

Cation localization and movement within DNA thrombin binding aptamer in solution

Marko Trajkovski,^a Primož Šket,^a and Janez Plavec,^{*,a,b}

^a Slovenian NMR Centre, National Institute of Chemistry, Hajdrihova 19, SI-1000 Ljubljana, Slovenia

^b Faculty of Chemistry and Chemical Technology, University of Ljubljana, SI-1000 Ljubljana, Slovenia

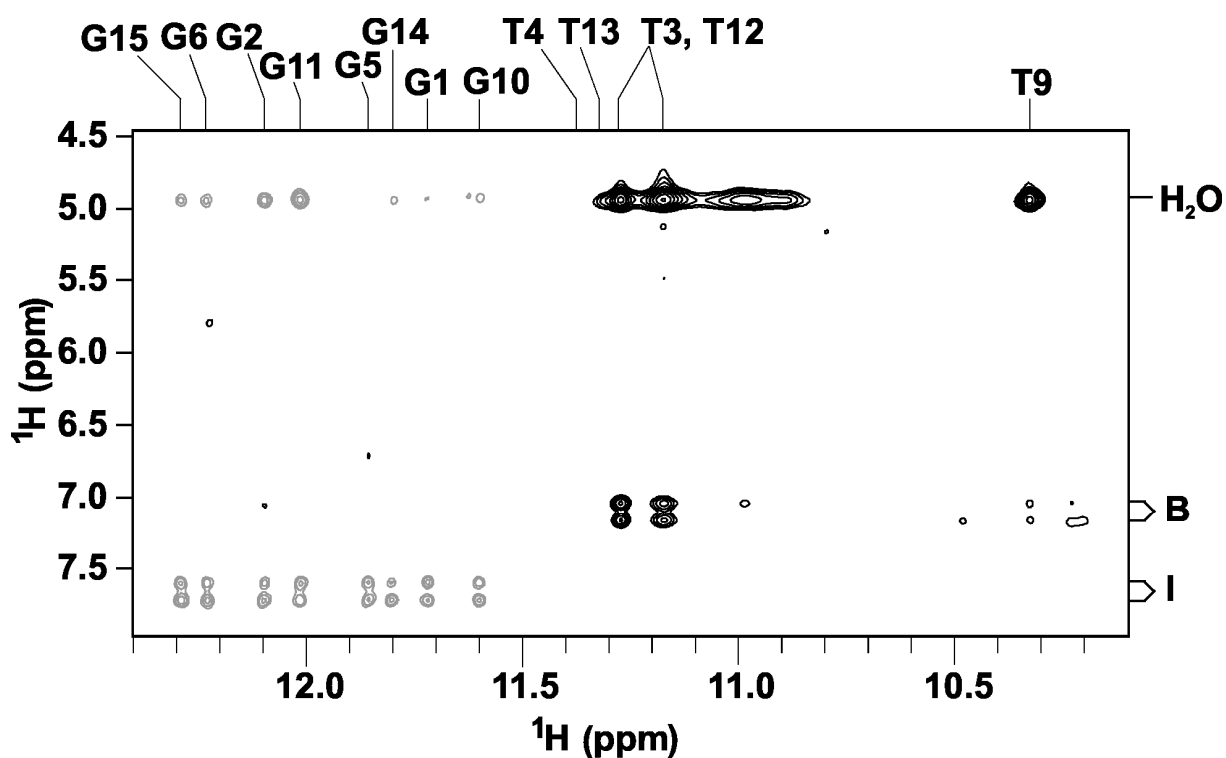


Figure S1. Region of ROESY spectrum of TBA with mixing time of 40 ms in the presence of 36 mM $^{15}\text{NH}_4\text{Cl}$ in 5% $^2\text{H}_2\text{O}$ at 5 °C and pH 4.5. The oligonucleotide concentration was 1.8 mM. Nitrogen-15 has not been decoupled along f1 dimension. Imino proton assignments are shown on the top, while resonance positions of water, ammonium ions in bulk solution (**B**) and at the inner binding site (**I**) are indicated on the right side of the spectrum.

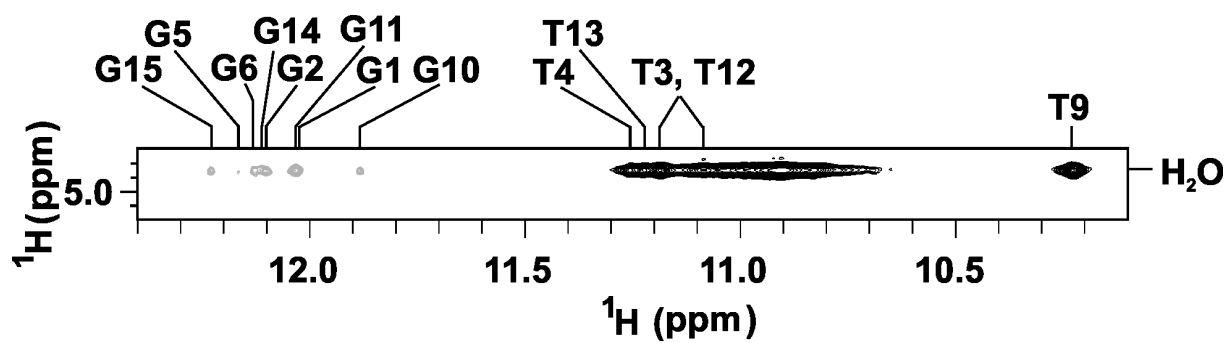


Figure S2. Region of ROESY spectrum of TBA with mixing time of 40 ms in the presence of one molar equivalent of KCl with respect to oligonucleotide at 1.9 mM concentration, 5% $^2\text{H}_2\text{O}$, 15 °C and pH 5.0. Imino proton assignments are shown on the top.