

# Synthesis of 2'-*O*-Methoxyethyl-Guanosine Using a Novel Silicon-Based Protecting Group

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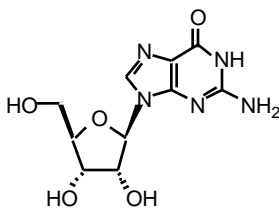
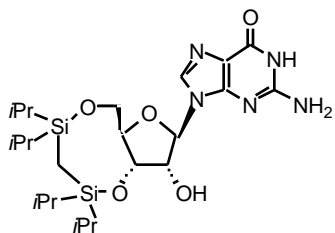
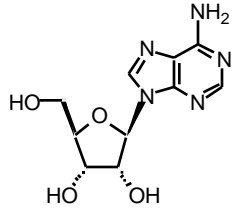
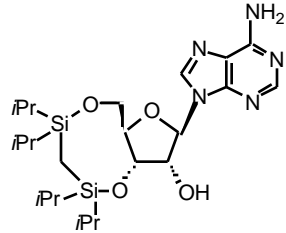
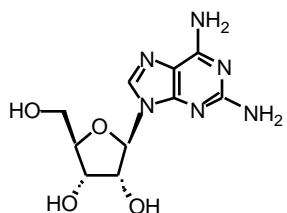
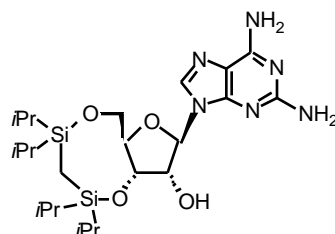
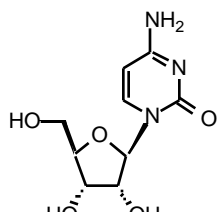
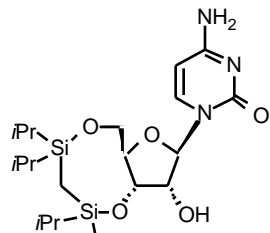
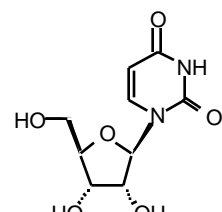
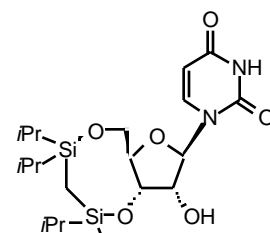
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## Supporting Information

### *Table of Contents*

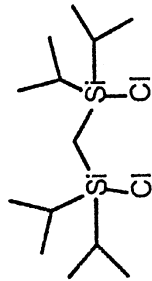
	<i>page</i>
i. Table of protection of nucleosides with <b>2</b>	2
ii. <sup>1</sup> H and <sup>13</sup> C NMR spectra (compounds <b>2-4</b> , <b>6-8</b> )	3-12
iii. X-Ray structure of compound <b>6</b>	13-29

**Table for protection of different nucleosides using MDPSCl<sub>2</sub>**

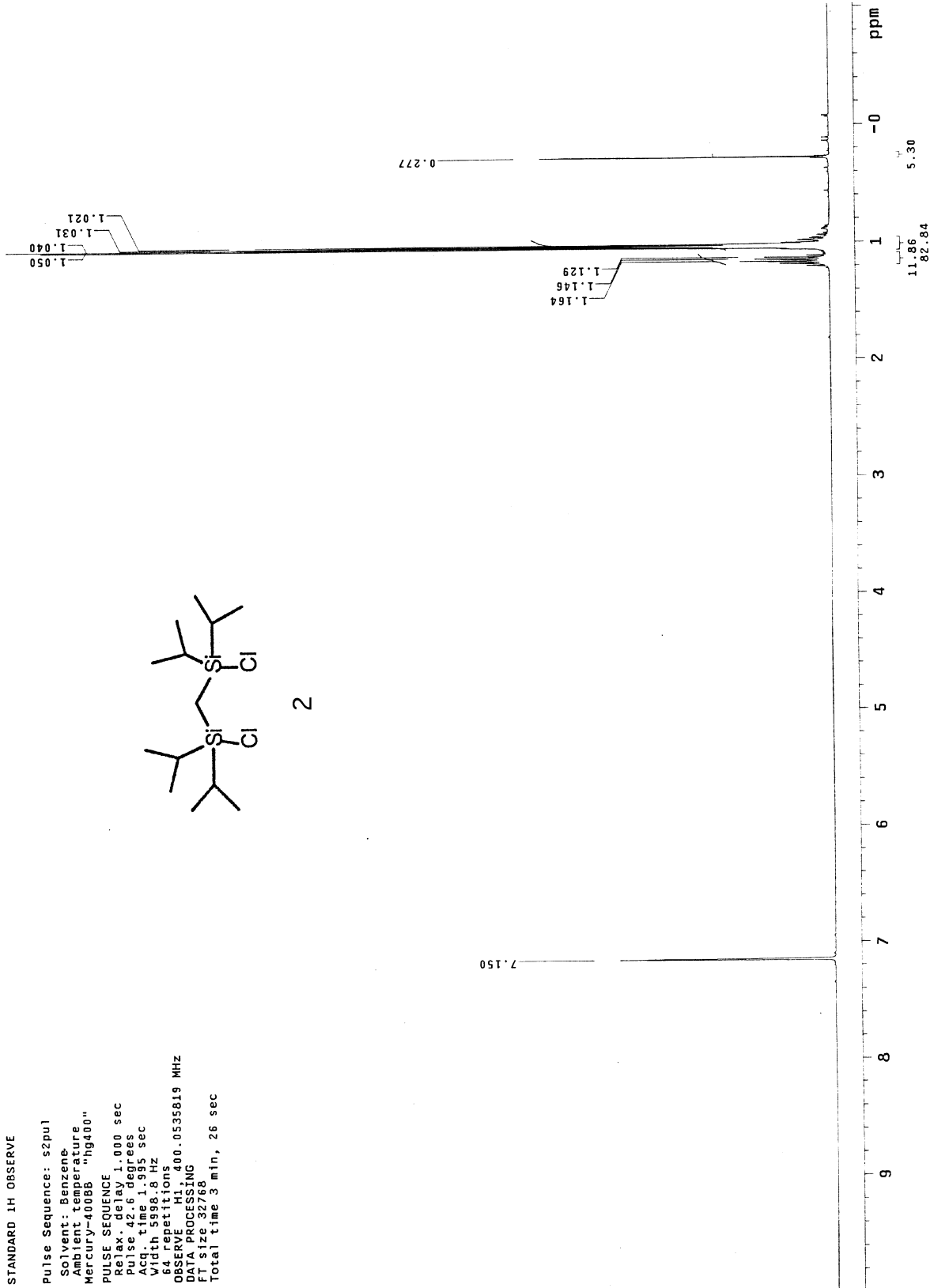
nucleoside	3',5'-O-protected nucleoside	Yield
		79%
		91%
		82%
		87%
		92%

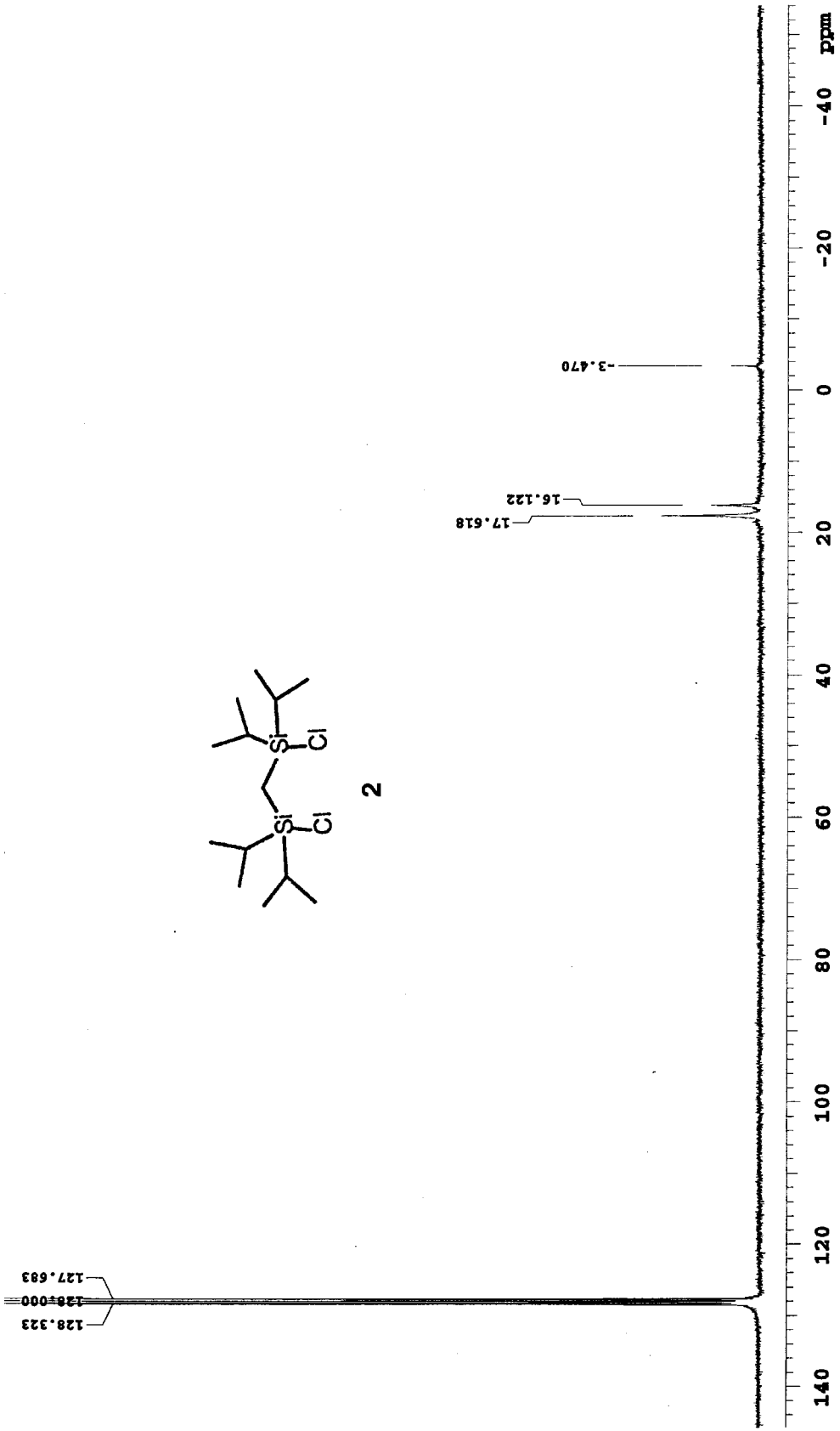
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Pulse 42.6 degrees  
Acq. time 1.955 sec  
Width 5998.8 Hz  
64 repetitions  
OBSERVE H1, 400.0535819 MHz  
DATA PROCESSING  
FT size 32768  
Total time 3 min, 26 sec



2





STANDARD 1H OBSERVE

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Solvent: CDCl3

Ambient temperature

File: KW-19

Mercury-300 "hg300"

PULSE SEQUENCE

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Acq. time 1.998 sec

Width 4500.5 Hz

64 repetitions

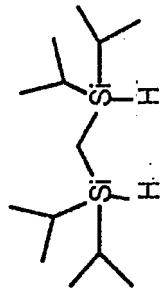
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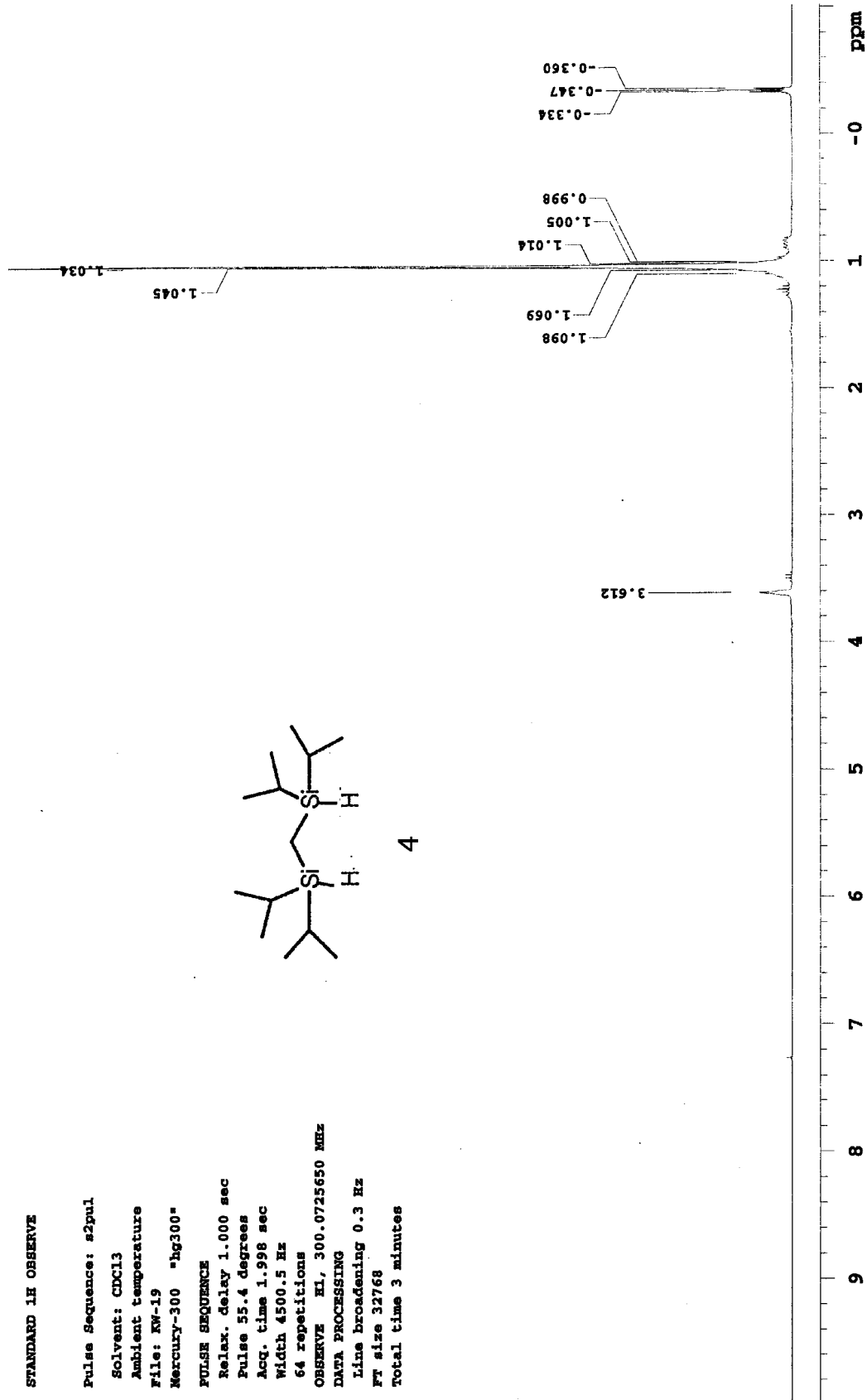
Line broadening 0.3 Hz

FT size 32768

Total time 3 minutes



4



13C OBSERVE

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

File: KW-19C

Mercury-300 "hg300"

PULSE SEQUENCE

Pulse 50.6 degrees

Acq time 1.95 sec

Width 18761.7 Hz

200 repetitions

OBSERVE C13, 75.4533063 MHz

DECOUPLE H1, 300.0740762 MHz

Power 40 dB

continuously on

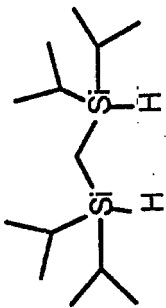
WALTZ-16 modulated

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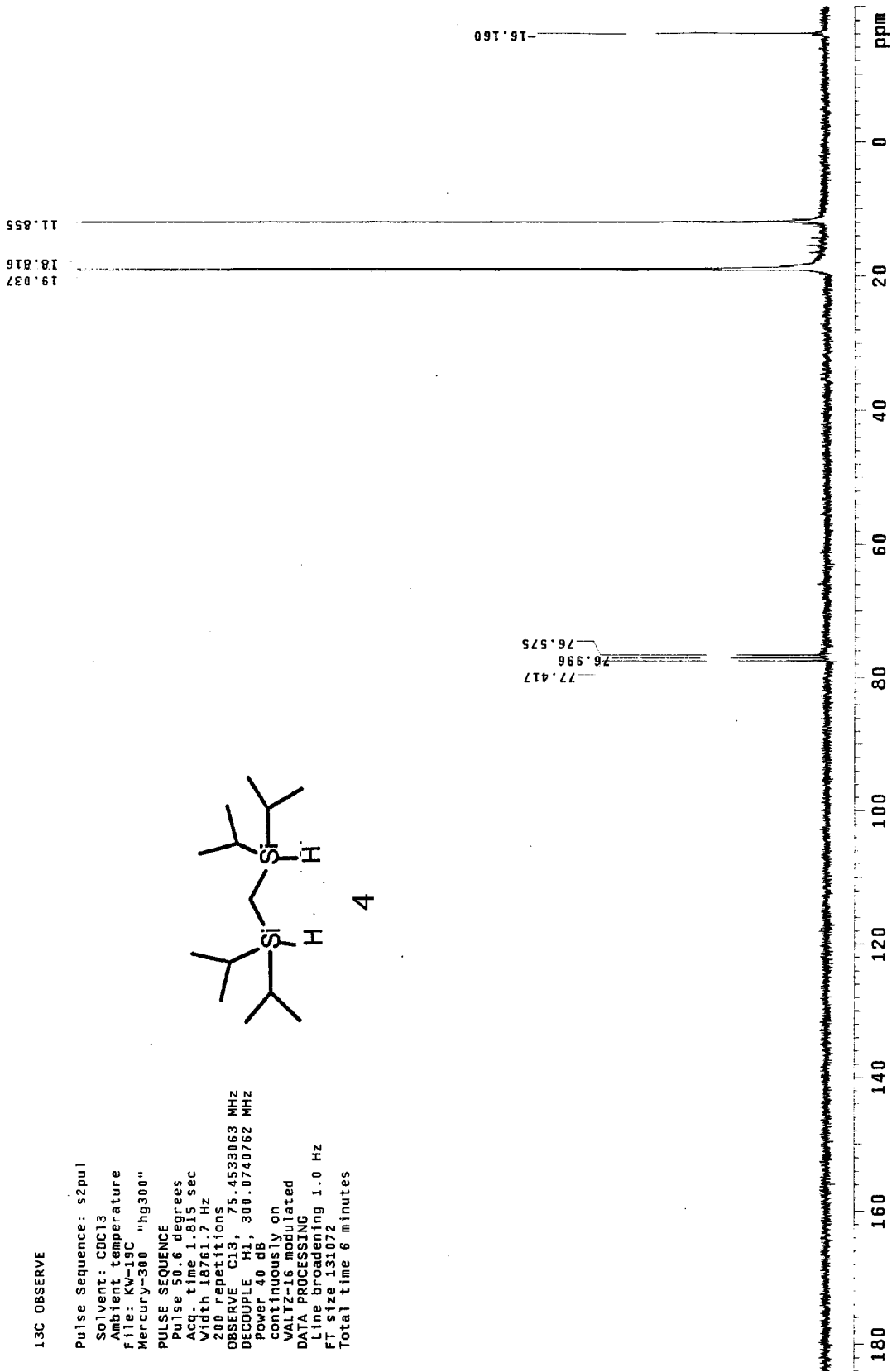
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FT size 131072

Total time 6 minutes

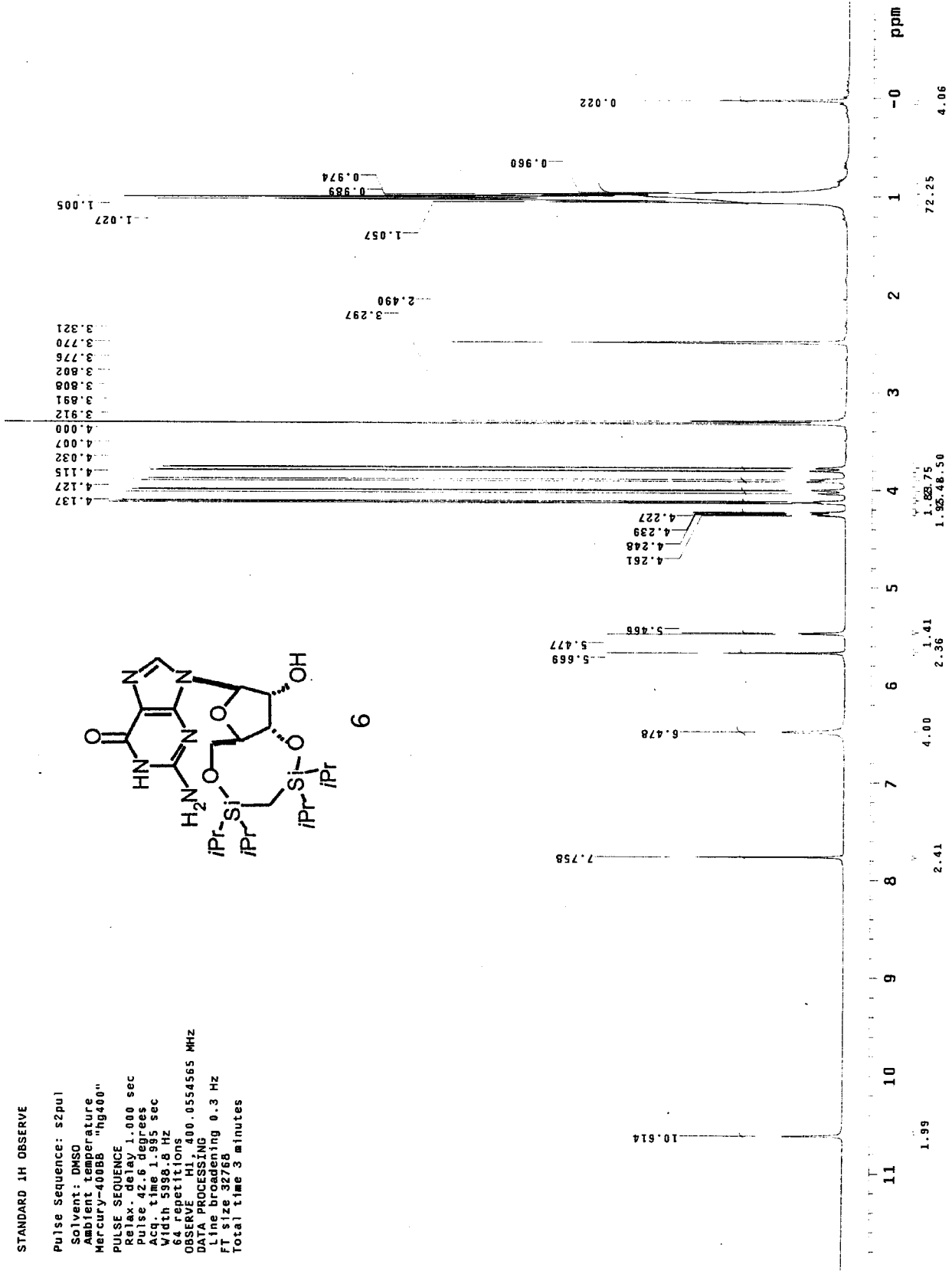
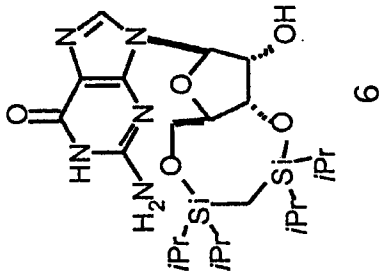


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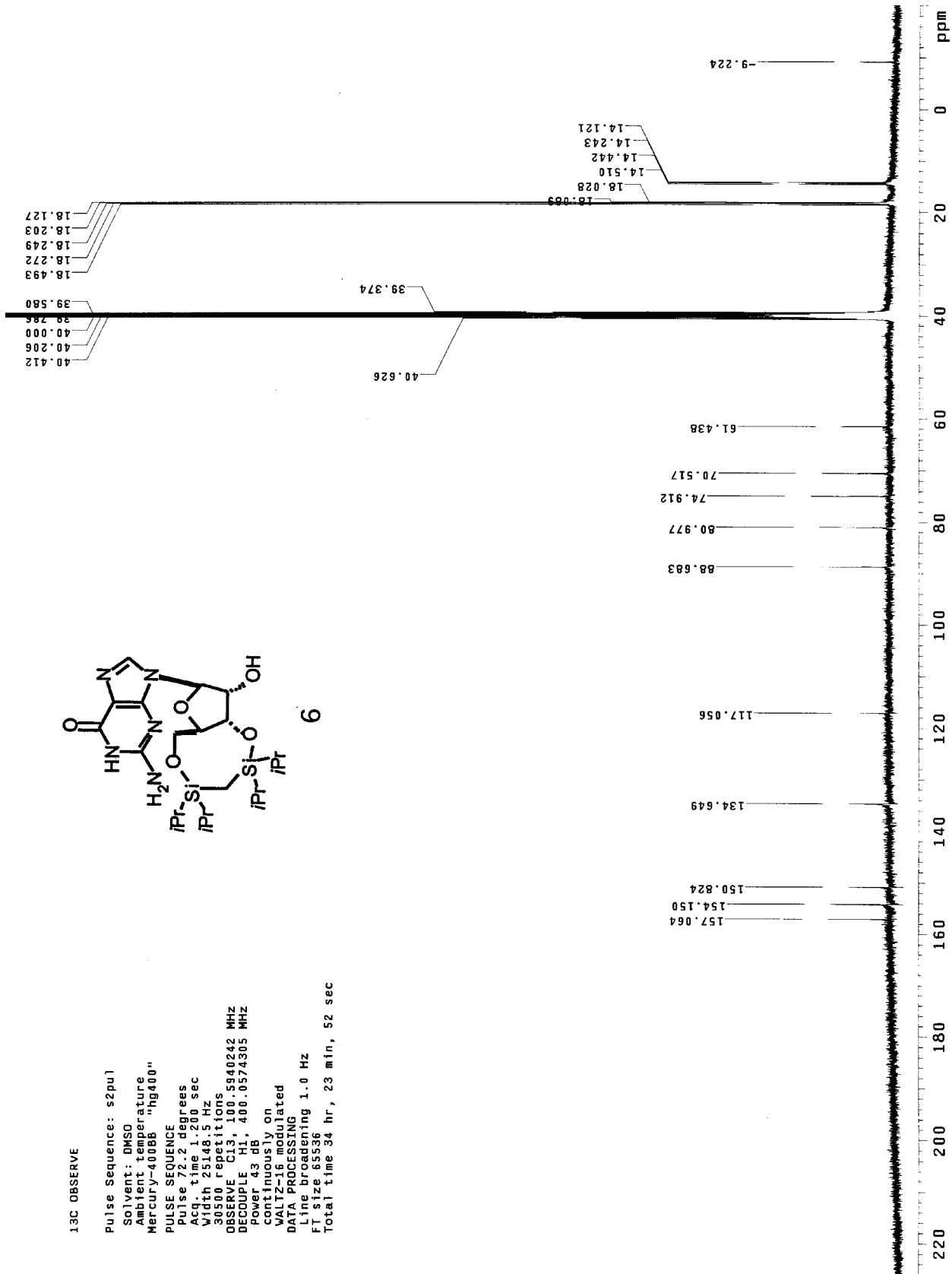
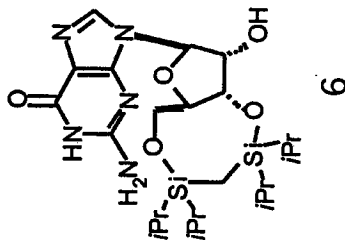
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 Ambient temperature  
 Mercury-400BB "hg400"  
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 Pulse 42.6 degrees  
 Acq. time 1.995 sec  
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 64 repetitions  
 OBSERVE RL 400.0554565 MHz  
 DATA PROCESSING  
 Line broadening 0.3 Hz  
 FT size 32788  
 Total time 3 minutes

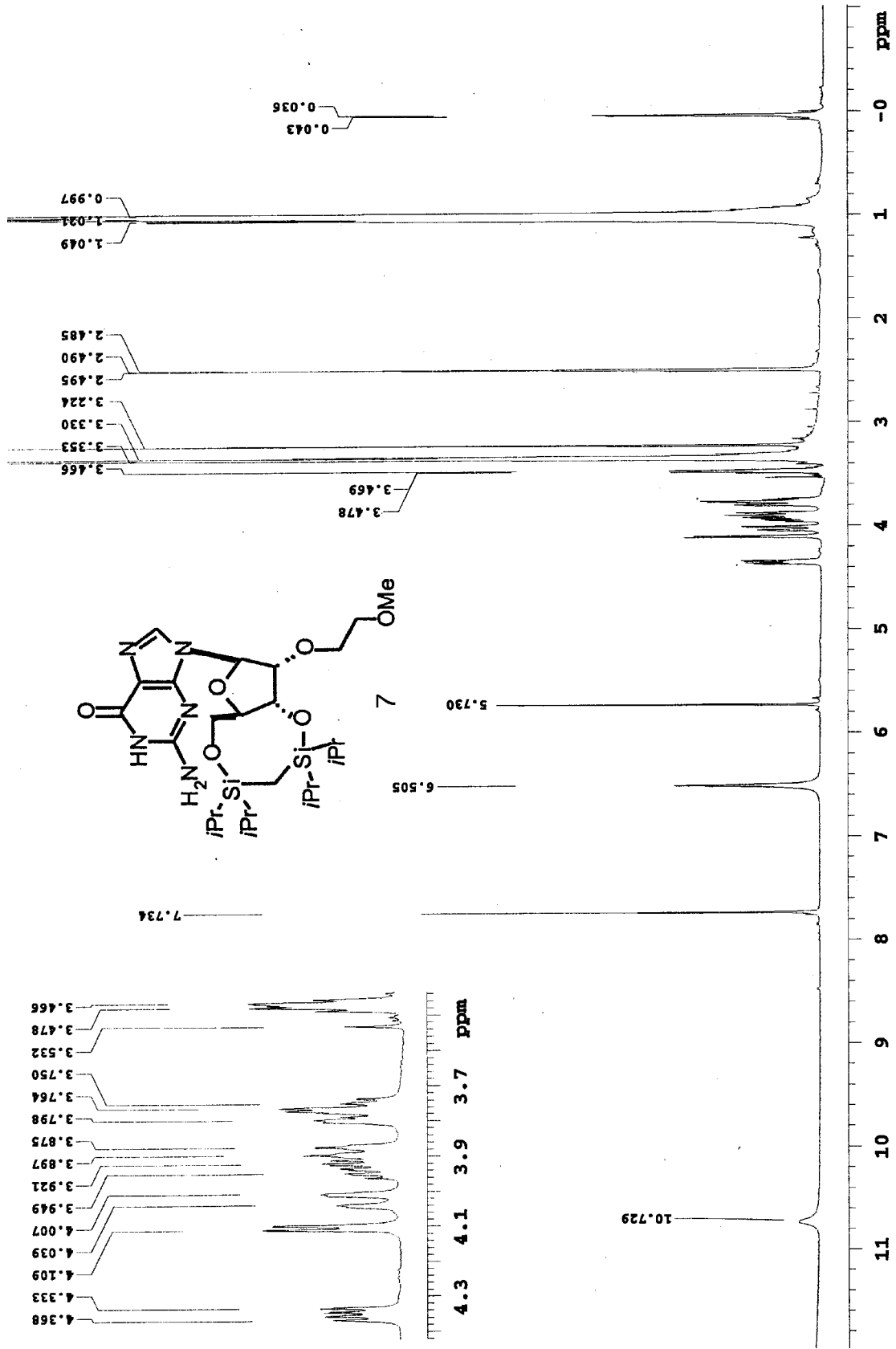


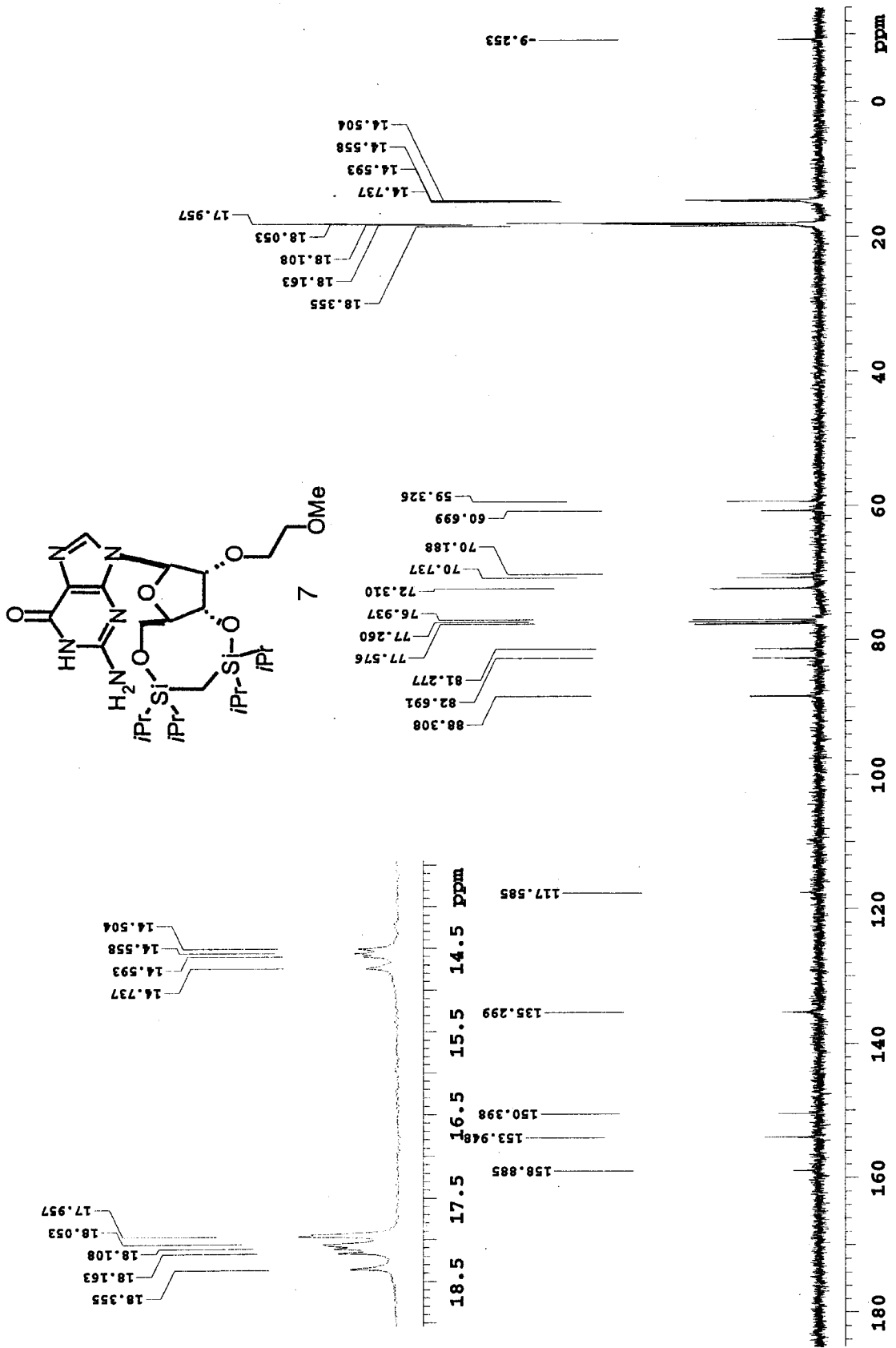
13C OBSERVE

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Solvent: DMSO  
Ambient temperature  
Mercury-400BB "hg400"  
PULSE SEQUENCE  
Pulse 72.2 degrees  
Acq. time 1.200 sec  
Width 25148.5 Hz  
30500 repetitions  
OBSERVE C13, 100.5940242 MHZ  
DECOUPLE H1, 400.0574305 MHZ  
Power 43 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 1.0 Hz  
FT size 65536  
Total time 34 hr, 23 min, 52 sec



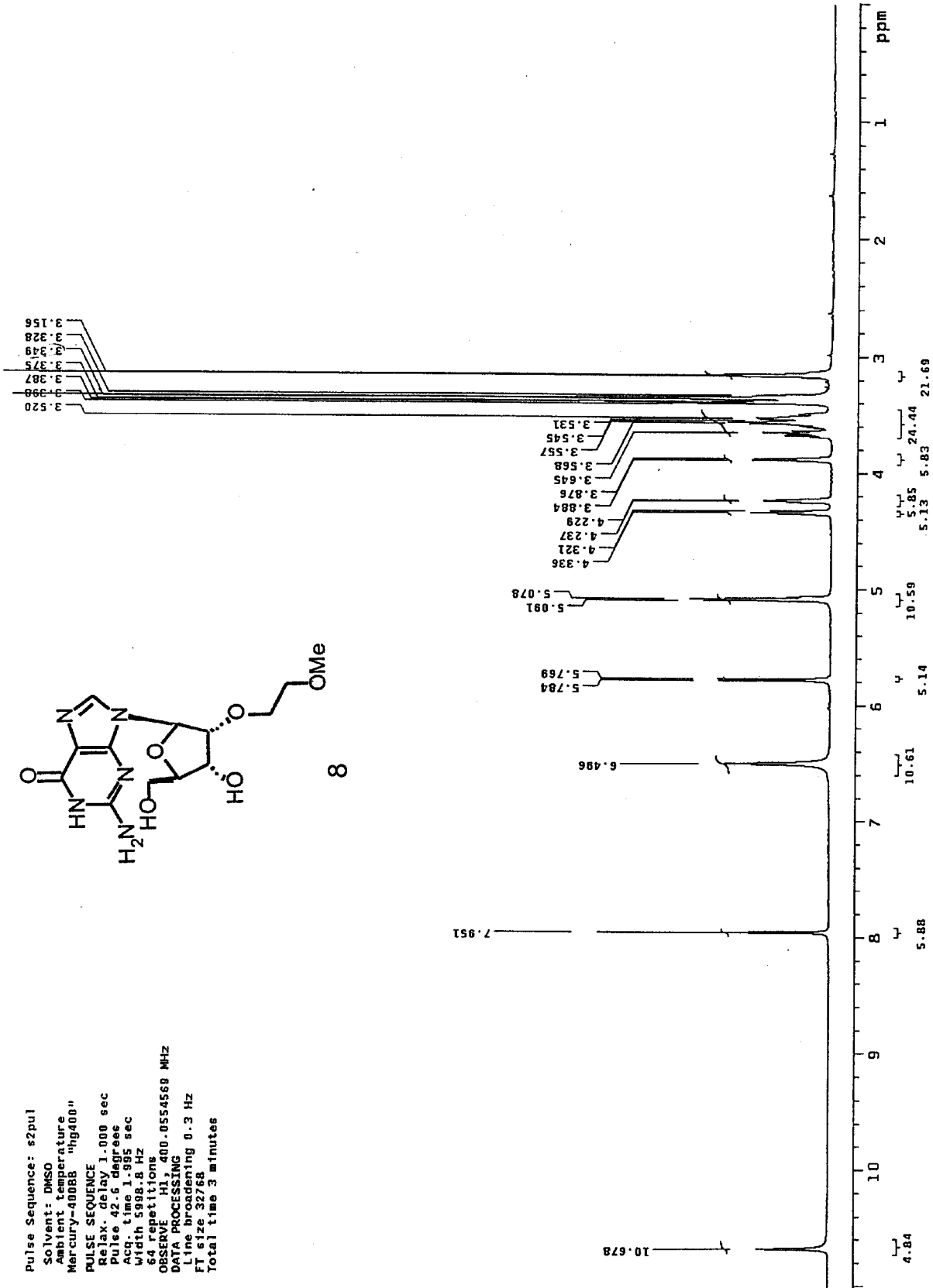
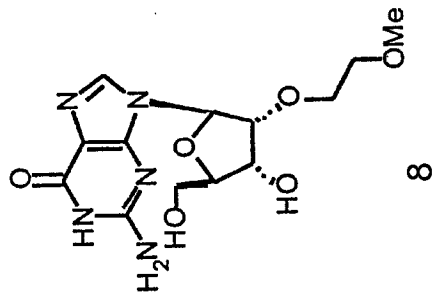


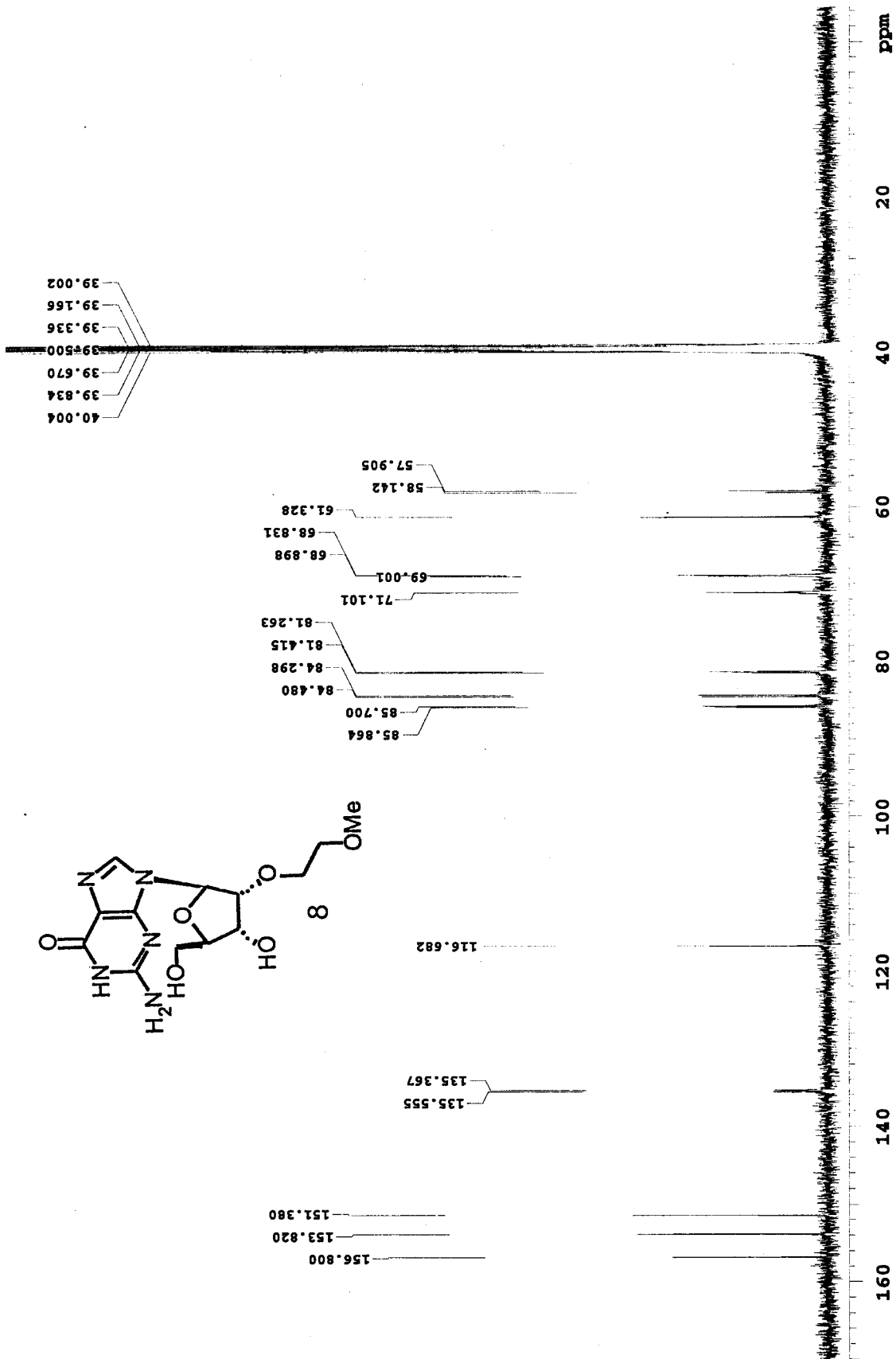




STANDARD 1H OBSERVE

Pulse Sequence: s2pul  
 Solvent: DMSO  
 Ambient temperature  
 Mercury-48088 "hg400"  
 PULSE SEQUENCE  
 Relax. delay 1.000 sec  
 Pulse 42.5 degrees  
 Acq. time 1.995 sec  
 Width 5998.8 Hz  
 64 repetitions  
 OBSERVE H1, 400.0554569 MHz  
 DATA PROCESSING  
 Line broadening 0.3 Hz  
 FT size 32768  
 Total time 3 minutes





Crystal structure of compound 6

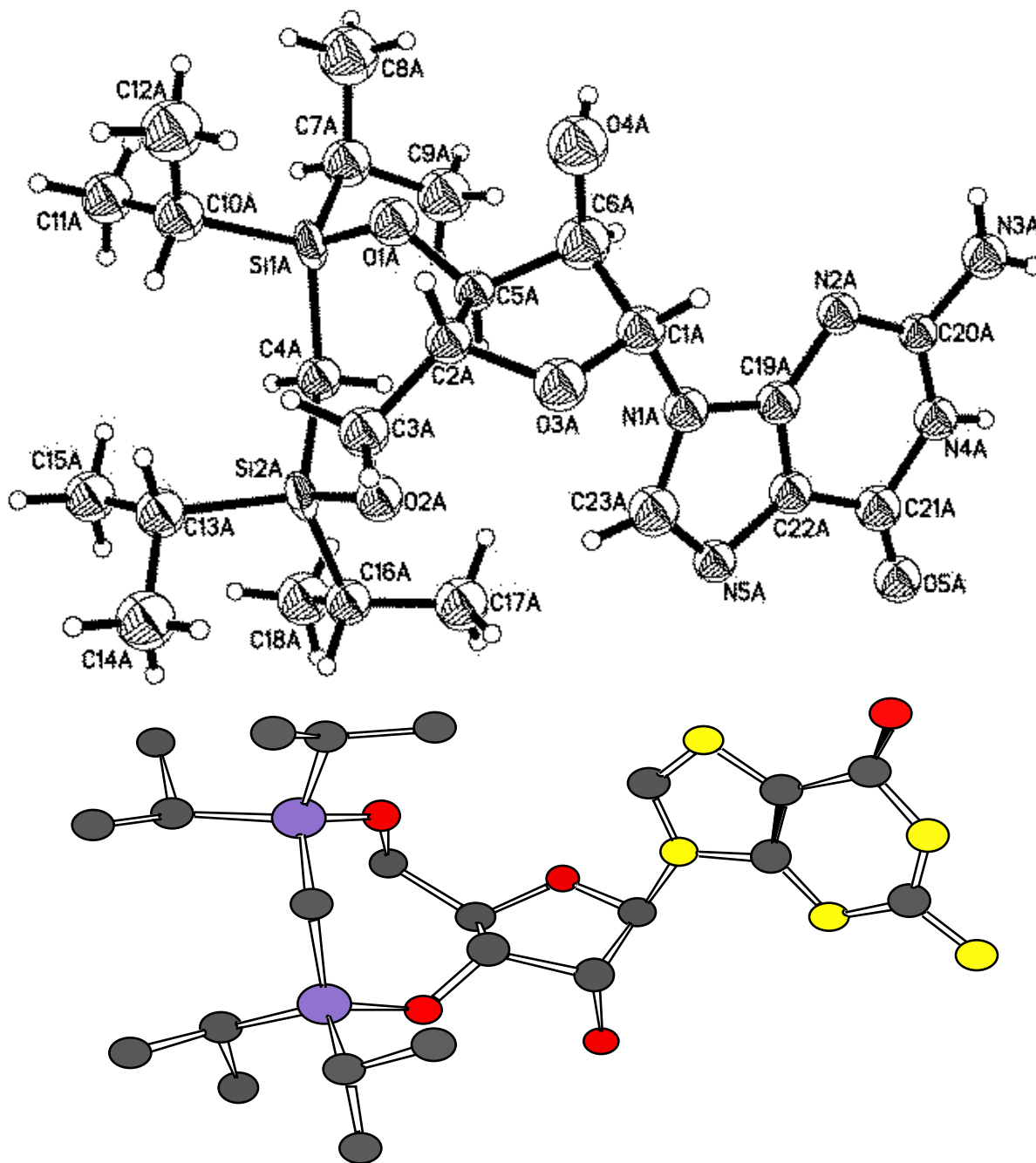


Table 1. Crystal data and structure refinement for **KW5**.

Identification code	campana	
Empirical formula	C <sub>23</sub> H <sub>42.14</sub> N <sub>5</sub> O <sub>5.72</sub> Si <sub>2</sub>	
Formula weight	536.53	
Temperature	373(2) K	
Wavelength	0.71073	
Crystal system	Triclinic	
Space group	P1	
Unit cell dimensions	a = 9.8401(10)	a = 85.235(2) .
	b = 10.7462(11)	b = 85.610(2) .
	c = 28.183(3)	g = 89.108(2) .
Volume	2961.0(5) <sup>3</sup>	
Z	4	
Density (calculated)	1.204 Mg/m <sup>3</sup>	
Absorption coefficient	0.161 mm <sup>-1</sup>	
F(000)	1156	
Crystal size	0.2 x 0.2 x 0.10 mm <sup>3</sup>	
Theta range for data collection	1.98 to 23.34 .	
Index ranges	-10<=h<=10, -11<=k<=11, -31<=l<=31	
Reflections collected	18522	
Independent reflections	15921 [R(int) = 0.0447]	
Completeness to theta = 23.34	99.3 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	15921 / 3 / 657	
Goodness-of-fit on F <sup>2</sup>	1.052	
Final R indices [I>2sigma(I)]	R1 = 0.1218, wR2 = 0.2886	
R indices (all data)	R1 = 0.1833, wR2 = 0.3321	
Absolute structure parameter	0.0(3)	
Largest diff. peak and hole	1.612 and -0.565 e. <sup>-3</sup>	

Table 2. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\times 10^3$ ) for **KW-5**. U(eq) is defined as one third of the trace of the orthogonalized  $U^{ij}$  tensor.

	x	y	z	U(eq)
Si(1A)	5018(4)	8129(3)	1187(2)	38(1)
Si(2A)	6828(4)	10027(3)	1762(2)	36(1)
O(1A)	6353(9)	7567(8)	889(3)	41(2)
O(2A)	8301(9)	9669(8)	1467(3)	36(2)
O(3A)	9992(9)	7837(9)	885(3)	42(2)
O(4A)	8272(11)	5920(10)	479(4)	56(3)
O(5A)	11846(9)	4559(9)	2883(3)	41(2)
N(1A)	10224(11)	6323(10)	1509(4)	33(3)
N(2A)	10562(10)	4062(10)	1546(4)	31(3)
N(3A)	11033(11)	1962(10)	1730(4)	37(3)
N(4A)	11415(11)	3323(10)	2283(4)	35(3)
N(5A)	10897(10)	6726(9)	2218(4)	31(3)
C(1A)	9870(14)	6531(13)	1019(5)	37(3)
C(2A)	8611(13)	8385(12)	800(5)	33(3)
C(3A)	8494(15)	9688(13)	961(5)	38(3)
C(4A)	5524(14)	8775(13)	1748(5)	36(3)
C(5A)	7679(12)	7405(11)	1053(4)	27(3)
C(6A)	8399(15)	6189(14)	957(5)	48(4)
C(7A)	3871(16)	6788(14)	1333(5)	45(4)
C(8A)	3515(19)	6185(17)	899(6)	68(5)
C(9A)	4487(18)	5822(16)	1703(6)	59(4)
C(10A)	4300(15)	9390(14)	781(5)	44(4)
C(11A)	2793(15)	9663(14)	941(5)	47(4)
C(12A)	4512(18)	9204(16)	267(6)	62(5)
C(13A)	6201(14)	11586(13)	1497(5)	41(4)
C(14A)	7259(17)	12564(15)	1551(6)	57(4)
C(15A)	4783(15)	11915(14)	1690(5)	46(4)
C(16A)	7288(14)	10066(13)	2392(5)	39(3)
C(17A)	8186(16)	8951(15)	2551(6)	53(4)
C(18A)	6038(17)	10160(16)	2739(6)	56(4)
C(19A)	10610(13)	5210(12)	1742(5)	32(3)
C(20A)	11016(13)	3167(11)	1859(4)	27(3)
C(21A)	11504(14)	4496(13)	2482(5)	38(3)
C(22A)	10974(13)	5466(12)	2170(5)	33(3)
C(23A)	10452(14)	7195(14)	1821(5)	42(4)
Si(1B)	-8818(4)	1905(4)	8825(2)	50(1)
Si(2B)	-6826(4)	-30(4)	8221(2)	47(1)
O(1B)	-7558(10)	2533(9)	9062(3)	49(3)
O(2B)	-5458(9)	314(8)	8496(3)	40(2)
O(3B)	-3952(9)	2193(8)	9009(3)	36(2)
O(4B)	-5792(12)	4189(11)	9418(4)	62(3)
O(5B)	-1323(9)	5464(8)	6999(3)	34(2)
N(1B)	-3456(11)	3698(10)	8391(4)	35(3)
N(2B)	-3096(11)	5974(10)	8342(4)	36(3)
N(3B)	-2600(12)	8048(11)	8167(4)	44(3)
N(4B)	-1996(11)	6693(10)	7600(4)	33(3)
N(5B)	-2500(11)	3285(10)	7666(4)	38(3)
C(1B)	-4029(14)	3501(13)	8868(5)	40(4)
C(2B)	-5271(14)	1726(13)	9110(5)	39(3)

C(3B)	-5406(15)	356(13)	8990(5)	43(4)
C(4B)	-8191(17)	1214(15)	8252(6)	54(4)
C(5B)	-6200(13)	2643(12)	8875(5)	34(3)
C(6B)	-5538(15)	3871(14)	8937(5)	48(4)
C(7B)	-9990(17)	3237(15)	8687(6)	52(4)
C(8B)	-10480(20)	3943(19)	9108(7)	81(6)
C(9B)	-9312(19)	4158(17)	8307(6)	71(5)
C(10B)	-9619(18)	680(17)	9259(6)	64(5)
C(11B)	-11060(20)	350(20)	9145(8)	90(6)
C(12B)	-9540(30)	810(20)	9747(9)	115(8)
C(13B)	-7495(17)	-1552(15)	8486(6)	58(4)
C(14B)	-6490(20)	-2620(20)	8345(8)	89(6)
C(15B)	-8883(18)	-1898(17)	8324(6)	64(5)
C(16B)	-6149(17)	-61(16)	7590(6)	54(4)
C(17B)	-5360(20)	1149(18)	7412(7)	73(5)
C(18B)	-7237(18)	-238(17)	7249(6)	65(5)
C(19B)	-2998(13)	4827(12)	8156(4)	31(3)
C(20B)	-2537(14)	6859(13)	8030(5)	36(3)
C(21B)	-1799(14)	5505(13)	7406(5)	40(3)
C(22B)	-2422(14)	4560(13)	7727(5)	38(3)
C(23B)	-3105(13)	2827(12)	8071(4)	31(3)
Si(1C)	18447(4)	12346(3)	4138(2)	54(1)
Si(2C)	16760(4)	14600(3)	3528(2)	51(1)
O(1C)	17063(9)	11574(9)	4348(3)	41(2)
O(2C)	15242(9)	14147(8)	3804(3)	40(2)
O(3C)	13484(8)	12045(8)	4264(3)	31(2)
O(4C)	15206(9)	9770(8)	4624(3)	34(2)
O(5C)	11693(9)	9685(8)	2250(3)	38(2)
N(1C)	13220(10)	10834(9)	3633(3)	26(2)
N(2C)	12966(10)	8590(9)	3582(3)	29(2)
N(3C)	12585(11)	6584(11)	3391(4)	43(3)
N(4C)	12171(11)	8198(10)	2839(4)	33(3)
N(5C)	12560(10)	11569(9)	2930(4)	28(2)
C(1C)	13611(13)	10805(12)	4127(4)	31(3)
C(2C)	14749(13)	12417(12)	4401(5)	34(3)
C(3C)	14954(16)	13832(13)	4273(5)	44(4)
C(4C)	18086(16)	13341(14)	3559(5)	47(4)
C(5C)	15783(12)	11633(11)	4142(4)	25(3)
C(6C)	15081(13)	10367(12)	4178(4)	29(3)
C(7C)	19748(16)	11116(14)	3991(5)	48(4)
C(8C)	20022(15)	10261(13)	4416(5)	43(4)
C(9C)	19286(17)	10348(15)	3587(6)	57(4)
C(10C)	18940(20)	13302(18)	4586(6)	71(5)
C(11C)	20460(20)	13690(20)	4505(8)	90(6)
C(12C)	18660(20)	12750(20)	5097(7)	88(6)
C(13C)	17365(18)	15993(16)	3773(6)	61(5)
C(14C)	16330(20)	17085(18)	3745(7)	76(6)
C(15C)	18772(18)	16419(17)	3616(6)	67(5)
C(16C)	16413(17)	14944(16)	2890(6)	57(4)
C(17C)	15553(17)	13947(15)	2716(6)	58(4)
C(18C)	17680(20)	15162(19)	2542(7)	82(6)
C(19C)	12885(13)	9779(12)	3401(4)	29(3)
C(20C)	12546(13)	7846(12)	3278(5)	30(3)
C(21C)	12063(12)	9443(11)	2645(4)	28(3)



C(22C)	12538(12)	10238(11)	2982(4)	27(3)
C(23C)	12985(12)	11819(12)	3333(4)	28(3)
Si(1D)	5984(4)	7533(3)	5919(2)	38(1)
Si(2D)	3947(4)	5268(3)	6412(2)	43(1)
O(1D)	4732(9)	8249(8)	5625(3)	40(2)
O(2D)	2575(9)	5798(9)	6130(3)	41(2)
O(3D)	1142(9)	7991(8)	5633(3)	36(2)
O(4D)	2993(10)	10186(9)	5287(3)	45(2)
O(5D)	-1737(10)	10277(9)	7644(3)	44(2)
N(1D)	604(11)	9156(10)	6271(4)	32(3)
N(2D)	248(11)	11384(10)	6326(4)	33(3)
N(3D)	-270(12)	13384(11)	6515(4)	47(3)
N(4D)	-967(11)	11774(10)	7059(4)	34(3)
N(5D)	-405(11)	8414(10)	6976(4)	35(3)
C(1D)	1169(13)	9198(12)	5788(5)	31(3)
C(2D)	2479(14)	7552(13)	5523(5)	38(3)
C(3D)	2585(15)	6111(13)	5640(5)	40(3)
C(4D)	5258(16)	6539(14)	6435(5)	47(4)
C(5D)	3396(12)	8286(11)	5791(4)	23(3)
C(6D)	2714(13)	9582(12)	5752(5)	32(3)
C(7D)	7000(14)	8786(13)	6130(5)	38(3)
C(8D)	7480(20)	9751(19)	5729(7)	79(6)
C(9D)	6253(18)	9472(16)	6513(6)	60(5)
C(10D)	6998(14)	6575(13)	5495(5)	40(3)
C(11D)	8312(16)	6090(15)	5714(6)	54(4)
C(12D)	7330(20)	7230(20)	5001(7)	94(7)
C(13D)	4723(16)	3924(14)	6100(6)	50(4)
C(14D)	3630(20)	2930(20)	6046(7)	88(6)
C(15D)	5994(19)	3383(18)	6329(7)	72(5)
C(16D)	3252(15)	4800(14)	7025(5)	46(4)
C(17D)	2143(16)	5775(15)	7185(6)	55(4)
C(18D)	4290(18)	4705(17)	7398(6)	64(5)
C(19D)	87(13)	10192(12)	6504(4)	30(3)
C(20D)	-359(13)	12128(12)	6630(5)	32(3)
C(21D)	-1138(13)	10523(11)	7255(4)	29(3)
C(22D)	-494(13)	9727(12)	6937(4)	30(3)
C(23D)	235(13)	8141(12)	6575(4)	30(3)
O(1S)	205(14)	2815(13)	10708(5)	50
O(2S)	1460(30)	-3200(30)	4524(10)	50
O(3S)	7970(19)	3601(17)	316(6)	50
O(4S)	2393(18)	3101(18)	10221(6)	50
O(5S)	-4160(20)	7000(20)	9180(8)	50

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Table 3. Bond lengths [ ] and angles [ ] for **KW-5**.

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Si(1A)-O(1A)	1.639(10)
Si(1A)-C(7A)	1.845(15)
Si(1A)-C(10A)	1.865(15)
Si(1A)-C(4A)	1.882(13)
Si(2A)-O(2A)	1.671(9)
Si(2A)-C(16A)	1.868(14)
Si(2A)-C(4A)	1.879(14)
Si(2A)-C(13A)	1.892(14)
O(1A)-C(5A)	1.420(15)
O(2A)-C(3A)	1.421(15)
O(3A)-C(1A)	1.428(15)
O(3A)-C(2A)	1.501(16)
O(4A)-C(6A)	1.414(17)
O(5A)-C(21A)	1.210(15)
N(1A)-C(23A)	1.371(17)
N(1A)-C(19A)	1.378(16)
N(1A)-C(1A)	1.448(16)
N(2A)-C(20A)	1.344(16)
N(2A)-C(19A)	1.396(16)
N(3A)-C(20A)	1.373(16)
N(4A)-C(20A)	1.311(15)
N(4A)-C(21A)	1.428(17)
N(5A)-C(23A)	1.293(16)
N(5A)-C(22A)	1.372(16)
C(1A)-C(6A)	1.53(2)
C(2A)-C(5A)	1.505(17)
C(2A)-C(3A)	1.509(18)
C(5A)-C(6A)	1.511(19)
C(7A)-C(8A)	1.50(2)
C(7A)-C(9A)	1.56(2)
C(10A)-C(12A)	1.48(2)
C(10A)-C(11A)	1.55(2)
C(13A)-C(15A)	1.51(2)
C(13A)-C(14A)	1.51(2)
C(16A)-C(18A)	1.52(2)
C(16A)-C(17A)	1.54(2)
C(19A)-C(22A)	1.333(18)
C(21A)-C(22A)	1.426(19)
Si(1B)-O(1B)	1.634(11)
Si(1B)-C(7B)	1.859(16)
Si(1B)-C(10B)	1.862(18)
Si(1B)-C(4B)	1.889(16)
Si(2B)-O(2B)	1.664(10)
Si(2B)-C(13B)	1.850(17)
Si(2B)-C(16B)	1.855(16)
Si(2B)-C(4B)	1.883(16)
O(1B)-C(5B)	1.401(16)
O(2B)-C(3B)	1.402(16)
O(3B)-C(2B)	1.399(16)
O(3B)-C(1B)	1.431(16)
O(4B)-C(6B)	1.427(17)
O(5B)-C(21B)	1.210(15)

N(1B)-C(23B)	1.376(16)
N(1B)-C(19B)	1.396(16)
N(1B)-C(1B)	1.418(17)
N(2B)-C(20B)	1.336(17)
N(2B)-C(19B)	1.379(16)
N(3B)-C(20B)	1.363(17)
N(4B)-C(20B)	1.310(16)
N(4B)-C(21B)	1.434(17)
N(5B)-C(23B)	1.309(16)
N(5B)-C(22B)	1.400(17)
C(1B)-C(6B)	1.53(2)
C(2B)-C(5B)	1.484(19)
C(2B)-C(3B)	1.548(19)
C(5B)-C(6B)	1.51(2)
C(7B)-C(8B)	1.51(2)
C(7B)-C(9B)	1.52(2)
C(10B)-C(12B)	1.40(3)
C(10B)-C(11B)	1.53(3)
C(13B)-C(15B)	1.53(2)
C(13B)-C(14B)	1.56(3)
C(16B)-C(18B)	1.51(2)
C(16B)-C(17B)	1.55(2)
C(19B)-C(22B)	1.345(18)
C(21B)-C(22B)	1.417(19)
Si(1C)-O(1C)	1.650(10)
Si(1C)-C(10C)	1.790(19)
Si(1C)-C(7C)	1.875(16)
Si(1C)-C(4C)	1.929(15)
Si(2C)-O(2C)	1.690(10)
Si(2C)-C(13C)	1.826(18)
Si(2C)-C(16C)	1.862(17)
Si(2C)-C(4C)	1.866(15)
O(1C)-C(5C)	1.424(15)
O(2C)-C(3C)	1.348(16)
O(3C)-C(2C)	1.405(16)
O(3C)-C(1C)	1.419(15)
O(4C)-C(6C)	1.377(14)
O(5C)-C(21C)	1.205(14)
N(1C)-C(23C)	1.327(15)
N(1C)-C(19C)	1.410(16)
N(1C)-C(1C)	1.471(16)
N(2C)-C(20C)	1.313(15)
N(2C)-C(19C)	1.340(15)
N(3C)-C(20C)	1.367(16)
N(4C)-C(20C)	1.342(16)
N(4C)-C(21C)	1.407(16)
N(5C)-C(23C)	1.290(15)
N(5C)-C(22C)	1.426(16)
C(1C)-C(6C)	1.527(18)
C(2C)-C(5C)	1.496(17)
C(2C)-C(3C)	1.546(19)
C(5C)-C(6C)	1.528(17)
C(7C)-C(8C)	1.49(2)
C(7C)-C(9C)	1.56(2)

C(10C)-C(12C)	1.52(3)
C(10C)-C(11C)	1.56(3)
C(13C)-C(15C)	1.49(2)
C(13C)-C(14C)	1.54(3)
C(16C)-C(17C)	1.51(2)
C(16C)-C(18C)	1.54(2)
C(19C)-C(22C)	1.310(17)
C(21C)-C(22C)	1.436(17)
Si(1D)-O(1D)	1.677(10)
Si(1D)-C(4D)	1.838(15)
Si(1D)-C(7D)	1.854(14)
Si(1D)-C(10D)	1.863(14)
Si(2D)-O(2D)	1.686(10)
Si(2D)-C(16D)	1.842(15)
Si(2D)-C(13D)	1.875(16)
Si(2D)-C(4D)	1.902(15)
O(1D)-C(5D)	1.363(14)
O(2D)-C(3D)	1.392(15)
O(3D)-C(1D)	1.405(15)
O(3D)-C(2D)	1.412(16)
O(4D)-C(6D)	1.423(15)
O(5D)-C(21D)	1.217(14)
N(1D)-C(23D)	1.365(16)
N(1D)-C(19D)	1.408(16)
N(1D)-C(1D)	1.428(16)
N(2D)-C(20D)	1.322(16)
N(2D)-C(19D)	1.343(16)
N(3D)-C(20D)	1.364(17)
N(4D)-C(20D)	1.337(16)
N(4D)-C(21D)	1.418(16)
N(5D)-C(23D)	1.304(16)
N(5D)-C(22D)	1.408(16)
C(1D)-C(6D)	1.575(18)
C(2D)-C(5D)	1.495(18)
C(2D)-C(3D)	1.560(19)
C(5D)-C(6D)	1.536(17)
C(7D)-C(9D)	1.50(2)
C(7D)-C(8D)	1.52(2)
C(10D)-C(12D)	1.52(2)
C(10D)-C(11D)	1.54(2)
C(13D)-C(15D)	1.54(2)
C(13D)-C(14D)	1.56(3)
C(16D)-C(18D)	1.52(2)
C(16D)-C(17D)	1.57(2)
C(19D)-C(22D)	1.365(18)
C(21D)-C(22D)	1.399(17)
O(1A)-Si(1A)-C(7A)	105.0(6)
O(1A)-Si(1A)-C(10A)	106.3(6)
C(7A)-Si(1A)-C(10A)	113.5(7)
O(1A)-Si(1A)-C(4A)	110.5(6)
C(7A)-Si(1A)-C(4A)	110.6(6)
C(10A)-Si(1A)-C(4A)	110.6(6)
O(2A)-Si(2A)-C(16A)	103.6(5)
O(2A)-Si(2A)-C(4A)	111.7(5)

C(16A)-Si(2A)-C(4A)	108.2(6)
O(2A)-Si(2A)-C(13A)	108.6(6)
C(16A)-Si(2A)-C(13A)	113.2(6)
C(4A)-Si(2A)-C(13A)	111.4(6)
C(5A)-O(1A)-Si(1A)	126.0(8)
C(3A)-O(2A)-Si(2A)	124.0(8)
C(1A)-O(3A)-C(2A)	109.5(9)
C(23A)-N(1A)-C(19A)	104.0(11)
C(23A)-N(1A)-C(1A)	128.1(11)
C(19A)-N(1A)-C(1A)	127.2(11)
C(20A)-N(2A)-C(19A)	108.7(10)
C(20A)-N(4A)-C(21A)	125.3(11)
C(23A)-N(5A)-C(22A)	104.3(11)
O(3A)-C(1A)-N(1A)	107.3(10)
O(3A)-C(1A)-C(6A)	106.6(11)
N(1A)-C(1A)-C(6A)	112.9(11)
O(3A)-C(2A)-C(5A)	102.0(10)
O(3A)-C(2A)-C(3A)	110.4(10)
C(5A)-C(2A)-C(3A)	117.8(11)
O(2A)-C(3A)-C(2A)	111.5(11)
Si(2A)-C(4A)-Si(1A)	124.4(7)
O(1A)-C(5A)-C(2A)	109.6(10)
O(1A)-C(5A)-C(6A)	116.3(11)
C(2A)-C(5A)-C(6A)	103.8(11)
O(4A)-C(6A)-C(5A)	110.1(12)
O(4A)-C(6A)-C(1A)	109.7(12)
C(5A)-C(6A)-C(1A)	100.6(12)
C(8A)-C(7A)-C(9A)	111.4(13)
C(8A)-C(7A)-Si(1A)	112.6(11)
C(9A)-C(7A)-Si(1A)	110.6(11)
C(12A)-C(10A)-C(11A)	112.9(13)
C(12A)-C(10A)-Si(1A)	114.9(11)
C(11A)-C(10A)-Si(1A)	110.7(10)
C(15A)-C(13A)-C(14A)	114.2(13)
C(15A)-C(13A)-Si(2A)	113.0(10)
C(14A)-C(13A)-Si(2A)	108.5(10)
C(18A)-C(16A)-C(17A)	110.4(12)
C(18A)-C(16A)-Si(2A)	112.2(10)
C(17A)-C(16A)-Si(2A)	112.5(10)
C(22A)-C(19A)-N(1A)	107.2(11)
C(22A)-C(19A)-N(2A)	129.5(12)
N(1A)-C(19A)-N(2A)	123.3(11)
N(4A)-C(20A)-N(2A)	126.5(12)
N(4A)-C(20A)-N(3A)	116.2(11)
N(2A)-C(20A)-N(3A)	117.3(11)
O(5A)-C(21A)-C(22A)	128.2(13)
O(5A)-C(21A)-N(4A)	121.3(12)
C(22A)-C(21A)-N(4A)	109.9(11)
C(19A)-C(22A)-N(5A)	110.8(11)
C(19A)-C(22A)-C(21A)	119.8(12)
N(5A)-C(22A)-C(21A)	129.0(12)
N(5A)-C(23A)-N(1A)	113.7(13)
O(1B)-Si(1B)-C(7B)	104.2(7)
O(1B)-Si(1B)-C(10B)	109.4(7)

C(7B)-Si(1B)-C(10B)	112.8(8)
O(1B)-Si(1B)-C(4B)	110.4(7)
C(7B)-Si(1B)-C(4B)	109.4(7)
C(10B)-Si(1B)-C(4B)	110.5(8)
O(2B)-Si(2B)-C(13B)	108.9(7)
O(2B)-Si(2B)-C(16B)	102.9(6)
C(13B)-Si(2B)-C(16B)	113.4(8)
O(2B)-Si(2B)-C(4B)	112.6(6)
C(13B)-Si(2B)-C(4B)	110.6(8)
C(16B)-Si(2B)-C(4B)	108.2(7)
C(5B)-O(1B)-Si(1B)	127.5(9)
C(3B)-O(2B)-Si(2B)	125.6(8)
C(2B)-O(3B)-C(1B)	109.3(10)
C(23B)-N(1B)-C(19B)	104.1(10)
C(23B)-N(1B)-C(1B)	128.6(11)
C(19B)-N(1B)-C(1B)	127.0(11)
C(20B)-N(2B)-C(19B)	110.6(11)
C(20B)-N(4B)-C(21B)	125.0(12)
C(23B)-N(5B)-C(22B)	103.0(11)
N(1B)-C(1B)-O(3B)	108.0(11)
N(1B)-C(1B)-C(6B)	114.4(12)
O(3B)-C(1B)-C(6B)	106.3(11)
O(3B)-C(2B)-C(5B)	106.4(11)
O(3B)-C(2B)-C(3B)	113.2(11)
C(5B)-C(2B)-C(3B)	115.8(12)
O(2B)-C(3B)-C(2B)	109.8(11)
Si(2B)-C(4B)-Si(1B)	123.2(9)
O(1B)-C(5B)-C(2B)	113.1(11)
O(1B)-C(5B)-C(6B)	115.1(11)
C(2B)-C(5B)-C(6B)	102.2(11)
O(4B)-C(6B)-C(5B)	110.1(12)
O(4B)-C(6B)-C(1B)	107.4(12)
C(5B)-C(6B)-C(1B)	100.4(12)
C(8B)-C(7B)-C(9B)	108.1(15)
C(8B)-C(7B)-Si(1B)	114.9(12)
C(9B)-C(7B)-Si(1B)	110.2(12)
C(12B)-C(10B)-C(11B)	112.1(18)
C(12B)-C(10B)-Si(1B)	117.7(15)
C(11B)-C(10B)-Si(1B)	112.8(13)
C(15B)-C(13B)-C(14B)	106.1(15)
C(15B)-C(13B)-Si(2B)	114.8(12)
C(14B)-C(13B)-Si(2B)	109.6(13)
C(18B)-C(16B)-C(17B)	108.3(13)
C(18B)-C(16B)-Si(2B)	113.7(12)
C(17B)-C(16B)-Si(2B)	111.5(11)
C(22B)-C(19B)-N(2B)	127.7(12)
C(22B)-C(19B)-N(1B)	106.8(11)
N(2B)-C(19B)-N(1B)	125.5(11)
N(4B)-C(20B)-N(2B)	125.9(13)
N(4B)-C(20B)-N(3B)	117.7(12)
N(2B)-C(20B)-N(3B)	116.4(12)
O(5B)-C(21B)-C(22B)	130.3(13)
O(5B)-C(21B)-N(4B)	119.4(12)
C(22B)-C(21B)-N(4B)	109.6(12)

C(19B)-C(22B)-N(5B)	111.5(12)
C(19B)-C(22B)-C(21B)	121.0(13)
N(5B)-C(22B)-C(21B)	127.6(12)
N(5B)-C(23B)-N(1B)	114.6(12)
O(1C)-Si(1C)-C(10C)	108.5(7)
O(1C)-Si(1C)-C(7C)	105.3(6)
C(10C)-Si(1C)-C(7C)	113.2(8)
O(1C)-Si(1C)-C(4C)	109.5(6)
C(10C)-Si(1C)-C(4C)	111.3(8)
C(7C)-Si(1C)-C(4C)	108.8(7)
O(2C)-Si(2C)-C(13C)	110.9(7)
O(2C)-Si(2C)-C(16C)	104.5(6)
C(13C)-Si(2C)-C(16C)	110.6(8)
O(2C)-Si(2C)-C(4C)	112.9(6)
C(13C)-Si(2C)-C(4C)	110.0(8)
C(16C)-Si(2C)-C(4C)	107.8(7)
C(5C)-O(1C)-Si(1C)	126.1(8)
C(3C)-O(2C)-Si(2C)	127.3(9)
C(2C)-O(3C)-C(1C)	108.7(9)
C(23C)-N(1C)-C(19C)	106.1(10)
C(23C)-N(1C)-C(1C)	128.5(10)
C(19C)-N(1C)-C(1C)	125.1(10)
C(20C)-N(2C)-C(19C)	109.8(10)
C(20C)-N(4C)-C(21C)	125.0(11)
C(23C)-N(5C)-C(22C)	101.5(10)
O(3C)-C(1C)-N(1C)	106.9(9)
O(3C)-C(1C)-C(6C)	108.3(10)
N(1C)-C(1C)-C(6C)	112.8(10)
O(3C)-C(2C)-C(5C)	105.1(10)
O(3C)-C(2C)-C(3C)	110.4(11)
C(5C)-C(2C)-C(3C)	112.8(11)
O(2C)-C(3C)-C(2C)	114.1(12)
Si(2C)-C(4C)-Si(1C)	123.7(8)
O(1C)-C(5C)-C(2C)	113.0(10)
O(1C)-C(5C)-C(6C)	112.7(10)
C(2C)-C(5C)-C(6C)	102.1(10)
O(4C)-C(6C)-C(5C)	109.6(10)
O(4C)-C(6C)-C(1C)	110.2(10)
C(5C)-C(6C)-C(1C)	99.5(10)
C(8C)-C(7C)-C(9C)	109.8(13)
C(8C)-C(7C)-Si(1C)	112.1(10)
C(9C)-C(7C)-Si(1C)	110.6(11)
C(12C)-C(10C)-C(11C)	109.1(16)
C(12C)-C(10C)-Si(1C)	115.3(14)
C(11C)-C(10C)-Si(1C)	112.0(13)
C(15C)-C(13C)-C(14C)	111.4(15)
C(15C)-C(13C)-Si(2C)	117.8(13)
C(14C)-C(13C)-Si(2C)	112.7(13)
C(17C)-C(16C)-C(18C)	108.9(14)
C(17C)-C(16C)-Si(2C)	112.0(11)
C(18C)-C(16C)-Si(2C)	115.2(13)
C(22C)-C(19C)-N(2C)	130.0(12)
C(22C)-C(19C)-N(1C)	104.4(11)
N(2C)-C(19C)-N(1C)	125.5(11)

N(2C)-C(20C)-N(4C)	125.8(12)
N(2C)-C(20C)-N(3C)	118.9(11)
N(4C)-C(20C)-N(3C)	115.1(11)
O(5C)-C(21C)-N(4C)	121.0(11)
O(5C)-C(21C)-C(22C)	130.8(12)
N(4C)-C(21C)-C(22C)	108.0(10)
C(19C)-C(22C)-N(5C)	112.6(11)
C(19C)-C(22C)-C(21C)	121.0(12)
N(5C)-C(22C)-C(21C)	126.1(11)
N(5C)-C(23C)-N(1C)	115.3(11)
O(1D)-Si(1D)-C(4D)	110.1(6)
O(1D)-Si(1D)-C(7D)	106.4(6)
C(4D)-Si(1D)-C(7D)	109.3(7)
O(1D)-Si(1D)-C(10D)	107.8(6)
C(4D)-Si(1D)-C(10D)	110.5(7)
C(7D)-Si(1D)-C(10D)	112.6(7)
O(2D)-Si(2D)-C(16D)	104.1(6)
O(2D)-Si(2D)-C(13D)	108.8(6)
C(16D)-Si(2D)-C(13D)	112.6(7)
O(2D)-Si(2D)-C(4D)	112.1(6)
C(16D)-Si(2D)-C(4D)	108.6(7)
C(13D)-Si(2D)-C(4D)	110.5(7)
C(5D)-O(1D)-Si(1D)	125.1(8)
C(3D)-O(2D)-Si(2D)	124.3(9)
C(1D)-O(3D)-C(2D)	110.5(10)
C(23D)-N(1D)-C(19D)	105.0(10)
C(23D)-N(1D)-C(1D)	128.9(11)
C(19D)-N(1D)-C(1D)	125.2(11)
C(20D)-N(2D)-C(19D)	109.2(11)
C(20D)-N(4D)-C(21D)	125.5(11)
C(23D)-N(5D)-C(22D)	104.5(10)
O(3D)-C(1D)-N(1D)	108.6(10)
O(3D)-C(1D)-C(6D)	106.2(10)
N(1D)-C(1D)-C(6D)	110.7(10)
O(3D)-C(2D)-C(5D)	106.4(11)
O(3D)-C(2D)-C(3D)	111.0(11)
C(5D)-C(2D)-C(3D)	113.9(11)
O(2D)-C(3D)-C(2D)	111.6(11)
Si(1D)-C(4D)-Si(2D)	125.3(8)
O(1D)-C(5D)-C(2D)	114.0(10)
O(1D)-C(5D)-C(6D)	115.4(10)
C(2D)-C(5D)-C(6D)	101.4(10)
O(4D)-C(6D)-C(5D)	110.6(10)
O(4D)-C(6D)-C(1D)	106.3(10)
C(5D)-C(6D)-C(1D)	100.2(10)
C(9D)-C(7D)-C(8D)	107.5(13)
C(9D)-C(7D)-Si(1D)	113.4(11)
C(8D)-C(7D)-Si(1D)	112.5(11)
C(12D)-C(10D)-C(11D)	110.5(14)
C(12D)-C(10D)-Si(1D)	114.6(12)
C(11D)-C(10D)-Si(1D)	110.1(10)
C(15D)-C(13D)-C(14D)	113.6(15)
C(15D)-C(13D)-Si(2D)	112.7(11)
C(14D)-C(13D)-Si(2D)	110.6(12)



C(18D)-C(16D)-C(17D)	106.9(13)
C(18D)-C(16D)-Si(2D)	115.1(11)
C(17D)-C(16D)-Si(2D)	109.4(10)
N(2D)-C(19D)-C(22D)	129.5(12)
N(2D)-C(19D)-N(1D)	124.1(11)
C(22D)-C(19D)-N(1D)	106.3(11)
N(2D)-C(20D)-N(4D)	126.1(12)
N(2D)-C(20D)-N(3D)	117.6(12)
N(4D)-C(20D)-N(3D)	116.1(12)
O(5D)-C(21D)-C(22D)	129.9(12)
O(5D)-C(21D)-N(4D)	121.4(11)
C(22D)-C(21D)-N(4D)	108.7(11)
C(19D)-C(22D)-C(21D)	120.7(12)
C(19D)-C(22D)-N(5D)	109.9(11)
C(21D)-C(22D)-N(5D)	129.2(11)
N(5D)-C(23D)-N(1D)	114.2(11)

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Table 4. Anisotropic displacement parameters ( $\times 10^3$ ) for **KW-5**. The anisotropic displacement factor exponent takes the form:  $-2p^2[ h^2 a^*U^{11} + \dots + 2 h k a^* b^* U^{12} ]$

	U <sup>11</sup>	U <sup>22</sup>	U <sup>33</sup>	U <sup>23</sup>	U <sup>13</sup>	U <sup>12</sup>
Si(1A)	28(2)	16(2)	69(3)	-1(2)	-7(2)	2(2)
Si(2A)	20(2)	18(2)	70(3)	-4(2)	0(2)	4(2)
Si(1B)	30(2)	25(2)	94(4)	0(2)	0(2)	-4(2)
Si(2B)	36(2)	26(2)	78(3)	-6(2)	-2(2)	4(2)
Si(1C)	23(2)	14(2)	126(4)	-11(2)	-12(2)	1(2)
Si(2C)	35(2)	15(2)	105(4)	-8(2)	-6(2)	-1(2)
Si(1D)	30(2)	13(2)	70(3)	3(2)	3(2)	5(2)
Si(2D)	30(2)	8(2)	86(3)	5(2)	7(2)	7(2)

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Table 5. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\times 10^{-3}$ ) for **KW-5**.

	x	y	z	U(eq)
H(4AA)	7759	5327	476	84
H(3AA)	11296	1361	1924	45
H(3AB)	10781	1808	1455	45
H(4AB)	11642	2665	2455	42
H(1AA)	10495	6061	811	44
H(2AB)	8490	8424	457	39
H(3AC)	9316	10146	851	46
H(3AD)	7731	10119	820	46
H(4AC)	4691	9081	1907	43
H(4AD)	5827	8067	1950	43
H(5AB)	7629	7499	1397	33
H(6AA)	8078	5501	1186	57
H(7AA)	3020	7106	1485	55
H(8AA)	2756	5638	982	102
H(8AB)	4284	5713	779	102
H(8AC)	3276	6818	658	102
H(9AA)	3902	5110	1761	89
H(9AB)	4565	6200	1996	89
H(9AC)	5372	5561	1580	89
H(10A)	4800	10148	826	53
H(11A)	2442	10312	728	71
H(11B)	2734	9926	1260	71
H(11C)	2267	8920	936	71
H(12A)	4338	9975	83	94
H(12B)	3901	8577	189	94
H(12C)	5436	8940	194	94
H(13A)	6162	11516	1154	49
H(14A)	7042	13322	1366	86
H(14B)	8142	12267	1439	86
H(14C)	7263	12723	1881	86
H(15A)	4486	12675	1524	69
H(15B)	4785	12027	2025	69
H(15C)	4173	11254	1646	69
H(16A)	7822	10823	2406	46
H(17A)	8166	8865	2894	79
H(17B)	9106	9089	2420	79
H(17C)	7848	8203	2440	79
H(18A)	6315	10351	3044	84
H(18B)	5566	9379	2774	84
H(18C)	5443	10809	2619	84
H(23A)	10299	8046	1754	51
H(4BA)	-6585	4029	9511	92
H(3BA)	-2291	8656	7973	53
H(3BB)	-2950	8189	8446	53
H(4BB)	-1738	7346	7421	40
H(1BA)	-3503	3961	9077	48
H(2BB)	-5482	1739	9455	47
H(3BC)	-4632	-132	9097	52
H(3BD)	-6228	-3	9154	52
H(4BC)	-8985	881	8124	65

H(4BD)	-7878	1907	8031	65
H(5BB)	-6159	2518	8533	41
H(6BA)	-5798	4541	8703	58
H(7BA)	-10793	2906	8557	63
H(8BA)	-11017	4648	9003	122
H(8BB)	-9703	4227	9256	122
H(8BC)	-11015	3404	9335	122
H(9BA)	-9848	4911	8283	106
H(9BB)	-9241	3799	8006	106
H(9BC)	-8418	4347	8394	106
H(10B)	-9080	-75	9202	76
H(11D)	-11451	-230	9392	136
H(11E)	-11018	-15	8845	136
H(11F)	-11610	1097	9125	136
H(12D)	-10068	178	9932	173
H(12E)	-9882	1622	9821	173
H(12F)	-8603	733	9823	173
H(13B)	-7569	-1543	8835	69
H(14D)	-6896	-3412	8444	133
H(14E)	-5659	-2547	8499	133
H(14F)	-6292	-2550	8005	133
H(15D)	-9316	-2498	8557	96
H(15E)	-8755	-2250	8022	96
H(15F)	-9446	-1163	8293	96
H(16B)	-5508	-765	7571	65
H(17D)	-5133	1159	7074	109
H(17E)	-4533	1172	7573	109
H(17F)	-5912	1865	7479	109
H(18D)	-6842	-135	6926	97
H(18E)	-7950	370	7294	97
H(18F)	-7607	-1062	7312	97
H(23B)	-3283	1980	8137	38
H(4CA)	14469	9784	4781	51
H(3CA)	12881	6290	3658	51
H(3CB)	12313	6084	3196	51
H(4CB)	11982	7620	2662	39
H(1CA)	12992	10260	4336	37
H(2CB)	14787	12230	4746	41
H(3CC)	14132	14272	4379	53
H(3CD)	15691	14109	4447	53
H(4CC)	18942	13727	3438	57
H(4CD)	17874	12759	3331	57
H(5CB)	15911	11958	3807	30
H(6CA)	15418	9852	3922	35
H(7CA)	20601	11535	3874	58
H(8CA)	20543	9554	4316	64
H(8CB)	19173	9982	4578	64
H(8CC)	20526	10695	4628	64
H(9CA)	19803	9584	3581	86
H(9CB)	19435	10826	3285	86
H(9CC)	18334	10160	3646	86
H(10C)	18395	14073	4554	86
H(11G)	20588	14462	4644	135
H(11H)	20721	13794	4168	135

H(11I)	21025	13052	4652	135
H(12G)	19080	13259	5308	132
H(12H)	19024	11920	5129	132
H(12I)	17692	12732	5177	132
H(13C)	17393	15755	4116	73
H(14G)	16716	17806	3862	114
H(14H)	15513	16854	3937	114
H(14I)	16125	17274	3420	114
H(15G)	18933	17196	3747	100
H(15H)	18872	16533	3274	100
H(15I)	19417	15804	3727	100
H(16C)	15874	15719	2871	69
H(17G)	15588	14038	2373	87
H(17H)	14627	14034	2843	87
H(17I)	15899	13138	2819	87
H(18G)	17414	15539	2242	123
H(18H)	18130	14378	2494	123
H(18I)	18294	15707	2672	123
H(23C)	13117	12633	3409	34
H(4DA)	3732	9944	5173	67
H(3DA)	169	13666	6254	56
H(3DB)	-653	13895	6705	56
H(4DB)	-1281	12353	7231	41
H(1DA)	649	9781	5584	37
H(2DB)	2711	7739	5180	46
H(3DC)	1826	5711	5516	48
H(3DD)	3421	5801	5484	48
H(4DC)	4862	7104	6660	57
H(4DD)	6027	6135	6582	57
H(5DB)	3321	7957	6127	27
H(6DA)	2934	10098	6006	39
H(7DA)	7810	8396	6264	45
H(8DA)	8055	10345	5852	118
H(8DB)	6708	10175	5602	118
H(8DC)	7989	9341	5481	118
H(9DA)	6835	10097	6611	91
H(9DB)	5992	8895	6782	91
H(9DC)	5453	9865	6392	91
H(10D)	6450	5843	5453	48
H(11J)	8692	5419	5541	81
H(11K)	8104	5794	6042	81
H(11L)	8959	6755	5697	81
H(12J)	7681	6633	4787	140
H(12K)	7996	7863	5019	140
H(12L)	6514	7609	4884	140
H(13D)	5029	4258	5775	60
H(14J)	4061	2128	6017	133
H(14K)	3155	3158	5765	133
H(14L)	2988	2882	6321	133
H(15J)	6386	2737	6144	108
H(15K)	5742	3042	6648	108
H(15L)	6648	4034	6336	108
H(16D)	2816	3986	7026	55
H(17J)	1816	5556	7511	82

H(17K)	1398	5773	6984	82
H(17L)	2536	6592	7159	82
H(18J)	3827	4570	7710	96
H(18K)	4797	5466	7377	96
H(18L)	4902	4019	7342	96
H(23D)	423	7325	6502	36
H(1SA)	-132	3528	10630	50
H(2SA)	2316	-3234	4458	50
H(3SA)	7404	3126	209	50
H(3SB)	7781	3821	596	50
H(6SA)	2222	2497	10059	50
H(6SB)	2235	3815	10081	50
H(5SA)	-3656	6882	9412	50
H(5SB)	-4759	6431	9197	50

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