Supporting Information

Comparative evaluation and design of G-triplex/thiflavin T-based molecular beacon

Jingru Gao, Qiang Liu, Wei Liu, Yan Jin and Baoxin Li*

Key Laboratory of Applied Surface and Colloid Chemistry, Ministry of Education; Key Laboratory of Analytical Chemistry for Life Science of Shaanxi Province, School of Chemistry & Chemical Engineering, Shaanxi Normal University, Xi'an 710062, China

Table S1. Oligonucleotide sequences for forming G3

Name	Sequence (5′-3′)
G3	TGGGAAGGGAGGG
G3-T_3	TGGGAAGGGAGGGTTT
G3-T_4	TGGGAAGGGAGGGTTTT
G3-T_5	TGGGAAGGGAGGGTTTTT
G3-T_6	TGGGAAGGGAGGGTTTTTT
G3-T_7	TGGGAAGGGAGGGTTTTTTT
G3-A_3	TGGGAAGGGAGGGAAA
G3-A_4	TGGGAAGGGAGGGAAAA
G3-A_5	TGGGAAGGGAGGGAAAAA
G3-A_6	TGGGAAGGGAGGGAAAAAA
G3-A_7	TGGGAAGGGAGGGAAAAAAA
G3-$(AT)_2$	TGGGAAGGGAGGGATAT
G3-$(AT)_3$	TGGGAAGGGAGGGATATAT
G3-$(AT)_4$	TGGGAAGGGAGGGATATATAT
G3-$(AT)_5$	TGGGAAGGGAGGGATATATATAT

Table S2. Oligonucleotide sequences of target DNA and related DNA in this work

Name	Sequence (5′-3′)
p 53 DNA	TCATCACACTGGAAGACTC
smT	TCATCACACCGGAAGACTC
dmT	TCATCATACTGGCAGACTC
ncT	ATGGGTCAGATTACGTTG A

Table S3. Oligonucleotide sequences of MB used in this work*

Name	Sequence (5′-3′)
G3M53	TGGGAAGGGAGGGAAAAAGAGTCTTCCAGTGTGATGATTTTTCCC
G3M43	TGGGAAGGGAGGGAAAAAGAGTCTTCCAGTGTGATGATTTTCCC
G3M42	TGGGAAGGGAGGGAAAAAGAGTCTTCCAGTGTGATGATTTTCC
G3M41	TGGGAAGGGAGGGAAAAAGAGTCTTCCAGTGTGATGATTTTC
G3M35	TGGGAAGGGAGGGAAAAAGAGTCTTCCAGTGTGATGATTTCCCTC
G3M33	TGGGAAGGGAGGGAAAAAGAGTCTTCCAGTGTGATGATTTCCC
G3M32	TGGGAAGGGAGGGAAAAAGAGTCTTCCAGTGTGATGATTTCC
G3M26	TGGGAAGGGAGGGAAAAAGAGTCTTCCAGTGTGATGATTCCCTCC
G3M25	TGGGAAGGGAGGGAAAAAGAGTCTTCCAGTGTGATGATTCCCTC
G3M23	TGGGAAGGGAGGGAAAAAGAGTCTTCCAGTGTGATGATTCCC
G3M17	TGGGAAGGGAGGGAAAAAGAGTCTTCCAGTGTGATGATCCCTCCC
G3M16	TGGGAAGGGAGGGAAAAAGAGTCTTCCAGTGTGATGATCCCTCC
G3M15	TGGGAAGGGAGGGAAAAAGAGTCTTCCAGTGTGATGATCCCTC
G3M07	TGGGAAGGGAGGGAAAAAGAGTCTTCCAGTGTGATGACCCTCCC
G3M06	TGGGAAGGGAGGGAAAAAGAGTCTTCCAGTGTGATGACCCTCC
G3M05	TGGGAAGGGAGGGAAAAAGAGTCTTCCAGTGTGATGACCCTC
G4-MB	AGGGTTAGGGTTAGGGTTAGGGCTTGAGGAGTCTTCCAGTGTGATGACTCAAGCCCTAAC
G4-MB-1	AGGGTTAGGGTTAGGGTTAGGGCTTGAGTCTTCCAGTGTGATGAAAGCCC

* Underlined bases denote the stem of G3-based MB.

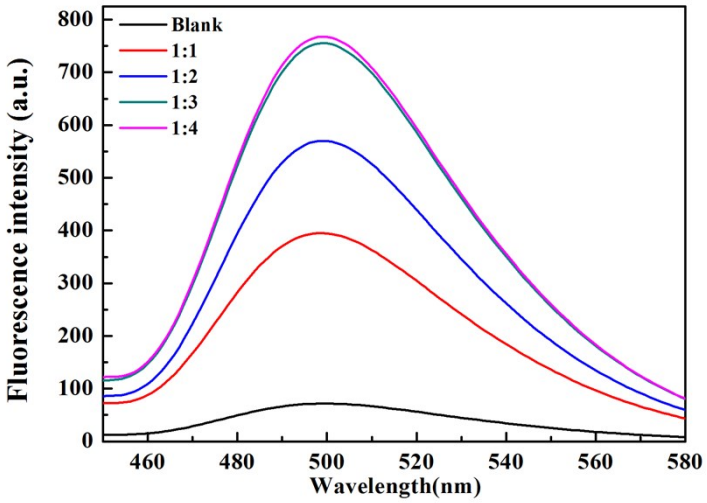

Figure S1. Fluorescence emission spectra of the G4-based MB under the different MB-to-target ratios. MB probe concentration was 0.45 μM. Reaction media were 75 mM KCl, and 20 mM Tris-HCl (pH 8.3).

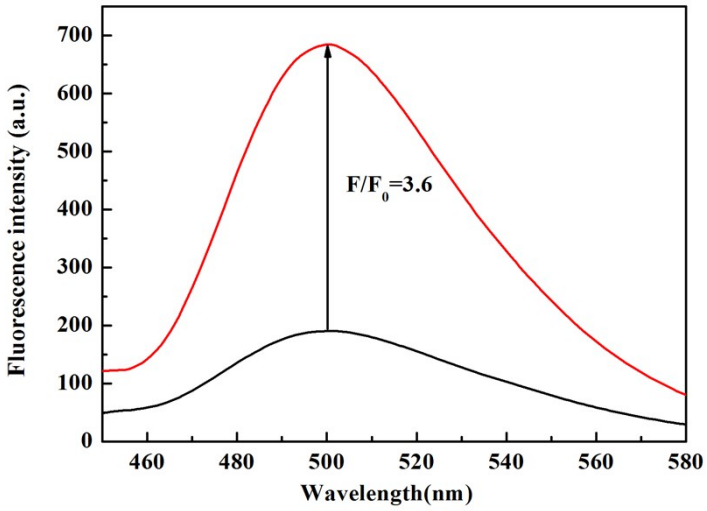

Figure S2. Fluorescence spectra of the G4-based MB-1 in the absence (black line) and presence (red line) of target p53.

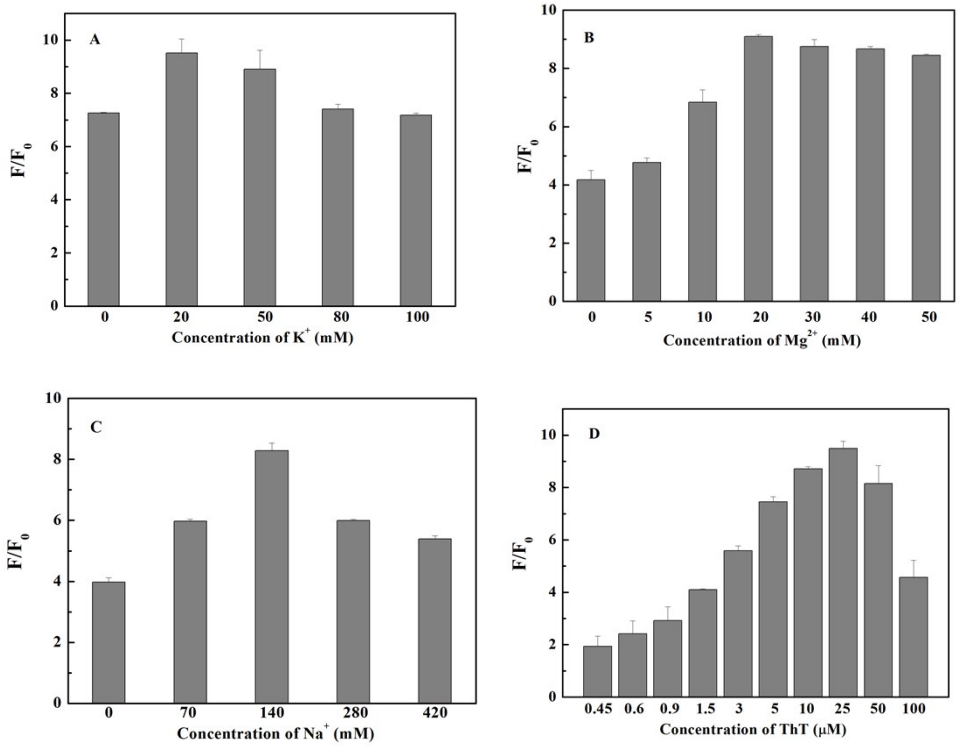

Figure S3. Effect of ions and ThT concentrations on the response of G3-based MB.

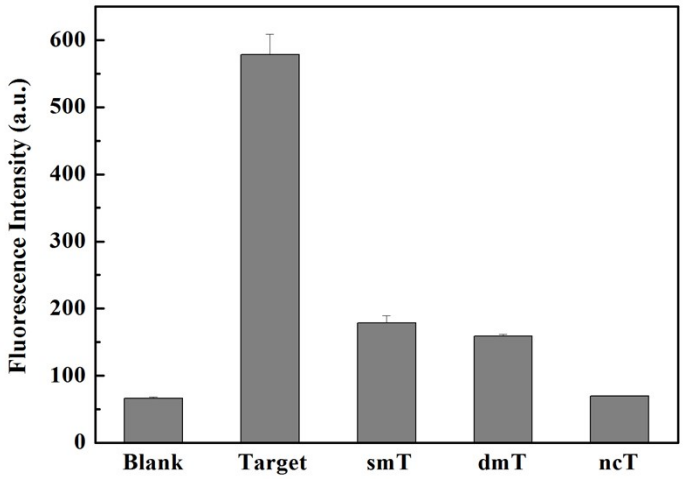

Figure S4. Fluorescence response of G3/ThT-based MB system to different DNA sequence: single-base mismatch DNA (smT), double-base mismatch DNA (dmT), random sequence (ncT), and target DNA.

Table S4. Detection of target DNA in 1% human serum samples (n=3).

Samples	Added	Found	Recovery (%)	RSD (%)
No. 1	50 nM	49 nM	98	6.4
No. 2	90 nM	89.8 nM	99	1.2
No. 3	200 nM	201 nM	101	1.2