Effect of Silver Nanoparticles on the Photophysics of Riboflavin: Consequences on the ROS Generation.

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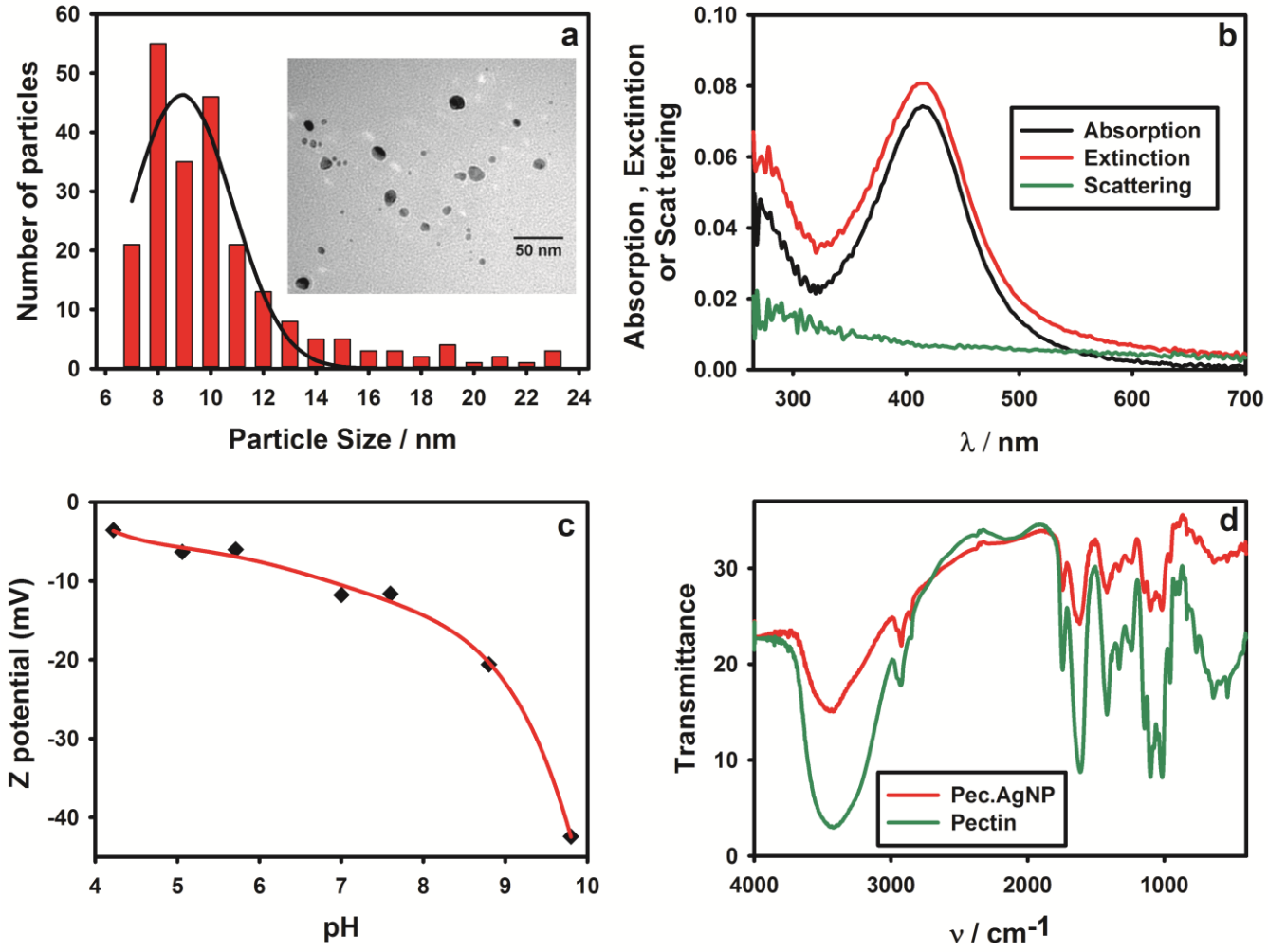

Figure S1: a) Size distribution histogram of Pec.AgNP. Inset: TEM image of Pec.AgNP. b) UV-vis absorption, extinction, and scattering spectra of a 11.7 M suspension of Pec.AgNP. c) Zeta potential measurements of Pec.AgNP as a function of pH. d) FTIR spectra of pectin and Pec.AgNP.

[Ag] / M	Lifetime / ns
0	4.73
4.55E-08	4.75
6.83E-08	4.75
7.88E-08	4.73
9.11E-08	4.75
1.18E-07	4.72
1.58E-07	4.72
4.55E-07	4.70
4.55E-07	4.75
6.83E-07	4.68
7.88E-07	4.72
9.11E-07	4.69
4.55E-06	4.73

Table S1: Fluorescence lifetimes of Rf in the absence and presence of Pec.Ag NP (λ^{exc} = 388 nm).

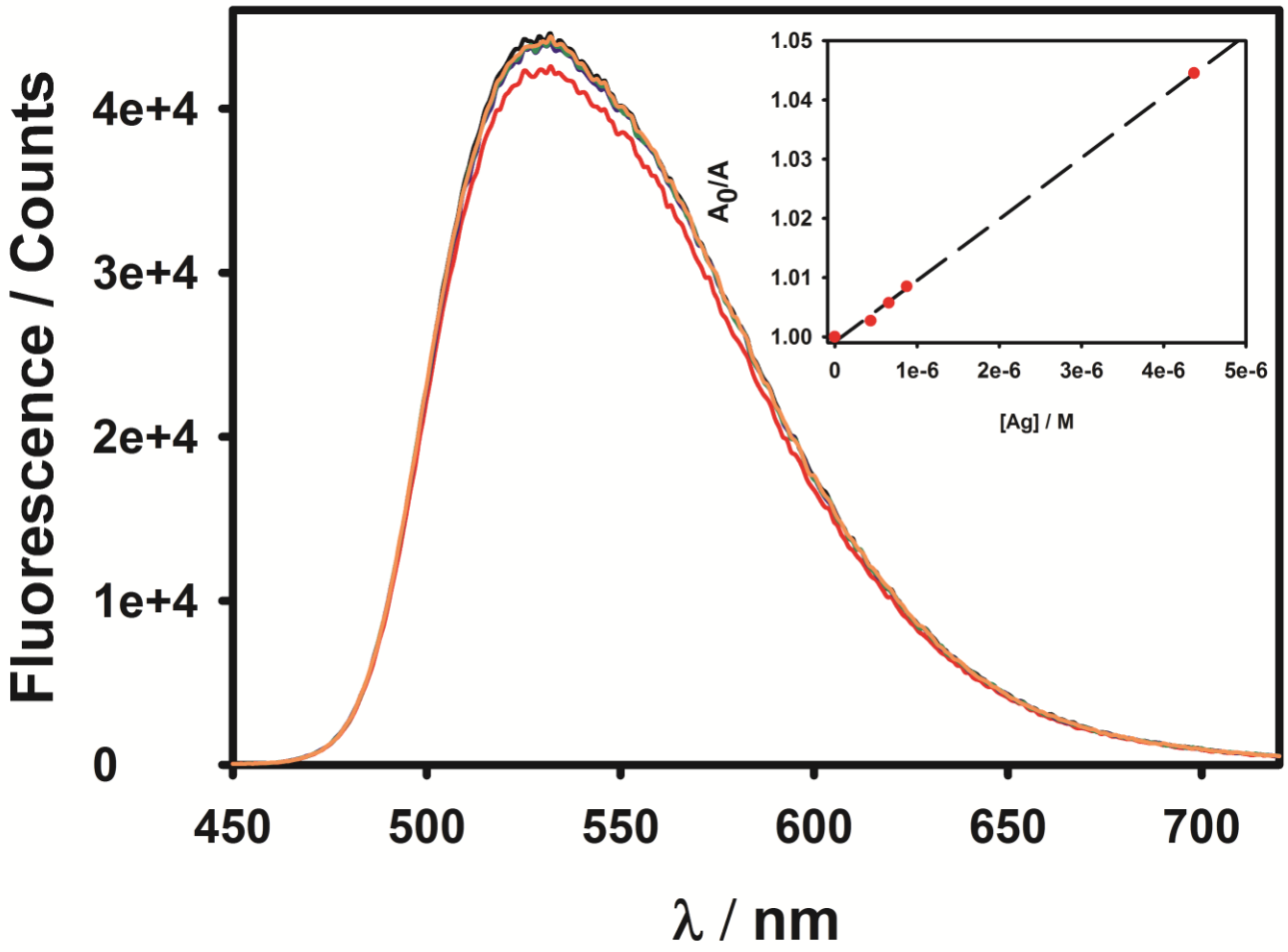

Figure S2: Fluorescence emission spectra (λ^{exc} = 420nm) of Rf (16 μM) in the absence (black) and presence of various amounts of Pec.AgNP. The Ag concentrations are: 4.37 μM (red), 0.87 μM (blue), 0.65 μM (green), 0.44 μM (orange). Inset: Plot of (A_0/A) vs. [Ag]. A_0 and A are the emission areas without and with nanoparticles, respectively.

Calculation of the diffusion-controlled rate constant with the Smoluchowski equation

Rates of reaction at an interface, with one reactant immobilized at a spherical surface, as derived from the Smoluchowski equation are given by equation (S1)[1]

$$k_{q,P} = \frac{4\pi N_{AV} R_{P+Rf} D_{P+Rf}}{1000 n_{q/P}} e^{(-E_a/kt)} \qquad \text{(S1)}$$

Where N_{AV} is the Avogadro constant, R_{P+Rf} is the encounter radius, D_{P+Rf} is the mutual diffusion coefficient given by the sum of D_P and D_{Rf}, $n_{q,P}$ is the average number of surface Ag atoms per particle. The pre-exponential factor represents the diffusion-controlled rate constant, and E_a is the activation energy of the reaction.

The average number of Ag atoms per particle calculated from the density of silver and the diameter of the particles is 2.2×10^4. Considering that the amount of surface Ag atoms for particles of 9 nm diameter is about 15%,[2] the average value of $n_{q,P}$ yields 3.35×10^3. Taking $R_{P+Rf} \sim R_P = 4.5 \times 10^{-7}$ cm, $D_{P+Rf} \sim D_{Rf} = 2.6 \times 10^{-5}$ cm^2s^{-1},[3] and $n_{q,P} = 3.3 \times 10^3$, the calculated diffusion-controlled rate constant between silver atoms and any species in solution is 2.7×10^7 $M^{-1}s^{-1}$.

References

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