Theoretical Investigation of the Cooperation of Iminoguanidine with the Enzymes-Binding Domain of Covid-19 and Bacterial Lysozyme Inhibitors and their Pharmacokinetic Properties

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Received January 24th, 2022; Accepted August 1st, 2022.

DOI for the article: http://dx.doi.org/10.29356/jmcs.v66i4.1726
Fig. S1. The connection between the observed and predicted activities by GA-MLR.

Fig. S2. Residuals of iminoguanidine derivatives against the experimental values of pIC50 using GA-MLR model.
Fig. S3. Plot of Y-randomization test: All gotten values for $R^2$ and $Q^2$ test are approximately 0.11 and −0.31, respectively.

Fig. S4. William plot for the developed 2D-QSAR model.
**Fig. S5.** Insubria plot for the 2D-QSAR model, using the two descriptors.
Fig. S6. 2D interaction contour map with the key protein residues after MD simulation.
Fig. S7. MDs simulations study of modeled SARS-CoV-2 and compound 15 (A) Total energy, (B) Kinetic energy, and (C) Potential energy.