Supporting Information

4'-epi-DNA: A DNA mimic containing 4'-hydroxymethyl- α -L-xylo-thymidine with compact backbone like RNA

Seema Bagmare¹, Vedvati G. Puranik,² Moneesha Fernandes¹ and
Vaijayanti A. Kumar^{1*}

¹Organic Chemistry Division, ²Center for Material Characterization, CSIR-National Chemical Laboratory, Pune 411008 India

	Page No.
Crystal data	S2-S4
Compound 2 : ¹ H, ¹³ C NMR and DEPT NMR	S5
Compound 3 : ¹ H, ¹³ C NMR and DEPT NMR	S6
Compound 4 : ¹ H, ¹³ C NMR and DEPT NMR	S7
Compound 6 : ¹ H, ¹³ C NMR and DEPT NMR	S8
Compound 7 : ¹ H, ¹³ C NMR and DEPT NMR	S9
Compound 8 : ¹ H, ¹³ C NMR and DEPT NMR	S10
Compound 9 : ¹ H, ¹³ C NMR and DEPT NMR	S11
Compound 10 : ¹ H, ¹³ C NMR and DEPT NMR	S12
HRMS of compounds 2-4, 6-10	S13-16
³¹ P NMR Compound 11	S17
HPLC and MALDI-TOF analysis of ON1 and ON2	S18-19
Melting curves for ON1-ON2 oligomers with complementary DNA/RNA and corresponding first derivative curves.	S20

Crystal Data:

Single crystals of the compound were grown by slow evaporation of the solution in CDCl_3 . Colourless crystal of approximate size $0.19 \times 0.14 \times 0.11 \text{ mm}^3$, was used for data collection on *Bruker SMART APEX* CCD diffractometer using $\text{Mo K}\alpha$ radiation with fine focus tube with 50kV and 30mA. Crystal to detector distance 6.05 cm, 512 x 512 pixels / frame, quadrant data acquisition. Total frames = 2424, Oscillation / frame -0.3° , exposure / frame = 10.0 sec / frame, maximum detector swing angle = -30.0° , beam center = (260.2, 252.5), in plane spot width = 1.24, SAINT integration, θ range = 1.69 to 25.00° , completeness to θ of 25.0° is 99.9.0 %. SADABS correction applied, $\text{C}_{17}\text{H}_{30}\text{N}_2\text{O}_6\text{Si}$, $M = 386.52$. Crystals belong to Monoclinic, space group $P2_1$, $a = 10.4579(5)$, $b = 16.8927(8)$, $c = 12.7383(6) \text{ \AA}$, $V = 2125.20(17) \text{ \AA}^3$, $Z = 4$, $D_c = 1.208 \text{ g/cc}$, $\mu (\text{MoK}\alpha) = 0.143 \text{ mm}^{-1}$, $T = 293(2) \text{ K}$, 20740 reflections measured, 7468 unique [$I > 2\sigma(I)$], R value 0.0543, $wR2 = 0.1287$. All the data were corrected for Lorentzian, polarisation and absorption effects. SHELX-97 (ShelxTL)^{ref} was used for structure solution and full matrix least squares refinement on F^2 . Hydrogen atoms were included in the refinement as per the riding model. Largest diff. peak and hole 0.353 and $-0.289 \text{ e.\AA}^{-3}$. Data collection and refinement parameters are listed in table 1.

X-ray analysis revealed that there are two molecules in the asymmetric unit with slight change in conformation for silyl group. The conformation of the molecule at C1', C3' and C4' for both molecules is R, S and R respectively.

Table 1. Crystal data and structure refinement for compound **9**

Empirical formula	$\text{C}_{17}\text{H}_{30}\text{N}_2\text{O}_6\text{Si}$
Formula weight	386.52
Temperature	273(2) K
Wavelength	0.71073 $\text{\AA}$
Crystal system	Monoclinic
Space group	$P2_1$
Unit cell dimensions	$a = 10.4579(5) \text{ \AA}$ $\alpha = 90^\circ$.
	$b = 16.8927(8) \text{ \AA}$ $\beta = 109.200(1)^\circ$.
	$c = 12.7383(6) \text{ \AA}$ $\gamma = 90^\circ$.
Volume	$2125.20(17) \text{ \AA}^3$

Z	4
Density (calculated)	1.208 g/cc
Absorption coefficient	0.143 mm ⁻¹
F(000)	832
Crystal size	0.19 x 0.14 x 0.11 mm ³
Theta range for data collection	1.69 to 25.00°.
Index ranges	-12<=h<=12, -20<=k<=20, -15<=l<=15
Reflections collected	20740
Independent reflections	7468 [R(int) = 0.0265]
Completeness to theta = 25.00°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9845 and 0.9734
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	7468 / 1 / 485
Goodness-of-fit on F ²	1.071
Final R indices [I>2sigma(I)]	R1 = 0.0543, wR2 = 0.1285
R indices (all data)	R1 = 0.0656, wR2 = 0.1360
Absolute structure parameter	0.22(14)
Largest diff. peak and hole	0.353 and -0.289 e.Å ⁻³

Crystal data for compound 9

Table 1. Geometrical parameters obtained from X-ray crystal structure for compound **9**

Torsional angles	Torsional angle (deg)
v0 =[C4'- O4'- C1'- C2']	-15.3
v1 =[O4'- C1'- C2'- C3']	30.3
v2 =[C1'- C2'- C3'- C4']	-33.6
v3 =[C2'- C3'- C4'- O4']	-25.3
v4 =[C1'- O4'- C4'- C3']	6.7
χ =[O4'- C1'- N1- C2]	-147

G. M. Sheldrick, SHELX-97 program for crystal structure solution and refinement, University of Göttingen, Germany, 1997

s2 #1403 RT: 6.25 AV: 1 NL: 8.48E6
T: FTMS + p ESI Full ms [66.70-1000.00]

ALDS-7 #1-15 RT: 0.01-0.20 AV: 15 NL: 5.84E5
T: FTMS + p ESI Full ms [200.00-1200.00]

HPLC chromatogram for ON1 and ON2

Melting curves for ON1-ON2 oligomers with complementary DNA/RNA and corresponding first derivative curves.