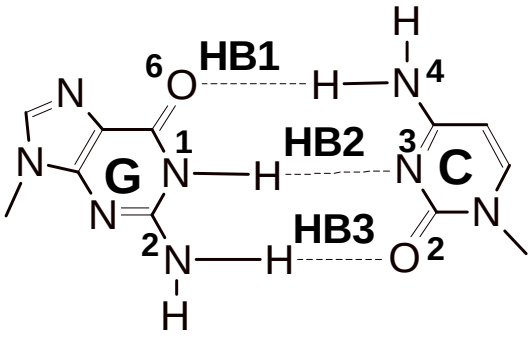
Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

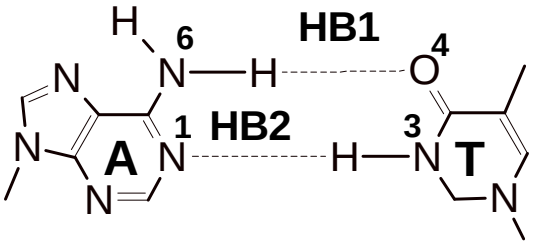
Supplementary Materials

Effects of (5'S)-5',8-cyclo-2'-deoxyadenosine on the base excision repair of oxidatively generated clustered DNA damage. A biochemical and theoretical study.

Boleslaw T. Karwowski, Sophie Bellon, Peter O'Neill, Martine E. Lomax and Jean Cadet

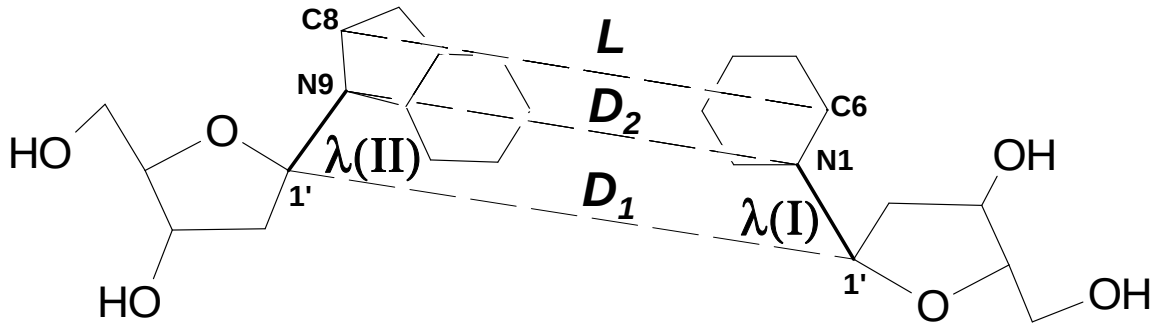
Graphical representation of hydrogen bonds.





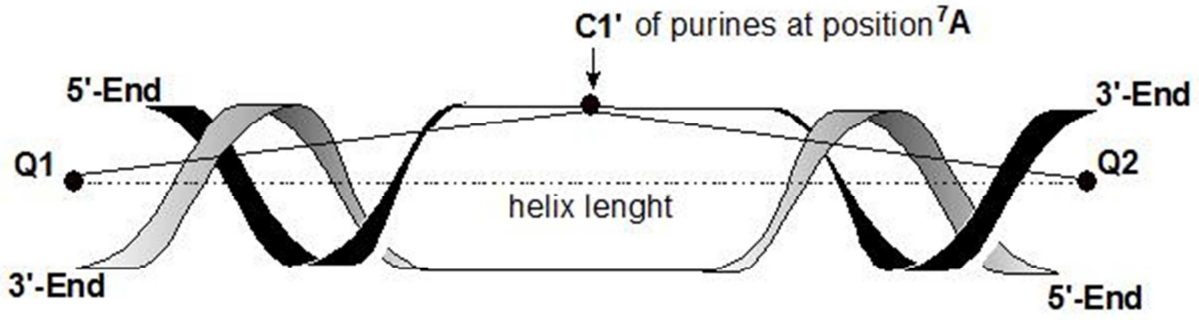
BASE PAIR	Hydrogen Bond		
	HB1	HB2	HB3
A::T	O4---N6	N3---N1	
A::U	O4---N6	N3---N1	
G:::C	N4---O6	N3---N1	O2---N2

Graphical representation of idealized base pair parameters



Base Pairs Parameters	
λ(I) [°]	**N1** --- **C1'** (pyrimidine) --- **C1'** (purine)
λ(II) [°]	**N9** --- **C1'** (purine) --- **C1'** (pyrimidine)
D1 [Å]	**C1' ---- C1'**
D2 [Å]	**N9 --- N1**
L [Å]	**C8 --- C6**

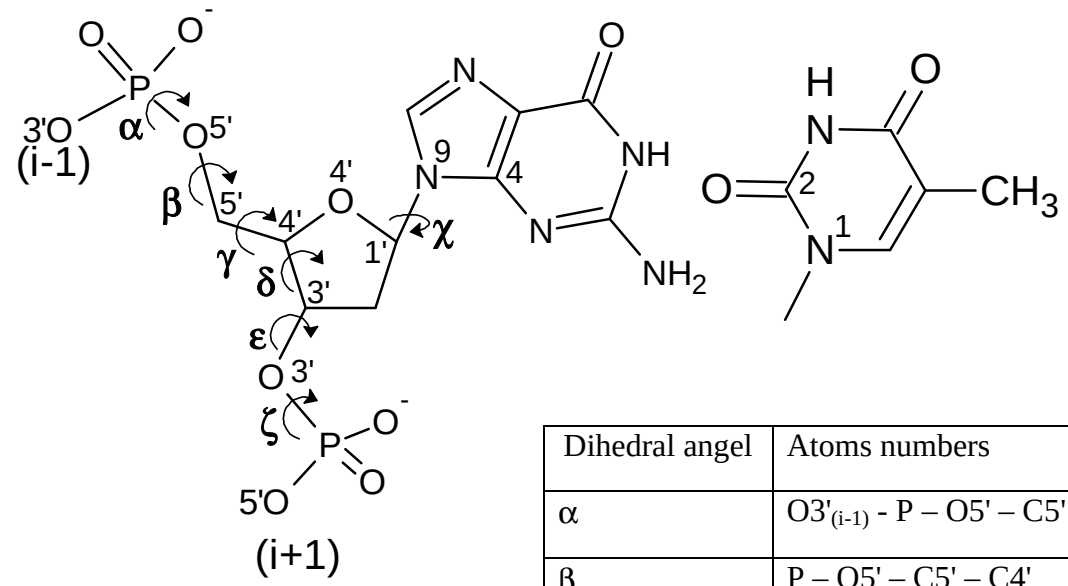
Graphical representation of helix length and helix bent.



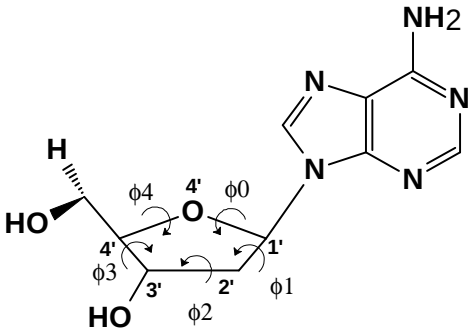
Helix length has been measured as distance between positions of points: **Q1** and **Q2**, assigned by W3DNA analysis.

Helix bending has been measured as the angle between: **Q1** point, **C1'** atom of purines located at position ^{7}**A**, and **Q2** point. The position/coordinates of **Q1** and **Q2** has been taken from W3DNA analysis of suitable *ds*-oligodeoxynucleotide.

The graphical representation of dihedral angles and sugar pseudorotation phase used for conformational analysis, data of the analysis are presented in Table 7S in supplementary material.

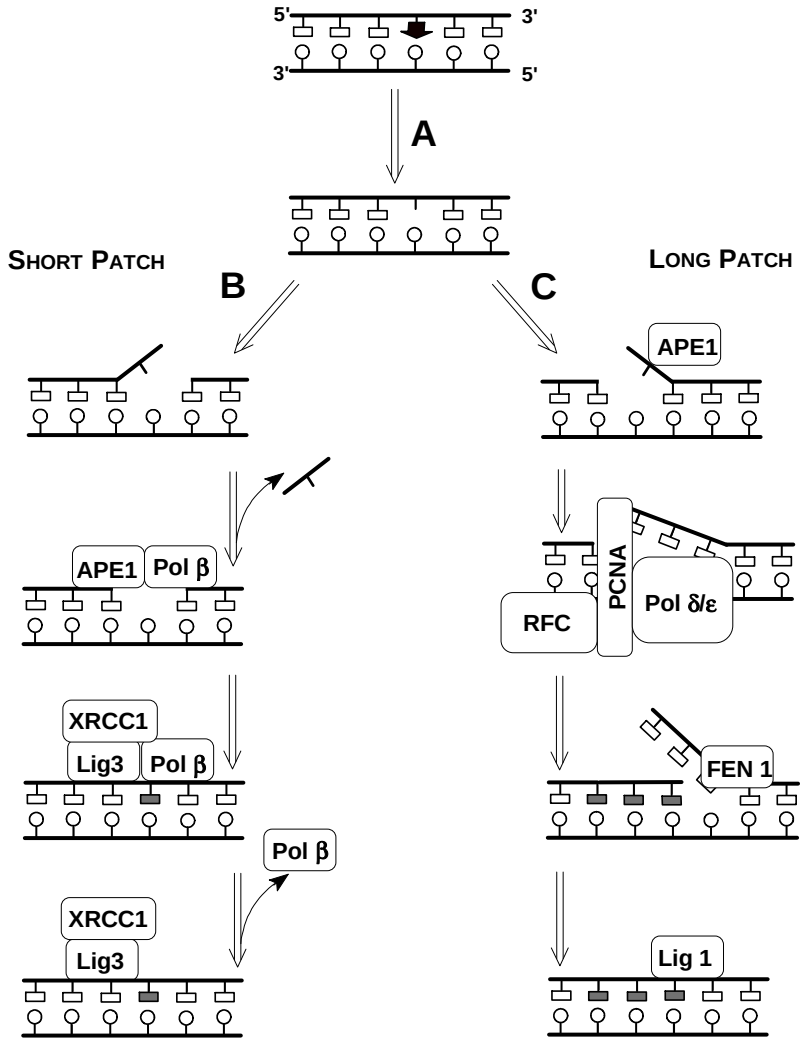


Dihedral angel	Atoms numbers
α	$O3'_{(i-1)}$ - P – O5' – C5'
β	P – O5' – C5' – C4'
γ	O5' – C5' – C4' – C3'
δ	C5' – C4' – C3' – O3'
ε	C4' – C3' – O3' – $P_{(i+1)}$
ζ	C3' – O3' – $P_{(i+1)}$ – $O5'_{(i+1)}$
χ (purines)	O4' – C1' – N9 – C4
χ (pyrimidines)	O4' – C1' – N1 – C2



Sugar pseudorotation phase equation: $\tan(P)=[(\phi_4+\phi_1)-(\phi_3+\phi_0)]/[2\phi_2\ (\sin(36)+\sin(72)]$	
Dihedral angel	Atoms numbers
ϕ_0	C4' – O4' – C1' – C2'
ϕ_1	O4' – C1' – C2' – C3'
ϕ_2	C1' – C2' – C3' – C4'
ϕ_3	C2' – C3' – C4' – O4'
ϕ_4	C3' – C4' – O4' – C1'

Scheme 1S. The schematic overviev of Base Excision Repair paths.

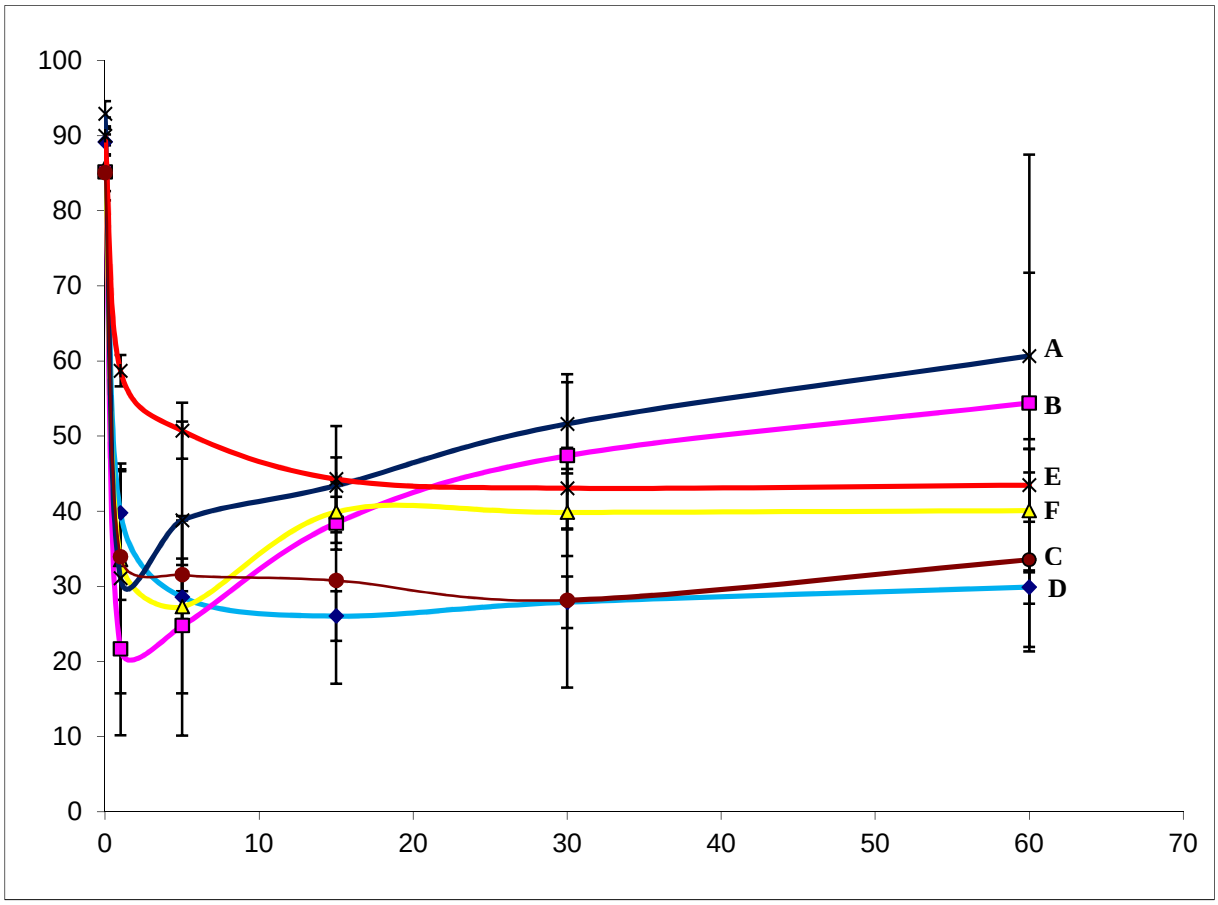


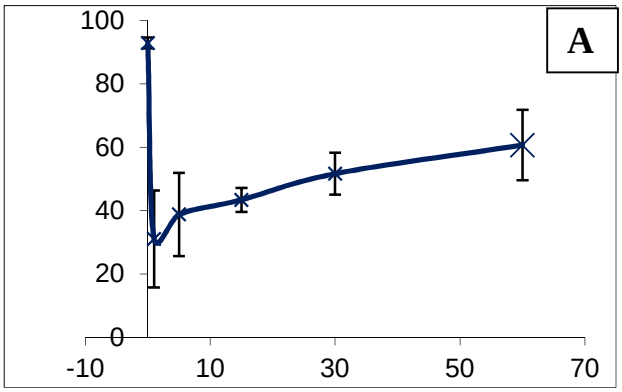
Abreviations: **APE1** – Human apurinic/apyrimidinc endonuclease, **Polβ** – Polymerase β(beta), **XRCC1** - X-ray repair cross-complementing protein 1, **Lig3** – Ligase III, **RFC** - replication factor C, **PCNA** – Proliferating cell nuclear antigen, Polδ – Polimerase δ (delta), Polε- Polimerase ε (epsilon), FEN1 – Flap structure-specific endonuclease 1, Lig1 – Ligase I. Black arow ⬇ represented the damage nucleobase, ⊤ represents the apurinic/apyrimidinic site.

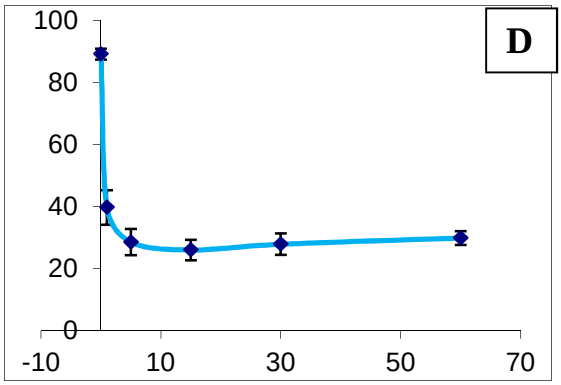
(For more details: A. Sancar, L. A. Lindsey-Boltz, K. Ünsal-Kaçmaz, S. Linn, ***M****olecular mechanisms of mammalian dna repair and the dna damage checkpoints.*, Annual Review of Biochemistry, 2004, **73**, 39-85)

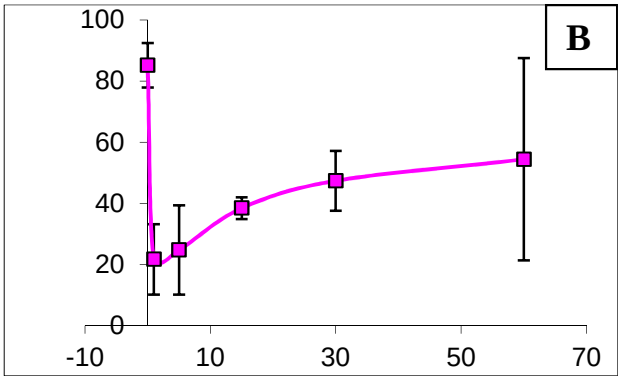
Figure 1S Time scale for the rejoining of an AP-site, formed from conversion of the uracil by UDG prior to exposure to NE, following incubation with NE at 37 ^{o}C for upto 60 min. The repair protocol is shown in the Experimental. Thenumbers in parentheses corresponding to sequence of double stranded 40-mer oligonucleosides given in Table 1 and schematically depicted in Figure 1:

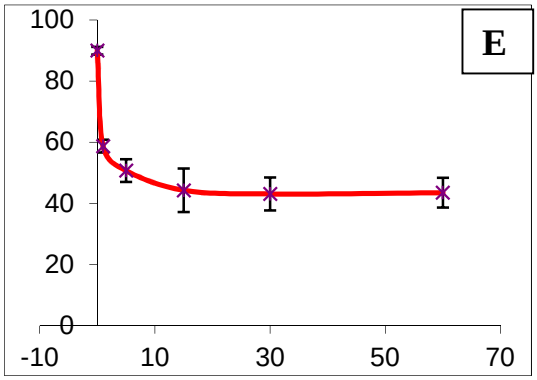
A) dark blue curve - AP-site control (no (5'*S*)-cdA) i.e. correspond to the distance between dU and dA equal 0 bases, present in reference *ds*-oligonucleoside Con.1; **B**) violet curve - correspond to the distance between dU and dA equal to -5 bases present in *ds*-oligonucleoside U_{-5}; **C**) brown curve - correspond to the distance between dU and (5'*S*)-cdA equal to -1 base present in *ds*- oligonucleoside U_{-1}; **D**) light blue - correspond to the opposite position of dU versus (5'*S*)-cdA present in *ds*-oligonucleoside U0, **E**) red curve - correspond to the distance between dU and dA equal to +1 base present in *ds*-oligonucleoside U_{+1}; **F**) yellow curve - correspond to the distance between dU and dA equal to +5 bases present in construct U_{+5}.

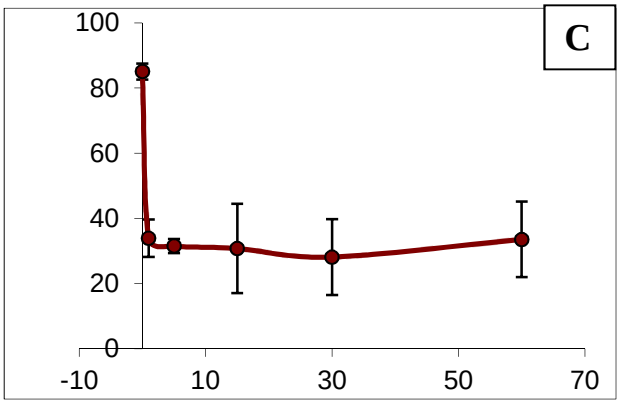



A
100
80
60
40
20
0
-10
10
30
50
70


D
100
80
60
40
20
0
-10
10
30
50
70


B
100
80
60
40
20
0
-10
10
30
50
70


E
100
80
60
40
20
0
-10
10
30
50
70


C
100
80
60
40
20
0
-10
10
30
50
70

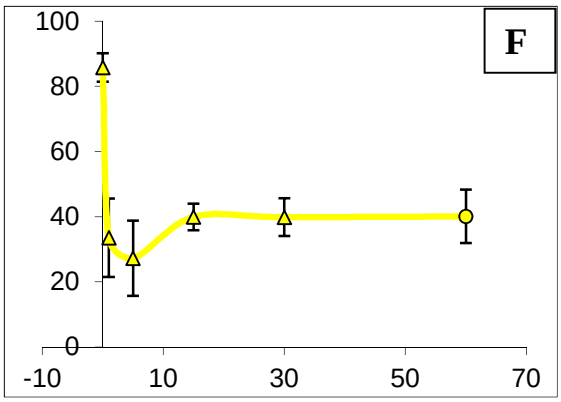

F
100
80
60
40
20
0
-10
10
30
50
70

Figure 2S. Graphical representation of oligodeoxynucleotide structures obtained under Molecular Mechanics optimization. Oligodeoxynucleotides contain only one modification: 2'-deoxyuridine or AP-site or single DNA strand brake at different positions namely 0, -1, +1.

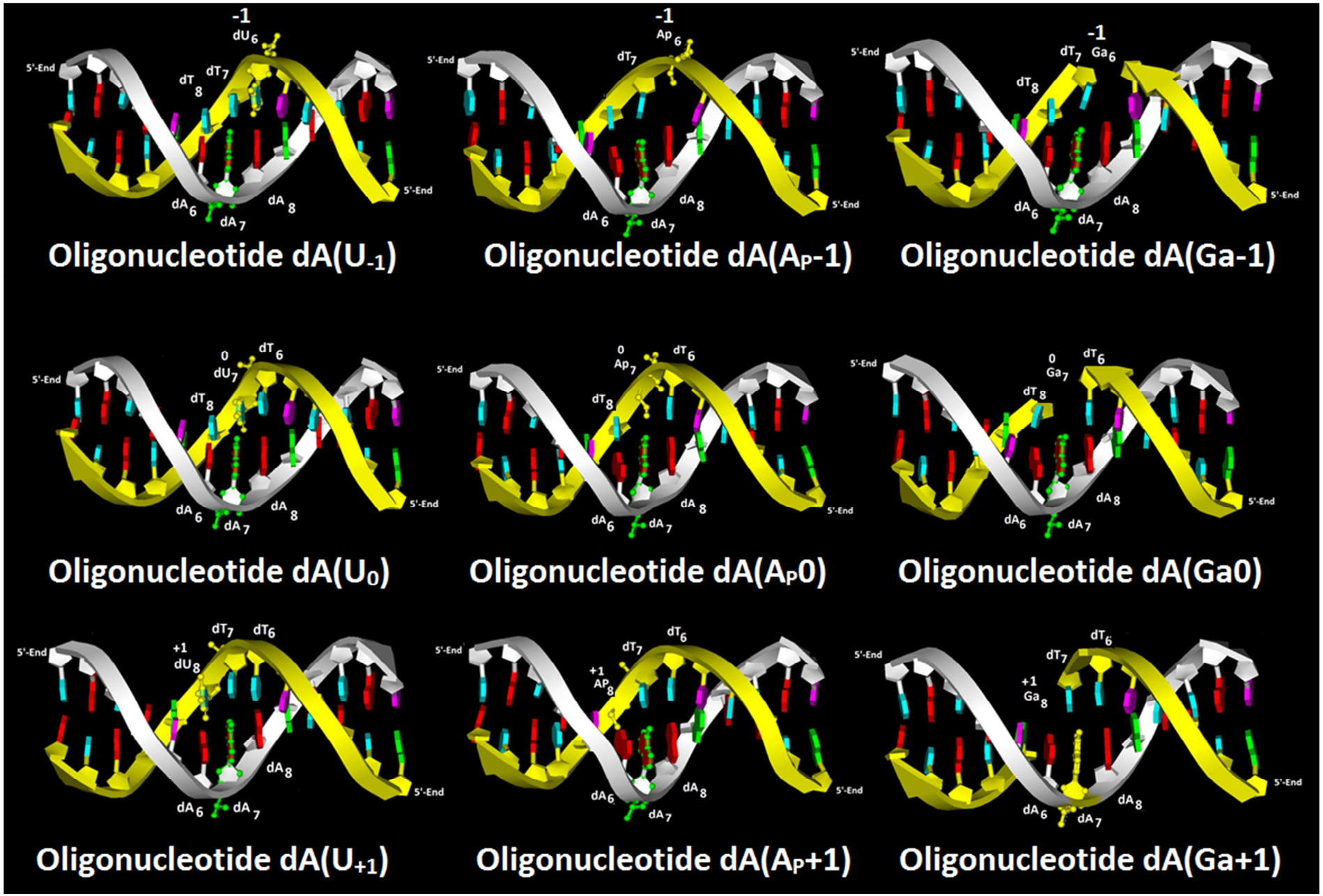


Figure 2S continued. Graphical representation of oligodeoxynucleotide structures obtained under Molecular Mechanics optimization. Oligodeoxynucleotides contain (5'*S*)-cdA in one strand and another modification i.e. 2'-deoxyuridine, AP-site or single DNA strand break in the complementary one, at different positions namely 0, -1, +1.

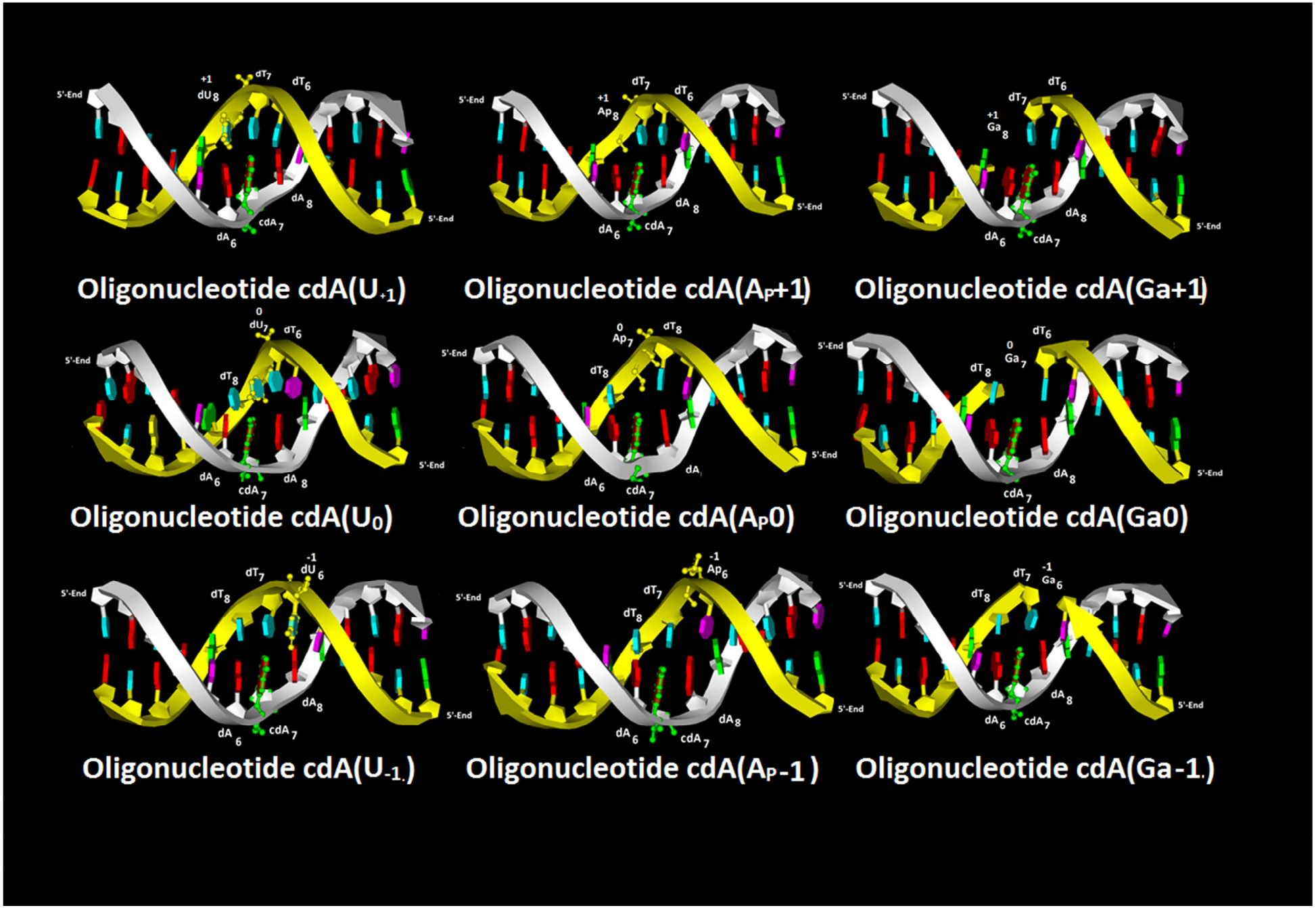
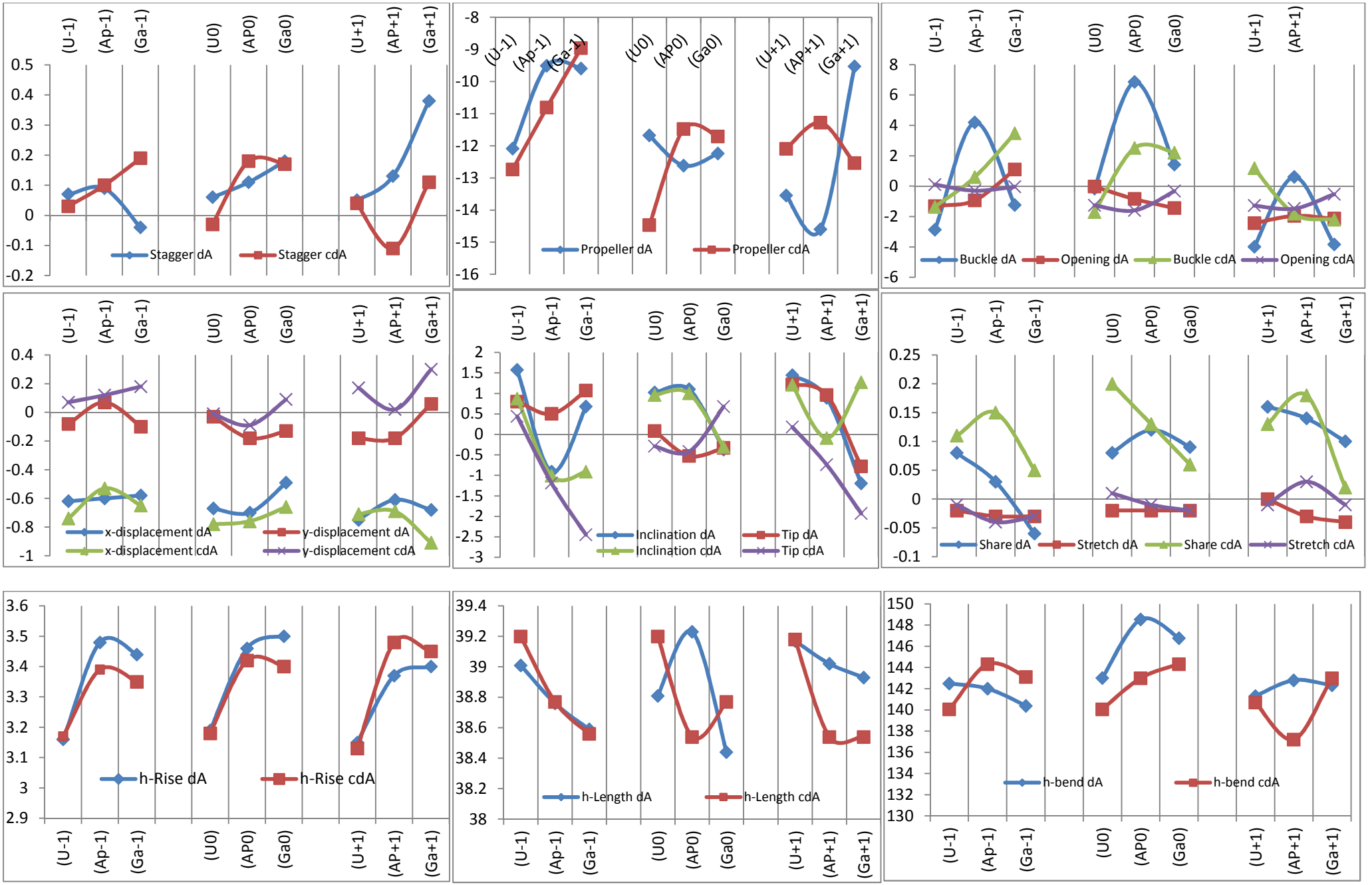
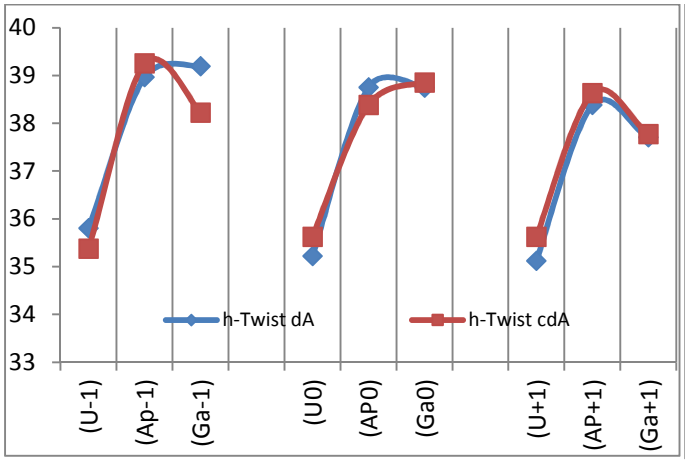


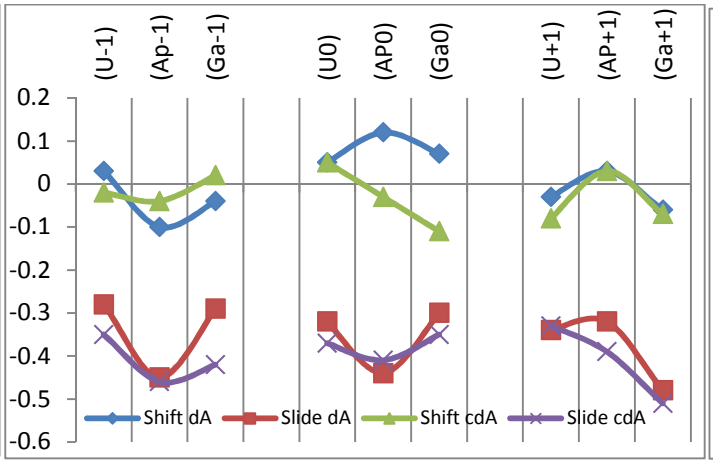
Table 1S. Average values of: **a)** base pair parameters, **b)** complementary base-pair parameters, **c)** local helical parameters of double stranded oligodeoxynucleotides that contained at positions **7A** 2'-deoxyadenosine (dA) or (5'S) 5',8-cyclo-2'-deoxyadenosine (cdA) in one strand and at different positions **T6** (U-1) or **T7** (U0) or **T8**(U+1) the 2'-deoxyuridine in the opposite chain which after conversion gives first an apurinic/apyrimidinic site **T6**(Ap+1) or **T7** (Ap0) or **T8**(Ap+1), and then a single strand break e.i. gap **T6**(Ga+1) or**T7** (Ga0) or **T8**(Ga+1). The structures of *ds*-oligodeoxynucleotides obtained under Molecular Mechanics (Amber 94 force field) calculation in solvation box, the sodium ions have been used as counterions to neutralize the negative charge of *ds*-DNA.

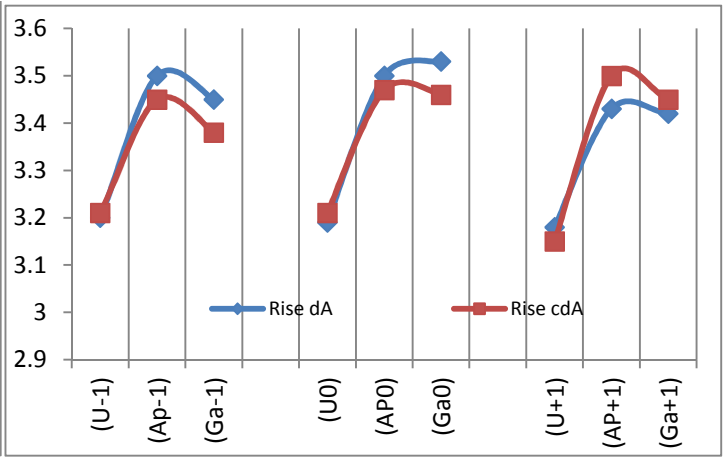
OLIGODEOXYNUCLEOTIDE	Average values																			
	Complementarybase-pareparameters						Base-pair parameters						Local helical parameters							
	Share	**Stretch**	**Stagger**	**Buckle**	**Propeller**	**Opening**	**Shift**	**Slide**	**Rise**	**Tilt**	**Roll**	**Twist**	**x-displacement**	**y-displacement**	**h-Rise**	**Inclination**	**Tip**	**h-Twist**	**h-Length**	**h-bend**
dA(U-1)	0.08	-0.02	0.07	-2.88	-12.09	-1.32	0.03	-0.28	3.2	-0.52	0.96	35.52	-0.62	-0.08	3.16	1.57	0.8	35.8	39.01	142.49
dA(Ap-1)	0.03	-0.03	0.09	4.19	-9.51	-0.94	-0.1	-0.45	3.5	-0.3	0.03	38.54	-0.6	0.07	3.48	-0.91	0.5	38.96	38.76	142.01
dA(Ga-1)	-0.06	-0.03	-0.04	-1.25	-9.6	1.09	-0.04	-0.29	3.45	0.38	1.29	38.51	-0.58	-0.1	3.44	0.68	1.07	39.19	38.59	140.39
dA(U0)	0.08	-0.02	0.06	-0.17	-11.68	-0.03	0.05	-0.32	3.19	-0.03	0.76	35.07	-0.67	-0.03	3.19	1.02	0.08	35.22	38.81	143.01
dA(A_P0)	0.12	-0.02	0.11	6.85	-12.62	-0.85	0.12	-0.44	3.5	0.2	0.98	38.43	-0.7	-0.18	3.46	1.1	-0.53	38.75	39.23	148.54
dA(Ga0)	0.09	-0.02	0.18	1.42	-12.24	-1.44	0.07	-0.3	3.53	0.77	-0.28	38.50	-0.49	-0.13	3.5	-0.37	-0.33	38.74	38.44	146.78
dA(U+1)	0.16	0.00	0.05	-4.00	-13.55	-2.44	-0.03	-0.34	3.18	-0.51	1.08	34.81	-0.75	-0.18	3.15	1.44	1.22	35.12	39.17	141.30
dA(A_P+1)	0.14	-0.03	0.13	0.6	-14.6	-1.96	0.03	-0.32	3.43	-0.52	0.97	38.00	-0.61	-0.18	3.37	0.89	0.96	38.38	39.02	142.80
dA(Ga+1)	0.1	-0.04	0.38	-3.85	-9.53	-2.14	-0.06	-0.48	3.42	0.89	-0.73	37.45	-0.68	0.06	3.4	-1.2	-0.78	37.7	38.93	142.33
cdA(U-1)	0.11	-0.01	0.03	-1.37	-12.74	0.1	-0.02	-0.35	3.21	-0.32	0.58	35.15	-0.74	0.07	3.17	0.87	0.44	35.37	39.20	140.06
cdA(Ap-1)	0.15	-0.04	0.1	0.59	-10.81	-0.3	-0.04	-0.46	3.45	1.02	-0.21	38.81	-0.53	0.12	3.39	-1.01	-1.19	39.25	38.77	144.31
cdA(Ga-1)	0.05	-0.03	0.19	3.47	-8.96	-0.04	0.02	-0.42	3.38	1.89	-0.51	37.61	-0.65	0.18	3.35	-0.91	-2.45	38.22	38.56	143.12
cdA(U0)	0.20	0.01	-0.03	-1.71	-14.47	-1.26	0.05	-0.37	3.21	0.04	0.78	35.17	-0.78	-0.01	3.18	0.96	-0.29	35.62	39.20	140.06
cdA(A_P0)	0.13	-0.01	0.18	2.51	-11.48	-1.6	-0.03	-0.41	3.47	0.31	0.77	38.12	-0.76	-0.09	3.42	1	-0.42	38.38	38.54	143.00
cdA(A_P0)	0.06	-0.02	0.17	2.2	-11.71	-0.33	-0.11	-0.35	3.46	-0.39	-0.04	38.54	-0.66	0.09	3.4	-0.31	0.68	38.85	38.77	144.31
cdA(U+1)	0.13	-0.01	0.04	1.17	-12.1	-1.28	-0.08	-0.33	3.15	-0.31	0.83	35.38	-0.71	0.17	3.13	1.21	0.18	35.62	39.18	140.71
cdA(A_P+1)	0.18	0.03	-0.11	-1.83	-11.28	-1.48	0.03	-0.39	3.5	0.27	0.27	38.49	-0.69	0.02	3.48	-0.09	-0.74	38.63	38.54	137.20
cdA(Ga+1)	0.02	-0.01	0.11	-2.22	-12.54	-0.54	-0.07	-0.51	3.45	1.18	0.71	37.62	-0.91	0.3	3.45	1.27	-1.93	37.77	38.54	142.99

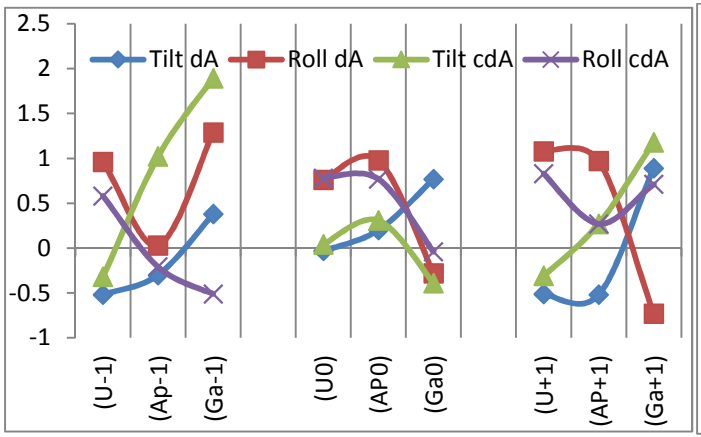
Graph 1S. Graphical representation of data presented in **Table 1S**




40
39
38
37
36
35
34
33
h-Twist dA
h-Twist cdA
(U-1)
(Ap-1)
(Ga-1)
(U0)
(AP0)
(Ga0)
(U+1)
(AP+1)
(Ga+1)


0.2
0.1
0
-0.1
-0.2
-0.3
-0.4
-0.5
-0.6
Shift dA
Slide dA
Shift cdA
Slide cdA
(U-1)
(Ap-1)
(Ga-1)
(U0)
(AP0)
(Ga0)
(U+1)
(AP+1)
(Ga+1)


3.6
3.5
3.4
3.3
3.2
3.1
3
2.9
Rise dA
Rise cdA
(U-1)
(Ap-1)
(Ga-1)
(U0)
(AP0)
(Ga0)
(U+1)
(AP+1)
(Ga+1)


2.5
2
1.5
1
0.5
0
-0.5
-1
Tilt dA
Roll dA
Tilt cdA
Roll cdA
(U-1)
(Ap-1)
(Ga-1)
(U0)
(AP0)
(Ga0)
(U+1)
(AP+1)
(Ga+1)

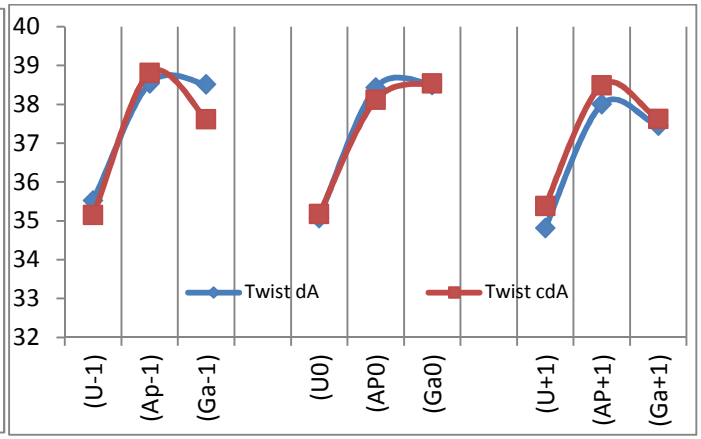

40
39
38
37
36
35
34
33
32
Twist dA
Twist cdA
(U-1)
(Ap-1)
(Ga-1)
(U0)
(AP0)
(Ga0)
(U+1)
(AP+1)
(Ga+1)

Table 2S. Base pairs parameters, complementary base-pair parameters and local helical parameters of double stranded oligodeoxynucleotides that contained at position **7A** 2'-deoxyadenosine (dA) or (5'S)-5',8-cyclo-2'-deoxyadenosine (cdA) in one strand and at different positions **T6** (U-1) or **T7** (U0) or **T8** (U+1) the 2'-deoxyuridine in the opposite strand. The structures of *ds*-oligodeoxynucleotides obtained under Molecular Mechanics (Amber 94 force field) calculation in solvation box, the sodium ions have been used as counterions to neutralize the negative charge of *ds*-DNA.

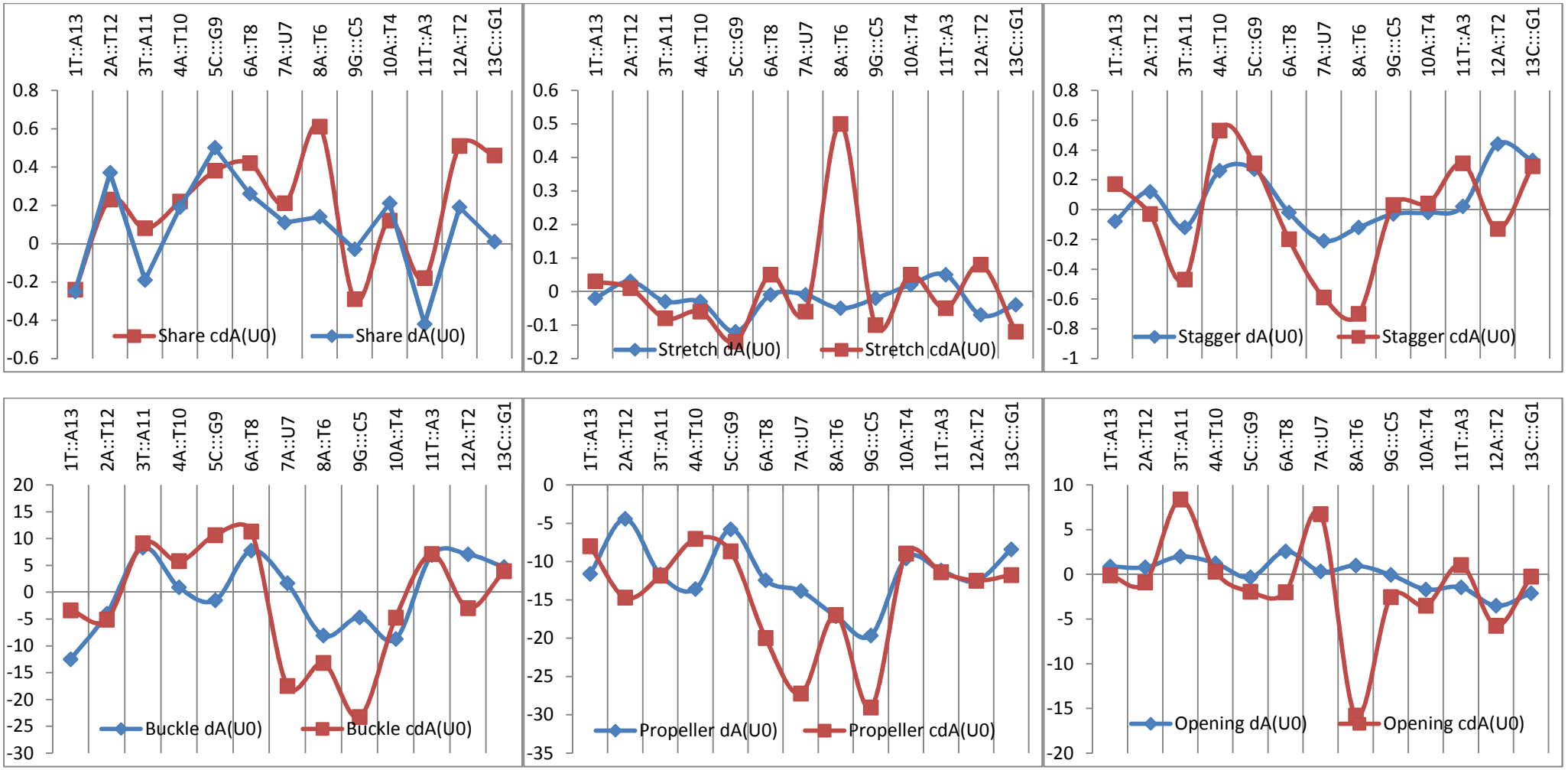
BASE PAIR																			
		dA(U0)						dA(U-1)						dA(U+1)					
		Share	**Stretch**	**Stagger**	**Buckle**	**Propeller**	**Opening**	**Share**	**Stretch**	**Stagger**	**Buckle**	**Propeller**	**Opening**	**Share**	**Stretch**	**Stagger**	**Buckle**	**Propeller**	**Opening**
5'	3'																		
^{1}T	A_{13}	-0.25	-0.02	-0.08	-12.51	-11.61	0.87	-0.27	0.05	-0.06	-7.66	-12.82	-4.29	-0.23	0.13	0.34	-12.85	-10.75	-7.83
^{2}A	T_{12}	0.37	0.03	0.12	-4.02	-4.42	0.79	0.2	0.01	0.05	-4.56	-10.33	-2.03	0.36	-0.02	0.23	-4.52	-19.03	-2.68
^{3}T	A_{11}	-0.19	-0.03	-0.12	8.32	-11.7	1.99	-0.18	-0.05	-0.23	4.17	-7.19	1.75	-0.12	0.04	-0.13	4.86	-3.35	8.69
^{4}A	T_{10}	0.19	-0.03	0.26	0.91	-13.58	1.24	0.17	-0.01	0.09	-8.36	-8.96	1.44	0.44	0.02	-0.23	-7.56	-7.66	-1.98
^{5}C	G_{9}	0.5	-0.12	0.27	-1.53	-5.79	-0.34	0.19	-0.06	0.23	3.82	-3.07	-1.34	0.32	-0.11	-0.06	6.74	-8.64	-1.63
^{6}A	**T_{8}**	0.26	-0.01	-0.02	7.76	-12.44	2.58	0.46	0	-0.14	7.48	-16.44	1.19	0.38	0.03	-0.28	-6.09	-10.24	-3.3
^{7}A	**T_{7}**	0.11	-0.01	-0.21	1.67	-13.85	0.32	0.06	-0.03	0.17	4.44	-21.28	-4.5	0.26	0	-0.13	-5.16	-23.06	-2.82
^{8}A	**T_{6}**	0.14	-0.05	-0.12	-8.1	-17.12	0.97	0.13	-0.04	0.13	-11.07	-22.28	0.8	0.13	-0.02	0.14	-9.46	-20.14	-6.15
^{9}G	C_{5}	-0.03	-0.02	-0.03	-4.68	-19.65	-0.06	-0.46	-0.1	0.01	-8.34	-23.54	0.65	-0.13	-0.07	0.14	-5.56	-21.86	-1.47
^{10}A	T_{4}	0.21	0.02	-0.02	-8.73	-9.59	-1.69	0.36	0.07	-0.34	-15.95	-12.46	-4.94	0.4	0.14	-0.21	-13.53	-14.8	-8.73
^{11}T	A_{3}	-0.42	0.05	0.02	6.92	-11.17	-1.45	-0.03	-0.01	0.21	-3.79	-10.63	-0.81	-0.16	-0.05	0.58	-4.87	-8.5	2.32
^{12}A	T_{2}	0.19	-0.07	0.44	7.07	-12.52	-3.52	0.3	0.01	0.26	-3.24	-8.2	-4.99	0.07	0.04	-0.02	0.26	-12.27	-4.95
^{13}C	G_{1}	0.01	-0.04	0.33	4.69	-8.41	-2.11	0.16	-0.09	0.56	5.56	-0.02	-0.13	0.36	-0.14	0.36	5.79	-15.82	-1.22
3'	5'																		
		cdA(U0)						cdA(U-1)						cdA(U+1)					
5'	3'																		
^{1}T	A_{13}	-0.24	0.03	0.17	-3.36	-8.01	-0.12	-0.34	-0.01	-0.02	-3.37	-12.97	-0.31	-0.31	0.07	0.12	-8.98	-11.63	-3.92
^{2}A	T_{12}	0.23	0.01	-0.03	-5.12	-14.71	-0.92	0.29	0.01	0.22	-2.54	-9.86	0.25	0.25	-0.02	0.18	-5.88	-9.42	2.17
^{3}T	A_{11}	0.08	-0.08	-0.47	9.11	-11.84	8.36	-0.08	-0.02	-0.22	8.93	-5.98	-0.22	-0.22	-0.02	-0.08	3.06	-6.5	1.31
^{4}A	T_{10}	0.22	-0.06	0.53	5.77	-7.03	0.3	-0.1	-0.05	0.25	0.26	-10.98	0.28	0.28	-0.01	0.23	2.21	-9.73	-0.21
^{5}C	G_{9}	0.38	-0.15	0.31	10.64	-8.66	-1.94	0.63	-0.19	0.13	6.43	-8.94	0.35	0.35	-0.11	0.01	8.91	-9.13	-2.4
^{6}A	**T_{8}**	0.42	0.05	-0.2	11.33	-19.97	-1.99	0.34	-0.01	-0.29	-0.45	-12.14	0.55	0.55	0.01	-0.07	11.36	-17.29	-1.25
^{7}A	**T_{7}**	0.21	-0.06	-0.59	-17.46	-27.23	6.74	0.33	0.13	-0.41	-19.2	-23.73	0.46	0.46	0	-0.35	-14.63	-18.73	6.38
^{8}A	**T_{6}**	0.61	0.5	-0.7	-13.19	-16.96	-15.81	0.26	0.14	-0.16	-4.04	-12.22	0.35	0.35	0.11	0.21	7	-11	-6.72
^{9}G	C_{5}	-0.29	-0.1	0.03	-23.26	-29.05	-2.55	-0.46	-0.13	0.06	-4.97	-19.5	-0.39	-0.39	-0.18	0.36	0.34	-19.5	-2.37
^{10}A	T_{4}	0.12	0.05	0.04	-4.75	-8.96	-3.52	0.21	0.02	-0.11	-8.63	-9.92	0	-0.00	0.05	-0.37	-15.69	-13.54	-4.51
^{11}T	A_{3}	-0.18	-0.05	0.31	7.1	-11.37	1.05	0.01	-0.1	0.55	-0.33	-9.39	-0.05	-0.05	-0.02	0.2	0.65	-10.14	0.56
^{12}A	T_{2}	0.51	0.08	-0.13	-2.96	-12.49	-5.74	0.36	0.13	-0.03	1.55	-15.43	0.14	0.14	0.07	0.04	5.68	-5.61	-4.64
^{13}C	G_{1}	0.46	-0.12	0.29	3.93	-11.77	-0.26	-0.08	-0.05	0.39	8.6	-14.63	0.29	0.29	-0.04	-0.02	21.13	-15.03	-0.99
3'	5'																		

BASE PAIR STEP																		
	dA(U_0)						dA(U-1)						dA(U+1)					
	Shift	**Slide**	**Rise**	**Tilt**	**Roll**	**Twist**	**Shift**	**Slide**	**Rise**	**Tilt**	**Roll**	**Twist**	**Shift**	**Slide**	**Rise**	**Tilt**	**Roll**	**Twist**
TA/TA	0.5	0.57	3.08	0.14	1.36	42.99	0.9	0.64	3.11	0.92	1.61	41.74	0.49	0.18	3.17	-1.14	4.57	33.13
AT/AT	-0.56	-0.26	2.92	2.13	-1.79	27.32	-0.09	-0.23	2.98	2.41	-1.27	29.88	0.66	-0.29	3.02	4.14	-2.93	30.94
TA/TA	0.56	0.13	3.32	-0.02	4.79	40.48	0.27	-0.32	3.46	-2.44	7.32	41.32	-0.74	0.17	3.56	-0.99	5.38	45.89
AC/GT	0.4	-0.6	3.31	-0.69	-0.36	33.44	-0.21	-0.4	3.01	-0.71	3.84	31.86	0.32	-0.39	2.93	-1.09	1.75	27.97
CA/TG	-0.49	0.38	3.12	2.82	5.45	36.98	-0.67	0.34	3.25	3.67	0.62	38.29	-1.19	-0.58	3.49	-0.46	7.47	38.02
AA/TT	-0.41	-0.82	3.36	-1.4	-0.17	31.07	0.04	-0.33	3.14	-3.36	-2.07	31.23	-0.62	-0.22	3.22	-1.67	-4.39	36.26
AA/TT	0.45	-0.45	3.36	2.28	0.34	38.79	0.15	-0.82	3.51	-0.38	-2.49	39.11	-0.19	-0.81	3.19	-3.1	0.18	29.84
AG/CT	-0.27	0.24	3.19	-1.13	4.8	33.11	0.27	-0.24	3.2	0.23	9.34	31.42	0.41	-0.1	3.3	-0.43	1.9	36.19
GA/TC	-0.29	-1.18	3.29	-2.12	-0.06	30.52	-0.75	-1.01	3.44	-0.09	0.07	32.29	-0.94	-1.07	3.32	0.98	0.83	34.01
AT/AT	-0.15	-0.48	2.8	0.33	-2.88	29.55	0.4	-0.23	2.95	-2.12	-3.24	34.36	0.81	-0.79	2.98	-4.87	-3.54	26.31
TA/TA	0.79	0	3.15	-0.43	-1.87	40.71	-0.41	-0.27	3.18	-0.14	0.46	34.77	0.01	0.35	2.98	6.58	0.06	43.85
AC/GT	0.1	-1.35	3.32	-2.28	-0.45	35.93	0.48	-0.43	3.14	-4.2	-2.64	39.95	0.64	-0.56	3.04	-4.05	1.67	35.33
	cdA(U_0)						cdA(U-1)						cdA(U+1)					
TA/TA	0.73	0.37	3.18	3.57	4.31	42.67	0.85	0.56	3.17	2.24	-0.26	42.34	0.48	0.64	3.11	-0.13	-0.81	46.34
AT/AT	0.25	-0.25	2.8	4.14	-0.46	29	-0.05	-0.39	2.93	3.2	-1.85	31.35	-0.15	-0.43	2.97	1.8	-2.49	27.52
TA/TA	0.23	0.01	3.37	-3.57	3.41	39.86	0.59	-0.55	3.31	-1.4	6.16	35.33	0.55	-0.1	3.21	0.15	6.52	38.31
AC/GT	0.16	-0.88	3.21	1.37	-2.5	35.09	-0.01	-0.2	3.24	0.39	-2.14	40.86	-0.2	-0.45	3.12	1.74	0.31	33.98
CA/TG	-0.1	-0.27	3.24	6.19	3.63	28.49	-0.33	-0.49	3.53	2.47	1.63	28.47	0.28	-0.02	3.26	4.04	2.44	33.51
AA/TT	-0.56	0.09	3.74	-6	6	47.46	0.13	0.2	3.68	-3.78	3.89	45.35	-1.05	-0.22	3.65	-6.13	3.48	43.62
AA/TT	-1.21	-0.61	3.14	2.91	2.03	28.09	-1.23	-0.63	3.03	1.12	0.84	26.47	-0.27	-0.49	2.77	0.03	1.38	26.2
AG/CT	0.32	-0.92	3.54	-5.86	3.48	32.47	-0.04	-0.56	3.25	-3.42	1.85	34.42	-0.18	-0.72	3.29	-3.26	0	37.04
GA/TC	-0.73	-0.85	3	-3.48	-7.91	30.19	-0.87	-0.93	3.31	-1.28	-1.27	35.77	-0.75	-1.41	3.62	3.83	0.99	32.76
AT/AT	0.38	-0.67	2.93	-2.15	-2.74	30.2	0.7	-0.46	3.04	-3.97	-5.28	32.09	0.54	-0.19	2.83	-3.47	-5.19	34.02
TA/TA	0.1	0.15	3.4	5.66	-1.56	45.14	-0.87	-0.15	3.11	3.64	2.64	38.07	-0.62	-0.26	3.09	-0.46	3.73	34.53
AC/GT	1.02	-0.65	3.03	-2.31	1.61	33.36	0.86	-0.65	2.96	-3.1	0.76	31.28	0.42	-0.27	2.91	-1.82	-0.45	36.76

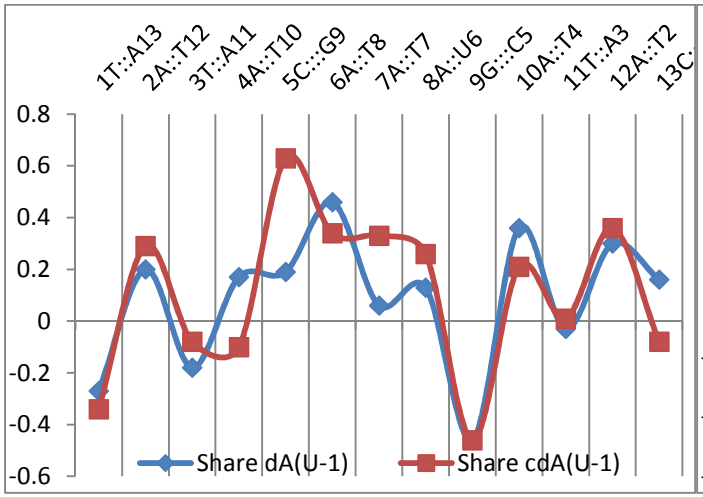
BASE PAIR STEP	Local helical parameters																	
	dA(U0)						dA(U-1)						dA(U+1)					
	x-displacement	y-displacement	h-Rise	Inclination	Tip	h-Twist	x-displacement	y-displacement	h-Rise	Inclination	Tip	h-Twist	x-displacement	y-displacement	h-Rise	Inclination	Tip	h-Twist
TA/TA	0.66	-0.67	3.1	1.86	-0.2	43.02	0.74	-1.17	3.15	2.26	-1.29	41.78	-0.41	-1.03	3.15	7.96	1.98	33.45
AT/AT	-0.15	1.65	2.88	-3.78	-4.49	27.46	-0.21	0.63	2.97	-2.45	-4.66	30	-0.02	-0.49	3.09	-5.44	-7.7	31.34
TA/TA	-0.36	-0.81	3.32	6.9	0.03	40.75	-1.25	-0.65	3.33	10.26	3.42	42	-0.29	0.85	3.58	6.87	1.26	46.2
AC/GT	-0.98	-0.81	3.31	-0.63	1.2	33.45	-1.36	0.27	2.95	6.96	1.28	32.09	-1.18	-0.89	2.89	3.61	2.25	28.05
CA/TG	-0.1	1.12	3.1	8.52	-4.42	37.47	0.43	1.46	3.18	0.95	-5.58	38.47	-1.83	1.73	3.33	11.33	0.7	38.72
AA/TT	-1.5	0.48	3.38	-0.31	2.61	31.1	-0.23	-0.68	3.13	-3.82	6.21	31.47	0.26	0.76	3.24	-7.01	2.68	36.55
AA/TT	-0.72	-0.38	3.37	0.51	-3.43	38.85	-0.9	-0.28	3.55	-3.71	0.57	39.19	-1.6	-0.26	3.19	0.35	6.01	30
AG/CT	-0.35	0.28	3.2	8.36	1.97	33.47	-1.99	-0.44	3.01	16.79	-0.4	32.75	-0.43	-0.72	3.29	3.05	0.7	36.24
GA/TC	-2.23	0.12	3.3	-0.12	4.03	30.59	-1.83	1.33	3.44	0.12	0.17	32.29	-1.96	1.76	3.27	1.42	-1.68	34.03
AT/AT	-0.41	0.35	2.83	-5.62	-0.65	29.69	0.06	-0.97	2.93	-5.46	3.58	34.57	-0.88	-2.85	2.87	-7.65	10.53	26.98
TA/TA	0.2	-1.19	3.14	-2.69	0.61	40.76	-0.52	0.67	3.18	0.76	0.24	34.78	0.46	0.55	2.95	0.09	-8.75	44.32
AC/GT	-2.13	-0.5	3.33	-0.73	3.69	36.01	-0.34	-1.16	3.1	-3.84	6.12	40.25	-1.14	-1.58	2.92	2.74	6.64	35.59
	cdA(U0)						cdA(U-1)						cdA(U+1)					
1TA/TA	0.08	-0.65	3.25	5.9	-4.89	43.02	0.8	-0.95	3.21	-0.36	-3.09	42.39	0.88	-0.62	3.09	-1.03	0.16	46.35
AT/AT	-0.41	0.28	2.81	-0.92	-8.22	29.29	-0.4	0.62	2.93	-3.41	-5.89	31.56	-0.35	0.71	2.99	-5.21	-3.76	27.69
TA/TA	-0.39	-0.76	3.33	4.97	5.21	40.15	-1.77	-1.16	3.15	10.05	2.29	35.88	-0.93	-0.81	3.16	9.85	-0.22	38.84
AC/GT	-1.09	-0.07	3.27	-4.14	-2.26	35.2	-0.06	0.06	3.24	-3.06	-0.56	40.91	-0.82	0.6	3.1	0.53	-2.98	34.02
CA/TG	-1.3	1.5	3.09	7.24	-12.32	29.37	-1.39	1.27	3.46	3.29	-5.01	28.62	-0.43	0.17	3.26	4.21	-6.97	33.83
AA/TT	-0.43	0.14	3.76	7.39	7.39	48.17	-0.12	-0.54	3.66	5.03	4.88	45.66	-0.67	0.75	3.73	4.64	8.19	44.16
AA/TT	-1.69	3.1	2.96	4.17	-5.98	28.3	-1.58	2.96	2.96	1.83	-2.45	26.5	-1.4	0.61	2.74	3.05	-0.07	26.24
AG/CT	-2.24	-1.6	3.32	6.15	10.34	33.16	-1.22	-0.45	3.2	3.11	5.76	34.64	-1.12	-0.16	3.29	0	5.12	37.18
GA/TC	-0.13	0.71	3.18	-14.81	6.51	31.38	-1.32	1.23	3.37	-2.06	2.08	35.82	-2.67	2.04	3.47	1.74	-6.76	32.99
AT/AT	-0.78	-1.12	2.94	-5.23	4.11	30.4	0.04	-1.88	2.97	-9.43	7.08	32.74	0.37	-1.38	2.76	-8.77	5.86	34.57
TA/TA	0.34	0.38	3.38	-2.02	-7.34	45.5	-0.54	1.76	3	4.03	-5.55	38.32	-0.97	0.97	3.06	6.26	0.78	34.73
AC13/GT	-1.38	-2.11	2.92	2.8	4.02	33.48	-1.32	-2.11	2.85	1.41	5.73	31.44	-0.37	-0.88	2.89	-0.72	2.88	36.81

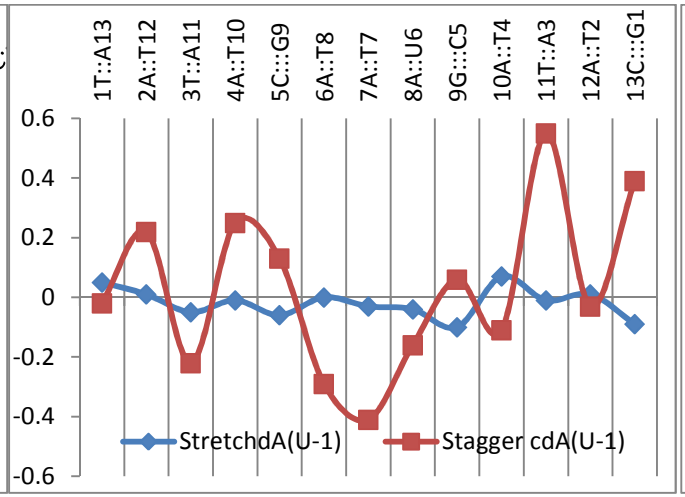
Graph 2S. Graphical representation of data presented in **Table 2S**

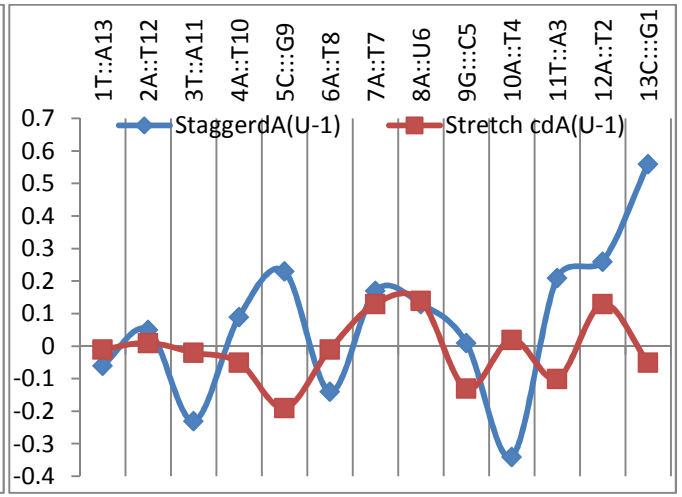
Oligodeoxynucleotide dA(U0) versus cdA(U0)

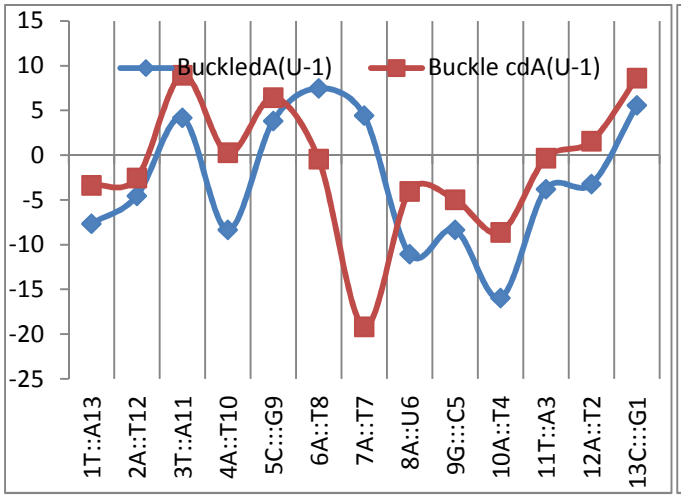


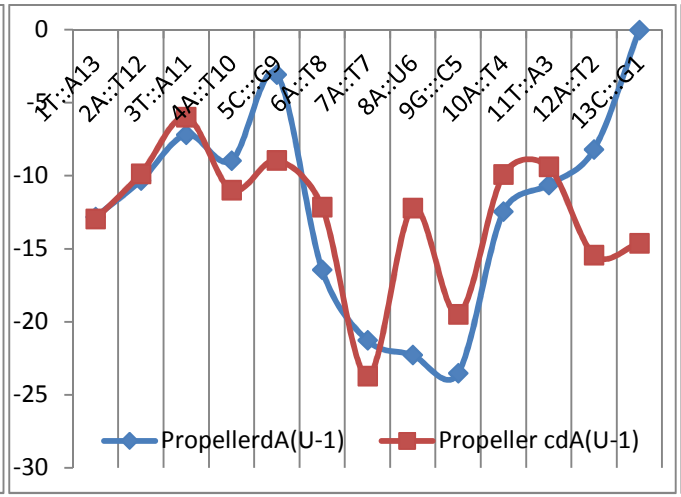
Oligodeoxynucleotide dA(U-1) versus cdA(U-1)

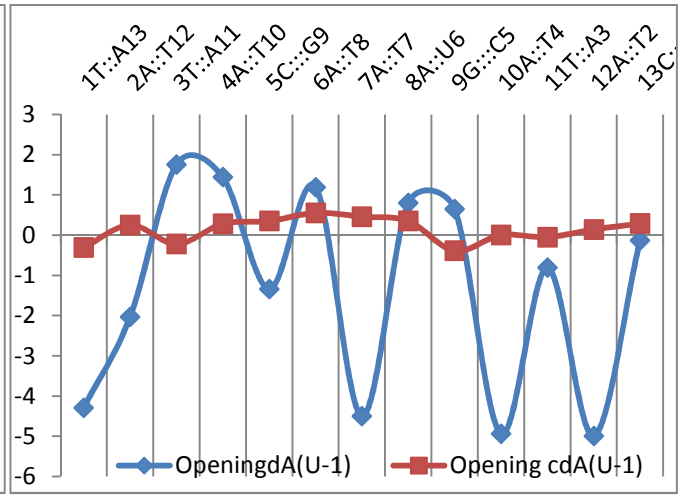




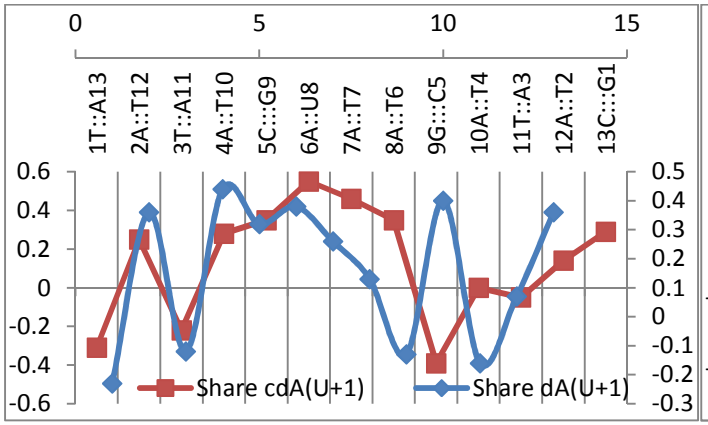


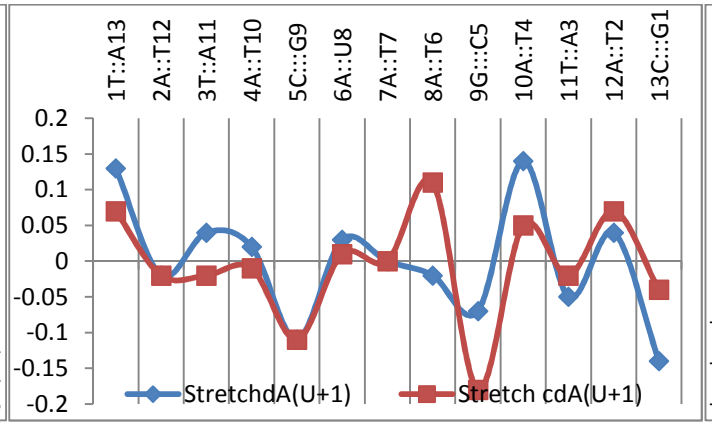


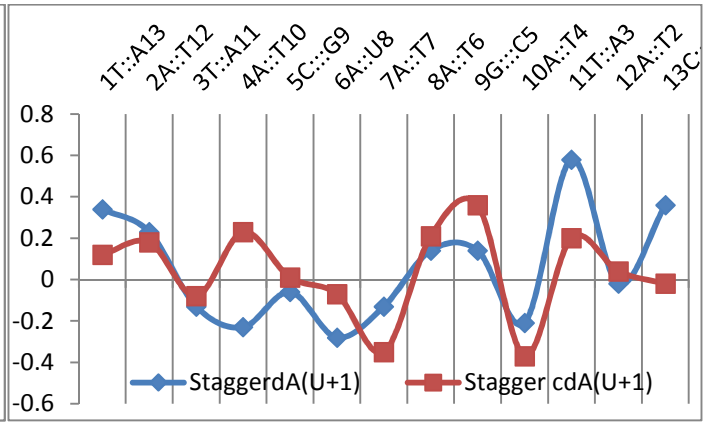


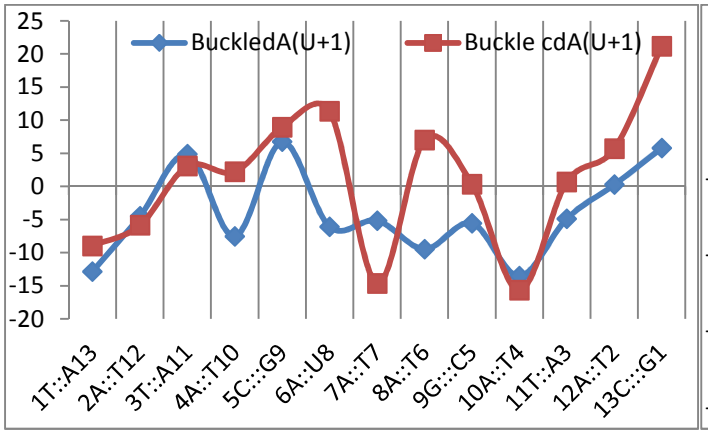


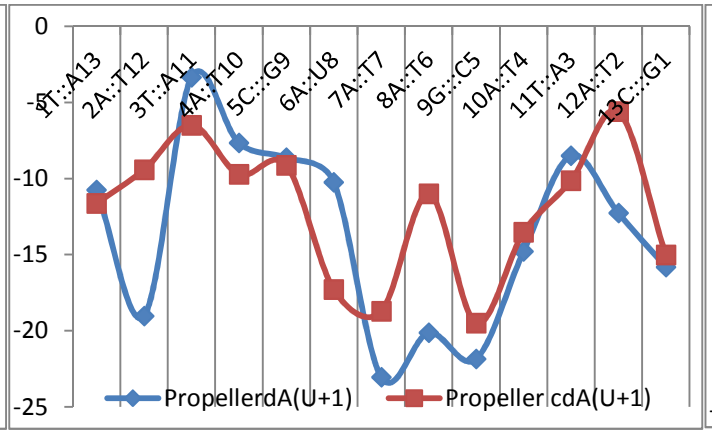
Oligodeoxynucleotide dA(U+1) versus cdA(U+1)

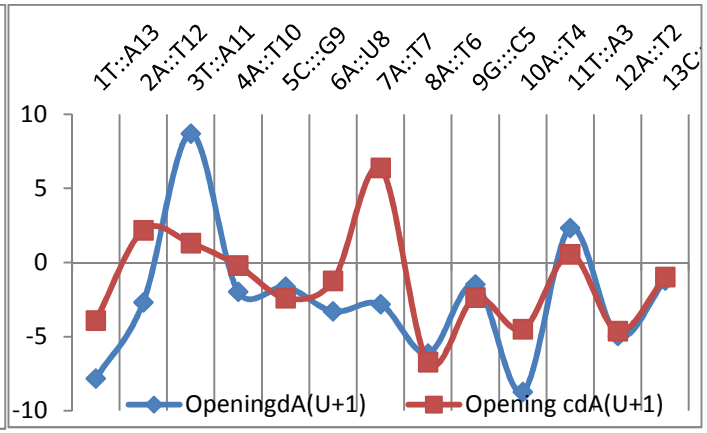




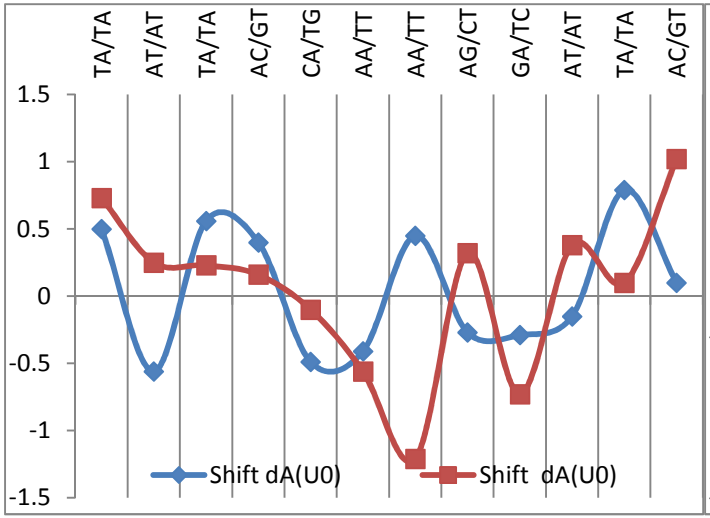


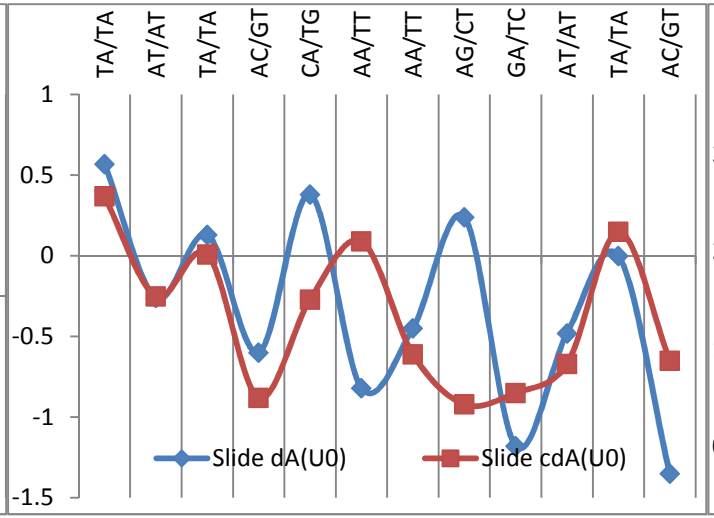


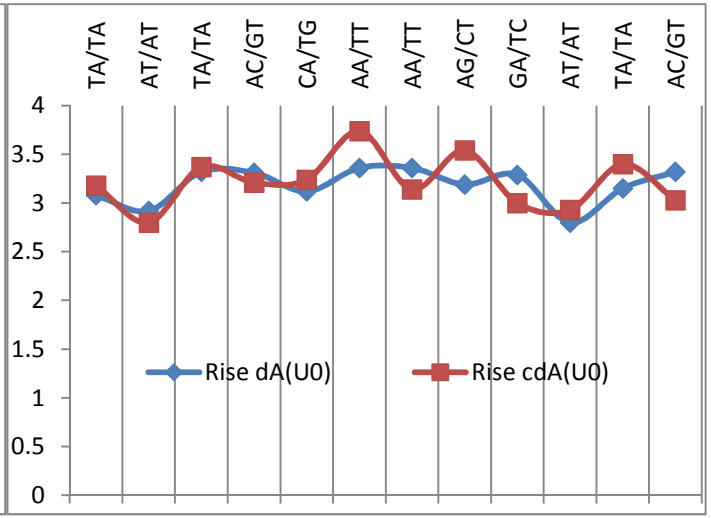


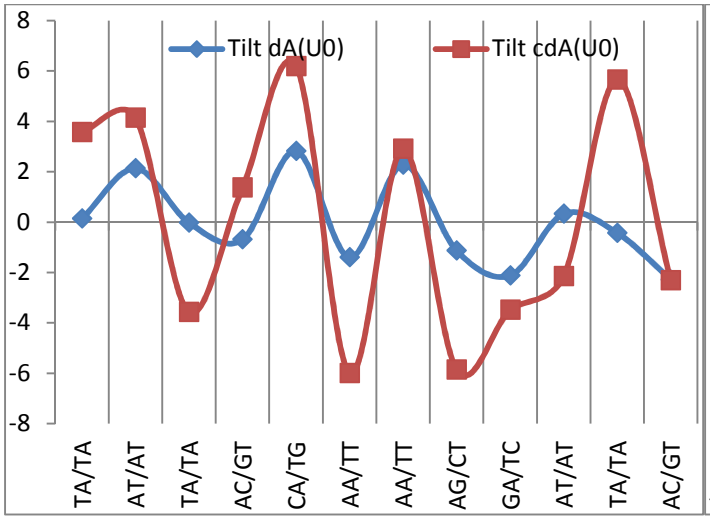


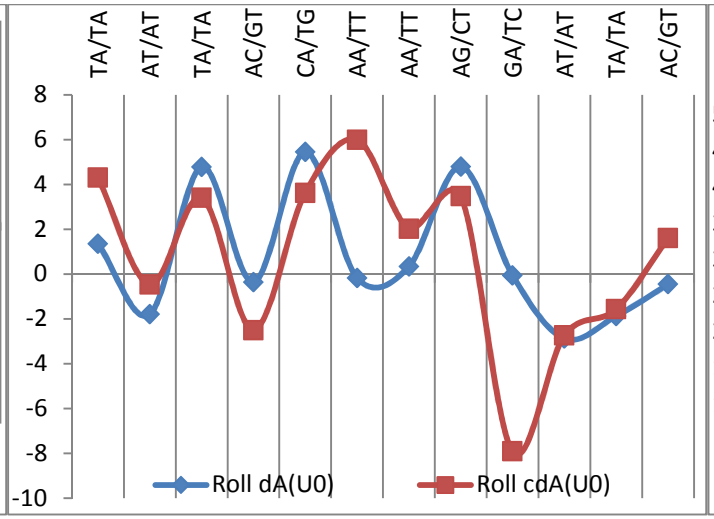
Oligodeoxynucleotide dA(U0) versus cdA(U0)

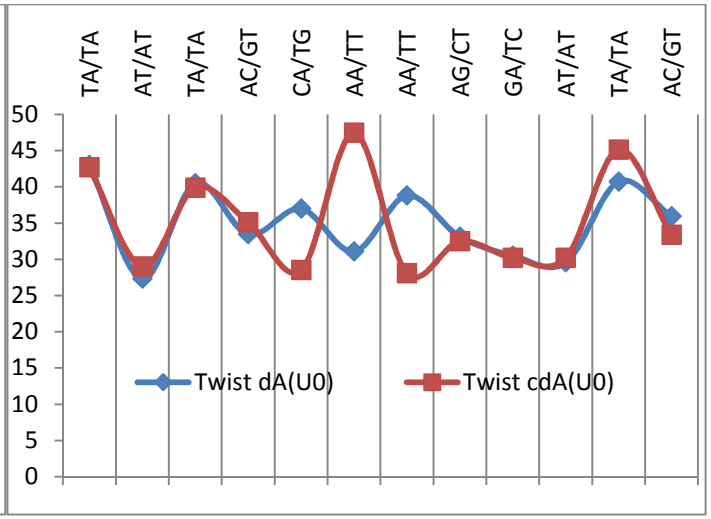




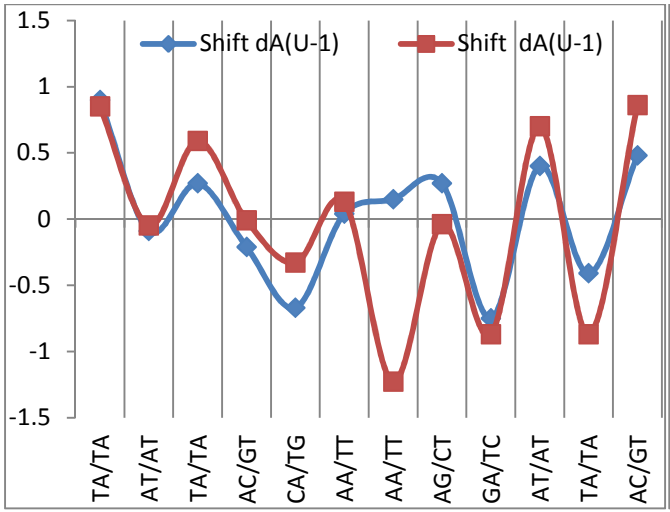


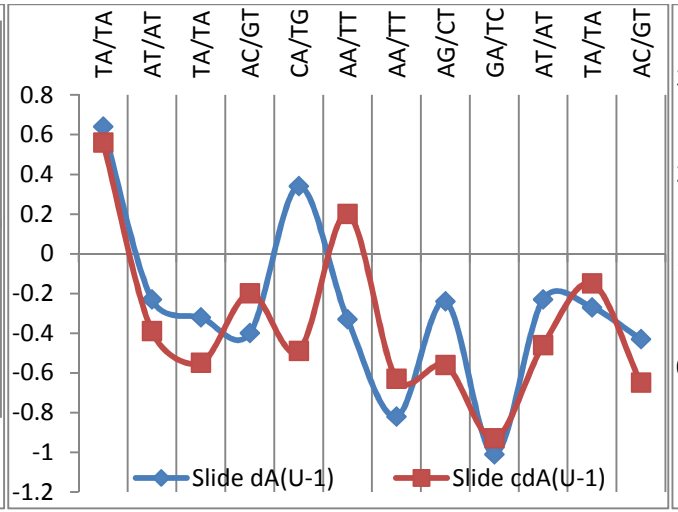


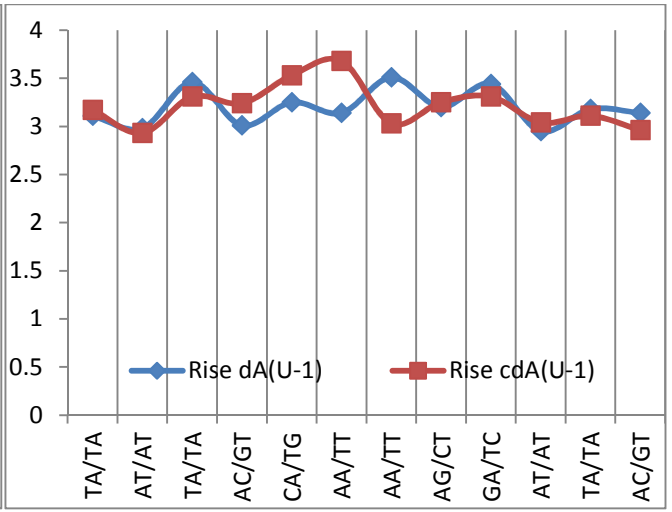


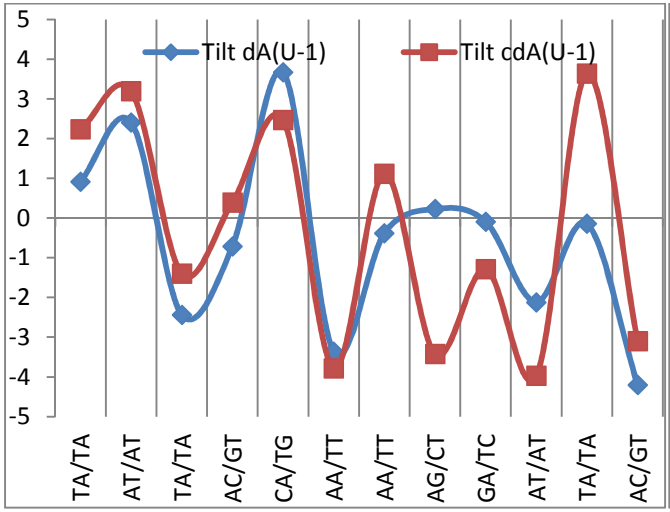


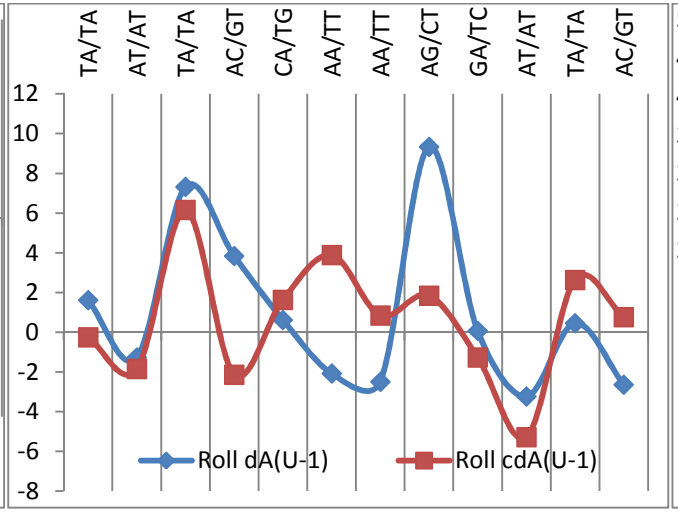
Oligodeoxynucleotide dA(U-1) versus cdA(U-1)

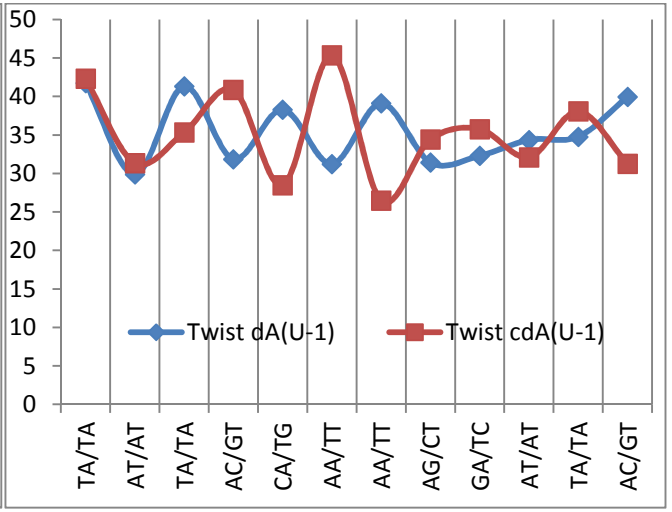




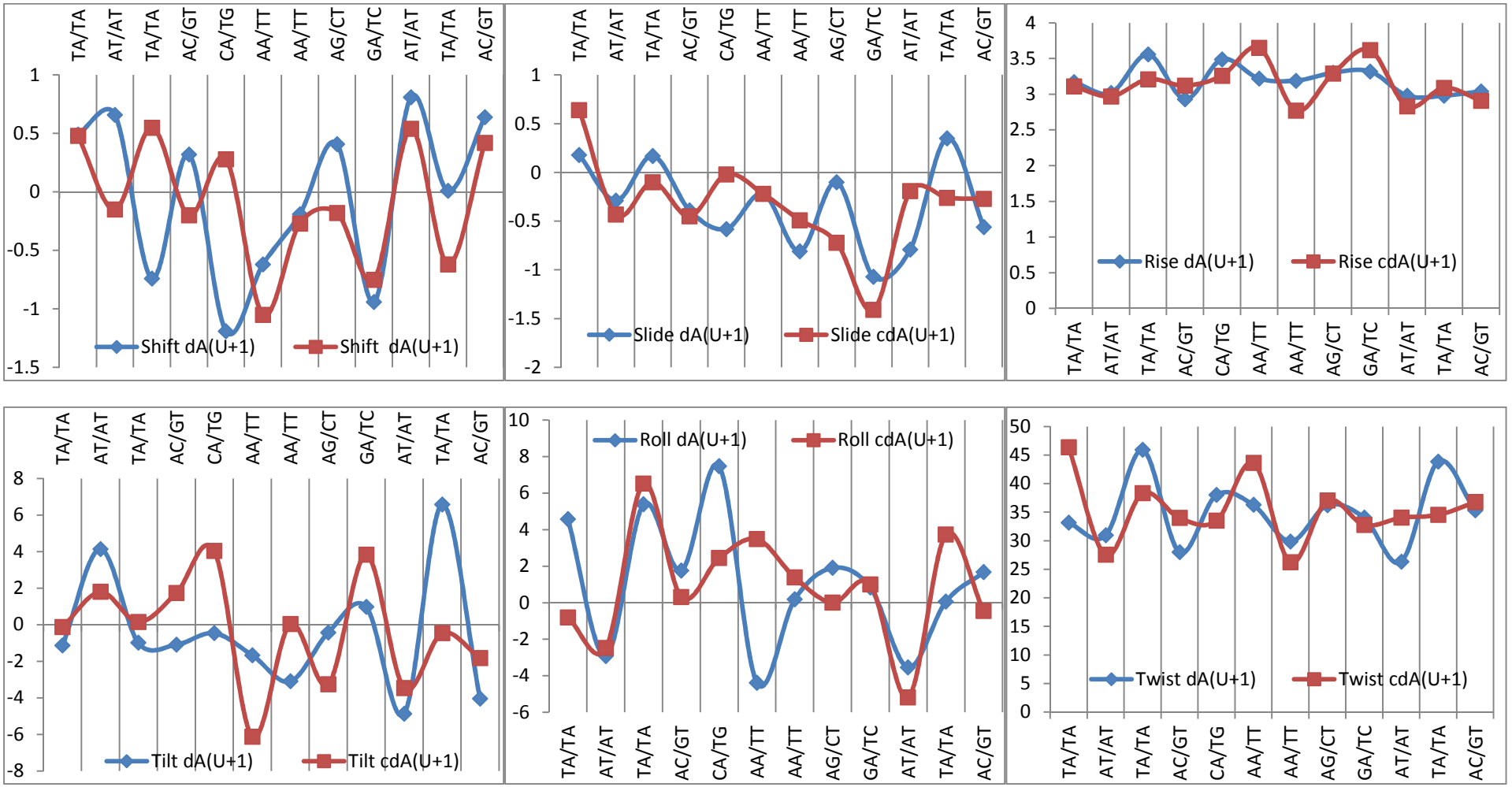




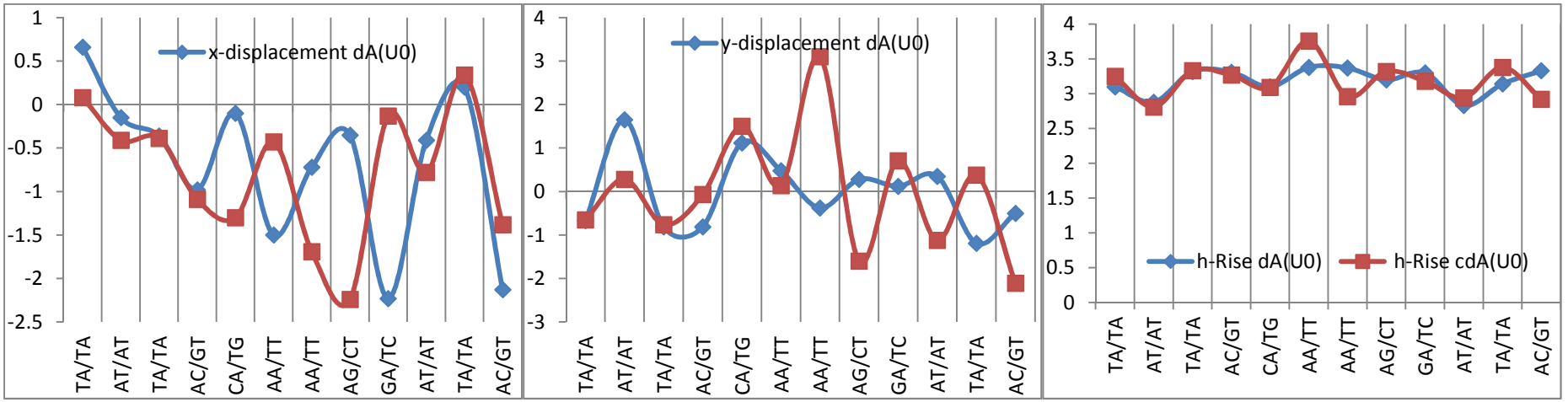


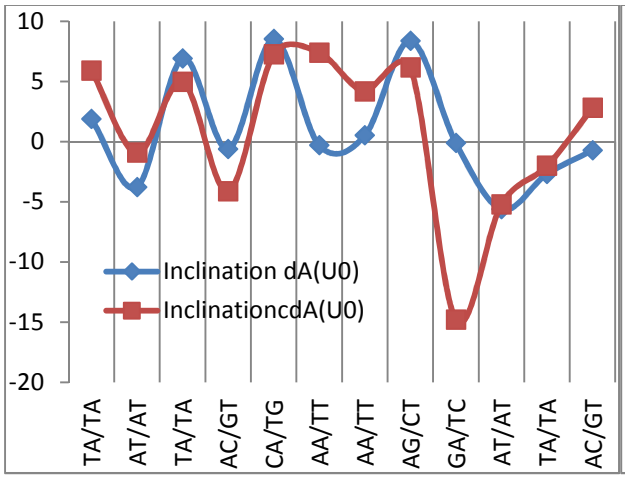


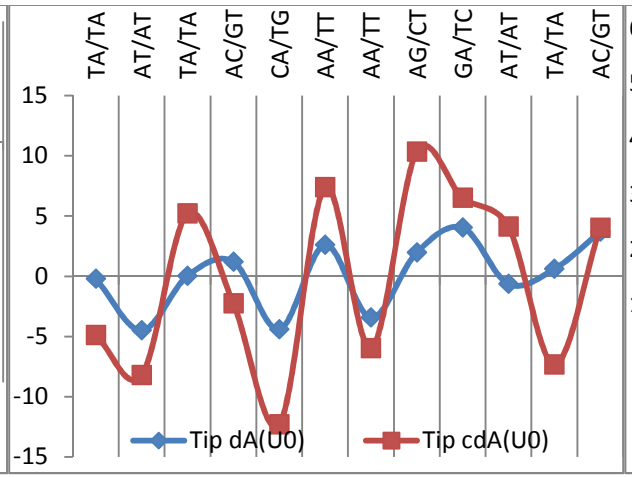
Oligodeoxynucleotide dA(U+1) versus cdA(U+1)

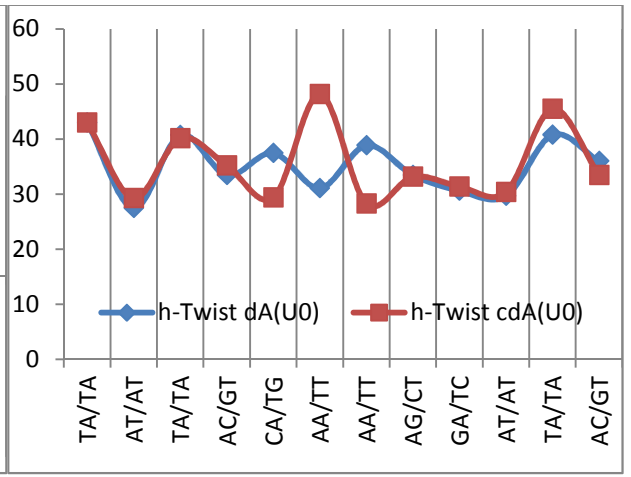


Oligodeoxynucleotide dA(U0) versus cdA(U0)

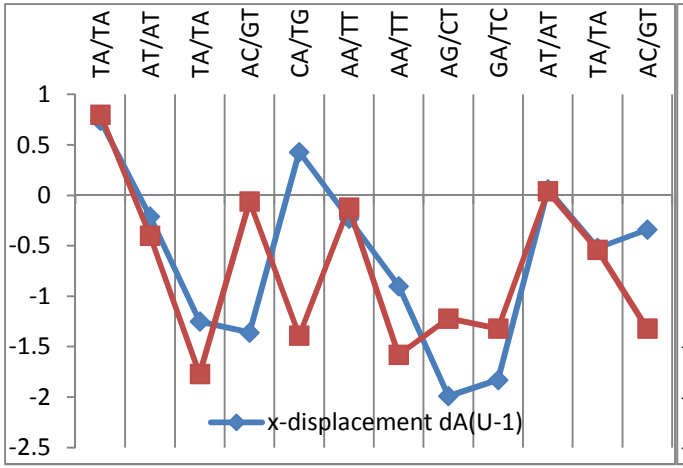


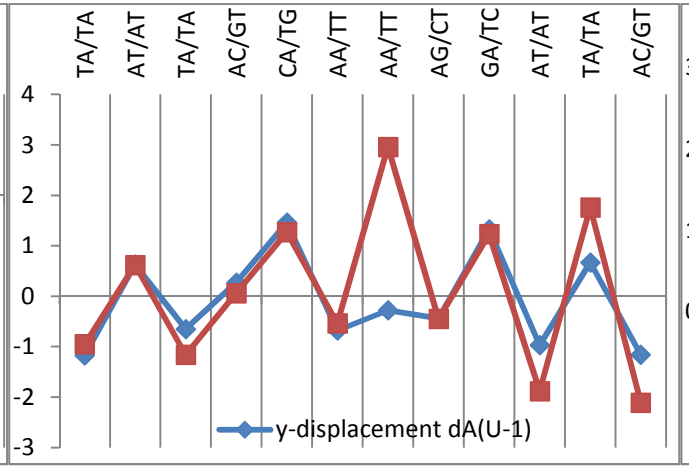


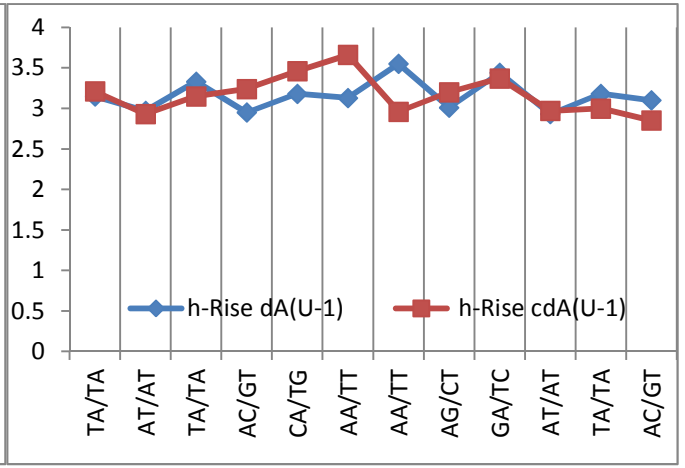


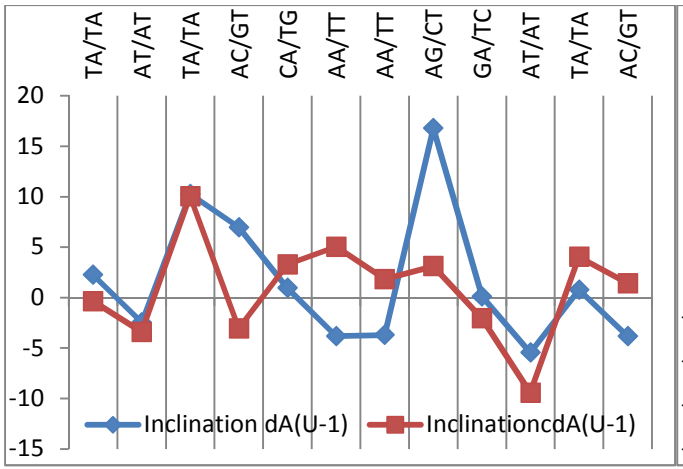


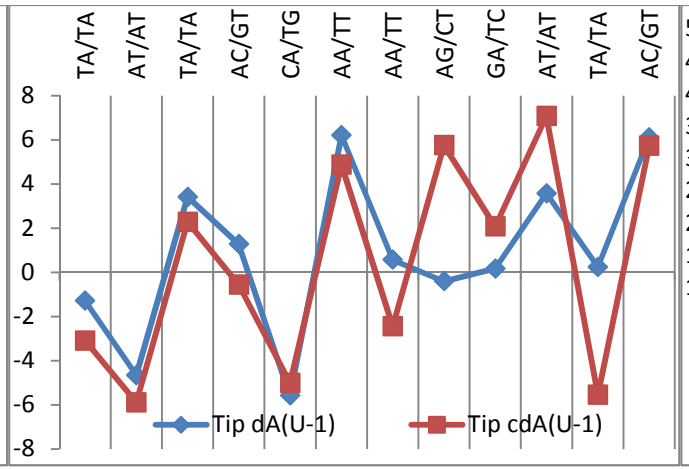
Oligodeoxynucleotide dA(U-1) versus cdA(U-1)

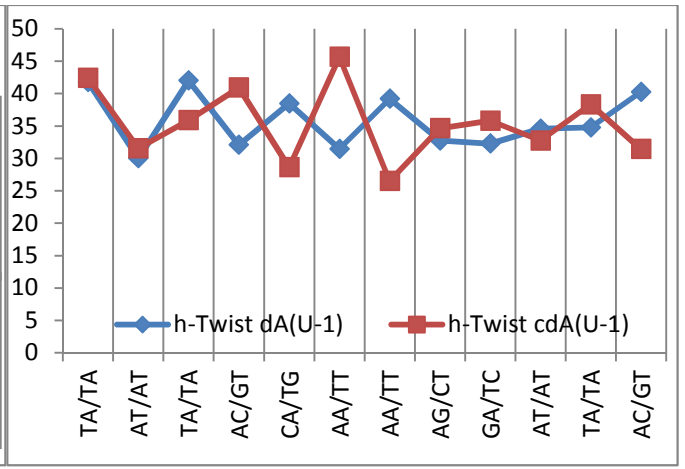




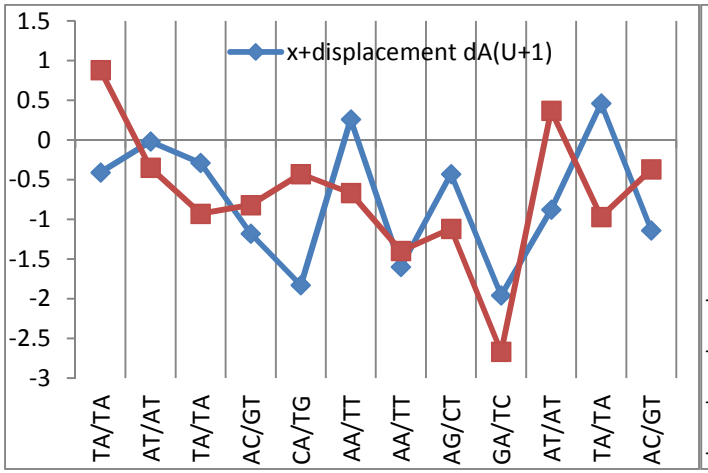


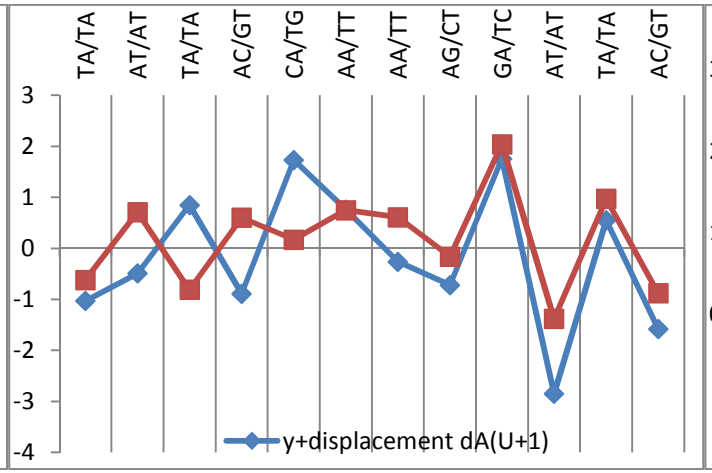


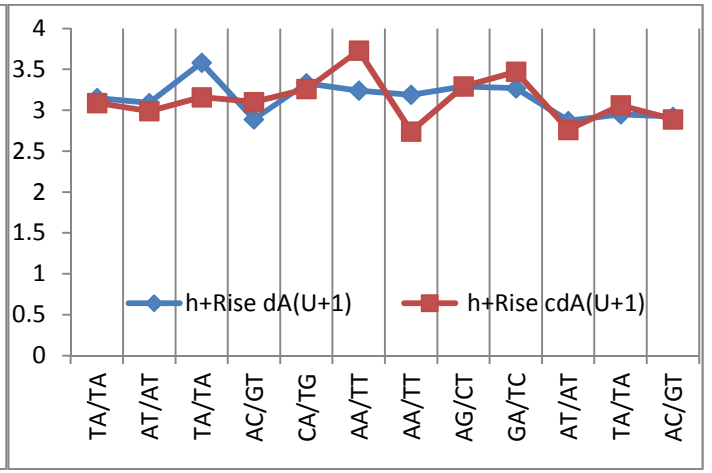


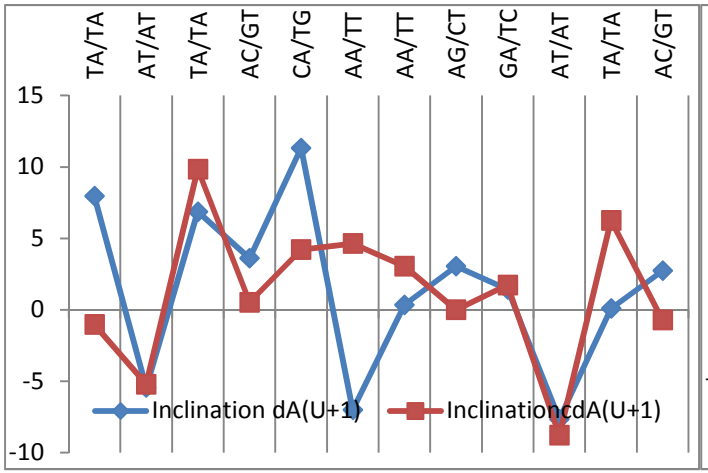


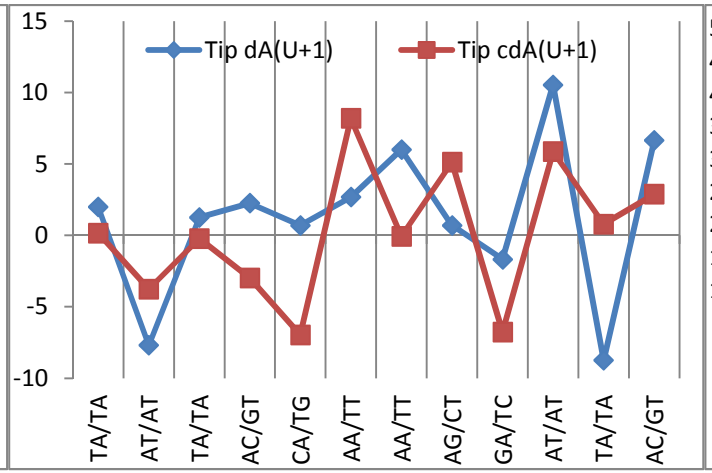
Oligodeoxynucleotide dA(U+1) versus cdA(U+1)











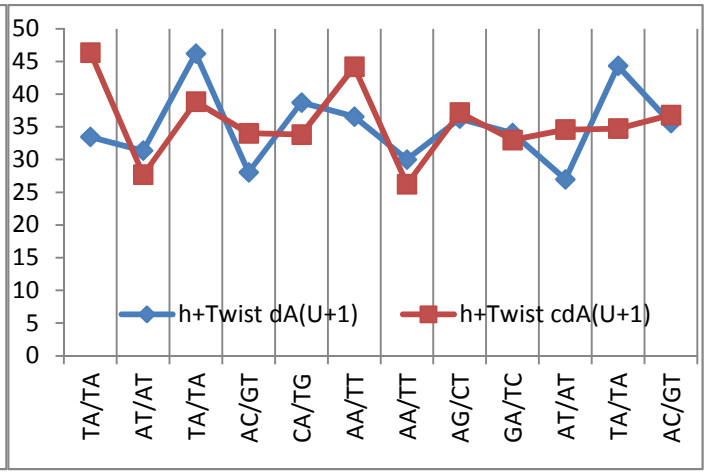


Table 3S. Base pair parameters, complementary base-pair parameters and local helical parameters of double stranded oligodeoxynucleotide that contained at position **7A** 2'-deoxyadenosine (dA) or (5'S)-5',8-cyclo-2'-deoxyadenosine (cdA) in one strand and at different positions **T6** (Ap-1) or **T7** (Ap0) or **T8** (Ap+1) apurinic/apyrimidininc sites in the opposite strand. The structures of *ds*-oligodeoxynucleotides obtained under Molecular Mechanics (Amber 94 force field) calculation in solvation box, the sodium ions have been used as counterions to neutralize the negative charge of *ds*-DNA.

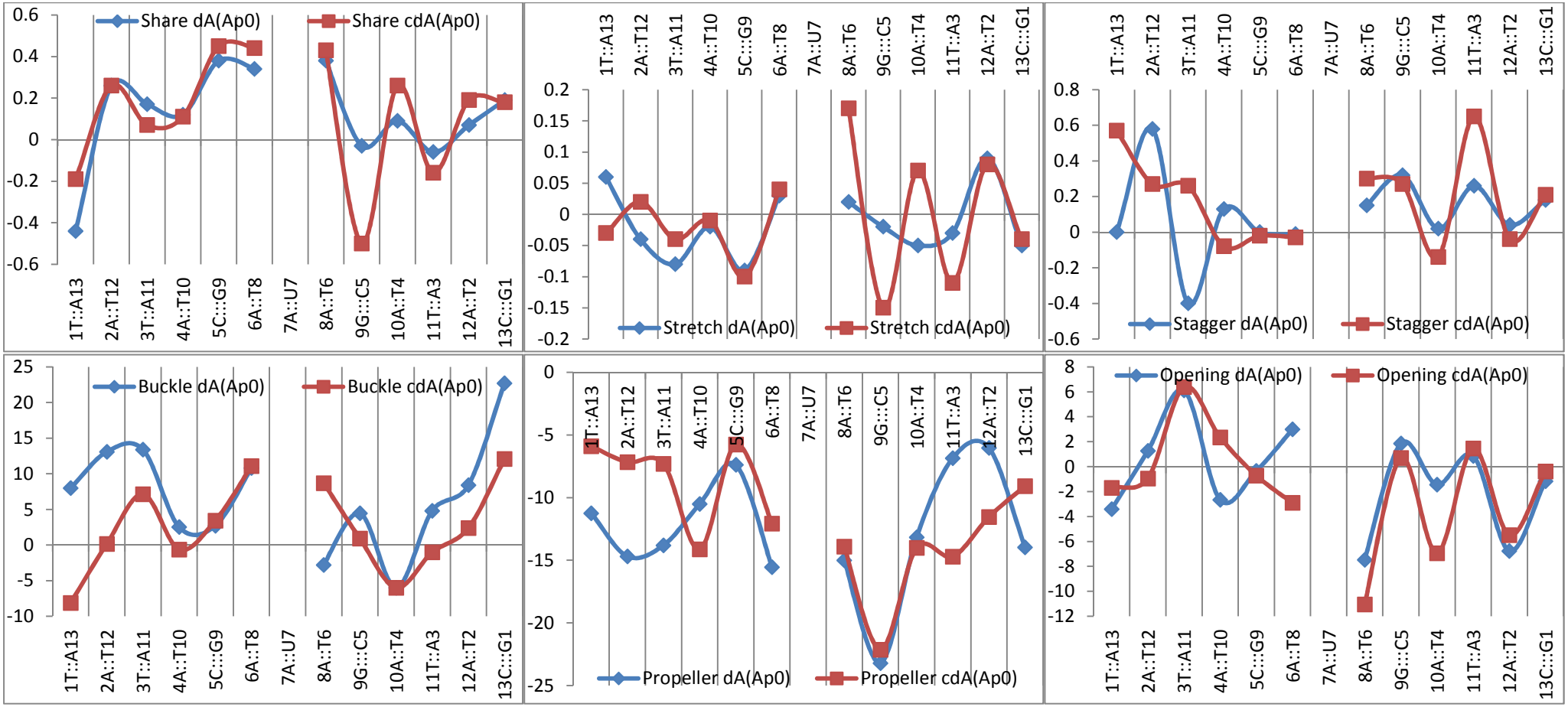
BASE PAIR		Oligodeoxynucleotides																	
		dA(Ap0)						dA(Ap-1)						dA(Ap+1)					
		Share	**Stretch**	**Stagger**	**Buckle**	**Propeller**	**Opening**	**Share**	**Stretch**	**Stagger**	**Buckle**	**Propeller**	**Opening**	**Share**	**Stretch**	**Stagger**	**Buckle**	**Propeller**	**Opening**
5'	3'																		
^{1}T	A_{13}	-0.44	0.06	0	8.01	-11.24	-3.41	-0.32	0	0.37	-11.24	-3.36	-1.63	-0.09	0.05	0.35	-12.82	-9.49	-6.38
^{2}A	T_{12}	0.26	-0.04	0.58	13.08	-14.69	1.26	0.23	0	0.48	0.81	-4.99	-2,94	0.16	0	0.28	5.41	-11.84	-0.83
^{3}T	A_{11}	0.17	-0.08	-0.4	13.38	-13.81	6.12	-0.12	-0.01	0.01	10.22	-6.8	2.12	-0.25	-0.05	-0.27	10.91	-13.11	0.16
^{4}A	T_{10}	0.12	-0.02	0.13	2.52	-10.51	-2.66	0.02	-0.03	-0.06	-0.01	-8.19	-1.96	-0.11	-0.01	0.09	-5.8	-12.92	-2.29
^{5}C	G_{9}	0.38	-0.09	0	2.7	-7.38	-0.35	0.19	-0.07	0.05	7.84	-10.43	-3.24	0.8	-0.23	0.18	3.13	-10.14	-0.69
^{6}A	**T_{8}**	0.34	0.03	-0.01	10.83	-15.56	2.99	0.27	-0.02	-0.22	7.24	-8.14	-0.42						
^{7}A	**T_{7}**							-0.02	-0.08	0.48	16.92	-9.3	-1.16	0.25	-0.03	0	1.72	-27.55	-4.83
^{8}A	**T_{6}**	0.38	0.02	0.15	-2.79	-15	-7.47							0.15	-0.05	0.24	-4.36	-22.8	-3.66
^{9}G	C_{5}	-0.03	-0.02	0.32	4.47	-23.21	1.86	-0.31	-0.13	0.26	2.31	-22.3	-1.98	-0.09	-0.01	-0.18	-19.61	-20.74	0.13
^{10}A	T_{4}	0.09	-0.05	0.02	-6	-13.17	-1.44	0.1	0.02	-0.03	-3.87	-4.49	0.20	0.17	0	0.2	-7.03	-10.65	-1.25
^{11}T	A_{3}	-0.06	-0.03	0.26	4.81	-6.84	0.86	-0.26	0.03	0.04	14.64	-9.52	-1.77	-0.13	-0.01	0.4	5.6	-9.23	1.27
^{12}A	T_{2}	0.07	0.09	0.04	8.4	-6.03	-6.76	0.18	-0.03	-0.23	-0.54	-12.52	-1.86	0.18	0.12	0.1	10.43	-8.66	-6.79
^{13}C	G_{1}	0.19	-0.05	0.18	22.72	-13.96	-1.17	0.4	-0.09	-0.03	5.94	-14.1	0.16	0.65	-0.12	0.13	19.66	-18.03	1.6
3'	5'																		
		cdA(Ap0)						cdA(Ap-1)						cdA(Ap+1)					
5'	3'																		
^{1}T	A_{13}	-0.19	-0.03	0.57	-8.13	-5.9	-1.69	0.09	-0.07	0.3	-6.63	-10.77	1.24	-0.34	0.13	-0.24	6.4	-3.34	-8.3
^{2}A	T_{12}	0.26	0.02	0.27	0.16	-7.16	-0.95	0.14	0	0.22	-8.45	-4.61	-2.03	0.44	0.02	0.13	2.85	-11.09	0.46
^{3}T	A_{11}	0.07	-0.04	0.26	7.12	-7.3	6.39	0.03	-0.07	-0.25	5.75	-8.18	1.13	-0.03	-0.06	-0.16	5.96	-12	4.79
^{4}A	T_{10}	0.11	-0.01	-0.08	-0.62	-14.13	2.35	0.07	-0.01	0.11	-3.14	-8.95	-1.6	0.03	-0.06	0.35	-2.79	-9.01	0.6
^{5}C	G_{9}	0.45	-0.1	-0.02	3.43	-5.75	-0.72	0.29	-0.11	0.38	-1.66	-7.5	-1.28	0.55	-0.09	0	9.33	-3.71	0.1
^{6}A	**T_{8}**	0.44	0.04	-0.03	11.08	-12.07	-2.9	0.2	0.02	0.05	10.55	-10.21	0.19						
^{7}A	**T_{7}**							0.33	-0.02	-0.43	-4.3	-10.54	4.47	0.39	0.06	-0.65	-25.67	-24.98	5.1
^{8}A	**T_{6}**	0.43	0.17	0.3	8.7	-13.91	-11.04							0.45	0.33	-0.46	-10.2	-12.78	-11.33
^{9}G	C_{5}	-0.5	-0.15	0.27	0.9	-22.14	0.7	0.04	-0.05	0.33	-3.41	-26.28	-1.26	-0.03	-0.02	-0.13	-15.66	-16.91	-2.18
^{10}A	T_{4}	0.26	0.07	-0.14	-5.98	-14.01	-6.94	0.13	-0.03	0.19	-0.8	-11.86	-2.22	0.35	0.01	-0.11	-13.08	-11.94	-0.5
^{11}T	A_{3}	-0.16	-0.11	0.65	-1.02	-14.71	1.46	-0.14	0	0.02	7.22	-13.38	-0.85	-0.26	0.04	0.04	3.12	-10.53	0.14
^{12}A	T_{2}	0.19	0.08	-0.04	2.38	-11.54	-5.48	0.12	-0.03	0.18	-0.17	-5.56	-2.41	0.18	0.1	-0.04	2.36	-6.4	-6.95
^{13}C	G_{1}	0.18	-0.04	0.21	12.07	-9.08	-0.39	0.54	-0.1	0.07	12.14	-11.81	1.05	0.43	-0.07	-0.05	15.44	-12.73	0.3
3'	5'																		

BASE PAIR STEP	Oligodeoxynucleotides																	
	dA(Ap0)						dA(Ap-1)						dA(Ap+1)					
	Shift	**Slide**	**Rise**	**Tilt**	**Roll**	**Twist**	**Shift**	**Slide**	**Rise**	**Tilt**	**Roll**	**Twist**	**Shift**	**Slide**	**Rise**	**Tilt**	**Roll**	**Twist**
TA/TA	0.71	0.31	3.11	-2.95	-0.35	37.7	-0.18	-0.03	2.96	-0.36	-8.02	42.11	0.27	0.76	2.83	0.02	-1.27	33.69
AT/AT	0.12	-0.39	3.25	6.44	-3.39	33.64	-0.1	-0.66	3.04	3.26	-2.16	26.48	-0.47	0.12	3.06	1.86	-5.3	35.01
TA/TA	-0.14	-0.49	3.47	-2.61	10.83	37.33	-0.44	0.02	3.41	0.59	6.32	44.53	0.54	-0.94	3.42	-0.75	13.31	38.02
AC/GT	0.23	-0.76	3.3	1.76	-1.82	33.36	0.3	-0.6	3.1	-1.09	-1.1	31.06	-0.19	-0.38	3.03	0.1	1.71	33.54
CA/TG	0.04	0.57	3.3	2.07	-0.4	35.18	-0.67	0.01	3.33	2.58	5.21	36.39	-0.7	0.14	6.58	-1.31	3.61	69.66
AA/TT	-0.48	-1.49	6.68	-0.64	3.71	73.15	0.19	-0.35	2.95	-7.07	-3.06	33.02						
AA/TT							-0.57	-1.26	6.77	-0.34	10.45	70.02	0.24	-0.54	3.25	-1.78	-0.36	31.98
AG/CT	0.55	-0.05	3.17	2.62	0.47	32							-0.1	-0.6	3.6	-1.14	6.45	39.54
GA/TC	-0.63	-0.76	3.35	-0.82	1.13	34.91	-0.75	-0.77	3.48	-2.88	-7.26	36.85	-0.42	-0.78	2.96	-2.44	-3.71	28.78
AT/AT	0.74	-0.75	2.94	-0.73	-3.96	31.68	0.17	-0.46	2.8	-0.93	-2.01	26.76	0.35	-0.81	2.94	-1.68	-2.3	29.94
TA/TA	-0.34	-0.37	3.06	1.48	2.81	37.07	0.58	-0.29	3.65	4.76	0.53	39.99	0.37	0.09	3.07	4.59	-1.44	40.81
AC/GT	0.58	-0.66	2.89	-4.36	1.76	36.76	0.39	-0.51	3.04	-1.76	1.46	36.71	0.46	-0.64	3.04	-3.25	-0.02	37.01
	cdA(Ap0)						**cdA(Ap-1)**						**cdA(Ap+1)**					
TA/TA	0.03	0.26	2.96	3.83	-4.94	46.41	0.03	-0.01	3.25	0.44	-4.53	41.02	0.71	0.52	3.31	0.44	-0.56	47.11
AT/AT	0.28	-0.63	3.05	0.28	-2.94	27.37	-0.36	-0.1	2.92	3.71	-0.19	29.17	0.1	-0.31	3.12	1.92	-3.07	27.67
TA/TA	0.25	-0.32	3.3	5.08	6.26	37.94	0.06	-0.22	3.4	-1.22	7.9	41.14	0.57	-0.31	3.33	-1.91	4.66	37.38
AC/GT	-0.05	-0.35	3.15	-0.23	4.56	35.68	0.27	-0.69	3.24	-1.99	-1.01	31.92	-0.13	-0.31	3.06	3.58	0.07	35.74
CA/TG	-0.11	0	3.1	0.87	1.62	29.74	-0.05	0.22	3.1	3.67	-2.57	34.51	-0.84	-0.5	7.3	-1.69	4.68	79.3
AA/TT	-1.1	-0.72	6.49	-3.41	2.68	74.34	-0.61	0.41	3.77	-6.3	-5.87	47.54						
AA/TT							-0.53	-2.55	5.74	12.55	10.44	61.55	-0.72	-0.77	2.94	3.52	2.03	25.91
AG/CT	0.51	-0.67	3.52	0.11	1.98	31.89							0.12	-1.08	3.43	-2.45	-0.6	30.98
GA/TC	-1.14	-0.79	3.37	-1.47	1.65	37.55	-0.61	-0.83	3.21	-3.53	-4.81	31.83	-0.68	-0.78	3.19	-1.24	-0.04	34.99
AT/AT	0.81	-0.69	3.1	-4.67	-3.55	29.08	0.39	-0.74	3.03	1.15	-1.53	29.96	0.06	-0.43	2.74	-0.38	-2.81	27.68
TA/TA	-0.96	-0.02	3.1	5.16	0.6	36.85	0.46	-0.13	3.33	1.28	1.1	41.03	0.33	0.08	3.18	1.54	1.11	39.27
AC/GT	1.15	-0.55	2.99	-2.17	0.59	32.45	0.55	-0.39	2.99	1.52	-1.28	37.19	0.84	-0.43	2.93	-0.39	-2.52	37.33

BASE PAIR STEP	Oligodeoxynucleotides																	
	dA(Ap0)						dA(Ap-1)						dA(Ap+1)					
	x-displacement	y-displacement	h-Rise	Inclination	Tip	h-Twist	x-displacement	y-displacement	h-Rise	Inclination	Tip	h-Twist	x-displacement	y-displacement	h-Rise	Inclination	Tip	h-Twist
TA/TA	0.52	-1.46	3.04	-0.54	4.56	37.82	0.68	0.22	2.92	-11.04	0.5	42.84	0.27	0.76	2.83	0.02	-1.27	33.69
AT/AT	-0.13	0.8	3.24	-5.78	-10.97	34.39	-0.9	1	3.05	-4.69	-7.06	26.76	-0.47	0.12	3.06	1.86	-5.3	35.01
TA/TA	-2.1	-0.12	3.21	16.48	3.96	38.9	-0.57	0.63	3.38	8.3	-0.78	44.96	0.54	-0.94	3.42	-0.75	13.31	38.02
AC/GT	-1.01	-0.1	3.35	-3.17	-3.05	33.46	-0.93	-0.77	3.1	-2.05	2.04	31.1	-0.19	-0.38	3.03	0.1	1.71	33.54
CA/TG	1	0.25	3.29	-0.66	-3.42	35.24	-0.7	1.42	3.25	8.28	-4.1	36.83	-0.7	0.14	6.58	-1.31	3.61	69.66
AA/TT	-1.5	0.36	6.62	3.11	0.53	73.24	-0.15	-1.36	2.87	-5.3	12.23	33.88						
AA/TT							-1.83	0.47	6.55	9.05	0.29	70.69	0.24	-0.54	3.25	-1.78	-0.36	31.98
AG/CT	-0.18	-0.53	3.2	0.85	-4.74	32.1							-0.1	-0.6	3.6	-1.14	6.45	39.54
GA/TC	-1.44	0.93	3.34	1.89	1.36	34.94	-0.17	0.76	3.61	-11.33	4.5	37.64	-0.42	-0.78	2.96	-2.44	-3.71	28.78
AT/AT	-0.7	-1.46	2.99	-7.22	1.34	31.93	-0.55	-0.58	2.82	-4.33	2.01	26.85	0.35	-0.81	2.94	-1.68	-2.3	29.94
TA/TA	-0.92	0.72	3.01	4.4	-2.32	37.2	-0.49	-0.23	3.69	0.78	-6.92	40.27	0.37	0.09	3.07	4.59	-1.44	40.81
AC/GT	-1.25	-1.42	2.77	2.77	6.88	37.05	-0.99	-0.83	2.99	2.32	2.79	36.78	0.46	-0.64	3.04	-3.25	-0.02	37.01
	cdA(Ap0)						cdA(Ap-1)						cdA(Ap+1)					
1TA/TA	0.7	0.25	2.91	-6.24	-4.83	46.81	0.48	0	3.23	-6.44	-0.63	41.26	0.69	-0.85	3.31	-0.71	-0.55	47.11
AT/AT	-0.65	-0.53	3.1	-6.2	-0.59	27.53	-0.17	1.41	2.85	-0.37	-7.33	29.4	0.06	0.23	3.13	-6.38	-4	27.9
TA/TA	-1.25	0.25	3.22	9.5	-7.7	38.75	-1.15	-0.22	3.3	11.12	1.72	41.88	-1.09	-1.13	3.23	7.22	2.97	37.71
AC/GT	-1.19	0.05	3.08	7.41	0.37	35.96	-1.07	-0.84	3.24	-1.83	3.61	32	-0.51	0.69	3.03	0.11	-5.82	35.92
CA/TG	-0.33	0.38	3.09	3.15	-1.68	29.79	0.74	0.61	3.05	-4.31	-6.15	34.79	-0.67	0.55	7.28	3.67	1.32	79.43
AA/TT	-0.76	0.7	6.5	2.22	2.82	74.45	1.03	0.18	3.75	-7.21	7.74	48.27						
AA/TT							-3.2	1.43	5.11	10.01	-12.04	63.47	-2.18	2.41	2.75	4.48	-7.79	26.22
AG/CT	-1.61	-0.9	3.47	3.59	-0.21	31.95							-1.89	-0.73	3.43	-1.12	4.58	31.08
GA/TC	-1.44	1.57	3.38	2.55	2.28	37.61	-0.63	0.47	3.34	-8.67	6.37	32.37	-1.29	0.95	3.21	-0.07	2.06	35.01
AT/AT	-0.65	-2.51	3	-6.99	9.19	29.65	-1.13	-0.53	3.07	-2.96	-2.22	30.01	-0.32	-0.2	2.77	-5.86	0.8	27.82
TA/TA	-0.11	2.14	2.94	0.95	-8.12	37.2	-0.31	-0.51	3.34	1.58	-1.82	41.06	-0.01	-0.31	3.19	1.64	-2.29	39.31
AC13/GT	-1.07	-2.39	2.9	1.06	3.87	32.53	-0.46	-0.68	3.02	-2.01	-2.37	37.24	-0.37	-1.36	2.94	-3.94	0.6	37.41

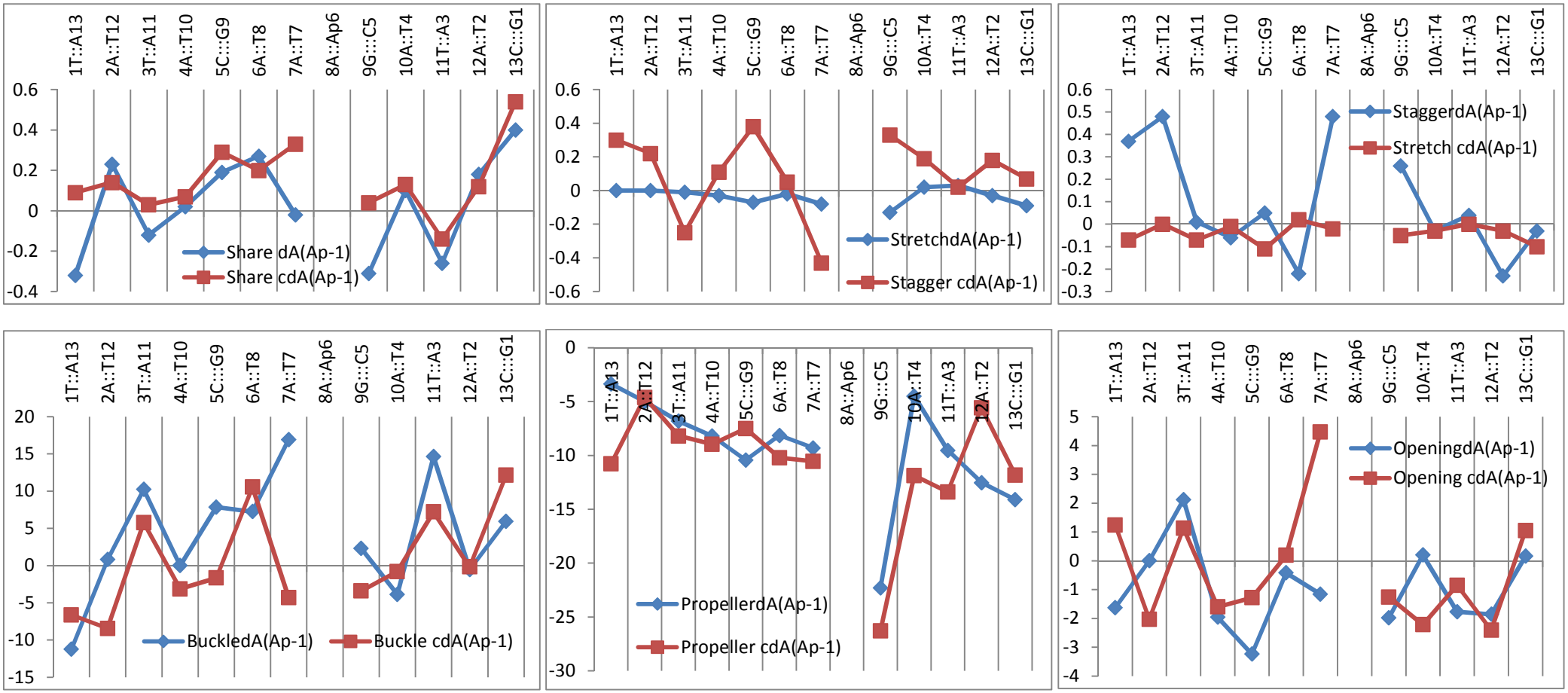
Graph 3S. Graphical representation of data presented in **Table 3S**

Oligodeoxynucleotide dA(Ap0) versus cdA(Ap0)



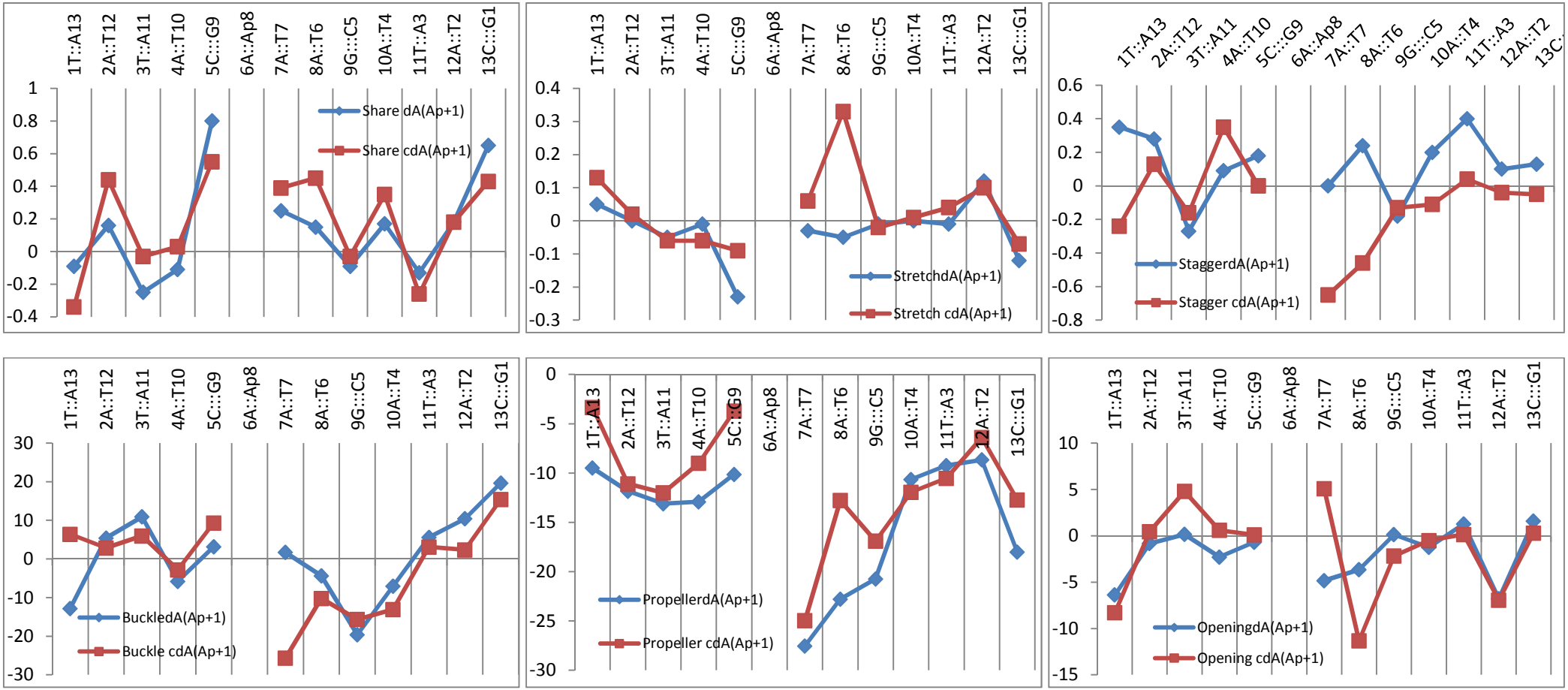
Graph 3S. Graphical representation of data presented in **Table 3S**

Oligodeoxynucleotide dA(Ap-1) versus cdA(Ap-1)



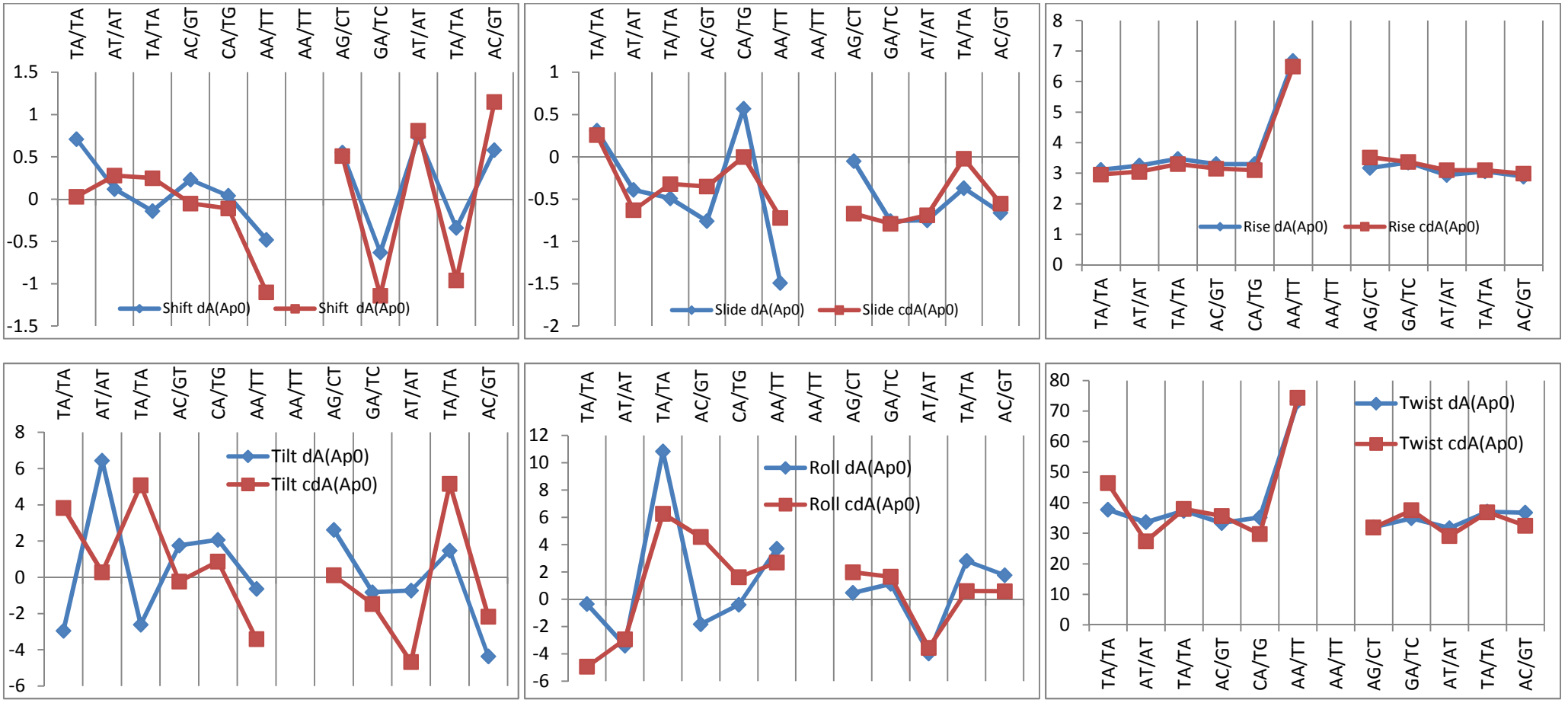
Graph 3S. Graphical representation of data presented in **Table 3S**

Oligodeoxynucleotide dA(Ap+1) versus cdA(Ap+1)



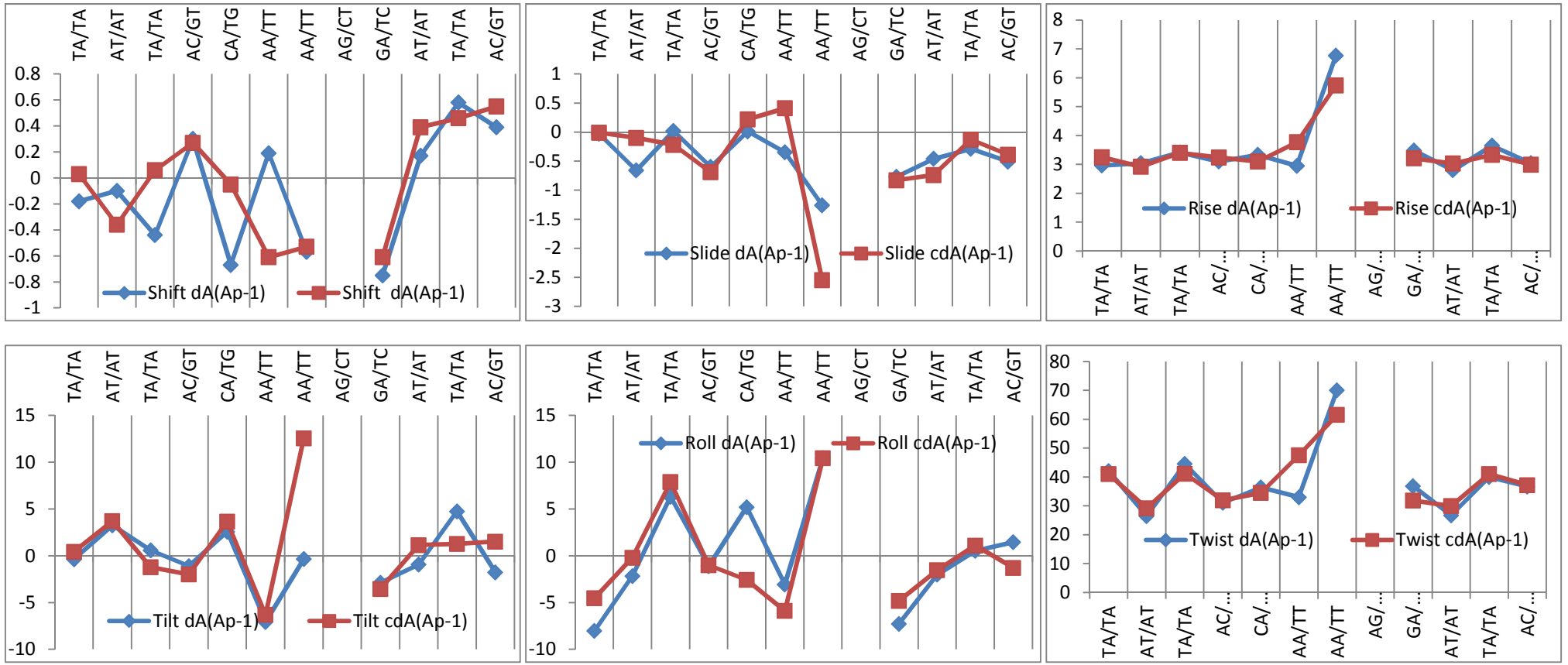
Graph 3S. Graphical representation of data presented in **Table 3S**

Oligodeoxynucleotide dA(Ap0) versus cdA(Ap0)



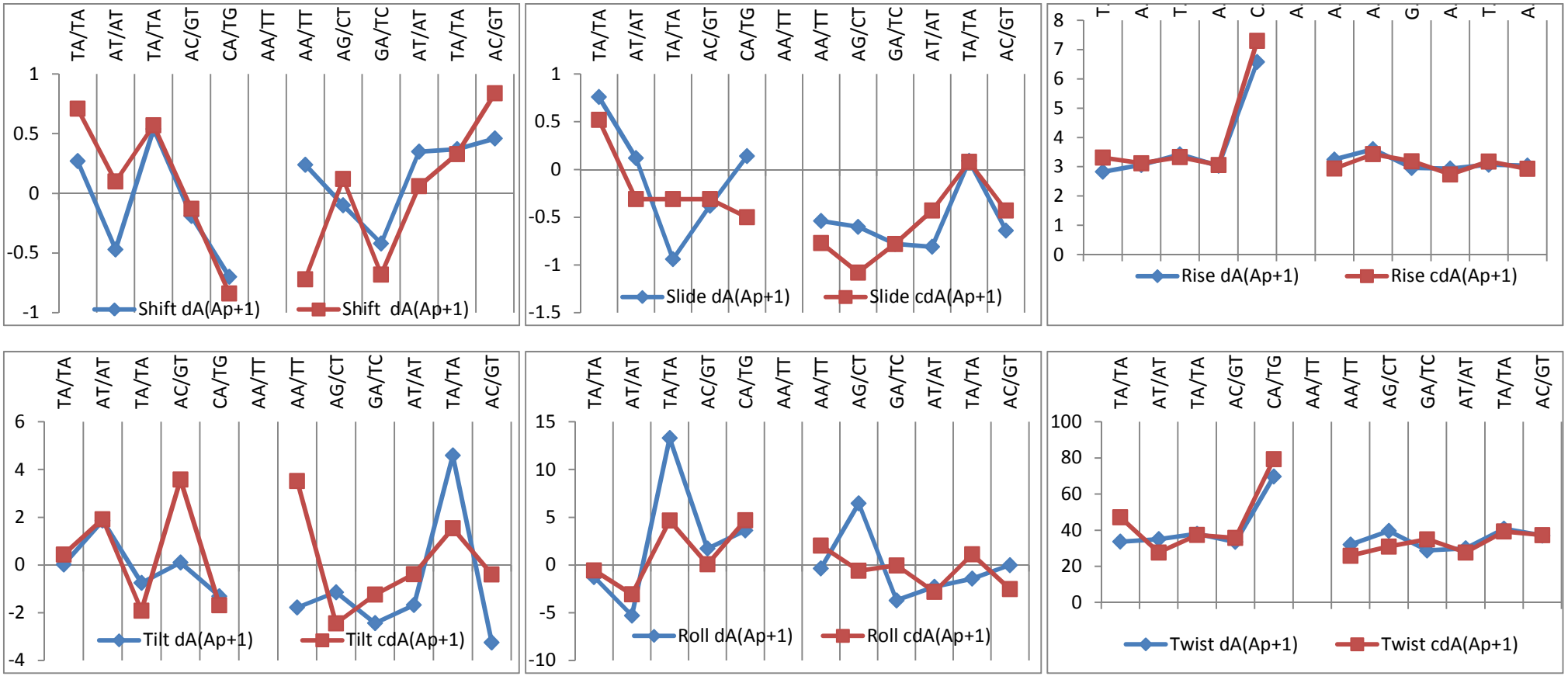
Graph 3S. Graphical representation of data presented in **Table 3S**

Oligodeoxynucleotide dA(Ap-1) versus cdA(Ap-1)



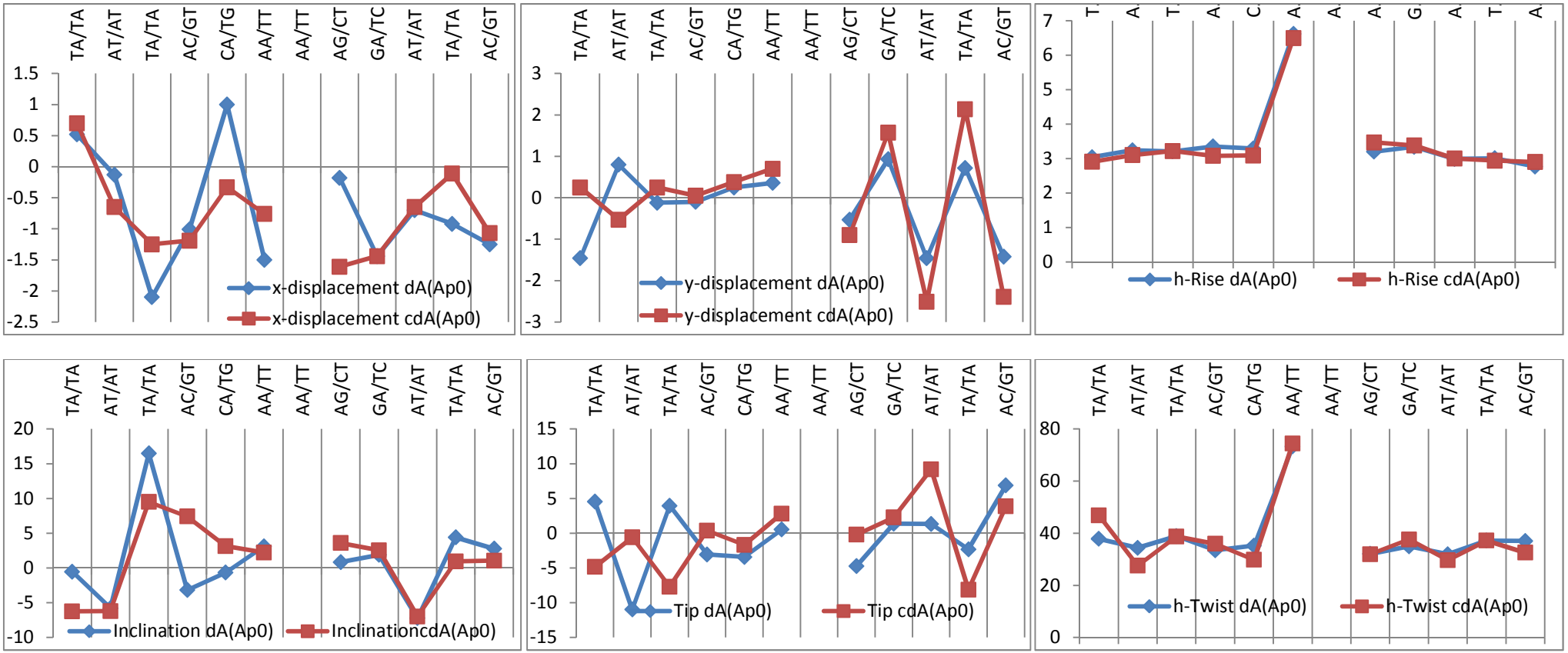
Graph 3S. Graphical representation of data presented in **Table 3S**

Oligodeoxynucleotide dA(Ap-1) versus cdA(Ap-1)



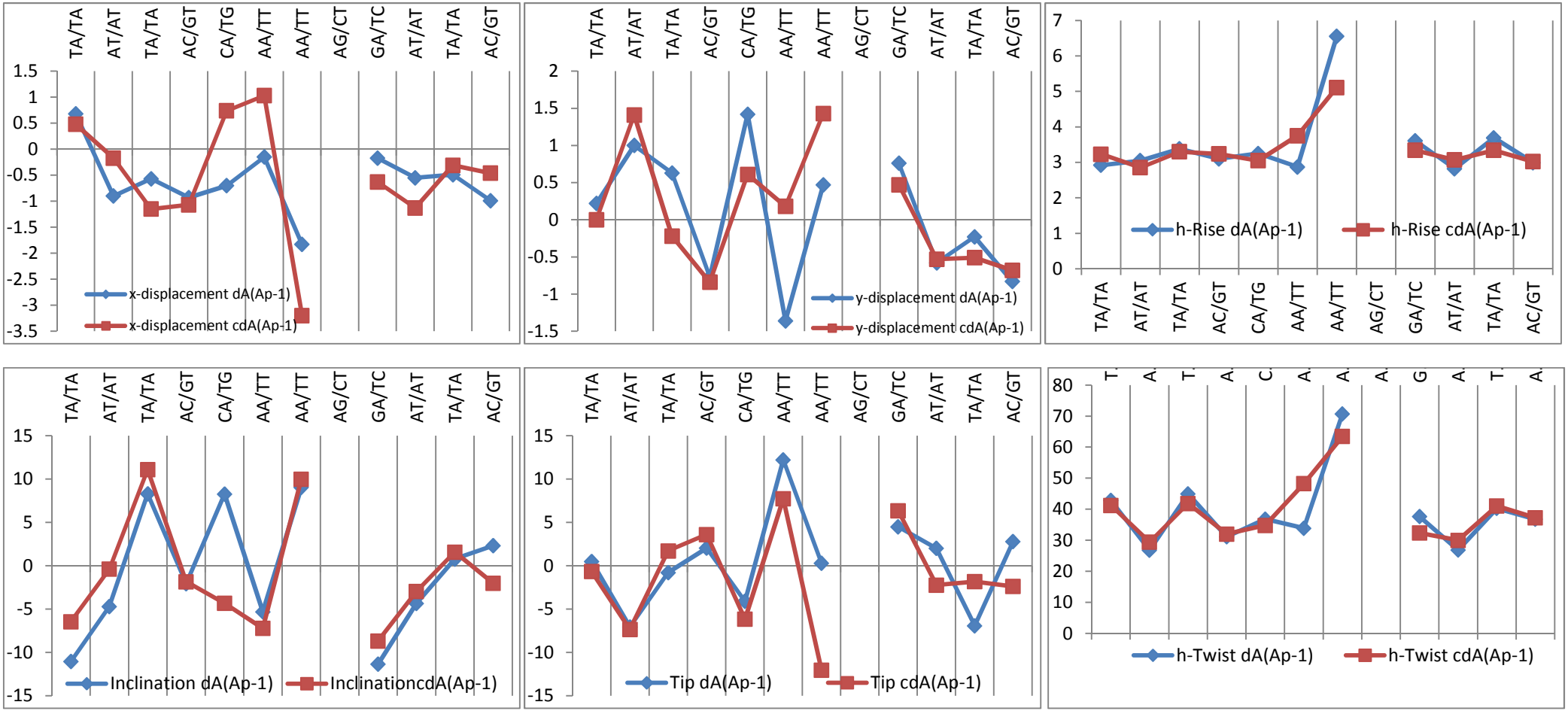
Graph 3S. Graphical representation of data presented in **Table 3S**

Oligodeoxynucleotide dA(Ap0) versus cdA(Ap0)



Graph 3S. Graphical representation of data presented in **Table 3S**

Oligodeoxynucleotide dA(Ap-1) versus cdA(Ap-1)



Graph 3S. Graphical representation of data presented in **Table 3S**

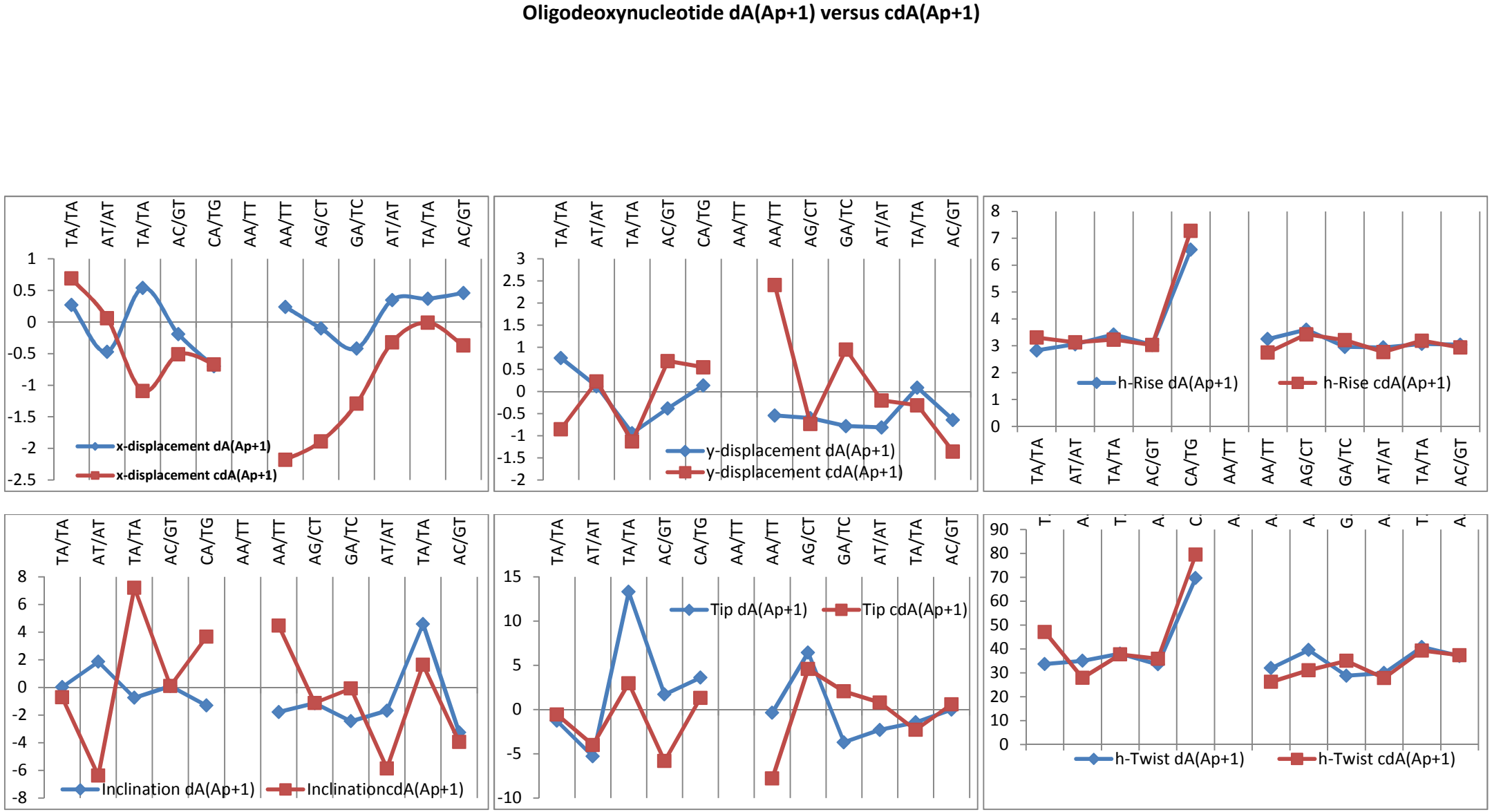


Table 4S. Base pair parameters, complementary base-pair parameters and local helical parameters of double stranded oligodeoxynucleotides that contained at position 7A 2'-deoxyadenosine (dA) or (5'S)-5',8-cyclo-2'-deoxyadenosine (cdA) in one strand and at different positions **T6** (Ga-1) or **T7** (Ga0) or **T8** (Ga+1) a single strand break e.i. gap (Ga) in the opposite strand. The structures of *ds*-oligodeoxynucleotides obtained under Molecular Mechanics (Amber 94 force field) calculation in solvation box, the sodium ions have been used as counterions to neutralize the negative charge of *ds*-DNA.

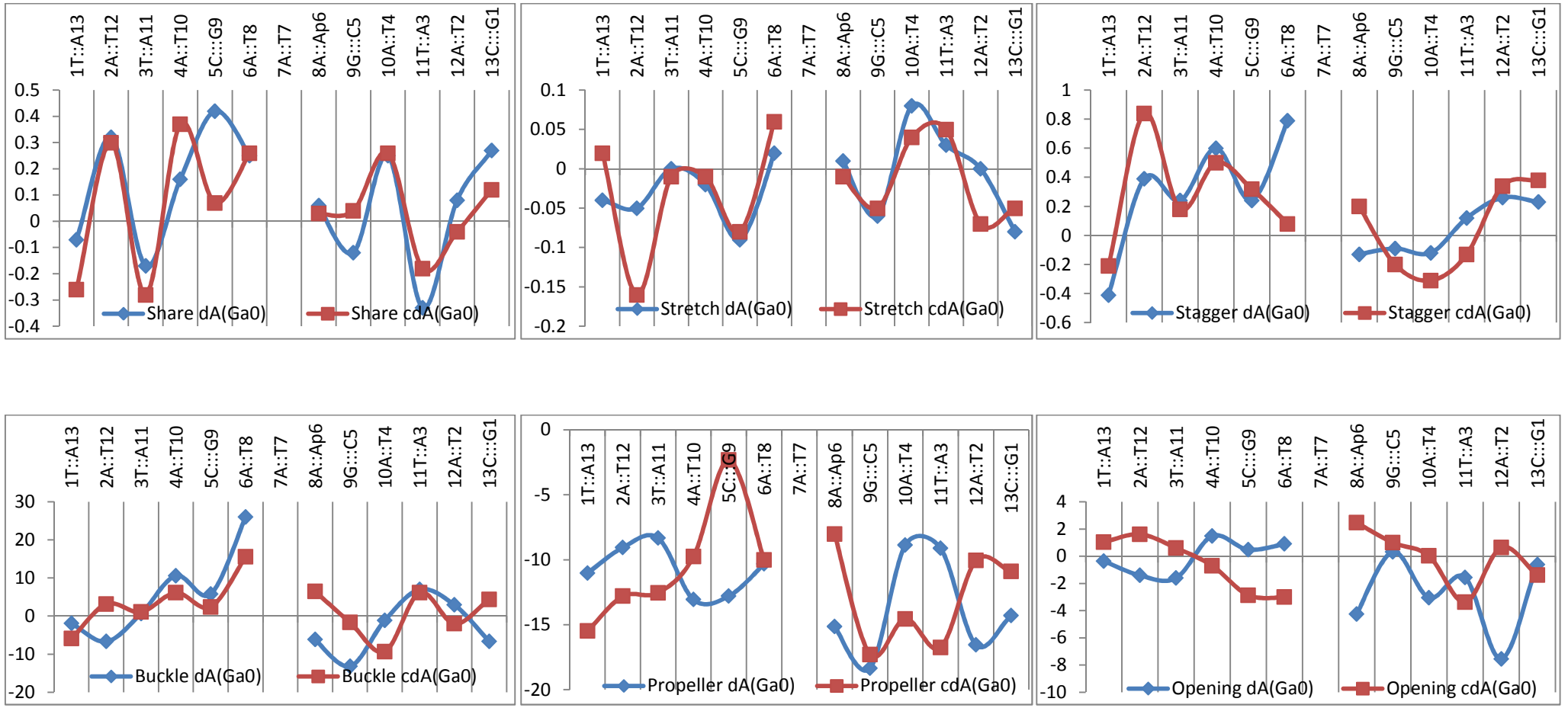
BASE PAIR		Oligodeoxynucleotides																	
		dA(Ga0)						dA(**Ga**-1)						dA(**Ga**+1)					
		Share	**Stretch**	**Stagger**	**Buckle**	**Propeller**	**Opening**	**Share**	**Stretch**	**Stagger**	**Buckle**	**Propeller**	**Opening**	**Share**	**Stretch**	**Stagger**	**Buckle**	**Propeller**	**Opening**
5'	3'																		
^{1}T	A_{13}	-0.07	-0.04	-0.41	-1.96	-11.02	-0.36	-0.23	-0.03	-0.19	1.69	-11.58	3.56	-0.36	-0.05	0.88	-20.38	-7.66	0.21
^{2}A	T_{12}	0.32	-0.05	0.39	-6.7	-9.06	-1.41	0.14	-0.02	-0.28	-14.82	-11.99	6.5	0.31	0.13	-0.12	-9.16	-12.53	-4.81
^{3}T	A_{11}	-0.17	0	0.24	0.64	-8.33	-1.61	-0.29	0.03	0.01	-1	-13.72	2.01	-0.3	0.05	0.06	-0.06	-14.24	-3.71
^{4}A	T_{10}	0.16	-0.02	0.6	10.59	-13.06	1.48	-0.05	-0.03	0.23	-2.48	0.4	-1.99	0.11	-0.05	0.58	3.79	1.15	-0.59
^{5}C	G_{9}	0.42	-0.09	0.24	5.78	-12.8	0.48	-0.27	-0.06	0.38	17.5	-15.66	-2.34	0.38	-0.12	0.31	8.08	0.35	0.19
^{6}A	**T_{8}**	0.25	0.02	0.79	26	-10.32	0.9	0.35	-0.01	-0.64	-2.88	-6.13	-1.21						
^{7}A	**T_{7}**							-0.03	-0.01	0.24	11.26	-3.08	-3.53	0.05	-0.17	0.77	-5.49	-5.84	-4.16
^{8}A	**T_{6}**	0.06	0.01	-0.13	-6.17	-15.14	-4.26							0.33	0	0.44	-4.38	-8.82	-1.39
^{9}G	C_{5}	-0.12	-0.06	-0.09	-13.17	-18.35	0.32	-0.67	-0.17	-0.66	-17.62	-17.95	5.08	-0.33	-0.17	0.25	-6.56	-28.01	-1.12
^{10}A	T_{4}	0.25	0.08	-0.12	-1.16	-8.87	-3.05	0.19	0.03	-0.11	-9.77	-10.61	-1.17	0.26	0.03	0.07	-13.19	-19.46	-6.45
^{11}T	A_{3}	-0.33	0.03	0.12	6.97	-9.11	-1.56	-0.19	-0.02	0.45	-3.1	-11.11	7.35	-0.25	-0.03	0.77	-14.52	-6.32	0.92
^{12}A	T_{2}	0.08	0	0.26	2.92	-16.54	-7.55	0.26	0.01	0.02	0.98	-9.76	0.26	0.42	0	0.36	3.53	-7.02	-4.17
^{13}C	G_{1}	0.27	-0.08	0.23	-6.65	-14.3	-0.61	0.06	-0.04	0.02	5.3	-4.04	-1.45	0.54	-0.14	0.18	12.15	-5.98	-0.62
3'	5'																		
		cdA(Ga0)						cdA(**Ga**-1)						cdA(**Ga**+1)					
5'	3'																		
^{1}T	A_{13}	-0.26	0.02	-0.21	-5.92	-15.47	1.04	-0.04	-0.02	0.21	-8.31	-3.03	1.63	-0.21	0.01	0.35	-7.66	-2.36	0.53
^{2}A	T_{12}	0.3	-0.16	0.84	3.14	-12.8	1.61	0.21	-0.01	0.38	-3.84	-6.32	3.84	-0.07	-0.06	0.09	-4.19	-8.81	1.01
^{3}T	A_{11}	-0.28	-0.01	0.18	1.07	-12.55	0.61	0.12	-0.1	0.56	-3.34	-14.14	1.31	-0.08	-0.03	-0.23	5.55	-12.74	-1.33
^{4}A	T_{10}	0.37	-0.01	0.5	6.14	-9.76	-0.7	0.17	-0.01	0.32	2.3	-12.55	-1.63	0.58	0.01	0.08	-7.59	-7.69	-3.43
^{5}C	G_{9}	0.07	-0.08	0.32	2.39	-2.32	-2.87	-0.05	-0.06	0.31	8.59	-13.46	-1.75	0.1	-0.01	0	9.26	-3.88	-2.62
^{6}A	**T_{8}**	0.26	0.06	0.08	15.58	-10.02	-3.01	0.12	-0.01	-0.07	8.87	-12.64	-1.18						
^{7}A	**T_{7}**							0.3	0.01	-0.38	9.88	15.02	8.07	0.22	0.13	0.17	-22.38	-27.59	10.38
^{8}A	**T_{6}**	0.03	-0.01	0.2	6.45	-8.03	2.46							0.27	-0.07	0.48	-5.74	-14.68	-5.38
^{9}G	C_{5}	0.04	-0.05	-0.2	-1.68	-17.29	1	-0.4	-0.14	0.14	-6.67	-18.33	-1.58	-0.44	-0.17	0.15	-10.61	-22.68	-0.77
^{10}A	T_{4}	0.26	0.04	-0.31	-9.34	-14.55	0.02	0.11	0.05	0.1	0.12	-12.02	-4.62	0.26	0.04	0.12	-7.11	-8.8	-1.8
^{11}T	A_{3}	-0.18	0.05	-0.13	6.15	-16.75	-3.38	-0.03	-0.08	0.35	4.16	-11	-2.41	-0.36	0.05	0.23	1.95	-4.93	-1.59
^{12}A	T_{2}	-0.04	-0.07	0.34	-2.01	-10.06	0.64	0.07	-0.05	0.58	10.78	-8.68	-0.22	0.12	0.01	0.08	16.73	-17.61	-1.82
^{13}C	G_{1}	0.12	-0.05	0.38	4.38	-10.9	-1.39	0.02	0	-0.21	19.15	-10.34	-1.94	-0.12	-0.04	-0.21	5.07	-18.73	0.39
3'	5'																		

BASE PAIR STEP	Oligodeoxynucleotides																	
	dA(Ga0)						dA(Ga-1)						dA(Ga+1)					
	Shift	**Slide**	**Rise**	**Tilt**	**Roll**	**Twist**	**Shift**	**Slide**	**Rise**	**Tilt**	**Roll**	**Twist**	**Shift**	**Slide**	**Rise**	**Tilt**	**Roll**	**Twist**
TA/TA	0.51	-0.12	3.47	-4.49	-1.46	38.05	0.32	0.6	3.51	1.96	8.16	47.44	-1.2	-0.07	2.84	4.62	1.3	35.71
AT/AT	-0.72	-0.72	3.03	0.91	-1.41	30.19	-0.34	-0.51	2.77	-2.05	0.23	27.38	-0.03	-0.4	2.92	-0.75	-2.75	28.71
TA/TA	1.25	0.49	2.86	1.59	-1.19	40.68	-0.43	-0.12	3.15	-3.66	5.55	41.94	-0.14	0.05	3.17	-5.27	0.81	39.29
AC/GT	0.47	-0.74	3.42	1.39	-4.13	37.34	0.58	-0.48	2.93	-0.38	-4.17	28.67	0.32	-0.72	3.4	0.94	-5.69	34.44
CA/TG	-0.3	0.37	2.86	-2.08	0.64	31.95	-0.79	-0.63	3.96	4.16	-2.87	38.25						
AA/TT							0.29	-0.93	2.85	-7.88	-6.36	30.68	-0.43	-1.18	6.16	7.28	-0.26	68.57
AA/TT	-0.78	-0.68	7.07	11.34	0.51	71.45							-0.34	-0.34	3.37	2.89	3.99	36.26
AG/CT	0.34	-0.84	3.48	-0.99	3.02	26.01	0.29	-0.49	6.77	18.5	9.08	67.26	0.04	-0.4	3.41	-0.66	3.09	29.3
GA/TC	-0.59	0.26	2.99	1.55	0.69	38.93	-1.01	0.27	2.88	-7.5	1.8	41.36	-0.62	-0.49	3.33	-0.95	-2.06	36.92
AT/AT	0.13	-0.65	3.01	-1.83	-3.96	31.19	0.5	-0.82	3.02	-2.85	-1.88	26.89	0.74	-0.92	3.26	-2.37	-3.31	29.6
TA/TA	0.49	-0.54	3.23	1.31	6.87	36.81	-0.26	0.58	3.04	4.59	3.25	45.53	0.19	0.24	2.75	4.5	-3.48	43.48
AC/GT	-0.02	-0.07	3.42	-0.24	-2.63	40.88	0.42	-0.63	3.12	-0.77	1.43	28.22	0.75	-1.03	3.08	-0.46	0.34	29.67
	cdA(Ga0)						cdA(Ga-1)						cdA(Ga+1)					
TA/TA	0.57	0.66	3.05	-8.27	-3.56	39.79	0.33	0.04	3.05	0.02	-1.03	44.32	0.22	-0.46	3.12	1.72	2.4	32.49
AT/AT	-0.66	-0.92	3.25	3.62	-1.83	31.39	-0.7	-1.28	3.26	-1.32	-2.24	26.78	-0.71	-0.51	2.96	2.51	-0.98	31.87
TA/TA	1.08	0.26	3	1.67	-0.86	38.55	-0.2	0.31	2.97	3.07	1.65	39.26	0.51	-0.5	3.57	-0.05	1.82	38.09
AC/GT	-0.14	-1.06	3.45	-1.11	-1.73	37.14	0.84	-0.19	3.09	0.99	-7.46	35.96	0.19	-0.39	2.92	1.23	-1.73	33.39
CA/TG	0.29	-0.51	2.95	2.58	-1.41	27.97	0.25	-0.56	3.22	2.1	2.58	30.29						
AA/TT							-0.27	-0.54	3.48	-6.05	-7.74	44.64	-0.04	-1.44	6.71	1.98	-1.67	76.01
AA/TT	-0.86	-0.17	6.52	6.22	6.37	71.75							-0.57	-0.27	2.89	1.44	3.99	28.43
AG/CT	-0.46	-0.95	3.48	1.64	0.22	29.04	-0.21	-1.45	5.83	19.82	2.18	58.29	0.22	-0.99	3.44	2.34	0.78	31.5
GA/TC	-1.05	0.13	3.22	-2.94	0.89	42.1	-0.48	0.51	3.07	-1.9	4.46	39.92	-0.55	-0.24	3.07	0.15	-0.58	40.4
AT/AT	0.1	-0.49	2.72	-1.8	-1.23	30.24	0.47	-0.97	3.11	-2.01	0.24	25.57	-0.03	-0.86	3.03	-0.17	-2.94	27.46
TA/TA	0.5	-0.94	3.25	-3.06	6.84	30.72	-0.25	-0.23	2.96	-0.96	2.45	44.37	0.43	0.68	2.92	3.62	5.41	37.19
AC/GT	-0.6	0.12	3.14	-2.8	-4.18	45.29	0.4	-0.3	3.1	7.09	-0.73	24.32	-0.38	-0.68	3.37	-1.73	1.34	37.03

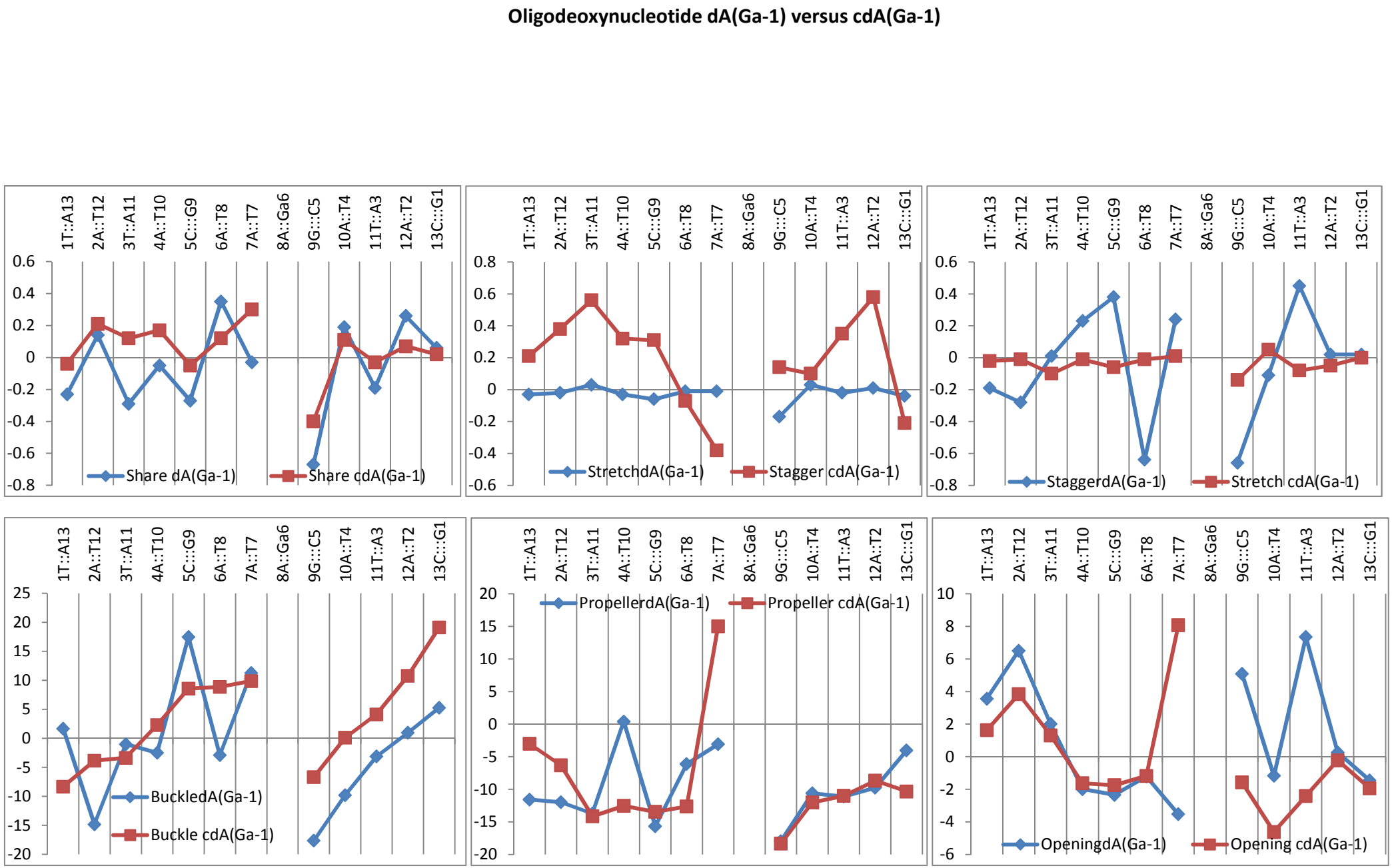
BASE PAIR	Oligodeoxynucleotides																	
	dA(Ga0)						cdA(Ga-1)						cdA(Ga+1)					
	x-displacement	y-displacement	h-Rise	Inclination	Tip	h-Twist	x-displacement	y-displacement	h-Rise	Inclination	Tip	h-Twist	x-displacement	y-displacement	h-Rise	Inclination	Tip	h-Twist
TA/TA	0.01	-1.36	3.4	-2.23	6.85	38.33	0.04	-0.22	3.57	10.05	-2.41	48.13	-0.27	2.49	2.67	2.11	-7.5	36.02
AT/AT	-1.11	1.56	3.04	-2.7	-1.75	30.24	-1.12	0.28	2.78	0.48	4.32	27.46	-0.26	-0.09	2.94	-5.53	1.5	28.85
TA/TA	0.81	-1.64	2.89	-1.71	-2.29	40.73	-0.71	0.24	3.13	7.69	5.07	42.44	-0.02	-0.4	3.16	1.21	7.79	39.64
AC/GT	-0.58	-0.53	3.5	-6.42	-2.16	37.58	-0.13	-1.23	2.96	-8.37	0.76	28.96	-0.29	-0.39	3.47	-9.53	-1.57	34.91
CA/TG	0.58	0.22	2.89	1.16	3.78	32.02	-0.52	1.81	3.89	-4.36	-6.31	38.57						
AA/TT	-0.62	1.47	6.89	0.43	-9.65	72.22	-0.67	-1.77	2.83	-11.64	14.4	32.27	-1.02	0.88	6.09	-0.23	-6.44	68.91
AA/TT							-1.1	1.12	6.55	8.01	-16.32	69.99	-1.1	0.95	3.28	6.38	-4.61	36.58
AG/CT	-2.72	-1.03	3.34	6.68	2.2	26.2							-1.46	-0.23	3.35	6.08	1.29	29.47
GA/TC	0.32	1.05	2.97	1.04	-2.33	38.96	0.2	0.7	3.02	2.52	10.51	42.04	-0.49	0.85	3.36	-3.24	1.49	36.98
AT/AT	-0.51	-0.55	3.06	-7.32	3.38	31.49	-1.3	-1.72	3	-4.01	6.09	27.1	-1.1	-1.93	3.27	-6.45	4.62	29.88
TA/TA	-1.73	-0.59	3.1	10.77	-2.05	37.45	0.48	0.7	3.04	4.18	-5.91	45.86	0.6	0.1	2.73	-4.67	-6.04	43.84
AC/GT	0.2	0	3.42	-3.76	0.34	40.96	-1.59	-1.03	3.07	2.93	1.58	28.27	-2.07	-1.55	3.05	0.66	0.9	29.68
	cdA(Ga0)						cdA(Ga-1)						cdA(Ga+1)					
1TA/TA	1.31	-1.65	2.81	-5.16	11.96	40.75	0.14	-0.44	3.05	-1.36	-0.02	44.33	-1.22	-0.1	3.09	4.28	-3.07	32.62
AT/AT	-1.34	1.87	3.2	-3.37	-6.65	31.64	-2.16	1.16	3.39	-4.82	2.84	26.91	-0.77	1.7	2.91	-1.79	-4.56	31.98
TA/TA	0.49	-1.45	3.03	-1.3	-2.52	38.59	0.28	0.62	2.96	2.46	-4.56	39.41	-1.02	-0.78	3.54	2.79	0.07	38.13
AC/GT	-1.41	0.06	3.5	-2.72	1.74	37.19	0.68	-1.2	3.09	-11.92	-1.58	36.72	-0.43	-0.16	2.94	-3.01	-2.13	33.46
CA/TG	-0.76	-0.04	2.99	-2.91	-5.32	28.12	-1.57	-0.06	3.18	4.93	-4	30.47						
AA/TT							0.04	-0.22	3.52	-10.04	7.85	45.66	-1.06	0.15	6.73	-1.36	-1.6	76.05
AA/TT	-0.56	1.14	6.41	5.41	-5.29	72.23							-1.33	1.43	2.8	8.06	-2.92	28.74
AG/CT	-1.94	1.3	3.44	0.44	-3.27	29.09	-1.61	1.87	5.46	2.17	-19.73	61.32	-1.97	0.06	3.42	1.44	-4.31	31.6
GA/TC	0.09	1.16	3.28	1.23	4.09	42.21	0.26	0.49	3.12	6.5	2.78	40.2	-0.28	0.81	3.07	-0.83	-0.21	40.41
AT/AT	-0.74	-0.5	2.73	-2.35	3.44	30.32	-2.25	-1.6	3.05	0.54	4.54	25.65	-1.13	0.02	3.1	-6.17	0.36	27.61
TA/TA	-2.94	-1.46	2.91	12.68	5.68	31.6	-0.51	0.25	2.94	3.24	1.27	44.44	0.42	-0.23	3.01	8.4	-5.62	37.73
AC13/GT	0.51	0.53	3.15	-5.41	3.62	45.55	-0.49	1.07	3.09	-1.69	-16.39	25.33	-1.25	0.35	3.36	2.11	2.73	37.09

Graph 4S. Graphical representation of data presented in **Table 4S**

Oligodeoxynucleotide dA(Ga0) versus cdA(Ga0)

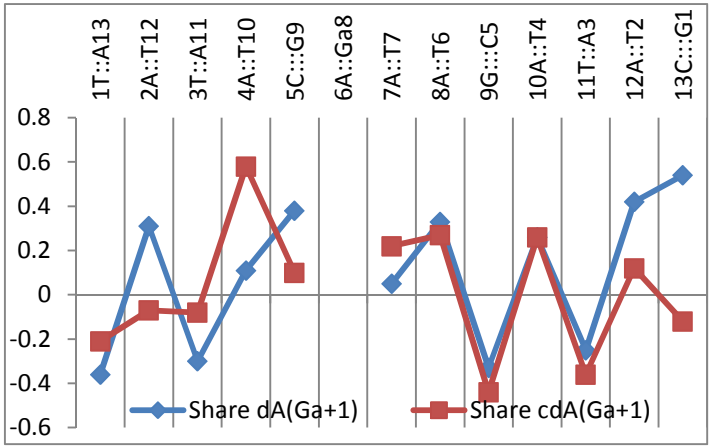


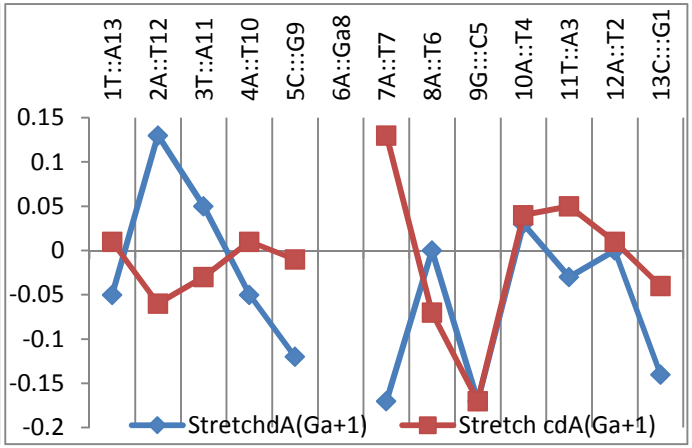
Graph 4S. Graphical representation of data presented in **Table 4S**

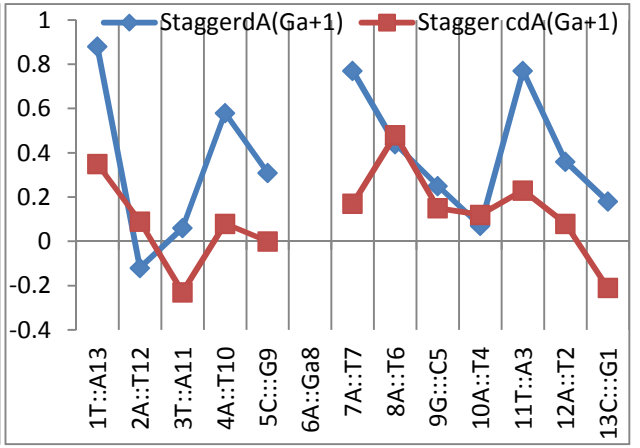


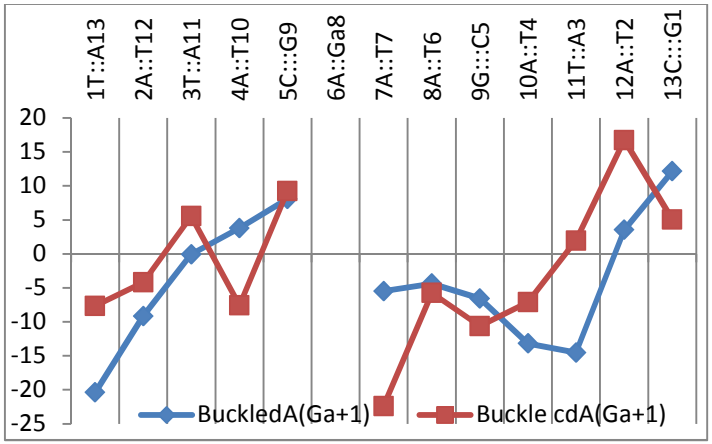
Graph 4S. Graphical representation of data presented in **Table 4S**

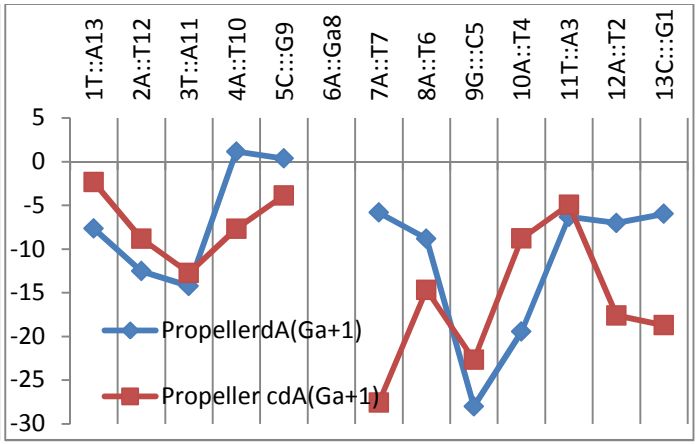
Oligodeoxynucleotide dA(Ga+1) versus cdA(Ga+1)

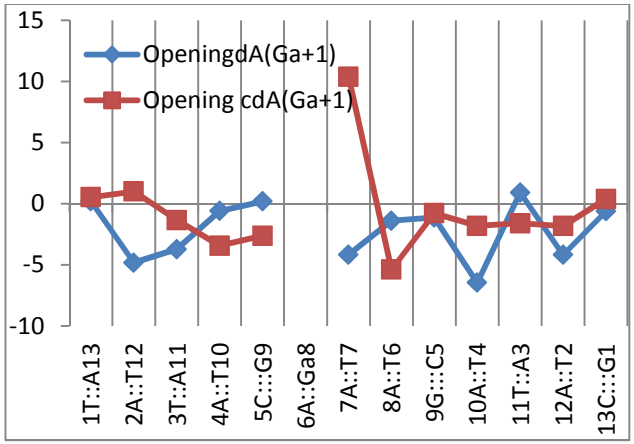






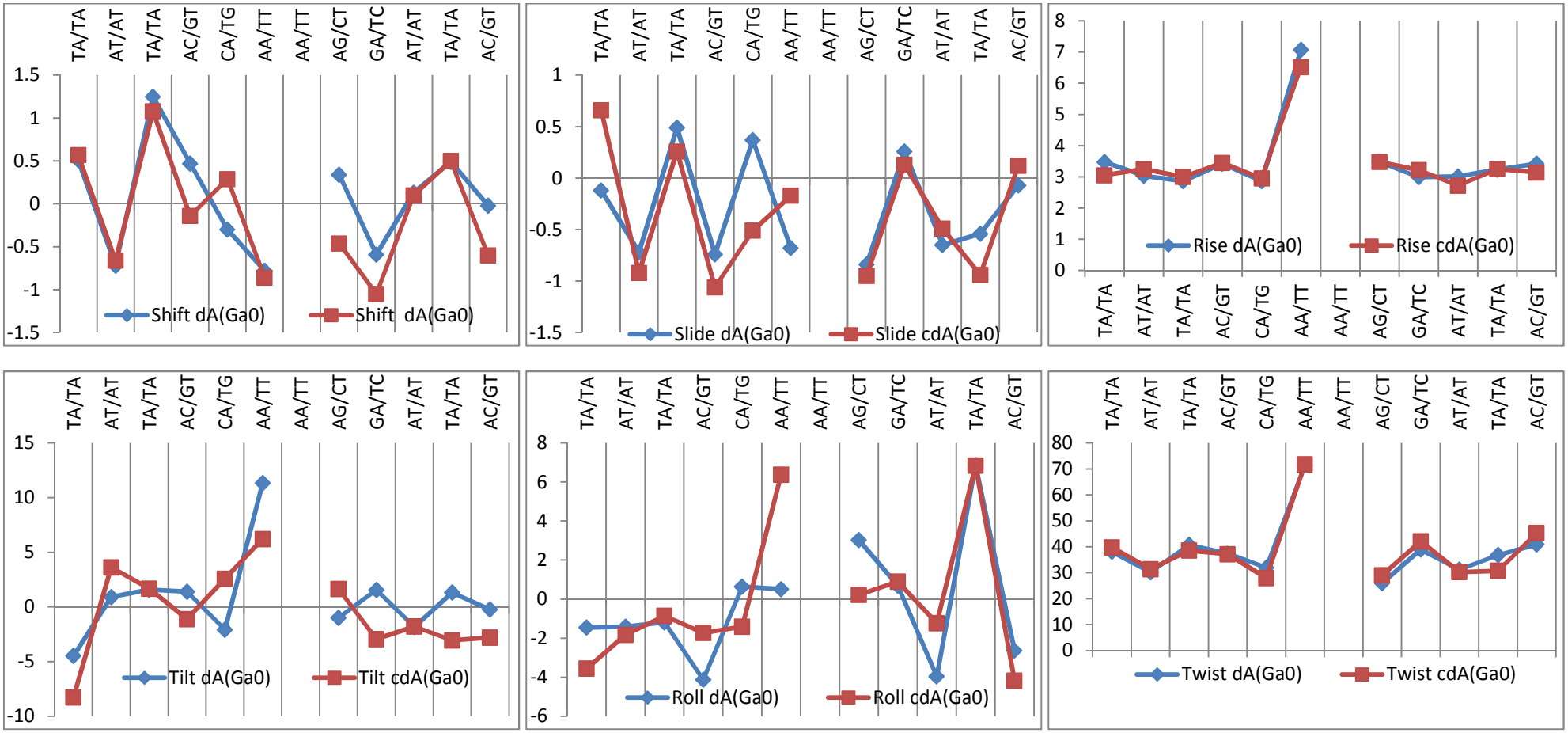






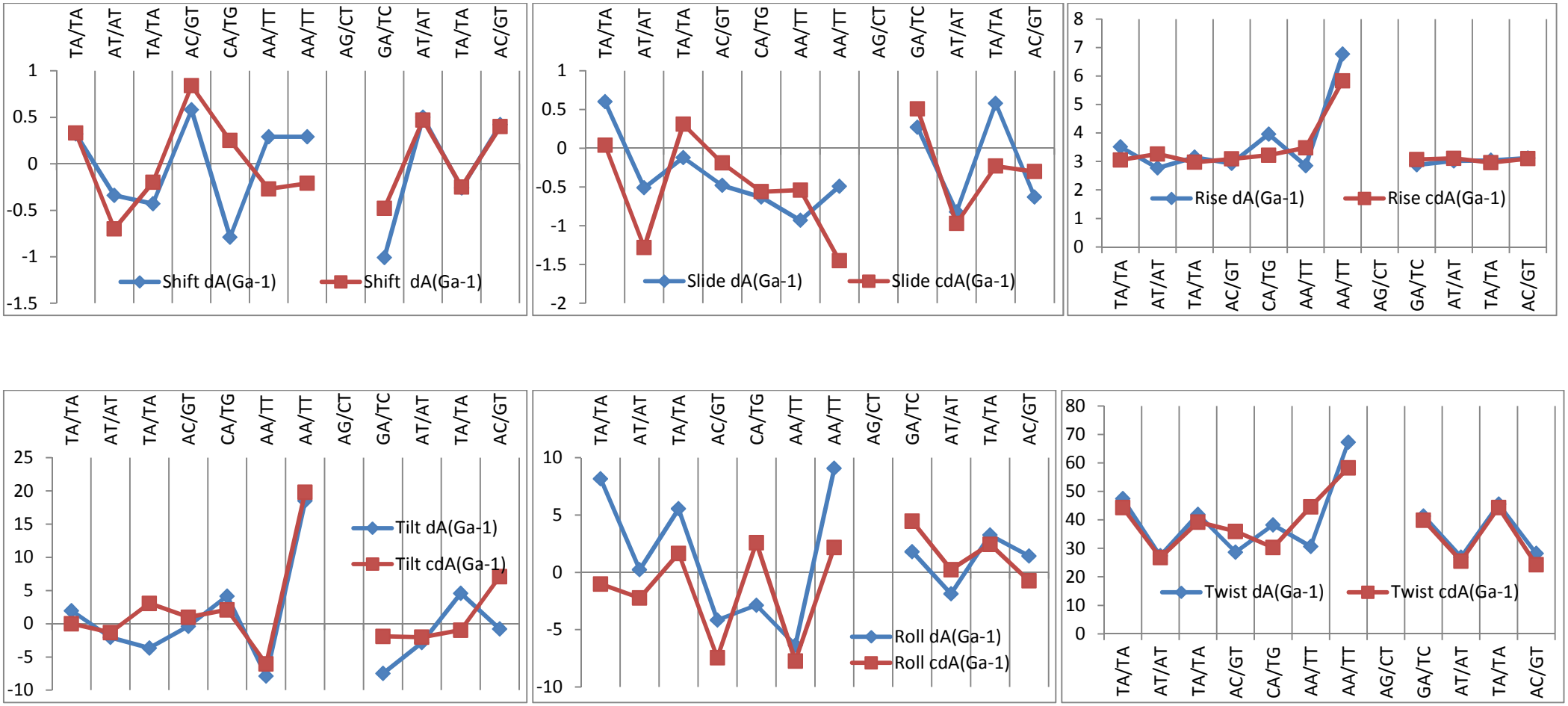
Graph 4S. Graphical representation of data presented in **Table 4S**

Oligodeoxynucleotide dA(Ga0) versus cdA(Ga0)



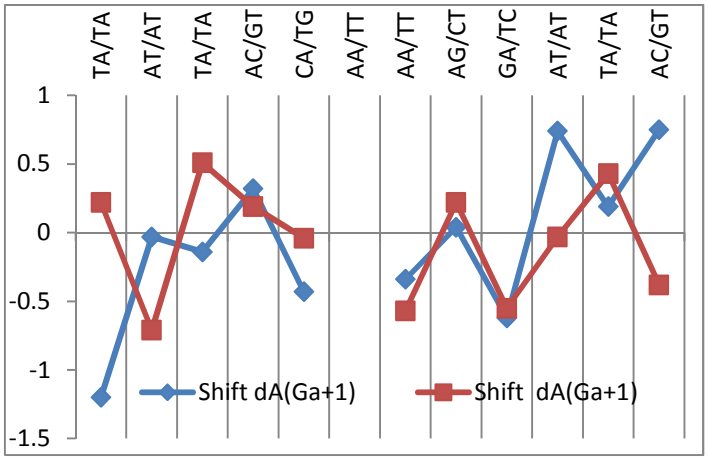
Graph 4S. Graphical representation of data presented in **Table 4S**

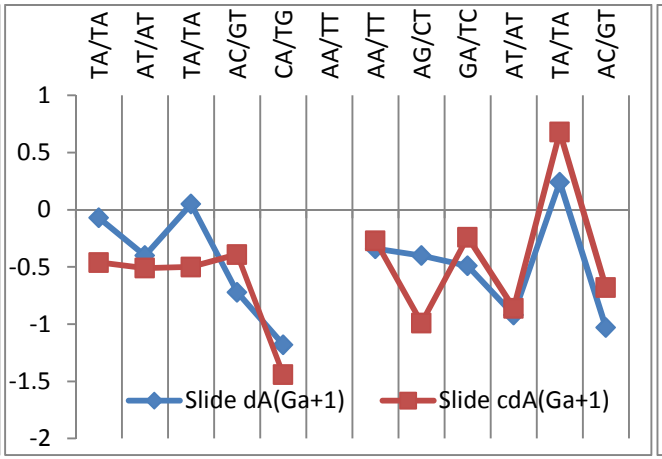
Oligodeoxynucleotide dA(Ga-1) versus cdA(Ga-1)

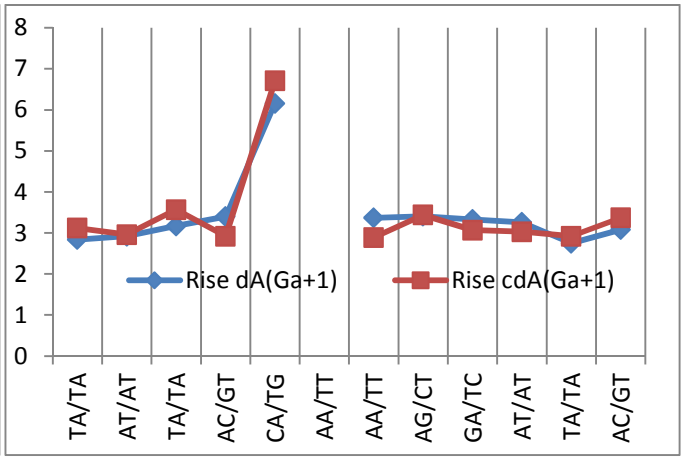


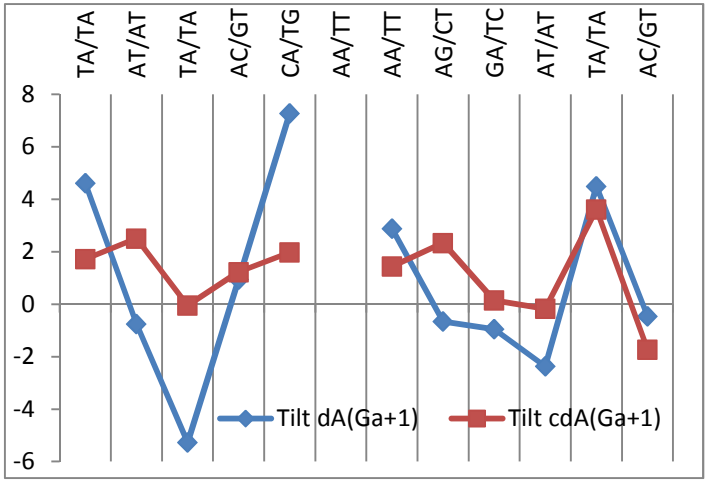
Graph 4S. Graphical representation of data presented in **Table 4S**

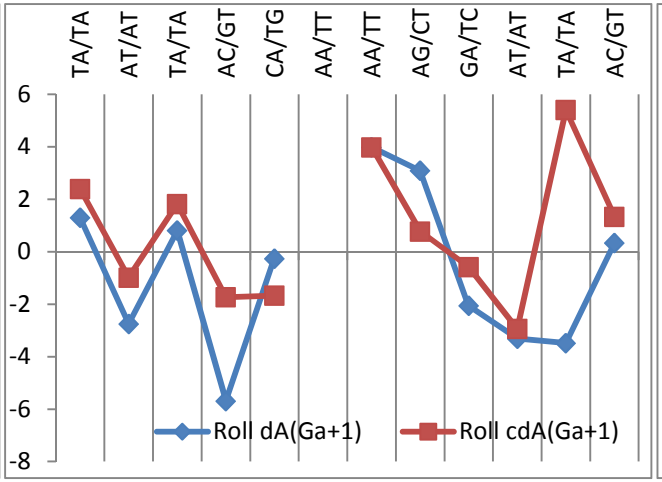
Oligodeoxynucleotide dA(Ga+1) versus cdA(Ga+1)

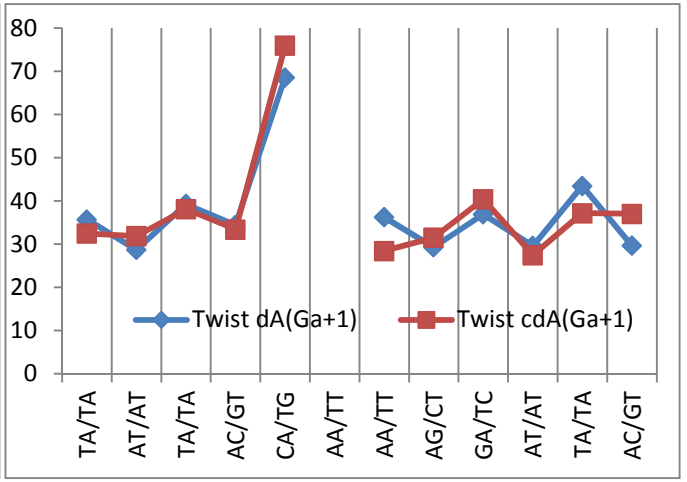






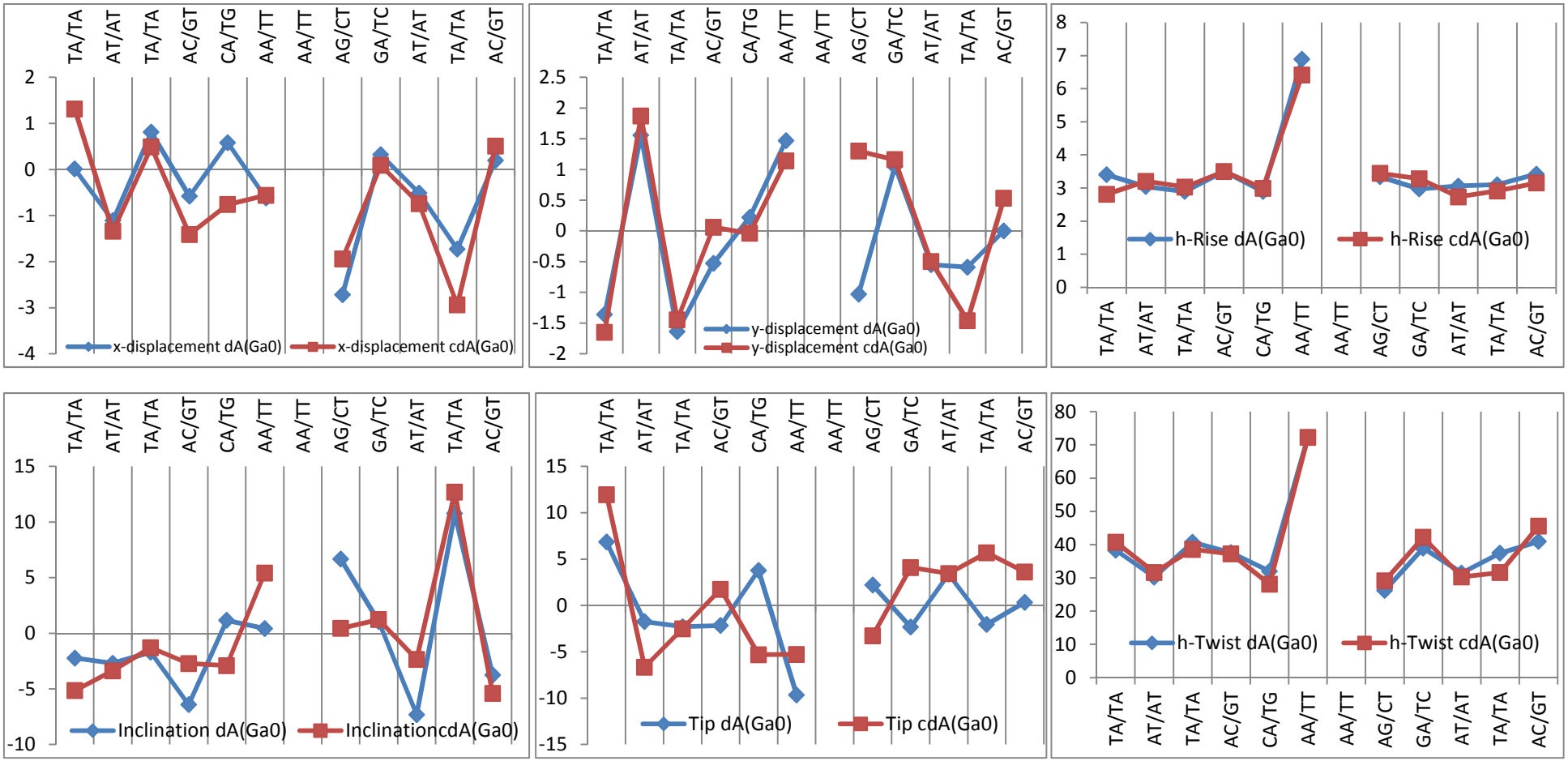






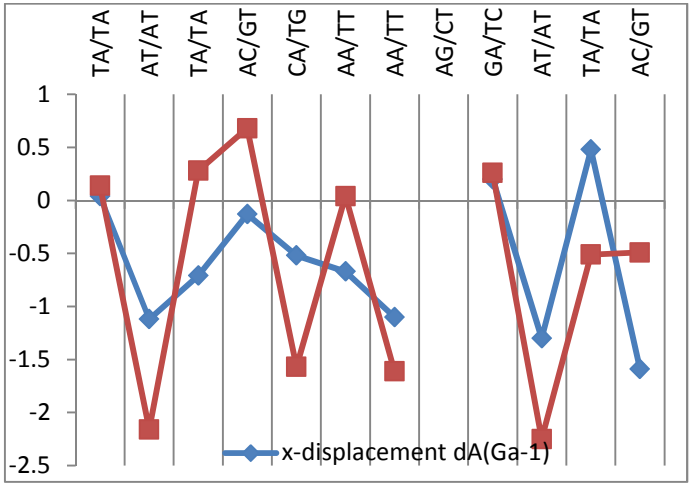
Graph 4S. Graphical representation of data presented in **Table 4S**

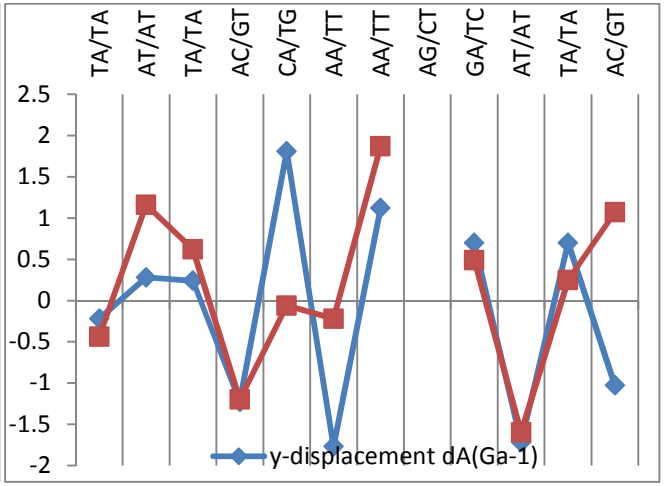
Oligodeoxynucleotide dA(Ga0) versus cdA(Ga0)

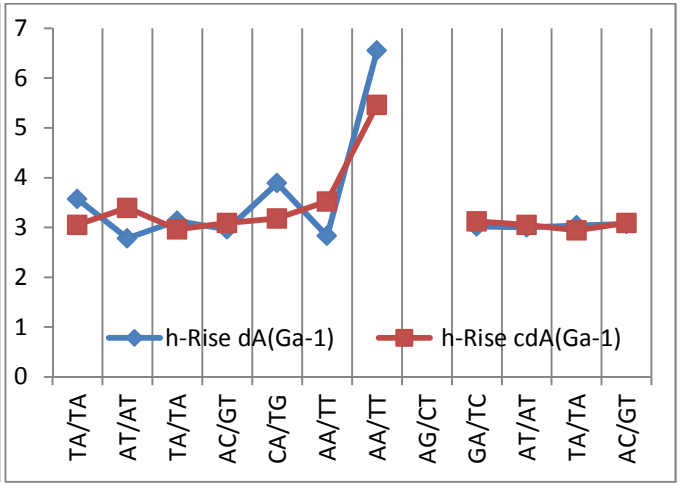


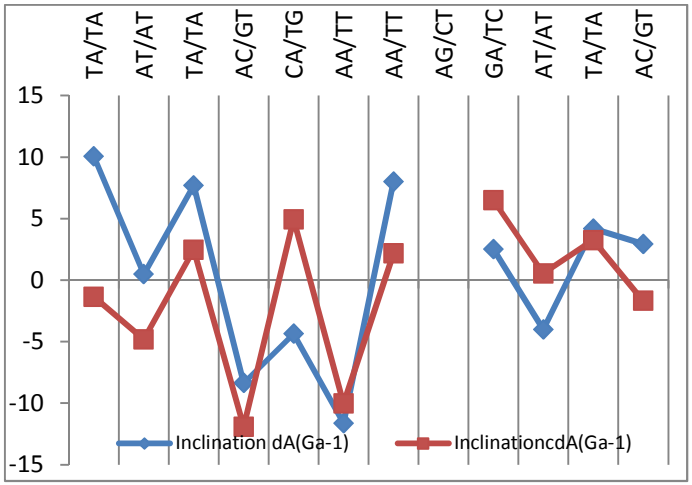
Graph 4S. Graphical representation of data presented in **Table 4S**

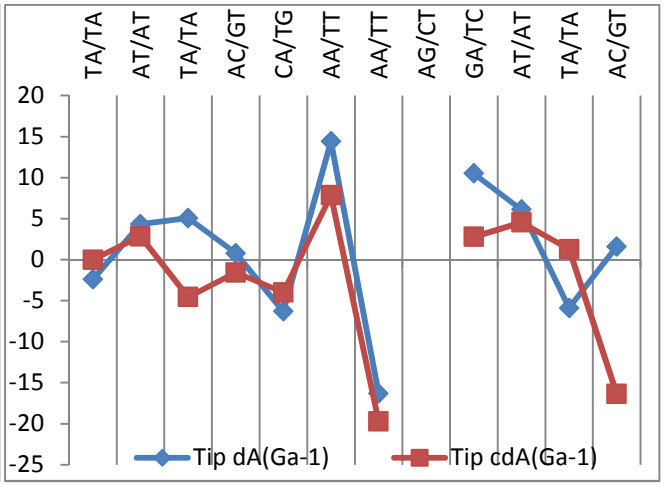
Oligodeoxynucleotide dA(Ga-1) versus cdA(Ga-1)

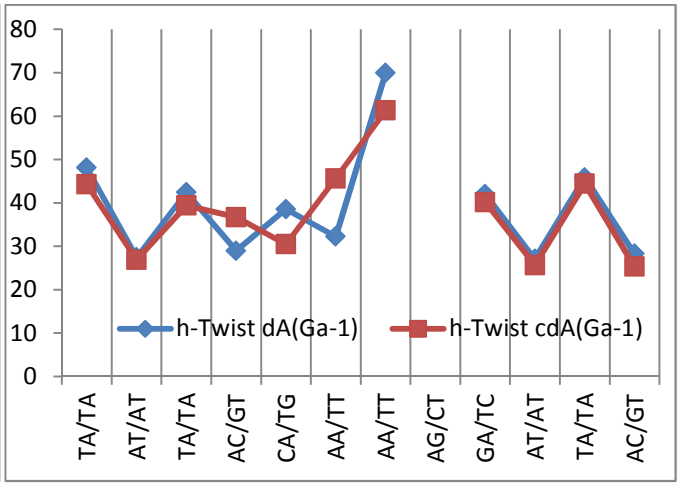






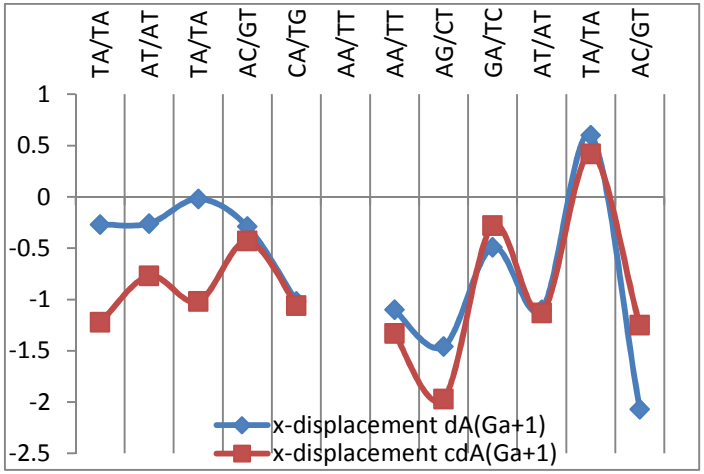


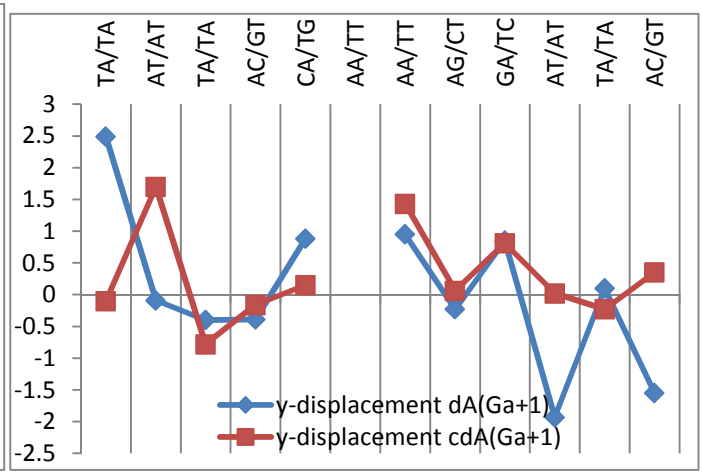


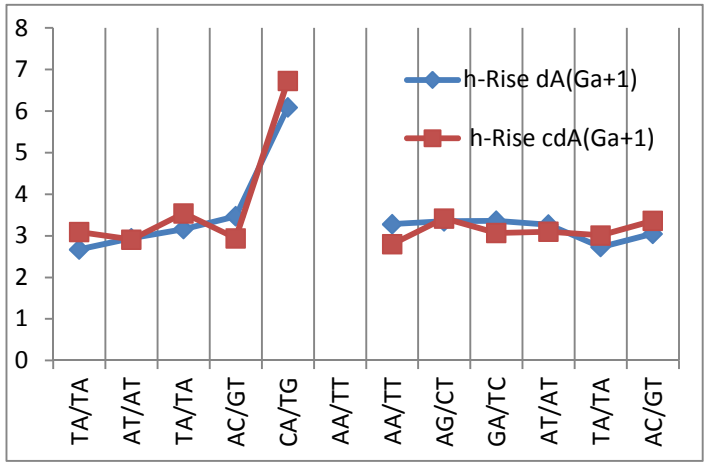


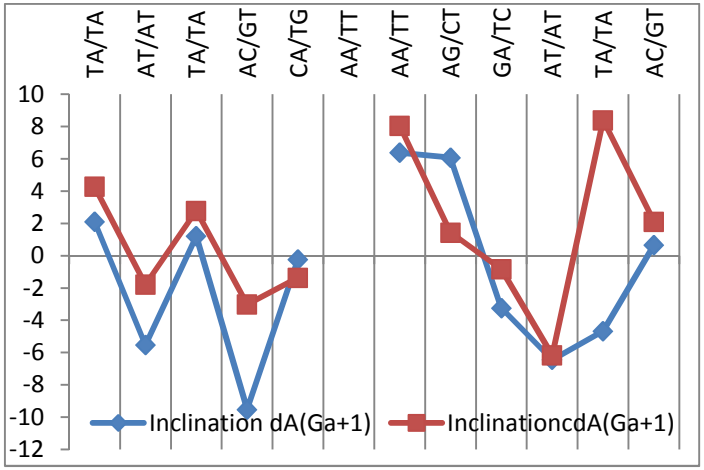
Graph 4S. Graphical representation of data presented in **Table 4S**

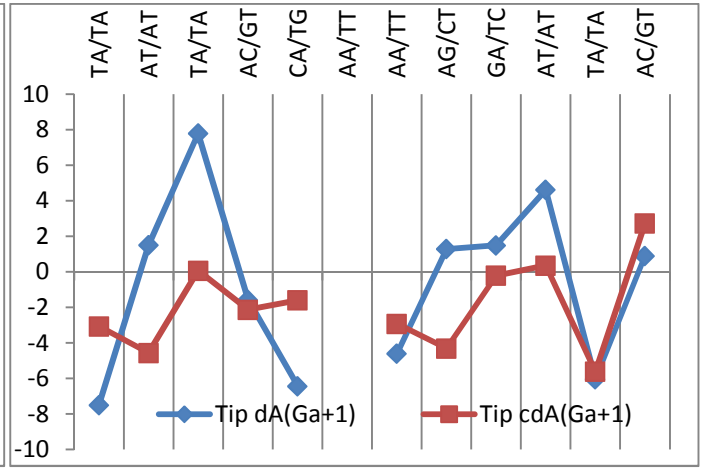
Oligodeoxynucleotide dA(Ga+1) versus cdA(Ga+1)











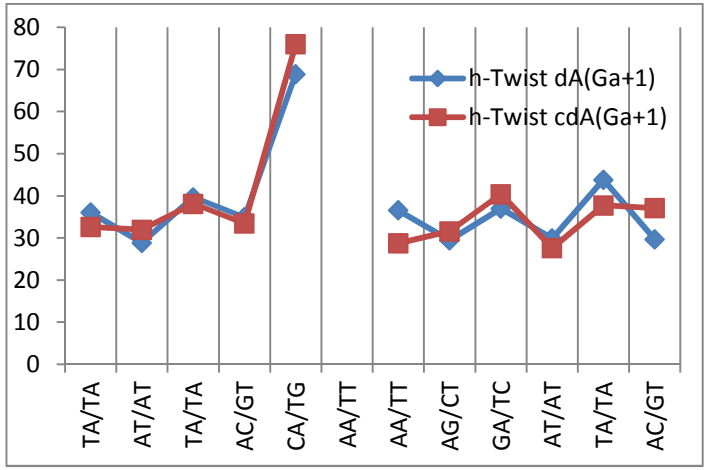
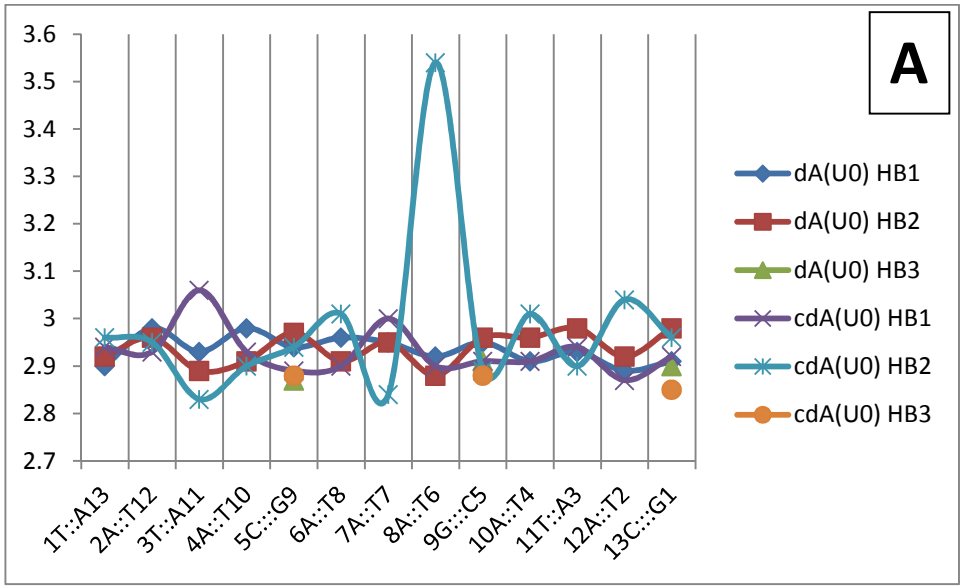
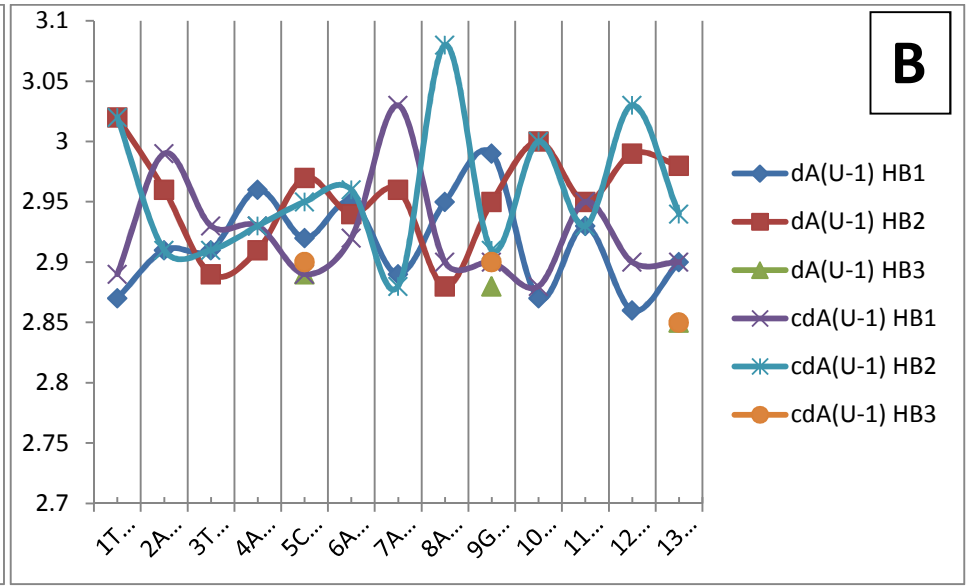


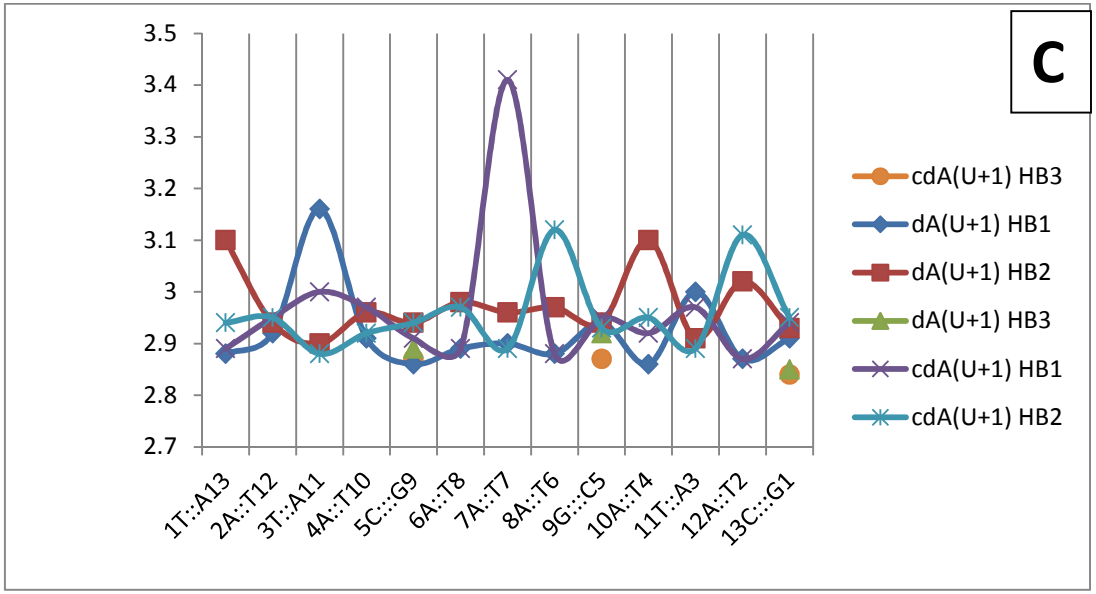
Table 5S. Base pair hydrogen bond length (HB) analysis in double stranded (*ds*) oligodeoxynucleotides that contained at position **7A** 2'-deoxyadenosine or (5'*S*)-5',8-cyclo-2'-deoxyadenosine in one strand and at different positions **T6** (U-1) or **T7** (U0) or **T8** (+1) 2'-deoxyuridine in the opposite strand which were first converted to an apurinic/apyrimidinic site (**Ap-1**, **Ap0**, **Ap+1**) and subsequently to a single strand break e.i. gaps (**Ga-1**, **Ga0**, **Ga+1**). The structures of *ds*-oligodeoxynucleotudes obtained under Molecular Mechanics (Amber 94 force field) calculation in solvation box, the sodium ions have been used as counterions to neutralize the negative charge of *ds*-DNA. Hydrogen bond for base pair **A::T**: **HB1**: O4-N6; **HB2**: N3-N1 and for **C:::G HB1**: N4-O6; **HB2**: N3-N1; **HB3**: O2-N2.

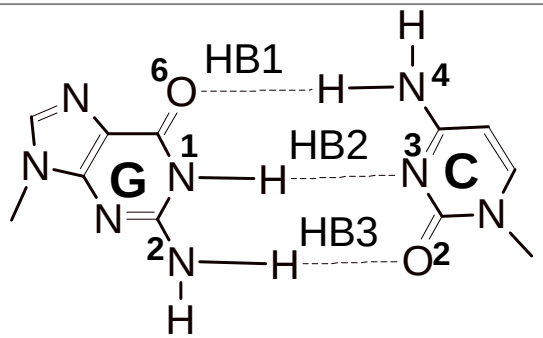
BASE PAIR		**2'-deoxyAdenosine at position 7A in double stranded oligodeoxynucleotide**																								
		cdA(U0)			**cdA(U-1)**			**cdA(U+1)**			**cdA(Ap0)**			**cdA(Ap-1)**			**cdA(Ap+1)**			**cdA(Ga0)**			**cdA(Ga-1)**			**cdA(Ga+1)**		
5'	**3'**	HB1	HB2	HB3	HB1	HB2	HB3	HB1	HB2	HB3	HB1	HB2	HB3	HB1	HB2	HB3	HB1	HB2	HB3	HB1	HB2	HB3				HB1	HB2	HB3
^{1}T	**A_{13}**	2.9	2.92		2.87	3.02		2.88	3.1		2.89	3.01		2.93	2.91		2.86	3.04		2.9	2.95		2.96	2.89		2.94	2.87	
^{2}A	**T_{12}**	2.98	2.96		2.91	2.96		2.92	2.94		2.98	2.89		2.9	2.98		2.93	2.95		2.9	2.93		3.05	2.85		2.91	3.08	
^{3}T	**A_{11}**	2.93	2.89		2.91	2.89		3.16	2.9		3	2.84		2.97	2.91		2.88	2.88		2.94	2.96		2.99	2.94		2.91	3	
^{4}A	**T_{10}**	2.98	2.91		2.96	2.91		2.91	2.96		2.89	2.94		2.9	2.95		2.93	2.98		3.01	2.91		2.91	2.96		2.89	2.94	
^{5}C	**G_{9}**	2.94	2.97	2.87	2.92	2.97	2.89	2.86	2.94	2.89	2.92	2.96	2.86	2.88	2.96	2.96	2.95	2.97	2.85	3	2.96	2.85	2.93	2.93	2.85	2.92	2.95	2.85
^{6}A	**T_{8}**	2.96	2.91		2.95	2.94		2.89	2.98		2.99	2.93		2.9	2.94					2.97	2.89		2.91	2.98		2.88	2.93	
^{7}A	**T_{7}**	2.95	2.95		2.89	2.96		2.9	2.96					2.9	2.88		2.91	2.95					2.88	2.97				
^{8}A	**T_{6}**	2.92	2.88		2.95	2.88		2.88	2.97		2.84	3					2.91	2.93		2.87	2.99					2.96	2.97	
^{9}G	**C_{5}**	2.95	2.96	2.91	2.99	2.95	2.88	2.94	2.94	2.92	3.06	2.95	2.86	2.92	2.93	2.93	2.96	2.94	2.89	2.93	2.91	2.87	2.97	2.92	2.84	2.95	2.89	2.9
^{10}A	**T_{4}**	2.91	2.96		2.87	3		2.86	3.1		2.89	2.91		2.97	2.96		2.93	2.95		2.93	3.03		2.92	2.97		2.86	2.99	
^{11}T	**A_{3}**	2.93	2.98		2.93	2.95		3	2.91		2.96	2.92		2.9	2.96		2.99	2.94		2.92	2.96		3.14	2.88		2.95	2.92	
^{12}A	**T_{2}**	2.89	2.92		2.86	2.99		2.87	3.02		2.88	3.08		2.88	2.94		2.89	3.09		2.88	3.01		2.95	2.94		2.87	2.96	
^{13}C	**G_{1}**	2.91	2.98	2.9	2.9	2.98	2.85	2.91	2.93	2.85	2.89	2.93	2.84	2.94	2.95	2.86	2.95	2.93	2.82	2.94	2.95	2.87	2.9	2.96	2.88	2.9	2.96	2.83
3'	**5'**																											
BASE PAIR		**(5'*S*) 5',8-cyclo-2'-deoxyAdenosine at position 7A in double stranded oligodeoxynucleotide**																								
		cdA(U0)			**cdA(U-1)**			**cdA(U+1)**			**cdA(Ap0)**			**cdA(Ap-1)**			**cdA(Ap+1)**			**cdA(Ga0)**			**cdA(Ga-1)**			**cdA(Ga+1)**		
5'	**3'**	HB1	HB2	HB3	HB1	HB2	HB3	HB1	HB2	HB3	HB1	HB2	HB3	HB1	HB2	HB3	HB1	HB2	HB3	HB1	HB2	HB3	HB1	HB2	HB3	HB1	HB2	HB3
^{1}T	**A_{13}**	2.94	2.96		2.89	3.02		2.89	2.94		2.91	2.94		2.95	2.90		2.86	3.11		2.94	2.97		2.94	2.91		2.94	2.94	
^{2}A	**T_{12}**	2.93	2.95		2.99	2.91		2.95	2.95		2.95	2.97		2.91	2.97		2.96	2.95		2.96	2.85		3.04	2.92		2.93	2.91	
^{3}T	**A_{11}**	3.06	2.83		2.93	2.91		3	2.88		3.07	2.88		2.94	2.89		2.98	2.86		2.94	2.92		3.00	2.9		2.90	2.93	
^{4}A	**T_{10}**	2.93	2.90		2.93	2.93		2.97	2.92		2.99	2.92		2.92	2.95		2.94	2.91		2.95	2.94		2.92	2.94		2.87	2.96	
^{5}C	**G_{9}**	2.89	2.94	2.88	2.89	2.95	2.9	2.91	2.94	2.87	2.93	2.97	2.88	2.91	2.96	2.87	2.98	2.98	2.87	2.87	2.96	2.94	2.92	2.94	2.88	2.89	3.00	2.93
^{6}A	**T_{8}**	2.90	3.01		2.92	2.96		2.89	2.97		2.87	2.99		2.95	2.95					2.89	2.99		2.91	2.95				
^{7}A	**T_{7}**	3.00	2.84		3.03	2.88		3.41	2.89					3.01	2.90		3.00	2.91					3.16	2.89		3.46	2.92	
^{8}A	**T_{6}**	2.9			2.90	3.08		2.88	3.12		2.88	3.16					2.90	3.33		3.00	2.92					2.88	2.94	
^{9}G	**C_{5}**	2.91	2.89	2.88	2.9	2.91	2.9	2.95	2.93	2.87	3.00	2.92	2.87	2.99	2.94	2.93	2.90	2.95	2.94	2.93	2.94	2.89	2.92	2.93	2.89	2.94	2.90	2.86
^{10}A	**T_{4}**	2.91	3.01		2.88	3.00		2.92	2.95		2.86	3.05		2.92	2.94		2.92	2.92		2.96	2.96		2.90	3.02		2.94	2.98	
^{11}T	**A_{3}**	2.94	2.90		2.95	2.93		2.97	2.89		2.99	2.88		2.94	2.94		2.97	2.97		2.92	3.01		2.89	2.92		2.94	2.99	
^{12}A	**T_{2}**	2.87	3.04		2.90	3.03		2.87	3.11		2.87	3.05		2.88	2.94		2.87	3.09		2.93	2.91		2.95	2.91		2.90	2.96	
^{13}C	**G_{1}**	2.92	2.96	2.85	2.90	2.94	2.85	2.94	2.95	2.84	2.94	2.97	2.85	2.95	2.96	2.82	2.92	2.95	2.85	2.93	2.97	2.87	2.87	2.95	2.89	2.93	2.94	2.89
3'	**5'**																											

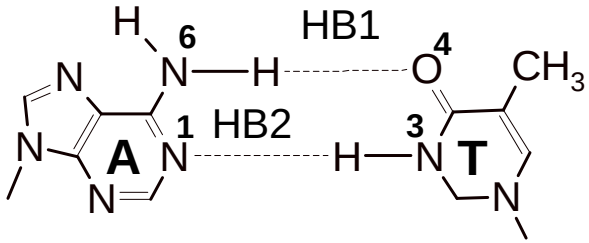
Graph 5S. Graphical representation of hydrogen bond lengths analysis, presented in **Table 5S**. **Y-axis** represents the hydrogen bond length in Å, **X-axis** represents the position and composition of base pair in investigated *ds*-oligodeoxynucleotide.

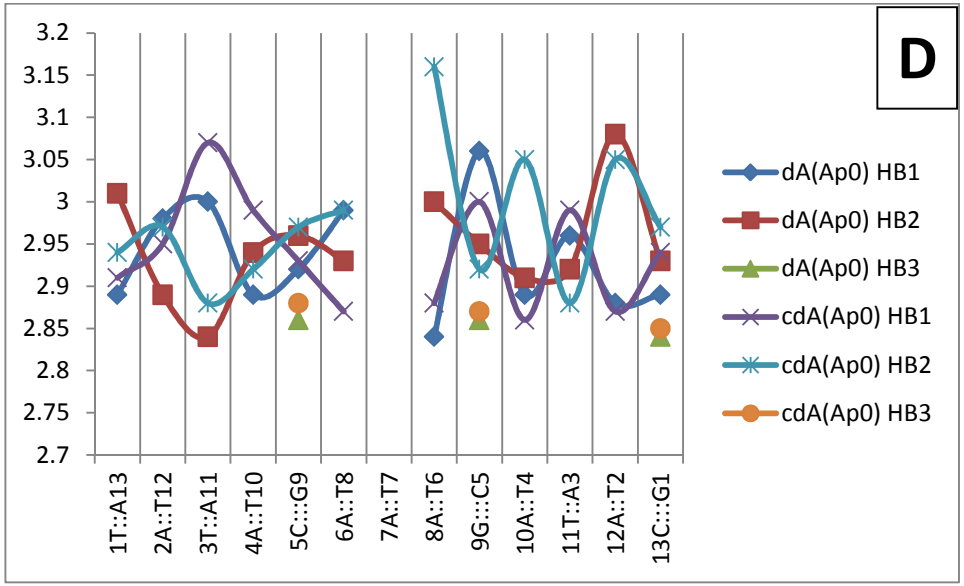


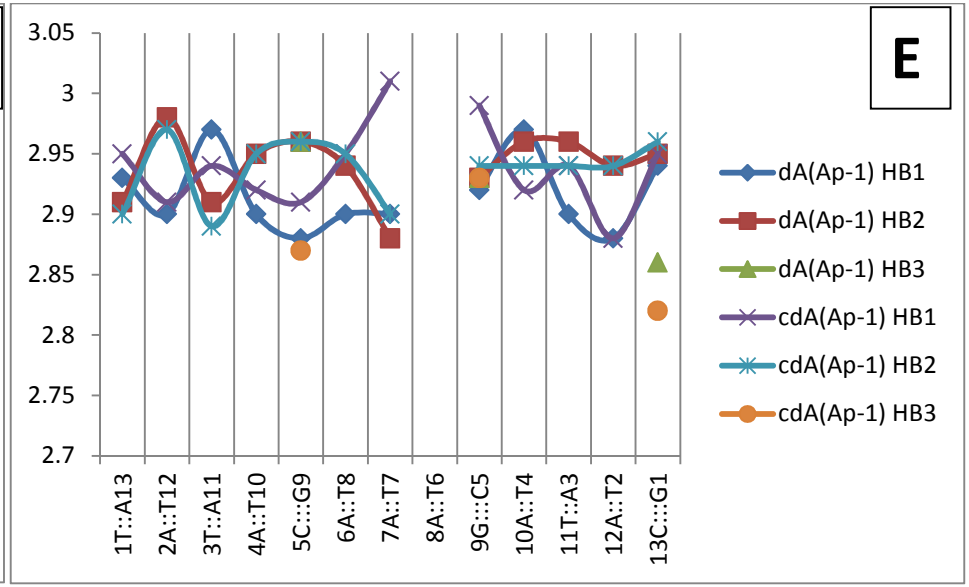


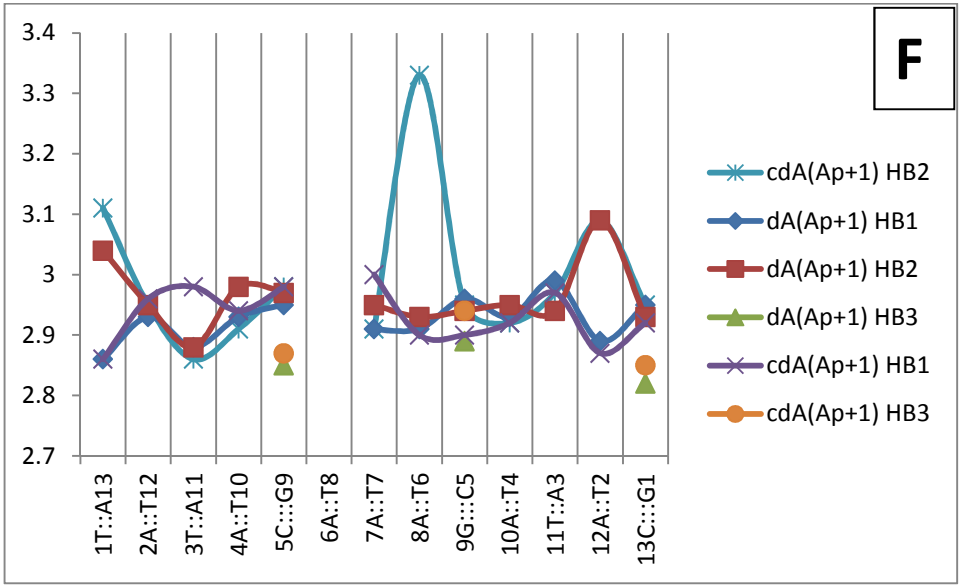


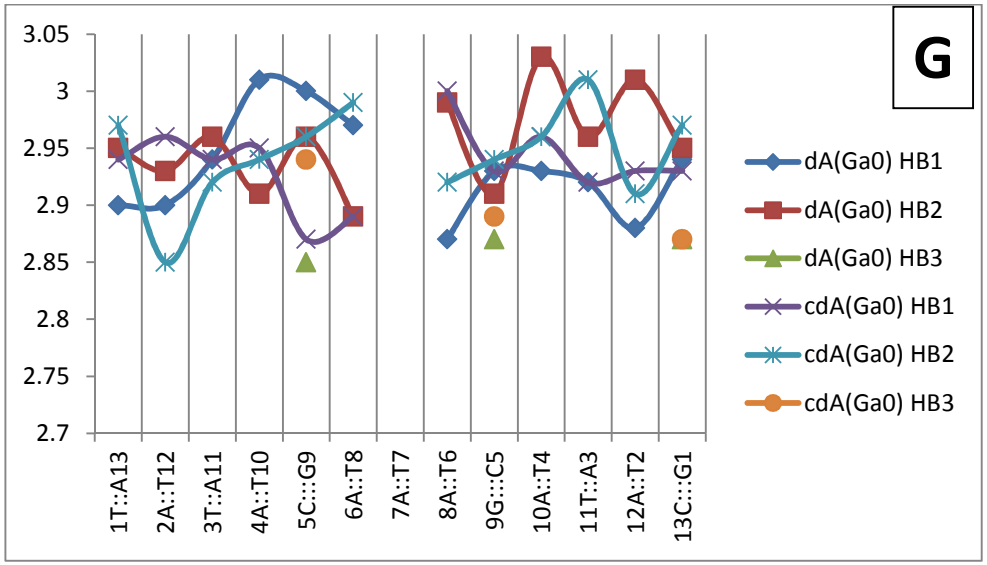


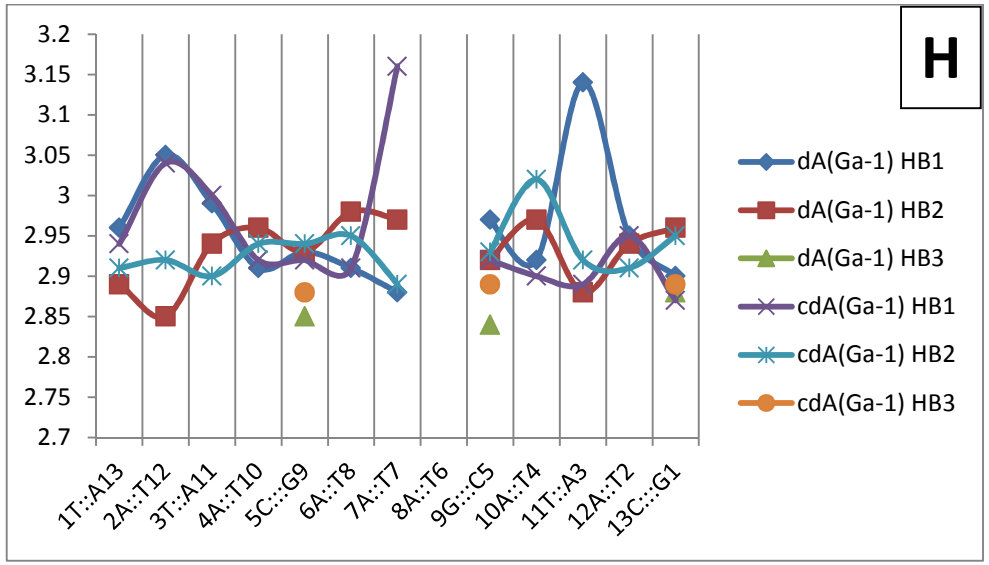



D
3.2
3.15
3.1
3.05
3
2.95
2.9
2.85
2.8
2.75
2.7
1T::A13
2A::T12
3T::A11
4A::T10
5C:::G9
6A::T8
7A::T7
8A::T6
9G:::C5
10A::T4
11T::A3
12A::T2
13C:::G1
dA(Ap0) HB1
dA(Ap0) HB2
dA(Ap0) HB3
cdA(Ap0) HB1
cdA(Ap0) HB2
cdA(Ap0) HB3


E
3.05
3
2.95
2.9
2.85
2.8
2.75
2.7
1T::A13
2A::T12
3T::A11
4A::T10
5C:::G9
6A::T8
7A::T7
8A::T6
9G:::C5
10A::T4
11T::A3
12A::T2
13C:::G1
dA(Ap-1) HB1
dA(Ap-1) HB2
dA(Ap-1) HB3
cdA(Ap-1) HB1
cdA(Ap-1) HB2
cdA(Ap-1) HB3


F
3.4
3.3
3.2
3.1
3
2.9
2.8
2.7
1T::A13
2A::T12
3T::A11
4A::T10
5C:::G9
6A::T8
7A::T7
8A::T6
9G:::C5
10A::T4
11T::A3
12A::T2
13C:::G1
cdA(Ap+1) HB2
dA(Ap+1) HB1
dA(Ap+1) HB2
dA(Ap+1) HB3
cdA(Ap+1) HB1
cdA(Ap+1) HB3


G
3.05
3
2.95
2.9
2.85
2.8
2.75
2.7
1T::A13
2A::T12
3T::A11
4A::T10
5C:::G9
6A::T8
7A::T7
8A::T6
9G:::C5
10A::T4
11T::A3
12A::T2
13C:::G1
dA(Ga0) HB1
dA(Ga0) HB2
dA(Ga0) HB3
cdA(Ga0) HB1
cdA(Ga0) HB2
cdA(Ga0) HB3


H
3.2
3.15
3.1
3.05
3
2.95
2.9
2.85
2.8
2.75
2.7
1T::A13
2A::T12
3T::A11
4A::T10
5C:::G9
6A::T8
7A::T7
8A::T6
9G:::C5
10A::T4
11T::A3
12A::T2
13C:::G1
dA(Ga-1) HB1
dA(Ga-1) HB2
dA(Ga-1) HB3
cdA(Ga-1) HB1
cdA(Ga-1) HB2
cdA(Ga-1) HB3

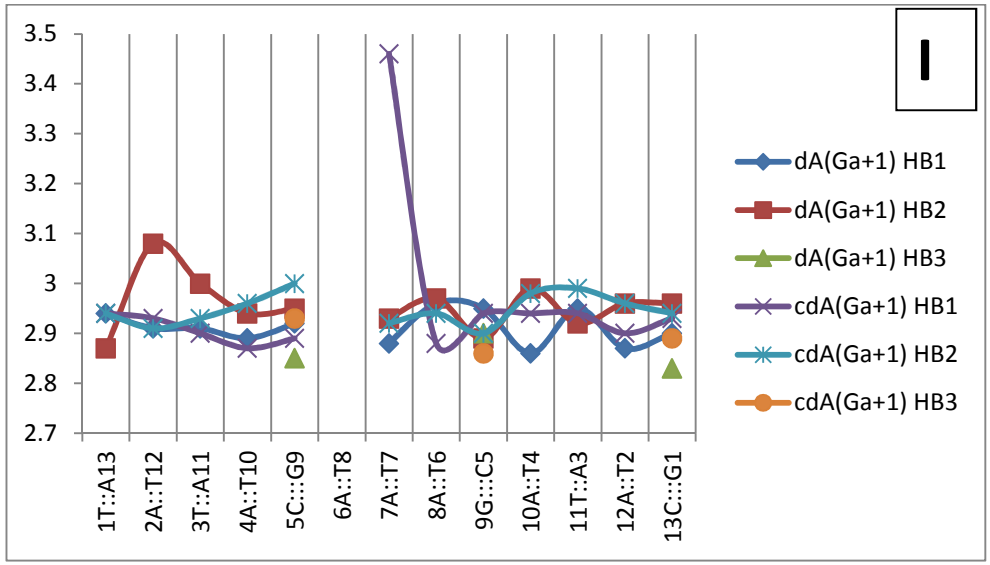
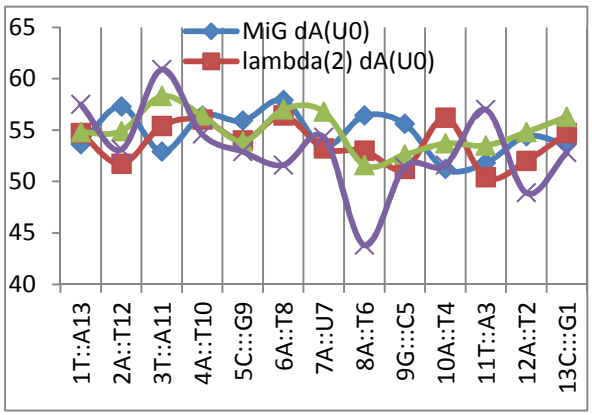
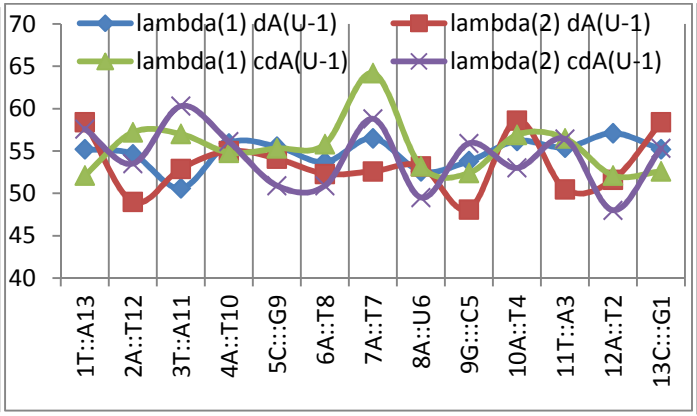

I
3.5
3.4
3.3
3.2
3.1
3
2.9
2.8
2.7
1T::A13
2A::T12
3T::A11
4A::T10
5C:::G9
6A::T8
7A::T7
8A::T6
9G:::C5
10A::T4
11T::A3
12A::T2
13C:::G1
dA(Ga+1) HB1
dA(Ga+1) HB2
dA(Ga+1) HB3
cdA(Ga+1) HB1
cdA(Ga+1) HB2
cdA(Ga+1) HB3

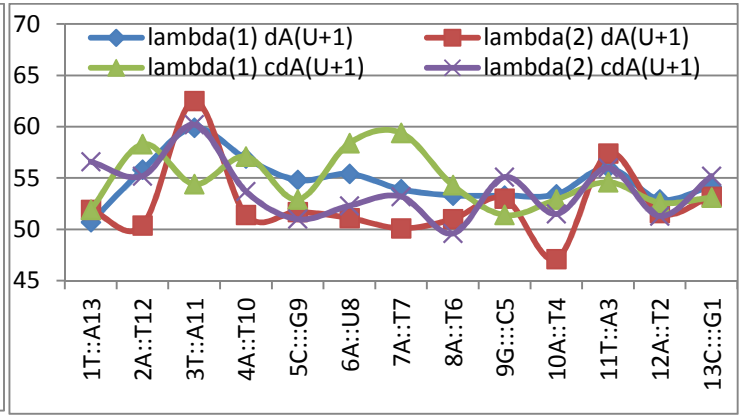
Table 6S. Base pairs and base step (MaG-major groove, MiG-minor groove width and adopted form) parameters of double stranded oligodeoxynucleotides that contained at position **7A** 2'-deoxyadenosine (dA) or (5'*S*)-5',8-cyclo-2'-deoxyadenosine (cdA) in one strand and at different positions **T6** (Ap-1) or **T7** (Ap0) or **T8** (AP+1) 2'-deoxyuridine in the opposite strand. The structures of *ds*-oligodeoxynucleotudes obtained under Molecular Mechanics (Amber 94 force field) calculation in solvation box, the sodium ions have been used as counterions to neutralize the negative charge of *ds*-DNA.

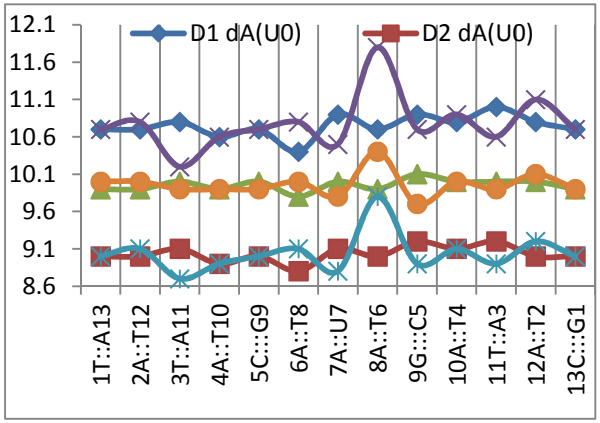
BASE PAIR		Oligodeoxynucleotides																									
		dA(U0)									dA(U-1)									dA(U+1)							
5'	3'	λ(1) (°)	λ(2) (°)	D1 Å	D2 Å	L Å	Step	MiG Å	MaG Å	Form	λ(1)	λ(2)	D1	D2	L	Step	MiG	MaG	Form	λ(1)	λ(2)	D1	D2	L	Step	MiG	MaG	Form
^{1}T	A_{13}	53.6	54.7	10.7	9.0	9.9	TA/TA			B	55.2	58.4	10.5	8.9	9.8	TA/TA			B	50.7	51.9	11.1	9.3	10	TA/TA			B
^{2}A	T_{12}	57.3	51.7	10.7	9.0	9.9	AT/AT			B	54.6	49	11.1	9.2	10.1	AT/AT			B	55.8	50.4	10.8	9.1	10	AT/AT			B
^{3}T	A_{11}	52.9	55.4	10.8	9.1	10.0	TA/TA	12.0	18.9	B	50.6	52.9	11	9.2	10	TA/TA	13.0	17.5	B	59.9	62.5	10.3	8.8	10	TA/TA	12.1	18.5	B
^{4}A	T_{10}	56.4	56.0	10.6	8.9	9.9	AC/GT	12.9	18.2	B	55.9	55	10.7	9	9.9	AC/GT	13.4	17.8		56.9	51.4	10.8	9.1	10	AC/GT	12.1	18.5	B
^{5}C	G_{9}	55.9	54.0	10.7	9.0	10.0	CA/TG	13.4	18.3	B	55.5	54.1	10.7	9	9.9	CA/TG	13.2	17.7		54.8	51.7	10.8	9	9.9	CA/TG	11.6	18	
^{6}A	**T_{8}**	57.9	56.4	10.4	8.8	9.8	AA/TT	12.9	17.4		53.7	52.3	10.7	8.9	9.8	AA/TT	13.4	17.4	B	55.4	51.1	10.9	9.1	10	AA/TT	11.7	17.6	B
^{7}A	**T_{7}**	53.4	53.2	10.9	9.1	10.0	AA/TT	12.6	17.4	B	56.5	52.6	10.8	9.1	10	AA/TT	12.5	17.9	B	53.9	50.1	10.9	9.1	10	AA/TT	11.6	16.9	B
^{8}A	**T_{6}**	56.4	53.0	10.7	9.0	9.9	AG/CT	11.9	17.4	B	52.6	53.2	10.7	9	9.9	AG/CT	11.5	17.8	B	53.3	51	10.9	9.1	9.9	AG/CT	11.4	18	
^{9}G	C_{5}	55.6	51.2	10.9	9.2	10.1	GA/TC	11.7	18.4	B	53.8	48.1	11	9.1	9.9	GA/TC	11.4	18.1	B	53.3	53	10.8	9.1	10	GA/TC	12.3	19	B
^{10}A	T_{4}	51.2	56.2	10.8	9.1	10.0	AT/AT	11.5	17.9	B	56.2	58.6	10.5	8.9	9.9	AT/AT			B	53.4	47.1	11.2	9.3	10	AT/AT	12.4	17.1	B
^{11}T	A_{3}	51.8	50.4	11.0	9.2	10.0	TA/TA			B	55.4	50.5	10.9	9.1	10	TA/TA			B	56	57.4	10.5	8.9	9.9	TA/TA			B
^{12}A	T_{2}	54.4	52.0	10.8	9.0	10.0	AC/GT			B	57.1	51.6	10.7	9	9.9	AC/GT			B	52.9	51.6	11	9.2	10	AC/GT			B
^{13}C	G_{1}	53.6	54.7	10.7	9.0	9.9					55.2	58.4	10.5	8.9	9.8					54.2	53.2	10.7	9	9.9				
3'	5'																											
		cdA(U0)									cdA(U-1)									cdA(U+1)							
5'	3'	λ(1) (°)	λ(2) (°)	D1 Å	D2 Å	L Å	Step	MiG Å	MaG Å	Form	λ(1)	λ(2)	D1	D2	L	Step	MiG	MaG	Form	λ(1)	λ(2)	D1	D2	L	Step	MiG	MaG	Form
^{1}T	A_{13}	54.8	57.5	10.7	9	10	TA/TA			B	52.1	57.6	10.7	9	10	TA/TA			B	51.9	56.6	10.9	9.1	10	TA/TA			B
^{2}A	T_{12}	54.9	53.1	10.8	9.1	10	AT/AT			B	57.2	53.5	10.7	9	10	AT/AT			B	58.3	55.2	10.6	8.9	9.9	AT/AT			B
^{3}T	A_{11}	58.3	60.9	10.2	8.7	9.9	TA/TA	11.4	20.0	B	57	60.3	10.4	8.9	9.9	TA/TA	11.7	18.1	B	54.4	60.2	10.6	9	10	TA/TA	13	17.4	B
^{4}A	T_{10}	56.4	54.6	10.6	8.9	9.9	AC/GT	11.5	18.3		54.8	56.1	10.6	8.9	9.9	AC/GT	11.2	18.3	B	57.1	53.7	10.7	9	10	AC/GT	12.2	19.4	B
^{5}C	G_{9}	53.9	52.9	10.7	9	9.9	CA/TG	12.1	18.6	B	55.3	50.9	10.7	9	9.9	CA/TG	11.8	18.9	B	52.9	51	10.9	9	9.9	CA/TG	11.9	18.8	B
^{6}A	**T_{8}**	57	51.6	10.8	9.1	10	AA/TT	11.9	18.5	B	55.8	50.9	10.9	9.1	10	AA/TT	12.7	17.9	B	58.4	52.3	10.7	9	10	AA/TT	12.5	17.1	B
^{7}A	**T_{7}**	56.8	54.3	10.5	8.8	9.8	AA/TT	11	18.2	B	64.2	58.8	10	8.6	9.9	AA/TT	12.1	18.8		59.4	53.2	10.5	8.8	9.9	AA/TT	11.7	17.4	
^{8}A	**T_{6}**	51.6	43.8	11.8	9.8	10.4	AG/CT	11.3	19.5	B	53.2	49.5	11.2	9.3	10.1	AG/CT	11.3	17.5	B	54.3	49.6	11.1	9.3	10.1	AG/CT	10.7	16.7	
^{9}G	C_{5}	52.6	51.4	10.7	8.9	9.7	GA/TC	11.5	17.6	B	52.4	55.9	10.7	9	9.9	GA/TC	11.7	18.0	B	51.4	55.1	10.7	9	9.9	GA/TC	11.2	17.5	B
^{10}A	T_{4}	53.7	51.6	10.9	9.1	10	AT/AT	11.4	17.6	B	56.9	53	10.7	9	10	AT/AT	11.5	17.5	B	52.9	51.5	10.9	9.1	9.9	AT/AT	11.9	17.1	B
^{11}T	A_{3}	53.5	57	10.6	8.9	9.9	TA/TA			B	56.5	56.4	10.5	8.9	9.9	TA/TA			B	54.6	56	10.7	9	10	TA/TA			B
^{12}A	T_{2}	54.8	48.9	11.1	9.2	10.1	AC/GT			B	52.1	48	11.2	9.3	10.1	AC/GT			B	52.6	51.3	11	9.2	10	AC/GT			B
^{13}C	G_{1}	56.3	52.8	10.7	9	9.9					52.6	55.3	10.8	9.1	10					53.1	55.2	10.7	8.9	9.8				
3'	5'																											

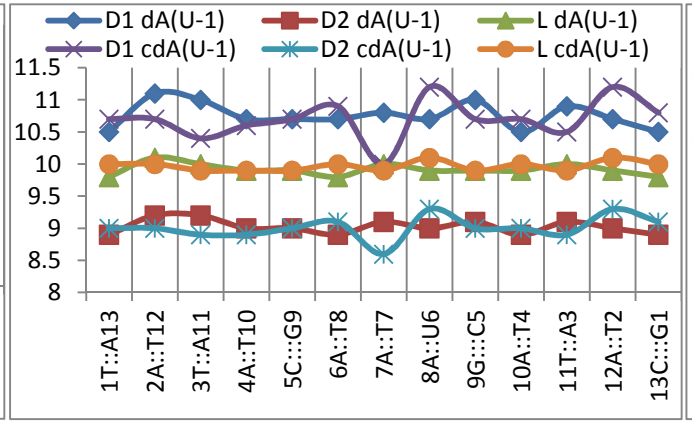
Graph 6S Graphical representation of data presented in **Table 6S**

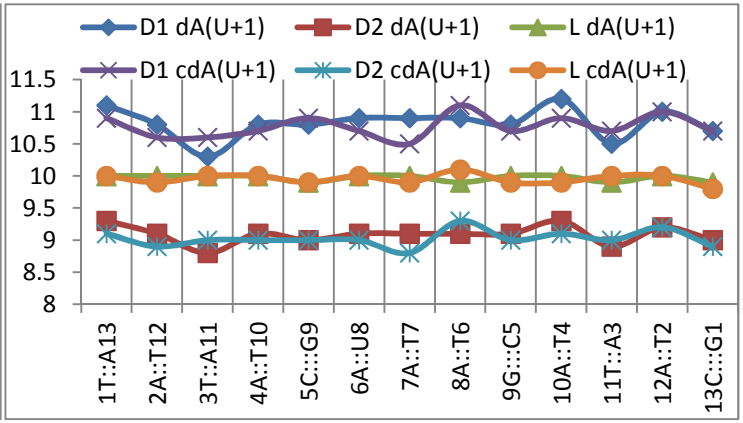


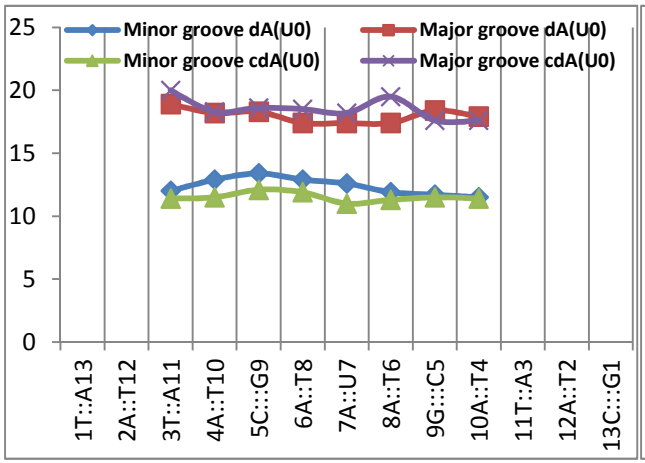


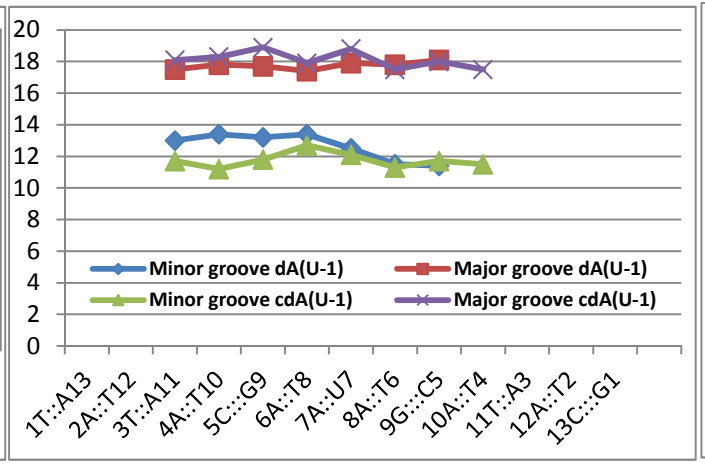












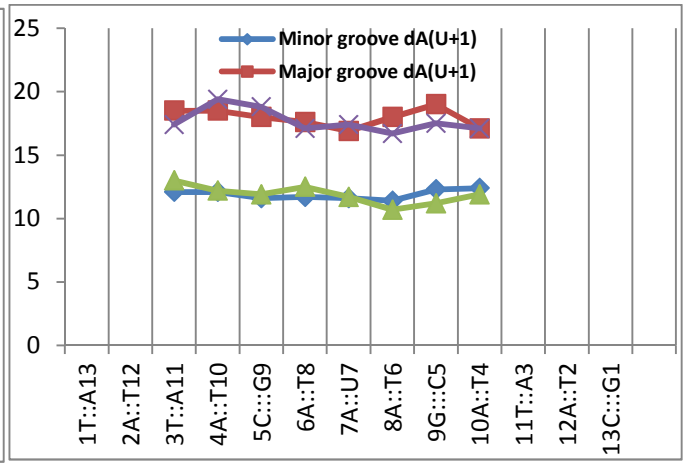
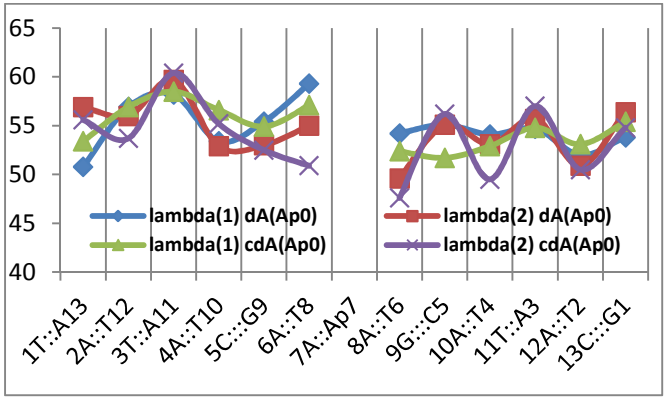
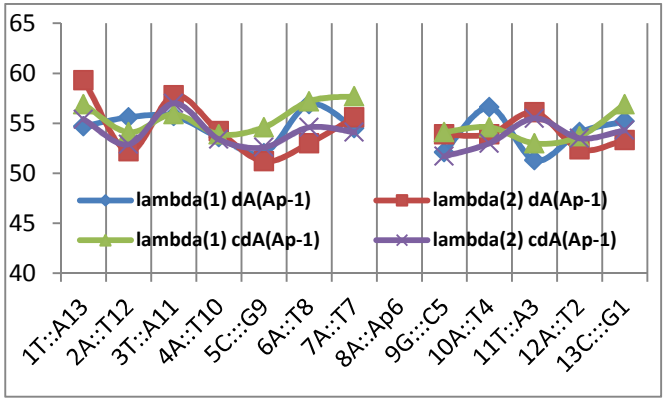


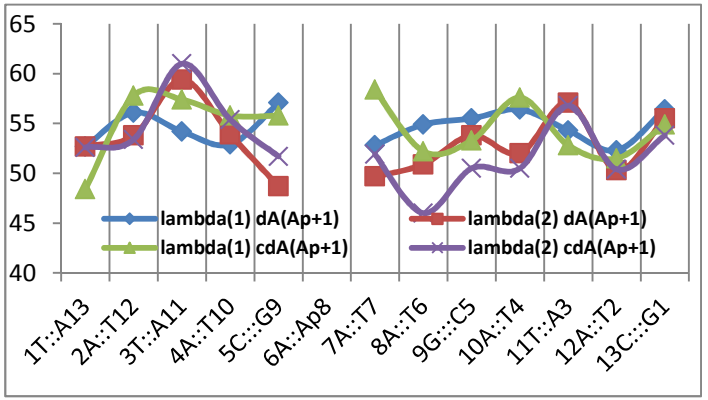
Table 6S continued. Base pairs and base step (MaG-major groove, MiG-minor groove width and adopted form) parameters of double stranded oligodeoxynucleotides that contained at position **7A** 2'-deoxyadenosine(dA) or (5'*S*) -5',8-cyclo-2'-deoxyadenosine (cdA) in one strand and at different positions **T6** (U-1) or **T7** (U0) or **T8** (U+1) an apurinic/apyrimidinic site in the opposite strand. The structures of *ds*-oligodeoxynucleotudes obtained under Molecular Mechanics (Amber 94 force field) calculation in solvation box, the sodium ions have been used as counterions to neutralize the negative charge of *ds*-DNA.

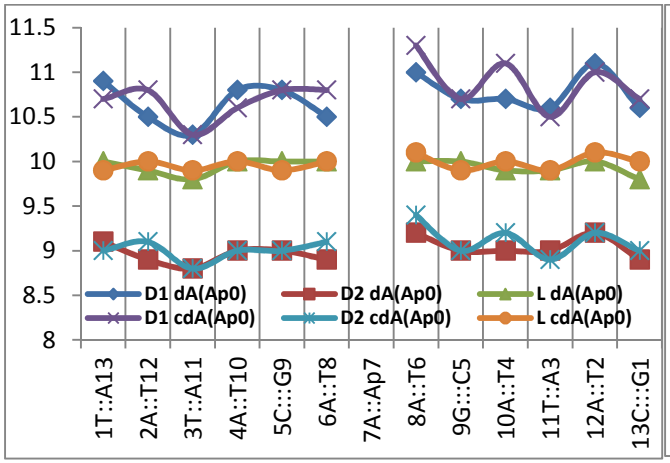
BASE PAIR		**Oligodeoxynucleotudes**																									
		dA(Ap0)									**dA(Ap-1)**									**dA(Ap+1)**								
5'	3'	**λ(1) (°)**	**λ(2) (°)**	**D1 Å**	**D2 Å**	**L Å**	Step	MiG **Å**	MaG **Å**	Form	λ(1)	λ(2)	D1	D2	L		MiG	MaG	Form	λ(1)	λ(2)	D1	D2	L		MiG	MaG	Form
[1]T	A_{13}	50.8	56.9	10.9	9.1	10	TA/TA			B	54.7	59.3	10.6	8.9	9.9	TA/TA				52.7	52.7	10.9	9.1	10	TA/TA			B
[2]A	T_{12}	56.9	56	10.5	8.9	9.9	AT/AT			B	55.6	52.2	10.8	9.1	10	AT/AT			B	56.1	53.8	10.7	9	10	AT/AT			B
[3]T	A_{11}	58.2	59.7	10.3	8.8	9.8	TA/TA	12.1	18.2	B	55.7	57.8	10.5	8.9	9.9	TA/TA	12.4	17.6	B	54.2	59.4	10.6	8.9	9.9	TA/TA	12.6	17.6	B
[4]A	T_{10}	53.4	52.9	10.8	9	10	AC/GT	12.9	18	B	53.6	54.2	10.8	9	10	AC/GT	11.7	18	B	52.9	53.9	10.8	9.1	10	AC/GT	13.2	16.6	B
[5]C	G_9	55.4	53	10.8	9	10	CA/TG	13.8	17.8	B	52	51.2	10.9	9.1	9.9	CA/TG	12.9	17.3	B	57.1	48.7	10.7	8.9	9.8	CA/TG	13.5	17.4	
[6]A	**T_8**	59.3	55	10.5	8.9	10	AA/TT	13.6	17.5	B	56.9	53	10.7	9	9.9	AA/TT	14.4	17.1	B						AA/TT			
[7]A	**T_7**						AA/TT				54.5	55.6	10.6	8.9	9.8	AA/TT	13.8	17.9		52.8	49.7	11	9.1	9.9	AA/TT	13.1	17.3	B
[8]A	**T_6**	54.2	49.6	11	9.2	10	AG/CT	13.2	16.1	B						AG/CT				54.9	50.9	10.8	9	9.9	AG/CT	12.1	20	B
[9]G	C_5	55.1	55.1	10.7	9	10	GA/TC	12.3	17.6	B	52.1	53.9	10.8	9	9.9	GA/TC	13.4	18.1	B	55.5	53.8	10.7	9	9.9	GA/TC	12	18.4	B
[10]A	T_4	54.1	53.1	10.7	9	9.9	AT/AT	11.5	17.4	B	56.6	53.9	10.7	9	10	AT/AT	12.8	18	B	56.4	52.0	10.7	9	10	AT/AT	12.6	17.4	B
[11]T	A_3	54.7	55.7	10.6	9	9.9	TA/TA			B	51.3	56.1	10.8	9	9.9	TA/TA			B	54.3	57.1	10.6	9	10	TA/TA			
[12]A	T_2	52	50.9	11.1	9.2	10	AC/GT				54.1	52.4	10.8	9	9.9	AC/GT			B	52.3	50.3	11.1	9.2	10	AC/GT			
[13]C	G_1	53.8	56.4	10.6	8.9	9.8					55.2	53.3	10.7	9	9.9					56.4	55.5	10.5	8.8	9.8				
3'	5'																											
		cdA(Ap0)									**cdA(Ap-1)**									**cdA(Ap+1)**								
5'	3'	**λ(1) (°)**	**λ(2) (°)**	**D1 Å**	**D2 Å**	**L Å**	Step	MiG **Å**	MaG **Å**	Form	λ(1)	λ(2)	D1	D2	L	Step	MiG	MaG	Form	λ(1)	λ(2)	D1	D2	L	Step	MiG	MaG	Form
[1]T	A_{13}	53.4	55.6	10.7	9	9.9	TA/TA				56.9	55.4	10.6	8.9	9.9	TA/TA			B	48.4	52.6	11.2	9.3	10.1	TA/TA			B
[2]A	T_{12}	56.9	53.7	10.8	9.1	10	AT/AT			B	54.1	52.9	10.8	9	10	AT/AT			B	57.8	53.4	10.7	9	10	AT/AT			B
[3]T	A_{11}	58.5	60.4	10.3	8.8	9.9	TA/TA	12.2	17.2	B	55.9	57	10.6	8.9	9.9	TA/TA	12.5	17.3	B	57.4	61	10.4	8.8	9.9	TA/TA	13	17.7	B
[4]A	T_{10}	56.6	55.2	10.6	9	10	AC/GT	13.0	19.2	B	53.9	53.4	10.8	9	10	AC/GT	11.9	17.8	B	55.8	55.4	10.6	8.9	9.9	AC/GT	13.6	18	
[5]C	G_9	54.9	52.5	10.8	9	9.9	CA/TG	14.1	18.0	B	54.6	52.6	10.8	9	9.9	CA/TG	13.0	17.9	B	55.8	51.7	10.8	9	9.9	CA/TG	14.1	17.4	
[6]A	**T_8**	57.1	50.9	10.8	9.1	10	AA/TT	13.9	17.4		57.2	54.6	10.7	9	10	AA/TT	14.0	17.3							AA/TT			
[7]A	**T_7**						AA/TT				57.7	54.1	10.6	8.9	10	AA/TT	13.2	17.3		58.4	51.9	10.5	8.8	9.8	AA/TT	13.4	17.2	B
[8]A	**T_6**	52.4	47.6	11.3	9.4	10.1	AG/CT	13.2	16.8	B						AG/CT				52.2	46	11.5	9.6	10.3	AG/CT	11.8	19.1	B
[9]G	C_5	51.7	56.2	10.7	9	9.9	GA/TC	12.6	18.2	B	54.1	51.7	10.9	9.1	10	GA/TC	12.9	16.8	B	53.3	50.5	10.9	9.1	9.9	GA/TC	11.7	17.7	B
[10]A	T_4	52.9	49.5	11.1	9.2	10	AT/AT	12.0	17.4	B	54.6	53	10.8	9	10	AT/AT	12.3	17.2	B	57.6	50.5	10.7	9	9.9	AT/AT	12.6	17.3	B
[11]T	A_3	54.8	57	10.5	8.9	9.9	TA/TA			B	53	55.5	10.7	9	10	TA/TA			B	52.8	56.8	10.8	9.1	10	TA/TA			B
[12]A	T_2	53.1	50.5	11	9.2	10.1	AC/GT			B	53.7	53.5	10.8	9	10	AC/GT			B	51.5	50.4	11.1	9.3	10.1	AC/GT			
[13]C	G_1	55.4	54.8	10.7	9	10					56.9	54.3	10.6	9	9.9					54.9	53.8	10.7	9	9.9				
3'	5'																											

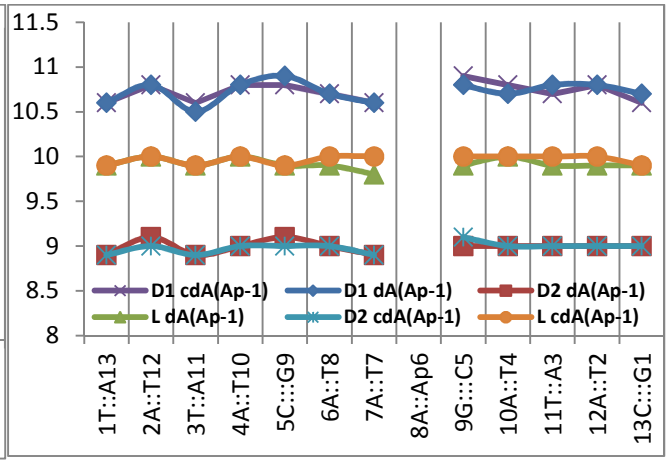
Graph 6S continued. Graphical representation of data presented in **Table 6S continued**

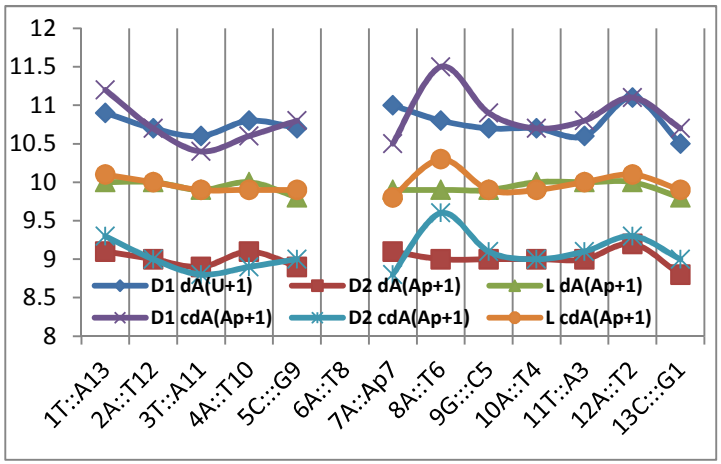


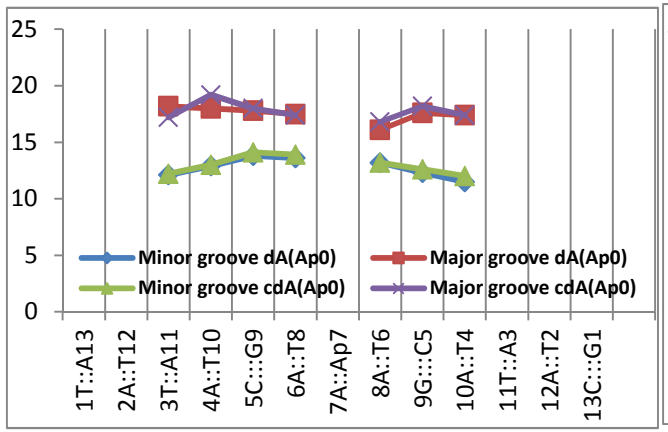


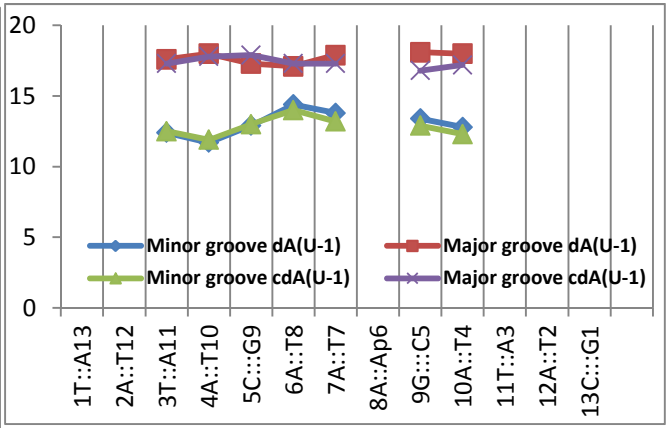












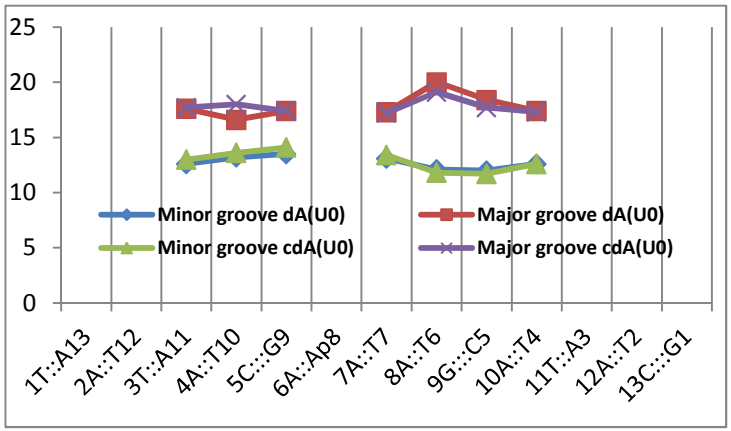


Table 6 continued. Base pairs and base step (MaG-major groove, MiG-minor groove width and adopted form) parameters of double stranded oligodeoxynucleotides that contained at position **7A** 2'-deoxyadenosine(dA) or (5'S)-5',8-cyclo-2'-deoxyadenosine (cdA) in one strand and at different positions **T6** (Ga-1) or **T7** (Ga0) or **T8** (Ga+1) a single strand break e.i gap (Ga) in the opposite strand. The structures of *ds*-oligodeoxynucleotudes obtained under Molecular Mechanics (Amber 94 force field) calculation in solvation box, the sodium ions have been used as counterions to neutralize the negative charge of *ds*-DNA.

BASE PAIR		Oligodeoxynucleotudes																									
		dA(Ga0)									dA(Ga+1)									dA(Ga-1)							
5'	3'	**λ(1) (º)**	**λ(2) (º)**	**D1 Å**	**D2 Å**	**L Å**	Step	MiG **Å**	MaG **Å**	Form	λ(1)	λ(2)	D1	D2	L		MiG	MaG	Form	λ(1)	λ(2)	D1	D2	L		MiG	MaG	Form
[1]T	A_{13}	53.6	54.7	10.7	9	9.9	TA/TA			B	55.2	58.4	10.5	8.9	9.8	TA/TA			B	56.5	60.2	10.5	8.9	10	TA/TA			B
[2]A	T_{12}	57.3	51.7	10.7	9	9.9	AT/AT			B	54.6	49	11.1	9.2	10.1	AT/AT			B	61.2	57.7	10.3	8.8	9.9	AT/AT			B
[3]T	A_{11}	52.9	55.4	10.8	9.1	10	TA/TA	12.0	18.9	B	50.6	52.9	11	9.2	10	TA/TA	13		B	54.2	56.9	10.7	9	10	TA/TA	12.1	18.1	B
[4]A	T_{10}	56.4	56	10.6	8.9	9.9	AC/GT	12.9	18.2	B	55.9	55	10.7	9	9.9	AC/GT	13.4	17.6		53.1	54.4	10.8	9	10	AC/GT	11.5	18.7	
[5]C	G_9	55.9	54	10.7	9	10	CA/TG	13.4	18.3	B	55.5	54.1	10.7	9	9.9	CA/TG	13.2	17.6		50.4	58	10.7	9	9.9	CA/TG	12.1	19.1	B
[6]A	**T_8**	57.9	56.4	10.4	8.8	9.8	AA/TT	12.9	17.3							AA/TT				56.5	51.9	10.8	9.1	10	AA/TT	13.2	16.7	B
[7]A	**T_7**						AA/TT				53.7	52.3	10.7	8.9	9.8	AA/TT	13.4	17.4	B	53.2	52.8	10.8	9	9.9	AA/TT	13.2	17.4	
[8]A	**T_6**	53.4	53.2	10.9	9.1	10	AG/CT	12.6	17.2	B	56.5	52.6	10.8	9.1	10	AG/CT	12.5	17.5	B						AG/CT			
[9]G	C_5	56.4	53	10.7	9	9.9	GA/TC	11.9	17.0	B	52.6	53.2	10.7	9	9.9	GA/TC	11.5	17.5	B	54.7	60.6	10.4	8.8	9.8	GA/TC	12.6	18.0	B
[10]A	T_4	55.6	51.2	10.9	9.2	10.1	AT/AT	11.7		B	53.8	48.1	11	9.1	9.9	AT/AT	11.4		B	56	52.7	10.8	9	10	AT/AT	12.0	17.4	B
[11]T	A_3	51.2	56.2	10.8	9.1	10	TA/TA			B	56.2	58.6	10.5	8.9	9.9	TA/TA			B	58.8	61.4	10.3	8.8	10	TA/TA			B
[12]A	T_2	51.8	50.4	11	9.2	10	AC/GT			B	55.4	50.5	10.9	9.1	10	AC/GT			B	57.2	54.3	10.7	9	10	AC/GT			B
[13]C	G_1	54.4	52	10.8	9	10					57.1	51.6	10.7	9	9.9					53.4	55	10.8	9.1	10				
3'	5'																											
		dA(Ga0)									dA(Ga+1)									dA(Ga-1)							
5'	3'	**λ(1) (º)**	**λ(2) (º)**	**D1 Å**	**D2 Å**	**L Å**	Step	MiG **Å**	MaG **Å**	Form	λ(1)	λ(2)	D1	D2	L	Step	MiG	MaG	Form	λ(1)	λ(2)	D1	D2	L	Step	MiG	MaG	Form
[1]T	A_{13}	54.8	58.6	10.7	9	10	TA/TA			B	54.8	57.2	10.7	9	10	TA/TA			B	56.7	58.2	10.5	8.9	9.9	TA/TA			
[2]A	T_{12}	58.6	54.4	10.4	8.8	9.9	AT/AT			B	55.5	55.5	10.6	8.9	9.9	AT/AT			B	58.6	56.4	10.5	8.9	10	AT/AT			B
[3]T	A_{11}	53.9	58.1	10.6	9	10	TA/TA	11.8	19.3	B	53.5	54.5	10.8	9	9.9	TA/TA	13.4	17.5	B	57.3	54.9	10.5	8.9	9.9	TA/TA	11.5	17.3	B
[4]A	T_{10}	57.7	53.1	10.7	9	10	AC/GT	12.7	19.0		56.5	49.3	10.9	9.1	10	AC/GT	13.8	18.1	B	55.1	54.2	10.7	9	10	AC/GT	11	18.1	B
[5]C	G_9	51.3	53.5	10.9	9.1	10	CA/TG	14.2	19.2		52.1	52.3	11	9.1	10	CA/TG	13.5	18.1		51.5	55.1	10.8	9.1	10	CA/TG	12.4	18.6	B
[6]A	**T_8**	56.5	52.3	10.8	9.1	9.9	AA/TT	13.8	18.0							AA/TT				58.7	54	10.6	9	9.9	AA/TT	13.3	16.9	
[7]A	**T_7**						AA/TT				60.9	55.9	10.3	8.7	9.9	AA/TT	13.4	16.9		59.3	56	10.3	8.8	9.9	AA/TT	13.1	18.3	
[8]A	**T_6**	57.5	56.8	10.5	8.9	10	AG/CT	12.6	17.6	B	54.4	50.5	10.9	9.1	9.9	AG/CT	12.3	17.0	B						AG/CT			
[9]G	C_5	56.2	53.3	10.8	9.1	10	GA/TC	11.4	18.6	B	52.7	53.8	10.7	8.9	9.8	GA/TC	11.4	17.4	B	51.1	54.7	10.8	9	9.9	GA/TC	12.6	16.4	B
[10]A	T_4	57.1	52.1	10.8	9	10	AT/AT	10.7	17.5	B	56.3	52.3	10.8	9.1	10	AT/AT	12.2	18.2	B	53	52.2	11	9.2	10	AT/AT	12.0	17.8	B
[11]T	A_3	50.7	53.9	11	9.1	10	TA/TA			B	52.1	57.3	10.8	9.1	10	TA/TA			B	54.5	54.7	10.7	9	9.9	TA/TA			B
[12]A	T_2	56.8	55.7	10.6	8.9	9.9	AC/GT			B	55.3	54.7	10.7	9	9.9	AC/GT			B	56.6	56.1	10.6	8.9	9.9	AC/GT			B
[13]C	G_1	53.9	53.9	10.8	9.1	10					52.2	57	10.8	9.1	10					55.9	55.4	10.7	9	9.9				
3'	5'																											

Table 7S. Sugar-phosphate backbone torsion angles and sugar ring pseudorotation phase of double stranded oligodeoxynucleotides that contained at position **7A** 2'-deoxyadenosine in one strand and at different positions **T6** (**U-1**) or **T7** (**U0**) or **T8** (**U+1**) 2'-deoxyuridine in the opposite strand. The structures of *ds*-oligodeoxynucleotides obtained under Molecular Mechanics (Amber 94 force field) calculation in solvation box, the sodium ions have been used as counterions to neutralize the negative charge of *ds*-DNA.

STRAND	double stranded oligodeoxynucleotide																					
	dA(U0)								**dA(U-1)**								**dA(U+1)**							
5'	α	β	γ	δ	ε	ζ	χ	P	α	β	γ	δ	ε	ζ	χ	P	α	β	γ	δ	ε	ζ	χ	P
^{1}T	---	-176.4	50.9	141.6	-178.7	-97.3	-110.4	175.7	---	-177.3	56	138.3	177.6	-91.2	-103.3	177.1	---	-179.3	54.6	133.2	-178.1	-89.8	-108.5	167.8
^{2}A	-61.8	-179.9	53.2	127	178.8	-101.6	-106.5	155.7	-58.7	172.6	56	128	-179.2	-101.2	-109.1	142.8	-59.6	163.8	58.1	118.1	179.1	-92.9	-119.7	129.3
^{3}T	-55.5	171.2	54.9	119	-178.5	-87.4	-112	127.9	-61.4	175.3	51.7	130.6	-178.9	-102.2	-104.8	143.6	-62.8	-178.2	50.9	137.8	-173.5	-124.6	-98.2	154.7
^{4}A	-60.3	171.4	51.5	118.4	-174.9	-91.5	-114.7	125.9	-68.7	173	54.8	109.6	-171.2	-85.1	-133.6	109.4	-62.7	179.9	48.7	138.6	-169.4	-94.2	-112.1	182.1
^{5}C	-55	160.1	53.8	107.5	-171.9	-106	-128.6	112.7	-64.2	170.7	56.7	122.3	173.4	-99.3	-120.4	136.2	-63.3	159.6	57.9	122.7	-175.6	-124.6	-116.4	130.3
^{6}A	-63.1	-176	51.7	140.2	171.9	-93.3	-93.9	183.6	**-58.9**	**-159.5**	**46**	**141.2**	**174.5**	**-88.9**	**-91**	208.7	-59.6	-175	48.3	141.4	173.7	-97.1	-117.3	185
^{7}A	**-65.6**	**-178.7**	**48.1**	**118.2**	**173.3**	**-91.2**	**-116.1**	129.6	-61	168.7	49.7	120.3	169.1	-94.1	-114.8	132.8	-59.6	-178.1	53.9	133.2	-173.2	-85	-112.5	160.5
^{8}A	-48.5	175.4	46.2	103	-171.3	-83.1	-132.6	86.6	-59.7	-179.7	41.9	82.2	-168.6	-67.4	-147.7	18.1	**-70.4**	**166.3**	**54.9**	**93.4**	**176.6**	**-86.3**	**-135.7**	95.2
^{9}G	-65.5	169.4	62	130	179.2	-90.6	-111.8	150.5	-62.3	172.6	66.7	128.2	-179.8	-86.3	-123.2	154.7	-49	174.1	51.2	135.3	178.5	-90.8	-114.4	156.3
^{10}A	-63	177	46.6	92.7	-177.4	-86.3	-135.6	86.5	-59.7	174.8	47.8	103.3	-174.4	-89.2	-137	104.1	-64.8	-164.8	34.3	122.7	174.1	-88.8	-112.9	138
^{11}T	-59.5	166.9	58.7	108	-179.8	-83.2	-124.9	111.1	-57.6	164.9	61.4	110.8	-174.3	-89.9	-129.2	114.5	-51.9	165.7	54.5	90.2	-179.7	-82.1	-145.1	83
^{12}A	-58.3	170.1	51.3	134.7	-177.5	-105.9	-116.6	151.7	-64.4	172.3	52.6	132.8	180	-109.1	-115	146.7	-61.3	179.2	54.4	137.7	176.6	-90.7	-106.2	172.3
^{13}C	-63.8	178.4	55.7	136.1	---	---	-122.8	148.3	-61.4	-177.7	52.4	139.8	---	---	-111.5	161	-60.4	170.7	56.3	127.8	---	---	-120.2	135
3'																								
3'	**2'-deoxyUracy at position T7**								**2'-deoxyUracyl at position T6**								**2'-deoxyUracyl at position T8**							
A_{13}	-63.2	170.4	49.4	144.9	---	---	-103.2	191.1	-66.3	171.2	50.4	148.4	---	---	-101.5	192.5	-64.1	175.5	52.8	133	---	---	-100.8	149.9
T_{12}	-53.7	170.7	49.5	135.1	-160.6	-139.6	-106.7	144.4	-57.8	173.6	49.5	137.7	-159.8	-140.3	-104.9	148.7	-61.6	156.7	64.4	92.3	-167.1	-79.5	-132.8	83.3
A_{11}	-60.4	-140.3	28.5	149.1	171.3	-86.9	-93.7	216.3	-72.8	-110.8	14	154.6	163.7	-86.8	-83.6	229.1	-65.9	-138.8	34.9	142.1	176.7	-99.8	-93	215.8
T_{10}	-62.9	-177.8	52.2	135.1	171.2	-96.1	-113.1	152.1	-60.5	168.5	58.6	136.6	168.7	-83.6	-111.7	150	-58	168.3	55.6	137.5	171.1	-92.3	-112.3	152.7
G_{9}	-53.9	169.1	54.6	129.8	175.5	-96.3	-114.2	150.6	-56.5	168.1	54.4	121.7	-175.1	-96.4	-120.5	133.9	-55.6	166	53	97.6	-172	-87.1	-140.3	93.3
T_{8}	-58	172.4	44.2	94.4	-174.1	-87.4	-134.3	89.3	-63.6	170.6	50.8	105.6	-178.8	-87.3	-122.2	106.9	**-64**	**169.6**	**50.4**	**114.9**	**-179**	**-89.2**	**-116.9**	121.8
T_{7}	**-55.5**	**-177.6**	**44.8**	**136.1**	**-177.8**	**-86.8**	**-115.9**	164.2	-56.1	174.8	55.5	115.3	-174.2	-89.9	-126.6	122	-57.3	168.1	54.9	103.6	-174.4	-83.7	-127.4	107.6
T_{6}	-65	166.8	54.3	127	178	-112.7	-104.6	140	**-65.8**	**171.8**	**54.6**	**126.1**	**175.9**	**-98.2**	**-106.4**	140	-57.7	-177.1	54.2	131.9	179	-85.9	-108.5	167
C_{5}	-49.8	170.1	53.2	99.4	-162.5	-87.2	-134.2	101.4	-52.4	160.5	55.5	88.4	-164.2	-84.6	-138.7	86.2	-58.3	162.2	50.2	82.1	-178.9	-83.9	-143.6	71.9
T_{4}	-68.2	172.4	51	109.4	168.5	-83.6	-113.2	116.1	-59.7	178.5	54	134.3	179.5	-87.8	-102.2	162.6	-60.5	167.5	58.1	118.7	-177.5	-86.6	-116.3	128.1
A_{3}	-59.4	-178.5	52.1	140.3	-174.7	-88.1	-113.4	184.6	-63.4	-179.5	45.1	125.4	179.6	-111.7	-109	138.1	-63.9	-170.3	41.2	134	177.6	-90.4	-109.9	203.5
T_{2}	-65.3	-172	54.7	135.5	-176.9	-112.6	-122.6	153.9	-63.5	179.6	57.6	134.6	176.8	-89.9	-108.4	159.7	-65.3	175.9	59.8	138.9	-174.6	-113.8	-114.4	155.3
G_{1}	---	168.1	57.7	142.6	179.2	-99	-131.8	165.4	---	-179.5	47.4	132.4	-170	-112	-135.3	145.5	---	177.6	59.9	91.4	-173.1	-82.1	-153.1	79
5'																								

Table 7S continued. Sugar-phosphate backbone torsion angles and sugar ring pseudorotation phase of double stranded oligodeoxynucleotides contained at position **7A** (5'*S*)-5',8-cyclo-2'-deoxyadenosine in one strand and at different positions **T6** (**U-1**) or **T7** (**U0**) or **T8** (**U+1**) 2'-deoxyuridine in the opposite strand. The structures of *ds*-oligodeoxynucleotides obtained under Molecular Mechanics (Amber 94 force field) calculation in solvation box, the sodium ions have been used as counterions to neutralize the negative charge of *ds*-DNA.

STRAND	double stranded oligodeoxynucleotide																							
	cdA(U0)								**cdA(U-1)**								**cdA(U+1)**							
5'	α	β	γ	δ	ε	ζ	χ	P	α	β	γ	δ	ε	ζ	χ	P	α	β	γ	δ	ε	ζ	χ	P
^{1}T	---	-176.9	50.6	139.4	-175.7	-94.4	-106.2	174.5	---	164.7	49.7	133.8	-178	-92.1	-116.6	166	---	166.3	50.8	142.3	175.9	-98.9	-113.5	169
^{2}A	-70.3	168.1	60.6	115	176.2	-91	-117.7	125.2	-56.1	169.9	55	131.4	-179.7	-101.8	-111.3	150.9	-61.4	-166	45.6	142	178.3	-95.3	-102.8	195.1
^{3}T	-55.7	171.7	52.7	111.5	-177	-87.1	-117.5	112.5	-63.6	179.6	52.1	122.5	179.8	-89.1	-107.7	135.6	-62.8	166.2	58.4	107.7	-173.6	-87.5	-122.9	108.5
^{4}A	-60.8	173.3	54	125.4	-177	-95	-112.9	140	-59.8	164.1	54.5	96	-177.5	-87.1	-135.7	93.4	-67.8	165.7	56.1	97.7	179.4	-87.5	-131.8	83.5
^{5}C	-61.6	171	54.7	100.9	-173.4	-86.7	-123.9	101.1	-58.1	169.5	57.4	114.8	-174	-88.1	-124.4	121.9	-60.1	167.5	59.7	112.1	-171.7	-85.8	-128.8	113.7
^{6}A	-62.5	165.8	56.1	133.4	178.9	-85.1	-104.5	149.4	-57.6	175.1	43.3	142.8	-179.9	-81.3	-107.4	158.5	-60.9	171	53	142.1	178.2	-86.3	-101.4	161.8
^{7}A	-50.8	-80.5	-68.4	140	-157.4	-59.8	-158.7	**288.5**	-54.2	-80.7	-74.8	143.1	-162.5	-63.3	-163.9	**286.2**	-54.7	-79.1	-66.8	139.1	-155.4	-60.7	-159.2	**288.2**
^{8}A	-72.1	170.2	68.8	144.8	171.3	-91.4	-120.8	174.4	-71.8	170.3	69.5	142.3	-178.4	-106	-122.2	169.3	-69.9	169.5	67.5	147.9	-176.6	-116.5	-117.8	175
^{9}G	-61.9	-164.3	46.4	132.1	-172.9	-89.6	-126.2	155.4	-63.6	-174.4	50.9	144.5	169.2	-87.3	-117.1	170.3	-60.8	-176.9	49.6	145.4	177.8	-86	-122.8	178.1
^{10}A	-62.4	177.5	48	108	178.2	-88.4	-121	116.4	-68.5	-145.9	33.8	136.3	176.9	-92.4	-104.1	173.3	-67	-173	43.8	117.5	-171.4	-92.8	-125.5	126.8
^{11}T	-56.9	165.3	61	99.7	-175.7	-85.1	-136	99.6	-56.7	163	55.2	86.8	175.9	-85.1	-141.6	70.4	-63.4	162.4	58.6	94.2	178.1	-84.1	-135.4	83.5
^{12}A	-60.2	174.7	50.3	134.2	179	-91.3	-107	158	-57.3	173.7	62.2	139.7	-175	-86	-114.7	172.2	-59.5	-178.3	48	133.8	-179.3	-98.8	-112.5	163.8
^{13}C	-58.4	172.9	52.3	126.6	---	---	-115.5	131.6	-64.2	171	49.1	131.5	---	---	-111.2	136.2	-61.9	170.9	60.7	137.6	---	---	-110.1	151.3
3'																								
3'	**2'-deoxyUracy at position T7**								**2'-deoxyUracyl at position T6**								**2'-deoxyUracyl at position T8**							
A_{13}	-62.1	178.8	47	140.9	---	---	-103.2	188.3	-64	168.4	53.2	149	---	---	-107.8	186.4	-65	175.5	50.1	142	---	---	-98.1	191.5
T_{12}	-55.1	166.3	54.1	132.2	-164.2	-132.5	-110.4	142	-54.9	-179.2	47.1	140	-164.6	-137.5	-105.6	152.3	-53	178.7	47	138.7	-164.3	-132.8	-103.9	153.6
A_{11}	-69.6	-136.7	37.4	142.1	171.3	-88	-92.8	217.9	-65.7	-128.3	16.3	152.3	161.9	-88	-94	217.4	-69.5	-117.8	16.8	153.2	157.3	-85.4	-84	226.8
T_{10}	-60.6	-176.6	57	142.4	169.5	-97.3	-118.5	164.3	-64.1	173.8	59.6	141.1	173	-91.5	-112.5	159.4	-60.8	176	54	135.7	172.3	-88.6	-114.1	149.7
G_{9}	-68.9	167.5	48.5	118.1	173.6	-103.3	-122.8	128.4	-50.8	167.9	52.2	122.2	-174.1	-102.3	-128.5	133.7	-57	169.8	53.1	122.8	-179.4	-93.8	-124.5	136.6
T_{8}	-63.2	172.8	64.1	127	-169.2	-82.6	-122	147.4	-62.3	-179.7	54	123.3	178.8	-86.3	-113.6	146.3	**-62.2**	**167.5**	**55**	**96.7**	**-179.5**	**-85.9**	**-131.2**	**95.4**
T_{7}	**-58.7**	**161.1**	**53.1**	**87**	**-176.4**	**-77.2**	**-139.9**	**77.5**	-59.2	163.5	52.3	86.7	-174.7	-79.2	-134.9	**73**	-58.2	169.8	55.1	117.1	-176.4	-84.1	-115.4	126.8
T_{6}	-68.3	168.8	55.9	116	-179.6	-90	-110.8	125.3	**-63**	**166.9**	**56.4**	**117**	**-179.6**	**-87.5**	**-118.6**	**126.6**	-61.9	170	52.6	113.7	-178.2	-90	-126	123.4
C_{5}	-46.2	161.5	63.6	88.1	-168.3	-81.6	-126.5	90.6	-59.7	165.5	55.1	91.2	-168.8	-87.4	-136	89.2	-57.2	164.7	54.7	86.4	-169.8	-81.4	-148.4	84.7
T_{4}	-73.7	173.2	51	109.4	173.1	-86.8	-111.1	117.3	-56.1	179.1	54.4	135.9	-179.6	-85.8	-107.9	162.5	-62	169.3	63.2	131.8	178.4	-84.4	-106.6	154.6
A_{3}	-56.7	179.6	52.7	142	-170.1	-84.8	-120	184.6	-68.6	-177	42.9	122.2	173.1	-104.3	-113.3	134.8	-61.2	179.8	48.2	118.7	-179	-103.7	-116	128.6
T_{2}	-75.6	173.7	62.2	139.5	178.3	-116.7	-112.7	156	-65	169.7	61.6	130.2	-176.1	-92.1	-118	141.8	-65.6	-178.3	58	129.7	177.4	-88.7	-116.3	149.8
G_{1}	---	-172.7	56.9	128.1	-165.4	-104.6	-132.5	141.9	---	-176.4	58.5	110.2	-172.7	-92.5	-136.4	111	---	172.8	57.5	86.6	-173.7	-80	-157.6	70.4
5'																								

Table 7S continued. Sugar-phosphate backbone torsion angles and sugar ring pseudorotation phase of double stranded oligodeoxynucleotides contained at position **7A** 2'-deoxyadenosine in one strand and at different positions **T6** (**Ap-1**) or **T7** (**Ap0**) or **T8** (**Ap+1**) the apurinic/apyrimidinic site (**Ap**) in the opposite strand. The structures of *ds*-oligodeoxynucleotides obtained under Molecular Mechanics (Amber 94 force field) calculation in solvation box, the sodium ions have been used as counterions to neutralize the negative charge of *ds*-DNA.

STRAND	double stranded oligodeoxynucleotide																							
	dA(Ap0)								**dA(Ap-1)**								**dA(Ap+1)**							
5'	α	β	γ	δ	ε	ζ	χ	P	α	β	γ	δ	ε	ζ	χ	P	α	β	γ	δ	ε	ζ	χ	P
^{1}T	---	167	50.1	139.5	179.9	-90.8	-100.6	178.5	---	-171.1	41.4	142.7	177.2	-101	-118.7	175	---	170.8	50.2	136.9	-174.3	-95.7	-108.2	173.9
^{2}A	-60.1	168	53.8	124	-173.7	-106	-107.6	135.3	-61.4	-176.9	54.3	136	-178.7	-97.9	-109.4	166.7	-62.5	168.3	56.3	135.9	-172.2	-131.5	-97.6	149.4
^{3}T	-65.4	163.7	59.1	103.1	-176.2	-81.2	-124.1	94	-65.4	173.7	55.6	131.8	-174.3	-119.3	-107.9	142.9	-58.9	167.7	54.1	141.6	179.2	-88.9	-101.8	165.1
^{4}A	-69	174	55.9	115.4	-176.5	-85.2	-126.3	124.4	-64.8	-174	49.4	136.8	-179.9	-86.1	-108.4	182.1	-74.5	177.4	53.3	104.6	-171.9	-86.2	-129.5	107
^{5}C	-62.9	167.6	53.2	93.5	-179.5	-88.1	-137	80.3	-60.8	168.4	53.8	112.2	174.4	-97.4	-121.3	120.5	-65.5	167	55.3	92.9	173.9	-89.2	-130.6	80.8
^{6}A	-56.1	176.2	57.8	143.1	177	-87.3	-100.3	183.8	-57.9	-161.3	46.3	145.7	176.5	-95.7	-92.6	192.1	-49.2	179.6	56.7	143	178.1	-94	-93.2	194.6
^{7}A	-61.5	168.2	50.1	84.6	-174.9	-85.3	-146.3	78.7	-65.3	175.3	48.2	127.5	179.1	-105.4	-108.8	140.9	-62.2	179.8	40.5	125.7	171.4	-90	-103.9	143.8
^{8}A	-63.4	-174.6	50.4	132.7	173.9	-94.4	-112.1	171.6	-63.3	175	54.1	118.1	-174.1	-88.2	-132.1	126.4	-54.6	177.9	46.7	133.3	172.8	-104.8	-115.1	145.4
^{9}G	-51.9	172.6	58.8	135	-177.7	-96.2	-107.9	154	-57.1	176.8	46.9	136.8	162.7	-88.6	-109.9	156.7	-62.2	-161.1	43.9	140	175.2	-88.5	-113	179.8
^{10}A	-69.1	-175.2	45	118.7	177.4	-83.8	-118	133.4	-62.8	-134.9	31.3	139.6	-179.3	-88.2	-103.4	201.7	-58.9	178.6	50.4	110.7	-175.1	-90.8	-123.9	117.4
^{11}T	-57.4	168	54.3	100.3	-175.6	-89.4	-133.9	97.7	-58.1	161.9	57.3	100.7	176.4	-83.7	-122	105.3	-61.2	165	55.5	94.1	-177.1	-85.4	-131.9	89.9
^{12}A	-62.5	179	47.2	140.4	-174.8	-107.4	-106.5	163.1	-56.8	171.4	52.3	122.2	-175.8	-95.1	-121.7	133.5	-62.5	172.8	54.1	134.6	173.4	-104	-107.1	157
^{13}C	-67.8	169.4	61.4	132.9	---	---	-114.7	141.5	-60	167.1	58	131.8	---	---	-117.4	139.3	-58	172.3	60.3	141.2	---	---	-115	154.1
3'																								
3'	**Ap at position T7**								**Ap at position T6**								**Ap at position T8**							
A_{13}	-61	173.4	56.3	142.1	---	---	-108.5	157.8	-59.7	168.7	59	146.1	---	---	-117.2	176.4	-59.9	172.8	51.6	136.9	---	---	-96.8	155.6
T_{12}	-59.1	170.9	57.4	98.8	-179.6	-88.1	-137.9	92.6	-58.2	170.9	50.6	129.1	-176.7	-127.8	-115.5	139.1	-55.2	167.1	52.9	94	-178.2	-84.5	-125	87.7
A_{11}	-64.7	-129.2	22.6	150.1	168	-89.6	-93.5	210.7	-62.2	-150.7	32.3	143.7	173.8	-89.1	-100.1	202.3	-72.7	-109.1	14.1	153.4	172.3	-86.5	-93.1	222.8
T_{10}	-62.7	176.7	55.4	138.2	171.8	-88.5	-118.4	151.1	-58.4	179.9	50.2	136.9	175.3	-97.8	-112.5	150.7	-60.1	165.9	59.3	132.3	165.6	-82.7	-116.3	145.4
G_{9}	-58.8	175.1	54.2	136	175.9	-99.3	-109.1	162.8	-59.5	156.7	63.1	107.8	179	-88.7	-134.6	115.7	---	171.2	70.2	124.8	-177.1	-90.6	-115.8	144.7
T_{8}	-110.2	-179.6	60.5	100.2	-174.4	-81.8	-137.6	86.2	-63.2	-179.2	52.6	118.9	-175.9	-91.7	-112.7	127.7	---	---	---	---	---	---	---	---
T_{7}	---	---	---	---	---	---	---	---	---	-171.8	55.4	130.4	176.8	-95.3	-117.9	153.1	-55.4	164.3	57.9	110.8	---	---	-127.5	116.3
T_{6}	-63	170.2	54.7	135.4	---	---	-109	148.9	---	---	---	---	---	---	---	---	-60.8	173.9	53.6	112.9	-178.7	-88.6	-122	117.6
C_{5}	-57	164.6	55.3	89.4	-169.6	-84.9	-138.6	85.1	-51.7	164.7	56.7	82.6	---	---	-142.3	72.8	-54.2	163.9	53.3	102.8	-177.1	-94.2	-118	108
T_{4}	-59	-176.1	53.1	130.1	-179.4	-89	-111.7	152	-62.2	172.2	46.7	109.5	170.1	-84.6	-111.6	116.9	-68.5	173.8	53.6	108.2	179	-86	-114.8	115.3
A_{3}	-70.7	-173.4	51	131	172.4	-100.2	-116.9	156.1	-59.1	-179.4	48.9	130.9	-169	-89.8	-122.2	159.6	-66.2	179.9	57.3	141.5	-173.9	-91.2	-115.6	178.4
T_{2}	-65.9	-178.5	61.6	140.2	177.7	-97.1	-116.7	162.9	-70.2	179.2	57.9	137.3	-178.1	-112.9	-110.8	152.9	-66.1	173.3	68.4	144.1	-173.9	-120.6	-123.5	161.5
G_{1}	---	173.4	52.3	80.1	-172.3	-78.9	-168.3	58.9	---	-171.1	52.1	138.7	-174.4	-100.8	-122.7	161.6	---	162.4	54	84.1	-167	-71.2	-164	31
5'																								

Table 7S continued. Sugar-phosphate backbone torsion angles and sugar ring pseudorotation phase of double stranded oligodeoxynucleotides that contained at position **7A** (5'S)-5',8-cyclo-2'-deoxyadenosine in one strand and at different positions **T6** (**Ap-1**) or **T7** (**Ap0**) or **T8** (**Ap+1**) an apurinic/apyrimidinic site (**Ap**) in the opposite strand. The structures of *ds*-oligodeoxynucleotides obtained under Molecular Mechanics (Amber 94 force field) calculation in solvation box, the sodium ions have been used as counterions to neutralize the negative charge of *ds*-DNA.

STRAND	double stranded oligodeoxynucleotide																							
	cdA(Ap0)								**cdA(Ap-1)**								**cdA(Ap+1)**							
5'	α	β	γ	δ	ε	ζ	χ	P	α	β	γ	δ	ε	ζ	χ	P	α	β	γ	δ	ε	ζ	χ	P
^{1}T	---	174.2	50.9	142.6	-178.6	-109.1	-125.1	164.3	---	-178.7	43.3	142.1	178.7	-98.8	-109.7	181.1	---	168.3	45.9	145.8	179.4	-98.9	-111.2	171.5
^{2}A	-63.5	-172.7	51.4	140.7	174.7	-90	-104.2	192.4	-62.4	174.4	57.4	126.4	-176.6	-95.8	-120.6	146.8	-63.1	-173.7	50.7	136.3	177.1	-89.1	-100.6	179.2
^{3}T	-64.1	169	57.4	105	-177.3	-87	-128.7	103.8	-71.6	177.6	57.3	131.8	177.5	-104.7	-105	147.3	-63.1	174.3	47.9	112.9	-178	-93.1	-113.1	114.9
^{4}A	-63.9	170.2	54.3	108.7	-175.7	-86.2	-123.7	110.3	-61.8	-178.7	54	129	-176.6	-87.3	-114.8	154.2	-61.6	163.3	56.3	96.2	-176	-85.8	-137.8	85.8
^{5}C	-60.2	171	54.7	106.1	-172.1	-86.2	-124.2	107	-62.4	165	57.6	97	-177.3	-89.6	-135.5	96.2	-61	172.4	58.9	113.6	-176.5	-88.1	-122	118.5
^{6}A	-62.6	166	56.8	140.9	-179.3	-83.4	-102.7	157	-62.9	179.1	53.6	141.9	178	-85.1	-97.4	167.9	-55.8	170.4	47.3	138.1	-178.7	-82.1	-110.1	153.6
^{7}A	-51.1	-82.7	-70.7	137.5	-157.4	-68.7	-153.7	**290.9**	-52.9	-87.5	-72.9	143.2	-156.5	-56.7	-167	**286**	-54.6	-83.7	-70.3	143.7	-160.2	-57.9	-166.1	**284.4**
^{8}A	-66.7	172.1	63	142.3	173.1	-97	-108.3	177.1	-73	165.4	69.5	136.6	-178.6	-103.1	-135.7	155.9	-73.8	171	69.5	138.6	176.3	-95.7	-121.2	166.9
^{9}G	-59.1	-178.1	53.6	138.3	-177.6	-93.7	-116.5	159.2	-64.5	-167.8	52.9	141	175.9	-87	-112.3	177.5	-60.8	-175.8	51	131.2	-179.9	-93.8	-129.5	148.7
^{10}A	-64.2	-156.9	27.2	140.5	178.1	-95.2	-103	175.7	-63	-165.2	35.5	125.8	179.2	-92.7	-110.9	143.7	-69	-168.6	48.6	114.9	-176.6	-87	-119.9	125.5
^{11}T	-57.8	162.9	57.4	86.7	179.6	-86	-145.9	71.5	-59.1	164.1	59.3	99.5	-175.4	-86.2	-130.6	97.1	-58.6	164.7	57.9	100	-173	-85.3	-125.9	100.4
^{12}A	-58.1	179.2	58.3	143.5	-176.7	-85.2	-108.3	178	-65.6	168	59.8	119.4	177.3	-87.6	-127.2	135	-66.5	169.1	51.7	120.7	170.2	-96	-115.6	136.1
^{13}C	-63.4	170.2	47.1	127.6	---	---	-107.1	132.6	-57.3	175.7	52.7	137.2	---	---	-106.9	147.4	-53.9	169	63.8	138.6	---	---	-118.9	154.2
3'																								
3'	**Ap at position T7**								**Ap at position T6**								**Ap at position T8**							
A_{13}	-58.9	169.9	55.9	145.9	---	---	-113	179	-60.5	175.9	54.7	140	---	---	-117.8	171.5	-70.6	165.2	59.1	140	---	---	-118.4	170.7
T_{12}	-53.8	174.4	47.3	131.7	-172.8	-129.7	-111.3	144	-57.5	167.6	56.2	124.5	178.2	-115.9	-111.6	137.3	-53.7	179.6	44.1	138.9	-162.9	-139.6	-101.4	153.9
A_{11}	-70.6	-120.8	25.6	148.2	165.6	-85.1	-94.4	222.1	-67.6	-123.8	22.1	151.2	172.3	-88.2	-91.4	220.9	-76.7	-110.9	16.8	152.6	158.1	-83.2	-83.8	228.9
T_{10}	-65.5	174.1	53.6	136.8	165	-89.4	-109	151.7	-66.8	175.4	53.8	132.4	168	-90.7	-112.9	145.2	-60.7	174.6	62.4	137.3	166.7	-82.7	-117.2	153.3
G_{9}	-50.7	165.6	53.2	128.9	-172.6	-102.5	-118.5	142.8	-59	165.1	62.9	122.6	-176.9	-92.2	-121.1	137.3	-71.2	173	64.6	129.9	174.3	-96.2	-113	153.2
T_{8}	-120.9	172.1	56.9	98.7	178.9	-88.2	-128.8	97.4	-61.0	171.2	59.6	115.1	-177.7	-91.2	-122.5	121.2	---	---	---	---	---	---	---	---
T_{7}	---	---	---	---	---	---	---	---	---	179.6	54.1	99.8	-169.6	-85.2	-144.3	97.5	-54.6	163.5	55.6	111.2	---	---	-123.7	119.4
T_{6}	-65	168.8	54.9	129	---	---	-120.1	141.8	---	---	---	---	---	---	---	---	-58.3	169.4	51.7	106.1	-179.1	-87.2	-122.8	113.6
C_{5}	-53.7	163.2	56.1	94.2	-166.5	-86.5	-138.8	91.4	-49.6	162.3	59.5	91.6	---	---	-132.6	94.8	-51.9	170	45.8	99.2	-179	-85	-119.5	104.6
T_{4}	-55.4	171.7	54.6	128	-178.8	-88.7	-114.4	143.9	-64.5	-178.1	49.4	117.6	177.8	-87.6	-111.7	129.4	-59.5	166.7	54.2	109.1	-179.3	-82.1	-117.4	117.2
A_{3}	-67.1	160	54.6	87.6	177.1	-84.7	-135.8	74.4	-57.5	-175.2	45.9	140.6	176.8	-91.1	-113.4	177.3	-56.7	-170	47.1	135.3	-177.3	-88.5	-109.6	188.8
T_{2}	-63.2	179.2	58.2	128.3	-172.4	-89	-113.4	143.5	-70.1	178.3	54.6	135.8	179.3	-115	-108.9	152.7	-69.7	177.2	59	137.4	174.8	-108.5	-114.3	159.5
G_{1}	---	176.9	48.7	127.4	-176.9	-102.6	-125.6	145.3	---	171.8	51.5	125.6	-169.1	-101.6	-130.7	135.9	---	173.8	51.6	133.6	-171.5	-108.9	-129	149.7
5'																								

Table 7S continued. Sugar-phosphate backbone torsion angles and sugar ring pseudorotation phase of double stranded oligodeoxynucleotides that contained at position **7A** 2'-deoxyadenosine in one strand and at different positions **T6** (**Ga-1**) or **T7** (**Ga0**) or **T8**(**Ga+1**) a single strand break e.i. gap (**Ga**) in the opposite strand. The structures of *ds*-oligodeoxynucleotides obtained under Molecular Mechanics (Amber 94 force field) calculation in solvation box, the sodium ions have been used as counterions to neutralize the negative charge of *ds*-DNA.

STRAND	double stranded oligodeoxynucleotide																							
	dA(Ga0)								**dA(Ga-1)**								**dA(Ga+1)**							
5'	α	β	γ	δ	ε	ζ	χ	P	α	β	γ	δ	ε	ζ	χ	P	α	β	γ	δ	ε	ζ	χ	P
^{1}T	---	172.1	43.5	139.9	-177.2	-85.6	-112.4	177.8	---	-167.8	46.4	138.2	178.4	-105.2	-105	155.7	---	-177.3	44.6	137.7	179	-101.6	-116	174.2
^{2}A	-61.4	168.3	54.2	109.2	-175.4	-97.7	-127.3	113.2	-55.4	-160.9	34.2	145.9	174.7	-93.2	-100.9	205.3	-61.1	177.2	56.1	128.1	-179.8	-92	-109.8	150.1
^{3}T	-61.1	173.9	55.2	116	-178.1	-85.4	-118.7	126.5	-59.5	170.5	53.6	126.5	-175.1	-105.1	-113.9	136.8	-64	171.8	56	121	-179.9	-100.7	-113.3	130.4
^{4}A	-58.6	169.4	51.6	118.8	174	-94.4	-104.8	131.5	-71.1	-161.4	35.9	131.7	174.3	-88.9	-109.6	183.6	-64.1	-165.1	39.5	137.6	169.3	-90	-106.3	181.8
^{5}C	-56.3	170.9	49	93.3	-177.2	-88	-130.6	78.5	-54.1	162.2	61.6	117.3	172.5	-96.1	-121.8	128.2	-57.2	176.1	55.1	115.6	-176	-91.1	-124.1	123.1
^{6}A	-59.4	-179.1	53.3	132	175.6	-87.9	-100.8	176.7	-58.5	-162	43.8	137.1	178.4	-88.3	-109.6	175.3	-58.2	173.3	51.8	131	-176.9	-110.4	-103.8	147.2
^{7}A	-55.8	163.2	50.7	88.1	-177	-85.3	-145.2	81.2	-55.4	173.1	43.2	106.2	-178	-86.7	-127.3	110.4	-65	179.6	49.6	133.3	-179.9	-101.4	-116.9	152.5
^{8}A	-58.4	177.9	56.2	142.3	-174.9	-88.8	-107	177	-55.1	164.3	55.6	101.3	-173.8	-87.2	-134.7	105.5	-65.6	-172.8	52.4	125.2	176.6	-92.9	-109.3	152.3
^{9}G	-65.3	160.9	56.7	85.9	179.3	-88.2	-143.1	80.5	-59.9	171.3	51.1	136.8	-177	-121.4	-109.2	151.2	-54.9	160.5	61.7	103.5	-177.7	-86.9	-135	105
^{10}A	-61.7	-174.4	54.6	136	172.4	-93.3	-104.2	171.8	-62.1	-176.8	49.9	141.2	178.3	-92.9	-111.7	179.8	-57.5	172.9	49.5	125.9	-174.4	-93.2	-121.1	139.3
^{11}T	-59.7	176.8	53.5	123.1	-174	-85.2	-118.6	137.3	-60	163.8	59.2	95.9	-177.6	-88.2	-142.8	90.4	-62	166.9	60	94.5	-179.5	-86.3	-143.7	93.6
^{12}A	-62	173	44.8	128.8	-172.5	-128.9	-110.2	137.9	-60	-171.7	48.9	140.5	-178.4	-92.2	-95.4	182.9	-56.1	179.4	48.1	137.5	-177.2	-94.7	-102.4	160.6
^{13}C	-59	160.2	63.8	139.9	---	---	-125.6	159.6	-59.2	164.6	55.4	119.4	---	---	-118	125	-63.2	165	56.3	104.7	---	---	-127.3	103.1
3'																								
3'	**Ga at position T7**								**Ga at position T6**								**Ga at position T8**							
A_{13}	-62.1	176.6	54.6	141.3	---	---	-107.3	157.4	-64.3	-174.1	42.6	143.9	---	---	-99.2	202.5	-64	173.1	43.3	137.9	---	---	-101.7	146.7
T_{12}	-53.6	164.8	58.5	105.7	-179.8	-94.3	-132.6	108.7	-62.2	177.1	48.7	133.8	-169.1	-125.3	-99	143.1	-53.5	165.2	53.7	116.2	-173.3	-84	-117	124.7
A_{11}	-67.9	-170.8	50.4	141.3	174.8	-85.8	-102.5	196.1	-61.4	179	53.8	133.5	178.4	-87.7	-110.4	160	-56.9	169.3	54.4	110.6	179.8	-90.2	-117.4	117
T_{10}	-58.9	178.8	57.9	137.9	-174.8	-119.8	-120.6	158.7	-59.4	176.9	57.7	133.4	179.5	-102.1	-114.8	152.9	-62	-174.7	53.2	113.4	-179.1	-87.4	-124.8	121.5
G_{9}	-58.2	162.8	59.8	137	178.8	-118.5	-111.3	150.9	-57.8	162.6	53.5	81.2	-174.1	-81.6	-153.8	65.5	-72	---	54.9	142.3	173.3	-95.8	-114.1	178.9
T_{8}	---	-164.7	48	123.9	-173.6	-90.8	-127	150	-53.9	-173.5	52.3	133.8	-179.2	-88	-110.7	159.8	-26.2	---	---	---	---	---	---	---
T_{7}	---	---	---	---	---	---	---	---	---	179	46.8	135.8	170.0	-95.9	-127.7	165.6	-62.5	173.4	51.5	123.2	---	---	-118.6	128
T_{6}	-61.9	171.3	45.2	131.4	---	---	-108.8	136.4	---	---	---	---	---	---	---	---	-60.4	174.7	50.5	118.8	-177.8	-88.9	-113.1	130.2
C_{5}	-61	167.9	56.7	119.8	-172.1	-87.4	-112.6	130.5	-65.3	169.2	42.7	88.6	---	---	-109.9	51.9	-62	166.2	54.5	95.9	-171.9	-81.8	-129.5	91.9
T_{4}	-62.5	173.6	56.4	110.1	-176.3	-89.3	-122.4	113.8	-61.1	167.7	54.3	107.5	-174.9	-89.1	-116.5	113	-61.2	171.3	58.1	115.3	-177.1	-85.1	-117.5	124.9
A_{3}	-68.2	-165.1	47	135.7	176.3	-91.7	-111.4	173.4	-61.4	-165.4	48.8	140.6	177.8	-89.4	-97.2	197.4	-65.1	-164.2	44.6	141	172.6	-97.1	-94.8	197.5
T_{2}	-66.1	172.4	60.7	139.4	178.9	-105	-115.7	155	-63.4	-178.5	50.1	134.7	174	-107.7	-107.7	150.8	-62.9	176.7	55.4	130	-178	-105.1	-124.5	140.2
G_{1}	---	-178.6	49.8	127.6	178.5	-103.9	-106.2	142.9	---	-173.8	48.6	147.2	175.3	-96.5	-105.4	190.9	---	178.3	54.3	139.2	-175	-93.8	-127.2	172.8
5'																								

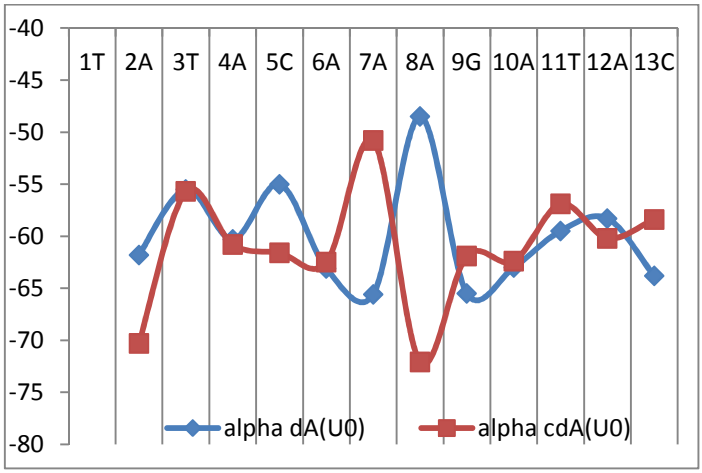
Table 7S continued. Sugar-phosphate backbone torsion angles and sugar ring pseudorotation phase of double stranded oligodeoxynucleotides that contained at position **7A** (5'S)-5',8-cyclo-2'-deoxyadenosine in one strand and at different positions **T6** (**Ga-1**) or **T7** (**Ga0**) or **T8** (**Ga+1**) a single strand break e.i. gap (**Ga**) in the opposite strand. The structures of ds-oligodeoxynucleotides obtained under Molecular Mechanics (Amber 94 force field) calculation in solvation box, the sodium ions have been used as counterions to neutralize the negative charge of *ds*-DNA.

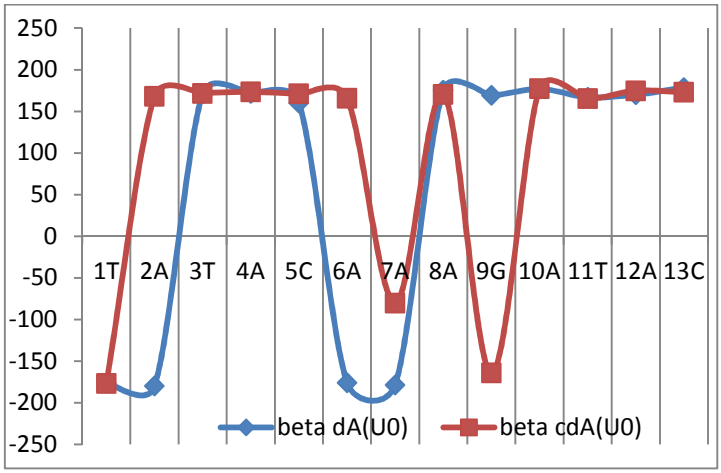
STRAND	double stranded oligodeoxynucleotide																					
	cdA(Ga0)								**cdA(Ga-1)**								**cdA(Ga+1)**							
5'	α	β	γ	δ	ε	ζ	χ	P	α	β	γ	δ	ε	ζ	χ	P	α	β	γ	δ	ε	ζ	χ	P
^{1}T	---	177.1	45.3	140.6	-173.5	-88.8	-104.4	185.9	---	160.7	52.8	144.1	176.2	-107.5	-110	167.7	---	168.2	51.2	139.8	174.9	-91	-106.3	176.3
^{2}A	-67	156.3	73.7	114.5	-173.9	-96	-124.7	123.9	-60.7	-175.9	53	137.4	178.4	-91.1	-112	175.2	-63	175.8	51.6	115.7	180	-102.1	-120.2	123.7
^{3}T	-70.9	179	50.6	115.9	-179.3	-88.9	-111.7	123.9	-66.8	170.8	58.5	91.6	-175.9	-82.8	-140.4	84.9	-64.2	179.9	53.5	124.1	-179.1	-93	-109.6	137.8
^{4}A	-54.9	163.6	55.6	119.5	-175.8	-107.9	-111.4	128.3	-61.7	-178.1	49	131.8	-179.9	-98.6	-103.9	159.9	-58.7	163.7	56.2	96.1	-175.8	-83.5	-139.4	89.4
^{5}C	-58.7	179.7	42.4	115	-177.7	-83.2	-126	124	-57	152.6	73.7	114.5	-166.2	-81.6	-130.7	123	-61.4	172.9	59.8	123.9	-174	-87.8	-116	140.5
^{6}A	-60	165.2	55.7	136.7	-177.4	-80.2	-110.1	151.6	-74.5	175.4	42.7	135.8	174.6	-89.9	-101.1	151	-58.8	162.9	51.8	127.9	179.1	-86.3	-118.2	138.7
^{7}A	-55.2	-82.4	-64.9	144	-162.9	-64	-154.2	281.4	-46.4	-72.4	-48.1	173.6	176.2	-69.7	-138.5	236.4	-52.3	-76.3	-70.9	138	-156.5	-63	-164.9	289.8
^{8}A	-71.9	168	70.9	136.8	178.2	-95.2	-104.4	172	-57.5	162.4	41.4	121.1	-178.1	-105.4	-111.6	135	-65.9	166.9	69.9	142.1	179.5	-89.6	-122.8	179.4
^{9}G	-64.4	174.1	54.1	133.7	-164.2	-134.3	-114.5	143.6	-58.9	161.5	63.8	105.2	-171.4	-86	-138.3	100	-65.7	179.8	50	129.9	-179.4	-103.5	-119.6	140.8
^{10}A	-61.3	179.1	45.4	136.5	-177.6	-91.8	-112.4	182.8	-73.4	-177.4	52.2	134.5	175.6	-85.5	-108.2	173	-65.9	-168.5	48.2	135	178.4	-94.8	-103.8	166.4
^{11}T	-57.5	165.4	57.2	116.7	-178.3	-87.2	-119.6	126.6	-58.4	167.2	53.8	124.2	-176.4	-116.7	-124.6	132.9	-64.3	170.6	57.4	96.7	-172.6	-83	-129.4	94.8
^{12}A	-57.9	170	50	120.3	-168.2	-123.1	-127.8	126.4	-64.9	-163.8	49.3	144.6	-172.6	-88.8	-98	198.2	-62.4	170.9	54.7	132.4	169.8	-106.4	-99.1	154.7
^{13}C	-59.6	177.8	52.8	143.5	---	---	-101.9	179.1	-65.4	166.7	50.6	130.1	---	---	-92.5	135.9	-59.9	179.4	57.1	140.1	---	---	-117.9	159.1
3'																								
3'	**Ga at position T7**								**Ga at position T6**								**Ga at position T8**							
A_{13}	-59.7	-176.9	48.6	141.4	---	---	-93.2	184.8	-60.4	176.9	43.4	142	---	---	-111.5	191.4	-56.9	170.8	52.5	138.9	---	---	-114.5	154.4
T_{12}	-56.8	168.2	57.5	95.7	-177.1	-88.7	-141.8	90.6	-61.4	178.3	48.3	127.8	-164.6	-136.1	-115.3	134.5	-56.6	163.4	56.3	96.1	-175.9	-86.8	-135.2	91.3
A_{11}	-67.1	-167.7	45.9	143.2	173.5	-88.2	-103.1	190.8	-69.7	177.9	55.1	137.7	173.2	-86.8	-103.7	162.9	-65.5	-159.4	39.7	135.7	-179.2	-90.8	-108.4	167.1
T_{10}	-57.1	-173.2	53.9	138.7	-178.3	-110.8	-117.6	163.1	-57.9	-175.3	51.4	144.4	-177.4	-106.3	-104.4	173.7	-70.5	175.6	59.6	132	171.7	-94.4	-113.9	151.2
G_{9}	-70.7	168.9	58.7	125.9	173.7	-103.2	-123.2	137.9	-53.7	167.4	55.2	116.9	179.2	-104.3	-130.4	124.7	---	174.7	50.3	144.2	-172	-100.6	-124.8	179.6
T_{8}	---	-178.1	43.7	135.4	-172.9	-90.1	-121.8	176.9	-56.5	-170.9	52.3	126.3	179.8	-90.9	-119	152.4	---	---	---	---	---	---	---	---
T_{7}	---	---	---	---	---	---	---	---	---	176	38.8	141.7	170.5	-94.1	-122.1	175.5	-57.7	162.7	55.1	115.2	---	---	-116.2	117.6
T_{6}	-69.5	169.3	54.3	118.1	---	---	-128	121.5	---	---	---	---	---	---	---	192.3	-60.7	179.5	45.3	109.6	-176.1	-87.7	-120.3	114.4
C_{5}	-60.5	162.8	58.4	122.4	-174.2	-88.5	-117	131.8	-55.4	177	46.8	135	---	---	-97	148.9	-59.1	166	56.1	112	-174.4	-85.9	-119.5	119.8
T_{4}	-56.8	172.7	55.9	121.2	-176.4	-91.2	-113.2	132.4	-60.2	167.4	55.7	97.6	-179.2	-87.5	-128.1	100.3	-58.4	172.9	56.4	108.9	-179.1	-87.6	-121.7	115.8
A_{3}	-66.5	167.8	54.6	101.1	179.7	-90.1	-130.2	102	-63.7	-178.1	54.4	126.4	-178.5	-90.4	-111.7	146	-63.4	-171	43.4	136.7	169.8	-89.3	-99.1	183.4
T_{2}	-65.4	178.5	60.2	134.6	-177.6	-95.5	-108.7	161	-62.3	175.2	51.1	125.9	178.2	-106.5	-118.6	136.6	-60.1	173.9	56.9	103.9	-173	-84.1	-139.3	99.2
G_{1}	---	-177.3	54.5	125.2	-177	-105.4	-126.5	135.6	---	---	43.5	146.3	169.5	-86.1	-97.8	204.3	---	166.3	47.2	146.7	170.1	-92.5	-100	188.8
5'																								

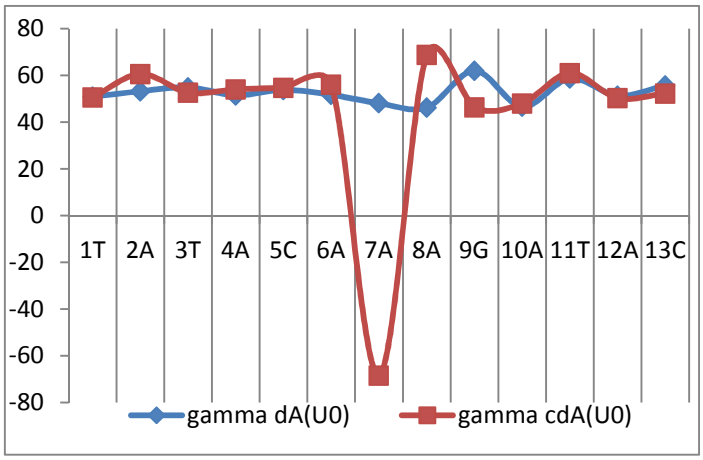
Graph 7S Graphical representation of data presented in Table 7S

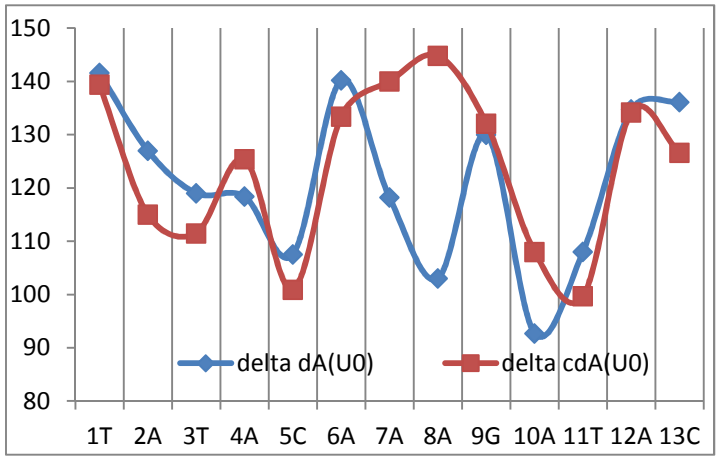
5'-^{1}T^{2}A^{3}T^{4}A^{5}C^{6}A^{7}**A**^{8}A^{9}G^{10}A^{11}T^{12}A^{13}C-3'

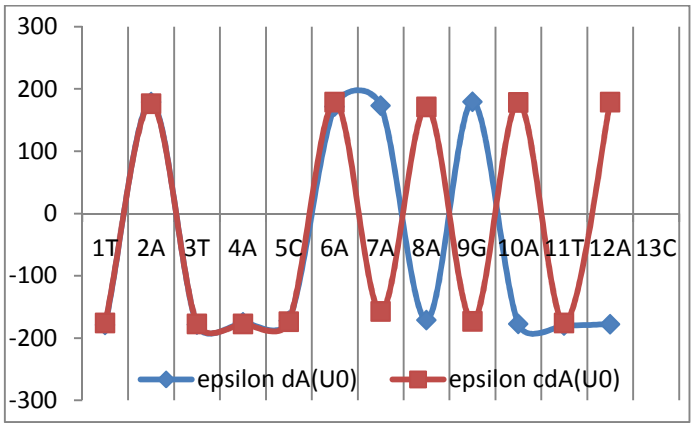
dA(U0)/cdA(U0). Comparison of dihedral angles (α, β, γ, δ, ε, ζ, χ) and sugar pseudorotation phase (P) vales obtained for the strand with the following base sequence: 5'-^{1}T^{2}A^{3}T^{4}A^{5}C^{6}A^{7}**A**^{8}A^{9}G^{10}A^{11}T^{12}A^{13}C-3' as a part of a double stranded oligodeoxynucleotide that contained at position **7A** 2'-deoxyadenosine in one strand and at **T7** (**U0**) 2'-deoxyuridine in the opposite strand (**dA(U0)**) with a double stranded oligodeoxynucleotide that contained at position 7**A** (5′*S*)-5',8-cyclo-2'-deoxyadenosine and 2'-deoxyuridine at position **T7** (**cdA(U0**)).

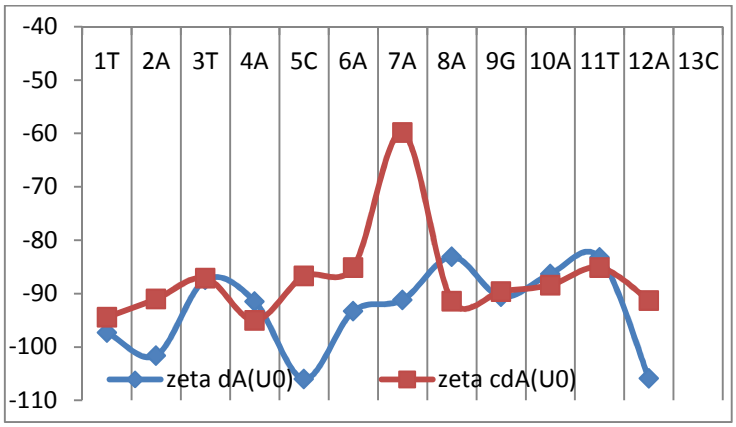


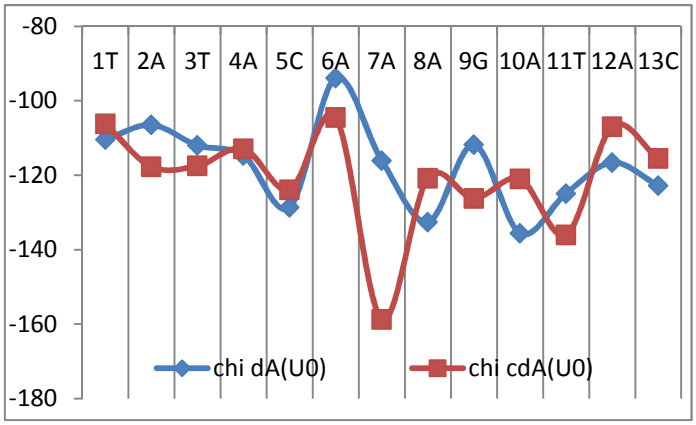


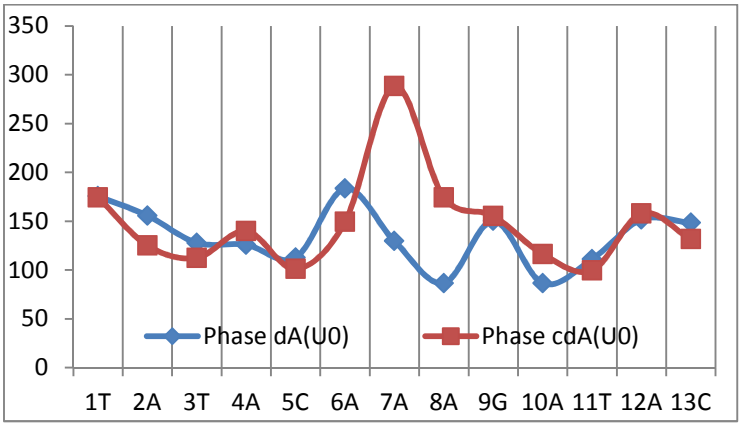








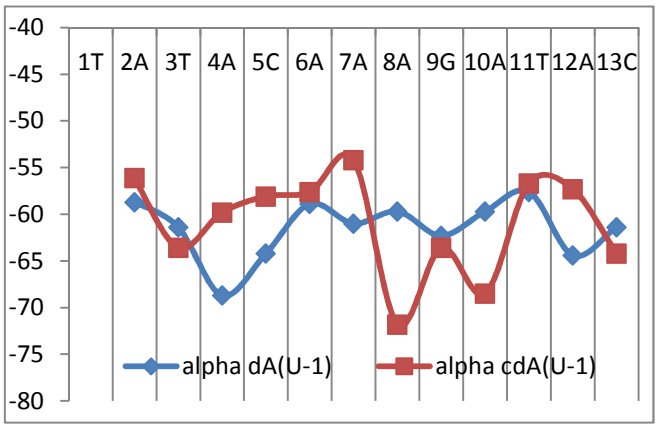


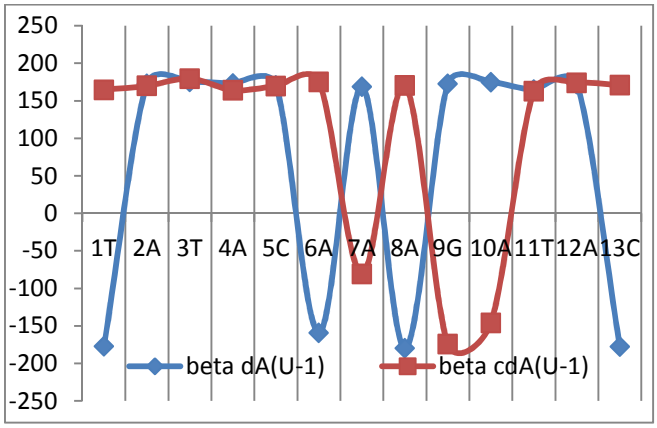


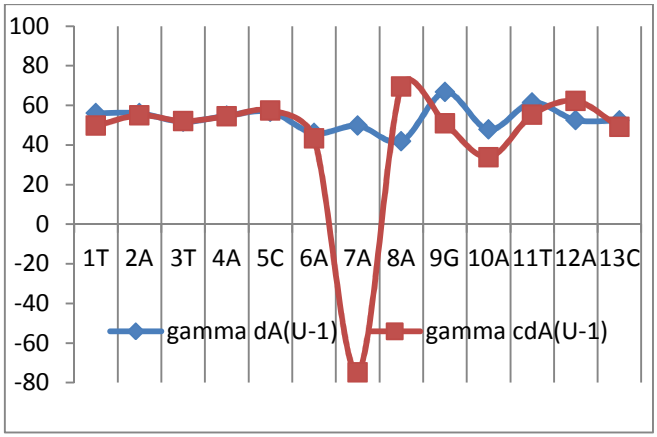
Graph 7S Graphical representation of data presented in Table 7S

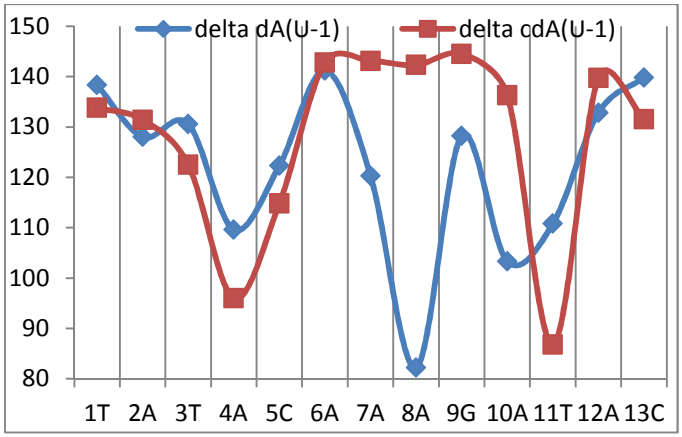
5'-^{1}T^{2}A^{3}T^{4}A^{5}C^{6}A^{7}**A**^{8}A^{9}G^{10}A^{11}T^{12}A^{13}C-3'

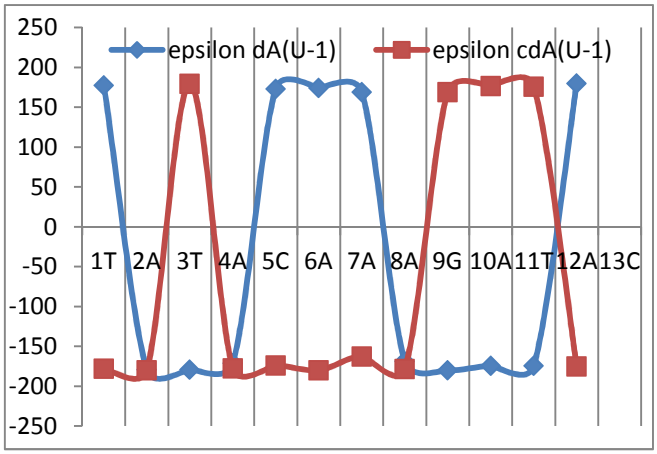
dA(U-1)/cdA(U-1). Comparison of dihedral angles (α, β, γ, δ, ε, ζ, χ) and sugar pseudorotation phase (P) vales obtained for the strand with the following base sequence: 5'-^{1}T^{2}A^{3}T^{4}A^{5}C^{6}A^{7}**A**^{8}A^{9}G^{10}A^{11}T^{12}A^{13}C-3' as a part of a double stranded oligodeoxynucleotide that contained at position **7A** 2'-deoxyadenosine in one strand and at **T6** (**U-1**) 2'-deoxyuridine in the opposite strand (**dA(U-1)**) with a double stranded oligodeoxynucleotide that contained at position **7A** (5′*S*)-5',8-cyclo-2'-deoxyadenosine and 2'-deoxyuridine at position **T6** (**cdA(U-1)**).

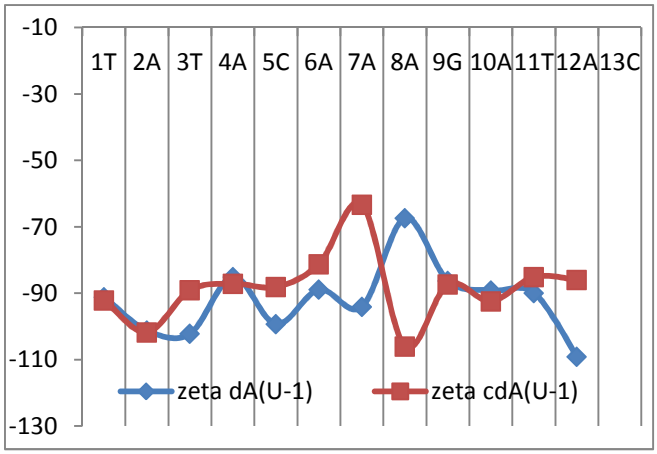


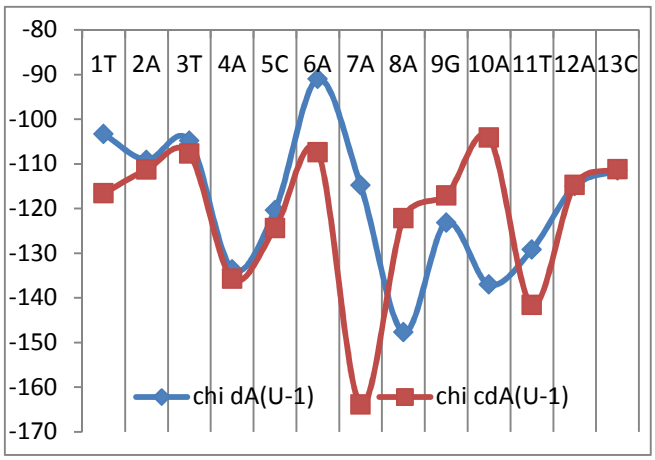


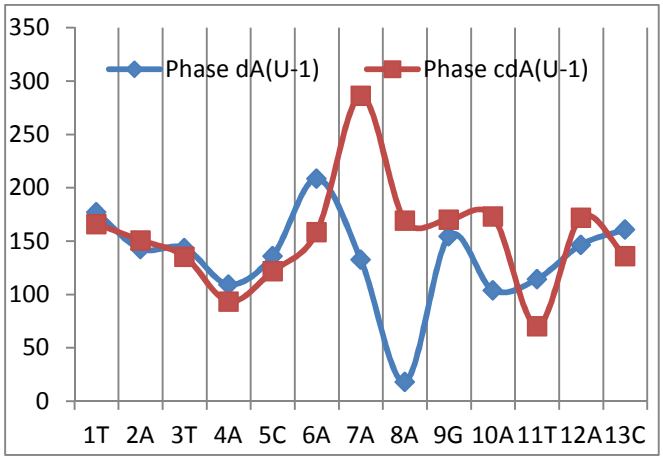








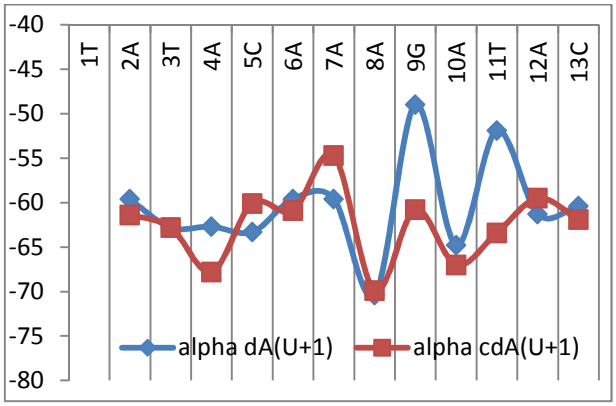


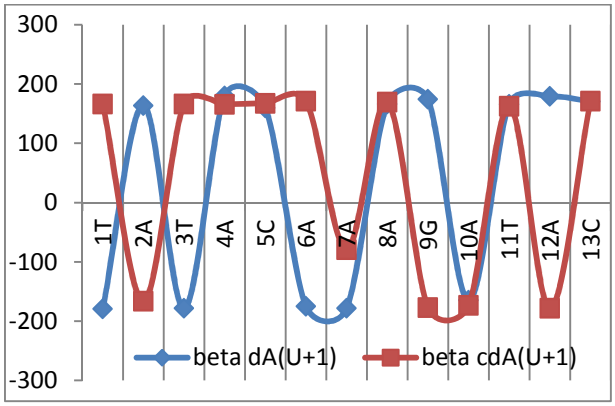


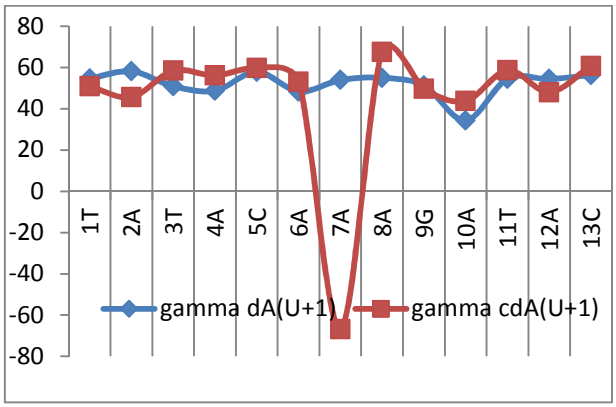
Graph 7S Graphical representation of data presented in Table 7S

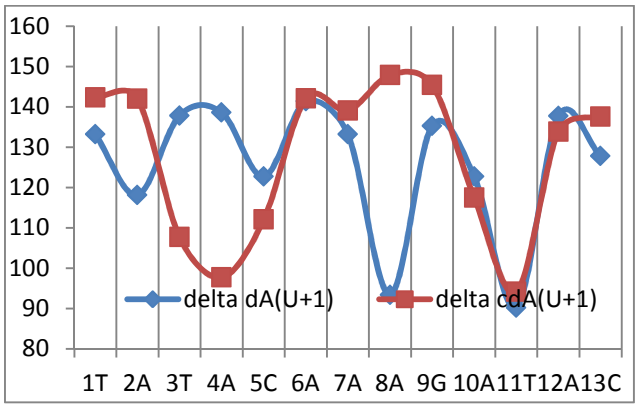
5'-^{1}T^{2}A^{3}T^{4}A^{5}C^{6}A^{7}**A**^{8}A^{9}G^{10}A^{11}T^{12}A^{13}C-3'

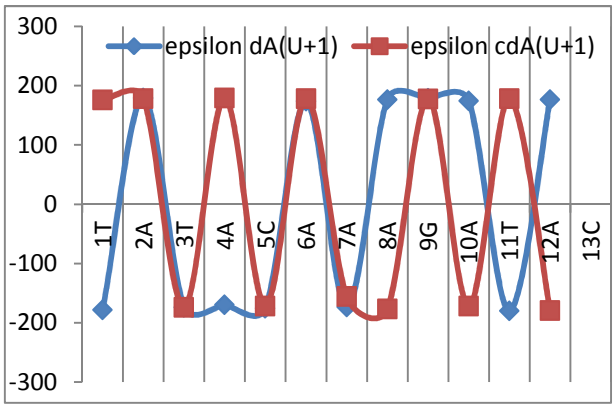
dA(U+1)/cdA(U+1). Comparison of dihedral angles (α, β, γ, δ, ε, ζ, χ) and sugar pseudorotation phase (P) vales obtained for the strand with the following base sequence: 5'-^{1}T^{2}A^{3}T^{4}A^{5}C^{6}A^{7}**A**^{8}A^{9}G^{10}A^{11}T^{12}A^{13}C-3' as a part of double stranded oligodeoxynucleotides contained at position **7A** 2'-deoxyadenosine in one strand and at **T8** (**U+1**) 2'-deoxyuridine in the opposite strand (**dA(U+1)**) with a double stranded oligodeoxynucleotide that contained at position **7A** (5′*S*) 5',8-cyclo-2'-deoxyadenosine and 2'-deoxyuridine**T8 (cdA(U+1))**.

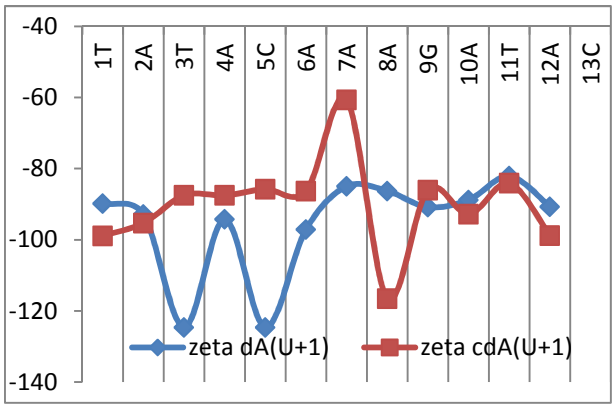


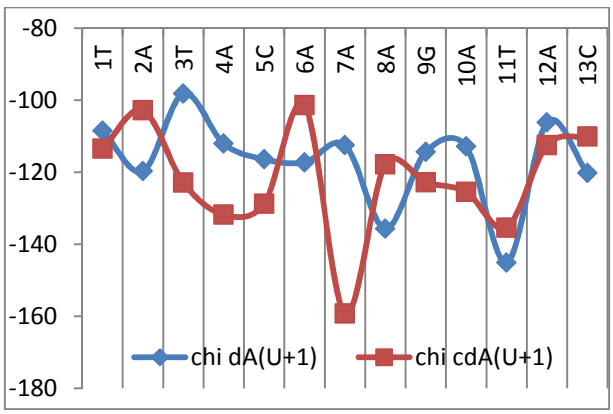


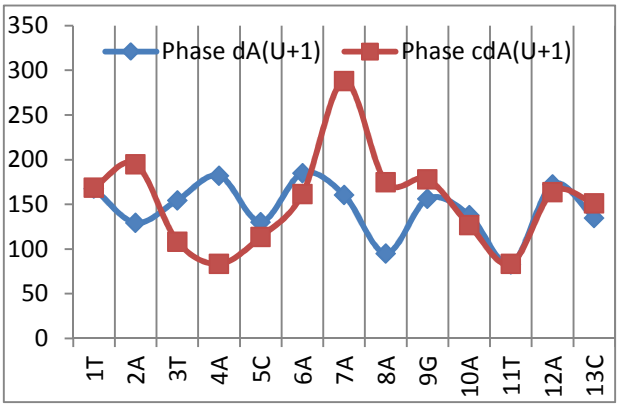








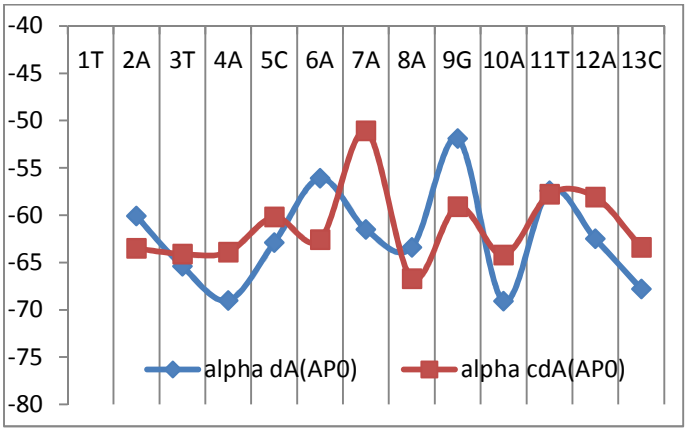


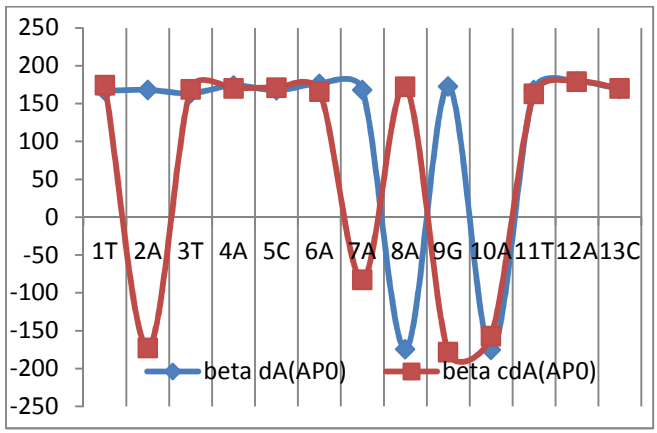


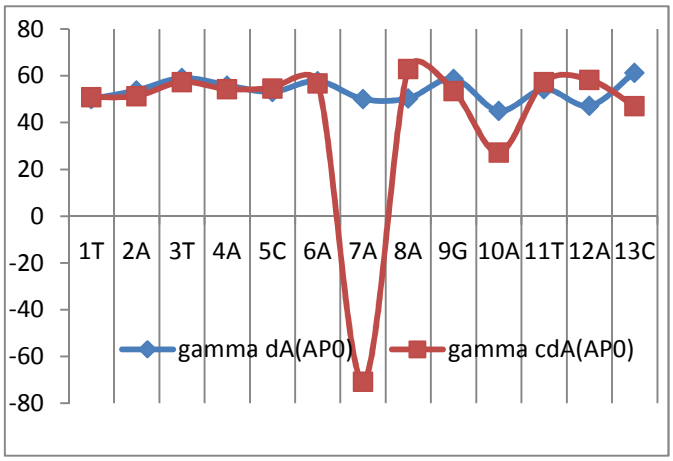
Graph 7S Graphical representation of data presented in Table 7S

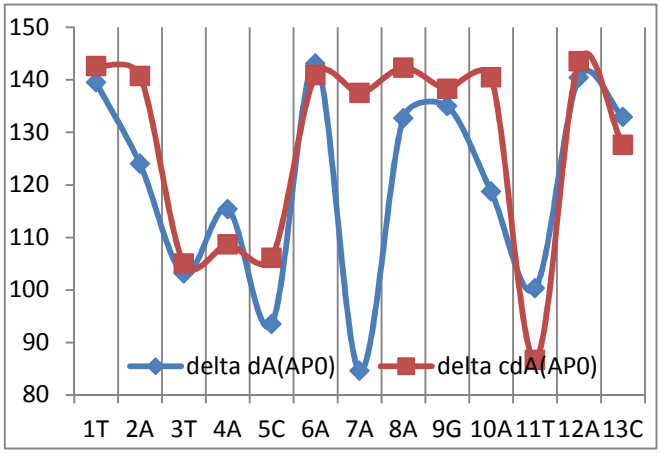
5'-^{1}T^{2}A^{3}T^{4}A^{5}C^{6}A^{7}**A**^{8}A^{9}G^{10}A^{11}T^{12}A^{13}C-3'

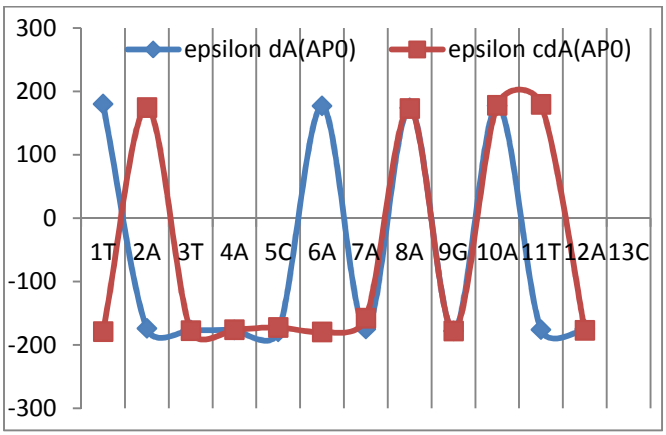
dA(Ap0)/cdA(Ap0). Comparison of dihedral angles (α, β, γ, δ, ε, ζ, χ) and sugar pseudorotation phase (P) vales obtained for the strand with the following base sequence: 5'-^{1}T^{2}A^{3}T^{4}A^{5}C^{6}A^{7}**A**^{8}A^{9}G^{10}A^{11}T^{12}A^{13}C-3' as a part of double stranded oligodeoxynucleotides contained at position **7A** 2'-deoxyadenosine in one strand and at **T7** (**Ap0**) an apurinic/apyrimidinic site in the opposite strand (**dA(Ap0)**) with a double stranded oligodeoxynucleotide that contained at position **7A** (5′*S*)-5',8-cyclo-2'-deoxyadenosine and an apurinic/apyrimidinic site at the position **T7 (cdA(Ap0))**.

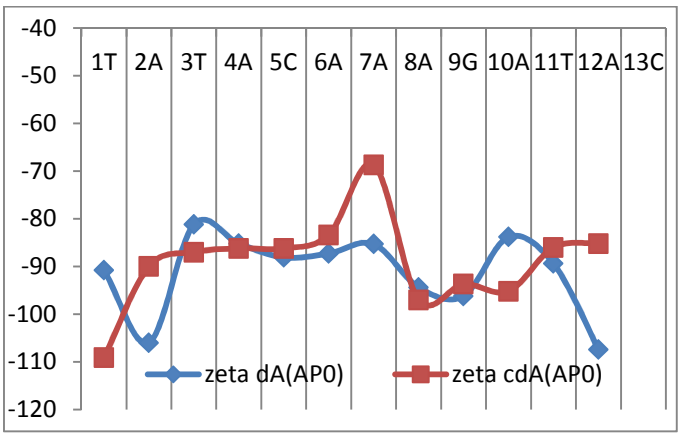


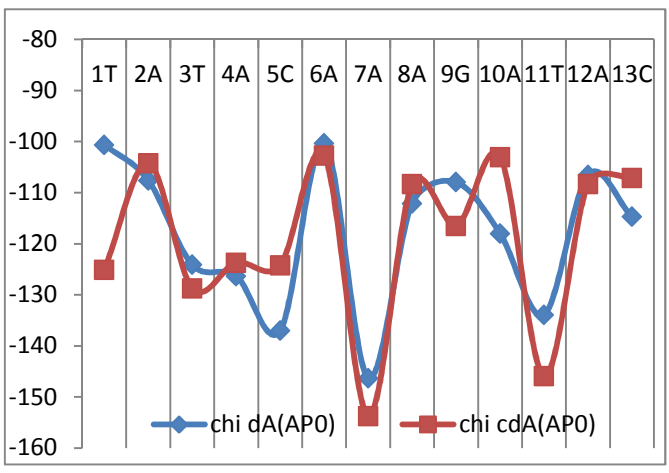


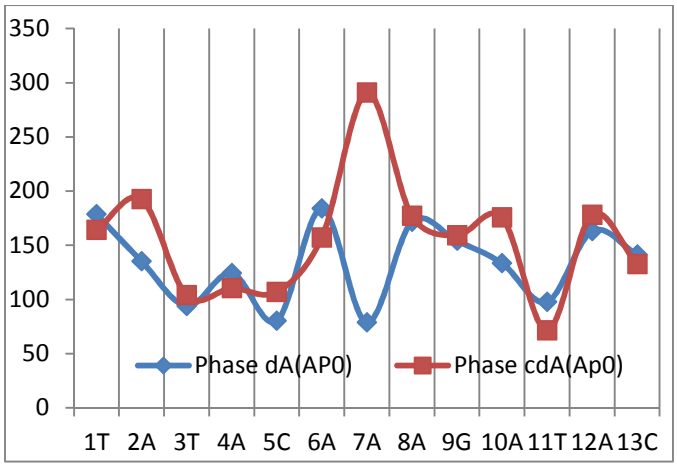








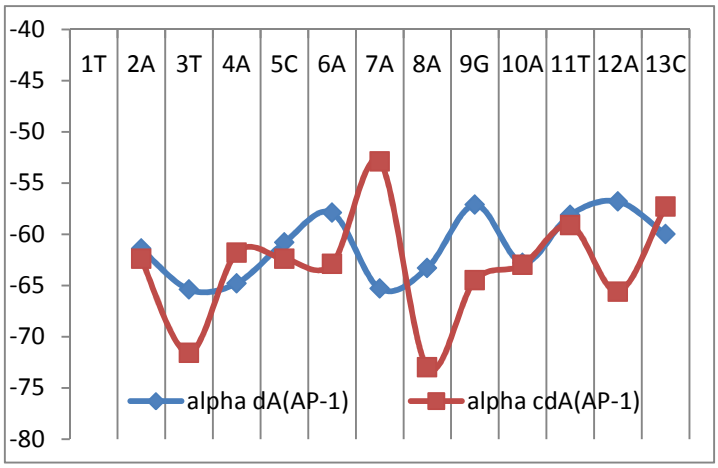


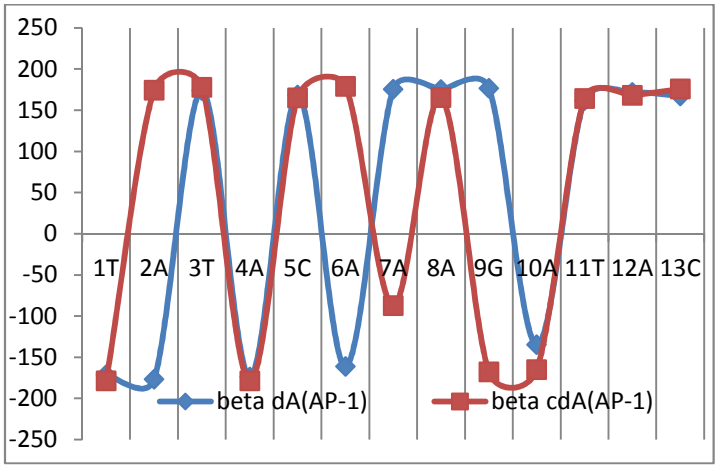


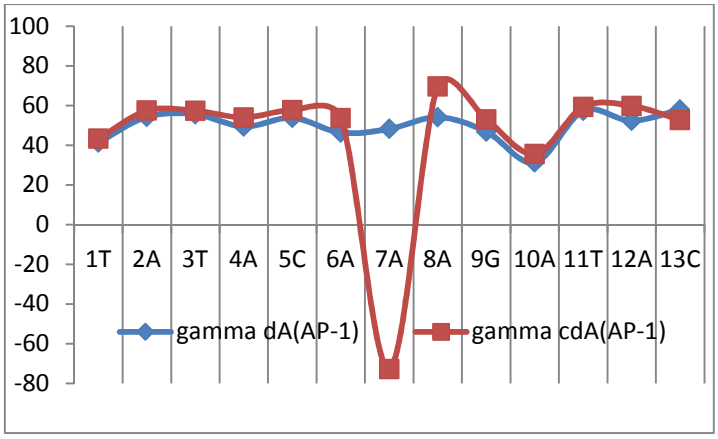
Graph 7S Graphical representation of data presented in Table 7S

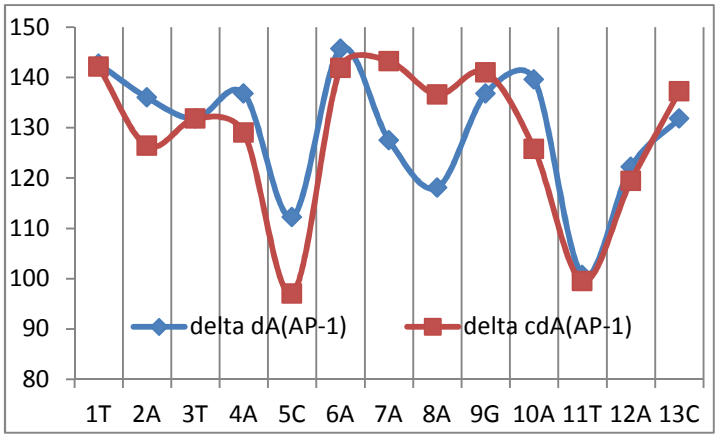
5'-^{1}T^{2}A^{3}T^{4}A^{5}C^{6}A^{7}**A**^{8}A^{9}G^{10}A^{11}T^{12}A^{13}C-3'

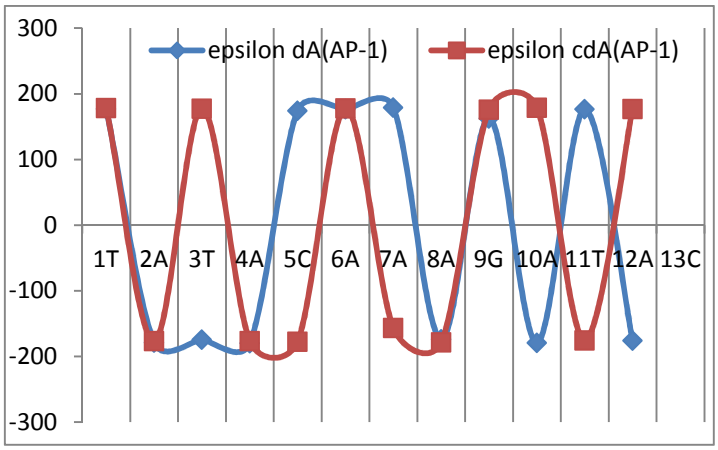
dA(Ap-1)/cdA(Ap-1). Comparison of dihedral angles (α, β, γ, δ, ε, ζ,χ) and sugar pseudorotation phase (P) vales obtained for the strand with the following base sequence: 5'-^{1}T^{2}A^{3}T^{4}A^{5}C^{6}A^{7}**A**^{8}A^{9}G^{10}A^{11}T^{12}A^{13}C-3' as a part of double stranded oligodeoxynucleotides contained at position **7A** 2'-deoxyadenosine in one strand and at **T6** (**Ap-1**) an apurinic/apyrimidinic site in the opposite strand (**dA(Ap-1)**) with a double stranded oligodeoxynucleotide that contained at position **7A** (5′*S*)-5',8-cyclo-2'-deoxyadenosine and an apurinic/apyrimidinic site at position **T6 (cdA(Ap-1))**.

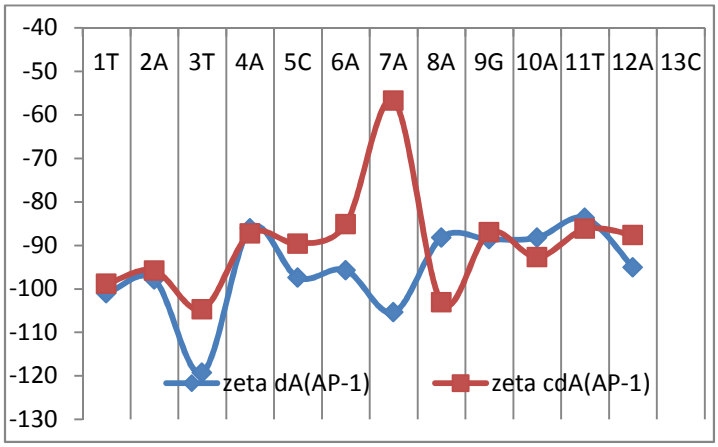


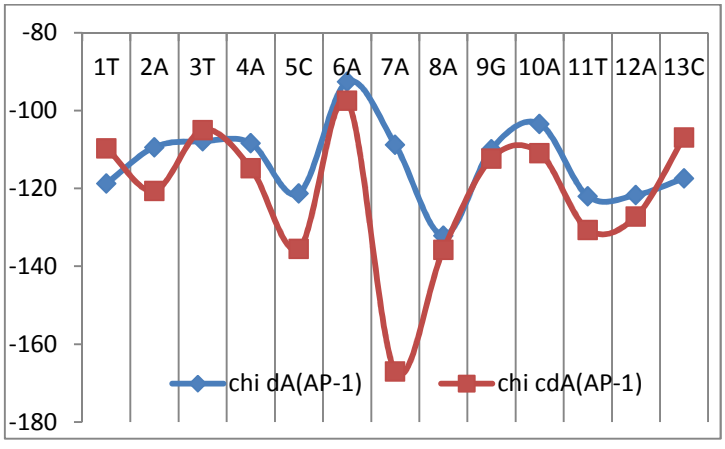


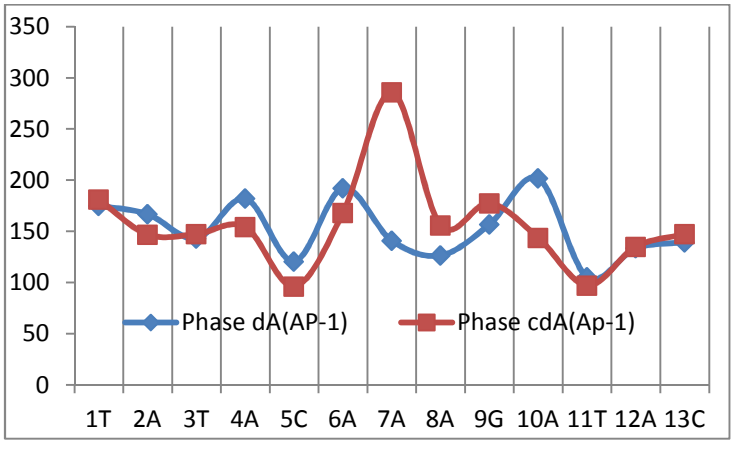








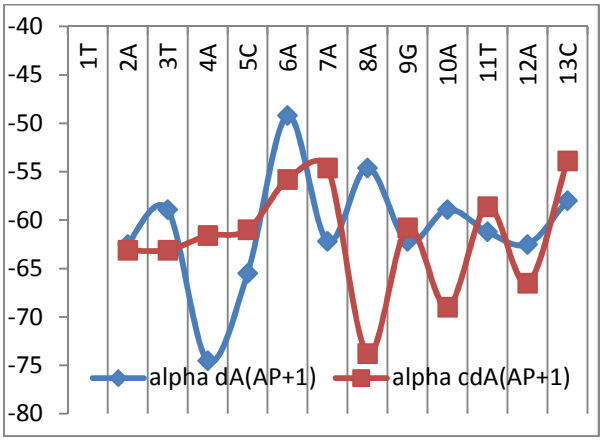


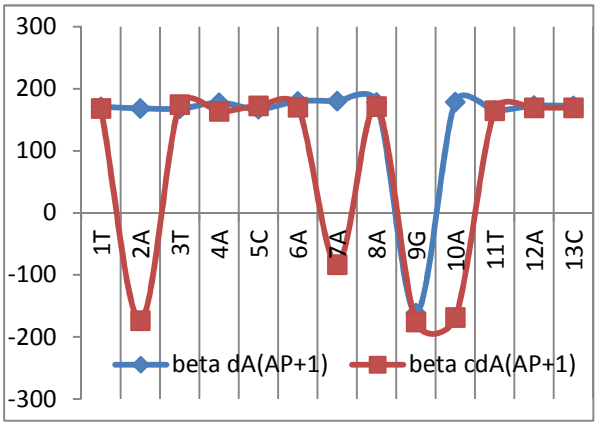


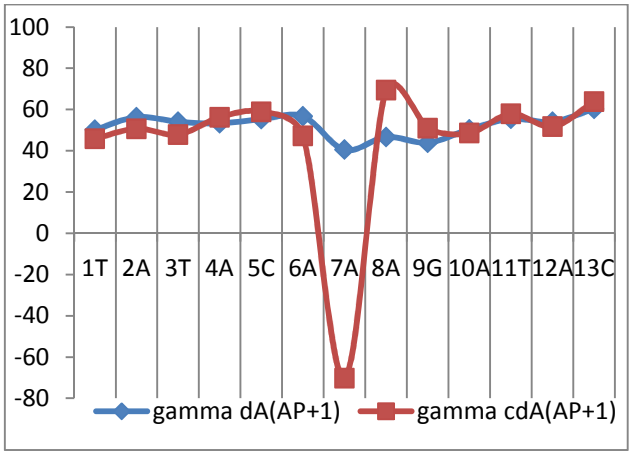
Graph 7S Graphical representation of data presented in Table 7S

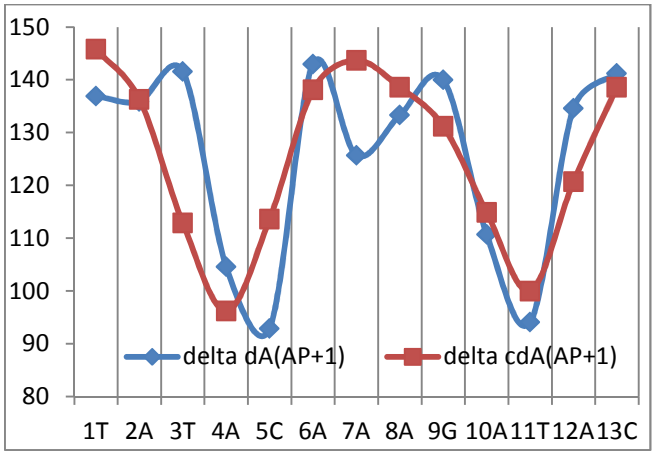
5'-^{1}T^{2}A^{3}T^{4}A^{5}C^{6}A^{7}**A**^{8}A^{9}G^{10}A^{11}T^{12}A^{13}C-3'

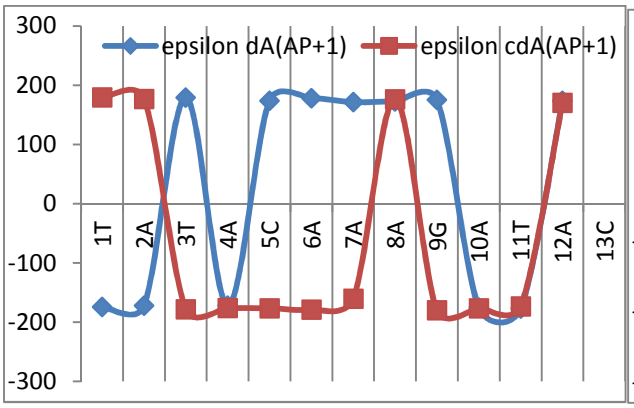
dA(Ap+1)/cdA(Ap+1). Comparison of dihedral angles (α, β, γ, δ, ε, ζ, χ) and sugar pseudorotation phase (P) vales obtained for the strand with the following base sequence: 5'-^{1}T^{2}A^{3}T^{4}A^{5}C^{6}A^{7}**A**^{8}A^{9}G^{10}A^{11}T^{12}A^{13}C-3' as a part of double stranded oligodeoxynucleotide that contained at position **7A** 2'-deoxyadenosine in one strand and at **T8** (**Ap+1**) an apurinic/apyrimidinic site in the opposite strand (**dA(Ap+1)**) with a double stranded oligodeoxynucleotide that contained at position **7A** (5′*S*)-5',8-cyclo-2'-deoxyadenosine and an apurinic/apyrimidinic site at position **T8 (cdA(Ap+1))**.

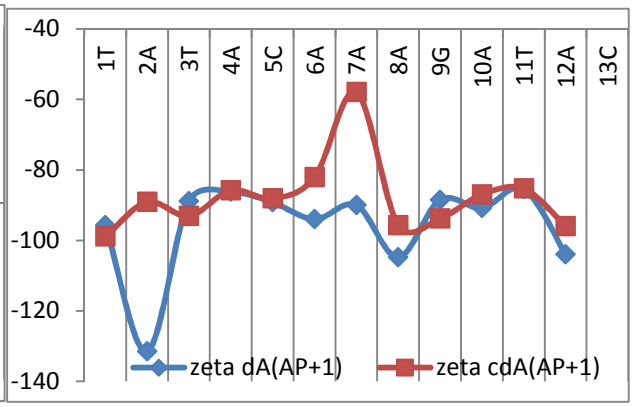


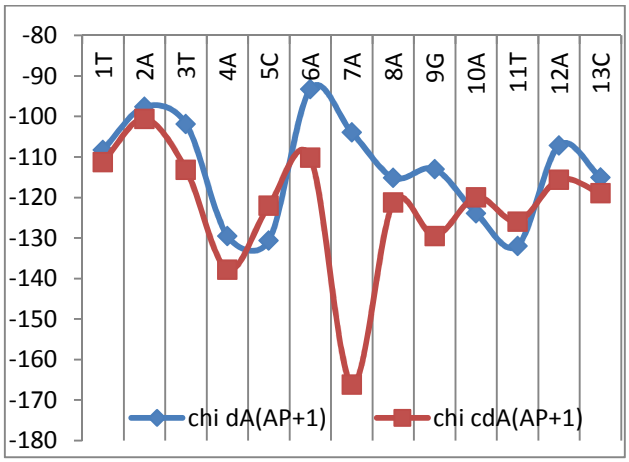


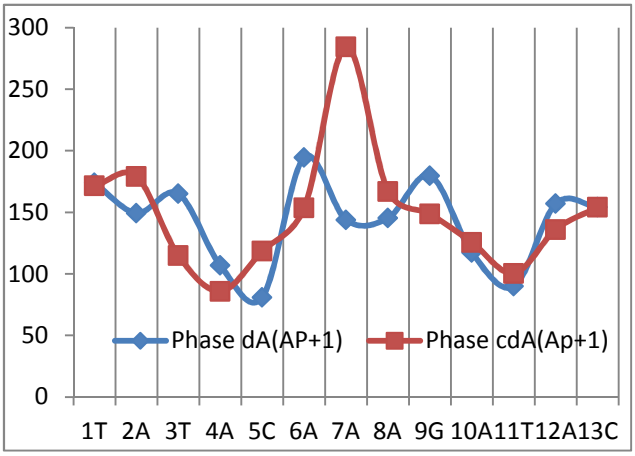








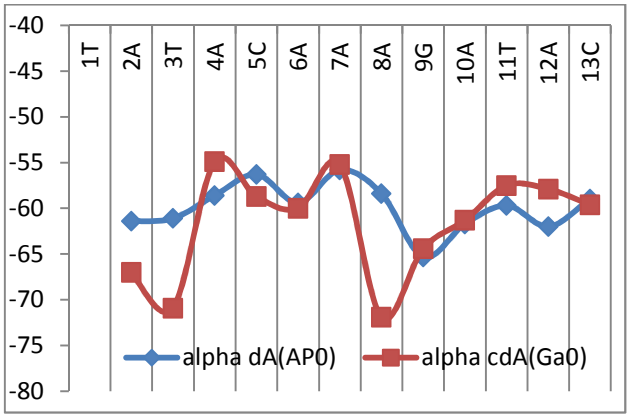


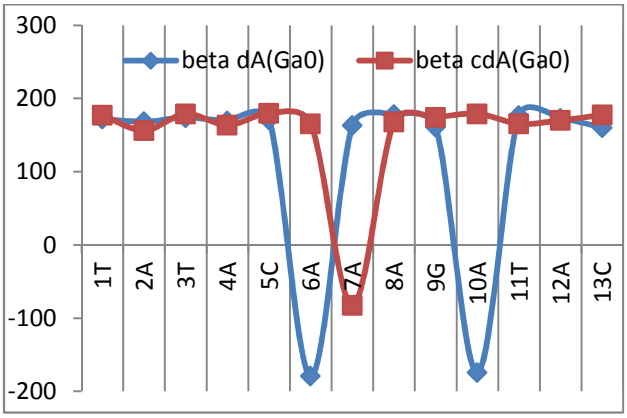


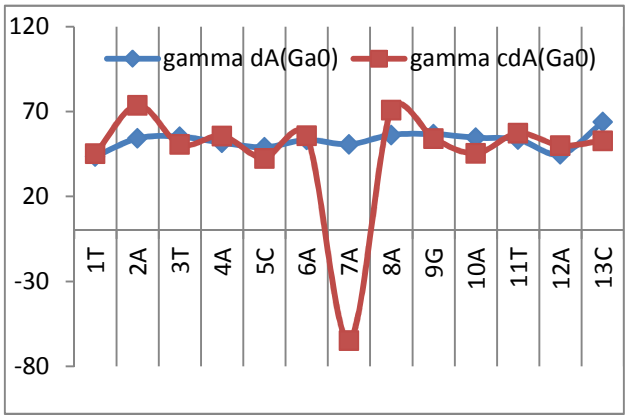
Graph 7S Graphical representation of data presented in Table 7S

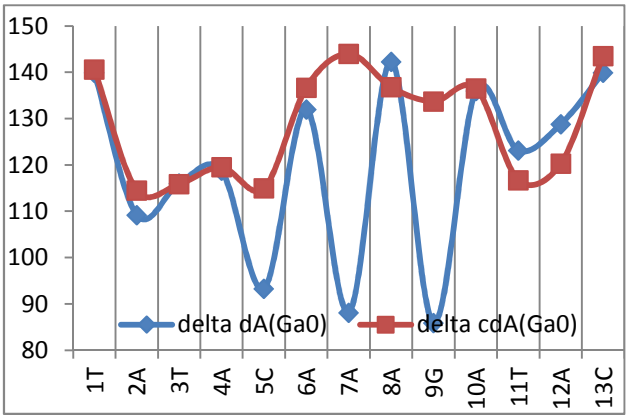
5'-^{1}T^{2}A^{3}T^{4}A^{5}C^{6}A^{7}**A**^{8}A^{9}G^{10}A^{11}T^{12}A^{13}C-3'

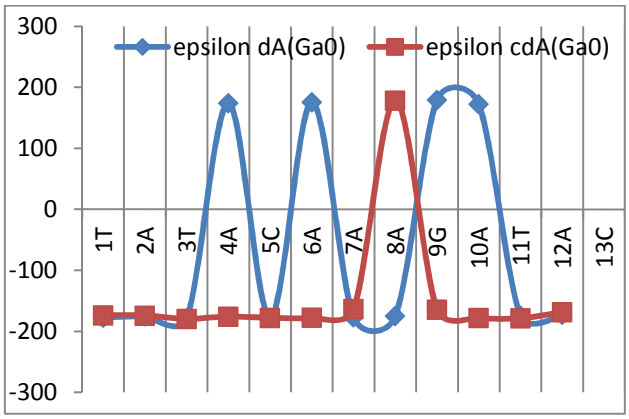
dA(Ga0)/cdA(Ga0). Comparison of dihedral angles (α, β, γ, δ, ε, ζ, χ) and sugar pseudorotation phase (P) vales obtained for the strand with the following base sequence: 5'-^{1}T^{2}A^{3}T^{4}A^{5}C^{6}A^{7}**A**^{8}A^{9}G^{10}A^{11}T^{12}A^{13}C-3' as a part of double stranded oligodeoxynucleotide that contained at position **7A** 2'-deoxyadenosine in one strand and at **T7** (**Ga0**) a single strand break e.i. gap in the opposite strand (**dA(Ga0)**) with a double stranded oligodeoxynucleotide that contained at position **7A** (5′*S*)-5',8-cyclo-2'-deoxyadenosine and a single strand break at position **T7 (cdA(Ga0))**.

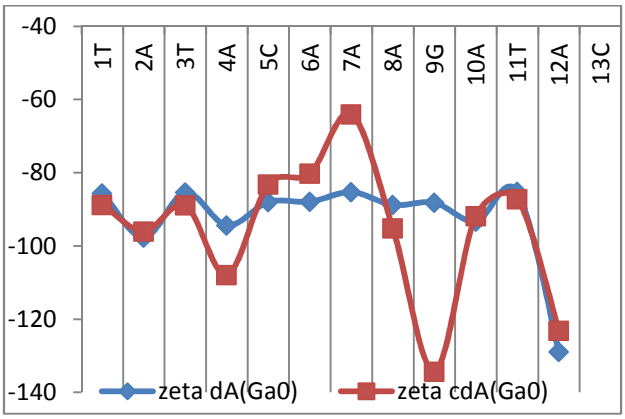


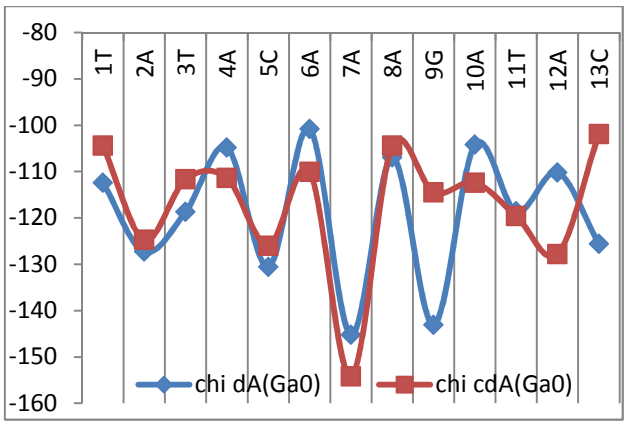


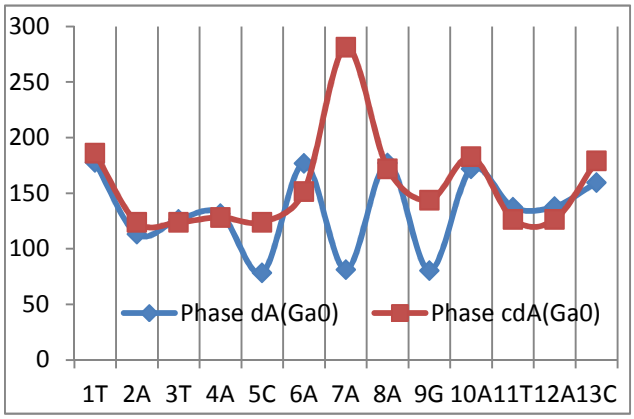








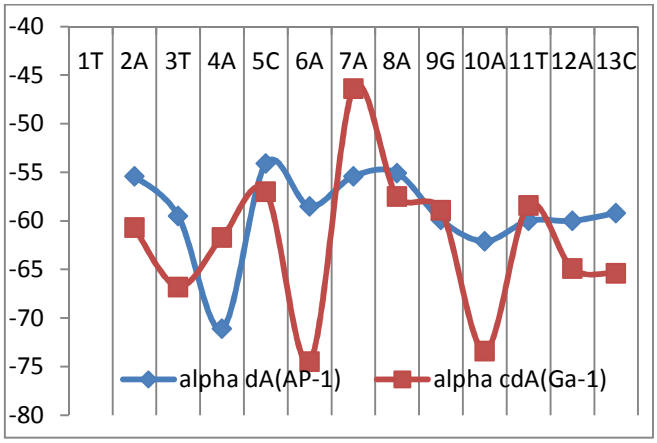


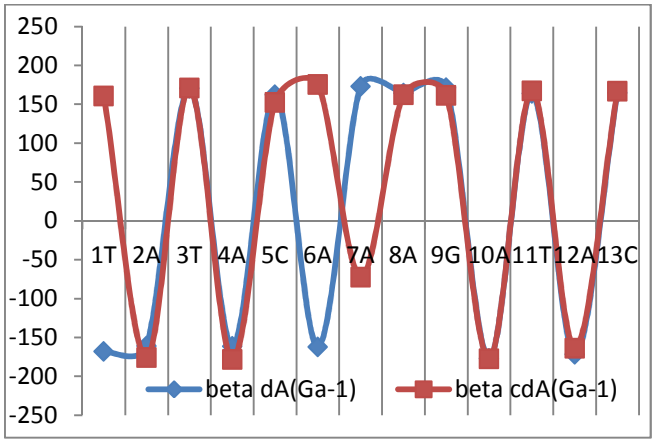


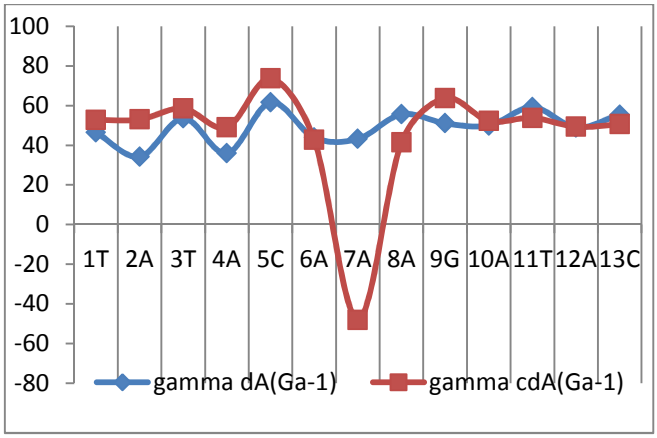
Graph 7S Graphical representation of data presented in Table 7S

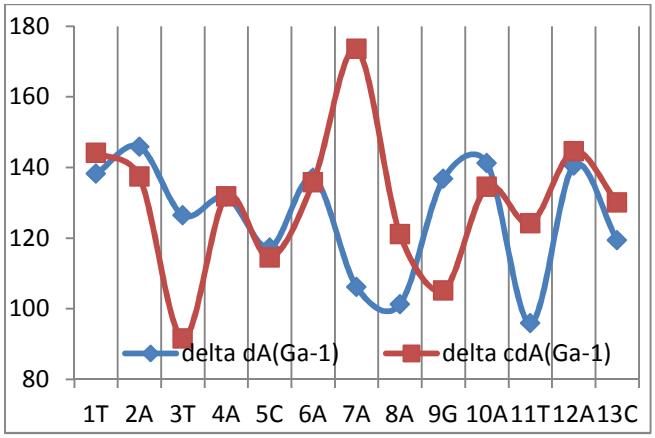
5'-^{1}T^{2}A^{3}T^{4}A^{5}C^{6}A^{7}**A**^{8}A^{9}G^{10}A^{11}T^{12}A^{13}C-3'

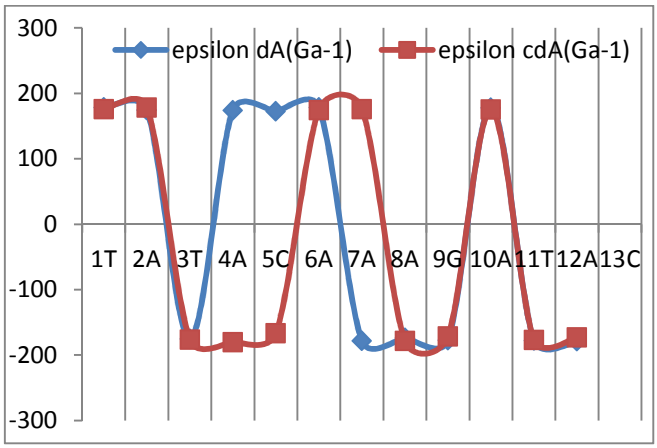
dA(Ga-1)/cdA(Ga-1). Comparison of dihedral angles (α, β, γ, δ, ε, ζ, χ) and sugar pseudorotation phase (P) vales obtained for the strand with the following base sequence: 5'-^{1}T^{2}A^{3}T^{4}A^{5}C^{6}A^{7}**A**^{8}A^{9}G^{10}A^{11}T^{12}A^{13}C-3' as a part of double stranded oligodeoxynucleotide that contained at position **7A** 2'-deoxyadenosine in one strand and at **T6** (**Ga-1**) a single strand break e.i. gap in the opposite strand (**dA(Ga-1)**) with a double stranded oligodeoxynucleotide that contained at position **7A** (5′*S*)-5',8-cyclo-2'-deoxyadenosine and a single strand brake at position **T6 (cdA(Ga-1))**.

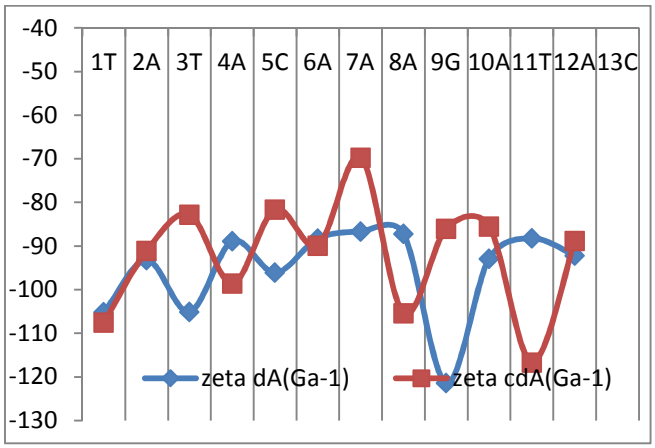


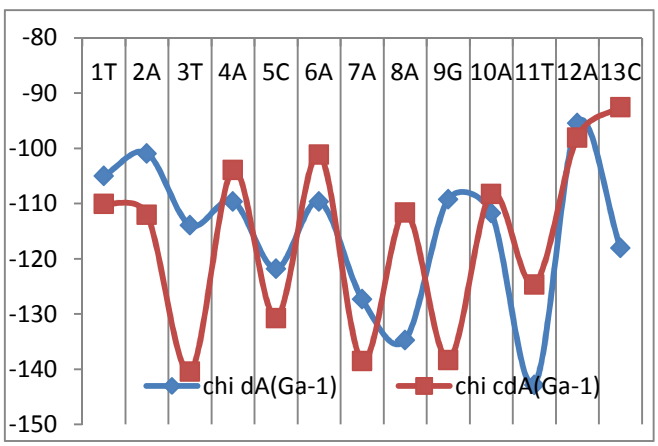


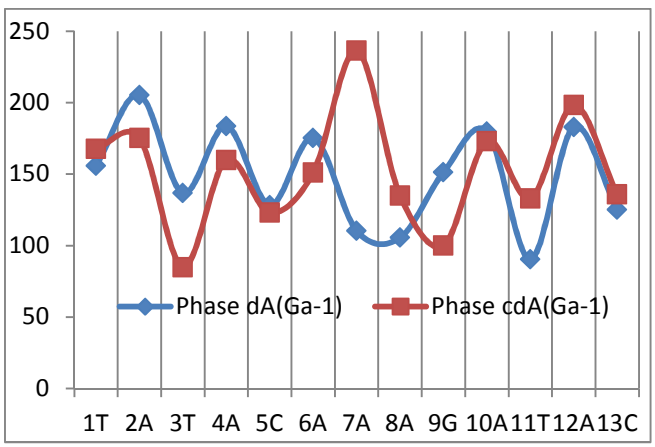








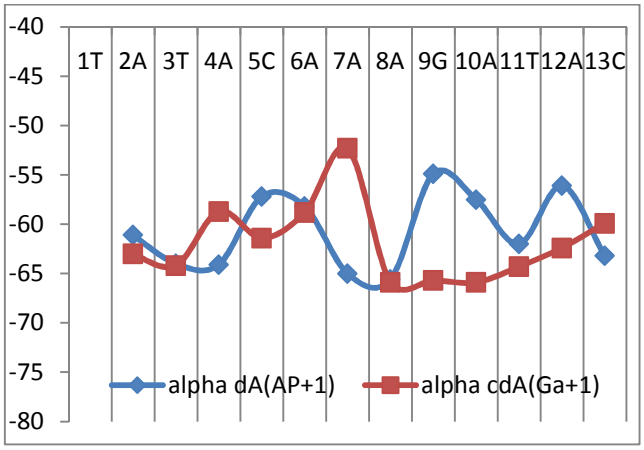


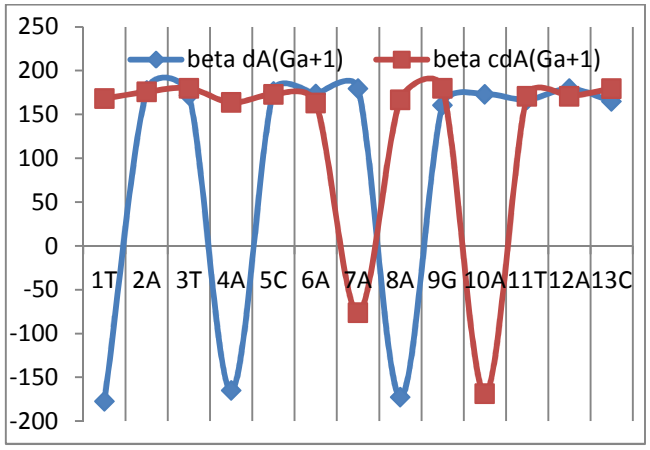


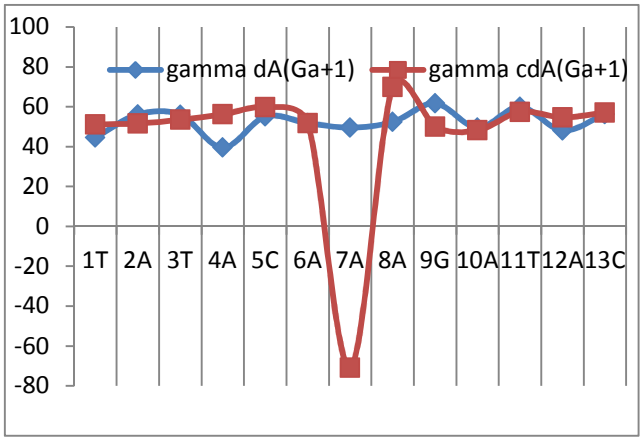
Graph 7S Graphical representation of data presented in Table 7S

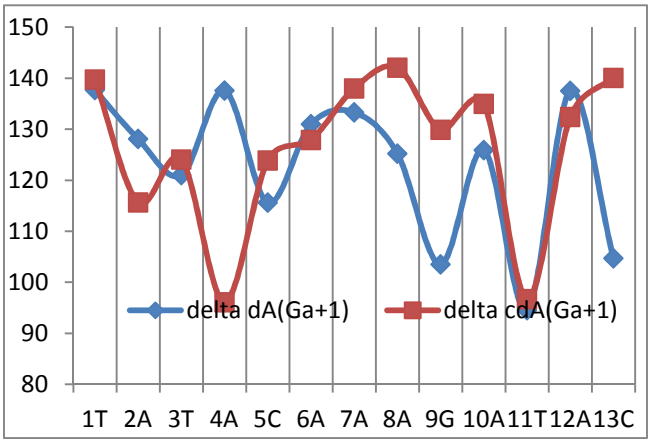
5'-^{1}T^{2}A^{3}T^{4}A^{5}C^{6}A^{7}**A**^{8}A^{9}G^{10}A^{11}T^{12}A^{13}C-3'

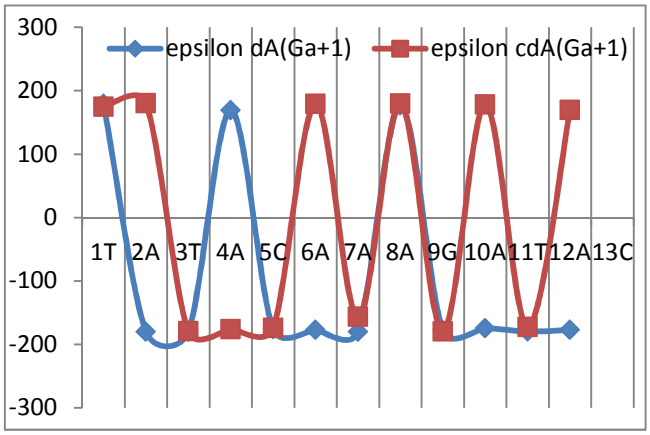
dA(Ga+1)/cdA(Ga+1). Comparison of dihedral angles (α, β, γ, δ, ε, ζ, χ) and sugar pseudorotation phase (P) vales obtained for the strand with the following base sequence: 5'-^{1}T^{2}A^{3}T^{4}A^{5}C^{6}A^{7}**A**^{8}A^{9}G^{10}A^{11}T^{12}A^{13}C-3' as a part of double stranded oligodeoxynucleotide that contained at position **7A** 2'-deoxyadenosine in one strand and at **T8** (**Ga+1**) a single strand break e.i. gap in the opposite strand (**dA(Ga+1))** with a double stranded oligodeoxynucleotide that contained at position **7A** (5′*S*)-5',8-cyclo-2'-deoxyadenosine and a single strand brake at position **T6 (cdA(Ga+1))**.

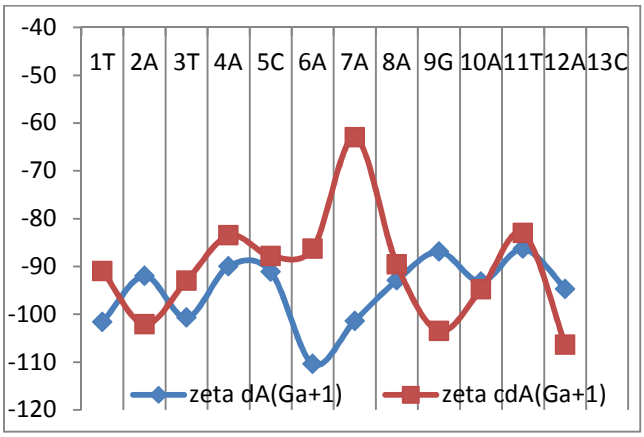


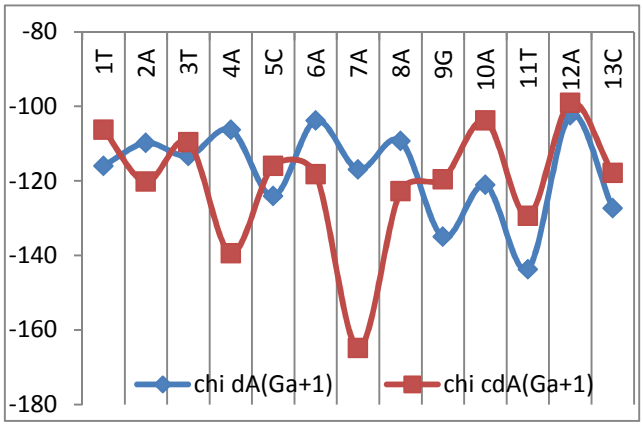


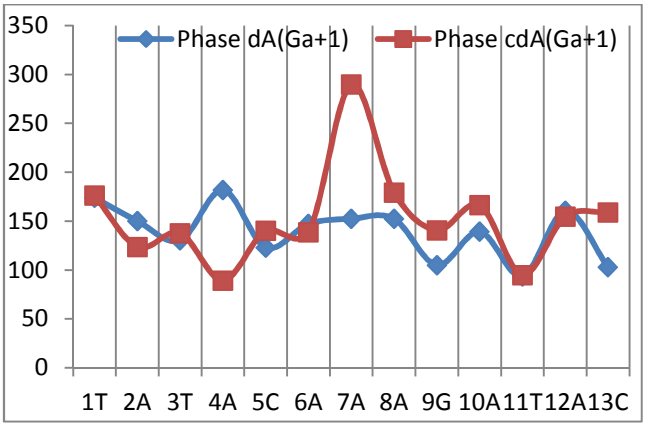








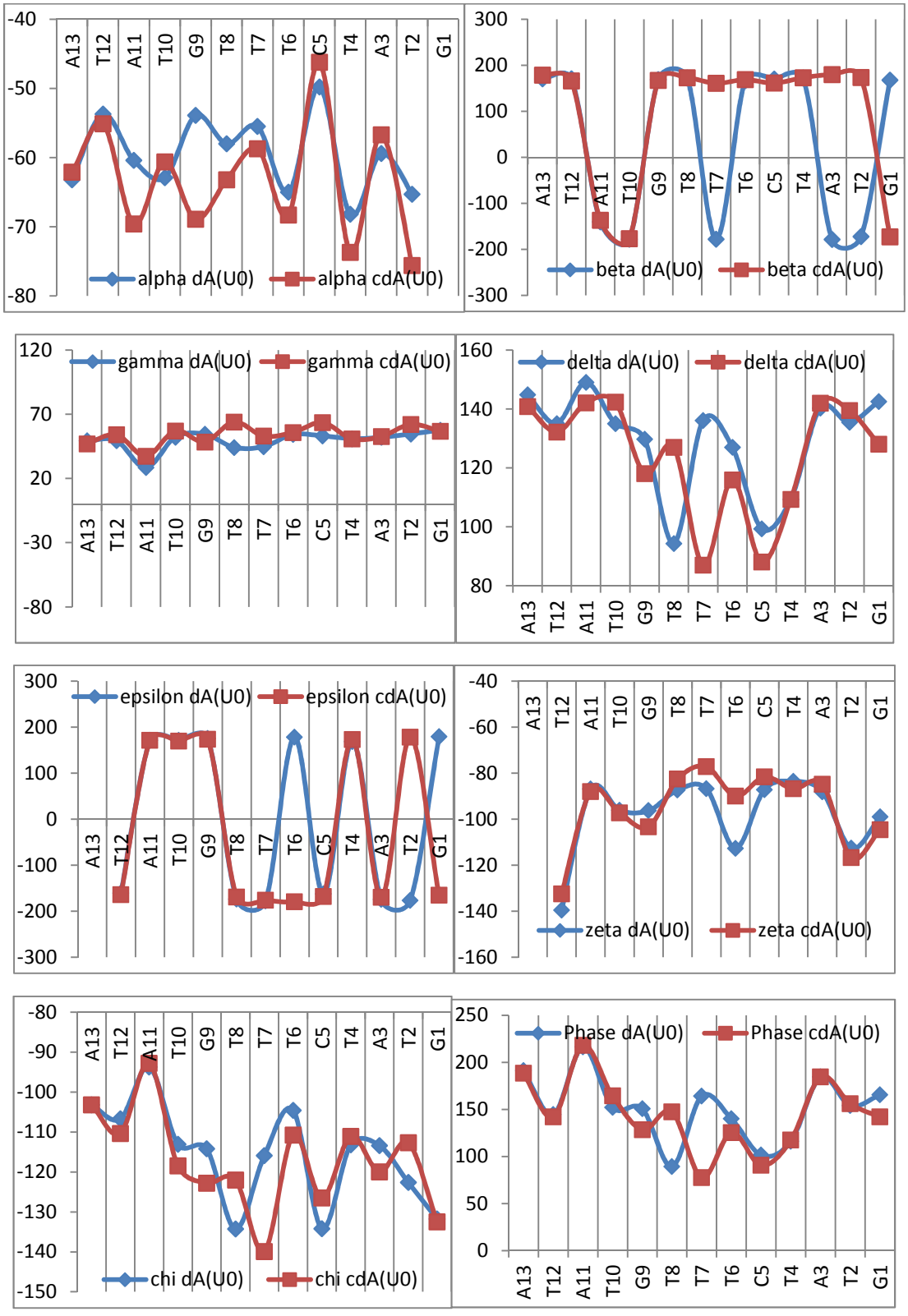




Graph 7S Graphical representation of data presented in Table 7S

5'-^{13}A^{12}T^{11}A^{10}T^{9}G^{8}T^{7}**T**^{6}T^{5}C^{4}T^{3}A^{2}T^{1}G-3'

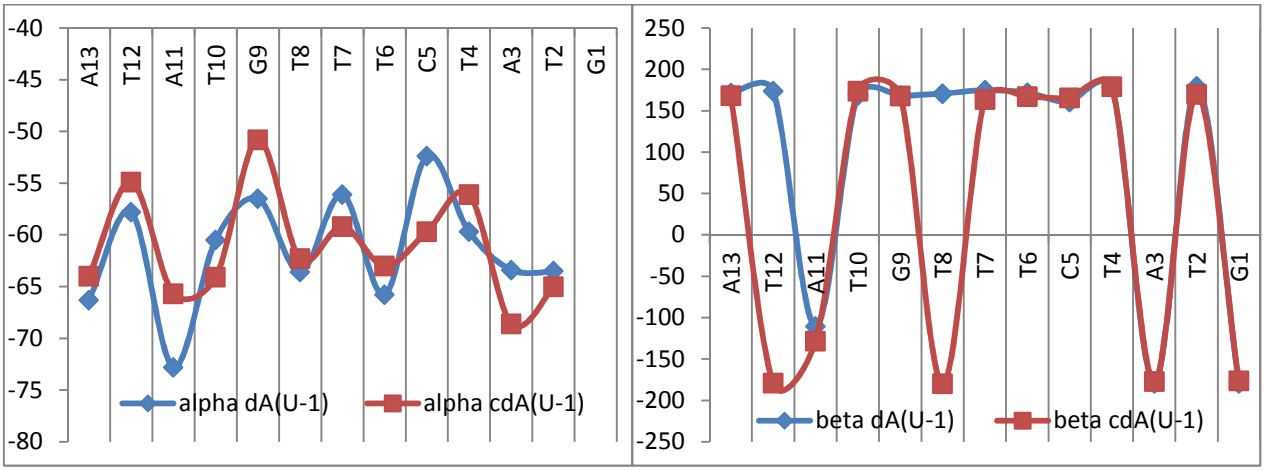
dA(U0)/cdA(U0). Comparison of dihedral angles (α, β, γ, δ, ε, ζ, χ) and sugar pseudorotation phase (P) vales obtained for the strand with the following base sequence: 5'-^{13}A^{12}T^{11}A^{10}T^{9}G^{8}T^{7}**T**^{6}T^{5}C^{4}T^{3}A^{2}T^{1}G-3', as a part of double stranded oligodeoxynucleotide contained at position **7A** 2'-deoxyadenosine in one strand and at **T7** (**U0**) 2'-deoxyuridine in the opposite strand (**dA(U0)**) with a double stranded oligodeoxynucleotide that contained at position **7A** (5′*S*)-5',8-cyclo-2'-deoxyadenosine and 2'-deoxyuridine at position **T7 (cdA(U0))**.

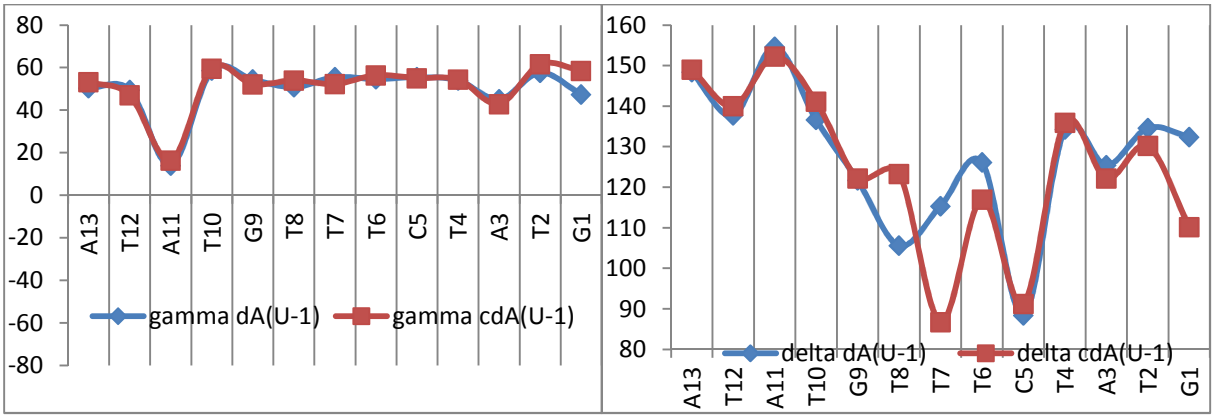


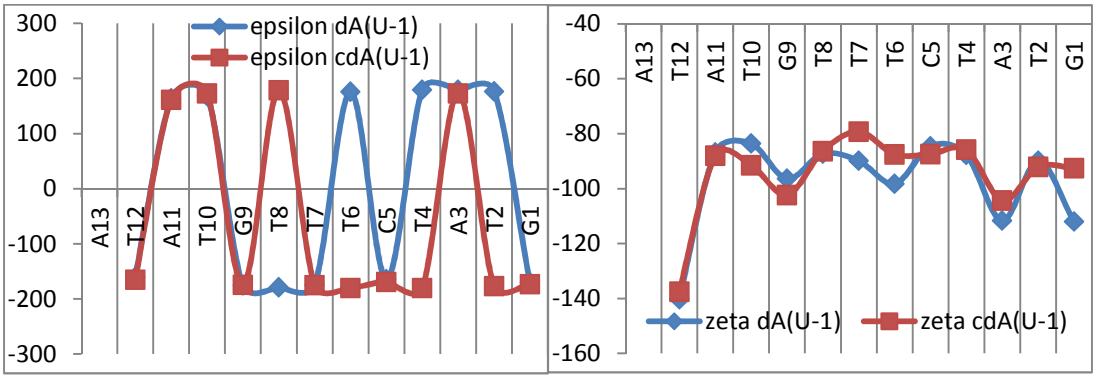
Graph 7S Graphical representation of data presented in Table 7S

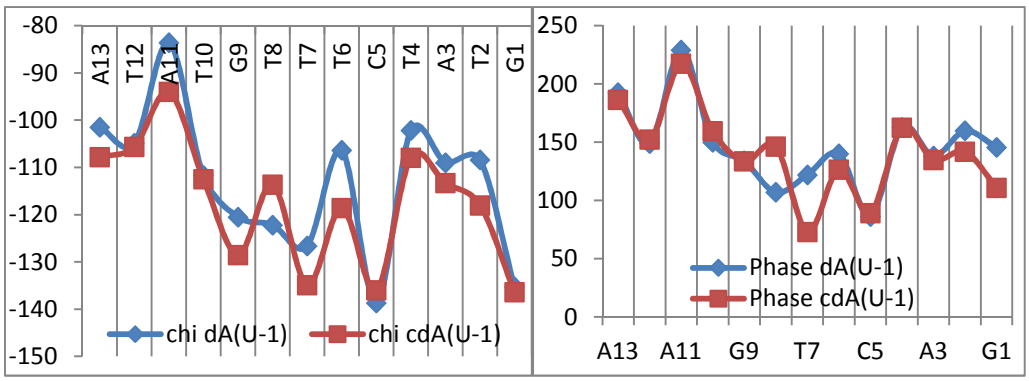
5'-^{13}A^{12}T^{11}A^{10}T^{9}G^{8}T^{7}**T**^{6}T^{5}C^{4}T^{3}A^{2}T^{1}G-3'

dA(U-1)/cdA(U-1). Comparison of dihedral angles (α, β, γ, δ, ε, ζ, χ) and sugar pseudorotation phase (P) vales obtained for the strand with the following base sequence: 5'-^{13}A^{12}T^{11}A^{10}T^{9}G^{8}T^{7}**T**^{6}T^{5}C^{4}T^{3}A^{2}T^{1}G-3', as a part of double stranded oligodeoxynucleotide contained at position **7A** 2'-deoxyadenosine in one strand and at **T6** (**U-1**) 2'-deoxyuridine in the opposite strand (**dA(U-1)**) with a double stranded oligodeoxynucleotide that contained at position **7A** (5′*S*)-5',8-cyclo-2'-deoxyadenosine and 2'-deoxyuridine at position **T6 (cdA(U-1))**.





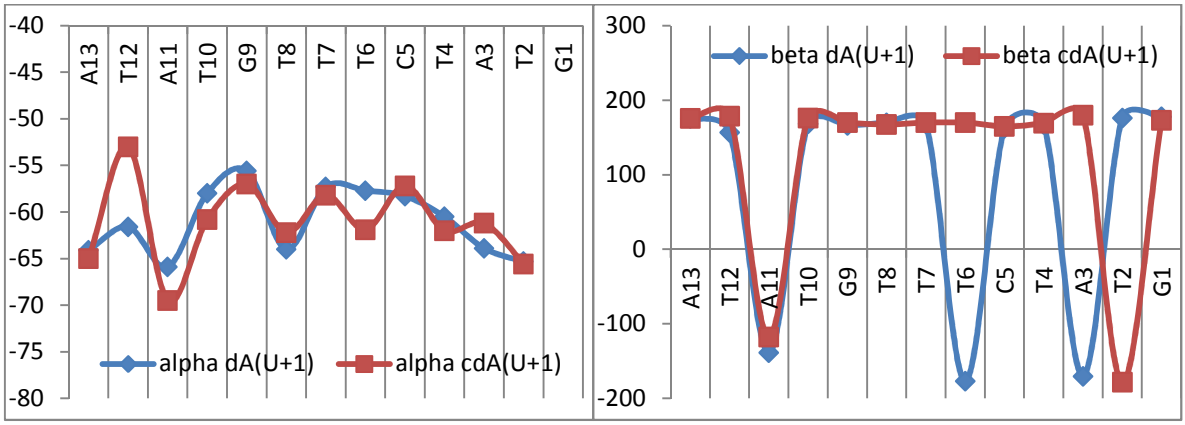


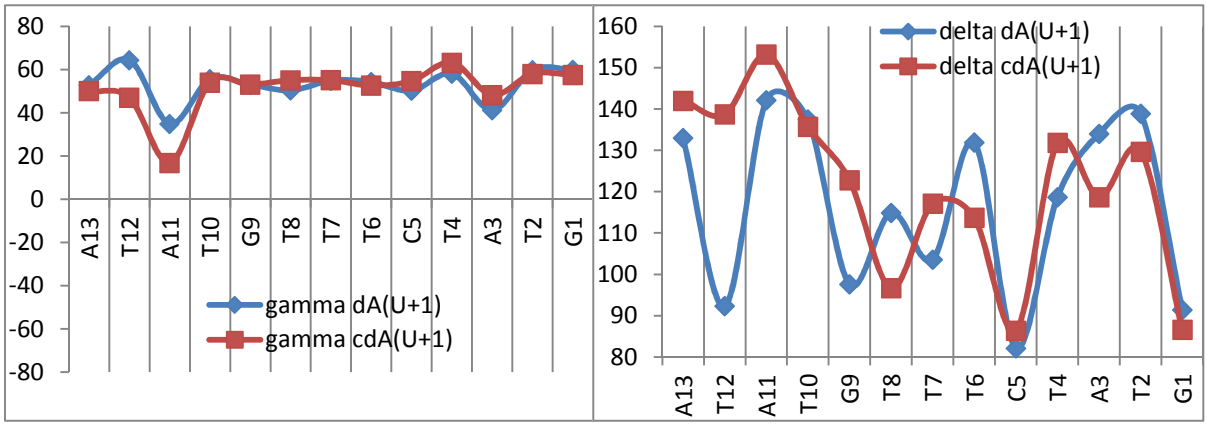


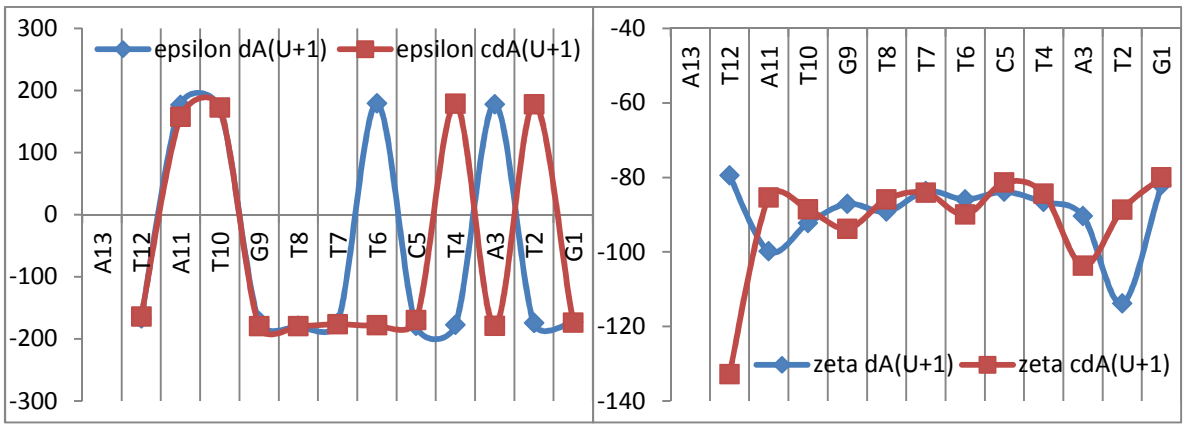
Graph 7S Graphical representation of data presented in Table 7S

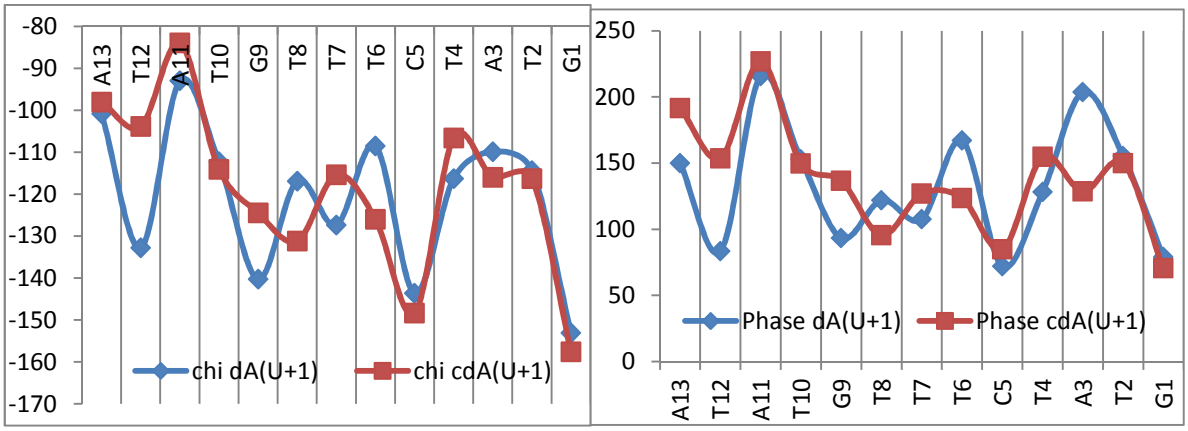
5'-^{13}A^{12}T^{11}A^{10}T^{9}G^{8}T^{7}**T**^{6}T^{5}C^{4}T^{3}A^{2}T^{1}G-3'

dA(U+1)/cdA(U+1). Comparison of dihedral angles (α, β, γ, δ, ε, ζ, χ) and sugar pseudorotation phase (P) vales obtained for the strand with the following base sequence: 5'-^{13}A^{12}T^{11}A^{10}T^{9}G^{8}T^{7}**T**^{6}T^{5}C^{4}T^{3}A^{2}T^{1}G-3', as a part of double stranded oligodeoxynucleotide contained at position **7A** 2'-deoxyadenosine in one strand and at **T8** (**U+1**) 2'-deoxyuridine in the opposite strand (**dA(U+1)**) with a double stranded oligodeoxynucleotide that contained at position **7A** (5′*S*)-5',8-cyclo-2'-deoxyadenosine and 2'-deoxyuridine at position **T8** (**cdA(U+1)**)."





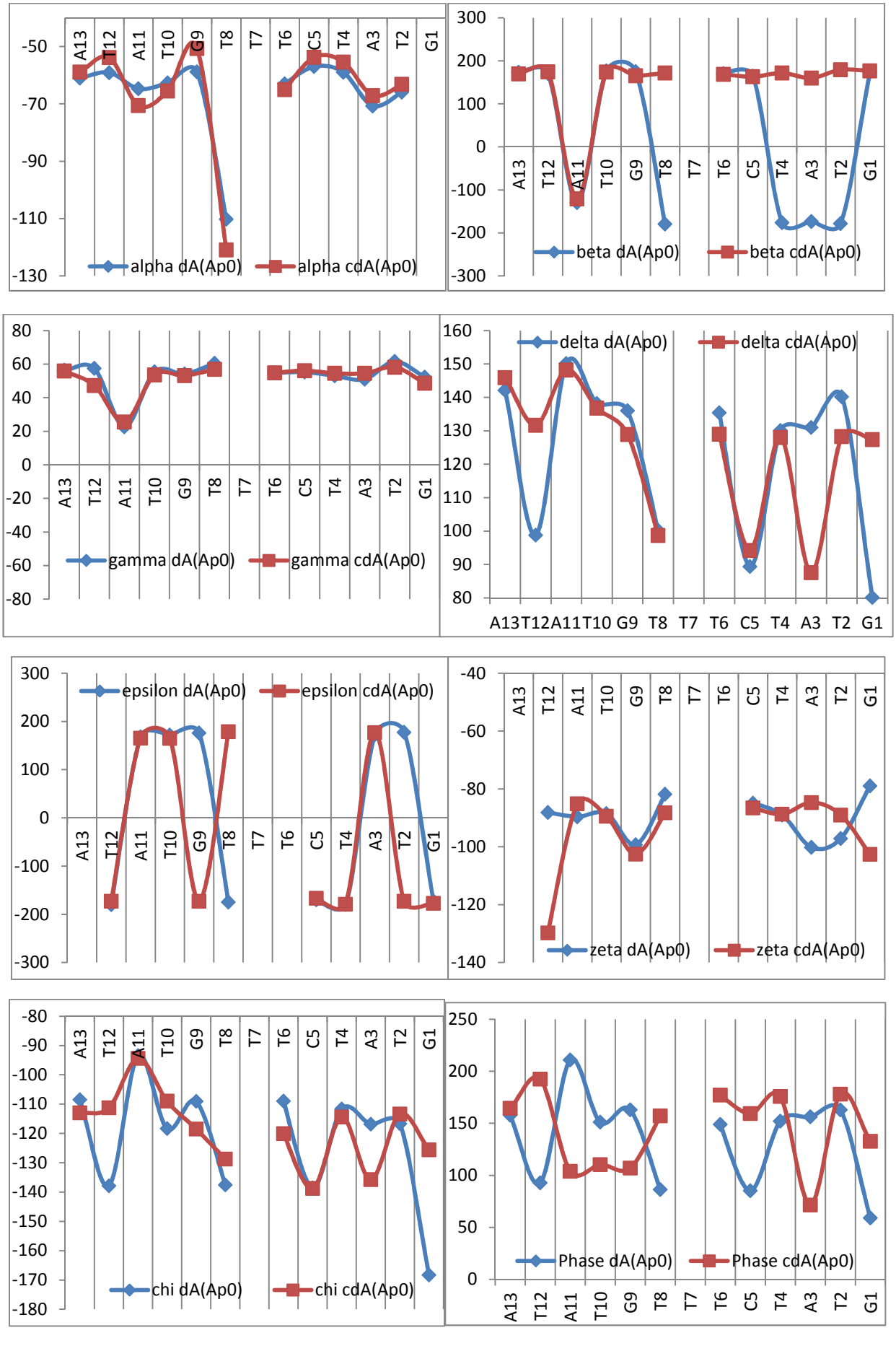




Graph 7S Graphical representation of data presented in Table 7S

5'-^{13}A^{12}T^{11}A^{10}T^{9}G^{8}T^{7}**T**^{6}T^{5}C^{4}T^{3}A^{2}T^{1}G-3'

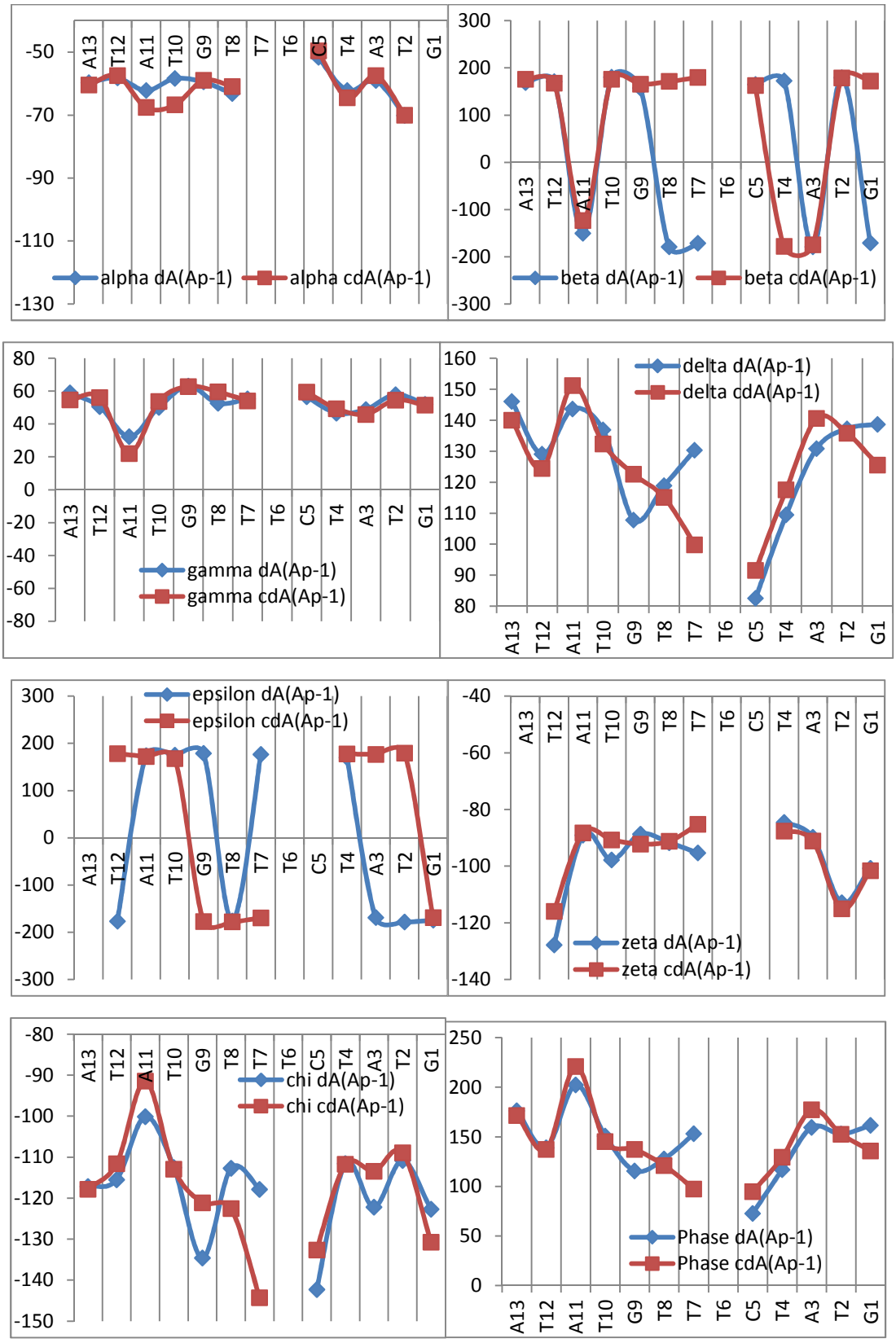
dA(Ap0)/cdA(Ap0). Comparison of dihedral angles (α, β, γ, δ, ε, ζ, χ) and sugar pseudorotation phase (P) vales obtained for the strand with the following base sequence: 5'-^{13}A^{12}T^{11}A^{10}T^{9}G^{8}T^{7}**T**^{6}T^{5}C^{4}T^{3}A^{2}T^{1}G-3' as a part of double stranded oligodeoxynucleotide contained at position **7A** 2'-deoxyadenosine in one strand and at **T7** (**Ap0**) the apurinic/apyrimidinic site in the opposite strand (**dA(Ap+1)**) with a double stranded oligodeoxynucleotide that contained at position **7A** (5′*S*)-5',8-cyclo-2'-deoxyadenosine and an apurinic/apyrymidinic site at position **T7 (cdA(Ap0))**.



Graph 7S Graphical representation of data presented in Table 7S

5'-^{13}A^{12}T^{11}A^{10}T^{9}G^{8}T^{7}**T**^{6}T^{5}C^{4}T^{3}A^{2}T^{1}G-3'

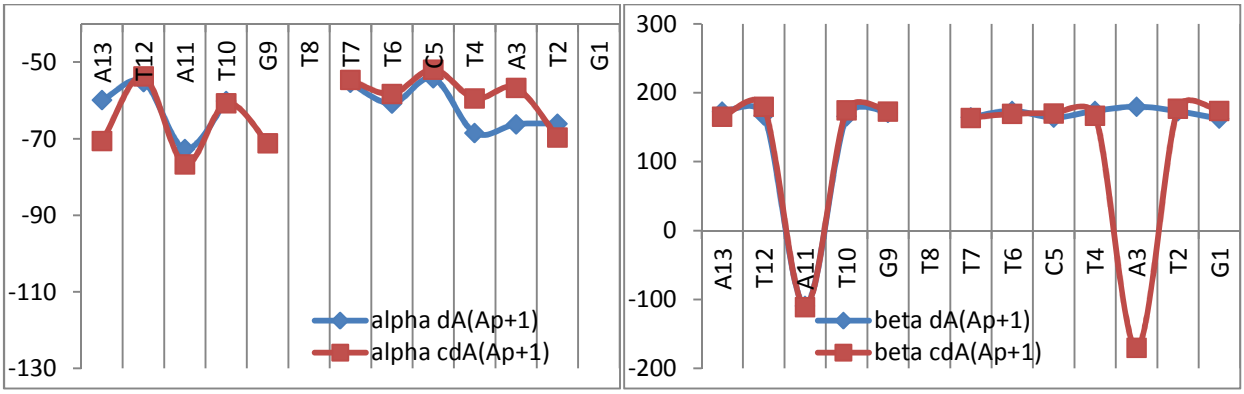
dA(Ap-1)/cdA(Ap-1). Comparison of dihedral angles (α, β, γ, δ, ε, ζ, χ) and sugar pseudorotation phase (P) vales obtained for the strand with the following base sequence: 5'-^{13}A^{12}T^{11}A^{10}T^{9}G^{8}T^{7}**T**^{6}T^{5}C^{4}T^{3}A^{2}T^{1}G-3' as a part of double stranded oligodeoxynucleotide that contained at position **7A** 2'-deoxyadenosine in one strand and at **T6** (**Ap-1**) an apurinic/apyrimidinic site in the opposite strand (**dA(Ap-1)**) with a double stranded oligodeoxynucleotide that contained at position **7A** (5′*S*)-5',8-cyclo-2'-deoxyadenosine and an apurinic/apyrimidinic site at position **T6 (cdA(Ap-1))**.

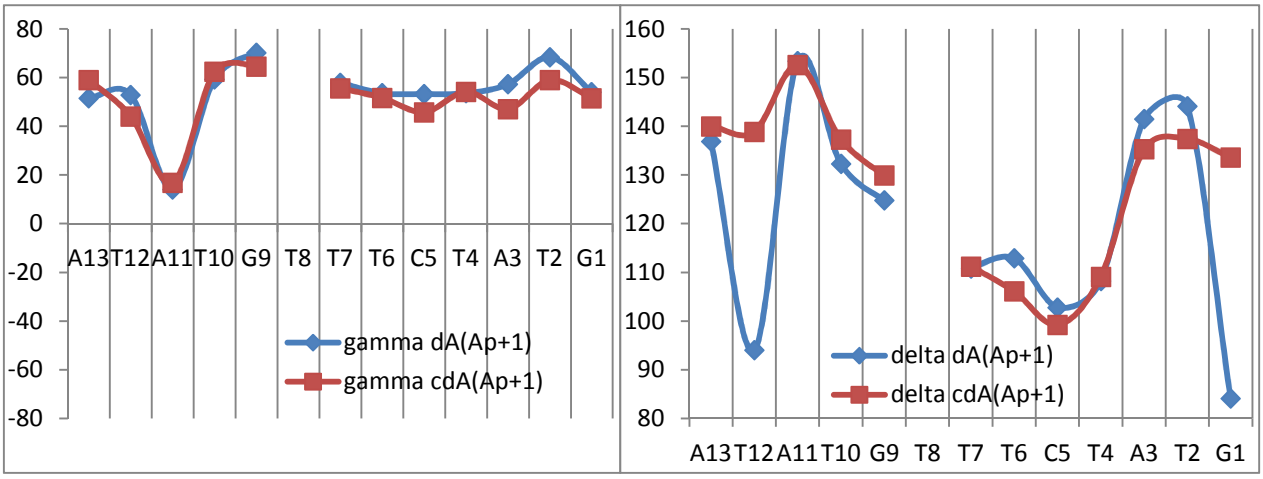


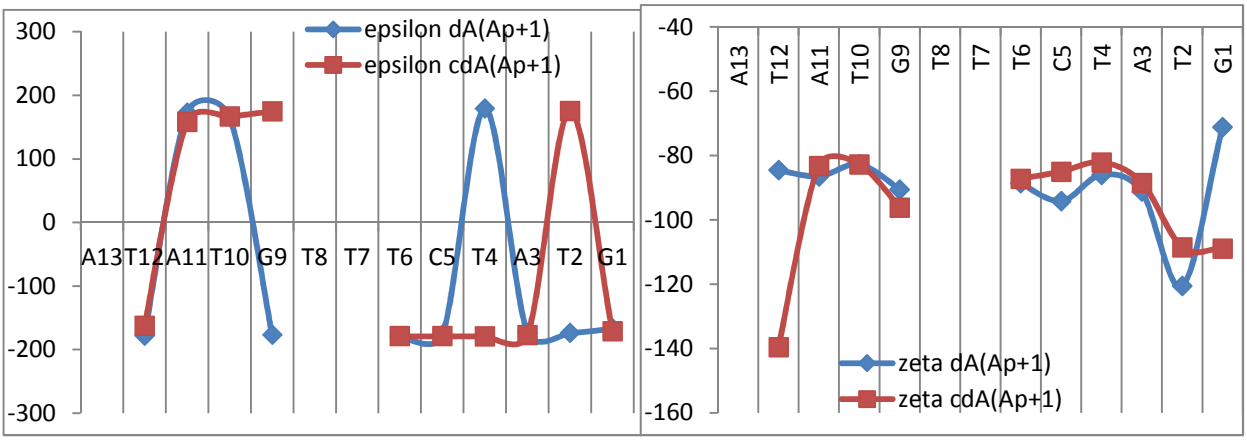
Graph 7S Graphical representation of data presented in Table 7S

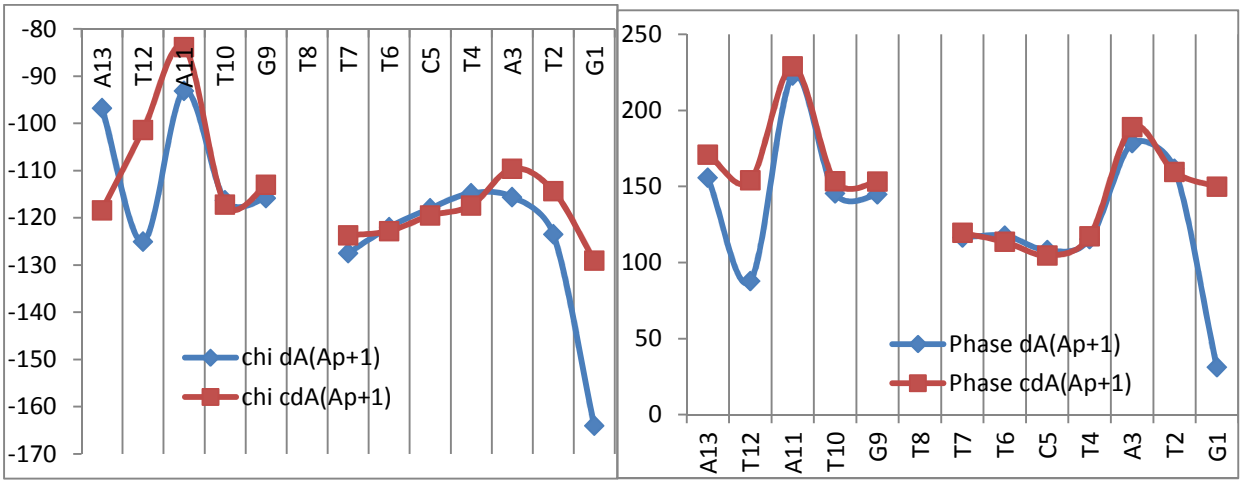
5'-^{13}A^{12}T^{11}A^{10}T^{9}G^{8}T^{7}**T**^{6}T^{5}C^{4}T^{3}A^{2}T^{1}G-3'

dA(Ap+1)/cdA(Ap+1). Comparison of dihedral angles (α, β, γ, δ, ε, ζ, χ) and sugar pseudorotation phase (P) vales obtained for the strand with the following base sequence: 5'-^{13}A^{12}T^{11}A^{10}T^{9}G^{8}T^{7}**T**^{6}T^{5}C^{4}T^{3}A^{2}T^{1}G-3' as a part of double stranded oligodeoxynucleotide that contained at position **7A** 2'-deoxyadenosine in one strand and at **T8** (**Ap+1**) an apurinic/apyrimidinic site in the opposite strand (**dA(Ap+1)**) a with double stranded oligodeoxynucleotide that contained at position **7A** (5′*S*)-5',8-cyclo-2'-deoxyadenosine and an apurinic/apyrimidinic site at position **T8 (cdA(Ap+1))**.





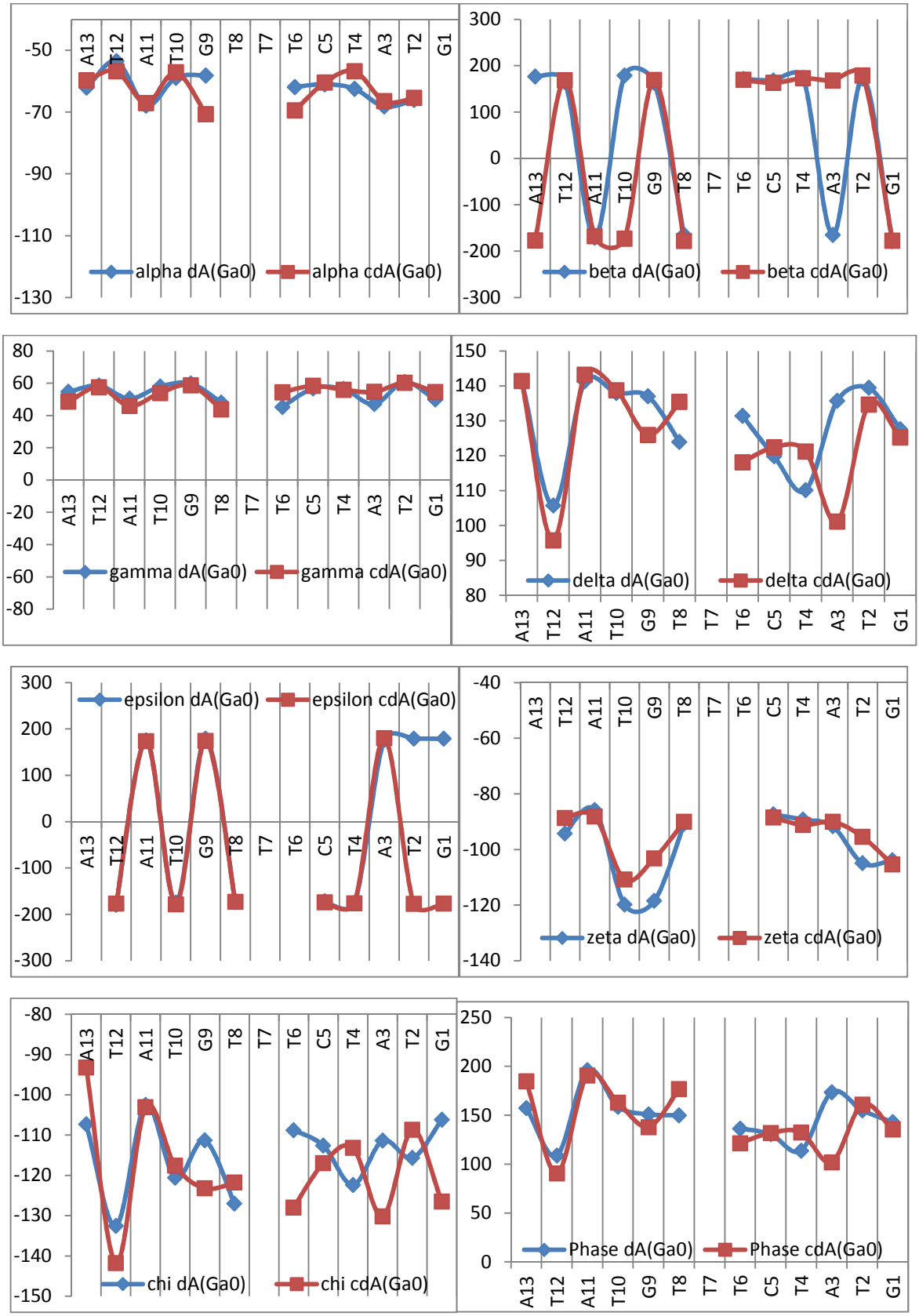




Graph 7S Graphical representation of data presented in Table 7S

5'-^{13}A^{12}T^{11}A^{10}T^{9}G^{8}T^{7}**T**^{6}T^{5}C^{4}T^{3}A^{2}T^{1}G-3'

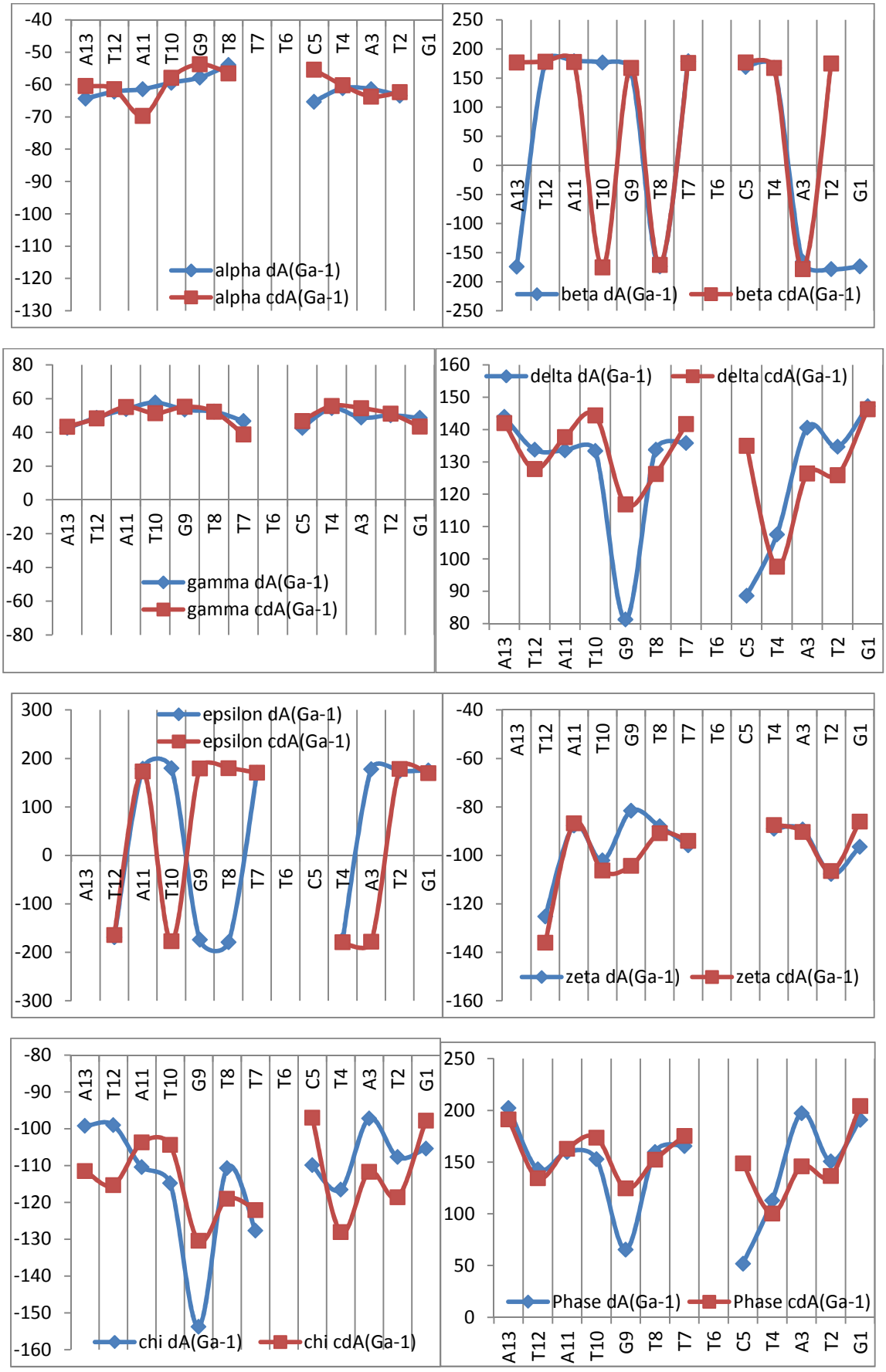
dA(Ga0)/cdA(Ga0). Comparison of dihedral angles (α, β, γ, δ, ε, ζ, χ) and sugar pseudorotation phase (P) vales obtained for the strand with the following base sequence: 5'-^{13}A^{12}T^{11}A^{10}T^{9}G^{8}T^{7}**T**^{6}T^{5}C^{4}T^{3}A^{2}T^{1}G-3' as a part of double stranded oligodeoxynucleotide contained at position **7A** 2'-deoxyadenosine in one strand and at position **T7** (**Ga0**) a single strand break e.i. gap in the opposite strand (**dA(Ga0)**) with a double stranded oligodeoxynucleotide that contained at position **7A** (5′*S*)-5',8-cyclo-2'-deoxyadenosine and a single strand break at position **T7 (cdA(Ga0))**.



Graph 7S Graphical representation of data presented in Table 7S

5'-^{13}A^{12}T^{11}A^{10}T^{9}G^{8}T^{7}**T**^{6}T^{5}C^{4}T^{3}A^{2}T^{1}G-3'

dA(Ga-1)/cdA(Ga-1). Comparison of dihedral angles (α, β, γ, δ, ε, ζ, χ) and sugar pseudorotation phase (P) vales obtained for the strand with the following base sequence: 5'-^{13}A^{12}T^{11}A^{10}T^{9}G^{8}T^{7}**T**^{6}T^{5}C^{4}T^{3}A^{2}T^{1}G-3' as a part of double stranded oligodeoxynucleotide contained at position **7A** 2'-deoxyadenosine in one strand and at **T6** (Ga-1) the single strand brake e.i. gap opposite chain (**dA(Ga-1)**) a with double stranded oligodeoxynucleotide that contained at position **7A** (5′*S*)-5',8-cyclo-2'-deoxyadenosine and a single strand break at position **T6 (cdA(Ga-1))**.



Graph 7S Graphical representation of data presented in Table 7S

5'-^{13}A^{12}T^{11}A^{10}T^{9}G^{8}T^{7}**T**^{6}T^{5}C^{4}T^{3}A^{2}T^{1}G-3'

dA(Ga+1)/cdA(Ga+1). Comparison of dihedral angles (α, β, γ, δ, ε, ζ, χ) and sugar pseudorotation phase (P) vales obtained for the strand with the following base sequence: 5'-^{13}A^{12}T^{11}A^{10}T^{9}G^{8}T^{7}**T**^{6}T^{5}C^{4}T^{3}A^{2}T^{1}G-3' as a part of double stranded oligodeoxynucleotide that contained at position **7A** 2'-deoxyadenosine in one strand and at **T8** (**Ga+1**) a single strand break e.i. gap in the opposite strand (**dA(Ga+1)**) with a double stranded oligodeoxynucleotide that contained at position **7A** (5′*S*)-5',8-cyclo-2'-deoxyadenosine and a single strand break at position **T8** (**cdA(Ga+1)**).