Supplemental Material for

Altered Structural Fluctuations in Duplex RNA versus DNA:

A conformational switch involving base pair opening

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Table S1. Base opening events in all the simulations[a]

	(0.3M NaCl)		(1 M NaCl)	
Base Pair	# of events	Duration (ps)	# of events	Duration (ps)
duplex **I**				
A2U7	2	88	0	0
G3C6	1	4172	4	710
U4A5	2	2110	8	1732
A5U4	18	2124	3	858
C6G3	6	1414	2	4834
U7A2	1	1498	4	826
duplex **II**				
G5C8	7	1454	0	0
U6A7	3	852	1	1290
A7U6	10	1022	1	124
C8G5	4	804	4	124
duplex **V**				
C6G3	1	10	0	0
duplex **VII**				
C3G8	1	90	1	38
G4C7	3	60	0	0
A5U6	3	1928	4	276
U6A5	5	2176	1	3656
C7G4	8	3230	4	1022
G8C3	5	4194	5	3420
duplex **VIII**				
U4A9	5	826	0	0
C6G7	1	396	5	980
G7C6	4	328	7	2006
A8U5	1	160	1	422
A9U4	1	140	1	584
duplex **IX**				
G5C8	3	416	3	144
A6U7	0	0	2	44
G7C6	3	78	0	0
G8C5	2	484	0	0
U9A4	1	2770	0	0

a. Only the simulations with base opening events of longer than 10 ps are included. Duration was the total time for all the events for a particular base pair.

Table S2. Average distances of H2’(n)-O4’(n+1) during the base pair opened states

	basepair	Start (ps)	End (ps)	Duration (ps)	Strand 1 (Å)	Strand 2 (Å)
Duplex I (0.3 M)						
1	2-7	1472	1544	72	2.4±0.3	2.3±0.3
2	2-7	3552	3568	16	2.2±0.3	2.5±0.3
3	3-6	606	4778	4172	3.3±1.0	2.4±0.3
4	4-5	1594	1622	28	4.0±0.3	5.2±0.4
5	4-5	2918	5000	2082	2.5±04	4.8±0.5
6	5-4	540	782	242	2.4±0.4	2.4±0.2
7	5-4	2298	2332	34	2.3±0.4	2.4±0.2
8	5-4	2534	2562	28	4.0±1.0	2.6±0.2
9	5-4	2568	2696	128	4.2±0.6	2.5±0.3
10	5-4	2702	2820	118	4.3±0.8	2.4±0.2
11	5-4	2830	3278	448	2.7±0.7	2.4±0.2
12	5-4	3362	3442	80	2.5±0.2	2.4±0.2
13	5-4	3522	3622	100	2.6±0.4	2.4±0.2
14	5-4	3626	3672	46	2.6±0.4	2.4±0.2
15	5-4	3712	3740	28	2.6±0.4	2.4±0.2
16	5-4	3746	3898	152	2.6±0.4	2.4±0.2
17	5-4	3902	3952	50	2.6±0.4	2.4±0.2
18	5-4	3978	4166	188	2.5±0.3	2.4±0.2
19	5-4	4176	4206	30	2.5±0.3	2.4±0.2
20	5-4	4210	4270	60	2.5±0.4	2.4±0.2
21	5-4	4416	4460	44	2.3±0.3	2.5±0.2
22	5-4	4466	4648	182	2.4±0.3	2.4±0.2
23	5-4	4714	4780	66	2.5±0.3	2.4±0.2
24	6-3	342	376	34	2.5±0.4	2.6±0.6
25	6-3	1320	2238	918	2.3±0.3	2.5±0.5
26	6-3	2408	2420	12	2.3±0.2	2.6±0.3
27	6-3	2424	2436	12	2.3±0.2	2.4±0.3
28	6-3	2456	2862	406	2.4±0.3	3.5±0.8
29	6-3	2870	2902	32	2.4±0.4	4.4±0.5
30	7-2	3502	5000	1498	5.4±0.6	3.8±0.7
	All	0	5000	5000	3.4±1.0	3.5±1.1
Duplex I (1 M)						
31	3-6	460	482	22	2.7±0.5	2.6±0.6
32	3-6	496	514	18	2.4±0.7	2.3±0.3
33	3-6	4326	4340	14	2.2±0.3	2.2±0.4
34	3-6	4344	5000	654	2.7±0.6	2.4±0.3
35	4-5	1718	1814	96	2.5±0.3	2.5±0.3
36	4-5	1924	2388	464	2.4±0.2	2.4±0.3
37	4-5	2466	2704	238	2.5±0.2	2.4±0.4
38	4-5	2758	2888	130	2.4±0.2	2.2±0.2
39	4-5	2942	3414	472	2.4±0.2	2.4±0.3
40	4-5	3418	3696	278	2.4±0.2	2.3±0.3
41	4-5	3700	3712	12	2.4±0.3	2.8±0.2
42	4-5	3768	3810	42	2.3±0.2	2.4±0.2
43	5-4	2	132	130	4.7±0.3	4.3±0.5
44	5-4	2818	3528	710	4.8±0.4	2.7±0.5
45	5-4	4532	4550	18	5.2±0.2	4.9±0.6
46	6-3	118	1202	1084	2.4±0.3	2.7±0.6
47	6-3	1250	5000	3750	2.4±0.3	3.0±0.9
48	7-2	2084	2100	16	3.0±0.7	2.6±0.2
49	7-2	2110	2174	64	2.6±0.4	2.6±0.3
50	7-2	4242	4288	46	2.4±0.2	2.4±0.3
	All	0	5000	5000	3.3±1.0	3.3±0.9

Table S2. (continued)

	basepair	Start (ps)	End (ps)	Duration (ps)	Strand 1 (Å)	Strand 2 (Å)
Duplex II (0.3 M)						
51	3-10	2990	3748	758	3.4±0.8	3.9±0.6
52	5-8	2	92	90	2.4±0.5	2.2±0.3
53	5-8	596	728	132	2.4±0.4	2.4±0.3
54	5-8	1894	2164	270	2.5±0.6	2.3±0.3
55	5-8	2504	2634	130	2.3±0.4	2.1±0.2
56	5-8	2758	3154	396	2.6±0.7	2.3±0.3
57	5-8	3630	3650	20	3.2±0.8	2.2±0.3
58	5-8	4314	4730	416	4.2±0.7	2.5±0.5
59	6-7	478	526	48	2.6±0.4	2.5±0.3
60	6-7	4040	4420	380	2.4±0.2	2.8±0.8
61	6-7	4424	4848	424	2.6±0.5	3.6±1.2
62	7-6	1700	1744	44	2.2±0.4	2.6±0.3
63	7-6	2034	2064	30	2.3±0.3	2.4±0.3
64	7-6	2092	2138	46	2.3±0.7	2.5±0.2
65	7-6	2142	2194	52	2.3±0.4	2.4±0.2
66	7-6	2198	2404	206	2.2±0.3	2.4±0.3
67	7-6	2732	2752	20	2.3±0.3	2.3±0.2
68	7-6	2756	2772	16	2.3±0.1	2.4±0.2
69	7-6	3054	3170	116	2.6±0.3	2.4±0.3
70	7-6	3174	3476	302	2.6±0.4	2.5±0.4
71	7-6	3528	3718	190	2.5±0.3	2.4±0.2
72	8-5	3764	3810	46	2.3±0.3	2.5±0.9
73	8-5	3858	3954	96	2.2±0.3	3.1±0.8
74	8-5	4332	4398	66	2.1±0.2	2.4±0.5
75	8-5	4404	5000	596	2.2±0.3	2.5±0.4
76	10-3	2990	3748	758	2.5±0.3	2.7±0.7
77	10-3	4544	5000	456	2.5±0.3	2.5±0.5
	All	0	5000	5000	3.3±0.9	3.3±0.9
Duplex II (1 M)						
78	3-10	1296	1316	20	3.9±0.5	2.3±0.2
79	3-10	2954	4880	1926	2.8±0.7	2.5±0.3
80	5-8	4270	4278	8	3.8±0.7	3.7±0.4
81	6-7	1380	2670	1290	2.4±0.3	2.4±0.4
82	7-6	1192	1316	124	2.3±0.3	2.4±0.3
83	8-5	2756	2776	20	2.5±0.2	2.3±0.2
84	8-5	2836	2862	26	2.1±0.2	3.0±0.3
85	8-5	3584	3648	64	2.3±0.3	2.7±0.6
86	8-5	4520	4534	14	2.3±0.3	2.3±0.3
	All	0	5000	5000	3.3±0.8	3.4±0.8

Table S2. (continued)

	basepair	Start (ps)	End (ps)	Duration (ps)	Strand 1 (Å)	Strand 2 (Å)
Duplex VII (0.3 M)						
87	3-8	1956	2046	90	4.4±0.4	4.5±04
88	4-7	3494	3522	28	4.1±0.8	2.5±0.3
89	4-7	3550	3562	12	4.2±0.4	2.5±0.2
90	4-7	3708	3728	20	3.8±0.5	2.4±0.2
91	5-6	14	54	40	4.0±0.6	3.9±0.8
92	5-6	3000	3016	16	2.4±0.2	2.2±0.3
93	5-6	3108	4980	1872	2.6±0.4	2.4±0.3
94	6-5	1234	3170	1936	5.1±0.5	4.7±0.4
95	6-5	3972	4038	66	5.2±0.5	4.7±0.4
96	6-5	4790	4832	42	4.8±0.4	4.8±0.3
97	6-5	4856	4876	20	4.8±0.2	4.7±0.2
98	6-5	4888	5000	112	5.0±0.4	5.0±0.3
99	7-4	1386	1614	228	2.4±0.3	2.3±0.2
100	7-4	1628	1764	136	2.5±0.4	2.3±0.2
101	7-4	2048	2194	146	2.5±0.2	2.3±0.2
102	7-4	2200	2582	382	2.5±0.3	2.3±0.2
103	7-4	2592	2708	116	2.6±0.3	2.3±0.2
104	7-4	2712	2728	16	2.8±0.2	2.2±0.3
105	7-4	2790	4816	2026	2.5±0.3	2.3±0.4
106	7-4	4820	5000	180	2.5±0.3	2.3±0.2
107	8-3	698	1008	310	2.3±0.4	2.4±0.3
108	8-3	1054	1160	106	3.9±0.6	2.7±0.4
109	8-3	1164	1260	96	4.3±0.4	2.7±0.3
110	8-3	1314	2052	738	4.5±0.6	2.4±0.3
111	8-3	2056	5000	2944	4.3±0.6	2.5±0.2
	all	0	5000	5000		
Duplex VII (1 M)						
112	3-8	1428	1466	38	4.5±0.6	4.3±0.3
113	5-6	1310	1368	58	2.5±0.3	2.3±0.3
114	5-6	1378	1492	114	2.7±0.4	2.4±0.2
115	5-6	1676	1694	18	2.6±0.3	2.2±0.3
116	5-6	1698	1784	86	2.6±0.3	2.4±0.3
117	6-5	1348	5000	3652	5.0±0.4	5.0±0.4
118	7-4	792	1064	272	3.3±0.3	2.4±0.4
119	7-4	1068	1088	20	2.6±0.4	3.0±0.7
120	7-4	1102	1780	678	2.4±0.3	2.4±0.3
121	7-4	1794	1846	52	2.6±0.4	2.5±0.3
122	8-3	1404	1478	74	4.4±0.5	2.7±0.3
123	8-3	1522	1534	12	4.7±0.5	2.7±0.2
124	8-3	1542	1908	366	4.4±0.5	2.6±0.3
125	8-3	1940	1954	14	4.0±0.3	2.3±0.2
126	8-3	2046	5000	2954	3.8±0.6	2.4±0.3
	all	0	5000	5000		

Table S2. (continued)

	basepair	Start (ps)	End (ps)	Duration (ps)	Strand 1 (Å)	Strand 2 (Å)
Duplex VIII (0.3 M)						
127	4-9	1968	2082	114	2.4±0.3	2.5±0.5
128	4-9	4276	4740	464	3.2±0.7	2.4±0.3
129	4-9	4744	4774	30	2.3±0.2	2.3±0.3
130	4-9	4778	4860	82	2.5±0.3	2.9±0.6
131	4-9	4864	5000	136	2.4±0.4	2.5±0.5
132	6-7	1866	2262	396	2.4±0.3	2.6±0.4
133	7-6	1184	1208	24	3.1±0.8	2.6±0.2
134	7-6	1212	1224	12	3.4±0.3	2.3±0.1
135	7-6	1228	1484	256	2.4±0.2	2.3±0.2
136	7-6	2420	2456	36	2.3±0.3	2.2±0.1
137	8-5	828	988	160	2.7±0.3	2.2±0.2
138	9-4	1160	1300	140	2.4±0.2	2.3±0.2
	all	0	5000	5000		
Duplex VIII (1 M)						
139	6-7	3006	3026	20	4.2±0.2	4.8±0.4
140	6-7	3030	3140	110	4.3±0.5	4.5±0.4
141	6-7	3224	3318	94	2.3±0.3	2.9±0.5
142	6-7	3322	3362	40	2.3±0.2	2.9±0.5
143	6-7	3366	4082	716	2.4±0.2	2.6±0.4
144	7-6	396	646	250	2.7±0.3	2.4±0.3
145	7-6	650	824	174	2.5±0.3	2.4±0.3
146	7-6	1224	2318	1094	4.8±0.4	4.4±0.3
147	7-6	2644	2672	28	4.1±0.3	2.5±0.4
148	7-6	2726	2760	34	3.7±0.6	2.3±0.3
149	7-6	4556	4578	22	3.1±0.4	2.3±0.2
150	7-6	4596	5000	404	2.4±0.3	2.3±0.2
152	8-5	2530	2952	422	2.5±0.3	2.6±0.7
153	9-4	4416	5000	584	2.6±0.4	2.4±0.2
	all	0	5000	5000		

Table S2. (continued)

	basepair	Start (ps)	End (ps)	Duration (ps)	Strand 1 (Å)	Strand 2 (Å)
Duplex IX (0.3 M)						
154	5-8	344	366	22	3.4±0.7	2.2±0.2
155	5-8	3756	3776	20	2.7±0.4	3.0±1.0
156	5-8	4626	5000	374	2.7±0.6	2.4±0.3
157	7-6	470	520	50	2.6±0.7	2.5±0.3
158	7-6	4246	4258	12	2.3±0.3	2.4±0.2
159	7-6	4262	4278	16	2.5±0.2	2.3±0.4
160	8-5	80	114	34	2.8±0.2	2.3±0.4
161	8-5	2134	2584	450	2.6±0.7	2.4±0.3
162	9-4	1898	1974	76	2.9±0.5	2.4±0.3
163	9-4	2306	5000	2694	4.7±0.4	4.9±0.4
164	10-3	496	852	356	2.5±0.5	2.4±0.3
165	10-3	1562	1610	48	2.4±0.4	4.6±0.5
	all	0	5000	5000	3.3±0.8	3.4±0.9
Duplex IX (1 M)						
166	3-10	3916	4428	512	4.4±0.5	5.0±0.5
167	3-10	4432	5000	568	4.4±0.5	5.0±0.5
168	5-8	3982	4014	32	3.4±0.4	2.5±0.4
169	5-8	4020	4042	22	2.9±0.4	2.8±0.4
170	5-8	4126	4216	90	3.7±0.7	2.7±0.4
171	6-7	4776	4798	22	2.3±0.4	2.4±0.2
172	6-7	4846	4868	22	2.1±0.5	2.5±0.2
	all	0	5000	5000	3.5±0.8	3.4±0.9

Table S3. Time sequence of the N1-N3 and 2’OH-O4’ hydrogen bond distances during selected base pair opening and re-closure events in duplex **II** (1 M NaCl) and duplex **VIII** (0.3 M NaCl) simulations

Duplex **II** (1380 – 2670 ps)				Duplex **VIII** (1160 – 1300 ps)			
Time(ps)	N1-N3	H2’-O4’	O2’-H2’-O4’	Time (ps)	N1-N3	H2’-O4’	O2’-H2’-O4’
Base pair opening							
1372	3.19	4.25	62.3	1156	2.95	2.60	121.3
1378	3.17	3.01	94.1	1158	2.90	2.88	140.1
1380	**3.77**	**2.43**	**135.6**	**1160**	**4.68**	**2.16**	**138.6**
1382	4.82	2.65	120.6	1162	4.52	2.31	135.8
1384	3.91	2.44	133.8	1164	4.66	2.40	154.3
1386	4.84	2.29	127.7	1166	4.75	2.07	169.6
Base pair closing							
2666	4.33	2.51	121.9	1296	4.43	2.37	131.7
2668	4.98	2.01	128.2	1298	5.02	2.84	120.7
2670	**4.23**	**1.85**	**150.3**	**1300**	**4.04**	**2.27**	**123.2**
2672	3.44	1.77	168.1	1302	3.16	2.10	149.2
2674	3.11	1.95	156.3	1304	3.28	1.97	153.8
2676	3.26	1.94	162.9	1306	3.35	2.40	109.0
:				:			
2688	2.89	3.09	99.9	1332	2.97	3.38	105.5

Distances are in Å, and angles in degrees.

Table S4. Number of water molecules within 3.5 Å of both the (Pu)N1 and (Py)N3 atoms for each base pair in the duplexes when the base pair was in the closed state[a]

	(Base pair)[b]					
	1	**2**	**3**	**4**	**5**	**6**
			(0.3 M NaCl)			
I	0.02	0.13	0.35	0.17	0.10	0.17
II	0.01	0.01	0.07	0.07	0.03	0.01
III	0.01	0	0.01	0	0	0.01
IV	0	0	0	0	0	0
V	0.02	0	0	0	0	0.01
VI	0	0.01	0	0	0	0.01
VII	0.01	0.03	0.43	0.03	0.22	0.04
VIII	0.01	0.01	0.01	0.14	0.01	0.01
IX	0	0	0.03	0	0.37	0.25
			(1 M NaCl)			
I	0.02	0.02	0.08	0.46	0.01	0.13
II	0.02	0.05	0.02	0.02	0.01	0.01
III	0	0	0.01	0.01	0	0.02
IV	0	0	0.01	0.01	0	0
V	0.02	0	0.01	0	0	0.01
VI	0.01	0	0	0.02	0.01	0
VII	0	0.01	0.17	0.03	0.05	0.03
VIII	0	0	0.18	0.03	0.16	0.01
IX	0.02	0	0.01	0	0	0.03

a. The number of water molecules was the sum of water molecules averaged over the total number of time points. The closed state was defined as when the N1-N3 distance for a base pair was less than 3.5 Å.

b. Only the central 6 base pairs were included in the analysis for all the sequences and are labeled from 1 to 6 accordingly.

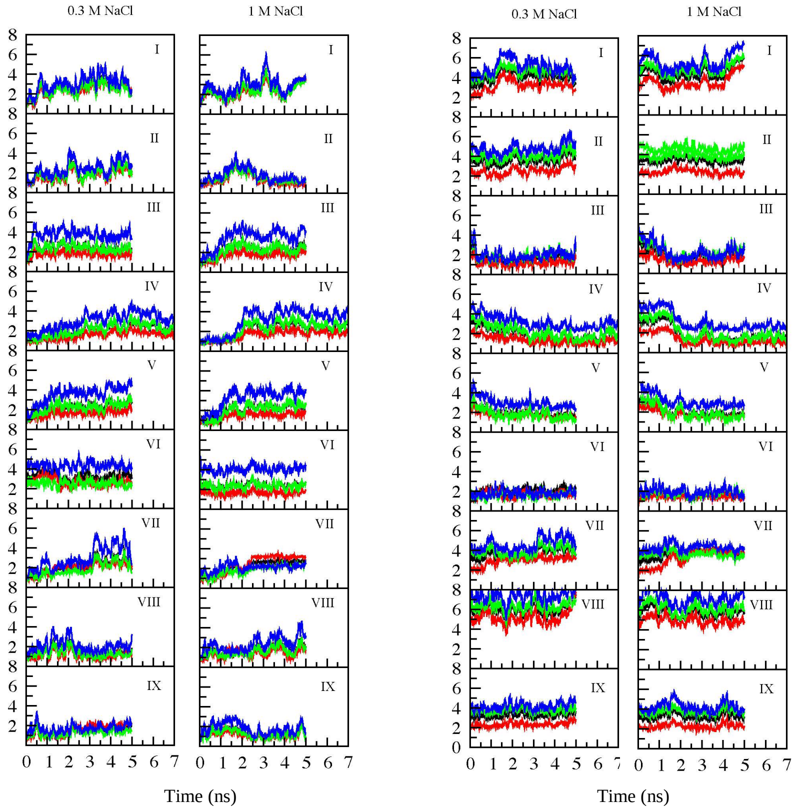
Supplemental Figure Legends

Figure S1. RMS differences at 0.3 and 1 M salt concentrations with the canonical A form (left panel) and B form (right panel) structure as the reference state. The black, red, green and blue colors represent all, base, sugar and phosphate, respectively.

Figure S2. N1-N3 distance versus time for the MD simulations. Only the central 6 residues are included. The colors black, red, green, blue, yellow and tan sequentially represent the central 6 base pairs.

Figure S3. Hydrogen bonding interactions between water molecules and the (A7)N1 and (U6)H3 base atoms in the base pair opened state (from 1380 to 2670 ps) from the duplex **II** simulation at 1 M NaCl. The two bars show the presence of hydrogen bond and the gaps within the bars show that there is no hydrogen bond. The colors stand for different water molecules that were involved in hydrogen bonding with the bases. In many cases, the two bases were bridged by the same water molecules as annotated W1, W2 and so on.

Figure S1.



0.3 M NaCl
1 M NaCl
0.3 M NaCl
1 M NaCl
I
II
III
IV
V
VI
VII
VIII
IX
0
2
4
6
8
0 1 2 3 4 5 6 7
Time (ns)
Time (ns)

Figure S2

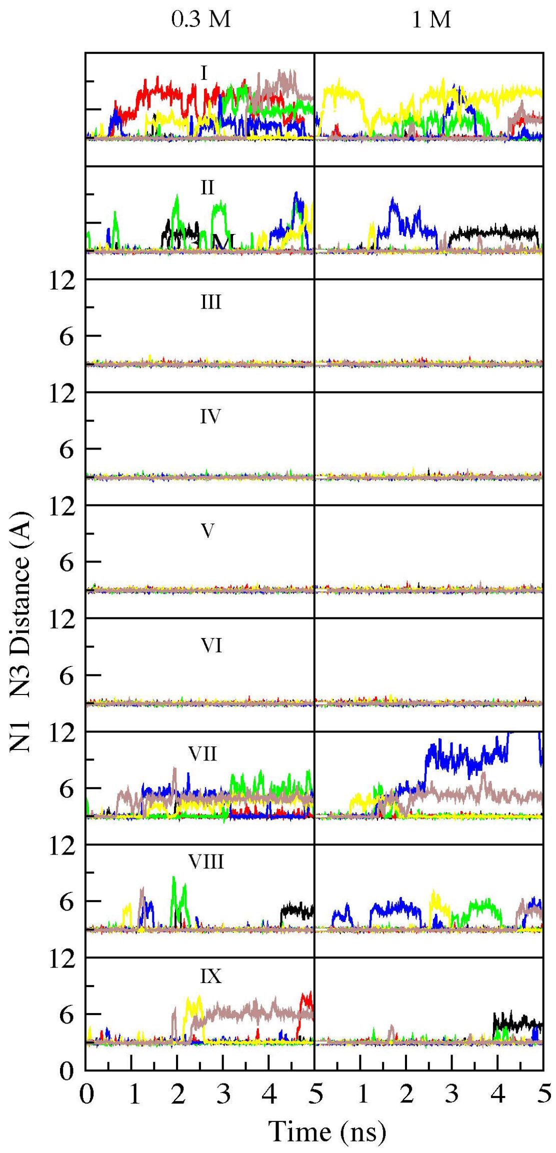

0.3 M
1 M
I
II
III
IV
V
VI
VII
VIII
IX
12
6
0
N1 N3 Distance (A)
0
1
2
3
4
5
Time (ns)

Figure S3