

Supplementary materials

Molecular Mechanisms behind the Anti Corona Virus Activity of Small Metal Oxide Nanoparticles

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Table S1. Calculated probability values from one-way ANOVA statistical analysis with Tukey post-hoc test of experimental results for TGEV and EMCV viruses inactivation by TATT titania and POM NPs. P-values are expressed as differences between log pfu/ml at NP exposures and negative (non-exposed) controls. Null hypothesis suggested statistical identity of NP exposures and non-exposed control unless shown otherwise. P-values < 0.05 (highlighted) were considered statistically significant.

TGEV			
TATT NPs	p-value	POM NPs	p-value
1.25 mM vs control	4.52186·10 ⁻⁸	1.25 mM vs control	0.9674
0.125 mM vs control	6.31492·10 ⁻⁵	0.125 mM vs control	0.81529
0.013 mM vs control	0.96317	0.013 mM vs control	1
0.001 mM vs control	0.77279	0.001 mM vs control	0.99999
0.125 mM vs. 1.25 mM	0		
EMCV			
TATT NPs	p-value	POM NPs	p-value
1.25 mM vs control	0.99995	1.25 mM vs control	1
0.125 mM vs control	1	0.125 mM vs control	1
0.013 mM vs control	1	0.013 mM vs control	1

Table S2. Crystallographic data for (HEPES)₃(H₃O)SiW₁₂O₄₀.

Chemical formula	C ₅ H ₉ N ₅ O ₃₆ S ₃ Si ₃ W ₁₂
Formula weight	3101.82 g/mol
Temperature	273(2) K
Wavelength	0.71073 Å
Crystal system	monoclinic
Space group	P 1 21/c 1
Unit cell dimensions	a = 32.191(3) Å α = 90° b = 14.8183(12) Å β = 91.018(2)° c = 15.3532(13) Å γ = 90°
Volume	7322.6(11) Å ³
Z	4
Theta range for data collection	2.28 to 32.49°
Index ranges	-48 ≤ h ≤ 47, -21 ≤ k ≤ 22, -23 ≤ l ≤ 22
Reflections collected	119465
Independent reflections	25909 [R(int) = 0.0967]
Nr. of obs. independent refl; I > 2σ(I)	17682
Final R indices, observed	R1 = 0.0744, wR2 = 0.1830
Final R-indices, all data	R1 = 0.1114, wR2 = 0.1997

Table S3. Crystallographic data for (HGly₃)₄SiW₁₂O₄₀.

Chemical formula	C ₂₄ H ₄₄ N ₁₂ O ₅₆ SiW ₁₂	
Formula weight	3631.00 g/mol	
Temperature	273(2) K	
Wavelength	0.71073 Å	
Crystal system	triclinic	
Space group	P -1	
Unit cell dimensions	a = 10.8473(5) Å	α = 99.7051(8)°
	b = 12.4152(5) Å	β = 91.9863(9)°
	c = 13.1760(6) Å	γ = 103.7460(9)°
Volume	1693.76(13) Å ³	
Z	1	
Theta range for data collection	2.84 to 25.02°	
Index ranges	-12 ≤ h ≤ 12, -14 ≤ k ≤ 14, -15 ≤ l ≤ 15	
Reflections collected	16418	
Independent reflections	5757 [R(int) = 0.0377]	
Nr. of obs. independent refl; I > 2σ(I)	5605	
Final R indices, observed	R1 = 0.0655, wR2 = 0.1564	
Final R-indices, all data	R1 = 0.0666, wR2 = 0.1570	

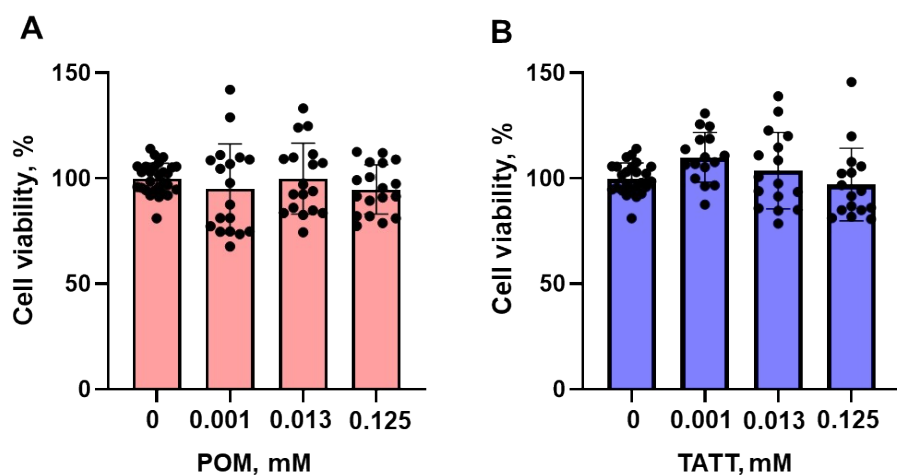


Figure S1. Viability of cell lines used for viral infection in the presence of POM and TATT NPs. The highest exposure concentration (0.125 mM) is equal to the highest concentration of NPs used during viral infection.

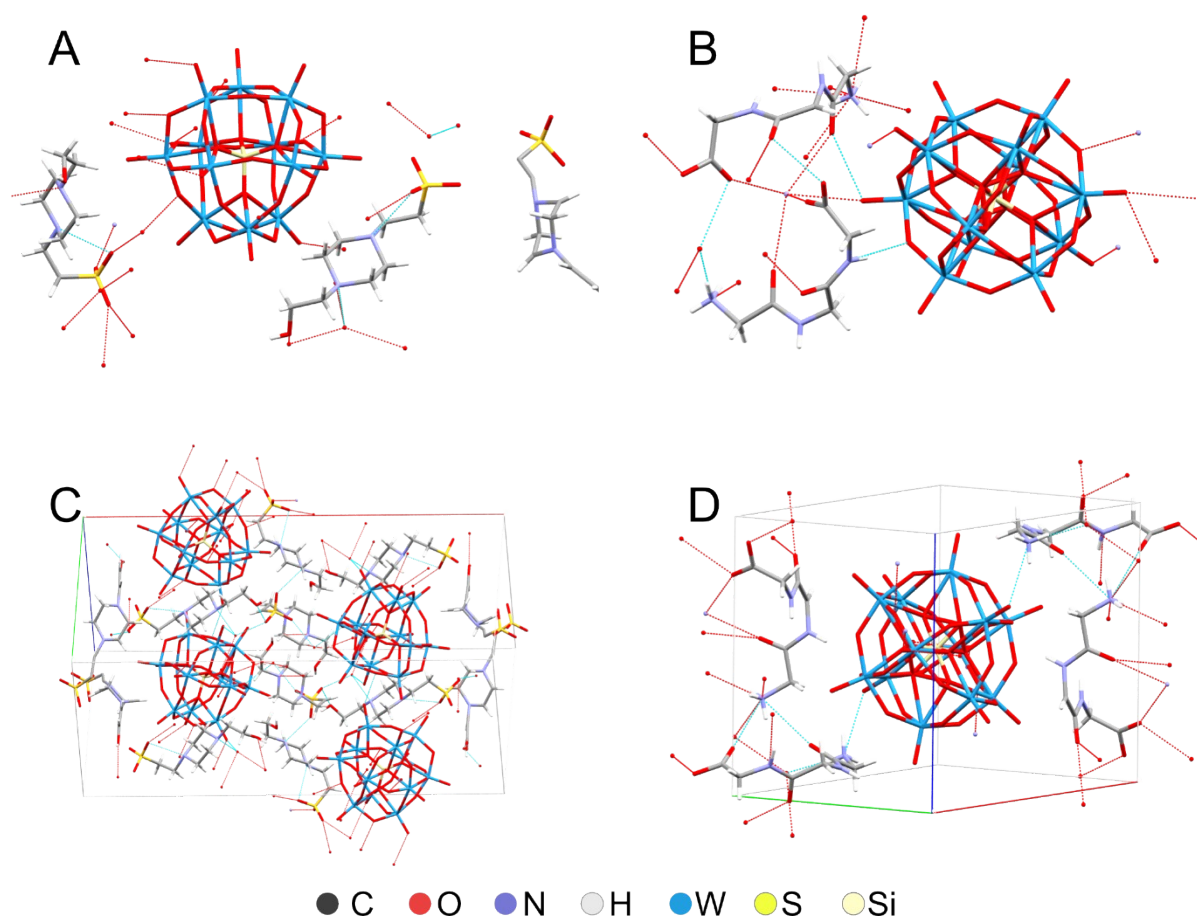


Figure S2. Showing hydrogen bonds for $(\text{HEPES})_3(\text{H}_3\text{O})\text{SiW}_{12}\text{O}_{40}$ (A), $(\text{HGly})_3\text{SiW}_{12}\text{O}_{40}$ (B) in their asymmetric unit and unit cell (C-D)