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Table S1: Backbone, Glycosidic Tosion, and Pseudorotation Phase Angles of the Final Structures.

				isomer 1					
	residue	alpha	beta	gamma	delta	epsilon	zeta	chi	phase
strand 1	C1	na	na	47.9	74.2	222.1	285.4	194.1	8.1
	G2	288.3	170.7	57.5	77.6	199.9	298.0	194.6	7.2
	C3	291.3	173.0	59.9	75.8	207.7	298.2	200.2	11.4
	G4	285.6	174.9	51.6	72.2	199.5	294.9	198.5	15.3
	A5	291.3	173.7	59.3	76.8	196.6	293.7	193.7	12.8
	A6	290.3	171.8	61.3	82.9	198.5	293.5	197.0	19.1
	T7	289.8	170.8	58.5	83.3	194.5	290.1	204.6	25.8
	T8	288.8	173.7	58.1	82.7	192.4	293.0	210.1	29.8
	C9	288.4	169.3	65.3	80.8	203.6	300.0	208.8	25.5
	G10	279.2	174.5	54.0	79.2	192.3	295.8	197.9	38.8
	C11	289.2	170.8	63.4	74.3	199.2	289.6	196.9	34.3
	G12	289.3	173.7	58.6	86.1	na	na	206.5	31.4
strand 2	C1	na	na	48.7	74.3	216.5	289.2	194.3	8.3
	G2	289.0	168.8	61.4	80.0	195.5	295.4	195.5	12.7
	C3	290.3	171.6	62.7	75.4	208.2	299.0	201.7	12.8
	G4	284.7	174.9	50.8	71.8	199.3	294.6	198.2	16.1
	A5	291.4	173.4	59.5	76.9	196.7	294.0	193.9	12.5
	A6	290.1	172.0	61.0	82.8	198.3	293.6	197.0	19.1
	T7	289.8	170.8	58.7	83.4	194.3	290.1	204.7	26.1
	T8	288.7	173.7	58.1	82.6	192.4	293.1	210.0	29.6
	C9	288.3	169.6	65.2	81.0	203.8	299.8	208.8	26.3
	G10	279.0	173.8	55.1	80.6	192.3	296.7	197.8	42.1
	C11	287.7	170.1	63.9	66.5	85.7	70.7	196.5	32.7
	G12	231.9	163.6	44.7	77.9	na	na	221.8	50.4
average		285.5	171.7	57.7	78.2	194.9	284.0	200.9	22.8
				isomer 2					
strand 1	C1	na	na	57.2	75.2	221.7	286.8	194.8	12.8
	G2	282.7	170.8	59.1	78.3	192.6	306.4	196.9	7.3
	C3	282.7	170.8	59.1	78.3	192.6	306.4	196.9	7.3
	G4	270.7	179.2	56.9	71.4	194.7	303.5	201.7	14.6
	A5	285.9	176.7	61.1	73.8	188.4	304.2	194.5	11.1
	A6	283.2	177.8	63.0	82.3	190.5	305.3	197.3	19.8
	T7	277.9	174.9	62.7	76.8	174.8	310.5	202.7	26.5
	T8	270.6	185.6	62.7	80.7	184.7	300.9	213.0	33.2
	C9	282.0	173.2	67.2	78.7	195.4	304.5	211.6	31.0
	G10	278.3	174.8	60.3	81.6	184.0	306.5	198.8	52.9
	C11	279.1	175.1	66.3	74.4	181.3	308.4	204.7	48.3
	G12	246.1	200.5	63.4	85.7	na	na	225.7	39.6
strand 2	C1	na	na	55.0	76.3	230.0	294.6	202.4	18.9
	G2	251.0	182.4	58.5	75.4	191.8	303.9	194.4	12.7
	C3	286.9	175.6	62.0	72.6	195.9	302.4	198.6	9.1
	G4	285.1	178.6	55.5	71.2	194.7	302.4	197.7	13.3
	A5	285.9	177.1	60.2	74.3	190.6	301.6	195.0	12.4
	A6	285.8	175.1	64.7	82.6	187.2	304.1	196.3	20.0
	T7	280.3	176.5	60.4	81.0	187.1	299.7	206.9	27.1
	T8	275.9	178.9	63.6	79.9	182.6	303.9	211.1	28.7
	C9	281.3	174.7	68.5	78.5	184.0	322.2	211.7	26.4
	G10	241.9	186.9	64.2	77.2	182.4	302.4	204.8	42.3
	C11	284.2	171.3	68.3	74.0	191.5	301.0	201.0	36.0
	G12	275.8	181.8	59.7	86.1	na	na	210.7	33.0
average		275.9	178.3	61.8	77.5	192.0	303.5	203.1	24.5
A-form		276	207	45	84	179	310	205	13
B-form		313	213	36	156	154	264	262	191

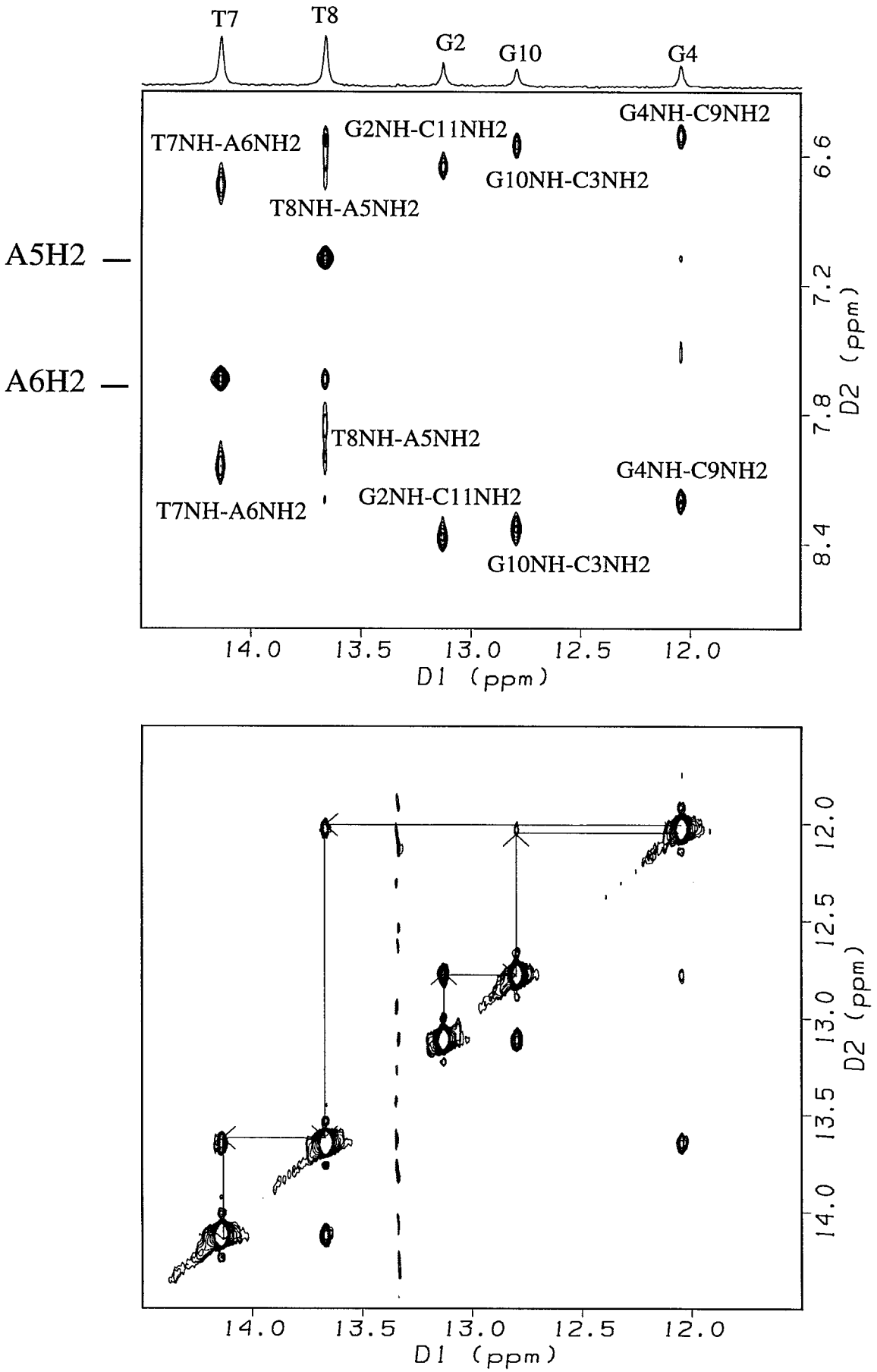

FIGURE S1 Watergate NOESY spectra of N3' -> P5' phosphoramidate DNA at 2 ^{o}C in *90% H2O/ 10% D2O*, imino to imino (top) and imino to aromatic (bottom) proton regions.

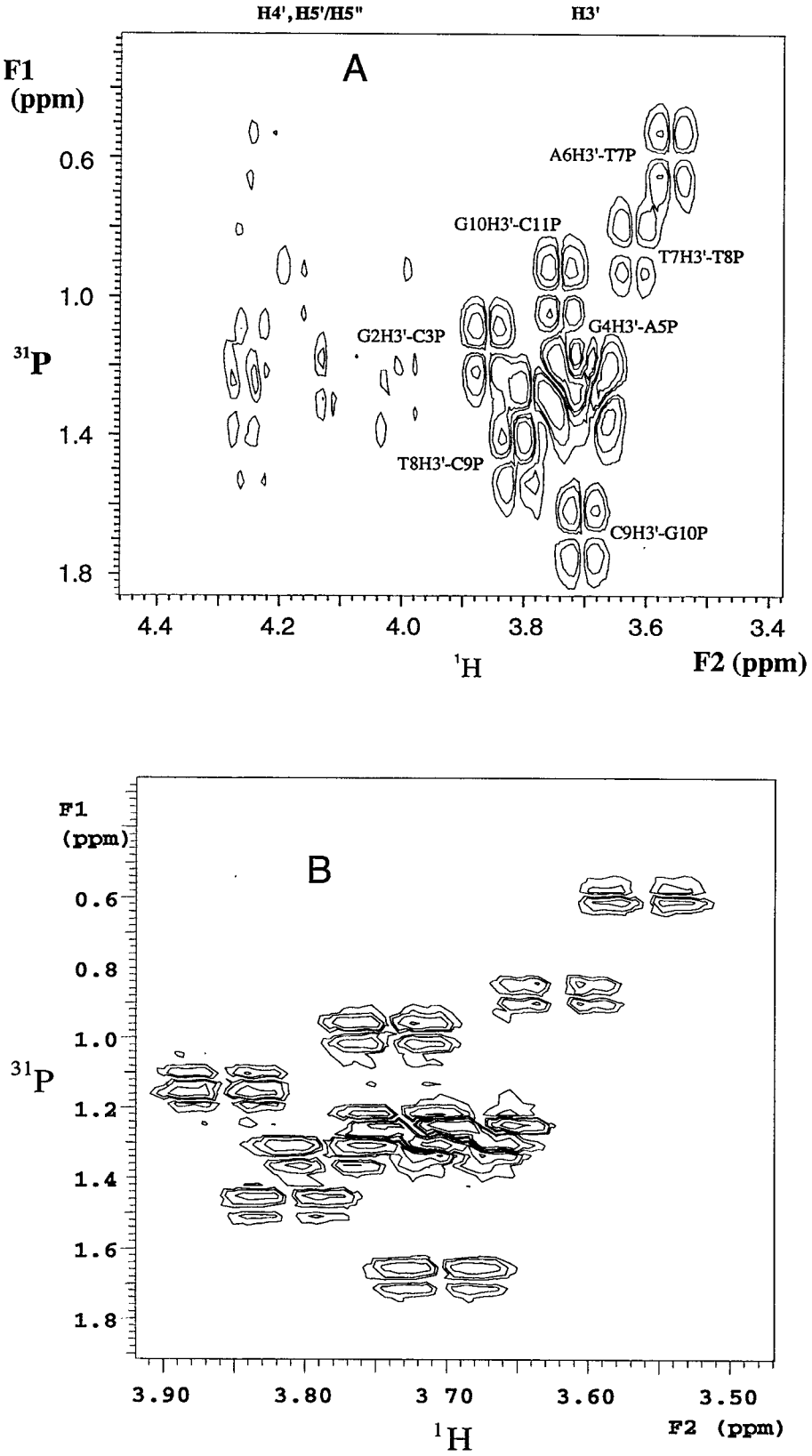

FIGURE S2. Phosphorus-proton (A) and selective (B) heteronuclear correlation spectra of N3'-> P5' phosphoramidate DNA at 25 ^{o}C. Phosphorus chemical shift assignments are based on connections to H3' protons, and are referenced to TMP.

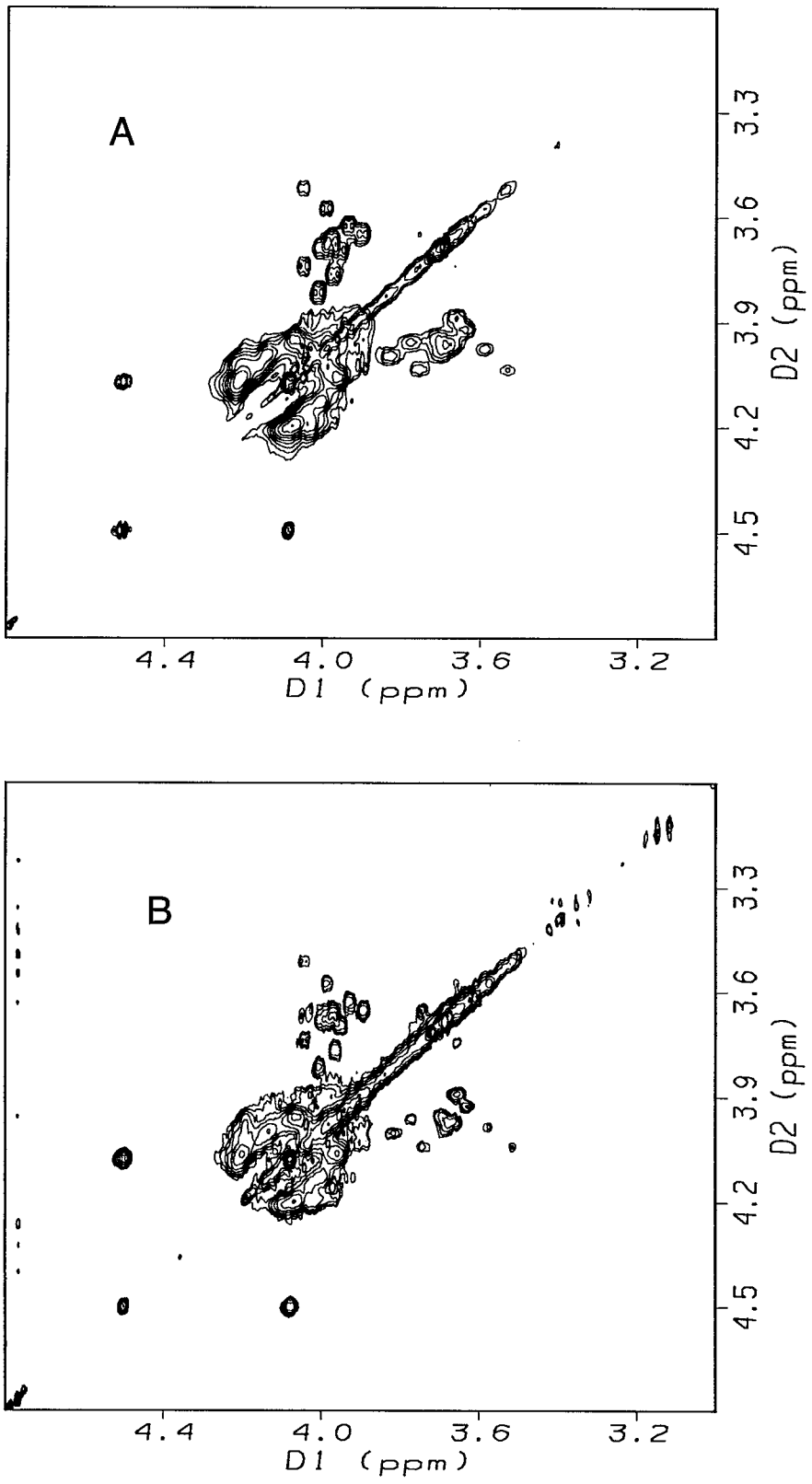

FIGURE S3. The TOCSY spectra of N3' -> P5' phosphoramidate (CGCGAATTCGCG) with the mixing times of 40 ms (A) and 120 ms (B) at 25 °C.