

Letter to Editor

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Dose prediction of lopinavir/ritonavir for 2019-novel coronavirus (2019-nCoV) infection based on mathematic modeling

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Wuhan novel coronavirus or 2019-novel coronavirus (2019-nCoV) infection is a rapidly emerging respiratory viral disease[1]. 2019nCoV infection is characterized as febrile illness with possible severe lung complication[1]. The disease was firstly reported in China in December 2019 and then spread to many countries (such as Thailand, Japan and Singapore)[2,3]. As a new disease, there is a limited knowledge of treatment for the infection. Lu recently proposed that some drug might be useful in treatment of 2019-nCoV infection[3]. Lu noted that "lopinavir/ritonavir, nucleoside analogues, neuraminidase inhibitors, remdesivir, peptide (EK1), abidol, RNA synthesis inhibitors (such as TDF, 3TC), anti-inflammatory drugs (such as hormones and other molecules), Chinese traditional medicine, such ShuFengJieDu capsules and LianHuaQingWen capsule might be useful[3]." Of those mentioned drugs, lopinavir/ritonavir is a widely used antiviral for management of another important virus infection, human immunodeficiency virus (HIV) infection. Since 2019-nCoV infection is an RNA virus similar to HIV, lopinavir/ritonavir is proposed for management of 2019-nCoVinfection.

At present, lopinavir/ritonavir is widely used for possible treatment of 2019-nCoV infection in countries that the emerging infection exists. Here, the authors used a mathematical modelling theoretical approach to predict the expected proper dosage of lopinavir/ritonavir for possible treatment of 2019-nCoV infection. The protocol for mathematical modeling in this work is the same as previous report by Wiwanitkit *et al*[4]. Briefly, the primary agreement was there had to be a specific amount of required energy for reaction between lopinavir/ritonavir and its target enzyme and this energy is a specific constant for the reaction. Based on bonding theory, the required amount of lopinavir/ritonavir was varied to the two substrates, lopinavir/ritonavir and target, protease. Here, the simple equation 'A + B \rightarrow C where A was the target enzyme, B was lopinavir/ritonavir and C was end product' could be written.

For HIV, the molecular mass of protease is equal to 21.6 kDa.

For 2019-nCoV, the molecular weight was calculated from the functional motif showing protease function within the sequence of the virus. From molecular weight calculation tool (https://www.bioinformatics.org/sms/prot_mw.html; version 1 by Stothard[4]), the molecular mass of protease of 2019-nCoV is equal to 33.8 kDa. By standard comparison technique as used in the previous report[5], the required dosage of lopinavir /ritonavir for 2019-nCoV infection was about 1.56 times higher than that for HIV infection. Hence, based on the modeling study, if lopinavir/ritonavirs used for management of 2019-nCoV, a doubled dosage of the present dosage for HIV infection is recommended.

Conflict of interest statement

We declare that we have no conflict of interest.

Authors' contributions

SY and VW conceived the idea, performed the data collection. SY wrote the manuscript and all authors discussed the results and contributed to the final manuscript.

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