Formation of 5',8-cyclo-2'-deoxyadenosine in single strand DNA. Theoretical quantum mechanics study

Supplementary materials:

Table 1

Values of torsion angles in [^{o}] of 2-deoxyribose, for pseudorotation parameters calculation, obtained by DFT method (B3LYP/6-31++G**) in gaseous phase.

Dihedral angle	MOLECULE						
	1	**4**	**7**	**10**	**13**	**16**	**19**
υ_0	-15.7542	-0.82696	-13.8069	17.29648	36.70653	45.33845	43.55132
υ_1	31.37153	22.99658	32.6296	6.16924	-13.1502	-27.0456	-21.6066
υ_2	-33.8727	-34.5906	-37.8251	-25.3004	-13.707	-0.31766	-7.10976
υ_3	25.72718	34.91506	30.75327	35.92665	35.25305	26.87284	32.58279
υ_4	-6.56219	-21.8108	-11.0215	-33.9605	-45.5901	-45.4503	-47.9212
	2	**5**	**8**	**11**	**14**	**17**	**(5*S*')cdA**
υ_0	-16.7278	-9.75081	-11.0319	30.99414	41.49181	41.54146	45.50527
υ_1	33.0298	28.93577	28.88789	-26.5567	-26.3295	-16.9335	-28.8637
υ_2	-35.6788	-36.0515	-34.509	12.59076	2.64291	-12.4422	2.0557
υ_3	27.02625	30.76825	29.08006	4.73664	21.4326	37.00905	24.14854
υ_4	-6.76286	-13.4139	-11.6205	-22.5145	-39.8067	-49.5404	-43.6152
	3	**6**	**9**	**12**	**15**	**18**	**(5*R*')cdA**
υ_0	-11.2528	-3.17193	-3.78936	41.02927	40.98794	46.91446	47.08884
υ_1	30.40536	24.338	23.30184	-24.9909	-23.7949	-29.7694	-31.4138
υ_2	-36.7697	-34.8916	-32.2857	0.99809	-1.23062	2.69745	4.62543
υ_3	31.07042	33.43128	30.93818	22.935	24.69016	24.82854	22.3038
υ_4	-12.8215	-19.3728	-17.481	-40.4234	-41.424	-45.2122	-43.3334

Description of dihedral angles	
υ_0	C4' – O4' – C1' – C2'
υ_1	O4' – C1' – C2' – C3'
υ_2	C1' – C2' – C3' – C4'
υ_3	C2' – C3' – C4' – O4'
υ_4	C3' – C4' – O4' – C1'

Table 2

Natural Population Analysis (NPA) charges for each atom in anionic and anionic-radical form of 2'-deoxyadenosine-3',5'-diphosphate, calculated in gaseous phase (DFT B3LYP / 6-31++G**).

	1	2	3	4	5	6	7	8	9
5'-Phospate									
$CH_3$3''	0.28	0.28	0.28	0.29	0.30	0.29	0.28	0.29	0.29
O5'c	-0.84	-0.88	-0.88	-0.87	-0.88	-0.88	-0.88	-0.88	-0.86
P5'	2.55	2.55	2.55	2.55	2.55	2.5	2.55	2.55	2.56
O5'a	-1.18	-1.17	-1.19	-1.16	-1.16	-1.15	-1.17	-1.17	-1.16
O5'b	-1.18	-1.17	-1.16	-1.16	-1.16	-1.17	-1.19	-1.17	-1.09
2-Deoxyribose									
O5'	-0.86	-0.89	-0.86	-0.81	-0.82	-0.81	-0.86	-0.89	-0.86
C5'	-0.11	-0.11	-0.12	0.07	0.12	0.11	-0.11	-0.11	-0.11
H5'a	0.20	0.20	0.19			0.18	0.20	0.21	0.20
H5'b	0.23	0.23	0.23	0.20	0.20		0.23	0.23	0.23
C4'	0.05	0.05	0.06	0.03	-0.03	0.03	0.06	0.06	0.05
H4'	0.24	0.23	0.25	0.24	0.25	0.25	0.25	0.24	0.24
O4'	-0.59	-0.61	-0.61	-0.60	-0.61	-0.60	-0.60	-0.60	-0.59
C3'	0.07	0.07	0.07	0.07	0.07	0.07	0.07	0.07	0.07
H3'	0.24	0.25	0.26	0.25	0.25	0.24	0.26	0.24	0.23
O3'	-0.87	-0.89	-0.87	-0.88	-0.89	-0.86	-0.86	-0.89	-0.86
C2'	-0.5	-0.5	-0.5	-0.51	-0.51	-0.50	-0.5	-0.51	-0.50
H2' a	0.24	0.26	0.23	0.23	0.25	0.23	0.24	0.26	0.24
H2' b	0.28	0.28	0.28	0.29	0.29	0.29	0.28	0.28	0.28
C1'	0.28	0.28	0.27	0.27	0.27	0.27	0.26	0.27	0.27
H1'	0.24	0.24	0.26	0.25	0.24	0.24	0.26	0.24	0.25
Adenine									
N9	-0.43	-0.42	-0.42	-0.42	-0.42	-0.43	-0.47	-0.48	-0.49
C8	0.25	0.26	0.25	0.25	0.25	0.25	0.56	0.61	0.56
H8	0.29	0.29	0.25	0.25	0.27	0.29			
N7	-0.50	-0.52	-0.51	-0.51	-0.52	-0.51	-0.56	-0.55	-0.56
C4	0.37	0.37	0.37	0.37	0.37	0.37	0.38	0.378	0.37
C5	-0.01	-0.01	-0.01	-0.01	-0.01	-0.01	-0.01	-0.01	-0.01
C6	0.40	0.40	0.40	0.40	0.40	0.40	0.40	0.40	0.39
N6	-0.85	-0.85	-0.84	-0.84	-0.85	-0.85	-0.84	-0.84	-0.85
H6a	0.42	0.43	0.42	0.42	0.42	0.43	0.42	0.43	0.42
H6b	0.41	0.41	0.41	0.41	0.41	0.41	0.41	0.41	0.41
N3	-0.51	-0.52	-0.50	-0.51	-0.51	-0.51	-0.5	-0.51	-0.57
C2	0.22	0.22	0.23	0.23	0.23	0.25	0.23	0.23	0.22
H2	0.20	0.20	0.20	0.2	0.19	0.20	0.2	0.20	0.20
N1	-0.58	-0.58	-0.57	-0.58	-0.58	-0.58	-0.57	-0.57	-0.58
3'-Phospate									
O3'a	-1.19	-1.19	-1.19	-1.19	-1.19	-1.19	-1.19	-1.19	-1.19
O3'b	-1.16	-1.16	-1.17	-1.16	-1.16	-1.16	-1.17	-1.16	-1.16
P3'	2.55	2.55	2.54	2.55	2.55	2.55	2.54	2.55	2.55
O3'c	-0.88	-0.87	-0.87	-0.87	-0.87	-0.80	-0.86	-0.87	-0.88
$CH_3$5''	0.28	0.28	0.28	0.29	0.30	0.28	0.28	0.29	0.28

Table 3

Natural Population Analysis (NPA) charges for each atom in anionic and anionic-radical form of 2'-deoxyadenosine-3',5'-diphosphate and 5',8-cyclo-2'-deoxynucleotide-3',5'-diphosphate calculated in gaseous phase (DFT B3LYP / 6-31++G**).

	10	**11**	**12**	**13**	**14**	**15**	**16**	**17**	**18**	**19**	**(5*S*')cdA**	**(5*R*')cdA**
5'-Phospate												
$CH_3$3''	0.29	0.29	0.30	0.30	0.29	0.29	0.28	0.29	0.29	0.29	0.29	0.29
O5'c	-0.87	-0.87	-0.87	-0.87	-0.86	-0.87	-0.88	-0.88	-0.87	-0.87	-0.87	-0.87
P5'	2.54	2.54	2.54	2.54	2.56	2.54	2.55	2.55	2.57	2.55	2.55	2.55
O5'a	-1.18	-1.17	-1.15	-1.15	-1.17	-1.14	-1.16	-1.16	-1.18	-1.19	-1.17	-1.18
O5'b	-1.14	-1.16	-1.15	-1.15	-1.16	-1.17	-1.17	-1.16	-1.18	-1.16	-1.16	-1.15
2-Deoxyribose												
O5'	-0.81	-0.82	-0.79	-0.79	-.81	-0.81	-0.86	-0.87	-0.87	-0.87	-0.85	-0.86
C5'	-0.07	-0.07	0.15	0.14	0.13	0.14	0.07	0.07	0.07	0.06	0.02	0.03
H5'a	0.25	**0.20**	0.23	0.2			0.25	0.25			0.28	
H5'b	**0.19**	0.25			0.23	0.24			0.26	0.25		0.28
C4'	0.05	0.06	0.05	0.01	-0.00	-0.1	0.04	0.05	0.05	0.04	0.05	0.05
H4'	0.25	0.26	0.26	0.25	0.25	0.26	0.27	0.25	0.26	0.27	0.27	0.27
O4'	-0.59	0.58	-0.59	-0.59	-0.58	-0.59	-0.58	-0.59	-0.58	-0.59	-0.59	-0.578
C3'	0.07	0.06	0.07	0.07	0.07	0.07	0.07	0.07	0.06	0.07	0.07	0.07
H3'	0.25	0.24	0.24	0.26	0.24	0.24	0.25	0.26	0.23	0.24	0.25	0.23
O3'	-0.88	-0.87	-0.88	-0.89	-0.88	-0.88	-0.87	-0.89	-0.86	-0.86	-0.87	-0.86
C2'	-0.52	-0.51	-0.62	-0.52	-0.51	-0.51	-0.52	-0.52	-0.5	-0.5	-0.51	-0.49
H2' a	0.24	0.25	0.24	0.25	0.24	0.26	0.24	0.24	0.24	0.25	0.24	0.25
H2' b	0.30	0.28	0.29	0.29	0.28	0.28	0.29	0.29	0.27	0.28	0.29	0.27
C1'	0.27	0.27	0.26	0.29	0.26	0.29	0.27	0.28	0.25	0.28	0.27	0.27
H1'	0.25	0.25	0.25	0.23	0.25	0.23	0.25	0.24	0.25	0.24	0.25	0.25
Adenine												
N9	-0.47	-0.48	-0.46	-0.46	-0.47	-0.46	-0.45	-0.46	-0.48	-0.46	-0.44	-0.44
C8	0.42	0.45	0.15	0.15	0.15	0.15	0.086	0.09	0.08	0.09	0.44	0.44
H8			0.25	0.25	0.24	0.27	0.26	0.25	0.24	0.27		
N7	-0.55	-0.54	-0.5	-0.50	-0.48	-0.50	-0.42	-0.4	-0.4	-0.39	-0.49	-0.47
C4	0.37	0.37	0.38	0.37	0.38	0.37	0.43	0.42	0.43	0.42	0.037	0.36
C5	-0.01	-0.01	-0.01	0.02	0.01	0.01	0.02	0.03	0.03	0.02	0.00	0.00
C6	0.40	0.40	0.39	0.38	0.41	0.38	0.386	0.38	0.41	0.39	0.40	0.41
N6	-0.84	-0.84	-0.85	-0.85	-0.84	0.85	-0.84	-0.83	-0.82	-0.84	-0.84	-0.85
H6a	0.42	0.43	0.43	0.43	0.46	0.43	0.43	0.45	0.47	0.44	0.43	0.43
H6b	0.41	0.41	0.40	0.40	0.40	0.41	0.41	0.4	0.4	0.41	0.41	0.41
N3	-0.52	-0.52	-0.54	-0.54	-0.55	-0.54	-0.56	-0.56	-0.56	-0.56	-0.53	-0.53
C2	0.23	0.23	0.21	0.22	0.21	0.22	0.23	0.23	0.23	0.232	0.22	0.22
H2	0.20	0.20	0.19	0.19	0.19	0.19	0.2	0.19	0.19	0.2	0.2	0.20
N1	-0.57	-0.57	-0.57	-0.57	-0.57	-0.57	-0.56	-0.57	-0.58	-0.58	-0.58	-0.58
3'-Phospate												
O3'a	-1.19	-1.19	-1.19	-1.19	-1.19	-1.18	-1.18	-1.16	-1.19	-1.19	-1.16	-1.16
O3'b	-1.16	-1.17	-1.16	-1.16	-1.17	-1.17	-1.17	-1.19	-1.16	-1.16	-1.19	-1.19
P3'	2.55	2.55	2.55	2.55	2.55	2.55	2.55	2.55	2.55	2.55	2.55	2.55
O3'c	-0.87	-0.87	-0.87	-0.87	-0.87	-0.87	-0.87	-0.87	-0.88	-0.88	-0.87	-0.88
$CH_3$5''	0.29	0.29	0.29	0.28	0.29	0.29	0.29	0.28	0.28	0.28	0.29	0.28