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Supplementary Material
(Six pages)

Figure 1S. The expanded aromatic to H1', H2', H2", methyl region of the non-exchangeable proton 2D-NOESY spectrum of the $d(CGATCG)_2$ duplex collected at 2 °C shows the nucleotide conformation. Note the similar intensity patterns between those of $d(CGATCG)_2$ and $d(CG[iA]TCG)_2$ (see **Figure 2**), suggesting similar structures. **Experimental**: The hexamer DNA d(CGATCG) was synthesized on an Applied Biosystems DNA synthesizer at the Genetic Facility of UIUC. It was purified and desalted on a Sepharose S100 column equilibriated with 20 mM NH_4OH. Solutions of the DNA oligomers were prepared as described earlier.[11] For the d(CGATCG) sample, 3.18 mg lyophilized powder was dissolved in 0.55 ml of H_2O containing 20 mM phosphate buffer at pH 7.0, resulting in a 1.4 mM duplex solution. For the d(CG[iA]TCG), a ~0.4 mM DNA duplex solution was similarly prepared. NMR spectra were collected on a Varian VXR500 500 MHz spectrometer and the data were processed with FELIX v1.1 (Hare Research, Woodinville, WA). The non-exchangeable 2D NOE spectra were collected at 2 °C at a mixing time of 150 ms and a total recycle delay of 2.9 seconds where the average T1 relaxation was 1.8 seconds. The data were collected by the States/TPPI technique[12] with 256 t_1 increments and 2048 t_2 complex points each the average of 128 transients. TOCSY spectra were used together with the NOE spectra to derive the assignment. 2D NOESY spectra at 2 °C in 90% H_2O were collected with the 1 not 1 pulse sequence as the read pulse of the NOESY. 24 transients were averaged with a recycle delay of 2.9 seconds and a mixing time of 100 ms. The

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excitation offset was set to one quarter of the spectral bandwidth which was set to 12000 Hz so that the imino resonances around 13 ppm were nearly maximally excited. DNA models were prepared and energy-minimized using X-PLOR.[15]

Figure 2S. The expanded aromatic to H1', H2', H2", methyl region of the *simulated* non-exchangeable proton 2D-NOESY spectra of the d(CG[iA]TCG)$_2$ duplex, calculated from the refined model.

Table 1S. The chemical shift assignments of all non-exchangeable proton resonances and some exchangeable proton resonances.

Table 2S. The coupling constants derived from the PE-COSY spectra of d(CGATCG)$_2$ and d(CG[iA]TCG)$_2$. These values are consistent with the S-type (C2'-endo) sugar puckers.

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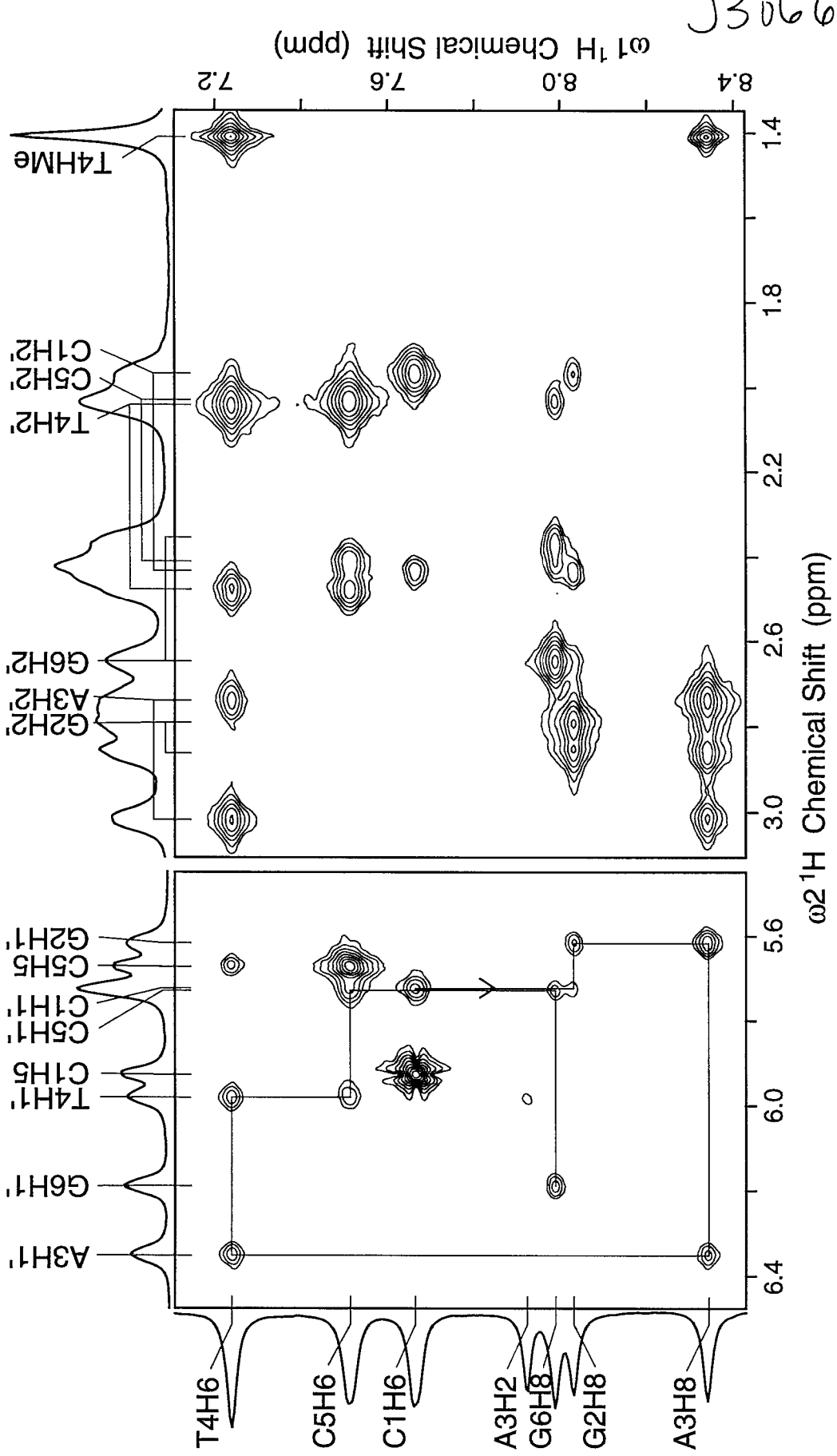

Figure 1s

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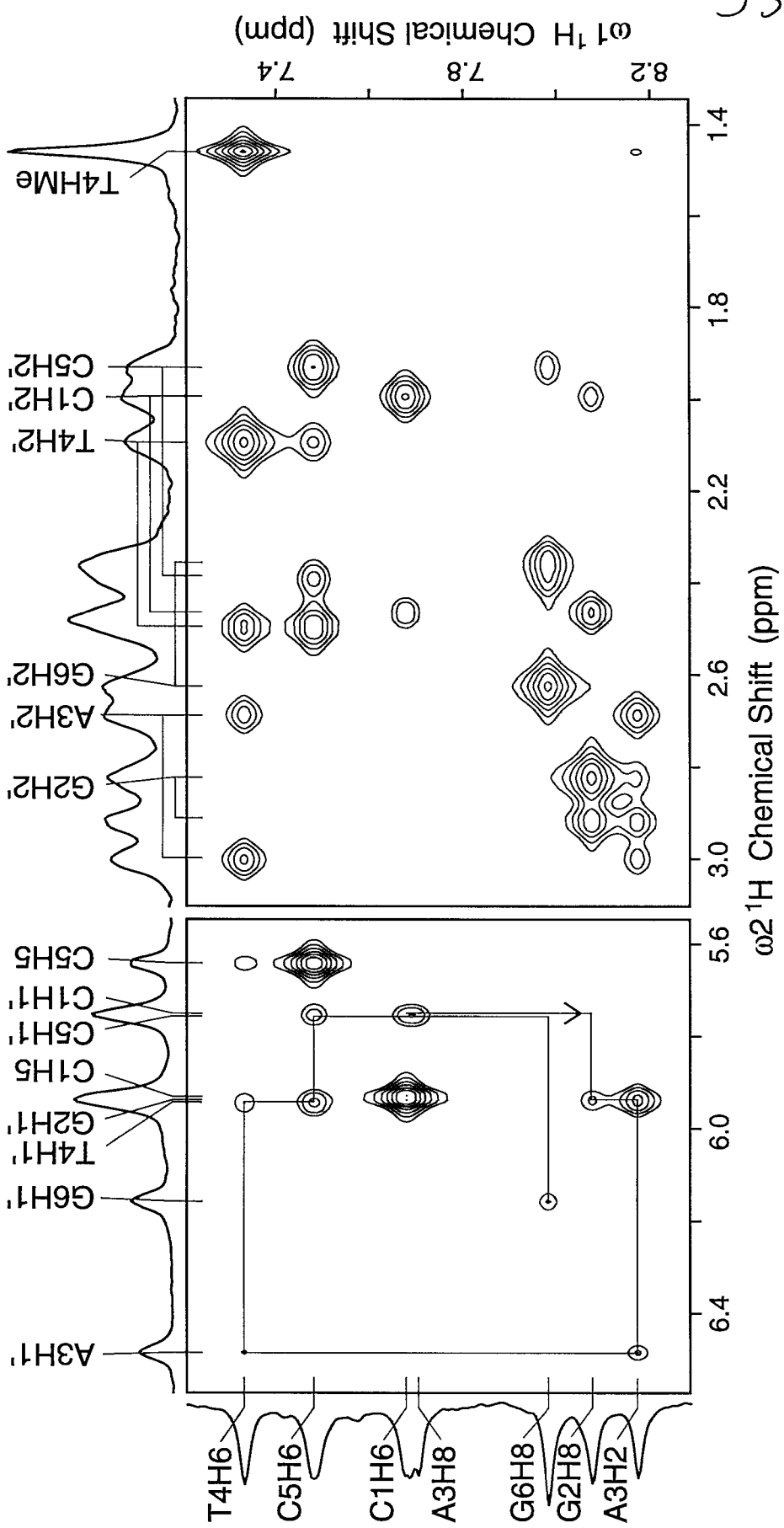

Figure 2S

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Table 1S

Chemical Shifts (ppm) for d(CGATCG)$_2$ at 2°C

	H5/Me /H2	H8/6	H1'	H2'	H2"	H3'	H4'	H5'	H5"	H1/3	H2/4 /6(a)	H2/4 /6(b)
C 1	5.92	7.67	5.72	1.97	2.44	4.73	4.07	3.73	3.73		8.30	7.16
G 2		8.03	5.62	2.79	2.86	5.04	4.36	4.11	4.01	12.95	na	na
A 3	7.92	8.34	6.35	2.74	3.02	5.07	4.54	4.27	4.27		7.73	7.73
T 4	1.41	7.24	5.98	2.04	2.48	4.88	4.21	4.35	4.18	13.73		
C 5	5.61	7.52	5.73	2.03	2.41	4.86	4.15	4.19	4.08		8.65	7.13
G 6		7.99	6.19	2.65	2.36	4.70	4.21	4.10	4.10	13.22	na	na

H2/4/6(a) are base-pair hydrogen bonded amino protons, H2/4/6(b) are not.

Chemical Shifts (ppm) for d(CG[iA]TCG)$_2$ at 2°C

	H5/Me /H2	H8/6	H1'	H2'	H2"	H3'	H4'	H5'	H5"	H1/3	H2/4 /6(a)	H2/4 /6(b)
C 1	5.93	7.68	5.76	2.00	2.47	4.75	4.07	3.74	3.74		8.31	7.17
G 2		8.07	5.94	2.83	2.92	5.06	4.42	4.15	4.04	12.87	na	na
A 3	8.17	7.70	6.49	2.69	3.00	4.78	4.55	4.38	4.35		8.30	6.93
T 4	1.46	7.33	5.95	2.10	2.50	4.84	4.27	4.27	4.14	14.96		
C 5	5.64	7.48	5.76	1.93	2.39	4.84	4.12	4.15	4.09		8.69	7.13
G 6		7.98	6.16	2.63	2.35	4.70	4.20	4.11	4.07	13.23	na	na

H2/4/6(a) are base-pair hydrogen bonded amino protons, H2/4/6(b) are not.

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Table 2S.
Coupling Constants in Hz for H1′-H2′ and H1′-H2″ for $d(CGATCG)_2$ and $d(CG[iA]TCG)_2$

	$d(CGATCG)_2$		$d(CG[iA]TCG)_2$	
	H1′-H2′	H1′-H2″	H1′-H2′	H1′-H2″
C1	na	6.1	8.3	7.2
G2	10.7	5.5	10.0	4.6
A3/iA3	9.2	5.9	6.9	7.2
T4	9.1	5.5	9.3	6.1
C5	na	6.4	7.4	7.3
G6	8.5	6.3	8.3	6.3