# Supplementary material

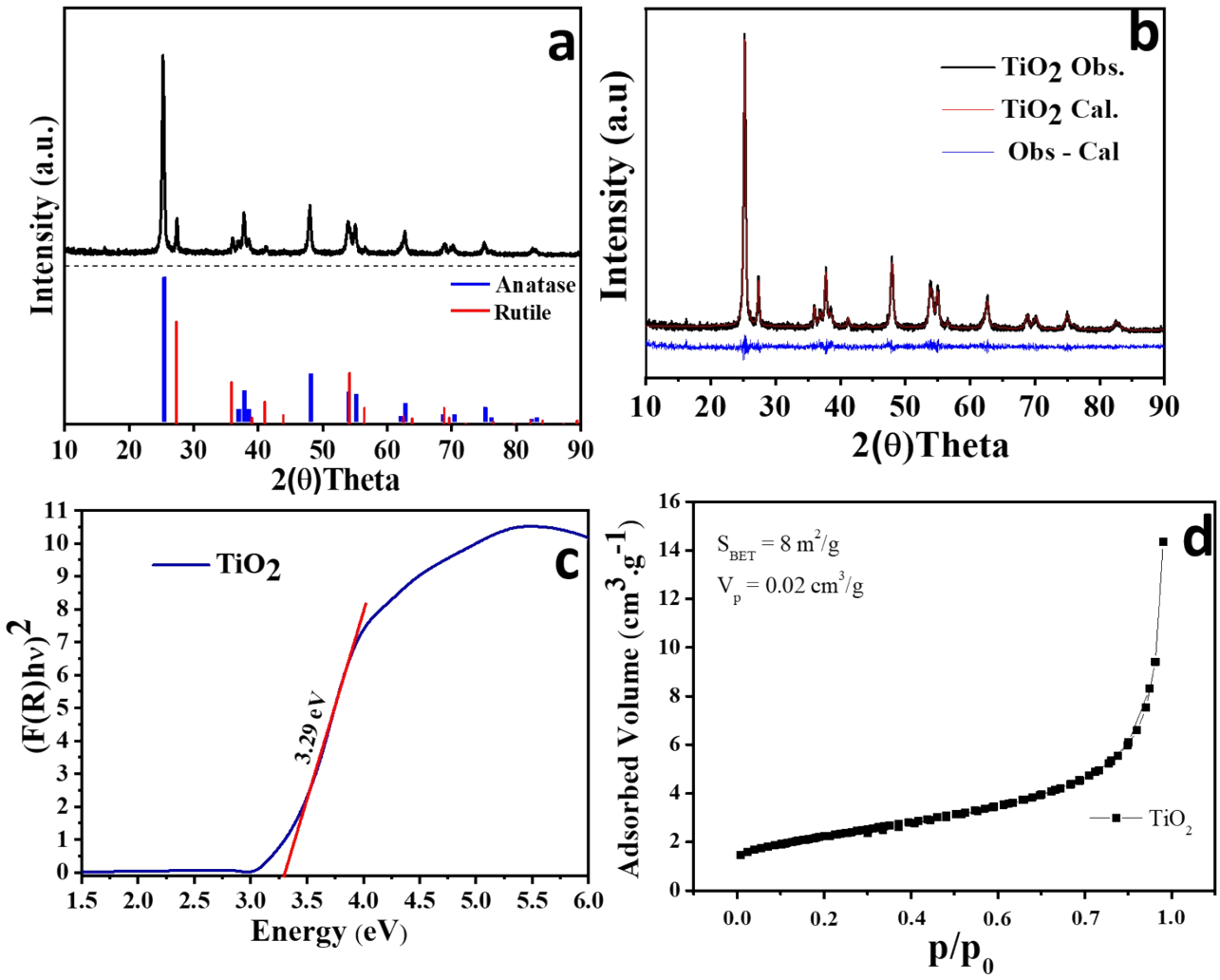



**Figure S1.** **(a)** X-Ray Diffractogram for titanium dioxide sample; **(b)** Rietveld refinement for $TiO_2$ diffractogram; **(c)** Band-gap energy for indirect allowed transitions; **(d)** $N_2$ adsorption-desorption isotherm of the $TiO_2$ photocatalyst.

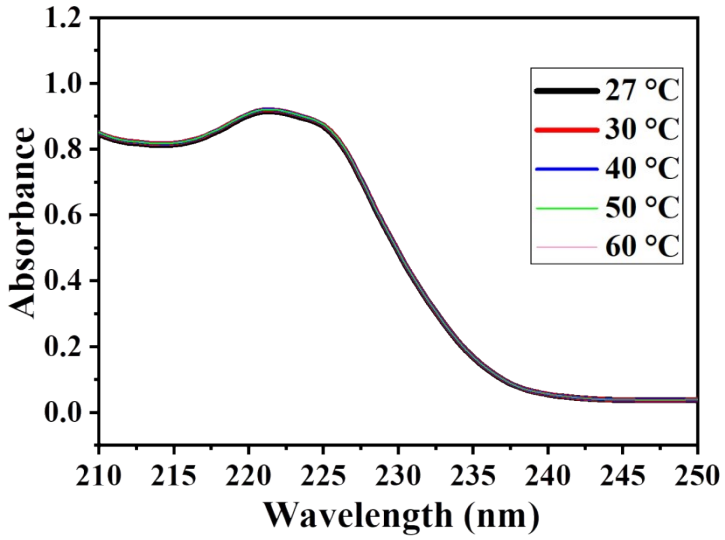



**Figure S2.** Ibuprofen thermal stability analysis in different temperatures.

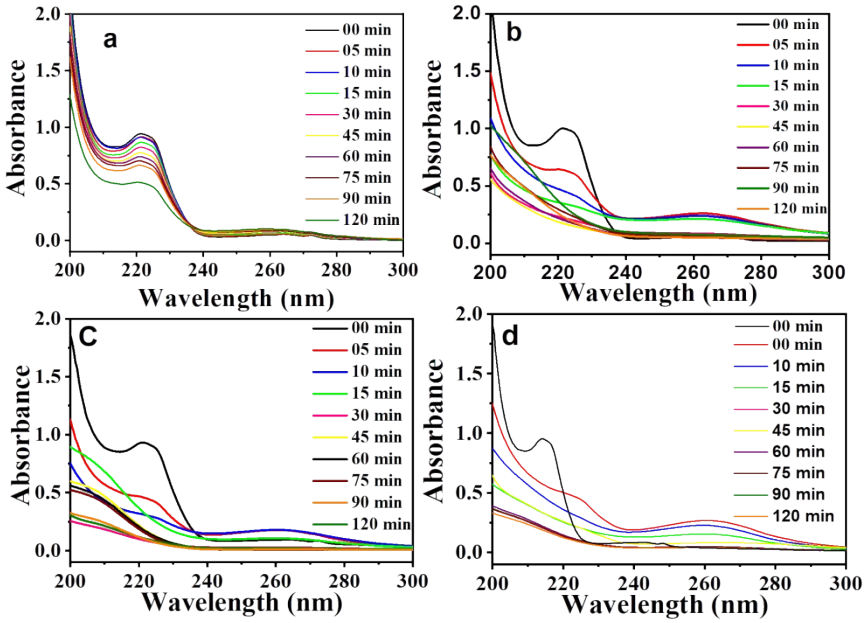



**Figure S3.** (a) Ibuprofen photolysis; (b) Photodegradation of ibuprofen using 0.01g of $TiO_2$; (c) using 0.03g of $TiO_2$; (d) using 0.05g of $TiO_2$.

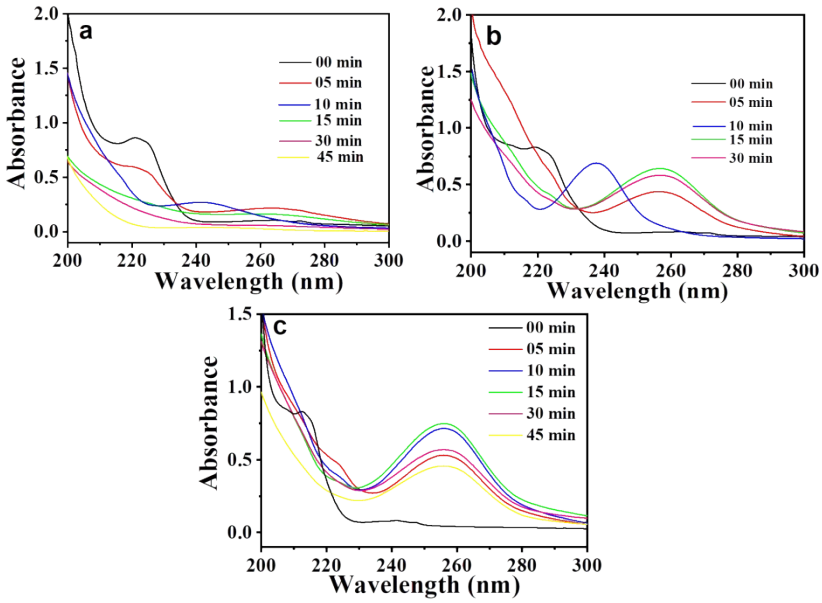



**Figure S4.** Ibuprofen photodegradation: (a) at pH 9.0; (b) at pH 5.0; (c) at pH 3.0.

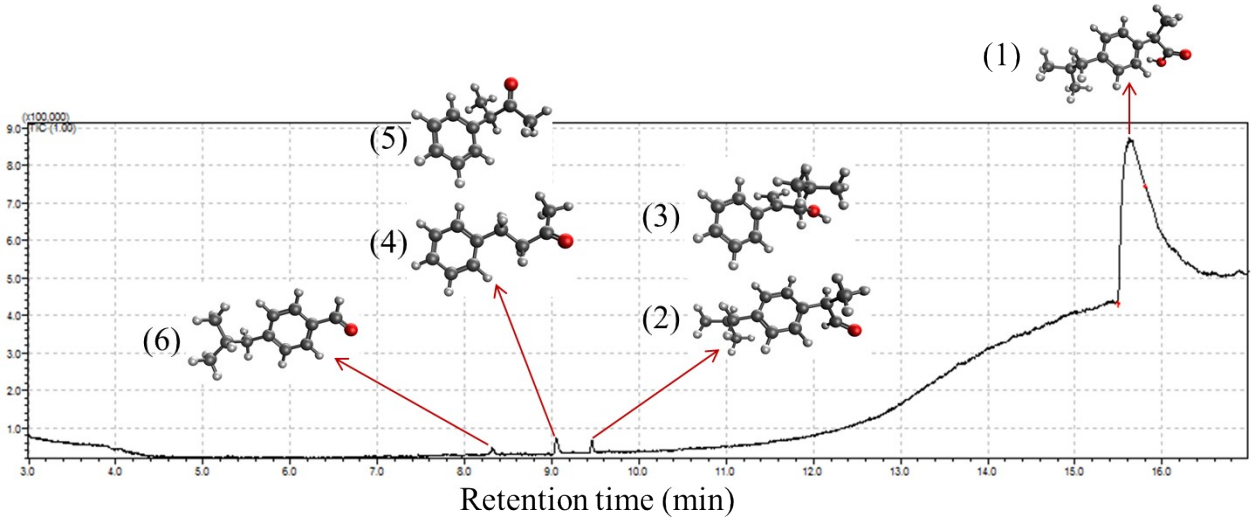



**Figure S5.** Chromatogram identifying the main by-products and intermediates of the reaction, where ibuprofen (1), 4-isobutylacetophenone (2), 4-methyl-2-phenyl-1-penten-3-ol (3), 4-phenyl-benzylacetone (4), 3-phenyl-2-butanone (5) and p-isobutylbenzaldehyde (6).

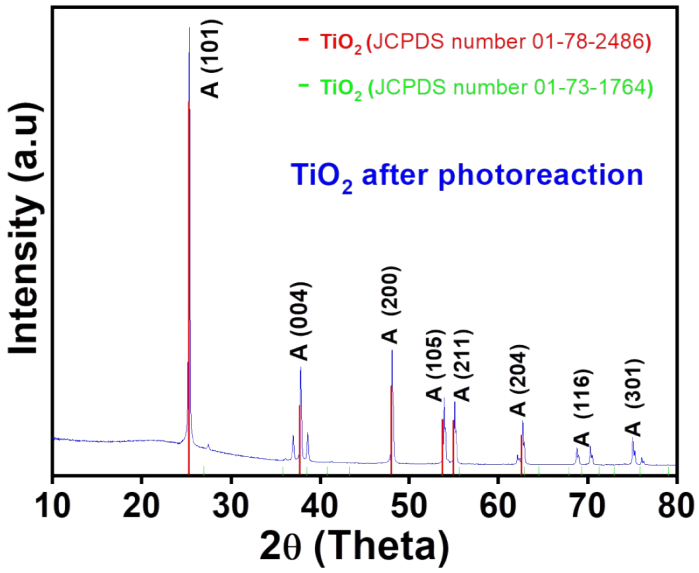



**Figure S6.** XRD result for the $TiO_2$ solid after photocatalytic test.

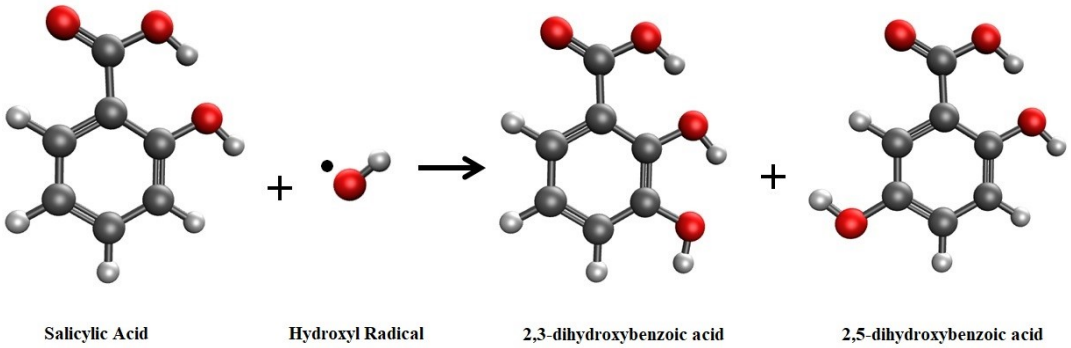



**Figure S7.** Products from the reaction between salicylic acid and hydroxyl radical.

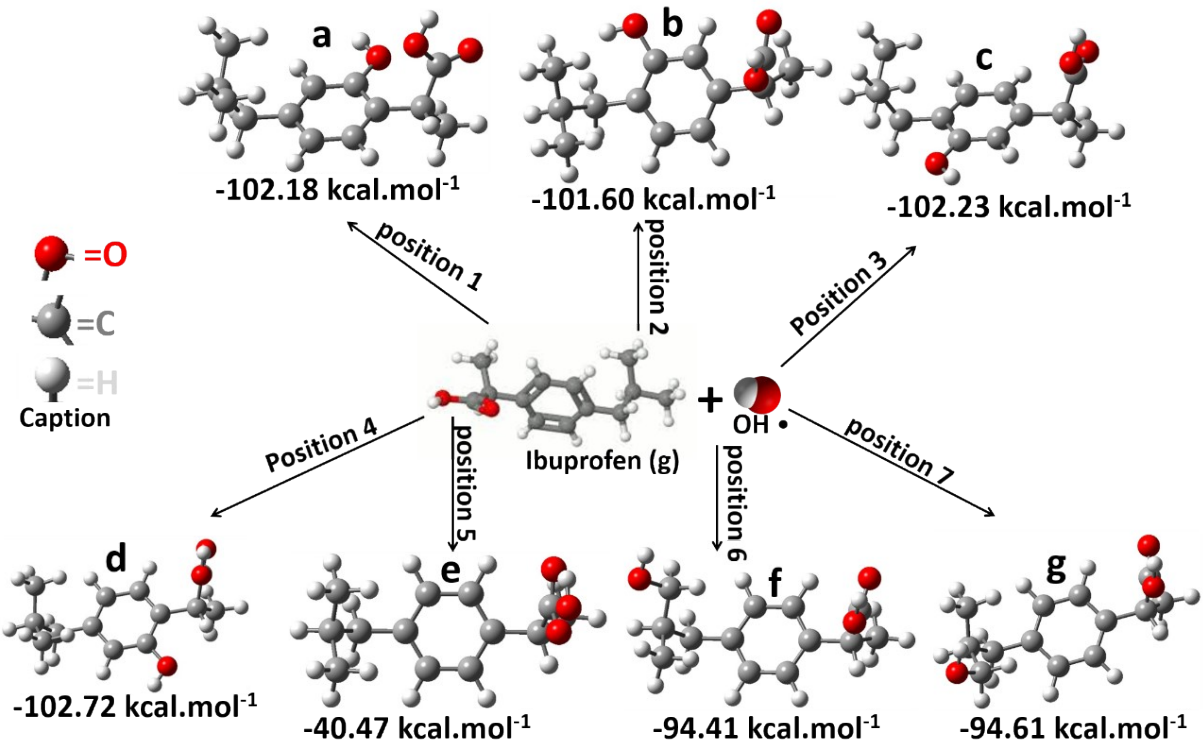
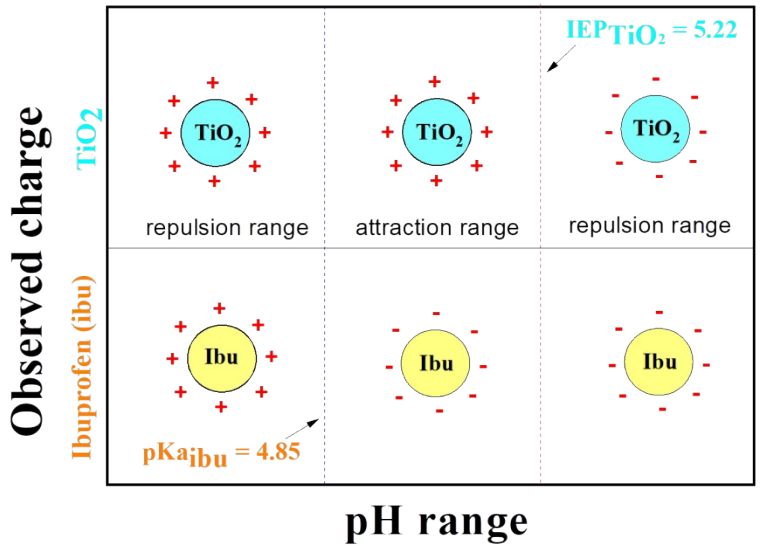



**Figure S8.** Schematic representation of ibuprofen/•OH radical system taking into account the presence of water after optimization used to calculate free energy for the seven different positions.




**Scheme S1.** Representation of the interaction between $TiO_2$ and ibuprofen charges, depending on the pH range.

**Table S1.** Kinetic parameters obtained for different $TiO_2$ mass.

| $TiO_2$ mass (g) | $R^2$ | k' ($min^{-1}$) | $T_{1/2}$ (min) |
|---|---|---|---|
| 00.1 | 0.9964 | 0.0318 | 21.7970 |
| 0.03 | 0.9708 | 0.1193 | 5.8101 |

**Table S2.** Kinetic parameters obtained for different pHs of ibuprofen solution.

| pH | $R^2$ | k' ($min^{-1}$) | $T_{1/2}$ (min) |
|---|---|---|---|
| 3.0 | 0.9030 | 0.0768 | 9.0253 |
| 7.0 | 0.9708 | 0.1193 | 5.8101 |

**Table S3.** Comparison of ibuprofen degradation between different studies using $TiO_2$ catalysts.

| Ibuprofen degradation | | | | |
|---|---|---|---|---|
| Concentration ($mg.L^{-1}$) | Catalyst | Time (min) | Performance (%) | Reference |
| 100 | $TiO_2$ | 90 | 99.99 | 1 |
| 0.05 | $TiO_2$ | 240 | 100 | 2 |
| 0.1 | $TiO_2$ | 45 | 100 | 3 |
| 20 | $TiO_2$ | 300 | 100 | 4 |
| 213 | $TiO_2$ | 240 | 100 | 5 |
| 15 | $TiO_2$ | 60 | 100 | 6 |
| 20 | $TiO_2$ | 30 | 100 | 7 |
| 20 | $TiO_2$ | 15 | 100 | this work |