Supporting Information

Toward a Designed Genetic System With Expanded-size Base Pairs: Solution Structure of the 8-base xDNA Double Helix

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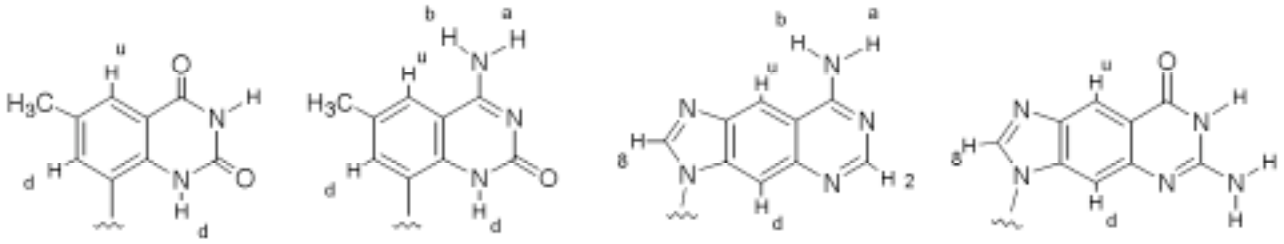
Table S1. ^{1}H Chemical Shift Assignments.

	(C)H3	H1'	H2	H2'	H2''	H3'	H4'	H5	H5'	H5''	H6	H8	Hd	Hu	NH	NH2 a	NH2 b
xT1	1.969	4.588	-	1.501	1.791	4.374	3.409	-	3.522	3.537	-	-	7.07	6.477	-	-	-
G2	-	5.332	-	2.564	2.475	4.765	4.217	-	3.812	3.645	-	7.718	-	-	12.96	8.767	5.736
xT3	2.318	4.152	-	2.247	2.549	4.898	4.066	-	3.899	4.013	-	-	7.668	7.127	13.71	-	-
A4	-	5.98	7.894	2.551	2.295	4.984	4.33	-	4.033	3.86	-	7.939	-	-	-	7.508	5.518
xC5	2.353	3.756	-	2.274	2.416	4.918	4.133	-	3.983	4.078	-	-	7.546	7.049	-	8.587	7.132
xG6	-	6.061	-	2.853	2.796	5.073	4.455	-	4.162	4.077	-	8.533	6.842	6.702	-	-	-
C7	-	5.567	-	2.371	2.02	4.884	4.157	5.284	4.229	4.137	7.361	-	-	-	-	7.406	6.409
xA8	-	5.849	7.159	2.866	2.787	5.065	4.362	-	4.148	4.022	-	8.597	6.793	7.7	-	8.235	7.603
xG9	-	6.213	-	2.784	2.602	4.999	4.487	-	4.246	4.283	-	8.307	6.856	6.762	-	-	-
T10	1.17	6.175	-	2.291	2.111	4.709	4.231	-	4.308	4.154	7.193	-	-	-	-	-	-
xA11	-	6.337	8.099	2.954	2.802	4.904	4.313	-	4.152	3.79	-	8.718	7.534	8.217	-	-	-
C12	-	6.019	-	2.538	2.122	4.813	4.332	5.27	4.187	4.151	7.494	-	-	-	-	7.503	6.687
T13	1.64	5.839	-	2.606	2.203	4.948	4.212	-	4.152	-	7.434	-	-	-	13.08	-	-
xG14	-	6.065	-	2.816	2.79	5.069	4.448	-	4.152	4.215	-	8.579	6.916	7.689	-	-	-
C15	-	5.741	-	2.38	2.14	4.919	4.265	5.282	4.271	4.188	7.474	-	-	-	-	7.682	6.453
G16	-	5.536	-	2.318	2.13	4.915	4.196	-	4.072	3.916	-	7.587	-	-	12.9	8.695	5.763
xT17	2.3	4.015	-	2.177	2.436	4.855	4.052	-	3.885	-	-	-	7.6	7.117	13.76	-	-
A18	-	6.046	8.021	2.406	2.08	4.949	4.315	-	4.019	3.85	-	7.71	-	-	-	7.388	5.509
xC19	2.337	4.834	-	2.136	-	4.958	4.263	-	3.967	4.083	-	-	7.187	7.081	-	8.696	7.184
A20	-	6.352	7.874	2.691	2.632	4.89	4.398	-	4.086	4.137	-	8.287	-	-	-	-	-



xT xC xA xG

Table S2. ^{13}C Chemical Shift Assignments.

	C(H3)	C1'	C2	C2'	C3'	C4'	C5	C5'	C6	C8	Cd	Cu
xT1	19.58	79.3	-	40.46	77.34	86.64	-	61.28	-	-	135.1	125.6
G2	-	82.36	-	-	77.61	85.65	-	65.65	-	135.1	-	-
xT3	19.79	73.07	-	37.22	74.32	85.23	-	-	-	-	134.3	127.2
A4	-	82.67	152.3	37.12	78.2	85.41	-	65.73	-	138.9	-	-
xC5	19.94	73.17	-	37.29	75.54	84.86	-	-	-	-	133.6	123.7
xG6	-	83.7	-	-	77.11	85.15	-	-	-	144.4	-	116.3
C7	-	83.32	-	36.91	74.4	83.16	95.87	-	140.1	-	-	-
xA8	-	83.39	149.8	38.1	76.06	84.63	-	65.56	-	145.9	102.7	112.9
xG9	-	83.35	-	38.54	75.4	84.24	-	65.26	-	143	99.73	115.7
T10	10.82	83.39	-	38.04	72.33	83.86	-	64.74	136.6	-	-	-
xA11	-	84.51	151.7	37.89	76.06	86.38	-	-	-	146	103.9	113.8
C12	-	84.23	-	37.33	74.19	83.17	95.5	64.62	140	-	-	-
T13	11.63	82.89	-	36.51	75.38	83.38	-	-	137.2	-	-	-
xG14	-	83.26	-	38.1	75.99	84.6	-	-	-	144.2	-	117.2
C15	-	83.59	-	37.09	75.17	83.58	95.57	-	140.2	-	-	-
G16	-	81.85	-	37.19	77.42	84.55	-	65.67	-	135.4	-	-
xT17	19.82	73.12	-	37.12	75.81	84.75	-	-	-	-	134.4	127.2
A18	-	82.6	152.7	-	77.97	85.48	-	-	-	138.6	-	-
xC19	19.94	74.3	-	-	76.85	85.06	-	65.61	-	-	132.8	123.3
A20	-	83.72	152.2	38.42	76.25	85.18	-	65.37	-	139.5	-	-

Table S3. Full list of NOE data.

Assgnment	w1	w2	Volume
xA11H1'-H3'	6.335	4.905	1.42E+06
xA11H1'-H8	6.337	8.718	4.20E+05
xA11H1'-Hd	6.337	7.535	1.29E+07
xA11H1'-C12H1'	6.336	6.024	
xA11H1'-C12H5	6.337	5.272	2.76E+06
xA11H1'-C12H6	6.327	7.503	4.81E+07
xA11H2-Hd	8.097	7.534	2.90E+05
xA11H2'-H1'	2.956	6.338	1.00E+07
xA11H2'-H3'	2.954	4.905	7.48E+06
xA11H2'-H4'	2.959	4.311	3.62E+05
xA11H2'-H5"	2.952	3.79	1.16E+06
xA11H2'-H8	2.953	8.718	1.26E+06
xA11H2'-Hd	2.955	7.535	2.68E+06
xA11H2'-C12H3'	2.949	4.815	
xA11H2'-C12H4'	2.953	4.325	4.54E+06
xA11H2'-C12H5	2.954	5.27	3.61E+06
xA11H2'-C12H5'	2.95	4.19	
xA11H2'-C12H6	2.955	7.495	5.41E+06
xA11H2"-H1'	2.804	6.338	5.78E+06
xA11H2"-H2'	2.801	2.956	
xA11H2"-H3'	2.802	4.904	
xA11H2"-H4'	2.801	4.314	2.88E+06
xA11H2"-H5"	2.801	3.791	2.47E+06
xA11H2"-H8	2.801	8.718	3.22E+06
xA11H2"-Hd	2.802	7.535	2.32E+06
xA11H2"-C12H6	2.806	7.496	3.96E+06
xA11H3'-H1'	4.901	6.339	1.22E+06
xA11H3'-H8	4.905	8.715	7.58E+05
xA11H3'-Hd	4.913	7.528	8.47E+06
xA11H3'-C12H6	4.906	7.497	
xA11H4'-H1'	4.311	6.337	1.66E+06
xA11H4'-H3'	4.31	4.906	
xA11H4'-H8	4.31	8.718	
xA11H4'-Hd	4.325	7.535	1.59E+06
xA11H5'-xA8H8	4.152	8.598	6.46E+05
xA11H5"-H1'	3.792	6.339	1.07E+06
xA11H5"-H3'	3.79	4.904	
xA11H5"-H4'	3.789	4.313	
xA11H5"-H8	3.79	8.718	7.13E+05
xA11H5"-Hd	3.791	7.535	6.47E+05
xA11H8-H1'	8.717	6.338	4.61E+05
xA11H8-Hd	8.72	7.532	
xA11Hd-H1'	7.534	6.338	1.66E+07
xA11Hd-H2	7.534	8.098	5.15E+05
xA11Hd-H8	7.533	8.719	
xA11Hd-C12H1'	7.534	6.021	2.12E+06
xA11Hd-C12H5	7.534	5.278	7.52E+07
xT1CH3-H1'	1.959	4.587	3.36E+06
xT1CH3-Hd	1.959	7.064	1.14E+07
xT1CH3-Hu	1.96	6.475	1.39E+07
xT1CH3-xC19CH3	1.959	2.338	
xT1CH3-xC19Hd	1.961	7.187	6.18E+05
xT1CH3-xC19Hu	1.961	7.076	6.83E+06
xT1CH3-A20H2	1.959	7.871	5.56E+05
xT1CH3-A20H8	1.96	8.288	
xT1H1'-Hd	4.587	7.065	1.12E+07
xT1H2'-H1'	1.495	4.587	1.16E+07
xT1H2'-H2"	1.495	1.79	
xT1H2'-H3'	1.494	4.372	1.79E+07
xT1H2'-H4'	1.493	3.41	2.13E+06
xT1H2'-H5'	1.492	3.536	1.97E+06
xT1H2'-Hd	1.495	7.065	5.12E+06
xT1H2'-G2H5'	1.49	3.808	
xT1H2'-G2H8	1.494	7.718	6.99E+05
xT1H2'-A20H2	1.493	7.87	3.01E+05
xT1H2"-H1'	1.79	4.588	1.56E+07
xT1H2"-H3'	1.79	4.372	1.19E+07
xT1H2"-H4'	1.79	3.411	2.00E+06
xT1H2"-H5'	1.79	3.529	
xT1H2"-Hd	1.79	7.065	5.74E+06
xT1H2"-G2H4'	1.788	4.215	
xT1H2"-G2H5'	1.792	3.815	
xT1H2"-G2H5"	1.789	3.646	
xT1H2"-G2H8	1.789	7.718	9.04E+05
xT1H2"-A20H2	1.783	7.87	
xT1H3'-H1'	4.371	4.586	4.09E+06
xT1H3'-Hd	4.371	7.064	1.18E+06
xT1H3'-G2H8	4.371	7.718	5.10E+05
xT1H4'-H1'	3.41	4.588	6.04E+06
xT1H4'-H3'	3.41	4.372	8.26E+06
xT1H4'-Hd	3.41	7.065	9.51E+05
xT1H4'-G2H1'	3.409	5.332	6.19E+05
xT1H4'-G2H4'	3.41	4.218	1.27E+06
xT1H4'-G2H5'	3.41	3.812	2.32E+06
xT1H4'-G2H5"	3.411	3.644	3.51E+06
xT1H4'-G2H8	3.41	7.718	4.98E+05
xT1H4'-A20H2	3.411	7.872	
xT1H5'-H1'	3.526	4.586	
xT1H5'-G2H1'	3.525	5.334	
xT1H5"-H3'	3.531	4.372	1.49E+07
xT1H5"-Hd	3.53	7.065	8.55E+05
xT1H5"-G2H4'	3.532	4.218	2.95E+06
xT1Hd-Hu	7.068	6.475	1.82E+06
xT1Hu-Hd	6.474	7.064	8.88E+05

xT1Hu-xC19Hd	6.476	7.188	8.11E+04
xT1Hu-xC19Hu	6.475	7.077	9.18E+05
xT1Hu-A20H8	6.473	8.287	1.90E+05
C12H1'-xA11H1'	6.019	6.343	
C12H1'-xA11H2	6.017	8.098	
C12H1'-xA11Hd	6.02	7.535	1.73E+06
C12H1'-H3'	6.02	4.815	2.51E+06
C12H1'-H5	6.021	5.27	
C12H1'-H6	6.019	7.496	2.80E+06
C12H1'-T13H6	6.019	7.433	1.46E+06
C12H2'-H1'	2.538	6.021	1.22E+07
C12H2'-H3'	2.538	4.814	7.17E+06
C12H2'-H4'	2.543	4.332	5.47E+06
C12H2'-H5	2.536	5.27	
C12H2'-H6	2.537	7.495	5.54E+06
C12H2'-T13H6	2.538	7.433	4.78E+06
C12H2''-H1'	2.124	6.02	6.22E+06
C12H2''-H2'	2.122	2.539	
C12H2''-H3'	2.121	4.816	
C12H2''-H4'	2.119	4.329	6.40E+06
C12H2''-H5	2.12	5.263	2.81E+06
C12H2''-H5''	2.126	4.153	
C12H2''-H6	2.124	7.495	
C12H2''-T13H6	2.123	7.433	
C12H3'-H6	4.815	7.496	
C12H4'-xA11H1'	4.328	6.338	3.18E+06
C12H4'-H1'	4.333	6.02	4.35E+06
C12H4'-H3'	4.332	4.814	8.66E+06
C12H4'-H6	4.331	7.495	2.76E+06
C12H4'-T13H6	4.335	7.433	6.30E+05
C12H5-xA11H1'	5.268	6.337	4.05E+05
C12H5-xA11Hd	5.279	7.529	2.64E+07
C12H5-H6	5.269	7.496	9.84E+06
C12H5'-xA11H1'	4.184	6.342	
C12H5'-xA11Hd	4.187	7.535	
C12H5'-H1'	4.192	6.022	3.00E+06
C12H5'-H3'	4.186	4.816	
C12H5'-H4'	4.186	4.333	
C12H5'-H6	4.187	7.493	3.88E+06
C12H6-xA11H1'	7.493	6.336	2.20E+06
C12H6-xA11H8	7.492	8.716	
C12H6-H1'	7.495	6.02	2.58E+06
C12H6-H5	7.496	5.27	1.09E+07
G2H1'-H3'	5.332	4.767	3.49E+06
G2H1'-H8	5.331	7.718	2.37E+06
G2H1'-xT3Hd	5.331	7.668	1.49E+06
G2H1'-xT3Hu	5.331	7.128	3.55E+05
G2H2'-H1'	2.566	5.333	1.08E+07
G2H2'-H3'	2.566	4.765	7.91E+06
G2H2'-H4'	2.562	4.225	2.34E+07
G2H2'-H5'	2.569	3.817	
G2H2'-H5''	2.565	3.646	3.64E+06
G2H2'-H8	2.563	7.717	
G2H2'-xT3H5'	2.565	3.9	2.09E+06
G2H2'-xT3Hu	2.558	7.129	1.21E+06
G2H2''-H1'	2.476	5.332	7.00E+06
G2H2''-H2'	2.477	2.566	
G2H2''-H3'	2.475	4.766	9.41E+06
G2H2''-H4'	2.467	4.217	1.47E+06
G2H2''-H5'	2.476	3.811	5.17E+06
G2H2''-H5''	2.476	3.646	4.92E+06
G2H2''-H8	2.477	7.721	
G2H2''-xT3Hd	2.48	7.668	
G2H2''-xT3Hu	2.47	7.128	1.07E+06
G2H4'-xT1Hd	4.217	7.062	
G2H4'-H1'	4.217	5.333	1.70E+06
G2H4'-H3'	4.217	4.763	
G2H4'-H8	4.216	7.718	8.75E+05
G2H5'-xT1H1'	3.812	4.587	
G2H5'-xT1Hd	3.814	7.064	5.60E+05
G2H5'-H1'	3.811	5.332	4.51E+05
G2H5'-H3'	3.812	4.765	7.57E+06
G2H5'-H4'	3.812	4.218	
G2H5'-H8	3.811	7.718	3.64E+06
G2H5''-xT1H1'	3.651	4.588	
G2H5''-H1'	3.642	5.334	
G2H5''-H3'	3.645	4.766	7.41E+06
G2H5''-H4'	3.646	4.218	9.34E+06
G2H5''-H5'	3.645	3.814	
G2H5''-H8	3.645	7.718	4.11E+06
G2H8-H1'	7.717	5.333	3.31E+06
G2H8-xT3Hu	7.717	7.129	1.37E+06
T13CH3-C12H1'	1.64	6.02	2.25E+06
T13CH3-C12H2'	1.639	2.539	5.60E+06
T13CH3-C12H2''	1.64	2.126	1.45E+07
T13CH3-C12H3'	1.64	4.814	3.41E+06
T13CH3-C12H4'	1.639	4.334	8.53E+05
T13CH3-C12H5	1.64	5.27	3.21E+06
T13CH3-C12H5'	1.64	4.178	2.06E+06
T13CH3-C12H6	1.639	7.495	5.49E+06
T13CH3-H1'	1.639	5.84	7.02E+05
T13CH3-H2'	1.638	2.607	
T13CH3-H2''	1.65	2.225	6.11E+07
T13CH3-H3'	1.64	4.949	9.05E+05
T13CH3-H4'	1.639	4.206	
T13CH3-H5'	1.64	4.145	2.90E+06
T13CH3-H6	1.64	7.433	1.10E+07
T13CH3-xG14H8	1.644	8.579	

T13CH3-xG14Hu	1.64	7.688	2.38E+06
T13H1'-C12H1'	5.836	6.022	
T13H1'-H3'	5.84	4.949	2.88E+06
T13H1'-H6	5.84	7.433	2.39E+06
T13H1'-xG14H8	5.84	8.579	1.03E+06
T13H2'-H1'	2.606	5.841	1.38E+07
T13H2'-H3'	2.607	4.949	
T13H2'-H4'	2.6	4.213	3.13E+06
T13H2'-H5'	2.608	4.153	1.33E+07
T13H2'-H6	2.606	7.433	6.81E+06
T13H2'-xG14H3'	2.607	5.067	2.39E+06
T13H2'-xG14H4'	2.609	4.448	1.09E+06
T13H2'-xG14H8	2.607	8.579	2.65E+06
T13H2"-H1'	2.202	5.841	7.55E+06
T13H2"-H2'	2.202	2.607	
T13H2"-H3'	2.199	4.949	
T13H2"-H4'	2.199	4.212	
T13H2"-H5'	2.2	4.153	
T13H2"-H6	2.201	7.433	
T13H2"-xG14H2"	2.204	2.789	
T13H2"-xG14H8	2.202	8.579	1.89E+06
T13H3'-H1'	4.948	5.841	1.85E+06
T13H3'-H6	4.948	7.433	1.98E+06
T13H3'-xG14H8	4.948	8.579	5.57E+05
T13H4'-C12H1'	4.218	6.018	2.32E+05
T13H4'-H1'	4.212	5.84	4.98E+06
T13H4'-H3'	4.212	4.949	
T13H4'-H6	4.212	7.433	9.39E+05
T13H5'-C12H1'	4.15	6.02	1.84E+06
T13H5'-H3'	4.15	4.949	
T13H5'-H6	4.152	7.433	1.54E+06
T13H6-C12H1'	7.433	6.02	2.09E+06
T13H6-H1'	7.432	5.84	3.36E+06
T13H6-xG14H8	7.434	8.579	6.49E+05
xT3CH3-G2H2"	2.319	2.474	
xT3CH3-G2H3'	2.319	4.767	1.93E+06
xT3CH3-G2H5"	2.316	3.644	
xT3CH3-G2H8	2.319	7.719	
xT3CH3-Hd	2.319	7.668	
xT3CH3-Hu	2.318	7.13	1.73E+07
xT3CH3-A4H2'	2.315	2.551	
xT3H1'-Hd	4.151	7.669	2.35E+06
xT3H1'-A4H8	4.15	7.94	1.30E+06
xT3H2'-H1'	2.245	4.151	
xT3H2'-H2"	2.249	2.545	
xT3H2'-H3'	2.246	4.897	
xT3H2'-H4'	2.246	4.067	
xT3H2'-H5'	2.253	3.891	
xT3H2'-Hd	2.245	7.668	
xT3H2"-H1'	2.542	4.152	1.27E+07
xT3H2"-H3'	2.547	4.899	
xT3H2"-H5'	2.557	3.897	6.93E+06
xT3H3'-Hd	4.897	7.669	1.17E+06
xT3H4'-G2H1'	4.066	5.331	5.03E+05
xT3H4'-H3'	4.066	4.893	
xT3H4'-Hd	4.064	7.669	7.36E+05
xT3H4'-A4H8	4.064	7.939	3.84E+05
xT3H5'-G2H1'	3.898	5.333	2.53E+06
xT3H5'-H3'	3.901	4.908	
xT3H5'-Hd	3.896	7.667	
xT3H5"-G2H1'	4.009	5.331	1.63E+06
xT3H5"-H3'	4.012	4.908	
xT3H5"-Hd	4.015	7.669	4.30E+05
xT3Hd-G2H1'	7.669	5.332	2.14E+06
xT3Hd-H1'	7.668	4.152	4.12E+06
xT3Hd-H3'	7.668	4.898	4.80E+06
xT3Hd-H4'	7.669	4.066	9.55E+05
xT3Hd-Hu	7.667	7.129	1.01E+06
xT3Hd-A4H8	7.666	7.939	4.08E+05
xT3Hu-G2H8	7.129	7.718	7.82E+05
xT3Hu-Hd	7.129	7.668	7.27E+05
A4H1'-H2	5.98	7.878	6.71E+05
A4H1'-H3'	5.981	4.985	3.30E+06
A4H1'-H8	5.981	7.94	2.62E+06
A4H1'-xC5Hd	5.98	7.547	1.07E+06
A4H1'-xC5Hu	5.982	7.046	
A4H2-A18H2	7.878	8.001	1.08E+06
A4H2'-xT3H4'	2.549	4.067	
A4H2'-xT3H5"	2.55	4.014	
A4H2'-xT3Hd	2.549	7.669	
A4H2'-H1'	2.551	5.982	1.20E+07
A4H2'-H3'	2.552	4.985	
A4H2'-H5"	2.553	3.86	
A4H2'-H8	2.55	7.94	7.83E+06
A4H2'-xC5Hd	2.549	7.545	
A4H2'-xC5Hu	2.552	7.045	
A4H2"-H1'	2.294	5.982	9.47E+06
A4H2"-H3'	2.295	4.986	
A4H2"-H4'	2.292	4.33	2.71E+06
A4H2"-H5"	2.286	3.86	
A4H2"-H8	2.294	7.94	1.39E+07
A4H3'-H1'	4.984	5.983	2.13E+06
A4H3'-H8	4.984	7.94	1.86E+06
A4H3'-xC5Hd	4.983	7.545	5.01E+05
A4H4'-H1'	4.331	5.983	2.51E+06
A4H4'-H3'	4.331	4.985	
A4H4'-H8	4.33	7.94	5.32E+05
A4H5'-H3'	4.035	4.984	

A4H5'-H4'	4.035	4.33	
A4H5'-H8	4.027	7.939	6.02E+05
A4H5''-H1'	3.859	5.979	
A4H5''-H3'	3.86	4.984	5.00E+06
A4H5''-H4'	3.859	4.33	
A4H5''-H5'	3.858	4.032	
A4H5''-H8	3.862	7.94	7.79E+05
A4H8-xT3H1'	7.939	4.152	2.73E+06
A4H8-xT3H4'	7.94	4.066	8.87E+05
A4H8-xT3Hd	7.939	7.668	9.83E+05
A4H8-H1'	7.939	5.982	3.47E+06
A4H8-xC5Hd	7.939	7.547	9.05E+05
A4H8-xC5Hu	7.939	7.046	1.09E+06
xG14H1'-H3'	6.062	5.072	5.69E+06
xG14H1'-H8	6.064	8.579	1.27E+06
xG14H1'-Hd	6.064	6.916	1.65E+07
xG14H1'-C15H1'	6.066	5.735	
xG14H1'-C15H5	6.062	5.285	4.59E+06
xG14H1'-C15H6	6.065	7.474	2.89E+06
xG14H1'-xA8H2	6.066	7.16	
xG14H2''-H1'	2.79	6.064	2.61E+07
xG14H2''-H4'	2.788	4.45	6.18E+06
xG14H2''-H5''	2.794	4.212	1.61E+07
xG14H2''-H8	2.789	8.579	1.28E+07
xG14H2''-Hd	2.787	6.916	3.52E+06
xG14H2''-Hu	2.792	7.687	
xG14H2''-C15H4'	2.784	4.259	7.17E+06
xG14H2''-C15H5	2.79	5.283	1.05E+07
xG14H2''-C15H6	2.786	7.474	5.74E+06
xG14H3'-H1'	5.07	6.065	3.41E+06
xG14H3'-H8	5.068	8.579	1.56E+06
xG14H3'-Hd	5.068	6.916	4.36E+05
xG14H3'-C15H5	5.07	5.283	3.34E+06
xG14H3'-C15H6	5.069	7.467	5.38E+06
xG14H4'-T13H1'	4.445	5.839	
xG14H4'-H1'	4.45	6.064	5.38E+06
xG14H4'-H3'	4.448	5.069	8.04E+06
xG14H4'-H8	4.447	8.578	4.76E+05
xG14H4'-Hd	4.447	6.916	7.21E+05
xG14H5'-T13H1'	4.152	5.842	4.13E+06
xG14H5'-H4'	4.152	4.449	
xG14H5'-H5''	4.151	4.216	
xG14H5'-H8	4.153	8.579	4.31E+05
xG14H5''-H1'	4.218	6.061	3.27E+07
xG14H5''-H3'	4.215	5.07	6.23E+06
xG14H5''-H4'	4.217	4.45	
xG14H5''-H8	4.214	8.579	4.31E+05
xG14H8-T13H3'	8.579	4.948	1.13E+06
xG14H8-T13H6	8.578	7.434	5.65E+05
xG14H8-Hd	8.577	6.915	3.67E+05
xG14H8-Hu	8.588	7.689	1.11E+06
xG14H8-C15H6	8.578	7.473	
xG14Hd-H1'	6.916	6.065	1.86E+07
xG14Hd-H8	6.915	8.579	4.49E+05
xG14Hd-Hu	6.912	7.687	5.31E+05
xG14Hd-C15H1'	6.916	5.741	1.08E+06
xG14Hd-C15H5	6.915	5.28	3.04E+06
xG14Hd-C15H6	6.916	7.472	3.48E+06
xG14Hd-xA8H2	6.916	7.16	1.19E+06
C15H1'-xG14H1'	5.741	6.061	
C15H1'-xG14Hd	5.741	6.916	6.88E+05
C15H1'-H3'	5.741	4.92	3.43E+06
C15H1'-H5	5.738	5.282	
C15H1'-H6	5.741	7.474	2.89E+06
C15H1'-G16H8	5.741	7.587	2.13E+06
C15H2'-xG14H2''	2.374	2.789	4.87E+06
C15H2'-H1'	2.38	5.742	1.25E+07
C15H2'-H3'	2.388	4.918	
C15H2'-H4'	2.383	4.265	4.01E+06
C15H2'-H5''	2.376	4.192	
C15H2'-H6	2.378	7.475	
C15H2'-G16H5''	2.38	3.918	
C15H2'-G16H8	2.376	7.586	
C15H2''-H1'	2.14	5.742	7.82E+06
C15H2''-H2'	2.139	2.381	
C15H2''-H5	2.138	5.283	
C15H2''-H5	2.137	5.283	5.16E+06
C15H2''-H6	2.137	7.475	
C15H2''-G16H5''	2.138	3.916	
C15H3'-H1'	4.919	5.742	1.80E+06
C15H3'-H5	4.918	5.284	
C15H3'-H6	4.918	7.476	2.94E+06
C15H4'-xG14H1'	4.263	6.053	1.19E+06
C15H4'-xG14H3'	4.269	5.066	3.59E+07
C15H4'-xG14Hd	4.266	6.917	6.27E+05
C15H4'-H1'	4.265	5.742	4.60E+06
C15H4'-H3'	4.266	4.92	
C15H4'-H6	4.266	7.475	1.86E+06
C15H4'-G16H8	4.264	7.587	3.49E+05
C15H5-xG14H1'	5.284	6.063	4.50E+06
C15H5-xG14H8	5.282	8.579	6.43E+05
C15H5-xG14Hd	5.282	6.916	5.78E+05
C15H5-H6	5.283	7.475	1.12E+07
C15H5''-H4'	4.19	4.265	
C15H5''-H6	4.187	7.476	
C15H6-xG14H1'	7.475	6.066	3.19E+06
C15H6-xG14H8	7.472	8.579	3.55E+05
C15H6-xG14Hd	7.473	6.916	1.01E+06

C15H6-H1'	7.474	5.741	3.09E+06
C15H6-H5	7.475	5.283	1.32E+07
C15H6-G16H8	7.475	7.585	
xC5CH3-A4H1'	2.358	5.973	2.22E+06
xC5CH3-A4H2'	2.35	2.551	
xC5CH3-A4H3'	2.352	4.985	
xC5CH3-A4H8	2.356	7.939	3.24E+06
xC5CH3-Hd	2.355	7.547	
xC5CH3-Hu	2.354	7.046	1.33E+07
xC5CH3-xG6Hu	2.354	6.701	1.03E+06
xC5H1'-A4H1'	3.753	5.979	
xC5H1'-A4H2	3.757	7.877	
xC5H1'-H3'	3.758	4.919	
xC5H1'-H4'	3.756	4.131	
xC5H1'-H5"	3.761	4.072	
xC5H1'-Hd	3.757	7.547	2.52E+06
xC5H1'-xG6H8	3.758	8.533	1.43E+06
xC5H1'-xG6Hu	3.753	6.7	
xC5H2'-H1'	2.272	3.758	9.59E+06
xC5H2'-H2"	2.277	2.41	
xC5H2'-H3'	2.276	4.916	
xC5H2'-H5'	2.277	3.987	
xC5H2'-H5"	2.271	4.08	
xC5H2'-Hd	2.274	7.546	
xC5H2'-xG6H8	2.27	8.534	1.68E+06
xC5H2"-A4H5"	2.403	3.851	8.44E+07
xC5H2"-H1'	2.412	3.759	6.77E+06
xC5H2"-H4'	2.404	4.131	
xC5H2"-H5'	2.407	3.98	
xC5H2"-Hd	2.409	7.547	
xC5H2"-xG6H5"	2.409	4.072	
xC5H2"-xG6H8	2.412	8.531	1.82E+06
xC5H3'-H1'	4.909	3.769	2.20E+07
xC5H3'-Hd	4.921	7.547	2.45E+06
xC5H3'-xG6H8	4.918	8.534	
xC5H4'-A4H1'	4.13	5.982	1.74E+06
xC5H4'-H1'	4.13	3.757	
xC5H4'-H3'	4.132	4.92	
xC5H4'-Hd	4.13	7.547	5.92E+05
xC5H4'-xG6H8	4.133	8.532	
xC5H5'-A4H1'	3.983	5.982	4.04E+06
xC5H5'-H3'	3.988	4.92	
xC5H5'-H5"	3.979	4.081	
xC5H5'-H5"	3.977	4.082	
xC5H5'-Hd	3.984	7.545	5.64E+05
xC5H5"-A4H1'	4.077	5.983	3.27E+06
xC5H5"-H3'	4.076	4.918	
xC5H5"-H4'	4.08	4.133	
xC5H5"-Hd	4.078	7.545	1.63E+06

xC5Hd-A4H1'	7.546	5.981	1.90E+06
xC5Hd-A4H8	7.546	7.94	8.54E+05
xC5Hd-H1'	7.546	3.758	3.47E+06
xC5Hd-H3'	7.553	4.918	2.90E+07
xC5Hd-Hu	7.546	7.046	1.03E+06
xC5Hd-xG6H8	7.547	8.533	
xC5Hd-xG6Hu	7.546	6.701	4.58E+05
xC5Hu-A4H8	7.045	7.939	7.68E+05
xC5Hu-Hd	7.045	7.546	6.00E+05
xC5Hu-xG6Hu	7.045	6.7	8.98E+05
G16H1'-H3'	5.536	4.914	3.20E+06
G16H1'-H8	5.534	7.585	1.45E+06
G16H1'-xT17Hd	5.537	7.599	2.14E+06
G16H2'-G2H1'	2.318	5.332	1.76E+06
G16H2'-H1'	2.318	5.538	1.29E+07
G16H2'-H3'	2.322	4.912	
G16H2'-H4'	2.317	4.195	
G16H2'-H5"	2.313	3.92	
G16H2'-xT17H5'	2.313	3.892	4.99E+06
G16H2'-xT17Hd	2.319	7.595	
G16H2"-H1'	2.128	5.538	7.77E+06
G16H2"-H3'	2.132	4.916	
G16H2"-H4'	2.129	4.196	
G16H2"-H8	2.132	7.586	
G16H2"-xT17Hd	2.13	7.601	
G16H3'-H1'	4.913	5.537	1.90E+06
G16H3'-H5'	4.922	4.078	4.73E+08
G16H3'-H8	4.914	7.586	8.01E+05
G16H3'-xT17Hd	4.915	7.592	2.34E+06
G16H4'-xG14Hd	4.199	6.915	
G16H4'-C15H1'	4.194	5.739	3.48E+06
G16H4'-H1'	4.196	5.537	3.09E+06
G16H4'-H3'	4.195	4.916	
G16H4'-H8	4.195	7.587	8.13E+05
G16H5'-C15H1'	4.069	5.741	
G16H5'-H4'	4.075	4.196	
G16H5'-H8	4.066	7.587	7.10E+06
G16H5"-C15H1'	3.918	5.741	2.46E+06
G16H5"-H3'	3.918	4.913	
G16H5"-H4'	3.915	4.195	
G16H5"-H8	3.911	7.586	8.74E+05
G16H8-C15H1'	7.586	5.742	2.81E+06
G16H8-C15H6	7.586	7.476	
G16H8-H1'	7.59	5.537	4.49E+06
G16H8-xT17Hu	7.591	7.118	2.41E+06
xG6H1'-H8	6.059	8.533	1.40E+06
xG6H1'-Hd	6.059	6.837	1.77E+07
xG6H1'-C7H1'	6.061	5.562	
xG6H1'-C7H6	6.059	7.362	2.92E+06

xG6H2'-H1'	2.853	6.061	8.71E+06	C7H2'-H3'	2.369	4.886	
xG6H2'-H4'	2.849	4.456	3.62E+06	C7H2'-H4'	2.371	4.158	
xG6H2'-H5'	2.862	4.156	5.81E+06	C7H2'-H5	2.375	5.285	3.58E+06
xG6H2'-H5"	2.857	4.079		C7H2'-H5"	2.371	4.137	
xG6H2'-H8	2.856	8.534	9.38E+06	C7H2'-H6	2.37	7.362	7.28E+06
xG6H2'-Hd	2.852	6.837	2.07E+06	C7H2'-xA8H3'	2.369	5.065	6.47E+06
xG6H2'-C7H5	2.851	5.285	5.09E+06	C7H2'-xA8H4'	2.373	4.363	
xG6H2'-C7H6	2.855	7.363	3.45E+06	C7H2'-xA8H8	2.371	8.598	1.93E+06
xG6H2"-H5'	2.789	4.153	5.70E+06	C7H2"-xG6H2"	2.021	2.794	
xG6H2"-H5"	2.801	4.077	1.92E+06	C7H2"-H1'	2.02	5.567	6.28E+06
xG6H2"-H8	2.794	8.535	8.52E+06	C7H2"-H2'	2.021	2.37	
xG6H2"-Hd	2.792	6.844	6.38E+06	C7H2"-H3'	2.022	4.885	
xG6H2"-C7H6	2.795	7.362	4.23E+06	C7H2"-H4'	2.019	4.16	2.44E+06
xG6H3'-H1'	5.071	6.056	1.24E+06	C7H2"-H5	2.02	5.286	4.97E+06
xG6H3'-H8	5.072	8.534	1.96E+06	C7H2"-H5'	2.021	4.231	
xG6H3'-C7H6	5.073	7.362		C7H2"-H5"	2.025	4.137	2.70E+06
xG6H4'-H3'	4.457	5.076	4.95E+06	C7H2"-H6	2.02	7.362	1.31E+07
xG6H4'-H3'	4.452	5.084	########	C7H2"-xA8H8	2.021	8.598	1.45E+06
xG6H4'-H8	4.455	8.531		C7H3'-H1'	4.881	5.57	5.08E+05
xG6H4'-Hd	4.456	6.837		C7H3'-H6	4.883	7.371	4.48E+06
xG6H4'-C7H5	4.449	5.286		C7H3'-xA8H8	4.88	8.597	
xG6H5'-H3'	4.163	5.074	5.06E+06	C7H4'-xG6H1'	4.155	6.06	1.18E+06
xG6H5'-H4'	4.163	4.457		C7H4'-xG6Hd	4.156	6.835	5.38E+05
xG6H5'-H8	4.163	8.533		C7H4'-H1'	4.158	5.567	5.33E+06
xG6H5"-H3'	4.077	5.072	4.50E+06	C7H4'-H3'	4.159	4.887	
xG6H5"-H4'	4.076	4.454		C7H4'-H5	4.156	5.284	
xG6H5"-H5'	4.076	4.174		C7H4'-H6	4.155	7.359	4.37E+06
xG6H5"-H8	4.077	8.532		C7H5-xG6H1'	5.284	6.061	
xG6H8-xC5H1'	8.533	3.758	2.33E+06	C7H5-xG6H8	5.285	8.533	7.35E+05
xG6H8-xC5Hd	8.534	7.546	5.45E+05	C7H5-xG6Hd	5.284	6.835	
xG6H8-H3'	8.544	5.069	3.31E+07	C7H5-H6	5.286	7.362	1.24E+07
xG6H8-H4'	8.533	4.457	7.01E+05	C7H5-xA8H8	5.285	8.595	
xG6H8-Hd	8.531	6.836		C7H5-xA8Hu	5.284	7.69	9.52E+05
xG6H8-C7H6	8.532	7.348	1.56E+06	C7H5'-xG6H1'	4.218	6.061	
xG6Hd-H1'	6.836	6.06	1.81E+07	C7H5'-xG6Hd	4.231	6.837	
xG6Hd-H8	6.831	8.531		C7H5'-H1'	4.232	5.565	
xG6Hd-C7H1'	6.829	5.569	6.40E+05	C7H5'-H3'	4.224	4.885	
xG6Hd-C7H5	6.836	5.284		C7H5'-H6	4.228	7.362	
xG6Hd-C7H6	6.834	7.364		C7H6-xG6H1'	7.361	6.06	2.89E+06
xG6Hu-xG14Hu	6.699	7.686	4.78E+05	C7H6-xG6H8	7.361	8.536	1.54E+06
xG6Hu-xC5Hu	6.7	7.045	7.05E+05	C7H6-xG6Hd	7.36	6.835	1.08E+06
xG6Hu-H8	6.705	8.535		C7H6-H1'	7.361	5.567	2.72E+06
C7H1'-xG6H1'	5.563	6.055		C7H6-H5	7.361	5.286	1.39E+07
C7H1'-xG6Hd	5.566	6.834	8.98E+05	C7H6-xA8H8	7.362	8.598	5.04E+05
C7H1'-H3'	5.566	4.885	2.84E+06	xT17CH3-G16H8	2.3	7.586	
C7H1'-H5	5.572	5.282		xT17CH3-H1'	2.303	4.016	
C7H1'-H6	5.566	7.362	3.05E+06	xT17CH3-H4'	2.305	4.057	
C7H1'-xA8H8	5.566	8.598	8.71E+05	xT17CH3-Hd	2.299	7.603	
C7H2'-H1'	2.371	5.568	1.20E+07	xT17CH3-Hu	2.297	7.117	1.38E+07

xT17H1'-G16H1'	4.011	5.538	2.21E+06
xT17H1'-H3'	4.013	4.854	
xT17H1'-Hd	4.015	7.602	2.49E+06
xT17H1'-A18H1'	4.019	6.045	1.27E+06
xT17H1'-A18H8	4.019	7.711	2.69E+06
xT17H2'-H1'	2.177	4.017	
xT17H2'-H2"	2.172	2.426	
xT17H2'-H3'	2.178	4.857	
xT17H2'-H4'	2.175	4.05	
xT17H2'-H5'	2.171	3.885	
xT17H2'-Hd	2.174	7.601	
xT17H2'-A18H8	2.173	7.71	
xT17H2"-H1'	2.428	4.014	
xT17H2"-H3'	2.434	4.855	
xT17H2"-H4'	2.426	4.05	
xT17H2"-Hd	2.429	7.602	
xT17H3'-Hd	4.856	7.598	
xT17H4'-G16H1'	4.055	5.537	1.87E+06
xT17H4'-H3'	4.05	4.854	
xT17H5'-G16H1'	3.884	5.537	4.19E+06
xT17H5'-H1'	3.886	4.015	
xT17H5'-H3'	3.882	4.855	
xT17H5'-H4'	3.884	4.056	
xT17H5'-Hd	3.886	7.6	
xT17Hd-H1'	7.6	4.021	9.63E+06
xT17Hd-H3'	7.601	4.854	4.27E+06
xT17Hu-G16H8	7.117	7.586	7.22E+05
xT17Hu-Hd	7.118	7.6	8.59E+05
A18H1'-H2	6.044	8.001	4.47E+05
A18H1'-H3'	6.044	4.95	4.32E+06
A18H1'-H8	6.044	7.711	3.05E+06
A18H1'-xC19Hd	6.046	7.188	8.30E+05
A18H2-A4H2	8	7.877	1.76E+06
A18H2'-H1'	2.406	6.046	1.37E+07
A18H2'-H3'	2.409	4.948	
A18H2'-H4'	2.407	4.316	2.20E+06
A18H2'-H8	2.407	7.71	
A18H2'-xC19Hd	2.405	7.187	3.34E+06
A18H2"-H1'	2.082	6.046	1.10E+07
A18H2"-H2'	2.082	2.407	
A18H2"-H3'	2.082	4.949	
A18H2"-H4'	2.076	4.315	1.66E+06
A18H2"-H5'	2.079	4.017	
A18H2"-H5"	2.081	3.847	
A18H2"-H8	2.08	7.71	
A18H2"-xC19H4'	2.074	4.26	
A18H3'-H1'	4.95	6.046	2.57E+06
A18H3'-H8	4.948	7.711	1.92E+06
A18H4'-H1'	4.316	6.043	1.97E+06
A18H4'-H3'	4.316	4.949	
A18H4'-H8	4.315	7.711	5.98E+05
A18H5'-H3'	4.018	4.949	
A18H5'-xA8H8	4.021	8.6	7.92E+05
A18H5"-H1'	3.852	6.046	
A18H5"-H3'	3.851	4.949	6.03E+06
A18H5"-H4'	3.85	4.316	
A18H5"-H8	3.842	7.702	1.68E+07
A18H8-xT17H1'	7.711	4.019	4.34E+06
A18H8-xT17H3'	7.711	4.852	2.22E+06
A18H8-H1'	7.71	6.045	4.00E+06
A18H8-xC19Hd	7.71	7.188	9.87E+05
A18H8-xC19Hu	7.71	7.077	1.45E+06
xA8H1'-H2	5.846	7.16	4.68E+05
xA8H1'-H3'	5.847	5.066	3.09E+06
xA8H1'-H8	5.848	8.598	1.47E+06
xA8H1'-Hd	5.848	6.792	1.54E+07
xA8H1'-xG9H8	5.849	8.308	1.40E+06
xA8H1'-xG9Hd	5.852	6.853	1.09E+07
xA8H2-xG14Hd	7.159	6.916	8.20E+05
xA8H2-xG14Hu	7.158	7.686	4.01E+05
xA8H2-xG9Hd	7.156	6.852	4.20E+05
xA8H2'-H1'	2.87	5.849	1.01E+07
xA8H2'-H3'	2.862	5.07	2.63E+07
xA8H2'-H4'	2.869	4.363	2.12E+06
xA8H2'-H5"	2.866	4.025	
xA8H2'-H8	2.868	8.598	6.16E+06
xA8H2'-Hd	2.87	6.792	2.47E+06
xA8H2'-xG9H4'	2.86	4.485	
xA8H2'-xG9H8	2.87	8.307	2.81E+06
xA8H2"-H1'	2.787	5.848	8.11E+06
xA8H2"-H2'	2.788	2.867	
xA8H2"-H3'	2.789	5.069	4.47E+07
xA8H2"-H4'	2.787	4.362	2.39E+06
xA8H2"-H5"	2.786	4.023	
xA8H2"-H8	2.787	8.598	1.09E+07
xA8H2"-Hd	2.787	6.792	1.94E+06
xA8H2"-xG9H8	2.785	8.308	6.13E+06
xA8H3'-H1'	5.065	5.847	2.12E+06
xA8H3'-H8	5.065	8.598	1.75E+06
xA8H3'-Hd	5.064	6.791	2.97E+05
xA8H3'-xG9H8	5.064	8.308	4.89E+05
xA8H4'-C7H1'	4.36	5.567	
xA8H4'-H1'	4.362	5.849	3.09E+06
xA8H4'-H3'	4.362	5.066	6.17E+06
xA8H4'-H8	4.362	8.598	3.78E+05
xA8H4'-Hd	4.361	6.792	6.52E+05
xA8H4'-xG9H8	4.361	8.307	2.17E+05
xA8H5'-H3'	4.149	5.067	1.11E+07

xA8H5'-H4'	4.15	4.362	
xA8H5"-C7H1'	4.024	5.569	1.26E+06
xA8H5"-A18H4'	4.022	4.314	
xA8H5"-H1'	4.02	5.848	
xA8H5"-H3'	4.022	5.066	4.66E+06
xA8H5"-H4'	4.019	4.362	
xA8H5"-H5'	4.021	4.15	
xA8H8-C7H1'	8.598	5.568	1.66E+06
xA8H8-C7H6	8.598	7.372	7.29E+06
xA8H8-Hd	8.597	6.792	4.99E+05
xA8H8-xG9H8	8.598	8.307	5.45E+05
xA8H8-xG9Hu	8.598	6.763	
xA8Hd-H1'	6.791	5.849	1.72E+07
xA8Hd-H2	6.791	7.159	4.45E+05
xA8Hd-H8	6.791	8.598	3.94E+05
xA8Hd-Hu	6.795	7.69	3.96E+05
xA8Hd-xG9H1'	6.792	6.213	1.59E+06
xA8Hd-xG9H8	6.792	8.307	5.04E+05
xA8Hu-C7H5	7.689	5.284	
xA8Hu-H2	7.686	7.159	3.34E+05
xA8Hu-xG9Hu	7.69	6.763	1.38E+06
xC19CH3-xT1Hu	2.339	6.475	6.95E+05
xC19CH3-A18H8	2.337	7.71	
xC19CH3-H1'	2.34	4.837	
xC19CH3-Hd	2.338	7.188	1.11E+07
xC19CH3-Hu	2.339	7.077	1.66E+07
xC19CH3-A20H2	2.338	7.871	9.69E+05
xC19CH3-A20H8	2.339	8.286	
xC19H1'-Hd	4.835	7.188	6.27E+05
xC19H1'-A20H8	4.84	8.287	
xC19H2'-CH3	2.132	2.335	
xC19H2'-H1'	2.138	4.835	
xC19H2'-H3'	2.137	4.958	
xC19H2'-H4'	2.137	4.263	
xC19H2'-H5'	2.14	3.955	9.41E+06
xC19H2'-H5"	2.136	4.082	
xC19H2'-Hd	2.139	7.188	2.13E+07
xC19H2'-A20H1'	2.131	6.351	
xC19H2'-A20H2'	2.137	2.691	
xC19H2'-A20H4'	2.139	4.399	7.11E+05
xC19H2'-A20H8	2.139	8.288	1.46E+06
xC19H3'-H1'	4.958	4.838	2.70E+06
xC19H3'-Hd	4.957	7.188	2.25E+06
xC19H3'-A20H8	4.959	8.287	4.53E+05
xC19H4'-H1'	4.261	4.837	
xC19H4'-H3'	4.262	4.958	
xC19H4'-Hd	4.261	7.188	6.02E+05
xC19H4'-A20H8	4.261	8.287	5.06E+05
xC19H5'-A18H1'	3.967	6.047	3.69E+06
xC19H5'-H1'	3.969	4.838	
xC19H5'-H3'	3.967	4.957	
xC19H5'-H4'	3.966	4.261	
xC19H5'-Hd	3.967	7.187	3.35E+05
xC19H5"-A18H1'	4.081	6.048	3.68E+06
xC19H5"-H3'	4.081	4.958	
xC19H5"-H4'	4.08	4.261	
xC19Hd-xT1Hu	7.187	6.474	8.28E+05
xC19Hd-A18H1'	7.187	6.046	1.76E+06
xC19Hd-A18H8	7.186	7.711	8.59E+05
xC19Hd-H1'	7.187	4.837	4.86E+06
xC19Hd-H3'	7.187	4.958	4.67E+06
xC19Hd-Hu	7.187	7.077	
xC19Hd-A20H2	7.195	7.866	2.31E+06
xC19Hd-A20H8	7.186	8.288	4.88E+05
xC19Hu-A18H8	7.076	7.711	1.17E+06
xC19Hu-Hd	7.076	7.187	
xC19Hu-A20H2	7.073	7.87	9.05E+05
xG9H1'-xA8H1'	6.211	5.848	
xG9H1'-xA8H2	6.215	7.161	
xG9H1'-xA8Hd	6.212	6.792	1.15E+06
xG9H1'-H3'	6.211	5	2.51E+06
xG9H1'-H8	6.211	8.308	1.17E+06
xG9H1'-Hd	6.21	6.854	1.82E+07
xG9H1'-A20H8	6.256	8.286	
xG9H1'-T10H6	6.211	7.193	1.36E+06
xG9H2'-H1'	2.785	6.212	1.13E+07
xG9H2'-H3'	2.785	5	1.02E+07
xG9H2'-H4'	2.785	4.488	2.77E+06
xG9H2'-Hd	2.783	6.854	2.02E+06
xG9H2'-Hu	2.782	6.763	
xG9H2'-T10H6	2.785	7.193	4.00E+06
xG9H2"-xA8Hd	2.596	6.792	
xG9H2"-H1'	2.594	6.212	7.74E+06
xG9H2"-H2'	2.593	2.785	
xG9H2"-H3'	2.592	4.999	
xG9H2"-H4'	2.595	4.488	1.95E+06
xG9H2"-H8	2.595	8.308	7.30E+06
xG9H2"-Hd	2.594	6.854	1.68E+06
xG9H2"-T10H5"	2.606	4.164	
xG9H2"-T10H6	2.595	7.193	3.02E+06
xG9H3'-H1'	5	6.212	1.90E+06
xG9H3'-H8	4.999	8.308	1.16E+06
xG9H3'-Hd	4.999	6.854	3.68E+05
xG9H3'-T10H6	4.999	7.193	6.79E+05
xG9H4'-xA8H1'	4.488	5.849	
xG9H4'-xA8Hd	4.486	6.792	2.44E+05
xG9H4'-H1'	4.487	6.212	3.17E+06
xG9H4'-H3'	4.487	5	4.88E+06

xG9H4'-H8	4.486	8.308	7.93E+05
xG9H4'-Hd	4.487	6.854	6.76E+05
xG9H5'-xA8H1'	4.248	5.846	2.66E+06
xG9H5'-xA8Hd	4.248	6.791	5.35E+05
xG9H5'-H3'	4.252	4.999	
xG9H5'-H4'	4.246	4.487	
xG9H5'-H8	4.243	8.31	8.01E+05
xG9H5''-xA8H1'	4.291	5.848	1.48E+06
xG9H5''-H3'	4.287	5.001	
xG9H5''-H4'	4.289	4.487	
xG9H5''-H8	4.288	8.308	5.79E+07
xG9H8-xA8H1'	8.307	5.85	2.56E+06
xG9H8-xA8H8	8.308	8.598	4.87E+05
xG9H8-xA8Hd	8.307	6.793	6.78E+05
xG9H8-H1'	8.307	6.212	1.90E+06
xG9H8-Hd	8.307	6.854	4.92E+05
xG9H8-Hu	8.306	6.764	5.66E+05
xG9H8-T10H6	8.306	7.193	4.39E+05
xG9Hd-xA11H2	6.854	8.099	
xG9Hd-xA8H2	6.853	7.159	6.48E+05
xG9Hd-H1'	6.854	6.212	2.05E+07
xG9Hd-H8	6.854	8.307	3.85E+05
xG9Hd-T10H6	6.854	7.193	7.41E+05
xG9Hu-xA8H8	6.762	8.597	
xG9Hu-xA8Hu	6.762	7.691	1.30E+06
A20H1'-H2	6.353	7.871	5.19E+05
A20H1'-H3'	6.353	4.89	2.82E+06
A20H1'-H8	6.353	8.288	2.49E+06
A20H2-H1'	7.871	6.354	2.33E+05
A20H2'-xT1Hu	2.69	6.474	1.07E+06
A20H2'-xC19Hd	2.688	7.188	1.36E+06
A20H2'-H1'	2.688	6.353	9.57E+06
A20H2'-H3'	2.688	4.889	
A20H2'-H4'	2.691	4.398	1.79E+06
A20H2'-H5'	2.688	4.09	4.03E+06
A20H2'-H5''	2.693	4.132	1.08E+07
A20H2'-H8	2.692	8.288	1.16E+07
A20H2''-xT1Hu	2.634	6.475	9.22E+05
A20H2''-H1'	2.629	6.353	1.68E+07
A20H2''-H2'	2.631	2.692	
A20H2''-H3'	2.635	4.888	
A20H2''-H4'	2.631	4.398	2.13E+06
A20H2''-H8	2.632	8.288	5.51E+06
A20H3'-H1'	4.892	6.352	6.48E+05
A20H3'-H8	4.888	8.288	1.11E+06
A20H4'-H1'	4.398	6.353	3.43E+06
A20H4'-H3'	4.397	4.889	7.02E+06
A20H4'-H8	4.398	8.288	5.74E+05
A20H5'-xC19H1'	4.084	4.838	
A20H5'-xC19Hd	4.085	7.187	8.47E+05
A20H5'-H1'	4.092	6.355	3.66E+05
A20H5'-H4'	4.086	4.399	
A20H5'-H8	4.085	8.288	1.10E+06
A20H5''-xC19H1'	4.134	4.84	
A20H5''-xC19Hd	4.136	7.189	4.33E+05
A20H5''-xG9H8	4.142	8.307	
A20H5''-H1'	4.132	6.352	3.52E+05
A20H5''-H3'	4.139	4.89	
A20H5''-H4'	4.139	4.398	
A20H5''-H8	4.137	8.288	9.98E+05
A20H8-xT1Hu	8.288	6.476	2.92E+05
A20H8-xC19H1'	8.287	4.836	2.11E+06
A20H8-xC19H3'	8.287	4.959	1.47E+06
A20H8-xC19Hd	8.287	7.187	5.78E+05
A20H8-H1'	8.287	6.353	3.19E+06
A20H8-H3'	8.287	4.889	3.49E+06
T10CH3-xA11H2	1.168	8.101	
T10CH3-xA8H8	1.169	8.597	
T10CH3-xA8Hd	1.169	6.791	
T10CH3-xG9H1'	1.171	6.212	1.99E+06
T10CH3-xG9H2'	1.171	2.786	4.73E+06
T10CH3-xG9H2''	1.171	2.596	3.95E+06
T10CH3-xG9H3'	1.171	5	1.63E+06
T10CH3-xG9H4'	1.172	4.487	5.09E+05
T10CH3-xG9H8	1.171	8.308	2.49E+06
T10CH3-xG9Hd	1.17	6.854	7.36E+05
T10CH3-xG9Hu	1.171	6.763	7.57E+05
T10CH3-H1'	1.17	6.176	2.91E+05
T10CH3-H2'	1.17	2.29	6.00E+05
T10CH3-H2''	1.171	2.111	2.25E+06
T10CH3-H3'	1.171	4.71	7.96E+05
T10CH3-H4'	1.168	4.231	
T10CH3-H5'	1.167	4.307	
T10CH3-H6	1.171	7.194	1.11E+07
T10H1'-xA11H2	6.172	8.099	
T10H1'-H3'	6.176	4.711	2.61E+06
T10H1'-H6	6.175	7.193	2.42E+06
T10H2'-xG9Hd	2.286	6.853	
T10H2'-H1'	2.293	6.176	1.58E+07
T10H2'-H3'	2.292	4.71	7.56E+06
T10H2'-H4'	2.292	4.231	
T10H2'-H5'	2.286	4.306	
T10H2'-H6	2.292	7.193	7.32E+06
T10H2''-xG9Hd	2.107	6.854	
T10H2''-H1'	2.112	6.176	8.03E+06
T10H2''-H2'	2.115	2.296	
T10H2''-H3'	2.111	4.71	1.05E+07
T10H2''-H4'	2.112	4.231	

T10H2"-H6	2.107	7.193	1.59E+07	T10H5'-H6	4.312	7.195	1.41E+05
T10H3'-H6	4.706	7.193	4.93E+05	T10H5"-xG9H1'	4.154	6.212	
T10H4'-xG9H1'	4.235	6.209	2.38E+06	T10H5"-xG9Hd	4.152	6.854	5.45E+05
T10H4'-xG9Hd	4.232	6.854	6.77E+05	T10H5"-H1'	4.153	6.176	
T10H4'-H1'	4.231	6.175	4.06E+06	T10H5"-H3'	4.152	4.71	5.39E+06
T10H4'-H3'	4.231	4.71	5.29E+06	T10H5"-H4'	4.153	4.232	
T10H4'-H6	4.231	7.193	6.42E+05	T10H5"-H5'	4.154	4.306	
T10H5'-xG9H1'	4.308	6.211	3.04E+06	T10H5"-H6	4.156	7.193	5.59E+05
T10H5'-xG9Hd	4.31	6.854	7.14E+05	T10H6-xG9H1'	7.193	6.212	2.40E+06
T10H5'-H1'	4.308	6.177		T10H6-xG9H8	7.192	8.307	4.62E+05
T10H5'-H3'	4.312	4.711	3.72E+06	T10H6-xG9Hd	7.193	6.854	9.89E+05
T10H5'-H6	4.312	7.192	6.96E+05	T10H6-H1'	7.193	6.175	2.89E+06

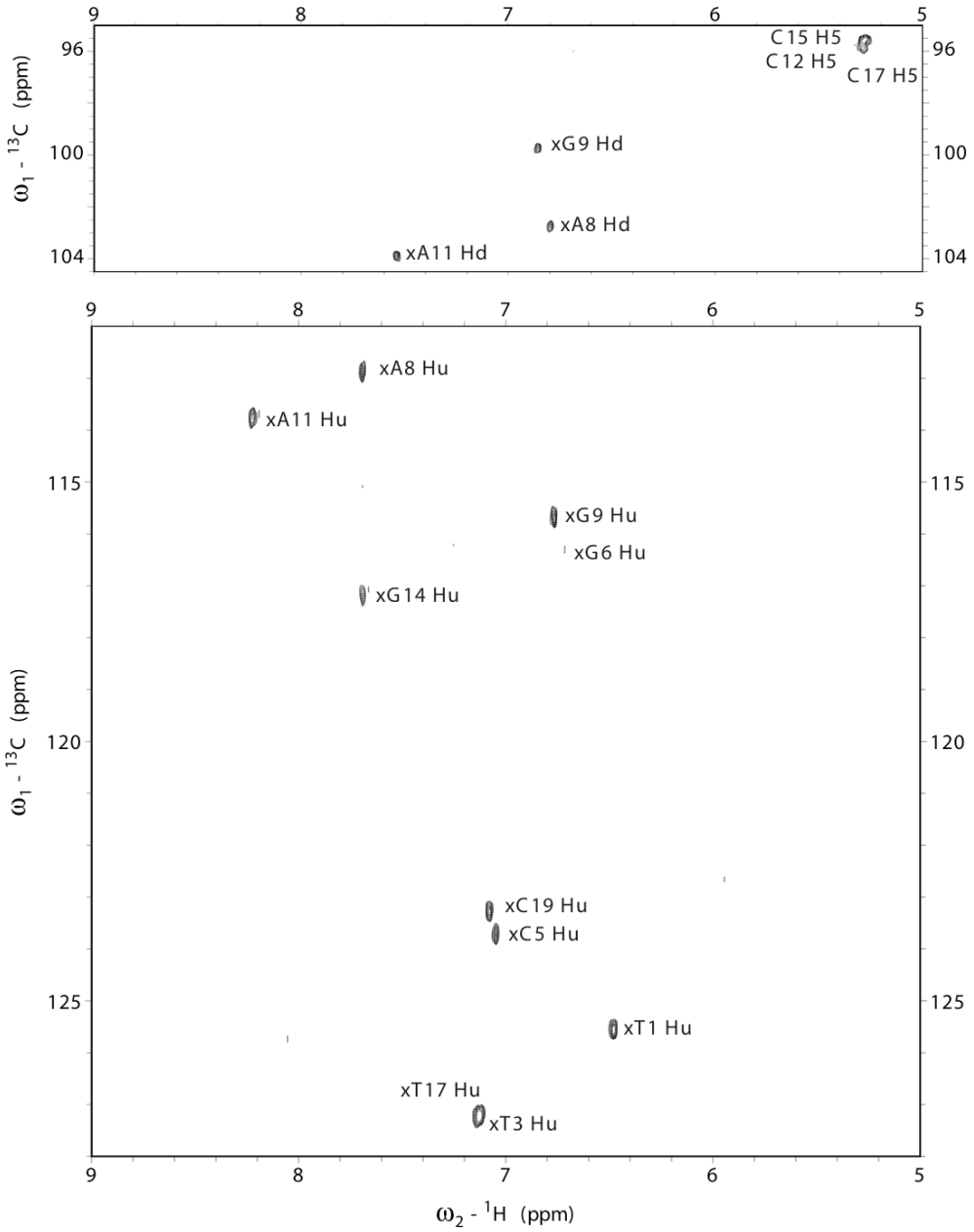


Figure S1A. $^{1}H/^{13}C$ HSQC spectrum of xDNA decamer duplex acquired at 25°C in 20 mM sodium phosphate buffer in D_2O, pH 7.0, showing the upfield aromatic proton/carbon correlations.

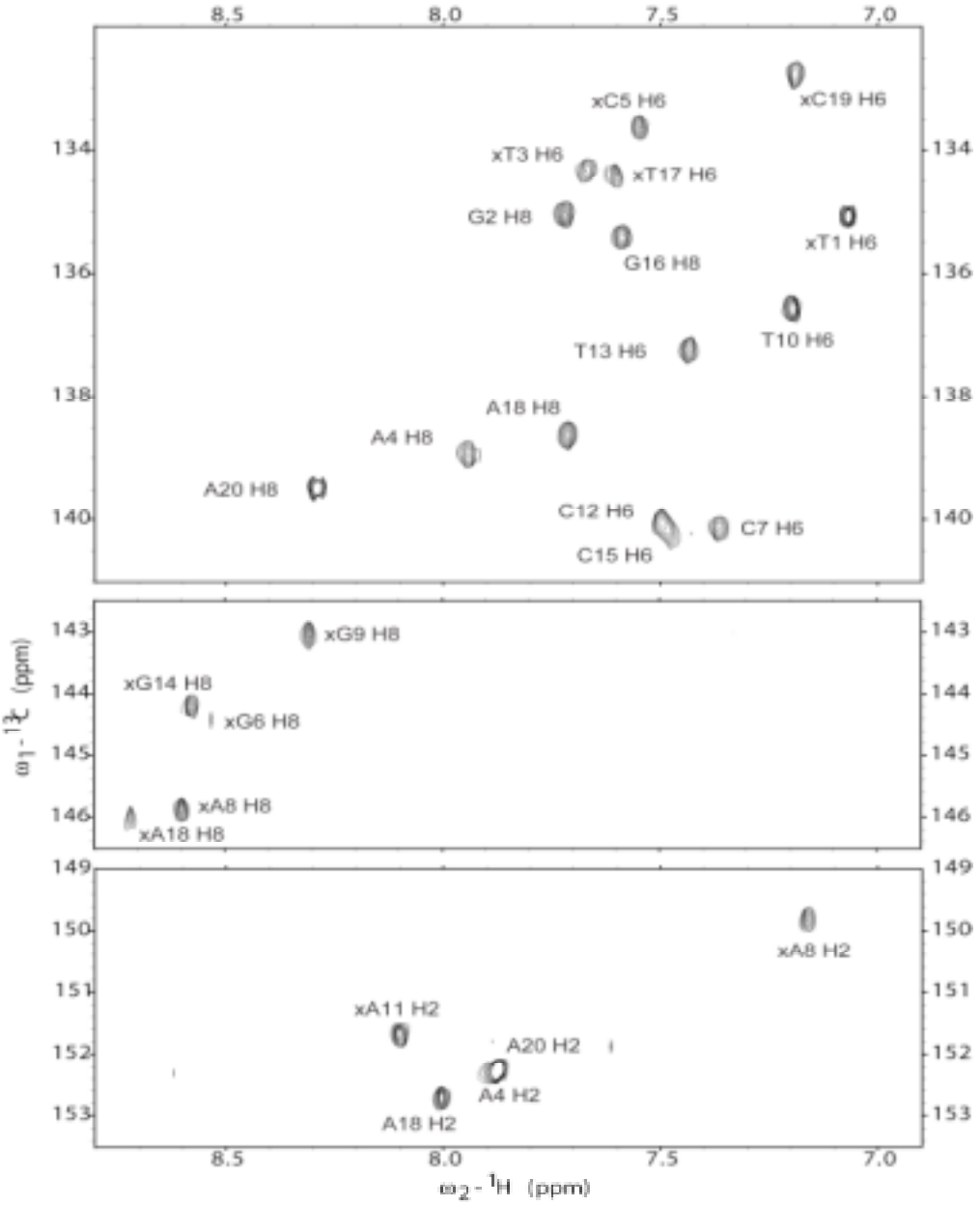


Figure S1B. $^{1}H/^{13}C$ HSQC spectrum of xDNA decamer duplex acquired at 25°C in 20 mM sodium phosphate buffer in D_2O, pH 7.0, showing the downfield aromatic proton/carbon correlations.

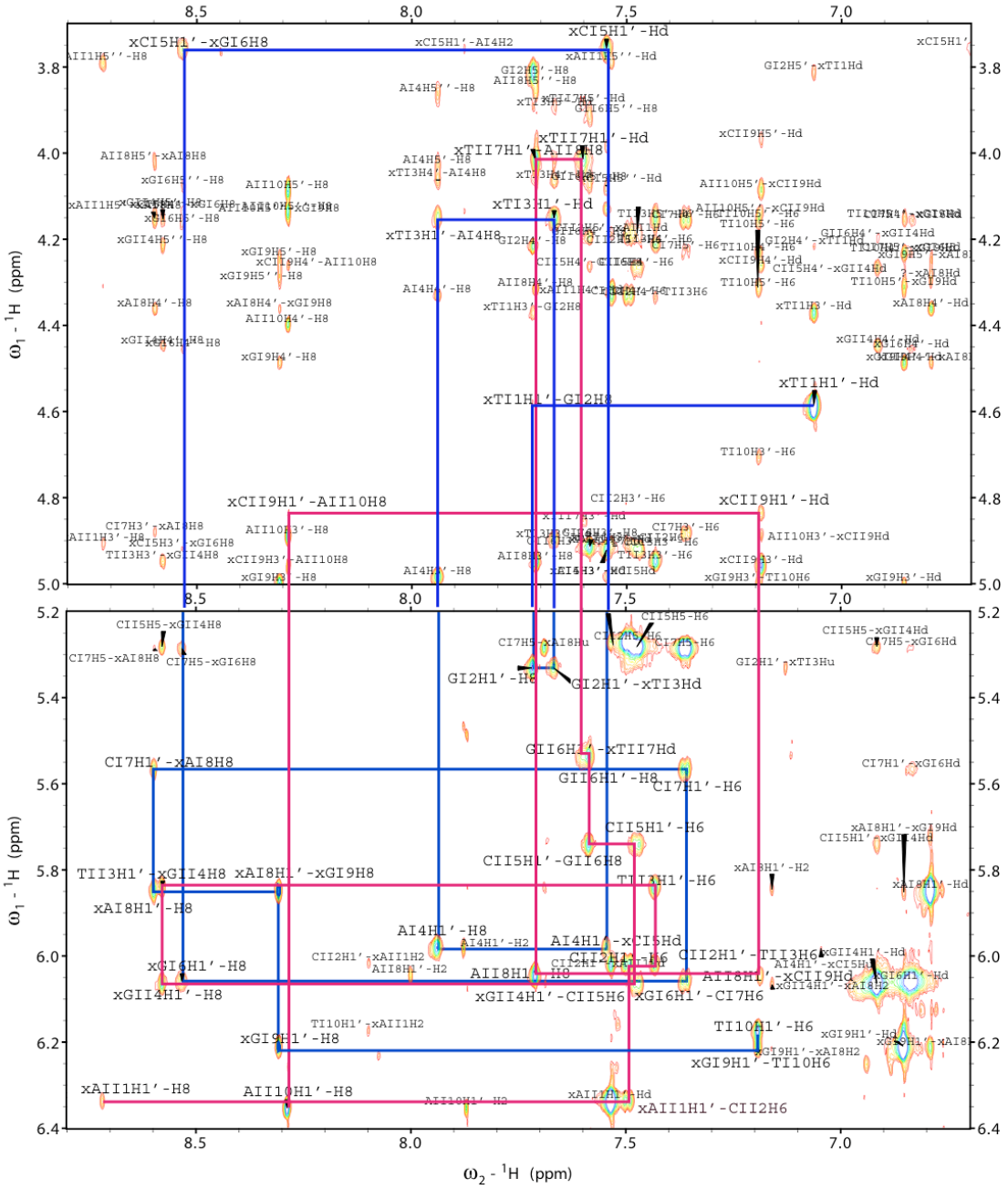


Figure S2. 1H/1H NOESY spectrum of xDNA 10 nucleotide duplex acquired at 25°C in 20 mM Sodium Phosphate buffer in D2O, pH 7.0, with a mixing time of 300 ms, and a recycle delay of 1.84 s, highlighting the aromatic proton to anomeric proton NOEs. The blue lines indicate the NOESY H1'/aromatic walk on strand 1, the red line on strand 2.

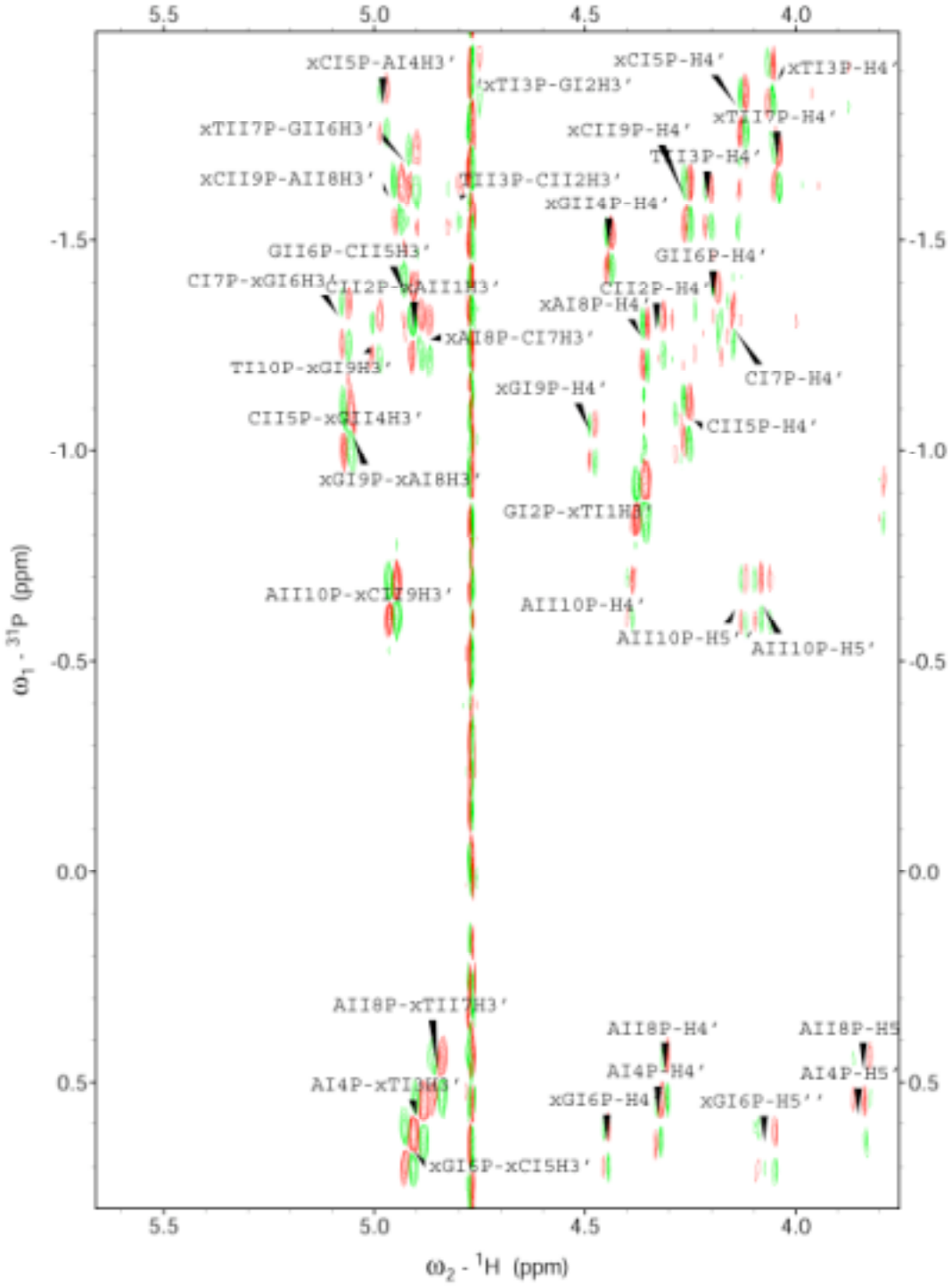


Figure S3. 1H/31P Heteronuclear COSY spectrum of xDNA 10 nucleotide duplex acquired at 25°C in 20 mM Sodium Phosphate buffer in D2O, pH 7.0, showing the large 3-bond H3'(i)-P(i+1), and 4-bond H4'(i)-P(i) coupling.

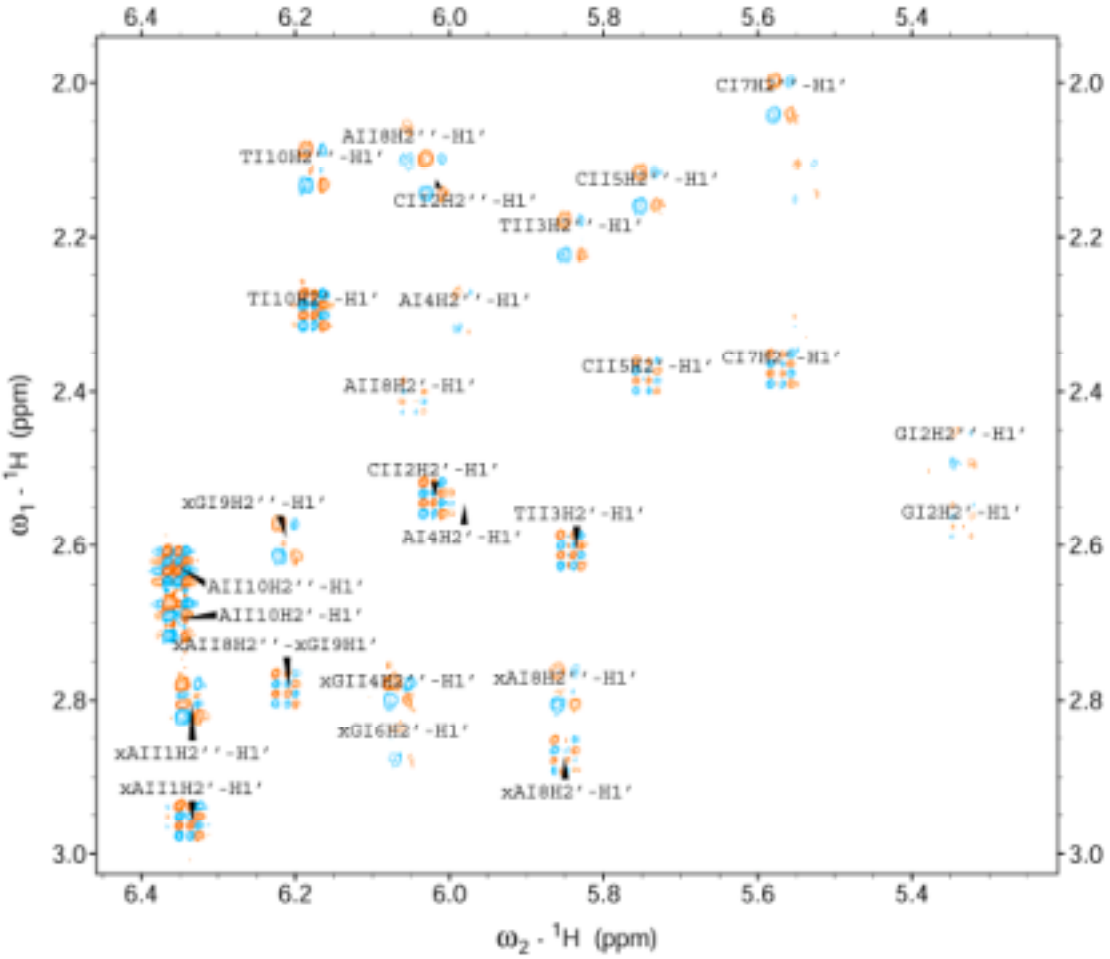


Figure S4. 1H/1H DQF-COSY spectrum of xDNA 10 nucleotide duplex acquired at 25°C in 20 mM Sodium Phosphate buffer in D2O, pH 7.0, showing the 3-bond coupling of the H1 to the H2' and H2".