Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Umbrella Sampling Molecular Dynamics Simulations Reveal Concerted Ion Movement through G-Quadruplex DNA Channels

Parisa Akhshi and Gang Wu*

Department of Chemistry, Queen's University, 90 Bader Lane,
Kingston, Ontario, Canada K7L 3N6
*Corresponding author: wugang@queensu.ca

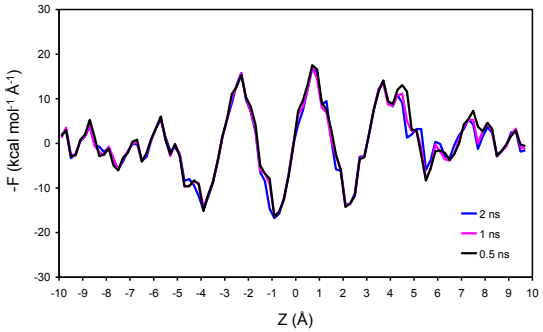

Figure S1. Comparison of the force profiles for a K^+ ion moving across the entire $[d(TG_4T)]_4$ G-quadruplex channel obtained with 0.5, 1.0, and 2.0 ns US simulation time for each window (0.25 Å wide). As there are a total of 80 windows between Z = –10 and 10 Å, the total simulation time was 40, 80, and 160 ns for the three cases, respectively.

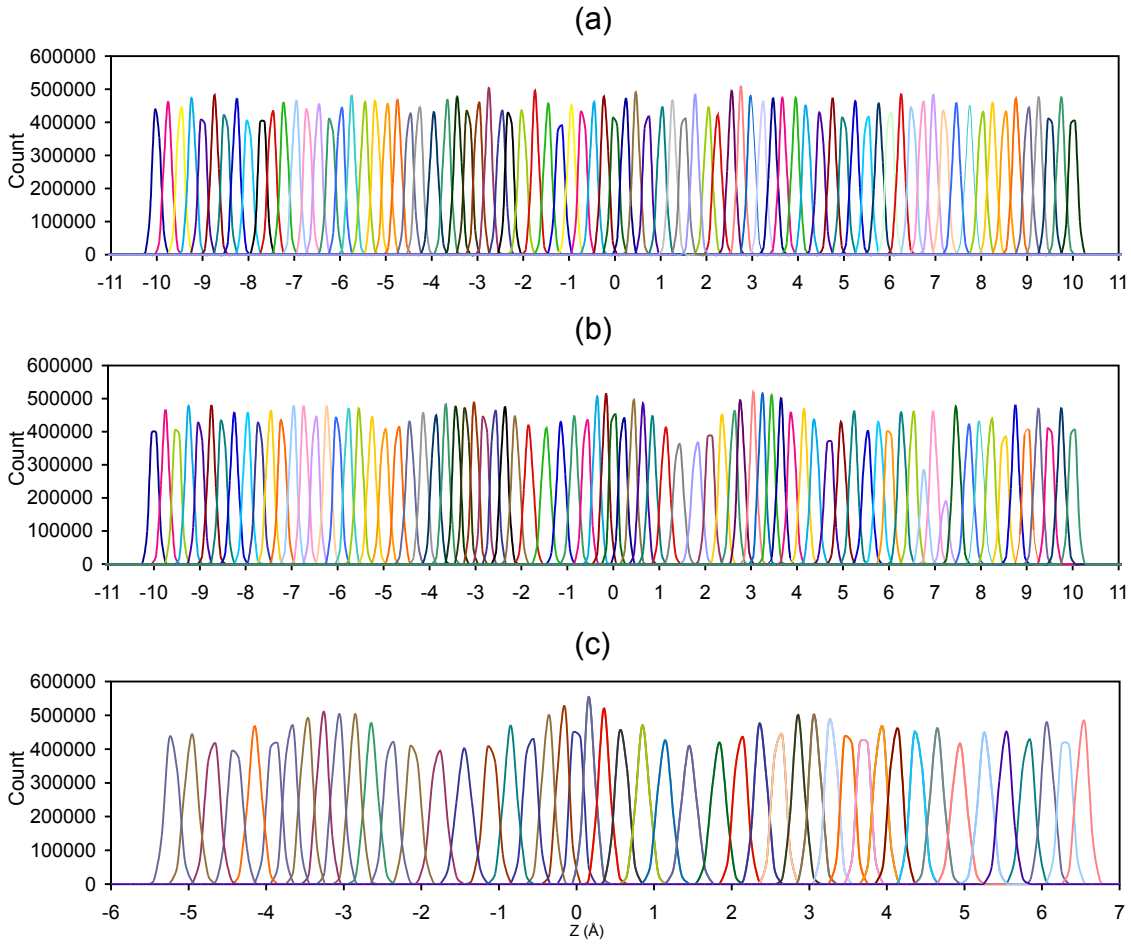

Figure S2. Window sampling histograms from US MD simulations for (a) Na^+ ion moving through the $[d(TG_4T)]_4$ channel, (b) K^+ ion moving through the $[d(TG_4T)]_4$ channel, and (c) NH_4^+ ion moving through the $[d(G_3T_4G_4)]_2$ channel. In each window, a harmonic biasing force constant of 100 kcal/(mol $Å^2$) was applied. In (a) and (b), the origin of the reaction coordinate (Z) is defined by the center of mass from the eight carbonyl oxygen atoms from the two central G-quartets, $[G4]_4$ and $[G3]_4$. In (c), the origin of Z is defined by the center of mass from four carbonyl oxygen atoms from the G1-G13-G9-G21 quartet. For the three US MD data sets, the aggregate simulation time was 24, 24, and 14 ns in (a), (b), and (c), respectively.