

Supplementary data for the article:

Savić, T. D.; Ćomor, M. I.; Abazović, N. D.; Šaponjić, Z. V.; Marinović-Cincović, M. T.; Veljković, D. Ž.; Zarić, S. D.; Janković, I. A. Anatase Nanoparticles Surface Modified with Fused Ring Salicylate-Type Ligands (1-Hydroxy-2-Naphthoic Acids): A Combined DFT and Experimental Study. *Journal of Alloys and Compounds* **2015**, *630*, 226–235.

<https://doi.org/10.1016/j.jallcom.2015.01.041>

Supporting Information

Anatase nanoparticles surface modified with fused ring salicylate-type ligands (1-hydroxy-2-naphthoic acids): a combined DFT and experimental study

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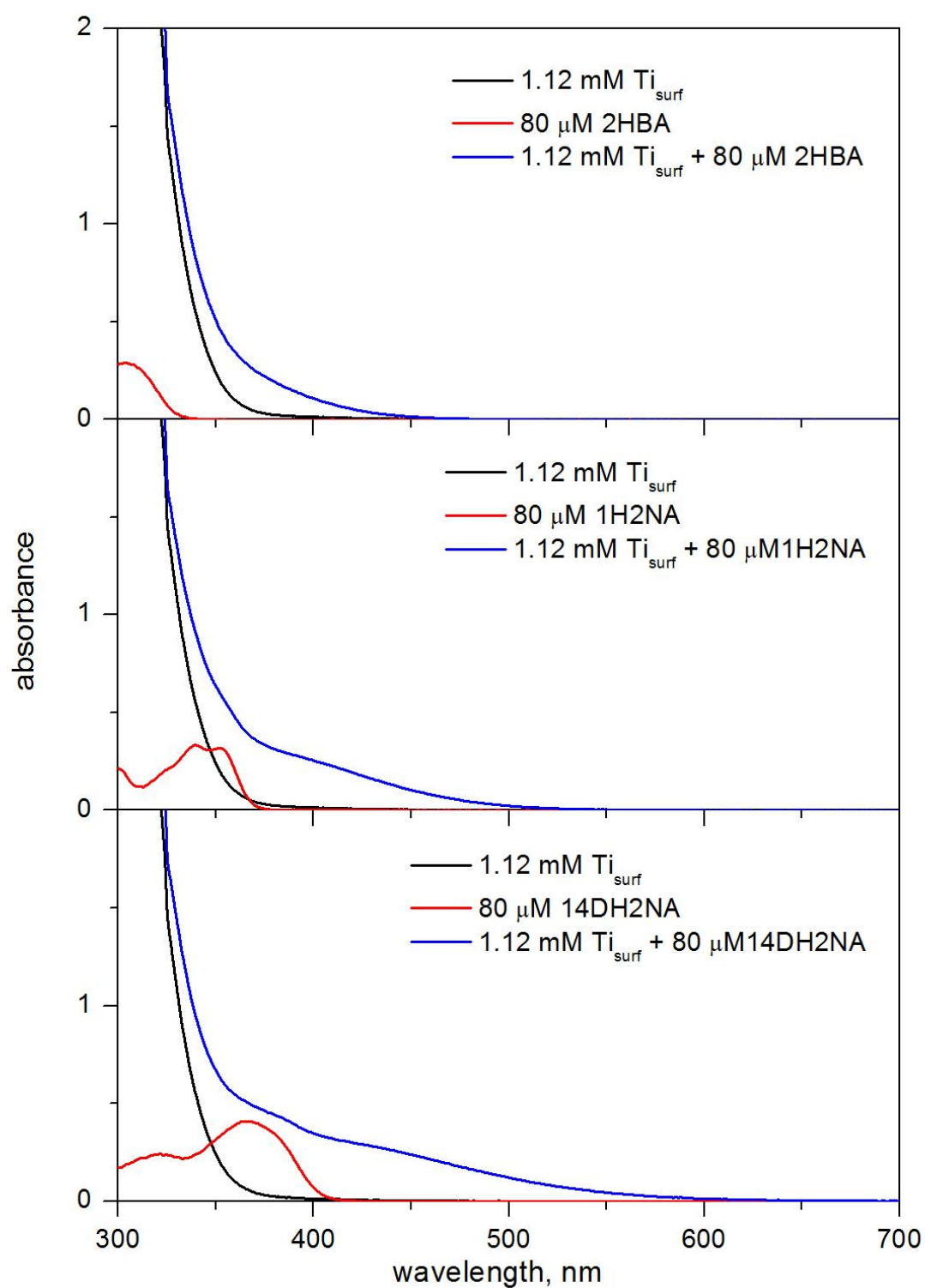


Fig. SM1 Absorption spectra of TiO_2 nanoparticles (black), free ligands (red) and ligand- TiO_2 CT-complexes with 15% coverage (blue) in methanol/water=90/10, pH 2

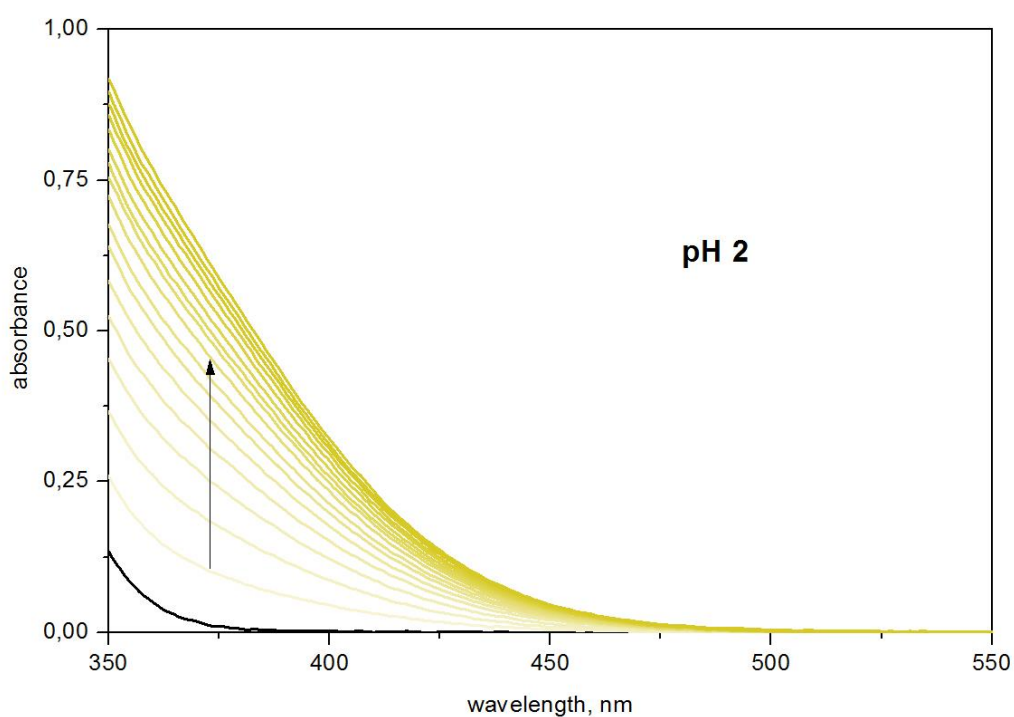
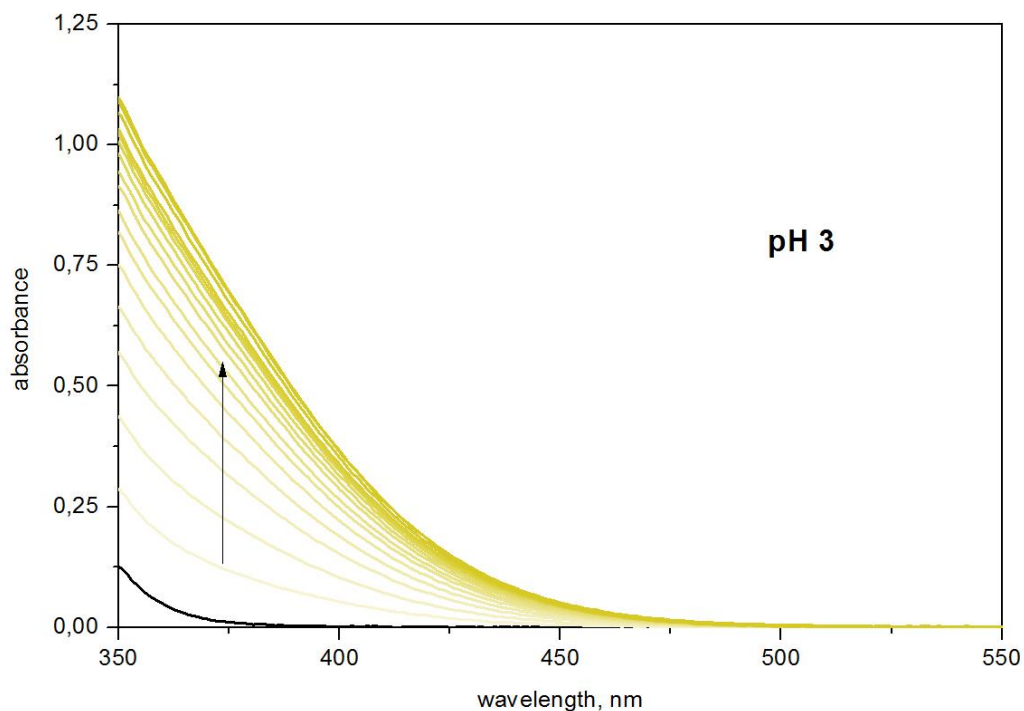


Fig. SM2 Absorption spectra of 3.6 mM TiO₂ (1 mM Ti_{surf}) nanoparticles before and after surface modification with 2HBA (0 – 560 μM in 35 μM steps) in methanol/water=90/10, at pH 2 and pH 3 (data recorded 20 h after surface modification)

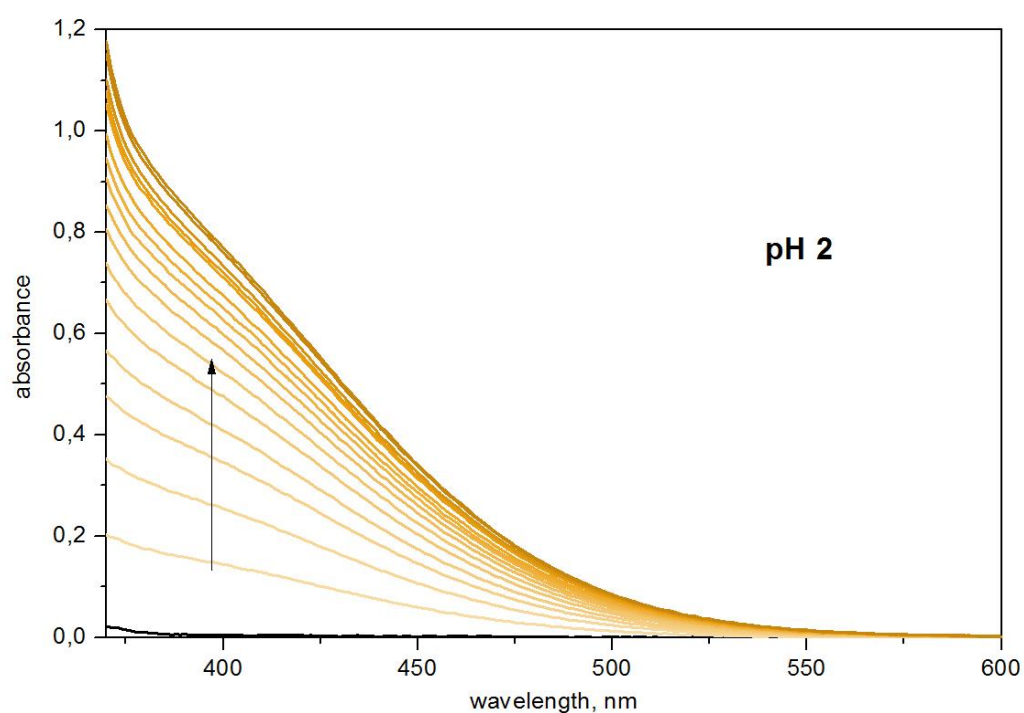
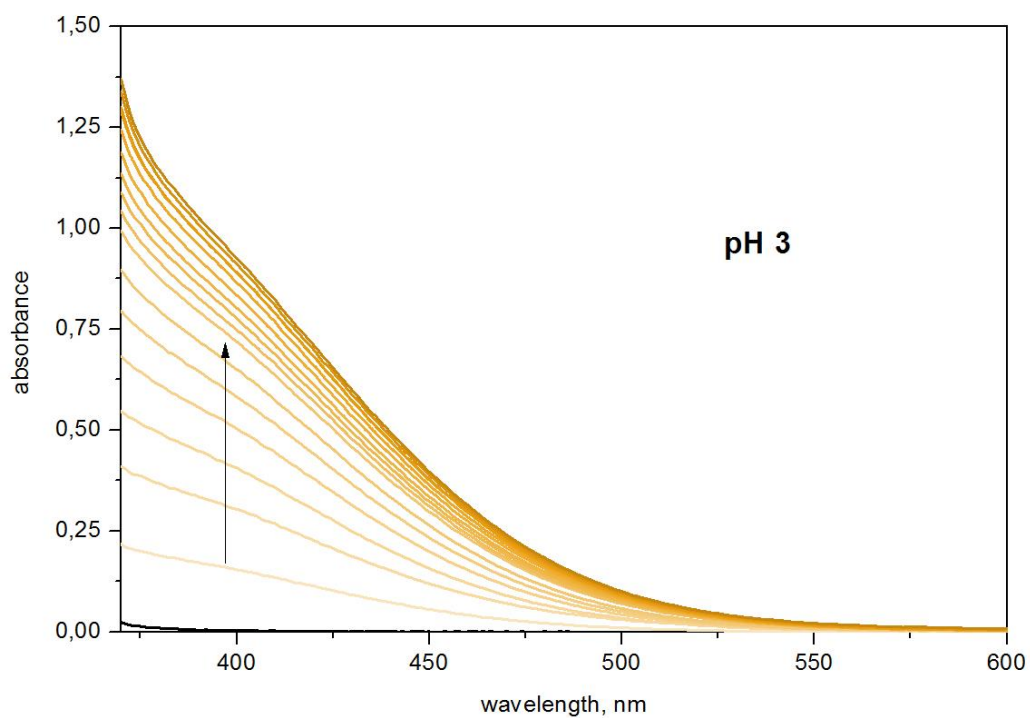


Fig. SM3 Absorption spectra of 3.6 mM TiO₂ (1 mM Ti_{surf}) nanoparticles before and after surface modification with 1H2NA (0 – 560 μM in 35 μM steps) in methanol/water=90/10, at pH 2 and pH 3 (data recorded 20 h after surface modification)

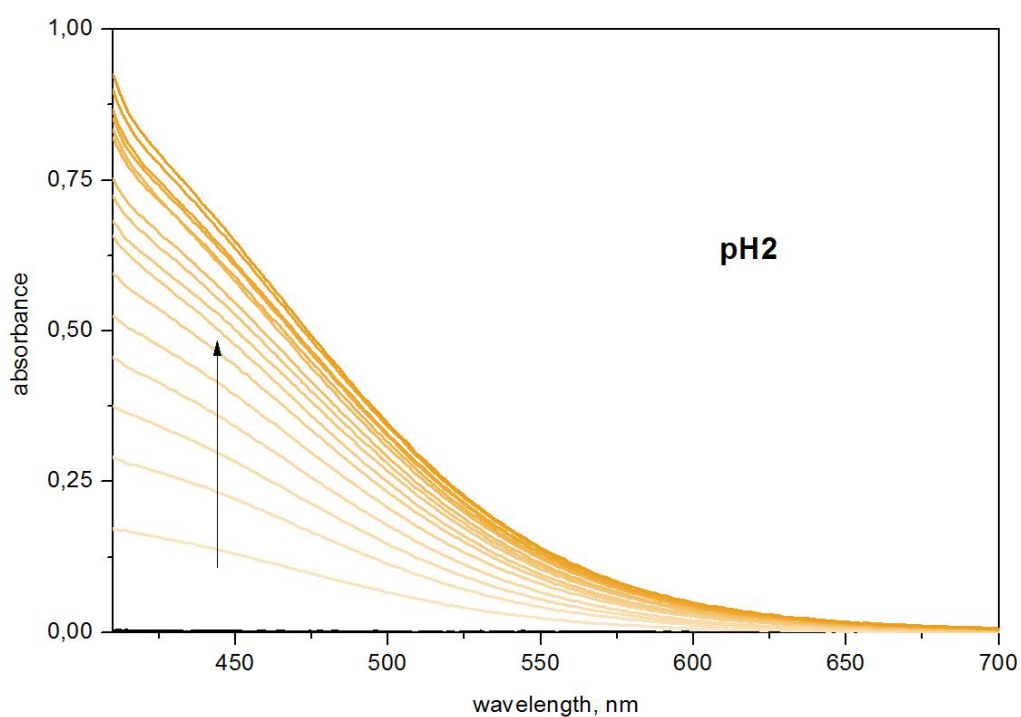
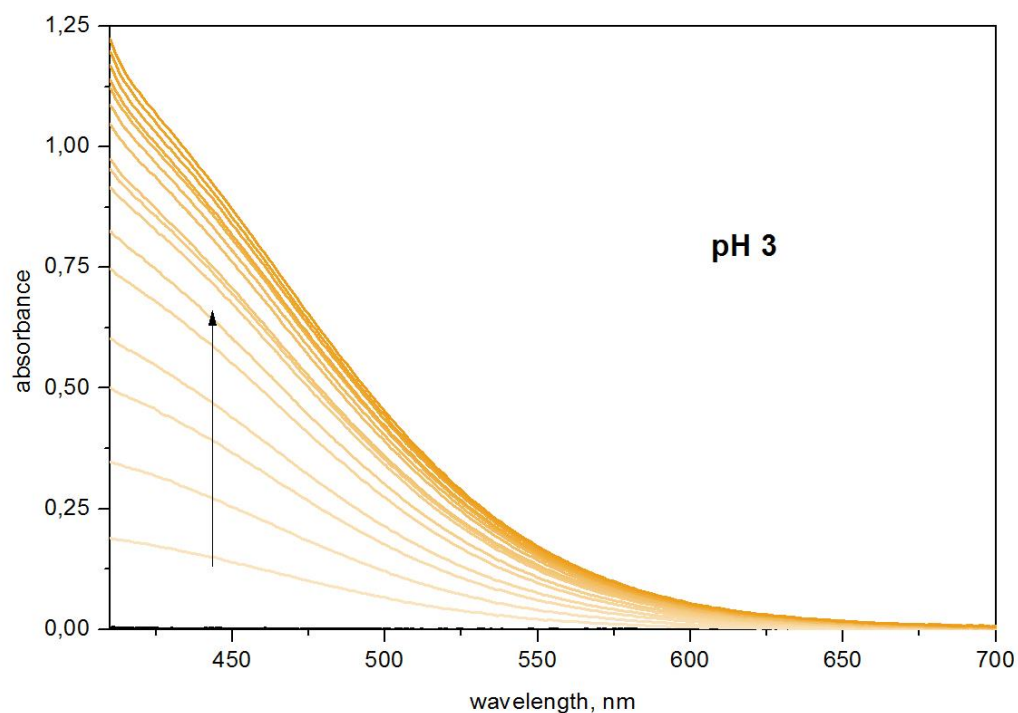


Fig. SM4 Absorption spectra of 3.6 mM TiO₂ (1 mM Ti_{surf}) nanoparticles before and after surface modification with 1,4DH2NA (0 – 560 μM in 35 μM steps) in methanol/water=90/10, at pH 2 and pH 3 (data recorded 20 h after surface modification)

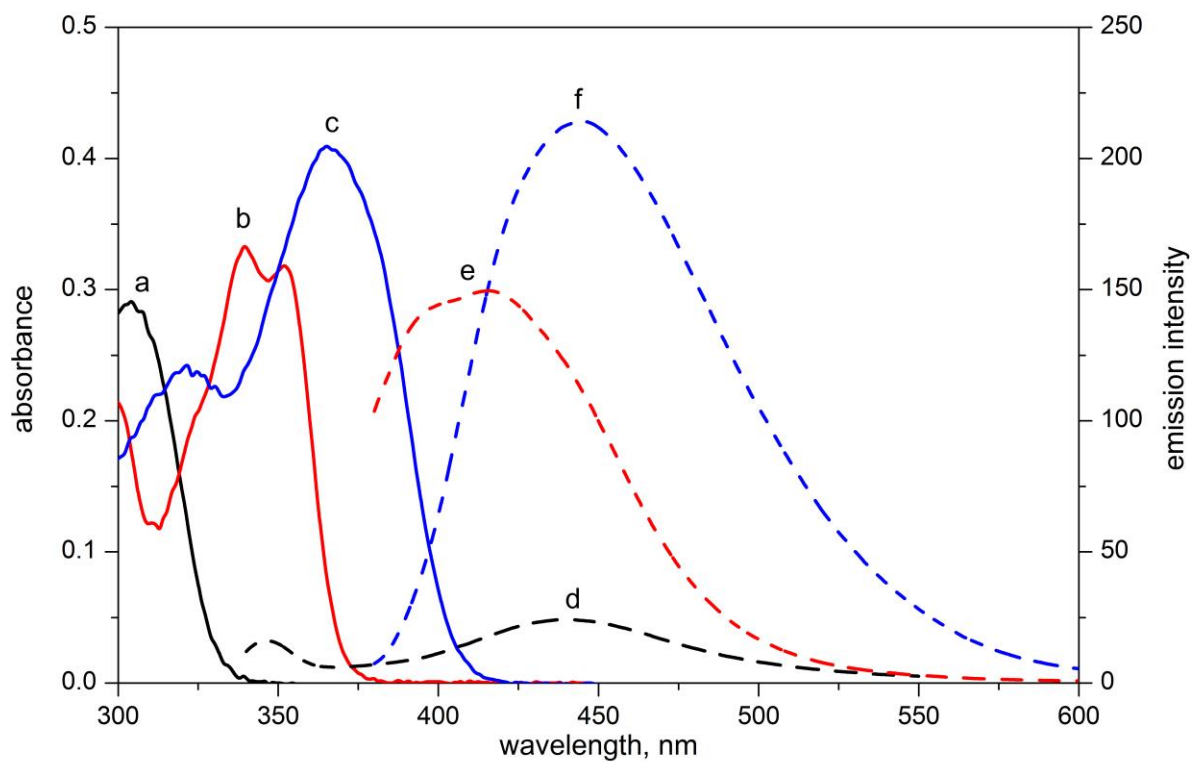


Fig. SM5. Absorption (80 μM ; a, b, c) and emission (1 μM ; d, e, f) spectra of 2HBA, 1H2NA and 1,4DH2NA, respectively in methanol/water =90/10 solutions at pH 2

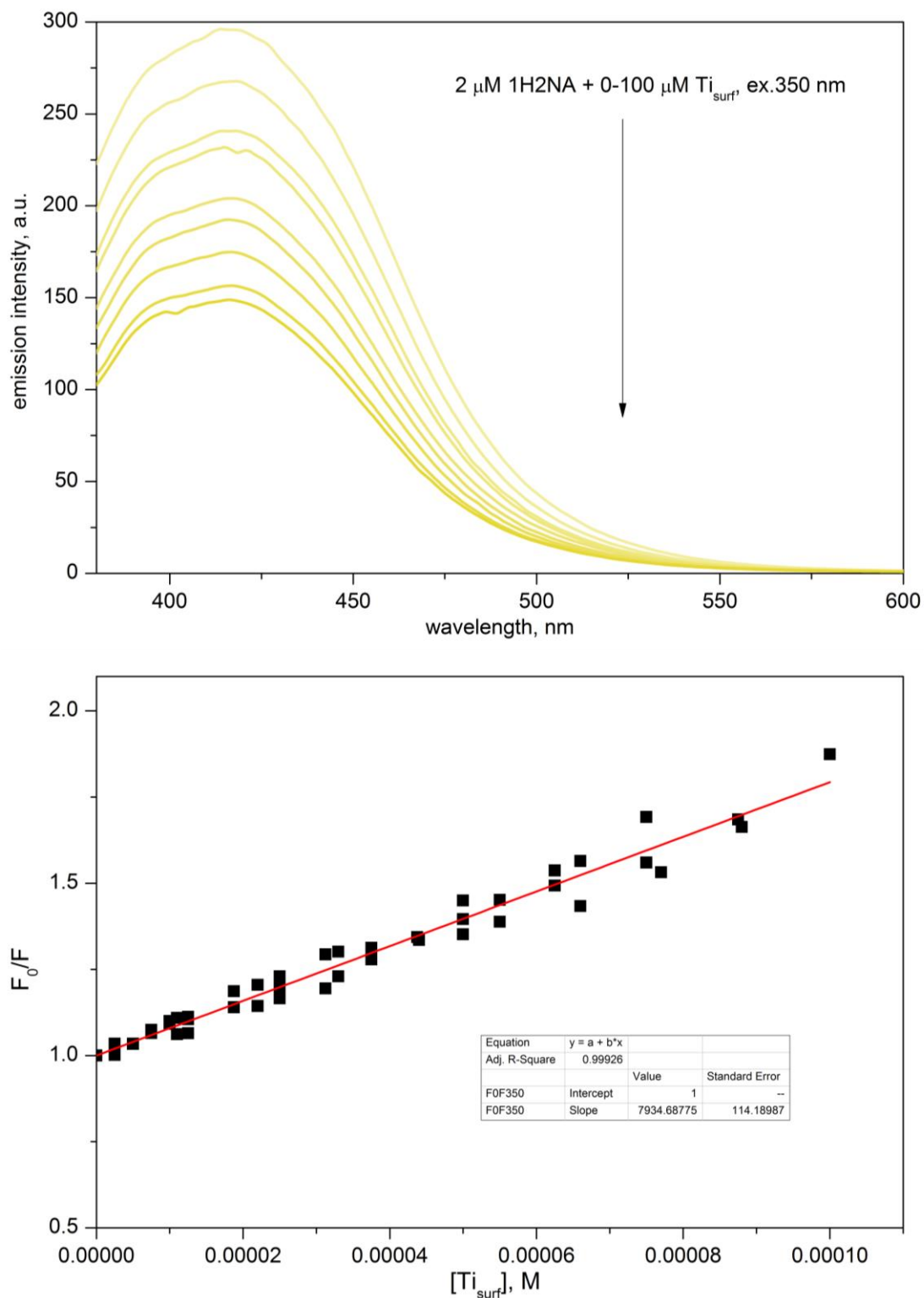


Fig. SM6 Emission spectra of 1H2NA (2 μM) in the presence of various concentrations of Ti_{surf} (0-100 μM in 12.5 μM steps) in methanol/water=90/10 solutions, at pH 2 (data recorded 20 h after surface modification) and Stern-Volmer plot for five series of measurements ($\lambda_{\text{ex}}=350 \text{ nm}$ / $\lambda_{\text{em}}=415 \text{ nm}$)

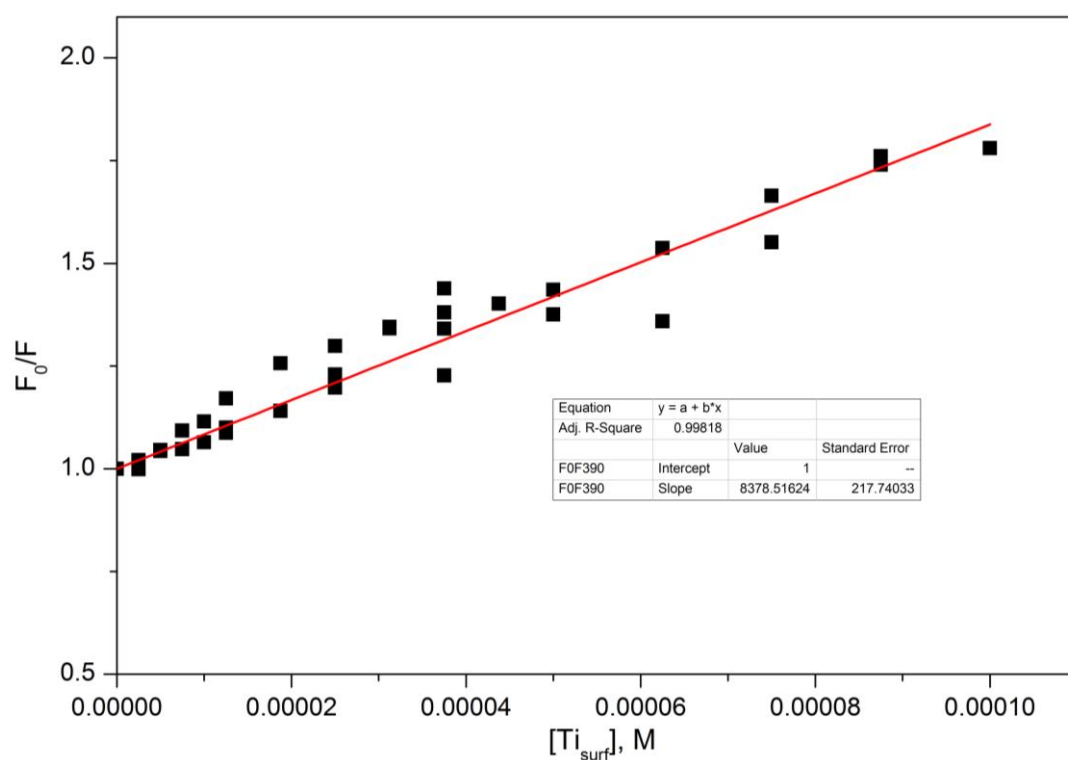
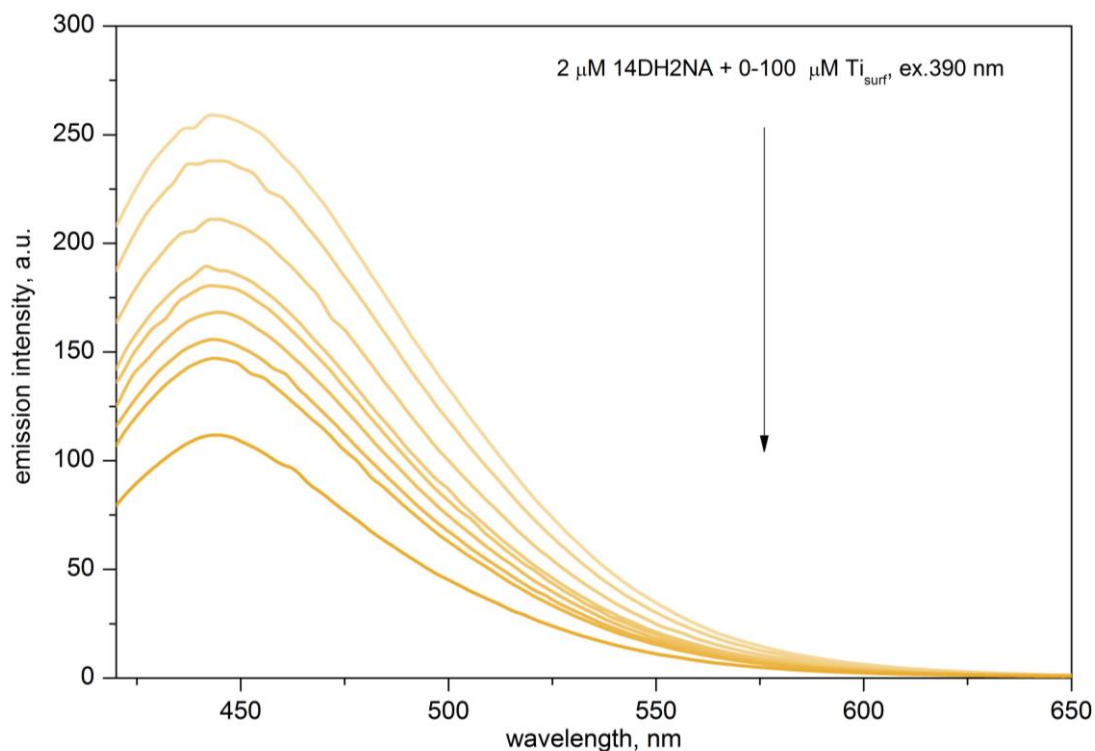


Fig. SM7 Emission spectra of 1,4DH2NA (2 μM) in the presence of various concentrations of Ti_{surf} (0-100 μM in 12.5 μM steps) in methanol/water=90/10 solutions, at pH 2 (data recorded 20 h after surface modification) and Stern-Volmer plot for four series of measurements ($\lambda_{\text{ex}}=390 \text{ nm}$ / $\lambda_{\text{em}}=445 \text{ nm}$)

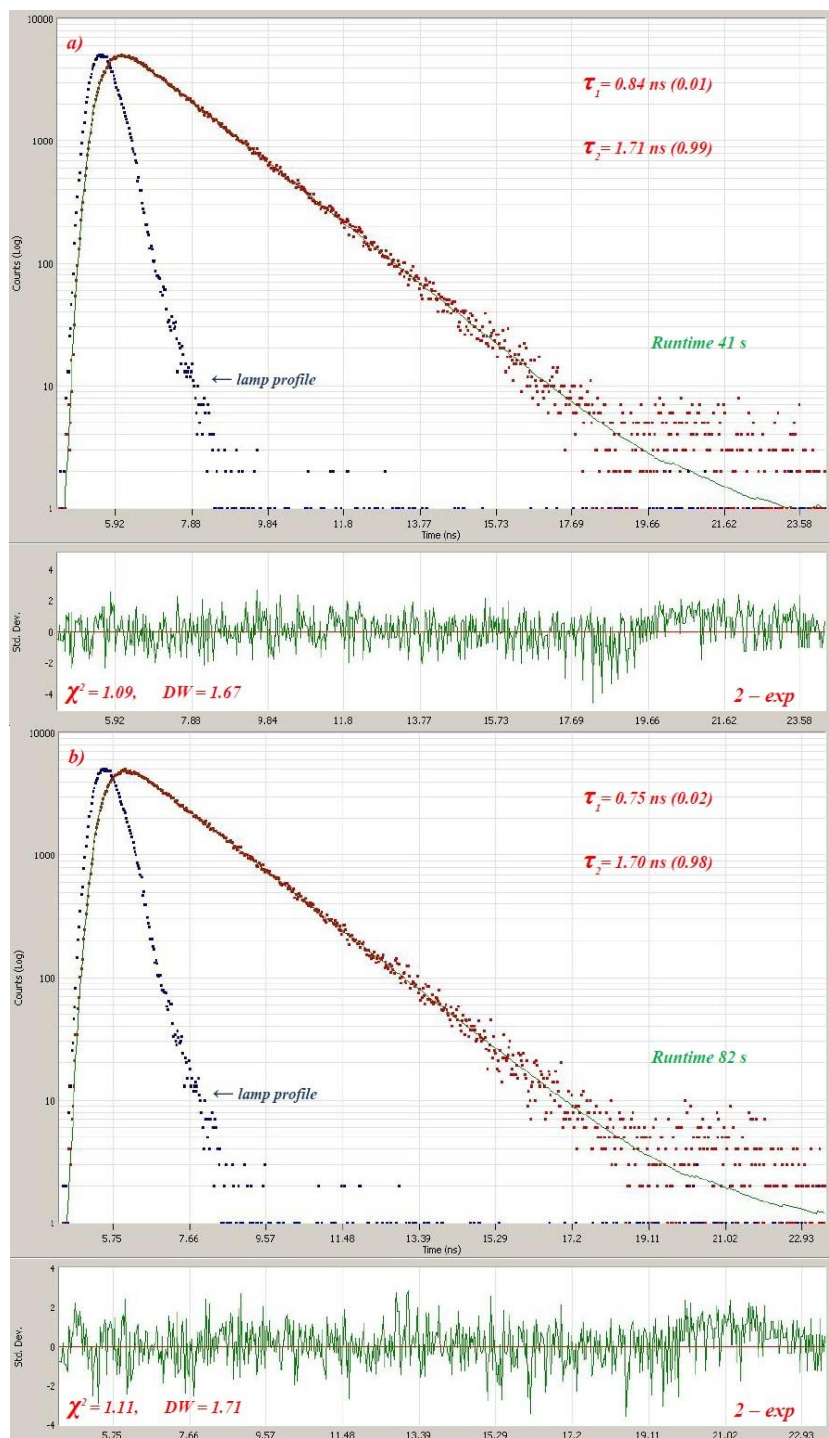


Fig. SM8 Time-resolved fluorescence decay profiles of 50 μM 1H2NA (a) and 50 μM 1H2NA + 130 μM Ti_{surf} (b) in methanol/water=90/10 solutions at pH 2. Excitation and emission wavelengths are 342 nm and 420 nm, respectively. The respective distribution of residuals, chi-square (χ^2) and Durbin-Watson (DW) parameters for biexponential fits are given below the fitted decay curves

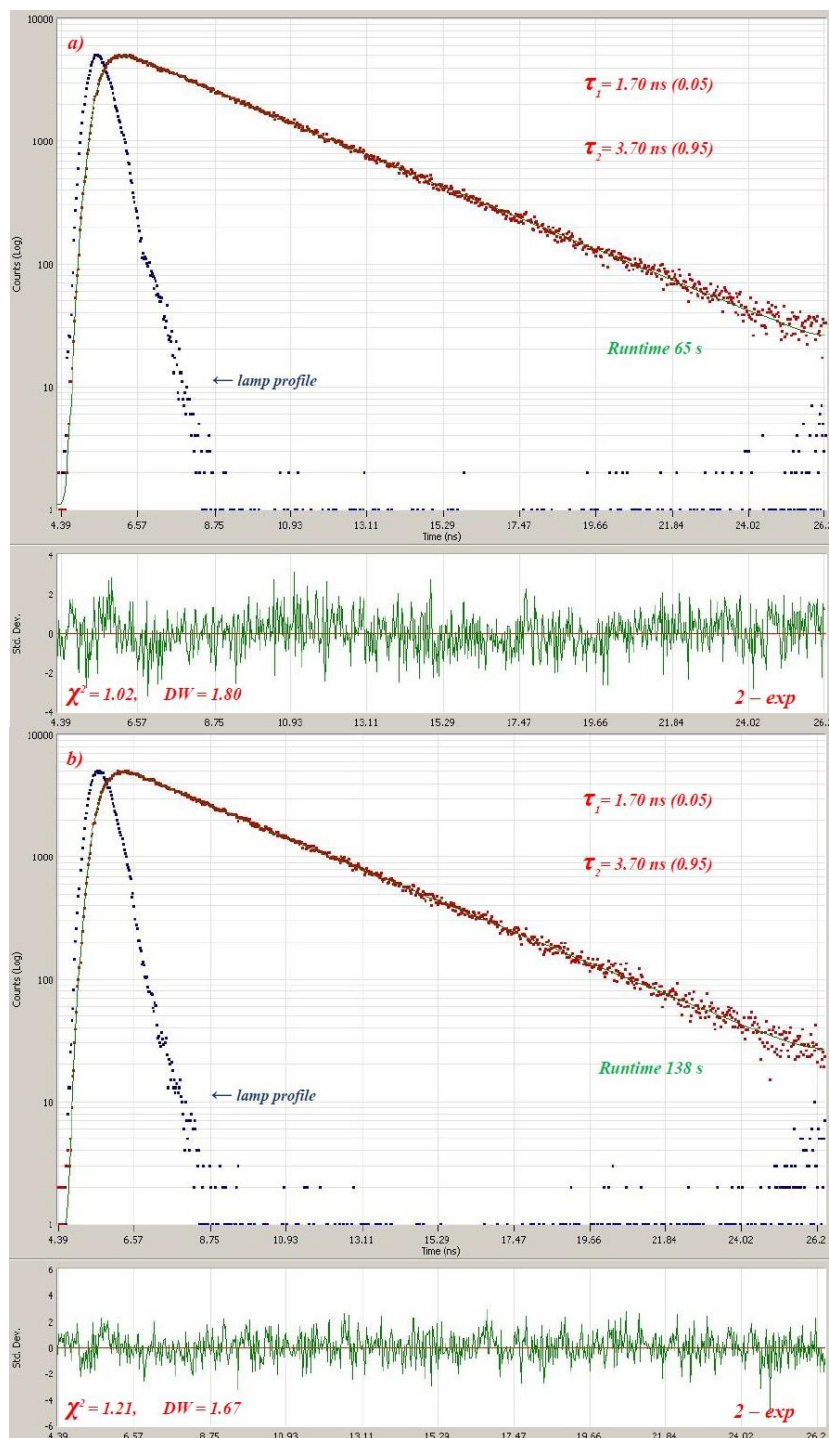


Fig. SM9 Time-resolved fluorescence decay profiles of 50 μM 1,4DH2NA (a) and 50 μM 1,4DH2NA + 130 μM Ti_{surf} (b) in methanol/water=90/10 solutions at pH 2. Excitation and emission wavelengths are 342 nm and 450 nm, respectively. The respective distribution of residuals, chi-square (χ^2) and Durbin-Watson (DW) parameters for biexponential fits are given below the fitted decay curves

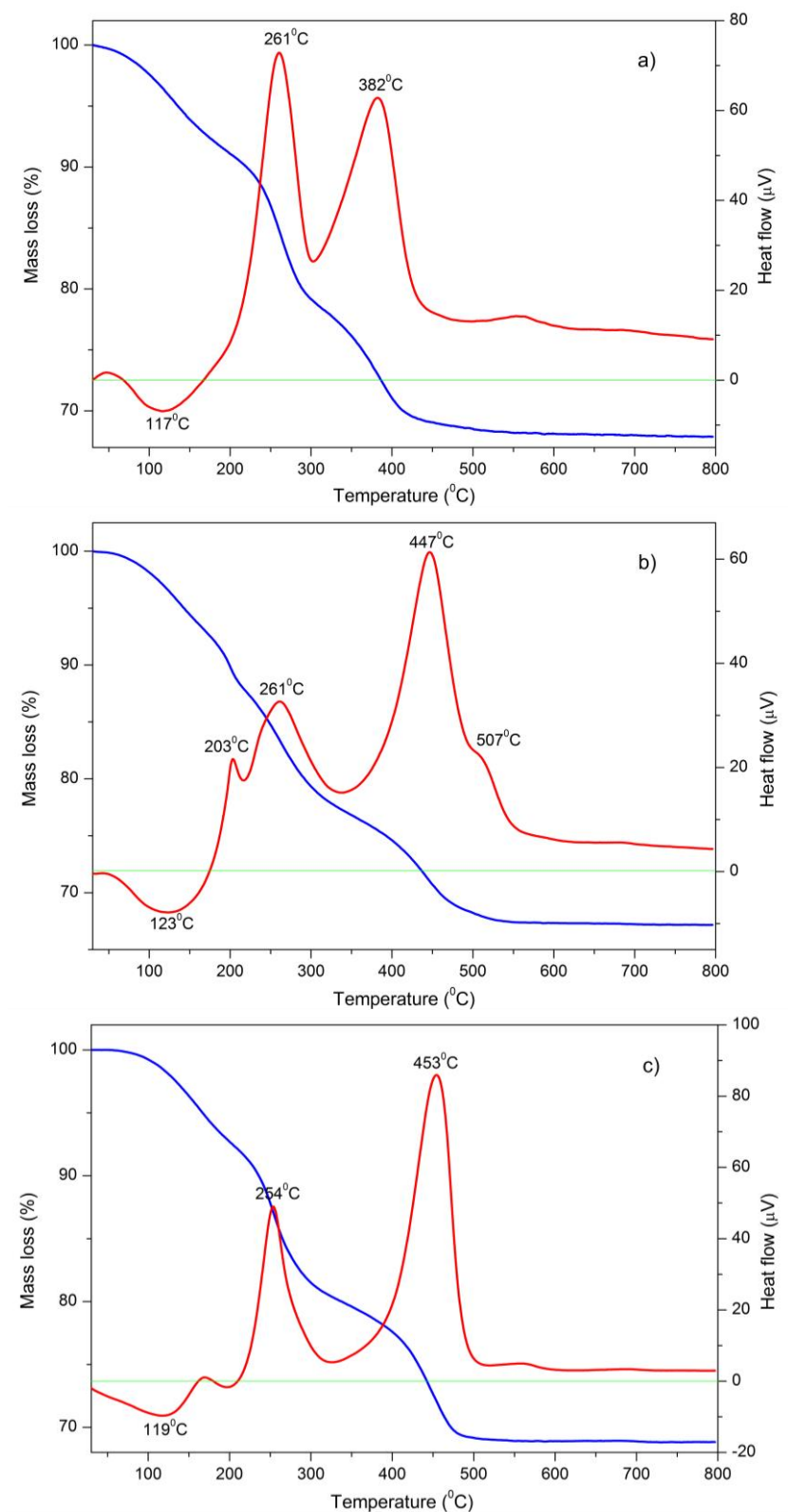


Fig. SM10 TG (blue line) and heat flow (red line) curves of TiO₂ nanoparticles modified with 2HBA (a), 1H₂NA (b) and 1,4DH₂NA (c) recorded at the heating rate of 20°C min⁻¹ in air