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## Do the omeprazole family compounds exert a protective effect against influenza? Insights from molecular docking and molecular dynamics

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Influenza is an important public health issue, which has a huge impact on healthcare systems and on society, both in terms of disease burden and costs. Although vaccines are a fairly effective weapon against influenza, antiviral drugs could offer an opportunity to alleviate the burden of influenza. Since Omeprazole Family Compounds (OFC) block the “proton pump”, we hypothesized that they could interfere with the mechanism of fusion of the virus envelope and endosomal membrane, thereby hindering the M2 proton pump mechanism of influenza viruses, as M2 is an integral membrane tetrameric pH-gated protein. We carried out an Molecular Dynamics (MD) simulation in order to gain further insights into the putative mechanisms of OFC. We simulated the M2 protein (PDB code 3C9J) and the ligands (amantadine, rimantadine as positive controls; oseltamivir as a negative control; omeprazole as a putative ligand) by means of the program Gromacs, version 4.5 for MD simulations and DOCK6 for docking. Our model confirmed the interaction between amantadine, rimantadine and the M2 protein, while no interaction was found for oseltamivir. Our molecular docking and MD simulation seems to confirm our previous epidemiological findings. However, further confirmation and research in the field are necessary in order to replicate our results in a robust and consistent way.