Supplemental material to the manuscript

DNATCO: Assignment of DNA conformers at dnatco.org

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SUPPLEMENTARY DATA

Figure S1. The top part of the dnatco.org home page summarizes the purpose of the web service and defines the nomenclature of the dinucleotide step. The PDB formatted structure file can be uploaded either from user's disk or by typing a PDB four-letter code and pressing the respective SUBMIT button.

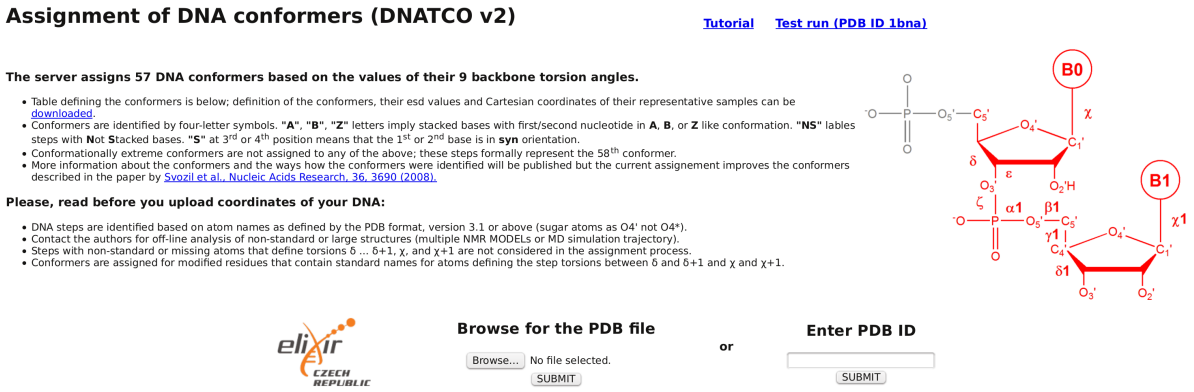

Table S1. The table summarizes the names and brief annotations of the 57 ntC DNA conformers and their grouping into 12 classes of the ntA structural alphabet together with the values of their torsion angles. These are seven torsions defining the backbone conformation of the step from δ of the first nucleotide to δ of the second one (labeled δ1), plus two torsion values around the glycosidic bonds of the first and second bases (χ and χ1). ntC are identified by four-letter symbols. The first letter aims to characterize the main feature(s) of the first nucleotide, the second of the second one. A, B, Z letters imply stacked bases with the first/second nucleotide in a conformation bearing features typical of the A, B, or Z DNA forms such as sugar pucker, torsion around the glycosidic bond, combination of torsions zeta and alpha and other torsions. The first two letters "NS" label steps with Not Stacked bases. Numbers at the third or fourth positions just guarantee the uniqueness of the ntC symbol, "S" at these positions means that the 1st or 2nd base is in the syn orientation. The last column "count" contains numbers of dinucleotide steps used for the definition of each ntC in the "golden set".

ntA	ntC	Annotation	δ	ε	ζ	α1	β1	γ1	δ1	χ	χ1	count
AAA	AA00	The most frequent, "canonical" A-DNA (identical to A-RNA)	83	206	287	293	174	55	83	199	202	296
	AA01	A-DNA with α1/γ1 crank (150/180)	82	194	291	149	193	182	87	205	188	55
	AA02	A-DNA with BI-like χ/χ1	88	203	275	294	161	54	88	244	245	168
A-B	AB01	A-to-B: δ C3'-endo, δ1 C2'-endo, χ/χ1 have A/B pattern	86	193	283	299	180	55	142	221	255	101
	AB02	A-to-B: δ~O4'-endo, extremely low ε, χ/χ1 are B-like	92	61	59	208	185	64	133	237	253	21
B1A	BA01	BI-to-A complex conformer with δ1 from C3' to O4'-endo, χ/χ1 are B-like	135	188	253	303	159	53	87	258	225	20
	BA02		122	185	271	279	186	48	89	233	238	9
	BA03		130	194	263	282	178	48	89	238	236	15
	BA04		137	190	258	296	165	54	90	249	226	16
	BA05		128	183	257	297	169	52	97	243	222	14
	BA06		129	185	267	296	170	53	101	249	236	86
	BA07		137	181	271	289	177	53	107	256	242	19
	BA08	B-to-A: β1~120, χ1 A-like	141	212	188	302	129	55	85	271	211	12
	BA09	BI-to-A: β1~60, α1/γ1 crank (250/170), χ1 A-like	135	199	287	254	71	168	86	265	187	13
	BA10		129	189	223	131	219	184	94	252	198	13
	BA11	B-to-A complex cluster: α1~100, γ1~180, χ1 A-like	133	203	233	100	218	199	88	252	199	15
	BA12		141	208	202	89	244	199	85	267	191	21
B2A	BA13	BII-to-A complex cluster: α1~60, γ1~180, χ1 A-like	142	224	191	80	237	196	92	271	197	20
	BA14		143	230	209	69	231	204	87	262	200	23
	BA15		142	240	187	75	227	189	88	267	201	19
	BA16	BII-to-A: χ1 A-like	145	255	187	63	226	196	87	260	201	7
	BA17	BII-to-A: δ1~O4'-endo, β1~120	148	255	177	294	130	44	96	272	234	27
BBB	BB00	The most frequent DNA conformer, "canonical" B form, also called BI	138	183	259	303	180	44	138	252	258	1960
2B1	BB01	Less populated variant of BI form	132	181	265	301	177	49	121	248	244	142
3B1	BB02	BI with α1/γ1 crank (30/300)	140	194	246	32	194	297	150	252	253	134
	BB03	BI with α1/γ1 crank (170/170)	145	176	276	166	164	173	146	239	232	31
B12	BB04	BI-to-BII conformer	140	201	214	315	153	46	140	263	253	244
	BB05	BI-to-BII with α1/γ1 crank (70/230), χ1 A-like	143	214	217	57	229	237	119	272	216	8
	BB06		143	223	193	73	233	212	126	265	205	14
BB2	BB07	BII form, typical by ε/ζ switch compared to BI	144	245	171	297	141	46	141	270	259	371
	BB08	BII form, variant, α1/γ1 crank (60/210)	145	259	184	61	223	205	140	268	235	11
	BB09		140	238	207	67	237	215	145	255	226	11
miB	BB10	B form with extremely low values of α1, β1, γ1	139	195	191	23	106	19	129	257	258	49
	BB11	B form with α1/γ1 crank (120/180)	144	200	199	121	226	189	143	258	222	22
	BB12	BI with α1/γ1 crank (250/170), low β1 70, χ1 A-like	140	196	287	248	73	172	144	263	212	18
	BB13	BI with α1/γ1 crank (210/160), low β1 100, χ1 A-like	143	186	291	216	104	161	147	252	219	17
	BB14	B-form with extremely low ε	121	104	303	229	260	73	132	264	263	8
	BB15	BI with high α1 and γ1 near 0	149	187	261	341	192	354	148	250	261	18
	BB16		144	215	301	278	180	42	144	194	281	11
	BB17		141	249	288	287	155	47	137	201	286	13
	BB18	Complex cluster of B-like conformers: A-like χ, bases may be unstacked to incorporate intercalated drug, occurs where backbone accommodates deformation (metal ion near, strand crossing in Holliday junctions, ends of duplexes)	147	226	274	286	168	53	145	199	278	30
	BB19		145	218	274	295	182	55	142	191	245	38
	BB20		142	233	295	294	165	50	139	188	257	7
	BB21		143	237	283	283	173	47	143	207	276	18
SQX	AB1S	A-to-B-like but χ1 syn, mostly in duplexes	91	214	280	295	176	56	139	238	67	14
	BBS1	BI-like but c syn, may be in duplex but many G-G in quadruplexes	146	189	275	294	174	52	135	62	261	47
	BB1S	G-G in quadruplexes, unusual β1, γ1, χ1 syn	140	202	282	307	258	304	151	236	65	17
	BB2S	BI-like but χ1 syn, mostly G-G in quadruplexes, α1 g+, γ1 g-	137	196	225	33	187	295	145	257	70	8
	NS1S	Partially unstacked T-G/G-T in quadruplexes, χ1 syn, unusual ζ, α1, γ1	143	206	61	82	204	192	146	242	68	13
	NS02	Start of loop in quadruplex or hairpin, G-X, untypical ζ, α1, γ1	145	225	67	74	189	191	137	264	258	14
	NS03	Partially unstacked T-T in quadruplexes, unusual combination of ε, ζ, α1, γ1, χ1	143	294	111	153	197	53	151	262	185	13
	NS04	Unstacked, in 4-way junction, ε, ζ high values	140	275	279	304	191	56	150	266	210	12
	NS05	5'-end of dsDNA, base open (unstacked), ζ, α1 ~60	154	242	77	63	177	64	137	237	249	10
ZZZ	ZZ1S	Z form, Y-R step	148	264	76	66	186	179	95	205	60	20
	ZZ2S	Z form, Y-R step, δ1 C2'-endo	141	263	71	78	179	185	148	208	77	41
	ZZS1	ZI form, R-Y step	97	242	294	209	230	55	144	63	205	48
	ZZS2	ZII form, R-Y step	95	186	63	169	162	44	144	58	213	17

Table S2. Estimated standard deviations of torsion averages for the 57 ntC DNA conformers defined in Table S1.

ntA	ntC	esd δ	esd ε	esd ζ	esd α1	esd β1	esd γ1	esd δ1	esd χ	esd χ1
AAA	AA00	4.8	7.7	5.9	6.2	8.0	6.1	4.4	7.3	6.9
	AA01	3.7	7.6	5.9	8.3	6.6	5.8	3.7	4.7	4.6
	AA02	5.9	8.9	9.9	6.9	8.2	4.9	5.5	7.8	7.4
A-B	AB01	3.8	12.7	7.9	7.8	8.6	6.0	4.4	11.8	8.6
	AB02	8.5	10.9	11.6	11.4	11.5	8.0	7.7	12.5	8.5
B1A	BA01	3.3	4.7	5.7	3.4	5.0	3.8	2.0	5.8	4.5
	BA02	5.4	6.1	6.2	4.1	4.2	5.1	6.7	4.3	3.3
	BA03	8.5	6.1	7.3	5.4	9.0	4.5	5.0	5.9	5.5
	BA04	3.8	2.7	4.0	4.9	3.3	3.3	3.7	3.9	4.8
	BA05	7.8	6.4	8.7	11.8	9.3	7.8	10.2	7.6	6.9
	BA06	8.1	7.4	5.8	6.2	4.8	5.4	7.9	8.2	6.2
	BA07	6.0	7.8	6.1	8.5	5.3	12.6	4.8	7.4	5.9
	BA08	6.6	6.8	4.9	4.8	6.0	5.8	5.5	5.5	3.1
	BA09	4.4	5.7	5.2	5.7	10.0	6.0	4.6	4.7	4.7
	BA10	12.1	7.8	11.5	8.4	6.8	7.9	6.6	9.1	6.1
	BA11	8.1	7.3	15.5	12.4	8.3	12.8	3.5	8.8	5.0
	BA12	9.3	6.9	14.8	7.0	9.6	7.5	6.9	13.4	4.8
B2A	BA13	5.5	10.6	7.6	9.3	8.2	8.1	7.8	9.6	6.3
	BA14	7.2	10.3	8.5	10.2	7.0	7.0	6.0	7.5	5.5
	BA15	6.0	7.9	7.0	7.9	6.1	8.4	6.4	8.7	8.3
	BA16	5.1	11.4	4.4	8.2	6.9	2.8	3.2	3.3	3.2
	BA17	8.1	8.6	10.1	9.5	9.0	7.4	7.8	9.4	8.1
BBB	BB00	5.8	9.3	10.2	9.2	10.5	6.0	5.1	9.0	9.9
2B1	BB01	8.1	6.9	6.0	7.7	5.6	6.4	3.8	8.6	6.0
3B1	BB02	5.6	7.0	7.8	8.8	14.2	8.5	4.8	8.9	9.3
	BB03	5.6	7.4	8.2	14.5	12.1	8.6	6.5	12.1	9.1
B12	BB04	4.4	9.6	9.1	8.0	9.0	6.5	4.5	8.9	8.7
	BB05	6.5	6.5	6.5	6.5	9.4	4.1	9.1	10.7	7.5
	BB06	5.8	7.5	7.7	7.4	7.0	4.7	7.4	9.9	7.7
BB2	BB07	5.1	12.3	9.6	8.8	7.6	6.0	5.5	9.7	11.2
	BB08	6.3	10.1	6.6	8.0	9.4	4.6	10.5	6.4	7.4
	BB09	8.7	6.6	8.1	6.6	7.0	7.4	8.0	7.5	8.2
miB	BB10	5.2	10.3	9.2	11.4	9.0	9.6	7.5	10.3	9.6
	BB11	6.2	9.6	9.0	12.5	11.3	10.2	7.0	10.0	9.9
	BB12	4.6	6.0	11.7	13.7	3.8	4.2	4.4	8.0	9.0
	BB13	7.3	7.9	11.4	9.4	10.5	7.0	7.9	7.9	7.5
	BB14	6.0	6.8	5.6	7.2	4.2	8.6	4.6	8.7	5.9
	BB15	4.8	6.4	10.4	10.4	11.6	12.5	5.2	10.7	7.6
	BB16	5.0	7.4	8.4	6.8	6.9	6.2	5.8	7.6	10.9
	BB17	4.7	6.6	5.1	4.8	5.1	6.9	3.8	6.6	7.5
	BB18	7.0	5.5	6.7	6.3	5.4	5.4	4.6	6.1	7.9
	BB19	8.1	8.8	5.5	6.8	5.6	8.3	4.7	9.0	8.1
	BB20	8.7	5.2	6.7	10.0	9.0	4.9	6.7	6.6	11.0
	BB21	7.9	7.1	5.9	7.4	6.7	6.7	4.2	5.3	8.0
SQX	AB1S	2.4	3.3	4.4	4.6	4.4	3.6	4.9	4.2	3.7
	BBS1	5.1	8.7	7.7	9.6	6.9	7.7	6.8	9.4	10.8
	BB1S	6.6	9.3	6.8	5.6	6.7	4.9	3.5	12.7	3.9
	BB2S	2.6	3.1	2.3	6.4	3.7	3.1	1.9	4.8	2.6
	NS1S	2.5	6.3	7.0	7.9	6.0	6.1	4.8	4.5	4.7
	NS02	2.8	9.3	6.6	12.1	7.9	7.7	9.1	12.5	8.3
	NS03	3.2	3.9	6.2	8.5	4.7	6.4	4.4	5.9	2.3
	NS04	3.5	6.2	7.3	9.3	7.9	7.1	2.6	6.4	3.9
	NS05	2.1	2.0	4.0	5.3	2.2	4.2	1.3	4.7	3.1
ZZZ	ZZ1S	3.5	5.3	4.0	3.8	4.4	3.5	5.0	5.5	6.1
	ZZ2S	4.5	5.5	6.2	7.0	6.7	4.7	6.6	6.8	4.7
	ZZS1	5.8	7.2	8.7	6.9	10.1	5.8	4.9	4.9	6.4
	ZZS2	2.0	5.6	6.4	6.0	6.6	5.1	2.9	4.3	4.6