

SUPPORTING INFORMATION

Double Threading through DNA: NMR Structural Study of a Bis-Naphthalene Macrocycle Bound to a Thymine–Thymine Mismatch

Muriel Jourdan,^{,†} Anton Granzhan,[‡] Regis Guillot,[§] Pascal Dumy[†] and Marie-Paule Teulade-Fichou^{*,‡}*

[†] CNRS UMR5250, ICMG FR2607, Département de Chimie Moléculaire, Université Joseph Fourier, 570 rue de la Chimie, 38041 Grenoble Cedex 9, France

[‡] CNRS UMR176, Institut Curie, Centre de Recherche, 91405 Orsay, France

[§] CNRS UMR8182, Institut de Chimie Moléculaire et des Matériaux d'Orsay, Université Paris-Sud XI, 91405 Orsay, France

Table S1. ^1H and ^{31}P chemical shifts (ppm) of TT-DNA duplex at 10 °C.

DNA Base	H8	H6	H5/Me/H2	H1'	H2'	H2''	H3'	H4'	H5'/H5''	NH	NH ₂	^{31}P
C1	–	7.70	5.94	5.78	2.12	2.50	4.75	4.09	3.76	–	7.13/8.14	–
G2	8.05	–	–	6.06	2.75	2.86	5.02	4.42	4.15/4.07	12.94	–	–4.62
T3	–	7.34	1.45	6.10	2.19	2.54	4.90	4.28	4.19	13.86	–	–4.51
C4	–	7.46	5.62	5.62	2.04	2.43	4.84	4.13	na ^a	–	6.96/8.52	–4.84
G5	7.92	–	–	6.00	2.60	2.73	4.83	4.28	4.12/4.07	13.00	–	–4.51
T6	–	6.95	1.50	5.52	1.29	2.00	4.77	4.30	4.04/4.10	10.56	–	–5.03
A7	8.29	–	7.79	6.07	2.92	2.92	5.04	4.21	na	–	–	–4.61
G8	7.63	–	–	5.88	2.51	2.73	4.88	4.40	na	12.82	–	–4.51
T9	–	7.17	1.29	5.88	2.04	2.46	4.89	4.22	na	13.79	–	–4.84
G10	7.92	–	–	5.96	2.65	2.75	5.01	4.40	na	12.94	–	–4.82
C11	–	7.48	5.45	6.21	2.21	2.21	4.52	4.28	4.09/4.13	–	6.77/8.27	–4.50
G12	7.98	–	–	5.99	2.65	2.81	4.87	4.27	3.73/3.73	13.12	–	–
C13	–	7.48	5.45	5.66	2.16	2.47	4.90	4.23	4.15	–	6.62/8.53	–5.03
A14	8.34	–	7.80	6.29	2.81	2.95	5.07	4.49	4.12	–	–	–4.50
C15	–	7.34	5.26	5.85	2.06	2.55	4.70	4.28	na	–	6.80/8.07	–4.82
T16	–	7.42	1.57	6.07	2.19	2.57	4.86	4.25	4.12/4.12	13.79	–	–4.96
T17	–	7.31	1.59	5.75	1.89	2.33	4.87	4.11	na	10.61	–	–5.14
C18	–	7.68	5.75	5.01	2.42	2.42	4.88	4.21	na	–	7.13/8.47	na
G19	7.93	–	–	5.66	2.72	2.83	5.05	4.35	na	12.82	–	–3.72
A20	8.24	–	7.92	6.24	2.69	2.92	5.06	4.48	4.24/4.18	–	–	–4.87
C21	–	7.26	5.31	5.63	1.87	2.30	4.82	4.26	4.13	–	6.77/8.39	–4.84
G22	7.93	–	–	6.17	2.62	2.37	4.69	4.19	4.11	12.92	–	–4.51

^a na: not assigned

Table S2. ^1H and ^{31}P chemical shifts of the **2,7-BisNP**–TT-DNA complex. Assignments are at 10 °C for sample in D_2O , 10 °C or 5 °C for exchangeable protons in 90% H_2O / 10% D_2O .

DNA Base	H8	H6	H5/Me/H2	H1'	H2'	H2''	H3'	H4'	NH	NH ₂	^{31}P
C1	–	7.70	5.94	5.77	2.12	2.48	4.75	4.08	–	7.12/8.14	-
G2	8.02	–	–	6.03	2.72	2.83	4.87	4.39	12.90	–	–4.67
T3	–	7.27	1.40	6.03	2.12	2.47	4.88	4.25	13.72	–	–4.63
C4	–	7.26	5.50	5.62	2.04	2.13	4.73	4.15	–	6.90/8.50	–4.88
G5	7.91	–	–	6.07	2.57	2.86	5.10	na ^a	11.63	–	na
T6	–	7.16	1.40	5.50	1.50	2.12	4.75	4.17	10.56 or 10.49 ^b	–	na
A7	7.88	–	na	6.04	2.89	2.89	4.88	4.31	–	–	–4.23
G8	7.80	–	–	5.95	2.57	2.75	4.47	4.23	12.44	–	–4.91
T9	–	7.25	1.34	5.90	2.12	2.50	4.91	4.25	13.72	–	na
G10	7.92	–	–	5.96	2.65	2.75	5.01	4.38	12.89	–	–4.82
C11	–	7.48	5.48	6.21	2.18	2.18	4.51	4.14	–	6.77/8.26	–4.58
G12	7.97	–	–	5.99	2.66	2.80	4.85	4.24	13.10	–	-
C13	–	7.48	5.43	5.69	2.19	2.47	4.90	4.23	–	6.59/8.48	na
A14	8.25	–	7.77	6.22	2.71	2.85	5.08	4.44	–	–	na
C15	–	7.15	5.07	5.78	2.32	1.72	4.70	4.28	–	6.65/8.02	na
T16	–	7.11	1.11	6.10	2.20	2.40	4.75	4.24	12.82	–	na
T17	–	7.89	2.04	5.97	2.42	2.55	5.04	4.12	10.56 or 10.49 ^b	–	na
C18	–	7.65	5.92	5.42	2.19	2.37	4.76	4.22	–	6.95/7.84	na
G19	7.92	–	–	5.54	2.73	2.78	5.03	4.37	12.71	–	na
A20	8.23	–	7.88	6.25	2.70	2.91	5.06	4.49	–	–	–4.76
C21	–	7.26	5.30	5.63	1.87	2.30	4.83	4.26	–	6.75/8.37	na
G22	7.92	–	–	6.16	2.62	2.36	4.67	4.19	12.90	–	–4.56

^a na: not assigned; ^b not differentiated.

Table S3. Table of distance restraints used for the molecular dynamics of the free TT-DNA duplex. The values are in Å. (a) distance in the final structure; (b) upper or lower restraint; (c) deviation from the upper or lower restraint in the final structure. The deviations are highlighted as followed: yellow (0.2–0.3 Å), grey (0.3–0.5 Å) and red (> 0.5 Å).

First atom	Last atom		current value (a)	upper/lower restraint (b)	deviation (c)						
H1' DC5	1 -- H6 DC5	1:	3.625	3.800	0.000	*H73 DT	9 -- H1' DG	8:	4.115	3.840	0.275
H2'1 DC5	1 -- H1' DC5	1:	2.442	2.520	0.000	*H73 DT	9 -- H8 DG	8:	2.689	2.880	0.191
H2'1 DC5	1 -- H6 DC5	1:	2.898	3.600	0.000	*H73 DT	9 -- H6 DT	9:	2.426	2.450	0.024
H2'1 DC5	1 -- H8 DG	2:	1.940	2.050	0.110	H2'1 DG	10 -- H5 DC3	11:	2.171	2.610	0.000
H2'2 DC5	1 -- H1' DC5	1:	3.048	3.210	0.000	H2'1 DG	10 -- H6 DC3	11:	2.687	2.610	0.077
H2'2 DC5	1 -- H6 DC5	1:	2.082	2.510	0.000	H8 DG	10 -- H1' DG	10:	3.843	4.000	0.000
H2'2 DC5	1 -- H8 DG	2:	3.582	3.440	0.142	H8 DG	10 -- H2'1 DG	10:	3.096	3.000	0.096
H5 DC5	1 -- H6 DC5	1:	2.428	2.450	0.000	H8 DG	10 -- H2'2 DG	10:	2.258	2.220	0.038
H2'1 DG	2 -- H8 DG	2:	2.458	2.270	0.188	H8 DG	10 -- H2'1 DT	9:	2.045	2.490	0.000
H2'1 DG	2 -- H6 DT	3:	2.242	2.400	0.158	H8 DG	10 -- H2'2 DT	9:	3.560	3.700	0.000
H2'2 DG	2 -- H8 DG	2:	2.153	2.380	0.000	H8 DG	10 -- H6 DT	9:	3.970	4.000	0.030
H2'2 DG	2 -- H6 DT	3:	3.861	3.700	0.161	H1' DC3	11 -- H5 DC3	11:	5.134	5.000	0.134
H8 DG	2 -- H1' DC5	1:	2.816	2.720	0.096	H1' DC3	11 -- H6 DC3	11:	3.626	3.720	0.000
H8 DG	2 -- H1' DG	2:	3.653	4.000	0.000	H2'1 DC3	11 -- H1' DC3	11:	2.171	2.060	0.111
H8 DG	2 -- H6 DT	3:	4.162	5.000	0.000	H2'1 DC3	11 -- H6 DC3	11:	3.181	3.000	0.181
H1' DT	3 -- H6 DT	3:	3.750	3.700	0.050	H2'2 DC3	11 -- H1' DC3	11:	2.975	3.000	0.000
H1' DT	3 -- H6 DC	4:	3.315	3.300	0.015	H2'2 DC3	11 -- H6 DC3	11:	1.938	2.190	0.000
H2'1 DT	3 -- H6 DT	3:	3.374	3.500	0.000	H2'2 DC3	11 -- H2'1 DC3	11:	4.895	5.000	0.000
H2'1 DT	3 -- H6 DC	4:	2.045	2.220	0.175	H5 DC3	11 -- H2'2 DC3	11:	4.125	4.000	0.125
H2'2 DT	3 -- H6 DT	3:	2.238	2.350	0.000	H6 DC3	11 -- H5 DG5	11:	2.363	2.450	0.000
H2'2 DT	3 -- H6 DC	4:	3.727	3.700	0.027	H1' DG5	12 -- H8 DG5	12:	3.662	3.800	0.000
H6 DT	3 -- H1' DG	2:	2.470	2.520	0.000	H2'1 DG5	12 -- H8 DG5	12:	2.828	2.870	0.058
H6 DT	3 -- H5 DC	4:	3.803	3.800	0.003	H8 DG5	12 -- H2'2 DG5	12:	1.864	2.210	0.000
*H73 DT	3 -- H8 DG	2:	2.931	3.210	0.000	H1' DC	13 -- H8 DA	14:	2.841	2.750	0.091
*H73 DT	3 -- H6 DT	3:	2.740	3.070	0.000	H2'1 DC	13 -- H1' DC	13:	2.340	2.620	0.000
H2'1 DC	4 -- H6 DC	4:	3.020	3.000	0.020	H2'1 DC	13 -- H6 DC	13:	3.443	3.330	0.113
H2'2 DC	4 -- H6 DC	4:	2.080	2.590	0.000	H2'1 DC	13 -- H8 DA	14:	2.111	2.280	0.169
H6 DC	4 -- H1' DC	4:	3.677	3.900	0.000	H2'2 DC	13 -- H5 DC	13:	4.045	3.970	0.075
H6 DC	4 -- H5 DC	4:	2.438	2.450	0.000	H2'2 DC	13 -- H6 DC	13:	2.076	2.510	0.000
H8 DG	5 -- H1' DC	4:	2.498	2.410	0.088	H2'2 DC	13 -- H8 DA	14:	3.741	3.630	0.111
H8 DG	5 -- H2'1 DC	4:	2.107	2.490	0.000	H6 DC	13 -- H2'2 DG5	12:	2.914	2.630	0.284
H8 DG	5 -- H2'2 DC	4:	3.802	3.700	0.102	H2'1 DA	14 -- H5 DC	15:	3.076	3.050	0.026
H8 DG	5 -- H6 DC	4:	4.638	5.000	0.000	H2'2 DA	14 -- H5 DC	15:	2.555	2.930	0.000
H8 DG	5 -- H1' DG	5:	3.901	3.900	0.001	H8 DA	14 -- H1' DA	14:	3.796	3.660	0.136
H8 DG	5 -- H2'1 DG	5:	3.604	3.700	0.000	H8 DA	14 -- H2'2 DA	14:	2.468	2.370	0.098
H8 DG	5 -- H2'2 DG	5:	2.353	2.390	0.000	H8 DA	14 -- H5 DC	15:	3.161	3.060	0.101
H2'1 DT	6 -- H1' DT	6:	2.323	2.600	0.000	H1' DC	15 -- H2'2 DC	15:	2.653	2.390	0.263
H2'2 DT	6 -- H1' DT	6:	2.858	2.440	0.418	H1' DC	15 -- H6 DC	15:	3.330	2.980	0.350
H6 DT	6 -- H1' DG	5:	2.886	2.790	0.096	H1' DC	15 -- H6 DT	16:	3.005	2.910	0.095
H6 DT	6 -- H2'1 DG	5:	2.126	2.390	0.264	H1' DC	15 -- *H73 DT	16:	4.228	3.990	0.238
H6 DT	6 -- H2'2 DG	5:	3.744	3.700	0.044	H5 DC	15 -- H1' DA	14:	3.375	3.230	0.145
H6 DT	6 -- H8 DG	5:	4.832	5.000	0.000	H6 DC	15 -- H1' DA	14:	2.962	2.830	0.132
H6 DT	6 -- H1' DT	6:	3.495	3.700	0.000	H6 DC	15 -- H2'2 DA	14:	2.967	2.740	0.227
H6 DT	6 -- H2'1 DT	6:	2.575	2.490	0.085	H6 DC	15 -- H2'1 DC	15:	3.397	3.000	0.397
H6 DT	6 -- H2'2 DT	6:	2.124	2.300	0.179	H6 DC	15 -- H2'2 DC	15:	2.138	2.350	0.000
H6 DT	6 -- *H73 DT	6:	2.776	3.170	0.000	H6 DC	15 -- H5 DC	15:	2.473	2.370	0.103
*H73 DT	6 -- H8 DG	5:	3.551	3.470	0.081	H2'1 DT	16 -- H6 DT	16:	3.257	3.000	0.257
H1' DA	7 -- H8 DG	8:	2.808	2.660	0.148	H6 DT	16 -- H2'1 DC	15:	2.802	2.970	0.968
H2'1 DA	7 -- H8 DA	7:	3.240	3.170	0.070	H6 DT	16 -- H2'2 DC	15:	2.832	2.440	0.392
H2'1 DA	7 -- H8 DG	8:	2.279	2.770	0.000	H6 DT	16 -- H1' DT	16:	3.708	3.790	0.000
H2'2 DA	7 -- H8 DA	7:	2.051	2.160	0.000	H6 DT	16 -- H2'2 DT	16:	2.140	2.440	0.000
H2'2 DA	7 -- H8 DG	8:	3.768	3.770	0.000	*H73 DT	16 -- H5 DC	15:	3.422	3.580	0.000
H8 DA	7 -- H1' DA	7:	3.642	3.470	0.172	*H73 DT	16 -- H6 DC	15:	2.870	3.490	0.000
H8 DA	7 -- H8 DG	8:	4.387	5.000	0.000	*H73 DT	16 -- H6 DT	16:	2.681	3.120	0.000
H1' DG	8 -- H2'1 DG	8:	2.108	2.610	0.000	H1' DT	17 -- H6 DC	18:	3.263	3.150	0.113
H2'2 DG	8 -- H1' DG	8:	2.739	2.460	0.279	H2'1 DT	17 -- H5 DC	18:	3.145	3.050	0.095
H2'2 DG	8 -- H8 DG	8:	2.068	2.210	0.142	H2'1 DT	17 -- H6 DC	18:	2.159	2.570	0.411
H2'2 DG	8 -- H6 DT	9:	2.990	3.610	0.000	H2'2 DT	17 -- H6 DC	18:	2.998	2.900	0.098
H8 DG	8 -- H1' DG	8:	3.515	3.920	0.000	H6 DT	17 -- H2'1 DT	16:	2.750	2.730	0.020
H8 DG	8 -- H2'1 DG	8:	3.479	3.710	0.000	H6 DT	17 -- H2'2 DT	16:	2.694	2.640	0.054
H1' DT	9 -- H8 DG	10:	2.823	2.740	0.083	H6 DT	17 -- H6 DT	16:	3.225	2.910	0.315
H1' DT	9 -- H2'1 DT	9:	2.458	2.510	0.000	H6 DT	17 -- H1' DT	17:	3.200	2.520	0.680
H2'1 DT	9 -- H6 DT	9:	3.102	3.000	0.102	H6 DT	17 -- H2'1 DT	17:	3.149	2.580	0.569
H2'2 DT	9 -- H6 DT	9:	2.062	2.390	0.000	H6 DT	17 -- H2'2 DT	17:	1.878	2.140	0.262
H6 DT	9 -- H2'1 DG	8:	2.238	2.690	0.000	H6 DT	17 -- H3' DT	17:	2.769	2.630	0.139
H6 DT	9 -- H8 DG	8:	3.490	3.190	0.309	H6 DT	17 -- *H73 DT	17:	2.830	3.190	0.000
*H73 DT	9 -- H8 DG	10:	4.972	4.820	0.152	H6 DT	17 -- H5 DC	18:	3.268	3.080	0.188
						H1' DC	18 -- H6 DC	18:	3.480	3.380	0.100
						H5 DC	18 -- H2'2 DT	17:	2.755	3.000	0.000
						H5 DC	18 -- *H73 DT	17:	3.371	4.160	0.000
						H5 DC	18 -- H6 DC	18:	2.451	2.440	0.011
						H6 DC	18 -- H2'1 DC	18:	2.584	2.390	0.194

H6	DC	18	--	H2'2	DC	18:	1.924	2.720	0.796
H6	DC	18	--	H8	DG	19:	5.237	5.000	0.237
H1'	DG	19	--	H2'2	DG	19:	2.778	2.530	0.248
H1'	DG	19	--	H8	DG	19:	3.618	3.480	0.138
H1'	DG	19	--	H8	DA	20:	2.819	2.670	0.149
H2'1	DG	19	--	H8	DG	19:	3.371	3.000	0.371
H2'2	DG	19	--	H8	DG	19:	1.986	2.380	0.000
H2'1	DA	20	--	H1'	DA	20:	2.019	2.100	0.081
H2'2	DA	20	--	H1'	DA	20:	2.739	2.540	0.199
H2'2	DA	20	--	H8	DA	20:	2.073	2.430	0.000
H2'2	DA	20	--	H5	DC	21:	3.003	2.950	0.053
H2'2	DA	20	--	H6	DC	21:	3.321	2.830	0.491
H3'	DA	20	--	H1'	DA	20:	3.246	2.920	0.326
H8	DA	20	--	H2'2	DG	19:	2.839	2.590	0.249
H8	DA	20	--	H8	DG	19:	3.730	4.000	0.270
H8	DA	20	--	H1'	DA	20:	3.216	3.410	0.194
H8	DA	20	--	H2'1	DA	20:	2.572	2.270	0.302
H8	DA	20	--	H5	DC	21:	2.699	3.060	0.361
H1'	DC	21	--	H2'1	DC	21:	2.191	2.550	0.000
H2'1	DC	21	--	H6	DC	21:	2.602	2.440	0.162
H2'2	DC	21	--	H6	DC	21:	2.088	2.580	0.000
H5	DC	21	--	H1'	DA	20:	3.349	3.240	0.109
H5	DC	21	--	H2'1	DA	20:	2.027	2.420	0.393
H5	DC	21	--	H6	DC	21:	2.422	2.310	0.112
H6	DC	21	--	H1'	DA	20:	3.004	2.910	0.094
H6	DC	21	--	H2'1	DA	20:	1.888	2.380	0.492
H6	DC	21	--	H8	DG3	22:	4.815	5.000	0.000
H1'	DG3	22	--	H2'1	DG3	22:	2.182	2.120	0.062
H1'	DG3	22	--	H2'2	DG3	22:	2.940	3.000	0.000
H1'	DG3	22	--	H8	DG3	22:	3.168	3.000	0.168
H2'1	DG3	22	--	H8	DG3	22:	2.680	3.000	0.000
H2'2	DG3	22	--	H8	DG3	22:	2.050	1.880	0.170
C4'	DC	4	--	C4'	DG3	22:	15.083	15.000	0.083
C4'	DC	4	--	C4'	DC	21:	10.239	15.000	0.000
C4'	DG	5	--	C4'	DC	21:	12.524	15.000	0.000
C4'	DG	5	--	C4'	DA	20:	10.467	15.000	0.000
C4'	DT	6	--	C4'	DG	19:	11.512	15.000	0.000
C4'	DA	7	--	C4'	DG	19:	13.476	15.000	0.000
C4'	DA	7	--	C4'	DC	18:	12.323	15.000	0.000
C4'	DG	8	--	C4'	DC	18:	13.944	15.000	0.000
C4'	DT	9	--	C4'	DT	17:	13.457	15.000	0.000
C4'	DT	9	--	C4'	DT	16:	10.579	15.000	0.000
C4'	DG	10	--	C4'	DT	16:	11.826	15.000	0.000
C4'	DG	10	--	C4'	DC	15:	10.831	15.000	0.000
C4'	DC3	11	--	C4'	DC	15:	13.165	15.000	0.000
C4'	DC3	11	--	C4'	DA	14:	10.906	15.000	0.000
H42	DC5	1	--	O6	DG3	22:	1.813	2.000	0.000
N3	DC5	1	--	H1	DG3	22:	1.948	2.040	0.000
N3	DC5	1	--	N1	DG3	22:	2.943	3.050	0.000
N4	DC5	1	--	O6	DG3	22:	2.825	3.010	0.000
O2	DC5	1	--	H22	DG3	22:	1.871	1.950	0.000
H1	DG	2	--	N3	DC	21:	1.841	2.040	0.000
H22	DG	2	--	O2	DC	21:	1.762	1.950	0.000
N1	DG	2	--	N3	DC	21:	2.849	2.850	0.001
O6	DG	2	--	H42	DC	21:	1.875	2.000	0.000
O6	DG	2	--	N4	DC	21:	2.892	3.010	0.000
H3	DT	3	--	N1	DA	20:	1.922	1.910	0.012
N3	DT	3	--	N1	DA	20:	2.928	2.920	0.008
O4	DT	3	--	H61	DA	20:	2.061	2.040	0.021
H42	DC	4	--	O6	DG	19:	1.796	1.800	0.004
N3	DC	4	--	H1	DG	19:	1.908	2.040	0.000
N3	DC	4	--	N1	DG	19:	2.889	3.050	0.000
N4	DC	4	--	O6	DG	19:	2.791	2.810	0.019
O2	DC	4	--	H22	DG	19:	1.878	1.950	0.000
H1	DG	5	--	N3	DC	18:	1.883	2.040	0.000
H22	DG	5	--	O2	DC	18:	1.777	1.950	0.000
N1	DG	5	--	N3	DC	18:	2.878	3.050	0.000
O6	DG	5	--	H42	DC	18:	1.870	2.000	0.000
O6	DG	5	--	N4	DC	18:	2.868	3.010	0.000
H61	DA	7	--	O4	DT	16:	2.065	2.040	0.025
N1	DA	7	--	H3	DT	16:	1.826	1.910	0.000
N1	DA	7	--	N3	DT	16:	2.775	2.920	0.000
H1	DG	8	--	N3	DC	15:	1.979	2.040	0.000
H22	DG	8	--	O2	DC	15:	1.788	1.950	0.000
N1	DG	8	--	N3	DC	15:	2.965	3.050	0.000
O6	DG	8	--	H42	DC	15:	2.007	2.000	0.007
O6	DG	8	--	N4	DC	15:	3.019	3.010	0.009
H3	DT	9	--	N1	DA	14:	1.916	1.910	0.006
N3	DT	9	--	N1	DA	14:	2.923	2.920	0.003
O4	DT	9	--	H61	DA	14:	1.975	2.040	0.000
H1	DG	10	--	N3	DC	13:	1.923	2.040	0.000
H22	DG	10	--	O2	DC	13:	1.800	1.950	0.000
N1	DG	10	--	N3	DC	13:	2.918	3.050	0.000

O6	DG	10	--	H42	DC	13:	1.846	2.000	0.000
O6	DG	10	--	N4	DC	13:	2.869	3.010	0.000
H42	DC3	11	--	O6	DG5	12:	1.856	2.000	0.000
N3	DC3	11	--	H1	DG5	12:	1.944	2.040	0.000
N3	DC3	11	--	N1	DG5	12:	2.898	3.050	0.000
N4	DC3	11	--	O6	DG5	12:	2.860	3.010	0.000
O2	DC3	11	--	H22	DG5	12:	1.758	1.950	0.000

Table S4. Table of distance restraints used for the molecular dynamics of the **2,7-BisNP–TT-DNA** complex. **2,7-BisNP** is called ‘BNP’ in the table. The values are in Å: (a) distance in the final structure; b) upper or lower restraint; (c) deviation from the upper or lower restraint in the final structure. The deviations are highlighted as followed: yellow (0.2–0.3 Å), grey (0.3–0.5 Å) and red (> 0.5 Å).

First atom	Last atom		current value (a)	upper/lower restraint (b)	deviation (c)
H5	BNP	-- H1 DG	5: 3.425	4.000	0.000
H5	BNP	-- H5 DC	18: 4.910	5.000	0.000
H6	BNP	-- H1 DG	5: 3.119	4.000	0.000
H1	BNP	-- H1' DT	16: 3.880	4.000	0.190
H1	BNP	-- *H73 DT	16: 5.521	5.000	0.521
H1	BNP	-- H1' DT	17: 2.505	4.000	0.000
H1	BNP	-- H2'1 DT	17: 2.081	4.000	0.000
H1	BNP	-- H2'2 DT	17: 3.756	4.000	0.000
H2	BNP	-- H1' DT	17: 2.162	3.000	0.000
H2	BNP	-- H2'1 DT	17: 2.312	3.000	0.000
H2	BNP	-- H2'2 DT	17: 3.214	4.000	0.000
H2	BNP	-- H1' DT	16: 5.070	5.000	0.070
H2	BNP	-- *H73 DT	16: 4.108	4.000	0.108
H7	BNP	-- H1' DT	16: 3.548	3.000	0.548
H7	BNP	-- H2'1 DT	16: 3.557	3.000	0.557
H7	BNP	-- H2'2 DT	16: 2.709	3.000	0.000
H7	BNP	-- *H73 DT	16: 3.611	4.000	0.000
H8	BNP	-- H1' DT	16: 2.849	4.000	0.000
H8	BNP	-- H2'1 DT	16: 4.283	4.000	0.283
H8	BNP	-- H2'2 DT	16: 3.962	4.000	0.000
H8	BNP	-- *H73 DT	16: 5.104	4.000	1.104
CH2)18	BNP	-- *H73 DT	16: 5.090	5.000	0.090
CH2)18	BNP	-- *H73 DT	16: 3.939	5.000	0.000
CH2)24	BNP	-- H1' DA	7: 3.970	4.000	0.000
CH2)24	BNP	-- H1' DA	7: 4.049	4.000	0.049
H1'	DC5	1 -- H6 DC5	1: 3.734	3.800	0.000
H2'1	DC5	1 -- H1' DC5	1: 2.370	2.520	0.000
H2'1	DC5	1 -- H6 DC5	1: 3.366	3.600	0.000
H2'1	DC5	1 -- H8 DG	2: 1.999	2.050	0.051
H2'2	DC5	1 -- H1' DC5	1: 3.030	3.210	0.000
H2'2	DC5	1 -- H6 DC5	1: 2.110	2.510	0.000
H2'2	DC5	1 -- H8 DG	2: 3.608	3.440	0.168
H5	DC5	1 -- H6 DC5	1: 2.429	2.450	0.000
H2'1	DG	2 -- H8 DG	2: 2.476	2.270	0.206
H2'1	DG	2 -- H6 DT	3: 2.348	2.400	0.052
H2'2	DG	2 -- H8 DG	2: 2.168	2.380	0.000
H2'2	DG	2 -- H6 DT	3: 3.936	3.700	0.236
H8	DG	2 -- H1' DC5	1: 2.811	2.720	0.091
H8	DG	2 -- H1' DG	2: 3.619	4.000	0.000
H8	DG	2 -- H6 DT	3: 4.136	5.000	0.000
H1'	DT	3 -- H6 DT	3: 3.730	3.700	0.030
H1'	DT	3 -- H6 DC	4: 3.352	3.300	0.052
H2'1	DT	3 -- H6 DT	3: 3.177	3.500	0.000
H2'1	DT	3 -- H6 DC	4: 2.089	2.220	0.131
H2'2	DT	3 -- H6 DT	3: 2.258	2.350	0.000
H2'2	DT	3 -- H6 DC	4: 3.834	3.700	0.134
H6	DT	3 -- H1' DG	2: 2.424	2.520	0.000
H6	DT	3 -- H5 DC	4: 3.418	3.800	0.000
*H73	DT	3 -- H8 DG	2: 2.790	3.210	0.000
*H73	DT	3 -- H6 DT	3: 2.705	3.070	0.000
H2'1	DC	4 -- H6 DC	4: 2.986	3.000	0.000
H2'2	DC	4 -- H6 DC	4: 2.092	2.590	0.000
H6	DC	4 -- H1' DC	4: 3.671	3.900	0.000
H6	DC	4 -- H5 DC	4: 2.423	2.450	0.000
H8	DG	5 -- H1' DC	4: 2.527	2.410	0.117
H8	DG	5 -- H2'1 DC	4: 2.211	2.490	0.000
H8	DG	5 -- H2'2 DC	4: 3.749	3.700	0.049
H8	DG	5 -- H6 DC	4: 3.973	4.000	0.027
H8	DG	5 -- H1' DG	5: 3.884	3.900	0.000
H8	DG	5 -- H2'1 DG	5: 3.748	3.700	0.048
H8	DG	5 -- H2'2 DG	5: 2.335	2.390	0.000
H6	DT	6 -- H1' DG	5: 2.872	2.790	0.082
H6	DT	6 -- H2'1 DG	5: 2.384	2.390	0.006
H6	DT	6 -- H2'2 DG	5: 3.618	3.700	0.000
H6	DT	6 -- H8 DG	5: 4.611	5.000	0.000
H1'	DG	8 -- H2'1 DG	8: 2.064	2.090	0.026
H2'2	DG	8 -- H1' DG	8: 2.754	2.460	0.294
H2'2	DG	8 -- H8 DG	8: 2.148	2.210	0.062
H2'2	DG	8 -- H6 DT	9: 3.620	3.610	0.010
H8	DG	8 -- H1' DG	8: 3.208	3.920	0.000
H8	DG	8 -- H2'1 DG	8: 3.145	3.710	0.000
H1'	DT	9 -- H8 DG	10: 2.896	2.740	0.156
H1'	DT	9 -- H2'1 DT	9: 2.344	2.510	0.000
H2'1	DT	9 -- H6 DT	9: 3.138	3.000	0.138
H2'2	DT	9 -- H6 DT	9: 2.056	2.390	0.000
H6	DT	9 -- H2'1 DG	8: 2.520	2.690	0.000
H6	DT	9 -- H8 DG	8: 3.414	3.190	0.224
*H73	DT	9 -- H8 DG	10: 4.873	4.820	0.053
*H73	DT	9 -- H1' DG	8: 4.124	3.840	0.284
*H73	DT	9 -- H8 DG	8: 2.735	2.880	0.165
*H73	DT	9 -- H6 DT	9: 2.471	2.450	0.000
H2'1	DG	10 -- H5 DC3	11: 2.584	2.610	0.000
H2'1	DG	10 -- H6 DC3	11: 2.557	2.610	0.000
H8	DG	10 -- H1' DG	10: 3.811	4.000	0.000
H8	DG	10 -- H2'1 DG	10: 3.130	3.000	0.130
H8	DG	10 -- H2'2 DG	10: 2.170	2.220	0.000
H8	DG	10 -- H2'1 DT	9: 2.371	2.490	0.000
H8	DG	10 -- H2'2 DT	9: 3.729	3.700	0.029
H8	DG	10 -- H6 DT	9: 3.923	4.000	0.077
H1'	DC3	11 -- H5 DC3	11: 5.144	5.000	0.144
H1'	DC3	11 -- H6 DC3	11: 3.614	3.720	0.000
H2'1	DC3	11 -- H1' DC3	11: 2.192	2.060	0.132
H2'1	DC3	11 -- H6 DC3	11: 3.096	3.000	0.096
H2'2	DC3	11 -- H1' DC3	11: 2.983	3.000	0.000
H2'2	DC3	11 -- H6 DC3	11: 1.964	2.190	0.000
H5	DC3	11 -- H2'1 DC3	11: 4.757	5.000	0.000
H5	DC3	11 -- H2'2 DC3	11: 4.163	4.000	0.163
H6	DC3	11 -- H5 DC3	11: 2.359	2.450	0.000
H1'	DG5	12 -- H8 DG5	12: 3.692	3.800	0.000
H2'1	DG5	12 -- H8 DG5	12: 3.013	2.870	0.143
H8	DG5	12 -- H2'2 DG5	12: 1.852	2.210	0.000
H1'	DC	13 -- H8 DA	14: 2.866	2.750	0.116
H2'1	DC	13 -- H1' DC	13: 2.373	2.620	0.000
H2'1	DC	13 -- H6 DC	13: 3.392	3.330	0.062
H2'1	DC	13 -- H8 DA	14: 2.196	2.280	0.084
H2'2	DC	13 -- H5 DC	13: 4.141	3.970	0.171
H2'2	DC	13 -- H6 DC	13: 2.041	2.510	0.000
H2'2	DC	13 -- H8 DA	14: 3.746	3.630	0.116
H6	DC	13 -- H2'2 DG5	12: 2.900	2.630	0.270
H2'1	DA	14 -- H5 DC	15: 3.142	3.050	0.092
H2'2	DA	14 -- H5 DC	15: 2.698	2.930	0.000
H8	DA	14 -- H1' DA	14: 3.790	3.660	0.130
H8	DA	14 -- H2'2 DA	14: 2.413	2.370	0.043
H8	DA	14 -- H5 DC	15: 3.055	3.060	0.005
H1'	DC	15 -- H2'2 DC	15: 2.768	2.390	0.378
H1'	DC	15 -- H6 DC	15: 3.307	2.980	0.327
H1'	DC	15 -- H6 DT	16: 3.144	2.910	0.234
H1'	DC	15 -- *H73 DT	16: 4.179	3.990	0.189
H5	DC	15 -- H1' DA	14: 3.354	3.230	0.124
H6	DC	15 -- H1' DA	14: 2.952	2.830	0.122
H6	DC	15 -- H2'2 DA	14: 2.933	2.740	0.193
H6	DC	15 -- H2'1 DC	15: 3.102	3.000	0.102
H6	DC	15 -- H2'2 DC	15: 1.925	2.350	0.000
H6	DC	15 -- H5 DC	15: 2.390	2.370	0.020
H1'	DC	18 -- H6 DC	18: 3.443	3.380	0.063
H5	DC	18 -- H6 DC	18: 2.418	2.440	0.000
H6	DC	18 -- H2'1 DC	18: 2.485	2.390	0.095
H6	DC	18 -- H2'2 DC	18: 2.494	2.720	0.226
H6	DC	18 -- H8 DG	19: 3.974	4.000	0.026
H1'	DG	19 -- H2'2 DG	19: 2.754	2.530	0.224
H1'	DG	19 -- H8 DG	19: 3.555	3.480	0.075
H1'	DG	19 -- H8 DA	20: 2.818	2.670	0.148
H2'1	DG	19 -- H8 DG	19: 3.425	3.000	0.425
H2'2	DG	19 -- H8 DG	19: 1.932	2.380	0.000
H2'1	DA	20 -- H1' DA	20: 2.015	2.100	0.085
H2'2	DA	20 -- H1' DA	20: 2.769	2.540	0.229
H2'2	DA	20 -- H8 DA	20: 1.941	2.430	0.000
H2'2	DA	20 -- H5 DC	21: 3.150	2.950	0.200

H2'2	DA	20	--	H6	DC	21:	3.547	2.830	0.717
H3'	DA	20	--	H1'	DA	20:	3.321	2.920	0.401
H8	DA	20	--	H2'2	DG	19:	2.790	2.590	0.200
H8	DA	20	--	H8	DG	19:	3.860	4.000	0.140
H8	DA	20	--	H1'	DA	20:	3.212	3.410	0.198
H8	DA	20	--	H2'1	DA	20:	2.645	2.270	0.375
H8	DA	20	--	H5	DC	21:	2.934	3.060	0.126
H1'	DC	21	--	H2'1	DC	21:	2.146	2.550	0.000
H2'1	DC	21	--	H6	DC	21:	2.525	2.440	0.085
H2'2	DC	21	--	H6	DC	21:	2.073	2.580	0.000
H5	DC	21	--	H1'	DA	20:	3.406	3.240	0.166
H5	DC	21	--	H2'1	DA	20:	2.300	2.420	0.120
H5	DC	21	--	H6	DC	21:	2.385	2.310	0.075
H6	DC	21	--	H1'	DA	20:	2.930	2.910	0.020
H6	DC	21	--	H2'1	DA	20:	2.058	2.380	0.322
H6	DC	21	--	H8	DG3	22:	4.858	5.000	0.000
H1'	DG3	22	--	H2'1	DG3	22:	2.199	2.120	0.079
H1'	DG3	22	--	H2'2	DG3	22:	2.947	3.000	0.000
H1'	DG3	22	--	H8	DG3	22:	3.273	3.000	0.273
H2'1	DG3	22	--	H8	DG3	22:	2.511	3.000	0.000
H2'2	DG3	22	--	H8	DG3	22:	2.074	1.880	0.194
C4'	DC	4	--	C4'	DG3	22:	14.743	15.000	0.000
C4'	DC	4	--	C4'	DC	21:	10.661	15.000	0.000
C4'	DG	5	--	C4'	DC	21:	13.374	15.000	0.000
C4'	DG	5	--	C4'	DA	20:	11.347	15.000	0.000
C4'	DT	6	--	C4'	DG	19:	10.149	15.000	0.000
C4'	DA	7	--	C4'	DG	19:	12.639	15.000	0.000
C4'	DA	7	--	C4'	DC	18:	10.265	15.000	0.000
C4'	DG	8	--	C4'	DC	18:	13.483	15.000	0.000
C4'	DG	10	--	C4'	DC	15:	10.577	15.000	0.000
C4'	DC3	11	--	C4'	DC	15:	12.782	15.000	0.000
C4'	DC3	11	--	C4'	DA	14:	9.808	15.000	0.000
H42	DC5	1	--	O6	DG3	22:	1.873	2.000	0.000
N3	DC5	1	--	H1	DG3	22:	1.940	2.040	0.000
N3	DC5	1	--	N1	DG3	22:	2.922	3.050	0.000
N4	DC5	1	--	O6	DG3	22:	2.876	3.010	0.000
O2	DC5	1	--	H22	DG3	22:	1.806	1.950	0.000
H1	DG	2	--	N3	DC	21:	1.928	2.040	0.000
H22	DG	2	--	O2	DC	21:	1.864	1.950	0.000
N1	DG	2	--	N3	DC	21:	2.935	3.050	0.000
O6	DG	2	--	H42	DC	21:	1.865	2.000	0.000
O6	DG	2	--	N4	DC	21:	2.867	3.010	0.000
H3	DT	3	--	N1	DA	20:	1.884	1.910	0.000
N3	DT	3	--	N1	DA	20:	2.891	2.920	0.000
O4	DT	3	--	H61	DA	20:	1.859	2.040	0.000
H42	DC	4	--	O6	DG	19:	1.856	2.000	0.000
N3	DC	4	--	H1	DG	19:	1.906	2.040	0.000
N3	DC	4	--	N1	DG	19:	2.902	3.050	0.000
N4	DC	4	--	O6	DG	19:	2.859	3.010	0.000
O2	DC	4	--	H22	DG	19:	1.804	1.950	0.000
H1	DG	5	--	N3	DC	18:	1.924	2.040	0.000
H22	DG	5	--	O2	DC	18:	1.864	1.950	0.000
N1	DG	5	--	N3	DC	18:	2.891	3.050	0.000
O6	DG	5	--	H42	DC	18:	2.060	2.000	0.060
O6	DG	5	--	N4	DC	18:	2.880	3.010	0.000
H61	DA	7	--	O4	DT	16:	1.858	2.040	0.000
N1	DA	7	--	H3	DT	16:	1.980	1.910	0.070
N1	DA	7	--	N3	DT	16:	2.939	2.920	0.019
H1	DG	8	--	N3	DC	15:	1.991	2.040	0.000
H22	DG	8	--	O2	DC	15:	1.871	1.950	0.000
N1	DG	8	--	N3	DC	15:	2.934	3.050	0.000
O6	DG	8	--	H42	DC	15:	1.937	2.000	0.000
O6	DG	8	--	N4	DC	15:	2.942	3.010	0.000
H3	DT	9	--	N1	DA	14:	1.867	1.910	0.000
N3	DT	9	--	N1	DA	14:	2.859	2.920	0.000
O4	DT	9	--	H61	DA	14:	1.980	2.040	0.000
H1	DG	10	--	N3	DC	13:	1.932	2.040	0.000
H22	DG	10	--	O2	DC	13:	1.788	1.950	0.000
N1	DG	10	--	N3	DC	13:	2.924	3.050	0.000
O6	DG	10	--	H42	DC	13:	1.924	2.000	0.000
O6	DG	10	--	N4	DC	13:	2.932	3.010	0.000
H42	DC3	11	--	O6	DG5	12:	1.846	2.000	0.000
N3	DC3	11	--	H1	DG5	12:	1.969	2.040	0.000
N3	DC3	11	--	N1	DG5	12:	2.935	3.050	0.000
N4	DC3	11	--	O6	DG5	12:	2.842	3.010	0.000
O2	DC3	11	--	H22	DG5	12:	1.870	1.950	0.000

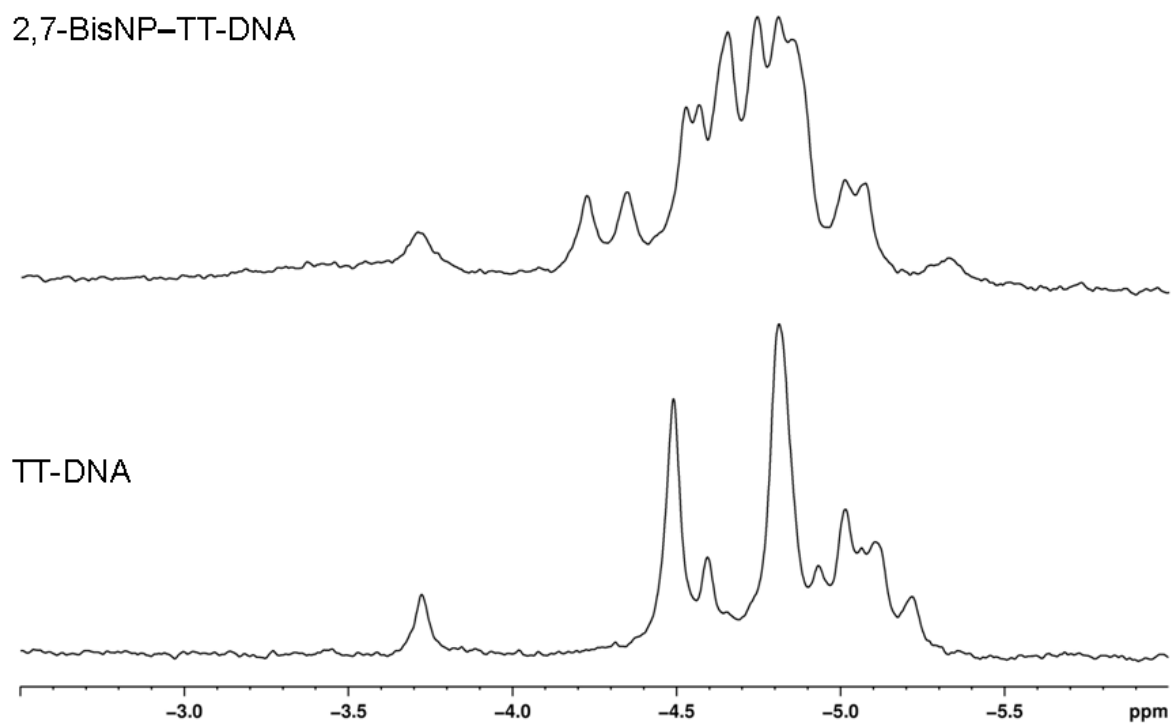


Figure S1. 1D ^{31}P spectra of the free TT-DNA and the **2,7-BisNP**-TT-DNA complex in D_2O at 10°C .

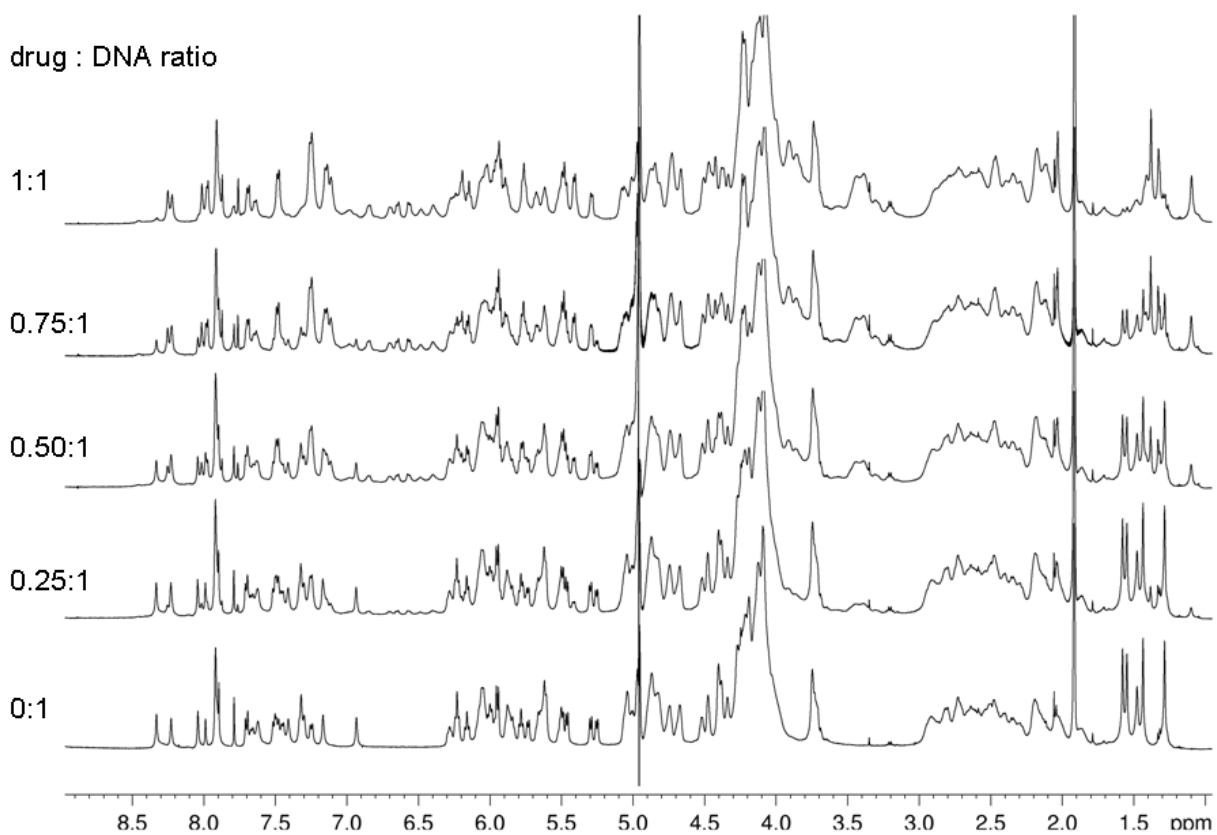


Figure S2. 1D NMR spectra of TT-DNA upon addition of **2,7-BisNP** in D₂O, at 10 °C and pH 6. The molar ligand-to-DNA ratio is indicated for each spectrum.

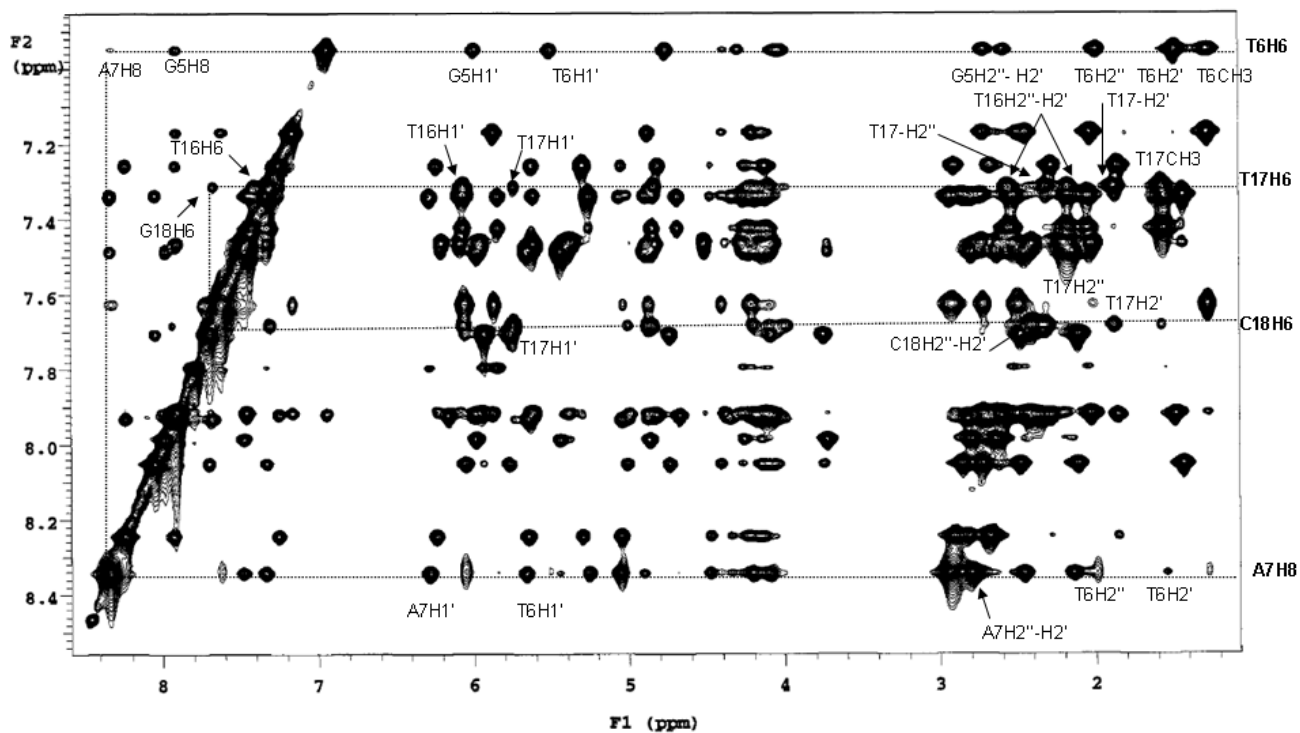


Figure S3. Expansion of the 250 ms NOESY spectrum of the free TT-DNA in D₂O at 10 °C. Correlations are between the aromatic protons and the sugar protons. The sequential walk between the mismatched thymine T₆ and the adjacent bases G₅ and A₇, and between the mismatched T₁₇ and the adjacent bases T₁₆ and C₁₈ is displayed.