

Views on Structure-based design of antiviral drug candidates targeting the SARS-CoV-2 main protease by Dai *et al.* (2020)

Hasanain Abdulhameed Odhar

Department of pharmacy, Al-Zahrawi University College, Karbala, Iraq; Hasanain Abdulhameed Odhar - Tel: 009647725300923; Email: hodhar3@gmail.com; *Corresponding author:

Received April 23, 2020; Accepted April 24, 2020; Published May 31, 2020

DOI: 10.6026/97320630016435

Declaration on Publication Ethics:

The authors state that they adhere with COPE guidelines on publishing ethics as described elsewhere at <https://publicationethics.org/>. The authors also undertake that they are not associated with any other third party (governmental or non-governmental agencies) linking with any form of unethical issues connecting to this publication. The authors also declare that they are not withholding any information that is misleading to the publisher in regard to this article.

Declaration on official E-mail:

The corresponding author declares that official e-mail from their institution is not available for all authors

Views:

The project for the report [1] seems to be well funded and the authors had access to many modern facilities and techniques. They were able to successfully design, synthesize and evaluate two lead inhibitors of SARS-CoV-2 main protease. Interestingly, they were able to crystallize protease-inhibitor complex to visualize real chemical interaction involved. According to x-ray diffraction images, they found that the aldehyde group of synthesized inhibitors is involved in covalent bond with Mpro active site. We can appreciate this finding by noting that computational modeling approaches like docking studies have difficulties in predicting covalent bonds. The design of these two novel inhibitors may be considered a continuation for several previous attempts of

structure-based design of coronavirus main protease inhibitors, for example the well-known peptide inhibitor N3. I am only concerned about the interaction between lead inhibitors and water molecules in crystallization images. These water molecules may be active site reserved water or merely the result of crystallization process. It would be interesting to prepare several derivatives of these two lead inhibitors and then establish a structure-activity relationship study. This seems to be crucial for elucidating the structure of core scaffold.

Reference:

[1] Dai W *et al.* 2020 Science. 2020 doi:10.1126/science.abb4489

Edited by P Kanguane

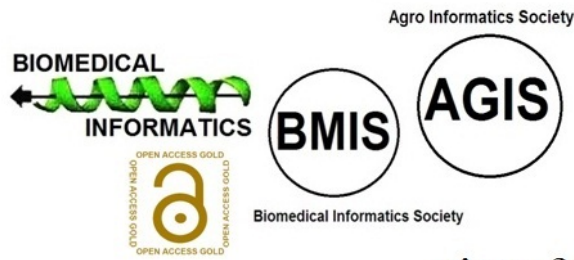
Citation: Odhar, Bioinformation 16(5): 435-437 (2020)

License statement: This is an Open Access article which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly credited. This is distributed under the terms of the Creative Commons Attribution License

Articles published in BIOINFORMATION are open for relevant post publication comments and criticisms, which will be published immediately linking to the original article for FREE of cost without open access charges. Comments should be concise, coherent and critical in less than 1000 words.

BIOINFORMATION

Discovery at the interface of physical and biological sciences



since 2005

BIOINFORMATION

Discovery at the interface of physical and biological sciences

indexed in



EBSCO

