Supporting Information

Stability of *N*-glycosidic bond of (5'*S*)-8,5'-cyclo-2'-deoxyguanosine

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Table S1. ^{1}H Chemical shifts (δ, ppm) of 2-deoxyribose after 24 h in 20% DCOOD, 10% DMSO-d_6 and 70% D_2O at 37 ^{o}C

	1' H (ppm)	2' Ha and 2' Hb (ppm)	3' H (ppm)	4' and 5' H (ppm)	1' C (ppm)	2' C (ppm)	3' C (ppm)
α deoxyribopyranose (35%)	5.11 (t, J = 3.4 Hz)	2.02 and 1.82 (m)	4.12 (m)	4.1-3.5	93.4	35.3	66.1
β deoxyribopyranose (30%)	4.61 (t, J = 9.0, 2.3 Hz)	2.00 and 1.76 (m)	3.92 (m)	4.1-3.5	95.6	36.8	69.0
α-deoxyribopyranose oligomer (15%)	5.43 (t, J = 4.3 Hz)	1.96 (m)	4.19 (m)	4.1-3.5	100.0	42.8	72.7
β -deoxyribopyranose oligomer (15%)	5.38 (t, J = 5.2, 1.5 Hz)	2.25 and 1.70 (ddd, J = 5.8, 5.2, 1.5 Hz)	4.06 (m)	4.1-3.5	100.4	42.8	72.6

Table S2. ^{13}C Chemical shifts (δ, ppm) of ddcdG with and without 10% DCOOD in DMSO-d_6

sugar carbon	purine carbon	ddcdG	ddcdG + 10% acid	Δ shift (ppm)
	2	153.6	156.6	3
	4	148.6	149.2	0.6
	5	115.3	109.9	-5.4
	6	156.2	156.8	0.6
	8	139.8	144.7	4.9
1’		83.4	86.7	3.3
2’		46	46.8	0.8
3’		73.2	75.1	1.9
4’		82.4	82.9	0.5
5’		29.8	28.7	-1.1

Table S3

Hydrolyzed *S*-cdG

^{1}H	^{13}C (HSQC)	^{13}C (HMBC – Carbons 2-3 bonds from proton)
6.33	88.2	147.5, 87.4, 69.8
5.42	100.7, 94.2	69.0, 65.9
5.28	69.4, 64.8	147.5, 152.2, 69.8, 87.4, 94.0
5.05	68.9	
4.85	73.5	147.8, 150.7
4.63	87.4	147.5, 88.0, 69.2
4.40	72.8	
4.32	88.4	
4.13	65.9	
4.11	88.5	
4.10	71.4	65.0
4.00	70.4	
3.93	69.3	
2.62/2.11	46.2	87.4
2.01	43.4	73.0, 100.7
2.14/1.72	43.3	70.1, 88.4
1.94/1.64	36.4	69.4, 96.3
1.86/1.76	33.6	65.5, 94.2, 71.3

COSY and HSQC put together

Starting material (19%) 6.33/88.2 ->2.62/2.11/46.2 ->4.63/87.4 ->5.28 (Unhydrolyzed *S*-cdG)
β-Pyranose derivative (10%) 5.42/100.4 -> 2.01/43.4 -> 4.40/72.8
α-Pyranose derivative (36%) 5.42/94.2 -> 1.86/1.76/33.6 -> 4.11/71.4
Suspected Septanose derivative (23%) 4.85/73.5 -> 1.94/1.64/36.4 -> 3.93/69.3
Furanose derivative (12%) 4.32/88.4 -> 2.14/1.72/43.3

Table S4

Hydrolyzed ddcdG

^{1}H	^{13}C (HSQC)	^{13}C (HMBC – Carbons 2-3 bonds from proton)
6.65		
6.47 (d, J=5.0 Hz)	88.7	
6.33 (d, J=5.4 Hz)	86.8	
6.21 (d, J=4.0 Hz)	75.8	
5.44 (dd, J=4.2, 4.3 Hz)		100.3
5.40 (dd, J=1.9, 5.2 Hz)		100.0
4.72 (d, J=6.6 Hz)		
4.39 (dd, J=2.9, 7.1 Hz)		
4.25 (m)		
4.04 (m)		
3.44 to 2.89 (m, H5'a+b)		
2.62/2.14	46.8	
2.70/2.14	47.4	
2.01	42.2	
2.24/1.73	42.0	
2.50/2.20	39.7	

COSY and HSQC Data

Starting material (23%) 6.33/86.8 -> 2.63/2.14/46.8 -> 4.40/75.3 -> 82 -> 3.39/3.00/28.7

HMBC 3.39/3.00 ->144 (C8)

α Furanose derivative (6%) 6.47/88.7 -> 2.70/2.14/47.4 -> 4.40

HMBC 4.40 → 146.3

β Furanose derivative (3%) 6.21/75.8 -> 2.50/2.20/39.7 -> 4.04

HMBC 4.04 → 149.1

Suspected α Septanose derivative (26%) 5.44/100.3 -> 2.01/42.2 -> 4.25/75.4 -> 83.8->

2.90/3.24/31.7 HMBC 2.90/3.24→149.6

Suspected β Septanose derivative (24%) 5.40/100.0 -> 2.24/1.73/42.0 -> 4.07/75.3 -->

3.04/3.31/33.0 HMBC 3.04/3.31→ 150.0

Figure S1. 1D and COSY ^{1}H-NMR spectra of *S*-cdG in DMSO-d_6

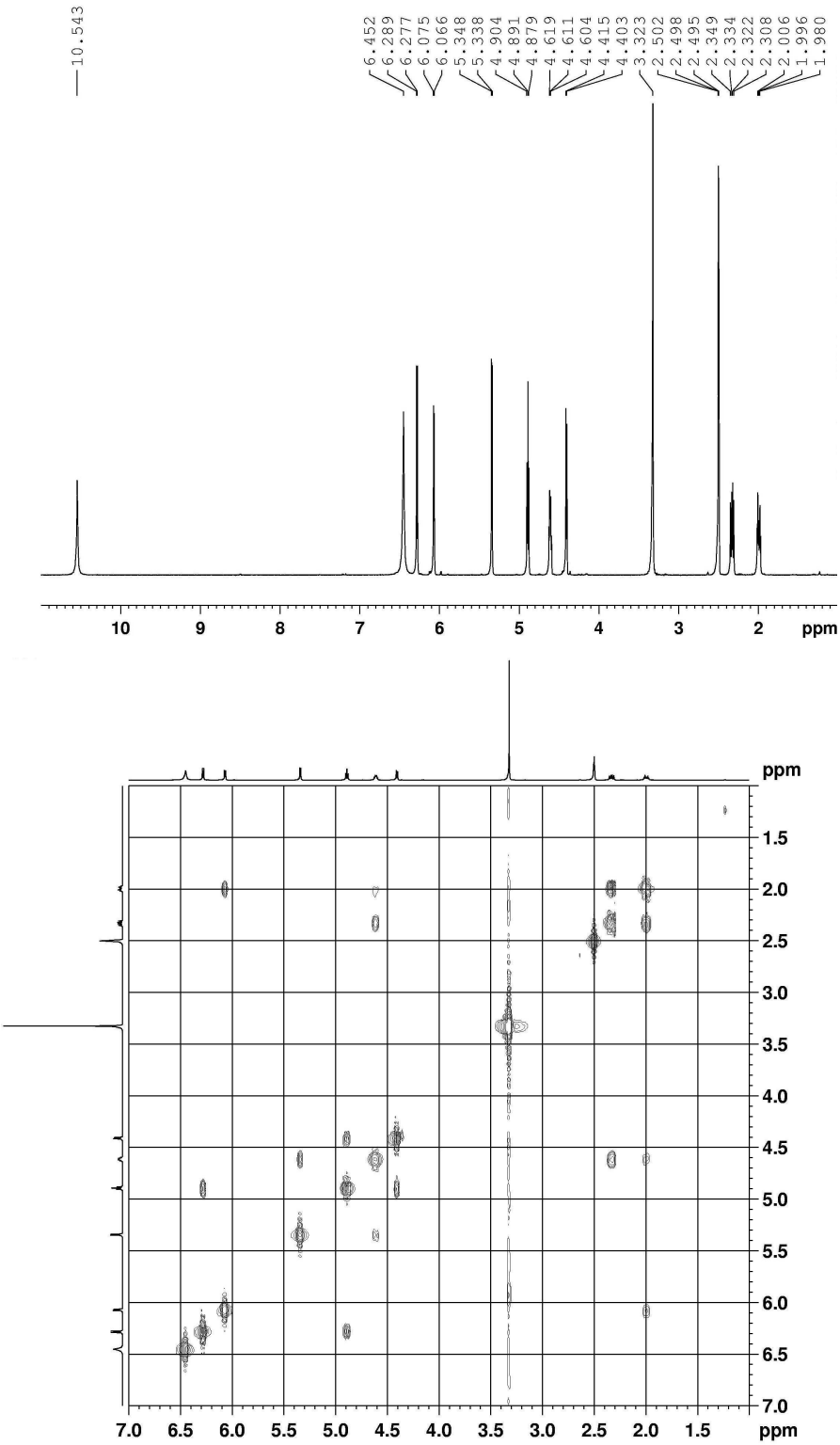

Figure S2A. ^{1}H-NMR spectra of ddcdG after 24 h in 20% DCOOD, 10% DMSO-d_6 and 70% D_2O at 37 ^{o}C

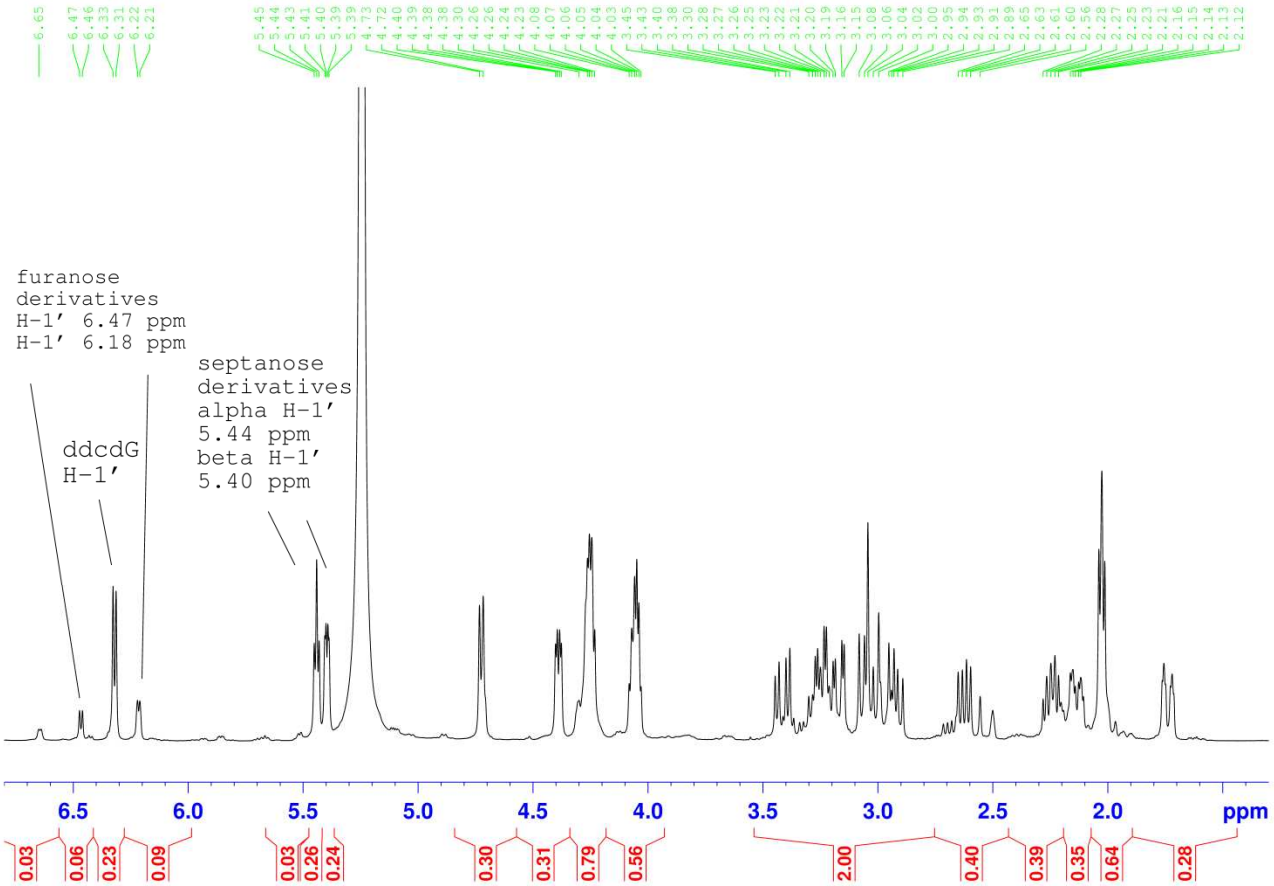
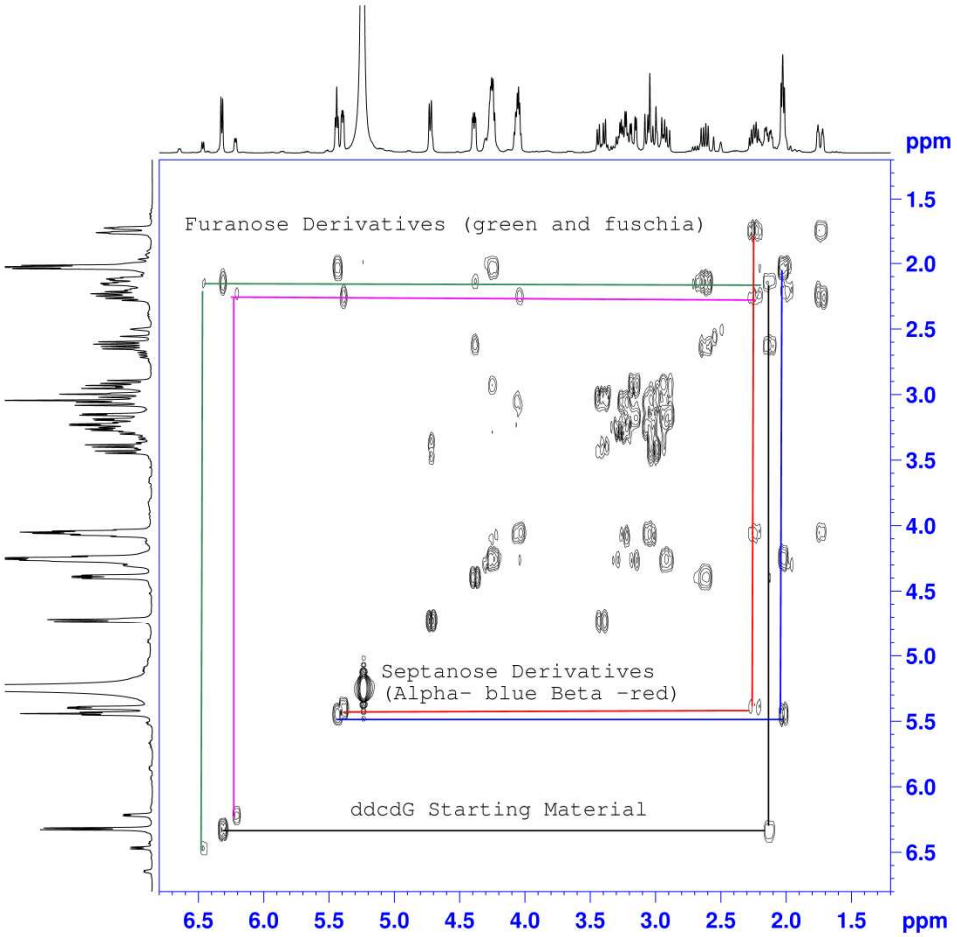
Figure S2B. COSY ^{1}H-NMR spectra of ddcdG after 24 h in 20% DCOOD, 10% DMSO-d_6 and 70% D_2O at 37 ^{o}C: α and β deoxyribofuranose (green and fuschia line), suspected septanose (α blue, β red line), unhydrolyzed ddcdG (black line).