Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supplementary Information

Considering both small and large scale motions of vascular endothelial growth factor (VEGF) is crucial for reliably predicting its binding affinities to DNA aptamers

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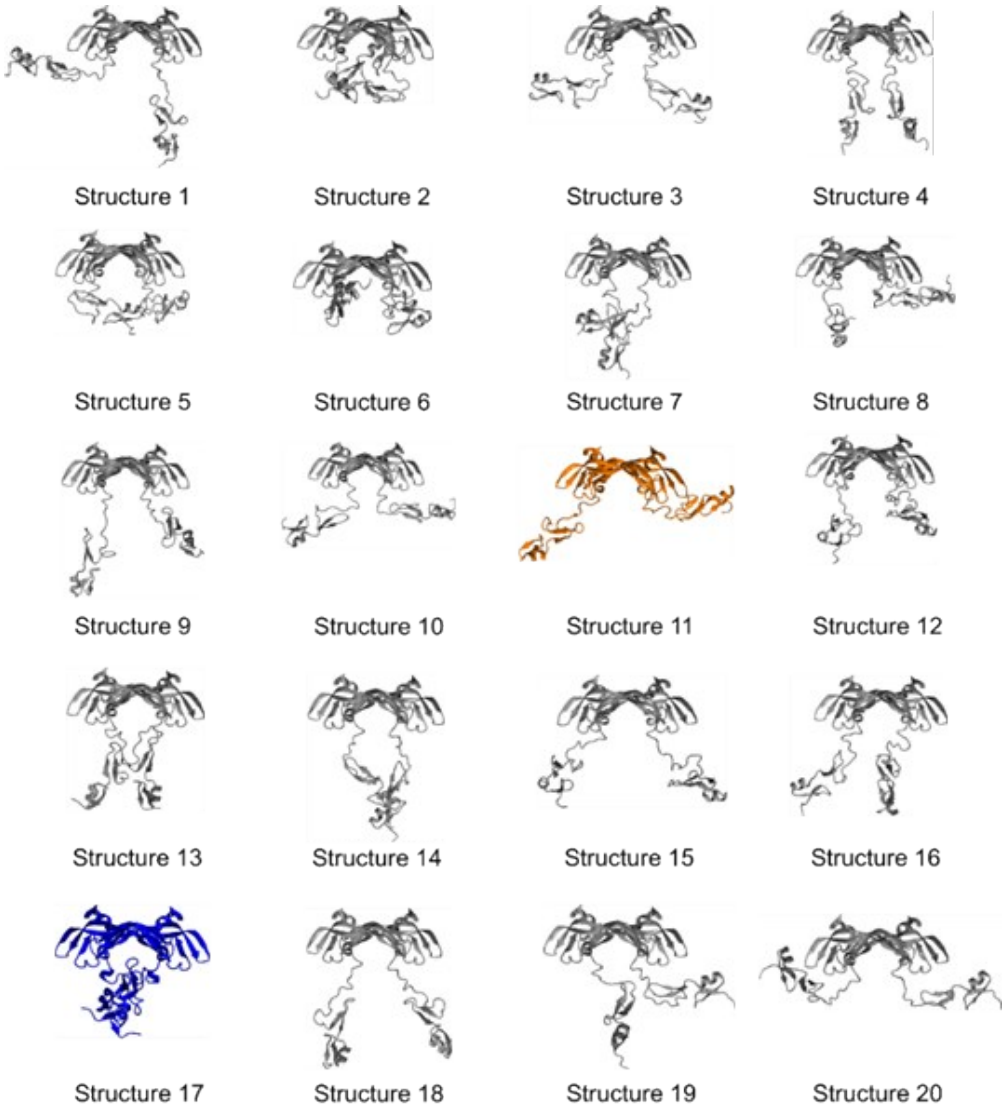

Figure S1. Twenty $VEGF_{165}$ conformations created by merging an RBD dimer and two HBD units. The conformation that was used for subsequent ensemble docking with the six DNA aptamer variants is colored in orange (Structure 11), and the conformation that was used for additional docking calculations for comparisons with Structure 11 is colored in blue (Structure 17).

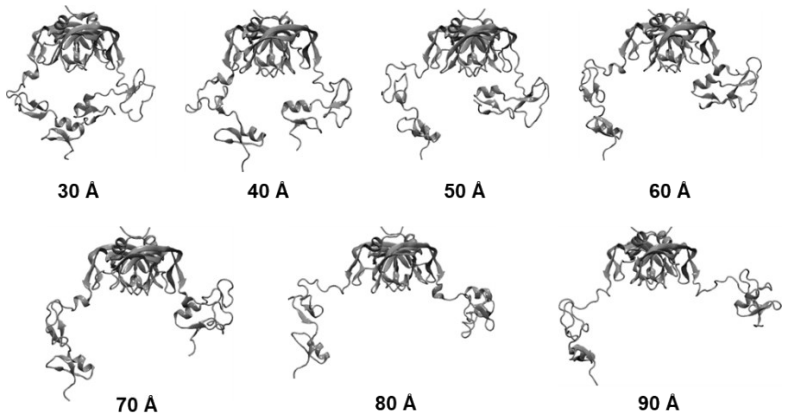

Figure S2. Seven $VEGF_{165}$ conformations from Structure 17, generated along the distance between the HBD units.

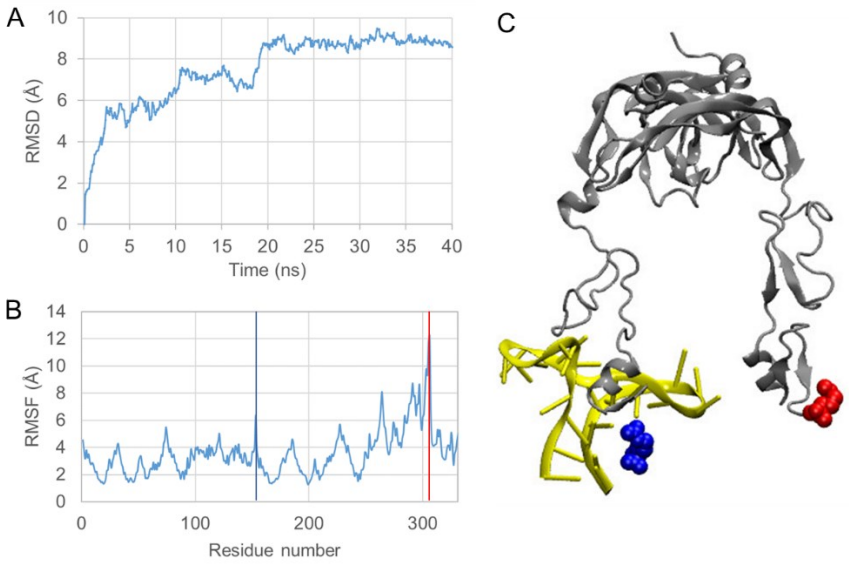

Figure S3. (A) Root mean square deviation (RMSD) of the $VEGF_{165}$–DNA aptamer complex structure over 40 ns of an MD simulation. RMSD was calculated in reference to the initial snapshot. (B) Root mean square fluctuation (RMSF) for the same simulation. (C) The position of two C-terminal residues, one of which exhibits the largest RMSF value. The converged RMSD value shown in (A) is rather large (~9 Å), and this is due to the fluctuation of the C-terminal residue (RMSF = ~12 Å) and its vicinity in one of the two HBDs which is not bound to DNA aptamer. The terminal group with the large RMSF is marked in red in B and C. The other C-terminal residue (RMSF = ~6 Å) and its vicinity do not fluctuate as much due to their interactions with the DNA aptamer, as marked in blue in B and C.