Supporting Information

# A bridged nucleic acid, 2′,4′-BNA$^{COC}$: Synthesis of fully modified oligonucleotides bearing thymine, 5-methylcytosine, adenine and guanine 2′,4′-BNA$^{COC}$ monomers, and RNA-selective nucleic acid recognition.

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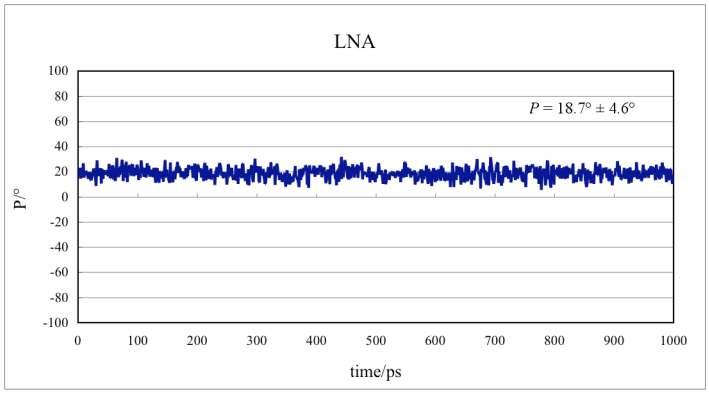
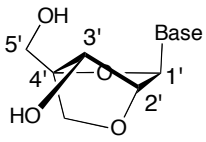
†The authors wish it to be known that, in their opinion, the first two authors should be regarded as joint First Authors.

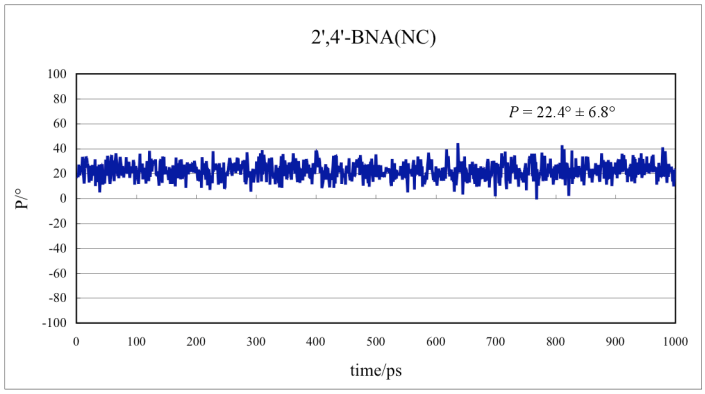
## Molecular Dynamics.

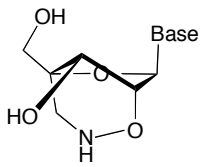
Molecular dynamics simulations were performed with the default parameters of MacroModel program (version 9.1). Partial charges for all atoms were assigned by using this force field and solvation in water was accounted for by the GB/SA continuum solvation model in conjunction with AMBER* force field. The simulation parameters of the stochastic dynamics were used as following; temperature of 300K, time step of 1.5 fs, equilibration of 1 ps, and simulation time of 1000 ps. The simulations were carried out for the single stranded trimer of each thymidine analogues, and data samples of the centered nucleotide were used for discussions. 1000 samples were collected and every torsion angles of their sugar moiety were measured. Pseudorotation phase angle (*P*) and the degree of pucker ($\upsilon_{max}$) were calculated based on reference 5.



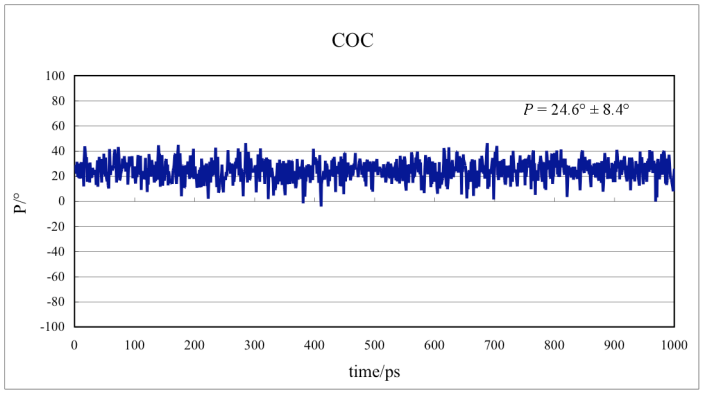



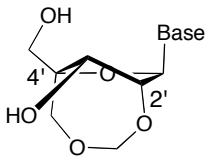

2',4'-BNA/LNA



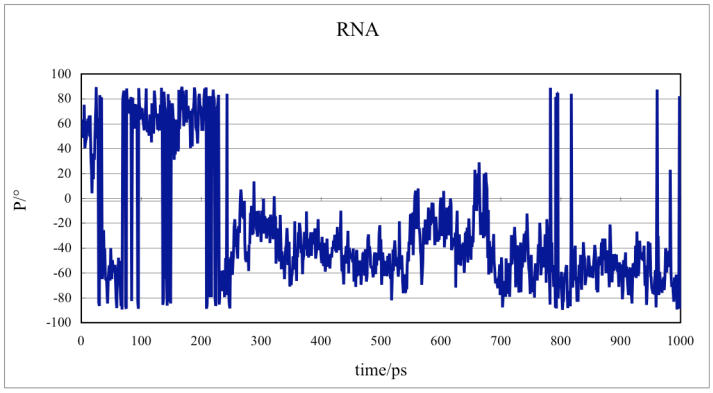



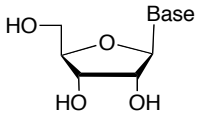

2',4'-BNA$^{NC}$



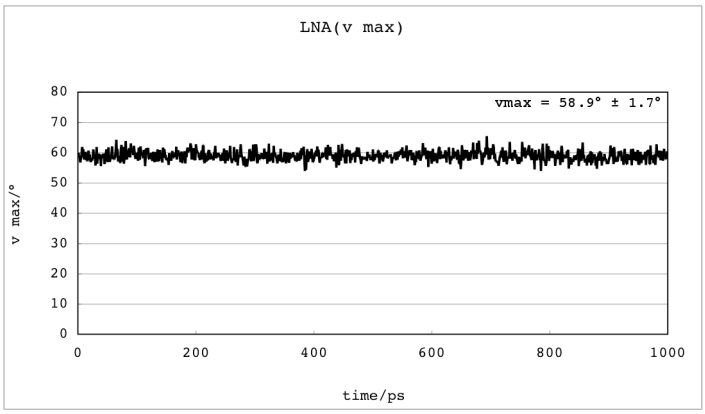

2',4'-BNA$^{COC}$

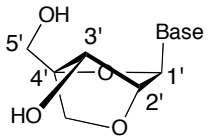


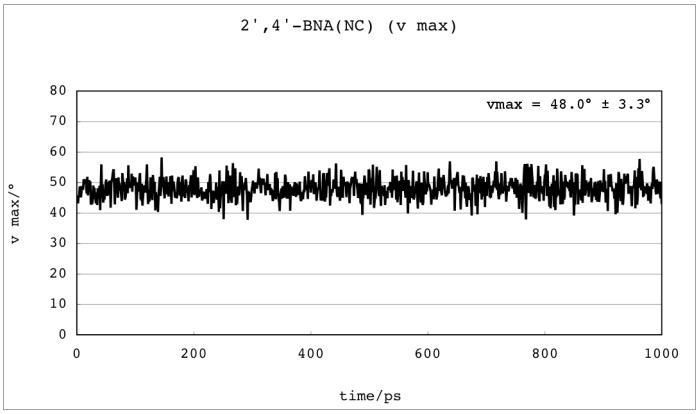

RNA

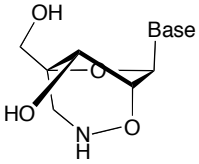
**Figure S1. Time course of pseudorotation phase angle (*P*).** Parameters of the stochastic dynamics; temperature of 300K, time step of 1.5 fs, equilibration of 1 ps, and simulation time of 1000 ps.



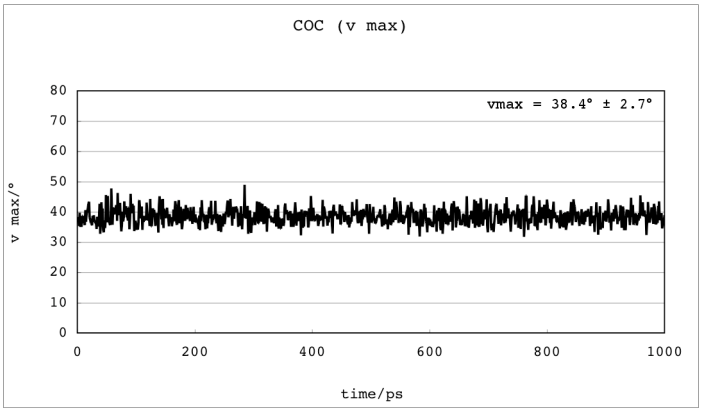



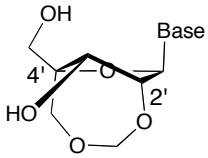

2',4'-BNA/LNA



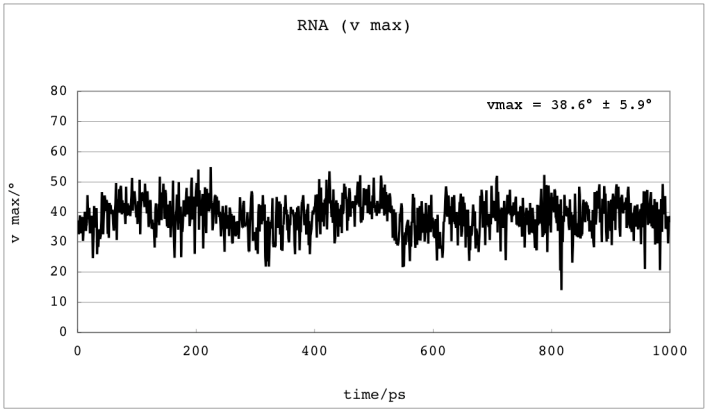



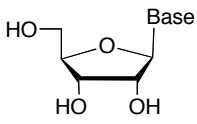

2',4'-BNA$^{NC}$




2',4'-BNA$^{COC}$




RNA

**Figure S1. Time course of sugar puckering amplitude ($\upsilon_{max}$).** Parameters of the stochastic dynamics; temperature of 300K, time step of 1.5 fs, equilibration of 1 ps, and simulation time of 1000 ps.