Electronic Supplementary Information (ESI†)

Substituents effect on the surface modification of anatase nanoparticles with catecholate-type ligands: a combined DFT and experimental study

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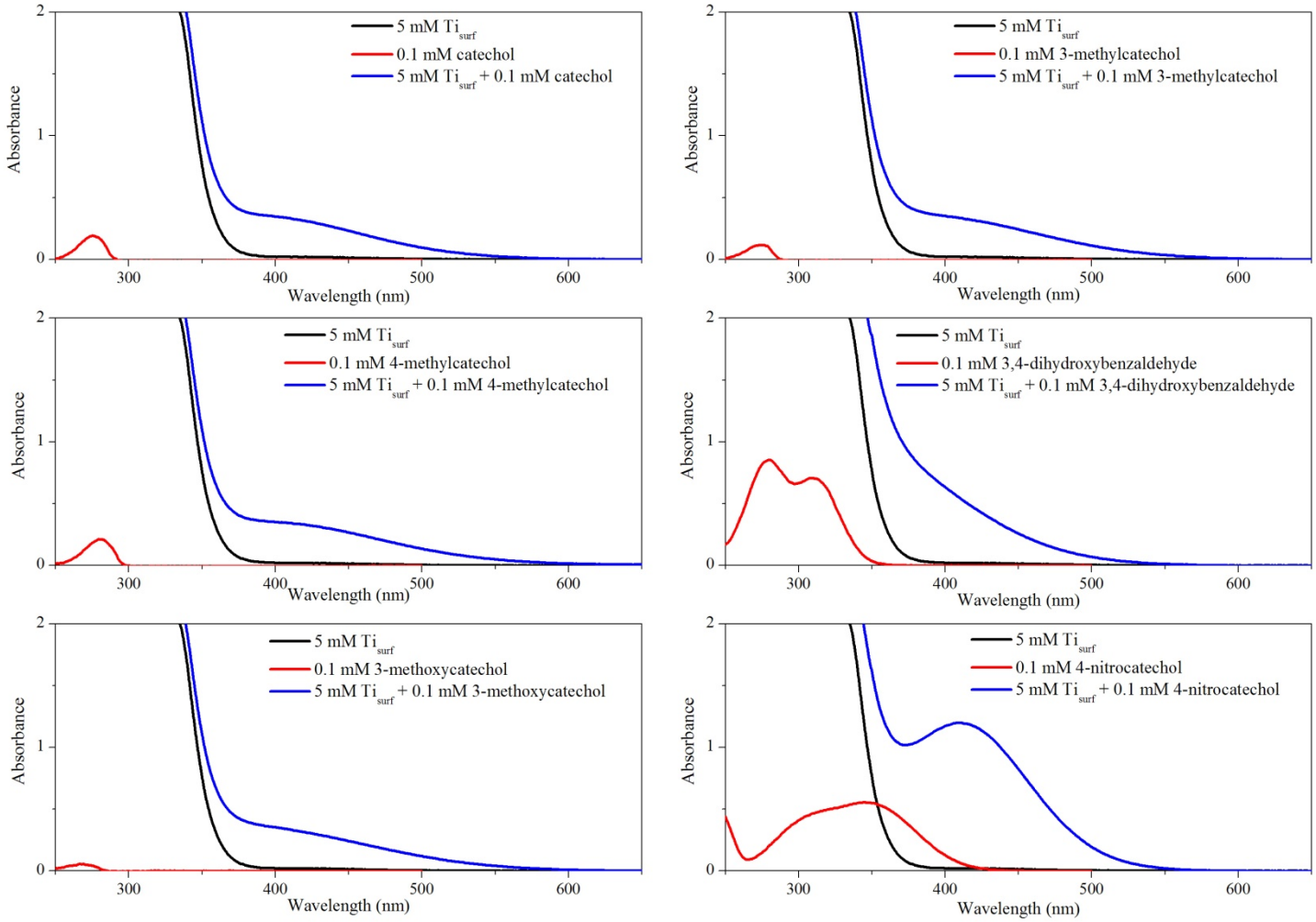

Figure S1. Absorption spectra of TiO_2 nanoparticles (black), free ligands (red) and ligand-TiO_2 CT-complexes (blue) with 4% coverage in methanol/water=90/10, pH 2.

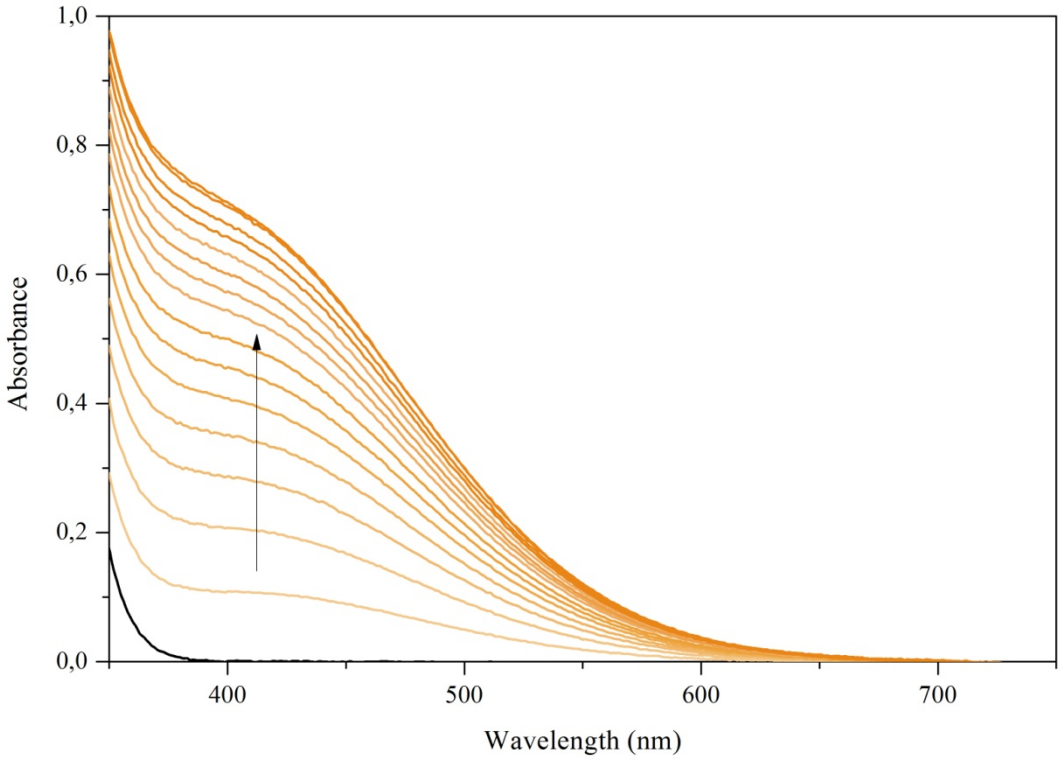

Figure S2 Absorption spectra of 3.6 mM TiO_2 (1 mM Ti_{surf}) nanoparticles before and after surface modification with 4-methylcatechol (0 – 0.6 mM in 0.04 mM steps) in methanol/water=90/10, pH = 2 (data recorded 20 h after surface modification).

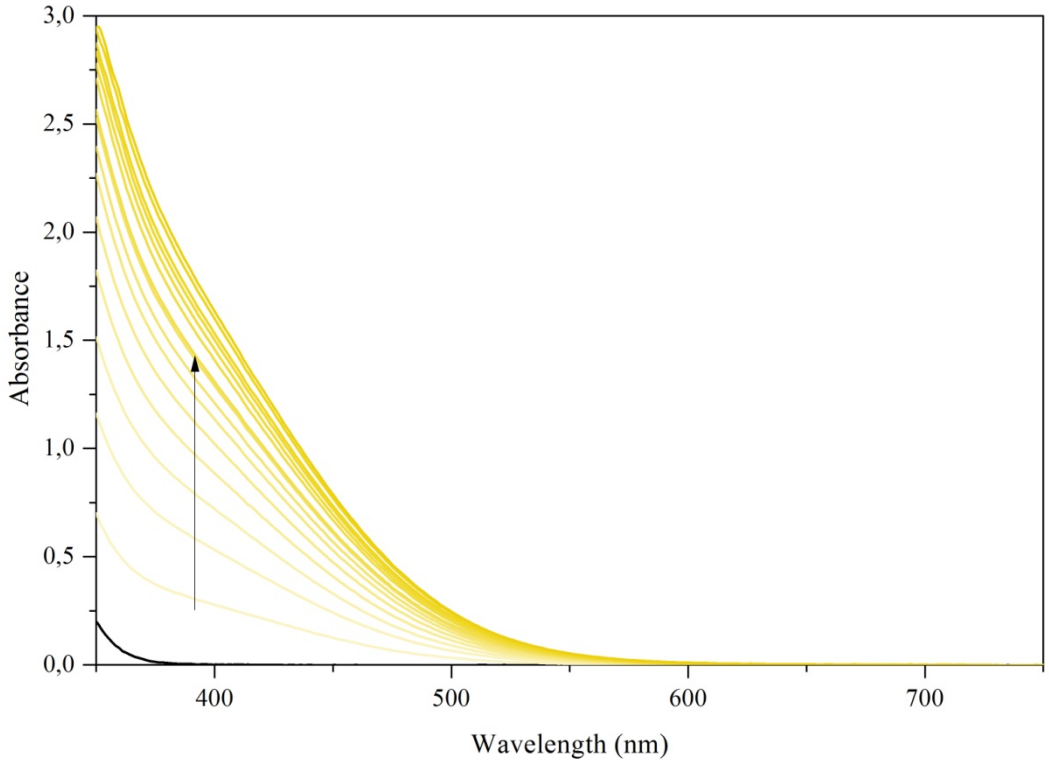

Figure S3 Absorption spectra of 3.6 mM TiO_2 (1 mM Ti_{surf}) nanoparticles before and after surface modification with 3,4-dihydroxybenzaldehyde (0 – 0.6 mM in 0.04 mM steps) in methanol/water=90/10, pH = 2 (data recorded 20 h after surface modification).

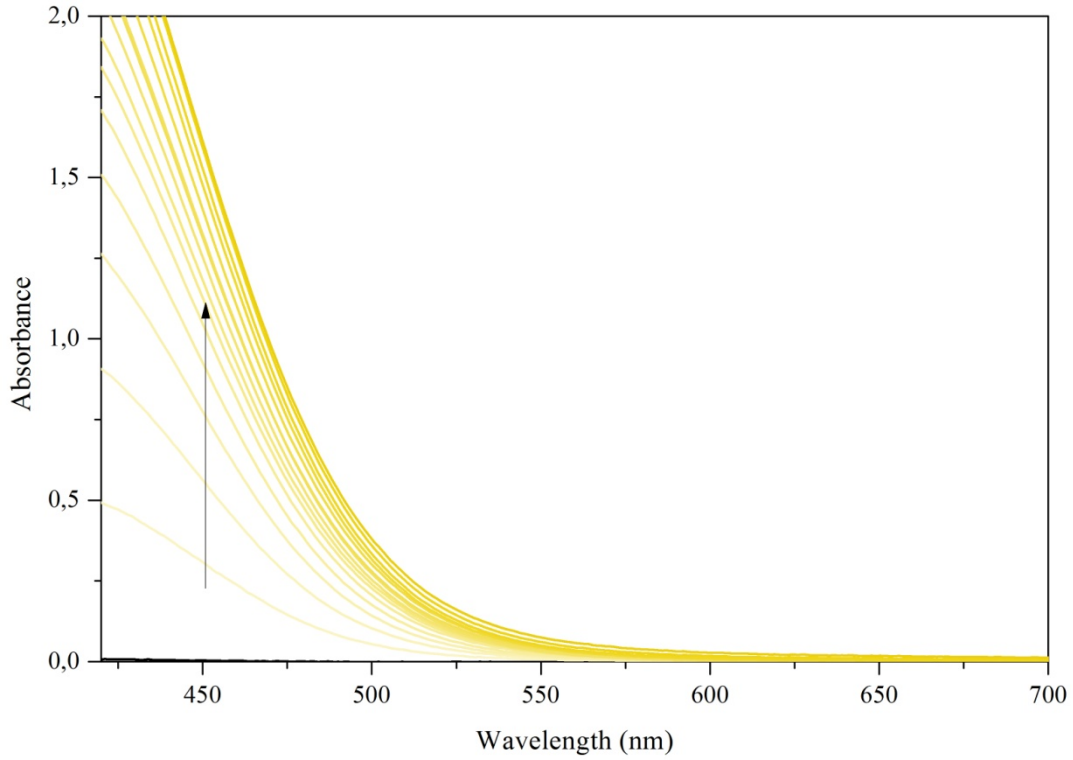

Figure S4 Absorption spectra of 3.6 mM TiO_2 (1 mM Ti_{surf}) nanoparticles before and after surface modification with 4-nitrocatechol (0 – 0.6 mM in 0.04 mM steps) in methanol/water=90/10, pH = 2 (data recorded 20 h after surface modification).

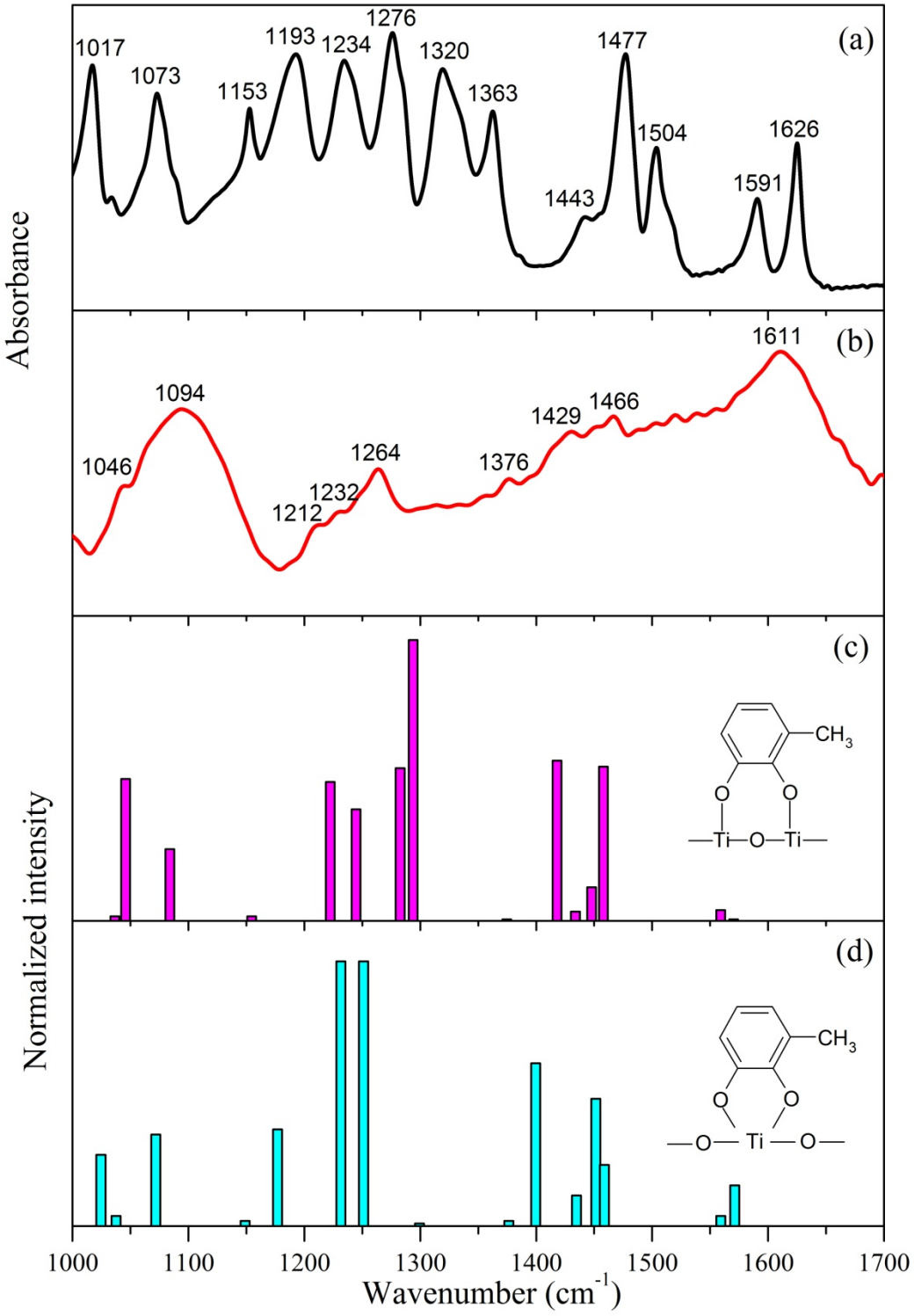

Figure S5 FTIR spectra of 3MetCat: Experimental spectra of free 3MetCat (a) and adsorbed on TiO_2 nanoparticles (b); scaled predicted spectra at the B3LYP/6-31G** level of theory for bridging (c) and chelating (d) bidentate binding structure

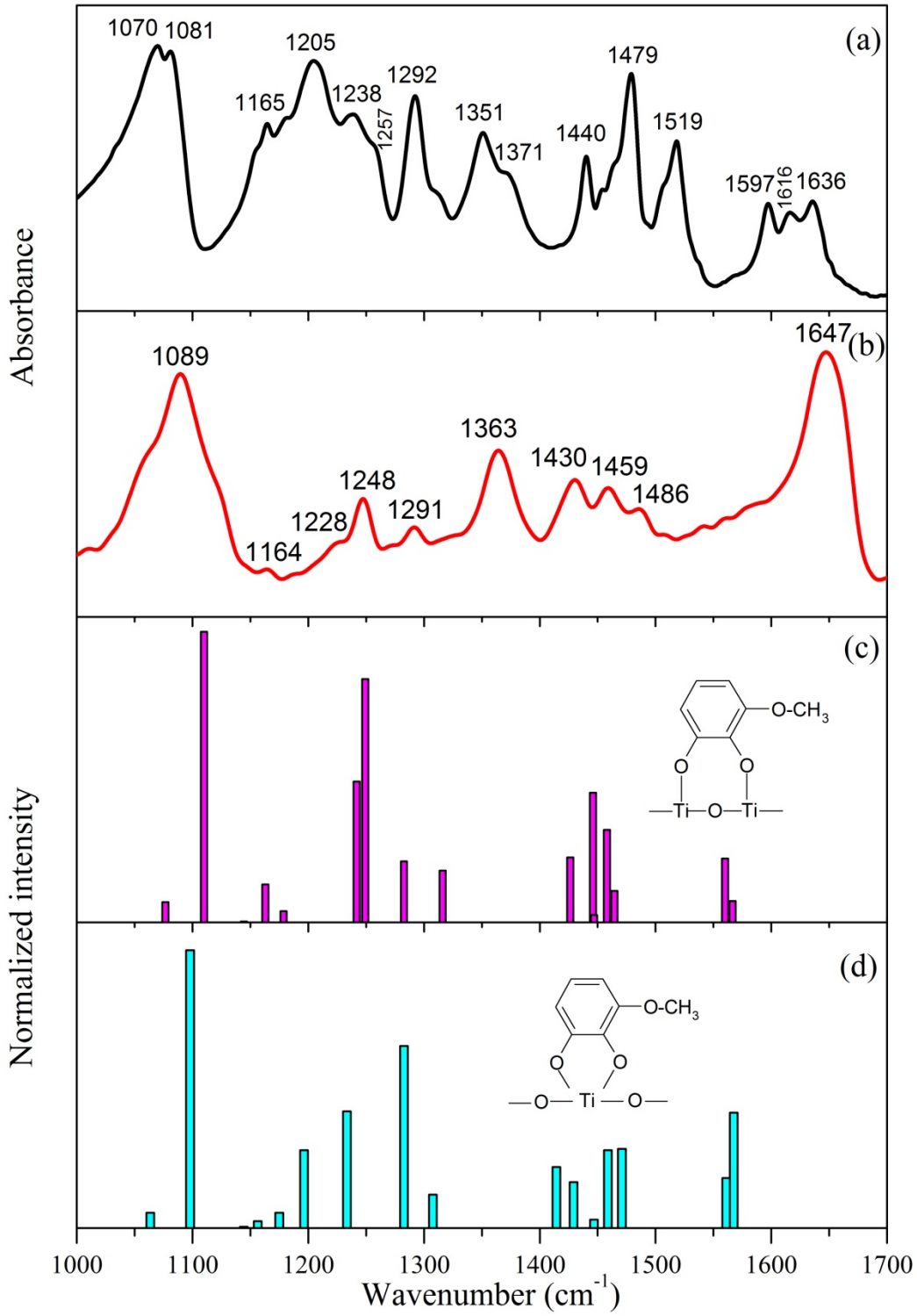

Figure S6 FTIR spectra of 3MethoxyCat: Experimental spectra of free 3MethoxyCat (a) and adsorbed on TiO_2 nanoparticles (b); scaled predicted spectra at the B3LYP/6-31G** level of theory for bridging (c) and chelating (d) bidentate binding structure

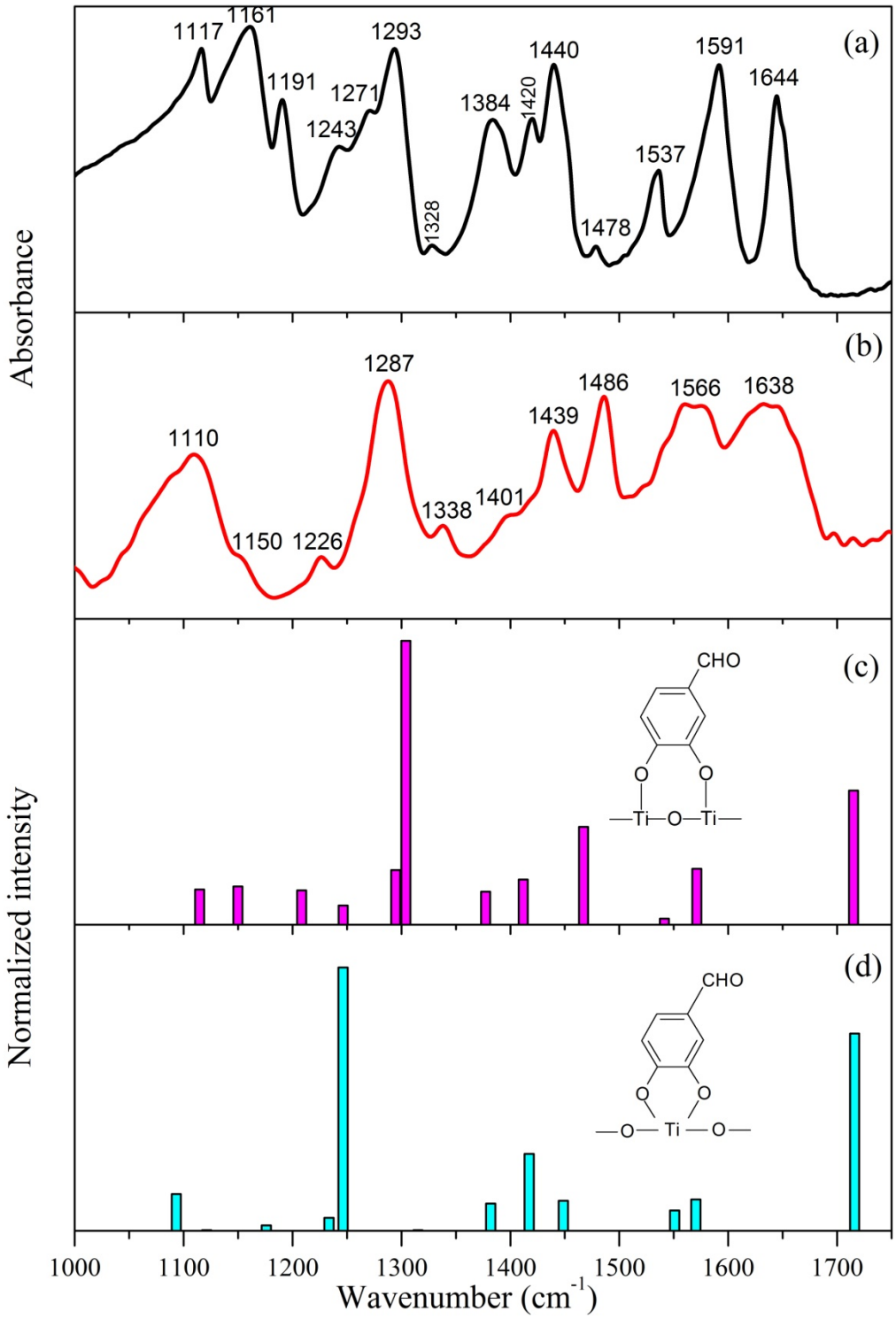

Figure S7 FTIR spectra of 34DHBA: Experimental spectra of free 34DHBA (a) and adsorbed on TiO_2 nanoparticles (b); scaled predicted spectra at the B3LYP/6-31G** level of theory for bridging (c) and chelating (d) bidentate binding structure

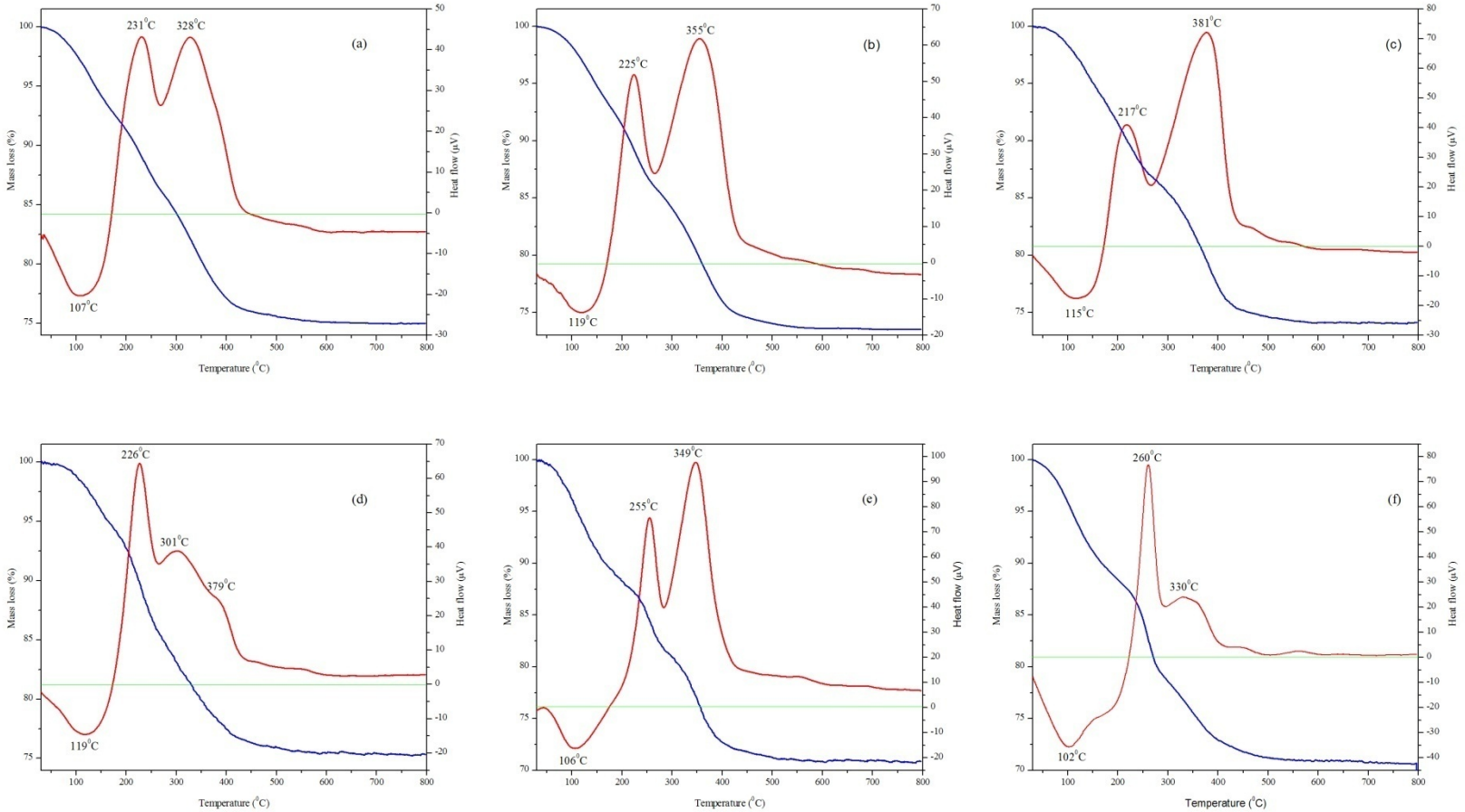

Figure S8. TG (blue line) and heat flow (red line) curves of TiO_2 nanoparticles modified with Cat (a), 3MetCat (b), 4MetCat (c), 3MethoxyCat (d), 34DHBA (e) and 4NitCat (f) recorded at the heating rate of 20^0C min^{-1} in air.