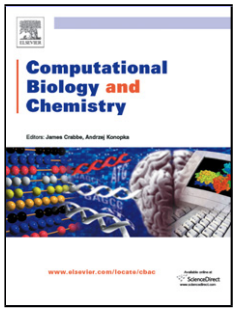

Title: Tetracyclines as a potential antiviral therapy against Crimean Congo Hemorrhagic Fever Virus: docking and molecular dynamic studies

Authors: Amirhossein Sharifi, Arash Amanlou, Faezeh Moosavi, Sahand Golestanian, Massoud Amanlou

PII: S1476-9271(16)30298-5
DOI: http://dx.doi.org/doi:10.1016/j.compbiolchem.2017.06.003
Reference: CBAC 6701

To appear in: *Computational Biology and Chemistry*

Received date: 20-6-2016
Revised date: 5-1-2017
Accepted date: 23-6-2017

Please cite this article as: Sharifi, Amirhossein, Amanlou, Arash, Moosavi, Faezeh, Golestanian, Sahand, Amanlou, Massoud, Tetracyclines as a potential antiviral therapy against Crimean Congo Hemorrhagic Fever Virus: docking and molecular dynamic studies.Computational Biology and Chemistry http://dx.doi.org/10.1016/j.compbiolchem.2017.06.003

Tetracyclines as a potential antiviral therapy against Crimean Congo Hemorrhagic Fever Virus: docking and molecular dynamic studies

Amirhossein Sharifi[1], Arash Amanlou[2], Faezeh Moosavi[1], Sahand Golestanian[1], Massoud Amanlou[1,*]

[1] Department of Medicinal Chemistry, Faculty of Pharmacy and Pharmaceutical Sciences Research Center, Tehran University of Medical Sciences, 16 Azar Ave., Tehran, Iran.

[2] Faculty of Specialized Veterinary Sciences, Science and Research Branch, Islamic Azad University, Tehran, Iran.

***Corresponding author**

Prof. Massoud Amanlou. Department of Medicinal Chemistry, Faculty of Pharmacy and Pharmaceutical Sciences Research Center, Tehran University of Medical Sciences, 16 Azar Ave., Tehran, Iran. amanlou@tums.ac.ir

Tel: +98 21 66959067

Abstract

Crimean-Congo Hemorrhagic Fever Virus (CCHFV) is one of the deadliest human diseases with mortality rate near 50%. Special attention should be paid to this virus since there is no approved treatment for it. On the other hand, the recent outbreak of Ebola virus which is a member of hemorrhagic fever viruses shows this group of viruses can be extremely dangerous. Previous studies have indicated that nucleoprotein of CCHFV, a pivotal protein in virus replication, is an appropriate target for antiviral drug development. The aim of this study is finding inhibitor(s) of this protein. Herein, a virtual screening procedure employing docking followed by molecular dynamic was used to identify small molecule inhibitors of the nucleoprotein from FDA-approved drugs. Regarding CCHFV, using in-silico method is a safe way to achieve its inhibitor(s) since this virus is categorized as a World Health Organization (WHO) biosafety level 4 pathogen and therefore investigation in general laboratories is restricted. In conclusion, considering docking and molecular dynamic results alongside with bioavailability of FDA-approved drugs, doxycycline and minocycline are proposed as potential inhibitors of CCHFV nucleoprotein. There is hope, this study encourage other research groups for in-vitro and in-vivo studies about the efficacy of those two medicines in CCHFV treatment.

Key words: Crimean Congo virus; Docking; Molecular dynamic; Doxycycline; Minocycline; FDA-approved drugs