Molecular Dynamics and Principal Components of Potassium Binding with Human Telomeric Intra-molecular G-Quadruplex

Zhiguo Wang *, 1, Ruping Chen 1, 2, Ling Hou 1, Jianfeng Li 1, Jun-Ping Liu *, 1, 2, 3, 4

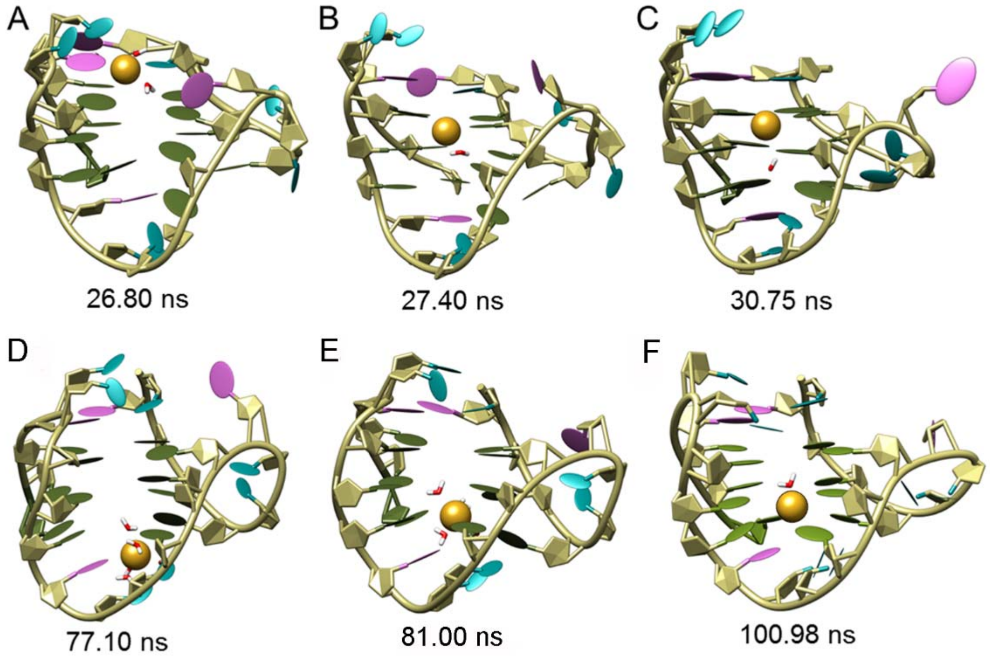

Figure S1

Binding processes of Na^+ ions with human telomeric hybrid [3+1] form-one G-quadruplex. Figures (A)-(C) represent the binding process through the top pathway in sim-Na1; (D)-(F) represent the binding process through the bottom pathway in sim-Na2. The bases of adenine, thymine and guanine nucleotides were colored orchid, cyan and olive green, respectively; the Na^+ ions were represented as yellow spheres.

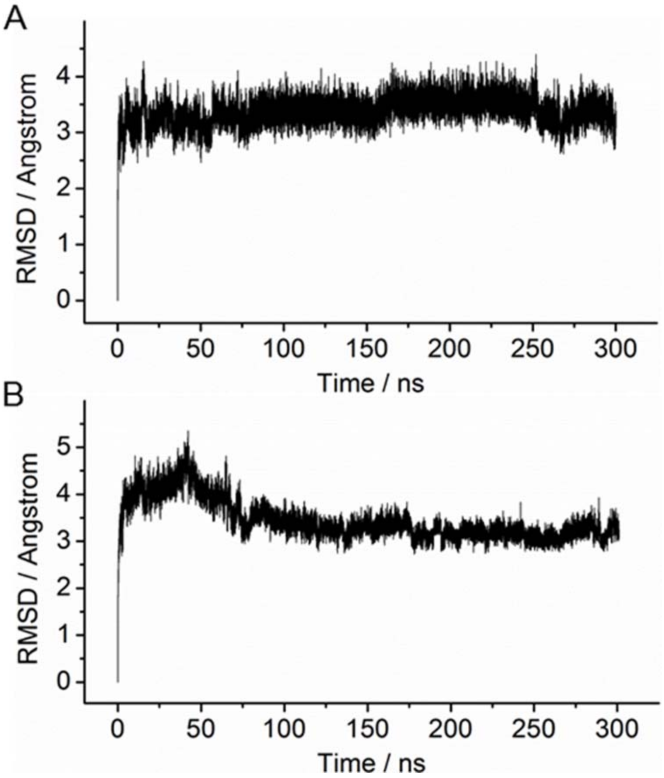

Figure S2

The RMSDs of human hybrid [3+1] form-one G-quadruplex in Na^+ containing solutions. (A) and (B) presented the RMSD values of sim-Na1 and sim-Na2, respectively.

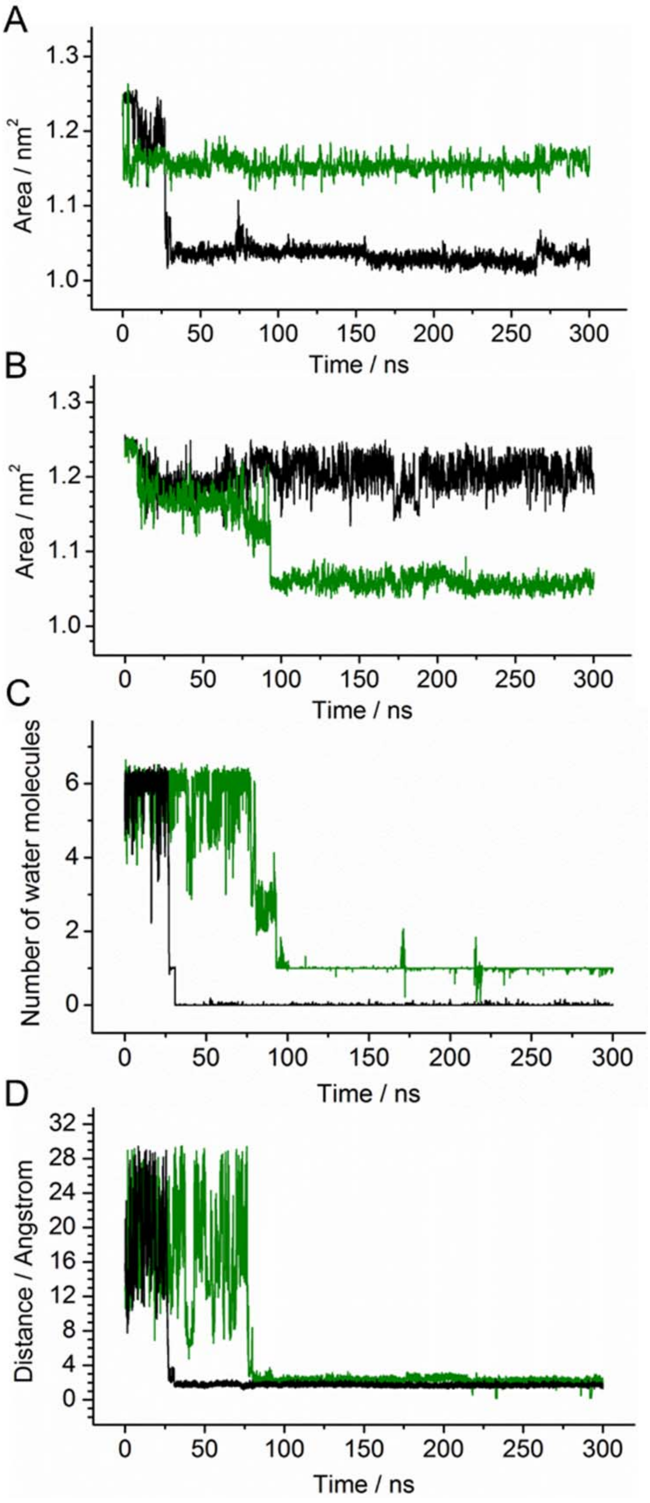

Figure S3

The variations of G-tetrad gate areas, coordinated waters and distances in the simulations of sim-Na1 and sim-Na2. (A) and (B) respectively showed the changes of G-tetrad gate areas of sim-Na1 and sim-Na2, in which the top and bottom areas were colored black and green, respectively; (C) and (D) respectively presented the number of waters within 3.5 Å of binding Na^+ ions and the distances between the binding Na^+ ions and CCG in sim-Na1 (black) and sim-Na2 (green).