



## Short Commentary

## A short Commentary on “Network Pharmacology, Molecular Docking and Molecular Dynamics Simulation Studies of the Molecular Targets and Mechanisms of ChuanKeZhi in the Treatment of COVID-19”

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COVID-19 is an infectious disease caused by the SARS-CoV-2 virus. Globally, as of 20 September 2022, there have been 609,848,852 confirmed cases of COVID-19, including 6,507,002 deaths, reported to WHO. Although almost 12,640,866,343 vaccine doses have been administered globally, the number of confirmed cases still continued to rise [1]. On November 24, 2021, a variant of the novel coronavirus (Omicron, B.1.1.529) was first reported in South Africa. On November 26, 2021, the World Health Organization (WHO) named it Omicron (Omicron) variant. The Omicron variant included several subtypes, including B.1.1.529, BA.1, BA.2, BA.3 and so on [2,3]. Compared with the original strain, the Spike (S) protein of Omicron variant has multiple mutation sites and is more capable of binding to angiotensin-converting enzyme 2 (ACE2), thus the virus is more capable of spreading and immune evasion [4]. Although the severity and mortal

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ity caused by Omicron infection are lower than those of the previous strains, due to its high transmissibility, the total number of Omicron infections, the death rate, and the daily number of new infections have reached a significant peak in the United States, the United Kingdom, and India [5-7].

Nowadays, Traditional Chinese Medicine (TCM) has been widely applied in most of COVID-19 patients in China and has shown obvious and effective results [8]. Chuankezhi Injection (CKZI) was mainly made up of two Chinese herbs: Yingyanghuo (YYH, dried leaves of *Epimedium brevicornis* Maxim., *Epimedium sagittatum* (Siebold and Zucc.) Maxim., *Epimedium pubescens* Maxim, and *Epimedium koreanum* Nakai) and Bajitian (BJT, *Morinda officinalis* FC How). CKZI has been proved to improve lung function, inhibit airway inflammation, reduce the expression of Gluco-Corticoids (GC) resistance-related factors in asthma and Chronic Obstructive Pulmonary Disease (COPD) [9,10]. A number of researches have revealed the potential of YYH and BJT in diseases. In our study, we made use of public databases and to explore the potential targets of two herbs: YYH and BJT. When compared the present data about COVID-19, we finally got 74 overlapped targets which could be considered as key targets, for instance, AKT1, TNF, IL6, VEGFA, IL1B, TP53, JUN and CASP3, etc. were supposed to be the main genes among those.

In addition, we also screened candidate compounds of YYH and BJT and made molecular docking with Spike protein S1, SARS-CoV-2-3CL pro and ACE2 (angiotensin converting enzyme2) for validating the binding energy. Excitingly, quercetin, anhydrocaritin and 8-Isopentenyl-kaempferol showed the most noticeable binding ability. Interestingly, quercetin, anhydrocaritin and 8-Isopentenyl-kaempferol all belong to flavonoids. Flavonoids has been proved to hold various treating potential for inhibiting inflammation, regulating immune responses, etc., [11]. The results of Molecular Dynamic (MD) simulation studies also showed that the complex of candidate compounds and COVID-19 related proteins were stable, which were consistent to our previous results.

GO function and KEGG pathway enrichment analyses were made to further explore potential involved functions and pathways. Positive regulation of cellular component movement was the most potential biological process. Membrane raft and cytokine receptor binding were the most essential cellular component and molecular functions, respectively. In addition, JAK-STAT signaling pathway and MAPK signaling pathway were considered to be strongly related to the treating mechanisms of COVID-19 by CKZ. In other words, the target genes influenced various cellular functions and process.

In conclusion, we initially found the potential value of CKZ in COVID-19 treatment. Quercetin, anhydrocaritin and 8-Isopentenyl-kaempferol may be the main active molecular in CKZ. Although CKZ has been widely used in clinical and proved safe and effective in many respiratory diseases, and our studies indicated the strong curative potential of YYH and BJT in COVID-19, the results still need further validation in clinical. COVID-19 still spreads around the world and greatly influenced the life and economy of us. A better and economic therapy needs to explore.

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