SUPPLEMENT INFORMATION

Limitations for colorimetric aggregation assay of metal ions and ways of their overcoming

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Numerical simulation of the system

For numerical simulation using the COPASI software, the following parameters were used:

>Model
>Biochemical
>Compartments
>Probe
Details: Simulation Type – fixed
Contained Species – A, A2Pb, APb, APbA, Pb

>Species

Name	Simulation Type	Initial Concentration (mmol/ml)
A	Reactions	1e-05
APb	Reactions	0
Pb	Reactions	1e-07
A2Pb	Reactions	0
APbA	Reactions	0

>Reactions:
>Reaction 1
A + Pb = APb
Rate Law: Mass action (reversible)

>Reaction 2
A + APb = A2Pb
Rate Law: Mass action (reversible)

>Reaction 3
A + APb = APbA
Rate Law: Mass action (reversible)

>Parameter Overview

k1(Reaction 1) ml/(mmol*s)	k2(Reaction 1) 1/s	k1(Reaction 2) ml/(mmol*s)	k2(Reaction 2) 1/s	k1(Reaction 3) ml/(mmol*s)	k2(Reaction 3) 1/s
10000	0.01	10000	0.01	10000	0.01

>Mathematical

>Differential equations

$$\frac{d([A]\cdot V_{compartment})}{dt} = -V_{compartment}\cdot((10000\cdot[A]\cdot[Pb]-0.01\cdot[APb])) - V_{compartment}\cdot((10000\cdot[A]\cdot[APb]-0.01\cdot[A2Pb])) - V_{compartment}\cdot((10000\cdot[A]\cdot[APb]-0.01\cdot[APbA]))$$

$$\frac{d([APb]\cdot V_{compartment})}{dt} = +V_{compartment}\cdot((10000\cdot[A]\cdot[Pb]-0.01\cdot[APb])) - V_{compartment}\cdot((10000\cdot[A]\cdot[APb]-0.01\cdot[A2Pb])) - V_{compartment}\cdot((10000\cdot[A]\cdot[APb]-0.01\cdot[APbA]))$$

$$\frac{d([Pb]\cdot V_{compartment})}{dt} = -V_{compartment}\cdot((10000\cdot[A]\cdot[Pb]-0.01\cdot[APb]))$$

$$\frac{d([A2Pb]\cdot V_{compartment})}{dt} = +V_{compartment}\cdot((10000\cdot[A]\cdot[APb]-0.01\cdot[A2Pb]))$$

$$\frac{d([APbA]\cdot V_{compartment})}{dt} = +V_{compartment}\cdot((10000\cdot[A]\cdot[APb]-0.01\cdot[APbA]))$$

>Tasks

>Time course

Duration (s) – 300, Interval size (s) – 3, Intervals – 100

>Parameter scan

Object – [Pb]_0

Intervals – 100, min – 1e-07, max – 4e-05

Task – Time course

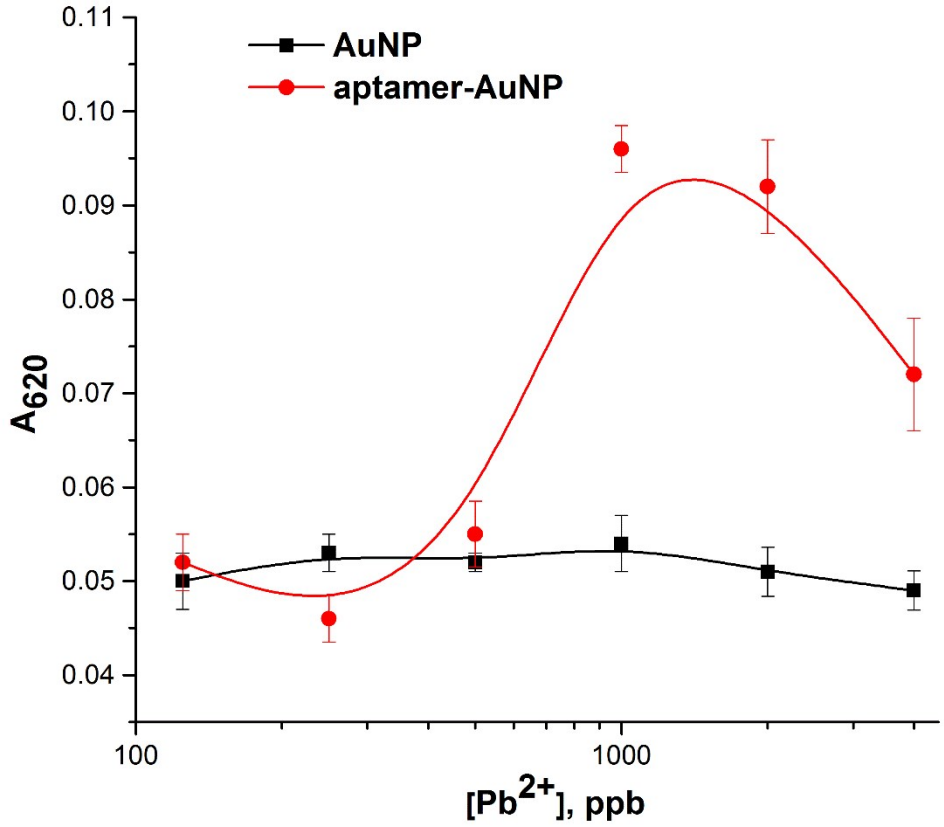

Fig. S1. Optical density versus Pb^{2+} ion concentration (n=3). Red curve corresponds to the gold nanoparticles conjugated with aptamer, black curve (below) corresponds to native citrate-capped gold nanoparticles