

# A potent virucidal activity of TiO<sub>2</sub> functionalized nanoparticles adsorbed with flavonoids against SARS-CoV-2

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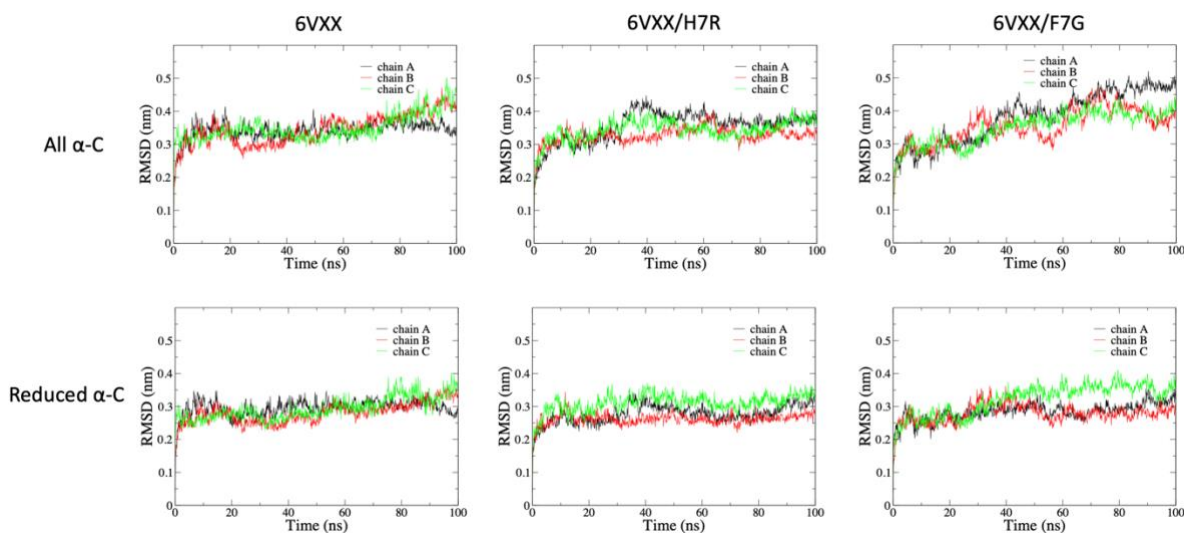
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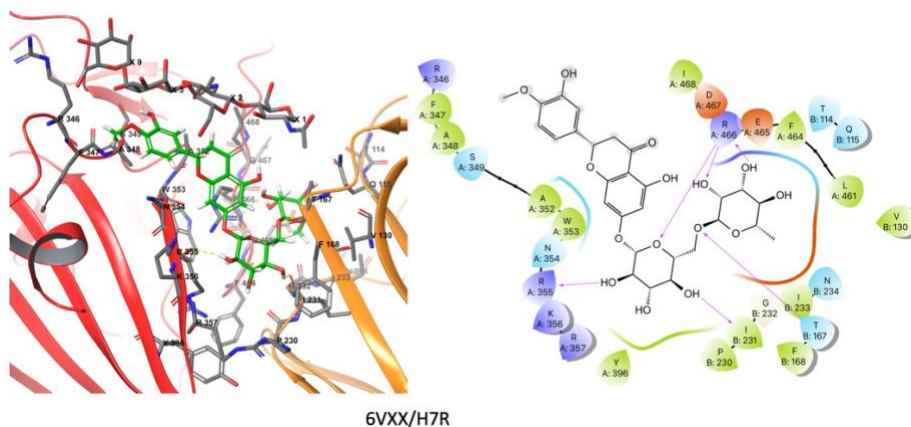
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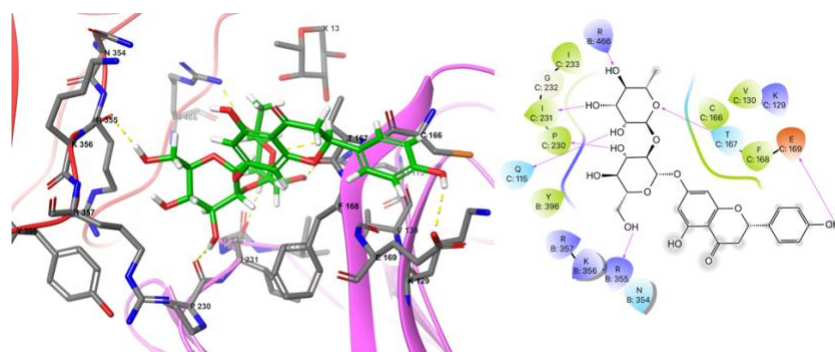


**Figure S1**  $\alpha$ -Carbon root mean square deviation (RMSD) along time.  $\alpha$ -Carbon of first and last 15 residues (amino and carboxyl terminal) and loop from 676 to 689 was not consider for the RMSD calculation on the reduced  $\alpha$ -carbon graphs



6VXX/H7R

**Figure S2** Three-dimensional interaction maps for SARS-CoV2 spike glycoprotein and interacting H7R. H7R is shown with carbons on green. All residues at least 5Å are shown on both representations. Sugars are named as X1, X2, X3, X9 and X13 and not shown on the interaction map. Hydrogen bonds are shown as dotted lines yellow on the three-dimensional representation and as pink arrows on the interaction maps

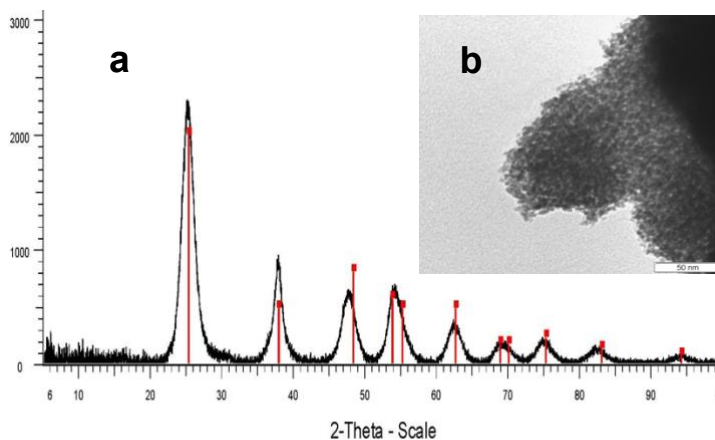


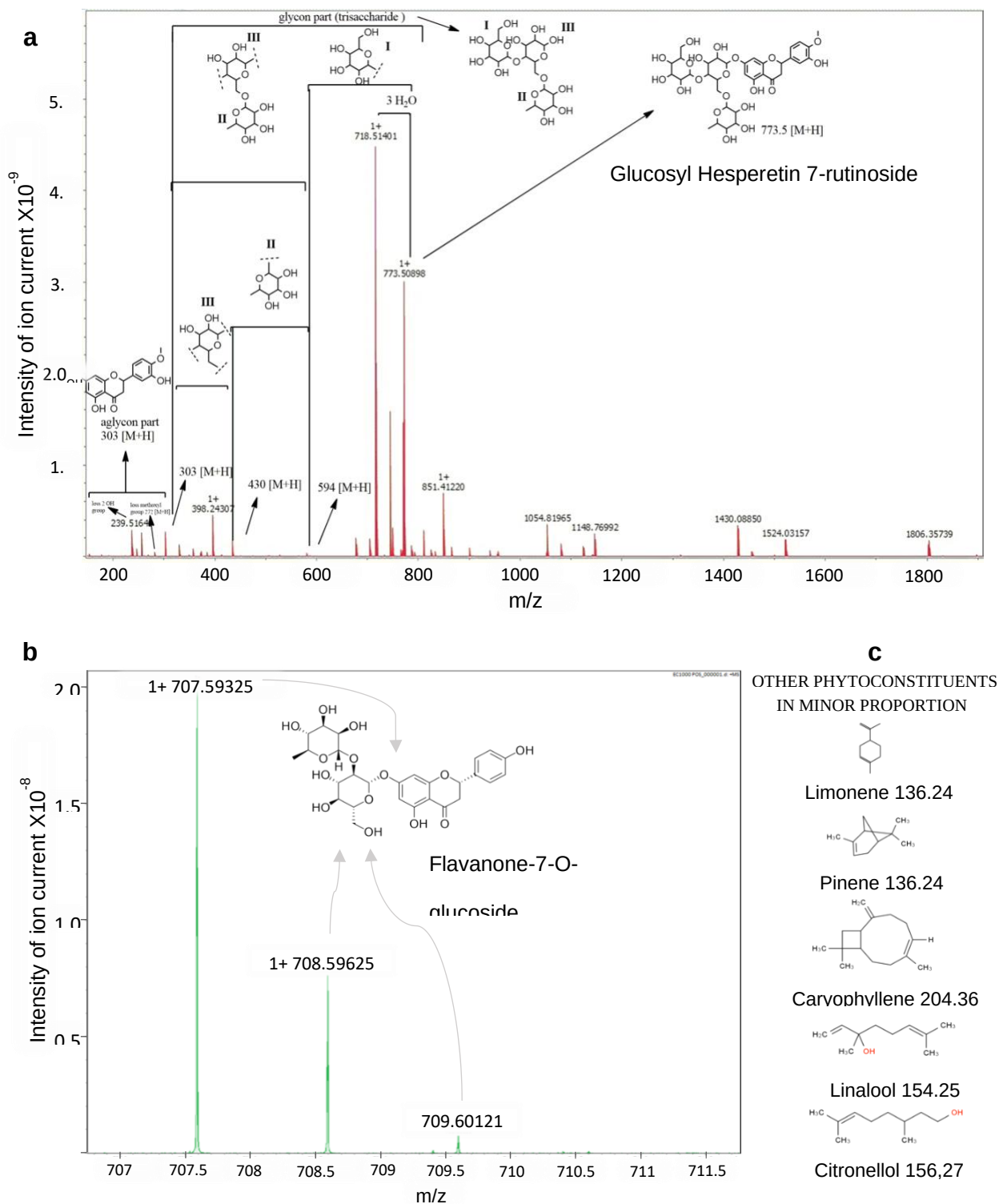
6VXX/F7G

**Figure S3** Three-dimensional and interaction maps for spike glycoprotein and interacting F7G. F7G is shown with carbons on green. All residues at least 5Å are shown on both representations. Sugars are named as X1, X2, X3, X9 and X13 and not shown on the interaction map. Hydrogen bonds are shown as dotted lines yellow on the three-dimensional representation and as pink arrows on the interaction maps

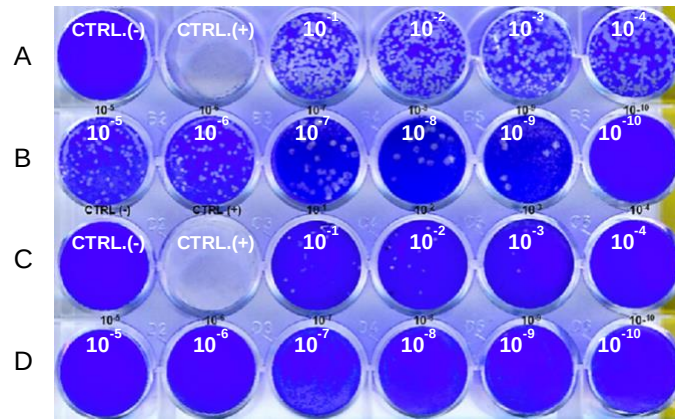
**Figure S4 a. X-ray diffraction peak of TiO<sub>2</sub> NPs.** XRD measurements show that TiO<sub>2</sub> NPs exhibit the anatase structure. The average grain size calculated from the broadening of the XRD peak of anatase was 2 nm.

**b. Transmission electron microscope (TEM) image of anatase TiO<sub>2</sub> NPs.** TEM showed the average size of nanoparticles suspended of 2 nm, consistent with the XRD results

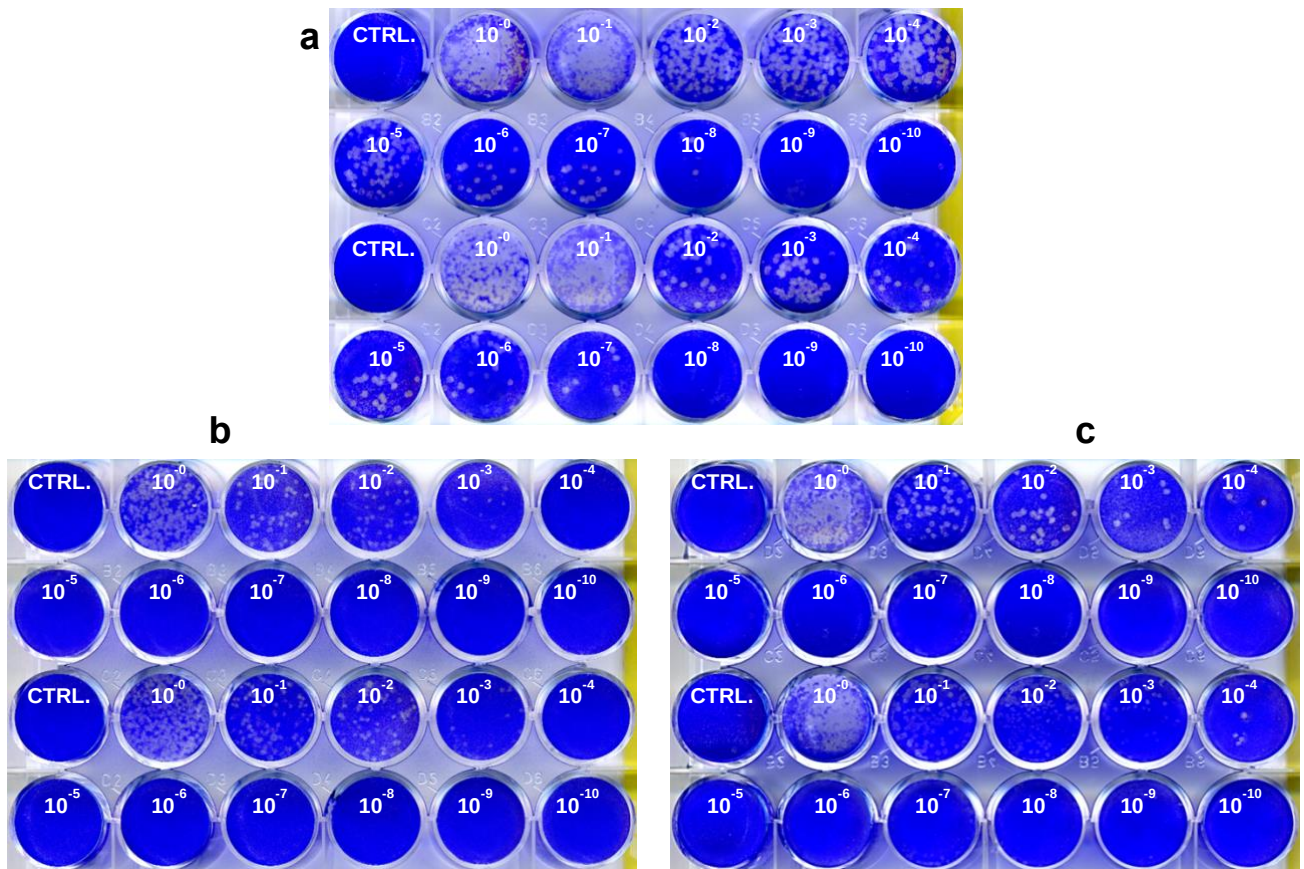




**Figure S5.** ESI FT-ICR. **a.** Representative positive ion mode mass spectra of (H7R) Glycosil-Hesperetin (isotopic pattern: 773.50, 774.51, 775.51). **b.** Representative negative ion mode mass spectra of (F7G) Naringin- $H^{++}$   $^{65}Cu^{2++}$   $2CH_3OH$  (isotopic pattern: 707.59, 708.59, 709.60). **c.** Representative positive ion mode mass spectra of terpenes



**Figure S6** Plaque assay virus titration. **Lane A and B.** Coronavirus ChoV-229E in VERO.E6 cells as control. PFU/mL=  $6 \times 10^{10}$ . **Lane C and D.** Coronavirus 229E pre-incubated for 5 minutes with F7G. PFU/mL=  $3 \times 10^4$



**Figure S7** Plaque assay virus titration. **a.** SARS-CoV-2 in VERO.E6 cells as control. PFU/mL=  $3 \times 10^9$  **b.** SARS-CoV-2 pre-incubated for 5 minutes with F7G. PFU/mL=  $5 \times 10^4$  **c.** SARS-CoV-2 pre-incubated for 5 minutes with H7R. PFU/mL=  $3 \times 10^5$