Supporting Material

Title: Imino proton exchange rates imply an induced-fit binding mechanism for the $VEGF_{165}$-targeting aptamer, Macugen

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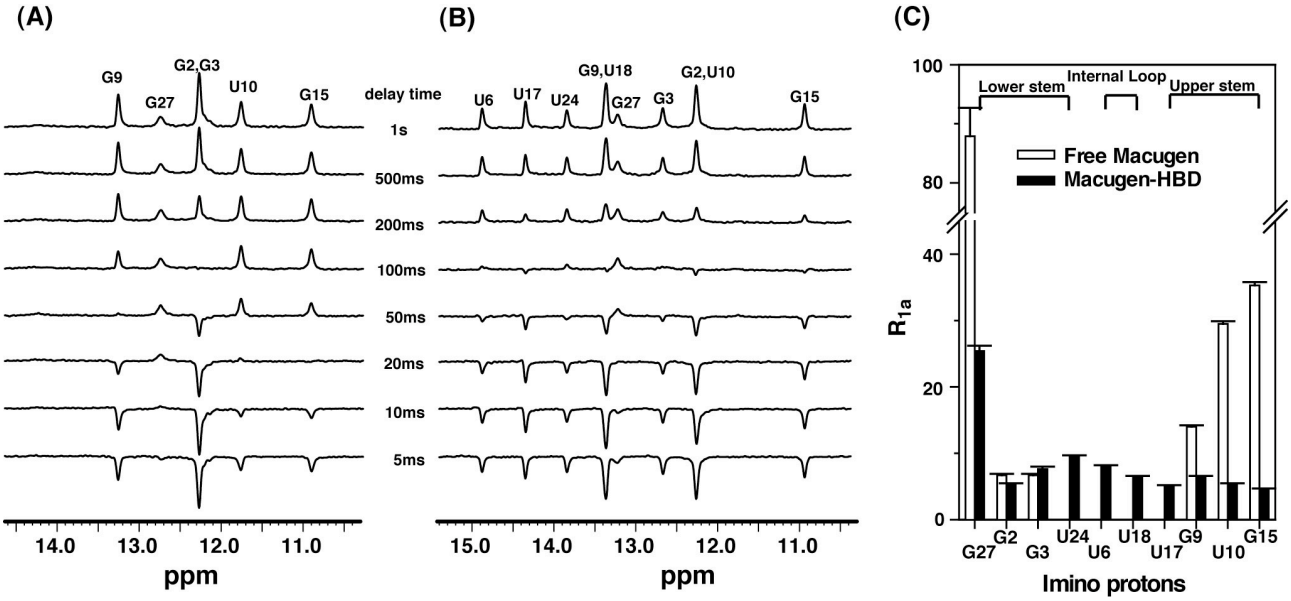

Figure 5S. Inversion recovery spectra of imino protons of (A) free Macugen and (B) the HBD-Macugen complex at 15 °C. (C) Apparent R_1 relaxation rates (R_{1a}) of the imino protons in free Macugen (open bars) and the HBD-Macugen complex (filled bars).

Table 2S: Apparent relaxation rate constants R_{1a} of the imino protons of free Macugen and the HBD- and VEGF-Macugen complexes (s^{-1})

Base Pair	Imino proton	Free Macugen	HBD-Macugen		VEGF-Macugen
		15 °C	15 °C	35 °C	35 °C
C1·G27	G27	87.9±4.8	25.4±0.8	n.a.[a]	n.a.[a]
G2·C26	G2	≤6.7±0.2[b]	≤5.3±0.2[c]	≤3.2±0.1[c]	n.d.[e]
G3·C25	G3	≤6.7±0.2[b]	7.6± 0.4	2.9±0.1	n.d.[e]
A4·U24	U24	n.a.[a]	9.5±0.2	38.4±1.7	40.0±5.0
	U20	n.a.[a]	n.a.[a]	n.a.[a]	61.8±3.3
U6·A19	U6	n.a.[a]	8.0±0.2	53.3±2.6	50.8±8.9
C7·U18	U18	n.a.[a]	≤6.3±0.3[d]	18.0±0.3[d]	19.5±1.0
A8·U17	U17	n.a.[a]	4.9±0.3	2.7±0.1	n.d.[e]
G9·C16	G9	14.0±0.2	≤6.3±0.3[d]	3.1±0.2[d]	n.d.[e]
U10·G15	U10	35.3±0.4	≤5.3±0.2[c]	≤3.2±0.1[c]	n.d.[e]
	G15	29.5±0.5	4.4±0.3	2.2±0.1	n.d.[e]

a) n.a.: no resonance.

b) The G2 and G3 resonances overlap in the free aptamer so the individual R_{1a} values could not be determined. The intensities fit well to a single exponential and thus only an upper limit for the R_{1a} of each proton is reported.

c) The G2 and U10 resonances overlap in the HBD- and VEGF-Macugen complexes so the individual R_{1a} values could not be determined. The intensities fit well to a single exponential and thus only an upper limit for the R_{1a} of each proton is reported.

d) The G9 and U18 resonances overlap in the HBD- and VEGF-Macugen complexes so the individual R_{1a} values could not be determined. The intensities fit well to a single exponential and thus only an upper limit for the R_{1a} of each proton is reported.

e) The R_{1a} could not be accurately determined because of double exponential relaxation behavior for the large VEGF-Macugen complex.