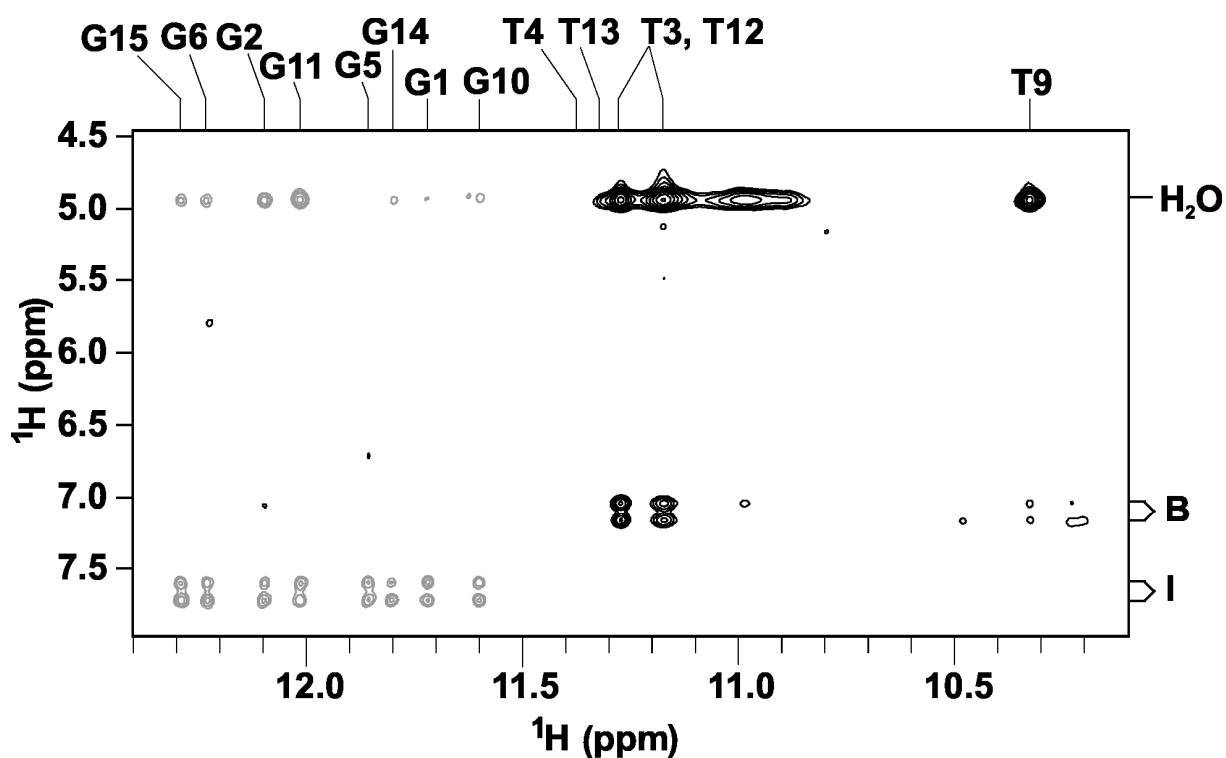


## Cation localization and movement within DNA thrombin binding aptamer in solution

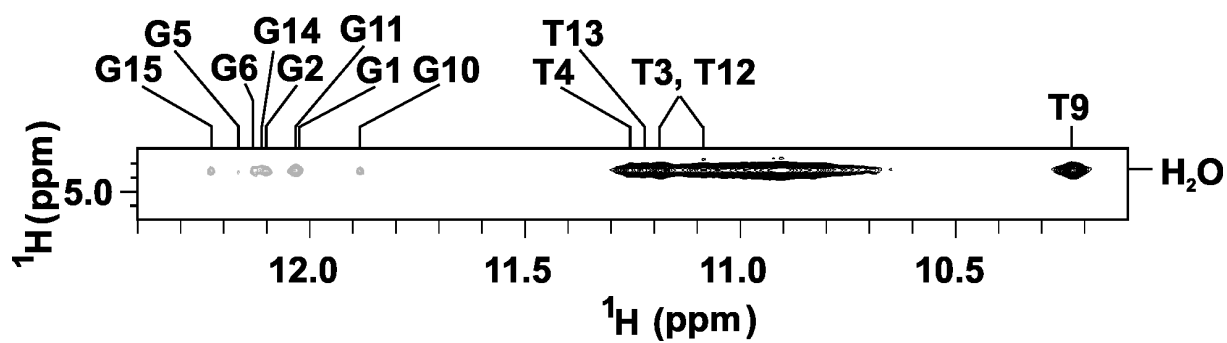
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**Figure S1.** Region of ROESY spectrum of TBA with mixing time of 40 ms in the presence of 36 mM  $^{15}\text{NH}_4\text{Cl}$  in 5%  $^2\text{H}_2\text{O}$  at 5 °C and pH 4.5. The oligonucleotide concentration was 1.8 mM. Nitrogen-15 has not been 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.