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Solution Structure of the Complex between the Head-To-Tail Dimer of Calicheamicin γ_1^I Oligosaccharide and a DNA Duplex Containing d(ACCT) and d(TCCT) High Affinity Binding Sites

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Supporting Information

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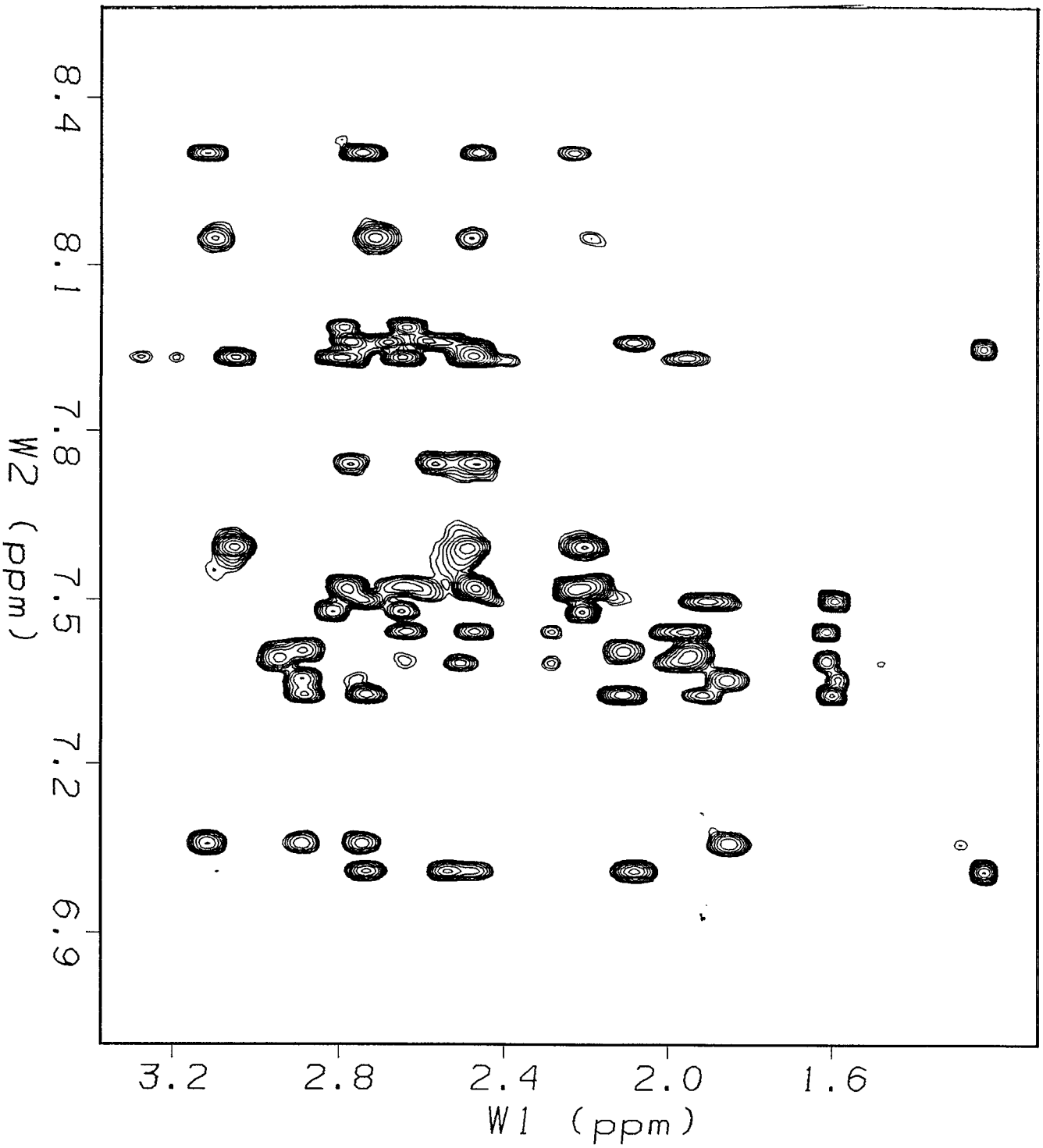
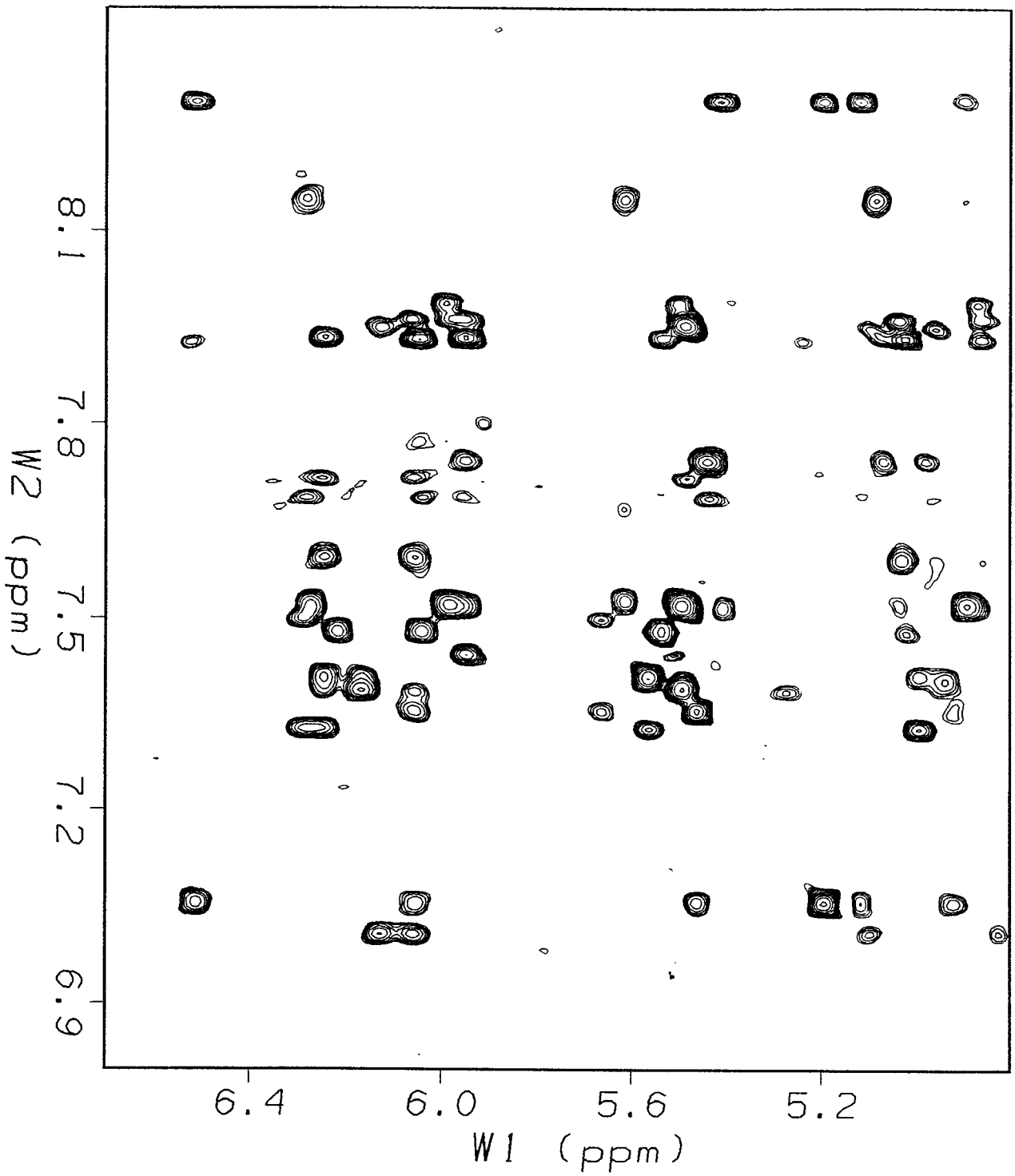
Figure Captions

Fig S1. Region from Hahn Echo NOESY of the HTD complex (τ_m =200 ms mixing time, 27 °C in D_2O) showing $d_i(6,8;2')$, $d_s(2";6,8)$, $d_i(5Me;6)$, $d_s(6,8;5Me)$ connectivities.

Fig S2. Region from Hahn Echo NOESY of the HTD complex (τ_m =200 ms mixing time, 27 °C in D_2O) showing $d_i(6,8;1')$, $d_s(1';6,8)$ connectivities.

Fig S3. Region from Hahn Echo NOESY of the HTD complex (τ_m =200 ms mixing time, 27 °C in D_2O) showing $d_i(1';4')$ connectivities.


8.4
8.1
7.8
7.5
7.2
6.9
W2 (ppm)
3.2
2.8
2.4
2.0
1.6
W1 (ppm)



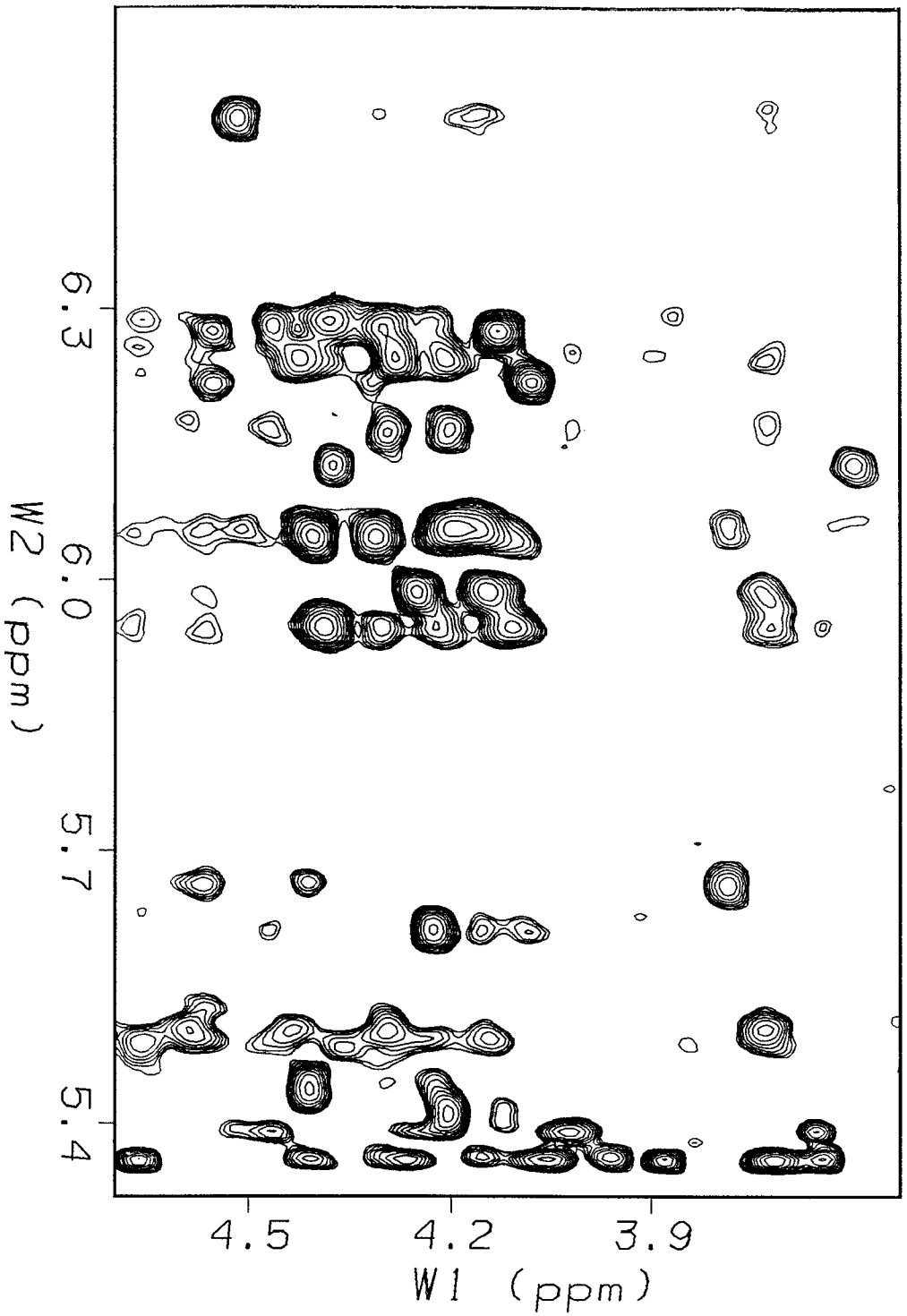

6.3
6.0
5.7
5.4
W2 (ppm)
4.5
4.2
3.9
W1 (ppm)

Table S1. Helical parameters of the twenty initial NAB-generated DNA conformations used in the structure calculations for the 1:1 complex of d(GCACCTTCCTGC)· d(GCAGGAAGGTGC) and HTD (**4**).

Structure Number	X displacement	Inclination	Twist	Rise
1	-2.0	22.0	32.7	2.6
2	2.2	5.8	36.0	3.4
3	2.5	-0.0	36.0	3.4
4	2.2	5.8	26.0	3.4
5	2.2	5.8	45.9	3.4
6	-2.0	22.0	36.9	2.6
7	-2.0	21.9	27.0	2.6
8	2.2	22.0	32.7	3.4
9	-2.0	22.0	32.7	3.4
10	-0.2	10.3	38.0	4.0
11	-1.4	16.0	32.5	3.8
12	-5.0	25.0	35.9	3.0
13	-0.7	25.0	35.9	4.0
14	-2.0	26.9	30.0	4.0
15	-1.3	16.0	33.0	3.0
16	-1.3	4.5	32.9	2.9
17	-0.5	6.2	39.9	3.6
18	-2.0	12.5	37.9	3.8
19	2.5	12.8	36.0	3.7
20	-0.0	12.8	36.0	3.7

Table S2. NMR derived distance constraints used in the structure calculation protocol for the 1:1 complex of d(GCACCTTCCTGC)·d(GCAGGAAGGTGC)-HTD (**4**).

Residue No.	Residue	Proton	Residue No.	Residue	Proton	Upper bound distance
1	GUA	H1'	1	GUA	H8	4.12
1	GUA	H1'	2	CYT	H6	3.42
1	GUA	H1'	2	CYT	H5	3.69
1	GUA	H8	2	CYT	H5	3.55
1	GUA	H8	2	CYT	H41	3.05
1	GUA	H8	2	CYT	H42	4.13
1	GUA	H1	23	GUA	H1	5.14
1	GUA	H1	24	CYT	H42	5.27
1	GUA	H3'	2	CYT	H6	5.07
1	GUA	H3'	2	CYT	H5	5.20
1	GUA	H2'	2	CYT	H6	3.15
1	GUA	H2'	2	CYT	H5	2.49
1	GUA	H2'	2	CYT	H41	4.47
1	GUA	H2"	2	CYT	H6	4.90
1	GUA	H2"	2	CYT	H5	3.86
1	GUA	H2"	2	CYT	H41	5.13
2	CYT	H4'	2	CYT	H6	4.75
2	CYT	H1'	2	CYT	H6	4.04
2	CYT	H1'	3	ADE	H8	3.99
2	CYT	H6	2	CYT	H5	2.69
2	CYT	H6	2	CYT	H41	4.87
2	CYT	H6	3	ADE	H8	5.28
2	CYT	H5	2	CYT	H41	2.70
2	CYT	H5	2	CYT	H42	3.95
2	CYT	H5	23	GUA	H1	5.25
2	CYT	H41	2	CYT	H42	2.04
2	CYT	H41	22	THY	Me	4.95
2	CYT	H41	23	GUA	H1	4.24
2	CYT	H42	22	THY	Me	4.83
2	CYT	H42	22	THY	H3	4.24
2	CYT	H42	23	GUA	H1	2.74
2	CYT	H42	24	CYT	H42	4.90
2	CYT	H3'	3	ADE	H8	5.05
2	CYT	H2'	3	ADE	H8	3.75
2	CYT	H2"	3	ADE	H8	2.45
3	ADE	H4'	3	ADE	H8	5.24
3	ADE	H1'	3	ADE	H8	4.19
3	ADE	H1'	3	ADE	H2	4.96
3	ADE	H1'	4	CYT	H6	3.55
3	ADE	H1'	4	CYT	H5	4.36
3	ADE	H8	4	CYT	H5	3.93
3	ADE	H8	4	CYT	H41	4.33
3	ADE	H2	21	GUA	H1	4.30
3	ADE	H2	22	THY	H3	3.16
3	ADE	H2	23	GUA	H1	4.63
3	ADE	H3'	4	CYT	H6	5.11
3	ADE	H2'	4	CYT	H6	4.10
3	ADE	H2'	4	CYT	H5	3.53

3	ADE	H2'	4	CYT	H41	5.15
3	ADE	H2"	4	CYT	H6	2.49
3	ADE	H2"	4	CYT	H5	2.99
3	ADE	H2"	4	CYT	H41	5.19
4	CYT	H4'	4	CYT	H6	4.84
4	CYT	H1'	4	CYT	H6	4.02
4	CYT	H1'	5	CYT	H6	3.66
4	CYT	H1'	5	CYT	H5	4.43
4	CYT	H6	4	CYT	H5	2.70
4	CYT	H6	4	CYT	H41	4.89
4	CYT	H6	5	CYT	H5	4.19
4	CYT	H6	5	CYT	H41	4.74
4	CYT	H5	4	CYT	H41	2.72
4	CYT	H5	4	CYT	H42	3.98
4	CYT	H5	5	CYT	H5	4.99
4	CYT	H5	5	CYT	H41	4.17
4	CYT	H5	5	CYT	H42	5.02
4	CYT	H41	4	CYT	H42	2.04
4	CYT	H41	5	CYT	H41	4.48
4	CYT	H41	5	CYT	H42	4.40
4	CYT	H41	21	GUA	H1	4.28
4	CYT	H42	5	CYT	H41	4.61
4	CYT	H42	5	CYT	H42	3.91
4	CYT	H42	20	GUA	H1	4.65
4	CYT	H42	21	GUA	H1	2.78
4	CYT	H42	22	THY	H3	5.15
4	CYT	H3'	5	CYT	H6	5.06
4	CYT	H2'	5	CYT	H6	4.02
4	CYT	H2'	5	CYT	H5	3.42
4	CYT	H2'	5	CYT	H41	5.08
4	CYT	H2"	5	CYT	H6	2.44
4	CYT	H2"	5	CYT	H5	2.99
4	CYT	H2"	5	CYT	H41	5.20
5	CYT	H4'	5	CYT	H6	4.85
5	CYT	H1'	5	CYT	H6	4.02
5	CYT	H1'	6	THY	H6	3.88
5	CYT	H6	5	CYT	H5	2.70
5	CYT	H6	5	CYT	H41	4.90
5	CYT	H6	6	THY	Me	4.61
5	CYT	H5	5	CYT	H41	2.72
5	CYT	H5	5	CYT	H42	3.98
5	CYT	H5	6	THY	Me	4.80
5	CYT	H41	5	CYT	H42	2.05
5	CYT	H41	20	GUA	H1	4.30
5	CYT	H41	21	GUA	H1	5.16
5	CYT	H42	6	THY	H3	4.81
5	CYT	H42	20	GUA	H1	2.79
5	CYT	H42	21	GUA	H1	4.30
5	CYT	H3'	6	THY	H6	5.14
5	CYT	H2'	6	THY	H6	3.98
5	CYT	H2'	6	THY	Me	4.32
5	CYT	H2"	6	THY	H6	2.49
5	CYT	H2"	6	THY	Me	4.43
6	THY	H4'	6	THY	H6	4.95

6	THY	H1'	6	THY	H6	4.03
6	THY	H1'	6	THY	H3	4.92
6	THY	H1'	7	THY	H6	3.95
6	THY	H6	6	THY	Me	3.97
6	THY	H6	6	THY	H3	5.11
6	THY	H6	7	THY	Me	4.47
6	THY	Me	6	THY	H3	4.94
6	THY	Me	7	THY	Me	4.87
6	THY	H3	7	THY	H3	3.81
6	THY	H3	18	ADE	H2	5.30
6	THY	H3	19	ADE	H2	3.14
6	THY	H3	20	GUA	H1	3.75
6	THY	H3'	7	THY	H6	5.16
6	THY	H2'	7	THY	H6	4.02
6	THY	H2'	7	THY	Me	4.34
6	THY	H2"	7	THY	H6	2.52
6	THY	H2"	7	THY	Me	4.41
7	THY	H4'	7	THY	H6	4.96
7	THY	H1'	7	THY	H6	4.03
7	THY	H1'	7	THY	H3	4.92
7	THY	H1'	8	CYT	H6	3.68
7	THY	H1'	8	CYT	H5	4.43
7	THY	H6	7	THY	Me	3.96
7	THY	H6	7	THY	H3	5.11
7	THY	H6	8	CYT	H5	3.98
7	THY	H6	8	CYT	H41	4.55
7	THY	Me	7	THY	H3	4.95
7	THY	Me	8	CYT	H41	3.86
7	THY	Me	8	CYT	H42	4.54
7	THY	H3	8	CYT	H5	5.22
7	THY	H3	8	CYT	H41	4.63
7	THY	H3	8	CYT	H42	4.08
7	THY	H3	17	GUA	H1	4.01
7	THY	H3	18	ADE	H2	3.14
7	THY	H3	19	ADE	H2	4.24
7	THY	H3'	8	CYT	H6	5.08
7	THY	H2'	8	CYT	H6	4.04
7	THY	H2'	8	CYT	H5	3.45
7	THY	H2'	8	CYT	H41	5.13
7	THY	H2"	8	CYT	H6	2.45
7	THY	H2"	8	CYT	H5	2.99
7	THY	H2"	8	CYT	H41	5.21
8	CYT	H4'	8	CYT	H6	4.84
8	CYT	H1'	8	CYT	H6	4.01
8	CYT	H1'	9	CYT	H6	3.67
8	CYT	H1'	9	CYT	H5	4.43
8	CYT	H1'	18	ADE	H2	5.23
8	CYT	H6	8	CYT	H5	2.70
8	CYT	H6	8	CYT	H41	4.89
8	CYT	H6	9	CYT	H5	4.15
8	CYT	H6	9	CYT	H41	4.71
8	CYT	H5	8	CYT	H41	2.72
8	CYT	H5	8	CYT	H42	3.97
8	CYT	H5	9	CYT	H5	4.97

8	CYT	H5	9	CYT	H41	4.15
8	CYT	H5	9	CYT	H42	5.01
8	CYT	H41	8	CYT	H42	2.04
8	CYT	H41	9	CYT	H41	4.40
8	CYT	H41	9	CYT	H42	4.33
8	CYT	H41	17	GUA	H1	4.31
8	CYT	H42	9	CYT	H41	4.59
8	CYT	H42	9	CYT	H42	3.90
8	CYT	H42	16	GUA	H1	4.66
8	CYT	H42	17	GUA	H1	2.80
8	CYT	H3'	9	CYT	H6	5.07
8	CYT	H2'	9	CYT	H6	4.00
8	CYT	H2'	9	CYT	H5	3.42
8	CYT	H2'	9	CYT	H41	5.08
8	CYT	H2"	9	CYT	H6	2.44
8	CYT	H2"	9	CYT	H5	3.00
8	CYT	H2"	9	CYT	H41	5.21
9	CYT	H4'	9	CYT	H6	4.85
9	CYT	H1'	9	CYT	H6	4.02
9	CYT	H1'	10	THY	H6	3.93
9	CYT	H6	9	CYT	H5	2.70
9	CYT	H6	9	CYT	H41	4.90
9	CYT	H6	10	THY	Me	4.58
9	CYT	H5	9	CYT	H41	2.72
9	CYT	H5	9	CYT	H42	3.98
9	CYT	H5	10	THY	Me	4.77
9	CYT	H41	9	CYT	H42	2.05
9	CYT	H41	16	GUA	H1	4.30
9	CYT	H41	17	GUA	H1	5.13
9	CYT	H42	10	THY	H3	4.79
9	CYT	H42	16	GUA	H1	2.79
9	CYT	H42	17	GUA	H1	4.27
9	CYT	H3'	10	THY	H6	5.15
9	CYT	H2'	10	THY	H6	3.98
9	CYT	H2'	10	THY	Me	4.31
9	CYT	H2"	10	THY	H6	2.50
9	CYT	H2"	10	THY	Me	4.44
10	THY	H4'	10	THY	H6	4.96
10	THY	H1'	10	THY	H6	4.03
10	THY	H1'	10	THY	H3	4.92
10	THY	H1'	11	GUA	H8	3.85
10	THY	H6	10	THY	Me	3.96
10	THY	H6	10	THY	H3	5.11
10	THY	H6	11	GUA	H8	5.19
10	THY	Me	10	THY	H3	4.95
10	THY	Me	14	CYT	H41	4.97
10	THY	Me	14	CYT	H42	4.84
10	THY	H3	11	GUA	H1	4.33
10	THY	H3	14	CYT	H42	4.29
10	THY	H3	15	ADE	H2	3.17
10	THY	H3	16	GUA	H1	3.74
10	THY	H3'	11	GUA	H8	5.12
10	THY	H2'	11	GUA	H8	3.93
10	THY	H2"	11	GUA	H8	2.46

11	GUA	H4'	11	GUA	H8	5.21
11	GUA	H1'	11	GUA	H8	4.19
11	GUA	H1'	12	CYT	H6	3.57
11	GUA	H1'	12	CYT	H5	4.33
11	GUA	H8	12	CYT	H5	3.97
11	GUA	H8	12	CYT	H41	4.34
11	GUA	H1	12	CYT	H42	4.39
11	GUA	H1	13	GUA	H1	5.16
11	GUA	H1	14	CYT	H5	5.26
11	GUA	H1	14	CYT	H41	4.24
11	GUA	H1	14	CYT	H42	2.74
11	GUA	H1	15	ADE	H2	4.62
11	GUA	H3'	12	CYT	H6	5.05
11	GUA	H2'	12	CYT	H6	4.08
11	GUA	H2'	12	CYT	H5	3.48
11	GUA	H2'	12	CYT	H41	5.15
11	GUA	H2"	12	CYT	H6	2.46
11	GUA	H2"	12	CYT	H5	2.95
11	GUA	H2"	12	CYT	H41	5.22
12	CYT	H4'	12	CYT	H6	4.88
12	CYT	H1'	12	CYT	H6	4.03
12	CYT	H6	12	CYT	H5	2.72
12	CYT	H6	12	CYT	H41	4.98
12	CYT	H5	12	CYT	H41	2.82
12	CYT	H5	12	CYT	H42	4.02
12	CYT	H41	12	CYT	H42	2.06
12	CYT	H42	13	GUA	H1	5.22
12	CYT	H42	14	CYT	H42	4.88
13	GUA	H1'	13	GUA	H8	4.14
13	GUA	H1'	14	CYT	H6	3.41
13	GUA	H1'	14	CYT	H5	3.67
13	GUA	H8	14	CYT	H5	3.60
13	GUA	H8	14	CYT	H41	3.06
13	GUA	H8	14	CYT	H42	4.15
13	GUA	H3'	14	CYT	H6	5.10
13	GUA	H3'	14	CYT	H5	5.20
13	GUA	H2'	14	CYT	H6	3.17
13	GUA	H2'	14	CYT	H5	2.50
13	GUA	H2'	14	CYT	H41	4.47
13	GUA	H2"	14	CYT	H6	4.91
13	GUA	H2"	14	CYT	H5	3.86
13	GUA	H2"	14	CYT	H41	5.12
14	CYT	H4'	14	CYT	H6	4.74
14	CYT	H1'	14	CYT	H6	4.03
14	CYT	H1'	15	ADE	H8	4.00
14	CYT	H6	14	CYT	H5	2.69
14	CYT	H6	14	CYT	H41	4.86
14	CYT	H6	15	ADE	H8	5.28
14	CYT	H5	14	CYT	H41	2.69
14	CYT	H5	14	CYT	H42	3.95
14	CYT	H41	14	CYT	H42	2.04
14	CYT	H3'	15	ADE	H8	5.06
14	CYT	H2'	15	ADE	H8	3.75
14	CYT	H2"	15	ADE	H8	2.46

15	ADE	H4'	15	ADE	H8	5.24
15	ADE	H1'	15	ADE	H8	4.20
15	ADE	H1'	15	ADE	H2	4.95
15	ADE	H1'	16	GUA	H8	3.70
15	ADE	H8	16	GUA	H8	5.19
15	ADE	H2	16	GUA	H1	4.77
15	ADE	H3'	16	GUA	H8	5.17
15	ADE	H2'	16	GUA	H8	4.01
15	ADE	H2"	16	GUA	H8	2.50
16	GUA	H4'	16	GUA	H8	5.18
16	GUA	H1'	16	GUA	H8	4.20
16	GUA	H1'	17	GUA	H8	3.76
16	GUA	H1	17	GUA	H1	3.73
16	GUA	H3'	17	GUA	H8	5.15
16	GUA	H2'	17	GUA	H8	3.99
16	GUA	H2"	17	GUA	H8	2.49
17	GUA	H4'	17	GUA	H8	5.21
17	GUA	H1'	17	GUA	H8	4.20
17	GUA	H1'	18	ADE	H8	3.71
17	GUA	H8	18	ADE	H8	5.28
17	GUA	H1	18	ADE	H2	4.31
17	GUA	H3'	18	ADE	H8	5.14
17	GUA	H2'	18	ADE	H8	4.00
17	GUA	H2"	18	ADE	H8	2.48
18	ADE	H4'	18	ADE	H8	5.19
18	ADE	H1'	18	ADE	H8	4.20
18	ADE	H1'	18	ADE	H2	4.94
18	ADE	H1'	19	ADE	H8	3.67
18	ADE	H8	19	ADE	H8	5.26
18	ADE	H2	19	ADE	H2	4.19
18	ADE	H3'	19	ADE	H8	5.13
18	ADE	H2'	19	ADE	H8	3.98
18	ADE	H2"	19	ADE	H8	2.47
19	ADE	H4'	19	ADE	H8	5.17
19	ADE	H1'	19	ADE	H8	4.19
19	ADE	H1'	19	ADE	H2	4.94
19	ADE	H1'	20	GUA	H8	3.72
19	ADE	H8	20	GUA	H8	5.26
19	ADE	H2	20	GUA	H1	4.72
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19	ADE	H2'	20	GUA	H8	3.95
19	ADE	H2"	20	GUA	H8	2.47
20	GUA	H4'	20	GUA	H8	5.20
20	GUA	H1'	20	GUA	H8	4.20
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20	GUA	H8	21	GUA	H8	5.29
20	GUA	H1	21	GUA	H1	3.76
20	GUA	H3'	21	GUA	H8	5.11
20	GUA	H2'	21	GUA	H8	3.99
20	GUA	H2"	21	GUA	H8	2.46
21	GUA	H4'	21	GUA	H8	5.19
21	GUA	H1'	21	GUA	H8	4.20
21	GUA	H1'	22	THY	H6	3.77
21	GUA	H8	22	THY	Me	4.44

21	GUA	H1	22	THY	H3	3.94
21	GUA	H3'	22	THY	H6	5.16
21	GUA	H2'	22	THY	H6	4.07
21	GUA	H2'	22	THY	Me	4.36
21	GUA	H2"	22	THY	H6	2.52
21	GUA	H2"	22	THY	Me	4.35
22	THY	H4'	22	THY	H6	4.95
22	THY	H1'	22	THY	H6	4.03
22	THY	H1'	22	THY	H3	4.92
22	THY	H1'	23	GUA	H8	3.82
22	THY	H6	22	THY	Me	3.97
22	THY	H6	22	THY	H3	5.12
22	THY	H6	23	GUA	H8	5.21
22	THY	Me	22	THY	H3	4.95
22	THY	H3	23	GUA	H1	4.32
22	THY	H3'	23	GUA	H8	5.12
22	THY	H2'	23	GUA	H8	3.94
22	THY	H2"	23	GUA	H8	2.46
23	GUA	H4'	23	GUA	H8	5.21
23	GUA	H1'	23	GUA	H8	4.19
23	GUA	H1'	24	CYT	H6	3.57
23	GUA	H1'	24	CYT	H5	4.33
23	GUA	H8	24	CYT	H5	3.98
23	GUA	H8	24	CYT	H41	4.35
23	GUA	H1	24	CYT	H42	4.38
23	GUA	H3'	24	CYT	H6	5.05
23	GUA	H2'	24	CYT	H6	4.08
23	GUA	H2'	24	CYT	H5	3.48
23	GUA	H2'	24	CYT	H41	5.15
23	GUA	H2"	24	CYT	H6	2.47
23	GUA	H2"	24	CYT	H5	2.95
23	GUA	H2"	24	CYT	H41	5.21
24	CYT	H4'	24	CYT	H6	4.88
24	CYT	H1'	24	CYT	H6	4.03
24	CYT	H6	24	CYT	H5	2.72
24	CYT	H6	24	CYT	H41	4.98
24	CYT	H5	24	CYT	H41	2.82
24	CYT	H5	24	CYT	H42	4.02
24	CYT	H41	24	CYT	H42	2.06
1	GUA	H8	1	GUA	H2'	3.39
1	GUA	H8	1	GUA	H2"	2.65
2	CYT	H6	2	CYT	H2'	2.31
2	CYT	H6	2	CYT	H2"	3.78
3	ADE	H8	3	ADE	H2'	2.28
3	ADE	H8	3	ADE	H2"	3.62
4	CYT	H6	4	CYT	H2'	2.21
4	CYT	H6	4	CYT	H2"	3.65
5	CYT	H6	5	CYT	H2'	2.20
5	CYT	H6	5	CYT	H2"	3.67
6	THY	H6	6	THY	H2'	2.17
6	THY	H6	6	THY	H2"	3.61
7	THY	H6	7	THY	H2'	2.15
7	THY	H6	7	THY	H2"	3.56
8	CYT	H6	8	CYT	H2'	2.16

8	CYT	H6	8	CYT	H2"	3.59
9	CYT	H6	9	CYT	H2'	2.17
9	CYT	H6	9	CYT	H2"	3.64
10	THY	H6	10	THY	H2'	2.12
10	THY	H6	10	THY	H2"	3.49
11	GUA	H8	11	GUA	H2'	2.24
11	GUA	H8	11	GUA	H2"	3.52
13	GUA	H8	13	GUA	H2'	3.53
13	GUA	H8	13	GUA	H2"	2.74
14	CYT	H6	14	CYT	H2'	2.28
14	CYT	H6	14	CYT	H2"	3.75
15	ADE	H8	15	ADE	H2'	2.28
15	ADE	H8	15	ADE	H2"	3.67
16	GUA	H8	16	GUA	H2'	2.33
16	GUA	H8	16	GUA	H2"	3.71
17	GUA	H8	17	GUA	H2'	2.27
17	GUA	H8	17	GUA	H2"	3.66
18	ADE	H8	18	ADE	H2'	2.26
18	ADE	H8	18	ADE	H2"	3.67
19	ADE	H8	19	ADE	H2'	2.30
19	ADE	H8	19	ADE	H2"	3.74
20	GUA	H8	20	GUA	H2'	2.29
20	GUA	H8	20	GUA	H2"	3.65
21	GUA	H8	21	GUA	H2'	2.25
21	GUA	H8	21	GUA	H2"	3.70
22	THY	H6	22	THY	H2'	2.11
22	THY	H6	22	THY	H2"	3.47
23	GUA	H8	23	GUA	H2'	2.25
23	GUA	H8	23	GUA	H2"	3.57
1	GUA	H8	1	GUA	H3'	4.97
2	CYT	H6	2	CYT	H3'	3.85
3	ADE	H8	3	ADE	H3'	4.36
4	CYT	H6	4	CYT	H3'	3.98
5	CYT	H6	5	CYT	H3'	3.82
6	THY	H6	6	THY	H3'	3.93
7	THY	H6	7	THY	H3'	4.03
8	CYT	H6	8	CYT	H3'	3.97
9	CYT	H6	9	CYT	H3'	3.83
10	THY	H6	10	THY	H3'	4.08
11	GUA	H8	11	GUA	H3'	4.43
12	CYT	H6	12	CYT	H3'	3.64
13	GUA	H8	13	GUA	H3'	5.00
14	CYT	H6	14	CYT	H3'	3.82
15	ADE	H8	15	ADE	H3'	4.29
16	GUA	H8	16	GUA	H3'	4.33
17	GUA	H8	17	GUA	H3'	4.29
18	ADE	H8	18	ADE	H3'	4.25
19	ADE	H8	19	ADE	H3'	4.20
20	GUA	H8	20	GUA	H3'	4.35
21	GUA	H8	21	GUA	H3'	4.18
22	THY	H6	22	THY	H3'	4.11
23	GUA	H8	23	GUA	H3'	4.43
24	CYT	H6	24	CYT	H3'	3.93
4	CYT	H5'	4	CYT	H6	4.13

4	CYT	H5"	4	CYT	H6	4.69
5	CYT	H5'	5	CYT	H6	4.10
9	CYT	H5'	9	CYT	H6	4.13
9	CYT	H5"	9	CYT	H6	4.59
18	ADE	H5'	18	ADE	H8	4.44
18	ADE	H5"	18	ADE	H8	4.99
22	THY	H5'	22	THY	H6	4.44
22	THY	H5"	22	THY	H6	4.95
1	GUA	H4'	1	GUA	H1'	2.60
2	CYT	H4'	2	CYT	H1'	3.07
3	ADE	H4'	3	ADE	H1'	2.99
4	CYT	H4'	4	CYT	H1'	2.95
5	CYT	H4'	5	CYT	H1'	2.99
6	THY	H4'	6	THY	H1'	2.92
7	THY	H4'	7	THY	H1'	2.91
8	CYT	H4'	8	CYT	H1'	2.97
9	CYT	H4'	9	CYT	H1'	3.02
10	THY	H4'	10	THY	H1'	2.92
11	GUA	H4'	11	GUA	H1'	3.17
12	CYT	H4'	12	CYT	H1'	3.11
13	GUA	H4'	13	GUA	H1'	2.36
14	CYT	H4'	14	CYT	H1'	3.06
15	ADE	H4'	15	ADE	H1'	2.99
16	GUA	H4'	16	GUA	H1'	2.99
17	GUA	H4'	17	GUA	H1'	3.12
18	ADE	H4'	18	ADE	H1'	3.09
19	ADE	H4'	19	ADE	H1'	3.06
20	GUA	H4'	20	GUA	H1'	3.00
21	GUA	H4'	21	GUA	H1'	3.21
22	THY	H4'	22	THY	H1'	2.95
23	GUA	H4'	23	GUA	H1'	3.17
24	CYT	H4'	24	CYT	H1'	3.10
3	ADE	H1'	4	CYT	H5'	3.04
4	CYT	H1'	5	CYT	H5'	3.08
8	CYT	H1'	9	CYT	H5'	3.17
17	GUA	H1'	18	ADE	H5'	2.93
21	GUA	H1'	22	THY	H5'	2.95
25	SUG	AMe	24	CYT	H4'	3.00
25	SUG	BMe	5	CYT	H4'	3.00
25	SUG	C7Me	5	CYT	H1'	3.00
25	SUG	H3B	22	THY	H3	3.00
25	SUG	C9Me	22	THY	H5'	4.00
25	SUG	C9Me	22	THY	H5"	4.00
25	SUG	H1D	22	THY	H5'	3.00
25	SUG	H1D	22	THY	H5"	3.00
25	SUG	C9Me	22	THY	H4'	3.00
25	SUG	H1D	22	THY	H4'	3.00
25	SUG	H2D	22	THY	H4'	3.00
25	SUG	H2D	22	THY	H5'	4.00
25	SUG	H2D	22	THY	H5"	4.00
25	SUG	DoMe	21	GUA	H4'	3.50
25	SUG	DoMe	20	GUA	H21	5.00
25	SUG	H1B	23	GUA	H4'	4.00
25	SUG	H1E	25	SUG	H2A	3.00

25	SUG	AMe	25	SUG	H2B1	5.00
25	SUG	BMe	25	SUG	C9Me	3.00
25	SUG	DMe	25	SUG	C8Me	4.00
25	SUG	H1D	25	SUG	C8Me	3.00
25	SUG	AMe	25	SUG	H1B	3.00
25	SUG	H1A	25	SUG	H3A	3.00
25	SUG	H1A	25	SUG	H5A	3.00
25	SUG	H3A	25	SUG	H5A	3.00
25	SUG	H2A	25	SUG	H4A	3.00
25	SUG	H1B	25	SUG	H5B	3.00
25	SUG	H2B1	25	SUG	H4B	3.00
25	SUG	H4E	25	SUG	H2E1	3.00
25	SUG	H3E	25	SUG	H5E1	3.00
27	SUG	AMe	20	GUA	H4'	4.00
27	SUG	BMe	9	CYT	H4'	5.00
27	SUG	C7Me	9	CYT	H1'	4.00
27	SUG	H2B1	18	ADE	H2	3.00
27	SUG	H2B2	18	ADE	H2	3.50
27	SUG	C9Me	18	ADE	H5'	5.00
27	SUG	C9Me	18	ADE	H5"	5.00
27	SUG	H1D	18	ADE	H5'	3.00
27	SUG	H1D	18	ADE	H5"	5.00
27	SUG	H2D	18	ADE	H5'	4.00
27	SUG	H2D	18	ADE	H5"	3.00
27	SUG	DoMe	17	GUA	H4'	4.00
27	SUG	DoMe	16	GUA	H21	5.00
27	SUG	H1B	19	ADE	H4'	3.00
27	SUG	H1B	19	ADE	H5'	3.00
27	SUG	H1E	27	SUG	H2A	3.00
27	SUG	AMe	27	SUG	H2B1	5.00
27	SUG	BMe	27	SUG	C9Me	3.00
27	SUG	DMe	27	SUG	C8Me	4.00
27	SUG	H1D	27	SUG	C8Me	3.00
27	SUG	AMe	27	SUG	H1B	3.00
27	SUG	H1A	27	SUG	H3A	3.00
27	SUG	H1A	27	SUG	H5A	3.00
27	SUG	H3A	27	SUG	H5A	3.00
27	SUG	H2A	27	SUG	H4A	3.00
27	SUG	H1B	27	SUG	H5B	3.00
27	SUG	H2B1	27	SUG	H4B	3.00
27	SUG	H4E	27	SUG	H2E1	3.00
27	SUG	H3E	27	SUG	H5E1	3.00
1	GUA	N1	24	CYT	N3	3.05
1	GUA	O6	24	CYT	N4	3.01
1	GUA	H1	24	CYT	N3	2.35
1	GUA	O6	24	CYT	H42	2.35
2	CYT	N3	23	GUA	N1	3.05
2	CYT	N4	23	GUA	O6	3.01
2	CYT	N3	23	GUA	H1	2.35
2	CYT	H42	23	GUA	O6	2.35
3	ADE	N1	22	THY	N3	2.92
3	ADE	N1	22	THY	H3	2.22
4	CYT	N3	21	GUA	N1	3.05
4	CYT	N4	21	GUA	O6	3.01

4	CYT	N3	21	GUA	H1	2.35
4	CYT	H42	21	GUA	O6	2.35
5	CYT	N3	20	GUA	N1	3.05
5	CYT	N4	20	GUA	O6	3.01
5	CYT	N3	20	GUA	H1	2.35
5	CYT	H42	20	GUA	O6	2.35
6	THY	N3	19	ADE	N1	2.92
6	THY	H3	19	ADE	N1	2.22
7	THY	N3	18	ADE	N1	2.92
7	THY	H3	18	ADE	N1	2.22
8	CYT	N3	17	GUA	N1	3.05
8	CYT	N4	17	GUA	O6	3.01
8	CYT	N3	17	GUA	H1	2.35
8	CYT	H42	17	GUA	O6	2.35
9	CYT	N3	16	GUA	N1	3.05
9	CYT	N4	16	GUA	O6	3.01
9	CYT	N3	16	GUA	H1	2.35
9	CYT	H42	16	GUA	O6	2.35
10	THY	N3	15	ADE	N1	2.92
10	THY	H3	15	ADE	N1	2.22
11	GUA	N1	14	CYT	N3	3.05
11	GUA	O6	14	CYT	N4	3.01
11	GUA	H1	14	CYT	N3	2.35
11	GUA	O6	14	CYT	H42	2.35
12	CYT	N3	13	GUA	N1	3.05
12	CYT	N4	13	GUA	O6	3.01
12	CYT	N3	13	GUA	H1	2.35
12	CYT	H42	13	GUA	O6	2.35