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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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Supplementary Information

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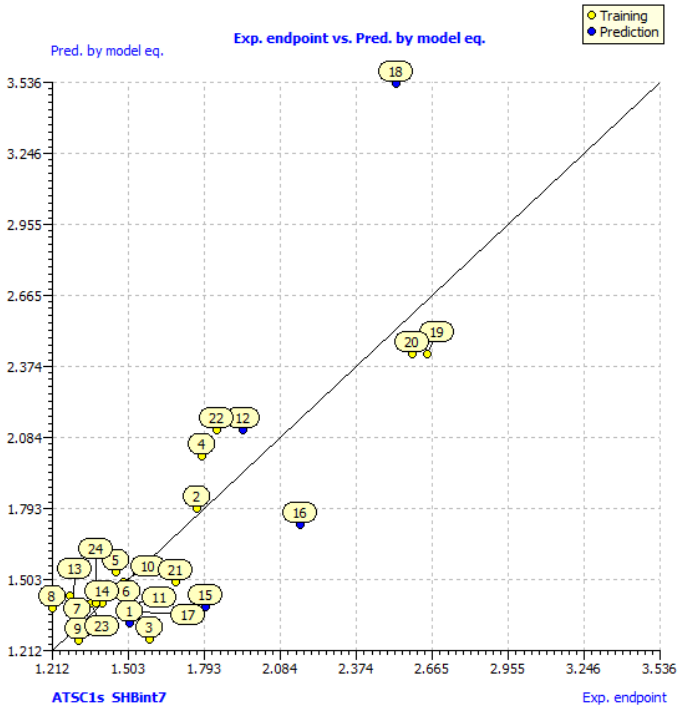

Fig. S1. The connection between the observed and predicted activities by GA-MLR.

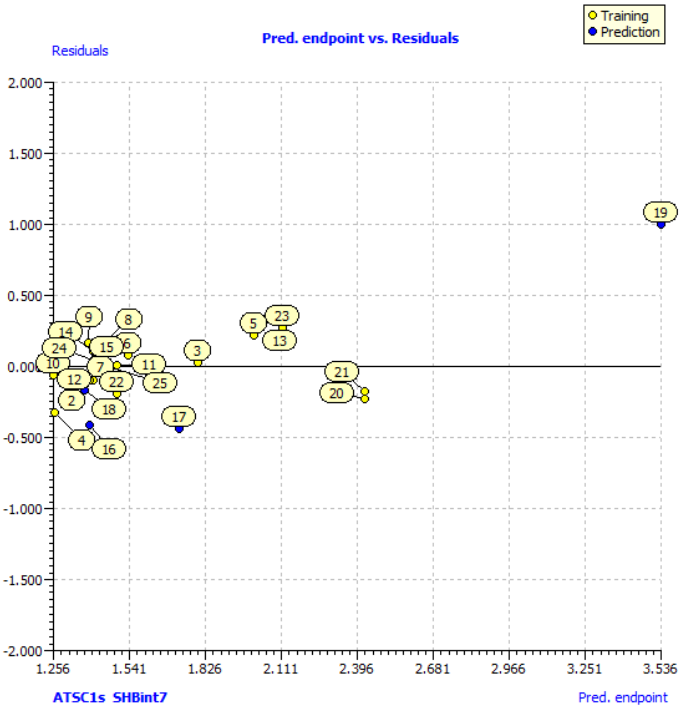

Fig. S2. Residuals of iminoguanidine derivatives against the experimental values of pIC50 using GA-MLR model.

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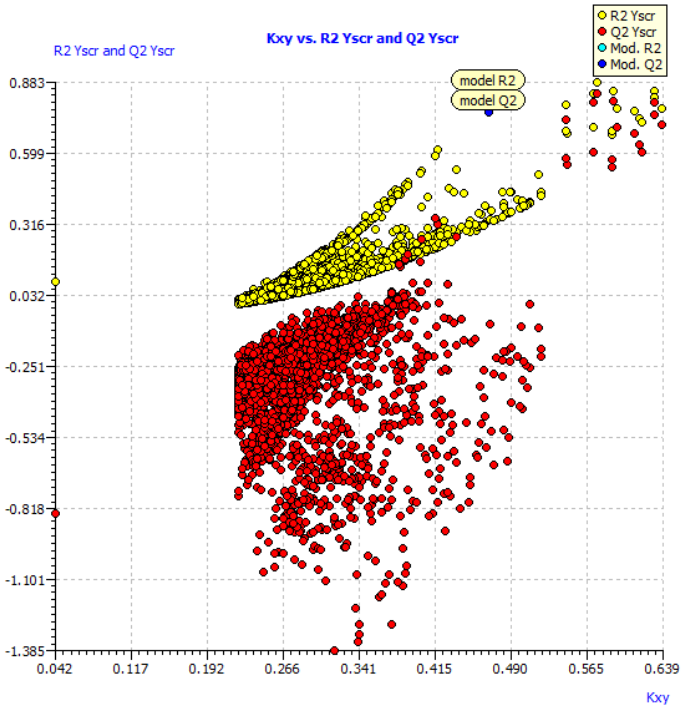

Fig. S3. Plot of Y-randomization test: All gotten values for R^2 and Q^2 test are approximately 0.11 and – 0.31, respectively.

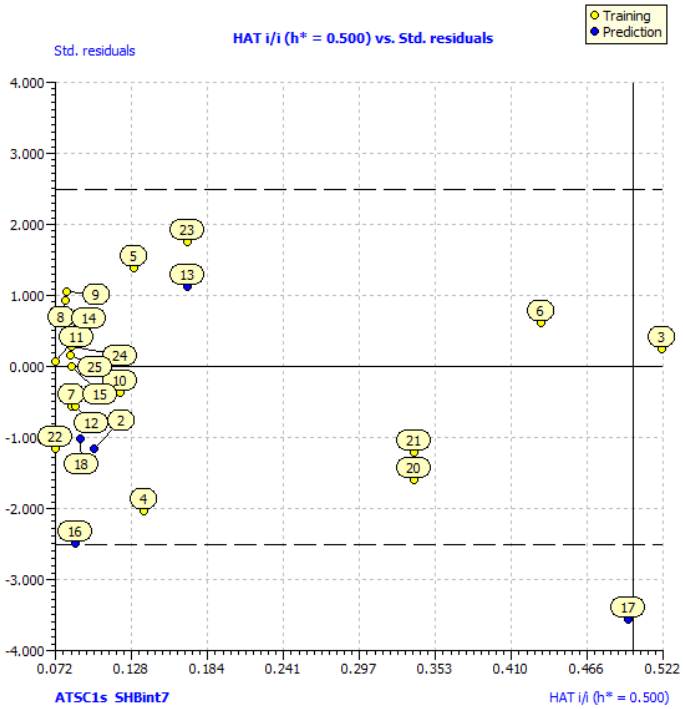

Fig. S4. William plot for the developed 2D-QSAR model.

J. Mex. Chem. Soc. **2022**, *66*(4)
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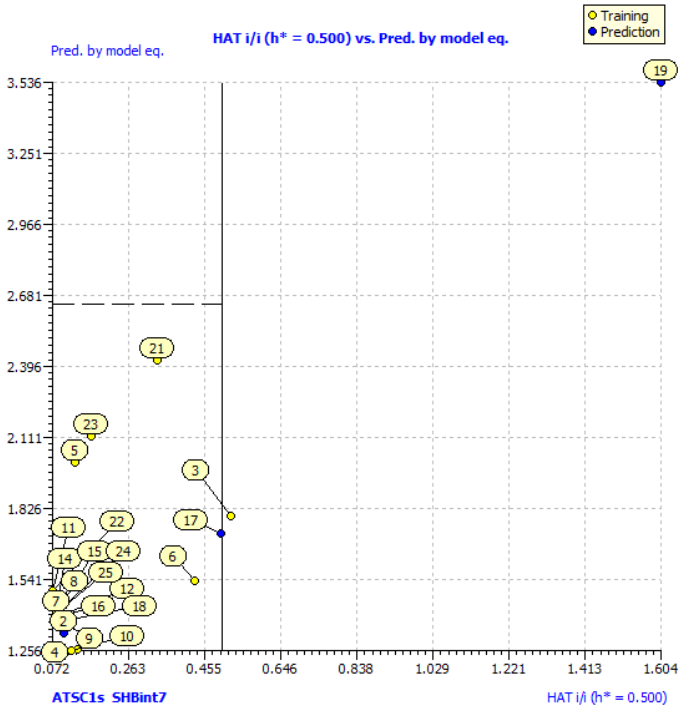
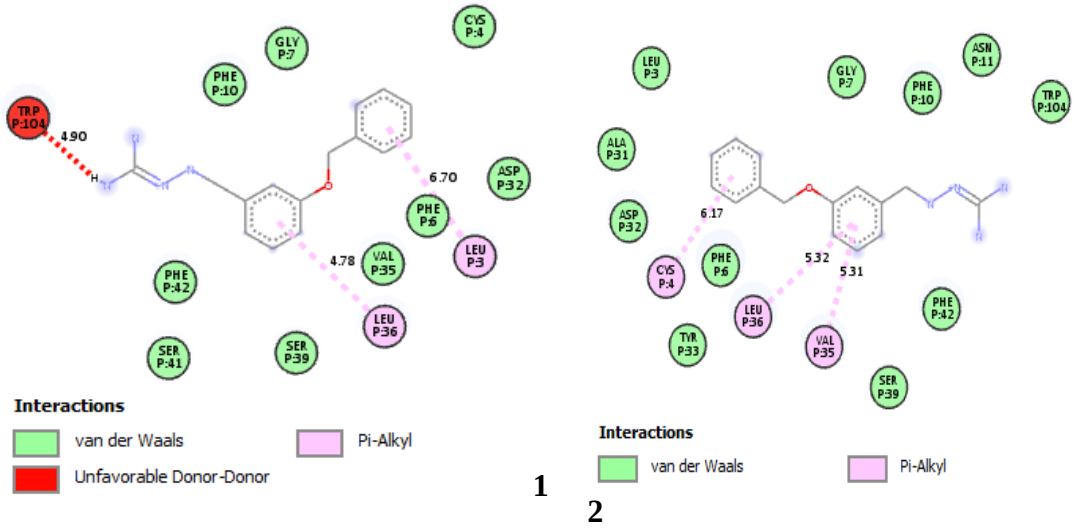


9.5

Fig. S5. Insubria plot for the 2D-QSAR model, using the two descriptors.



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J. Mex. Chem. Soc. **2022**, *66*(4)
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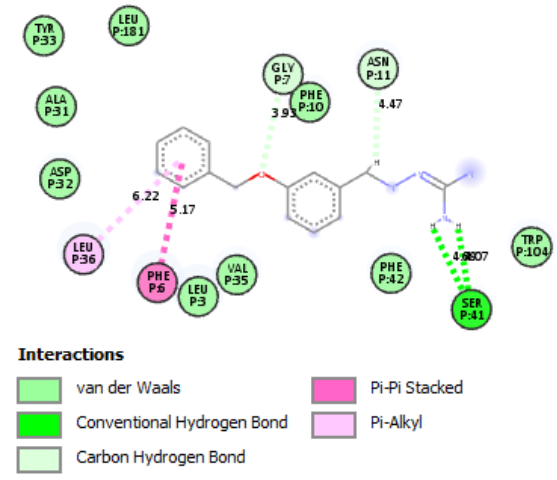

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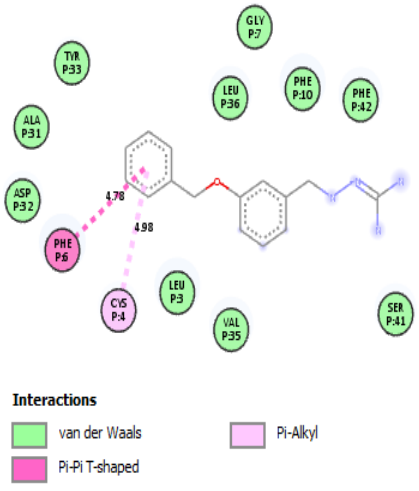

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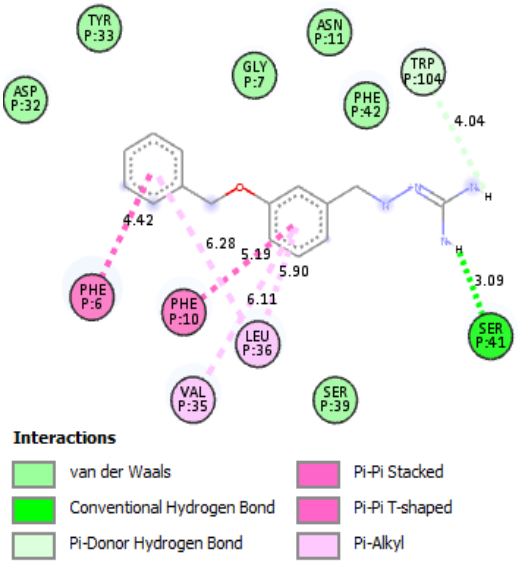

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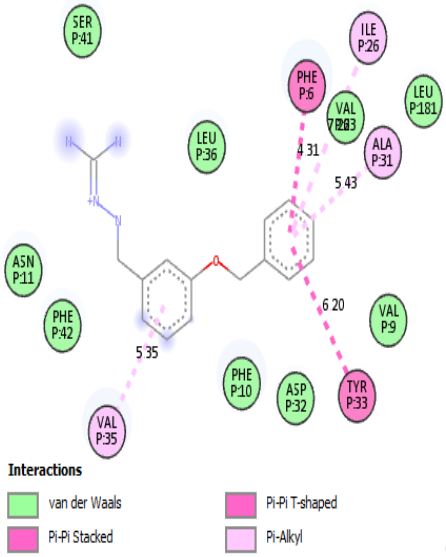

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J. Mex. Chem. Soc. **2022**, *66*(4)
Regular Issue

ISSN-e 2594-0317

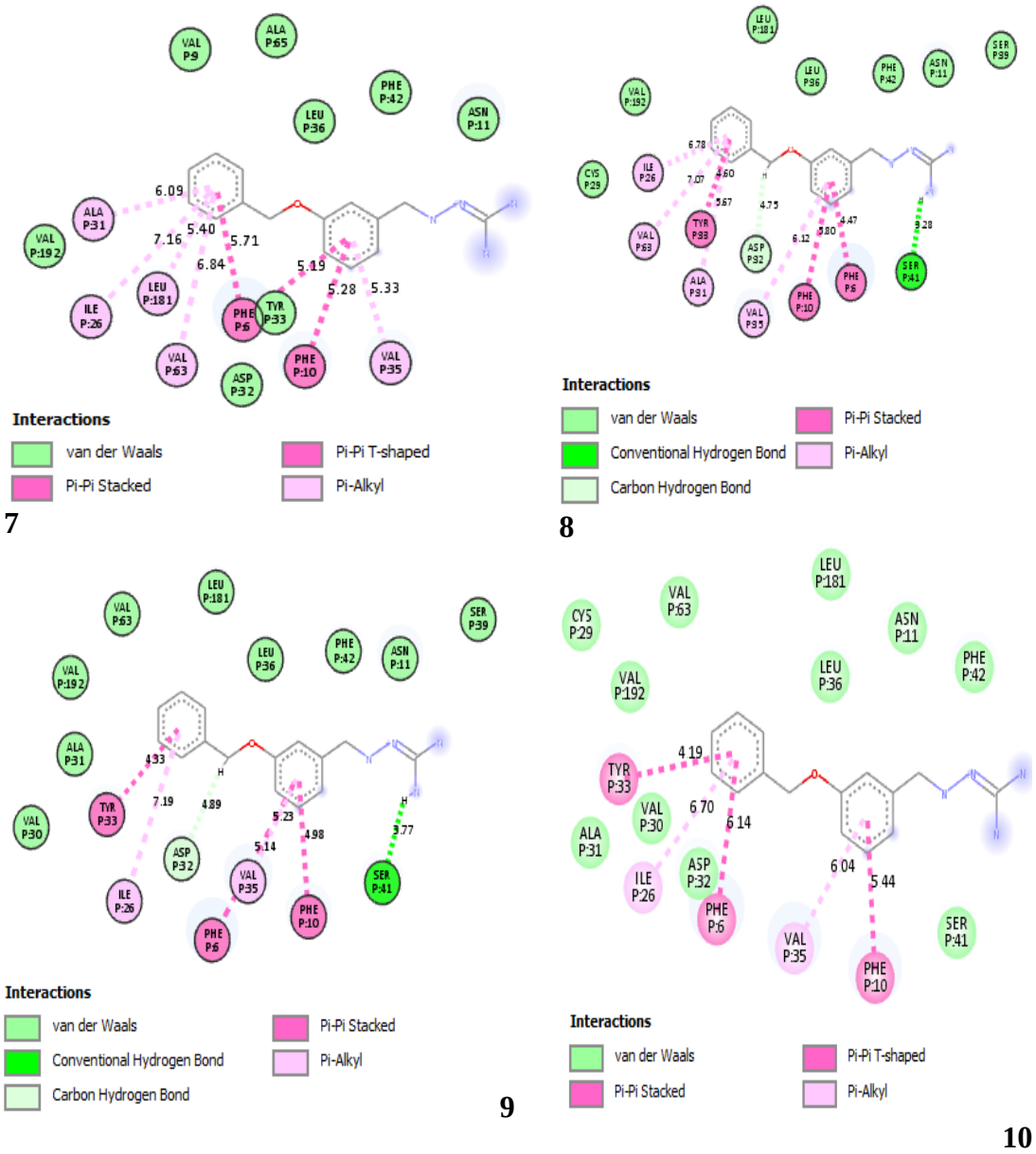

Fig. S6. 2D interaction contour map with the key protein residues after MD simulation.

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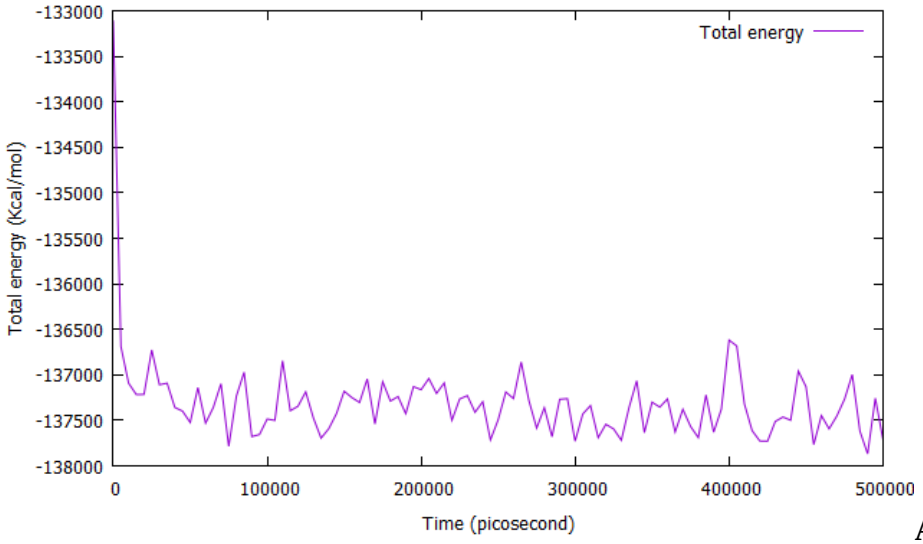
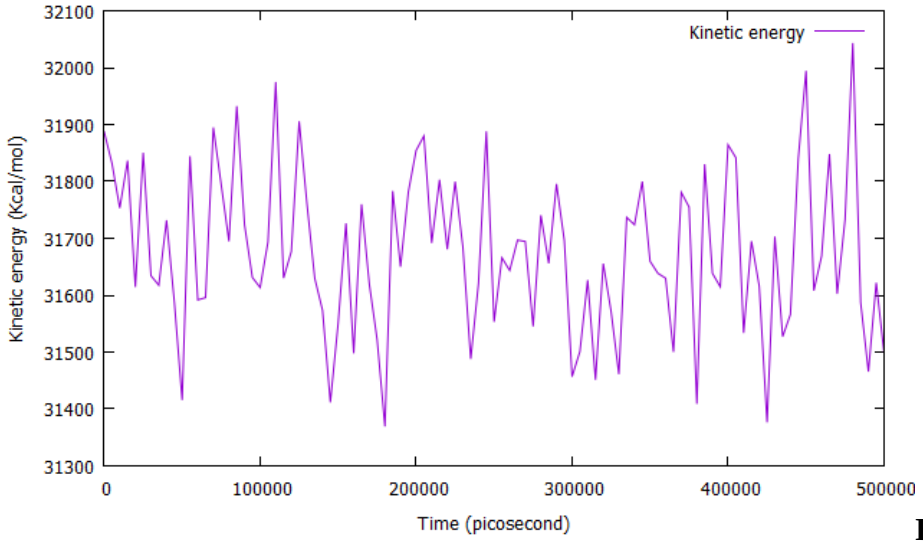


A



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J. Mex. Chem. Soc. **2022**, *66*(4)
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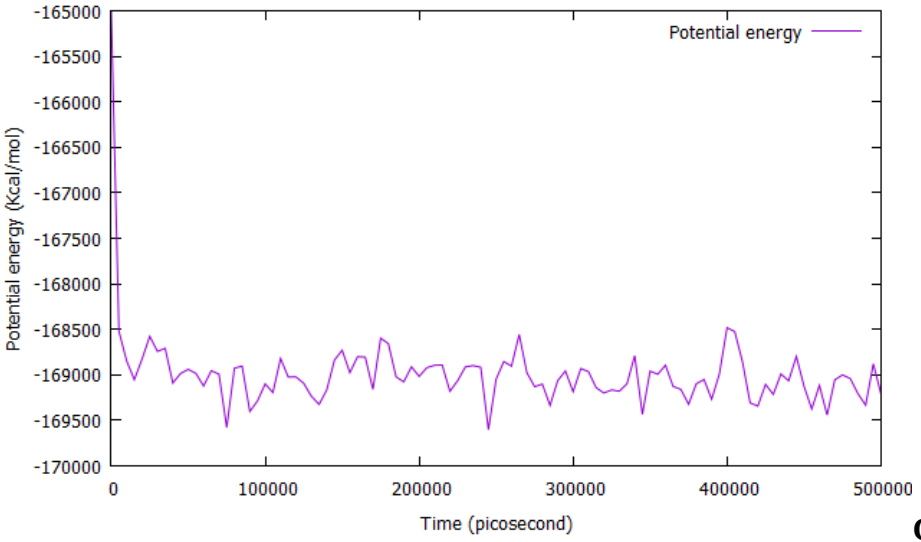

C

Fig. S7. MDs simulations study of modeled SARS-CoV-2 and compound 15 **(A)** Total energy, **(B)** Kinetic energy, and **(C)** Potential energy.