Identification of Potential Inhibitors of Severe Acute Respiratory Syndrome Coronavirus 2 Envelope Protein Ion Channel Activity Using Machine Learning Techniques

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Severe acute respiratory syndrome coronavirus 2 (SARS-CoV2) is a viral disease that has caused a major global pandemic. There are many developing treatments for SARS-CoV2 including vaccines from Pfizer or Moderna but the field lacks specific treatments that target viral pathogenesis. Quick screening of drug candidates is critical to reduce the fatality rate and societal impacts of the SARS-CoV2. Three machine learning models including Random Forest (RF), Support Vector Machine (SVM), and Multilayer Perceptron Neural Network (MPNN) were examined using previously identified inhibitors, and both RF and MPNN may serve as effective screening models. These models were used to screen potential drug candidates from a ZINC 15 FDA In-man database of 2374 compounds and the ChEMBL FDA database of 3369 compounds. The most promising inhibitors have been identified as Methylene Blue Cation and Piretanide. Further study with Molecular Docking confirmed that these two molecules could effectively block the ion channel of the viral transmembrane protein SARS-CoV2 E.