Supporting Information

DESIGN AND SYNTHESIS OF 4'-CYANO DIDEOXY ISONUCLEOSIDES AND THEIR ACTIVITY AGAINST HIV-1 AND HBV

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X-ray Structure Determination

Crystals of **11** was mounted on the top of a glass fiber, and the data collection was carried out on a Bruker SMART diffractometer equipped with a CCD area detector at 296 K. The data were corrected for Lorentz and polarization effects, and absorption corrections were applied with the *SADABS* probram.[1] The structure was solved by direct methods and subsequent difference Fourier syntheses using the program *SHELXTL*.[2] All non-H atoms were refined anisotropically, and H atoms were placed in calculated positions and thereafter refined with *U*iso(H) = 1.2*U*eq(C).

Figure S1. ORTEP of **11**

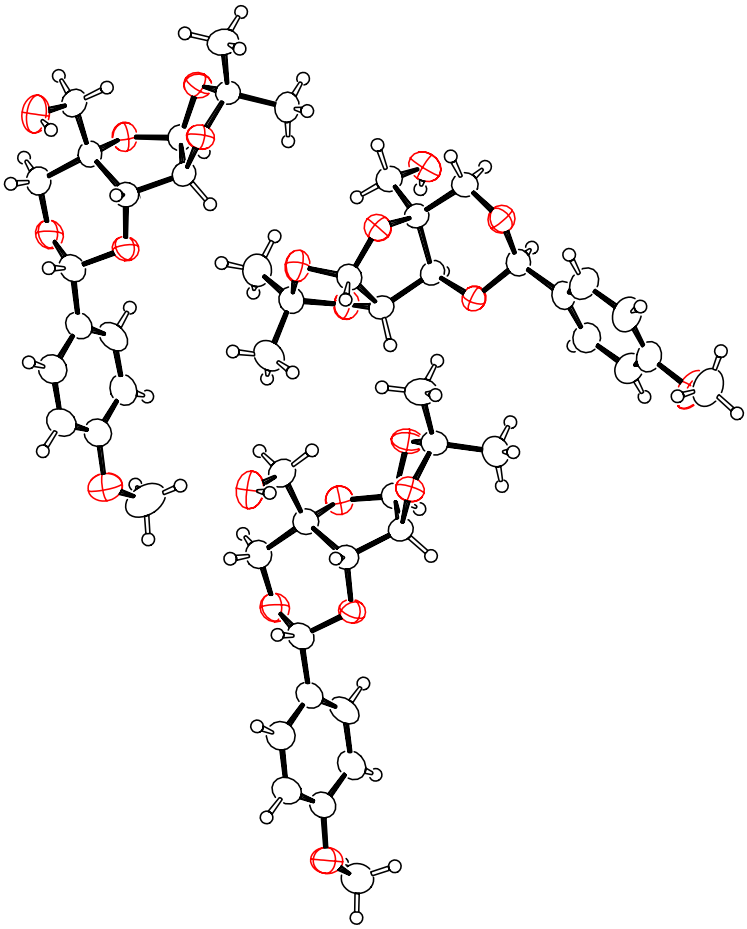

Table S1. Crystal data and structure refinement for **11**

Empirical formula	C17 H22 O7	
Formula weight	338.35	
Temperature	296 K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	*P*2(1)2(1)2(1)	
Unit cell dimensions	a = 5.5689(3) Å	$\alpha = 90°$.
	b = 29.8080(14) Å	$\beta = 90°$.
	c = 30.2386(14) Å	$\gamma = 90°$.
Volume	5019.5(4) Å^3	
Z	12	
Density (calculated)	1.343 Mg/m^3	
Absorption coefficient	0.104 mm^{-1}	
F(000)	2160	
Crystal size	0.36 x 0.23 x 0.16 mm^3	
Theta range for data collection	0.96 to 27.48°.	
Index ranges	$-5 <= h <= 7$, $-38 <= k <= 33$, $-38 <= l <= 39$	
Reflections collected	32330	
Independent reflections	11494 [R(int) = 0.0281]	
Completeness to theta = 27.48°	99.9 %	
Absorption correction	Empirical	
Max. and min. transmission	0.9834 and 0.9635	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11494 / 0 / 661	
Goodness-of-fit on F^2	1.040	
Final R indices [$I > 2$sigma(I)]	$R_1 = 0.0434$, $wR_2 = 0.1028$	
R indices (all data)	$R_1 = 0.0608$, $wR_2 = 0.1122$	
Absolute structure parameter	0.0(6)	
Largest diff. peak and hole	0.166 and -0.186 e.Å^{-3}	

References

(1) Sheldrick, G. M. Program for absorption correction of area detector frames; Bruker AXS, Inc.: Madison, WI, 1996.

(2) *SHELXTL*, *version 5.1*; Bruker AXS, Inc.: Madison, WI, 1997.