Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Reconfigurable DNA Triplex Structure for pH Responsive Logic Gates

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1. Supplementary of DNA triplex

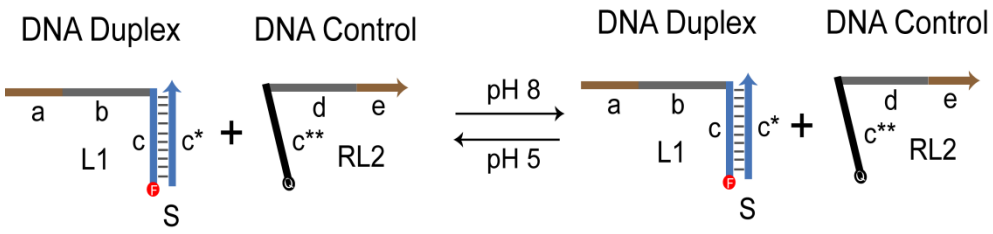

Fig. S1 Scheme of DNA triplex control at pH 5 and pH 8. The scheme contains the DNA Duplex and DNA Control with random sequence domain.

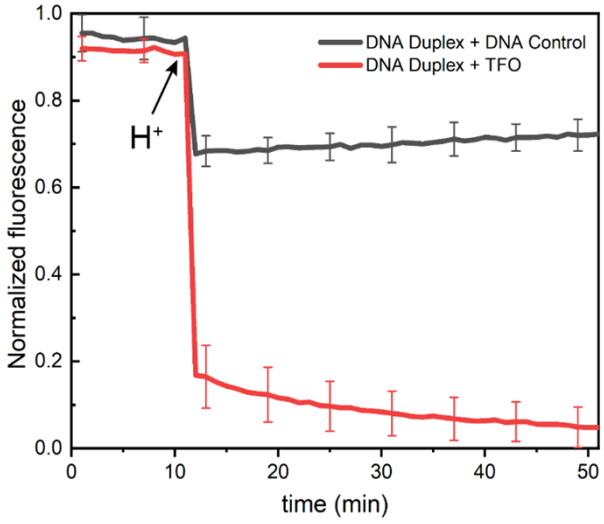

Fig. S2 Fluorescence kinetic experiments for the sequence specificity of triplex. Acetic acid was added to the DNA Control group and TFO group to adjust to pH 5 at 10 min. DNA strands involved in fluorescence kinetics measurements were all involved in reaction at 0.1 μM. Results are presented as means ± standard deviation (n=3).

In figure S2, it can be observed that the fluorescence value of the TFO group decreased significantly due to the formation of DNA triplex. The transformation was consistent with the effects of cyclic pH-jump experiments, while the fluorescence value of the DNA Control group did not change significantly. It indicates that DNA triplex is not formed at this time. In summary, the experimental results further prove the sequence specificity of DNA triplex.

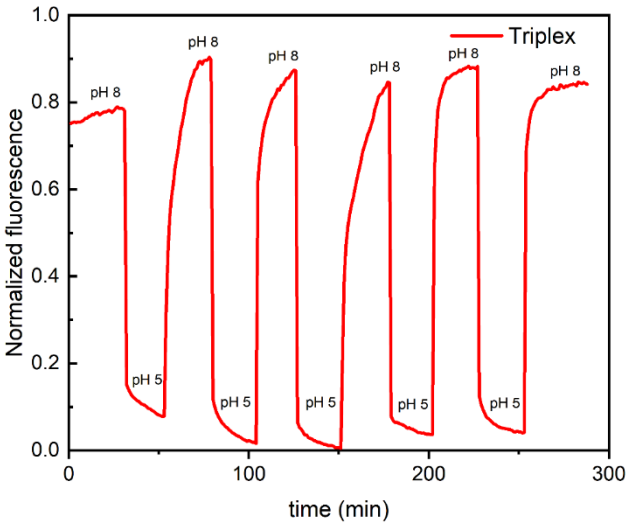

Fig. S3 The trend diagram of triplex with pH. sampling interval is 1 min, every 30 min is a cycle for 11 times, the 30 min include sampling and scanning. DNA strands involved in the fluorescence kinetic experiment all participated in the reaction at 0.1 μM. Results are presented as means ± standard deviation (n=3).

2. PAGE analysis of RDTS assembled

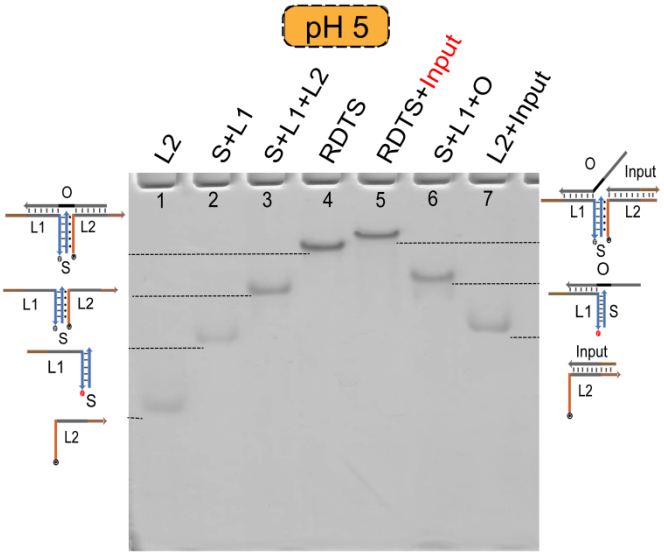

Fig. S4 PAGE analysis of RDTS at pH 5. The strands and complexes involved are marked above the lane number. DNA strands involved in PAGE experiment were all involved in reaction at 3 μM (pH 5).

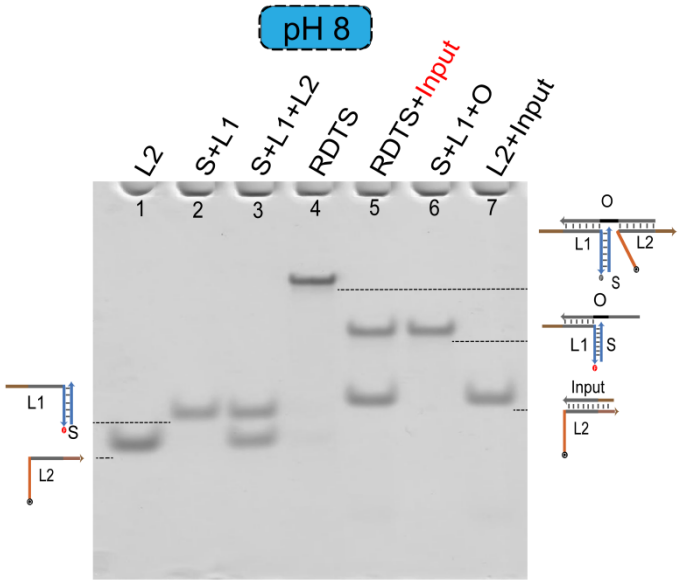

Fig. S5 PAGE analysis of RDTS at pH 8. The strands and complexes involved are marked above the lane number. DNA strands involved in PAGE experiment were all involved in reaction at 1.5 μM (pH 8).

3. pH responsive logic gates: AND Gate (State 2 to State 1)

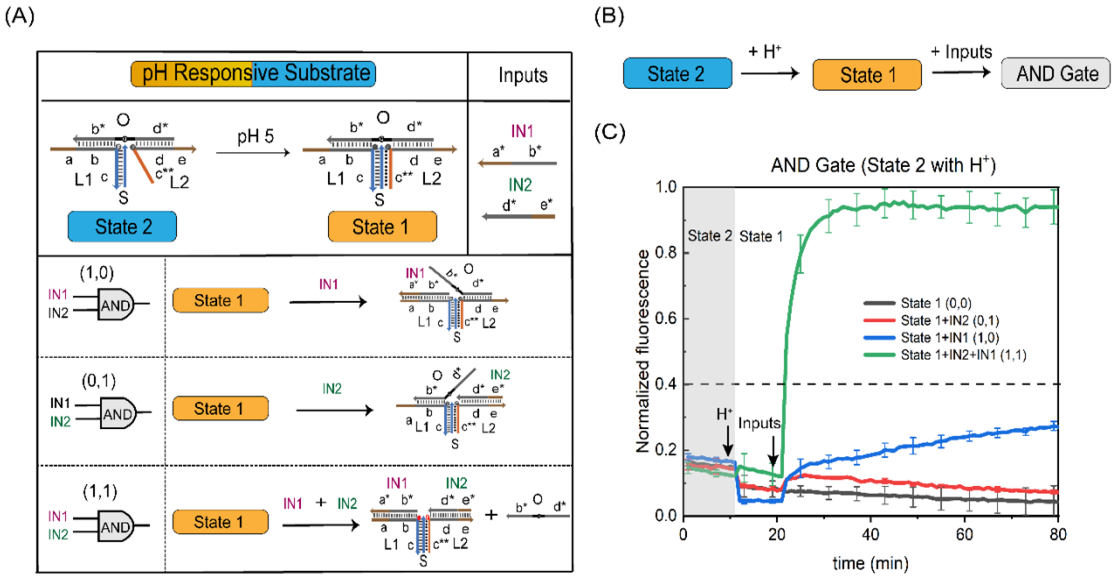

Fig. S6 (A) Scheme of pH responsive logic gates (State 2 to State 1). Acetic acid was added first to convert the substrate from State 2 to State 1, the pH responsive logic gates showed 'AND' gate after inputs were added (B) Abstract diagram of pH responsive logic gates (State 2 to State 1). Add the corresponding materials in arrow order. (C) Fluorescence kinetic experiments of pH responsive logic gates (State 2 to State 1). Acetic acid and Input are added at the arrow marks in the figure. DNA strands involved in fluorescence kinetics measurements were all involved in reaction at 0.1 μM.

4. pH responsive logic gates: OR Gate (State 1 to State 2)

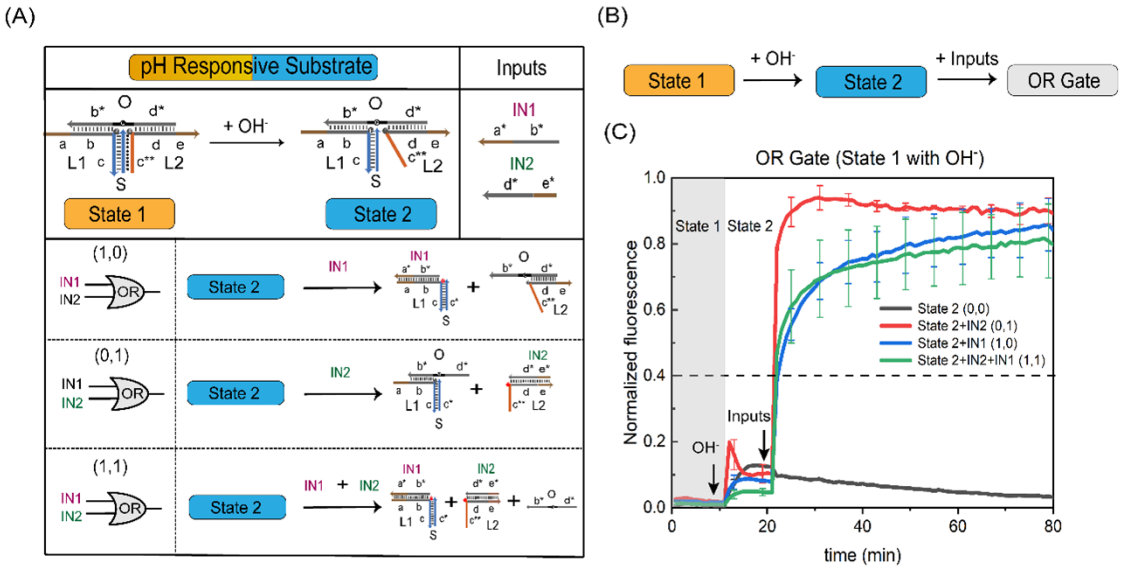

Fig. S7 (A) Scheme of pH responsive logic gates (State 1 to State 2). NaOH was added first to convert the substrate from State 2 to State 1, the pH responsive logic gates showed 'OR' gate after inputs were added (B) Abstract diagram of pH responsive logic gates (State 1 to State 2). Add the corresponding materials in arrow order. (C) Fluorescence kinetic experiments of pH responsive logic gates (State 1 to State 2). NaOH and Input are added at the arrow marks in the figure. DNA strands involved in fluorescence kinetics measurements were all involved in reaction at 0.1 μM.

5. The sequences used in the study

We use NUPACK to analyze all the DNA sequences to reduce undesired hybridization between DNA strands. DNA sequences are shown in Table S1 and S2.

Table S1 The sequences used in DNA Triplex & RDTS

Name	Sequences (from 5' to 3')	Length (n.t.)
L2	BHQ2-TTCCTTTCTCCTTCTTGAACTTACCTAACTCGTCCTTCT	39
L1	GCTGTCACTAGCTCAGTATTGATTGATTCTTCCTCTTTCCTT-Cy5	42
O+3T	GAGTTAGGTAAGTTCTTTTTTTCAATCAATACTGAGTTT	39
Input	AGAAGGACGAGTTAGGTAAGTTC	23
S	AAGGAAAGAGGAAGA	15
RL2	BHQ2-TTTTTTTTTTTTTTTTGAACTTACCTAACTCGTCCTTCT	39

Table S2 The sequences used in pH-responsive logic gates

Name	Sequences (from 5′ to 3′)	Length (n.t.)
L2	TTCCTTTCTCCTTCT-Cy5-GAACTTACCTAACTCGTCCTTCT	39
L1	GCTGTCACTAGCTCAGTATTGATTGA-Cy5-TCTTCCTCTTTCCTT	42
O	GAGTTAGGTAAGTTCTTT-BHQ2-TTTCAATCAATACTGAG	36
IN1	TCAATCAATACTGAGCTAGTGACAGC	26
IN2	AGAAGGACGAGTTAGGTAAGTTC	23
S	AAGGAAAGAGGAAGA	15