Histone Deacetylase (HDAC) Inhibitors as Potential Antivirals. In-Silico Study Based on Molecular Docking, Pharmacokinetics/Toxicity, and Molecular Dynamics

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Abstract:

The Zika virus belongs to the flavivirus family, which includes several major viruses with single-stranded RNA and positive-sense RNA. This virus is transmitted to humans by mosquito vectors. ZIKV infection is usually asymptomatic, but it can also cause mild flu-like illnesses or serious symptoms, posing a serious threat to human health. Several studies have shown that histone deacetylase 6 (HDAC6) inhibitors have antiviral effects on Zika virus. Therefore, we present a new study of a highly selective HDAC6 inhibitor, J27820. This study is based on computational chemistry and several in-silico techniques such as molecular docking, ADMET predictions, and molecular dynamics. First, the physicochemical and pharmacokinetic properties related to ADMET were evaluated. Then, molecular docking simulations were carried out to study the inhibitory therapeutic potential of the studied compounds J22352, and J27820 against three proteins (5H4I, 5TFR, and