Electronic Supplementary Material (ESI) for RSC Advances.

Supporting information

Ionic Liquid Prolongs DNA Translocation through Graphene Nanopore

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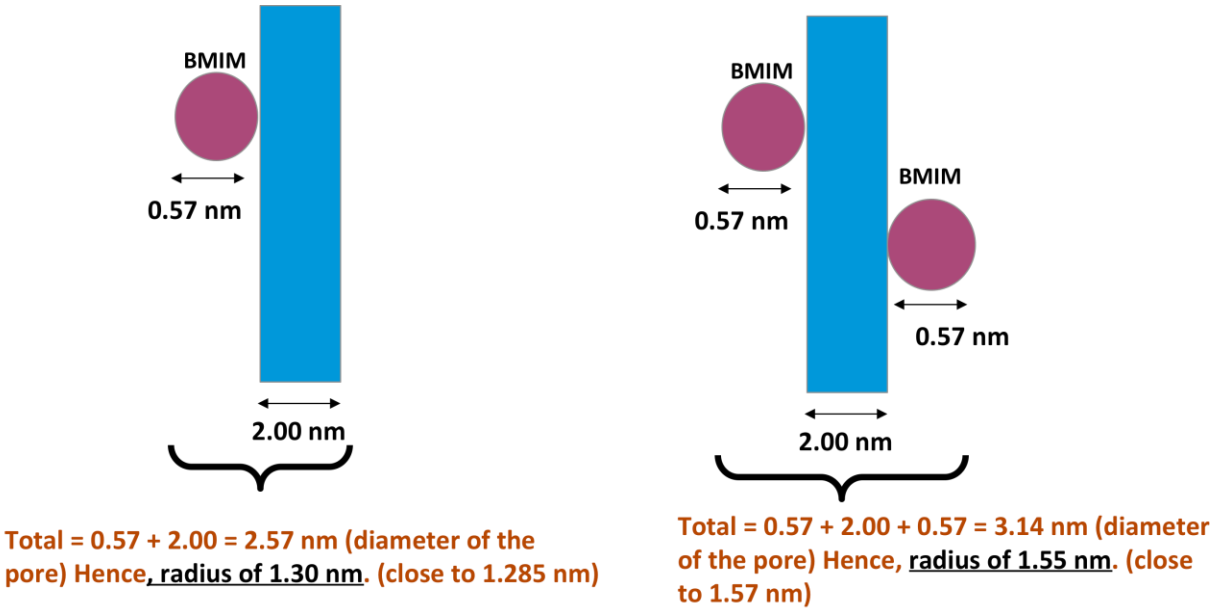

Figure S1. Schematic diagram showing choice of pore radius based on DNA and BMIM ion size.

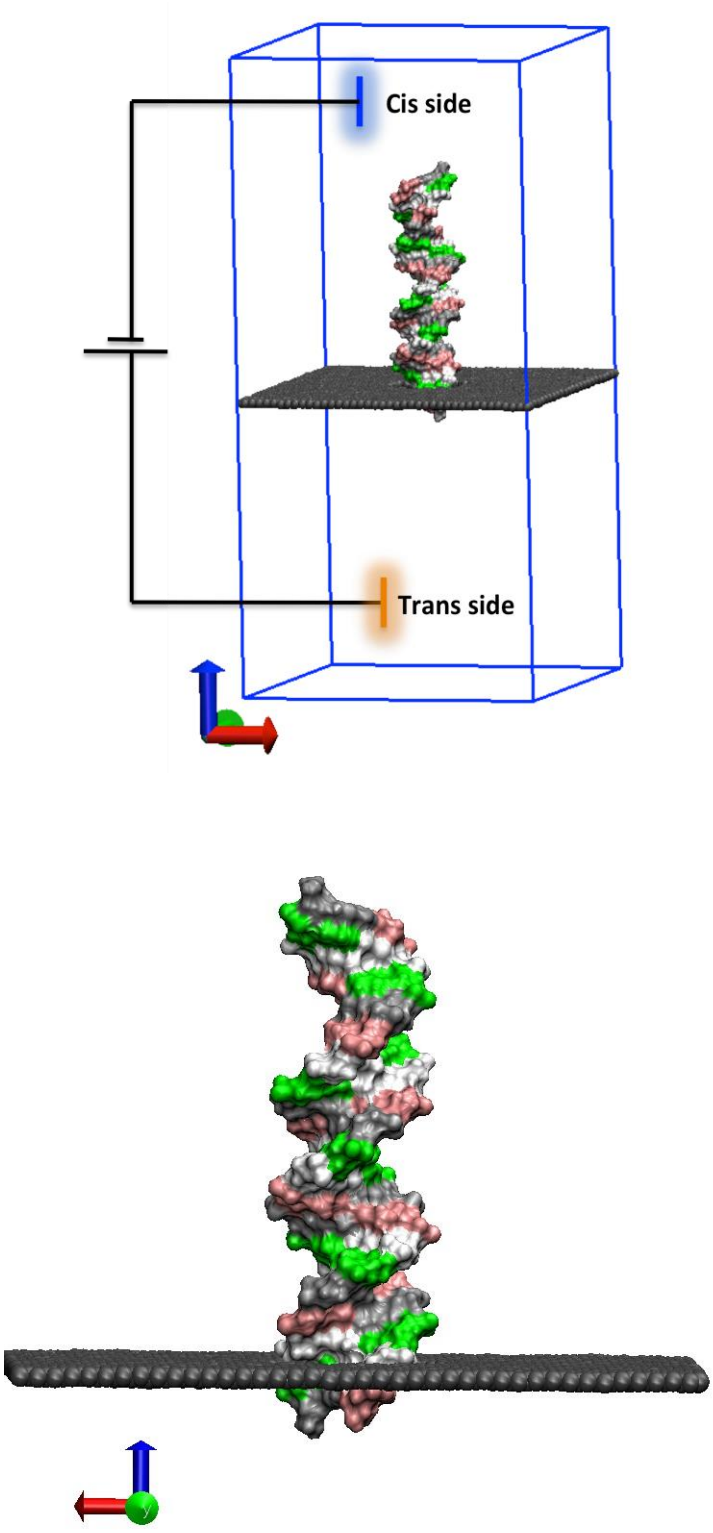

Figure S2. Snapshots showing initial configuration. Bottom panel is a zoomed view of the top panel.

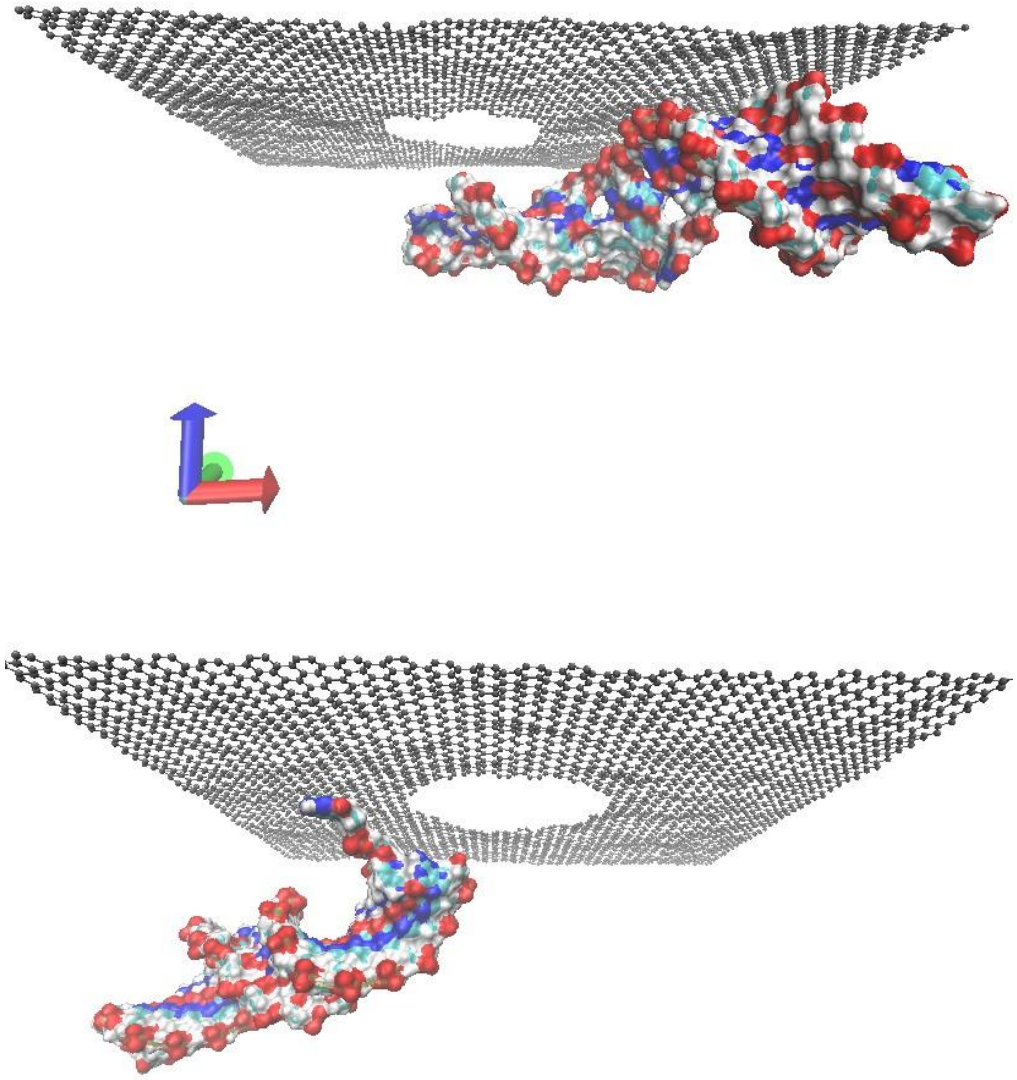

Figure S3. Configuration showing dG_{20} stuck to graphene surface for nanopore of 2.6 nm diameter and voltage of 0.05 V/nm.

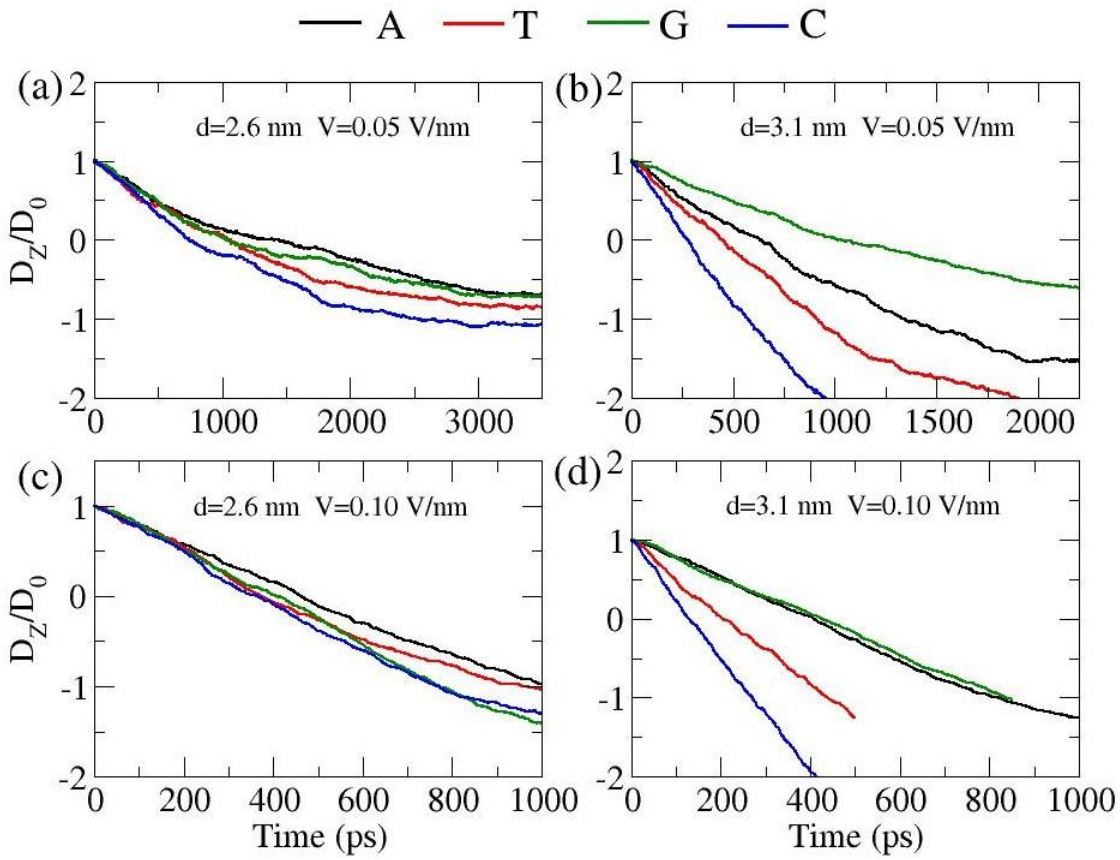

Figure S4. The Z-component of DNA movement ($D_!$) is normalized by its value at t=0 ($D_!$). We have plotted normalized movement ($\emptyset_!$ $D_!$) in all cases. The normalized DNA COM movements for polynucleotide systems (a) Diameter (d) = 2.6 nm, V=0.05 V/nm; (b) d =3.1 nm, V=0.05 V/nm; (c) d=2.6 nm, V=0.10 V/nm; (a) R=3.1 nm, V=0.10V/nm. Color indicators: A- black, T- red, G- green, C- blue.

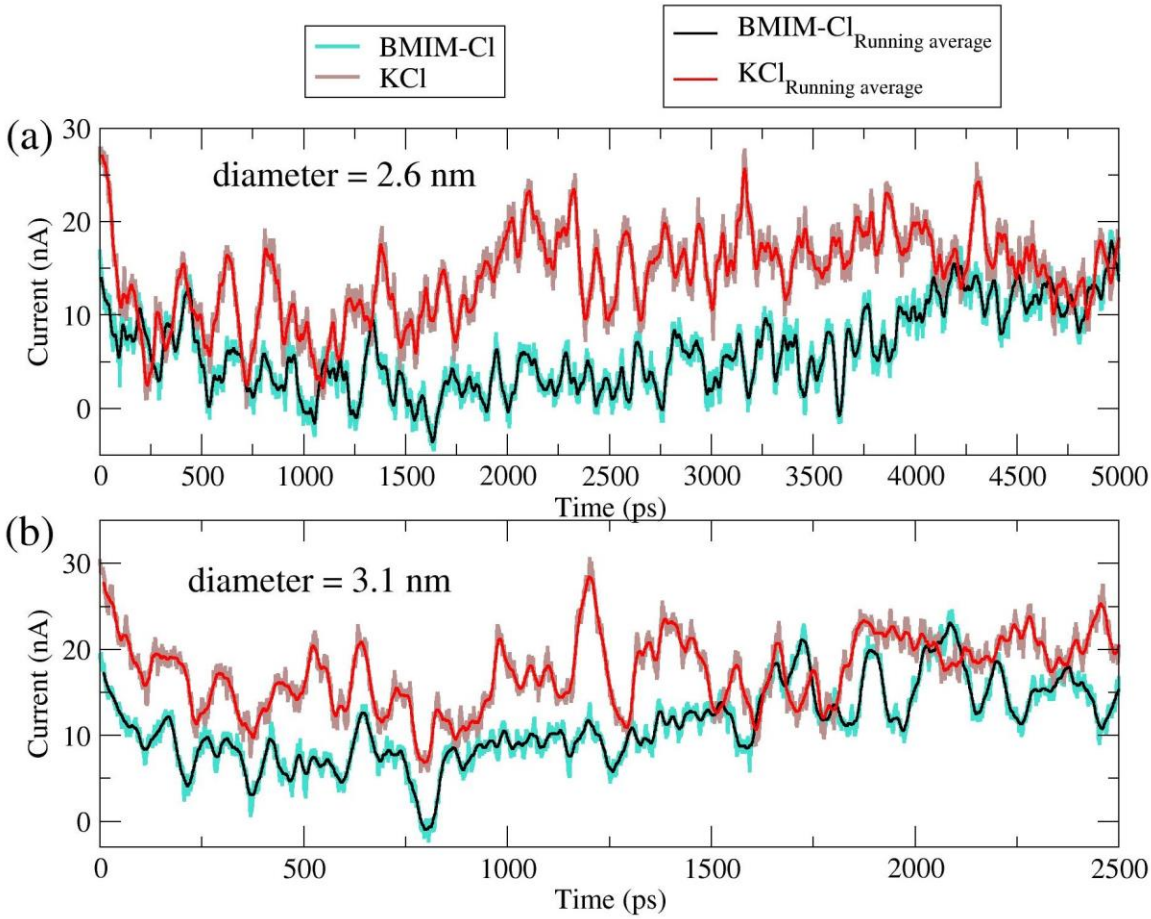

Figure S5. The current values for DNA translocation in case of (a) smaller nanopore (d =2.6 nm) and (b) larger nanopore (d=3.1 nm) using lag value of 50 ps in the presence of KCl (brown line) and BMIM-Cl (turquoise line). The running average are plotted for KCl (Red line) and BMIM-Cl simulations (Black line) to visually observe number of blockade events.

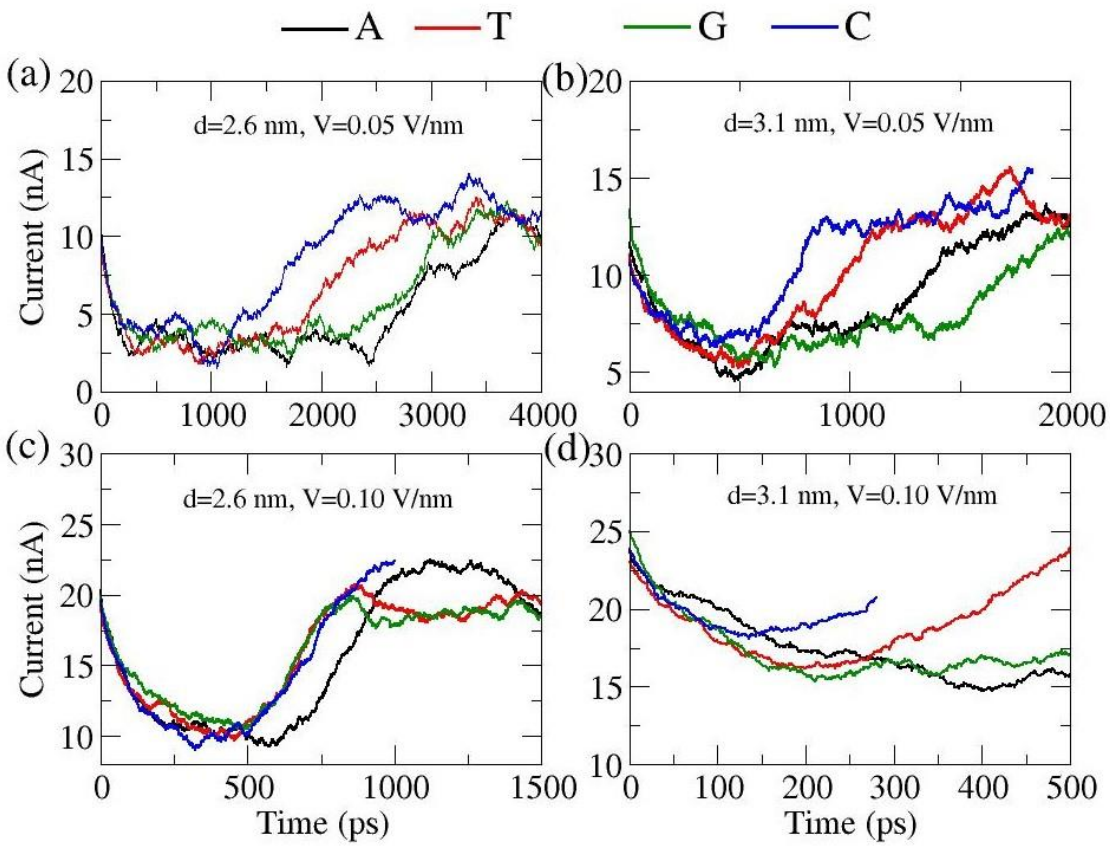

Figure S6. Ionic current of BMIM-Cl using lag of 250 ps for polynucleotide systems (a) Diameter (d) =2.6 nm, V=0.05 V/nm; (b) d=3.1 nm, V=0.05 V/nm; (c) d =2.6 nm, V=0.10 V/nm; (a) d=3.1 nm, V=0.10V/nm. Color indicators: A- black, T- red, G- green, C- blue.

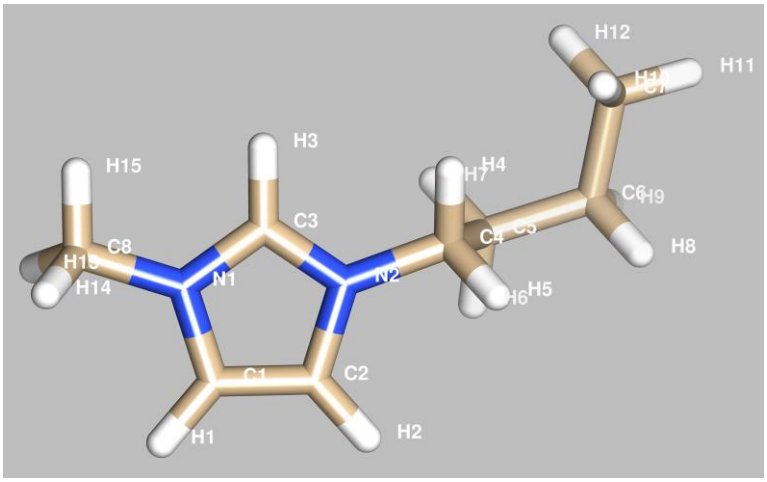

Figure S7. Structure of $BMIM^{+}$ cation

Table S1. Table showing details of the systems and simulations performed in this study.

Simulation ID	Sequence	Electrolyte	Voltage (V/nm)	Pore Diameter (nm)	Translocation time (ns)
1	dA_{20}	BMIM-Cl	0.05	2.6	5.0
2	dC_{20}	BMIM-Cl	0.05	2.6	5.0
3	dG_{20}	BMIM-Cl	0.05	2.6	5.0
4	dT_{20}	BMIM-Cl	0.05	2.6	5.0
5	dA_{20}	BMIM-Cl	0.05	3.10	2.50
6	dC_{20}	BMIM-Cl	0.05	3.10	2.50
7	dG_{20}	BMIM-Cl	0.05	3.10	2.50
8	dT_{20}	BMIM-Cl	0.05	3.10	2.50
9	dA_{20}	BMIM-Cl	0.10	2.6	1.50
10	dC_{20}	BMIM-Cl	0.10	2.6	1.50
11	dG_{20}	BMIM-Cl	0.10	2.6	1.50
12	dT_{20}	BMIM-Cl	0.10	2.6	1.50
13	dA_{20}	BMIM-Cl	0.10	3.10	1.00
14	dC_{20}	BMIM-Cl	0.10	3.10	1.00
15	dG_{20}	BMIM-Cl	0.10	3.10	1.00
16	dT_{20}	BMIM-Cl	0.10	3.10	1.00
17	$d(ACGT)_5$	BMIM-Cl	0.05	2.6	3.50
18	$d(ACGT)_5$	KCl	0.05	2.6	2.00
19	$d(ACGT)_5$	BMIM-Cl	0.05	3.10	1.70
20	$d(ACGT)_5$	KCl	0.05	3.10	1.10

Table S2. The translocation time of individual runs in each case of homo-polynucleotide sequence.

d=2.6 nm V=0.05 V/nm

Sequence	Run 1	Run 2	Run 3	average	SD
A	3090.0	2845.0	4580.0	3505.0	939.0
C	1888.0	2325.0	1737.0	1983.3	305.4
G	2810.0	3090.0	3190.0	3030.0	197.0
T	2980.0	2360.0	1950.0	2430.0	518.6

d=2.6 nm V=0.10 V/nm

Sequence	Run 1	Run 2	Run 3	average	SD
A	1040.0	1080.0	880.0	1000.0	105.8
C	980.0	840.0	790.0	870.0	98.5
G	890.0	920.0	990.0	933.3	51.3
T	770.0	890.0	910.0	856.7	75.7

d=3.1 nm V=0.05 V/nm

Sequence	Run 1	Run 2	Run 3	average	SD
A	1450.0	1990.0	1740.0	1726.7	270.2
C	1050.0	1695.0	900.0	1215.0	422.4
G	2253.0	2360.0	1961.0	2191.3	206.5
T	1263.0	1330.0	1020.0	1204.3	163.1

d=3.1 nm V=0.10 V/nm

Sequence	Run 1	Run 2	Run 3	average	SD
A	890.0	1026.0	844.0	920.0	94.6
C	374.0	488.0	506.0	456.0	71.6
G	842.0	840.0	840.0	840.7	1.2
T	626.0	540.0	685.0	617.0	72.9

Table S3. The blockade current of individual runs in each case of homo-polynucleotide sequence.

Blockade Current (nA) lag 250 ps

d=2.6 nm V=0.05 V/nm

Sequence	Run 1	Run 2	Run 3	average	SD
A	3.44	4.53	4.17	4.05	0.56
C	5.78	5.13	4.26	5.06	0.76
G	4.21	4.88	4.20	4.43	0.39
T	4.07	3.74	4.76	4.19	0.52

d=2.6 nm V=0.10 V/nm

Sequence	Run 1	Run 2	Run 3	average	SD
A	14.13	11.59	13.44	13.05	1.31
C	13.16	13.57	12.65	13.13	0.46
G	15.51	14.31	13.41	14.41	1.05
T	14.48	12.02	14.54	13.68	1.44

d=3.1 nm V=0.05 V/nm

Sequence	Run 1	Run 2	Run 3	average	SD
A	7.74	8.05	8.23	8.01	0.25
C	9.95	8.73	8.69	9.12	0.72
G	9.19	7.38	8.33	8.30	0.90
T	6.85	8.52	8.49	7.95	0.96

d=3.1 nm V=0.10 V/nm

Sequence	Run 1	Run 2	Run 3	average	SD
A	19.13	17.88	19.89	18.97	1.01
C	21.37	19.31	21.85	20.84	1.35
G	19.63	18.88	18.56	19.02	0.55
T	20.71	19.58	19.37	19.89	0.72