Recognition and discrimination of DNA quadruplexes by acridine-peptide conjugates

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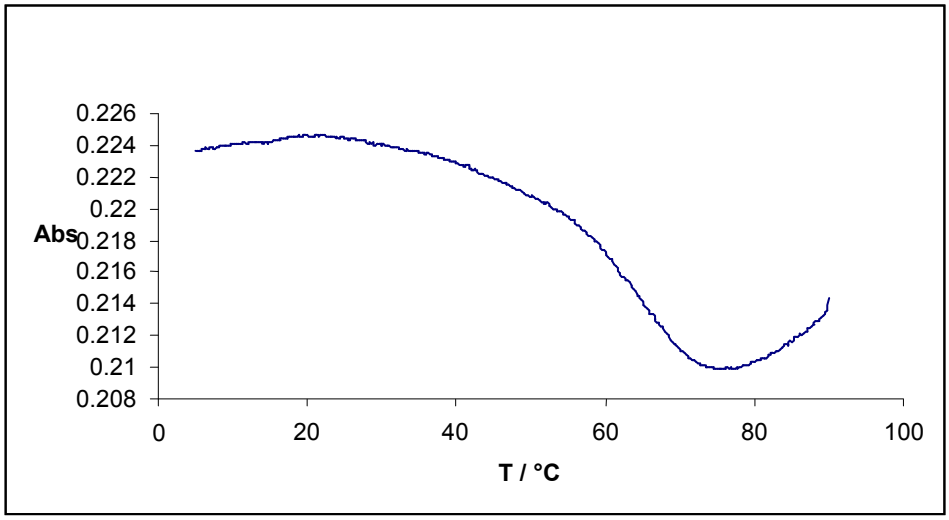
Compound	Observed *m/z*	r.t./min	Amino acid analysis mol.mol^{-1} (std devn)
7	912.4 $[M+2H]^{2+}$ 608.7 $[M+3H]^{3+}$	22.7[a]	F 2.04 (0.02), H 2.06 (0.00), R 3.90 (0.02)
8	843.0 $[M+2H]^{2+}$ 562.3 $[M+3H]^{3+}$	17.7[a]	S 1.92 (0.02), K 2.16 (0.00), R 3.94 (0.02)
9	827.0 $[M+2H]^{2+}$ 552.0 $[M+3H]^{3+}$	19.2[a]	V 1.98, K 4.00 (0.02), R 2.02 (0.02)
10	1190.6 $[M+H]^{+}$ 596.2 $[M+2H]^{2+}$	19.6[b]	F 1.03 (0.01), H 1.02 (0.01), R 1.94 (0.02)
11	1190.6 $[M+H]^{+}$ 596.0 $[M+2H]^{2+}$	19.0[b]	F 1.05 (0.00), H 1.04 (0.00), R 1.91 (0.00)
12	1190.7 $[M+H]^{+}$ 596.2 $[M+2H]^{2+}$	19.5[b]	F 1.00 (0.00), H 0.98 (0.01), R 2.02 (0.02)
13	562.0 $[M+2H]^{2+}$ 375.3 $[M+3H]^{3+}$	16.4[b]	S 0.96 (0.12), K 0.98 (0.09), R 2.07 (0.21)
14	1121.6 $[M+H]^{+}$ 561.5 $[M+2H]^{2+}$	15.3[b]	S 1.06 (0.00), K 1.05 (0.00), R 1.89 (0.00)
15	1122.1 $[M+H]^{+}$ 562.0 $[M+2H]^{2+}$	12.3[b]	S 0.98 (0.00), K 1.05 (0.01), R 1.97 (0.01)
16	596.7 $[M+2H]^{2+}$	20.2[b]	F 1.04 (0.03), H 0.98 (0.03), R 1.97 (0.06)
17	1192.6 $[M+H]^{+}$ 596.6 $[M+2H]^{2+}$	19.2[b]	F 1.05 (0.00), H 1.03 (0.01), R 1.92 (0.01)
18	1191.6 $[M+H]^{+}$ 596.7 $[M+2H]^{2+}$	19.5[b]	F 1.00 (0.01), H 1.02 (0.01), R 1.98 (0.02)
19	562.1 $[M+2H]^{2+}$	16.5[b]	S 0.89 (0.01), K 1.19 (0.03), R 1.93 (0.02)
20	1122.7 $[M+H]^{+}$ 562.0 $[M+2H]^{2+}$	15.6[b]	S 1.01 (0.00), K 1.06 (0.00), R 1.93 (0.00)
21	1123.1 $[M+H]^{+}$ 562.4 $[M+2H]^{2+}$	14.2[b]	S 0.98 (0.00), K 1.04 (0.00), R 1.98 (0.00)

HPLC methods: Solvent A = H_2O, 0.1% TFA, solvent B = MeCN, 0.1% TFA. Phenomenex C18 Luna 5 μM, 250 × 4.6 mm column, flow rate 1 mL min^{-1}. UV detection at 220 nm. Gradient [a] 0 – 2.5 min 5% B, 32.5 min 40% B. [b] 0 – 2.5 min 10% B, 32.5 min 40% B.

Table S1. Amino acid analysis and mass spectrometry of peptides **7** – **21**.



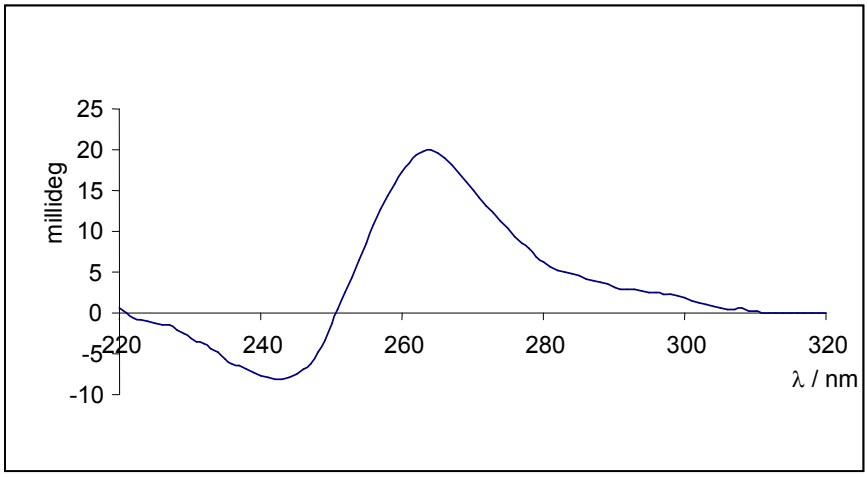


Figure S1. UV thermal melt and circular dichroism spectrum of *N-ras*. a) UV thermal melt at 295 nm of the *N-ras* (4 μM unbiotinylated oligonucleotide) in 100 mM KCl, 10 mM Tris-HCl, pH 7.4. Melting temperature, T_m = 61 °C, calculated as the point where the second derivative of the curve is zero. T_m was found to be independent of oligonucleotide concentration over the range 2 – 10 μM. b) Circular dichroism spectrum of *N-ras* (4 μM unbiotinylated oligonucleotide in 10 mM Tris-HCl, 100 mM KCl, pH 7.4, 4 °C).

a)

[K^+] mM	T_m °C
0	[a]
10	43
50	60
100	65
200	72

[a] No melting transition observed.

b)

Cation	T_m °C
K^+	66
Na^+	34.2
Li^+	[a]
NH_4^+	[a]

[a] No melting transition observed.

Table S2. a) T_m of *N-ras* (4 μM in 10 mM Tris-HCl, pH 7.4) as a function of KCl concentration. b) T_m of *N-ras* (4 μM in 10 mM Tris-HCl, pH 7.4) as a function of monovalent cation, supplied as 100 mM chloride salt.