Synthesis of Acyclothymidine Triphosphate and α -*P*-Boranotriphosphate and Their Substrate Properties with Retroviral Reverse Transcriptase

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Spectral data for compounds 5a and 5b.

NMR were obtained on a Varian spectrometer operating at 400 MHz for ^1H NMR and 161.9 MHz for ^{31}P NMR in D_2O . The chemical shift for ^{31}P NMR was reported in ppm relative to 85% H_3PO_4 as an external reference.

Acyclothymidine triphosphate (acTTP) 5a: ^1H NMR (D_2O) δ 7.44 (s, 1H, H-6), 5.09 (s, 2H, NCH_2), 3.96 (m, 2H, $\text{P}(\text{O})\text{OCH}_2$), 3.67 (m, 2H, CH_2O), 1.73 (s, 3H, CH_3 -5); ^{31}P NMR (D_2O) δ -9.72 (d, 1P, γ -P, $J_{\beta\gamma} = 13.11$ Hz), -10.07 (d, 1P, α -P, $J_{\alpha\beta} = 13.44$ Hz), -21.98 (m, 1P, β -P); UV (H_2O) λ_{max} 265.2 nm; FAB-MS m/z 438.9 [(M-H) $^-$]; HRMS found: m/z 438.9702, calcd for $\text{C}_8\text{H}_{14}\text{N}_2\text{O}_{13}\text{P}_3^-$: 438.9709.

Figure 1. RP-HPLC profile for ammonium salt of acyclothymidine triphosphate (acTTP) 5a

	Peak Name	RT	Area	% Area	Height
1	Peak1	18.131	49691646	98.48	750472
2	Peak2	20.493	769086	1.52	18188

*Acyclothymidine (α -P-borano)triphosphate (acTTP- α -BH₃) **5b***: ¹H NMR (D₂O) δ 7.42 (s, 1H, H-6), 5.06 (s, 2H, NCH₂), 3.94 (dt, J = 10, 4.8 Hz, 2H, P(O)OCH₂), 3.67 (t, J = 4.8 Hz, 2H, CH₂O), 1.72 (s, 3H, CH₃-5), 0.20 (br, 3H, BH₃); ³¹P NMR (D₂O) δ 84.58 (br, 1P, α -P), -6.13 (d, 1P, γ -P, $J_{\beta\gamma}$ = 24.45 Hz), -21.98 (t, 1P, β -P, J = 21.69 Hz); UV (H₂O) λ_{max} 265.2 nm; FAB-MS m/z 437.0 (M⁻); HRMS found: m/z 437.0101 (for ¹¹B), calcd for C₈H₁₇BN₂O₁₂P₃⁻: 437.0087.

Figure 2. RP-HPLC profile for ammonium salt of acyclothymidine (α -P-borano)triphosphate (acTTP- α -BH₃) **5b**