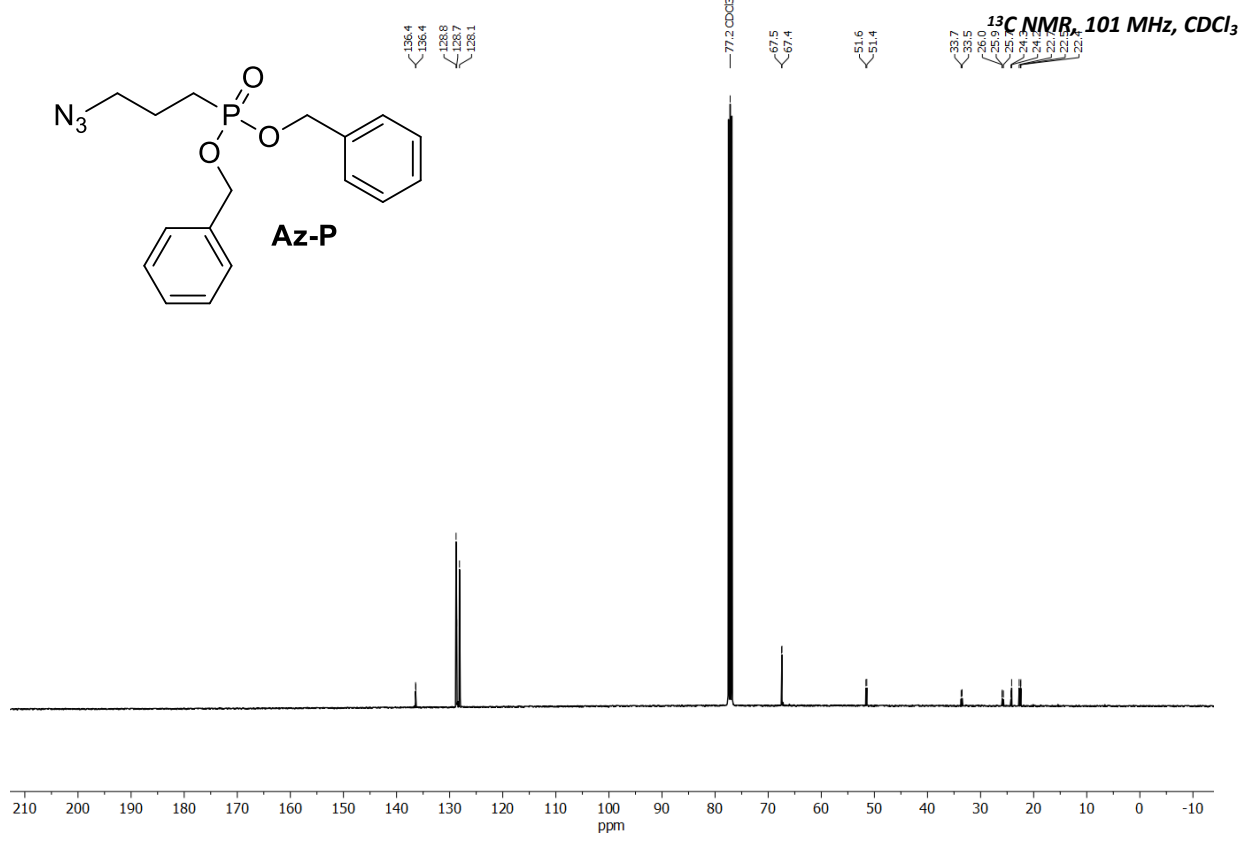
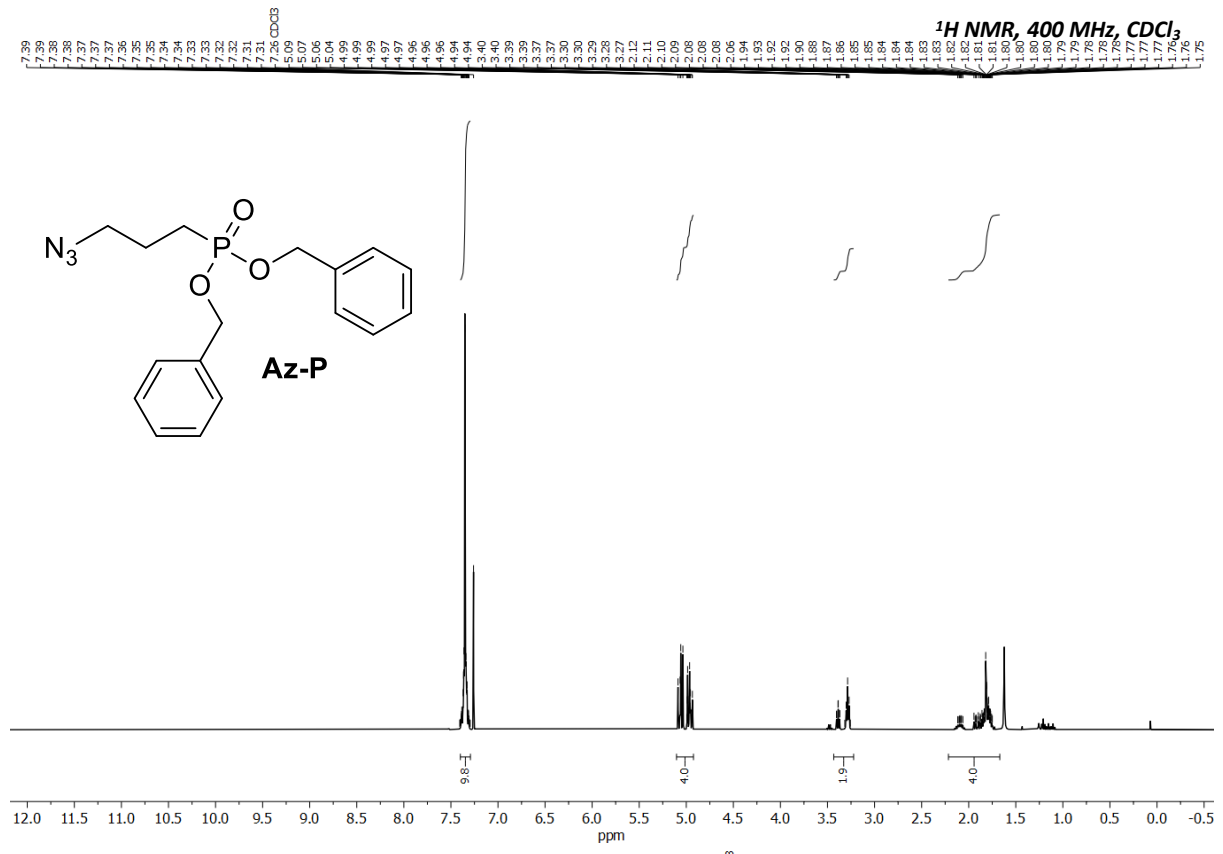
PNA2-H1

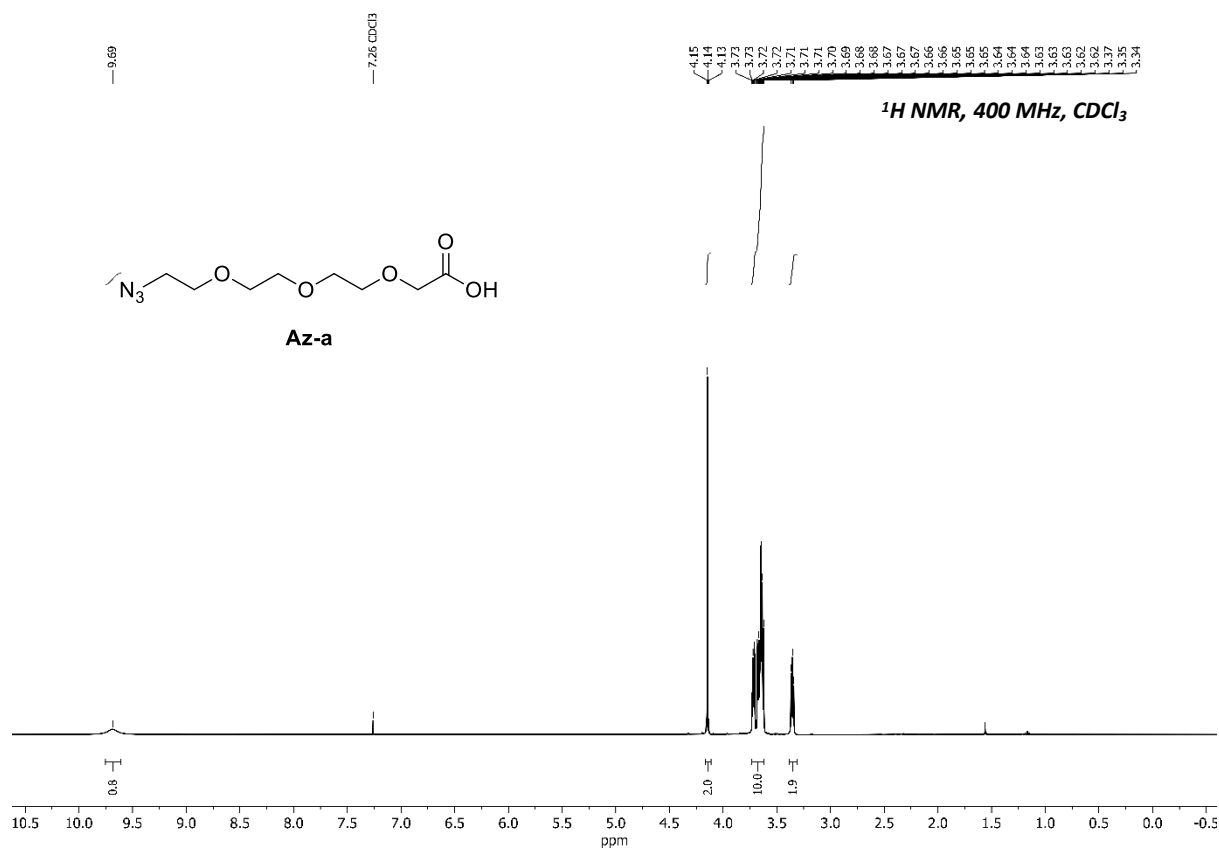


Copies of the ^1H and ^{13}C NMR spectra for compounds Az-A/H/N/G/P









References

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