Computer modeling of fluorescence enhancement

The study of fluorescence enhancement factor for a model fluorophore, which corresponds to the properties of aflatoxin molecules (excitation wavelength 365 nm, quantum yield 0.51 [1]), in the presence of a spherical silver nanoparticle of different sizes located on the dielectric substrate (flint glass, ε = 2.59) in a polymer membrane (ε = 2.22) using the Green's function approach[2]was performed (Fig. S1). The fluorescence enhancement factor was calculated as the product of excitation rate enhancement and the quantum yield modification in the presence of silver nanoparticle[2]:

$$\frac{\gamma_{em}}{\gamma^{0}_{em}} = \frac{\gamma_{exc}}{\gamma^{0}_{exc}}\frac{q}{q^{0}}, \tag{1}$$

where

$$\frac{\gamma_{exc}}{\gamma^{0}_{exc}} = \left|1 + \frac{k^{2}}{\varepsilon_{0}}\overleftrightarrow{\mathbf{G}}(\mathbf{r_m},\mathbf{r_p})\overleftrightarrow{\boldsymbol{\alpha}}(\varphi)\right|^{2}, \tag{2}$$

$$q = \frac{\gamma_{r}/\gamma^{0}_{r}}{\gamma_{r}/\gamma^{0}_{r} + \gamma_{abs}/\gamma^{0}_{r} + (1-q^{0})/q^{0}}. \tag{3}$$

Here, γ_{em} is the molecule emission rate, γ_{exc} is the molecule excitation rate, q is the molecule quantum yield, $\overleftrightarrow{\mathbf{G}}(\mathbf{r_m},\mathbf{r_p})$ is the Green's function for electromagnetic field, $\overleftrightarrow{\boldsymbol{\alpha}}$ is the nanoparticle polarizability, φ is the distance between the nanoparticle and the dielectric substrate, γ_{r} is the radiative decay rate, γ_{abs} is the rate of energy transfer between the molecule and the nanoparticle. All the variables with superscript 0 are related to the flurophore molecule properties in the absence of the nanoparticle.

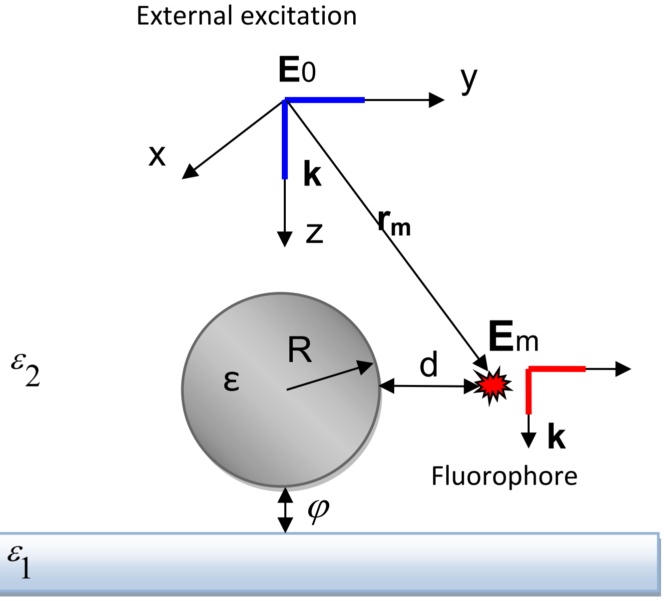

Fig. S1. Schematic drawing of a model system. Spherical nanoparticle with a radius of *R* is located on a dielectric substrate. Fluorophore molecule is located at a specific distance *d*from the nanoparticle surface.

It can be seen from the graph in Fig. S2 that the dependence of the fluorescence enhancement factor on the distance between the fluorophore and the nanoparticle surface is nonmonotonic and has a maximum depending on several factors: quantum yield of the fluorophore, nanoparticle size and the distance between the fluorophore. It can be also seen that the presence of a dielectric substrate somewhat reduces the magnitude of the fluorescence increase at an equidistant point, which increases in proportion to the size of the silver nanoparticle.

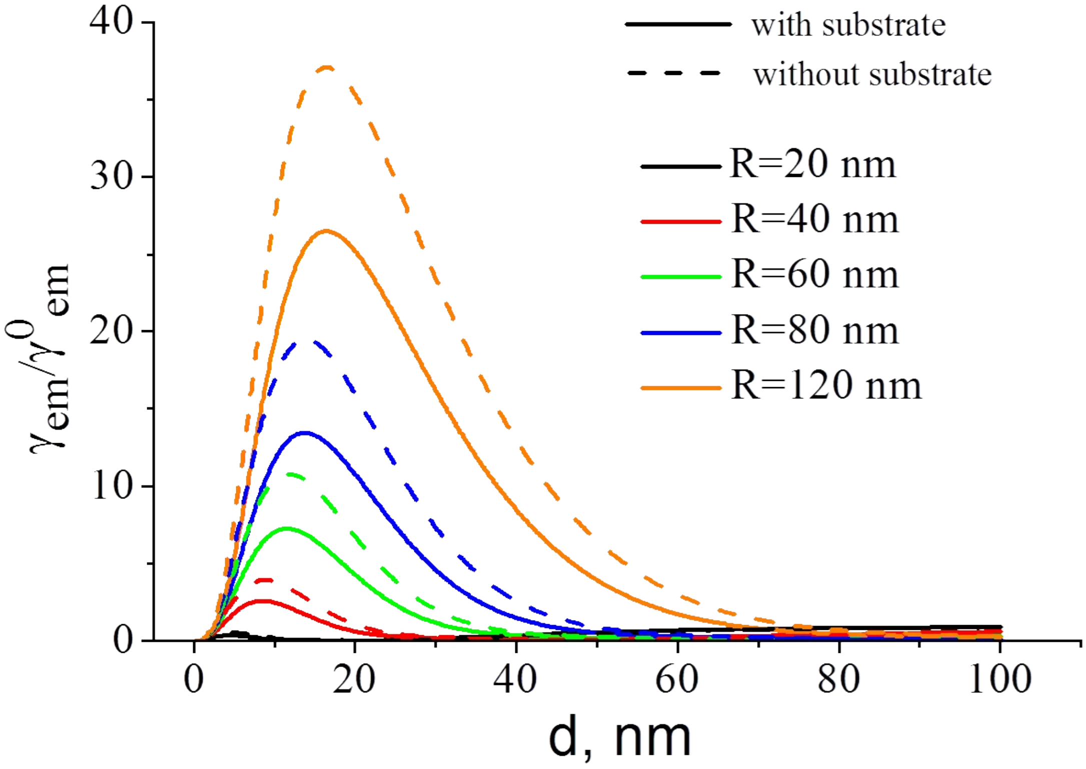

Fig. S2.The dependence of the fluorescence rate enhancement of a fluorophore molecule (q^0=0.51) on the distance from the molecule to the surface of a spherical silver nanoparticle of different radius.

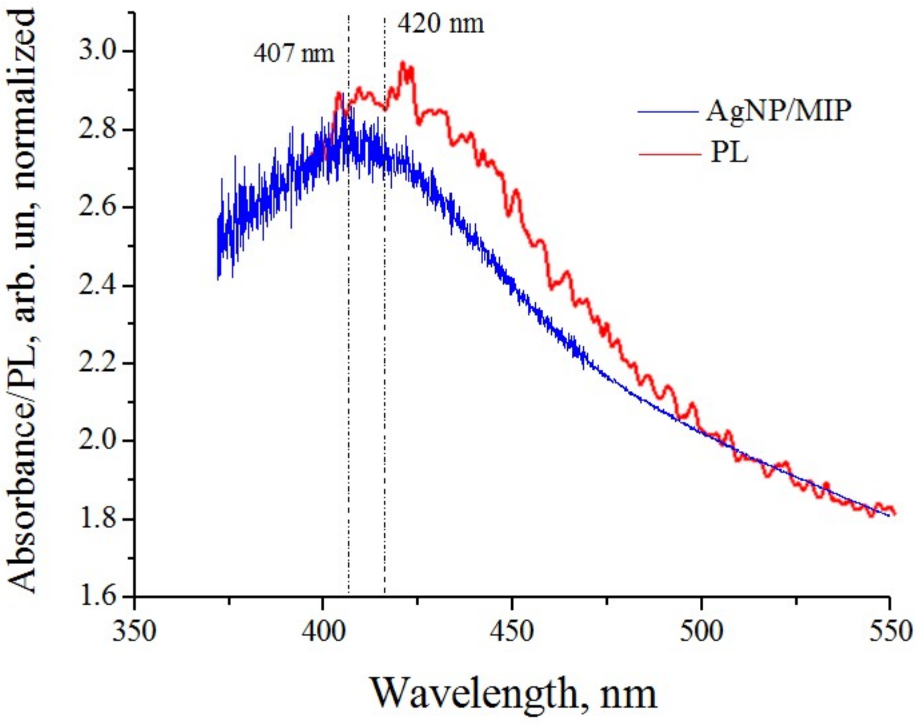

Fig. S3 The overlapping for absorbance spectra of MIP membrane with embedded Ag nanoparticles and emission spectra of molecules of aflatoxin B1, specifically bounded with MIP membrane.

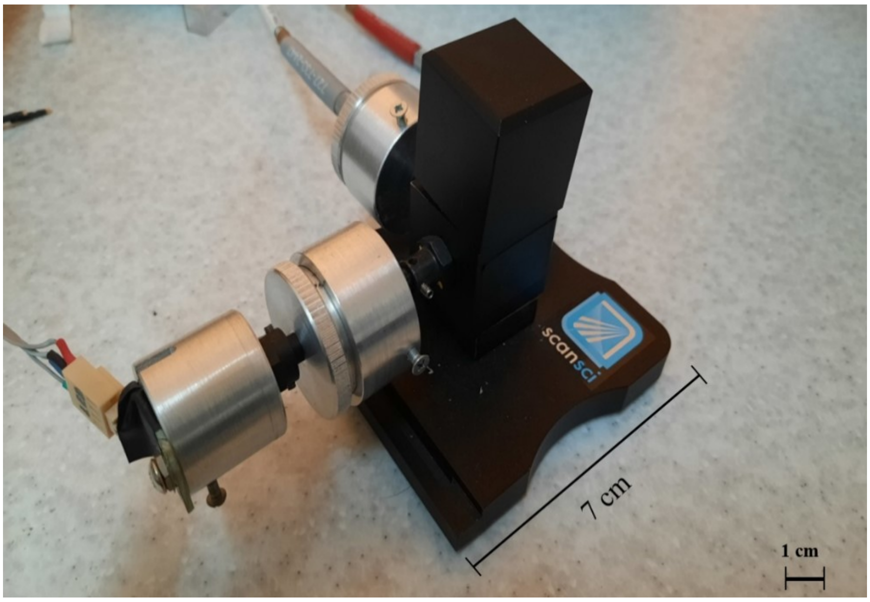

Fig. S4 The photograph of developed prototype of portable fluorimeter for LSPR/MIP detection of molecules of aflatoxin B1.

References

1. J. C.Netto-Ferreira, B.Heyne, J. C. Scaiano, *Photochemical &Photobiological Sciences*, 2011, **10(10)**, 1701-1708.

2. V. I. Chegel, O. M.Naum, A. M. Lopatynskyi, V. K. Lytvyn, *Nanoplasmonics, Nano-Optics, Nanocomposites, and Surface Studies*; Fesenko, O., Yatsenko, L., Eds.; Springer Proceedings in Physics; Springer International Publishing: Cham, 2015; Vol. **167**, pp 395–412.

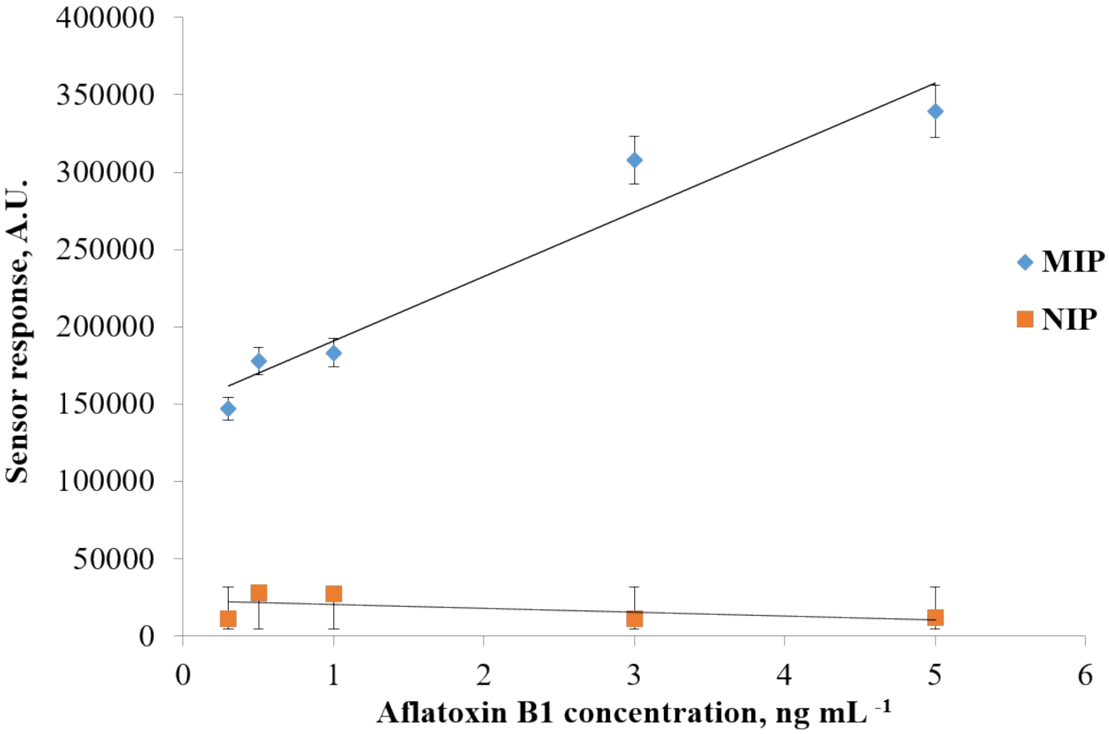

Figure S5 The fluorescent sensor signals obtained from AgNPs-containing MIP chips at low concentrations of aflatoxin B1 (0.3 - 5 ng mL $^{-1}$).