

Supporting information

Short-RNA selective binding of oligonucleotides modified using adenosine and guanosine derivatives that possess cyclohexyl phosphates as substituents

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General methods

The dry solvents were purchased and stored over molecular sieves 4A. ^1H , ^{13}C , and ^{31}P NMR spectra were obtained at 500, 126, and 203 MHz, respectively. The chemical shifts were measured from CDCl_3 (7.26 ppm), $\text{DMSO-}d_6$ (2.50 ppm) for ^1H NMR, CDCl_3 (77.0 ppm), $\text{DMSO-}d_6$ (39.5 ppm) for ^{13}C NMR and 85% phosphoric acid (0.0 ppm) for ^{31}P NMR. Oligonucleotides were purified on anion-exchange high performance liquid chromatography (HPLC) at 50 °C with a linear gradient (10–67%) of solvent I (1 M NaCl in 25 mM phosphate buffer (pH 6.0)) in solvent II (25 mM phosphate buffer (pH 6.0)) was used at a flow rate of 1.0 mL/min for 40 min. MALDI-TOF mass was performed using 3-hydroxypicolinic acid (100 mg/mL) in H_2O -diammoniumhydrogen citrate (100 mg/mL) in H_2O (10 : 1, v/v) as a matrix.

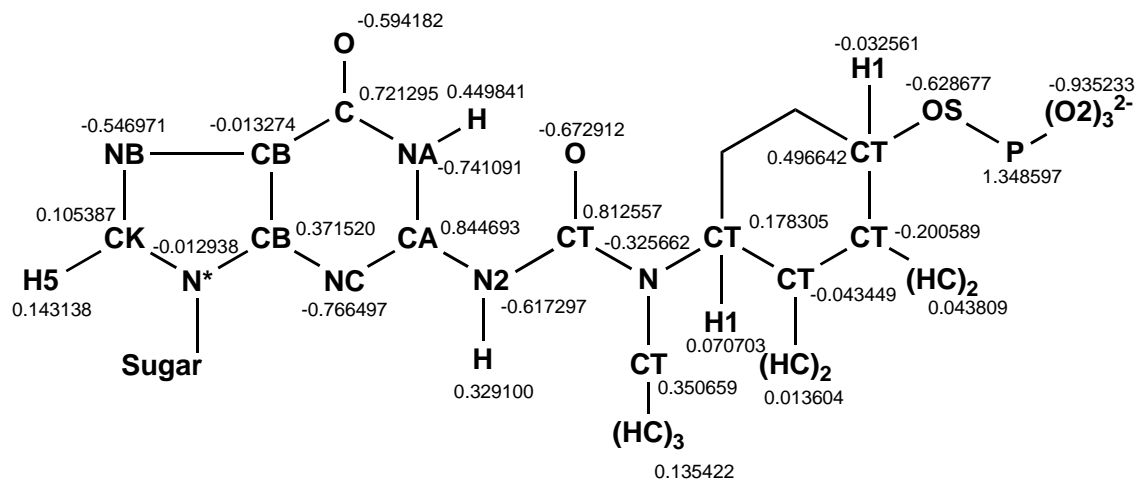
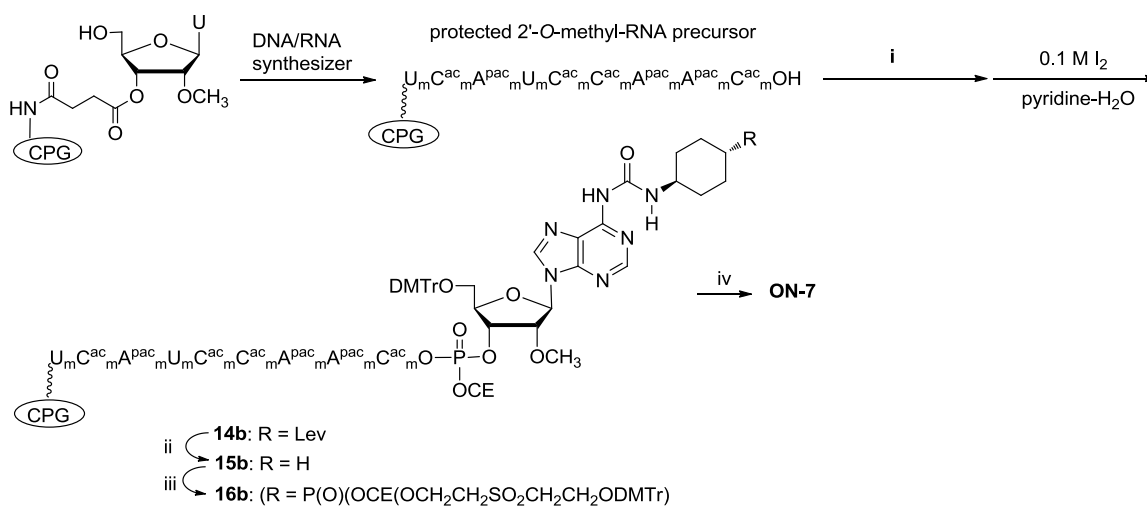
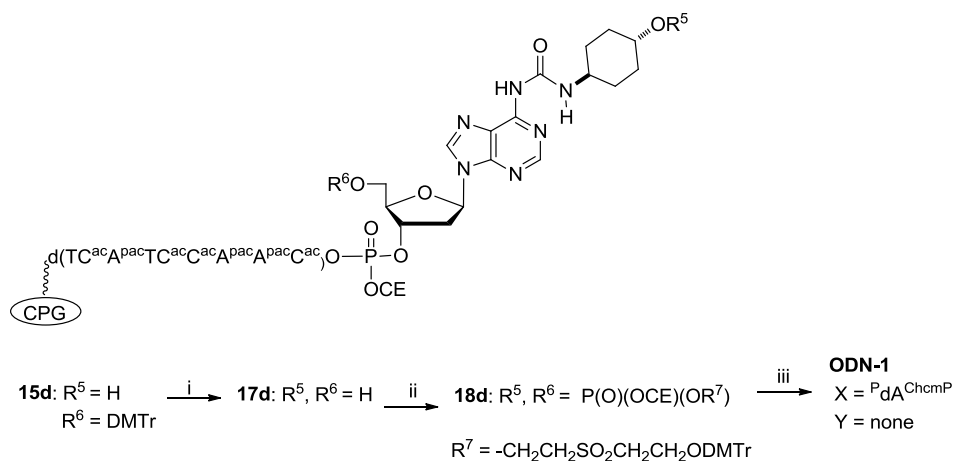
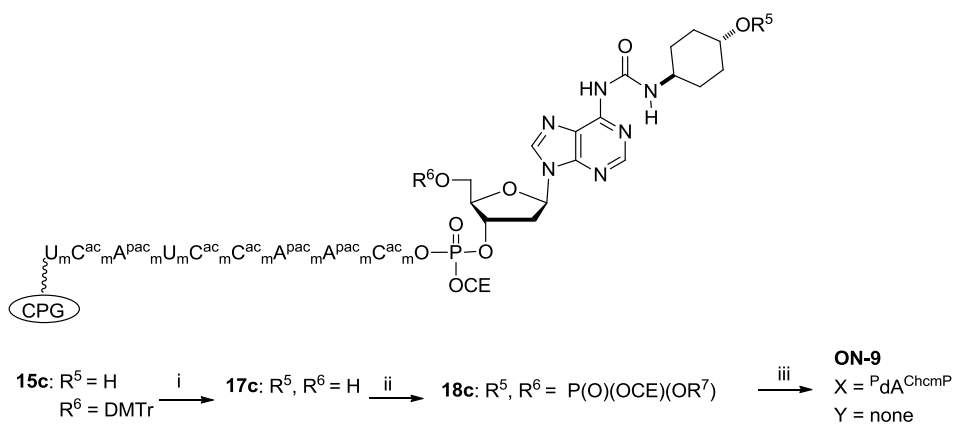


Figure S1. AMBER atom types and the partial charges of the base moiety of dG^{CmcMP}.



Reagents and conditions: i) **13b**, Activator42, CH_3CN , then 0.1 M DMAP, Ac_2O -pyridine (1:9, v/v); ii) 0.5 M NH_2NH_2 /pyridine- AcOH (3:2, v/v); iii) $\{(i\text{-Pr})_2\text{N-P(OCE)(OCH}_2\text{CH}_2\text{SO}_2\text{CH}_2\text{CH}_2\text{ODMTr})\}$, *l*H-tetrazole, CH_3CN , 1 min} x2, then 0.1 M I_2 /pyridine- H_2O (9:1, v/v); iv) 28% aq. NH_3 8h, then 2% aq. TFA on C18-cartridge column.

SCHEME S1. Preparation of **ON-7** incorporating A_m^{ChmP} .



Reagents and conditions: i) 3% dichloroacetic acid/ CH_2Cl_2 ; ii) $\{(i\text{-Pr})_2\text{N-P}(\text{OCE})(\text{OCH}_2\text{CH}_2\text{SO}_2\text{CH}_2\text{CH}_2\text{ODMTTr}), 1H\text{-tetrazole}, \text{CH}_3\text{CN}, 1 \text{ min}\} \times 2$, then 0.1 M I_2 /pyridine- H_2O (9:1, v/v); iv) 28% aq. NH_3 , then 2% aq. TFA on C18-cartridge column.

Scheme S2. Preparation of **ON-9** and **ODN-1**.

