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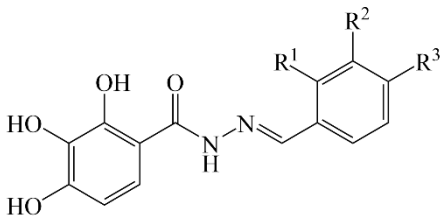
Selected Phenolic Hydrazones As Potential M^{pro} Inhibitors

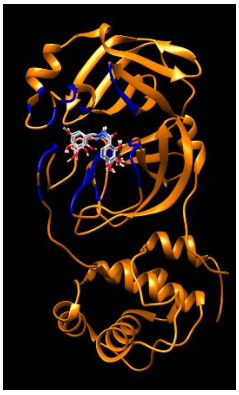
V. P. Petrović,* J. Branković and Z. D. Petrović

University of Kragujevac, Faculty of Science, Department of Chemistry, R. Domanovića 12, 34000 Kragujevac, Serbia

*vladimir.petrovic@pmf.kg.ac.rs

Hydrazone-type compounds are known for their versatile biological activities.[1] This encouraged us to subject six phenolic hydrazones (**1-6**) to *in silico* investigation of potential antiviral activity against SARS-CoV-2. For this purpose, molecular docking was performed on the protein involved in viral reproduction processes main protease (M^{pro}).[2]





The obtained results revealed that all compounds docked within the active site of M^{pro}. Binding affinities of all compounds were in the range of -7.6 to -8.1 kcal/mol. Considering that the binding energy of FDA approved drug Lopinavir amounts -7.7 kcal/mol, investigated phenolic hydrazones can be considered as promising M^{pro} inhibitors.

Keywords: phenolic hydrazones, SARS-CoV-2, molecular docking, M^{pro}

References

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