International Journal of Botany Studies
ISSN: 2455-541X; Impact Factor: RJIF 5.12
Received: 20-11-2020; Accepted: 05-12-2020: Published: 16-12-2020
www.botanyjournals.com
Volume 5; Issue 6; 2020; Page No. 669-670

Plant-derived biomolcules against 2019- nCoV main protease

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Abstract

2019 Novel corona-virus (2019-nCoV) also referred to as severe acute respiratory syndrome Corona-virus 2 (SARS-CoV-2) emerged as a global risk and put the entire globe into unrest. Unavailability of specific drug against the virus is more imperative. *In silico* Molecular Docking revealed that the phytochemical, Vasicine effectively binds at the active pocket of the SARS-CoV-2 main protease.

Keywords: 2019-nCoV, SARS-CoV-2, SARS-CoV-2 main protease, docking, phytochemicals, vasicine

Introduction

The pandemic situation caused due to the 2019-nCoV represents a severe public health calamity across the globe. The city of Wuhan was the epicentre where the outbreak of this human pathogen emerged, and resulted to human ailment, termed as COVID-19 [1, 2]. 2019-nCoV encodes at least 27 proteins, including 15 non-structural proteins, 4 structural proteins, and 8 auxiliary proteins. SARS-CoV-2 belongs to the beta corona-virus genus, closely related to the previously identified severe acute respiratory syndrome corona-virus (SARS-CoV) [3, 4]. Public Health Emergency of International Concern (PHEIC) was declared by the World Health Organization (WHO) owing to its fast rate of transmission within the humans [1, 5, 6]. Crystal structure of the SARS-CoV-2 main protease (M^{pro}) proves to be an exceptional ground for screening specific ligands [7]. Reportedly, M^{pro} and other known viral proteins are defining features paving the path of virus from entry to infection in the host cell [8, 9, 10].

Methods

Viral Protein Structure and Phytochemical dataset collection

The 3D structure of M^{pro} was accessed from Protein Data Bank accession 6Y2E. The phytochemical, Vasicine was obtained and consequently both the protein and the ligands were used for *in silico* analysis.

Molecular docking

For the *in silico* molecular docking, BIOVIA's Discovery Studio docking method [11] was used for molecular docking. The catalytic pocket of the M^{pro} protein was specified and targeted for binding of the ligand. CDOCKER Energy and CDOCKER Interaction Energy signify the affinity of the ligands with the protein receptors. Basically, high positive values of the CDOCKER Energy, CDOCKER Interaction Energy and a diminutive difference between the CDOCKER Energy and CDOCKER Interaction Energy are considered to be the most favourable [13-20].

Results and Discussion

It was found that vasicine; a common phytochemical specifically binds to the active pocket of the SARS-CoV-2 M^{pro} as apparent from higher CDOCKER energy and CDOCKER interaction energy (Table 1). Since, simple active bio molecule like Vasicine effectively binds into the active pocket of the M^{pro} under *in silico* conditions it is quite possible to design pharmacophore molecules based on the structural and functional identity of Vasicine and eventually can be used in the pharmaceutical sector.

Table 1: Cdocker energy and cdocker interaction energy values generated for the interaction of Vasicine with the active site of SARS-CoV-2 main protease (M^{pro}).

Ligand	**Receptor**			**Interaction status**	
Phytochemical	**Protein**	**PDB Accession**	**Docking Result**	**C Docker Energy**	**C Docker Interaction Energy**
Vasicine	Free Enzyme of the 2019-nCoV Main Protease	6Y2E	Positive	-8.91	-23.45

Conclusion and Future perspectives

The current *in silico* molecular docking based study reveals that vasicine can target the reported SARS-CoV-2 M^{pro}. It would be extremely noteworthy being confirmed *in vivo*. It is crucial to develop diagnostic tools, potential therapeutics and antibodies selectively for the COVID-19 proteins. Phytochemicals like Vasicine is commercially available and thus may be effectively prescribed to circumvent the current global scenario. Essentially, this study makes an attempt to reveal simple phytochemicals like vasicine which can be employed for designing novel therapeutics.

Author contribution statement

GKP conceived the idea. GKP, SKS, PKP performed the experiments. All authors have significant contribution in drafting the manuscript.

Funding

The present study was financially supported by Centurion University of Technology and Management, Odisha, India.

Acknowledgements

Authors are thankful to the administration and management of Centurion University of Technology and Management, Odisha, India for providing necessary facilities to conduct the experiment.

Conflict of interest

The authors declare that they have no conflict of interest.

References

1. Chen N, Zhou M, Dong X, *et al*. Epidemiological and clinical characteristics of 99 cases of 2019 novel coronavirus pneumonia in Wuhan, China: a descriptive study. Lancet. 2020; 395:507-513.
2. Huang C, Wang Y, Li X, *et al*. Clinical features of patients infected with 2019 novel coronavirus in Wuhan, China. Lancet. 2020; 395:497-506. https: //doi. org/10.1016/S0140-6736 (20)30183-5.
3. Lu R, Zhao X, Li J, *et al*. Genomic characterisation and epidemiology of 2019 novel coronavirus: implications for virus origins and receptor binding. Lancet. 2020; 395:565-574.
4. Wu F, Zhao S, Yu B, *et al*. A new coronavirus associated with human respiratory disease in China. Nature. 2020; 579:265-269.
5. Chan JFW, Yuan S, Kok KH, *et al*. A familial cluster of pneumonia associated with the 2019 novel coronavirus indicating person-to-person transmission: a study of a family cluster. Lancet. 2020; 395:514-523.
6. Li Q, Guan X, Wu P, *et al*. Early Transmission Dynamics in Wuhan, China, of Novel Coronavirus–Infected Pneumonia. N Engl J Med. 2020, 1-9.
7. Liu W, Morse JS, Lalonde T, Xu S. Learning from the Past: Possible Urgent Prevention and Treatment Options for Severe Acute Respiratory Infections Caused by 2019-nCoV. Chem Bio Chem, 2020, 730-738.
8. Wrapp D, Wang N, Corbett KS, *et al*. Cryo-EM structure of the 2019-nCoV spike in the prefusion conformation. Science. 2020; 1263:1260-1263.
9. Lung Jr hau, Yu-Shih Lin, Yao-Hsu Yang, *et al*. The potential chemical structure of anti-SARS-CoV-2 RNA-dependent RNA polymerase. J Med Virol, 2020, 0-1.
10. Ton A-T, Gentile F, Hsing M, *et al*. Rapid Identification of Potential Inhibitors of SARS- CoV-2 Main Protease by Deep Docking of 1.3 Billion Compounds. Mol Inform, 2020, 1-18.
11. Dassault Systèmes Biovia, discovery studio, San Diego: Dassault Systèmes, 2020.
12. Panigrahi Gagan Kumar, Sahoo Shraban Kumar and Satapathy Kunja Bihari. In silico Molecular Docking-Based Screening of Phytochemicals Targeted against Glypican-1. IJONS. 2020; 59(10):18708-18712.
13. Panigrahi GK and Satapathy KB. Sacrificed surveillance process favours plant defense: a review Plant Archives. 2020a; 20(1):2551-2559.
14. Panigrahi GK, Satapathy KB. Arabidopsis DCP5, a decapping complex protein interacts with Ubiquitin-5 in the processing bodies Plant Archives. 2020b; 20(1):2243-2247.
15. Panigrahi GK and Satapathy KB. Formation of Arabidopsis Poly (A)-Specific Ribonuclease associated processing bodies in response to pathogenic infection Plant Archives. 2020c; 20(2):4907-4912.
16. Panigrahi GK, Sahoo A, Satapathy KB. Insights to plant immunity: Defense signaling to epigenetics. Physiological and Molecular Plant Pathology. 2021; 113:1-7.
17. Panda S, Panigrahi GK, Padhi SN. Wild animals of India Anchor Academic Publishing. 2016; 1(1):105.
18. Panigrahi GK, Panda S, Padhi SN. Aquaponics: An innovative approach of symbiotic farming International Journal of Bioassays. 2016; 5(9):4808-4814
19. Panigrahi GK, Sahoo AS. A review on Natural Dye: Gift from bacteria International Journal of Bioassays. 2016; 5(9):4909-4912
20. Panigrahi GK, Sahoo AS, Panda S. A complex network of molecular events triggered upon environmental cues which decide the fate of gene expression: a review International Journal of Bioassays. 2016; 5(12):5185-5191.