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Structural Refinement of the S(61,3) Adduct

Mixing times 150, 200, 250 ms were used for the NOESY experiments as a function of mixing time. Overlapped cross peaks between styrene aromatic protons and DNA protons were not included in the NOE intensities used by MARDIGRAS. The magnitudes of expected NOEs between styrene aromatic protons and DNA were predicted by inspection of molecular models. Distances between styrene aromatic protons and DNA protons obtained from inspection of model structures were assigned as strong, medium, and weak distance restraints in MD calculations, with ranges 1.8-2.5 Å, 1.8-3.5 Å, and 1.8-5 Å, respectively. Restraints involving water-exchangeable protons were also incorporated in the MD calculations and were estimated by comparing these NOE intensities with those of known distances in the similar region.

Including NOE and empirical distance restraints, a total of 356 distance restraints were used for the MD calculations, of which 50 were base-pairing restraints, 3 were base-step restraints, between nucleotides G^3 and A^4, A^4 and C^5, and $^{S\text{-}SO}A^7$ and G^8. Three were internucleotide distance restraints between nucleotides G^3 and A^4, A^4 and C^5, and T^{17} and G^{18}, which were as follows: r[G^3 H2'-A^4 H8] = 3.50 ± 0.2Å, r[A^4 H1'-C^5 H5] = 3.50 ± 0.2 Å, and r[T^{17} H2''-G^{18} H8] = 2.45 ± 0.2 Å, and one was cross strand distance restraint between nucleotides A^6 and G^{18}, which was as follows: r[A^6 H2-G^{18} H1'] = 5.10 ± 0.2Å.

The MD calculations were initialized by assigning a random set of velocities that fit a Maxwell-Boltzmann distribution at 1300 K to all of the atoms. Sets of 5 MD calculations were initiated using random seeds, starting from both IniA and IniB. Simulated annealing was carried out for 7 ps, with the force constants of 10 kcal/mol.Å^2 for empirical hydrogen bonding and base-pair planarity restraints, and

50 kcal/mol.Å^2 as the maximum constant for NOE restraints. To control the temperature, the molecules were weakly coupled to a temperature bath with a target temperature of 1300 K and a coupling constant of 0.05 ps [Berendsen, H.J.C., Postma, J.P.M., van Gunsteren, W.F., DiNola, A., & Haak, J.R. (1984) *J. Phys. Chem. 81*, 3684-3690]. The force constants were scaled up to 100 and 150 kcal/mol.Å^2 for the empirical restraints and NOE restraints, respectively, during the next 7 ps with the temperature maintained at 1300 K. The temperature was maintained at 1300 K for 3 ps, and decreased to 300 K for a period of 3 ps, and then kept at 300 K for 2 ps using the high force constants. The force constants were scaled down to 20 and 50 kcal/mol.Å^2 for the empirical restraints and NOE restraints, respectively, for a period of 4 ps and kept at those values for 14 ps. The structures from the last 5 ps were averaged, and energy minimized for 300 iterations by the conjugated gradient method to give the final structures.

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Table S1. Assignments (ppm) of the base and deoxyribose protons of the S(61,2) adduct, corresponding to the major conformation.

	H2	H8	H6	H5	H1'	H2'	H2''	H3'	CH_3
C^1			7.35	5.60	5.45	1.57	2.11	4.45	
G^2		7.71			5.24	2.49	2.54	4.80	
G^3		7.63			5.46	2.48	2.59	4.86	
A^4	7.63	7.99			6.01	2.47	2.73	4.90	
C^5			6.97	5.05	5.40	1.63	2.15	4.60	
X^6	6.82	7.79			5.26	2.10	2.30		
A^7	7.47	7.84			5.86	2.36	2.65	4.86	
G^8		7.53			4.95	2.39	2.41		
A^9	7.15	7.93			5.80	2.46	2.73	4.88	
A^{10}	7.42	7.84			5.81	2.37	2.67	4.85	
G^{11}		7.36			5.74	2.17	2.07	4.42	
C^{12}			7.62	5.61	5.56	2.14	2.39	4.41	
T^{13}			7.51		6.02	2.09	2.45		1.45
T^{14}			7.34		6.01	2.09	2.47		1.47
C^{15}			7.51	5.60	5.74	2.00	2.37	4.65	
T^{16}			7.18		6.00	1.98	2.46		1.28
T^{17}			7.28		5.47	1.82	2.25	4.64	1.60
G^{18}		7.74			5.82	2.06	2.64		
T^{19}			7.16		5.88	1.98	2.36	4.63	1.17
C^{20}			7.39	5.47	5.74	1.96	2.21	4.64	
C^{21}			7.30	5.51	5.38	1.82	2.13	4.64	
G^{22}		7.76			5.96	2.48	2.20	4.51	

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Table S2. Assignments (ppm) of the base and deoxyribose protons of the S(61,3) adduct.

	H2	H8	H6	H5	H1'	H2'	H2''	H3'	H4'	CH_3
C^1			7.42	5.72	5.56	1.65	2.17	4.52	3.89	
G^2		7.74			5.28	2.51	2.57	4.81	4.13	
G^3		7.65			5.49	2.50	2.62	4.88	4.24	
A^4	7.65	8.00			6.04	2.50	2.74	4.87	4.30	
C^5			7.04	5.09	5.30	1.80	2.17	4.61	3.97	
A^6	7.14	7.86			5.87	2.32	2.69	4.83	4.20	
X^7	7.15	7.79			5.47	2.40	2.40	4.81	4.20	
G^8		7.52			5.51	2.32	2.57	4.84	4.24	
A^9	7.20	7.94			5.74	2.49	2.72	4.89	4.26	
A^{10}	7.52	7.87			5.87	2.42	2.70	4.87	4.26	
G^{11}		7.44			5.84	2.20	2.10	4.44	4.02	
C^{12}			7.73	5.77	5.72	2.16	2.45	4.51	3.95	
T^{13}			7.52		6.04	2.09	2.50	4.77		1.56
T^{14}			7.33		5.88	2.36	2.46			1.50
C^{15}			7.42	5.03	5.95	2.09	2.46			
T^{16}			7.22		5.66	1.84	2.32	4.64	3.94	1.57
T^{17}			7.32		5.77	2.18	2.44	4.77	3.88	1.51
G^{18}		7.69			5.81	2.44	2.63	4.78	4.22	
T^{19}			7.13		5.87	2.00	2.36	4.72	4.09	1.17
C^{20}			7.41	5.49	5.79	1.97	2.26	4.67	3.99	
C^{21}			7.33	5.55	5.47	1.84	2.18	4.67	3.95	
G^{22}		7.81			6.02	2.49	2.23	4.54	4.03	

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Table S3. Assignments (ppm) of the exchangeable imino and amino protons of the major conformation for the S(61,2) adduct.

base-pair	imino	amino	
	G N1H/ T N3H	C $N4H_{(a)}$ [a]	C $N4H_{(b)}$ [a]
G^{2}•C^{21}	13.03	6.94	8.56
G^{3}•C^{20}	12.64	6.68	8.24
A^{4}•T^{19}	13.63		
C^{5}•G^{18}	12.29	6.57	8.12
X^{6}•T^{17}	13.55		
A^{7}•T^{16}	13.11		
G^{8}•C^{15}	12.38	6.81	8.20
A^{9}•T^{14}	13.74		
A^{10}•T^{13}	14.14		

[a] C $N4H_{(a)}$: non-hydrogen-bonded proton of the amino group of cytosine; C $N4H_{(b)}$: hydrogen-bonded proton of the amino group of cytosine.

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Table S4. Assignments (ppm) of the exchangeable imino and amino protons of the S(61,3) adduct.

base-pair	imino	amino		
	G N1H/ T N3H	C $N4H_{(a)}$ [a]	C $N4H_{(b)}$[a]	A N6H
$G^2 \cdot C^{21}$	13.03	6.90	8.58	
$G^3 \cdot C^{20}$	12.65	6.61	8.25	
$A^4 \cdot T^{19}$	13.55			
$C^5 \cdot G^{18}$	12.29	6.38	7.98	
$A^6 \cdot T^{17}$	13.56			
$X^7 \cdot T^{16}$	13.76			7.36
$G^8 \cdot C^{15}$	12.19	4.19	8.06	
$A^9 \cdot T^{14}$	13.78			
$A^{10} \cdot T^{13}$	14.05			

[a] C $N4H_{(a)}$: non-hydrogen-bonded proton of the amino group of cytosine;

C $N4H_{(b)}$: hydrogen-bonded proton of the amino group of cytosine.

Table S5. Distance restraints derived from NOE data using MARDIGRAS for the S(61,3) adduct.

Class 1 Distance Restraints

Base 1	Atom 1	Base 2	Atom 2	Dist.	Lower	Upper
1	H1'	1	H4'	2.86	2.66	3.76
1	H6	1	H1'	2.81	2.61	3.81
1	H2'	1	H6	2.27	2.07	2.61
1	H2"	1	H4'	2.59	2.39	4.09
1	H2"	1	H6	2.6	2.05	3.6
1	H3'	1	H2'	2.15	1.95	2.35
1	H3'	1	H2"	2.18	1.98	2.78
2	H1'	2	H4'	3.12	2.92	3.62
2	H8	1	H2"	2.9	1.9	3.18
2	H2'	2	H8	2.49	2.29	2.69
2	H2"	2	H4'	3.04	2.84	3.94
2	H2"	2	H1'	2	1.8	2.2
2	H2"	2	H8	2.55	2.35	3.55
3	H1'	3	H4'	2.55	2.35	3.55
3	H2"	3	H4'	3.87	3.25	4.49
3	H2"	3	H1'	1.97	1.77	2.17
3	H3'	3	H1'	4.26	3.71	4.81
4	H1'	4	H4'	3.21	3.01	3.71
4	H2	4	H1'	4.89	4.39	5.09
4	H2'	4	H4'	3.89	3.56	4.22
4	H2"	4	H1'	2.51	2.21	2.71
4	H3'	4	H1'	4.27	3.87	4.47
4	H3'	4	H8	3.76	3.47	4.05
5	H1'	5	H4'	3.75	3.25	4.25
5	H6	4	H1'	3.55	3.35	3.75
5	H6	4	H2'	3.8	3.6	4.1
5	H6	4	H2"	2.57	2.17	2.77
5	H6	5	H4'	4.09	3.61	4.89
5	H5	4	H8	3.88	3.68	4.08
5	H5	4	H2'	3.52	3.02	3.72
5	H5	4	H2"	3	2.5	3.2
5	H2'	5	H1'	3.56	2.86	3.76
5	H2'	5	H6	2.56	2.36	2.76
5	H2'	5	H5	3.87	3.67	4.37
5	H3'	5	H6	4.04	3.84	4.24
5	H3'	5	H2'	2.76	2.26	2.96
5	H3'	5	H2"	2.96	2.76	3.16
6	H1'	6	H4'	2.81	2.61	3.61
6	H2'	6	H4'	3.54	3.28	3.8
6	H2'	6	H8	2.78	2.58	2.98
6	H2"	6	H4'	3.92	3.54	4.3

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6	H2"	6	H8	3.5	3	4
6	H3'	6	H1'	4.01	3.36	4.66
6	H8	5	H6	4.81	4.61	5.01
7	H1'	7	H4'	2.9	2.7	3.6
7	H8	6	H1'	4.64	3.64	4.84
7	H8	6	H2'	3.4	3.2	3.8
7	H8	6	H2"	3.02	2.52	3.52
7	H8	6	H3'	4.23	4.03	4.73
7	H3'	7	H1'	4.2	3.45	4.95
8	H1'	8	H4'	2.79	2.59	3.59
8	H2'	8	H1'	2.57	2.33	2.81
8	H2'	8	H8	2.69	2.49	2.89
8	H2"	8	H1'	1.95	1.75	2.15
8	H2"	8	H8	3.23	2.94	3.52
9	H1'	9	H4'	2.75	2.55	3.65
9	H2	9	H1'	4.35	4.15	4.55
9	H8	8	H1'	4.37	3.76	4.57
9	H8	8	H2'	3.54	3.32	3.76
9	H8	8	H2"	2.98	1.98	3.18
9	H8	8	H3'	4.7	4.26	5.1
9	H2'	9	H8	2.35	2.15	2.55
9	H2"	9	H4'	3.28	2.94	4.08
9	H2"	9	H8	3.33	2.85	3.92
10	H1'	10	H4'	2.85	2.65	3.65
10	H2	9	H2	3.91	3.71	4.11
10	H8	9	H2"	2.28	2.08	2.48
10	H2'	10	H4'	4.04	3.44	4.63
10	H2'	10	H8	2.62	2.12	2.82
10	H2"	10	H4'	3.01	2.81	4.01
10	H2"	10	H8	2.4	2.2	3.7
10	H3'	10	H1'	3.71	3.31	4.57
11	H8	10	H1'	3.28	3.08	3.48
11	H8	10	H2'	3.8	3.6	4
11	H2'	11	H8	2.89	2.09	3.09
11	H2"	11	H4'	2.67	2.47	4.07
11	H2"	11	H1'	2.05	1.85	2.25
11	H2"	11	H8	2.92	2.72	3.62
11	H3'	11	H2"	2.96	2.58	3.34
12	H1'	12	H4'	2.95	2.75	3.65
12	H2'	12	H1'	2.29	2.03	2.99
12	H2'	12	H6	2.44	2.17	2.71
12	H2"	12	H6	3.3	2.72	3.88
13	H6	12	H3'	3.4	2.95	5
13	H6	13	H1'	3.61	2.97	4.25
13	Me	12	H6	3.37	3.17	3.87
13	Me	12	H5	3.69	3.49	4.69
13	H3'	13	H6	2.98	2.78	3.78
14	H6	13	H1'	3.85	3.65	4.05
14	H6	13	H2"	2.17	1.97	2.37

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14	H6	14	H1'	3.87	3.48	4.26
14	Me	13	H2'	3.01	2.81	3.21
14	H3'	14	H1'	4.05	3.52	4.25
15	H6	14	H1'	3.03	2.83	3.73
15	H6	14	H2'	4	3.8	4.2
15	H5	14	H2'	2.84	2.64	3.34
15	H2'	15	H1'	2.58	2.38	2.78
15	H2'	15	H6	1.91	1.71	2.11
15	H2'	15	H5	3.1	2.74	4.3
15	H2"	15	H1'	2.31	2.11	2.51
16	H1'	16	H4'	2.65	2.45	3.75
16	H6	15	H1'	3.76	3.46	4.06
16	H6	15	H6	4.85	4.65	5.05
16	H6	15	H2'	3.53	3.33	3.73
16	H6	15	H2"	2.64	2.44	2.84
16	H6	16	H4'	3.57	3.35	4.87
16	H6	16	H1'	3.94	3.67	4.21
16	Me	15	H5	3.93	3.73	4.63
16	Me	16	H6	2.84	2.64	3.04
16	H2'	16	H1'	3.09	2.79	3.56
16	H2'	16	H6	2.71	2.51	2.91
16	H2"	16	H6	2.95	2.69	3.65
16	H3'	16	H2'	2.87	2.17	3.07
17	H6	16	H2'	4	3.25	4.75
17	Me	16	H6	3.3	3.1	4
17	H2'	17	H1'	2.64	2.4	2.84
17	H2'	17	Me	4.04	3.84	4.84
17	H2"	17	H1'	1.93	1.73	2.13
17	H3'	17	H1'	3.94	3.7	4.29
18	H1'	18	H4'	2.75	2.55	3.65
18	H2"	18	H4'	3.13	2.86	4.03
18	H2"	18	H8	2.94	2.16	3.72
18	H3'	18	H1'	4.01	3.81	4.69
18	H3'	18	H8	3.89	3.69	4.09
19	H6	18	H1'	3.52	2.99	4.28
19	H6	18	H2'	3.52	3.32	4.02
19	H6	18	H2"	2.48	2.28	2.68
19	H6	19	H4'	3.5	3.3	4.8
19	H6	19	H1'	3.92	3.57	4.12
19	Me	18	H8	3.52	3.32	3.92
19	Me	18	H2'	3.69	2.79	3.89
19	Me	18	H2"	3.58	2.78	3.78
19	Me	18	H3'	4.16	3.96	5.16
19	Me	19	H6	2.81	2.61	3.01
19	H2'	19	H6	2.29	2.09	2.49
19	H2"	19	H6	2.67	2.47	3.57
19	H3'	19	H2'	2.51	2.31	2.71
20	H6	19	H1'	3.7	3.5	3.9
20	H6	19	H2'	4	3.8	4.2

20	H6	20	H4'	3.73	3.23	4.83
20	H6	20	H1'	3.32	2.99	3.65
20	H5	19	H6	3.5	3.27	4
20	H2'	20	H4'	2.98	2.63	3.78
20	H2'	20	H1'	3.3	2.76	3.74
20	H2'	20	H6	2.11	1.91	2.31
20	H2'	20	H5	3.39	3.09	4.39
20	H2"	20	H6	2.88	2.21	3.55
21	H1'	21	H4'	2.6	2.4	3.6
21	H6	20	H1'	3.18	2.98	3.38
21	H6	20	H2'	4	3.8	4.2
21	H5	20	H6	3.9	3.7	4.1
21	H5	20	H2"	3.05	2.55	3.25
21	H2'	21	H6	2.11	1.91	2.31
21	H2'	21	H5	4.03	3.83	4.23
21	H2"	21	H1'	2	1.8	2.2
21	H2"	21	H6	2.3	2.1	3.6
22	H1'	22	H4'	2.53	2.33	3.73
22	H8	21	H2"	2.28	2.08	2.48
22	H2"	22	H1'	2	1.8	2.2
22	H2"	22	H8	2.37	2.12	3.67
22	H3'	22	H8	3.73	3.53	3.93
22	H3'	22	H2'	2.38	2.18	2.58
4	H8	3	H2'	3.5	3.3	4
7	H8	6	H8	5	4.6	5.4
18	H8	17	H2"	2.45	2.25	2.65
5	H6	4	H8	4.8	4.5	5
5	H5	4	H1'	3.5	3.3	3.7
18	H1'	6	H2	5.1	4.9	5.3
4	H8	3	H8	5	4.8	5.2
7	HB'	7	HA	2.85	2.65	3.05
7	HB"	7	HA	2.96	2.73	3.19
16	Me	7	HO	3.4	1.8	5
15	H5	7	HM	3.4	1.8	5
8	H1	7	HO	3.4	1.8	5
15	H41	7	HO	4.3	3.6	5
15	H41	7	HO'	4.3	3.6	5
7	H6	7	HA	3.75	3	4.5
7	HB'	7	H6	4	3.5	4.5
7	HB"	7	H6	4.25	3.5	5

Class 2 Distance Restraints

1	H2'	1	H4'	3.96	3.76	4.45
1	H2'	1	H5	4.19	3.99	4.39
2	H8	1	H3'	3.09	2.89	4.79
3	H8	2	H1'	3.83	3.63	4.03
3	H8	2	H2"	2.87	2.51	3.23
3	H2"	3	H8	3.32	2.56	3.74
4	H8	3	H1'	3.66	3.46	3.86

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4	H8	3	H2"	2.88	2.46	3.11
4	H8	3	H3'	4.6	4.4	4.8
4	H8	4	H1'	3.82	3.34	4.02
4	H2"	4	H4'	3.63	3.35	3.91
4	H2"	4	H8	3.46	2.94	3.98
5	H6	4	H3'	4.87	4.67	5.07
5	H6	5	H1'	3.88	3.64	4.12
5	H2"	5	H6	3.4	2.71	3.6
6	H8	5	H1'	3.5	3.3	3.7
6	H8	5	H2'	4.41	3.88	5.02
6	H8	5	H2"	3.41	1.91	3.61
6	H8	6	H1'	4.64	3.76	4.84
6	H3'	6	H8	3.96	3.76	4.16
7	H8	7	H1'	4.13	3.74	4.52
7	H3'	7	H8	4.02	3.82	4.22
8	H2'	8	H4'	4.11	3.56	4.66
8	H3'	8	H1'	3.9	3.69	4.1
9	H3'	9	H1'	3.99	3.69	4.29
9	H3'	9	H8	3.9	2.98	4.82
10	H8	9	H2'	3.67	3.47	3.87
10	H8	9	H3'	4.42	3.8	5.29
10	H8	10	H1'	4.08	3.67	4.49
10	H3'	10	H8	3.79	3.19	4.59
11	H8	10	H2"	3.77	2.07	4.47
11	H8	11	H4'	4.76	4.56	4.96
11	H8	11	H1'	4.03	3.53	4.23
11	H3'	11	H1'	4.4	3.86	4.94
12	H6	12	H4'	3.85	3.65	4.76
12	H6	12	H1'	3.09	2.89	3.53
12	H3'	12	H1'	3.92	3.72	4.12
12	H3'	12	H6	3.39	2.75	4.03
13	H6	12	H2'	4	3.8	4.2
13	Me	12	H2'	3.48	2.88	3.68
13	H2"	13	H6	2.5	2.3	3.6
13	H3'	13	H1'	4.22	3.67	4.42
14	Me	13	H6	4.02	3.26	4.22
14	H2'	14	H6	2.4	2.2	2.6
14	H2"	14	H6	2.1	1.9	3.6
15	H6	15	H1'	3.8	3.56	4
15	H5	14	H6	3.88	3.48	4.47
16	Me	15	H6	4.05	3.6	4.25
17	H6	16	H2"	2.16	1.86	2.58
17	H6	17	H1'	3.38	2.38	4.52
17	Me	16	H2'	3.48	2.78	3.68
17	Me	16	H2"	3	2.5	3.5
17	H2'	17	H6	1.95	1.75	2.15
17	H2"	17	H6	2.4	2.1	3.6
18	H8	17	H1'	3.68	3.48	4.08
18	H8	18	H1'	3.88	3.41	4.35

19	H6	18	H3'	4.66	3.96	5.36
19	Me	18	H1'	4	3.7	4.3
19	H3'	19	H1'	3.92	3.72	4.12
20	H6	19	H2"	2.29	2.09	2.49
20	H5	19	H2'	3.08	2.88	3.4
21	H6	20	H2"	2.46	2.26	2.66
21	H6	21	H1'	3.97	3.55	4.58
21	H5	20	H2'	3.28	3.08	3.83
22	H2'	22	H8	2.29	2.09	2.49

Class 3 Distance Restraints

1	H6	1	H4'	4.69	4.26	5.28
2	H8	1	H2'	3.99	3.69	4.29
5	H2"	5	H5	5.99	5.36	6.62
8	H8	8	H1'	3.88	3.68	4.08
10	H8	9	H1'	3.81	3.41	4.21
13	H6	12	H2"	2.73	2.13	3.32
15	H5	14	Me	5.18	4.98	5.38
15	H5	14	H2"	3.57	2.56	3.77
17	H6	16	H1'	3.62	3.42	4.02
17	Me	16	H3'	4.95	4.75	5.15
18	H8	17	H2'	3.8	3.5	4.1
18	H8	17	H3'	4.04	3.69	4.84
19	H1'	4	H2	5.01	4.81	5.21
19	H6	18	H8	5.09	4.89	5.29
19	H2'	19	Me	5.03	4.53	5.23
20	H6	19	H6	4.89	4.69	5.09
22	H8	22	H4'	4.58	4.38	5.08
22	H8	22	H1'	3.84	3.64	4.04

Class 4 Distance Restraints

1	H3'	1	H1'	4.01	3.77	4.25
1	H3'	1	H6	3.23	2.81	4.23
2	H8	1	H1'	3.53	3.23	3.83
2	H8	2	H4'	4.67	4.42	4.92
2	H8	2	H1'	3.85	3.65	4.05
2	H3'	2	H8	3.47	3.01	3.98
3	H8	2	H3'	4.32	4.12	5.02
3	H8	3	H4'	4.7	4.4	5
3	H8	3	H1'	3.69	3.48	3.9
3	H3'	3	H8	3.77	3.02	4.22
4	H8	4	H4'	4.72	4.29	5.15
5	H3'	5	H1'	3.92	3.72	4.12
6	H8	6	H4'	4.61	4.36	5.11
7	HA	6	H8	4.56	4.36	5.36
7	H8	7	H4'	4.9	4.5	5.3
8	H8	7	H1'	3.63	2.93	4.25
8	H8	7	H8	4.8	4.55	5.05
8	H8	7	H3'	4.39	3.61	5.17

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8	H8	8	H4'	4.69	4.44	4.94
8	H3'	8	H8	3.6	2.9	4.3
9	H8	9	H4'	4.82	4.41	5.23
9	H8	9	H1'	3.84	3.64	4.04
10	H8	10	H4'	4.65	4.26	5.23
11	H8	10	H8	4.71	4.43	4.99
11	H8	10	H3'	4.33	3.64	5.03
11	H3'	11	H8	3.54	3.1	3.98
13	H6	12	H1'	3.65	3.02	4.28
13	H6	12	H6	5.04	4.84	5.24
13	Me	12	H1'	4.07	3.87	4.27
13	H2'	13	H6	2.2	2	2.4
14	H6	13	H2'	3.85	3.46	4.24
14	Me	13	H1'	4.07	3.87	4.27
16	Me	15	H1'	4.03	3.83	4.23
16	H3'	16	H6	3.12	2.92	4.02
17	Me	16	H1'	4	3.7	4.2
18	H8	17	H6	4.8	4.5	5.1
18	H8	18	H4'	4.5	4.3	4.95
19	H3'	19	H6	3.15	2.95	3.85
19	H3'	19	Me	5.81	5.28	6.34
20	H6	19	H3'	4.29	3.65	4.93
22	H8	21	H1'	3.81	3.61	4.01
22	H8	21	H6	4.65	4.45	5.12
22	H8	21	H2'	3.8	3.6	4
22	H3'	22	H1'	3.94	3.74	4.14