Supplementary file 1

Stabilization of Hoogsteen H-bonds in G-quartet sheets by coordinated K⁺ ion for enhanced efficiency in guanine-rich DNA nanomotor

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Fig. S1. The 3D intramolecular tetraplex (TE) conformation of the 15-mer DNA nanomotor, captured from various perspectives. The labels A, B, and C correspond to the TE1K nanomotor, which features a K⁺ ion (depicted in purple) situated between G-quartet 1 and G-quartet 2 (pdb ID 4DII). Conversely, the configurations A', B', and C' represent ion-free structures designated as TE3 (pdb ID 1HUT). The conformation of all nucleotides is displayed in A and A' (front view), while the nucleotides of the G-quartets are exclusively depicted in B and B' (front view) as well as C and C' (side view).



Fig. S2. The MD simulation periodically boxes, consisted of TE1K, TE2K and TE3 in aqueous solution with 13 K^+ ion (magenta spheres). The crystal K^+ ion presented purple (indicated by arrows) in TE1K and TE2K.



Fig. S3. The G-quartet is stabilized by eight Hoogsteen hydrogen bonds between (NH)1...O6 and (NH)2...N7 groups. Potassium cation, K⁺, is coordinated to four guanine O6 carbonyl groups of G-quartet.



Fig. S4. Different MD simulations' snapshots of TE1K in front (left panels) and side views (right panels). The numbers of 13 neutralized K+ ions presented in magenta and the coordinated crystal K+ in the G-quartets' core indicated in purple (for clarifying, water molecules were removed).



Fig. S5. Different MD simulations' snapshots of TE2K in front (left panels) and side views (right panels). The numbers of 13 neutralized K+ ions presented in magenta and the coordinated crystal K+ in the G-quartets' core indicated in purple (for clarifying, water molecules were removed).



Fig. S6. Different MD simulations' snapshots of TE2 (free coordinated crystal K+) in front (left panels) and side views (right panels). The numbers of 14 neutralized K+ ions presented in magenta (for clarifying, water molecules were removed).

