

Targeting SARS-CoV-2 main protease (Mpro) and human ACE-2: a virtual screening of carotenoids and polyphenols from tomato (*Solanum lycopersicum* L.) to combat Covid-19

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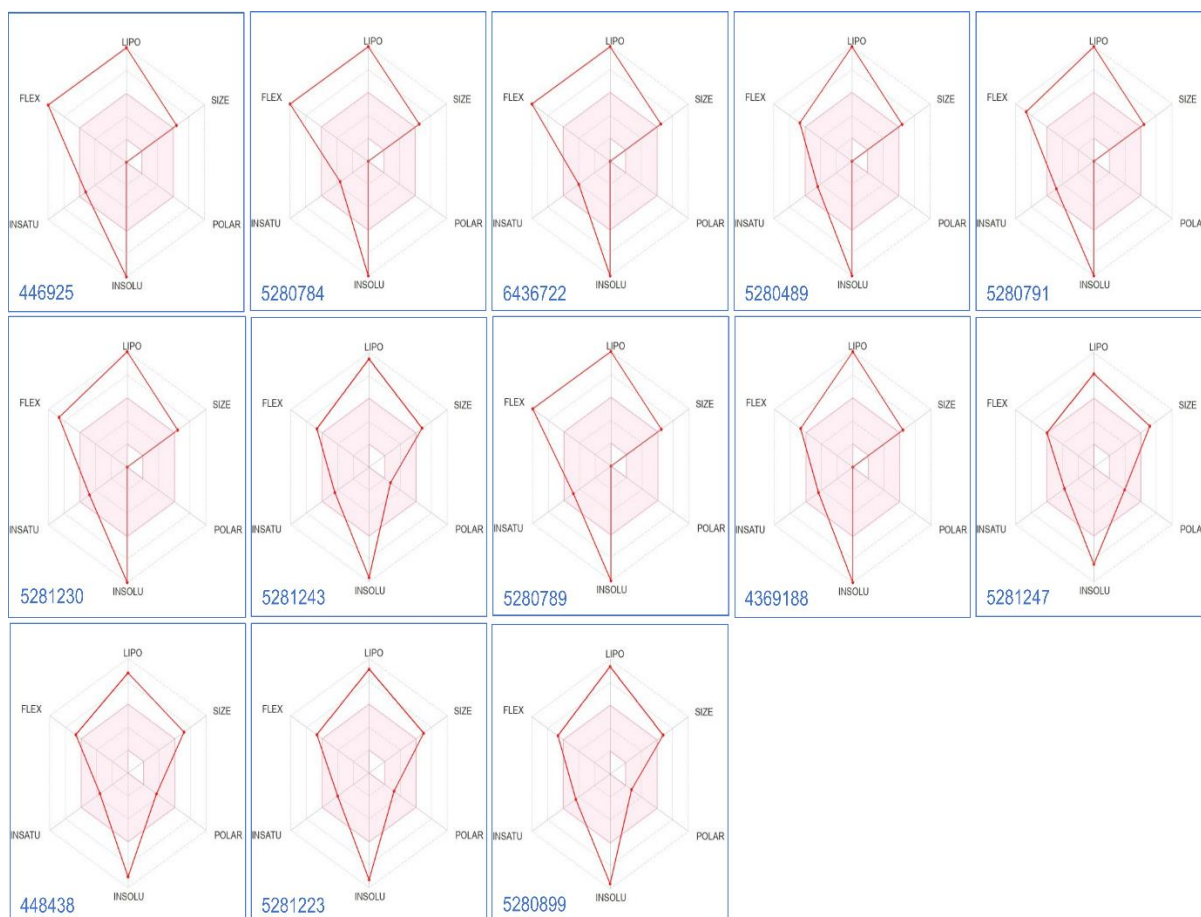
[#] These authors share equal authorship in this article.

from *S. lycopersicum* L.

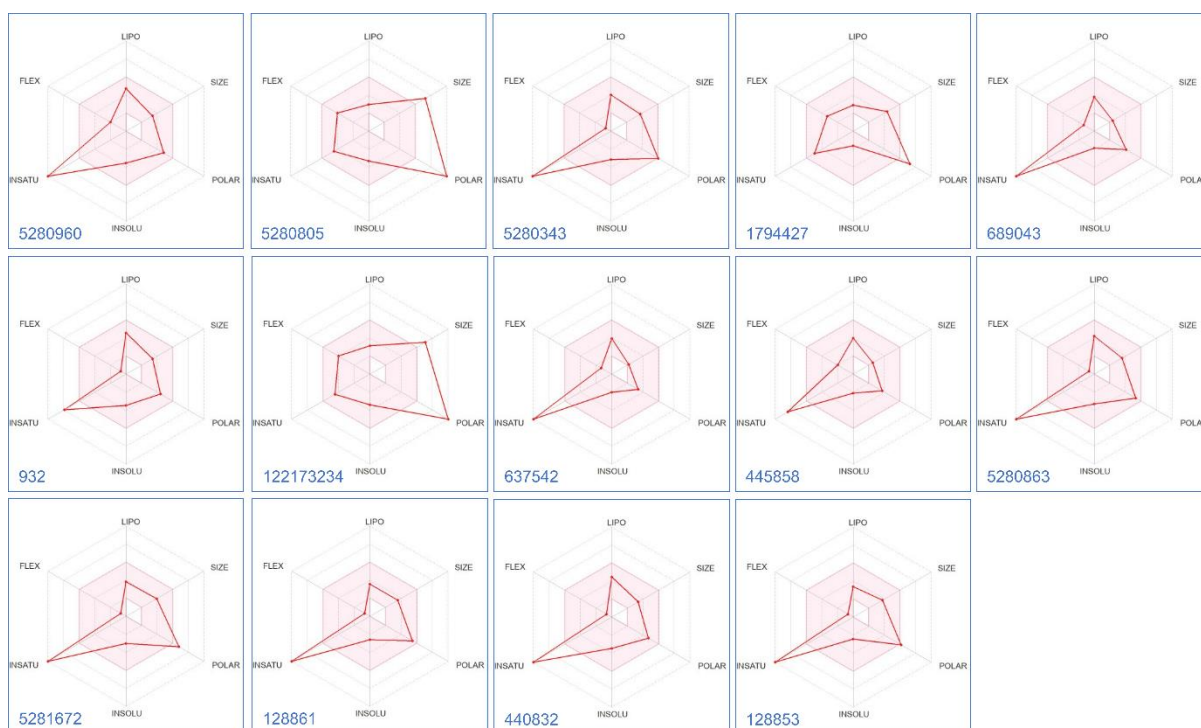
* Represents the reference standard antagonist of SARS-CoV-2 M ^{pro} activity.
Represents the reference standard antagonist of human ACE-2 activity.

Supplementary Table S2 Predicted toxicity of selected carotenoids and polyphenols from *S. lycopersicum* L.

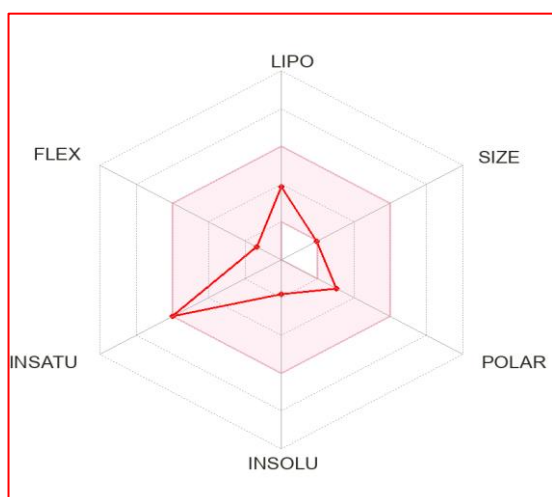
S.N.	Compound	Predicted LD ₅₀	Predicted Toxicity Class
Carotenoids			
1.	Neurosporene	5700 mg/kg	6
2.	Phytofluene	5700 mg/kg	6
3.	Phytoene	5700 mg/kg	6
4.	Lycopene	5700 mg/kg	6
5.	delta-Carotene	4390 mg/kg	5
6.	alpha-carotene	1510 mg/kg	4
7.	gamma-Carotene	1510 mg/kg	4
8.	beta-Carotene	1510 mg/kg	4
9.	Violaxanthin	55 mg/kg	3
10.	Zeaxanthin	10 mg/kg	2
11.	Antheraxanthin	37 mg/kg	2
12.	Neoxanthin	50 mg/kg	2
13.	Lutein	10 mg/kg	2
Polyphenols			
14.	Cyanidin	5000 mg/kg	5
15.	Kaempferol	3919 mg/kg	5
16.	p-coumaric acid	2850 mg/kg	5
17.	Caffeic acid	2980 mg/kg	5
18.	Chlorogenic acid	5000 mg/kg	5
19.	Kaempferol-3-rutinoside	5000 mg/kg	5
20.	Rutin	5000 mg/kg	5
21.	Naringenin chalcone	3600 mg/kg	5
22.	Delphinidin	5000 mg/kg	5
23.	Pelargonidin	3919 mg/kg	5
24.	Ferulic acid	1190 mg/kg	4
25.	naringenin	2000 mg/kg	4
26.	Myricetin	159 mg/kg	3
27.	Quercetin	159 mg/kg	3
28.	* 6-(ethylamino) pyridine-3-carbonitrile	330 mg/kg	3
29.	# Telmisartan	500 mg/kg	4
* Represents the reference standard antagonist of SARS-CoV-2 M ^{Pro} activity.			
# Represents the reference standard antagonist of human ACE-2 activity.			



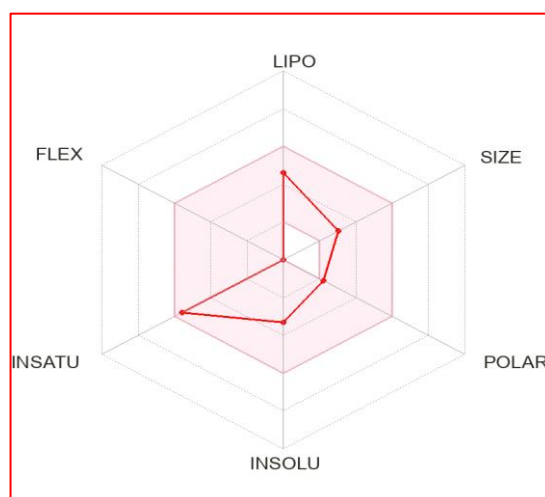
Supplementary Figure S1 Bioavailability radar chart for carotenoids. The pink area/zone represents the optimal range for each property and the redline represents the oral bioavailability properties of all the carotenoids. The optimal scores for each determinant are: **lipophilicity**: XLOGP3 between -0.7 and $+5.0$, **size**: MW between 150 and 500 g/mol, **polarity**: TPSA between 20 and $130\text{\AA}^2$, **solubility**: log S not higher than 6, **saturation**: fraction of carbons in the sp^3 hybridization not less than 0.25, and **flexibility**: no more than 9 rotatable bonds.



Supplementary Figure S2 Bioavailability radar chart for polyphenols. The pink area/zone represents the optimal range for each property and the redline represents the oral bioavailability properties of all the polyphenols. The optimal scores for each determinant are: **lipophilicity:** XLOGP3 between -0.7 and $+5.0$, **size:** MW between 150 and 500 g/mol, **polarity:** TPSA between 20 and $130\text{\AA}^2$, **solubility:** log S not higher than 6, **saturation:** fraction of carbons in the sp^3 hybridization not less than 0.25, and **flexibility:** no more than 9 rotatable bonds.



PubChem ID: 24701445



PubChem ID: 56999

Supplementary Figure S3 Bioavailability radar chart for EPC and telmisartan. The pink area/zone represents the optimal range for each property and the redline represents the oral bioavailability properties of EPC and telmisartan. The optimal scores for each determinant are: **lipophilicity**: XLOGP3 between -0.7 and $+5.0$, **size**: MW between 150 and 500 g/mol, **polarity**: TPSA between 20 and $130\text{\AA}^2$, **solubility**: log S not higher than 6, **saturation**: fraction of carbons in the sp^3 hybridization not less than 0.25, and **flexibility**: no more than 9 rotatable bonds.