

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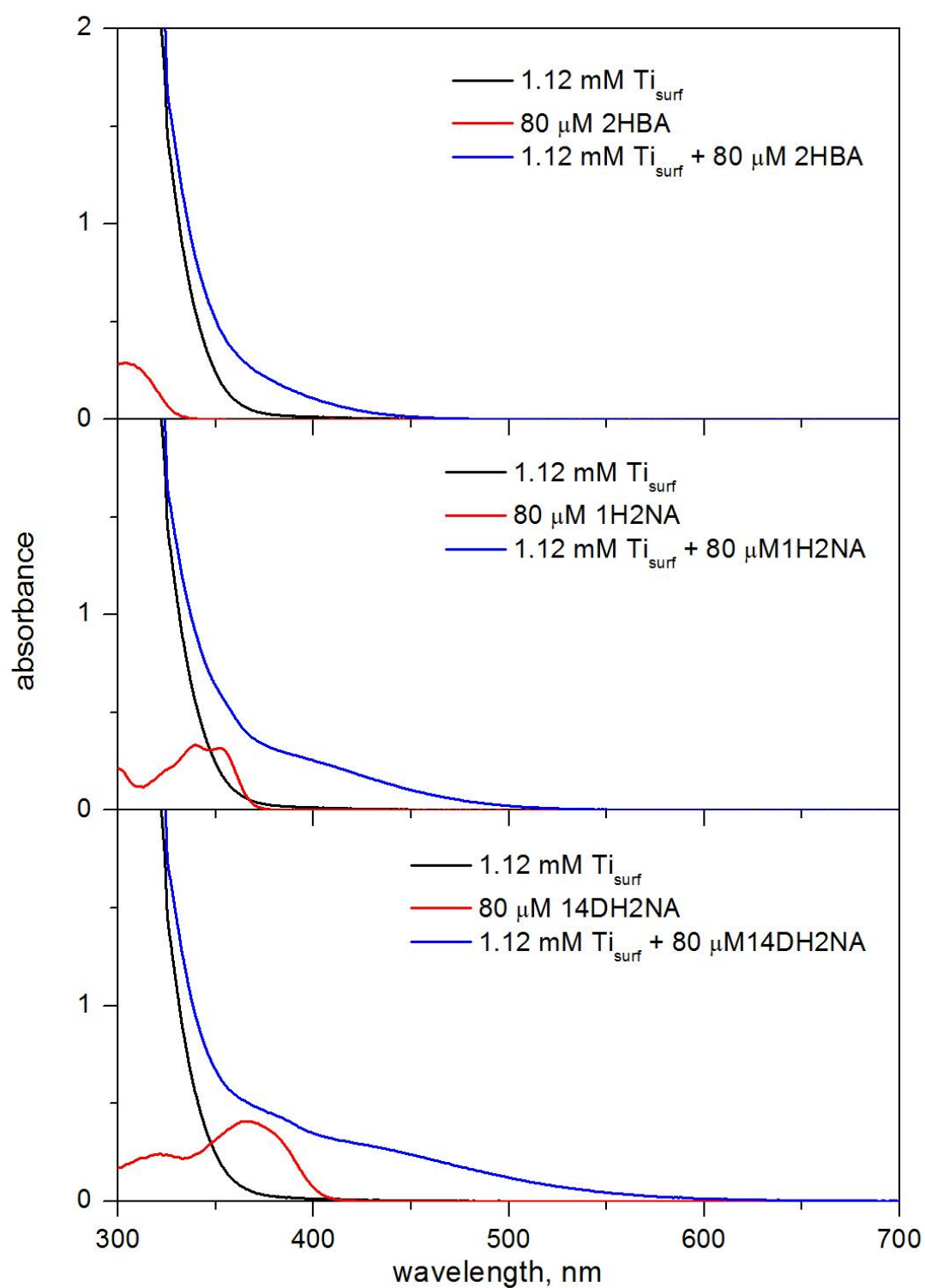
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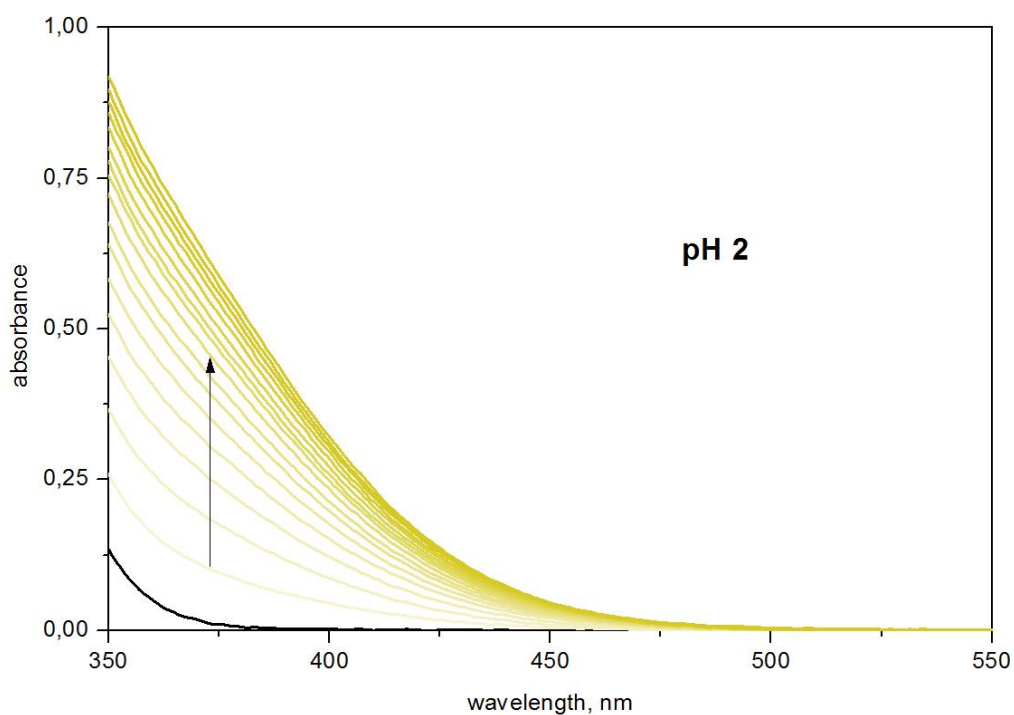
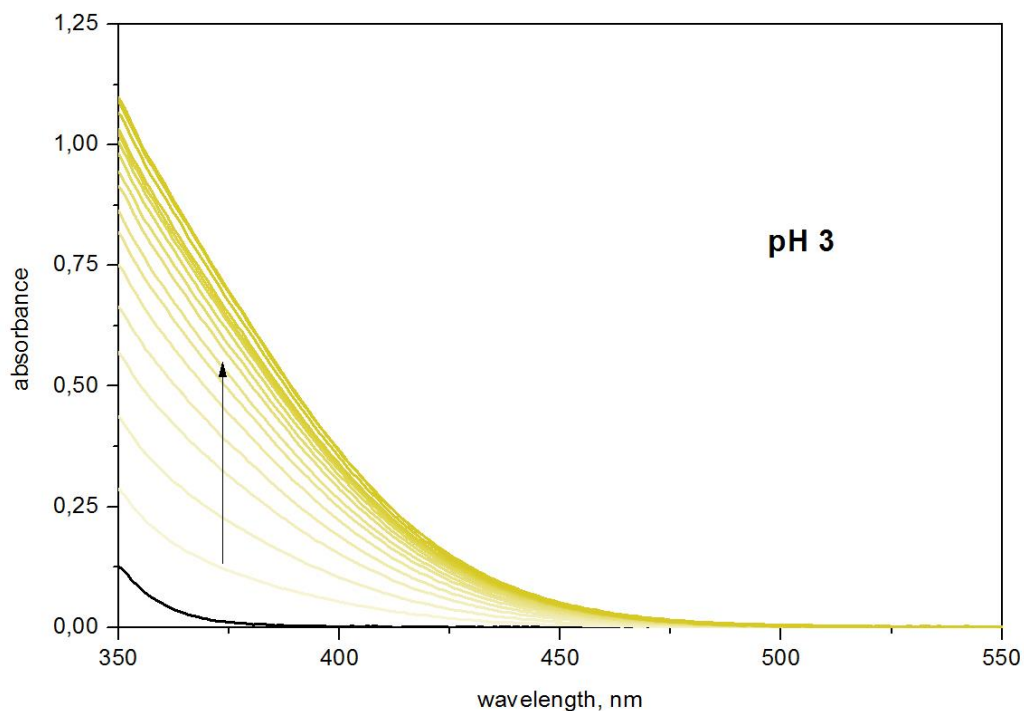
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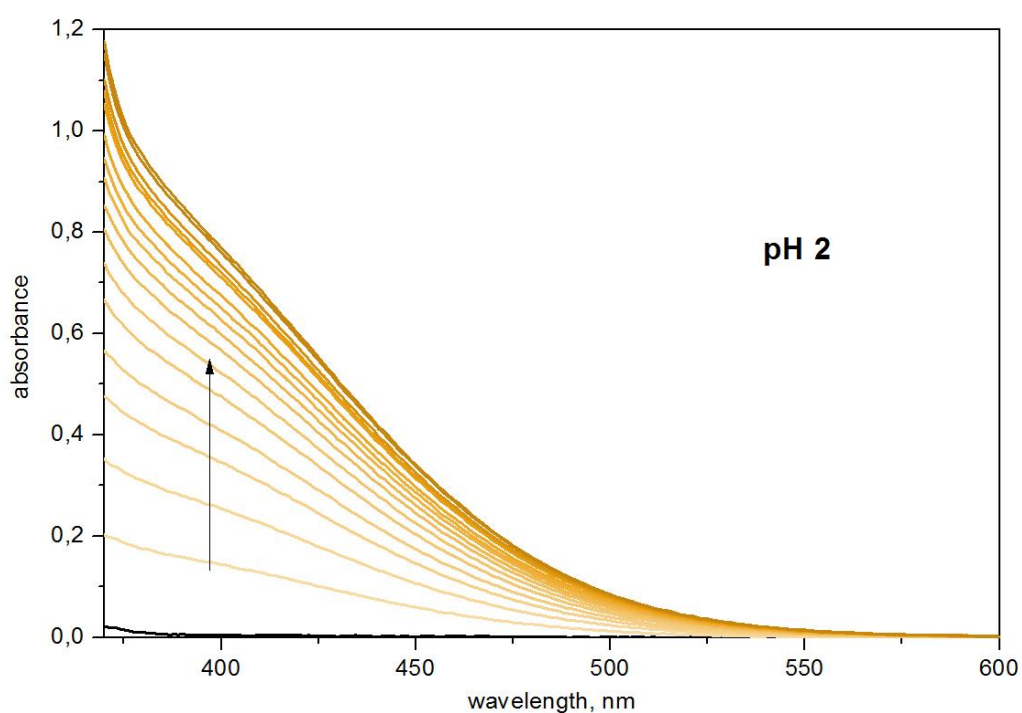
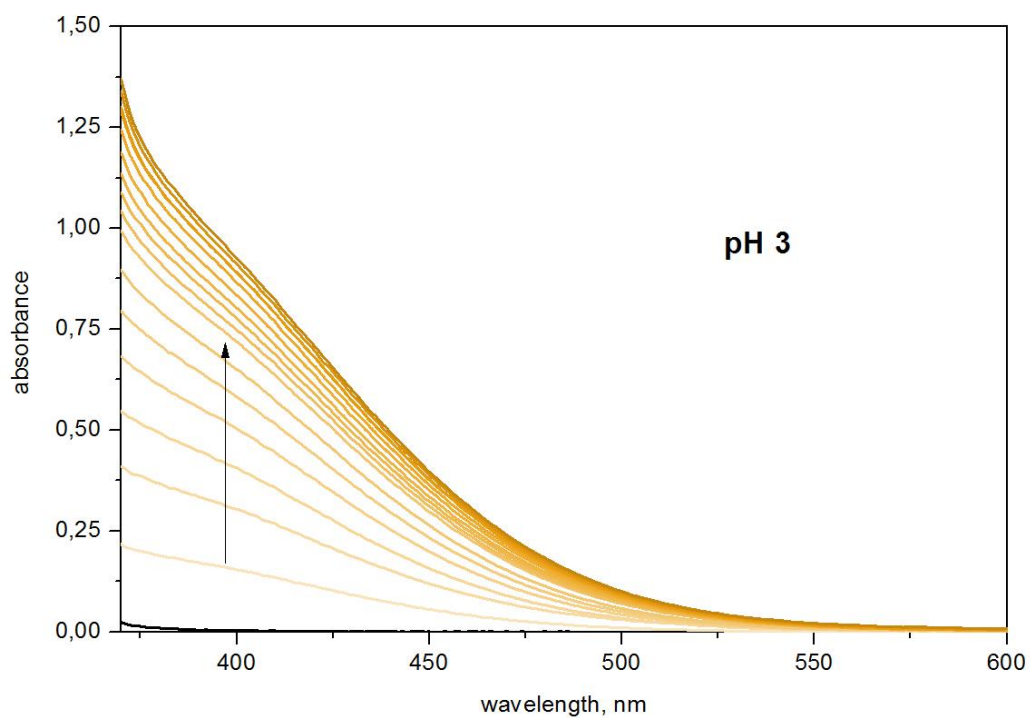
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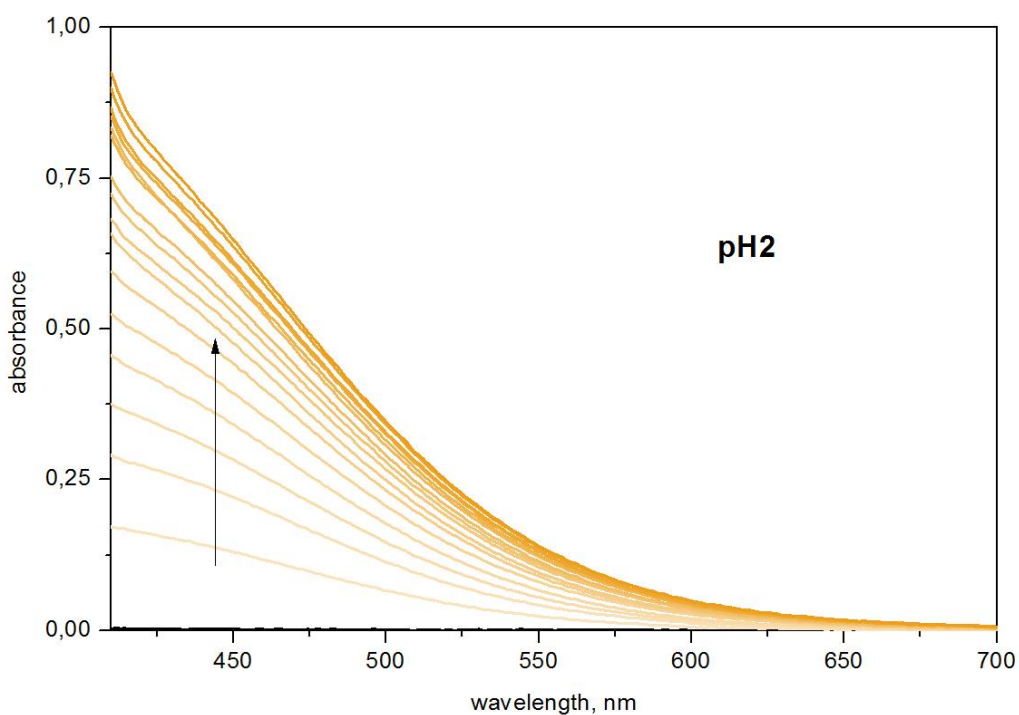
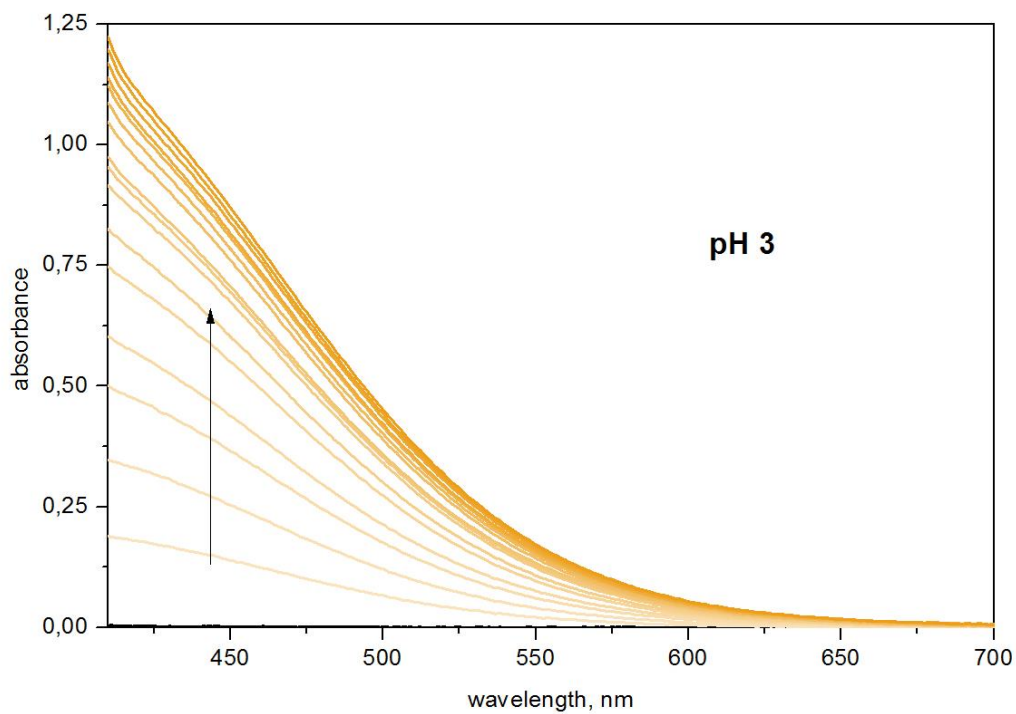
**Fig. SM1** Absorption spectra of  $TiO_2$  nanoparticles (black), free ligands (red) and ligand- $TiO_2$  CT-complexes with 15% coverage (blue) in methanol/water=90/10, pH 2



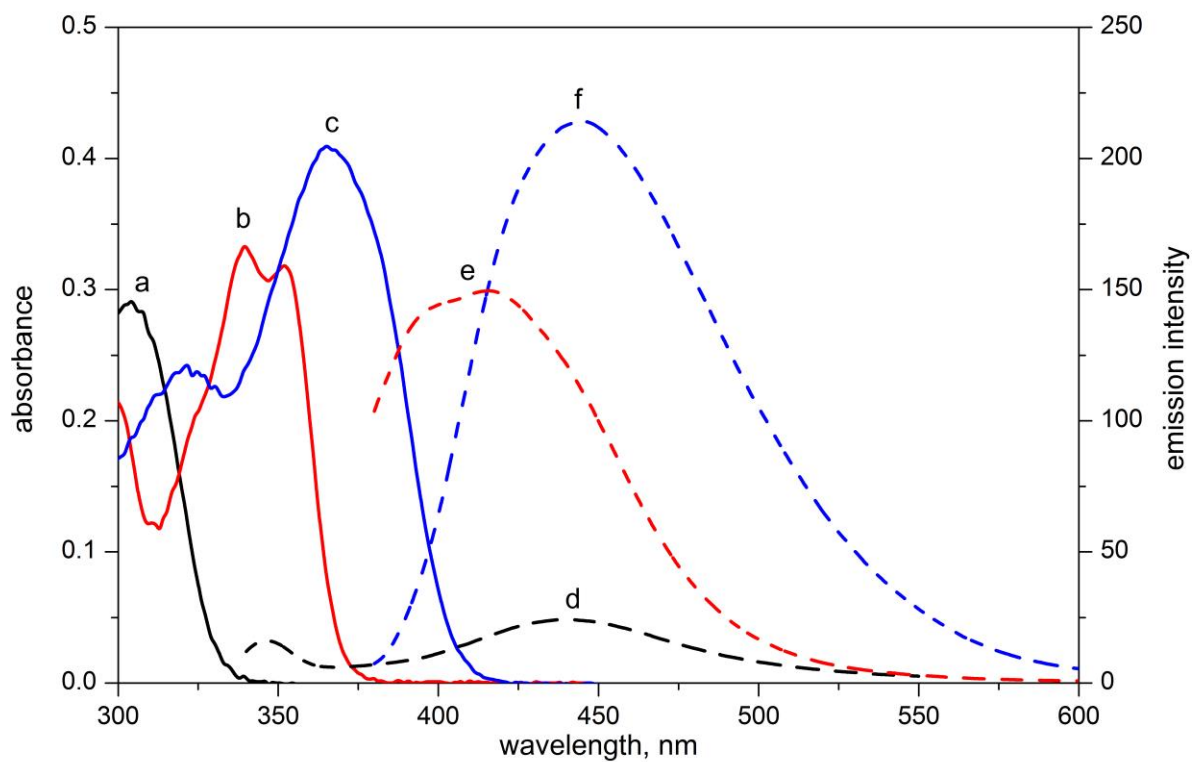
**Fig. SM2** Absorption spectra of 3.6 mM TiO<sub>2</sub> (1 mM Ti<sub>surf</sub>) nanoparticles before and after surface modification with 2HBA (0 – 560 μM in 35 μM steps) in methanol/water=90/10, at pH 2 and pH 3 (data recorded 20 h after surface modification)



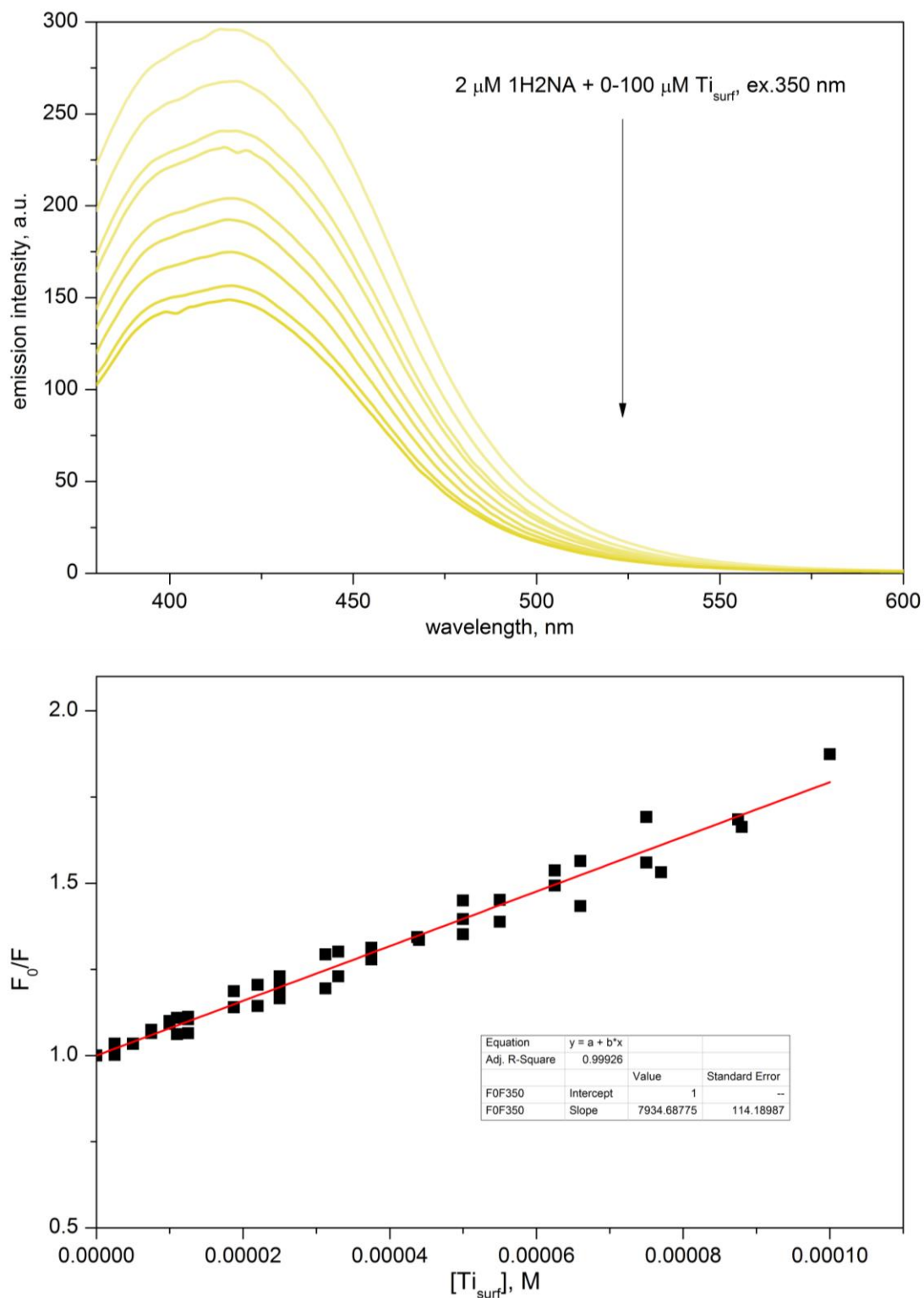
**Fig. SM3** Absorption spectra of 3.6 mM TiO<sub>2</sub> (1 mM Ti<sub>surf</sub>) nanoparticles before and after surface modification with 1H2NA (0 – 560 μM in 35 μM steps) in methanol/water=90/10, at pH 2 and pH 3 (data recorded 20 h after surface modification)



**Fig. SM4** Absorption spectra of 3.6 mM  $\text{TiO}_2$  (1 mM  $\text{Ti}_{\text{surf}}$ ) nanoparticles before and after surface modification with 1,4DH2NA (0 – 560  $\mu\text{M}$  in 35  $\mu\text{M}$  steps) in methanol/water=90/10, at pH 2 and pH 3 (data recorded 20 h after surface modification)

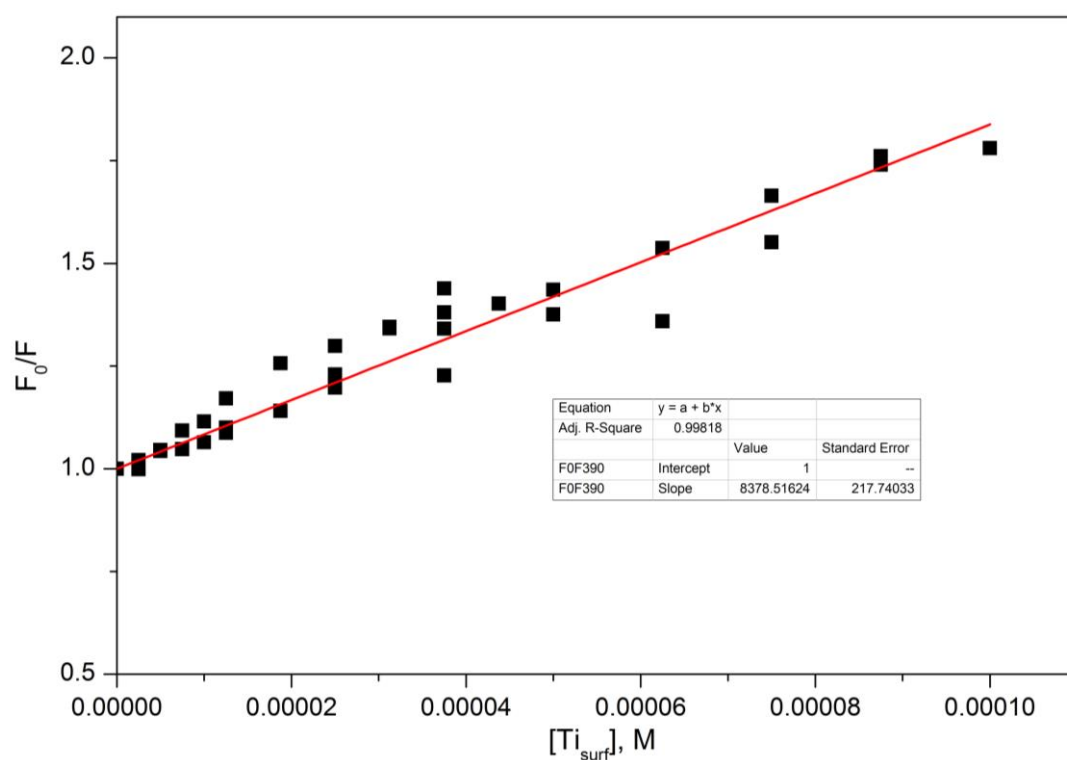
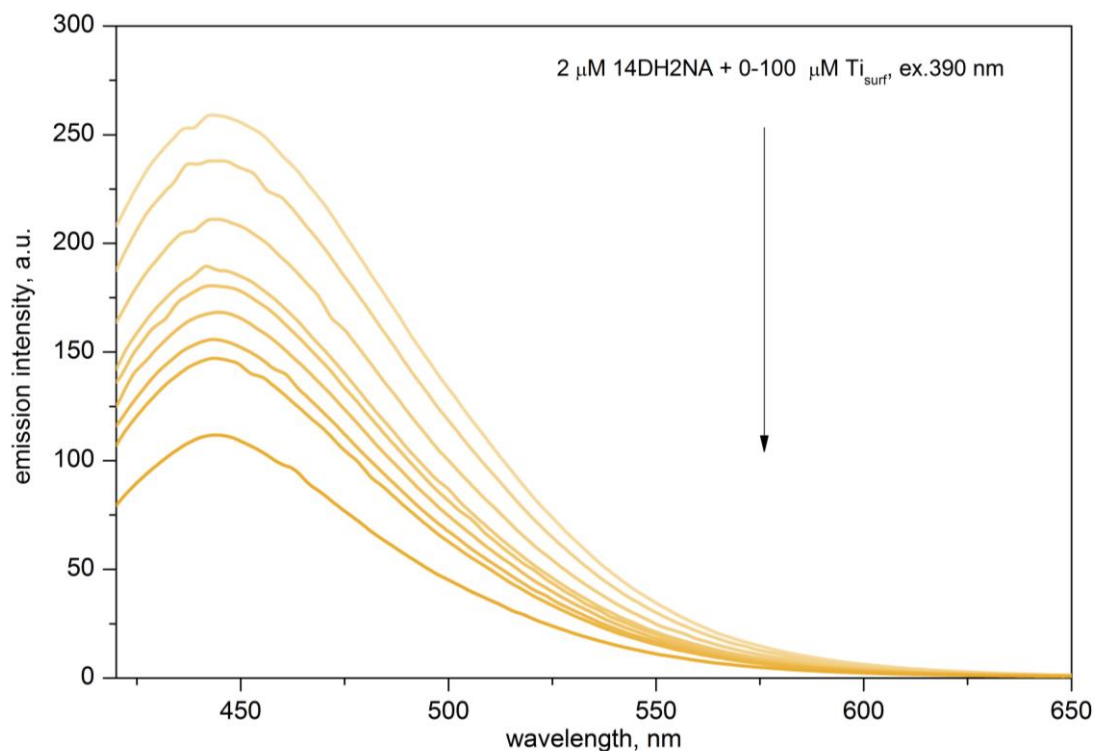


**Fig. SM5.** Absorption (80  $\mu\text{M}$ ; a, b, c) and emission (1  $\mu\text{M}$ ; d, e, f) spectra of 2HBA, 1H2NA and 1,4DH2NA, respectively in methanol/water =90/10 solutions at pH 2

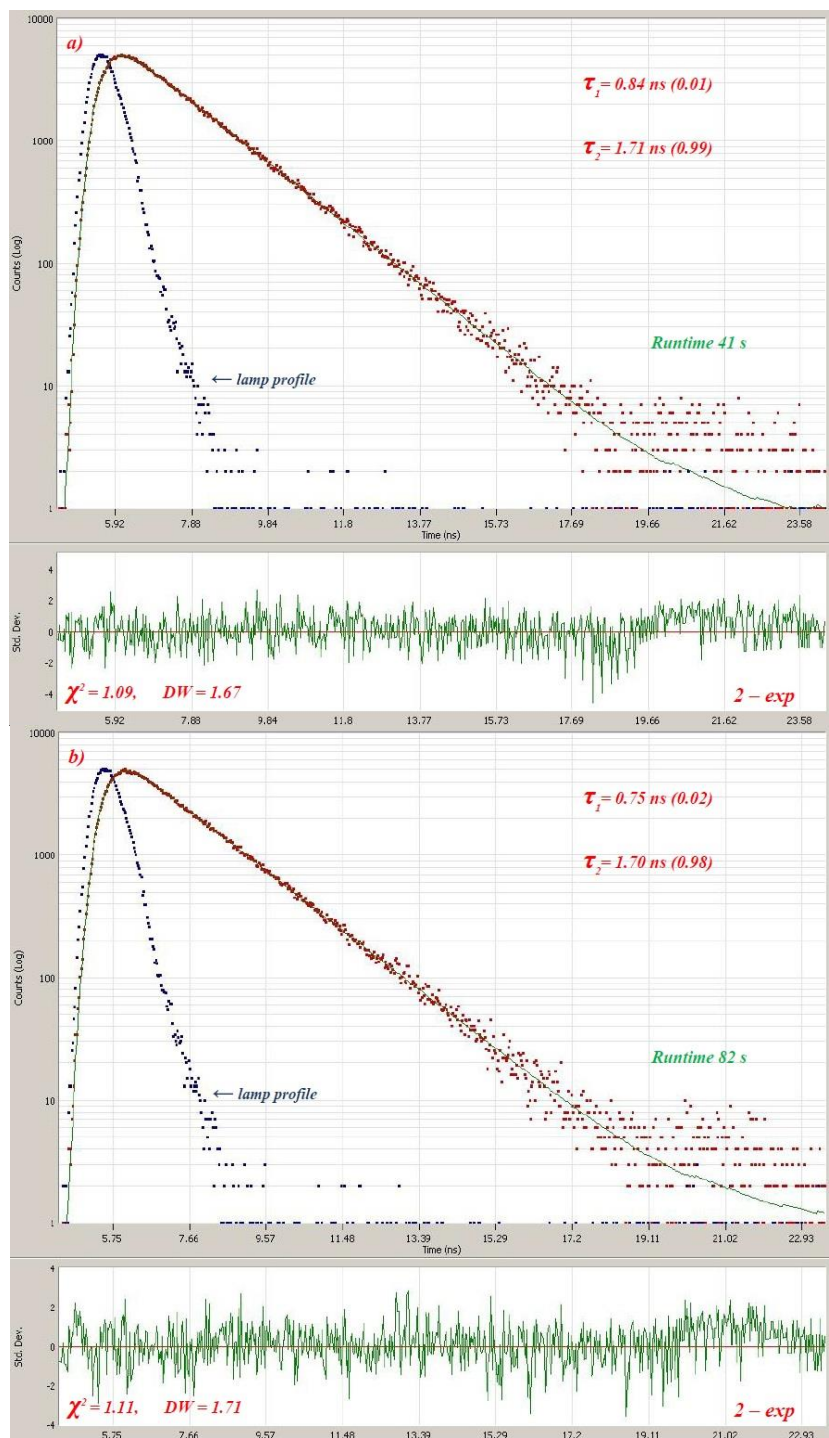


**Fig. SM6** Emission spectra of 1H2NA (2  $\mu\text{M}$ ) in the presence of various concentrations of  $\text{Ti}_{\text{surf}}$  (0-100  $\mu\text{M}$  in 12.5  $\mu\text{M}$  steps) in methanol/water=90/10 solutions, at pH 2 (data recorded 20 h after surface modification) and Stern-Volmer plot for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

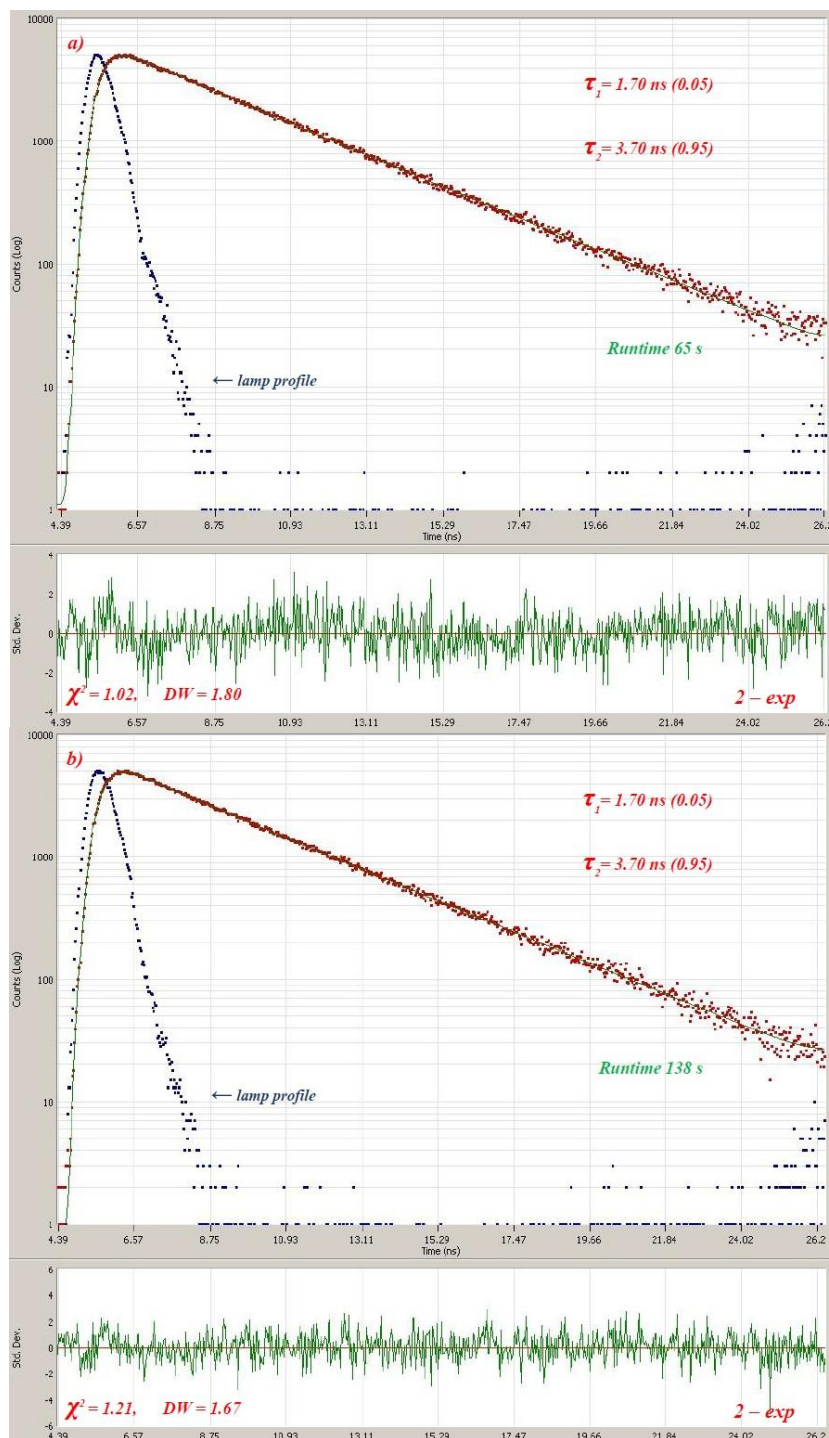




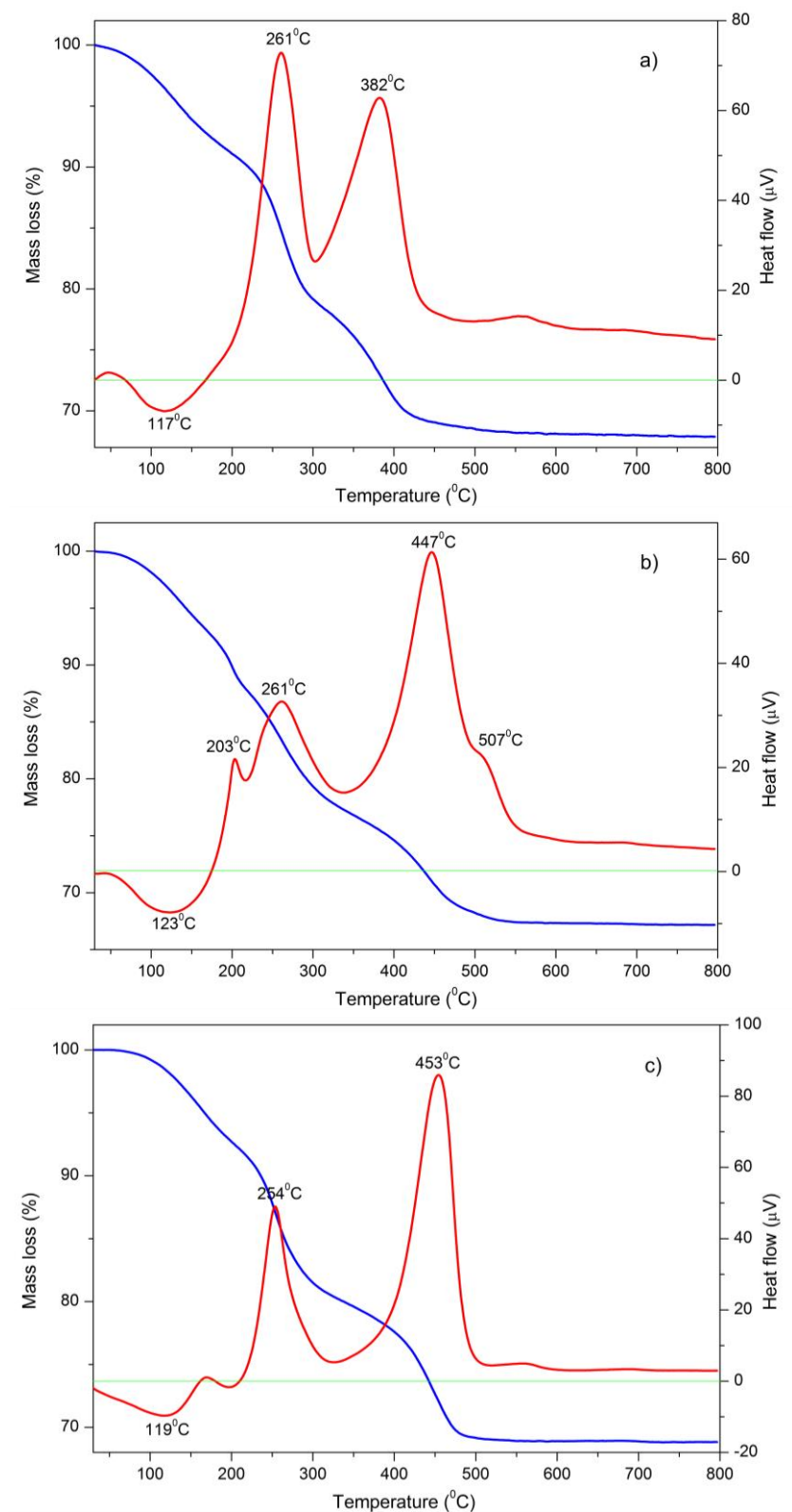
**Fig. SM7** Emission spectra of 1,4DH2NA (2  $\mu\text{M}$ ) in the presence of various concentrations of  $\text{Ti}_{\text{surf}}$  (0-100  $\mu\text{M}$  in 12.5  $\mu\text{M}$  steps) in methanol/water=90/10 solutions, at pH 2 (data recorded 20 h after surface modification) and Stern-Volmer plot 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  $\mu\text{M}$  1H2NA (a) and 50  $\mu\text{M}$  1H2NA + 130  $\mu\text{M}$   $\text{Ti}_{\text{surf}}$  (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 ( $\chi^2$ ) and Durbin-Watson (DW) parameters for biexponential fits are given below the fitted decay curves



**Fig. SM9** Time-resolved fluorescence decay profiles of 50  $\mu\text{M}$  1,4DH2NA (a) and 50  $\mu\text{M}$  1,4DH2NA + 130  $\mu\text{M}$   $\text{Ti}_{\text{surf}}$  (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 ( $\chi^2$ ) 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 TiO<sub>2</sub> nanoparticles modified with 2HBA (a), 1H<sub>2</sub>NA (b) and 1,4DH<sub>2</sub>NA (c) recorded at the heating rate of 20°C min<sup>-1</sup> in air