In-silico Design of Riboswitch Based Potent Inhibitors for Vibrio cholera

Authors : Somdutt Mujwar, Kamal Raj Pardasani

Abstract : Cholera pandemics are caused by facultative pathogenic Vibrio cholera bacteria persisting in the countries having warmer climatic conditions as well as the presence of large water bodies with huge amount of organic matter, it is responsible for the millions of deaths annually. Presently the available therapy for cholera is Oral Rehydration Therapy (ORT) with an antibiotic drug. Excessive utilization of life saving antibiotics drugs leads to the development of resistance by the infectious micro-organism against the antibiotic drugs resulting in loss of effectiveness of these drugs. Also, many side effects are also associated with the use of these antibiotic drugs. This riboswitch is explored as an alternative drug target for Vibrio cholera bacteria to overcome the problem of drug resistance as well as side effects associated with the antibiotics drugs. The bacterial riboswitch is virtually screened with 24407 legends to get possible drug candidates. The 10 ligands showing best binding with the riboswitch are selected to design a pharmacophore, which can be utilized to design lead molecules by using the phenomenon of bioisosterism.

Keywords : cholera, drug design, ligand, riboswitch, pharmacophore
Conference Title : ICSRD 2020 : International Conference on Scientific Research and Development
Conference Location : Chicago, United States
Conference Dates : December 12-13, 2020