

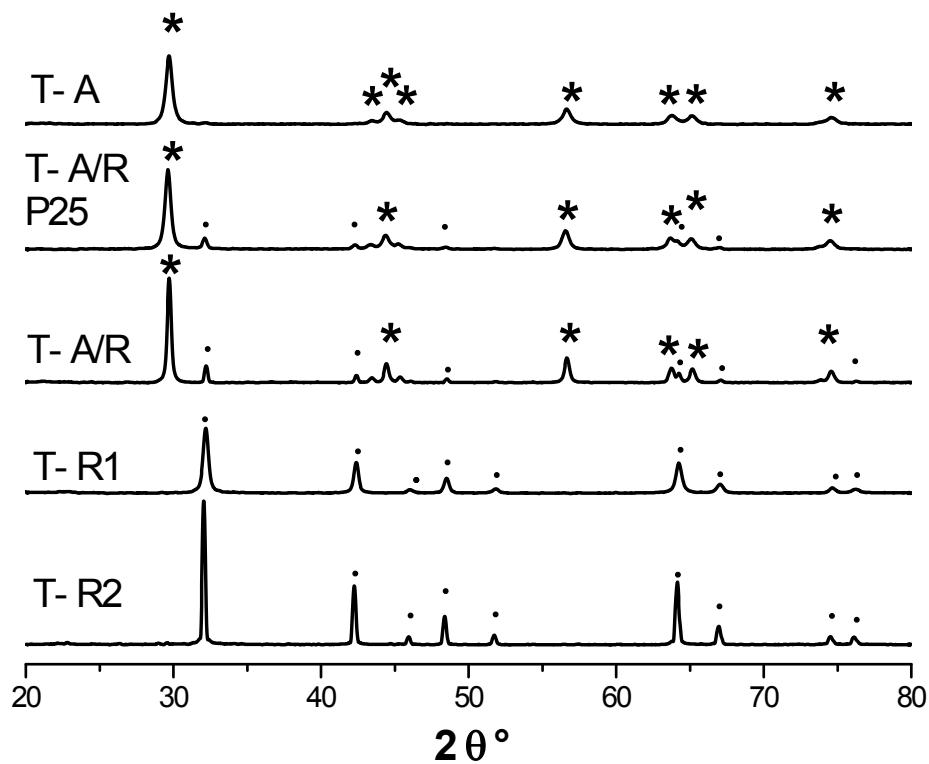
**A comparative study on the efficacy of different probes to predict the photo-activity of nano-titanium dioxide toward biomolecules**

*Marucco et al.*

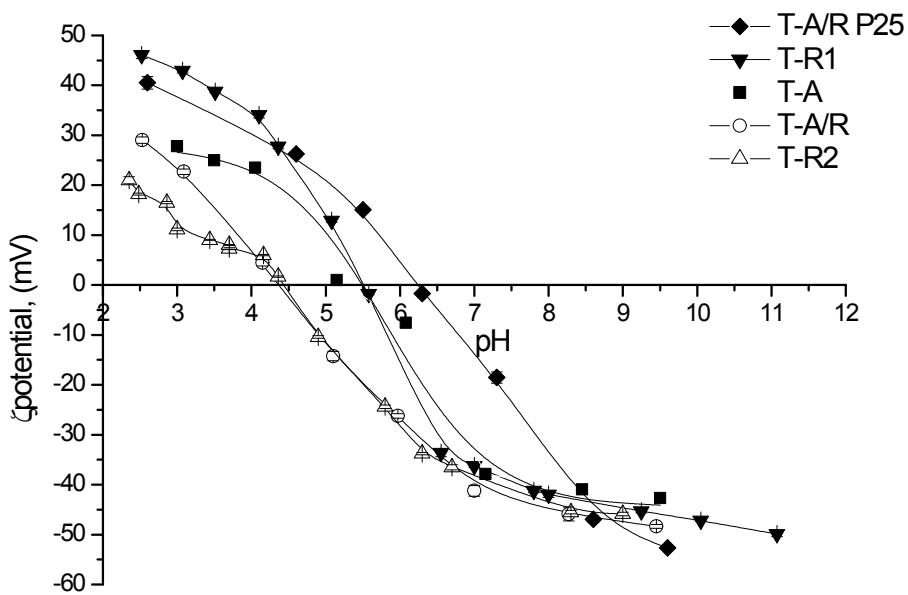
## **Supplementary information**

## **Summary of the content**

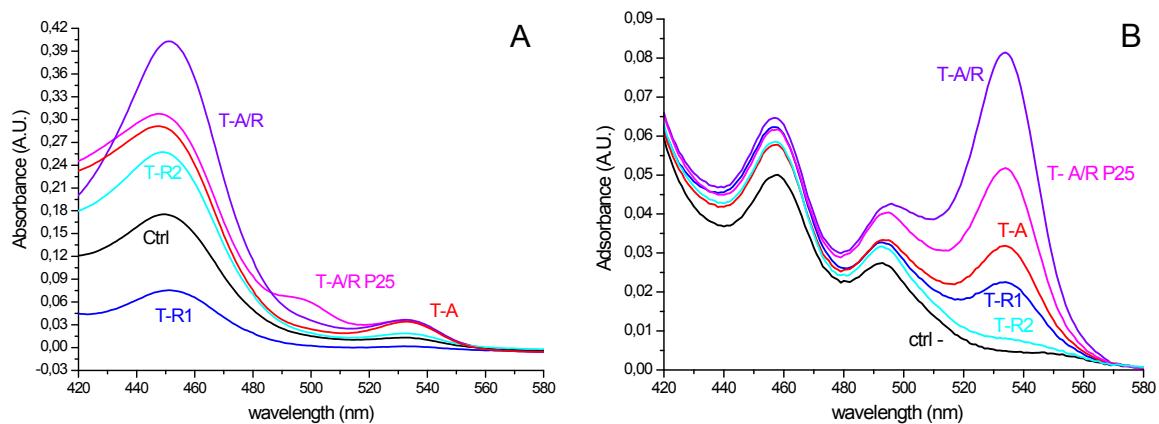
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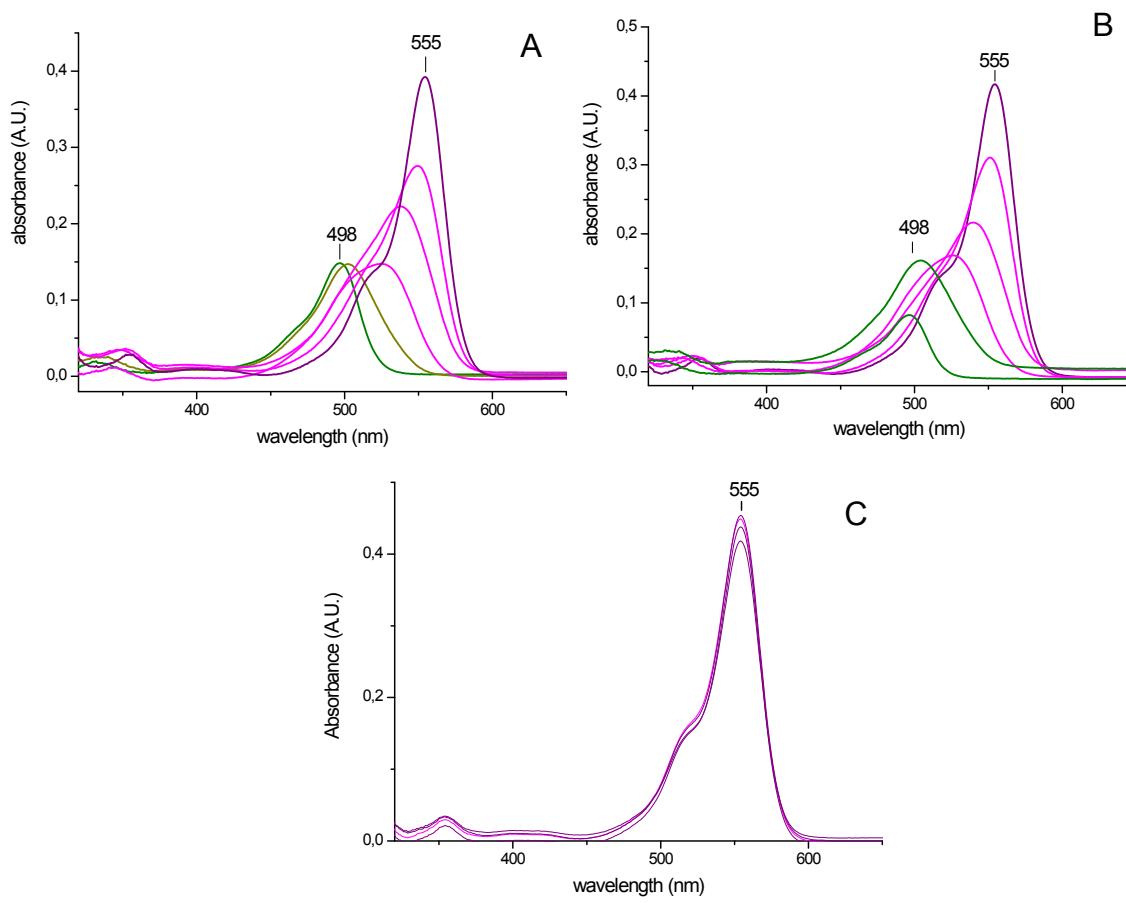
**Figure S 1.** X-ray diffractograms of the  $\text{TiO}_2$  powders in the  $20-80 = 2\theta$  range. The peaks of anatase (\*) and rutile (o) are showed above the diffractograms



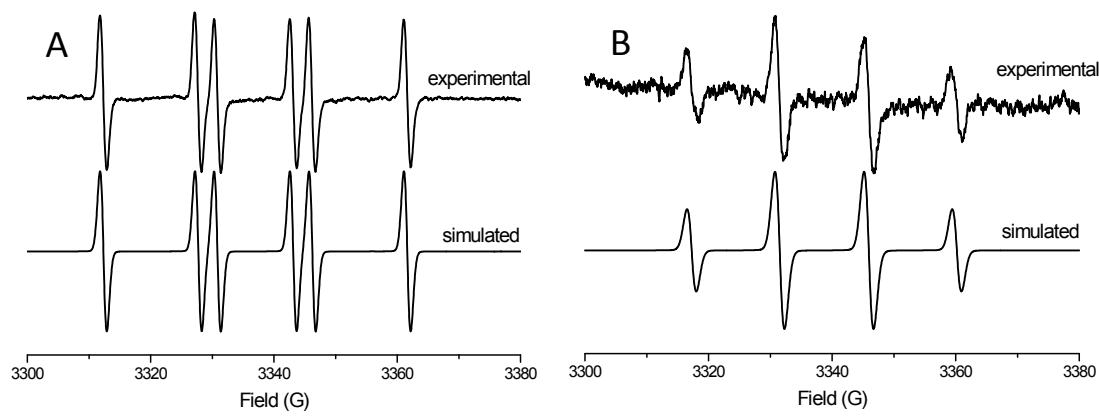
**Figure S2.**  $\zeta$  potential as a function of pH of the  $\text{TiO}_2$  powders.



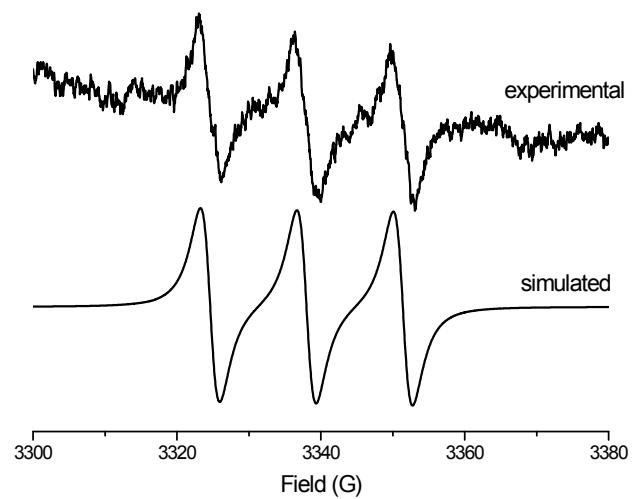
**Figure S3.** Degradation of A) linoleic acid; B) 2-deoxyribose. Representative UV/vis spectra after 1h of irradiation. The pick at 535 nm corresponds to the TBA adduct of MDA, while pick at 455 nm and 500 nm are due to the formation of other TBA-reactive species (TBARS) like mono-aldheydes (J. A. Knight, R. K. Pleper, L. McClellan, *Clinical Chemistry* 1988, **34**, 2433-2438.)



**Figure S4.** Degradation of rhodamine B. Representative **Uv-vis** spectra recorded at 90 minutes for (A)T-A; (B) T-A/R; (C) T-R2



**Figure S5.** Experimental and simulated EPR spectra of DMPO adducts. (A) DMPO/CO<sub>2</sub><sup>·-</sup>; (B) DMPO/HO<sup>·</sup>.



**Figure S6.** Experimental and simulated EPR spectra of PBN/O<sub>2</sub><sup>·</sup> adduct.

**Table 1S. Hyperfine splitting constants of the radicals species detected**

Radical specie	Solvent	Hyperfine splitting constants
DMPO/HO·	100 mM PB pH 7.4	$A_H$ 14.1G; $A_N$ 14.4G;
DMPO/CO <sub>2</sub> · <sup>-</sup>	125 mM PB pH 7.4	$A_H$ 15.4 G; $A_N$ 18.5 G;
PBN/O <sub>2</sub> · <sup>-</sup>	cyclohexane	$A_N$ 13.5 G;
PBN/HO <sub>2</sub> ·		
TEMPONE	cyclohexane	$A_N$ 14.0 G;
TEMPONE (from TMP)	water	$A_N$ 15.7 G;
TEMPONE (from TMPONE-H)	water	$A_N$ 15.7 G;
TEMPONE (from TMPONE-H)	phosphate buffer, pH 7.4	$A_N$ 15.7 G;

**Table 2S. Summary of the experimental conditions.**

Target molecule	Spin trapping/probe	Reactive specie/product detected	Solvent /buffer	pH	exposed surface area of TiO <sub>2</sub> m <sup>2</sup> /ml
Rhodamine B	-	-	H <sub>2</sub> O	5-6	0.105
H <sub>2</sub> O	DMPO	HO·	PB	7-7.4	1.12
		35 mM		100mM	
HCOOH 1M	DMPO	CO <sub>2</sub> ·-	PB	7-7.4	2.8
		75 mM		125mM	
-	TEMPONE-H	TEMPONE	H <sub>2</sub> O	4-6	0.7
		50μM			
-	TEMPONE-H	TEMPONE	PB	7-7.4	0.7
		50μM		10mM	
O <sub>2</sub>	4-oxoTMP	TEMPONE	cyclohexane	-	1.4
		50mM			
O <sub>2</sub>	4-oxo TMP	TEMPONE	PB	9	0.7
		50mM		10mM	
O <sub>2</sub>	PBN	O <sub>2</sub> ·-	cyclohexane	-	0.18
		20mM			
linoleic acid 1mM	-	MDA	PB	7-7.4	1.05
				10mM	
2-deoxyribose 1mM	-	MDA	PB	7-7.4	1.05
				10mM	