Electronic Supplementary Material (ESI) for Nanoscale Horizons.

Supporting Information

Enhancing DNA-based Nanodevices Activation through Cationic Peptide Acceleration of Strand Displacement

***Xianxue Zhang*, *Ruikai Du*, *Shichao Xu*, *Xinyue Wang* and *Zhen-Gang Wang* ***

Table S1. Oligonucleotide sequences used in this work

DNA	Sequence (5'-3')
1	Cy5-CAGATTGTGTACCTCAGTCGAAACC-BHQ2
2	GCTTTAAGGTTTCGACTGAGGTACACAATCTG
3	CAGATTGTGTACCTCAGTCGAAACCTTAAAGC
4	AGGTTTCGACTGAGGTACACAATCTG
5	CAGATTGTGTACCTCAGTCGAAACCT
6	TAAGGTTTCGACTGAGGTACACAATCTG
7	CAGATTGTGTACCTCAGTCGAAACCTTA
8	CTTTAAGGTTTCGACTGAGGTACACAATCTG
9	CAGATTGTGTACCTCAGTCGAAACCTTAAAG
10	TGCTTTAAGGTTTCGACTGAGGTACACAATCTG
11	CAGATTGTGTACCTCAGTCGAAACCTTAAAGCA
input A	CAAAACAAAACCTCATCTCATCCATTCCACTCA
input B	CAAAACAAAACCTCATCTCACCCTAAAATCTCA
gate A (partially complementary)	CACCACCAAACTTCATCTCAAAACAAAACCTCA TGAGATGAGGTTTTGTTTTGAGATG
threshold (partially complementary)	CACCACCAAACTTCA TGTTTTGAGATGAAGTTTGGTGGTG
gate B (partially complementary)	CATAACACAATCACATCTCACCACCAAACTTCA TGAGATGAAGTTTGGTGGTGAGATG
fuel	CAACATATCAATTCATCTCACCACCAAACTTCA
reporter B (partially complementary)	BHQ2-CATAACACAATCACA TGAGATGTGATTGTGTTATG-Cy5
a	Cy5-GCGGCAGAGCGACGCTCGGTCG
b	AACTCAGACGACCATCTCCTAA-BHQ2
c	ACAGGCCGGGATTAGGAGATGGTCGTCTGAGTTTTTT CGACCGAGCGTCGCTCTGCCGCCAAGTGCAATA
d	TATTGCACTTGTCCCGGCCTGTTTAAAGC
e	GCTTTAAACAGGCCGGGACAAGTGCAATA

Table S2. Peptides sequences used in this work

Name	Sequence
R5	NH_2-RRRRR-COOH
R10	NH_2-RRRRRRRRRR-COOH
R15	NH_2-RRRRRRRRRRRRRRR-COOH
K10	NH_2-KKKKKKKKKK-COOH
R5K5	NH_2-RRRRRKKKKK-COOH
(RK)5	NH_2-RKRKRKRKRK-COOH

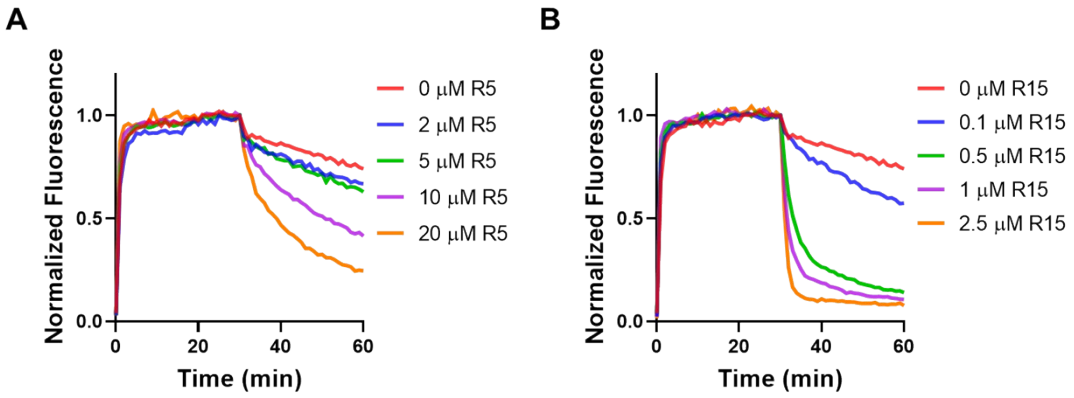

Figure S1. Effects of different concentrations of A) R5 and B) R15 on DNA strand displacement reaction. [DNA] = 1 μM.

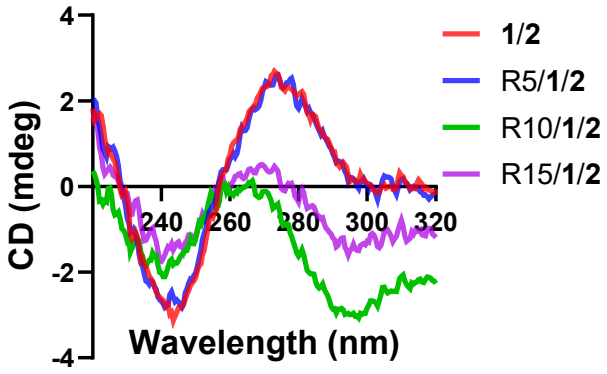

Figure S2. CD spectra of **1**/**2** in the presence of the R5, R10, or R15. [DNA] = 1 μM. [peptides] = 5 μM.

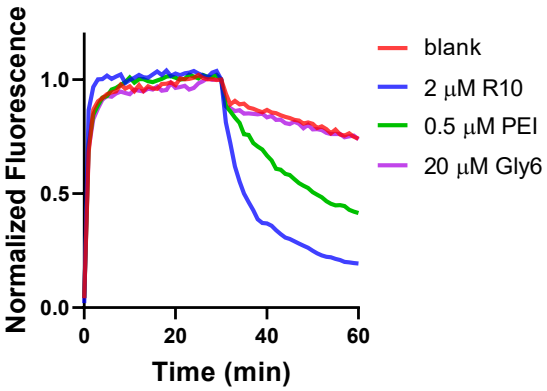

Figure S3. Effects of different concentrations of R10, PEI, and Gly6 on DNA strand displacement reaction. [DNA] = 1 μM.

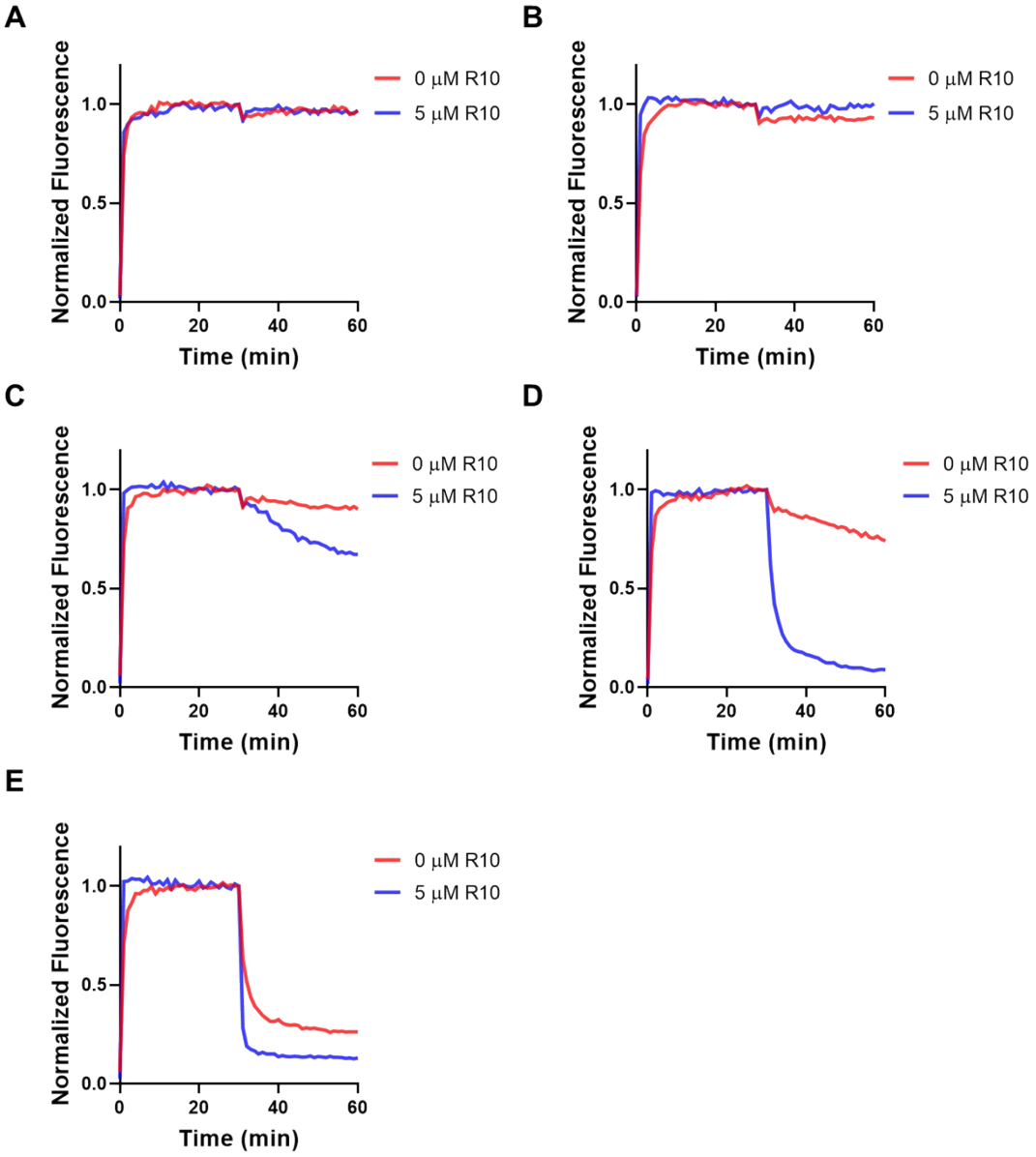

Figure S4. Effects of strand displacement reaction by R10 for different toehold length, A) 1 nt, B) 3 nt, C) 6 nt, D) 7 nt, E) 8nt. [DNA] = 1 μM.

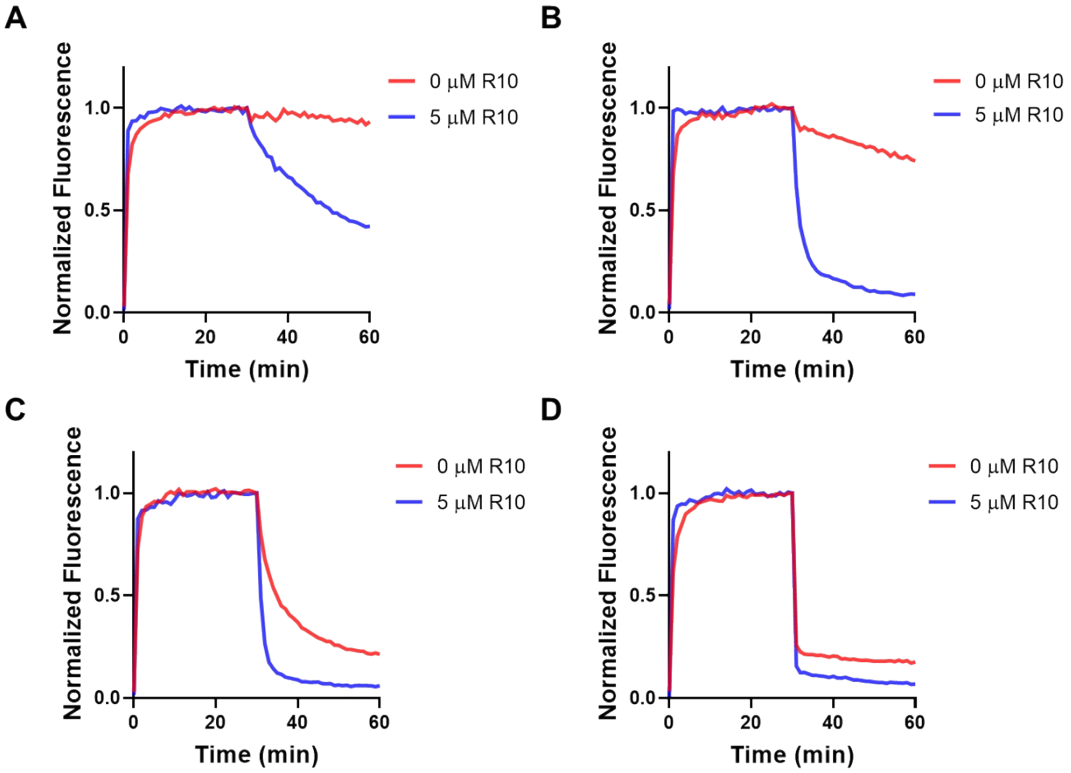

Figure S5. Effects of strand displacement reaction by R10 for different GC content in the toehold sequence, A) 0/7, B) 2/7, C) 4/7, D) 7/7. [DNA] = 1 μM.

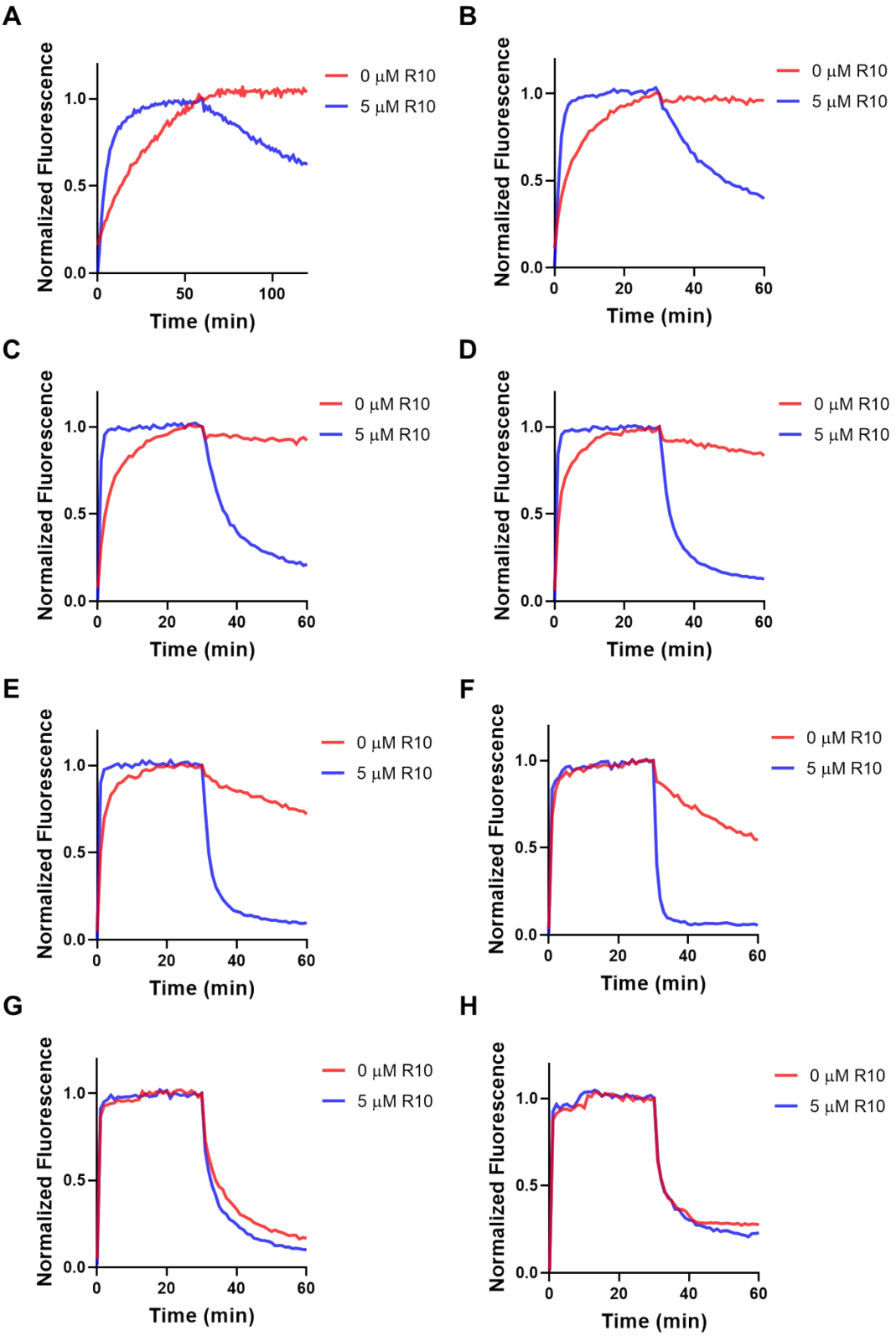

Figure S6. Effects of strand displacement reaction by R10 for different concentration of Na^+, A) [Na^+] = 10 mM, B) [Na^+] = 20 mM, C) [Na^+] = 30 mM, D) [Na^+] = 40 mM, E) [Na^+] = 50 mM, F) [Na^+] = 100 mM, G) [Na^+] = 500 mM, H) [Na^+] = 1000 mM. [DNA] = 1 μM.

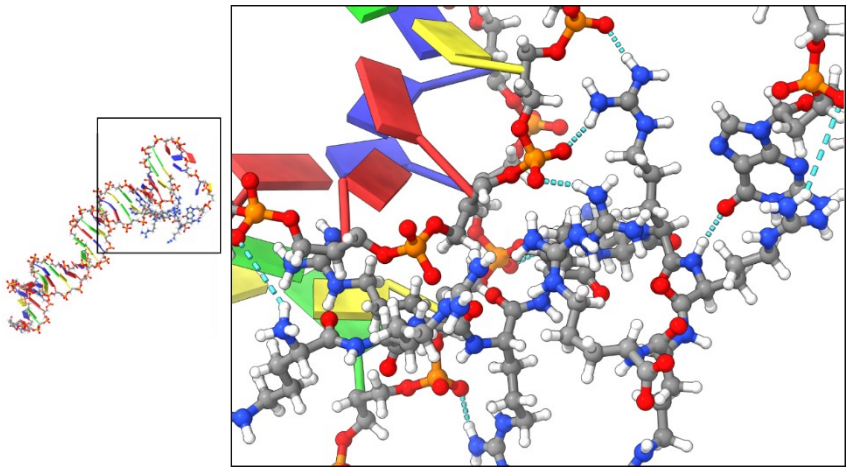

Figure S7. Representative structure of R10/DNA from the cluster analysis. The dotted line represents the electrostatic interaction of the guanidine group in R10 and the phosphate group in DNA.

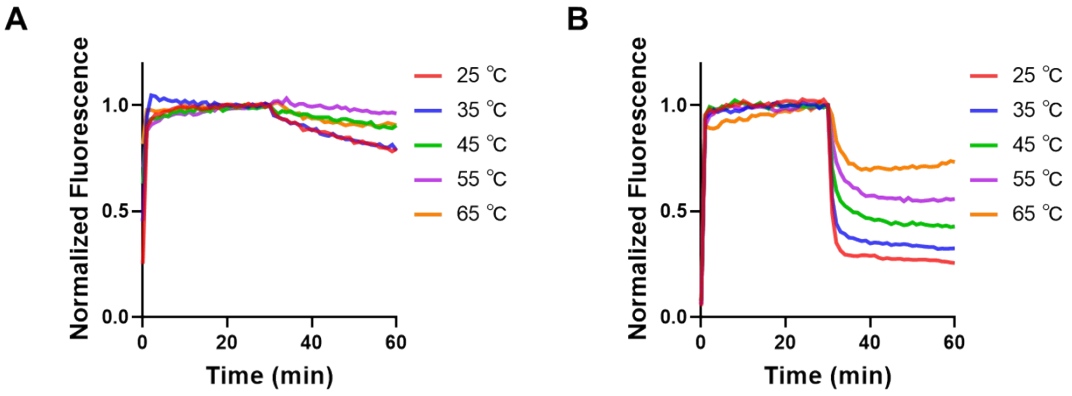

Figure S8. Effects of A) 0 µM R10 and B) 5 µM R10 on DNA strand displacement reaction at a range of temeratures. [DNA] = 1 µM.

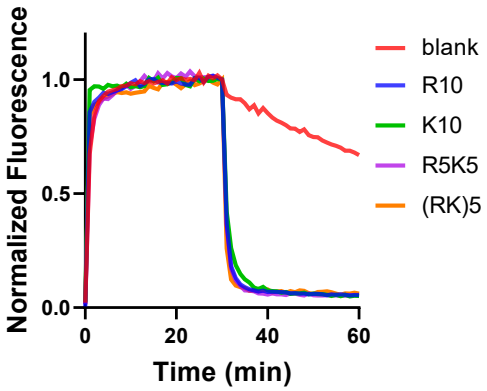

Figure S9. Effects of different cationic peptides on DNA strand displacement reaction. [DNA] = 1 μM, [peptide] = 5 μM.

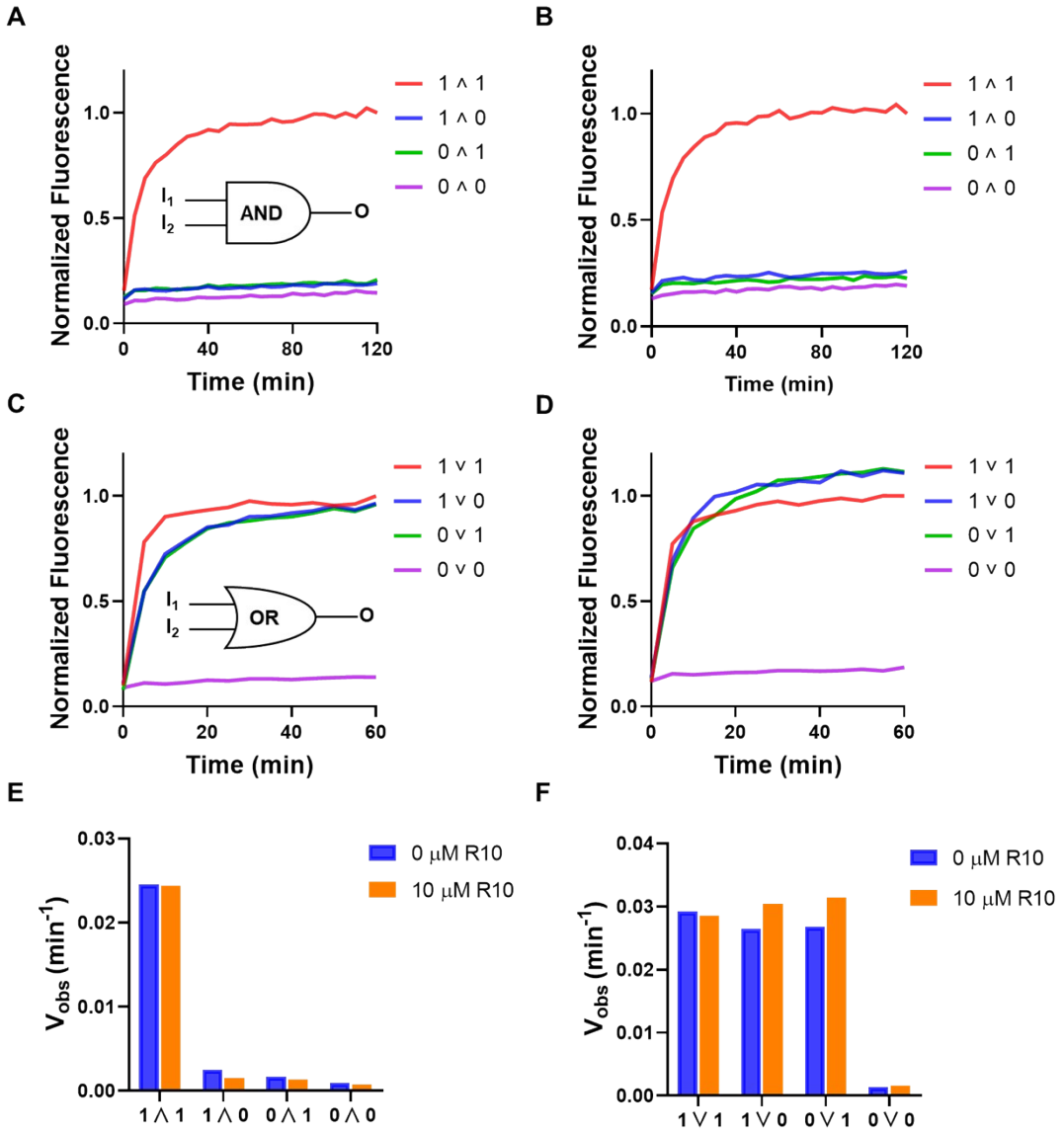

Figure S10. A-D) Output signal changes with time of A) AND gate and C) OR gate in the presence of R10 and of B) AND gate and D) OR gate in the absence of R10. The concentrations of gate A, gate B, fuel, and reporter B were 2 ×, 1 ×, 1 ×, 1.5 ×, respectively, with 1 × equal to 0.5×10^{-6} M. Concentrations of input strands were at 0.1 × (0, logic off) or 0.9 × (1, logic on). E,F) V_{obs} (taken from the first thirty minutes) of E) AND and F) OR gate by R10. Reactions were performed in 50 mM phosphate buffer (pH 7.0) containing 1 M NaCl.

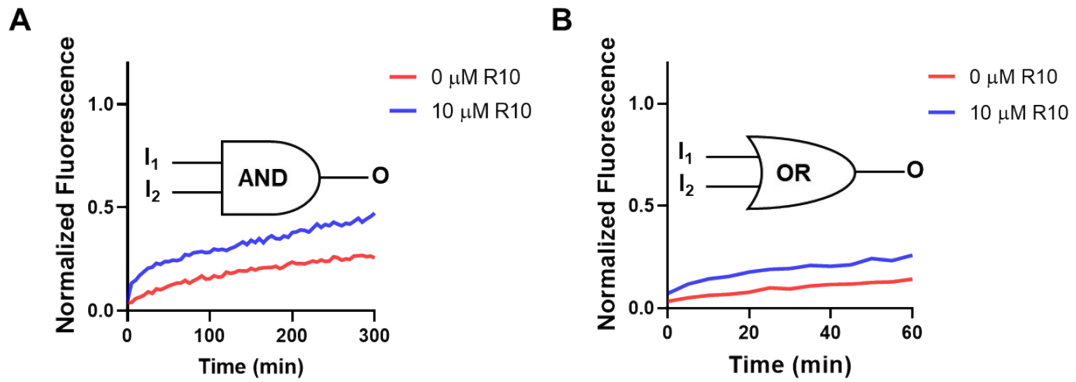

Figure S11. Time-dependent fluorescence signal changes for A) AND gate and B) OR gate in the absence and presence of R10. The concentrations of gate A, gate B, fuel, and reporter B were 2 ×, 1 ×, 1 ×, 1.5 ×, respectively, with 1 × equal to 0.5×10^{-6} M. Concentrations of input strands were 0 ×.