

Upconversion nanoparticle as elemental tag for the determination of alpha-fetoprotein in human serum by inductively coupled plasma mass spectrometry

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Supporting information

The number of lanthanides in UCNPs

It is known that the arrangement of atoms in NaYF₄ is hexagonal closest packing, which has an occupancy of 74.05%. Assuming that the diameter of a UCNP is 50 nm, we could obtain an approximate number of atoms. The details are listed below.

Firstly, assuming that all the lanthanide atoms are Y atoms.

For [YF₄]⁻, since it is sp³ hybridized, the distances from Y atom to each F atom are equal.

Assuming that [YF₄]⁻ is a sphere (Although sp³ hybridization means a tetrahedron), and its radius could be approximately calculated as

$$R([YF_4]^-) = R(F^-) + R(Y^{3+}) = 136 \text{ pm} + 93 \text{ pm} = 229 \text{ pm}$$

According to $V=4\pi R^3/3$

$$N([YF_4]^-) = N(Na^+) = 0.7405 V_{UCNP} / [V([YF_4]^-) + V(Na^+)] = 0.7405 R^3_{UCNP} / [R^3([YF_4]^-) + R^3(Na^+)]$$

Since $R_{UCNP} = 50 \text{ nm}$, $R([YF_4]^-) = 229 \text{ pm}$, $R(Na^+) = 95 \text{ pm}$

$N([YF_4]^-) = N(Na^+) = 7.19 \times 10^6$, which represent as the total lanthanide atoms in one UCNP.

The concentration of Y, Yb and Er in the prepared PAA modified UCNP dispersion was determined by calibrating standard solutions, and the concentrations of Y, Yb and Er were $3.38 \pm 0.12 \text{ g L}^{-1}$, $1.76 \pm 0.072 \text{ g L}^{-1}$ and $0.20 \pm 0.0089 \text{ g L}^{-1}$, corresponding to a molar ratio of 0.77:0.21:0.02. So the approximate number of Y, Yb and Er in one UCNP is 5.54×10^6 , 1.48×10^6 and 1.74×10^5 .

Table S1 Determination of ratio of Y and Yb in UCNP-antibody conjugates and eluent by ICP-MS in the same day. The samples were chosen randomly.

Serial	Ratio of Y/Yb signals in UCNP-antibody conjugates	Ratio of Y/Yb signals in eluent after the immunoassay
1	4.56	4.54
2	4.62	4.48
3	4.67	4.51
4	4.63	4.48
5	4.55	4.64
6	4.57	4.73
7	4.59	4.58
8	4.53	4.50
9	4.56	4.46
10	4.53	4.47
Average	4.58	4.54

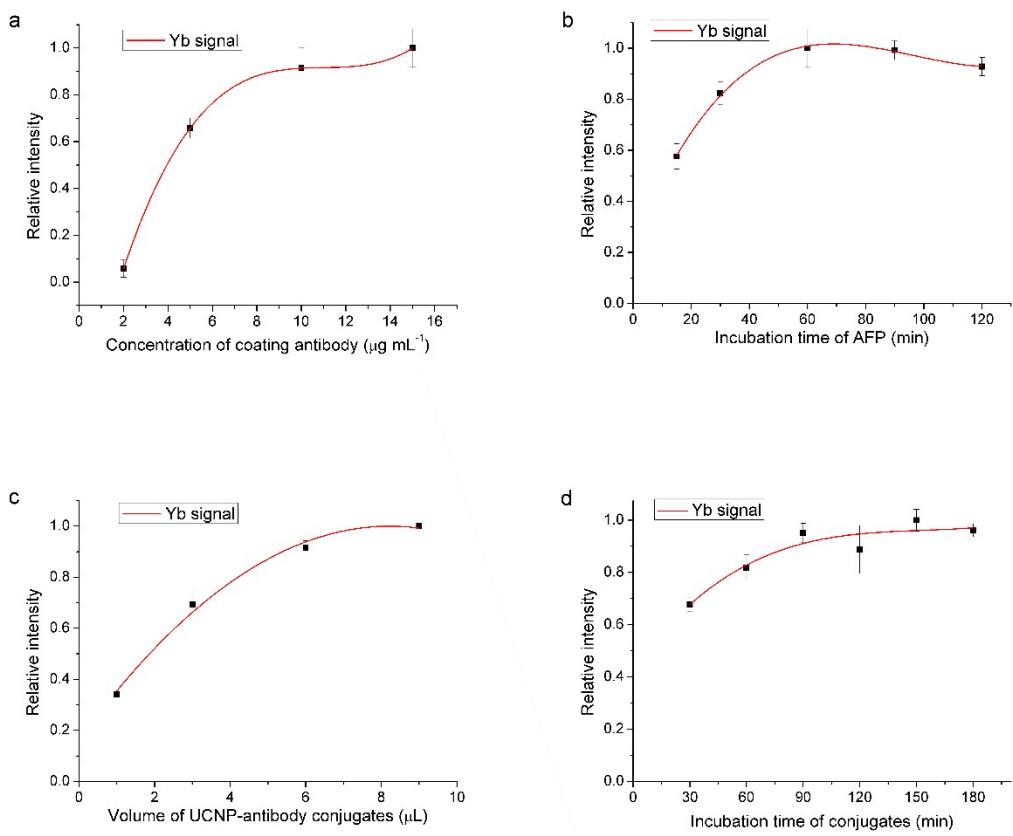


Fig. S1 Effect of concentration of coating antibody (a) as well as incubation time of AFP (b), and effect of volume (c) as well as incubation time of UCNP-antibody conjugates (d). All the results are based on the ICP-MS detection of Yb. The error bars in the figure represent standard deviations of three analyses.

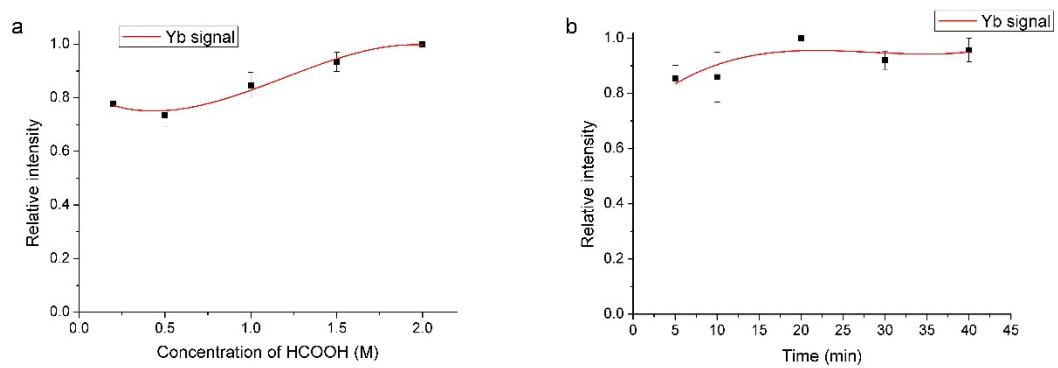


Fig. S2 Effect of concentration of formic acid (a), elution time (b) All the results are based on the ICP-MS detection of Yb. The error bars in the figure represent standard deviations of three analyses.