Electronic Supplementary Material (ESI) for Analyst

Supporting Information

Design of two and three input molecular logic gates using non-Watson-Crick base pairing-based molecular beacons

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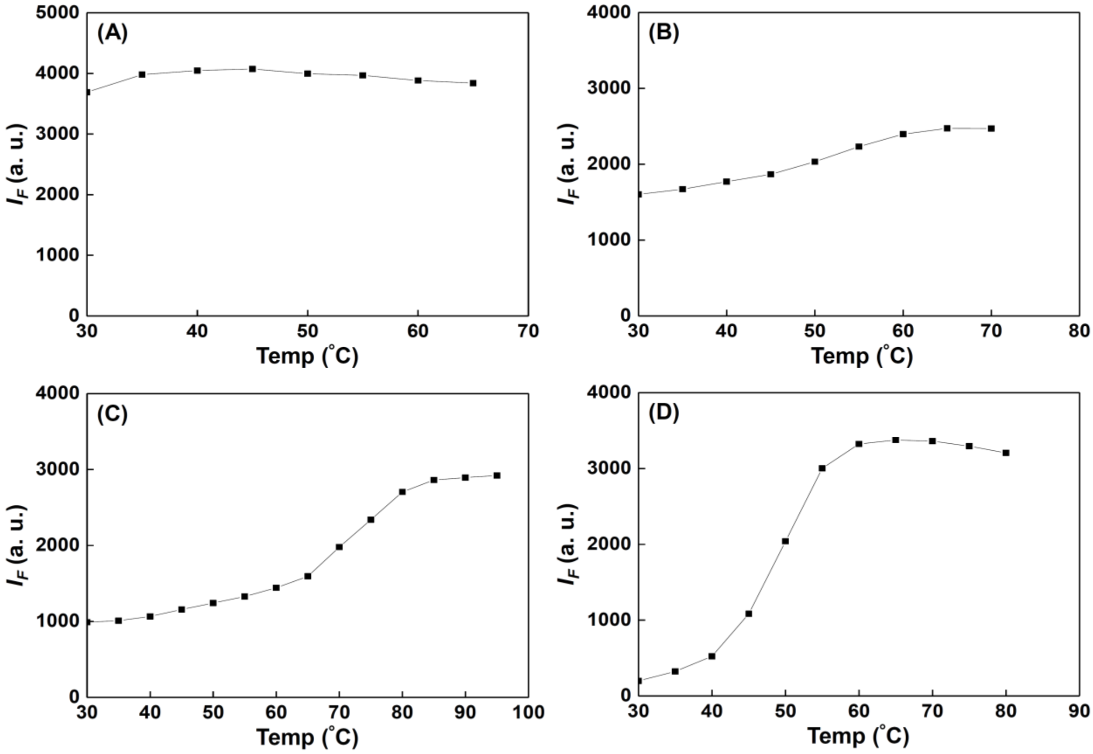

Figure S1. Effect of the increased temperature on the fluorescence intensity at 520 nm of 20 nM MB in the (A) absence and (B-D) presence of (B) 1 μM Hg2+, (C) 1 μM Ag+ and (D) 1 μM coralyne.

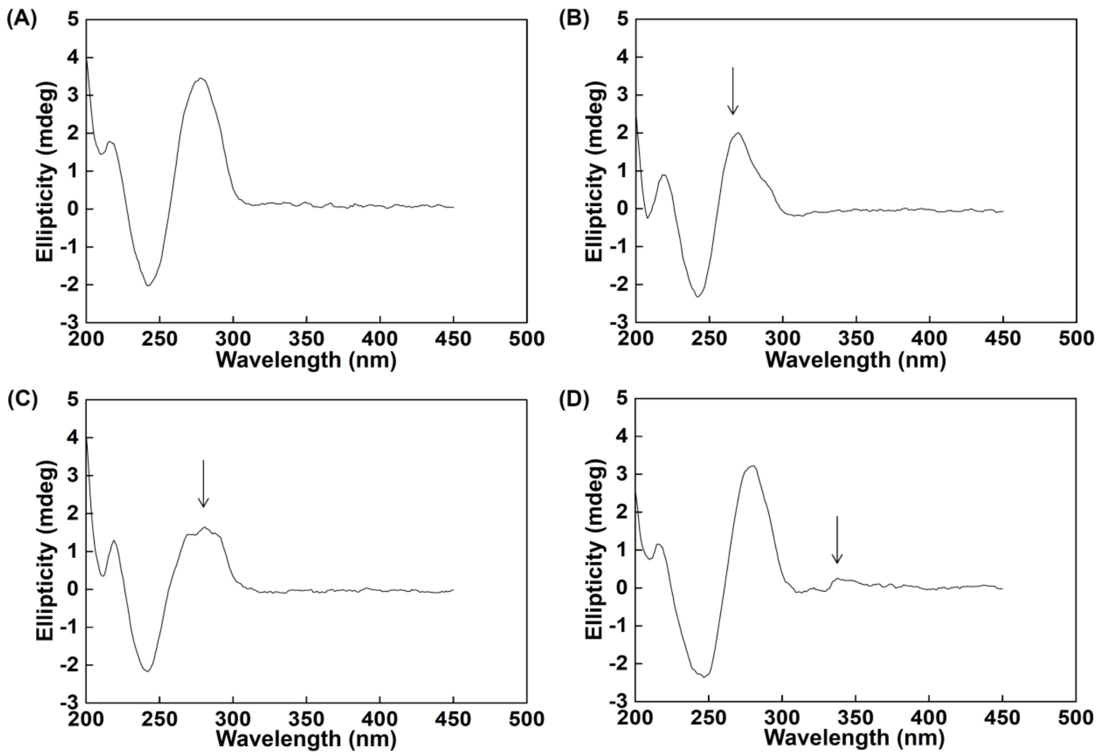

Figure S2. CD spectra of a solution of (A) MB, (B) MB and Hg2+, (C) MB and Ag+, and (D) MB and coralyne. The concentrations of MB, Hg2+, Ag+, and coralyne are 10, 50, 50, and 50 μM, respectively.

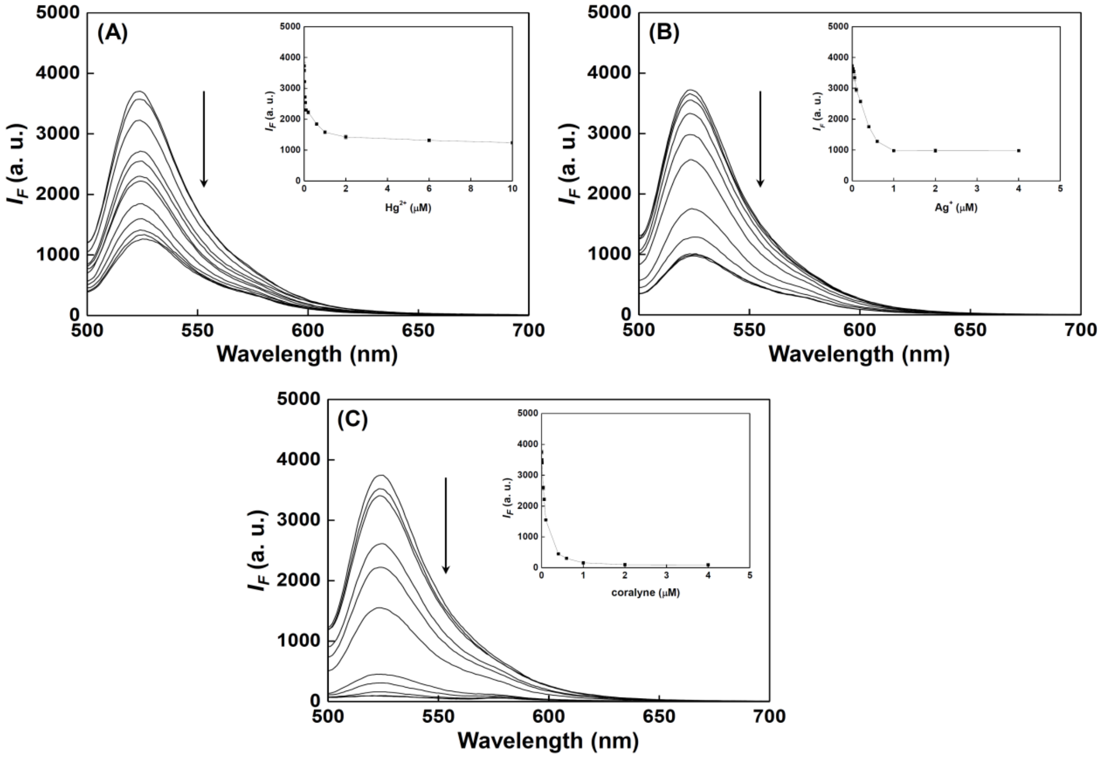

Figure S3. Fluorescence spectra of a solution of 20 nM MB in the presence of increasing concentration of (A) Hg2+, (B) Ag+, and (C) coralyne. The arrows indicate the signal changes with increase in analyte concentration (A: 0, 0.01, 0.02, 0.04, 0.06, 0.1, 0.2, 0.6, 1, 2, 6, and 10 μM; B: 0, 0.02, 0.04, 0.06, 0.1, 0.2, 0.4, 0.6, 1, 2, and 4 μM; C: 0, 0.006, 0.01, 0.04, 0.06, 0.1, 0.4, 0.6, 1, 2, and 4 μM). The MB probe was incubated with analyte in 5 mM phosphate buffer (pH 7.4) for 5 min at ambient temperature.

Table S1. Comparison of other sensors for the determination of Hg2+.

Sensor	detectiona	LOD	linear range	ref
thymine-rich molecular beacon based sensor	fluorescence	40 nM	20 to 600 nM	Angew. Chem. Int. Ed. 2004, 43, 4300-4302
TOTO-labeled polyT	fluorescence	3 nM	10 to 200 nM	Anal. Chem. 2008, 80, 3716-3721.
SG-labeled thymine-rich DNA	fluorescence	1 nM	3 to 66 nM	Chem. Commun., 2008, 4759-4761
[Pt(terpy)Cl]+-labeled polyT	phosphorescence	19 nM	300 to 6000 nM	Chem. Commun., 2009, 7479-7481
conjugated polymer-based T-rich DNA	fluorescence	42 nM	5 to 667 nM	Adv. Mater. 2007, 19, 1471-1474
polyT-modified gold nanoparticles	colorimetry	250 nM	500 to 5000 nM	Chem. Commun. 2008, 2242-2244
polyT-modified gold nanoparticles	colorimetry	10 nM	10 to 1000 nM	Biosens. & Bioelectron. 2009, 25, 204-210
ferrocence conjugated polyT DNA	DPV	0.5 nM	1 to 250 nM	Anal. Chem. 2009, 81, 5724–5730
ferrocence conjugated T-rich DNA	DPV	100 nM	100 to 2000 nM	Analyst 2009, 134, 1857-1862
T-rich FAM-ssDNA-absorbed gold nanoparticles	fluorescence	4 nM	100 to 6400 nM	Anal. Chem. 2008, 80, 9021-9028
T-rich FAM-ssDNA-absorbed SWNTs	fluorescence	14.5 nM	50 to 8000 nM	Chem. Commun., 2010,46, 1476-1478
polyT-modified gold nanoparticles	colorimetry	Not given	10 to 2000 nM	Angew. Chem. Int. Ed. 2007, 46, 4093-4096
polyT-modified gold nanoparticles	colorimetry	Not given	500 to 50000 nM	J. Am. Chem. Soc. 130, 3244-3245
T-Hg2+-T-based electron transfer sensor	CV	0.1 nM	0.1 to 1000 nM	J. Am. Chem. Soc., 2010, 132 , 6878-6879
T-rich modified DNA and gold nanoparticles amplification	DPV	0.5 nM	1-100 nM	Chem. Commun., 2009, 5633-5635
polyT-modified silver nanoparticles and SYBR green	Fluorescence	0.03 nM	0.01-0.5 nM	Biosens. & Bioelectron. 2012, 34, 185-190.
graphene oxide-based polythymine	fluorescence	0.5 nM	10 nM-2 μM	Analyst 2012, 137, 3300-3305

enzyme hybrided e-T-rich DNA	DPV	0.2 nM	Not given	Anal. Chem. 2013, 85, 4586–4593
thymine-rich DNA strands	EIS	0.1 nM	0.1 to 10 μM	Anal. Chem. 2011, 83, 6896-6901
metal/DNA-ligation and supermolecule	fluorescence	50 nM	200 nM to 5 μM	Analyst, 2013, 138, 2755–2760
thymine-rich DNA strands and GO	fluorescence	0.92 nM	1 to 50 nM	Biosens. & Bioelectron. 2013, 41, 889–893
hairpins conformation change of thymine-rich DNA	SWV	2.5 nM	5 to1000 nM	Biosens. & Bioelectron. 2013, 39, 315–319
target-induced conformation change of thymine-rich DNA	SWV	6.0 pM	0.01 to 1000 nM	Analyst, 2012, 137, 4425–4427
metal ion-triggered DNA-cleaving DNAzymes	colorimetry	4 nM	Not given	Biosens. & Bioelectron. 2012, 38, 331–336
Ru(bpy)2(dppz)2+ -labeled thymine rich DNA	ECL	20 pM	0.1 to 10 nM	Biosens. & Bioelectron.2012, 37, 37, 112–115
molecular beacon-based DNA sensor	fluorescence	2.5 nM	10 to 400 nM	Chem. Commun., 2011, 47, 12158–12160
mercury ion-induced FRET of quantum dots/DNA/gold nanoparticles	fluorescence	2 nM	2 to 60 nM	Anal. Chem. 2011, 83, 7061–7065
Hg2+-mediated structrure changing of G-quadruplex DNAzyme	colorimetry	9.2 nM	0 to 300 nM	Biosens. & Bioelectron. 2011, 26, 148-152
T-rich FAM-ssDNA and carbon dots	fluorescence	Not given	0 to 250 nM	Biosens. & Bioelectron. 2011, 26, 4656-4660
SYBR green-labeled thymine-rich DNA and single wall carbon nanotube	fluorescence	7.9 nM	20 to 1250 nM	Analyst, 2011, 136, 1632–1636
Ru(bpy)32+ dendrimer-labeled thymine-rich DNA	ECL	2.4 pM	7 pM to 50 nM	Biosens. & Bioelectron. 2012, 32, 37-42
FRET between dye-labeled ssDNA and	fluorescence	1.5 nM	0 to 20 nM	Biosens. & Bioelectron.2012, 36, 174-178

quantum dots				
T-Hg2+-T based molecular beacon probe	fluorescence	19 nM	Not given	Anal. Chem. 2012, 84, 4970−4978
T-Hg2+-T coordination with enzymatic signal amplification	electrochemical detection	0.3 nM	0.5 to 1 μM	Biosens. & Bioelectron. 2011, 26, 3320-3324
gold nanoparticle conjugated aptamer	fluorescence	57 pM	10 pM to 1 μM	Biosens. & Bioelectron. 2013, 41, 827-832
molecular beacon	fluorescence	3 nM	10 to 5000 nM	This study

a FRET, fluorescence resonance energy transfer; DPV, differential pulse voltammetry; CV, cyclic voltammograms; EIS, electrochemical impedance spectroscopy; SWV, square wave voltammetry; ECL, electrochemiluminescence.

Table S2. Comparison of other sensors for the determination of silver ions.

Sensors	detection	LOD	linear range	ref
Ru(bpy)2(dppz)2+ -labeled C-rich DNA and quantum dots	fluorescence	0.1 μM	2 to 10 μM	Analyst, 2013, 138, 421–424
SYBR Green-label polycytosine ssDNA	fluorescence	32 nM	50 to 700 nM	Chem. Commun., 2009, 6619–6621
SYBR Green-label cytosine-rich ssDNA	fluorescence	1 nM	1 to 100 nM	Analyst, 2013, 138, 2057-2060.
cytosine-rich DNA strands	electrochemistry	10 nM	100 to 800 nM	Anal. Chem., 2011, 83, 6896-6901
cytosine-rich oligonucleotide and graphene oxide	fluorescence	14 nM	20 to 1500 nM	Chem. Commun., 2012, 48, 82–84
cytosine-rich oligonucleotide and gaphene oxide nanoprobe	fluorescence	5 nM	Not given	Chem. Commun., 2010, 46, 2596–2598
G-rich FAM-ssDNA and graphene oxide	fluorescence	0.05 μM	0.1 to 10 μM	Talanta, 2013, 107, 277-283
G-rich DNAzyme	colorimetric	64 nM	100 to 3000 nM	Anal. Chem., 2010, 82, 789-793
silver-ion-induced DNAzyme switch	colorimetric	2.5 nM	5 to 100 nM	Chem. Eur. J., 2009, 15, 3347-3350
cytosine-based FRET sensor	fluorescence	Not given	Not given	Chem. Commun., 2008, 4825-4827
c-rich FAM-ssDNA and carbon dots	fluorescence	500 pM	0 to 400 nM	Langmuir, 2011, 27, 4305-4308
molecular beacon	fluorescence	6 nM	20 to 1000 nM	This study

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Table S3. Comparison of other sensors for the determination of coralyne.

Sensor	detection	LOD	linear range	ref
G-quadruplex DNAzyme	absorption	19 nM	0.06 to 10 μM	Anal. Method 2013, 5, 4671-4674
graphene oxide-based aptamer sensor	fluorescence	Not given	10 to 700 nM	Talanta 2013, 112, 117-122
poly(dA)-based DNA sensor	fluorescence	65 nM	0.1 to 10 μM	Chem. Commun., 2011, 47, 11134-11136
poly(dA)-adsorbed gold nanoparticle	absorption	Not given	0 to 728 nM	Analyst, 2009, 134, 1647–1651
coralyne-induced formation of peroxidasemimicking split DNAzyme	Absorption	31 nM	50 to 5000 nM	Analyst, 2013, 138, 4728-4731
molecular beacon	fluorescence	2 nM	6 to 1000 nM	This study

Table S1. The use of the proposed MB for creating truth tables of AND, OR, INHIBIT, NAND, NOR, and REVERSE IMPLICATION Boolean logic gates

AND		
$Input_1$	$Input_2$	Output (I_F)
SAH (10 μM)	SAHH (40 units/L)	
0	0	0 (1590)
1	0	0 (1417)
0	1	0 (1661)
1	1	1 (3274)

OR		
$Input_1$	$Input_2$	Output (I_F)
Cys (10 μM)	EDTA (100 μM)	
0	0	0 (1322)
1	0	1 (3694)
0	1	1 (3255)
1	1	1 (3671)

INH		
$Input_1$	$Input_2$	Output (I_F)
Cys (10 μM)	H_2O_2 (100 mM)	
0	0	0 (1052)
1	0	1 (3732)
0	1	0 (1128)
1	1	0 (1109)

NAND		
$Input_1$	$Input_2$	Output (I_F)
AgNPs (630 pM)	H_2O_2 (10 mM)	
0	0	1 (3715)
1	0	1 (2954)
0	1	1 (3497)
1	1	0 (720)

NOR		
$Input_1$	$Input_2$	Output (I_F)
Hg^{2+} (5 μM)	Ag^+ (1 μM)	
0	0	1 (3743)
1	0	0 (1342)
0	1	0 (974)
1	1	0 (1101)

REVERSE IMPLICATON		
$Input_1$	$Input_2$	Output (I_F)
Hg^{2+} (5 μM)	GSH (10 μM)	
0	0	1 (3708)
1	0	0 (1346)
0	1	1 (3692)
1	1	1 (3754)