

Supplementary materials for
Structure of DNA-Functionalized Dendrimer Nanoparticles
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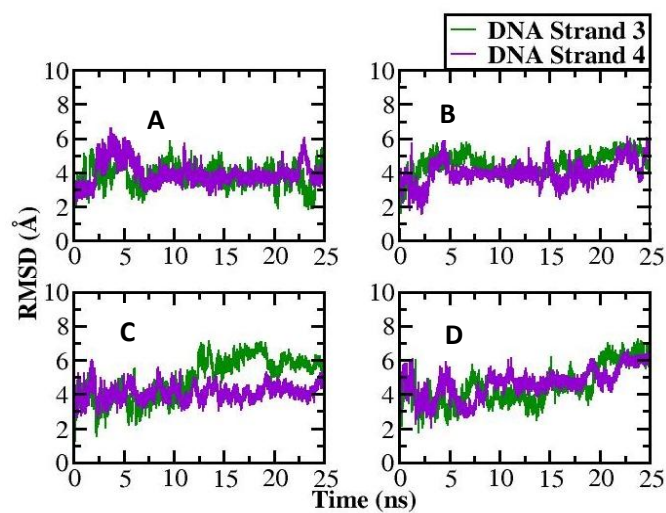


Figure S1: Root mean square deviation (RMSD) of ssDNAs (strand 3 & 4) of (a) G_3A_{10} (b) G_3C_{10} (c) G_4A_{10} (d) G_4C_{10} . In most of the cases the value of the RMSD becomes stable after 6 ns.

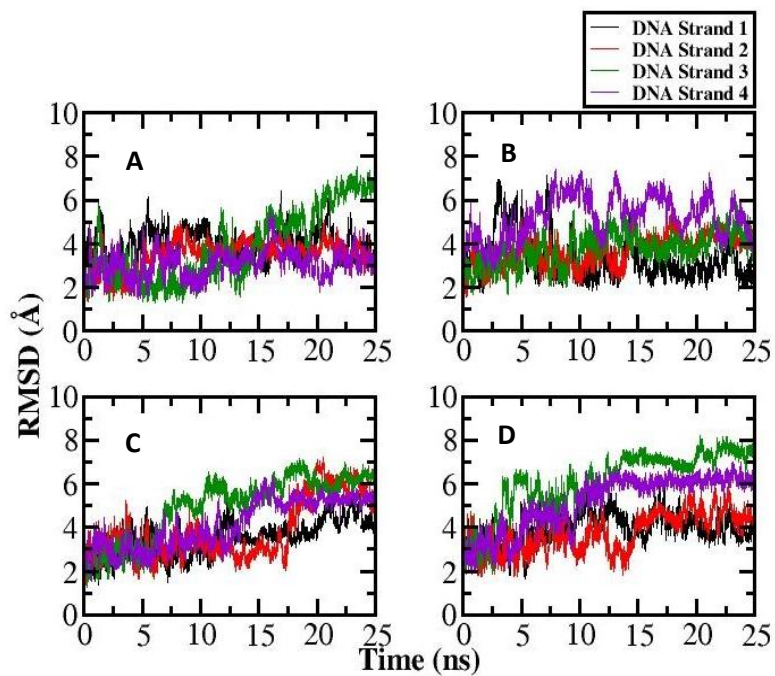


Figure S2: Root mean square deviation (RMSD) of ssDNAs of (A) $G_3^4G_{10}$ (B) $G_3^4T_{10}$ (C) $G_4^4G_{10}$ (D) $G_4^4T_{10}$. In most of the cases the value of the RMSD becomes stable after 6 ns.

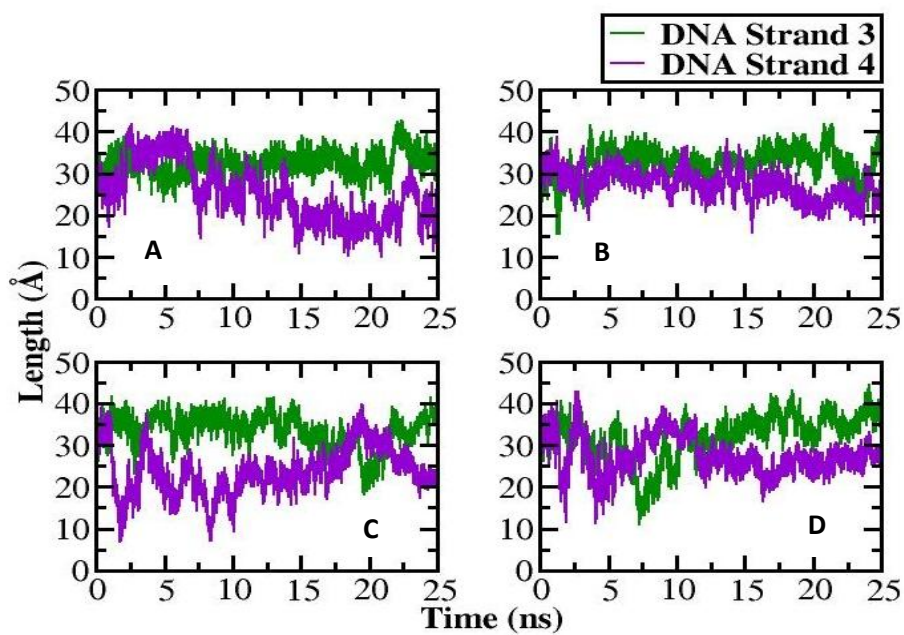


Figure S3: End to end distance (Length) of ssDNAs (strand 3 & 4) of (A) G_3A_{10} (B) G_3C_{10} (C) G_4A_{10} (D) G_4C_{10} .

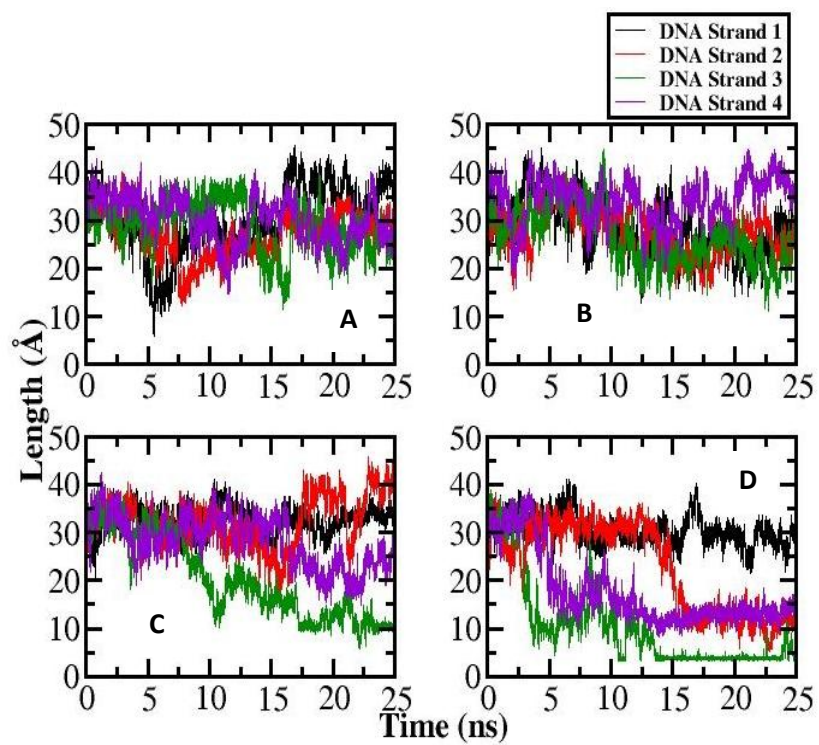


Figure S4: End to end distance (Length) of ssDNAs of (A) G_34G_{10} (B) G_34T_{10} (C) G_44G_{10} (D) G_44T_{10} .

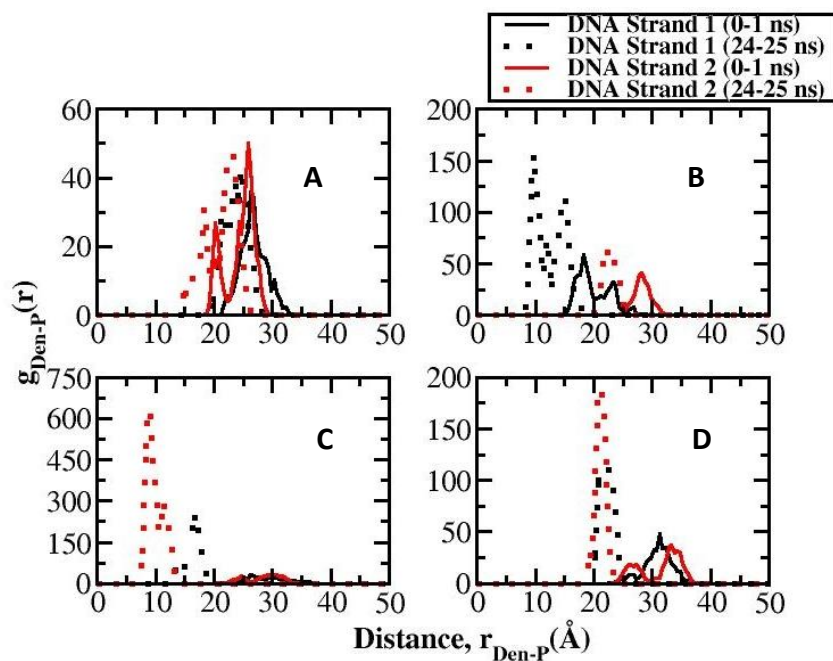


Figure S5: Radial distribution function of the Phosphorous atom of the first base next to the linker molecule relative to the center of the dendrimer particle for (A) G_34G_{10} (B) G_34T_{10} (C) G_44G_{10} (D) G_44T_{10} at the (0-1) ns (represented using continuous lines) and at (24-25) ns (represented using dashed lines) of the simulation. Radial distribution function of each of ssDNA is shown separately in different colours.

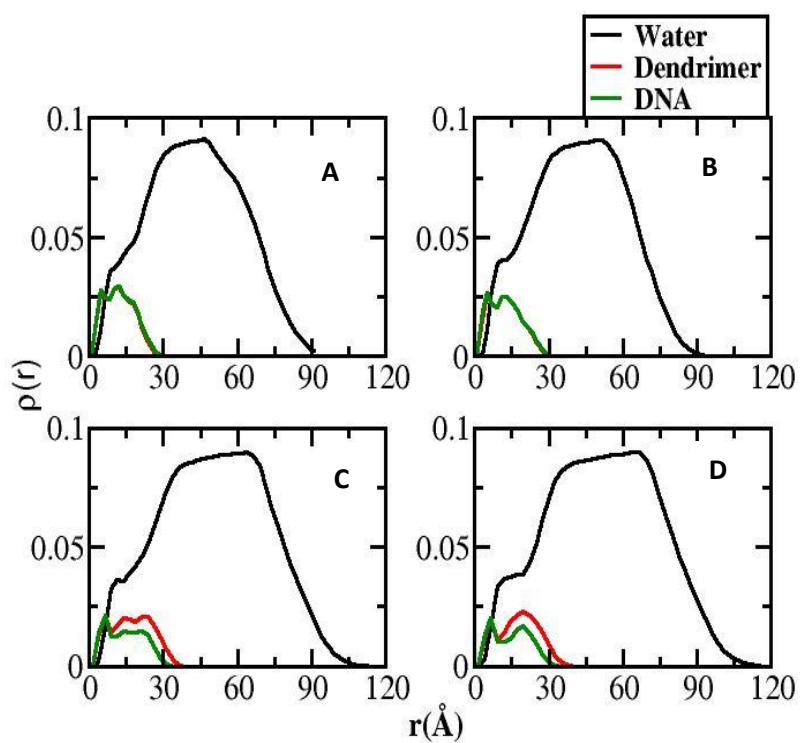


Figure S6: Density distribution for DNA, the dendrimer, and water in (A) G_34G_{10} (B) G_34T_{10} (C) G_44G_{10} (D) G_44T_{10} . The numbers shown were averaged from snapshots every 0.5 ps for the last 2 ns of the 25 ns long trajectory. The distribution has been calculated with respect to the center of mass of the dendrimer.