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# Mechanism of Sijunzi Stewing within the Treatment of Large Intestine Cancer Supported Network Medical Specialty and Experimental Validation

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### **Abstract**

**Ethno pharmacologic connexion:** Sijunzi Decoction(SJZD, as a noted classical prescription for the treatment of large intestine cancer(CRC) within the ancient Chinese drugs (TCM), has achieved smart curative effects in clinical follow. However, its specific ingredients and molecular mechanisms continue to be unclear.

**Aim of the study:** To analyze the effective ingredients and molecular mechanisms of SJZD within the treatment of CRC through network medical specialty technology and experimental validation.

**Materials and strategies:** First, the TCM Systems medical specialty information and analysis platform information were searched to screen the effective chemical elements of SJZD. Swiss Target Prediction was accustomed predict corresponding potential target genes of compounds. After that, we have a tendency to created a elements and corresponding target network by Cytoscape. at the same time, five sickness databases were accustomed search and filter CRC targets, then we have a tendency to created a drug-disease target protein-protein interaction (PPI) network. Cytoscape three.7 was used for image and cluster analysis, and Metascape information was used for GO and KEGG enrichment analysis. we have a tendency to histrion the most pathway-target network diagram. Autodock vina1.5.6 was applied to molecular arrival for the most compounds and target proteins. after, the potential mechanism of SJZD on carcinoma foretold by network pharmacologic analysis was by experimentation studied and verified in vivo and in vitro.

**Results:** 144 effective active chemical elements, 897 potential targets, and 2584 CRC target genes were screened out. the quantity of common targets between the SJZD and CRC was 414.3250 GO process things and 186 KEGG signal pathways were obtained when analysis. the most compounds and therefore the target macromolecule had an honest binding ability in molecular arrival. The results of cell and animal experiments showed that SJZD may promote programmed cell death and autophagy of CRC cells through PI3K/Akt/mTOR pathway.

**Conclusions:** SJZD will treat CRC through multiple elements, multiple targets and multiple pathways. we have a tendency to ab initio unconcealed the effective elements and molecular mechanisms of SJZD within the treatment of CRC, and that we used molecular arrival and experiment for preliminary verification.

**Keywords:** Sijunzi decoction; large intestine cancer; Network pharmacology; Molecular docking; Autophagy; programmed cell death

### Introduction

Colorectal cancer (CRC) could be a common metastatic tumor of the gastrointestinal system. in step with information from the International Agency for analysis on Cancer in 2018, CRC was hierarchal third worldwide within the incidence of malignant diseases, that was second in mortality. In the USA, CRC was hierarchal second within the range of the patients WHO died from cancer. in step with the yank medicine Society, 147,950 folks are freshly diagnosed with CRC in 2020, and 53,200 folks can die from the sickness within the USA. within the past 3 decades, the incidence of CRC in China has been increasing, and there's a unbroken upward trend. In 2020, Chinese official statistics ended that CRC incidence rate was hierarchal second and death rate was hierarchal fourth in malignant tumors. Despite many progress were created within the treatment of CRC, clinical test information continues to be for the most part missing and is desperately required to verify relevant effects and for the event of a lot of personalized treatment approaches [1].

Traditional Chinese medicine (TCM) has wealthy expertise and distinctive benefits within the treatment of CRC. Sijunzi stewing (SJZD) could be a classic prescription for the treatment of gi tumors in TCM. it had been derived from the Chinese Sung medical book 'Preions of the Bureau of Taiping People's Welfare Pharmacy, that was written quite 860 years past [2]. It will treat chassis weak, abdominal

distention, diarrhoea forcing out and alternative Pi's chi deficiency syndrome as well as CRC, referred to as Changxun by TCM. In step with TCM theory, Pi's chi deficiency results in a decline in immune perform and additional the formation of digestive tube tumorsits. SJZD perform square measure plenishing Pi's chi and removing wetness, thus its wide used as AN adjuvant treatment for CRC [3].

we used a mix of network medical specialty, molecular arrival and experiment to investigate the active ingredients, potential targets and molecular mechanisms of SJZD within the treatment of CRC, and that we conducted preliminary verification by cell and animal experiments [4]. The progress is shown in graphical abstract.

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### Materials and strategies

## Network pharmacology-based analysis

# Assortment and screening of active chemical composition in $\ensuremath{\mathsf{SJZD}}$

The Chinese drugs System pharmacologic information and Analysis Platform contains 499 Chinese flavoring medicines, 12144 compounds, 3311 targets and 837 connected diseases registered within the Chinese aggregation, users will screen them supported pharmacokinetic parameters of drug absorption, distribution, metabolism, and excretion. In TCMSP, all the active chemical composition of Ren Shen, Bai Zhu, Fu Ling, and Gan Cao were screened out, in step with oral bioavailability (OB)  $\geq\!30\%$  and drug-likeness (DL)  $\geq\!0.8$ . Then we have a tendency to else alternative main chemical ingredients by consulting connected literature [5].

# Predicting possible drug targets and creating a component-target network

The PubChem information was sought for SMILES of obtained compounds, and therefore the SMILES was entered into Swiss Target Prediction thus we are able to acquire the potential targets of the most active chemical composition [6]. The targets whose credibleness price was zero were removed. Cytoscape could be a helpful info image software package, it's presently chiefly used for visual analysis of biological info and social networks. Cytoscape3 [7]. was accustomed draw SJZD network diagrams. 'Network analysis' within the software package was accustomed calculate the degree, intermediate degree (BC), compactness (CC), average shortest path length (ASPL), they're successively representing the quantity of connections of a node with alternative nodes, the role of a counter within the affiliation of alternative nodes, the proximity of the counter to the middle of the network, and therefore the shortest path length between interruptions, all of them were accustomed assess the scenario of the network[8].

## **Experimental validation**

Fetal bovine body fluid (FBS) from Gibco (Grand Land, NY, USA); Dulbecco changed Eagle medium/high aldohexose (DMEM, SH30022.01) and phosphate buffered saline (PBS, SH30256.01) were obtained from GIBCO Life Technologies. Annexin V-FITC/PI programmed cell death Detection Kit (#3562) was purchased from Shanghai Beibo Biotechnology Co., LTD., China; Total macromolecule extraction kit, BCA macromolecule content detection kit and SDS PAGE Gel preparation Kit were purchased from Sigma-Aldrich[9].

### Discussion

The incidence of CRC has forever been high in developed countries in Western. However, the present development transformation countries as an example, China. The lifestyles and consumption habits of the inhabitants have bit by bit westernized. Factors like avoirdupois, lack of physical exertion, and high-fat diet are more and more evident square measure centered on, what causes the incidence of CRC to extend year by year, has made a larger economic burden of health. CRC could be a complex sickness caused by mode, genetic and environmental factors [10]. In general, the large intestine nonmalignant tumor can type CRC with development in 10–15 years. The clinical manifestations of CRC square measure various and Lacking specificity, like body part hurt, changes in intestine habits, abdominal pain, etc. Early

designation depends on the scrutiny; up to five hundredth of patients seem neoplasm metastasis at the primary time of designation [11]. The foremost common form of neoplasm metastasis is liver metastasis (50%). Existing treatment strategies embrace scrutiny and surgical native operation, therapy, radiation, biological targeted medical aid and therapy. Because of advances within the treatment of CRC, the survival time of patients with advanced CRC has been delayed from concerning five months to concerning thirty months however the 5-year survival rate of pathologic process patients continues to be but 100 percent and every treatment has its pathognomonic facet effects and complications [12].

### Conclusion

Our results demonstrate that SJZD induces autophagy and programmed cell death in carcinoma by modulating PI3K/Akt/mTOR sign in CRC and highlight SJZD as a promising adjuvant for CRC treatment

### Declaration of competitive interest

All authors state that they need no conflicts of interest relating to the publication of this paper.

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