

**Structure of an Oligodeoxynucleotide Containing a Butadiene Oxide-Derived N1
beta-Hydroxyalkyl Deoxyinosine Adduct in the Human *N-ras* Codon 61 Sequence[†]**

Supporting Information

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Table S1. ^1H NMR Assignments for the *ras6I* S-N1-BDO-(61,2) adduct.

Base	H1'	H2'	H2''	H3'	H4'	H5'	H5''	H5	H6	H8	CH ₃	BD	
C ¹	5.59	1.7	2.2	4.54		3.53	3.91	5.75	7.43			H _α	5.02
G ²	5.25	2.53	2.57	4		3.66	4.13			7.77		H _{α'}	5.12
G ³	5.54	2.65	2.64	4.82		3.96	4.02			7.68		H _β	5.58
A ⁴	6.05	2.45	2.69	4.9		4.07	4.27			8		H _γ	4.8
C ⁵	5.68	1.74	1.86	4.89		3.91		5.16	7.05			H _δ	3.4
X ⁶	5.44	2.13	2.2	4.63	4.02	3.81	3.72			7.66		H _{δ'}	3.22
A ⁷	5.42	2.53	2.2	4.71	3.81	4.14				8.02			
G ⁸	5.14	2.41	2.47	4.81		4.14	3.95			7.59			
A ⁹	5.77	2.72	2.47	4.8		4.05	4.27			7.98			
A ¹⁰	5.87	2.42	2.5	4.89		4.04	4.28			7.89			
G ¹¹	5.84	2.09	2.2	4.86	3.96	4.03	4.12			7.44			
C ¹²	5.76	1.54	2.15	4.44		3.73		5.82	7.76				
T ¹³	6.07	2.47	2.51	4.53						7.52		1.48	
T ¹⁴	6.01	2.09	1.52	4.77		4.07				7.34		1.46	
C ¹⁵	5.87	1.93	2.3	4.79				5.55	7.46				
T ¹⁶	5.98	2.21	1.95	4.7	4.02	3.97				7.22		1.45	
T ¹⁷	5.52	1.74	2	4.69		3.83	3.94			7.12		1.5	
G ¹⁸	5.75	2.59	2.65	4.61	4.17	3.84	3.89			7.86			
T ¹⁹	5.92	2.07	2.37	4.79		4	4.09			7.2		1.42	
C ²⁰	5.59	1.98	2.27	4.67		4		5.52	7.42				
C ²¹	5.45	1.86	2.19	4.68		3.82	4.02	5.63	7.36				
G ²²	6.04	2.5	2.66	4.54		3.92				7.83			

Table S2. NOE Restraints Used in the rMD Calculations for the *ras61* S-N1-BDO-(61,2) adduct.

Class 1						
Base 1	Atom 1	Base 2	Atom 2	Distance	Upper	Lower
1	H3'	1	H1'	4.66	0.7	0.7
1	H3'	1	H6	3.35	0.5	0.5
1	H3'	1	H2'	2.6	0.45	0.45
2	H8	1	H2'	3.69	0.81	0.81
2	H3'	2	H1'	4.42	0.66	0.66
2	H3'	2	H8	4.4	0.66	0.66
3	H8	2	H3'	4.39	0.64	0.64
3	H3'	3	H8	4.38	0.69	0.69
4	H8	3	H8	4.98	0.34	0.34
4	H2"	4	H1'	2.77	0.41	0.41
4	H3'	4	H1'	3.96	0.59	0.59
4	H3'	4	H8	4.35	0.8	0.8
5	H6	4	H1'	4.3	0.65	0.65
5	H6	4	H2'	3.61	0.51	0.51
5	H6	4	H2"	2.7	0.7	0.7
5	H6	4	H3'	4.95	0.74	0.74
5	H2'	5	H6	2.07	0.46	0.46
5	H2"	5	H6	3.52	0.53	0.53
5	H3'	5	H6	3.71	0.56	0.56
5	H5	5	H6	3	0.56	0.56
5	H6	5	H5'	3.2	0.56	0.56
6	H8	5	H2'	6.21	0.58	0.58
6	H8	5	H2"	5.23	0.47	0.47

6	H8	5	H3'	8.56	0.45	0.45
6	H2'	6	H8	4.49	0.55	0.55
6	H2''	6	H8	4.18	0.49	0.49
6	H3'	6	H8	5.63	0.59	0.59
7	H8	7	H4'	5.3	0.85	0.85
7	H8	6	H8	5	0.5	0.5
7	H8	7	H1'	3.67	0.55	0.55
7	H2'	7	H1'	2.53	0.38	0.38
7	H2''	7	H8	3.79	0.57	0.57
7	H3'	7	H8	4.37	0.84	0.84
8	H8	7	H1'	4.6	0.69	0.69
8	H8	8	H1'	3.55	0.53	0.53
8	H3'	8	H1'	4.44	0.67	0.67
8	H3'	8	H8	4.44	0.61	0.61
9	H8	8	H1'	4.42	0.66	0.66
9	H8	8	H8	4.46	0.67	0.67
9	H8	8	H3'	5	0.62	0.62
9	H8	9	H1'	3.88	0.58	0.58
9	H2''	9	H1'	2.46	0.37	0.37
9	H3'	9	H1'	3.72	0.77	0.77
10	H8	9	H1'	3.95	0.59	0.59
10	H8	9	H2'	2.71	0.41	0.41
10	H8	10	H1'	3.98	0.6	0.6
10	H2'	10	H1'	3.47	0.52	0.52
10	H2'	10	H8	2.5	0.67	0.67
10	H2''	10	H8	3.77	0.54	0.54
10	H3'	10	H1'	4.07	0.61	0.61

11	H8	10	H8	4.22	0.63	0.63
11	H8	10	H3'	4.49	0.67	0.67
11	H2'	11	H1'	2.63	0.4	0.4
11	H2"	11	H8	3.71	0.49	0.49
11	H3'	11	H1'	4.49	0.67	0.67
11	H3'	11	H8	4.29	0.79	0.79
11	H3'	11	H2'	2.81	0.57	0.57
11	H3'	11	H2"	2.83	0.43	0.43
12	H5	12	H6	2.23	0.33	0.33
12	H2'	12	H6	1.77	0.55	0.55
12	H3'	12	H6	3.88	0.58	0.58
12	H3'	12	H2'	1.85	0.47	0.47
13	H6	12	H2"	2.86	0.45	0.45
13	H6	12	H3'	4.04	0.62	0.62
13	H3'	13	H6	4.1	0.61	0.61
14	H6	13	H6	4.76	0.71	0.71
14	H6	14	H1'	4.12	0.62	0.62
14	H2'	14	H1'	2.95	0.44	0.44
14	H2"	14	H6	3.54	0.38	0.38
14	H3'	14	H1'	4.27	0.64	0.64
14	H3'	14	H6	4.01	0.63	0.63
15	H6	14	H1'	4.7	0.7	0.7
15	H6	14	H6	5.38	0.51	0.51
15	H6	14	H2"	4.04	0.61	0.61
15	H5	15	H6	2.4	0.36	0.36
15	H2'	15	H6	2.2	0.66	0.66
15	H2"	15	H6	3.43	0.51	0.51

15	H3'	15	H6	4.02	0.68	0.68
16	H6	15	H6	5.39	0.51	0.51
16	H6	15	H2'	3.59	0.57	0.57
16	H6	15	H2"	3.37	0.7	0.7
16	H6	16	H1'	3.7	0.56	0.56
16	H2'	16	H1'	2.38	0.36	0.36
16	H2'	16	H6	3.96	0.59	0.59
16	H2"	16	H1'	2.13	0.45	0.45
16	H2"	16	H6	4.36	0.65	0.65
16	H3'	16	H6	3.96	0.89	0.89
17	H6	16	H1'	4.62	0.69	0.69
17	H6	16	H2'	3.58	0.76	0.76
17	H6	16	H2"	3.98	0.6	0.6
17	H6	17	H1'	4.25	0.64	0.64
17	H2'	17	H1'	3.18	0.63	0.63
17	H2'	17	H6	2.39	0.66	0.66
17	H2"	17	H1'	1.85	0.58	0.58
17	H2"	17	H6	3.5	0.53	0.53
17	H3'	17	H1'	3.67	0.55	0.55
17	H3'	17	H6	3.21	0.48	0.48
17	H3'	17	H2"	2.87	0.23	0.23
18	H1'	18	H4'	3.46	0.67	0.67
18	H8	17	H1'	4.46	0.67	0.67
18	H8	17	H6	5.23	0.78	0.78
18	H8	17	H2'	3.69	0.76	0.76
18	H8	17	H2"	3.23	0.74	0.74
18	H8	17	H3'	4.96	0.74	0.74

18	H8	18	H4'	5.34	0.8	0.8
18	H8	18	H1'	3.9	0.58	0.58
18	H2'	18	H4'	4.31	0.65	0.65
18	H2'	18	H1'	3.05	0.56	0.56
18	H2''	18	H4'	4.07	0.69	0.69
18	H3'	18	H1'	4.67	0.7	0.7
18	H3'	18	H8	4.13	0.62	0.62
19	H6	18	H1'	4.38	0.66	0.66
19	H6	18	H8	5	0.39	0.39
19	H6	18	H2'	1.79	0.35	0.35
19	H6	18	H2''	3.36	0.22	0.22
19	H6	19	H1'	3.83	0.57	0.57
19	H2'	19	H1'	3.58	0.54	0.54
19	H2'	19	H6	2.82	0.2	0.2
19	H2''	19	H1'	1.74	0.52	0.52
19	H2''	19	H6	3.75	0.56	0.56
19	H3'	19	H6	3.75	0.83	0.83
20	H6	19	H1'	4.52	0.68	0.68
20	H5	20	H6	2.27	0.34	0.34
20	H2''	20	H6	3.36	0.44	0.44
20	H3'	20	H6	4.03	0.7	0.7
21	H6	20	H2'	3.58	0.62	0.62
21	H6	21	H1'	3.49	0.52	0.52
21	H2'	21	H1'	3.09	0.64	0.64
21	H2'	21	H6	2.97	0.45	0.45
21	H2''	21	H1'	2.34	0.5	0.5
21	H3'	21	H1'	3.99	0.6	0.6

21	H3'	21	H6	3.96	0.59	0.59
22	H8	21	H1'	4.11	0.62	0.62
22	H8	21	H2'	3.67	0.78	0.78
22	H8	21	H2"	3.86	0.33	0.33
22	H8	21	H3'	4.35	0.8	0.8
22	H8	22	H1'	4.08	0.61	0.61
22	H2"	22	H8	4.4	0.66	0.66
22	H3'	22	H1'	3.97	0.75	0.75
22	H3'	22	H8	3.96	0.59	0.59
1	H5"	1	H1'	4.38	0.66	0.66
1	H5'	1	H6	4.62	0.69	0.69
1	H5'	1	H2'	4	0.6	0.6
1	H5'	1	H3'	3.29	0.49	0.49
2	H5"	2	H1'	4.48	0.67	0.67
2	H5'	2	H8	4.39	0.66	0.66
2	H5'	2	H3'	2.52	0.38	0.38
2	H8	3	H8	5	0.3	0.3
3	H1'	3	H2'	2.62	0.39	0.39
3	H1'	3	H3'	4.23	0.64	0.64
3	H5'	3	H3'	3.9	0.73	0.73
4	H5'	4	H8	4.49	0.67	0.67
4	H8	5	H6	5	0.6	0.6
4	H5'	4	H2'	3.77	0.55	0.55
4	H5"	4	H1'	5.01	0.6	0.6
4	H5"	4	H8	4.77	0.72	0.72
4	H5"	4	H2'	4.33	0.65	0.65
5	H1'	5	H6	4.11	0.62	0.62

5	H1'	5	H2'	3.21	0.59	0.59
5	H1'	5	H3'	3.77	0.8	0.8
5	H1'	6	H8	5.91	0.32	0.32
6	H8	5	H6	6.61	0.51	0.51
6	H5'	6	H8	5.17	0.27	0.27
6	H5''	6	H8	6.82	0.48	0.48
6	H4'	6	H8	5.57	0.44	0.44
7	H5'	7	H1'	4.31	0.5	0.5
7	H8	8	H8	5	0.6	0.6
7	H5'	7	H8	3.97	0.6	0.6
8	H5'	8	H1'	4.12	0.62	0.62
8	H5'	8	H8	5.11	0.77	0.77
8	H5''	8	H8	5.14	0.77	0.77
8	H8	7	H8	5	0.2	0.2
9	H5''	9	H1'	5.05	0.61	0.61
9	H8	8	H8	5	0.5	0.5
9	H8	10	H8	5	0.6	0.6
10	H5'	10	H8	5.12	0.77	0.77
10	H5'	10	H2''	4.84	0.73	0.73
10	H5''	10	H1'	4.12	0.62	0.62
10	H5''	10	H8	5.18	0.78	0.78
11	H5'	11	H3'	3.96	0.59	0.59
11	H5''	11	H3'	2.79	0.72	0.72
11	H4'	11	H3'	2.41	0.38	0.28
12	H5'	12	H6	3.99	0.6	0.6
12	H5'	12	H3'	3.92	0.59	0.59
12	H5''	12	H6	4.69	0.7	0.7

12	H1'	12	H6	4.17	0.62	0.62
12	H1'	12	H2'	3.12	0.66	0.66
12	H1'	12	H2"	2.19	0.54	0.54
12	H1'	12	H3'	4.75	0.71	0.71
12	H1'	13	H6	3.35	0.5	0.5
13	H1'	13	H3'	4.59	0.69	0.69
13	H1'	14	H6	4	0.6	0.6
14	H5'	14	H6	4.67	0.7	0.7
15	H1'	15	H2'	3.93	0.59	0.59
15	H6	14	H6	5.05	0.51	0.51
15	H1'	15	H3'	4.75	0.71	0.71
15	H1'	16	H6	3.72	0.56	0.56
16	H5'	16	H1'	4.22	0.36	0.36
16	H5'	16	H6	3.5	0.82	0.82
16	H4'	16	H6	4.8	0.82	0.82
16	H5'	16	H2"	4.68	0.55	0.55
17	H5'	17	H1'	3.79	0.57	0.57
17	H5'	17	H6	4.71	0.71	0.71
17	H5'	17	H2'	4.07	0.61	0.61
17	H5'	17	H2"	4.88	0.58	0.58
17	H5'	17	H3'	3.61	0.54	0.54
17	H5"	17	H1'	4.13	0.62	0.62
17	H5"	17	H6	5.17	0.77	0.77
18	H5'	18	H4'	2.58	0.39	0.39
18	H5'	18	H8	4.43	0.66	0.66
18	H5"	18	H4'	2.44	0.52	0.52
18	H5"	18	H8	5.35	0.8	0.8

19	H5'	19	H1'	4.02	0.6	0.6
19	H5''	19	H1'	4.15	0.62	0.62
20	H5'	20	H6	4.83	0.72	0.72
20	H1'	20	H2'	3.01	0.57	0.57
20	H1'	20	H2''	2.17	0.61	0.61
21	H5'	21	H1'	4.19	0.63	0.63
21	H5''	21	H1'	4.35	0.65	0.65
22	H5'	22	H8	5.03	0.75	0.75
22	H8	21	H6	5.03	0.75	0.75
5	H6	4	H2	5.43	1	1
18	H8	19	H6	5.23	0.4	0.4
8	H2''	17	H5''	11	1	1
8	H1	9	H2	3.92	0.5	0.5
9	H2	10	H2	3.78	0.3	0.3
12	H6	13	H6	5.05	0.3	0.3
1	H6	2	H8	4.85	0.3	0.3
21	H6	22	H8	4.81	0.2	0.3
6	HAO1	6	HAO2	1.75	0.3	0.3
6	HAM1	6	HAO2	4.01	0.4	0.4
6	HAM2	6	HAO2	3.59	0.55	0.55
6	HAM2	6	HAM1	2.44	0.4	0.4
6	HAM2	6	HAL	2.68	0.44	0.44
6	HAM2	6	HAO1	4.35	0.5	0.5
6	H2	6	HAO1	4.62	0.95	0.95
6	H2	6	HAL	2.1	0.4	0.4
6	H2	6	HAO2	3.65	0.4	0.4
6	H2	6	HAN	3.8	0.4	0.4

6	H2	6	HAM2	4.36	0.48	0.48
6	H2	6	HAM1	2	0.38	0.38
6	HAN	6	HAO2	2.77	0.55	0.55
7	H2	16	H3	2.55	0.55	0.55
18	H1	4	H2	2.9	0.55	0.55
15	H42	16	H3	4.02	0.55	0.55

Class 2

1	H3'	1	H2"	3.52	0.53	0.53
2	H8	1	H2"	3.79	0.57	0.57
2	H2'	2	H8	2.13	0.42	0.42
2	H2"	2	H1'	2.77	0.42	0.42
2	H2"	2	H8	3.84	0.58	0.58
3	H8	2	H2'	2.7	0.41	0.41
3	H2'	3	H8	3	0.45	0.45
3	H3'	3	H2'	2.42	0.56	0.56
4	H2"	4	H8	3.38	0.51	0.51
5	H5	5	H6	2.49	0.37	0.37
8	H8	7	H2'	3.69	0.54	0.54
8	H2'	8	H1'	3.17	0.63	0.63
8	H2'	8	H8	2.08	0.61	0.61
8	H2"	8	H1'	2.22	0.48	0.48
9	H2'	9	H1'	3.12	0.47	0.47
9	H2'	9	H8	3.05	0.46	0.46
9	H3'	9	H8	4.35	0.73	0.73
10	H3'	10	H8	4.31	0.73	0.73

11	H8	10	H1'	3.65	0.55	0.55
12	H2''	12	H6	3.45	0.5	0.5
12	H3'	12	H2''	3.32	0.5	0.5
13	H2'	13	H6	3.49	0.52	0.52
13	H2''	13	H6	3.81	0.57	0.57
14	H6	13	H2'	1.72	0.53	0.53
14	H6	13	H2''	3.33	0.5	0.5
14	H2'	14	H6	1.79	0.49	0.49
15	H6	14	H2'	2.91	0.44	0.44
17	H3'	17	H2'	2.15	0.47	0.47
18	H2'	18	H8	2.58	0.39	0.39
18	H2''	18	H8	4.32	0.33	0.33
20	H6	19	H2''	4.02	0.6	0.6
20	H3'	20	H2'	2.81	0.42	0.42
21	H2''	21	H6	4.23	0.63	0.63
21	H3'	21	H2''	2.79	0.57	0.57
22	H2'	22	H1'	2.77	0.42	0.42
22	H2'	22	H8	2.67	0.4	0.4
4	H5''	4	H2''	3.96	0.59	0.59
7	H5'	7	H2'	3.75	0.56	0.56
8	H5'	8	H2'	3.78	0.54	0.54
9	H5'	9	H1'	3.89	0.58	0.58
10	H5''	10	H3'	2.88	0.43	0.43
14	H5'	14	H1'	4.41	0.47	0.47
15	H1'	15	H6	4.05	0.61	0.61
15	H1'	15	H2''	2.2	0.55	0.55
16	H5'	16	H2'	3.88	0.58	0.58

17	H5"	17	H2'	4.41	0.66	0.66
17	H5"	17	H3'	3.51	0.53	0.53
20	H5'	20	H2'	3.71	0.56	0.56
20	H1'	21	H6	2.93	0.44	0.44
22	H5'	22	H3'	2.58	0.39	0.39

Class 3

2	H2'	2	H1'	3.05	0.56	0.56
4	H2'	4	H1'	3.2	0.48	0.48
8	H2"	8	H8	4	0.6	0.6
9	H8	8	H2'	3.78	0.87	0.87
9	H8	8	H2"	3.02	0.6	0.6
10	H3'	10	H2'	2.46	0.47	0.47
11	H8	10	H2'	2.21	0.61	0.61
11	H8	11	H1'	3.85	0.65	0.65
11	H2'	11	H8	2.23	0.59	0.59
16	H3'	16	H2"	2.6	0.45	0.45
18	H2"	18	H1'	2.34	0.44	0.44
18	H3'	18	H4'	2.86	0.43	0.43
20	H3'	20	H2"	2.78	0.42	0.42
21	H3'	21	H2'	2.43	0.51	0.51
3	H5"	3	H3'	3.02	0.48	0.48
4	H5'	4	H2"	4.71	0.51	0.51
4	H5'	4	H3'	3.7	0.41	0.41
10	H5'	10	H1'	4.78	0.57	0.57
10	H5'	10	H3'	2.84	0.52	0.52

11	H5'	11	H1'	4.41	0.45	0.45
14	H5'	14	H3'	3.62	0.39	0.39
16	H5'	16	H3'	3.7	0.39	0.39
17	H5"	17	H2"	4.66	0.52	0.52
20	H5'	20	H3'	3.72	0.45	0.45
20	H1'	20	H6	3.57	0.68	0.68

Class 4

4	H3'	4	H2'	2.34	0.46	0.46
4	H3'	4	H2"	3.28	0.49	0.49
7	H2'	7	H8	2.71	0.26	0.26
8	H3'	8	H2'	2.5	0.53	0.53
8	H3'	8	H2"	3.45	0.52	0.52
13	H3'	13	H2"	2.62	0.39	0.39
4	H5'	4	H1'	4.44	0.5	0.5
8	H5'	8	H3'	3.71	0.35	0.35
8	H5"	8	H2"	4.71	0.56	0.56
8	H5"	8	H3'	2.82	0.47	0.47
20	H5'	20	H2"	4.8	0.51	0.51
22	H5'	22	H1'	4.35	0.65	0.65

Figure S1. Atomic Charges on the S-N1-BDO-(61,2) Adduct Calculated using Gaussian 03 and the Hartree-Fock, 3-21G* basis set.

