applied sciences

MDPI

SUPPORTING INFORMATION

Changing Cross-Reactivity for Different Immunoassays Using the Same Antibodies: Theoretical Description and Experimental Confirmation

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Numerical modeling of competitive immunochromatographic analysis

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

>Model
>Biochemical
>Compartments
>Probe
Details: Simulation Type – fixed
Contained Species – Ag, Ab, AgAb, Ag*, AbAg*

>Species

Name	Simulation Type	Initial Concentration (mmol/ml)	Expression (mmol/ml)
Ag	ode	1e-09	(reaction 1).k2*[AgAb]-(reaction 1).k1*[Ag]*[Ab]
Ab	ode	2e-10	(reaction 1).k2*[AgAb]-(reaction 1).k1*[Ag]*[Ab]
AgAb	ode	0	(reaction 1).k1*[Ag]*[Ab]) -(reaction 2).k2*[AgAb]
Ag*	ode	1.6e-10	(reaction 2).k2*[AbAg*]-(reaction 2).k1*[Ab]*[Ag*]
AbAg*	ode	0	((reaction 2).k1*[Ag*]*[Ab]-(reaction 2).k2*[AbAg*])

>Reactions:
>Reaction 1
Ag + Ab = AgAb
Rate Law: Mass action (reversible)

>Reaction 2

Ab + Ag* = AbAg*

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
1000000	0.0001	1000000	0.0001

>Mathematical

>Differential equations

$$\frac{d([Ab]\cdot V_{compartment})}{dt} = V_{compartment}\cdot("(reaction1).k2"\cdot[AgAb]-"(reaction1).k1"\cdot[Ag]\cdot[Ab])$$

$$\frac{d([Ag]\cdot V_{compartment})}{dt} = V_{compartment}\cdot("(reaction1).k2"\cdot[AgAb]-"(reaction1).k1"\cdot[Ab]\cdot[Ag])$$

$$\frac{d([AgAb]\cdot V_{compartment})}{dt} = V_{compartment}\cdot("(reaction1).k1"\cdot[Ag]\cdot[Ab]-"(reaction1).k2"\cdot[AgAb])$$

$$\frac{d([iAg]\cdot V_{compartment})}{dt} = V_{compartment}\cdot(("(reaction2).k2"\cdot[iAgAb]-"(reaction2).k1"\cdot[iAg]\cdot[Ab])$$

$$\frac{d([iAgAb]\cdot V_{compartment})}{dt} = V_{compartment}\cdot(("(reaction2).k1"\cdot[iAg]\cdot[Ab]-"(reaction2).k2"\cdot[iAgAb])$$

>Tasks

>Time course

Duration (s) – 600/3600, Interval size (s) – 60/360, Intervals – 10

>Parameter scan

Object – [A]_0

Intervals – 100, min – 2e-11, max – 2e-08

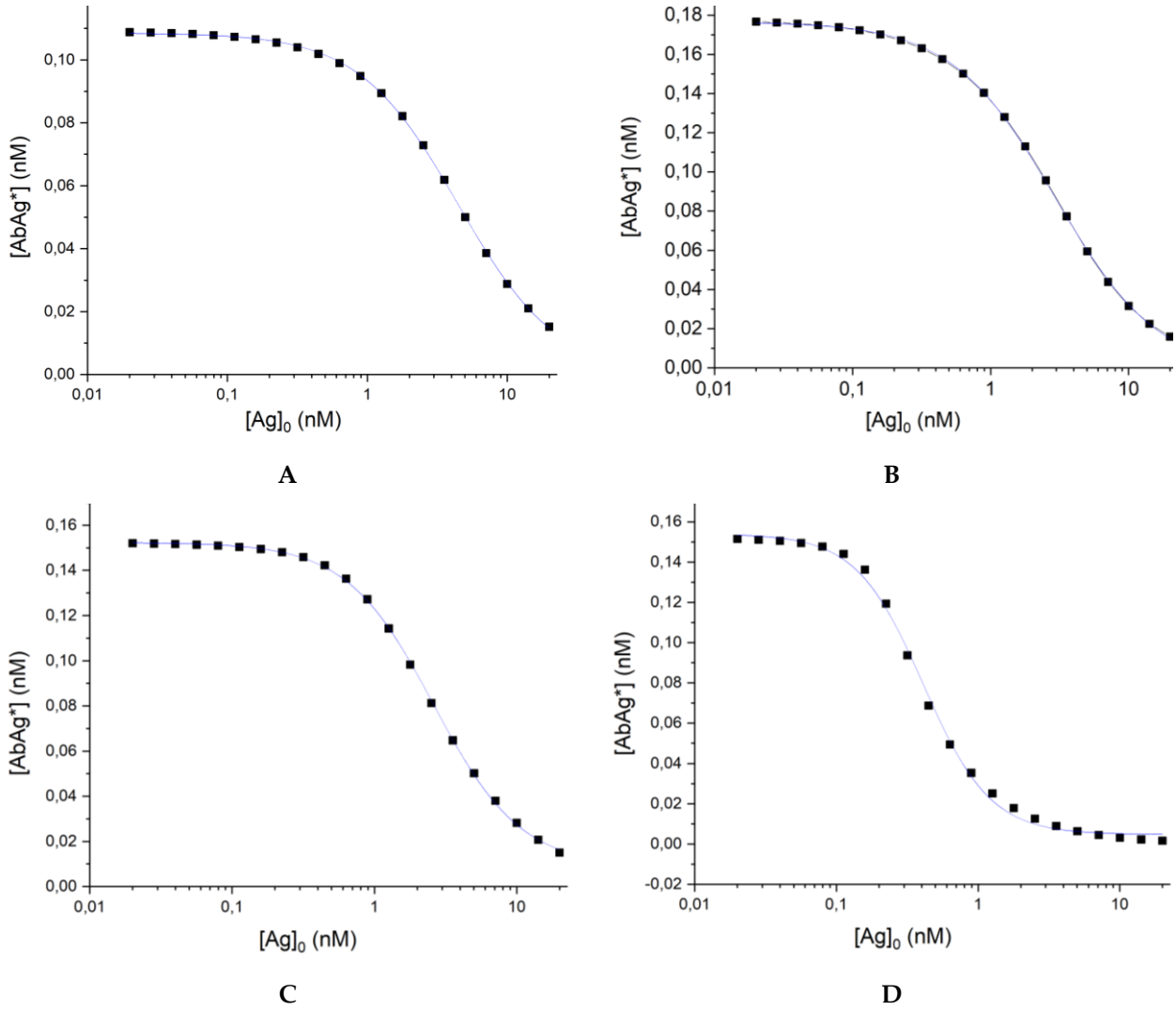


Figure S1. Theoretical calibration dependences of nonequilibrium competitive immunoassay at different reaction times (t) and different values of the kinetic association constant (ka): **A.** t = 600 s, ka = 10^6 1/(M*s); **B.** t = 600 s, ka = 10^7 1/(M*s); **C.** t = 3600 s, ka = 10^6 1/(M*s); **D.** t = 3600 s, ka = 10^7 1/(M*s). The concentration of antigen derivative $[Ag^*]_0$ - 0.16 nM, the concentration of specific antibodies $[Ab]_0$ - 0.2 nM, kinetic dissociation constant kd – 0.0001 1/s.