BioTech

Supplementary Materials: Development of the 12-Base Short Dimeric Myogenetic Oligodeoxynucleotide That Induces Myogenic Differentiation

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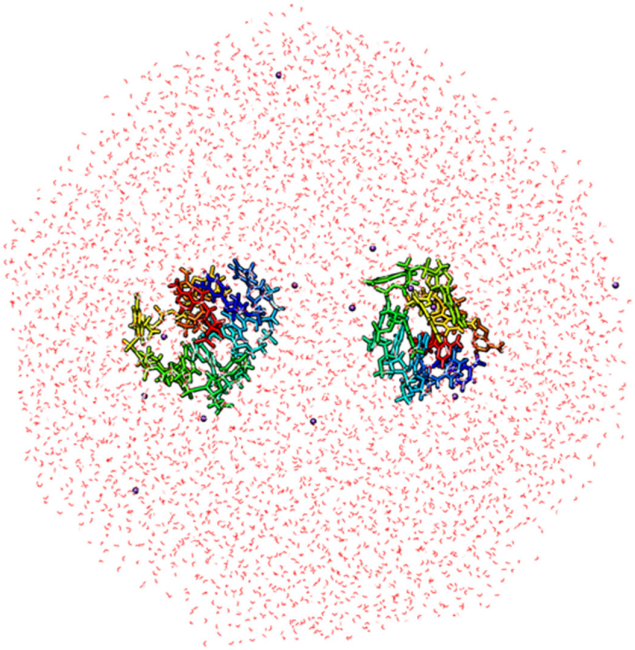
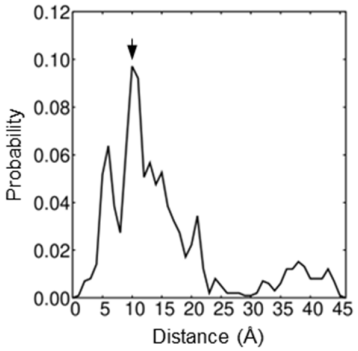
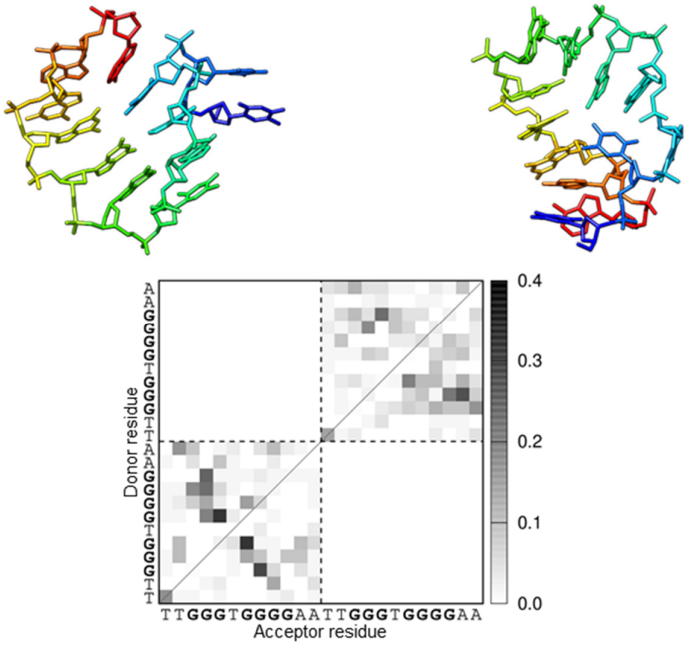


Supplementary Figure S1. The simulation system of the iMyo01-DNA dimer. iMyo01-DNA molecules are represented as a rainbow-colored stick model from the 5′ to the 3′ end. The solvent molecules are shown as red wires (oxygen atoms of water molecules), purple spheres (K^+ ions), and a green sphere (Cl^- ion).



Supplementary Figure S2. The probability of the center-of-mass distances between the two iMyo01-DNA molecules. The McMD simulation at 310 K provided 988 conformations as a canonical ensemble. Their center-of-mass distances and probability distribution are shown. The dimer state defined below 25 Å of the distance contains 855 conformations (86.5%), and the separated monomer state contains 133 conformations (13.5%). An arrow indicate the peak at $d_{com} \approx 10$ Å.



Supplementary Figure S3. The representative iMyo01-DNA structure in the separated monomer state. The structures (d_{com}, 37.8 Å) are shown as a rainbow-colored stick model from the 5′ to the 3′ end. The hydrogen bond pattern is plotted as a monochrome map. The gray scale indicates the probability of hydrogen bond formation between residues. The two iMyo01-DNA sequences are displayed sequentially on the axes.