

Supplementary Information to
Polyoxovanadates inhibition of *Escherichia coli* growth shows a reverse
correlation with Ca²⁺-ATPase inhibition

Dorinda Silva^{1,2}, Gil Fraqueza^{3,4}, Ricardo Lagoa^{1,2}, Anjana Anandan Vannathan⁵, Sib Sankar Mal^{5*} and
Manuel Aureliano^{4,6*}

¹ESTG, Polytechnic Institute of Leiria, Portugal; ² UCIBIO, Faculty of Science and Technology, University
NOVA of Lisbon, Portugal; ³ISE, University of Algarve, 8005-139 Faro, Portugal; ⁴CCMar, University of
Algarve, 8005-139 Faro, Portugal; ⁵Department of Chemistry, National Institute of Technology
Karnataka, Mangalore 575025, Karnataka, India; ⁶FCT, University of Algarve, 8005-139 Faro, Portugal

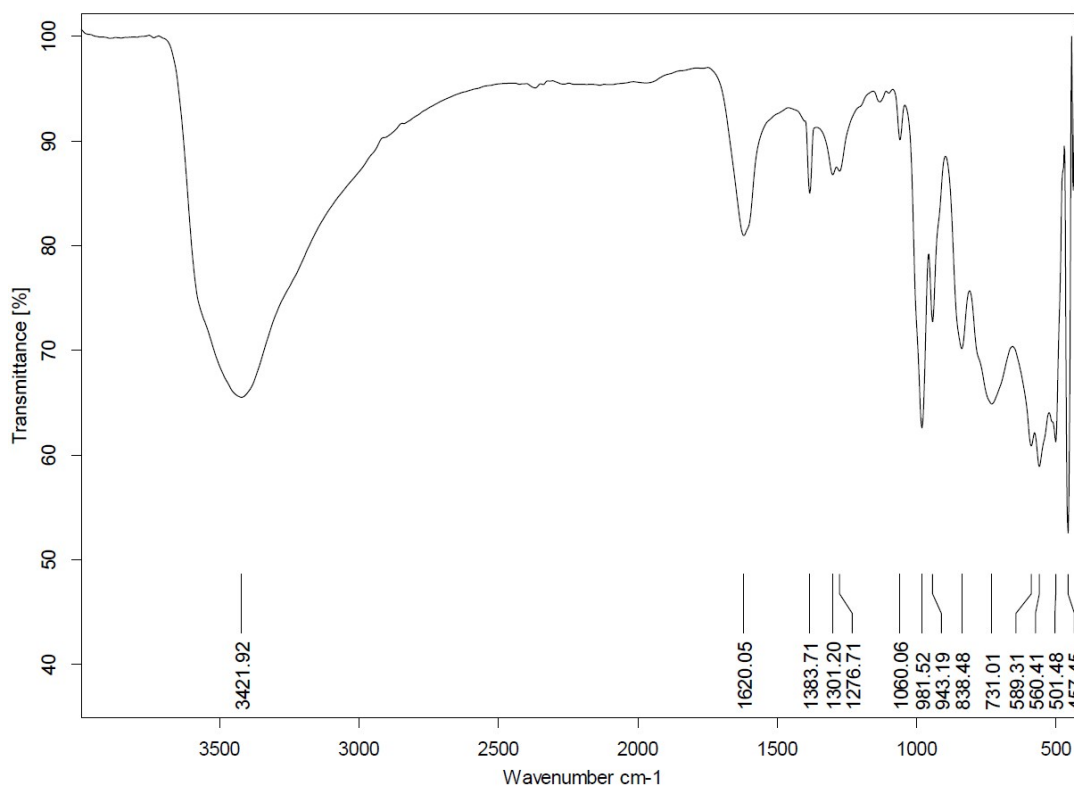


Fig. S1. FT-IR spectrum of the $K_5\text{Mn}^{\text{IV}}\text{V}_{11}\text{O}_{32}$ manganesepolyoxovanadate compound.

IR data (solid/KBr pellet, cm^{-1}): $K_5\text{Mn}^{\text{IV}}\text{V}_{11}\text{O}_{32}$: 982,943(vs) ($\text{V}=\text{O}_{\text{term}}$), 837, 589, 560 (m) ($\text{V}-\text{O}-\text{V}_{\text{as}}$), 731 (s).

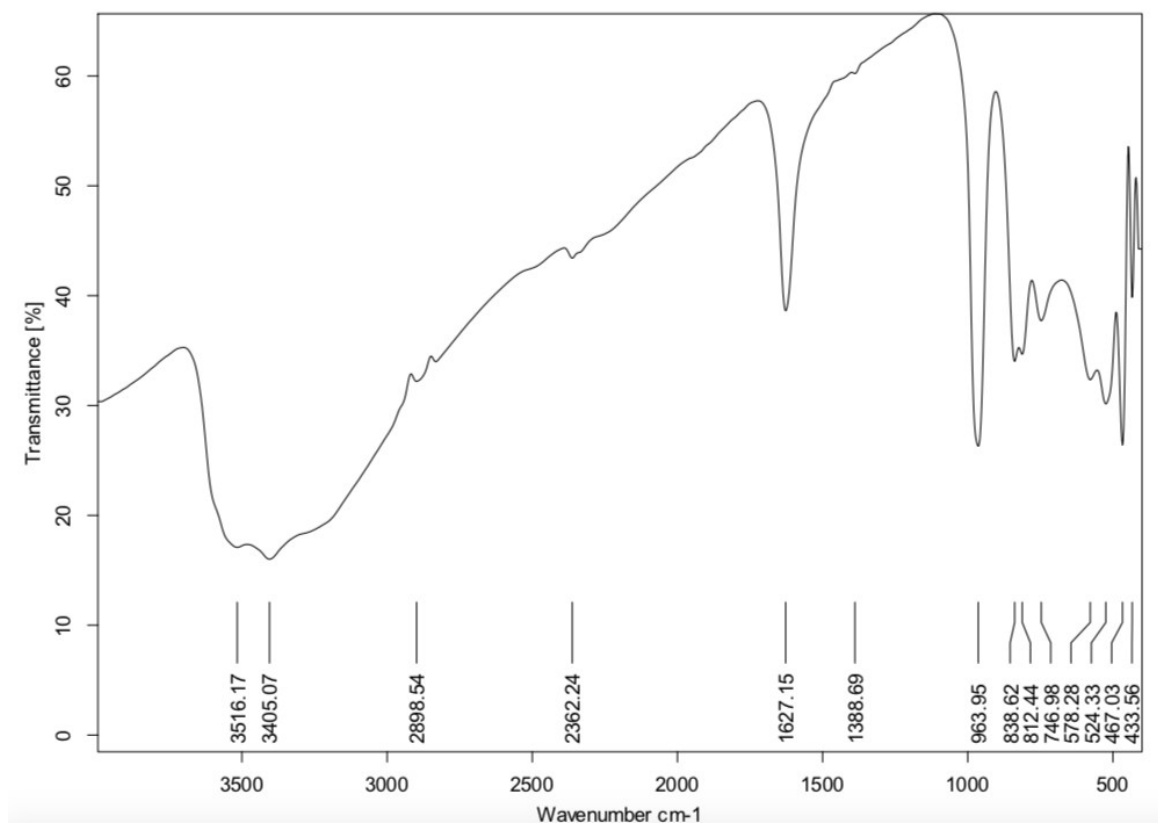


Fig. S2. FT-IR spectrum of the $K_7Mn^{IV}V_{13}O_{38}$ manganesepolyoxovanadate compound.

IR data (solid/KBr pellet, cm^{-1}): 964(s) ($V=O_{term}$), 839,812,578, 524 ($V-O-V_{as}$), 747 (s) ($Mn-O-V$).

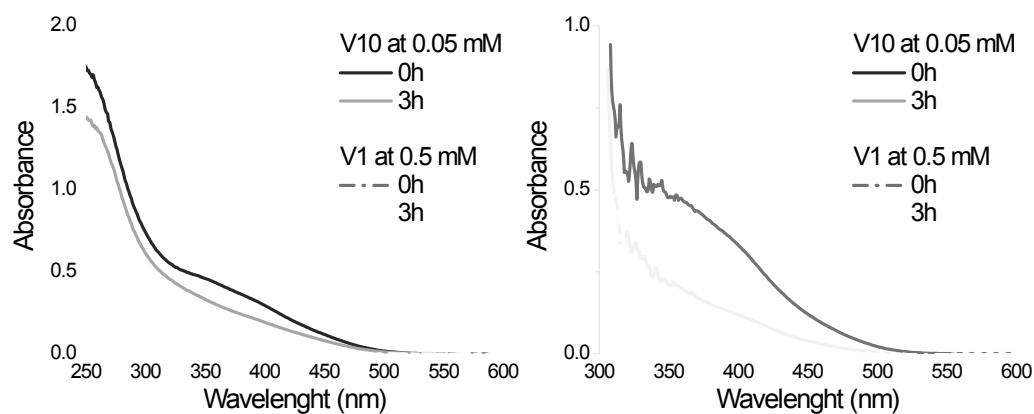


Figure S3. UV/vis spectra of decavanadate (V10, 0.05 mM) and vanadate (V1, 0.5 mM) after 0 and 3 hours incubation in water (left panel) as well as on the microbiological medium (right panel).

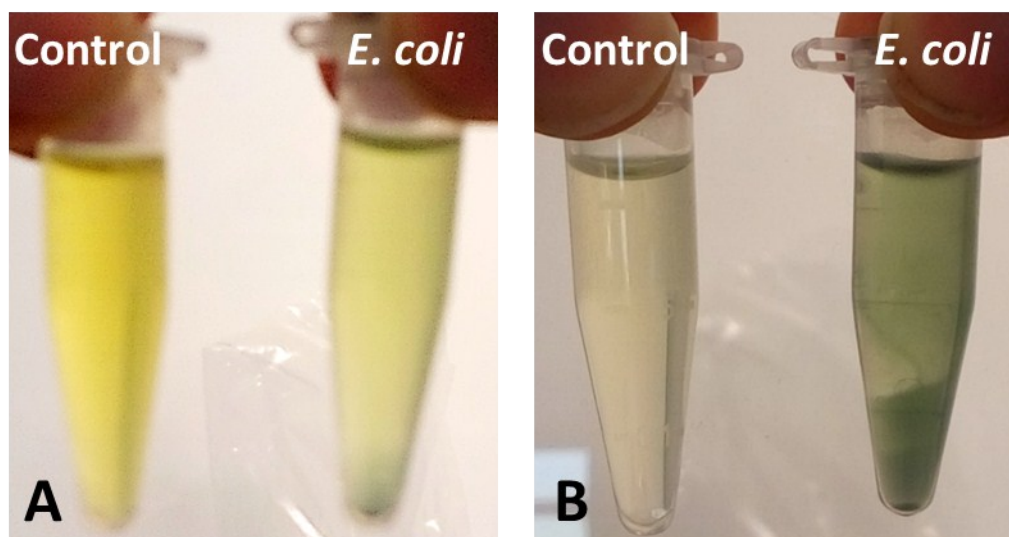


Figure S4. Decavanadate V_{10} concentration 1 mM (panel A) and vanadate V_1 concentration 10 mM (panel B), in culture medium LB, after 24 hours incubation at 37°C.

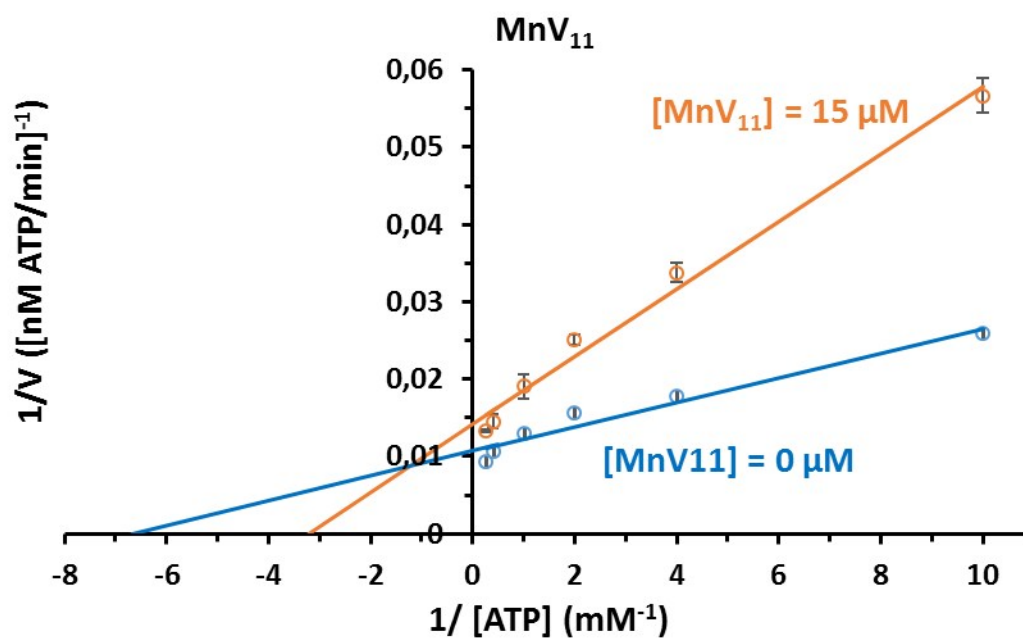


Figure S5. Lineweaver-Burk plot of Ca²⁺-ATPase activity in the absence (blue) and in the presence (orange) of 15 μM of the polyoxometalate MnV₁₁, used for determining the type of enzyme inhibition. The POV presented a mixed type of inhibition. Data are plotted as means ± SD. The results shown are the average of triplicate experiments.

Table S1. Antibacterial activity (MIC) of POMs alone, POM-hybrids and nanocomposites against *E. coli*.

POM/POM-hybrid	MIC ($\mu\text{g/ml}$)	Ref.
Polyoxometalate alone:		
$[\text{V}_{10}\text{O}_{28}]^{6-}$	50	48
$[\text{P}_5\text{W}_{30}]^{14-}$	>265	62
$[\text{P}_2\text{W}_{15}\text{V}_3]^{6-}$	>265	62
$[\text{P}_2\text{O}_7\text{Mo}_{18}]^{6-}$	>265	62
$[\text{As}_2\text{Mo}_{18}]^{6-}$	>265	62
Organic-inorganic-POM: organoantimony- polyoxotungstate:		
$[(\text{PhSb}^{\text{III}})_4(A-\alpha\text{-Ge}^{\text{IV}}\text{W}_9\text{O}_{34})_2]^{12-}$	80	45
$[(\text{PhSb}^{\text{III}})_4(A-\alpha\text{-P}^{\text{V}}\text{W}_9\text{O}_{34})_2]^{10-}$	110	45
$[\{2-(\text{Me}_2\text{NCH}_2\text{C}_6\text{H}_4)\text{Sb}^{\text{III}}\}_3(B-\alpha\text{-As}^{\text{III}}\text{W}_9\text{O}_{33})]^{3-}$	130	45
$[(\text{PhSb}^{\text{III}})\{\text{Na}(\text{H}_2\text{O})\}\text{As}^{\text{III}}_2\text{W}_{19}\text{O}_{67}]^{11-}$	500	46
$[(\text{PhSb}^{\text{III}})_2\text{As}^{\text{III}}_2\text{W}_{19}\text{O}_{67}]^{10-}$	250	46
$[(\text{PhSb}^{\text{III}})_3(B-\alpha\text{-As}^{\text{III}}\text{W}_9\text{O}_{33})_2]^{12-}$	125	46
Quinolone-based drug-POM:		
$[\text{Co}^{\text{II}}(\text{C}_{19}\text{FH}_{22}\text{N}_3\text{O}_4)_3][\text{C}_{19}\text{FH}_{23}\text{N}_3\text{O}_4][\text{HSiW}_{12}\text{O}_{40}]$	2.4	47
Nanocomposite: Bamboo charcoal-POM:		
BC/POM	4	50
Polymer-POM: PVA/PEI-POM:		
PVA-PEI- $\text{H}_5\text{PV}_2\text{Mo}_{10}\text{O}_{40}$	2	49
Chitosan-POM:		
CTS- $\text{Ca}_3\text{V}_{10}\text{O}_{28}$	12.5	48
Polyoxometalate ionic liquids:		
$[\text{N}(\text{C}_6\text{H}_{13})_4]_8[\alpha\text{-SiW}_{11}\text{O}_{39}]$	1000	51
$[\text{N}(\text{C}_7\text{H}_{15})_4]_8[\alpha\text{-SiW}_{11}\text{O}_{39}]$	25	51
$[\text{N}(\text{C}_8\text{H}_{17})_4]_8[\alpha\text{-SiW}_{11}\text{O}_{39}]$	50	51