Supporting Information for

Machine Learning Prediction of Electronic Coupling between the Guanine Bases of DNA

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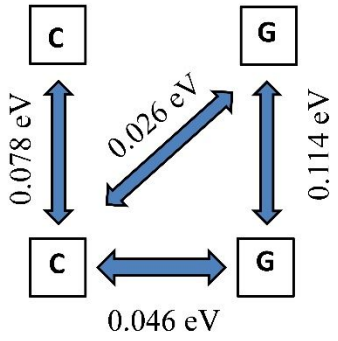

Figure S1: The root means square electronic coupling between the bases of the DNA with the sequence d(GGGG).

Structural Parameters	**Ranges in our Data set**	**Average Values for B DNA**
Twist	11.93° to 54.01°	33.75°
Buckle	-29.78° to 52.16°	-1.90°
Propeller	-34.37° to 38.36°	-7.17°
Helical Twist	13.1° to 53.89°	34.15°
Inclination Angle	-10.09° to 37.64°	6.33°
Tip	-11.61° to 24.66°	-0.33°
Roll	-15.66° to 28.78°	3.58°
Tilt	-14.75° to 18.07°	0.31°
Shift	-1.98 Å to 3.24 Å	0.12 Å

Slide	-2.21 Å to 3.32 Å	0.11 Å
Stretch	-0.37 Å to 1.61 Å	0.02 Å
Stagger	-1.34 Å to 1.88 Å	-0.02 Å
Shear	-0.8 Å to 4.07 Å	-0.008 Å
Helical rise	1.37 Å to 4.93 Å	3.34 Å
X-Displacement	-2.51 Å to 3.77 Å	-0.81 Å
Y-Displacement	-2.84 Å to 3.45 Å	-0.13 Å
Rise	2.19 Å to 4.94 Å	3.38 Å

Table S1: Ranges of DNA structural parameters in our dataset. The average values of these parameters for the B DNA are also quoted for comparison.

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