

Supporting Information

Fluorinated molecular beacons as functional DNA nanomolecules for cellular imaging

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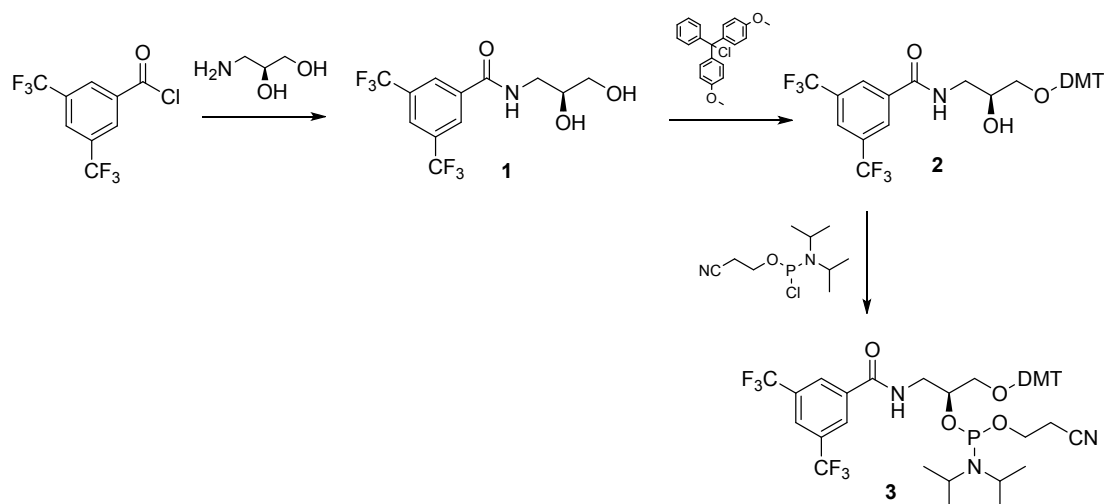
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Scheme S1. Synthesis route of F base phosphoramidite

The synthesis procedures of fluorinated base phosphoramidite monomer refer to the protocol developed in our laboratory.¹ ¹HNMR, ¹⁹FNMR, ³¹PNMR and ESI-MS data of 3,5-bis(trifluoromethyl) benzoyl phosphoramidite monomer (**3**) are as follows:

¹H NMR (300 MHz, CDCl₃) δ: 8.43 (s, 1H), 8.41 (s, 1H), 8.23 (s, 1H), 8.17 (s, 1H), 7.51 (d, J=6.0 Hz, 2H), 7.37 (d, J=6.6 Hz, 4H), 7.26-7.30 (m, 2H), 7.187.21 (m, 1H), 6.83-6.87 (m, 4H), 4.29-4.35 (m, 1H), 3.62-3.93 (m, 12H), 3.17-3.34 (m, 2H), 2.70-2.74 (m, 1H), 2.60-2.63 (m, 1H), 1.10-1.25 (m, 12H); ¹⁹F NMR (CDCl₃) δ: -64.23, -64.29; ³¹P NMR (CDCl₃) δ: 139.62, 140.99. MS (ESI⁺): m/z 833.3 (Calculated M+Na: 856.40).

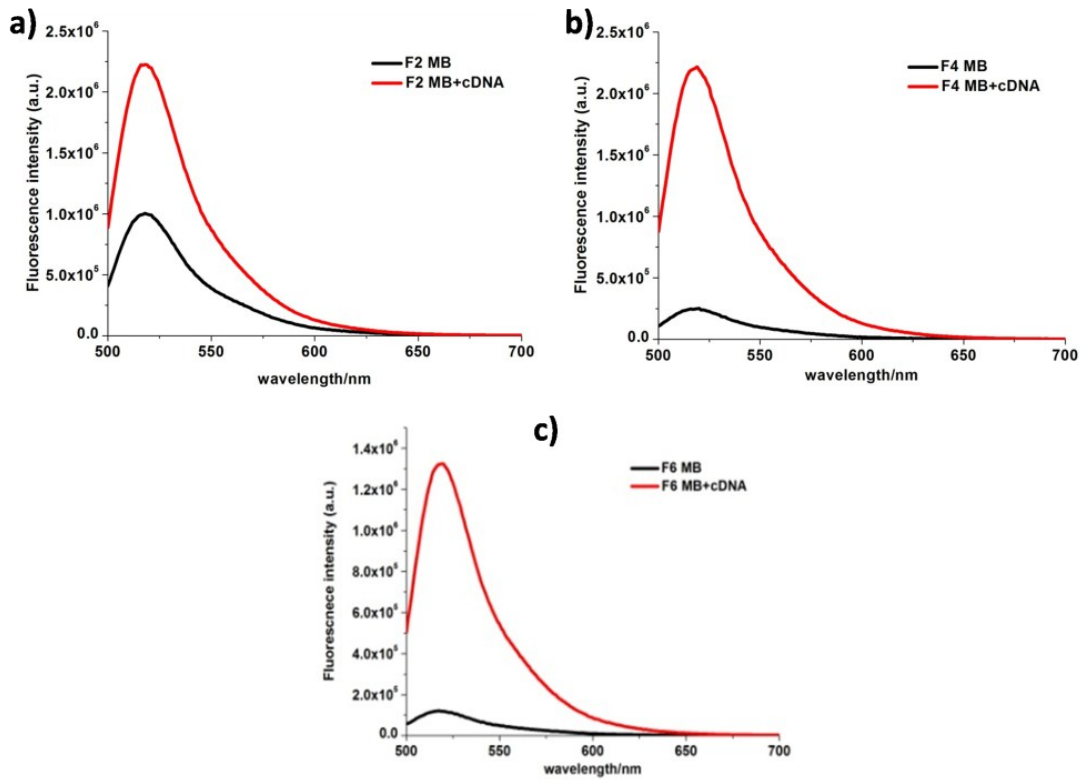


Figure S1. Fluorescence spectroscopy of FMBs before (black line) and after (red line) hybridization with cDNA. (a) F2 MB, (b) F4 MB and (c) F6 MB.

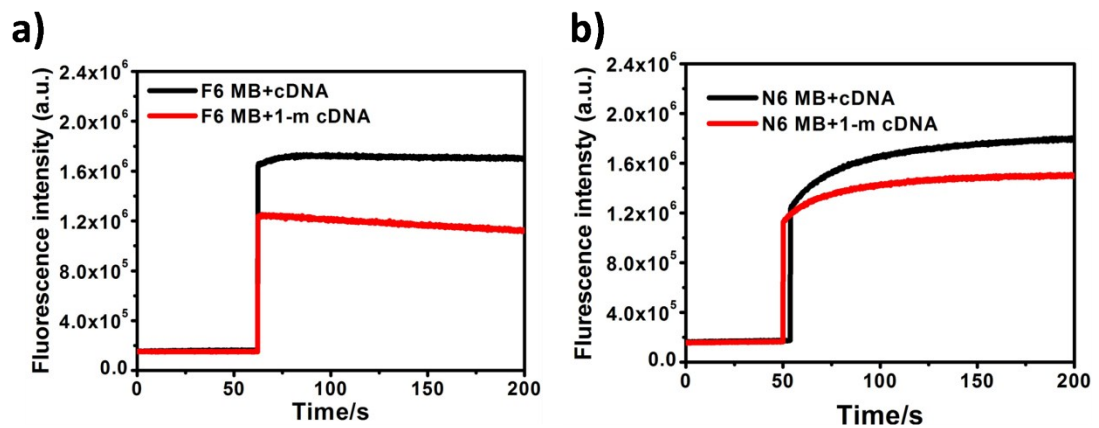


Figure S2. Fluorescence spectroscopy kinetics of F6 MB (a) and N6 MB (b) treated with cDNA (black line) and synthetic one-base mismatch target (1m-cDNA) (red line).

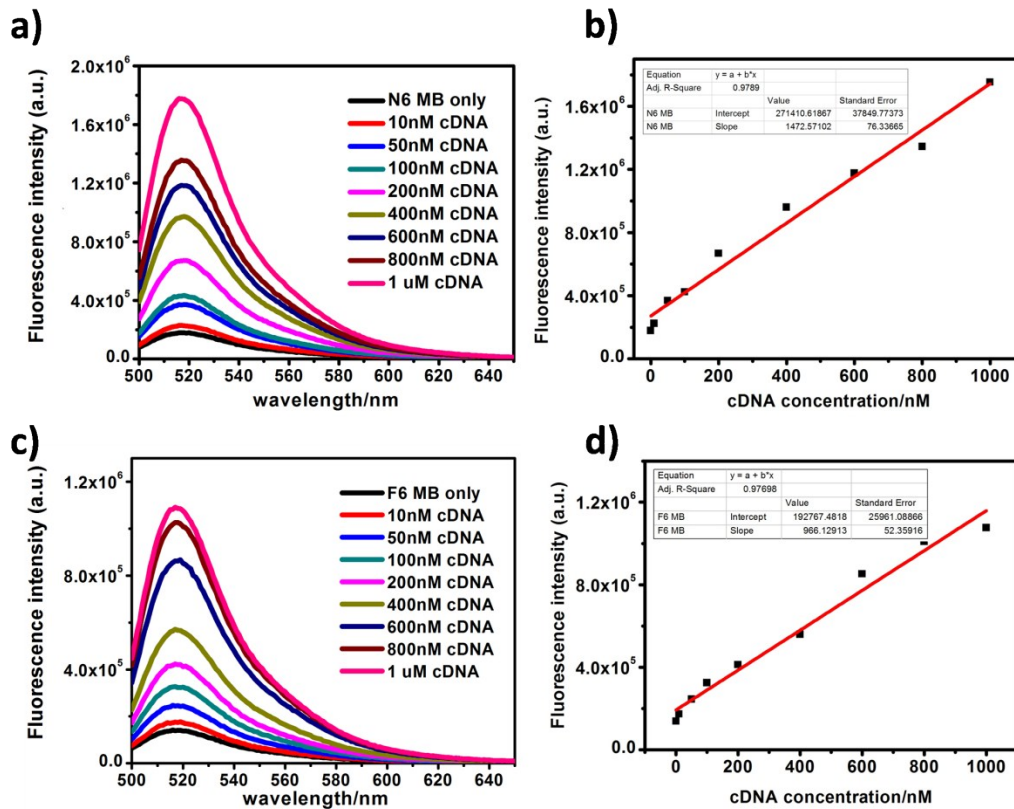


Figure S3. Fluorescence spectroscopy of 1 μ M N6 MB (a) and F6 MB (c) treated with cDNA. b & d) The fitted linear relation of N6 MB (b) and F6 MB (d) function to the concentration of cDNA. In both cases, the lowest detectable concentration of target DNA is 50 nM.

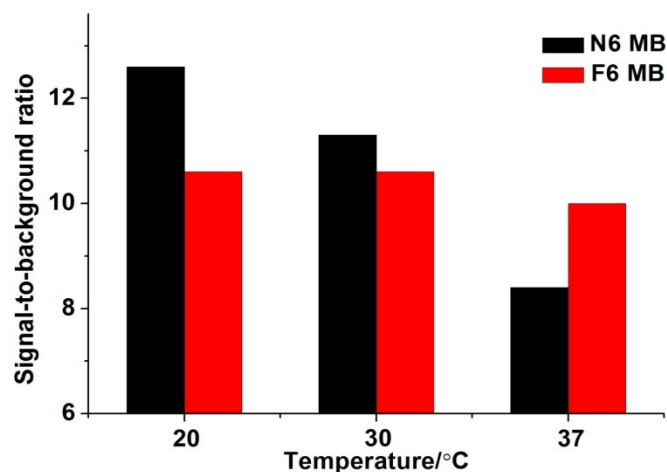


Figure S4. S/B ratios of F6 MB (red column) and N6 MB (black column) hybridized with cDNA at 20, 30 and 37 $^{\circ}$ C.

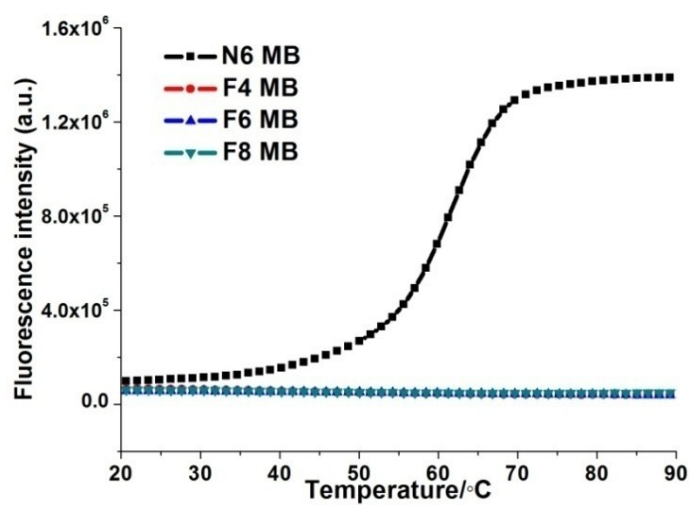


Figure S5. Melting curves of 200 nM FMBs and N6 MBs.

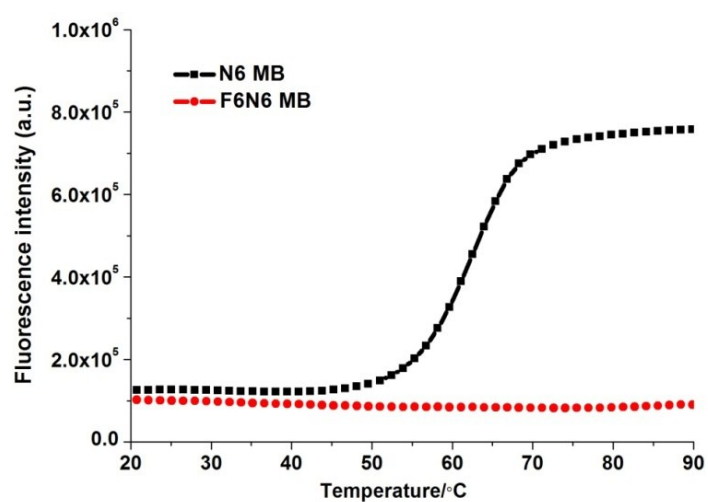


Figure S6. Melting curves of F6N6 MB and N6 MB. F6N6 MB represents FMBs with additional six natural base pairs in stem region.

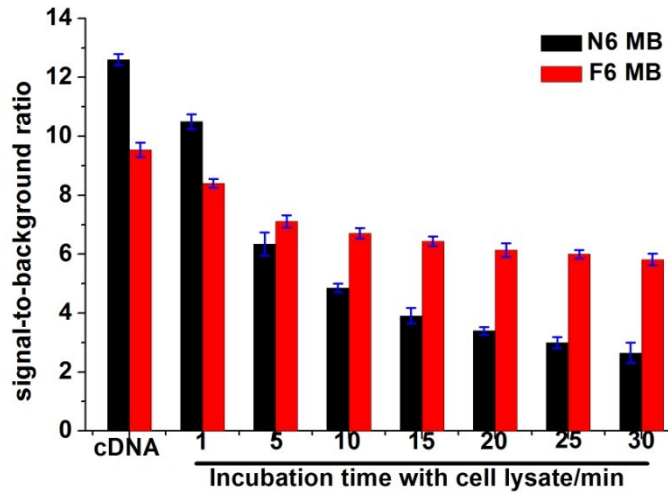


Figure S7. Comparison between the S/B ratio of F6 MB (red column) and N6 MB (black column) with various incubation times to CCRF-CEM cell lysate.

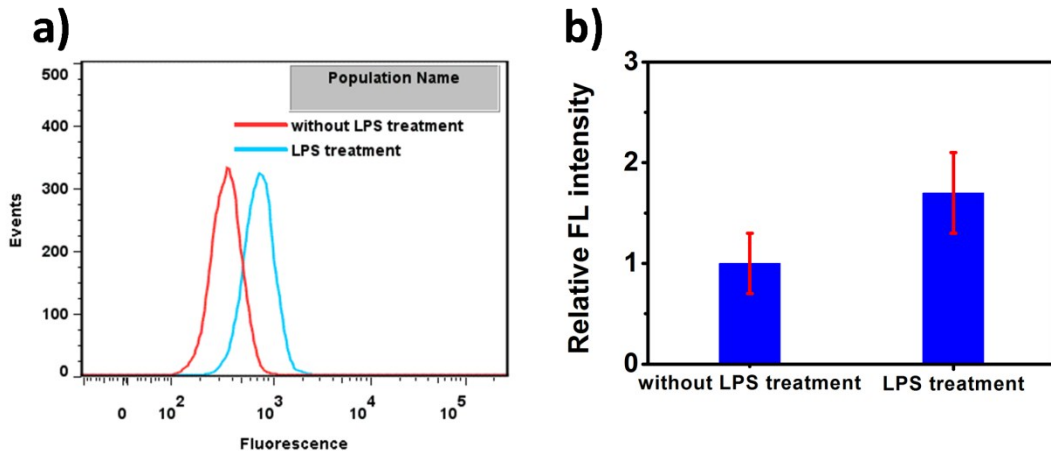


Figure S8. (a) Flow cytometry analysis and (b) the relative fluorescence intensity of MCF-7 cells (with and without LPS treatment) after incubation with AS1411-linked F6 MnSOD MBs.

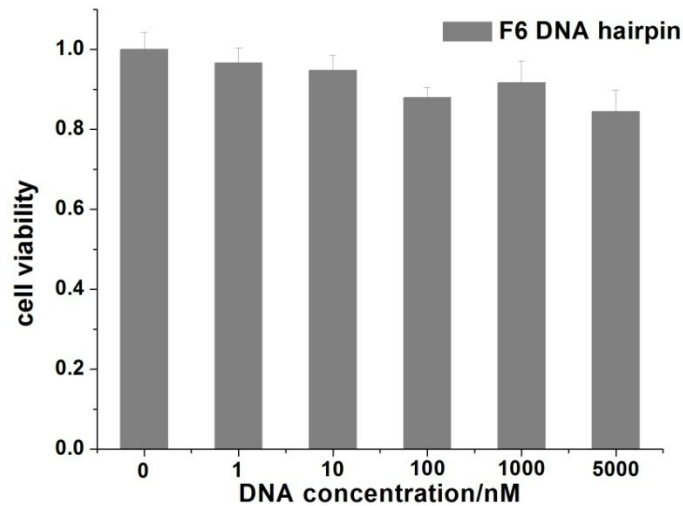


Figure S9. Cytotoxicity assay of MCF-7 cells treated with F6 DNA hairpin.

Table S1. DNA sequences designed in this article.

Name	Sequence (from 5' to 3')
F2 MB	FAM FF TCT AAA TCA CTA TGG TCG C FF Dabcyl
F4 MB	FAM FFFF TCT AAA TCA CTA TGG TCG C FFFF Dabcyl
F6 MB	FAM FFFFFF TCT AAA TCA CTA TGG TCG C FFFFFF Dabcyl
F8 MB	FAM FFFFFFF TCT AAA TCA CTA TGG TCG C FFFFFFF Dabcyl
F6N6 MB	FAM FFFFFF CCG AGC TCT AAA TCA CTA TGG TCG C GCT CGG FFFFFF Dabcyl
N6 MB	FAM CCG AGC TCT AAA TCA CTA TGG TCG C GCTCGG Dabcyl
cDNA	GCG ACC ATA GTG ATT TAG A
1m-cDNA	GCG ACC ATA GAG ATT TAG A
Oligo 2	CCA TAG TGA TTT AGA GCT CGG
Oligo3	TAG TGA TTT AGA GCT CGG
Oligo4	TGATTT AGA GCT CGG
AS1411- F6MnSOD MB	Dabcyl FFFFFF AGT TAC ATT CTC CCA GTT GAT T FFFFFF FAM TTT GGT GGT GGT GGT TGT GGT GGT GGT GGT TT
AS1411-F6 control MB	Dabcyl FFFFFF TCT AAA TCG CTA TGG TCG C FFFFFF FAM TTT GGT GGT GGT GGT TGT GGT GGT GGT GGT TT

MnSOD DNA	AAT CAA CTG GGA GAA TGT AAC T
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Note: **F** refers to F base

Reference

1. R. Wang, C. Wang, Y. Cao, Z. Zhu, C. Yang, J. Chen, F.-L. Qing and W. Tan, *Chemical Science*, 2014, **5**, 4076-4081.