Contents lists available at ScienceDirect

Asian Pacific Journal of Tropical Biomedicine

journal homepage: www.elsevier.com/locate/apjtb

Short communication http://dx.doi.org/10.1016/j.apjtb.2017.07.007

Cleft analysis of Zika virus non-structural protein 1

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ARTICLE INFO

Article history:
Received 4 Jul 2016
Received in revised form 4 Aug 2016
Accepted 26 Jul 2017
Available online 2 Aug 2017

Keywords:
Zika virus
Non-structural protein 1
Cleft
Flavivirus

ABSTRACT

The non-structural protein 1 is an important molecule of the viruses in flavivirus group including to Zika virus. Recently, the NS1 of Zika virus was discovered. There is still no complete information of the molecular interaction of NS1 of Zika virus which can be the clue for explanation for its pathogenesis and further drug search. Here the authors report the cleft analysis of NS1 of Zika virus and the result can be useful for future development of good diagnostic tool and antiviral drug finding for management of Zika virus.

1. Introduction

The non-structural protein 1 (NS1) is a widely mentioned protein in clinical virology [1]. Gibson *et al.* noted that 'studies with the flaviviruses have demonstrated that protective immunity can be elicited by NS1' [1]. For example, in dengue, Chen *et al.* recently found that DENV NS1 protein 'plays a critical role in viral pathogenesis and protective immunity' [2].

As noted NS1 is an important molecule of the viruses in flavivirus group including to Zika virus. Recently, the NS1 of Zika virus was discovered [3]. There is still no complete information of the molecular interaction of NS1 of Zika virus which can be the clue for explanation for its pathogenesis and further drug research. Here the authors report the cleft analysis of NS1 of Zika virus.

2. Materials and methods

The authors used the standard bioinformatics technique, cleft analysis, for assess the molecule of NS1 of Zika virus (5IY3). The online site at http://www.ebi.ac.uk/thornton-srv/databases/ProFunc/ [3] is used for analysis of the uploaded PDB structure of the NS1 of Zika virus. The specific tool namely 'RASMOL AB', which is developed by Pikora and Gieldon [4] is used for cleft analysis. In brief, RASMOL AB is a bioinformatics techniques for structure analysis based on 'identification of histidine isomers, and advanced structural selection and macro capabilities' [5].

3. Results

According to this study, there are 10 identified gap regions within the studied molecules with volumes from 353.53 to 1550.39 Å^3 (1550.39, 1441.55, 918.00, 904.08, 411.75, 403.73, 426.94, 369.98 and 353.53 Å^3, respectively). Focusing on the accessible vertices, the values range from 58.39% to 72.13%. For the buried vertices, the values range from 5.06% to 12.57%.

4. Discussion

Analysis of molecular surface of a molecule to find the cleft can be the starting point for finding the possible interaction site of a molecule. This can be the first clue for finding of fit molecule to interacting with the studied molecule that is the basic rule for finding of new drug in medicine. For Zika virus, as an emerging infection, searching for the new drug is an ongoing important research and development. The role of structural bioinformatics for the new antiviral drug search for Zika virus is proposed [6]. Focusing on Zika virus, NS1 protein becomes the

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Peer review under responsibility of Hainan Medical University. The journal implements double-blind peer review practiced by specially invited international editorial board members.

interesting drug target [4]. Also, it is proposed that 'NS1 proteins are unique to Zika virus highlighting possible challenges in vaccine design' [6].

Here, the author performs a cleft analysis on NS1 of Zika virus. Indeed, the NS1 of Zika virus is proposed to be similar but have significant different surface electrostatic pattern to NS1 of other similar viruses (such as dengue) [3]. It is no doubt that the details of surface cleft might be totally different. In this work, the authors used the standard bioinformatics technique for prediction of the cleft within the structure of NS1 of Zika virus. The results can be useful for future development of good diagnostic tool and antiviral drug finding for management of Zika virus.

Conflict of interest statement

We declare that we have no conflict of interest.

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