Supporting Information

Synthesis and Properties of 5-Cyano Substituted Nucleoside Analog with a Donor-Donor-Acceptor Hydrogen Bonding Pattern

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¹ H and ¹³ C NMR spectra of compound 14
¹ H and ¹³ C NMR spectra of compound 4
¹ H and ¹³ C NMR spectra of compound 15
¹ H and ³¹ P NMR spectra of compound 16

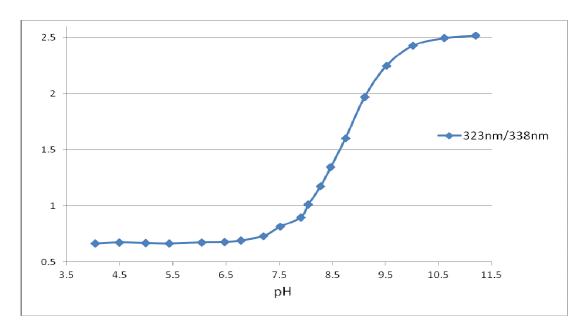


Figure S1. The ratio of absorbance at 323 nm and 338 nm measured as a function of pH give an estimate of the pK_a of 2'-deoxyribonucleoside **4** (cyano-d**Z**) to be 8.8.

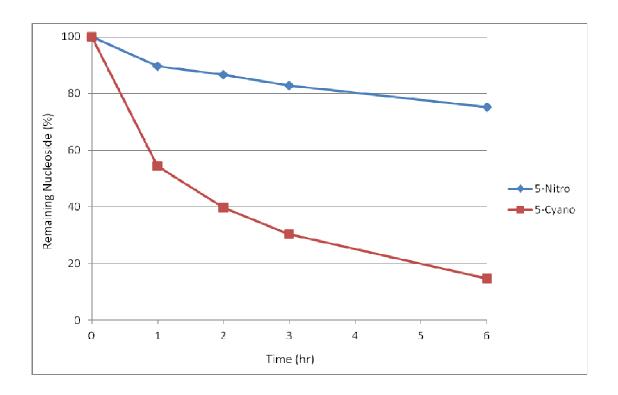


Figure S2. Epimerization of 5-nitro and 5-cyano (4) substituted pyDDA nucleosides at pH 2.1 and room temperature.

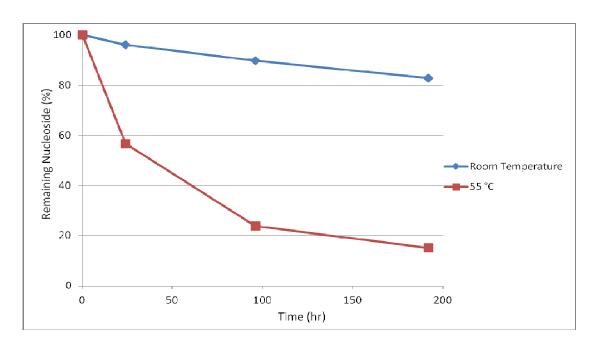


Figure S3. Time courses of epimerization of 5-cyano substituted py-DDA nucleoside (4) at pH 7.0 and room temperature or 55 °C.

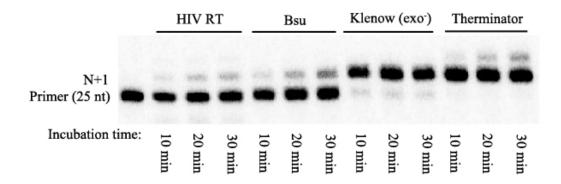
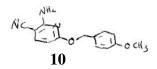
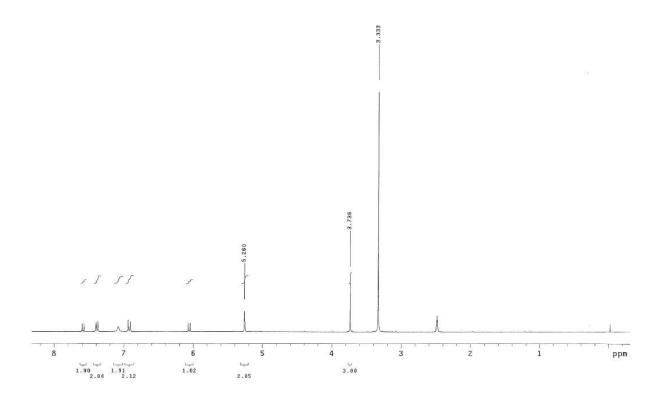
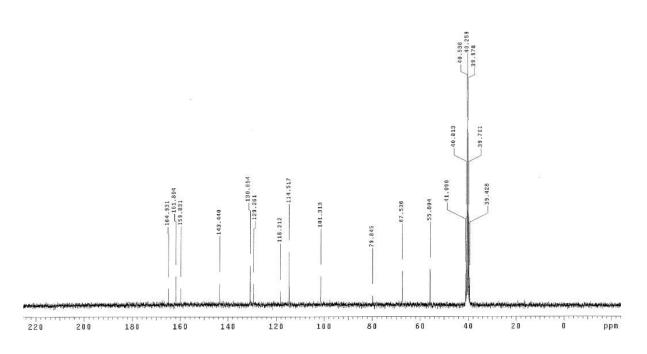


Figure S4. Standing-start primer extension showing the time course of polymerases as they incorprate cyano-d**ZTP** (**16**) opposite template d**P**.

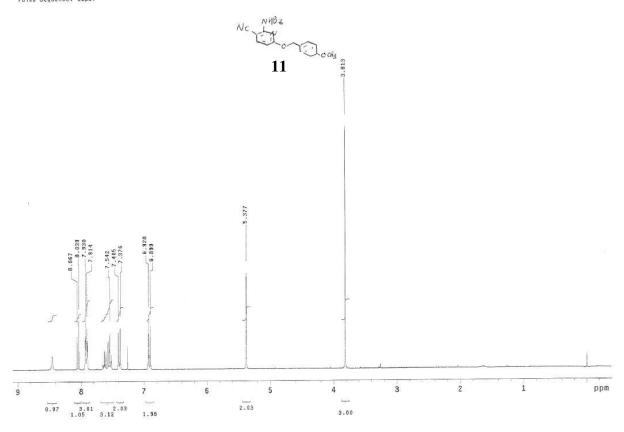


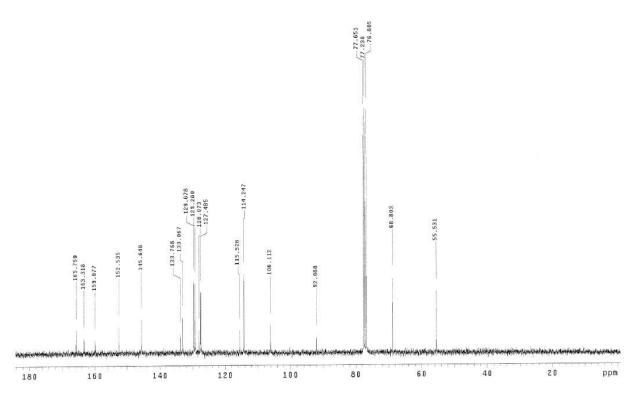


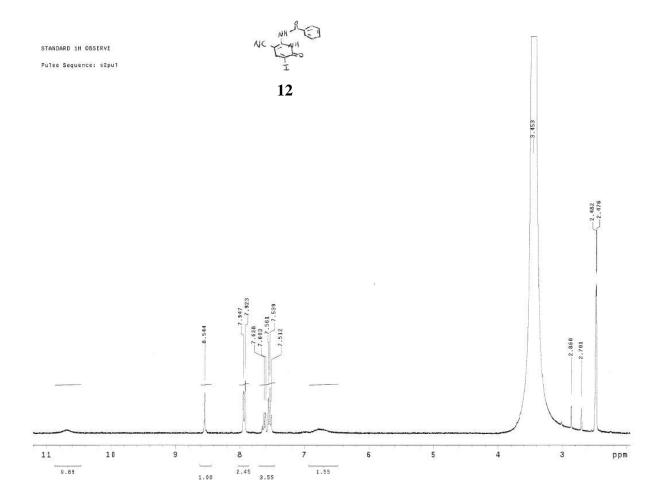




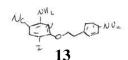
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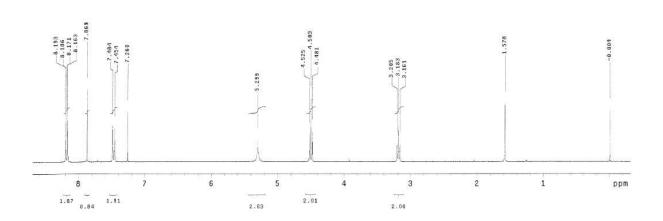


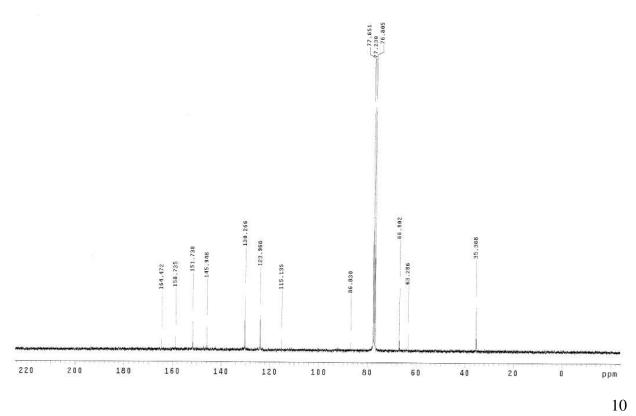




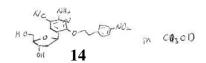
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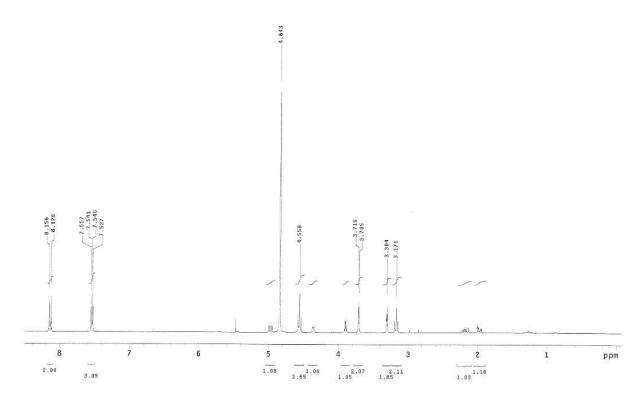


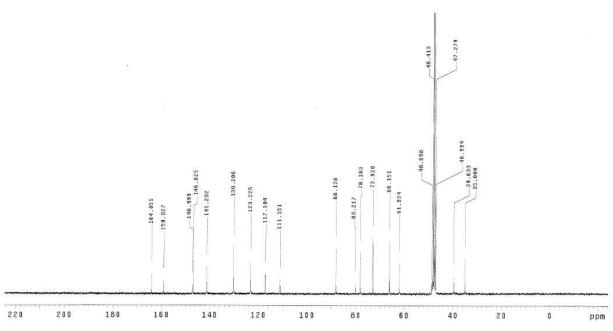


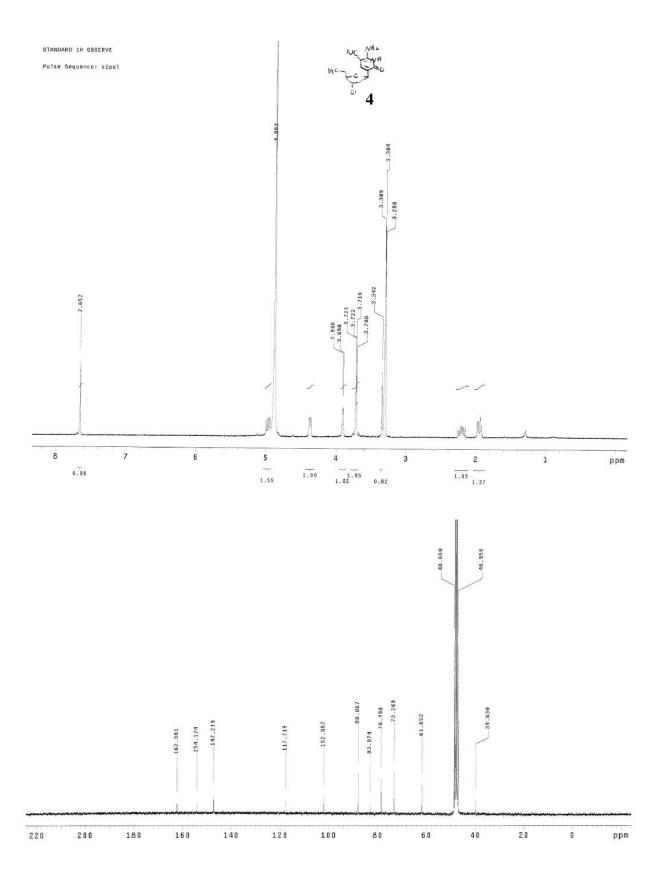












STANDARD 1H OBSERVE
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