

Supplemental Information

Elucidating Sequence-Assembly Relationships for Bilingual PNA Biopolymers

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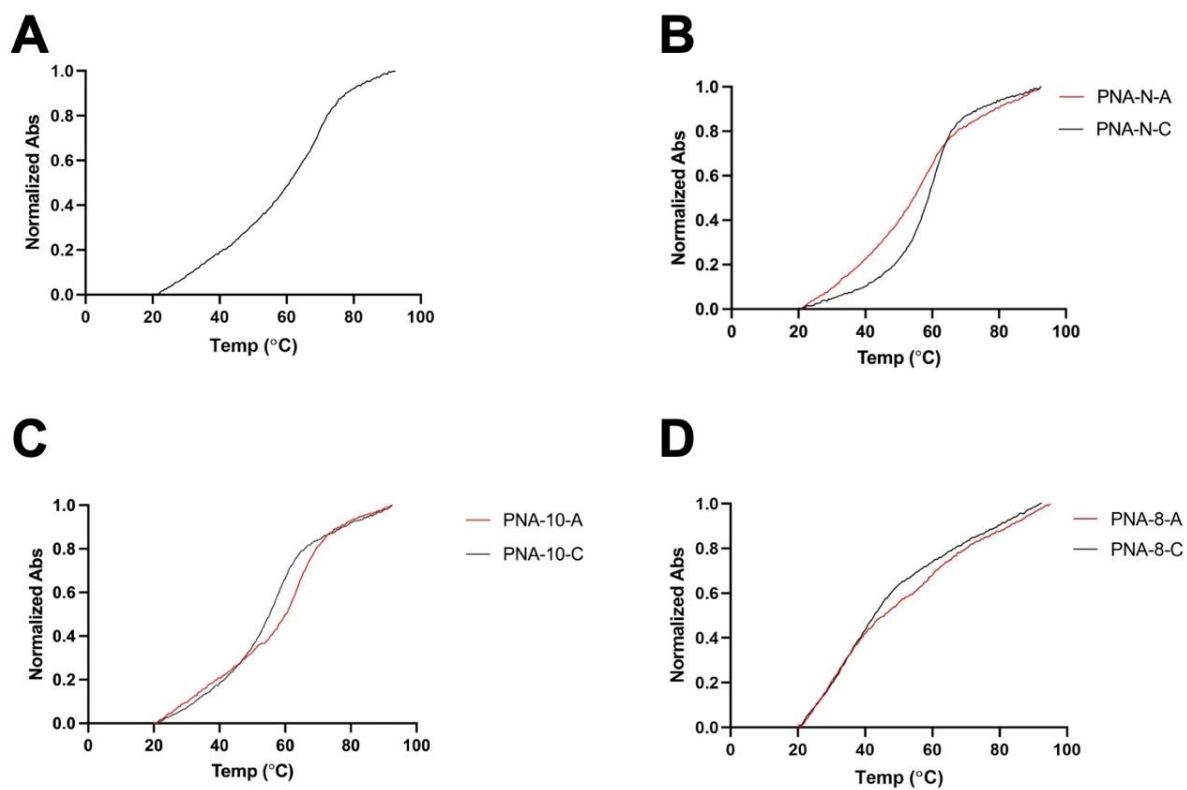


Fig S1 UV-Vis melting curves using normalized absorbance. PNA samples were prepared at 3 μ M in 1X PBS with 3 μ M of DNA, final concentrations. (A) PNA-B-A. (B) PNA-N-A and PNA-N-C. (C) PNA-10-A and PNA-10-C. (D) PNA-8-A and PNA-8-C.

Table S1 Melting temperature measurements using normalized absorbance using DNA

Strand	Melt Temp (°C)
PNA-B-A	61.96 ± 0.92
PNA-N-C	58.11 ± 0.09
PNA-N-A	55.74 ± 0.38
PNA-10-C	54.32 ± 0.33
PNA-10-A	60.1 ± 0.73
PNA-8-C	45.97 ± 1.4
PNA-8-A	48.08 ± 1.11

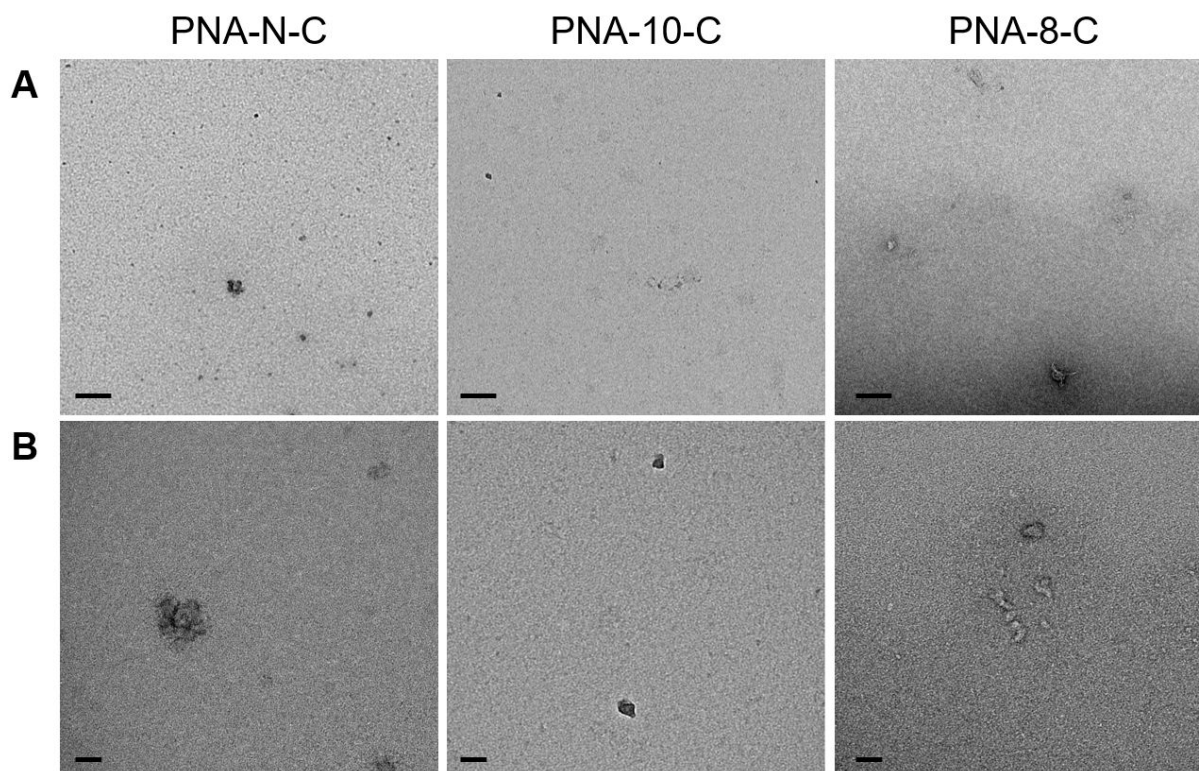


Fig S2. TEM images of PNA-N-C, PNA-10-C, and PNA-8-C assembled in water at 100 μ M. A) Scale bar = 200 nm. B) Scale bar = 50 nm.

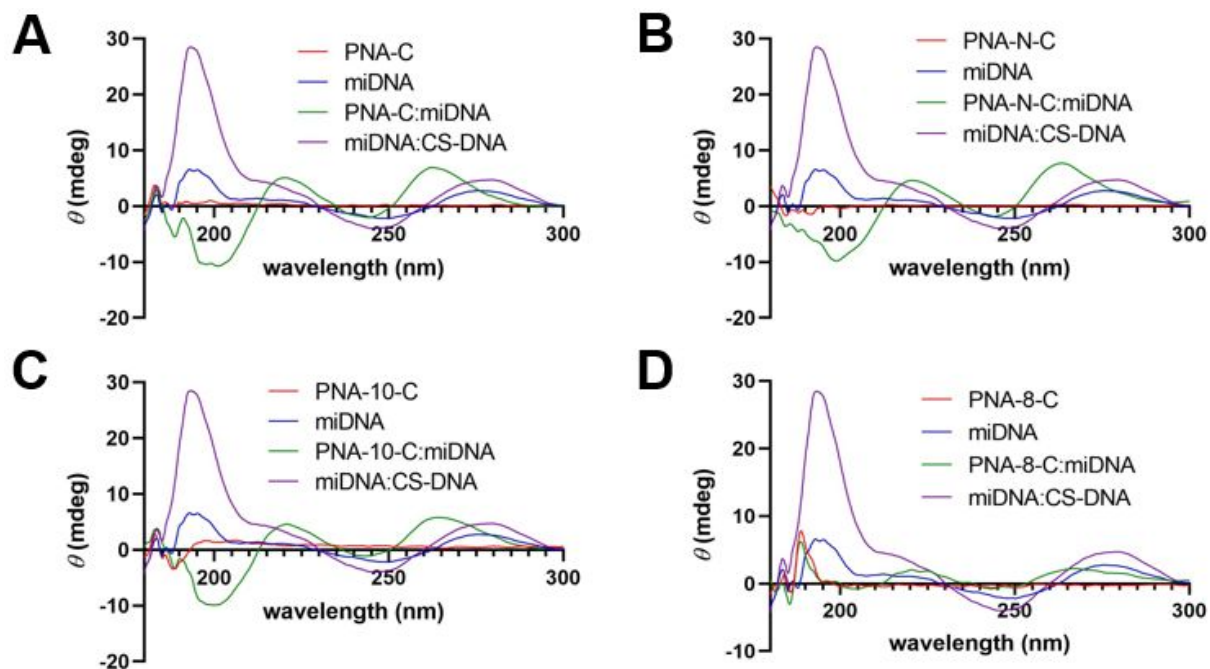


Fig S3 CD Spectroscopy of A) PNA-C B) PNA-N-C C) PNA-10-C, and D) PNA-8-C in 1x PBS at 100 μ M to demonstrate the change in maxima and minima up on the addition of DNA.

Table S2 Average Size of PNA Assembly Particles using DLS

Strand	Diameter
PNA-B-A	107.8 ± 47.0 nm
PNA-N-C	1.3 ± 0.1 nm 127.1 ± 36.3 nm
PNA-N-A	161.7 ± 44.4 nm
PNA-10-C	1.6 ± 0.3 nm 191.9 ± 79.1 nm
PNA-10-A	58.9 ± 17.8 nm
PNA-8-C	1.5 ± 0.3 nm 80.4 ± 22.8 nm
PNA-8-A	70.0 ± 43.1 nm

All sizes reported

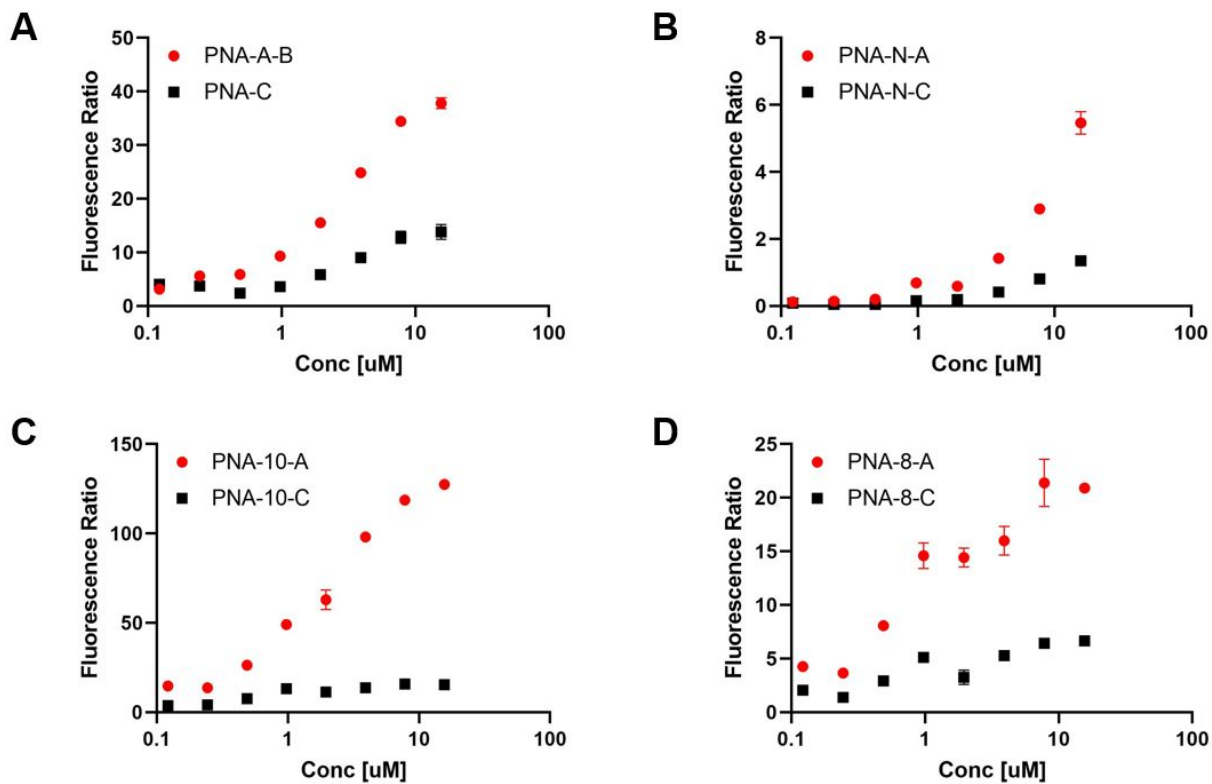


Fig S4 Fluorescence Ratio studies as a function of concentration, testing amphiphilic and control PNA sequences in. Top left: PNA-A-B and PNA-C; Top right: PNA-N-A and PNA-N-C; Bottom left: PNA-10-A and PNA-10-C; Bottom right: PNA-8-A and PNA-8-C. Samples tested in 1%DMSO/water.

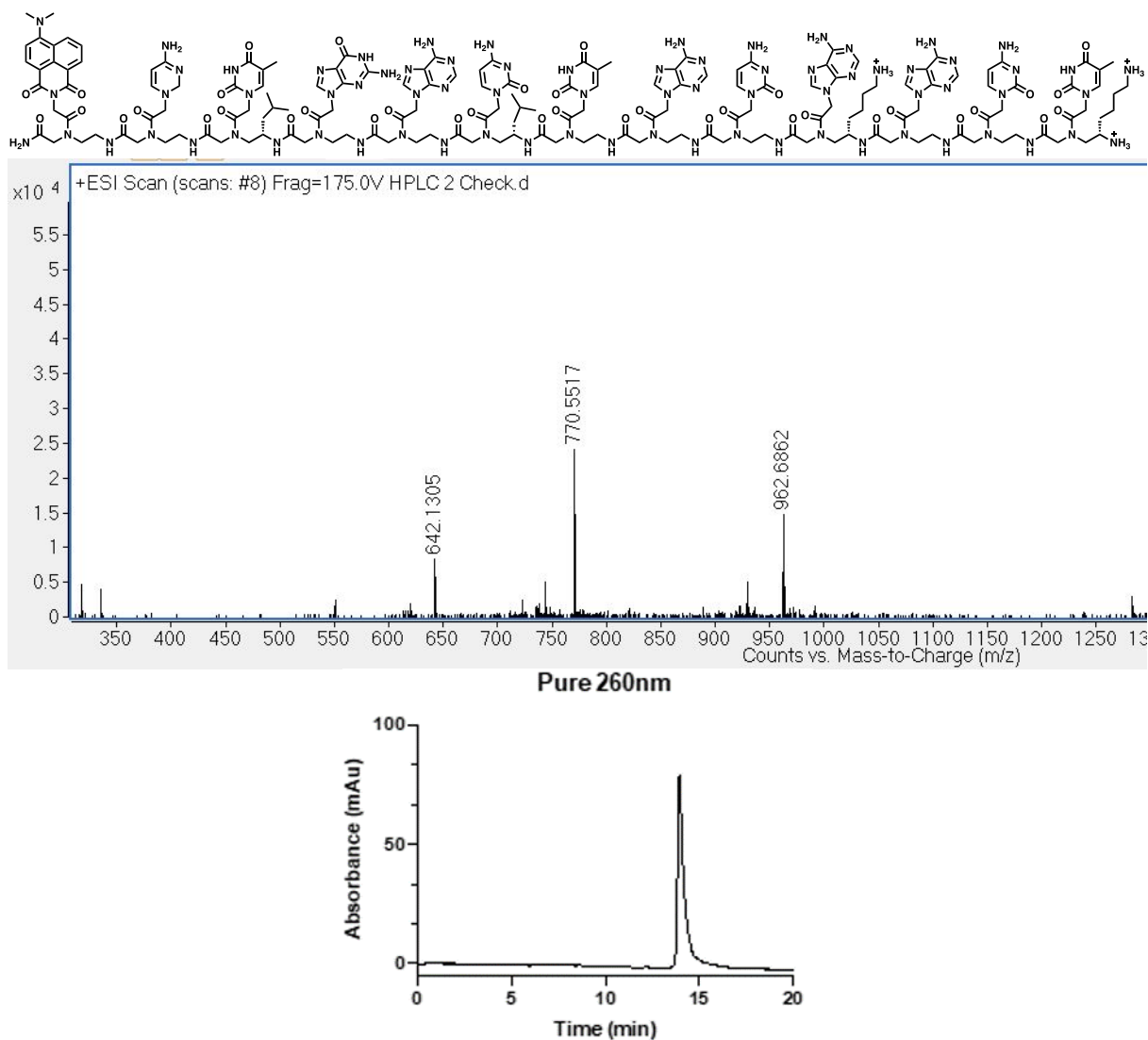


Fig S5 The chemical structure of PNA-B-A. The mass of the sequence was confirmed using ESI-TOF mass spectrometry and purified using RP-HPLC.

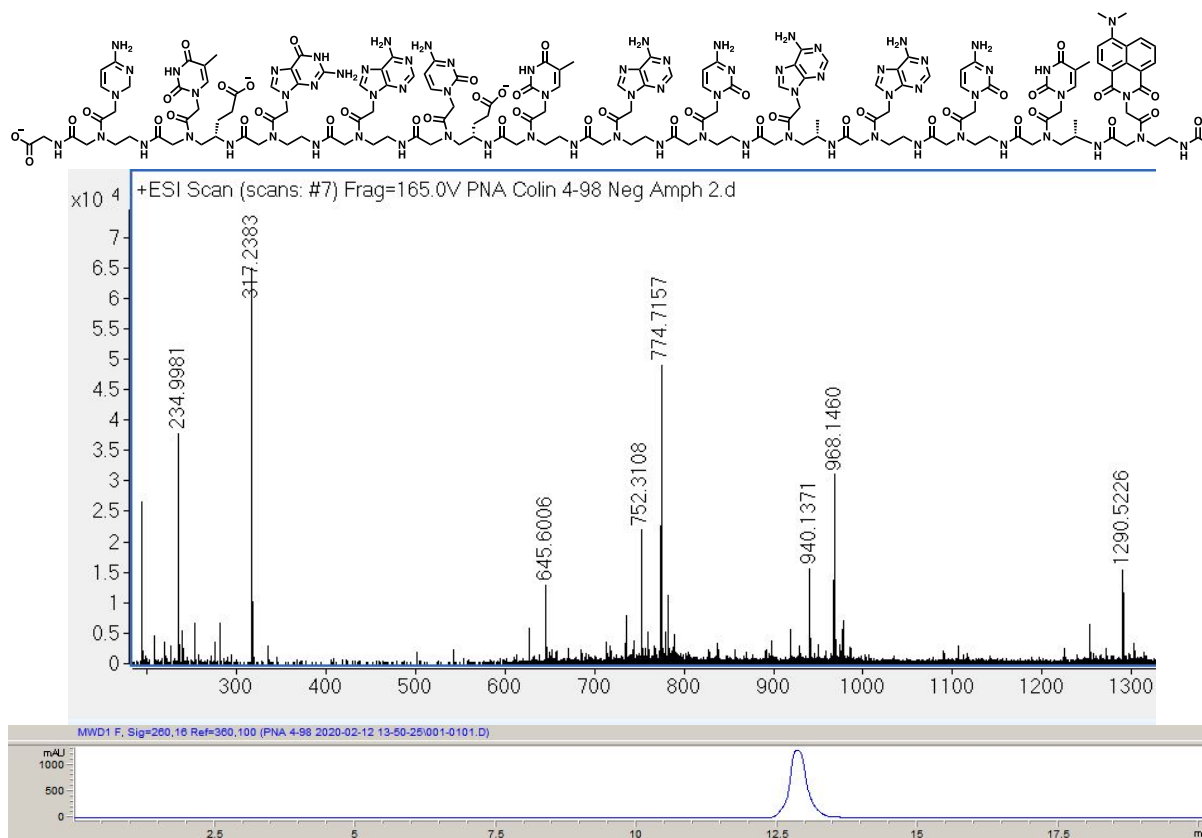


Fig S6 The chemical structure of PNA-N-A. The mass of the sequence was confirmed using ESI-TOF mass spectrometry and purified using RP-HPLC.

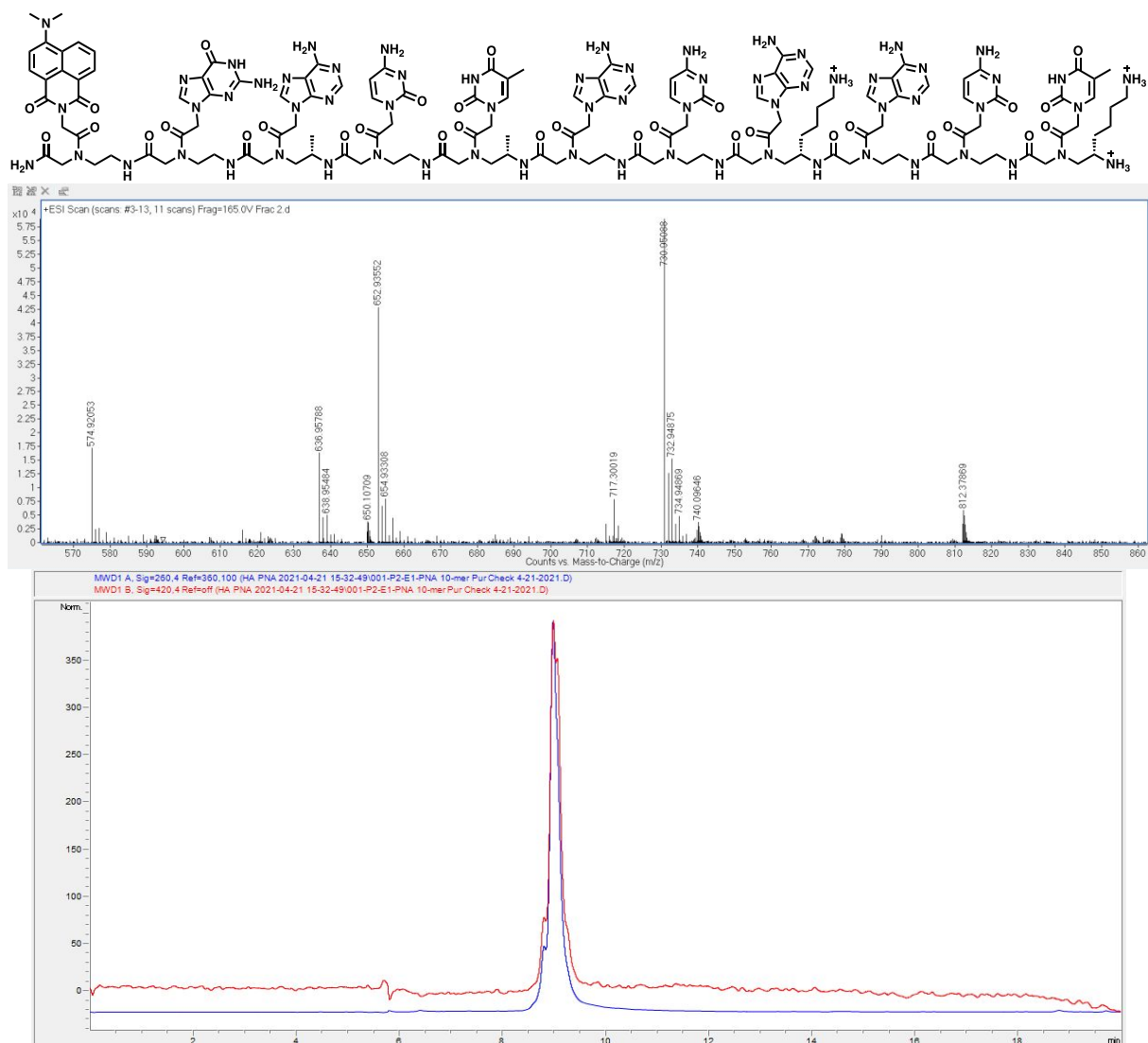


Fig S7 The chemical structure of PNA-10-A. The mass of the sequence was confirmed using ESI-TOF mass spectrometry and purified using RP-HPLC.

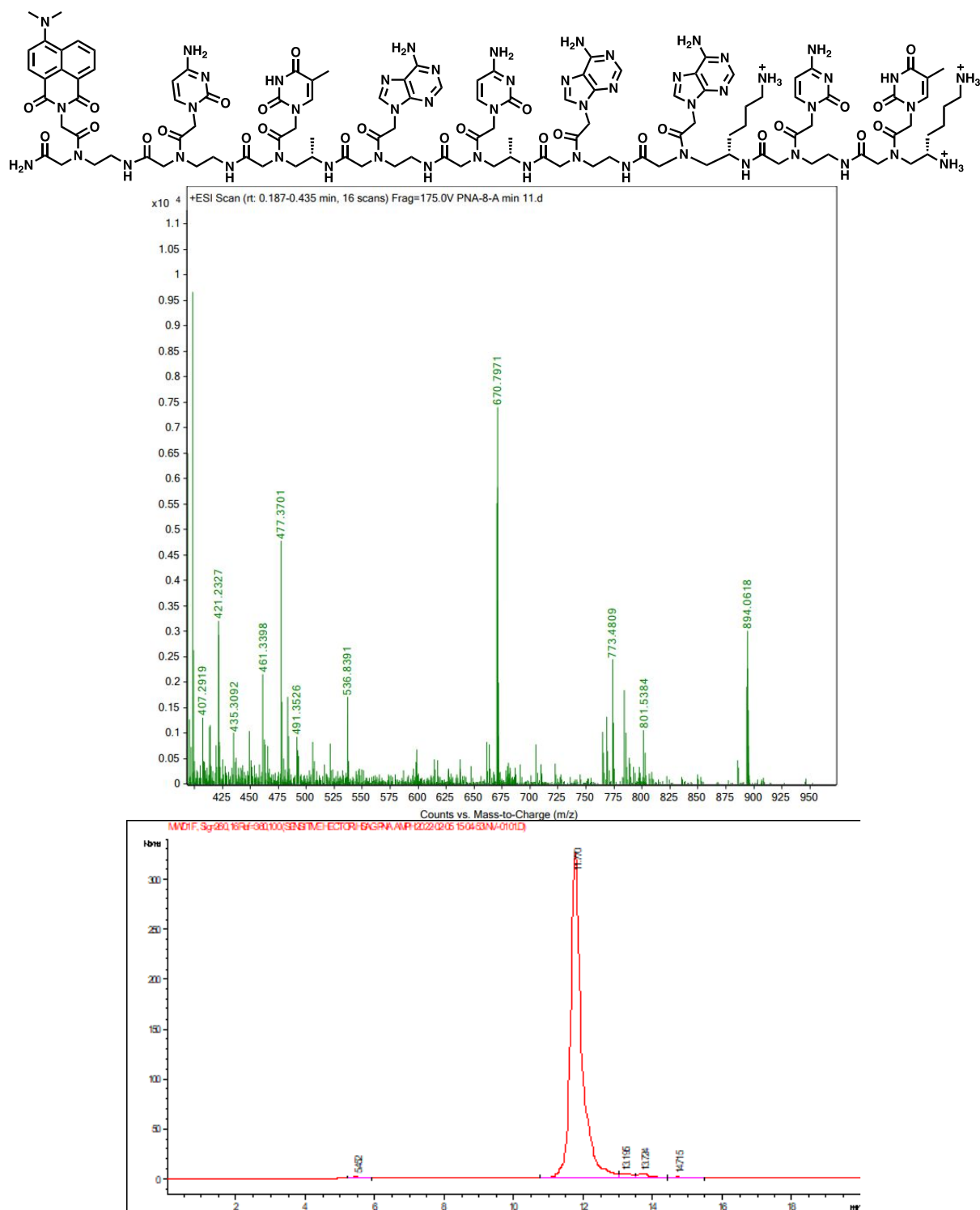


Fig S8 The chemical structure of PNA-8-A. The mass of the sequence was confirmed using ESI-TOF mass spectrometry and purified using RP-HPLC.

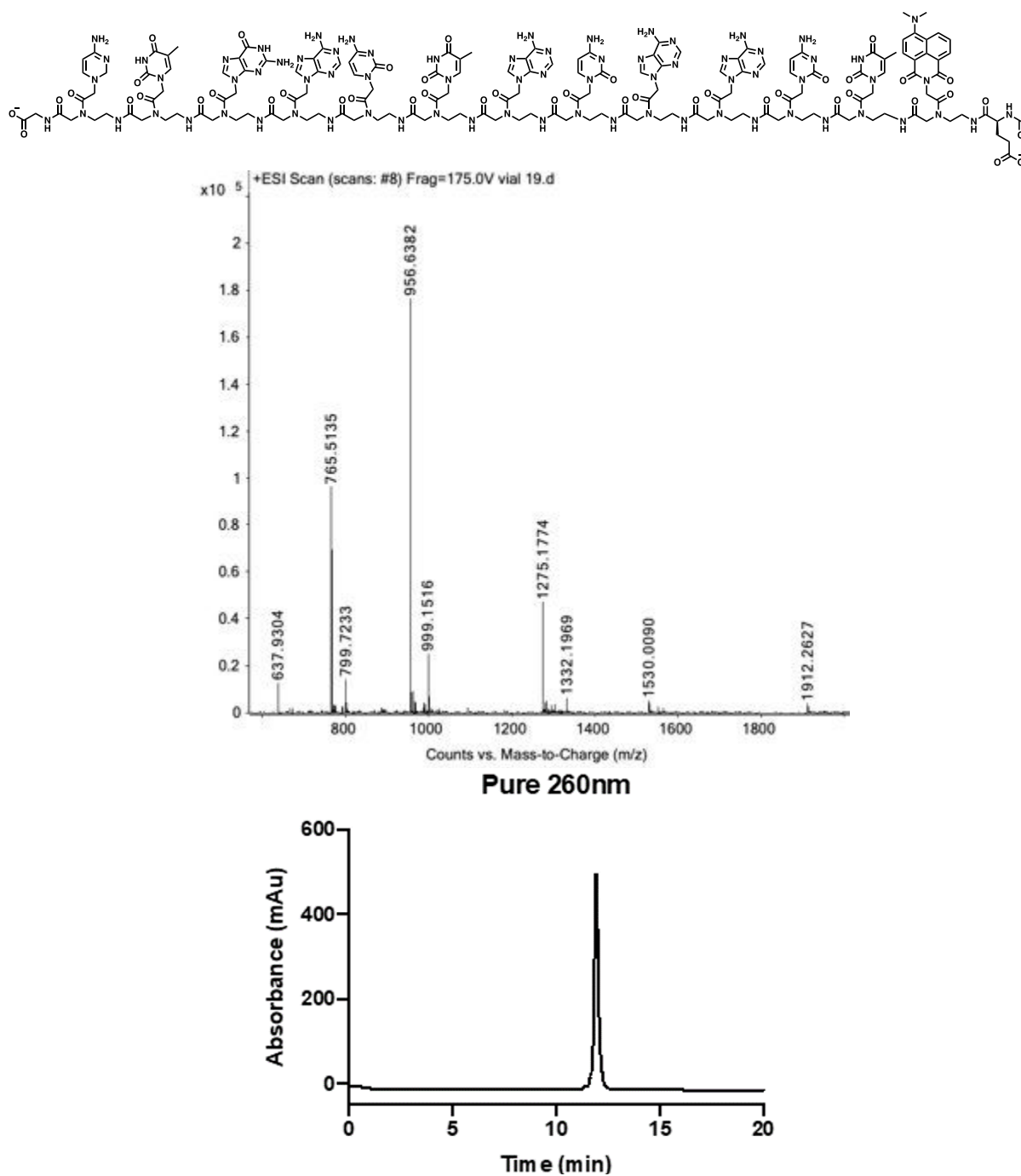


Fig S9 The chemical structure of PNA-N-C. The mass of the sequence was confirmed using ESI-TOF mass spectrometry and purified using RP-HPLC.

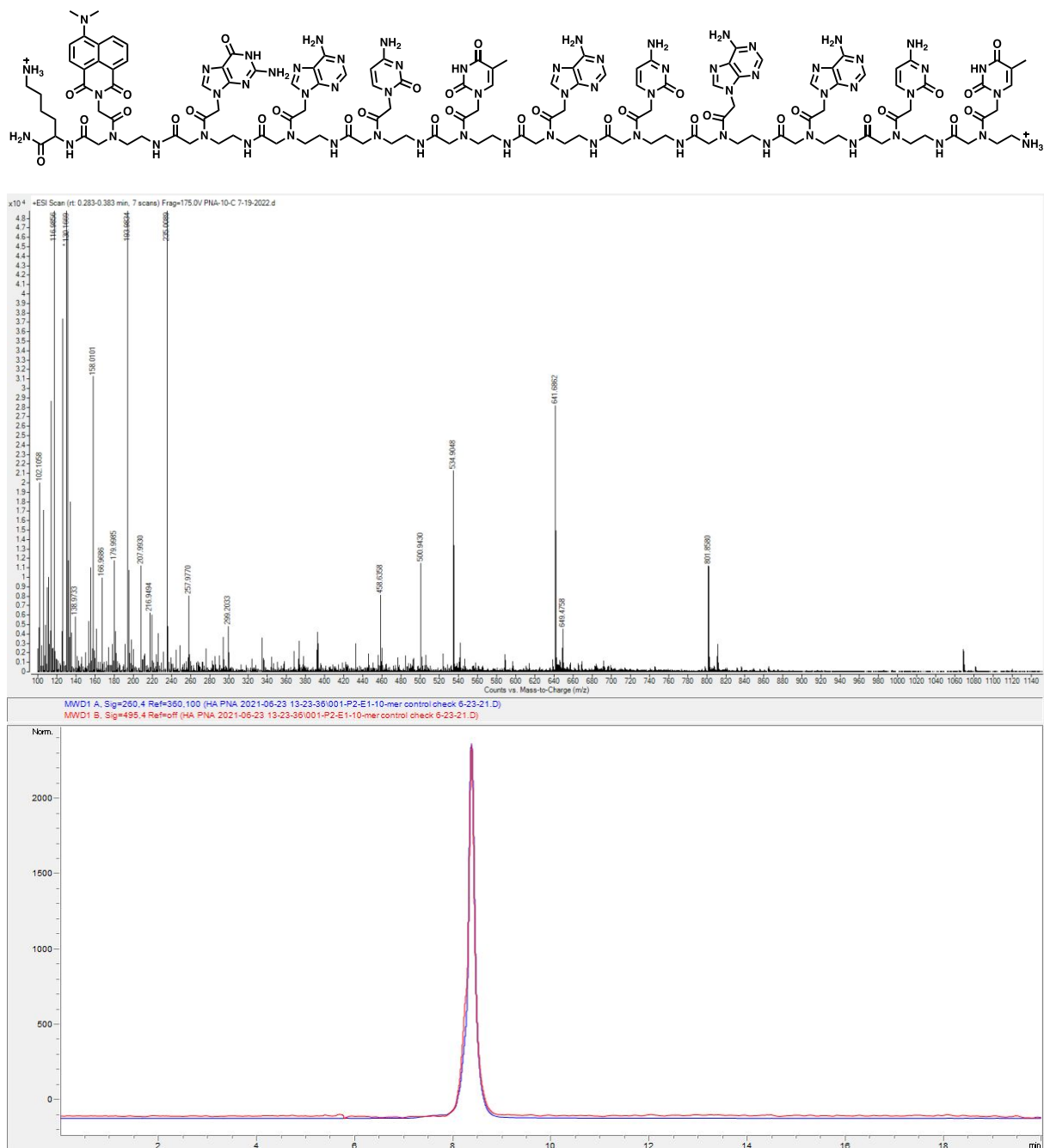


Fig S10 The chemical structure of PNA-10-C. The mass of the sequence was confirmed using ESI-TOF mass spectrometry and purified using RP-HPLC.

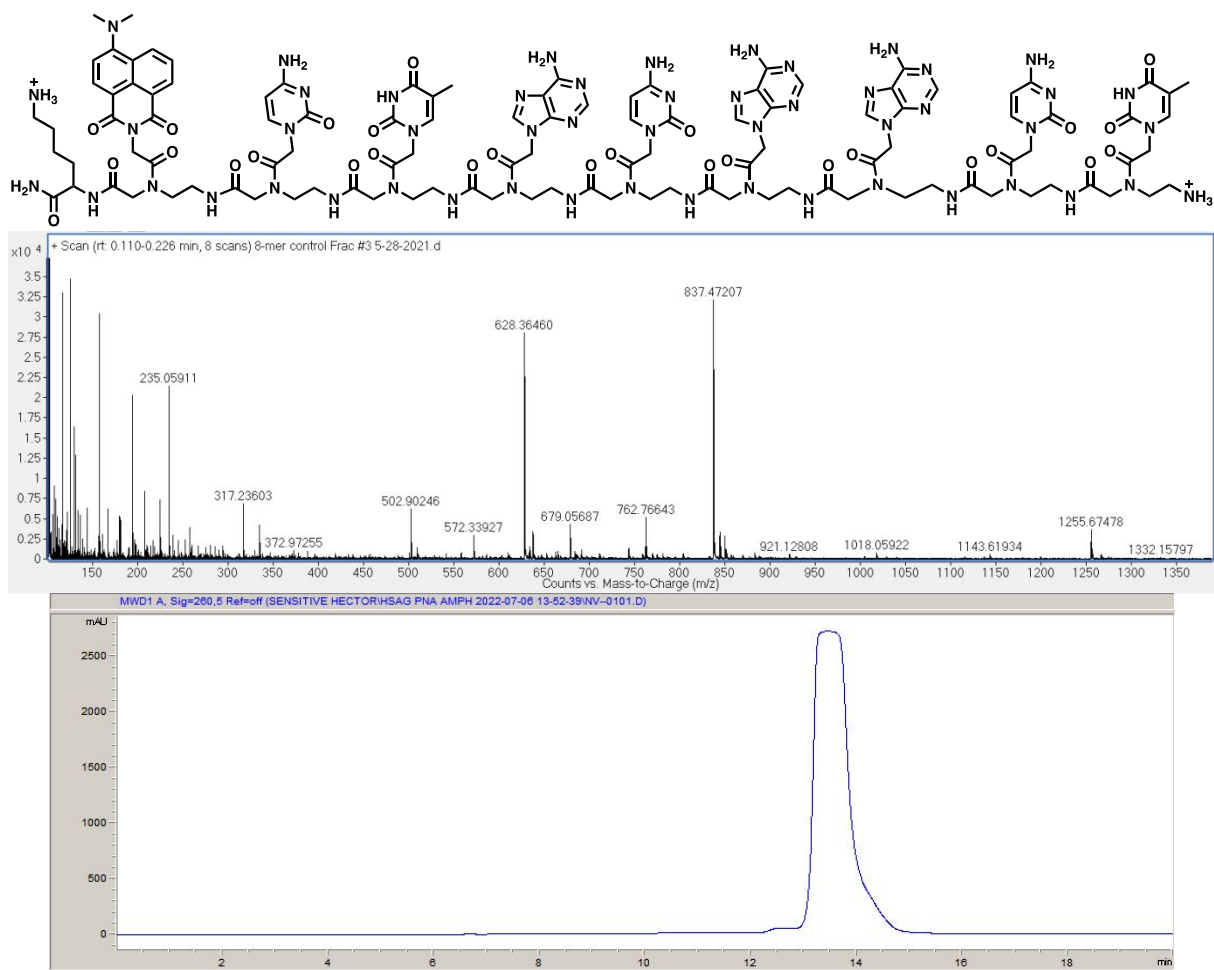


Fig S11 The chemical structure of PNA-8-C. The mass of the sequence was confirmed using ESI-TOF mass spectrometry and purified using RP-HPLC.

Table S3 PNA sequence, expected mass, and found mass

Strand	Expected Mass (M+3) ³⁺	Found Mass (M+3) ³⁺
PNA-B-A	962.212	962.686
PNA-N-C	955.943	956.638
PNA-N-A*	1288.572*	1290.523*
PNA-10-C	801.123	801.858
PNA-10-A	811.882	812.379
PNA-8-C	627.777	628.365
PNA-8-A	670.321	670.979

*Indicates mass expected and found were (M+2)²⁺