

## **Supplementary Information**

### **Novel Copper Oxide Bio-nanocrystals to Target Outer Membrane Lectin of Vancomycin-Resistant *Enterococcus faecium* (VREfm): *In silico*, Bioavailability, Antimicrobial, and Anticancer Potential**

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**Table S1:** ADME predicted calculations of Oleuropein

Physicochemical Properties	
Formula	C <sub>25</sub> H <sub>32</sub> O <sub>13</sub>
Molecular weight	540.51 g/mol
Num. heavy atoms	38
Num. arom. heavy atoms	6
Fraction Csp <sup>3</sup>	0.52
Num. rotatable bonds	11
Num. H-bond acceptors	13
Num. H-bond donors	6
Molar Refractivity	127.28
TPSA	201.67 Å <sup>2</sup>
Lipophilicity	
Log <i>P</i> <sub>o/w</sub> (iLOGP)	2.65
Log <i>P</i> <sub>o/w</sub> (XLOGP3)	-0.45
Log <i>P</i> <sub>o/w</sub> (WLOGP)	-0.63
Log <i>P</i> <sub>o/w</sub> (MLOGP)	-1.34
Log <i>P</i> <sub>o/w</sub> (SILICOS-IT)	-0.14
Consensus Log <i>P</i> <sub>o/w</sub>	0.02
Water Solubility	
Log <i>S</i> (ESOL)	-2.30
Solubility	2.72e+00 mg/ml ; 5.03e-03 mol/l
Class	Soluble
Log <i>S</i> (Ali)	-3.32
Solubility	2.59e-01 mg/ml ; 4.79e-04 mol/l
Class	Soluble
Log <i>S</i> (SILICOS-IT)	-0.66
Solubility	1.19e+02 mg/ml ; 2.19e-01 mol/l
Class	Soluble
Pharmacokinetics	
GI absorption	Low
BBB permeant	No
P-gp substrate	No
CYP1A2 inhibitor	No
CYP2C19 inhibitor	No
CYP2C9 inhibitor	No

CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log $K_p$ (skin permeation)	-9.92 cm/s

#### Druglikeness

Lipinski	No; 3 violations: MW>500, NorO>10, NHorOH>5
Ghose	No; 2 violations: MW>480, WLOGP<-0.4
Veber	No; 2 violations: Rotors>10, TPSA>140
Egan	No; 1 violation: TPSA>131.6
Muegge	No; 3 violations: TPSA>150, H-acc>10, H-don>5
Bioavailability Score	0.11

#### Medicinal Chemistry

PAINS	1 alert: catechol_A
Brenk	3 alerts: catechol, isolated_alkene, more_than_2_esters
Leadlikeness	No; 2 violations: MW>350, Rotors>7
Synthetic accessibility	6.22