Supporting Information

Detection of Benzo[a]pyrene-Guanine Adducts in Single-Stranded DNA using the α-Hemolysin Nanopore

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1. Characterization of the 4-mer and 41-mer BPDE DNA oligomers

HPLC was used to purify the adduct (4-mer BPDE and 41-mer BPDE) from the reaction mixture. Four product peaks are observed for the 4-mer, and these correspond to the four diastereomers of BPDE. For the 41-mer only one product peak was observed containing all four diastereomers.

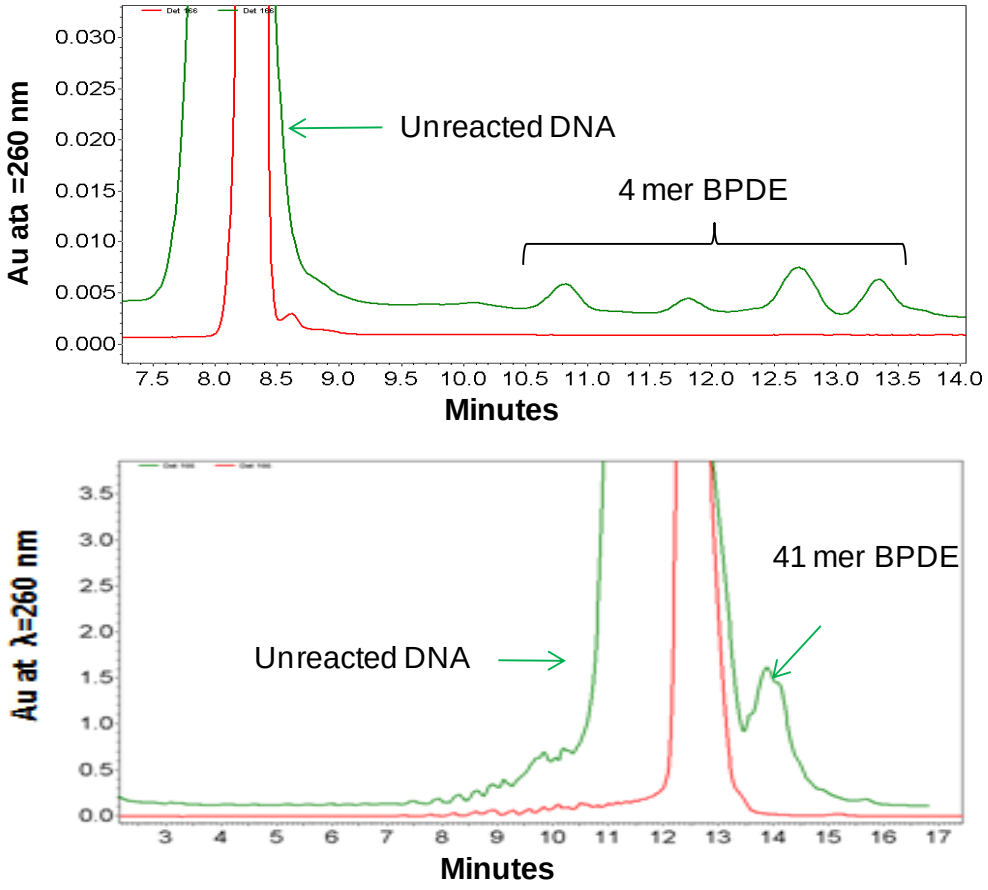

Figure S1. Ion-exchange HPLC traces for 4 mer-BPDE and 41-mer BPDE: The HPLC conditions utilized solvent A = 10% CH_3CN, 90% ddH_2O; B = 1 M NaCl in 10% CH_3CN 90% ddH_2O, 25 mM Tris pH 8; flow rate = 1 mL/min while monitoring the absorbance at 260 nm. The separation was initiated at 15% B followed by a linear increase to 100% B over 30 min.

2. *i-t* traces for the unmodified 41-mer and 41-mer BPDE in 1 M KCl

Open channel baseline current intervals longer than 20 ms were removed from the following *i–t* traces and indicated by the blue dashed lines.

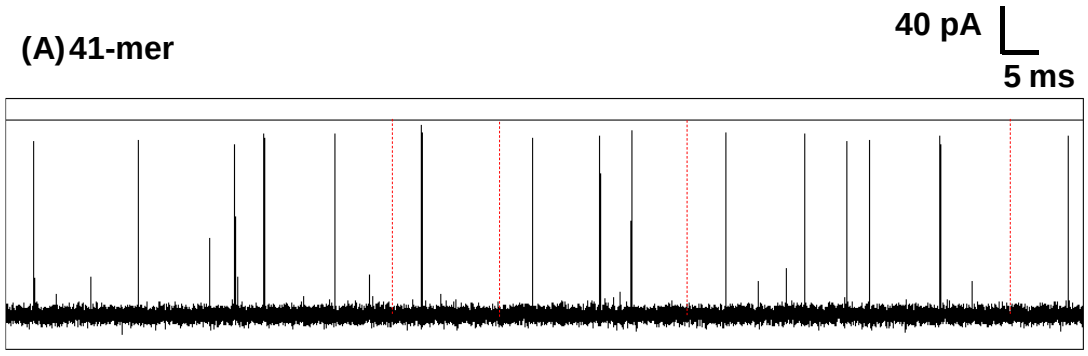

Figure S2. (A) Current vs. time profile for the 41-mer standard (4 μM) in 1 M KCl. The data were recorded at 180 mV (*trans* vs. *cis*) at 25.0 ± 0.5 °C.

(B) 41-mer BPDE

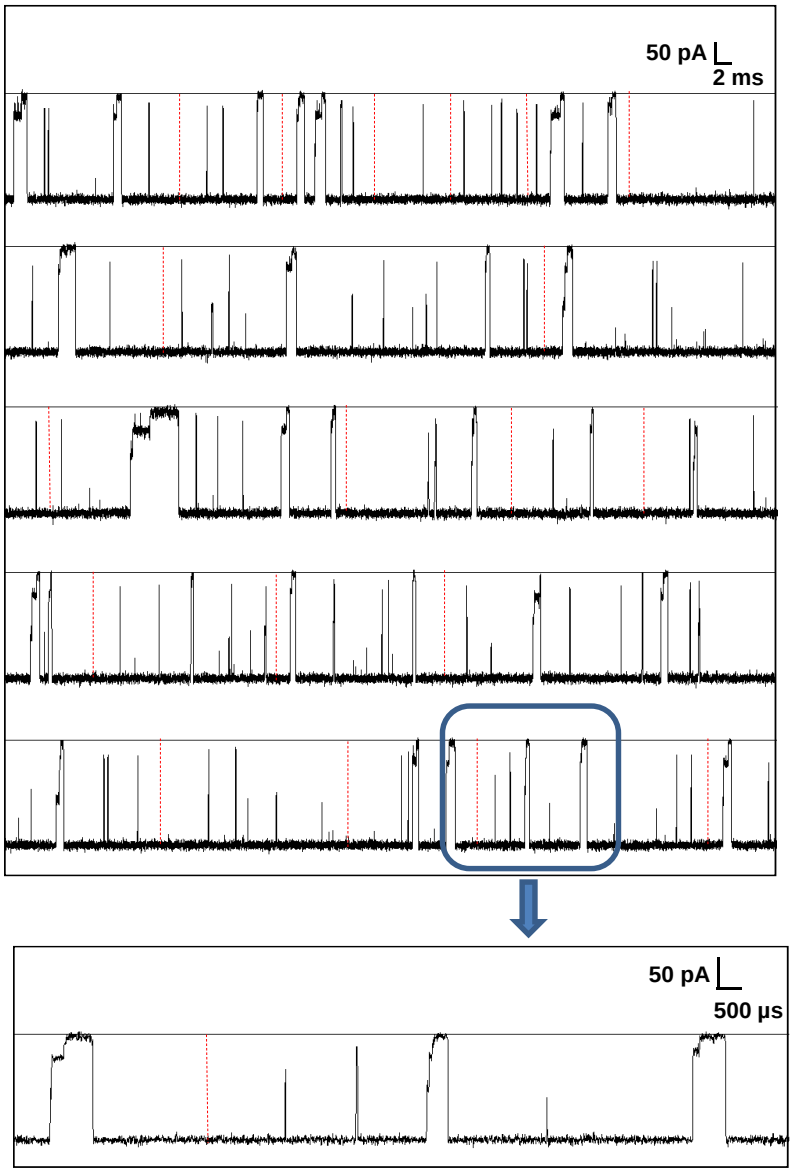

Figure S2. (B) Current vs. time profile for 41-mer BPDE (2 μM) in 1 M KCl. The data were recorded at 180 mV (*trans* vs. *cis*) at 25.0 ± 0.5 °C.

3. Current vs. time profile for the unmodified 41-mer and 41-mer BPDE in 3 M NaCl.

Open channel baseline current intervals longer than 20 ms were removed from the following *i–t* traces and indicated by the blue dashed lines.

(A) 41-mer

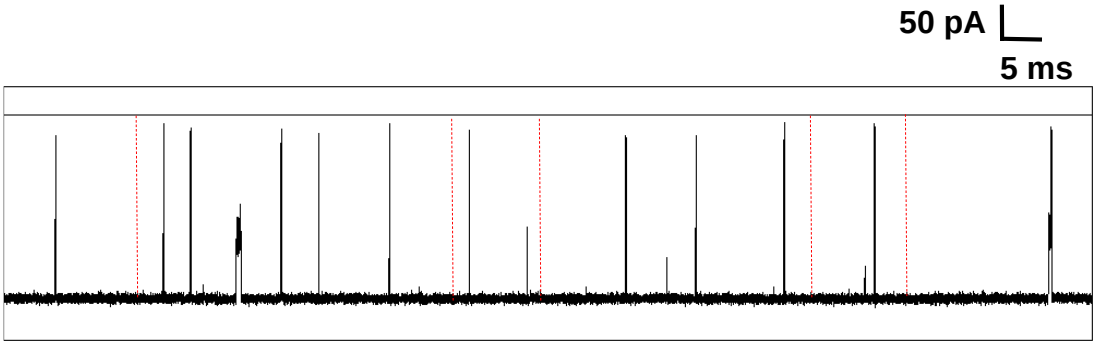

Figure S3.(A) Current vs. time profile for the 41-mer standard (4 μM) in 3 M NaCl. The data were recorded at 180 mV (*trans* vs. *cis*) at 25.0 ± 0.5 ^{o}C.

(B) 41-mer BPDE

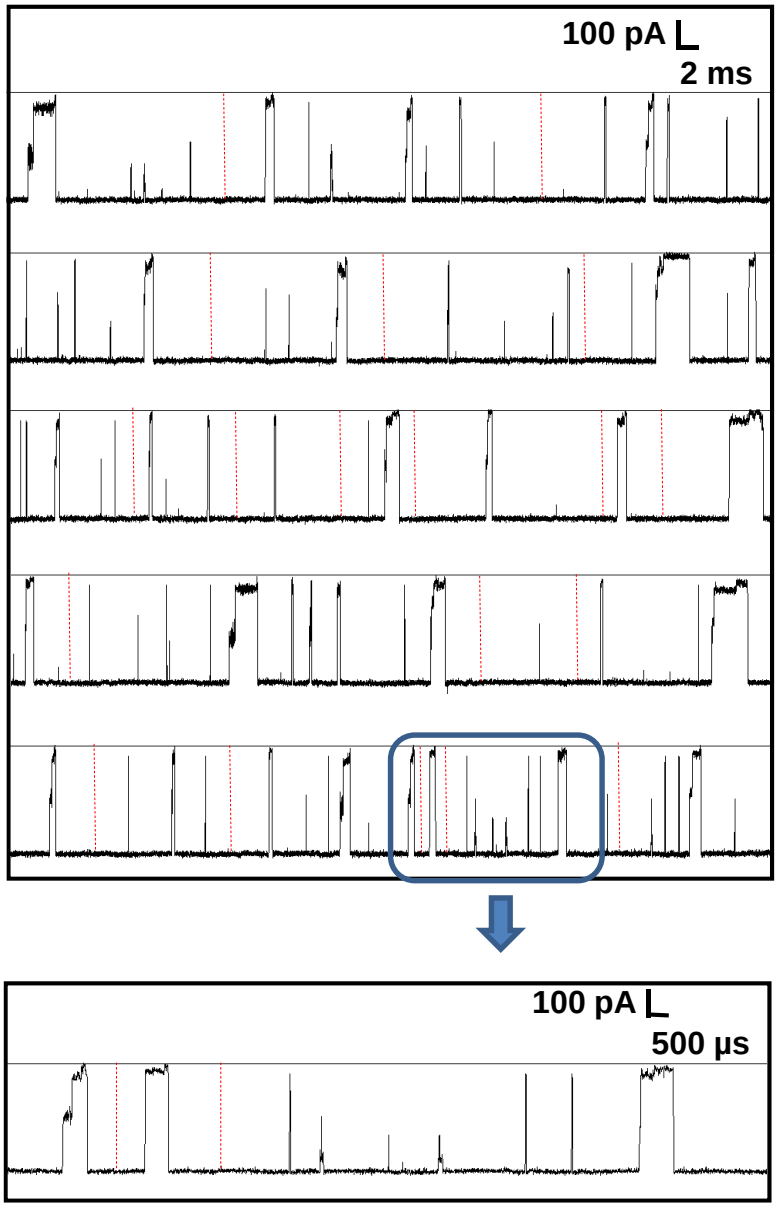

Figure S3.(B) Current vs. time profile for the 41-mer BPDE (2 μM) in 3 M NaCl. The data were recorded at 180 mV (*trans* vs. *cis*) at 25.0 ± 0.5 ºC.

4. Translocation analysis of the 41-mer and 41-mer BPDE in 1 M KCl and 3 M NaCl

The translocation time durations for (A) 41-mer and (B) 41-mer BPDE in 1 M KCl are shown below. The time distribution for translocation of 41-mer was fit with a Gaussian model. The modified 41-mer BPDE showed longer translocation times (325-375 events were analyzed), and its duration histogram exhibits an exponential decay.

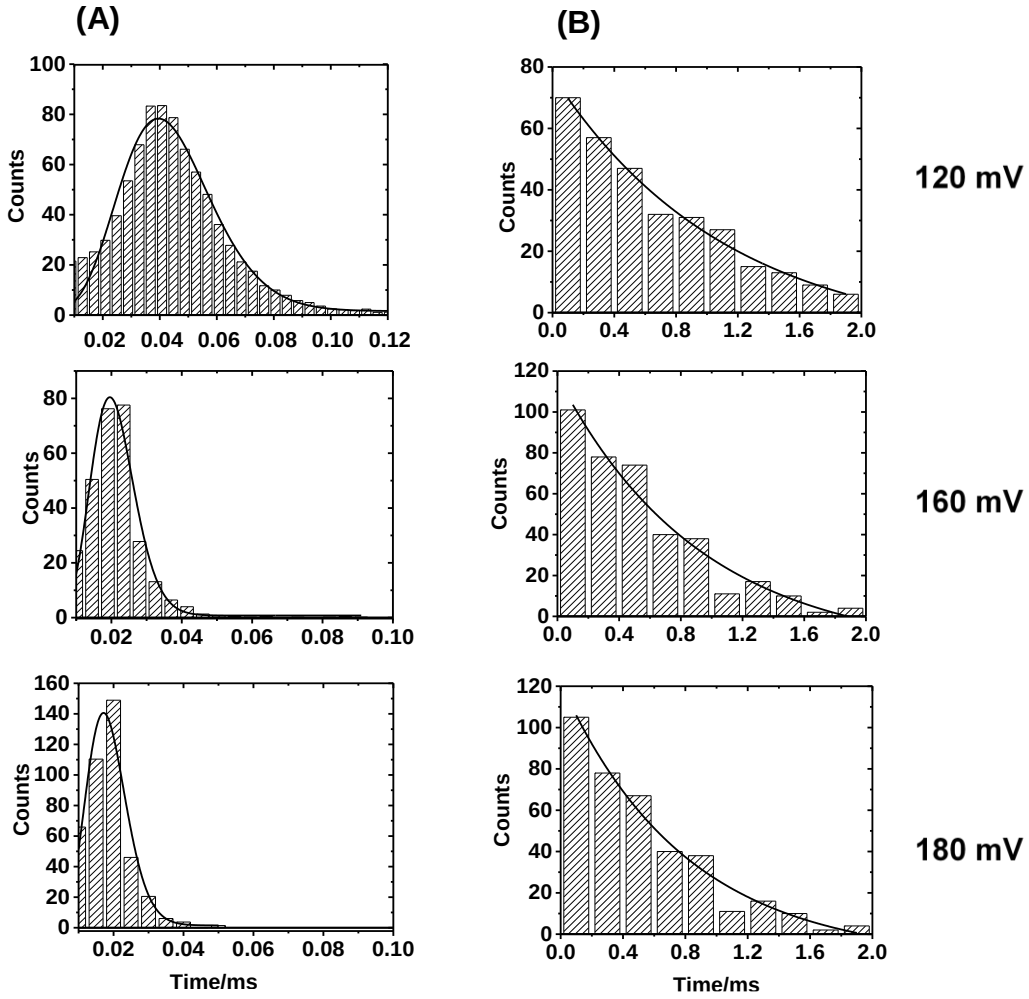

Figure S4. Translocation time analysis of the 41-mer and 41-mer BPDE in 1 M KCl.Only the events longer than 70 μs were used for translocation analysis of 41-BPDE. The data were recorded at 120,160 and 180 mV (*trans* vs. *cis*) at 25.0 ± 0.5 °C.