Supporting Information

for

Synthesis and optical properties of pyrroldinyl peptide nucleic acid carrying a clicked Nile red label

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NMR spectra, HPLC chromatogram, mass spectra and additional spectroscopic data
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Figure S8: (a) UV-vis and (b) fluorescence spectra of 10mer-Nr in MeCN-buffer (10 mM sodium phosphate, pH 7.0): 0% MeCN (black), 20% MeCN (blue), 50% MeCN (green), 100% MeCN (red). All spectra were measured at $[1] = 1.0 \, \mu \text{M}$, $\lambda_{\text{ex}} = 580$ nm, 700 PMT.
Figure S9: (a) UV-vis and (b) fluorescence spectra of 10mer-Nr: single stranded (black dotted), with 5'-d(AGTGATCTAC)-3' (blue), with 5'-d(AGTGTCTCTAC)-3' (red), with 5'-d(AGTCATCTAC)-3' (brown), with 5'-d(AGTGACCTAC)-3' (pink). All spectra were measured in 10 mM sodium phosphate buffer pH 7.0, [PNA] = 1.0 μM, [DNA] = 1.2 μM, λ_{ex} = 580 nm, 700 PMT.

Figure S10: (a) UV-vis and (b) fluorescence spectra of 10mer-Nr: single stranded (black dotted), with 5'-d(AGTGATCTAC)-3' (blue), with 5'-d(AGTGTCTCTAC)-3' (red), with 5'-d(AGTCATCTAC)-3' (brown), with 5'-d(AGTGACCTAC)-3' (pink), with 5'-d(AGTGATTCTAC)-3' (orange). All spectra were measured in 10 mM sodium phosphate buffer pH 7.0, [PNA] = 1.0 μM, [DNA] = 1.2 μM, λ_{ex} = 580 nm, 700 PMT.
Figure S11: (a) UV-vis and (b) fluorescence spectra of 10mer-Nr: single stranded (black dotted), with 5’-d(AGTGATCTAC)-3’ (blue), with 5’-d(AGTGACTCTAC)-3’ (red), with 5’-d(AGTCGATCTAC)-3’ (brown), with 5’-d(AGTGATCCTAC)-3’ (pink). All spectra were measured in 10 mM sodium phosphate buffer pH 7.0, [PNA] = 1.0 μM, [DNA] = 1.2 μM, λ<sub>ex</sub> = 580 nm, 700 PMT.

Figure S12: (a) UV-vis and (b) fluorescence spectra of 10mer-Nr: single stranded (black dotted), with 5’-d(AGTGATCTAC)-3’ (blue), with 5’-d(AGTGACTCTAC)-3’ (red), with 5’-d(AGTGCCCTCTAC)-3’ (brown), with 5’-d(AGTGACCCCTAC)-3’ (pink), with 5’-d(AGTGACTCCAC)-3’ (orange). All spectra were measured in 10 mM sodium phosphate buffer pH 7.0, [PNA] = 1.0 μM, [DNA] = 1.2 μM, λ<sub>ex</sub> = 580 nm, 700 PMT.
Figure S13: (a) UV-vis and (b) fluorescence spectra of 11merAA-Nr: single stranded (black dotted), with 5'-d(CGTATTTTATG)-3' (blue) and with 5'-d(CGTATTCTTTATG)-3' (red). All spectra were measured in 10 mM sodium phosphate buffer pH 7.0, [PNA] = 1.0 μM, [DNA] = 1.2 μM, λ_{ex} = 580 nm, 700 PMT.

Figure S14: (a) UV-vis and (b) fluorescence spectra of 11merCC-Nr: single stranded (black dotted), with 5'-d(CGTATAATATG)-3' (blue) and with 5'-d(CGTATACATATG)-3' (red). All spectra were measured in 10 mM sodium phosphate buffer pH 7.0, [PNA] = 1.0 μM, [DNA] = 1.2 μM, λ_{ex} = 580 nm, 700 PMT.
Figure S15: (a) UV-vis and (b) fluorescence spectra of 11merGG-Nr: single stranded (black dotted), with 5'-d(CGTATCCTATG)-3' (blue) and with 5'-d(CGTATCCCTATG)-3' (red). All spectra were measured in 10 mM sodium phosphate buffer pH 7.0, [PNA] = 1.0 µM, [DNA] = 1.2 µM, λ_ex = 580 nm, 700 PMT.

Figure S16: (a) UV-vis and (b) fluorescence spectra of 11merTT-Nr: single stranded (black dotted), with 5'-d(CGTATAATATG)-3' (blue) and with 5'-d(CGTATACATATG)-3' (red). All spectra were measured in 10 mM sodium phosphate buffer pH 7.0, [PNA] = 1.0 µM, [DNA] = 1.2 µM, λ_ex = 580 nm, 700 PMT.
Figure S17: (a) UV-vis and (b) fluorescence spectra of 10mer-Nr and its DNA hybrids before (---) and after (—) addition of β-cyclodextrin (10 mM): single stranded (black), with 5’-d(AGTGATCTAC)-3’ (blue), 5’-d(AGTGCTCTAC)-3’ (red), with 5’-d(AGTGACTCTAC)-3’ (green). All spectra were measured in 10 mM sodium phosphate buffer pH 7.0, [PNA] = 1.0 μM, [DNA] = 1.2 μM, λex = 580 nm, 700 PMT.

Figure S18: Photographs of 11merXX-Nr hybrids with DNA under black light (405 nm): (a) 11merAA-Nr and 5’-d(CGTATTTTATG)-3’ (b) (a) 11merAA-Nr and 5’-d(CGTATTTTATG)-3’ (c) 11merCC-Nr and 5’-d(CGTATGGTATG)-3’ (d) 11merCC-Nr and 5’-d(CGTATCTCTAG)-3’ (e) 11merTT-Nr and 5’-d(CGTATAATATG)-3’ (f) 11merTT-Nr and 5’-d(CGTATCCTATG)-3’ (g) 11merGG-Nr and 5’-d(CGTATCCTATG)-3’ (h) 11merGG-Nr and 5’-d(CGTATCCTATG)-3’; Conditions: 10 mM phosphate buffer pH 7.0, [PNA] = 10 μM and [DNA] = 12 μM