

Supporting Information

Probing the sequence effects on *NarI*-induced -2 frameshift mutagenesis by dynamic ^{19}F NMR, UV and CD spectroscopy

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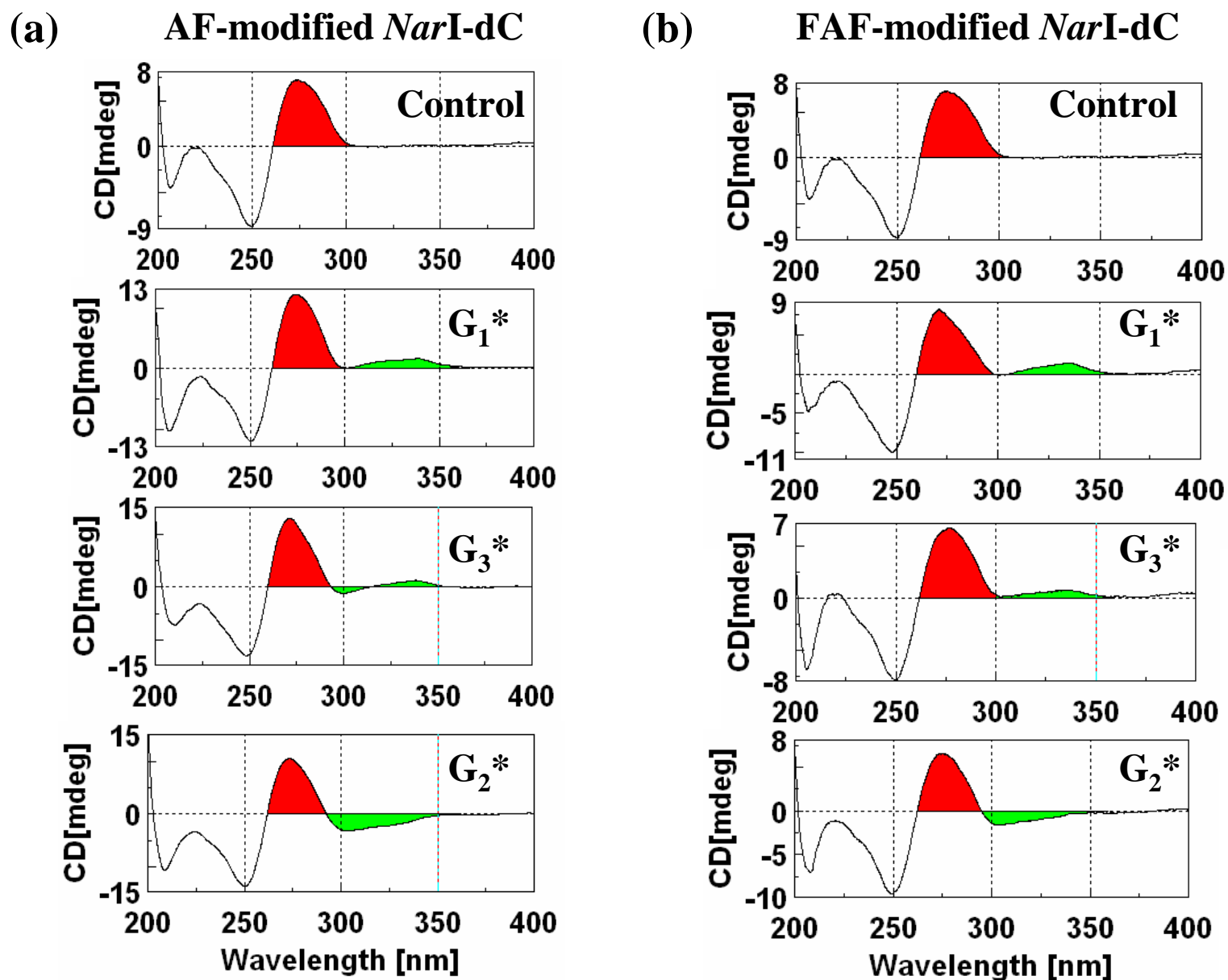


Figure S1. CD spectra of *NarI*-dC duplexes recorded at 15 °C for (a) the AF- and (b) FAF-modified duplex series (G^* denotes adduct site). See Figure 1 for structure and sequence details. The carcinogen-induced ellipticities in the 290-360 nm range ($ICD_{290-360nm}$) are highlighted with green.

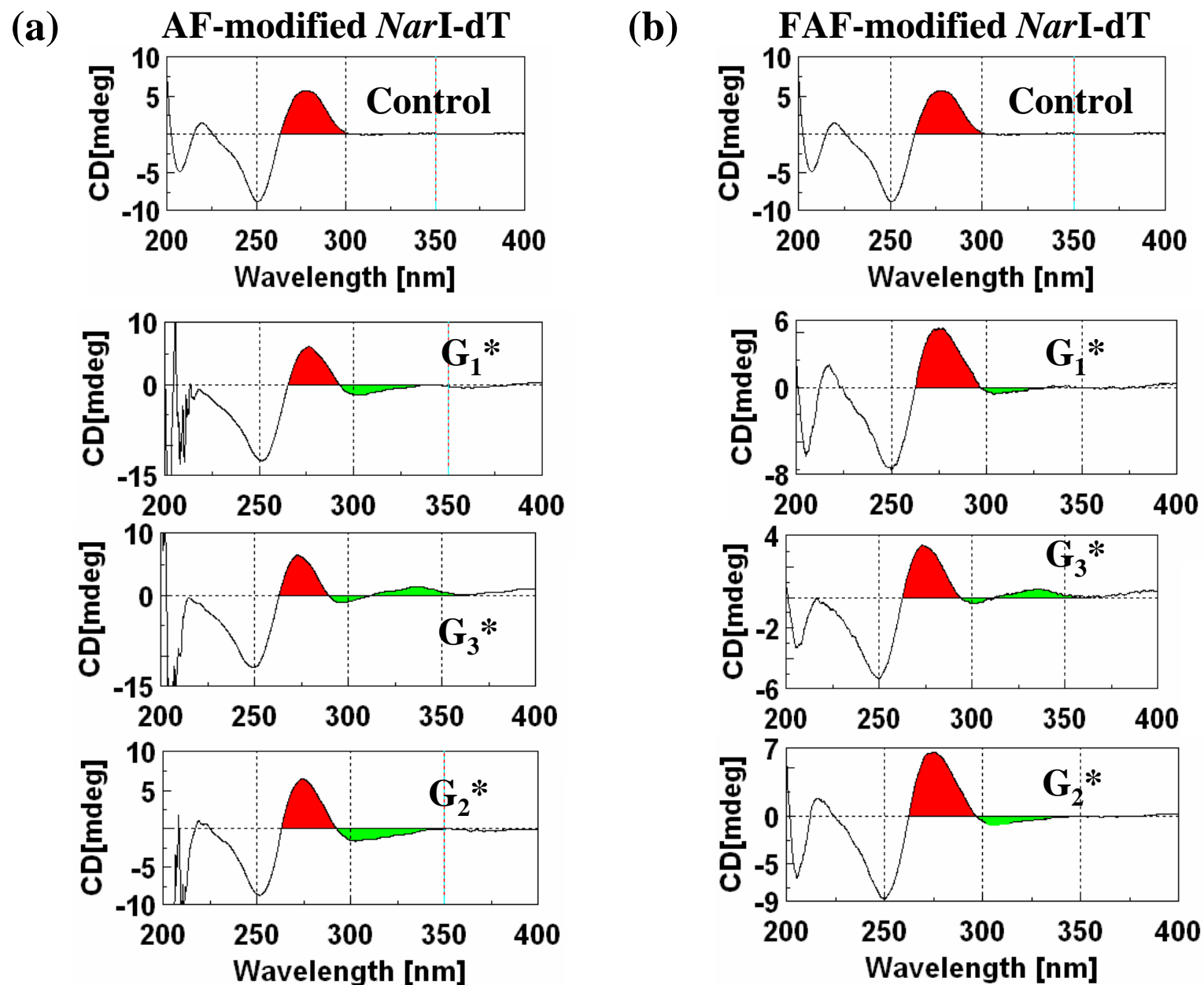
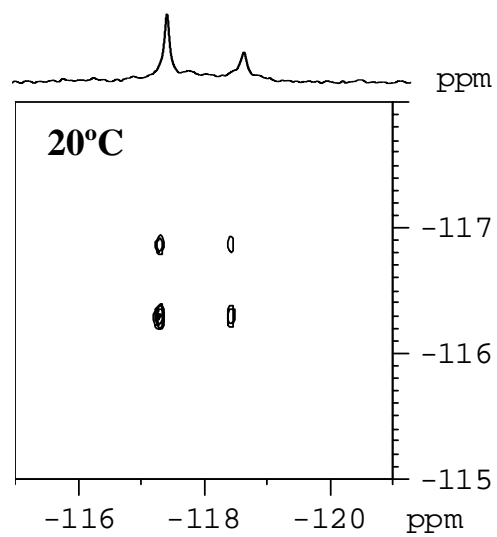


Figure S2. CD spectra of *NarI*-dT duplexes recorded at 15 °C for (A) the AF- and (B) FAF-modified series (G^* denotes adduct site). See Figure 1 for structure and sequence details. The carcinogen-induced ellipticities (either positive or negative) in the 290-360 nm range are highlighted with green.

(a)

CTCGG*CGCCATC
GAGCC GCGGTAG



(b)

CTCGG*CGCTATC
GAGCC GCGATAG

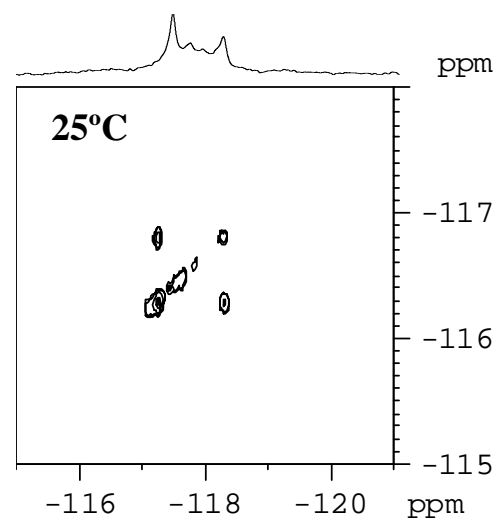


Figure S3. Examples of NOESY contour spectra: G2-FAF-modified (a) *NarI*-dC at 20°C (b) *NarI*-dT at 25°C.

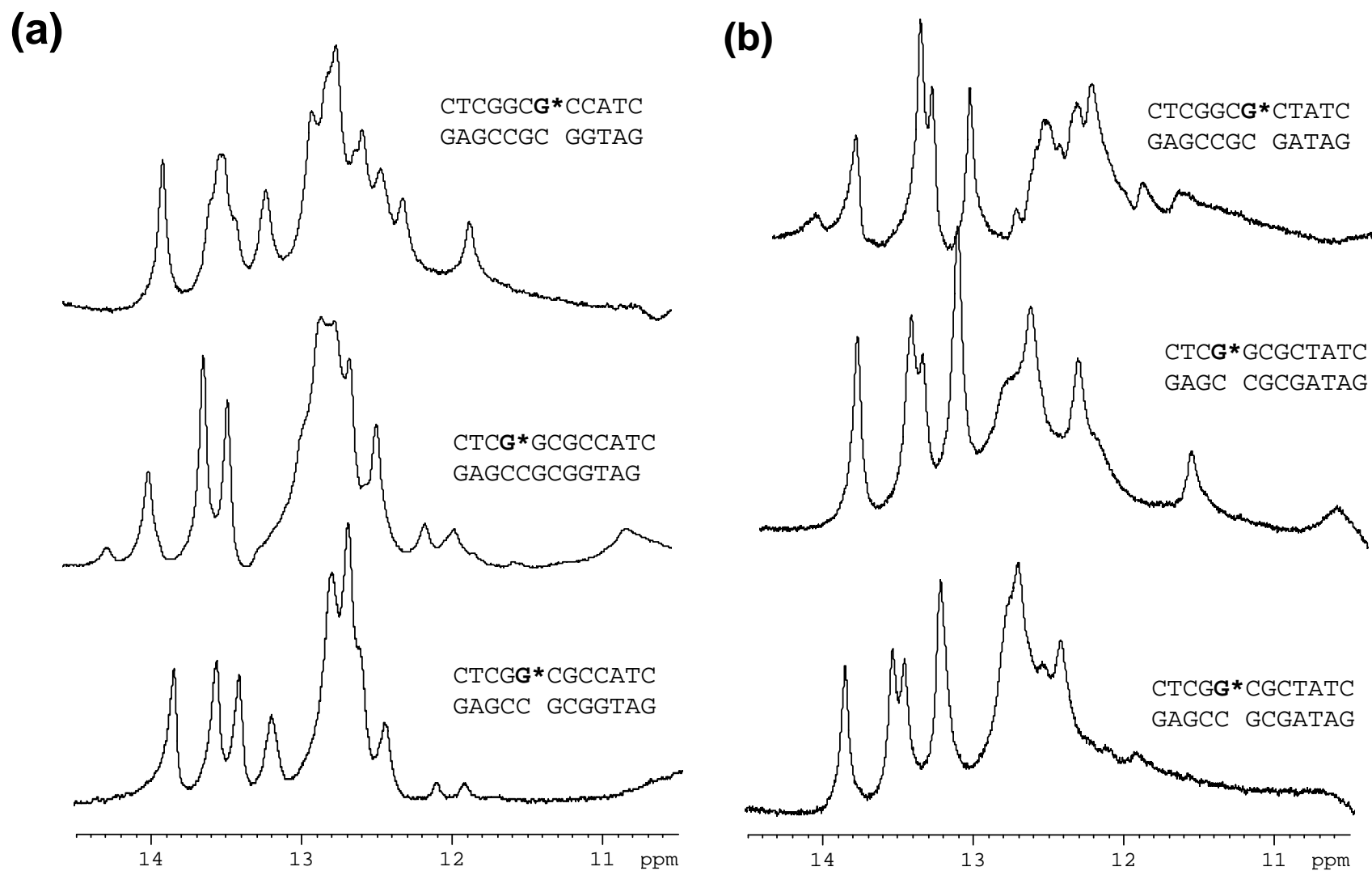


Figure S4. Imino proton spectra of fully-paired FAF-modified (a) *NarI*-dC and (b) *NarI*-dT duplexes recorded at 5° C

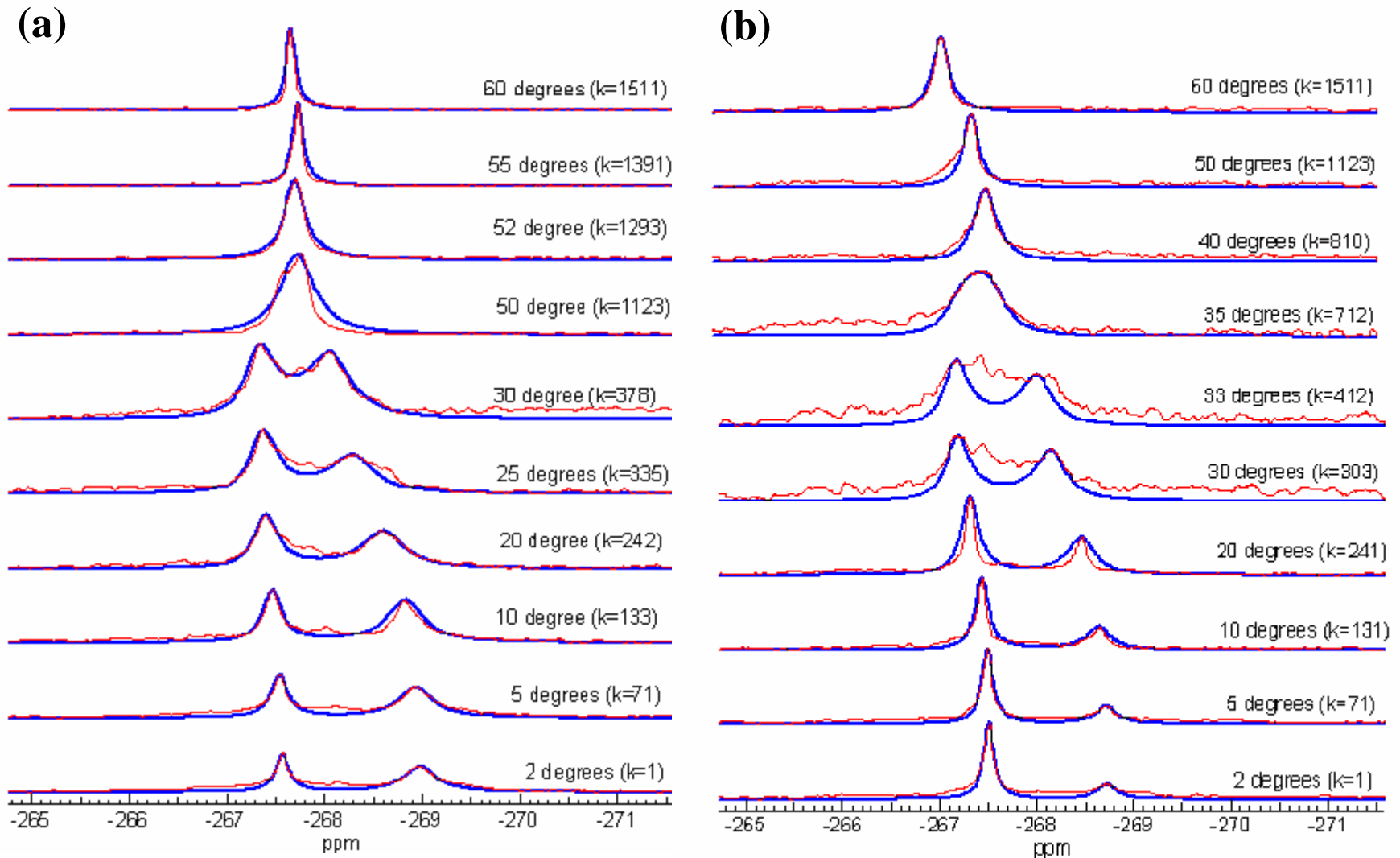


Figure S5. Complete line shape analysis of dynamic NMR spectra of (a) *NarI*-dC/G1 and (b) *NarI*-dC/G2 duplexes.

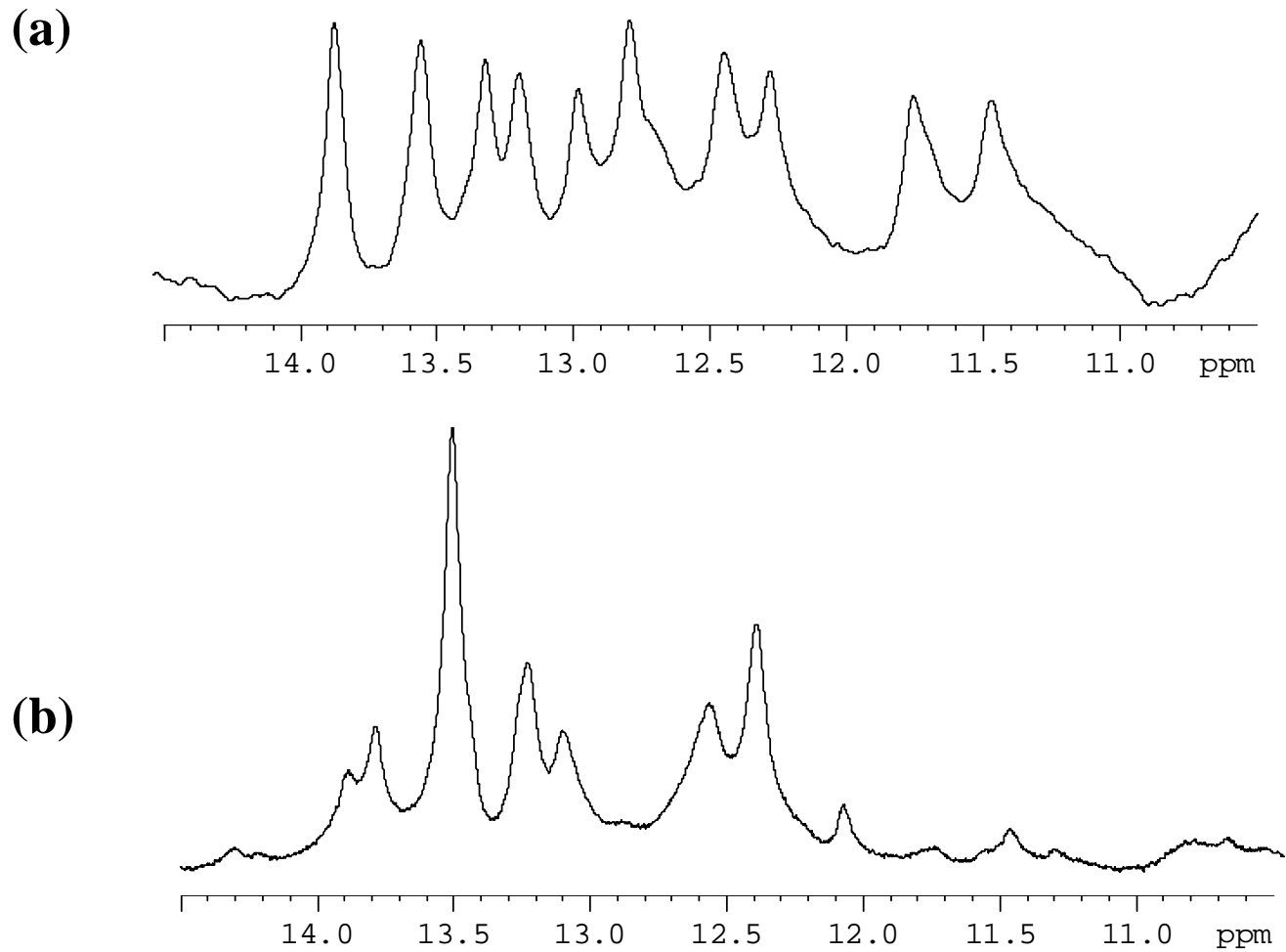


Figure S6. Imino proton spectra of (a) *NarI*-dC/-2 and (b) *NarI*-dT/-2 deletion duplexes recorded at 5 °C.

Table S1: Calculated and measured molecular weights for the AF- and FAF-modified 12-mer *NarI* sequences used in this study.

Sample	Sequence	Calculated Mass	Measured Mass
<i>NarI</i> -dC-G3[AF]	CTCGGCG(AF)CCATC	3,759.70	3,759.69
<i>NarI</i> -dC-G1[AF]	CTCG(AF)GCGCCATC	3,759.70	3,759.68
<i>NarI</i> -dC-G2[AF]	CTCGG(AF)CGCCATC	3,759.70	3,759.69
<i>NarI</i> -dT-G3[AF]	CTCGGCG(AF)CTATC	3,792.69	3,792.70
<i>NarI</i> -dT-G1[AF]	CTCG(AF)GCGCTATC	3,792.69	3,792.66
<i>NarI</i> -dT-G2[AF]	CTCGG(AF)CGCTATC	3,792.69	3,792.68
<i>NarI</i> -dC-G3[FAF]	CTCGGCG(FAF)CCATC	3,777.69	3,777.69
<i>NarI</i> -dC-G1[FAF]	CTCG(FAF)GCGCCATC	3,777.69	3,777.70
<i>NarI</i> -dC-G2[FAF]	CTCGG(FAF)CGCCATC	3,777.69	3,777.66
<i>NarI</i> -dT-G3[FAF]	CTCGGCG(FAF)CTATC	3,792.69	3,792.65
<i>NarI</i> -dT-G1[FAF]	CTCG(FAF)GCGCTATC	3,792.69	3,792.64
<i>NarI</i> -dT-G2[FAF]	CTCGG(FAF)CGCTATC	3,792.69	3,792.67

Table S2: Summary of the H/D Isotope effects for fully-paired and -2 deletion FAF-modified *NarI*-dC and *NarI*-dT duplexes^a

Duplex	¹⁹ FNMR δ in 90% H ₂ O/10% D ₂ O buffer at 20 ° C (ppm)	¹⁹ FNMR δ in 100% D ₂ O buffer at 20 ° C (ppm)	$\Delta\delta$ (ppm) ^b
<i>NarI</i> -dC/G3[FAF]	-117.33	-117.52	0.19
	-118.73	-118.80	0.07
<i>NarI</i> -dC/G1[FAF]	-117.38	-117.66	0.28
	-118.51	-118.74	0.18
<i>NarI</i> -dC/G2[FAF]	-117.30	-117.52	0.22
	-118.40	-118.51	0.11
<i>NarI</i> -dT/G3[FAF]	-117.46	-117.76	0.30
	-118.85	-118.99	0.14
<i>NarI</i> -dT/G1[FAF]	-117.45	-117.64	0.19
	-118.21	-118.28	0.07
	-119.05	-119.09	0.04
<i>NarI</i> -dT/G2[FAF]	-117.42	-117.65	0.23
	-118.60	-118.68	0.08
<i>NarI</i> -dC/G3[FAF]/-2 del	-118.073	-118.095	0.02
<i>NarI</i> -dT/G3[FAF]/-2 del	-116.47	-116.51	0.04
	-117.79	-117.94	0.15
	-119.19	-119.23	0.04

^aThe rationale for the H/D isotope effect is that the ¹⁹F resonance of the exposed FAF residue in a B-conformer should be more susceptible to solvent-induced shielding (usually > 0.2 ppm) than the buried FAF in an S-conformer (in most cases < 0.1 ppm) when the deuterium content is increased from 10 to 100% (9). ^b δ in H₂O buffer – δ in D₂O buffer at 20°C (ppm).