Restraining the Zika Virus in Brazil: A New Design and Analysis Method for Drugs through Computational and Biological Approaches

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The Zika Virus is a disease that has no cure. To date, approximately 100,000 Zika cases have been reported in Brazil in the current epidemic. The disease has been linked to serious neurological problems such as The Guillain Barré syndrome and microcephaly in newborn babies. While it takes pharmaceutical companies 10 years and an average of $2.6 billion to develop a single drug, pharmacological therapies to treat Zika are urgently needed in Brazil and around the world. We found a novel method to more quickly identify drugs that could be used in the fight against the Zika Virus, using both computational and biological approaches. First, using the “serendipity” method, we constructed fifty molecular structures of the Zika virus. Then, we developed a calculational method based on the Hamiltonian semiempirical models (AM1 and PM3) and compared it using other methods of calculation to test total molecular energy, HOMO-LUMO (Frontier Molecular Orbitals), Electrostatic Potential Map and physical-chemical properties. From the general analysis of the molecules, we isolated the NS1 protein from the Zika virus (ZIKV) using homology modeling. We then performed several docking simulations on the biological processes responsible for Zika virus proliferation, comparing them in vitro. A new molecule was found capable of inhibiting the proliferation of the Zika Virus in vitro and in silico with a rate of 94% binding-inhibition. With our method of calculation, new drugs could be developed in less time and with less money, saving millions of lives from an epidemic that is in dire need of a new vaccine.

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