Topic	Computational identification of Shenshao Ningxin Yin as an effective treatment for novel coronavirus infection (COVID-19) with myocarditis
Author	Ze-Yu Zhang, Zhu-Jun Mao, Ye-ping Ruan, and Xin Zhang
Link	https://www.aimspress.com/aimspress-data/mbe/2022/6/PDF/mbe-19-06-270.pdf
Source	AIMS
Date	06 April, 2022

English

Abstract:
Background: The newly identified betacoronavirus SARS-CoV-2 is the causative pathogen of the 2019 coronavirus disease (COVID-19), which has killed more than 4.5 million people. SARS-CoV-2 causes severe respiratory distress syndrome by targeting the lungs and also induces myocardial damage. Shenshao Ningxin Yin (SNY) has been used for more than 700 years to treat influenza. Previous randomized controlled trials (RCTs) have demonstrated that SNY can improve the clinical symptoms of viral myocarditis, reverse arrhythmia, and reduce the level of myocardial damage markers.
Methods: This work uses a rational computational strategy to identify existing drug molecules that target host pathways for the treatment of COVID-19 with myocarditis. Disease and drug targets were input into the STRING database to construct protein–protein interaction networks. The Metascape database was used for GO and KEGG enrichment analysis.
Results: SNY signaling modulated the pathways of coronavirus disease, including COVID-19, Ras signaling, viral myocarditis, and TNF signaling pathways. Tumor necrosis factor (TNF), cellular tumor antigen p53 (TP53), mitogen-activated protein kinase 1 (MAPK1), and the signal transducer and activator of transcription 3 (STAT3) were the pivotal targets of SNY. The components of SNY bound well with the pivotal targets, indicating there were potential biological activities.
Conclusion: Our findings reveal the pharmacological role and molecular mechanism of SNY for the treatment of COVID-19 with myocarditis. We also, for the first time, demonstrate that SNY displays multi-component, multi-target, and multi-pathway characteristics with a complex mechanism of action.

中文

摘要：
背景：新發現的 β 冠狀病毒 SARS-CoV-2 是 2019 年冠狀病毒病 (COVID-19) 的致病病原體，該病已導致超過 450 萬人死亡。 SARS-CoV-2 會通過靶向肺部引發嚴重的呼吸窘迫綜合症，並且引起心肌損傷。參芍寧心飲 (SNY) 應用於治療流感已有 700 多年的歷史。跟據以往的隨機對照試驗（RCTs）表明，參芍寧心飲可以改善病毒性心肌炎的臨床症狀，調節心律失常，降低心肌損傷標誌物水平。

方法：這研究工作使用了有理計算策略來分辨現有用於治療 COVID-19 心肌炎的靶向宿主途徑的藥物分子。疾病和藥物靶點被輸入到 STRING 數據庫中以構建蛋白質交互作用的網絡。 Metascape 數據庫則用於 GO 和 KEGG 的進階分析。

結果：參芍寧心飲信號調節了冠狀病毒疾病的傳遞路徑，包括 COVID-19、Ras 信號、病毒性心肌炎和腫瘤壞死因子信號傳遞路徑。腫瘤壞死因子 (TNF)、細胞腫瘤抗原 p53 (TP53)、絲裂原活化蛋白激酶 1 (MAPK1) 以及信號轉導及轉錄激活蛋白3 是參芍寧心飲的關鍵靶點。 參芍寧心飲的成分與關鍵靶點結合良好，反映出其擁有潛在的生物活性。

結論：我們的研究展示了參芍寧心飲在新冠肺炎引發的心肌炎的應用，包括在藥理作用以及分子機理，同時，我們第一次論證了參芍寧心飲中所展示的多組分、多靶點和多途徑的特徵，這包括了一系列複雜的活動機理。