Supplemetary Information

Synthesis of uracil containing nusleoside phosphonates substituted at C-6 position through aerobic ligand-free Suzuki-Miyaura cross-coupling

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Table S1 Optimization of Suzuki-Miyaura cross coupling of nucleoside **7** and boronic acid **10a**.

Entry	Product	Catalyst	Solvent system	Base	Time (min)	Temperature (°C)	Yield (%)[a]
1.	**8a**	$Ph(PPh_3)_4$	DMF:H_2O (8:1)	K_2CO_3	45	120	3
2.	**8a**	$Ph(PPh_3)_4$	THF	Cs_2CO_3	180	50	0
3.	**8a**	$Pd(dppf)Cl_2.CH_2Cl_2$	Toluene:H_2O (4:1)	K_2CO_3	45	100	66
4.	**8a**	$Pd(dppf)Cl_2.CH_2Cl_2$	CH_3CN:H_2O (4:1)	K_2CO_3	45	80	0
5.	**8a**	$Pd(dppf)Cl_2.CH_2Cl_2$	THF:H_2O (4:1)	K_2CO_3	45	70	trace

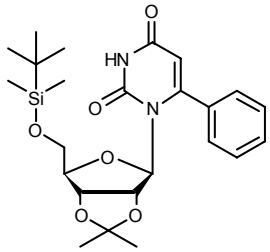
[a] Isolated yields.

Table S2 Screening of the reaction conditions for Suzuki-Miyaura coupling of substrate **18** with boronic acid **10b**.

Entry	Catalyst	Ligand	Solvent system	Base	Time (min)	Temperature (°C)	Yields (%)[a]
1.	$Pd(AcO)_2$ (30%)	TPPTS (30%)	CH_3CN:H_2O (2:1)	Cs_2CO_3	45	rt-90	43
2.	$Pd(AcO)_2$ (10%)	-	CH_3CN:H_2O (2:1)	Cs_2CO_3	45	90	21
3.	$Pd(dppf)Cl_2.CH_2Cl_2$ (10%)	-	Toluene:H_2O (4:1)	K_2CO_3	45	100	0
4.	$Pd(dppf)Cl_2.CH_2Cl_2$ (10%)	-	CH_3CN:H_2O (2:1)	Cs_2CO_3	45	90	5
5.	Pd/C (10%)	-	MeOH	Cs_2CO_3	90 and 45	rt and 90	14
6.	$Pd(AcO)_2$ (10%)	TPPTS (10%)	CH_3CN:H_2O (2:1)	Cs_2CO_3	45	90	0
7.	$Pd(AcO)_2$ (10%)	TPPTS (30%)	CH_3CN:H_2O (2:1)	Cs_2CO_3	45	90	0
8.	$Pd(AcO)_2$ (10%)	TPPTS (30%)	CH_3CN:H_2O (2:1)	Cs_2CO_3	45	55	14
9.	$Pd(AcO)_2$ (10%)	TPPTS (30%)	CH_3CN:H_2O (2:1)	Cs_2CO_3	60 and 40	rt and 40	15
10.	$Pd(AcO)_2$ (10%)	-	*i*PrOH:H_2O (2:1)	K_2CO_3	20	60	43

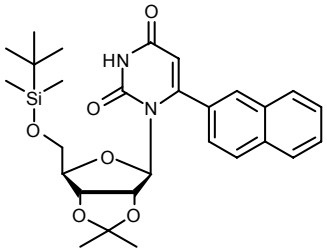
[a] Isolated yields of **13b**.

Yield, ^{1}H NMR, ^{13}C NMR and HR MS data of intermediates



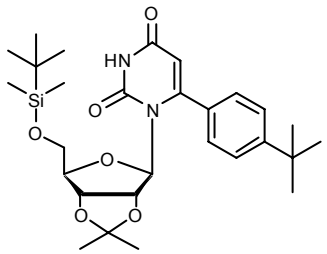
1-((3a*R*,4*R*,6*R*,6a*R*)-6-((tert-butyldimethylsilyloxy)methyl)-2,2-dimethyltetrahydro-furo[3,4-*d*][1,3]dioxol-4-yl)-6-phenylpyrimidine-2,4(1*H*,3*H*)-dione 8a

The product **8a** (75 mg, 83%) was isolated as beige oil. δ_H (300 MHz, DMSO-d_6, DMSO) 0.03 (6 H, s, 2×SiCH_3), 0.86 (9 H, s, *t*-Bu), 1.22 (3 H, s, *i* -Pr), 1.27 (3 H, s, *i* -Pr), 3.77 (2 H, br d, $J_{5',4'}$ 6.4, 5'-H), 3.89 (1 H, ddd, $J_{4',5'a}$ 5.8, $J_{4',5'b}$ 7.0, $J_{4',3'}$ 4.0, 4'-H), 4.70 (1 H, dd, $J_{3',2'}$ 6.3, $J_{3',4'}$ 3.9, 3'-H), 5.24 (1 H, dd, $J_{2',3'}$ 6.3, $J_{2',1'}$1.0, 2'-H), 5.29 (1 H, d, $J_{1',2'}$ 1.0,1'-H), 5.53 (1 H, s, 5-H), 7.44-7.50 (2 H, m, Ar), 7.53-7.59 (3 H, m, Ar), 11.59 (1 H, s, NH); δ_C (75 MHz, DMSO-d_6, DMSO) -5.27, -5.18, 18.07, 25.06, 25.78, 26.85, 63.78, 81.97, 83.73, 89.09, 92.47, 103.61, 112.37, 128.06, 129.01, 130.36, 132.76, 150.78, 155.17, 162.19; *m/z* 475.2259 (ESI) (M+H$^+$. $C_{24}H_{35}N_2O_6Si^+$ requires 475.2259).



1-((3a*R*,4*R*,6*R*,6a*R*)-6-((tert-butyldimethylsilyloxy)methyl)-2,2-dimethyltetrahydro-furo[3,4-*d*][1,3]dioxol-4-yl)-6-(naphthalen-2-yl)pyrimidine-2,4(1*H*,3*H*)-dione 8b

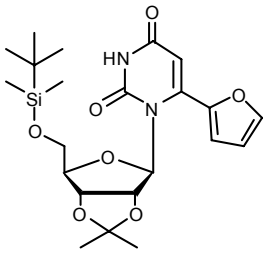
The product **8b** (81 mg, 81%) was isolated as slightly colored oil. δ_H (300 MHz, DMSO-d_6, DMSO) 0.03 (6 H, s, 2×SiCH_3), 0.86 (9 H, s, *t*-Bu), 1.22 (3 H, s, *i* -Pr), 1.27 (3 H, s, *i* -Pr), 3.77 (2 H,br d, $J_{5',4'}$ 6.4, 5'-H), 3.89 (1 H, ddd, $J_{4',5'a}$ 5.8, $J_{4',5'b}$ 7.0, $J_{4',3'}$ 4.0, 4'-H), 4.70 (1 H, dd, $J_{3',2'}$ 6.3, $J_{3',4'}$ 3.9, 3'-H), 5.24 (1 H, dd, $J_{2',3'}$ 6.3, $J_{2',1'}$1.0, 2'-H), 5.29 (1 H, d, $J_{1',2'}$ 1.0,1'-H), 5.53 (1 H, s, 5-H), 7.44-7.50 (2 H, m, Ar), 7.53-7.59 (3 H, m, Ar), 11.59 (1 H, s, NH); δ_C (75 MHz, DMSO-d_6, DMSO) -5.19, -5.28, 18.05, 25.01, 25.76, 26.79, 63.80, 81.90, 83.78, 89.12, 92.55, 103.97, 112.38, 127.27, 127.79, 128.37, 128.45, 130.12, 132.33, 133.15, 150.75, 155.15, 162.13; *m/z* 525,2425 (ESI) (M+H$^+$. $C_{28}H_{37}N_2O_6Si^+$ requires 525,2415).



1-((3a*R*,4*R*,6*R*,6a*R*)-6-((*tert*-Butyldimethylsilyloxy)methyl)-2,2-dimethyltetrahydro-furo[3,4-*d*][1,3]dioxol-4-yl)-6-(4-*tert*-butylphenyl)pyrimidine-2,4(1*H*,3*H*)-dione 8c

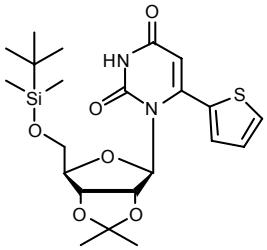
The product **8c** (83 mg ,82%) was isolated as beige oil. δ_H (300 MHz, DMSO-d_6, DMSO) 0.03 (6 H, s, 2×SiCH_3), 0.86 (9 H, s, Si*t*-Bu), 1.22 (2 H, s, *i* -Pr), 1.27 (3 H, s, *i* -Pr), 1.31 (8 H, s, *t*-Bu), 3.77 (2 H, d, $J_{5',4'}$ 6.6, 5'-H), 3.92 (1 H, dt, $J_{4',5'}$ 6.5, $J_{4',3'}$ 3.9, 4'-H), 4.71 (1 H, dd,

$J_{3',2'}$ 6.3, $J_{3',4'}$ 3.8, 3'-H), 5.23 (1 H, dd, $J_{2',3'}$ 6.3, $J_{2',1'}$ 1.1, 2'-H), 5.35 (1 H, d, , $J_{1',2'}$ 1.1, 1'-H), 5.51 (1 H, d, $J_{5,NH}$ 2.2, 5-H), 7.44 – 7.34 (2 H, m, Ph), 7.62 – 7.52 (2 H, m, Ph), 11.56 (1 H, d, $J_{NH,5}$ 1.9, NH); δ C (75 MHz, DMSO-d_6, DMSO) -5.20, -5.30, 18.04, 24.98, 25.76, 26.78, 30.88, 34.63, 63.77, 81.98, 83.70, 89.10, 92.41, 103.53, 112.29, 125.79, 127.82, 129.89, 150.79, 153.02, 155.22, 162.08; *m/z* 531.2882 (ESI) ($M+H^+$. $C_{28}H_{43}N_2O_6Si^+$ requires 531.2885).



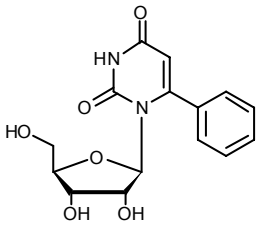
1-((3a*R*,4*R*,6*R*,6a*R*)-6-((tert-butyldimethylsilyloxy)methyl)-2,2-dimethyltetrahydro-furo[3,4-*d*][1,3]dioxol-4-yl)-6-(furan-2-yl)pyrimidine-2,4(1*H*,3*H*)-dione 8d

The product **8d** was obtained during modified procedure (using *o*-xylene instead toluene) as colourless oil (58 mg, 66 %). δ $_H$ (300 MHz, DMSO-d_6, DMSO) 0.01 (6 H, s, 2×SiCH_3), 0.85 (9 H, s, *t*-Bu), 1.26 (3 H, s, *i* -Pr), 1.39 (3 H, s, *i* -Pr), 3.76 (2 H, m, 5'-H), 4.01 (1 H, ddd, $J_{4',5'a}$ 6.2, $J_{4',5'b}$ 7.0, $J_{4',3'}$ 4.1, 4'-H), 4.75 (1 H, dd, $J_{3',2'}$ 6.2, $J_{3',4'}$ 4.1, 3'-H), 5.25 (1 H, dd, $J_{2',3'}$ 6.2, $J_{2',1'}$0.9, 2'-H), 5.63 (1 H, d, $J_{1',2'}$ 0.9,1'-H), 5.82 (1 H, d, $J_{1',2'}$ 2.2, 5-H), 6.75 (1 H, dd, $J_{4'',3''}$ 3.5, $J_{4'',5''}$ 1.6, 4''-H), 7.06 (1 H, dd, $J_{3'',4''}$ 3.5, $J_{3'',5''}$ 0.6, 3''-H), 7.56 (1 H, dd, $J_{5'',3''}$ 0.6, $J_{5'',4''}$ 0.6, 3''-H), 11.60 (1 H, d, $J_{NH,5}$ 1.8, NH); δ $_C$ (75 MHz, DMSO-d_6, DMSO) -5.32, –5.21, 18.03, 25.13, 25.77, 26.95, 63.78, 82.03, 84.01, 89.47, 93.02, 102.43, 112.38, 112.04, 114.77, 144.13, 144.36, 146.41, 150.69, 162.18; *m/z* 465,2050 (ESI) ($M+H^+$. $C_{22}H_{33}N_2O_7Si^+$ requires 465,2052).



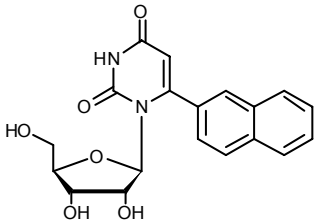
1-((3a*R*,4*R*,6*R*,6a*R*)-6-((*tert*-Butyldimethylsilyloxy)methyl)-2,2-dimethyltetrahydrofuro [3,4-*d*][1,3]dioxol-4-yl)-6-(thiophen-2-yl)pyrimidine-2,4(1*H*,3*H*)-dione 8e

The product **8e** was obtained during modified procedure (using *o*-xylene instead toluene) as colourless oil (9 mg, 10 %). δ $_H$ (300 MHz, DMSO-d_6, DMSO) 0.02 (6 H, s, 2×SiCH_3), 0.86 (9 H, s, *t*-Bu), 1.24 (3 H, s, *i* -Pr), 1.34 (3 H, s, *i* -Pr), 3.77 (2 H, d, $J_{5',4'}$ 6.5, 5'-H), 3.96 (1 H, dt, $J_{4',5'}$ 6.5, $J_{4',3'}$ 3.9, 4'-H), 4.72 (1 H, dd, $J_{3',2'}$ 6.3, $J_{3',4'}$ 3.9, 3'-H), 5.24 (1 H, dd, $J_{2',3'}$ 6.3, $J_{2',1'}$1.0, 2'-H), 5.60 (1 H,br s, 1'-H), 5.69 (1 H, d, $J_{5,NH}$ 2.2, 5-H), 7.25 (1 H, dd, *J* 5.1, 3.6, Ar), 7.42 (1 H, dd, *J* 3.6, 1.2, Ar), 7.88 (1 H, dd, *J* 5.1, 1.2, Ar), 11.62 (1 H, d, $J_{NH,5}$ 1.9, NH); δ $_C$ (75 MHz, DMSO-d_6, DMSO) -5.29, -5.19, 18.05, 25.08, 25.77, 25.88, 26.89, 63.82, 81.99, 83.82, 89.41, 92.39, 104.64, 112.32, 128.14, 130.16, 130.23, 132.36, 148.36, 150.64, 161.76; *m/z* 481.1804 (ESI) ($M+H^+$. $C_{22}H_{33}N_2O_6SSi^+$ requires 481.1823).



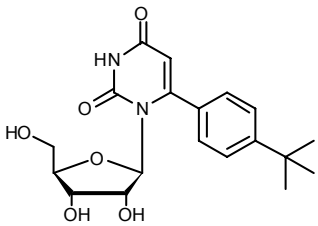
1-((2*R*,3*R*,4*S*,5*R*)-3,4-Dihydroxy-5-(hydroxymethyl)tetrahydrofuran-2-yl)-6-phenylpyrimidine-2,4(1*H*,3*H*)-dione 9a

The product **9a** (89 mg ,93%) was isolated as beige solid.δ_H (300 MHz, DMSO-d_6, DMSO) 3.37-3.63 (3 H, m, 4' and 5'-H), 4.02 (1 H, ddd, *J* 2.0, *J* 5.8, *J* 11.6, 3'-H), 4.60 (1 H, m, 2'-H and OH), 4.82 (1 H, d, *J* 6.1, OH), 5.05 (1 H, d, *J* 5.4, OH), 5.07 (1 H, d, *J* 3.9, 1'-H), 5.51 (1 H, s, 5-H), 7.46-7.58 (5 H, m, Ar), 11.47 (1 H, s, NH); δ_C (75 MHz, DMSO-d_6, DMSO) 62.15, 69.94, 70.93, 84.88, 93.63, 103.63, 128.08, 128.81, 130.17, 133.13, 150.62, 156.06, 162.13; *m/z* 319.0936 (negESI) ($M-H^+$. $C_{15}H_{15}N_2O_6^-$ requires 319.0936).



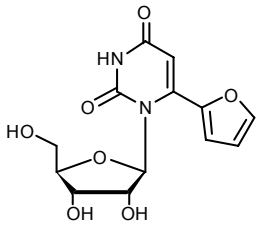
1-((2*R*,3*R*,4*S*,5*R*)-3,4-dihydroxy-5-(hydroxymethyl)tetrahydrofuran-2-yl)-6-(naphthalen-2-yl)pyrimidine-2,4(1*H*,3*H*)-dione 9b

The product **9b** (68 mg, 61%) was isolated as white solid. δ_H (300 MHz, DMSO-d_6, DMSO) 3.39-3.63 (3 H, m, 4' and 5'-H), 4.01 (1 H, dd, *J* 5.9, *J* 11.8, 3'-H), 4.62 (1 H, m, 2'-H and OH), 4.79 (1 H, d, *J* 6.1, OH), 5.05 (1 H, d, *J* 5.3, OH), 5.12 (1 H, d, *J* 3.9, 1'-H), 5.66 (1 H, d, *J* 1.9, 5-H), 7.55-7.69 (5 H, m, Ar), 7.98-8.12 (5 H, m, Ar), 11.54 (1 H,br s, NH); δ_C (75 MHz, DMSO-d_6, DMSO) 62.13, 69.92, 70.88, 84.89, 93.75,103.97, 127.11, 127.64, 127.71, 127.94, 128.23, 128.45, 130.56, 132.33, 133.16, 150.64, 156.08, 162.16; *m/z* 369,1090 (negESI) ($M-H^+$. $C_{19}H_{17}N_2O_6^-$ requires 369,1092).



6-**(4-tert-butylphenyl)-1-((2*R*,3*R*,4*S*,5*R*)-3,4-dihydroxy-5-(hydroxymethyl)tetrahydrofuran-2-yl)pyrimidine-2,4(1*H*,3*H*)-dione 9c**

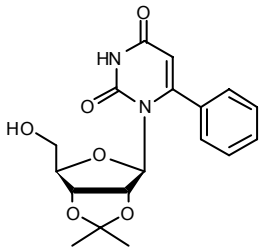
The product **9c** (103 mg, 91%) was isolated as pale yellow solid. δ_H (300 MHz, DMSO-d_6, DMSO) 1.32 (9 H, s), 3.39-3.64 (3 H, m, 4' and 5'-H), 4.00-4.08 (1 H, m, 3'-H), 4.52 – 4.67 (2 H, m, 2'-H and OH), 4.84 (1 H, d, *J* 6.2, OH), 5.07 (1 H, d, *J* 5.1, OH), 5.13 (1 H, d, *J* 3.8, 1'-H), 5.50 (1 H, d, *J* 1.9, 5-H), 7.41-7.58 (4 H, m, Ar), 11.47 (1 H, s, NH); δ_C (75 MHz, DMSO-d_6, DMSO) 30.93, 34.63, 62.19, 69.98, 71.00, 84.96, 93.64,103.52, 125.63, 127.84, 130.29, 150.68, 152.87, 156.10, 162.13; *m/z* 375,1565 (negESI) ($M-H^+$. $C_{19}H_{23}N_2O_6^-$ requires 375,1562).



1-((2R,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)tetrahydrofuran-2-yl)-6-(furan-2-yl)pyrimidine-2,4(1H,3H)-dione 9d

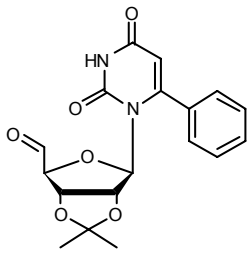
The product **9d** (91 mg, 98%) was isolated as white solid. δ_H (300 MHz, DMSO-d_6, DMSO) 3.45 (1H, dd, $J_{5'a,\ 5'b}$ 11.6, $J_{5'a,\ 4'}$ 6.3, 5'a -H), 3.61 (1H, dd, $J_{5'b,\ 5'a}$ 11.6, $J_{5'b,\ 4'}$ 3.7, 5'b-H), 3.69 (1H, ddd, $J_{4',3'}$ 6.0, $J_{4',5'a}$ 3.7, $J_{4',5'b}$ 6.3, 4'-H), 4.08 (1H, dd, $J_{3',2'} \sim J_{3',4'}$ 6.0, 3'-H), 4.60 (1H, dd, $J_{2',3'}$ 6.1, $J_{2',1'}$ 3.8 Hz, 2'-H), 5.39 (1H, d, $J_{1',2'}$ 3.8, H-1'), 5.81 (1H, d, $J_{5,NH}$ 2.1, 5-H), 6.75 (1H, dd, $J_{4'',3''}$ 3.5, $J_{4'',5''}$ 1.8, 4''-H); 7.12 (1H, dd, $J_{3'',4''}$ 3.5, $J_{3'',5''}$ 0.6, H-3''); 7.56 (1H, dd, $J_{5'',3''}$ 0.6, $J_{5'',4''}$ 1.8, H-4''); 11.60 (1H, d, $J_{NH,5}$ 1.8, NH);

δ_C (75 MHz, DMSO-d_6, DMSO) 62.11, 69.95, 71.02, 84.90, 93.98, 102.08, 112.36, 114.65, 144.30, 145.24, 146.20, 150.49, 162.19; *m/z* 309.0734 (negESI) ($M\text{-}H^+$, $C_{13}H_{13}N_2O_7^-$requires 309.0728).



1-((3a*R*,4*R*,6*R*,6a*R*)-6-(Hydroxymethyl)-2,2-dimethyltetrahydrofuro[3,4-*d*][1,3]dioxol-4-yl)-6-phenylpyrimidine-2,4(1*H*,3*H*)-dione 11

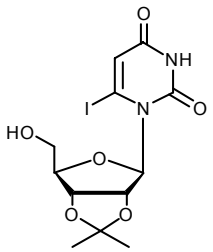
δ_H (300 MHz, DMSO-d_6, DMSO) 1.23 (3 H, s, *i* -Pr), 1.27 (3 H, s, *i* -Pr), 3.47 – 3.62 (2 H, m, 5'-H), 3.86 (1 H, ddd, $J_{4',5'a} \sim J_{4',5'b}$ 6.3, $J_{4',3'}$ 4.1, 4'-H), 4.72 (1 H, dd, $J_{3',2'}$ 6.3, $J_{3',4'}$ 4.1, 3'-H), 4.79 (1 H, t, *J* 5.6, OH), 5.24 (1 H, dd, $J_{2',3'}$ 6.3, $J_{2',1'}$1.4, 2'-H), 5.28 (1 H, d, $J_{1',2'}$ 1.5,1'-H), 5.53 (1 H, s, 5-H), 7.45-7.52 (2 H, m, Ar), 7.53-7.59 (3 H, m, Ar), 11.56 (1 H, s, NH); δ_C (75 MHz, DMSO-d_6, DMSO) 25.09,26.92, 61.92, 81.91, 83.50, 88.83, 92.33, 103.53, 112.40, 128.07, 128.97, 130.33, 132.74, 150.63, 155.20, 162.15; *m/z* 361,1397 (ESI) ($M+H^+$. $C_{18}H_{21}N_2O_6^+$ requires 361,1394).



(3a*S*,4*S*,6*R*,6a*R*)-6-(2,4-Dioxo-6-phenyl-3,4-dihydropyrimidin-1(2*H*)-yl)-2,2-dimethyltetrahydrofuro[3,4-*d*][1,3]dioxole-4-carbaldehyde 12

δ_H (300 MHz, DMSO-d_6, DMSO) 1.24 (3 H, s, *i* -Pr), 1.27 (3 H, s, *i* -Pr), 4.48 (1 H, d, *J* 1.2, 4'-H), 4.97 (1 H, dd, $J_{3',2'}$ 6.3, $J_{3',4'}$ 1.2, 3'-H), 5.17 (1 H, d, *J* 6.3, 2'-H), 5.43 (1 H, s,1'-H), 5.61 (1 H, s, 5-H), 7.46-7.66 (5 H, m, Ar), 9.37 (1H, s, 5'-H), 11.72 (1 H, s, NH); δ_C (75 MHz, DMSO-d_6, DMSO) 24.39.26.03, 84.05, 84.49, 93.28, 94.46, 103.87, 111.90, 128.55,

129.24, 130.49, 132.46, 151.71, 154.87, 162.12, 200.82; *m/z* 359,1239 (ESI) ($M+H^+$. $C_{18}H_{19}N_2O_6^+$ requires 359,1238).



1-((3a*R*,4*R*,6*R*,6a*R*)-6-(Hydroxymethyl)-2,2-dimethyltetrahydrofuro[3,4-*d*][1,3]dioxol-4-yl)-6-iodopyrimidine-2,4(1*H*,3*H*)-dione 16

δ_H (300 MHz, DMSO-d_6, DMSO) 1.28 (3 H, s, CH_3), 1.49 (3 H, s, CH_3), 3.50 (2 H, m, 5'-H), 3.98 (1 H, ddd, $J_{4',3'}$ 4.1, $J_{4',5'a} \sim J_{4',5'b}$ 6.4, 4'-H), 4.71 (1H, dd, $J_{3',2'}$ 6.4, $J_{3',4'}$ 4.1, 3'-H), 4.80 (1H, t, $J_{OH,5'}$ 6.4, OH), 5.21 (1H, dd, $J_{2',1'}$ 1.4, $J_{2',3'}$ 6.4, 2'-H), 6.00 (1H, d, , $J_{1',2'}$ 1.4, 1'-H), 6.35 (1H, d, $J_{5,NH}$ 2.1, 5-H), 11.62 (1H, d, $J_{NH,5} \sim$ 2.0, NH); δ_C (75 MHz, DMSO-d_6, DMSO) 25.18, 27.10, 61.83, 81.82, 83.79, 89.26, 100.52, 112.66 45, 115.32, 116.82, 147.58, 161.49; *m/z* 408,9896 (negESI) ($M-H^+$, $C_{12}H_{14}IN_2O_6^-$ requires 408,9902).

Conformational analysis

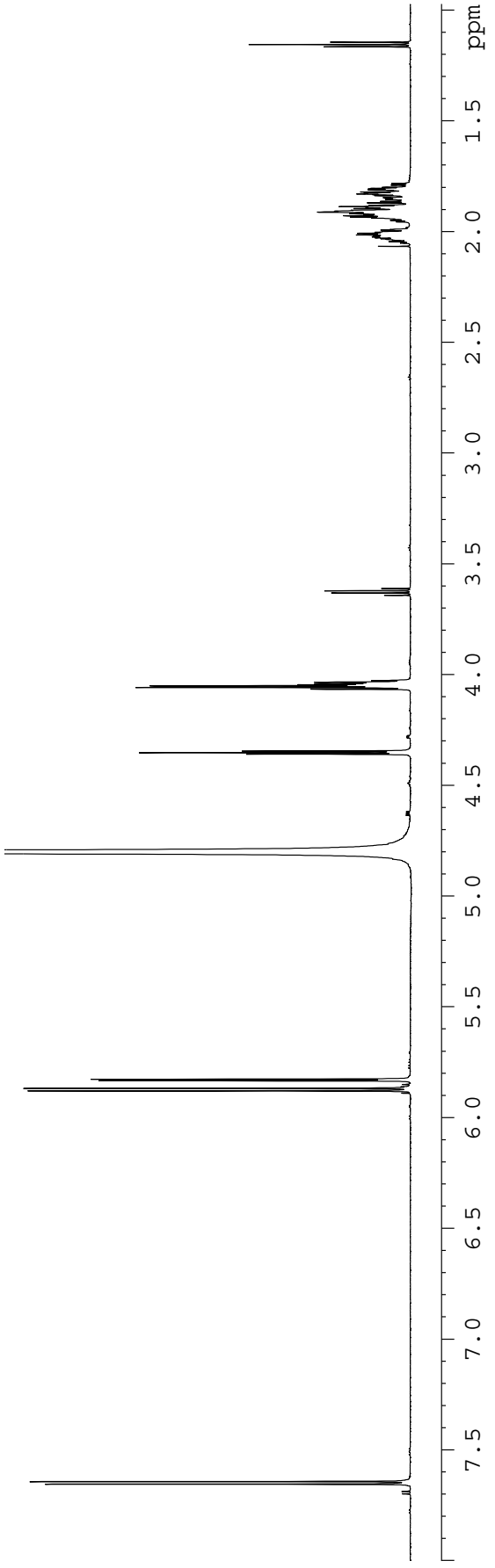


Figure S1: **5**, D_2O, 20 °C, 700 MHz

Figure S2: **22a**, D_2O, 20 °C, 700 MHz

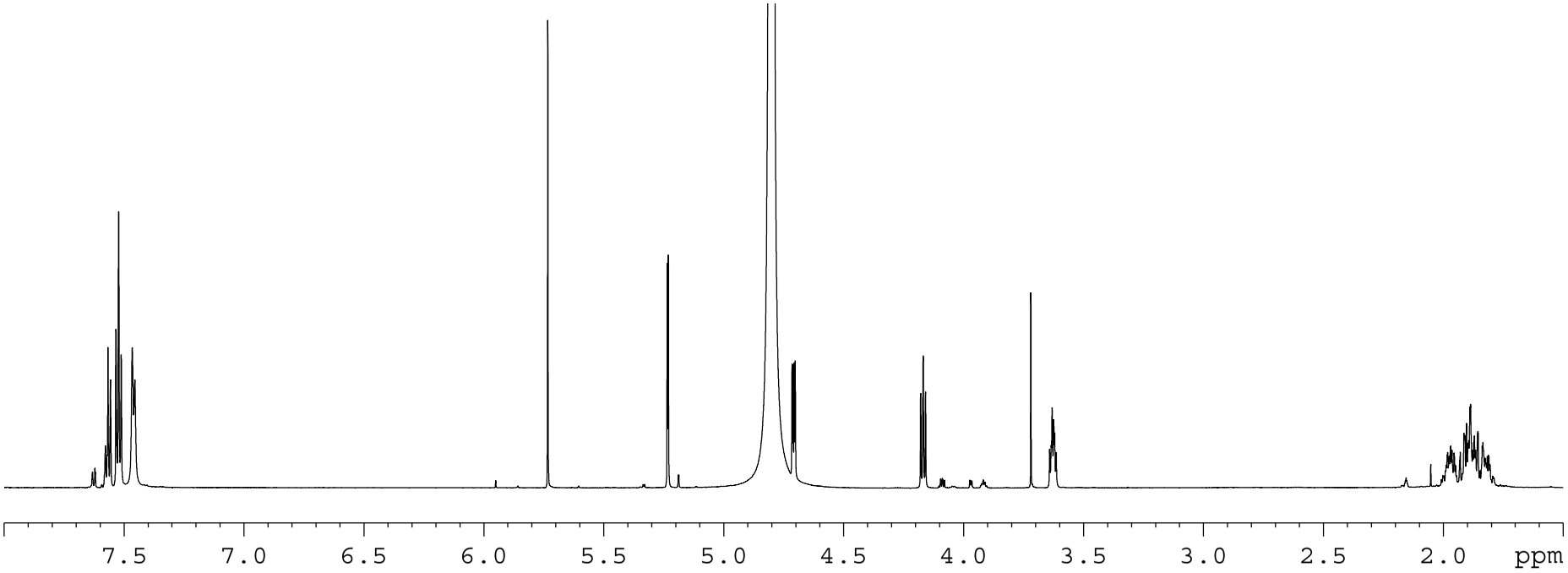


Figure S3: **9b**, DMSO-d6, 27°C, 700 MHz

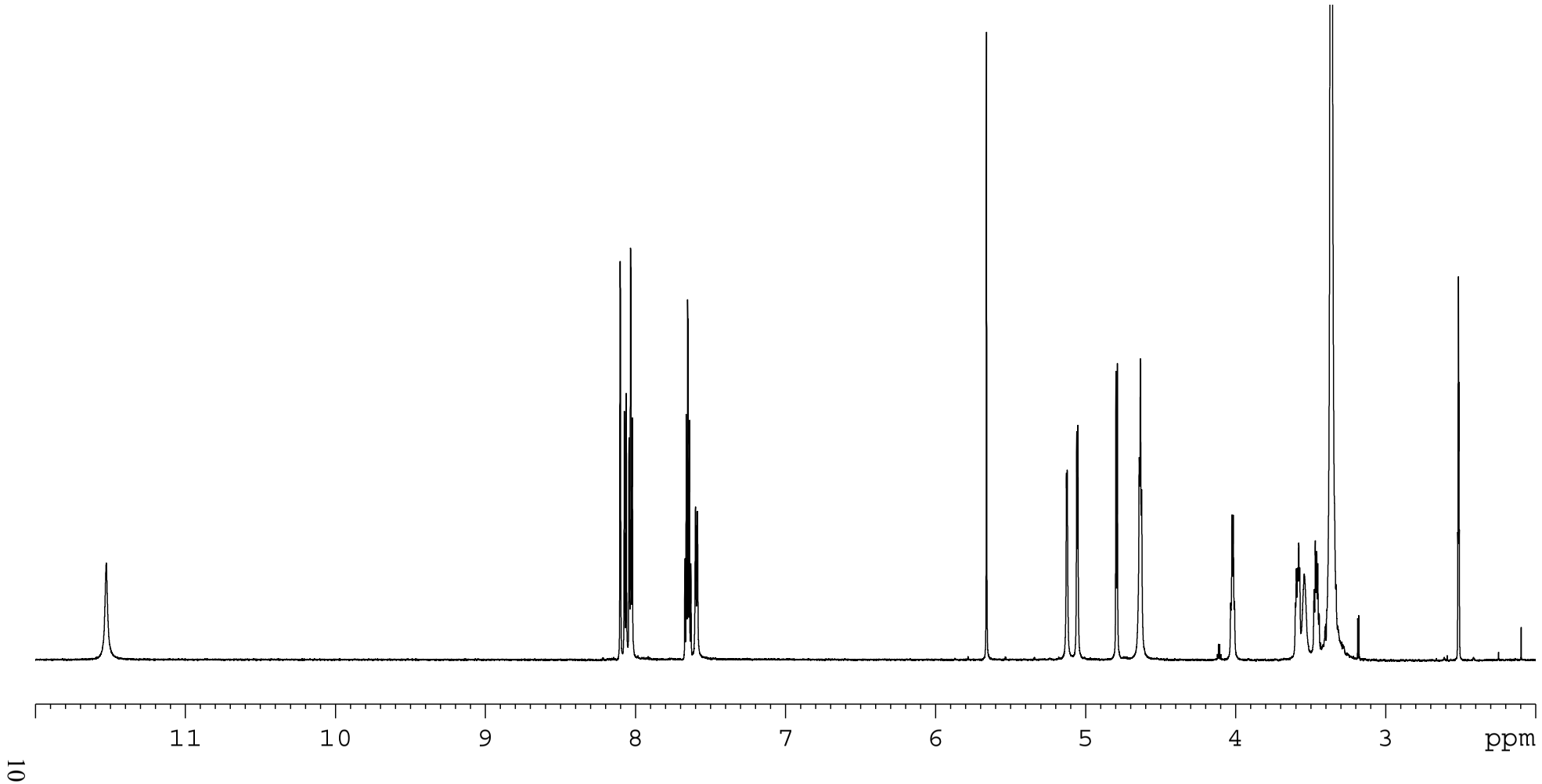


Table S3: Measured scalar couplings [Hz] for compound **5**.

T [°C]	20	27	35	42	50
H1'-H2'	4.551	4.621	4.621	4.621	4.691
H2'-H3'	5.181	5.251	5.251	5.391	5.391
H3'-H4'	5.601	5.531	5.461	5.426	5.461

Table S5: Measured scalar couplings [Hz] for compound **22a**.

T [°C]	20	27	35	42	50
H1'-H2'	3.011	3.115	3.115	3.115	3.115
H2'-H3'	6.476	6.406	6.547	6.547	6.546
H3'-H4'	7.736	7.737	7.631	7.526	7.526

Table S6: Measured scalar couplings [Hz] for compound **9b**.

T [°C]	27	35	42	50	60
H1'-H2'	3.991	3.921	3.921	3.991	4.061
H2'-H3'	5.904	6.184	5.951	5.881	5.904
H3'-H4'	6.721	6.861	5.951	5.648	5.764

Figure S4: Oberved nOe contacts for compounds **5**, **22a** and **9b**.