**Major Groove Orientation of the (2*S*)-*N*⁶-(2-hydroxy-3-buten-1-yl)-2'-Deoxyadenosine
DNA Adduct Induced by 1,2-Epoxy-3-butene**

Supporting Information

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Table S1. Parameter file for the (2*S*)-*N*⁶-HB-dA Adduct used for AMBER calculations

containing partial charges calculated from GAUSSIAN in the last column. For more information about the parameter file go to <http://ambermd.org/tutorials/> .

0	0	2								
HB	INT	1	N6dA.prep							
CORRECT	OMIT	DU	BEG							
0										
1	DUMM	DU	M	0	-1	-2	0	0	0	0
2	DUMM	DU	M	1	0	-1	1	0	0	0
3	DUMM	DU	M	2	1	0	1	90	0	0
4	P	P	M	3	2	1	1.6	119.04	200	1.073
5	O1P	O2	E	4	3	2	1.48	109.61	150	-0.754
6	O2P	O2	E	4	3	2	1.48	109.58	20	-0.754
7	O5'	OS	M	4	3	2	1.6	101.43	-98.89	-0.413
8	C5'	CT	M	7	4	3	1.44	119	-39.22	-0.111
9	H5'1	H1	E	8	7	4	1.09	109.5	60	0.066
10	H5'2	H1	E	8	7	4	1.09	109.5	-60	0.066
11	C4'	CT	M	8	7	4	1.52	110	180	0.072

12	H4'	H1	E	11	8	7	1.09	109.5	-200	0.089
13	O4'	OS	S	11	8	7	1.46	108.86	-86.31	-0.612
14	C1'	CT	B	13	11	8	1.39	110.04	105.6	0.079
15	H1'	H2	E	14	13	11	1.1	108.26	-240	0.162
16	N9	N*	B	14	13	11	1.47	111.71	-127.7	-0.498
17	C8	CK	B	16	14	13	1.38	131.04	127.86	0.221
18	H8	H5	E	17	16	14	1.08	121.18	-0.99	0.165
19	N7	NB	S	17	16	14	1.31	113.77	178.84	-0.539
20	C5	CB	S	19	17	16	1.39	104.32	0.39	0.238
21	C6	CA	S	20	19	17	1.42	134.53	179.49	0.56
22	N6	N2	B	21	20	19	1.35	125.77	0.67	-0.55
23	HN	H	E	22	21	20	1.01	115.27	-179.77	0.349
24	CA	CT	3	22	21	20	1.45	127.8	-1.98	-0.094

25	HA1	H1	E	24	22	21	1.1	110.1	-106.44	0.229
26	HA2	H1	E	24	22	21	1.09	110.23	12.15	0.168
27	CB	CT	3	24	22	21	1.53	102.3	133.89	0.117
28	OB	OH	S	27	24	22	1.44	105.19	56.02	-0.543
29	HOB	HO	E	28	27	24	0.97	107.62	-177.49	0.159
30	HB	HC	E	27	24	22	1.1	108.55	-61.94	0.13
31	CC	CE	B	27	24	22	1.5	112.19	176.52	-0.019
32	HC	HA	E	31	27	24	1.09	115.28	-60.65	0.14
33	CD	CE	B	31	27	24	1.33	124.3	120.33	-0.297
34	HD1	HA	E	33	31	27	1.09	121.65	-0.71	0.161
35	HD2	HA	E	33	31	27	1.09	121.9	179.78	0.156
36	C4	CB	S	16	14	13	1.37	123.06	-52.9	0.564
37	N3	NC	S	36	16	14	1.34	126.2	1.82	-0.46

38	C2	CQ	B	37	36	16	1.34	110.71	179.67	0.172
39	H2	H5	E	38	37	36	1.09	115.99	-179.97	0.145
40	N1	NC	E	38	37	36	1.34	128.5	-0.12	-0.522
41	C3'	CT	M	11	8	7	1.53	115.78	-329.11	0.164
42	H3'	H1	E	41	11	8	1.09	109.5	30	0.077
43	C2'	CT	B	41	11	8	1.53	102.8	-86.3	-0.056
44	H2'1	HC	E	43	41	11	1.09	109.5	120	0.1
45	H2'2	HC	E	43	41	11	1.09	109.5	240	0.1
46	O3'	OS	M	43	11	8	1.42	116.52	-203.47	-0.5
IMPROPER										
C8	C4	N9	C1'							
N7	N9	C8	H8							
N1	N3	C2	H2							
C5	N1	C6	N6							
N9	N3	C4	C5							
C5	N1	C6	N6							
CC	HD1	CD	HD2							

LOOP CLOSING EXPLICIT										
C1'	C2'									
C4	C5									
C4	N9									
N1	C6									
DONE										
STOP										

Table S2. Chemical Shifts (ppm) of the Base and Deoxyribose Protons of the (2*S*)-*N*⁶-HB-dA Duplex Obtained at 800 MHz, at 15 °C, and Referenced to the Chemical Shift of Water With Respect to DSS at This Temperature.

	H2	H8	H6	H5	H1'	H2'	H2''	H3'	CH ₃	H _{α/α'}	H _β	H _γ	H _{δ/δ'}
C ¹			7.59	5.90	5.74	1.85	2.35	4.69					
G ²		7.92			5.45	2.70	2.74	4.98					
G ³		7.82			5.70	2.69	2.82	5.06					
A ⁴	7.80	8.15			6.21	2.63	2.92	5.05					
C ⁵			7.14	5.21	5.51	1.86	2.31	4.81					
Y ⁶	6.95	8.20			5.59	2.64	2.69	5.01		3.96	4.29	5.89	5.30
										2.86			5.41
A ⁷	7.59	8.12			6.10	2.64	2.90	5.07					
G ⁸		7.62			5.24	2.49	2.60	4.97					
A ⁹	7.68	8.04			5.92	2.58	2.85	5.02					
A ¹⁰	7.33	8.02			6.03	2.56	2.86	5.01					
G ¹¹		7.57			6.00	2.26	2.35	4.60					
C ¹²			7.93	5.99	5.91	2.33	2.64	4.68					
T ¹³			7.69		6.22	2.29	2.67	4.93	1.71				
T ¹⁴			7.51		6.32	2.29	2.63	4.94	1.67				
C ¹⁵			7.65	5.68	5.00	2.14	2.55	4.83					
T ¹⁶			7.50		6.11	2.13	2.68	4.91	1.63				
T ¹⁷			7.42		5.72	2.18	2.49	4.89	1.75				
G ¹⁸		7.86			5.94	2.61	2.76	4.90					
T ¹⁹			7.33		6.05	2.18	2.53	4.43	1.34				
C ²⁰			7.57	5.65	5.95	2.13	2.42	4.83					

C ²¹			7.50	5.72	5.64	2.01	2.34	4.84					
G ²²		7.98			6.20	2.39	2.66	4.70					

Table S3. Chemical Shifts (ppm) of the Exchangeable Imino and Amino Protons of (2*S*)-*N*⁶-HB-dA Duplex Obtained at 600 MHz, at 10 °C, and Referenced to the Chemical Shift of Water With Respect to DSS at This Temperature.

Base pair	imino	amino	
	G H1/T H3	C NH _{2(a)} ^a	C NH _{2(b)} ^b
G ² :C ²¹	13.16	7.08	8.70
G ³ :C ²⁰	12.76	6.78	8.36
A ⁴ :T ¹⁹	13.72		
C ⁵ :G ¹⁸	12.35	6.69	8.18
Y ⁶ :T ¹⁷	13.95		
A ⁷ :T ¹⁶	13.92		
G ⁸ :C ¹⁵	12.47	6.97	8.20
A ⁹ :T ¹⁴	13.82		
A ¹⁰ :T ¹³	14.30		

^a Non-hydrogen-bonded cytosine amino proton. ^b Hydrogen-bonded cytosine amino proton.