

# Supporting Information

## Conformational Preferences of DNA in Reduced Dielectric Environments

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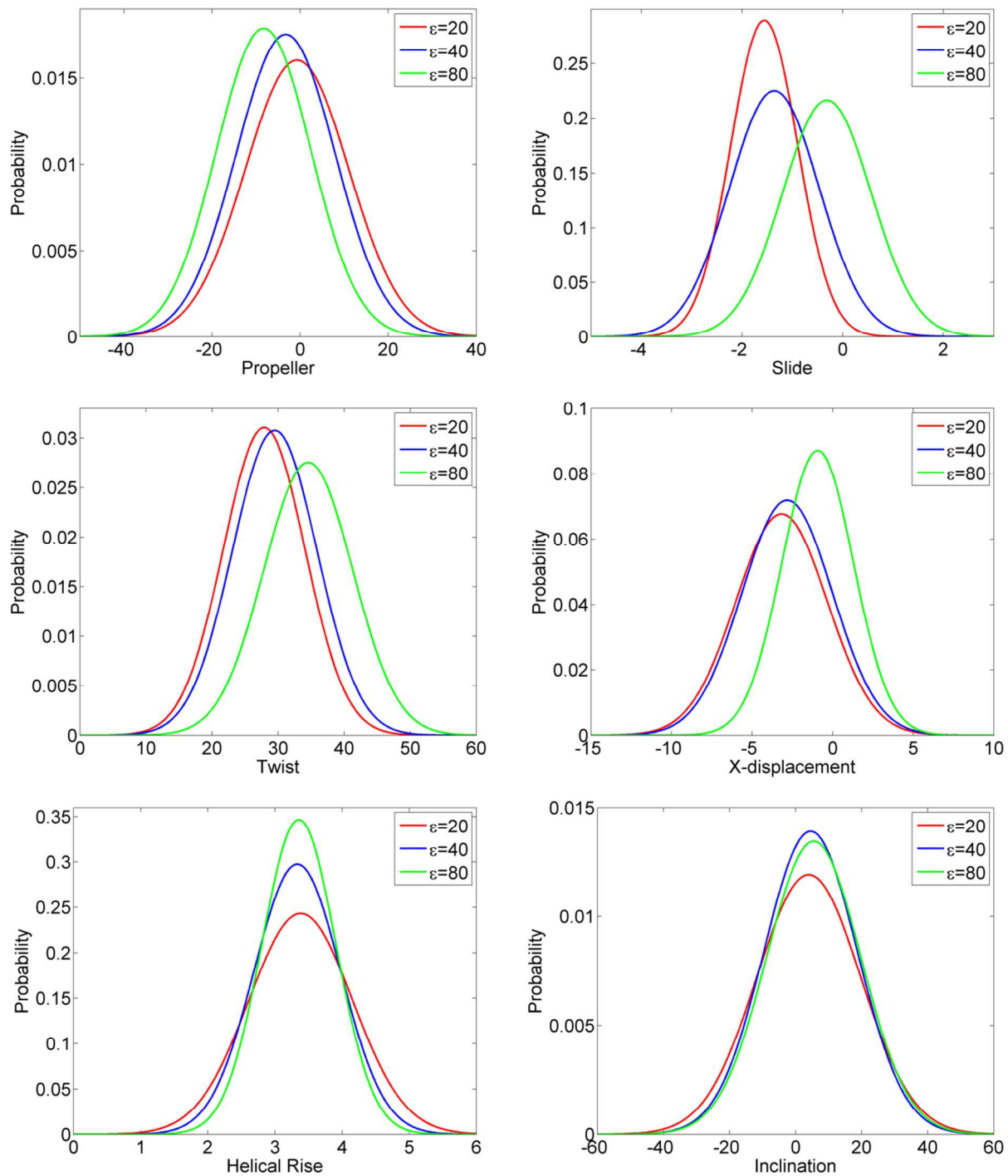
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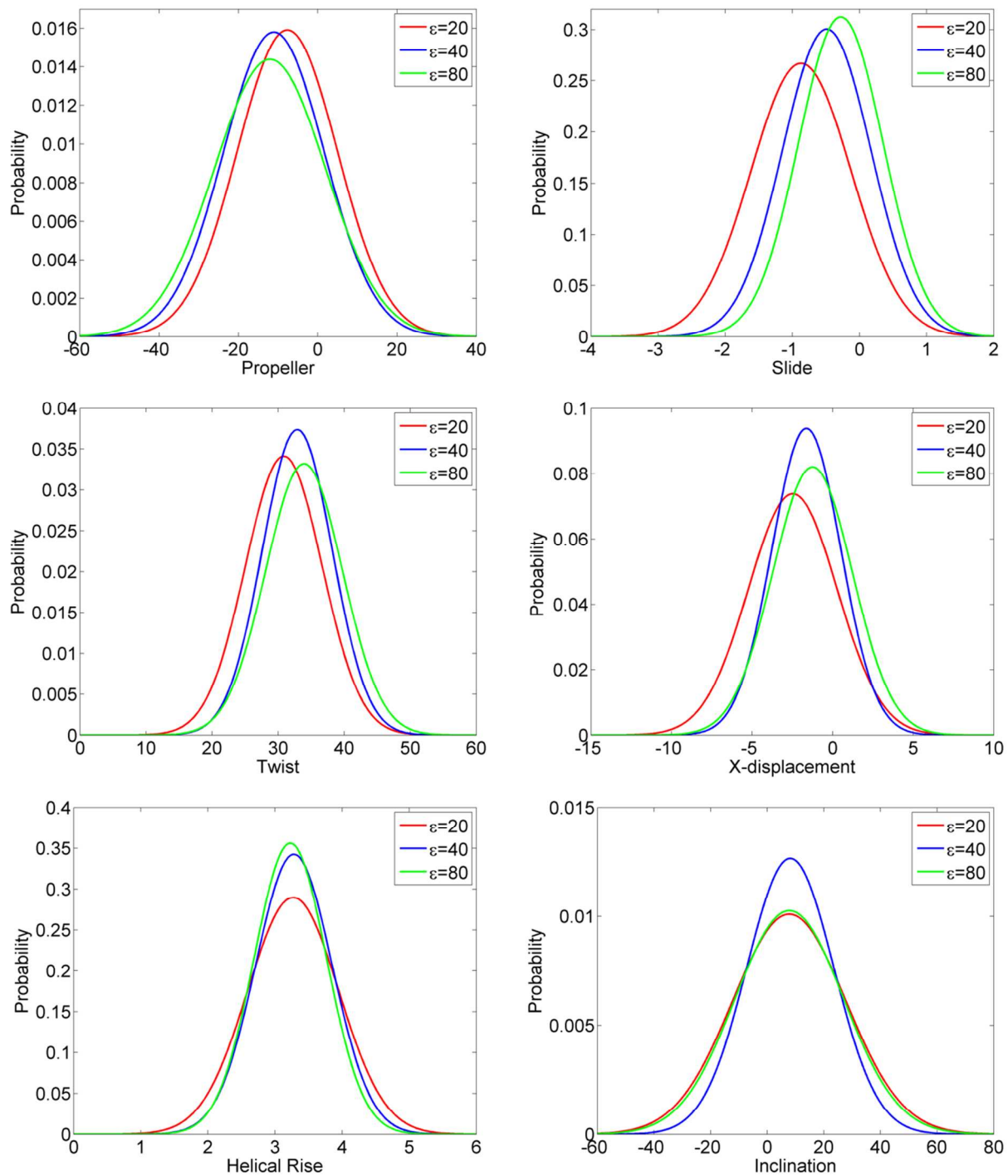
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**Figure S1.** Distributions of helical parameters for the GC-rich dodecamer in different dielectric environments with  $\epsilon=20$  (red), 40 (blue) and 80 (green).



**Figure S2.** Distributions of helicoidal parameters for the Drew-Dickerson dodecamer in different dielectric environments with  $\epsilon=20$  (red), 40 (blue) and 80 (green).

**Table S1.** Helicoidal Parameters for GC1, GC2, GC5 clusters compared to canonical A-, B- and C-DNA forms

	<b>A-DNA</b>	<b>B-DNA</b>	<b>C-DNA<sup>a</sup></b>	<b>GC1</b>	<b>GC2</b>	<b>GC5</b>
<b>Propeller</b>	-9.00 (7.08)	-11.72 (5.77)	-2.01	-2.67 (11.77)	-1.78 (9.73)	-8.07 (10.89)
<b>Slide</b>	-1.67 (0.42)	0.17 (0.68)	0.09	-1.23 (0.50)	-1.90 (0.45)	-0.21 (0.61)
<b>Twist</b>	30.24 (4.02)	34.81 (5.66)	38.06	30.55 (5.23)	27.48 (5.33)	34.11 (5.86)
<b>X-displacement</b>	-4.54 (1.26)	-0.13 (1.09)	0.82	-2.62 (2.29)	-3.95 (2.23)	-0.88 (1.71)
<b>H-rise</b>	2.77 (0.52)	3.25 (0.16)	3.31	3.40 (0.71)	3.46 (0.77)	3.39 (0.51)
<b>Inclination</b>	16.00 (10.68)	4.01 (6.74)	-8.07	3.22 (14.77)	1.65 (13.63)	4.85 (12.22)
<b>Minor Groove</b>	9.92 (0.72)	10.77 (0.91)	10.6	14.9 (0.37)	15.49 (0.42)	13.77 (1.20)
<b>Major Groove</b>	7.14 (2.38)	17.14 (0.93)	16.1	20.60 (0.90)	21.70 (0.92)	18.04 (1.25)

<sup>a</sup>Parameters are calculated for canonical C-DNA form using 3DNA program package.

**Table S2.** Helicoidal Parameters for DD1, DD2, DD3 clusters compared to canonical A-, B- and C-DNA forms

	<b>A-DNA</b>	<b>B-DNA</b>	<b>C-DNA<sup>a</sup></b>	<b>DD1</b>	<b>DD2</b>	<b>DD3</b>
<b>Propeller</b>	-9.00 (7.08)	-11.72 (5.77)	-2.01	-9.65 (10.93)	-5.32 (12.00)	-12.23 (12.33)
<b>Slide</b>	-1.67 (0.42)	0.17 (0.68)	0.09	-0.64 (0.50)	-1.04 (0.72)	-0.41 (0.52)
<b>Twist</b>	30.24 (4.02)	34.81 (5.66)	38.06	32.47 (4.81)	30.41 (6.21)	34.12 (4.85)
<b>X-displacement</b>	-4.54 (1.26)	-0.13 (1.09)	0.82	-1.80 (2.05)	-2.55 (2.84)	-1.12 (2.05)
<b>H-rise</b>	2.77 (0.52)	3.25 (0.16)	3.31	3.23 (0.56)	3.22 (0.71)	3.21 (0.49)
<b>Inclination</b>	16.00 (10.68)	4.01 (6.74)	-8.07	7.03 (17.42)	5.38 (20.32)	4.20 (18.65)
<b>Minor Groove</b>	9.92 (0.72)	10.77 (0.91)	10.6	14.42 (0.52)	14.86 (0.42)	13.74 (0.58)
<b>Major Groove</b>	7.14 (2.38)	17.14 (0.93)	16.1	19.16 (0.93)	21.38 (1.16)	18.23 (0.90)

<sup>a</sup>Parameters are calculated for canonical C-DNA form using 3DNA program package.