

Commentary

Promising Antiviral Molecules from Ayurvedic Herbs and Spices against COVID-19

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COVID-19 is caused by the novel coronavirus severe acute respiratory syndrome coronavirus-2 (SARS-CoV-2) and smashed our society severely. Many efforts/measures have been taken worldwide to control coronavirus disease 2019 (COVID-19) but it is spreading ceaselessly across the globe.⁽¹⁾ Interestingly, Chinese medicine was used to treat COVID-19 and they found better recovery results.^(2,3) This has also drawn the attention of the scientific community to Ayurveda where traditional knowledge of this domain can be explored for finding COVID-19 a cure or prevention.

This technical note provides a first-round result that has been done at the interface of Ayurveda and *in silico* biology regarding COVID-19. This article aims to provide the readers an understanding of the basic principles of ancient medicine and conjugation of *in silico* technology in Ayurveda for the development of core concepts of Ayurveda. Quick screening of traditional herbs/spices phytoconstituents can be done by *in silico* study in poly-herbal/Ayurvedic formulations. This inhibition/induction of phytoconstituents with target protein can quickly be identified by *in silico* study.^(4,5) Therefore, the authors have selected 11 herbs (*Allium sativum*, *Cinnamomum cassia*, *Cuminum cyminum*, *Piper nigrum*, *Curcuma longa*, *Ocimum sanctum*, *Zingiber officinale*, *Coriandrum sativum*, *Syzygium aromaticum*, *Trachyaspermum ammi*, *Mentha arvensis*) advised commonly in Ayurveda for *in silico* screening as an antimicrobial agent (Table 1). Total 26 major compounds were docked using AutoDock 4.2 simulator with the active site of the crystal structure of SARS-CoV-2 virus main protease (PDB ID: 6LU7, Table 1). Cinnzeylanol, cinnzeylanine, apigenin, and isobiflorin observed higher binding constant and inhibition activity against protease (PDB ID: 6LU7) denote a good antiviral property. The role and participation of protease in the endocytosis of SARS-CoV-2 into human cells are well established and they help in viral spread/infection in the host.⁽⁶⁾ Although this study was conducted with some individual compounds of ayurvedic herbs/spices to see the interaction and inhibitory properties with SARS-CoV-2 protease. But routinely, herbs are advised to take

collectively as a decoction (hot water extract of herbs), multiple phytoconstituents in the decoction formulation may synergize the inhibition results through single or multiple target sites. Further research is solicited for phytoconstituents interactions and their collective binding/inhibition behaviour against SARS-CoV-2 active sites. A docking study suggested that molecules of spices like curcumin and nimbin exhibited high interaction with SARS-CoV-2 target proteins viz., spike glycoprotein (MolDock score -141.36 and -148.62 kcal/mol) and angiotensin-converting enzyme 2 (ACE-2) receptor (MolDock score -142.64 and -140.10 kcal/mol).⁽⁷⁾ The above data pave a way for further research to extend the use of self-care advisory given by the Indian AYUSH ministry in prophylaxis and management of hotspot area, vulnerable, COVID-19 warriors, confirm positive contacts, and cases under home quarantine/isolation centers.

Since no medicine is available for COVID-19, therefore, we should rely on those things that have antiviral acreage, immune-boosting, and anti-inflammatory properties with fewer side effects and commonly available for all. In this regard, herbs/spices selected in this study provided its satisfactory anti-COVID-19 property. As per literature, they have also immune-boosting, and anti-inflammatory properties.^(5,8) At a time when the world is reeling under the effects of COVID-19, the result of the study indicated that these Ayurvedic herbs/spices should be looked as food therapeutics to protect individuals from various diseases. This is a short technical note and length does not permit to cover whole issues. The aim of the work is to simply attract/think researcher in this direction and to motivation for those who are working at the

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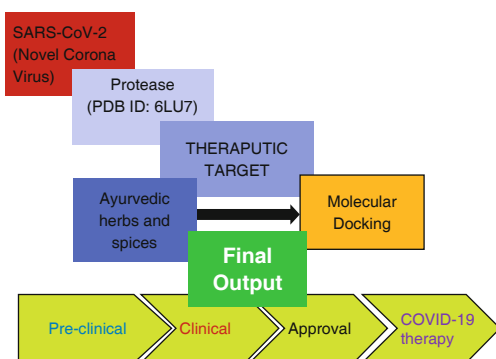
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Table 1. Binding and Inhibition Activity of Ayurvedic Herbs/Spices Phytoconstituents with Target Protease (PDB ID: 6LU7) of SARS-CoV-2

S. N.	Name of natural compound	Binding energy	Inhibition constant	Natural source (plant name)
1	Allicin	-3.37	3.38 mmol/L	
2	Allyl disulfide	-2.68	10.90 mmol/L	<i>Allium sativum</i>
3	Allyl trisulfide	-2.83	8.41 mmol/L	
4	Cinnamaldehyde	-4.16	893.38 μ mol/L	
5	Cinnazaylanol	-5.29	132.45 μ mol/L	<i>Cinnamomum cassia (Cinnamon)</i>
6	Cinnazaylanine	-5.12	178.04 μ mol/L	
7	2-Ethyl-6-heptylphenol	-3.38	3.30 mmol/L	
8	Cuminaldehyde	-4.5	506.19 μ mol/L	<i>Cuminum cyminum</i>
9	Cymene	-3.95	1.27 mmol/L	
10	Piperine	-4.94	240.08 μ mol/L	<i>Piper nigrum</i>
11	Bis demethoxycurcumin	-4.57	444.32 μ mol/L	
12	Curcumin	-3.36	3.44 mmol/L	<i>Curcuma longa</i>
13	1,2-Dimethoxy-4-prop-1-enylbenzene	-4.53	476.06 μ mol/L	
14	Apigenin	-5.27	139.94 μ mol/L	<i>Ocimum sanctum</i>
15	Eugenol	-4.9	255.14 μ mol/L	
16	Beta sitosterol	-4.1	987.25 μ mol/L	
17	Gingerol	-2.72	10.06 mmol/L	
18	Shagoals	-3.14	4.99 mmol/L	<i>Zingiber officinale</i>
19	Zingiberine	-4.13	933.32 μ mol/L	
20	(E)-dodec-2-en-1-ol	-3.16	4.86 mmol/L	
21	Methyl hexadecanoate	-1.91	39.90 mmol/L	<i>Coriandrum sativum</i>
22	Eugeniin	Not active	-	
23	Isobiflorin	-5.57	83.04 μ mol/L	<i>Syzygium aromaticum</i>
24	γ -Terpinene	-3.86	1.49 mmol/L	
25	Lingustilide	-4.93	245.31 μ mol/L	<i>Trachyspermum ammi</i>
26	(E)-3,7,11,15-tetramethylhexadec-2-en-1-ol	-2.4	17.38 mmol/L	<i>Mentha arvensis</i>

interface of Ayurveda and *in silico* biology. The reported result in this article (Table 1) is an Ayurveda phytoconstituents *in silico* efforts study which further necessitates the need for pre-clinical and clinical research of the active compounds (Figure 1) to increase the understanding in the development of effective future therapeutics in Ayurveda.

**Figure 1. Roadmap of Promising Antiviral Molecules Identification from Ayurvedic Herbs and Spices for COVID-19 Therapy**

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Conflict of Interest

None.

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