

## Supplementary Material

Table S1. Possible hydrogen bonds (Å and °) for compound **1**

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(2)-H(02)...O(3')#2	0.87(2)	2.19(4)	3.02(2)	160(7)
N(2)-H(02)...O(2)#2	0.87(2)	2.02(3)	2.877(16)	167(7)
C(2)-H(2)...O(2)#2	0.95	2.42	3.300(18)	153.2
C(36)-H(36)...O(3')#2	0.95	2.50	3.38(2)	154.0
C(4)-H(4)...O(4')#3	0.95	2.39	3.241(15)	149.5
C(14)-H(14)...O(4)#4	0.95	2.40	3.269(15)	151.6
C(14)-H(14)...O(4')#4	0.95	2.25	2.994(14)	134.9
C(25)-H(25)...O(3)#5	0.95	2.57	3.275(16)	131.1
C(26)-H(26)...O(2')#5	0.95	2.55	3.247(17)	130.8
C(17)-H(17A)...O(4)#5	0.98	2.56	3.304(16)	133.0
C(33)-H(33)...F(3')#6	0.95	2.35	3.217(15)	151.4
C(34)-H(34)...O(2')#7	0.95	2.47	3.288(16)	144.5
C(42)-H(42)...O(1)#4	0.95	2.62	3.414(8)	141.7

Symmetry transformations used to generate equivalent atoms: #1 -x+2,-y+1,-z+1; #2 x,y-1,z; #3 -x+2,-y+2,-z+1; #4 -x+1,-y+1,-z+1; #5 x-1,y-1,z; #6 -x,-y+1,-z; #7 -x+1,-y+1,-z

Table S2. Possible hydrogen bonds (Å and °) for compound **5**.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(12)-H(12)...O(3)	0.81(3)	2.17(3)	2.956(3)	164(3)
N(11)-H(11)...O(2)#1	0.78(3)	2.40(3)	3.150(3)	162(3)
C(8)-H(8)...O(1)#3	0.95	2.57	3.292(3)	133.2
C(2)-H(2)...O(2)#1	0.95	2.45	3.323(3)	152.7

Symmetry transformations used to generate equivalent atoms:

#1  $y, -x+1, z+1/4$ ; #2  $-y+1, x, z-1/4$ ; #3  $-y, x, z-1/4$