Use of an Artificial Intelligence Model for Drug Redirection Against Feline Rhinotracheitis

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This research presents a machine learning computational model capable of identifying potential inhibitors of the glycoprotein B (gB) of feline herpesvirus 1 (HVF-1), the cause of feline viral rhinotracheitis (FVR). FVR is an important viral disease in cats and one of the main reasons for animal abandonment in Brazil. The methodology used consisted of developing a computational model in Python, which searched for gB inhibitors in the ChEMBL database using descriptors capable of evaluating the inhibition concentration rate (IC50), oral bioavailability, and generation of the chemical structure of candidate molecules. A molecular docking simulation was performed to evaluate and validate the interactions between the inhibitors found by the model and also compare them to HVF-1 drugs. In silico toxicity assessment was also performed to verify the lethal dose (LD50), hepatotoxicity, carcinogenicity, immunotoxicity, mutagenicity, and cytotoxicity of the inhibitors. The results obtained showed that two inhibitors identified as CHEMBL2075962 and CHEMBL2077363 had biological activity with IC50 of 400 nM and 600 nM, respectively. In the molecular docking test, the structures showed high affinity for gB and correlation with the model created, with values of -8.3 and -9.4 kcal/mol. Additionally, in the toxicity assessment, the molecules showed no toxicity, and had LD50 data of 3250 mg/kg for CHEMBL2075962 and 2150 mg/kg for CHEMBL2077363, indicating a safety profile for oral animal use. These results are highly promising and can lead to the development of more effective therapies against FVR in cats, as there is currently no cure for the disease. This research can have a positive impact on animal health and potentially reduce the cases of cat abandonment in Brazil and worldwide.

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