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Supporting Information

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for

An Alternative Nucleobase Code: Characterization of Purine·Purine DNA Double Helices Bearing Guanine·iso-Guanine and Diaminopurine 7-Deaza-Xanthine Base-Pairs
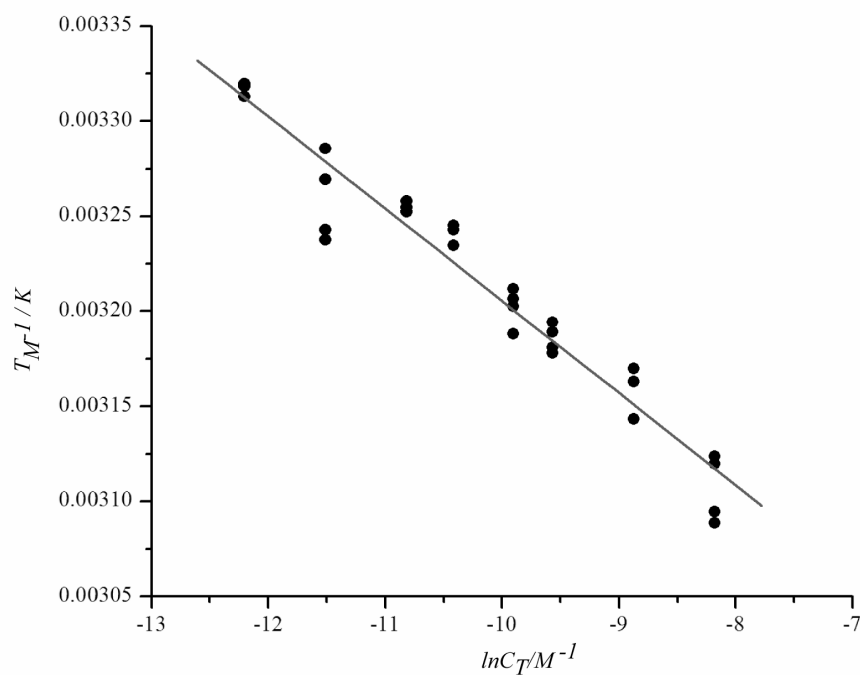
Benjamin D. Heuberger, and Christopher Switzer*

Figure S1. Van't Hoff plot with linear regression analysis for duplex **1**×**2** in 1.0 M NaCl, 10 mM NaH$_2$PO$_4$, pH 7.0.
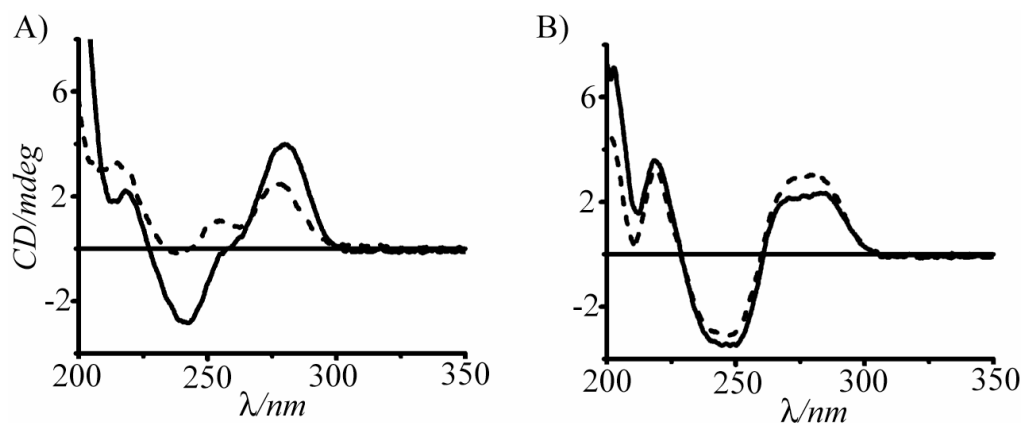
Figure S2. Circular dichroism spectra: A) **7•8**, B) **3•4**; solid line = 25 μM duplex, 1.0 M NaCl, 10 mM NaH$_2$PO$_4$, pH 7.0; dashed line = 25 μM duplex, 10 mM NaH$_2$PO$_4$, pH 7.0.
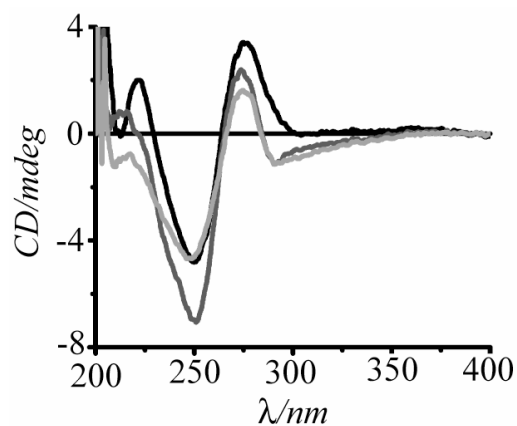

Figure S3. Circular dichroism spectra: Black = **11•12**, medium gray = **16•17**, light gray = **20•21**; 2.5 μM duplex, 1.0 M NaCl, 10 mM NaH$_2$PO$_4$, pH 7.0.

Table S1. MALDI-ToF data for oligonucleotides.

	Sequence[a]	Calculated mass	MALDI found
1	5'-diGDDiGDiGiGD-3'	2566.5	2566.9
2	5'-dXGGXGXXG-3'	2570.4	2572.4
5	5'-dGDDGDGGD-3'	2566.5	2566.6
6	5'-dXiGiGXiGXXiG-3'	2570.4	2571.3
9	5'-diGGXGDiGDX-3'	2568.5	2569.4
10	5'-dDXGXiGDiGG-3'	2568.5	2569.5
13	5'-diGX(G*)iGDiGX(G*)XDXG-3'	3882.6	3882.2
14	5'-diGDXDiGD(G*)X(G*)iGDG-3'	3880.7	3882.3
15	5'-diGAXAiGA(G*)X(G*)iGAG-3'	3820.7	3821.5
18	5'-diGD(G*)XDXiGG-3'	2567.5	2568.9
19	5'-diG(G*)DXDiGXG-3'	2567.5	2568.7

[a] X = 7-deaza-X; G* = 7-deaza-G