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Original Article

Shiquan Yuzhen Decoction inhibits angiogenesis and tumor apoptosis caused by non-small cell lung cancer and promotes immune response

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Abstract: Background: TCM treatment for lung carcinoma has been reported by many researches. Shiquan Yuzhen Decoction can be used in the clinical treatment of lung carcinoma, but its specific mechanism is still under exploration at present. Methods: The active ingredients and mechanism of Shiquan Yuzhen Decoction on non-small cell lung carcinoma were discussed by network pharmacology. The main active ingredients, targets and disease genes of non-small cell lung carcinoma of Shiquan Yuzhen Decoction were screened through relevant databases. Lewis lung carcinoma bearing mice model was established by inoculating Lewis lung carcinoma cells to C57BL/6 mice under the right armpit. Different doses of Shiquan Yuzhen Decoction were used to observe the apoptosis and angiogenesis changes of tumor tissues in mice. Results: A total of 26 key active compounds meeting the evaluation of generic properties and 182 main targets were screened out. The multi-level network model shows that Shiquan Yuzhen Decoction can regulate the target gene network of non-small cell lung carcinoma. And it can inhibit tumor growth in tumor-bearing mice, induce apoptosis of tumor cells, and evidently increase the activities of Caspase-3, 8 and 9. The dose of 17.4 g/kg can evidently inhibit the formation of microvessels in transplanted tumor tissues, improve the sensitivity of mice's diet and activities, increase the spleen index of tumor-bearing mice, and inhibit inflammatory factors. Conclusion: Shiquan Yuzhen Decoction can evidently improve the quality of life of Lewis lung carcinoma-bearing mice and inhibit tumor growth in mice, which is a potential clinical treatment plan.

Keywords: Non small cell lung carcinoma, Shiquan Yuzhen Decoction, KEGG, GO, PPI, angiogenesis, immunoprophylaxis

Introduction

Lung carcinoma (LC) ranks first in male malignant tumors in China and second in female malignant tumors, and it is the main cause of carcinoma death, ranking first in malignant tumors [1]. The incidence and mortality of LC in China are increasing year by year. It is estimated that by 2025, LC patients will reach 1 million, and China will have the highest incidence rate of LC in the world [2]. Non-small cell lung carcinoma (NSCLC) is most common in LC, accounting for more than 85% of LC cases [3]. Although modern scientific and medical technology is constantly developing in a breakthrough way, and modern clinical diagnosis and treatment of LC disease are increasingly rich, the morbidity and mortality of LC are still high, especially the overall treatment effect of middle and late LC is not satisfactory, which poses great danger to human life safety [4, 5].

In recent years, the role of Chinese medicine in preventing and treating LC has been attracted more attention [6, 7]. Chinese medicine acts in preventing and treating LC, improving the quality of life of LC patients, preventing metastasis and recurrence, and acts in palliative treatment, which fully embodies the characteristics and advantages of the holistic view of Chinese medicine. In particular, the complex components and multi-target effects of Chinese herbal medicine have many advantages in LC prevention and treatment [8, 9]. Many researches

revealed that Chinese medicine acts in regulating immune function, inhibiting tumor angiogenesis, inducing tumor cell apoptosis, directly killing tumor cells and inhibiting tumor cell proliferation [10, 11]. However, there are still different views on the treatment of Chinese medicine. It is considered that the composition of Chinese medicine is complex, and it is impossible to judge the way of the drugs which can improve the occurrence of tumor.

Network pharmacology is put forward on the basis of the theoretical development of multidirectional pharmacology, network biology, system biology, and big data analysis technology. It uses the holistic concept to explain the disease development process and the mechanism of drugs acting on the body, and at the same time, it provides new ideas and methods for new drug research and development [12]. Through big data technology, we analyzed the existing information including high-throughput sequencing, proteome, drugs, diseases and other related databases, and combined them with various data reports to establish a network of "drug-target-disease". Then, we applied related software tools to comprehensively display the relationship of drugs-targets, targets-diseases, diseases-diseases, and drugs-drugs. Therefore, we can observe the intervention and influence of drugs on diseases from multidimensional, all-round and deep-seated aspects, and can also find the possible targets and signal pathways of drugs for target diseases [13-15].

In this research, we explored the latent targets and signal pathways of Shiquan Yuzhen Decoction with the reference of network pharmacology, and verified it by animal models, which provided a basis for clinical use of Shiquan Yuzhen Decoction.

Methods and data

Screening of active ingredients

TCM chemical composition database TCMID (http://www.megabionet.org/tcmid) [16], TCMSP (http://tcmspw.com/tcmsp.php) [17], and HIT (http://lifecenter.sgst.cn/hit) were applied [18]. Referring to the articles on the research of ginseng, Astragalus membranaceus, raw dioscorea, rhizoma anemarrhenae, radix scrophulariae, Os Draconis, raw oyster, salvia, rhizoma sparganii, and curcuma zedoary in PubMed, CNKI and Wanfang websites, the chemical constituents of these ten herbs were searched, and the repeated parts were summarized and deleted as the chemical components of Shiquan Yuzhen decoction. The OB value and DL value of each chemical component of Shiquan Yuzhen Decoction were obtained by TCMID and TCMSP, and the chemical components with OB≥30% and DL≥0.18 were taken as the active components of Shiquan Yuzhen Decoction.

Target selection of active ingredients

Selected active ingredients were screened through uniprot database (http://www.uniprot.org/) [19] and Pubchem platform (https://pubchem.ncbi.nlm.nih.gov/) [20]. The "reviewed (Swiss prot)" was defined as "human" search, and the results were standardized to obtain the potential target of Shiquan Yuzhen decoction.

Query of NSCLC target gene

Through Genecards (https://www.genecards.org/) [21], OMIM (https://www.omim.org/) [22], DisGeNET (http://www.disgenet.org/) [23] and TTD (http://bidd.nus.edu.sg/group/cjttd/) [24] database, "NSCLC" and "Non-small-cell carcinoma" were applied as search terms, the target genes of NSCLC were obtained respectively, and then the differentially expressed genes obtained in all databases were merged and the duplicate parts were deleted, thus obtaining the genes related to NSCLC.

Screening and network construction of disease target of drug action

Gene mapping was carried out on the target points corresponding to the active ingredients in Shiquan Yuzhen Decoction and the disease gene information of NSCLC. Venny2.1 (http://bioinfogp.cnb.csic.es/tools/venny/index.html) [25] was used to visualize the Venn diagrams of the active ingredient target points of Shiquan Yuzhen Decoction and the disease gene of NSCLC, and the target points of Shiquan Yuzhen Decoction acting on NSCLC were obtained. The network analyzer plug-in in Cytoscape3.7.2 was used. According to the topological feature of degree of freedom, the main active ingredients with degree more than twice of the median were selected as the key active ingredients [26], and the target corresponding to the key

active components was called the core target. Based on this, the network diagram of "drug target disease" was constructed and visualized.

Analysis of biological pathways and biological targets

Enrichment analysis was performed using DAVID (https://david.ncifcrf.gov/) [27] online database. The key active components and core targets were introduced to the system, and the enrichment analysis of Gene Ontology (GO) and Kyoto Encyclopedia of Genes and Genomes (KEGG) were carried out. GO enrichment analysis (confidence value $P < 0.01$), Biological Process (BP), Cellular Component (CC) and Molecular Function (MF) were selected for core target enrichment and function annotation. In KEGG enrichment analysis, FDR < 0.01 was selected, and combined with the related literature of NSCLC, the signal pathway of Shiquan Yuzhen Decoction on NSCLC was screened out.

Analysis of protein co-expression

The functional protein association platform STRING V11.0 (https://string-db.org/) was used for protein co-expression analysis. The core target proteins of the key active components of Shiquan Yuzhen Decoction acting on NSCLC were uploaded to string. The target protein PPI network of Shiquan Yuzhen decoction was constructed by selecting "Homo sapiens" and setting minimum required interaction score > 0.9, so as to screen high confidence data.

Source of cell and animal

Altogether 40 healthy and clean C57BL/6 mice (with 20 males and 20 females) aged 4-6 weeks and weighed 17-20 g were obtained from Hunan SJA Laboratory Animal Co., Ltd, Changsha, Hunan, China. The mice were raised in the Experimental Animal Center of Shanghai University of Traditional Chinese Medicine, with four mice in a cage, which was circulated day and night, and the suitable activity space of mice was fully ensured. The indoor temperature was 17-24°C, and the mice were free to eat common standard feed and drink pure water. The mice were raised adaptively for one week, and the mice were grouped after they were applied to the environment. Lewis lung carcinoma cells were obtained from Shanghai Institute of Biochemistry and Cell Biology, Chinese Academy of Sciences.

Compatibility and preparation of prescriptions

Shiquan Yuzhen Decoction consisted of ginseng (12 g), Astragalus membranaceus (12 g), raw dioscorea (12 g), rhizoma anemarrhenae (12 g), radix scrophulariae (12 g), Os Draconis (12 g), raw oyster (12 g), Salvia miltiorrhiza (6 g), rhizoma anemarrhenae (4.5 g) and Curcuma zedoariae (4.5 g). All the above medicines were purchased from the outpatient Chinese medicine pharmacy of Pudong Branch of Longhua Hospital affiliated to Shanghai University of Traditional Chinese Medicine. The above medicinal herbs were obtained according to the prescribed amount. The Os Draconis and raw oyster were bathed in 10 times of water for 30 min, then decocted for 1 h in a medicine pot, then other medicines were bathed in 10 times of water for 30 min, then combined with the first decocted medicines and decocted for 1 h, filtered, the filtrate was stored, then 8 times of water was added and the medicines were decocted for 1 h, filtered, and the filtrates of the two times were combined, concentrated to contain 2 g/ml of crude drug, and stored in a refrigerator at 4°C for later use.

Animal model establishment and treatment

Lewis lung carcinoma cell line was cultivated in a cell culture dish with a radius of 5 cm. RPMI1640 culture medium including 10% FBS, 1% 100 mg/L streptomycin and 1% 100 mg/L penicillin was cultivated with constant temperature, constant humidity and with 5% CO_2, and the culture medium was changed every other day. After adherent growth, the cells were subcultured when reaching 75% of the bottom area of the culture dish. After a certain amount, Lewis lung carcinoma cells in logarithmic growth stage were digested, centrifuged and counted, and then re-suspended to prepare cell suspension with 5×10^6 cells/ml. Then, 0.2 ml Lewis lung carcinoma cell suspension was injected into the right armpit of the mice in model group and Shiquan Yuzhen Decoction group to establish Lewis lung carcinoma bearing mouse model. Nude mice in blank group were not injected with cells. Sixty-five mice were divided into two experimental samples (the first 40 mice were observed for weight changes and tumor tissues were collected, and the remaining 25 mice were observed for organ index changes), which were divided into blank control group, model group and low, medium and high dose groups of Shiquan Yuzhen

Decoction, with 8 or 5 mice in each group. Mice in Shiquan Yuzhen Decoction group and model group were inoculated with Lewis lung carcinoma cells in armpit, and were administered by gavage after successful model establishment. According to the "Equivalent dose ratio table converted by body surface area between human and animal", the model group was given 0.2 ml/of normal saline, the low dose group was given 8.7 g/kg daily, the middle dose group was given 17.4 g/kg daily, and the high dose group was given 34.8 g/kg daily. The mice in the model group and Shiquan Yuzhen Decoction groups applied intragastric administration once a day for 17 consecutive days, while the blank control group was not intervened. After 24 hours of the last administration, the mice were executed, and the subcutaneous transplanted tumor of the mice was quickly cut out with ophthalmic scissors, weighed and the tumor volume and tumor inhibition rate were obtained (tumor volume formula: $V = 1/2 \times a^2 \times b$, tumor inhibition rate calculation formula: (average tumor weight of model group-average tumor weight of Shiquan Yuzhen Decoction group)/ average tumor weight of model group × 100). Hair glossiness and softness, mental state, activity, diet, sleep and aggregation of mice in each group were observed every day, and the weight of mice was recorded every other day, and the curve of body mass change was visualized. The mice were executed 24 h after the last administration. The spleen and thymus tissues were cut out with ophthalmic scissors and weighed on an electronic microbalance. The spleen index and thymus index were calculated according to the formula of organ index (mg/g) = organ weight (mg)/body weight (g). This study was approved by the welfare and ethics committee of experimental animals in Shanghai University of Traditional Chinese Medicine.

Elisa

In this study, IL-6, TNF-α, t-PA, PAI-1 and FVii in tumor tissue or serum were detected by Elisa, and the detection steps were carried out according to the kit instructions.

TUNEL

In this study, TUNEL method was used to detect the apoptosis of mouse tumor tissues, which was briefly described as follows. The collected tumor tissues were fixed with 4% paraformaldehyde for 24 hours and embedded in paraffin to make sections. Paraffin sections were taken out and dewaxed in xylene. Gradient dehydration was carried out, 20 μg/ml protease K working solution and endogenous peroxidase strong blocking solution were cultivated for 20 min at room temperature. A 50 ul of biotin labeled solution was incubated at 37°C for 1 h in the dark. Labeled reaction stop solution was added and placed at room temperature for 10 min. A 50 ul of Streptavidin-HRP working solution was cultivated at room temperature for 30 min. Color developing solution was applied to observe the tissues under a microscope. Ten fields of vision were obtained under high magnification (× 400), and the number of apoptotic cells per unit was calculated.

Western blot

Total protein was extracted from tumor tissues of nude mice by RIP analysis lysis buffer, and the protein concentration was detected by BCA kit. A 50 μg of the protein was moved on sodium dodecyl sulfate polyacrylamide gel, and then moved into polyvinylidene fluoride membrane by wet transfer method. The membrane was sealed with 5% skimmed milk at room temperature for 1 h, and then sealed with the target (VEGFA 1:500, HIF-1α 1:500) at 4°C overnight. β-actin was applied as an internal reference. Next, the membrane was incubated with horseradish peroxidase labeled goat anti-rabbit secondary antibody (1:3000) for IgG H&L for 1 h. ECL kit was used for development, and Image J software was used for analysis.

Detection of apoptosis-related protein activity

Caspase-3, -8, -9 protein activity detection kit was used for detection. The collected subcutaneous transplanted tumor tissues were frozen in liquid nitrogen and placed in a refrigerator at -80°C for later use. RIP was used to crack the tissues, followed by homogenization. The BCA kit was used to adjust the protein concentration. In a 96-well plate, 50 ul of sample to be detected, 40 ul of detection buffer and 10 ul of Ac-DEVD-pNA (2 mm) were added to each well, mixed evenly, and incubated overnight at 37°C in the dark. Blank control was set according to the instructions. The absorbance at 405 nm was determined by spectrophotometer.

Immunohistochemical method

Paraffin sections were put into xylene and absolute ethanol for dewaxing, antigen repair and sealing. After blocking, BSA blocking solution was gently shaken off. CD31 (CD31 diluted 1:1000), CD8 (CD8 diluted 1:1000) and Anti-FOXP3 (FOXP3 diluted 1:1000) were added on the slice, placed at 4°C overnight. Secondary antibody (1:400) was put in and reacted for 1 h at room temperature in dark environment. DAPI dye solution was added dropwise, and placed for 10 min at room temperature away from light. And finally, these were sealed. The slices were counted according to Weidner evaluation standard, The microvessel density of each immunofluorescence section was observed under a low power microscope (× 40). After randomly selecting the most representative range of 10 microvessels, the number of microvessels in each range was observed and counted under the high power microscope (× 200 or × 400), and the average value was taken as the MVD value.

Statistical methods

The experimental results were expressed in ($\bar{x}$ ± s) and processed by SPSS23.0. One-way ANOVA analysis was applied between groups. Under the condition of satisfying normal distribution and homogeneous variance, independent sample t test was adopted between any two groups. If the variance was uneven, the corrected variance analysis was adopted. If it did not conform to the normal distribution, the Kruskal-Wallis H method of nonparametric test was adopted, and $P < 0.05$ means that the difference is statistically significant.

Results

Main activity formation and target prediction of Shiquan Yuzhen Decoction

Through database search and literature search, the duplicate items and chemical components without target points were removed, and 117 kinds of active components of Shiquan Yuzhen Decoction with OB > 30% and DL > 0.18 were found (Table S1), and 269 corresponding target points were obtained (Table S2), among which calcium carbonate and calcium phosphate, the main components of Os Draconis and Oyster, were eliminated because there were no effective targets. Then, we searched in Genecards, TTD, OMIM and DisGenet databases, and found 4082 expressed genes related to NSCLC diseases. We visualized Venn diagrams from 269 targets corresponding to the active ingredients of Shiquan Yuzhen Decoction, and found 188 intersecting differences with NSCLC related expressed genes (**Figure 1A**). Then, in order to further analyze the relationship between targets and main active ingredients, we selected the main active ingredients with a Degree more than twice the median for network topology, and screened out 26 active ingredients (Table S3). Then, according to the screened active ingredients and targets, a network diagram of "drug-target-disease" was constructed (**Figure 1B**).

Enrichment analysis of potential targets of Shiquan Yuzhen Decoction

In the above exploration, we identified the latent targets of Shiquan Yuzhen Decoction. In order to further analyze the mechanism of Shiquan Yuzhen Decoction in lung carcinoma, we respectively analyzed the biological function and signal pathway enrichment of 182 core target genes corresponding to 26 selected key active ingredients, and obtained 134 entries of biological processes by GO analysis, including 98 entries related to biological processes. The top 10 entries of biological processes according to the total number of genes mainly involved the positive regulation of RNA polymerase promoter II transcription, the negative regulation of DNA transcription template and apoptosis process (**Figure 2A-C**). KEGG analysis showed that 62 qualified KEGG pathways were obtained. Combined with the literature, 15 signaling pathways related to NSCLC diseases were screened out. Enriched signal pathways were mostly related to apoptosis, inflammation and angiogenesis (**Figure 2D**). It was suggested that Shiquan Yuzhen Decoction may treat non-small cell lung carcinoma by improving immunity, inhibiting angiogenesis and promoting apoptosis. At the end of the study, we visualized PPI network according to the predicted potential target genes (**Figure 3A**), in which 182 nodes contained 844 edges, and the top 30 key nodes were screened for display (**Figure 3B**). Among them, protein kinase (AKT1), signal transduction and transcription activator (STAT3), vascular endothelial growth

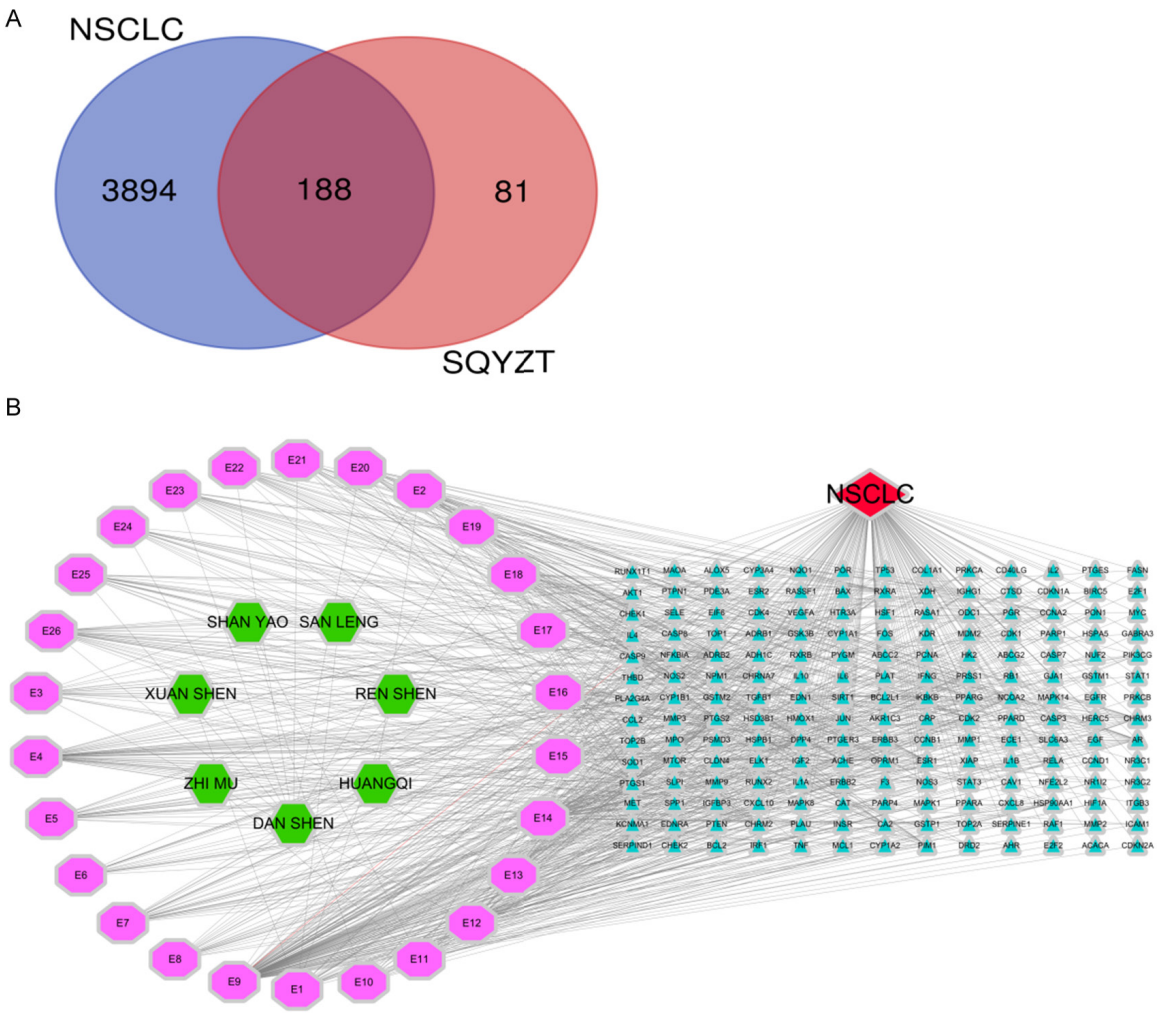

Figure 1. Activity formation and potential target prediction of Shiquan Yuzhen Decoction. A. Venn diagrams were visualized to analyze the common potential targets of NSCLC disease-related expressed genes and Shiquan Yuzhen Decoction. B. The network diagram of "drug-target-disease" was visualized by cytoscape software (orange diamond represents NSCLC, green hexagon represents effective composition of Shiquan Yuzhen Decoction, pink hexagon represents 26 key active components of Shiquan Yuzhen Decoction, and blue triangle represents potential target).

factor (VEGFA, EGFR) and interleukin (IL-2, IL-4, IL-6) of Shiquan Yuzhen Decoction acting in NSCLC targets had a high effect, suggesting that these target proteins act in the treatment of NSCLC.

Shiquan Yuzhen Decoction can hinder tumor forming in tumor-bearing mice

Through the above research, we identified the potential mechanism of Shiquan Yuzhen Decoction in the treatment of lung carcinoma. In order to further prove the role of Shiquan Yuzhen Decoction in LC treatment, we established C57BL/6 mouse model and used different doses of Shiquan Yuzhen Decoction for treatment. Through experiments, we observed that, except the blank control group, the model group and Shiquan Yuzhen Decoction groups could touch the subcutaneous tumor on the third day after subcutaneous inoculation, and the tumor volume gradually increased with time. In the first 9 days after modeling, the growth rate of tumor volume of tumor-bearing mice in model group and Shiquan Yuzhen Decoction groups was decreased, and there was no obvious difference among the groups. After modeling for 9 days, the growth rate of tumor volume of mice in each group was faster than before (**Figure 4A**). After the last administration, the mice were executed, and the tumor tissues were obtained and detected. Compared

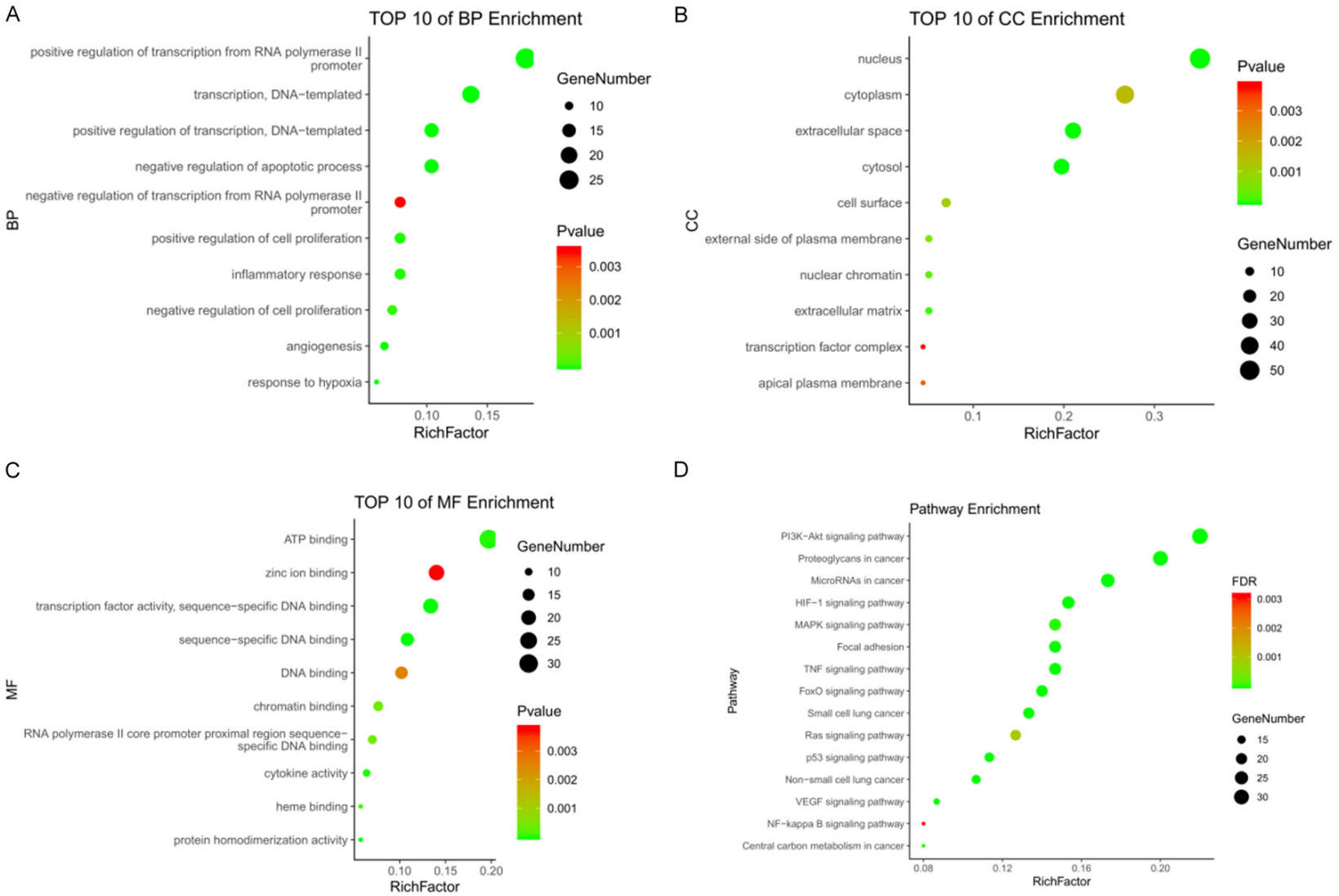

Figure 2. Analysis results of GO and KEGG. A-C. Functional analysis of 182 potential target genes by GO enrichment, including Biological Process (BP), Cellular Component (CC) and Molecular Function (MF). D. KEGG enrichment was used to analyze the potential signal pathways of 182 potential target genes.

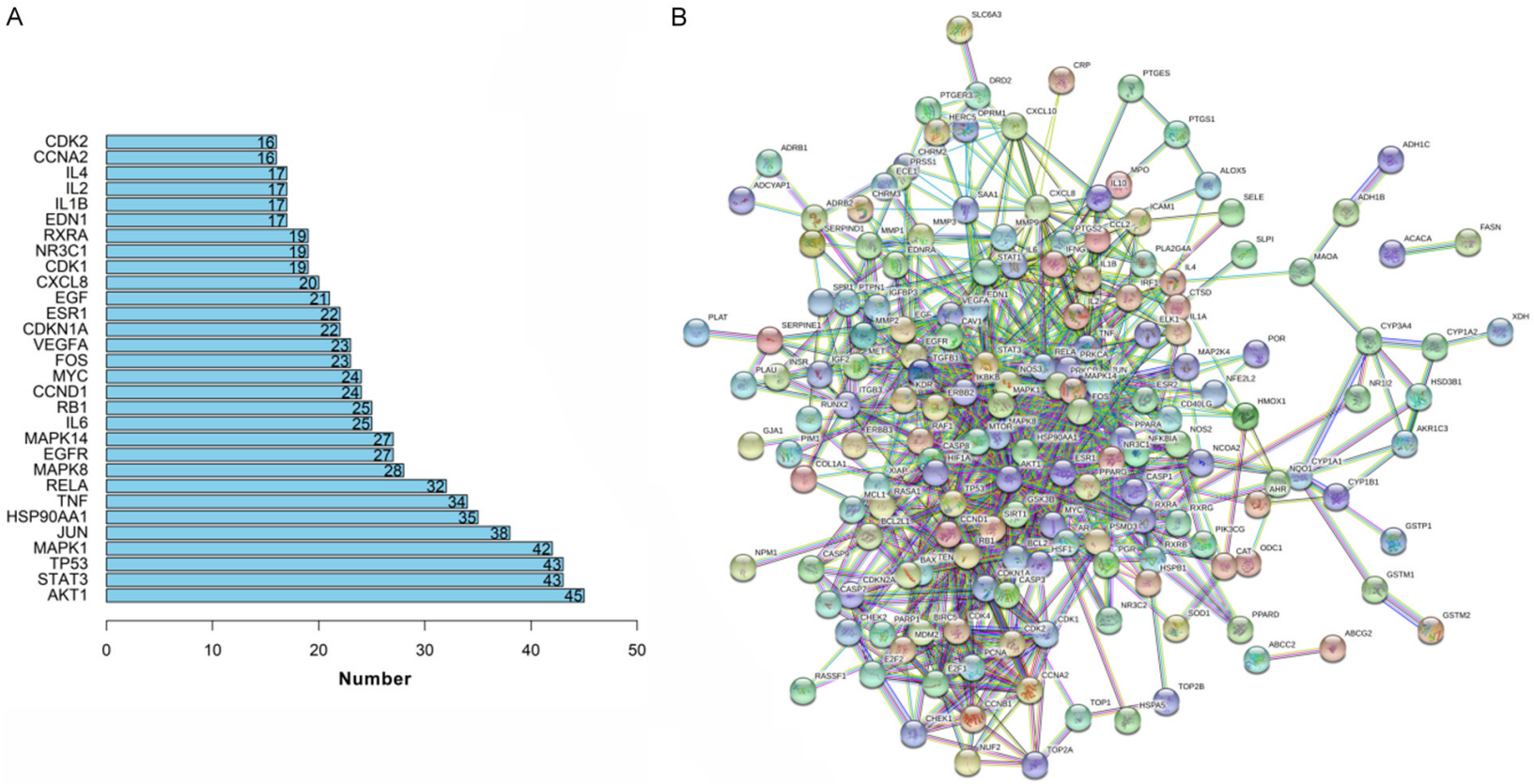

Figure 3. Analysis results of PPI. A. PPI was applied to filter the top 30 key nodes, and the numbers in the figure represent the number of intersecting edges. B. PPI network diagram.

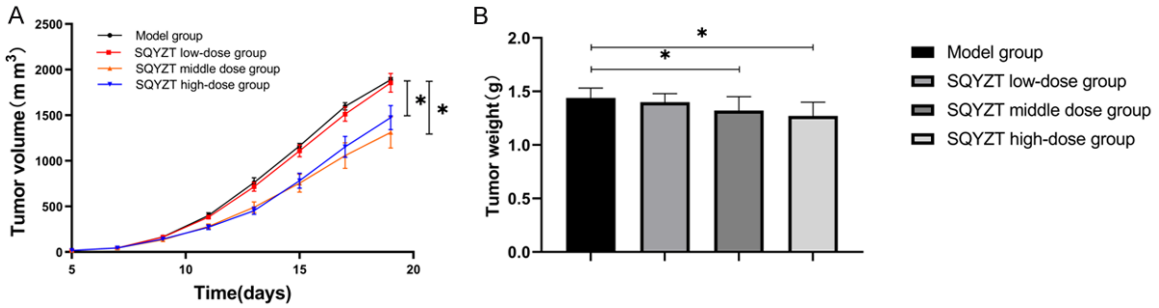

Figure 4. Shiquan Yuzhen Decoction inhibits tumor growth in tumor-bearing mice. A. Tumor growth of tumor-bearing mice after modeling. B. Detection of tumor quality in tumor bearing mice after the last Administration * indicates $P < 0.05$.

with the model group, the weight of subcutaneous transplanted tumor in the middle and high dose groups of Shiquan Yuzhen Decoction was lighter, but there was no difference compared with the low dose group (**Figure 4B**). In addition, the calculation showed that the tumor inhibition rates of low, middle and high dose groups of Shiquan Yuzhen Decoction were 2.43%, 8.43% and 11.74% respectively, indicating that Shiquan Yuzhen Decoction had a good effect on inhibiting tumor growth.

Shiquan Yuzhen Decoction promotes apoptosis of tumor tissue

Through observation and measurement, we found that Shiquan Yuzhen Decoction had a good effect on inhibiting tumor growth. Combined with network pharmacology, we analyzed the medicines and found that the effective components of Shiquan Yuzhen Decoction can directly act on apoptosis-related pathways of NSCLC, thus inducing tumor cells to produce apoptosis. In order to verify our hypothesis, the apoptosis of tumor tissue was detected by Tunel method. The results revealed that compared with the model group, the apoptosis of subcutaneous transplanted tumor tissues of tumor-bearing mice in the low Shiquan Yuzhen Decoction group increased slightly, and that in the middle and high-dose groups was evidently higher than that in the model group (**Figure 5A**). In addition, we also detected the expression of apoptosis-related proteins in tumor tissues. Compared with the model group, the activities of Caspase-3, -8 and -9 in subcutaneously transplanted tumor cells of tumor-bearing mice in the middle and high dose groups of Shiquan Yuzhen Decoction were evidently enhanced, and the activities of Caspase-3 and -9 in subcutaneously transplanted tumor cells of tumor-bearing mice in the low dose group of Shiquan Yuzhen Decoction were evidently increased (**Figure 5B**), suggesting that Shiquan Yuzhen Decoction could induce apoptosis of lung carcinoma tissues and play a role in inhibiting carcinoma.

Shiquan Yuzhen Decoction can inhibit tumor angiogenesis

Angiogenesis, as a difficult issue in LC treatment, puzzles clinicians. We found that Shiquan Yuzhen Decoction could regulate HIF-1 signal pathway and VEGF signal pathway, so we speculated that Shiquan Yuzhen Decoction may inhibit the expression of angiogenesis-related proteins to achieve the purpose of inhibiting tumor angiogenesis. At first, we detected the expression of CD31 in tumor tissues of mice. CD31 in subcutaneous transplanted tumor tissues of model group was evidently higher than that of Shiquan Yuzhen Decoction in middle and high dose groups, while the expression of CD31 in tumor tissues of low dose group was slightly lower than that of model group, but higher than that of middle and high dose groups (**Figure 6A**). In addition, MVD count showed that compared with the model group, the MVD in the middle and high dose groups of Shiquan Yuzhen Decoction was evidently lower (**Figure 6B**). Compared with the model group, the Western Blot indicated that Shiquan Yuzhen Decoction could evidently inhibit the expression of VEGFA and HIF-1a protein in subcutaneous transplanted tumor (**Figure 6C**), which suggested that Shiquan Yuzhen Decoction could effectively inhibit tumor angiogenesis.

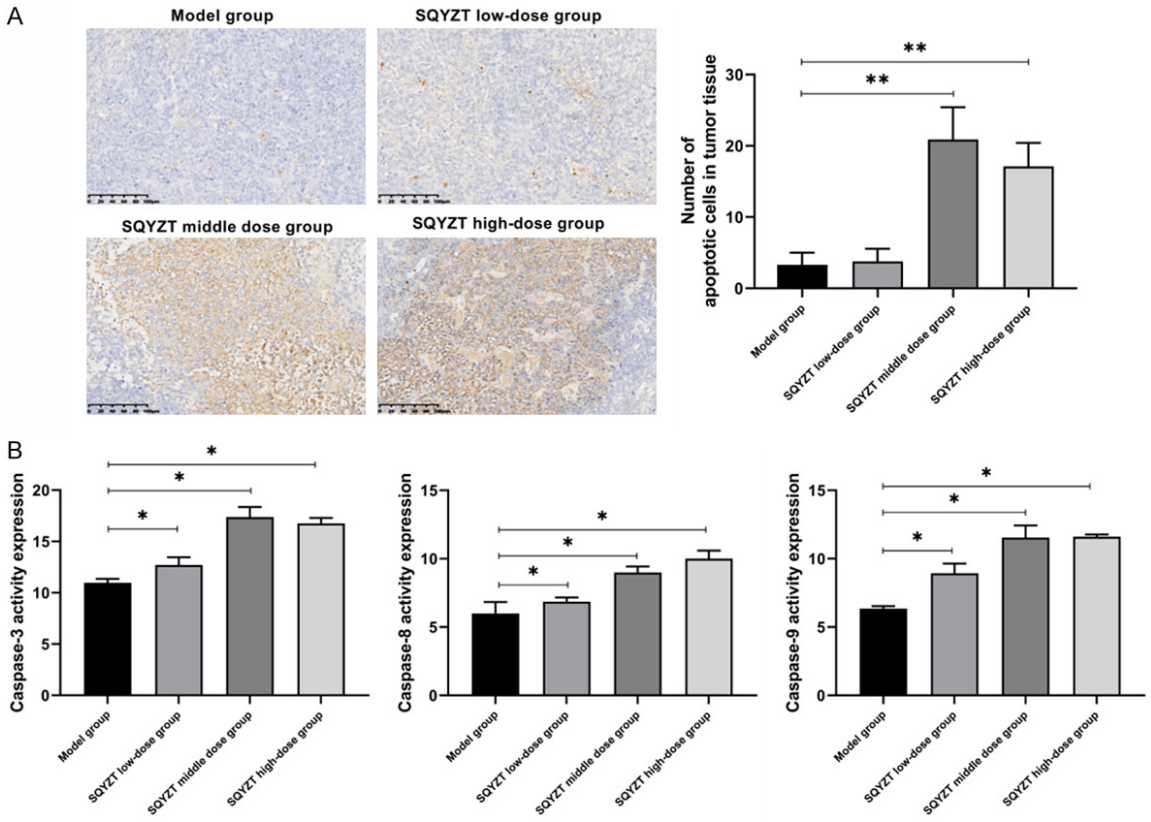

Figure 5. Shiquan Yuzhen Decoction promotes tumor apoptosis. A. Apoptosis of tumor tissue was detected by Tunel method. B. Caspase protein activity detection kit was used to detect Caspase-3, -8 and -9 activities in tissues. * indicates $P < 0.05$; ** indicates $P < 0.01$.

Shiquan Yuzhen Decoction can improve the immunity of tumor-bearing mice and prevent the metastasis of lung malignant tumor

At the end of the study, in order to further understand the immunity of Shiquan Yuzhen Decoction on tumor-bearing mice and prevent the metastasis of lung malignant tumor, we observed the behavior and weight of mice, and found that the blank control group mice were in good mental state, active and normal diet, and the weight showed a slow growth trend. On the third day after planting tumor, mice in other groups could touch subcutaneous tumor, and had low spirits, decreased food intake, sluggish action, lacked of luster of hair, and were conditioned to curling and gathering. In addition, the weight of tumor-bearing mice in the model group and Shiquan Yuzhen Decoction groups decreased evidently on the fourth day after modeling, but gradually returned to normal with time (**Figure 7A**). We also measured the immune organ index of mice. We found that compared with the blank group, the spleen index and thymus number of the tumor-bearing mice in the model group and Shiquan Yuzhen Decoction group were evidently higher. Compared with the model group, the spleen index of tumor-bearing mice in the middle and high dose groups of Shiquan Yuzhen Decoction was evidently increased (**Figure 7B**). Moreover, we found by Elisa that the expression of IL-6 in subcutaneous transplanted tumor tissues of tumor-bearing mice in the middle and high dose groups of Shiquan Yuzhen Decoction was evidently decreased, while the expression of TNF-α in serum of tumor-bearing mice in the middle and high dose groups of Shiquan Yuzhen Decoction was increased compared with the model group (**Figure 7C**). And we also found through comparison that the middle and high concentration of Shiquan Yuzhen Decoction significantly inhibited tumor growth in mice Effect (**Figure 7D**). In addition, we detected the expression of CD8+T and Treg (FOXP3) cells in mouse tumor tissues by IHC experiment. The results showed

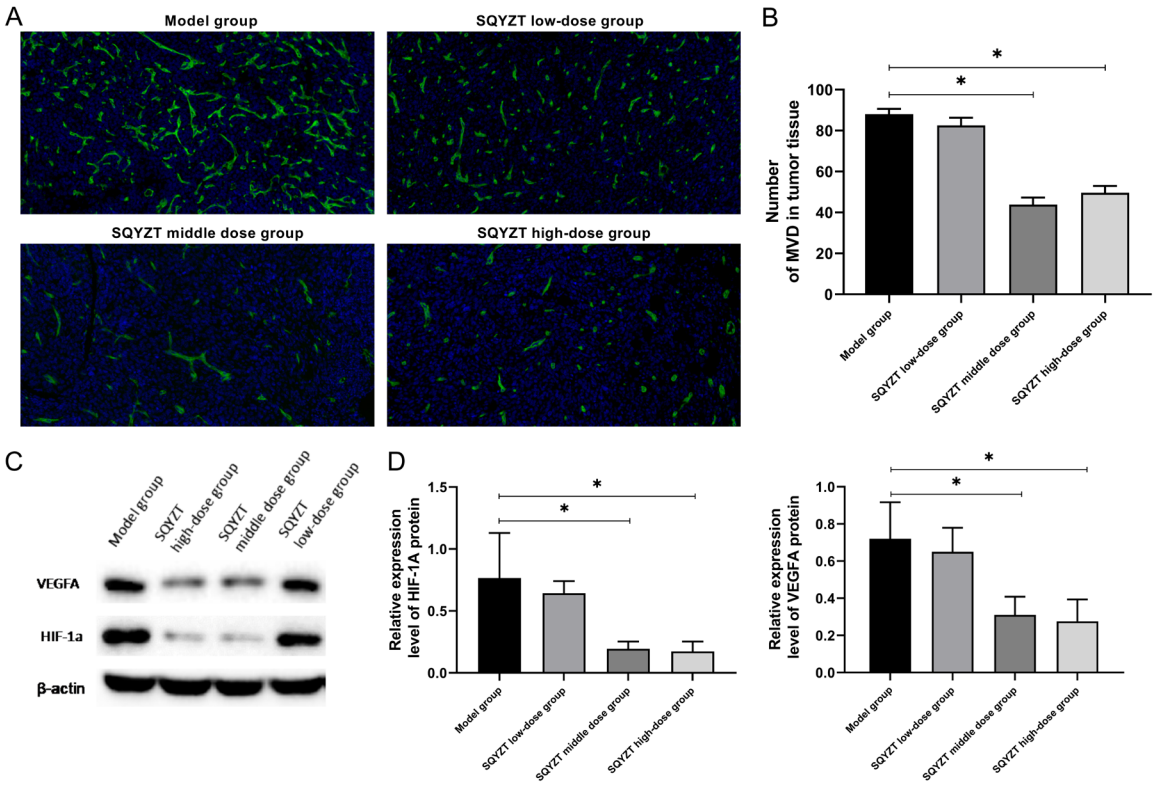

Figure 6. Effect of Shiquan Yuzhen Decoction on tumor angiogenesis. A. Effect of Shiquan Yuzhen Decoction on CD31 in tumor tissue was detected by immunofluorescence staining. B. Effect of Shiquan Yuzhen Decoction on MVD in tumor tissue was detected by MVD counting. C, D. Effect of Shiquan Yuzhen Decoction on VEGFA, HIF-1A in tumor tissue was detected by WB. * indicates $P < 0.05$.

that CD8+T positive rate in mice increased significantly with the increase of drug concentration, while FOXP3 positive rate in mice decreased gradually with the increase of drug concentration (**Figure 7E**). Finally, we also detected the factors related to coagulation and fibrinolysis in tumor-bearing mice. Compared with the blank group, PAI-1 was increased in the model group and the middle and low dose groups of Shiquan Yuzhen Decoction, and the expression of FVii was higher in the model group and the high and low dose groups of Shiquan Yuzhen Decoction. Compared with the model group, PAI-1 and FVii in plasma of mice in the middle and high dose groups of Shiquan Yuzhen Decoction decreased evidently (**Table 1**).

Discussion

The characteristic medical theory of Chinese medicine has been formulated and developed for thousands of years, and a variety of traditional Chinese medicines are combined with each other in a complex way to produce synergistic effect to improve the clinical curative effect [28]. The holistic view of TCM focuses on the recovery of overall function and the elimination of etiology. In recent years, there are many similarities between the proposal of network pharmacology and the basic theory of Chinese medicine [29]. Therefore, the network pharmacology can be applied to the research of Chinese medicine, and its compound prescription can be applied to explore the main components and possible mechanism of action of Chinese medicine and its compound prescription on diseases.

In this study, 26 key active ingredients and their corresponding 182 active targets were screened out, and the target network of active ingredients of Shiquan Yuzhen Decoction was constructed. The results showed that most of the single active ingredients of Shiquan Yuzhen Decoction can affect multiple targets, such as quercetin [30], luteolin [31] and kaempferol

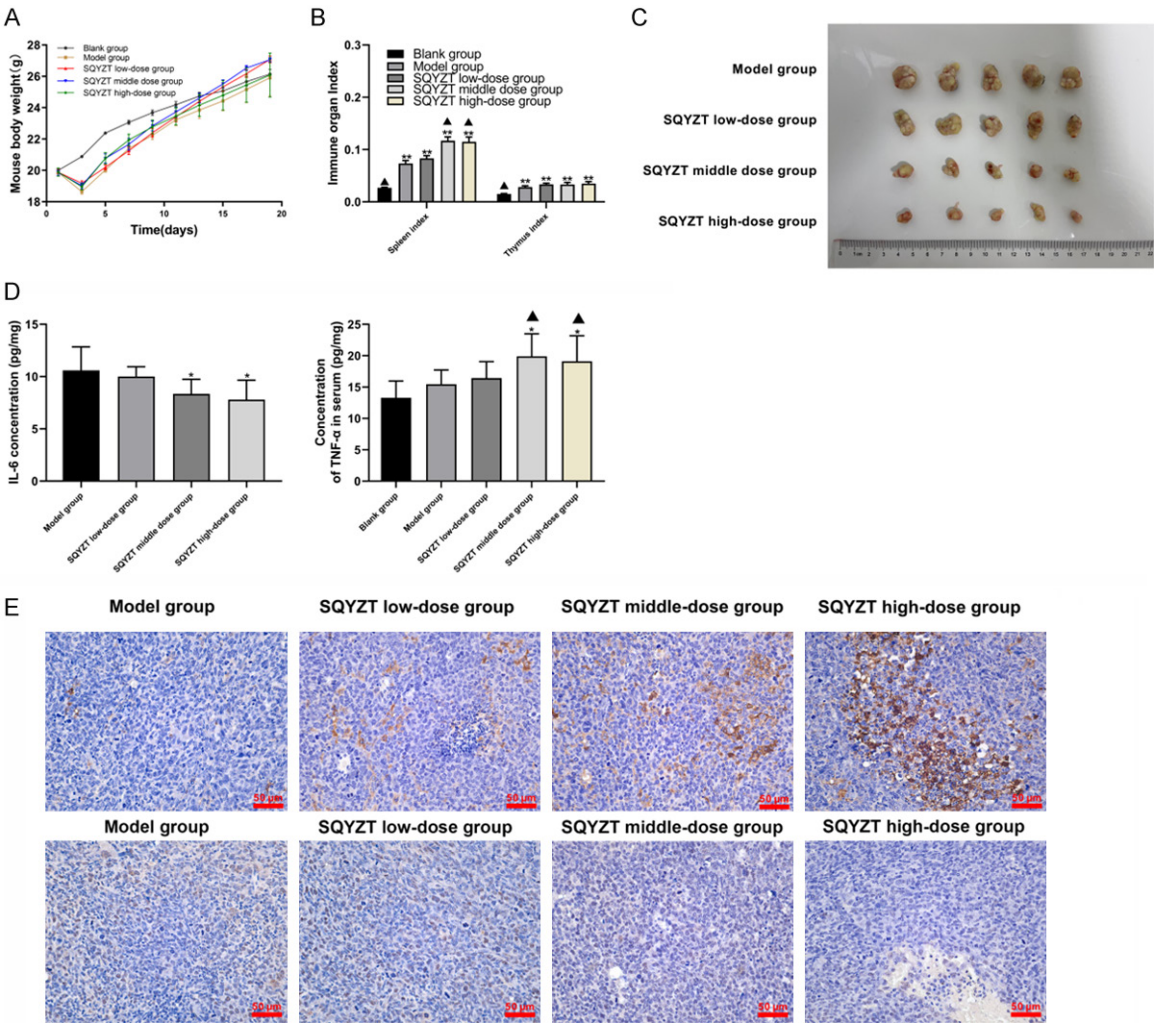

Figure 7. Effect of Shiquan Yuzhen Decoction on immunity and metastasis of malignant tumor in tumor-bearing mice. A. Effect of Shiquan Yuzhen Decoction on the body weight of tumor-bearing mice. B. Effect of Shiquan Yuzhen Decoction on the weight of immune organs in tumor-bearing mice. C. Comparison of tumor volumes collected after the mice were sacrificed. D. Effect of Shiquan Yuzhen Decoction on IL-6 in tumor tissue and TNF-α in serum of tumor-bearing mice. E. The expression of CD8+T and Treg(FOXP3) cells in mouse tumor tissues was detected by IHC test (400×). * indicates compared with the blank group, $P < 0.05$, and ▲ indicates compared with the model group, $P < 0.05$.

Table 1. Effect of SQYZT on the expression of t-PA, PAI-1 and FVii in plasma of tumor-bearing mice ($x \pm s$, $n = 8$)

Group	t-PA (ng/ml)	PAI-1 (ng/ml)	FVii (IU/ml)
Blank group	14.20±0.713	1.501±0.267▲	3.2290±0.5696▲
Model group	15.904±1.216	2.249±0.416*	4.6983±0.7120*
SQYZT low dose group	16.095±0.927	2.218±0.399*	4.3936±0.4950*
SQYZT medium dose group	17.586±2.197	1.869±0.145*,▲	3.8491±0.4348▲
SQYZT high dose group	17.544±1.323	1.806±0.284▲	4.0054±0.6033*,▲

Note: * indicates compared with the blank group, $P < 0.05$, and ▲ indicates compared with the model group, $P < 0.05$.

[32], which all played an ideal role in anti-tumor. Although putative targets in each single active ingredient are different, there are many overlapping targets in different active ingredients, and their coordinated action has produced immunomodulation, carcinoma cell apoptosis

promotion, tumor cell metastasis inhibition and tumor angiogenesis inhibition characteristics [33]. In addition, we enriched the predicted 182 targets, and found that Shiquan Yuzhen Decoction was involved in regulating the biological processes of cell proliferation, angiogenesis, gene expression and apoptosis [34]. The treatment of NSCLC may also influence some cell components and molecular functions, including nuclear matter, nucleus, cytoplasm, protein binding, enzyme binding and DNA binding [35]. Through KEGG enrichment analysis, a total of 15 NSCLC-related KEGG pathways containing PI3K-Akt signal pathway [36] and HIF-1 signal pathway [37] were evidently enriched. These signal pathways were mostly related to apoptosis, inflammation, proliferation, metastasis and angiogenesis. Finally, through PPI network analysis, we found that the core targets of Shiquan Yuzhen Decoction in treating NSCLC mainly focused on apoptosis, inflammation, angiogenesis, proliferation and cell cycle [38]. This suggested that Shiquan Yuzhen Decoction may improve the occurrence of NSCLC by regulating apoptosis and angiogenesis in related ways.

Over proliferation of cells and obstruction of apoptosis are important reasons for tumor formation. The formation of tumor microvessels provides a channel for nutrient transport of tumor cells, which greatly accelerates the proliferation and metastasis of tumor cells. In conclusion, tumor apoptosis and tumor angiogenesis act in judging malignant tumors [39, 40]. In order to verify the results of biological information analysis, we established the LC tumor-bearing mouse model. Through observation, we found that the medium and high doses of Shiquan Yuzhen Decoction could evidently hinder the growth of subcutaneous transplanted tumor in tumor-bearing mice, increase the incidence of apoptosis of tumor cells, and evidently increase the active expression of Caspase-3, Caspase-8 and Caspase-9. In addition, our experiment also found that Shiquan Yuzhen Decoction with medium and high dose concentration could evidently hinder the formation of blood vessels in transplanted tumor tissues, and reduce the expression of HIF-1a and downstream VEGFA in tissues. It showed that Shiquan Yuzhen Decoction had a good effect on inhibiting the formation of tumor microvessels. It was suggested that Shiquan Yuzhen Decoction could inhibit angiogenesis by promoting apoptosis of tumor cells, thus improving the occurrence of LC.

Tumor patients, whose physique is weak, suffer some damage to their immune function. Therefore, in the course of treatment, they should not only obtain anti-carcinoma effect, but also take care of the improvement of patients' quality of life and immune function [41]. In network pharmacology analysis, we predicted that TNF [42] and NF-kappa B [43] were the two main signal pathways of Shiquan Yuzhen Decoction. Therefore, at the end of the study, we analyzed the effects of Shiquan Yuzhen Decoction on immune function of tumor-bearing mice. Thymus is the place where T cells differentiate, develop and mature, and it is an important lymphoid organ [44]. Spleen is mainly involved in humoral immunity, which is the center of cellular immunity and humoral immunity and the largest immune organ of the body [45]. Both of them act in phagocytosis of tumor cells and clearance of necrotic tissues [46]. Through behavioral observation and immune organ index measurement, we found that Shiquan Yuzhen Decoction could improve the mental state and diet of tumor-bearing mice, maintain the body weight of mice in a state of continuous growth, and improve the spleen index of mice. Elisa revealed that Shiquan Yuzhen Decoction could reduce the expression of IL-6 in tumor tissue and increase the expression of TNF-α in serum. We speculated that Shiquan Yuzhen Decoction could improve the immune function, promote the release of TNF-α from NK cells and T cells, and play an anti-tumor role. As HIF-1a protein in tumor tissue was inhibited, IL-6 downstream of HIF-1a protein gene was also inhibited, so the content and expression of IL-6 in subcutaneous transplanted tumor tissue of tumor bearing mice in medium and high dose Shiquan Yuzhen Decoction groups were lower than those in model group.

Patients with malignant tumors often suffer from vascular endothelial cell damage due to stimulation of tumor cells, radiotherapy and chemotherapy, surgery and other factors, thus leading to hypercoagulable state [47]. Once the blood hypercoagulable state appears in malignant tumor, it can further promote the metastasis of tumor cells and thrombosis of the body,

and further aggravate the occurrence of hypercoagulable state [48]. Therefore, improving the coagulation status of malignant tumor patients can effectively prevent the metastasis of lung malignant tumor and prolong the life of tumor patients. In this study, the coagulation-related factors of tumor-bearing mice were also tested. The results revealed that t-PA in plasma of tumor-bearing mice in model group was no different from that in blank group, but FVI and PAI-1 were higher than those in blank group, indicating that tumor cells still had some influence on the coagulation of mice, while the expressions of FVI and PAI-1 in plasma of tumor-bearing mice in middle and high doses of Shiquan Yuzhen Decoction were evidently lower than those in model group. Therefore, we considered that Shiquan Yuzhen Decoction with a certain concentration can improve the hypercoagulability caused by tumor factors.

In the above research, we have basically determined the relevant mechanism of Shiquan Yuzhen Decoction in LC treatment, but there are still some shortcomings in this study. First, as a basic experiment, the application of Shiquan Yuzhen Decoction in clinic is less, which lacks accurate and sufficient clinical data support. Secondly, this study failed to make an in-depth study on the prevention and treatment of different stages of NSCLC with different concentrations of Shiquan Yuzhen Decoction. The interaction among immune function, angiogenesis, apoptosis and other related proteins in the progression of non-small cell lung carcinoma has not been discussed in depth. Therefore, we hope to carry out clinical research and related basic research in future to improve our experimental conclusions.

To sum up, Shiquan Yuzhen Decoction can evidently improve the quality of life of Lewis lung carcinoma-bearing mice and inhibit tumor growth in mice, which is a potential clinical treatment plan.

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Disclosure of conflict of interest

None.

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Table S1. Target screening

herb	pharmaceutical ingredients	No.	Gene
common buried rubber	trans-gondoic acid	C1	PTGS1
	trans-gondoic acid	C1	NCOA2
	trans-gondoic acid	C1	CHRM1
	trans-gondoic acid	C1	PTGS2
	trans-gondoic acid	C1	GABRA2
	trans-gondoic acid	C1	GABRA1
	trans-gondoic acid	C1	CHRNA7
	trans-gondoic acid	C1	GABRA6
	hederagenin	C2	PGR
	hederagenin	C2	NCOA2
	hederagenin	C2	CHRM3
	hederagenin	C2	CHRM1
	hederagenin	C2	GABRA2
	hederagenin	C2	GABRA3
	hederagenin	C2	CHRM2
	hederagenin	C2	ADRA1B
	hederagenin	C2	GABRA1
	hederagenin	C2	GRIA2
	hederagenin	C2	GABRA6
	hederagenin	C2	GABRA5
	hederagenin	C2	IGHG1
	hederagenin	C2	ADH1B
	hederagenin	C2	ADH1C
	hederagenin	C2	LYZ
	hederagenin	C2	COBT
	hederagenin	C2	PTGS1
	hederagenin	C2	SCN5A
	hederagenin	C2	PTGS2
	hederagenin	C2	RXRA
	hederagenin	C2	PDE3A
	hederagenin	C2	SLC6A2
	hederagenin	C2	NOR51B
	beta-sitosterol	C3	PGR
	beta-sitosterol	C3	NCOA2
	beta-sitosterol	C3	PTGS1
	beta-sitosterol	C3	PTGS2
	beta-sitosterol	C3	HSP90AA1
	beta-sitosterol	C3	PIK3CG
	beta-sitosterol	C3	KCNH2
	beta-sitosterol	C3	KAPCA
	beta-sitosterol	C3	DRD1
	beta-sitosterol	C3	CHRM3
	beta-sitosterol	C3	CHRM1
	beta-sitosterol	C3	SCN5A
	beta-sitosterol	C3	GABRA2
	beta-sitosterol	C3	CHRM4
	beta-sitosterol	C3	PDE3A
	beta-sitosterol	C3	HTR2A
	beta-sitosterol	C3	GABRA5
	beta-sitosterol	C3	ADRA1A
	beta-sitosterol	C3	GABRA3
	beta-sitosterol	C3	CHRM2
	beta-sitosterol	C3	ADRA1B
	beta-sitosterol	C3	ADRB2
	beta-sitosterol	C3	CHRNA2
	beta-sitosterol	C3	SLC6A4

beta-sitosterol	C3	OPRM1
beta-sitosterol	C3	GABRA1
beta-sitosterol	C3	CHRNA7
beta-sitosterol	C3	NOR51B
beta-sitosterol	C3	BCL2
beta-sitosterol	C3	BAX
beta-sitosterol	C3	CASP9
beta-sitosterol	C3	JUN
beta-sitosterol	C3	CASP3
beta-sitosterol	C3	CASP8
beta-sitosterol	C3	PRKCA
beta-sitosterol	C3	TGFB1
beta-sitosterol	C3	PON1
beta-sitosterol	C3	MAP2
formononetin	C4	NOS2
formononetin	C4	PTGS1
formononetin	C4	CHRM1
formononetin	C4	ESR1
formononetin	C4	AR
formononetin	C4	PPARG
formononetin	C4	PTGS2
formononetin	C4	RXRA
formononetin	C4	PDE3A
formononetin	C4	ADRA1A
formononetin	C4	SLC6A3
formononetin	C4	ADRB2
formononetin	C4	SLC6A4
formononetin	C4	ESR2
formononetin	C4	DPP4
formononetin	C4	MAPK14
formononetin	C4	GSK3B
formononetin	C4	HSP90AA1
formononetin	C4	CDK2
formononetin	C4	MAOB
formononetin	C4	CHEK1
formononetin	C4	KAPCA
formononetin	C4	PRSS1
formononetin	C4	PIM1
formononetin	C4	CCNA2
formononetin	C4	PCP4
formononetin	C4	PKIA
formononetin	C4	SERPIND1
formononetin	C4	NOS3
formononetin	C4	ACHE
formononetin	C4	LACTBL1
formononetin	C4	JUN
formononetin	C4	#N/A
formononetin	C4	IL4
formononetin	C4	SIRT1
formononetin	C4	ATP5B
formononetin	C4	ND6
formononetin	C4	HSD3B2
formononetin	C4	HSD3B1
Stigmasterol	C5	PGR
Stigmasterol	C5	NR3C2
Stigmasterol	C5	NCOA2
Stigmasterol	C5	ADH1C
Stigmasterol	C5	IGHG1

	Stigmasterol	C5	RXRA
	Stigmasterol	C5	NCOA1
	Stigmasterol	C5	PTGS1
	Stigmasterol	C5	PTGS2
	Stigmasterol	C5	ADRA2A
	Stigmasterol	C5	SLC6A2
	Stigmasterol	C5	SLC6A3
	Stigmasterol	C5	ADRB2
	Stigmasterol	C5	AKR1B1
	Stigmasterol	C5	PLAU
	Stigmasterol	C5	LTA4H
	Stigmasterol	C5	MAOB
	Stigmasterol	C5	MAOA
	Stigmasterol	C5	KAPCA
	Stigmasterol	C5	CTRB1
	Stigmasterol	C5	CHRM3
	Stigmasterol	C5	CHRM1
	Stigmasterol	C5	ADRB1
	Stigmasterol	C5	SCN5A
	Stigmasterol	C5	HTR2A
	Stigmasterol	C5	ADRA1A
	Stigmasterol	C5	GABRA3
	Stigmasterol	C5	CHRM2
	Stigmasterol	C5	ADRA1B
	Stigmasterol	C5	GABRA1
	Stigmasterol	C5	CHRNA7
ginseng	Diop	C6	SCN5A
	Diop	C6	ADRB2
	Diop	C6	CHRM3
	Stigmasterol	C5	PGR
	Stigmasterol	C5	NR3C2
	Stigmasterol	C5	NCOA2
	Stigmasterol	C5	ADH1C
	Stigmasterol	C5	IGHG1
	Stigmasterol	C5	RXRA
	Stigmasterol	C5	NCOA1
	Stigmasterol	C5	PTGS1
	Stigmasterol	C5	PTGS2
	Stigmasterol	C5	ADRA2A
	Stigmasterol	C5	SLC6A2
	Stigmasterol	C5	SLC6A3
	Stigmasterol	C5	ADRB2
	Stigmasterol	C5	AKR1B1
	Stigmasterol	C5	PLAU
	Stigmasterol	C5	LTA4H
	Stigmasterol	C5	MAOB
	Stigmasterol	C5	MAOA
	Stigmasterol	C5	KAPCA
	Stigmasterol	C5	CTRB1
	Stigmasterol	C5	CHRM3
	Stigmasterol	C5	CHRM1
	Stigmasterol	C5	ADRB1
	Stigmasterol	C5	SCN5A
	Stigmasterol	C5	HTR2A
	Stigmasterol	C5	ADRA1A
	Stigmasterol	C5	GABRA3
	Stigmasterol	C5	CHRM2
	Stigmasterol	C5	ADRA1B

Stigmasterol	C5	GABRA1
Stigmasterol	C5	CHRNA7
beta-sitosterol	C3	PGR
beta-sitosterol	C3	NCOA2
beta-sitosterol	C3	PTGS1
beta-sitosterol	C3	PTGS2
beta-sitosterol	C3	HSP90AA1
beta-sitosterol	C3	PIK3CG
beta-sitosterol	C3	KCNH2
beta-sitosterol	C3	KAPCA
beta-sitosterol	C3	DRD1
beta-sitosterol	C3	CHRM3
beta-sitosterol	C3	CHRM1
beta-sitosterol	C3	SCN5A
beta-sitosterol	C3	GABRA2
beta-sitosterol	C3	CHRM4
beta-sitosterol	C3	PDE3A
beta-sitosterol	C3	HTR2A
beta-sitosterol	C3	GABRA5
beta-sitosterol	C3	ADRA1A
beta-sitosterol	C3	GABRA3
beta-sitosterol	C3	CHRM2
beta-sitosterol	C3	ADRA1B
beta-sitosterol	C3	ADRB2
beta-sitosterol	C3	CHRNA2
beta-sitosterol	C3	SLC6A4
beta-sitosterol	C3	OPRM1
beta-sitosterol	C3	GABRA1
beta-sitosterol	C3	CHRNA7
beta-sitosterol	C3	NOR51B
beta-sitosterol	C3	BCL2
beta-sitosterol	C3	BAX
beta-sitosterol	C3	CASP9
beta-sitosterol	C3	JUN
beta-sitosterol	C3	CASP3
beta-sitosterol	C3	CASP8
beta-sitosterol	C3	PRKCA
beta-sitosterol	C3	TGFB1
beta-sitosterol	C3	PON1
beta-sitosterol	C3	MAP2
Inermin	C7	PTGS1
Inermin	C7	CHRM3
Inermin	C7	SCN5A
Inermin	C7	PTGS2
Inermin	C7	HTR3A
Inermin	C7	RXRA
Inermin	C7	ADRA1B
Inermin	C7	ADRB2
Inermin	C7	ADRA1D
Inermin	C7	SLC6A4
Inermin	C7	HSP90AA1
Inermin	C7	PIK3CG
Inermin	C7	CHRNA7
Inermin	C7	KAPCA
Inermin	C7	IGHG1
Inermin	C7	PRSS1
Inermin	C7	NCOA1

Inermin	C7	PCP4
kaempferol	C8	NOS2
kaempferol	C8	PTGS1
kaempferol	C8	AR
kaempferol	C8	PPARG
kaempferol	C8	PTGS2
kaempferol	C8	HSP90AA1
kaempferol	C8	PIK3CG
kaempferol	C8	KAPCA
kaempferol	C8	NCOA2
kaempferol	C8	DPP4
kaempferol	C8	PRSS1
kaempferol	C8	PGR
kaempferol	C8	SERPIND1
kaempferol	C8	CHRM1
kaempferol	C8	NOS3
kaempferol	C8	GABRA2
kaempferol	C8	ACHE
kaempferol	C8	SLC6A2
kaempferol	C8	CHRM2
kaempferol	C8	ADRA1B
kaempferol	C8	GABRA1
kaempferol	C8	TOP2B
kaempferol	C8	F7
kaempferol	C8	PCP4
kaempferol	C8	RELA
kaempferol	C8	IKBKB
kaempferol	C8	AKT1
kaempferol	C8	BCL2
kaempferol	C8	BAX
kaempferol	C8	TNF
kaempferol	C8	JUN
kaempferol	C8	AHSA1
kaempferol	C8	CASP3
kaempferol	C8	MAPK8
kaempferol	C8	XDH
kaempferol	C8	MMP1
kaempferol	C8	STAT1
kaempferol	C8	CDK1
kaempferol	C8	#N/A
kaempferol	C8	HMOX1
kaempferol	C8	CYP3A4
kaempferol	C8	CYP1A2
kaempferol	C8	CYP1A1
kaempferol	C8	ICAM1
kaempferol	C8	SELE
kaempferol	C8	VCAM1
kaempferol	C8	NR1I2
kaempferol	C8	CYP1B1
kaempferol	C8	ALOX5
kaempferol	C8	HAS2
kaempferol	C8	GSTP1
kaempferol	C8	AHR
kaempferol	C8	PSMD3
kaempferol	C8	SLC2A4
kaempferol	C8	NR1I3
kaempferol	C8	INSR

kaempferol	C8	DIO1
kaempferol	C8	PPP3CA
kaempferol	C8	PRXC1A
kaempferol	C8	GSTM1
kaempferol	C8	GSTM2
kaempferol	C8	AKR1C3
kaempferol	C8	SLPI
Aposiopolamine	C9	CHRM3
Aposiopolamine	C9	CHRM1
Aposiopolamine	C9	SLC6A2
Aposiopolamine	C9	SLC6A3
Aposiopolamine	C9	ADRB2
Aposiopolamine	C9	SLC6A4
Aposiopolamine	C9	GABRA1
Aposiopolamine	C9	DPP4
Deoxyharringtonine	C10	AR
Deoxyharringtonine	C10	NR3C2
Dianthramine	C11	PTGS1
Dianthramine	C11	PTGS2
Dianthramine	C11	HSP90AA1
arachidonate	C12	PTGS1
arachidonate	C12	PTGS2
arachidonate	C12	RXRG
arachidonate	C12	NCOA2
Frutinone A	C13	PTGS1
Frutinone A	C13	SERPIND1
Frutinone A	C13	AR
Frutinone A	C13	SCN5A
Frutinone A	C13	PPARG
Frutinone A	C13	PTGS2
Frutinone A	C13	RXRA
Frutinone A	C13	PDE3A
Frutinone A	C13	ADRB2
Frutinone A	C13	GABRA1
Frutinone A	C13	DPP4
Frutinone A	C13	HSP90AA1
Frutinone A	C13	PIK3CG
Frutinone A	C13	CHRNA7
Frutinone A	C13	KAPCA
Frutinone A	C13	ACHE
ginsenoside rh2	C14	BAX
ginsenoside rh2	C14	TNF
ginsenoside rh2	C14	CASP3
ginsenoside rh2	C14	PTGS2
ginsenoside rh2	C14	NFKBIA
ginsenoside rh2	C14	IL1B
ginsenoside rh2	C14	CASP1
ginsenoside rh2	C14	IFNG
ginsenoside rh2	C14	ADCYAP1
ginsenoside rh2	C14	PSMG1
ginsenoside rh2	C14	MAP2K4
ginsenoside rh2	C14	SLC2A4
Ginsenoside-Rh4_qt	C15	NR3C2
Ginsenoside-Rh4_qt	C15	NCOA2
Girinimbin	C16	PTGS1
Girinimbin	C16	SCN5A
Girinimbin	C16	PTGS2

	Girinimbin	C16	RXRA
	Girinimbin	C16	ADRB2
	Girinimbin	C16	GABRA1
	Girinimbin	C16	PIK3CG
	Girinimbin	C16	CHRNA7
	Girinimbin	C16	KAPCA
	Girinimbin	C16	NCOA2
	Panaxadiol	C17	NR3C1
	suchilactone	C18	KCNH2
	suchilactone	C18	SCN5A
	suchilactone	C18	FXa
	suchilactone	C18	PTGS2
	suchilactone	C18	F7
	suchilactone	C18	PTPN1
	suchilactone	C18	ADRB2
	suchilactone	C18	HSP90AA1
	suchilactone	C18	NCOA1
	suchilactone	C18	KCNMA1
	suchilactone	C18	PCP4
	suchilactone	C18	PTGS1
	suchilactone	C18	RXRA
	suchilactone	C18	PDE3A
	suchilactone	C18	ADRA1D
	suchilactone	C18	KAPCA
	alexandrin_qt	C19	PGR
	Fumarine	C20	PTGS1
	Fumarine	C20	CHRM3
	Fumarine	C20	KCNH2
	Fumarine	C20	CHRM1
	Fumarine	C20	SCN5A
	Fumarine	C20	FXa
	Fumarine	C20	CHRM5
	Fumarine	C20	PTGS2
	Fumarine	C20	HTR3A
	Fumarine	C20	F7
	Fumarine	C20	CHRM4
	Fumarine	C20	OPRD1
	Fumarine	C20	HTR2A
	Fumarine	C20	ADRA1B
	Fumarine	C20	ADRB2
	Fumarine	C20	ADRA1D
	Fumarine	C20	OPRM1
	Fumarine	C20	HSP90AA1
	Fumarine	C20	KAPCA
	Fumarine	C20	PCP4
	Fumarine	C20	SLC6A4
	Fumarine	C20	CACNA1S
	Fumarine	C20	PDE3A
	Fumarine	C20	SLC6A3
	Fumarine	C20	PDE4
	Fumarine	C20	TOP2B
	Fumarine	C20	DRD1
	Fumarine	C20	KDR
milkvetch root	Mairin	C21	PGR
	Jaranol	C22	NOS2
	Jaranol	C22	PTGS1
	Jaranol	C22	AR

Jaranol	C22	SCN5A
Jaranol	C22	PTGS2
Jaranol	C22	ESR2
Jaranol	C22	DPP4
Jaranol	C22	HSP90AA1
Jaranol	C22	CDK2
Jaranol	C22	CHEK1
Jaranol	C22	PRSS1
Jaranol	C22	NCOA2
Jaranol	C22	PCP4
hederagenin	C2	PGR
hederagenin	C2	NCOA2
hederagenin	C2	CHRM3
hederagenin	C2	CHRM1
hederagenin	C2	GABRA2
hederagenin	C2	GABRA3
hederagenin	C2	CHRM2
hederagenin	C2	ADRA1B
hederagenin	C2	GABRA1
hederagenin	C2	GRIA2
hederagenin	C2	GABRA6
hederagenin	C2	GABRA5
hederagenin	C2	IGHG1
hederagenin	C2	ADH1B
hederagenin	C2	ADH1C
hederagenin	C2	LYZ
hederagenin	C2	COBT
hederagenin	C2	PTGS1
hederagenin	C2	SCN5A
hederagenin	C2	PTGS2
hederagenin	C2	RXRA
hederagenin	C2	PDE3A
hederagenin	C2	SLC6A2
hederagenin	C2	NOR51B
(3S,8S,9S,10R,13R,14S,17R)-10,13-dimethyl-17-[(2R,5S)-5-propan-2-yloctan-2-yl]-2,3,4,7,8,9,11,12,14,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-3-ol	C23	PGR
isorhamnetin	C24	NOS2
isorhamnetin	C24	PTGS1
isorhamnetin	C24	ESR1
isorhamnetin	C24	AR
isorhamnetin	C24	PPARG
isorhamnetin	C24	PTGS2
isorhamnetin	C24	PTPN1
isorhamnetin	C24	ESR2
isorhamnetin	C24	DPP4
isorhamnetin	C24	MAPK14
isorhamnetin	C24	GSK3B
isorhamnetin	C24	HSP90AA1
isorhamnetin	C24	CDK2
isorhamnetin	C24	PIK3CG
isorhamnetin	C24	KAPCA
isorhamnetin	C24	PRSS1
isorhamnetin	C24	PIM1
isorhamnetin	C24	CCNA2
isorhamnetin	C24	NCOA2
isorhamnetin	C24	PCP4
isorhamnetin	C24	PYGM

isorhamnetin	C24	PPARD
isorhamnetin	C24	CHEK1
isorhamnetin	C24	AKR1B1
isorhamnetin	C24	NCOA1
isorhamnetin	C24	F7
isorhamnetin	C24	SERPIND1
isorhamnetin	C24	NOS3
isorhamnetin	C24	ACHE
isorhamnetin	C24	GABRA1
isorhamnetin	C24	MAOB
isorhamnetin	C24	GRIA2
isorhamnetin	C24	NOR51B
isorhamnetin	C24	RELA
isorhamnetin	C24	XDH
isorhamnetin	C24	NCF1
isorhamnetin	C24	OLR1
3,9-di-O-methylnissolin	C25	NOS2
3,9-di-O-methylnissolin	C25	PTGS1
3,9-di-O-methylnissolin	C25	CHRM3
3,9-di-O-methylnissolin	C25	SERPIND1
3,9-di-O-methylnissolin	C25	CHRM1
3,9-di-O-methylnissolin	C25	ESR1
3,9-di-O-methylnissolin	C25	ADRB1
3,9-di-O-methylnissolin	C25	SCN5A
3,9-di-O-methylnissolin	C25	PTGS2
3,9-di-O-methylnissolin	C25	NOS3
3,9-di-O-methylnissolin	C25	HTR3A
3,9-di-O-methylnissolin	C25	ADRA2C
3,9-di-O-methylnissolin	C25	RXRA
3,9-di-O-methylnissolin	C25	ACHE
3,9-di-O-methylnissolin	C25	PDE3A
3,9-di-O-methylnissolin	C25	ADRA1B
3,9-di-O-methylnissolin	C25	ADRB2
3,9-di-O-methylnissolin	C25	ADRA1D
3,9-di-O-methylnissolin	C25	OPRM1
3,9-di-O-methylnissolin	C25	GABRA1
3,9-di-O-methylnissolin	C25	PRSS1
3,9-di-O-methylnissolin	C25	NCOA2
3,9-di-O-methylnissolin	C25	PCP4
7-O-methylisomucronulatol	C26	NOS2
7-O-methylisomucronulatol	C26	PTGS1
7-O-methylisomucronulatol	C26	DRD1
7-O-methylisomucronulatol	C26	CHRM3
7-O-methylisomucronulatol	C26	SERPIND1
7-O-methylisomucronulatol	C26	KCNH2
7-O-methylisomucronulatol	C26	CHRM1
7-O-methylisomucronulatol	C26	ESR1
7-O-methylisomucronulatol	C26	AR
7-O-methylisomucronulatol	C26	ADRB1
7-O-methylisomucronulatol	C26	SCN5A
7-O-methylisomucronulatol	C26	PPARG
7-O-methylisomucronulatol	C26	FXa
7-O-methylisomucronulatol	C26	CHRM5
7-O-methylisomucronulatol	C26	PTGS2
7-O-methylisomucronulatol	C26	NOS3
7-O-methylisomucronulatol	C26	ADRA2C
7-O-methylisomucronulatol	C26	CHRM4

7-O-methylisomucronulatol	C26	RXRA
7-O-methylisomucronulatol	C26	OPRD1
7-O-methylisomucronulatol	C26	PDE3A
7-O-methylisomucronulatol	C26	HTR2A
7-O-methylisomucronulatol	C26	ADRA1A
7-O-methylisomucronulatol	C26	CHRM2
7-O-methylisomucronulatol	C26	ADRA1B
7-O-methylisomucronulatol	C26	SLC6A3
7-O-methylisomucronulatol	C26	ADRB2
7-O-methylisomucronulatol	C26	ADRA1D
7-O-methylisomucronulatol	C26	SLC6A4
7-O-methylisomucronulatol	C26	ESR2
7-O-methylisomucronulatol	C26	GABRA1
7-O-methylisomucronulatol	C26	DPP4
7-O-methylisomucronulatol	C26	MAPK14
7-O-methylisomucronulatol	C26	GSK3B
7-O-methylisomucronulatol	C26	HSP90AA1
7-O-methylisomucronulatol	C26	CDK2
7-O-methylisomucronulatol	C26	CHEK1
7-O-methylisomucronulatol	C26	KAPCA
7-O-methylisomucronulatol	C26	RXRB
7-O-methylisomucronulatol	C26	PRSS1
7-O-methylisomucronulatol	C26	PIM1
7-O-methylisomucronulatol	C26	CCNA2
7-O-methylisomucronulatol	C26	NCOA2
7-O-methylisomucronulatol	C26	KCNMA1
7-O-methylisomucronulatol	C26	PCP4
9,10-dimethoxypterocarpan-3-O-β-D-glucoside	C27	PTGS2
9,10-dimethoxypterocarpan-3-O-β-D-glucoside	C27	TOP2B
9,10-dimethoxypterocarpan-3-O-β-D-glucoside	C27	NCOA2
(6aR,11aR)-9,10-dimethoxy-6a,11a-dihydro-6H-benzofurano[3,2-c]chromen-3-ol	C28	NOS2
(6aR,11aR)-9,10-dimethoxy-6a,11a-dihydro-6H-benzofurano[3,2-c]chromen-3-ol	C28	PTGS1
(6aR,11aR)-9,10-dimethoxy-6a,11a-dihydro-6H-benzofurano[3,2-c]chromen-3-ol	C28	CHRM3
(6aR,11aR)-9,10-dimethoxy-6a,11a-dihydro-6H-benzofurano[3,2-c]chromen-3-ol	C28	SERPIND1
(6aR,11aR)-9,10-dimethoxy-6a,11a-dihydro-6H-benzofurano[3,2-c]chromen-3-ol	C28	CHRM1
(6aR,11aR)-9,10-dimethoxy-6a,11a-dihydro-6H-benzofurano[3,2-c]chromen-3-ol	C28	ESR1
(6aR,11aR)-9,10-dimethoxy-6a,11a-dihydro-6H-benzofurano[3,2-c]chromen-3-ol	C28	SCN5A
(6aR,11aR)-9,10-dimethoxy-6a,11a-dihydro-6H-benzofurano[3,2-c]chromen-3-ol	C28	PTGS2
(6aR,11aR)-9,10-dimethoxy-6a,11a-dihydro-6H-benzofurano[3,2-c]chromen-3-ol	C28	HTR3A
(6aR,11aR)-9,10-dimethoxy-6a,11a-dihydro-6H-benzofurano[3,2-c]chromen-3-ol	C28	RXRA
(6aR,11aR)-9,10-dimethoxy-6a,11a-dihydro-6H-benzofurano[3,2-c]chromen-3-ol	C28	ACHE
(6aR,11aR)-9,10-dimethoxy-6a,11a-dihydro-6H-benzofurano[3,2-c]chromen-3-ol	C28	ADRA1B
(6aR,11aR)-9,10-dimethoxy-6a,11a-dihydro-6H-benzofurano[3,2-c]chromen-3-ol	C28	ADRB2
(6aR,11aR)-9,10-dimethoxy-6a,11a-dihydro-6H-benzofurano[3,2-c]chromen-3-ol	C28	ADRA1D
(6aR,11aR)-9,10-dimethoxy-6a,11a-dihydro-6H-benzofurano[3,2-c]chromen-3-ol	C28	GABRA1
(6aR,11aR)-9,10-dimethoxy-6a,11a-dihydro-6H-benzofurano[3,2-c]chromen-3-ol	C28	HSP90AA1
(6aR,11aR)-9,10-dimethoxy-6a,11a-dihydro-6H-benzofurano[3,2-c]chromen-3-ol	C28	CHRNA7
(6aR,11aR)-9,10-dimethoxy-6a,11a-dihydro-6H-benzofurano[3,2-c]chromen-3-ol	C28	PRSS1
(6aR,11aR)-9,10-dimethoxy-6a,11a-dihydro-6H-benzofurano[3,2-c]chromen-3-ol	C28	NCOA2
(6aR,11aR)-9,10-dimethoxy-6a,11a-dihydro-6H-benzofurano[3,2-c]chromen-3-ol	C28	NCOA1
(6aR,11aR)-9,10-dimethoxy-6a,11a-dihydro-6H-benzofurano[3,2-c]chromen-3-ol	C28	PCP4
(6aR,11aR)-9,10-dimethoxy-6a,11a-dihydro-6H-benzofurano[3,2-c]chromen-3-ol	C28	CHRM4
Bifendate	C29	PTGS2
Bifendate	C29	KDR
Bifendate	C29	MET
Bifendate	C29	HSP90AA1
Bifendate	C29	KCNMA1

Bifendate	C29	PTGS1
Bifendate	C29	TOP2B
formononetin	C4	NOS2
formononetin	C4	PTGS1
formononetin	C4	CHRM1
formononetin	C4	ESR1
formononetin	C4	AR
formononetin	C4	PPARG
formononetin	C4	PTGS2
formononetin	C4	RXRA
formononetin	C4	PDE3A
formononetin	C4	ADRA1A
formononetin	C4	SLC6A3
formononetin	C4	ADRB2
formononetin	C4	SLC6A4
formononetin	C4	ESR2
formononetin	C4	DPP4
formononetin	C4	MAPK14
formononetin	C4	GSK3B
formononetin	C4	HSP90AA1
formononetin	C4	CDK2
formononetin	C4	MAOB
formononetin	C4	CHEK1
formononetin	C4	KAPCA
formononetin	C4	PRSS1
formononetin	C4	PIM1
formononetin	C4	CCNA2
formononetin	C4	PCP4
formononetin	C4	PKIA
formononetin	C4	SERPIND1
formononetin	C4	NOS3
formononetin	C4	ACHE
formononetin	C4	LACTBL1
formononetin	C4	JUN
formononetin	C4	#N/A
formononetin	C4	IL4
formononetin	C4	SIRT1
formononetin	C4	ATP5B
formononetin	C4	ND6
formononetin	C4	HSD3B2
formononetin	C4	HSD3B1
Calycosin	C30	NOS2
Calycosin	C30	PTGS1
Calycosin	C30	ESR1
Calycosin	C30	AR
Calycosin	C30	PPARG
Calycosin	C30	PTGS2
Calycosin	C30	RXRA
Calycosin	C30	PDE3A
Calycosin	C30	ESR2
Calycosin	C30	DPP4
Calycosin	C30	MAPK14
Calycosin	C30	GSK3B
Calycosin	C30	HSP90AA1
Calycosin	C30	CDK2
Calycosin	C30	CHEK1
Calycosin	C30	KAPCA

Calycosin	C30	PRSS1
Calycosin	C30	PIM1
Calycosin	C30	CCNA2
Calycosin	C30	NCOA2
Calycosin	C30	PCP4
Calycosin	C30	ADRB2
kaempferol	C8	NOS2
kaempferol	C8	PTGS1
kaempferol	C8	AR
kaempferol	C8	PPARG
kaempferol	C8	PTGS2
kaempferol	C8	HSP90AA1
kaempferol	C8	PIK3CG
kaempferol	C8	KAPCA
kaempferol	C8	NCOA2
kaempferol	C8	DPP4
kaempferol	C8	PRSS1
kaempferol	C8	PGR
kaempferol	C8	SERPIND1
kaempferol	C8	CHRM1
kaempferol	C8	NOS3
kaempferol	C8	GABRA2
kaempferol	C8	ACHE
kaempferol	C8	SLC6A2
kaempferol	C8	CHRM2
kaempferol	C8	ADRA1B
kaempferol	C8	GABRA1
kaempferol	C8	TOP2B
kaempferol	C8	F7
kaempferol	C8	PCP4
kaempferol	C8	RELA
kaempferol	C8	IKBKB
kaempferol	C8	AKT1
kaempferol	C8	BCL2
kaempferol	C8	BAX
kaempferol	C8	TNF
kaempferol	C8	JUN
kaempferol	C8	AHSA1
kaempferol	C8	CASP3
kaempferol	C8	MAPK8
kaempferol	C8	XDH
kaempferol	C8	MMP1
kaempferol	C8	STAT1
kaempferol	C8	CDK1
kaempferol	C8	#N/A
kaempferol	C8	HMOX1
kaempferol	C8	CYP3A4
kaempferol	C8	CYP1A2
kaempferol	C8	CYP1A1
kaempferol	C8	ICAM1
kaempferol	C8	SELE
kaempferol	C8	VCAM1
kaempferol	C8	NR1I2
kaempferol	C8	CYP1B1
kaempferol	C8	ALOX5
kaempferol	C8	HAS2
kaempferol	C8	GSTP1

kaempferol	C8	AHR
kaempferol	C8	PSMD3
kaempferol	C8	SLC2A4
kaempferol	C8	NR1I3
kaempferol	C8	INSR
kaempferol	C8	DIO1
kaempferol	C8	PPP3CA
kaempferol	C8	PRXC1A
kaempferol	C8	GSTM1
kaempferol	C8	GSTM2
kaempferol	C8	AKR1C3
kaempferol	C8	SLPI
FA	C31	CDK2
FA	C31	SERPIND1
FA	C31	GSK3B
isomucronulatol-7,2'-di-O-glucosiole	C32	TOP2B
1,7-Dihydroxy-3,9-dimethoxy pterocarpene	C33	PTGS2
1,7-Dihydroxy-3,9-dimethoxy pterocarpene	C33	RXRA
1,7-Dihydroxy-3,9-dimethoxy pterocarpene	C33	HSP90AA1
1,7-Dihydroxy-3,9-dimethoxy pterocarpene	C33	PRSS1
quercetin	C34	PTGS1
quercetin	C34	AR
quercetin	C34	PPARG
quercetin	C34	PTGS2
quercetin	C34	HSP90AA1
quercetin	C34	PIK3CG
quercetin	C34	NCOA2
quercetin	C34	DPP4
quercetin	C34	AKR1B1
quercetin	C34	PRSS1
quercetin	C34	TOP2B
quercetin	C34	SERPIND1
quercetin	C34	KCNH2
quercetin	C34	SCN5A
quercetin	C34	FXa
quercetin	C34	ADRB2
quercetin	C34	MMP3
quercetin	C34	KAPCA
quercetin	C34	F7
quercetin	C34	NOS3
quercetin	C34	RXRA
quercetin	C34	ACHE
quercetin	C34	GABRA1
quercetin	C34	MAOB
quercetin	C34	RELA
quercetin	C34	EGFR
quercetin	C34	AKT1
quercetin	C34	VEGFA
quercetin	C34	CCND1
quercetin	C34	BCL2
quercetin	C34	BCL2L1
quercetin	C34	FOS
quercetin	C34	CDKN1A
quercetin	C34	EIF6
quercetin	C34	BAX
quercetin	C34	CASP9
quercetin	C34	PLAU

quercetin	C34	MMP2
quercetin	C34	MMP9
quercetin	C34	MAPK1
quercetin	C34	IL10
quercetin	C34	EGF
quercetin	C34	RB1
quercetin	C34	TNF
quercetin	C34	JUN
quercetin	C34	IL6
quercetin	C34	CDKN2A
quercetin	C34	AHSA1
quercetin	C34	CASP3
quercetin	C34	TP53
quercetin	C34	ELK1
quercetin	C34	NFKBIA
quercetin	C34	POR
quercetin	C34	ODC1
quercetin	C34	XDH
quercetin	C34	CASP8
quercetin	C34	TOP1
quercetin	C34	RAF1
quercetin	C34	SOD1
quercetin	C34	PRKCA
quercetin	C34	MMP1
quercetin	C34	HIF1A
quercetin	C34	STAT1
quercetin	C34	RUNX1T1
quercetin	C34	HERC5
quercetin	C34	CDK1
quercetin	C34	HSPA5
quercetin	C34	ERBB2
quercetin	C34	#N/A
quercetin	C34	ACACA
quercetin	C34	HMOX1
quercetin	C34	CYP3A4
quercetin	C34	CYP1A2
quercetin	C34	CAV1
quercetin	C34	MYC
quercetin	C34	F3
quercetin	C34	GJA1
quercetin	C34	CYP1A1
quercetin	C34	ICAM1
quercetin	C34	IL1B
quercetin	C34	CCL2
quercetin	C34	SELE
quercetin	C34	VCAM1
quercetin	C34	PTGER3
quercetin	C34	CXCL8
quercetin	C34	PRKCB
quercetin	C34	BIRC5
quercetin	C34	DUOX2
quercetin	C34	#N/A
quercetin	C34	HSPB1
quercetin	C34	TGFB1
quercetin	C34	SULT1E1
quercetin	C34	MGAM
quercetin	C34	IL2

quercetin	C34	NR1I2
quercetin	C34	CYP1B1
quercetin	C34	CCNB1
quercetin	C34	PLAT
quercetin	C34	THBD
quercetin	C34	SERPINE1
quercetin	C34	COL1A1
quercetin	C34	IFNG
quercetin	C34	ALOX5
quercetin	C34	PTEN
quercetin	C34	IL1A
quercetin	C34	MPO
quercetin	C34	TOP2A
quercetin	C34	NCF1
quercetin	C34	ABCG2
quercetin	C34	HAS2
quercetin	C34	GSTP1
quercetin	C34	NFE2L2
quercetin	C34	NQO1
quercetin	C34	PARP1
quercetin	C34	AHR
quercetin	C34	PSMD3
quercetin	C34	SLC2A4
quercetin	C34	COL3A1
quercetin	C34	gyrB
quercetin	C34	CXCL11
quercetin	C34	CXCL2
quercetin	C34	DCAF5
quercetin	C34	NR1I3
quercetin	C34	CHEK2
quercetin	C34	INSR
quercetin	C34	CLDN4
quercetin	C34	PPARA
quercetin	C34	#N/A
quercetin	C34	HSF1
quercetin	C34	CRP
quercetin	C34	CXCL10
quercetin	C34	CHUK
quercetin	C34	SPP1
quercetin	C34	RUNX2
quercetin	C34	RASSF1
quercetin	C34	E2F1
quercetin	C34	E2F2
quercetin	C34	ACPP
quercetin	C34	CTSD
quercetin	C34	IGFBP3
quercetin	C34	IGF2
quercetin	C34	CD40LG
quercetin	C34	IRF1
quercetin	C34	ERBB3
quercetin	C34	PON1
quercetin	C34	DIO1
quercetin	C34	PCOLCE
quercetin	C34	NPEPPS
quercetin	C34	HK2
quercetin	C34	NKX3-1
quercetin	C34	RASA1

	quercetin	C34	PRXC1A
	quercetin	C34	GSTM1
	quercetin	C34	GSTM2
chinese yam	piperlonguminine	C35	CHRM1
	piperlonguminine	C35	NOS3
	piperlonguminine	C35	RXRA
	piperlonguminine	C35	PDE3A
	piperlonguminine	C35	ADRA1B
	piperlonguminine	C35	SLC6A3
	piperlonguminine	C35	ADRB2
	piperlonguminine	C35	SLC6A4
	piperlonguminine	C35	LTA4H
	piperlonguminine	C35	MAOB
	piperlonguminine	C35	SAA1
	(-)-taxifolin	C36	PTGS1
	(-)-taxifolin	C36	PTGS2
	(-)-taxifolin	C36	HSP90AA1
	(-)-taxifolin	C36	PIK3CG
	Kadsurenone	C37	PTGS1
	Kadsurenone	C37	CHRM3
	Kadsurenone	C37	SERPIND1
	Kadsurenone	C37	KCNH2
	Kadsurenone	C37	CHRM1
	Kadsurenone	C37	SCN5A
	Kadsurenone	C37	FXa
	Kadsurenone	C37	CHRM5
	Kadsurenone	C37	PTGS2
	Kadsurenone	C37	CA2
	Kadsurenone	C37	ACHE
	Kadsurenone	C37	CHRM2
	Kadsurenone	C37	ADRA1B
	Kadsurenone	C37	ADRB2
	Kadsurenone	C37	ADRA1D
	Kadsurenone	C37	TOP2B
	Kadsurenone	C37	OPRM1
	Kadsurenone	C37	DPP4
	Kadsurenone	C37	ITM2C
	Kadsurenone	C37	HSP90AA1
	Kadsurenone	C37	PRSS1
	Kadsurenone	C37	NCOA2
	Kadsurenone	C37	NCOA1
	Kadsurenone	C37	KCNMA1
	Kadsurenone	C37	PCP4
	Kadsurenone	C37	RXRA
	Kadsurenone	C37	PDE3A
	hancinone C	C38	NOS2
	hancinone C	C38	CHRM3
	hancinone C	C38	SERPIND1
	hancinone C	C38	KCNH2
	hancinone C	C38	CHRM1
	hancinone C	C38	ESR1
	hancinone C	C38	SCN5A
	hancinone C	C38	FXa
	hancinone C	C38	PTGS2
	hancinone C	C38	F7
	hancinone C	C38	PDE3A
	hancinone C	C38	ADRA1B

hancinone C	C38	ADRA1D
hancinone C	C38	TOP2B
hancinone C	C38	ESR2
hancinone C	C38	DPP4
hancinone C	C38	HSP90AA1
hancinone C	C38	PRSS1
hancinone C	C38	NCOA2
hancinone C	C38	NCOA1
hancinone C	C38	KCNMA1
hancinone C	C38	PCP4
24-Methylcholest-5-enyl-3beta-O-glucopyranoside_qt	C39	PGR
campesterol	C40	PGR
Isofucosterol	C41	PGR
Isofucosterol	C41	NR3C2
Isofucosterol	C41	ABAT
Isofucosterol	C41	GABRA1
Isofucosterol	C41	ADH1B
Isofucosterol	C41	ADH1C
Isofucosterol	C41	ADH1A
Isofucosterol	C41	NOR51B
Isofucosterol	C41	LYZ
Isofucosterol	C41	nprE
Isofucosterol	C41	COBT
Isofucosterol	C41	NCOA2
h-Met-h	C42	GABRA1
h-Met-h	C42	nprE
h-Met-h	C42	CTSD
h-Met-h	C42	ADH1C
h-Met-h	C42	MAT2A
Stigmasterol	C5	PGR
Stigmasterol	C5	NR3C2
Stigmasterol	C5	NCOA2
Stigmasterol	C5	ADH1C
Stigmasterol	C5	IGHG1
Stigmasterol	C5	RXRA
Stigmasterol	C5	NCOA1
Stigmasterol	C5	PTGS1
Stigmasterol	C5	PTGS2
Stigmasterol	C5	ADRA2A
Stigmasterol	C5	SLC6A2
Stigmasterol	C5	SLC6A3
Stigmasterol	C5	ADRB2
Stigmasterol	C5	AKR1B1
Stigmasterol	C5	PLAU
Stigmasterol	C5	LTA4H
Stigmasterol	C5	MAOB
Stigmasterol	C5	MAOA
Stigmasterol	C5	KAPCA
Stigmasterol	C5	CTRB1
Stigmasterol	C5	CHRM3
Stigmasterol	C5	CHRM1
Stigmasterol	C5	ADRB1
Stigmasterol	C5	SCN5A
Stigmasterol	C5	HTR2A
Stigmasterol	C5	ADRA1A
Stigmasterol	C5	GABRA3
Stigmasterol	C5	CHRM2

	Stigmasterol	C5	ADRA1B
	Stigmasterol	C5	GABRA1
	Stigmasterol	C5	CHRNA7
	Dioscoreside C_qt	C43	NR3C1
	Dioscoreside C_qt	C43	NCOA2
	diosgenin	C44	PGR
	diosgenin	C44	NR3C2
	diosgenin	C44	RELA
	diosgenin	C44	AKT1
	diosgenin	C44	VEGFA
	diosgenin	C44	CDKN1A
	diosgenin	C44	TP53
	diosgenin	C44	PTGS2
	diosgenin	C44	FASN
	diosgenin	C44	SOD1
	diosgenin	C44	CAT
	diosgenin	C44	HIF1A
	diosgenin	C44	NR1I2
	diosgenin	C44	PLA2G4A
	diosgenin	C44	ABCC2
	diosgenin	C44	MTOR
	AIDS180907	C45	NOS2
	AIDS180907	C45	ESR1
	AIDS180907	C45	AR
	AIDS180907	C45	FXa
	AIDS180907	C45	PTGS2
	AIDS180907	C45	F7
	AIDS180907	C45	TOP2B
	AIDS180907	C45	GSK3B
	AIDS180907	C45	PIM1
	AIDS180907	C45	CCNA2
	AIDS180907	C45	NCOA2
	AIDS180907	C45	NCOA1
	AIDS180907	C45	PCP4
	CLR	C46	PGR
	CLR	C46	NR3C2
	CLR	C46	NOR51B
	CLR	C46	NCOA2
common anemarrhena rhizome	asperglaucide	C47	SERPIND1
	asperglaucide	C47	KCNH2
	asperglaucide	C47	FXa
	asperglaucide	C47	PTGS2
	asperglaucide	C47	PRSS1
	kaempferol	C8	NOS2
	kaempferol	C8	PTGS1
	kaempferol	C8	AR
	kaempferol	C8	PPARG
	kaempferol	C8	PTGS2
	kaempferol	C8	HSP90AA1
	kaempferol	C8	PIK3CG
	kaempferol	C8	KAPCA
	kaempferol	C8	NCOA2
	kaempferol	C8	DPP4
	kaempferol	C8	PRSS1
	kaempferol	C8	PGR
	kaempferol	C8	SERPIND1

kaempferol	C8	CHRM1
kaempferol	C8	NOS3
kaempferol	C8	GABRA2
kaempferol	C8	ACHE
kaempferol	C8	SLC6A2
kaempferol	C8	CHRM2
kaempferol	C8	ADRA1B
kaempferol	C8	GABRA1
kaempferol	C8	TOP2B
kaempferol	C8	F7
kaempferol	C8	PCP4
kaempferol	C8	RELA
kaempferol	C8	IKBKB
kaempferol	C8	AKT1
kaempferol	C8	BCL2
kaempferol	C8	BAX
kaempferol	C8	TNF
kaempferol	C8	JUN
kaempferol	C8	AHSA1
kaempferol	C8	CASP3
kaempferol	C8	MAPK8
kaempferol	C8	XDH
kaempferol	C8	MMP1
kaempferol	C8	STAT1
kaempferol	C8	CDK1
kaempferol	C8	#N/A
kaempferol	C8	HMOX1
kaempferol	C8	CYP3A4
kaempferol	C8	CYP1A2
kaempferol	C8	CYP1A1
kaempferol	C8	ICAM1
kaempferol	C8	SELE
kaempferol	C8	VCAM1
kaempferol	C8	NR1I2
kaempferol	C8	CYP1B1
kaempferol	C8	ALOX5
kaempferol	C8	HAS2
kaempferol	C8	GSTP1
kaempferol	C8	AHR
kaempferol	C8	PSMD3
kaempferol	C8	SLC2A4
kaempferol	C8	NR1I3
kaempferol	C8	INSR
kaempferol	C8	DIO1
kaempferol	C8	PPP3CA
kaempferol	C8	PRXC1A
kaempferol	C8	GSTM1
kaempferol	C8	GSTM2
kaempferol	C8	AKR1C3
kaempferol	C8	SLPI
Anhydroicaritin	C48	NOS2
Anhydroicaritin	C48	PTGS1
Anhydroicaritin	C48	CHRM3
Anhydroicaritin	C48	SERPIND1
Anhydroicaritin	C48	KCNH2
Anhydroicaritin	C48	CHRM1
Anhydroicaritin	C48	ESR1

Anhydroicaritin	C48	AR
Anhydroicaritin	C48	SCN5A
Anhydroicaritin	C48	PPARG
Anhydroicaritin	C48	FXa
Anhydroicaritin	C48	CHRM5
Anhydroicaritin	C48	PTGS2
Anhydroicaritin	C48	NOS3
Anhydroicaritin	C48	RXRA
Anhydroicaritin	C48	ACHE
Anhydroicaritin	C48	ADRA1B
Anhydroicaritin	C48	ADRB2
Anhydroicaritin	C48	ESR2
Anhydroicaritin	C48	DPP4
Anhydroicaritin	C48	MAPK14
Anhydroicaritin	C48	GSK3B
Anhydroicaritin	C48	HSP90AA1
Anhydroicaritin	C48	CDK2
Anhydroicaritin	C48	CHEK1
Anhydroicaritin	C48	RXRB
Anhydroicaritin	C48	PRSS1
Anhydroicaritin	C48	PIM1
Anhydroicaritin	C48	NCOA2
Anhydroicaritin	C48	PCP4
Anhydroicaritin	C48	F7
Anhydroicaritin	C48	KDR
Anhydroicaritin	C48	TOP2B
Anhydroicaritin	C48	CCNA2
Anhydroicaritin	C48	NCOA1
Anhydroicaritin	C48	KCNMA1
Anhydroicaritin	C48	IGHG1
Anemarsaponin F_qt	C49	NR3C1
Hippeastrine	C50	CHRM3
Hippeastrine	C50	CHRM1
Hippeastrine	C50	AR
Hippeastrine	C50	SCN5A
Hippeastrine	C50	OPRD1
Hippeastrine	C50	ADRA1B
Hippeastrine	C50	OPRM1
Hippeastrine	C50	GABRA1
Hippeastrine	C50	HSP90AA1
Hippeastrine	C50	PIK3CG
Hippeastrine	C50	CHRNA7
Timosaponin B III_qt	C51	PGR
Timosaponin B III_qt	C51	NR3C1
Stigmasterol	C5	PGR
Stigmasterol	C5	NR3C2
Stigmasterol	C5	NCOA2
Stigmasterol	C5	ADH1C
Stigmasterol	C5	IGHG1
Stigmasterol	C5	RXRA
Stigmasterol	C5	NCOA1
Stigmasterol	C5	PTGS1
Stigmasterol	C5	PTGS2
Stigmasterol	C5	ADRA2A
Stigmasterol	C5	SLC6A2
Stigmasterol	C5	SLC6A3
Stigmasterol	C5	ADRB2

	Stigmasterol	C5	AKR1B1
	Stigmasterol	C5	PLAU
	Stigmasterol	C5	LTA4H
	Stigmasterol	C5	MAOB
	Stigmasterol	C5	MAOA
	Stigmasterol	C5	KAPCA
	Stigmasterol	C5	CTRB1
	Stigmasterol	C5	CHRM3
	Stigmasterol	C5	CHRM1
	Stigmasterol	C5	ADRB1
	Stigmasterol	C5	SCN5A
	Stigmasterol	C5	HTR2A
	Stigmasterol	C5	ADRA1A
	Stigmasterol	C5	GABRA3
	Stigmasterol	C5	CHRM2
	Stigmasterol	C5	ADRA1B
	Stigmasterol	C5	GABRA1
	Stigmasterol	C5	CHRNA7
	Icariin I	C52	TOP2B
	Anemarsaponin C_qt	C53	PGR
	Anemarsaponin C_qt	C53	NR3C2
	Anemarsaponin C_qt	C53	NR3C1
	(Z)-3-(4-hydroxy-3-methoxy-phenyl)-N-[2-(4-hydroxyphenyl)ethyl]acrylamide	C54	PTGS1
	(Z)-3-(4-hydroxy-3-methoxy-phenyl)-N-[2-(4-hydroxyphenyl)ethyl]acrylamide	C54	PTGS2
	(Z)-3-(4-hydroxy-3-methoxy-phenyl)-N-[2-(4-hydroxyphenyl)ethyl]acrylamide	C54	PDE3A
	(Z)-3-(4-hydroxy-3-methoxy-phenyl)-N-[2-(4-hydroxyphenyl)ethyl]acrylamide	C54	ADRA1B
	(Z)-3-(4-hydroxy-3-methoxy-phenyl)-N-[2-(4-hydroxyphenyl)ethyl]acrylamide	C54	ADRB2
	(Z)-3-(4-hydroxy-3-methoxy-phenyl)-N-[2-(4-hydroxyphenyl)ethyl]acrylamide	C54	HSP90AA1
	(Z)-3-(4-hydroxy-3-methoxy-phenyl)-N-[2-(4-hydroxyphenyl)ethyl]acrylamide	C54	LTA4H
	(Z)-3-(4-hydroxy-3-methoxy-phenyl)-N-[2-(4-hydroxyphenyl)ethyl]acrylamide	C54	PCP4
	diosgenin	C44	PGR
	diosgenin	C44	NR3C2
	diosgenin	C44	RELA
	diosgenin	C44	AKT1
	diosgenin	C44	VEGFA
	diosgenin	C44	CDKN1A
	diosgenin	C44	TP53
	diosgenin	C44	PTGS2
	diosgenin	C44	FASN
	diosgenin	C44	SOD1
	diosgenin	C44	CAT
	diosgenin	C44	HIF1A
	diosgenin	C44	NR1I2
	diosgenin	C44	PLA2G4A
	diosgenin	C44	ABCC2
	diosgenin	C44	MTOR
	coumaroyltyramine	C55	CHRM1
	coumaroyltyramine	C55	ADRB1
	coumaroyltyramine	C55	PTGS2
	coumaroyltyramine	C55	ADRB2
	coumaroyltyramine	C55	HSP90AA1
	coumaroyltyramine	C55	LTA4H
	coumaroyltyramine	C55	MAOB
	coumaroyltyramine	C55	KAPCA
	coumaroyltyramine	C55	PKIA
	coumaroyltyramine	C55	PTGS1
figwort root	sugiol	C56	CHRM3

sugiol	C56	CHRM1
sugiol	C56	SCN5A
sugiol	C56	CHRM5
sugiol	C56	PTGS2
sugiol	C56	CA2
sugiol	C56	CHRM4
sugiol	C56	OPRD1
sugiol	C56	ACHE
sugiol	C56	ADRA1A
sugiol	C56	CHRM2
sugiol	C56	ADRA1B
sugiol	C56	ADRB2
sugiol	C56	ADRA1D
sugiol	C56	DRD2
sugiol	C56	OPRM1
sugiol	C56	CHRNA7
beta-sitosterol	C3	PGR
beta-sitosterol	C3	NCOA2
beta-sitosterol	C3	PTGS1
beta-sitosterol	C3	PTGS2
beta-sitosterol	C3	HSP90AA1
beta-sitosterol	C3	PIK3CG
beta-sitosterol	C3	KCNH2
beta-sitosterol	C3	KAPCA
beta-sitosterol	C3	DRD1
beta-sitosterol	C3	CHRM3
beta-sitosterol	C3	CHRM1
beta-sitosterol	C3	SCN5A
beta-sitosterol	C3	GABRA2
beta-sitosterol	C3	CHRM4
beta-sitosterol	C3	PDE3A
beta-sitosterol	C3	HTR2A
beta-sitosterol	C3	GABRA5
beta-sitosterol	C3	ADRA1A
beta-sitosterol	C3	GABRA3
beta-sitosterol	C3	CHRM2
beta-sitosterol	C3	ADRA1B
beta-sitosterol	C3	ADRB2
beta-sitosterol	C3	CHRNA2
beta-sitosterol	C3	SLC6A4
beta-sitosterol	C3	OPRM1
beta-sitosterol	C3	GABRA1
beta-sitosterol	C3	CHRNA7
beta-sitosterol	C3	NOR51B
beta-sitosterol	C3	BCL2
beta-sitosterol	C3	BAX
beta-sitosterol	C3	CASP9
beta-sitosterol	C3	JUN
beta-sitosterol	C3	CASP3
beta-sitosterol	C3	CASP8
beta-sitosterol	C3	PRKCA
beta-sitosterol	C3	TGFB1
beta-sitosterol	C3	PON1
beta-sitosterol	C3	MAP2
sitosterol	C57	PGR
sitosterol	C57	NCOA2
sitosterol	C57	NR3C2

	14-deoxy-12(R)-sulfoandrographolide	C58	NR3C2
	harpagoside_qt	C59	SERPIND1
	harpagoside_qt	C59	ESR1
	harpagoside_qt	C59	CA2
	harpagoside_qt	C59	DPP4
	harpagoside_qt	C59	GSK3B
	harpagoside_qt	C59	CDK2
	harpagoside_qt	C59	LACTBL1
	harpagoside_qt	C59	PRSS1
	harpagoside_qt	C59	CCNA2
radix salviae miltiorrhizae	1,2,5,6-tetrahydrotanshinone	C60	PTGS1
	1,2,5,6-tetrahydrotanshinone	C60	CHRM3
	1,2,5,6-tetrahydrotanshinone	C60	CHRM1
	1,2,5,6-tetrahydrotanshinone	C60	SCN5A
	1,2,5,6-tetrahydrotanshinone	C60	CHRM5
	1,2,5,6-tetrahydrotanshinone	C60	PTGS2
	1,2,5,6-tetrahydrotanshinone	C60	HTR3A
	1,2,5,6-tetrahydrotanshinone	C60	CA2
	1,2,5,6-tetrahydrotanshinone	C60	CHRM4
	1,2,5,6-tetrahydrotanshinone	C60	RXRA
	1,2,5,6-tetrahydrotanshinone	C60	OPRD1
	1,2,5,6-tetrahydrotanshinone	C60	PDE3A
	1,2,5,6-tetrahydrotanshinone	C60	ADRA1A
	1,2,5,6-tetrahydrotanshinone	C60	CHRM2
	1,2,5,6-tetrahydrotanshinone	C60	ADRA1B
	1,2,5,6-tetrahydrotanshinone	C60	SLC6A3
	1,2,5,6-tetrahydrotanshinone	C60	ADRB2
	1,2,5,6-tetrahydrotanshinone	C60	ADRA1D
	1,2,5,6-tetrahydrotanshinone	C60	TOP2B
	1,2,5,6-tetrahydrotanshinone	C60	OPRM1
	1,2,5,6-tetrahydrotanshinone	C60	GABRA1
	1,2,5,6-tetrahydrotanshinone	C60	HSP90AA1
	1,2,5,6-tetrahydrotanshinone	C60	CHRNA7
	1,2,5,6-tetrahydrotanshinone	C60	NCOA2
	1,2,5,6-tetrahydrotanshinone	C60	NCOA1
	1,2,5,6-tetrahydrotanshinone	C60	DRD1
	1,2,5,6-tetrahydrotanshinone	C60	HTR2A
	1,2,5,6-tetrahydrotanshinone	C60	SLC6A4
	1,2,5,6-tetrahydrotanshinone	C60	IGHG1
	Poriferasterol	C61	PGR
	Poriferasterol	C61	NR3C2
	poriferast-5-en-3beta-ol	C62	PGR
	poriferast-5-en-3beta-ol	C62	NCOA2
	isoimperatorin	C63	PTGS2
	sugiol	C56	CHRM3
	sugiol	C56	CHRM1
	sugiol	C56	SCN5A
	sugiol	C56	CHRM5
	sugiol	C56	PTGS2
	sugiol	C56	CA2
	sugiol	C56	CHRM4
	sugiol	C56	OPRD1
	sugiol	C56	ACHE
	sugiol	C56	ADRA1A
	sugiol	C56	CHRM2
	sugiol	C56	ADRA1B

sugiol	C56	ADRB2
sugiol	C56	ADRA1D
sugiol	C56	DRD2
sugiol	C56	OPRM1
sugiol	C56	CHRNA7
Dehydrotanshinone II A	C64	DRD1
Dehydrotanshinone II A	C64	CHRM3
Dehydrotanshinone II A	C64	SERPIND1
Dehydrotanshinone II A	C64	CHRM1
Dehydrotanshinone II A	C64	ESR1
Dehydrotanshinone II A	C64	AR
Dehydrotanshinone II A	C64	SCN5A
Dehydrotanshinone II A	C64	PPARG
Dehydrotanshinone II A	C64	CHRM5
Dehydrotanshinone II A	C64	PTGS2
Dehydrotanshinone II A	C64	CHRM4
Dehydrotanshinone II A	C64	OPRD1
Dehydrotanshinone II A	C64	ACHE
Dehydrotanshinone II A	C64	HTR2A
Dehydrotanshinone II A	C64	ADRA1A
Dehydrotanshinone II A	C64	ADRB2
Dehydrotanshinone II A	C64	OPRM1
Dehydrotanshinone II A	C64	GABRA1
Dehydrotanshinone II A	C64	DPP4
Dehydrotanshinone II A	C64	CHRNA7
Dehydrotanshinone II A	C64	NCOA1
Baicalin	C65	FXa
Baicalin	C65	PTPN1
digallate	C66	PTGS2
digallate	C66	HSP90AA1
digallate	C66	AKR1B1
luteolin	C67	PTGS1
luteolin	C67	AR
luteolin	C67	PTGS2
luteolin	C67	HSP90AA1
luteolin	C67	PRSS1
luteolin	C67	NCOA2
luteolin	C67	KAPCA
luteolin	C67	DPP4
luteolin	C67	PIK3CG
luteolin	C67	RELA
luteolin	C67	EGFR
luteolin	C67	AKT1
luteolin	C67	VEGFA
luteolin	C67	CCND1
luteolin	C67	BCL2L1
luteolin	C67	CDKN1A
luteolin	C67	CASP9
luteolin	C67	MMP2
luteolin	C67	MMP9
luteolin	C67	MAPK1
luteolin	C67	IL10
luteolin	C67	RB1
luteolin	C67	CDK4
luteolin	C67	TNF
luteolin	C67	JUN
luteolin	C67	IL6

luteolin	C67	CASP3
luteolin	C67	TP53
luteolin	C67	NFKBIA
luteolin	C67	XDH
luteolin	C67	TOP1
luteolin	C67	MDM2
luteolin	C67	APBA3
luteolin	C67	MMP1
luteolin	C67	PCNA
luteolin	C67	ERBB2
luteolin	C67	#N/A
luteolin	C67	HMOX1
luteolin	C67	CASP7
luteolin	C67	ICAM1
luteolin	C67	MCL1
luteolin	C67	BIRC5
luteolin	C67	IL2
luteolin	C67	CCNB1
luteolin	C67	TYR
luteolin	C67	IFNG
luteolin	C67	IL4
luteolin	C67	TOP2A
luteolin	C67	GSTP1
luteolin	C67	XIAP
luteolin	C67	SLC2A4
luteolin	C67	INSR
luteolin	C67	CD40LG
luteolin	C67	PTGES
luteolin	C67	NUF2
luteolin	C67	ADCY2
luteolin	C67	MET
5,6-dihydroxy-7-isopropyl-1,1-dimethyl-2,3-dihydrophenanthren-4-one	C68	PTGS1
5,6-dihydroxy-7-isopropyl-1,1-dimethyl-2,3-dihydrophenanthren-4-one	C68	CHRM3
5,6-dihydroxy-7-isopropyl-1,1-dimethyl-2,3-dihydrophenanthren-4-one	C68	CHRM1
5,6-dihydroxy-7-isopropyl-1,1-dimethyl-2,3-dihydrophenanthren-4-one	C68	SCN5A
5,6-dihydroxy-7-isopropyl-1,1-dimethyl-2,3-dihydrophenanthren-4-one	C68	PTGS2
5,6-dihydroxy-7-isopropyl-1,1-dimethyl-2,3-dihydrophenanthren-4-one	C68	CA2
5,6-dihydroxy-7-isopropyl-1,1-dimethyl-2,3-dihydrophenanthren-4-one	C68	RXRA
5,6-dihydroxy-7-isopropyl-1,1-dimethyl-2,3-dihydrophenanthren-4-one	C68	ACHE
5,6-dihydroxy-7-isopropyl-1,1-dimethyl-2,3-dihydrophenanthren-4-one	C68	ADRA1A
5,6-dihydroxy-7-isopropyl-1,1-dimethyl-2,3-dihydrophenanthren-4-one	C68	ADRA1B
5,6-dihydroxy-7-isopropyl-1,1-dimethyl-2,3-dihydrophenanthren-4-one	C68	ADRB2
5,6-dihydroxy-7-isopropyl-1,1-dimethyl-2,3-dihydrophenanthren-4-one	C68	TOP2B
5,6-dihydroxy-7-isopropyl-1,1-dimethyl-2,3-dihydrophenanthren-4-one	C68	OPRM1
5,6-dihydroxy-7-isopropyl-1,1-dimethyl-2,3-dihydrophenanthren-4-one	C68	IGHG1
5,6-dihydroxy-7-isopropyl-1,1-dimethyl-2,3-dihydrophenanthren-4-one	C68	NCOA2
5,6-dihydroxy-7-isopropyl-1,1-dimethyl-2,3-dihydrophenanthren-4-one	C68	NCOA1
5,6-dihydroxy-7-isopropyl-1,1-dimethyl-2,3-dihydrophenanthren-4-one	C68	PCP4
2-isopropyl-8-methylphenanthrene-3,4-dione	C69	PTGS1
2-isopropyl-8-methylphenanthrene-3,4-dione	C69	DRD1
2-isopropyl-8-methylphenanthrene-3,4-dione	C69	CHRM3
2-isopropyl-8-methylphenanthrene-3,4-dione	C69	CHRM1
2-isopropyl-8-methylphenanthrene-3,4-dione	C69	ESR1
2-isopropyl-8-methylphenanthrene-3,4-dione	C69	AR
2-isopropyl-8-methylphenanthrene-3,4-dione	C69	SCN5A
2-isopropyl-8-methylphenanthrene-3,4-dione	C69	PPARG
2-isopropyl-8-methylphenanthrene-3,4-dione	C69	CHRM5

2-isopropyl-8-methylphenanthrene-3,4-dione	C69	PTGS2
2-isopropyl-8-methylphenanthrene-3,4-dione	C69	NOS3
2-isopropyl-8-methylphenanthrene-3,4-dione	C69	HTR3A
2-isopropyl-8-methylphenanthrene-3,4-dione	C69	CHRM4
2-isopropyl-8-methylphenanthrene-3,4-dione	C69	RXRA
2-isopropyl-8-methylphenanthrene-3,4-dione	C69	HTR2A
2-isopropyl-8-methylphenanthrene-3,4-dione	C69	ADRA1A
2-isopropyl-8-methylphenanthrene-3,4-dione	C69	CHRM2
2-isopropyl-8-methylphenanthrene-3,4-dione	C69	ADRA1B
2-isopropyl-8-methylphenanthrene-3,4-dione	C69	SLC6A3
2-isopropyl-8-methylphenanthrene-3,4-dione	C69	ADRB2
2-isopropyl-8-methylphenanthrene-3,4-dione	C69	ADRA1D
2-isopropyl-8-methylphenanthrene-3,4-dione	C69	SLC6A4
2-isopropyl-8-methylphenanthrene-3,4-dione	C69	OPRM1
2-isopropyl-8-methylphenanthrene-3,4-dione	C69	GABRA1
2-isopropyl-8-methylphenanthrene-3,4-dione	C69	CDK2
2-isopropyl-8-methylphenanthrene-3,4-dione	C69	PIK3CG
2-isopropyl-8-methylphenanthrene-3,4-dione	C69	CHRNA7
2-isopropyl-8-methylphenanthrene-3,4-dione	C69	KAPCA
2-isopropyl-8-methylphenanthrene-3,4-dione	C69	IGHG1
2-isopropyl-8-methylphenanthrene-3,4-dione	C69	PIM1
2-isopropyl-8-methylphenanthrene-3,4-dione	C69	CCNA2
2-isopropyl-8-methylphenanthrene-3,4-dione	C69	NCOA2
2-isopropyl-8-methylphenanthrene-3,4-dione	C69	PCP4
3α-hydroxytanshinonella	C70	SERPIND1
3α-hydroxytanshinonella	C70	CHRM1
3α-hydroxytanshinonella	C70	SCN5A
3α-hydroxytanshinonella	C70	CHRM5
3α-hydroxytanshinonella	C70	PTGS2
3α-hydroxytanshinonella	C70	OPRD1
3α-hydroxytanshinonella	C70	ACHE
3α-hydroxytanshinonella	C70	ADRB2
3α-hydroxytanshinonella	C70	OPRM1
3α-hydroxytanshinonella	C70	DPP4
3α-hydroxytanshinonella	C70	CHRNA7
3α-hydroxytanshinonella	C70	PRSS1
3α-hydroxytanshinonella	C70	NCOA1
(E)-3-[2-(3,4-dihydroxyphenyl)-7-hydroxy-benzofuran-4-yl]acrylic acid	C71	PTGS2
(E)-3-[2-(3,4-dihydroxyphenyl)-7-hydroxy-benzofuran-4-yl]acrylic acid	C71	PTPN1
(E)-3-[2-(3,4-dihydroxyphenyl)-7-hydroxy-benzofuran-4-yl]acrylic acid	C71	HSP90AA1
4-methylenemiltirone	C72	PTGS1
4-methylenemiltirone	C72	DRD1
4-methylenemiltirone	C72	CHRM3
4-methylenemiltirone	C72	CHRM1
4-methylenemiltirone	C72	ESR1
4-methylenemiltirone	C72	AR
4-methylenemiltirone	C72	SCN5A
4-methylenemiltirone	C72	PPARG
4-methylenemiltirone	C72	CHRM5
4-methylenemiltirone	C72	PTGS2
4-methylenemiltirone	C72	NOS3
4-methylenemiltirone	C72	ADRA2A
4-methylenemiltirone	C72	CA2
4-methylenemiltirone	C72	ADRA2C
4-methylenemiltirone	C72	CHRM4
4-methylenemiltirone	C72	RXRA
4-methylenemiltirone	C72	OPRD1

4-methylenemiltirone	C72	HTR2A
4-methylenemiltirone	C72	ADRA1A
4-methylenemiltirone	C72	CHRM2
4-methylenemiltirone	C72	ADRA1B
4-methylenemiltirone	C72	SLC6A3
4-methylenemiltirone	C72	ADRB2
4-methylenemiltirone	C72	ADRA1D
4-methylenemiltirone	C72	TOP2B
4-methylenemiltirone	C72	SLC6A4
4-methylenemiltirone	C72	DRD2
4-methylenemiltirone	C72	OPRM1
4-methylenemiltirone	C72	GABRA1
4-methylenemiltirone	C72	CHRNA7
4-methylenemiltirone	C72	KAPCA
4-methylenemiltirone	C72	NCOA2
4-methylenemiltirone	C72	NCOA1
2-(4-hydroxy-3-methoxyphenyl)-5-(3-hydroxypropyl)-7-methoxy-3-benzofurancarboxaldehyde	C73	NOS2
2-(4-hydroxy-3-methoxyphenyl)-5-(3-hydroxypropyl)-7-methoxy-3-benzofurancarboxaldehyde	C73	SERPIND1
2-(4-hydroxy-3-methoxyphenyl)-5-(3-hydroxypropyl)-7-methoxy-3-benzofurancarboxaldehyde	C73	ESR1
2-(4-hydroxy-3-methoxyphenyl)-5-(3-hydroxypropyl)-7-methoxy-3-benzofurancarboxaldehyde	C73	AR
2-(4-hydroxy-3-methoxyphenyl)-5-(3-hydroxypropyl)-7-methoxy-3-benzofurancarboxaldehyde	C73	PPARG
2-(4-hydroxy-3-methoxyphenyl)-5-(3-hydroxypropyl)-7-methoxy-3-benzofurancarboxaldehyde	C73	ESR2
2-(4-hydroxy-3-methoxyphenyl)-5-(3-hydroxypropyl)-7-methoxy-3-benzofurancarboxaldehyde	C73	MAPK14
2-(4-hydroxy-3-methoxyphenyl)-5-(3-hydroxypropyl)-7-methoxy-3-benzofurancarboxaldehyde	C73	GSK3B
2-(4-hydroxy-3-methoxyphenyl)-5-(3-hydroxypropyl)-7-methoxy-3-benzofurancarboxaldehyde	C73	HSP90AA1
2-(4-hydroxy-3-methoxyphenyl)-5-(3-hydroxypropyl)-7-methoxy-3-benzofurancarboxaldehyde	C73	CDK2
2-(4-hydroxy-3-methoxyphenyl)-5-(3-hydroxypropyl)-7-methoxy-3-benzofurancarboxaldehyde	C73	PIM1
2-(4-hydroxy-3-methoxyphenyl)-5-(3-hydroxypropyl)-7-methoxy-3-benzofurancarboxaldehyde	C73	CCNA2
formyltanshinone	C74	SERPIND1
formyltanshinone	C74	AR
formyltanshinone	C74	PTGS2
formyltanshinone	C74	RXRA
formyltanshinone	C74	DPP4
formyltanshinone	C74	PIK3CG
formyltanshinone	C74	KAPCA
formyltanshinone	C74	NCOA1
3-beta-Hydroxymethyllenetanshiquinone	C75	DRD1
3-beta-Hydroxymethyllenetanshiquinone	C75	SERPIND1
3-beta-Hydroxymethyllenetanshiquinone	C75	CHRM1
3-beta-Hydroxymethyllenetanshiquinone	C75	PTGS2
3-beta-Hydroxymethyllenetanshiquinone	C75	CA2
3-beta-Hydroxymethyllenetanshiquinone	C75	RXRA
3-beta-Hydroxymethyllenetanshiquinone	C75	OPRD1
3-beta-Hydroxymethyllenetanshiquinone	C75	ACHE
3-beta-Hydroxymethyllenetanshiquinone	C75	ADRA1A
3-beta-Hydroxymethyllenetanshiquinone	C75	ADRB2
3-beta-Hydroxymethyllenetanshiquinone	C75	OPRM1
3-beta-Hydroxymethyllenetanshiquinone	C75	DPP4
3-beta-Hydroxymethyllenetanshiquinone	C75	HSP90AA1
3-beta-Hydroxymethyllenetanshiquinone	C75	CHRNA7
3-beta-Hydroxymethyllenetanshiquinone	C75	IGHG1
3-beta-Hydroxymethyllenetanshiquinone	C75	PRSS1
3-beta-Hydroxymethyllenetanshiquinone	C75	NCOA1
Methylenetanshinquinone	C76	DRD1
Methylenetanshinquinone	C76	CHRM3
Methylenetanshinquinone	C76	SERPIND1
Methylenetanshinquinone	C76	CHRM1

Methylenetanshinquinone	C76	SCN5A
Methylenetanshinquinone	C76	CHRM5
Methylenetanshinquinone	C76	PTGS2
Methylenetanshinquinone	C76	CA2
Methylenetanshinquinone	C76	RXRA
Methylenetanshinquinone	C76	OPRD1
Methylenetanshinquinone	C76	ACHE
Methylenetanshinquinone	C76	HTR2A
Methylenetanshinquinone	C76	ADRA1A
Methylenetanshinquinone	C76	CHRM2
Methylenetanshinquinone	C76	ADRB2
Methylenetanshinquinone	C76	SLC6A4
Methylenetanshinquinone	C76	OPRM1
Methylenetanshinquinone	C76	GABRA1
Methylenetanshinquinone	C76	DPP4
Methylenetanshinquinone	C76	HSP90AA1
Methylenetanshinquinone	C76	CHRNA7
Methylenetanshinquinone	C76	IGHG1
Methylenetanshinquinone	C76	PRSS1
Methylenetanshinquinone	C76	NCOA1
przewalskin a	C77	NR3C2
przewalskin a	C77	NR3C1
przewalskin b	C78	PTGS2
przewalskin b	C78	PGR
przewalskin b	C78	NR3C2
przewalskin b	C78	NR3C1
przewalskin b	C78	NCOA2
przewalskin b	C78	NCOA1
Przewaquinone B	C79	SERPIND1
Przewaquinone B	C79	PTGS2
Przewaquinone B	C79	RXRA
Przewaquinone B	C79	DPP4
Przewaquinone B	C79	HSP90AA1
Przewaquinone B	C79	PIK3CG
Przewaquinone B	C79	IGHG1
Przewaquinone B	C79	PRSS1
Przewaquinone B	C79	NCOA1
przewaquinone c	C80	PTGS1
przewaquinone c	C80	DRD1
przewaquinone c	C80	CHRM3
przewaquinone c	C80	SERPIND1
przewaquinone c	C80	CHRM1
przewaquinone c	C80	SCN5A
przewaquinone c	C80	CHRM5
przewaquinone c	C80	PTGS2
przewaquinone c	C80	CA2
przewaquinone c	C80	CHRM4
przewaquinone c	C80	OPRD1
przewaquinone c	C80	ACHE
przewaquinone c	C80	ADRA1A
przewaquinone c	C80	CHRM2
przewaquinone c	C80	ADRB2
przewaquinone c	C80	OPRM1
przewaquinone c	C80	GABRA1
przewaquinone c	C80	DPP4
przewaquinone c	C80	HSP90AA1
przewaquinone c	C80	PIK3CG

przewaquinone c	C80	CHRNA7
przewaquinone c	C80	NCOA1
(6S,7R)-6,7-dihydroxy-1,6-dimethyl-8,9-dihydro-7H-naphtho[8,7-g]benzofuran-10,11-dione	C81	SERPIND1
(6S,7R)-6,7-dihydroxy-1,6-dimethyl-8,9-dihydro-7H-naphtho[8,7-g]benzofuran-10,11-dione	C81	PTGS2
(6S,7R)-6,7-dihydroxy-1,6-dimethyl-8,9-dihydro-7H-naphtho[8,7-g]benzofuran-10,11-dione	C81	CA2
(6S,7R)-6,7-dihydroxy-1,6-dimethyl-8,9-dihydro-7H-naphtho[8,7-g]benzofuran-10,11-dione	C81	ACHE
(6S,7R)-6,7-dihydroxy-1,6-dimethyl-8,9-dihydro-7H-naphtho[8,7-g]benzofuran-10,11-dione	C81	DPP4
(6S,7R)-6,7-dihydroxy-1,6-dimethyl-8,9-dihydro-7H-naphtho[8,7-g]benzofuran-10,11-dione	C81	HSP90AA1
(6S,7R)-6,7-dihydroxy-1,6-dimethyl-8,9-dihydro-7H-naphtho[8,7-g]benzofuran-10,11-dione	C81	PRSS1
(6S,7R)-6,7-dihydroxy-1,6-dimethyl-8,9-dihydro-7H-naphtho[8,7-g]benzofuran-10,11-dione	C81	NCOA1
przewaquinone f	C82	SERPIND1
przewaquinone f	C82	PTGS2
przewaquinone f	C82	DPP4
przewaquinone f	C82	PRSS1
przewaquinone f	C82	NCOA1
sclareol	C83	PTGS2
tanshinaldehyde	C84	DRD1
tanshinaldehyde	C84	SERPIND1
tanshinaldehyde	C84	CHRM1
tanshinaldehyde	C84	PTGS2
tanshinaldehyde	C84	OPRD1
tanshinaldehyde	C84	ACHE
tanshinaldehyde	C84	HTR2A
tanshinaldehyde	C84	ADRB2
tanshinaldehyde	C84	OPRM1
tanshinaldehyde	C84	DPP4
tanshinaldehyde	C84	CHRNA7
tanshinaldehyde	C84	PRSS1
tanshinaldehyde	C84	NCOA1
Danshenol B	C85	PTGS2
Danshenol B	C85	CA2
Danshenol B	C85	PGR
Danshenol B	C85	TOP2B
Danshenol B	C85	OPRM1
Danshenol B	C85	NR3C1
Danshenol B	C85	HSP90AA1
Danshenol B	C85	NCOA1
Danshenol A	C86	PTGS1
Danshenol A	C86	KCNH2
Danshenol A	C86	SCN5A
Danshenol A	C86	FXa
Danshenol A	C86	PTGS2
Danshenol A	C86	RXRA
Danshenol A	C86	PIK3CG
Danshenol A	C86	NCOA1
Danshenol A	C86	KCNMA1
Salvilenone	C87	PTGS1
Salvilenone	C87	ESR1
Salvilenone	C87	AR
Salvilenone	C87	CHRM5
Salvilenone	C87	PTGS2
Salvilenone	C87	HTR3A
Salvilenone	C87	ESR2
Salvilenone	C87	PIM1
cryptotanshinone	C88	PTGS1
cryptotanshinone	C88	DRD1
cryptotanshinone	C88	CHRM3

cryptotanshinone	C88	CHRM1
cryptotanshinone	C88	SCN5A
cryptotanshinone	C88	CHRM5
cryptotanshinone	C88	PTGS2
cryptotanshinone	C88	CA2
cryptotanshinone	C88	CHRM4
cryptotanshinone	C88	OPRD1
cryptotanshinone	C88	ADRA1A
cryptotanshinone	C88	CHRM2
cryptotanshinone	C88	ADRA1B
cryptotanshinone	C88	ADRB2
cryptotanshinone	C88	ADRA1D
cryptotanshinone	C88	TOP2B
cryptotanshinone	C88	OPRM1
cryptotanshinone	C88	CHRNA7
cryptotanshinone	C88	NCOA2
cryptotanshinone	C88	NCOA1
cryptotanshinone	C88	PGR
cryptotanshinone	C88	GABRA1
cryptotanshinone	C88	RELA
cryptotanshinone	C88	STAT3
cryptotanshinone	C88	CCND1
cryptotanshinone	C88	BCL2L1
cryptotanshinone	C88	TNF
cryptotanshinone	C88	APBA3
cryptotanshinone	C88	EDN1
cryptotanshinone	C88	BIRC5
dan-shexinkum d	C89	NOS2
dan-shexinkum d	C89	PTGS1
dan-shexinkum d	C89	SERPIND1
dan-shexinkum d	C89	KCNH2
dan-shexinkum d	C89	CHRM1
dan-shexinkum d	C89	ESR1
dan-shexinkum d	C89	AR
dan-shexinkum d	C89	SCN5A
dan-shexinkum d	C89	PPARG
dan-shexinkum d	C89	FXa
dan-shexinkum d	C89	PTGS2
dan-shexinkum d	C89	CA2
dan-shexinkum d	C89	RXRA
dan-shexinkum d	C89	ACHE
dan-shexinkum d	C89	ADRA1B
dan-shexinkum d	C89	ADRB2
dan-shexinkum d	C89	TOP2B
dan-shexinkum d	C89	ESR2
dan-shexinkum d	C89	DPP4
dan-shexinkum d	C89	GSK3B
dan-shexinkum d	C89	CDK2
dan-shexinkum d	C89	CHEK1
dan-shexinkum d	C89	IGHG1
dan-shexinkum d	C89	PRSS1
dan-shexinkum d	C89	PIM1
dan-shexinkum d	C89	CCNA2
dan-shexinkum d	C89	NCOA2
dan-shexinkum d	C89	NCOA1
dan-shexinkum d	C89	PCP4
danshenspiroketallactone	C90	PTGS1

danshenspiroketallactone	C90	DRD1
danshenspiroketallactone	C90	CHRM3
danshenspiroketallactone	C90	SERPIND1
danshenspiroketallactone	C90	CHRM1
danshenspiroketallactone	C90	ESR1
danshenspiroketallactone	C90	SCN5A
danshenspiroketallactone	C90	CHRM5
danshenspiroketallactone	C90	PTGS2
danshenspiroketallactone	C90	CA2
danshenspiroketallactone	C90	CHRM4
danshenspiroketallactone	C90	RXRA
danshenspiroketallactone	C90	ACHE
danshenspiroketallactone	C90	ADRA1A
danshenspiroketallactone	C90	CHRM2
danshenspiroketallactone	C90	ADRA1B
danshenspiroketallactone	C90	ADRB2
danshenspiroketallactone	C90	ADRA1D
danshenspiroketallactone	C90	CHRNA2
danshenspiroketallactone	C90	SLC6A4
danshenspiroketallactone	C90	OPRM1
danshenspiroketallactone	C90	GABRA1
danshenspiroketallactone	C90	DPP4
danshenspiroketallactone	C90	HSP90AA1
danshenspiroketallactone	C90	CHRNA7
deoxyneocryptotanshinone	C91	PTGS1
deoxyneocryptotanshinone	C91	DRD1
deoxyneocryptotanshinone	C91	CHRM3
deoxyneocryptotanshinone	C91	CHRM1
deoxyneocryptotanshinone	C91	ESR1
deoxyneocryptotanshinone	C91	AR
deoxyneocryptotanshinone	C91	SCN5A
deoxyneocryptotanshinone	C91	CHRM5
deoxyneocryptotanshinone	C91	PTGS2
deoxyneocryptotanshinone	C91	NOS3
deoxyneocryptotanshinone	C91	CA2
deoxyneocryptotanshinone	C91	CHRM4
deoxyneocryptotanshinone	C91	RXRA
deoxyneocryptotanshinone	C91	OPRD1
deoxyneocryptotanshinone	C91	ADRA1A
deoxyneocryptotanshinone	C91	CHRM2
deoxyneocryptotanshinone	C91	ADRA1B
deoxyneocryptotanshinone	C91	ADRB2
deoxyneocryptotanshinone	C91	ADRA1D
deoxyneocryptotanshinone	C91	TOP2B
deoxyneocryptotanshinone	C91	OPRM1
deoxyneocryptotanshinone	C91	GSK3B
deoxyneocryptotanshinone	C91	CDK2
deoxyneocryptotanshinone	C91	CHRNA7
deoxyneocryptotanshinone	C91	IGHG1
deoxyneocryptotanshinone	C91	PIM1
deoxyneocryptotanshinone	C91	NCOA2
deoxyneocryptotanshinone	C91	NCOA1
dihydrotanshinlactone	C92	NOS2
dihydrotanshinlactone	C92	PTGS1
dihydrotanshinlactone	C92	DRD1
dihydrotanshinlactone	C92	CHRM3
dihydrotanshinlactone	C92	SERPIND1

dihydrotanshinlactone	C92	CHRM1
dihydrotanshinlactone	C92	ESR1
dihydrotanshinlactone	C92	AR
dihydrotanshinlactone	C92	SCN5A
dihydrotanshinlactone	C92	PPARG
dihydrotanshinlactone	C92	CHRM5
dihydrotanshinlactone	C92	PTGS2
dihydrotanshinlactone	C92	HTR3A
dihydrotanshinlactone	C92	CA2
dihydrotanshinlactone	C92	RXRA
dihydrotanshinlactone	C92	ACHE
dihydrotanshinlactone	C92	PDE3A
dihydrotanshinlactone	C92	HTR2A
dihydrotanshinlactone	C92	ADRA1A
dihydrotanshinlactone	C92	ADRA1B
dihydrotanshinlactone	C92	PTPN1
dihydrotanshinlactone	C92	SLC6A3
dihydrotanshinlactone	C92	ADRB2
dihydrotanshinlactone	C92	ADRA1D
dihydrotanshinlactone	C92	SLC6A4
dihydrotanshinlactone	C92	OPRM1
dihydrotanshinlactone	C92	GABRA1
dihydrotanshinlactone	C92	DPP4
dihydrotanshinlactone	C92	GSK3B
dihydrotanshinlactone	C92	PIK3CG
dihydrotanshinlactone	C92	CHRNA7
dihydrotanshinlactone	C92	KAPCA
dihydrotanshinlactone	C92	IGHG1
dihydrotanshinlactone	C92	PRSS1
dihydrotanshinlactone	C92	PIM1
dihydrotanshinlactone	C92	CCNA2
dihydrotanshinone I	C93	PTGS1
dihydrotanshinone I	C93	SCN5A
dihydrotanshinone I	C93	PTGS2
dihydrotanshinone I	C93	HTR3A
dihydrotanshinone I	C93	RXRA
dihydrotanshinone I	C93	ADRA1A
dihydrotanshinone I	C93	ADRA1B
dihydrotanshinone I	C93	ADRB2
dihydrotanshinone I	C93	GABRA1
dihydrotanshinone I	C93	HSP90AA1
dihydrotanshinone I	C93	PIK3CG
dihydrotanshinone I	C93	CHRNA7
dihydrotanshinone I	C93	KAPCA
dihydrotanshinone I	C93	IGHG1
dihydrotanshinone I	C93	NCOA2
dihydrotanshinone I	C93	NCOA1
dihydrotanshinone I	C93	PCP4
epidanshenspiroketallactone	C94	PTGS1
epidanshenspiroketallactone	C94	DRD1
epidanshenspiroketallactone	C94	CHRM3
epidanshenspiroketallactone	C94	CHRM1
epidanshenspiroketallactone	C94	ESR1
epidanshenspiroketallactone	C94	SCN5A
epidanshenspiroketallactone	C94	CHRM5
epidanshenspiroketallactone	C94	PTGS2
epidanshenspiroketallactone	C94	NOS3

epidanshenspiroketallactone	C94	CHRM4
epidanshenspiroketallactone	C94	RXRA
epidanshenspiroketallactone	C94	OPRD1
epidanshenspiroketallactone	C94	PDE3A
epidanshenspiroketallactone	C94	HTR2A
epidanshenspiroketallactone	C94	ADRA1A
epidanshenspiroketallactone	C94	CHRM2
epidanshenspiroketallactone	C94	ADRA1B
epidanshenspiroketallactone	C94	ADRB2
epidanshenspiroketallactone	C94	ADRA1D
epidanshenspiroketallactone	C94	SLC6A4
epidanshenspiroketallactone	C94	OPRM1
epidanshenspiroketallactone	C94	GABRA1
epidanshenspiroketallactone	C94	HSP90AA1
epidanshenspiroketallactone	C94	CDK2
epidanshenspiroketallactone	C94	CHRNA7
epidanshenspiroketallactone	C94	PIM1
C09092	C95	CHRM3
C09092	C95	SERPIND1
C09092	C95	CHRM1
C09092	C95	SCN5A
C09092	C95	CA2
C09092	C95	ACHE
C09092	C95	ADRA1A
C09092	C95	CHRM2
C09092	C95	ADRA1B
C09092	C95	ADRB2
C09092	C95	ADRA1D
C09092	C95	OPRM1
isocryptotanshi-none	C96	NOS2
isocryptotanshi-none	C96	PTGS1
isocryptotanshi-none	C96	DRD1
isocryptotanshi-none	C96	CHRM3
isocryptotanshi-none	C96	CHRM1
isocryptotanshi-none	C96	ESR1
isocryptotanshi-none	C96	AR
isocryptotanshi-none	C96	SCN5A
isocryptotanshi-none	C96	FXa
isocryptotanshi-none	C96	CHRM5
isocryptotanshi-none	C96	PTGS2
isocryptotanshi-none	C96	CA2
isocryptotanshi-none	C96	CHRM4
isocryptotanshi-none	C96	RXRA
isocryptotanshi-none	C96	OPRD1
isocryptotanshi-none	C96	ACHE
isocryptotanshi-none	C96	ADRA1A
isocryptotanshi-none	C96	CHRM2
isocryptotanshi-none	C96	ADRA1B
isocryptotanshi-none	C96	ADRB2
isocryptotanshi-none	C96	ADRA1D
isocryptotanshi-none	C96	TOP2B
isocryptotanshi-none	C96	DRD2
isocryptotanshi-none	C96	OPRM1
isocryptotanshi-none	C96	GABRA1
isocryptotanshi-none	C96	CDK2
isocryptotanshi-none	C96	CHRNA7
isocryptotanshi-none	C96	PRSS1

isocryptotanshi-none	C96	PIM1
isocryptotanshi-none	C96	NCOA2
isocryptotanshi-none	C96	NCOA1
Isotanshinone II	C97	NOS2
Isotanshinone II	C97	DRD1
Isotanshinone II	C97	CHRM3
Isotanshinone II	C97	SERPIND1
Isotanshinone II	C97	CHRM1
Isotanshinone II	C97	ESR1
Isotanshinone II	C97	AR
Isotanshinone II	C97	SCN5A
Isotanshinone II	C97	CHRM5
Isotanshinone II	C97	PTGS2
Isotanshinone II	C97	RXRA
Isotanshinone II	C97	OPRD1
Isotanshinone II	C97	ACHE
Isotanshinone II	C97	ADRA1A
Isotanshinone II	C97	CHRM2
Isotanshinone II	C97	ADRB2
Isotanshinone II	C97	OPRM1
Isotanshinone II	C97	ESR2
Isotanshinone II	C97	GABRA1
Isotanshinone II	C97	DPP4
Isotanshinone II	C97	GSK3B
Isotanshinone II	C97	CDK2
Isotanshinone II	C97	CHRNA7
Isotanshinone II	C97	CHEK1
Isotanshinone II	C97	PIM1
Isotanshinone II	C97	CCNA2
manool	C98	NCOA2
miltionone I	C99	PTGS1
miltionone I	C99	CHRM3
miltionone I	C99	CHRM1
miltionone I	C99	ESR1
miltionone I	C99	AR
miltionone I	C99	SCN5A
miltionone I	C99	FXa
miltionone I	C99	PTGS2
miltionone I	C99	CA2
miltionone I	C99	RXRA
miltionone I	C99	OPRD1
miltionone I	C99	HTR2A
miltionone I	C99	ADRA1A
miltionone I	C99	CHRM2
miltionone I	C99	ADRA1B
miltionone I	C99	ADRB2
miltionone I	C99	TOP2B
miltionone I	C99	OPRM1
miltionone I	C99	NR3C1
miltionone I	C99	GSK3B
miltionone I	C99	CDK2
miltionone I	C99	LACTBL1
miltionone I	C99	CHRNA7
miltionone I	C99	IGHG1
miltionone I	C99	PIM1
miltionone I	C99	CCNA2
miltionone I	C99	NCOA2

miltionone I	C99	NCOA1
miltionone II	C100	SERPIND1
miltionone II	C100	PTGS2
miltionone II	C100	CA2
miltionone II	C100	ACHE
miltionone II	C100	PGR
miltionone II	C100	NR3C1
miltionone II	C100	NCOA2
miltionone II	C100	NCOA1
miltipolone	C101	ESR1
miltipolone	C101	ACHE
Miltirone	C102	PTGS1
Miltirone	C102	DRD1
Miltirone	C102	CHRM3
Miltirone	C102	CHRM1
Miltirone	C102	ESR1
Miltirone	C102	AR
Miltirone	C102	DRD5
Miltirone	C102	SCN5A
Miltirone	C102	CHRM5
Miltirone	C102	PTGS2
Miltirone	C102	NOS3
Miltirone	C102	CA2
Miltirone	C102	ADRA2C
Miltirone	C102	CHRM4
Miltirone	C102	RXRA
Miltirone	C102	OPRD1
Miltirone	C102	ADRA1A
Miltirone	C102	CHRM2
Miltirone	C102	ADRA1B
Miltirone	C102	SLC6A3
Miltirone	C102	ADRB2
Miltirone	C102	ADRA1D
Miltirone	C102	TOP2B
Miltirone	C102	OPRM1
Miltirone	C102	CHRNA7
Miltirone	C102	NCOA2
neocryptotanshinone ii	C103	PTGS1
neocryptotanshinone ii	C103	DRD1
neocryptotanshinone ii	C103	CHRM3
neocryptotanshinone ii	C103	CHRM1
neocryptotanshinone ii	C103	ESR1
neocryptotanshinone ii	C103	AR
neocryptotanshinone ii	C103	SCN5A
neocryptotanshinone ii	C103	PTGS2
neocryptotanshinone ii	C103	NOS3
neocryptotanshinone ii	C103	CA2
neocryptotanshinone ii	C103	CHRM4
neocryptotanshinone ii	C103	RXRA
neocryptotanshinone ii	C103	OPRD1
neocryptotanshinone ii	C103	PDE3A
neocryptotanshinone ii	C103	ADRA1A
neocryptotanshinone ii	C103	CHRM2
neocryptotanshinone ii	C103	ADRA1B
neocryptotanshinone ii	C103	SLC6A3
neocryptotanshinone ii	C103	ADRB2
neocryptotanshinone ii	C103	ADRA1D

neocryptotanshinone ii	C103	SLC6A4
neocryptotanshinone ii	C103	OPRM1
neocryptotanshinone ii	C103	GABRA1
neocryptotanshinone ii	C103	GSK3B
neocryptotanshinone ii	C103	HSP90AA1
neocryptotanshinone ii	C103	CDK2
neocryptotanshinone ii	C103	CHRNA7
neocryptotanshinone ii	C103	PIM1
neocryptotanshinone ii	C103	CCNA2
neocryptotanshinone	C104	PTGS1
neocryptotanshinone	C104	CHRM3
neocryptotanshinone	C104	CHRM1
neocryptotanshinone	C104	SCN5A
neocryptotanshinone	C104	PPARG
neocryptotanshinone	C104	PTGS2
neocryptotanshinone	C104	CA2
neocryptotanshinone	C104	ADRA1B
neocryptotanshinone	C104	ADRB2
neocryptotanshinone	C104	ADRA1D
neocryptotanshinone	C104	TOP2B
neocryptotanshinone	C104	OPRM1
neocryptotanshinone	C104	CHRNA7
neocryptotanshinone	C104	IGHG1
neocryptotanshinone	C104	NCOA2
neocryptotanshinone	C104	NCOA1
1-methyl-8,9-dihydro-7H-naphtho[5,6-g]benzofuran-6,10,11-trione	C105	PTGS1
1-methyl-8,9-dihydro-7H-naphtho[5,6-g]benzofuran-6,10,11-trione	C105	DRD1
1-methyl-8,9-dihydro-7H-naphtho[5,6-g]benzofuran-6,10,11-trione	C105	CHRM3
1-methyl-8,9-dihydro-7H-naphtho[5,6-g]benzofuran-6,10,11-trione	C105	SERPIND1
1-methyl-8,9-dihydro-7H-naphtho[5,6-g]benzofuran-6,10,11-trione	C105	SCN5A
1-methyl-8,9-dihydro-7H-naphtho[5,6-g]benzofuran-6,10,11-trione	C105	CHRM5
1-methyl-8,9-dihydro-7H-naphtho[5,6-g]benzofuran-6,10,11-trione	C105	PTGS2
1-methyl-8,9-dihydro-7H-naphtho[5,6-g]benzofuran-6,10,11-trione	C105	CA2
1-methyl-8,9-dihydro-7H-naphtho[5,6-g]benzofuran-6,10,11-trione	C105	RXRA
1-methyl-8,9-dihydro-7H-naphtho[5,6-g]benzofuran-6,10,11-trione	C105	ACHE
1-methyl-8,9-dihydro-7H-naphtho[5,6-g]benzofuran-6,10,11-trione	C105	ADRA1A
1-methyl-8,9-dihydro-7H-naphtho[5,6-g]benzofuran-6,10,11-trione	C105	ADRB2
1-methyl-8,9-dihydro-7H-naphtho[5,6-g]benzofuran-6,10,11-trione	C105	OPRM1
1-methyl-8,9-dihydro-7H-naphtho[5,6-g]benzofuran-6,10,11-trione	C105	GABRA1
1-methyl-8,9-dihydro-7H-naphtho[5,6-g]benzofuran-6,10,11-trione	C105	DPP4
1-methyl-8,9-dihydro-7H-naphtho[5,6-g]benzofuran-6,10,11-trione	C105	HSP90AA1
1-methyl-8,9-dihydro-7H-naphtho[5,6-g]benzofuran-6,10,11-trione	C105	PIK3CG
1-methyl-8,9-dihydro-7H-naphtho[5,6-g]benzofuran-6,10,11-trione	C105	CHRNA7
1-methyl-8,9-dihydro-7H-naphtho[5,6-g]benzofuran-6,10,11-trione	C105	IGHG1
1-methyl-8,9-dihydro-7H-naphtho[5,6-g]benzofuran-6,10,11-trione	C105	NCOA1
prolithospermic acid	C106	NOS2
prolithospermic acid	C106	PTGS1
prolithospermic acid	C106	SERPIND1
prolithospermic acid	C106	ESR1
prolithospermic acid	C106	AR
prolithospermic acid	C106	PTGS2
prolithospermic acid	C106	PTPN1
prolithospermic acid	C106	HSP90AA1
prolithospermic acid	C106	PRSS1
prolithospermic acid	C106	PCP4
(2R)-3-(3,4-dihydroxyphenyl)-2-[(Z)-3-(3,4-dihydroxyphenyl)acryloyl]oxy-propionic acid	C107	SERPIND1
(2R)-3-(3,4-dihydroxyphenyl)-2-[(Z)-3-(3,4-dihydroxyphenyl)acryloyl]oxy-propionic acid	C107	ESR1

(2R)-3-(3,4-dihydroxyphenyl)-2-[(Z)-3-(3,4-dihydroxyphenyl)acryloyl]oxy-propionic acid	C107	AR
(2R)-3-(3,4-dihydroxyphenyl)-2-[(Z)-3-(3,4-dihydroxyphenyl)acryloyl]oxy-propionic acid	C107	PPARG
(2R)-3-(3,4-dihydroxyphenyl)-2-[(Z)-3-(3,4-dihydroxyphenyl)acryloyl]oxy-propionic acid	C107	PTGS2
(2R)-3-(3,4-dihydroxyphenyl)-2-[(Z)-3-(3,4-dihydroxyphenyl)acryloyl]oxy-propionic acid	C107	DPP4
(2R)-3-(3,4-dihydroxyphenyl)-2-[(Z)-3-(3,4-dihydroxyphenyl)acryloyl]oxy-propionic acid	C107	PRSS1
(2R)-3-(3,4-dihydroxyphenyl)-2-[(Z)-3-(3,4-dihydroxyphenyl)acryloyl]oxy-propionic acid	C107	CCNA2
salvianolic acid g	C108	PTGS2
salvianolic acid j	C109	F7
salvianolic acid j	C109	PTPN1
salvianolic acid j	C109	PRSS1
salvilenone l	C110	PTGS2
salvilenone l	C110	RXRA
salvilenone l	C110	ACHE
salvilenone l	C110	PGR
salvilenone l	C110	PTPN1
salvilenone l	C110	NR3C1
salvilenone l	C110	NCOA2
salvilenone l	C110	NCOA1
salviolone	C111	PTGS1
salviolone	C111	DRD1
salviolone	C111	CHRM3
salviolone	C111	SERPIND1
salviolone	C111	CHRM1
salviolone	C111	DRD5
salviolone	C111	SCN5A
salviolone	C111	CHRM5
salviolone	C111	PTGS2
salviolone	C111	ADRA2A
salviolone	C111	HTR1A
salviolone	C111	HTR3A
salviolone	C111	GABRA2
salviolone	C111	CHRM4
salviolone	C111	OPRD1
salviolone	C111	ACHE
salviolone	C111	PDE3A
salviolone	C111	HTR2A
salviolone	C111	GABRA5
salviolone	C111	SLC6A2
salviolone	C111	ADRA1A
salviolone	C111	GABRA3
salviolone	C111	HTR2C
salviolone	C111	CHRM2
salviolone	C111	ADRA2B
salviolone	C111	ADRA1B
salviolone	C111	SLC6A3
salviolone	C111	ADRB2
salviolone	C111	CHRNA2
salviolone	C111	SLC6A4
salviolone	C111	DRD2
salviolone	C111	OPRM1
salviolone	C111	GABRA1
salviolone	C111	HTR1B
salviolone	C111	CHRNA7
salviolone	C111	GABRA6
salviolone	C111	GABRG3
salviolone	C111	GABRE
(6S)-6-hydroxy-1-methyl-6-methylol-8,9-dihydro-7H-naphtho[8,7-g]benzofuran-10,11-quinone	C112	SERPIND1

(6S)-6-hydroxy-1-methyl-6-methylol-8,9-dihydro-7H-naphtho[8,7-g]benzofuran-10,11-quinone	C112	PTGS2
(6S)-6-hydroxy-1-methyl-6-methylol-8,9-dihydro-7H-naphtho[8,7-g]benzofuran-10,11-quinone	C112	CA2
(6S)-6-hydroxy-1-methyl-6-methylol-8,9-dihydro-7H-naphtho[8,7-g]benzofuran-10,11-quinone	C112	ACHE
(6S)-6-hydroxy-1-methyl-6-methylol-8,9-dihydro-7H-naphtho[8,7-g]benzofuran-10,11-quinone	C112	DPP4
(6S)-6-hydroxy-1-methyl-6-methylol-8,9-dihydro-7H-naphtho[8,7-g]benzofuran-10,11-quinone	C112	HSP90AA1
(6S)-6-hydroxy-1-methyl-6-methylol-8,9-dihydro-7H-naphtho[8,7-g]benzofuran-10,11-quinone	C112	PRSS1
(6S)-6-hydroxy-1-methyl-6-methylol-8,9-dihydro-7H-naphtho[8,7-g]benzofuran-10,11-quinone	C112	NCOA1
Tanshindiol B	C113	SERPIND1
Tanshindiol B	C113	PTGS2
Tanshindiol B	C113	CA2
Tanshindiol B	C113	ACHE
Tanshindiol B	C113	DPP4
Tanshindiol B	C113	HSP90AA1
Tanshindiol B	C113	NCOA1
Przewaquinone E	C114	SERPIND1
Przewaquinone E	C114	PTGS2
Przewaquinone E	C114	CA2
Przewaquinone E	C114	ACHE
Przewaquinone E	C114	DPP4
Przewaquinone E	C114	HSP90AA1
Przewaquinone E	C114	NCOA1
tanshinone iia	C115	DRD1
tanshinone iia	C115	CHRM3
tanshinone iia	C115	SERPIND1
tanshinone iia	C115	CHRM1
tanshinone iia	C115	SCN5A
tanshinone iia	C115	CHRM5
tanshinone iia	C115	PTGS2
tanshinone iia	C115	CHRM4
tanshinone iia	C115	OPRD1
tanshinone iia	C115	ACHE
tanshinone iia	C115	ADRA1A
tanshinone iia	C115	CHRM2
tanshinone iia	C115	ADRB2
tanshinone iia	C115	OPRM1
tanshinone iia	C115	DPP4
tanshinone iia	C115	CHRNA7
tanshinone iia	C115	NCOA1
tanshinone iia	C115	RXRA
tanshinone iia	C115	RELA
tanshinone iia	C115	BCL2
tanshinone iia	C115	FOS
tanshinone iia	C115	CDKN1A
tanshinone iia	C115	MMP9
tanshinone iia	C115	JUN
tanshinone iia	C115	AHSA1
tanshinone iia	C115	CASP3
tanshinone iia	C115	TP53
tanshinone iia	C115	NFKBIA
tanshinone iia	C115	FASN
tanshinone iia	C115	EDNRA
tanshinone iia	C115	EDN1
tanshinone iia	C115	CYP3A4
tanshinone iia	C115	CYP1A2
tanshinone iia	C115	MYC
tanshinone iia	C115	CYP1A1

	tanshinone iia	C115	NR1I2
	tanshinone iia	C115	NPM1
	tanshinone iia	C115	ECE1
	tanshinone iia	C115	PARP4
	tanshinone iia	C115	CALCR
	tanshinone iia	C115	ITGB3
	(6S)-6-(hydroxymethyl)-1,6-dimethyl-8,9-dihydro-7H-naphtho[8,7-g]benzofuran-10,11-dione	C116	SERPIND1
	(6S)-6-(hydroxymethyl)-1,6-dimethyl-8,9-dihydro-7H-naphtho[8,7-g]benzofuran-10,11-dione	C116	CHRM1
	(6S)-6-(hydroxymethyl)-1,6-dimethyl-8,9-dihydro-7H-naphtho[8,7-g]benzofuran-10,11-dione	C116	SCN5A
	(6S)-6-(hydroxymethyl)-1,6-dimethyl-8,9-dihydro-7H-naphtho[8,7-g]benzofuran-10,11-dione	C116	PTGS2
	(6S)-6-(hydroxymethyl)-1,6-dimethyl-8,9-dihydro-7H-naphtho[8,7-g]benzofuran-10,11-dione	C116	OPRD1
	(6S)-6-(hydroxymethyl)-1,6-dimethyl-8,9-dihydro-7H-naphtho[8,7-g]benzofuran-10,11-dione	C116	ACHE
	(6S)-6-(hydroxymethyl)-1,6-dimethyl-8,9-dihydro-7H-naphtho[8,7-g]benzofuran-10,11-dione	C116	ADRA1A
	(6S)-6-(hydroxymethyl)-1,6-dimethyl-8,9-dihydro-7H-naphtho[8,7-g]benzofuran-10,11-dione	C116	ADRB2
	(6S)-6-(hydroxymethyl)-1,6-dimethyl-8,9-dihydro-7H-naphtho[8,7-g]benzofuran-10,11-dione	C116	OPRM1
	(6S)-6-(hydroxymethyl)-1,6-dimethyl-8,9-dihydro-7H-naphtho[8,7-g]benzofuran-10,11-dione	C116	DPP4
	(6S)-6-(hydroxymethyl)-1,6-dimethyl-8,9-dihydro-7H-naphtho[8,7-g]benzofuran-10,11-dione	C116	CHRNA7
	(6S)-6-(hydroxymethyl)-1,6-dimethyl-8,9-dihydro-7H-naphtho[8,7-g]benzofuran-10,11-dione	C116	PRSS1
	(6S)-6-(hydroxymethyl)-1,6-dimethyl-8,9-dihydro-7H-naphtho[8,7-g]benzofuran-10,11-dione	C116	NCOA1
	tanshinone VI	C117	PTGS1
	tanshinone VI	C117	ESR1
	tanshinone VI	C117	AR
	tanshinone VI	C117	SCN5A
	tanshinone VI	C117	PPARG
	tanshinone VI	C117	FXa
	tanshinone VI	C117	PTGS2
	tanshinone VI	C117	HSP90AA1
	tanshinone VI	C117	LACTBL1
	tanshinone VI	C117	IGHG1
	tanshinone VI	C117	NCOA2
	tanshinone VI	C117	NCOA1
	tanshinone VI	C117	PCP4
zedoray rhizome	hederagenin	C2	PGR
	hederagenin	C2	NCOA2
	hederagenin	C2	CHRM3
	hederagenin	C2	CHRM1
	hederagenin	C2	GABRA2
	hederagenin	C2	GABRA3
	hederagenin	C2	CHRM2
	hederagenin	C2	ADRA1B
	hederagenin	C2	GABRA1
	hederagenin	C2	GRIA2
	hederagenin	C2	GABRA6
	hederagenin	C2	GABRA5
	hederagenin	C2	IGHG1
	hederagenin	C2	ADH1B
	hederagenin	C2	ADH1C
	hederagenin	C2	LYZ
	hederagenin	C2	COBT
	hederagenin	C2	PTGS1
	hederagenin	C2	SCN5A
	hederagenin	C2	PTGS2
	hederagenin	C2	RXRA
	hederagenin	C2	PDE3A
	hederagenin	C2	SLC6A2
	hederagenin	C2	NOR51B

Table S2. Targets of Shiquan Yuzhen Decoction

common buried rubber	ginseng	milkvetch root	chinese yam	common anemarrhena rhizome	figwort root	radix salviae miltiorrhizae	zedoray rhizome
PTGS1	SCN5A	PGR	CHRM1	SERPIND1	CHRM3	PTGS1	PGR
NCOA2	ADRB2	NOS2	NOS3	KCNH2	CHRM1	CHRM3	NCOA2
CHRM1	CHRM3	PTGS1	RXRA	FXa	SCN5A	CHRM1	CHRM3
PTGS2	PGR	AR	PDE3A	PTGS2	CHRM5	SCN5A	CHRM1
GABRA2	NR3C2	SCN5A	ADRA1B	PRSS1	PTGS2	CHRM5	GABRA2
GABRA1	NCOA2	PTGS2	SLC6A3	NOS2	CA2	PTGS2	GABRA3
CHRNA7	ADH1C	ESR2	ADRB2	PTGS1	CHRM4	HTR3A	CHRM2
GABRA6	IGHG1	DPP4	SLC6A4	AR	OPRD1	CA2	ADRA1B
PGR	RXRA	HSP90AA1	LTA4H	PPARG	ACHE	CHRM4	GABRA1
CHRM3	NCOA1	CDK2	MAOB	HSP90AA1	ADRA1A	RXRA	GRIA2
GABRA3	PTGS1	CHEK1	SAA1	PIK3CG	CHRM2	OPRD1	GABRA6
CHRM2	PTGS2	PRSS1	PTGS1	KAPCA	ADRA1B	PDE3A	GABRA5
ADRA1B	ADRA2A	NCOA2	PTGS2	NCOA2	ADRB2	ADRA1A	IGHG1
GRIA2	SLC6A2	PCP4	HSP90AA1	DPP4	ADRA1D	CHRM2	ADH1B
GABRA5	SLC6A3	CHRM3	PIK3CG	PGR	DRD2	ADRA1B	ADH1C
IGHG1	AKR1B1	CHRM1	CHRM3	CHRM1	OPRM1	SLC6A3	LYZ
ADH1B	PLAU	GABRA2	SERPIND1	NOS3	CHRNA7	ADRB2	COBT
ADH1C	LTA4H	GABRA3	KCNH2	GABRA2	PGR	ADRA1D	PTGS1
LYZ	MAOB	CHRM2	SCN5A	ACHE	NCOA2	TOP2B	SCN5A
COBT	MAOA	ADRA1B	FXa	SLC6A2	PTGS1	OPRM1	PTGS2
SCN5A	KAPCA	GABRA1	CHRM5	CHRM2	HSP90AA1	GABRA1	RXRA
RXRA	CTRB1	GRIA2	CA2	ADRA1B	PIK3CG	HSP90AA1	PDE3A
PDE3A	CHRM1	GABRA6	ACHE	GABRA1	KCNH2	CHRNA7	SLC6A2
SLC6A2	ADRB1	GABRA5	CHRM2	TOP2B	KAPCA	NCOA2	NOR51B
NOR51B	HTR2A	IGHG1	ADRA1D	F7	DRD1	NCOA1	
HSP90AA1	ADRA1A	ADH1B	TOP2B	PCP4	GABRA2	DRD1	
PIK3CG	GABRA3	ADH1C	OPRM1	RELA	PDE3A	HTR2A	
KCNH2	CHRM2	LYZ	DPP4	IKBKB	HTR2A	SLC6A4	
KAPCA	ADRA1B	COBT	ITM2C	AKT1	GABRA5	IGHG1	
DRD1	GABRA1	RXRA	PRSS1	BCL2	GABRA3	PGR	
CHRM4	CHRNA7	PDE3A	NCOA2	BAX	CHRNA2	NR3C2	
HTR2A	HSP90AA1	SLC6A2	NCOA1	TNF	SLC6A4	ACHE	
ADRA1A	PIK3CG	NOR51B	KCNMA1	JUN	GABRA1	DRD2	
ADRB2	KCNH2	ESR1	PCP4	AHSA1	NOR51B	SERPIND1	
CHRNA2	DRD1	PPARG	NOS2	CASP3	BCL2	ESR1	
SLC6A4	GABRA2	PTPN1	ESR1	MAPK8	BAX	AR	
OPRM1	CHRM4	MAPK14	F7	XDH	CASP9	PPARG	
BCL2	PDE3A	GSK3B	ESR2	MMP1	JUN	DPP4	
BAX	GABRA5	PIK3CG	PGR	STAT1	CASP3	FXa	
CASP9	CHRNA2	KAPCA	NR3C2	CDK1	CASP8	PTPN1	
JUN	SLC6A4	PIM1	ABAT	#N/A	PRKCA	AKR1B1	
CASP3	OPRM1	CCNA2	GABRA1	HMOX1	TGFB1	PRSS1	
CASP8	NOR51B	PYGM	ADH1B	CYP3A4	PON1	KAPCA	
PRKCA	BCL2	PPARD	ADH1C	CYP1A2	MAP2	PIK3CG	
TGFB1	BAX	AKR1B1	ADH1A	CYP1A1	NR3C2	RELA	

PON1	CASP9	NCOA1	NOR51B	ICAM1	SERPIND1	EGFR
MAP2	JUN	F7	LYZ	SELE	ESR1	AKT1
NOS2	CASP3	SERPIND1	nprE	VCAM1	DPP4	VEGFA
ESR1	CASP8	NOS3	COBT	NR1I2	GSK3B	CCND1
AR	PRKCA	ACHE	CTSD	CYP1B1	CDK2	BCL2L1
PPARG	TGFB1	MAOB	MAT2A	ALOX5	LACTBL1	CDKN1A
SLC6A3	PON1	RELA	IGHG1	HAS2	PRSS1	CASP9
ESR2	MAP2	XDH	ADRA2A	GSTP1	CCNA2	MMP2
DPP4	HTR3A	NCF1	SLC6A2	AHR		MMP9
MAPK14	ADRA1D	OLR1	AKR1B1	PSMD3		MAPK1
GSK3B	PRSS1	ADRB1	PLAU	SLC2A4		IL10
CDK2	PCP4	HTR3A	MAOA	NR1I3		RB1
MAOB	NOS2	ADRA2C	KAPCA	INSR		CDK4
CHEK1	AR	ADRB2	CTRB1	DIO1		TNF
PRSS1	PPARG	ADRA1D	ADRB1	PPP3CA		JUN
PIM1	DPP4	OPRM1	HTR2A	PRXC1A		IL6
CCNA2	SERPIND1	DRD1	ADRA1A	GSTM1		CASP3
PCP4	NOS3	KCNH2	GABRA3	GSTM2		TP53
PKIA	ACHE	FXa	CHRNA7	AKR1C3		NFKBIA
SERPIND1	TOP2B	CHRM5	NR3C1	SLPI		XDH
NOS3	F7	CHRM4	RELA	CHRM3		TOP1
ACHE	RELA	OPRD1	AKT1	ESR1		MDM2
LACTBL1	IKBKB	HTR2A	VEGFA	SCN5A		APBA3
#N/A	AKT1	ADRA1A	CDKN1A	CHRM5		MMP1
IL4	TNF	SLC6A3	TP53	RXRA		PCNA
SIRT1	AHSA1	SLC6A4	FASN	ADRB2		ERBB2
ATP5B	MAPK8	RXRB	SOD1	ESR2		#N/A
ND6	XDH	KCNMA1	CAT	MAPK14		HMOX1
HSD3B2	MMP1	TOP2B	HIF1A	GSK3B		CASP7
HSD3B1	STAT1	CHRNA7	NR1I2	CDK2		ICAM1
NR3C2	CDK1	KDR	PLA2G4A	CHEK1		MCL1
NCOA1	#N/A	MET	ABCC2	RXRB		BIRC5
ADRA2A	HMOX1	PKIA	MTOR	PIM1		IL2
AKR1B1	CYP3A4	LACTBL1	AR	KDR		CCNB1
PLAU	CYP1A2	JUN	GSK3B	CCNA2		TYR
LTA4H	CYP1A1	#N/A	PIM1	NCOA1		IFNG
MAOA	ICAM1	IL4	CCNA2	KCNMA1		IL4
CTRB1	SELE	SIRT1		IGHG1		TOP2A
ADRB1	VCAM1	ATP5B		NR3C1		GSTP1
	NR1I2	ND6		OPRD1		XIAP
	CYP1B1	HSD3B2		OPRM1		SLC2A4
	ALOX5	HSD3B1		CHRNA7		INSR
	HAS2	IKBKB		NR3C2		CD40LG
	GSTP1	AKT1		ADH1C		PTGES
	AHR	BCL2		ADRA2A		NUF2
	PSMD3	BAX		SLC6A3		ADCY2
	SLC2A4	TNF		AKR1B1		MET
	NR1I3	AHSA1		PLAU		PCP4

INSR
DIO1
PPP3CA
PRXC1A
GSTM1
GSTM2
AKR1C3
SLPI
RXRG
NFKBIA
IL1B
CASP1
IFNG
ADCYAP1
PSMG1
MAP2K4
NR3C1
FXa
PTPN1
KCNMA1
CHRM5
OPRD1
CACNA1S
PDE4
KDR

CASP3
MAPK8
MMP1
STAT1
CDK1
HMOX1
CYP3A4
CYP1A2
CYP1A1
ICAM1
SELE
VCAM1
NR1I2
CYP1B1
ALOX5
HAS2
GSTP1
AHR
PSMD3
SLC2A4
NR1I3
INSR
DIO1
PPP3CA
PRXC1A
GSTM1
GSTM2
AKR1C3
SLPI
MMP3
EGFR
VEGFA
CCND1
BCL2L1
FOS
CDKN1A
EIF6
CASP9
PLAU
MMP2
MMP9
MAPK1
IL10
EGF
RB1
IL6
CDKN2A
TP53

LTA4H
MAOB
MAOA
CTRB1
ADRB1
HTR2A
ADRA1A
GABRA3
PDE3A
VEGFA
CDKN1A
TP53
FASN
SOD1
CAT
HIF1A
PLA2G4A
ABCC2
MTOR
PKIA

NOS3
CDK2
PIM1
CCNA2
ADRA2A
ADRA2C
NOS2
ESR2
MAPK14
GSK3B
NR3C1
KCNH2
KCNMA1
STAT3
EDN1
CHEK1
CHRNA2
LACTBL1
DRD5
F7
HTR1A
GABRA2
GABRA5
SLC6A2
GABRA3
HTR2C
ADRA2B
HTR1B
GABRA6
GABRG3
GABRE
BCL2
FOS
AHSA1
FASN
EDNRA
CYP3A4
CYP1A2
MYC
CYP1A1
NR1I2
NPM1
ECE1
PARP4
CALCR
ITGB3

ELK1
NFKBIA
POR
ODC1
CASP8
TOP1
RAF1
SOD1
PRKCA
HIF1A
RUNX1T1
HERC5
HSPA5
ERBB2
ACACA
CAV1
MYC
F3
GJA1
IL1B
CCL2
PTGER3
CXCL8
PRKCB
BIRC5
DUOX2
HSPB1
TGFB1
SULT1E1
MGAM
IL2
CCNB1
PLAT
THBD
SERPINE1
COL1A1
IFNG
PTEN
IL1A
MPO
TOP2A
ABCG2
NFE2L2
NQO1
PARP1
COL3A1
gyrB
CXCL11 PTGS1

CXCL2
DCAF5
CHEK2
CLDN4
PPARA
HSF1
CRP
CXCL10
CHUK
SPP1
RUNX2
RASSF1
E2F1
E2F2
ACPP
CTSD
IGFBP3
IGF2
CD40LG
IRF1
ERBB3
PON1
PCOLCE
NPEPPS
HK2
NKX3-1
RASA1

Table S3. Network parameters

Node	Type
NSCLC	disease
SAN LENG	Herb
REN SHEN	Herb
HUANGQI	Herb
SHAN YAO	Herb
ZHI MU	Herb
XUAN SHEN	Herb
DAN SHEN	Herb
EZHU	Herb
PTGS1	gene
NCOA2	gene
PTGS2	gene
CHRNA7	gene
PGR	gene
CHRM3	gene
GABRA3	gene
CHRM2	gene
IGHG1	gene
ADH1B	gene
ADH1C	gene
RXRA	gene
PDE3A	gene
HSP90AA1	gene
PIK3CG	gene
ADRB2	gene
OPRM1	gene
BCL2	gene
BAX	gene
CASP9	gene
JUN	gene
CASP3	gene
CASP8	gene
PRKCA	gene
TGFB1	gene
PON1	gene
NOS2	gene
ESR1	gene
AR	gene
PPARG	gene
SLC6A3	gene
ESR2	gene
DPP4	gene
MAPK14	gene
GSK3B	gene
CDK2	gene
CHEK1	gene
PRSS1	gene

PIM1	gene
CCNA2	gene
SERPIND1	gene
NOS3	gene
ACHE	gene
IL4	gene
SIRT1	gene
HSD3B1	gene
NR3C2	gene
PLAU	gene
MAOA	gene
ADRB1	gene
HTR3A	gene
TOP2B	gene
RELA	gene
IKBKB	gene
AKT1	gene
TNF	gene
MAPK8	gene
XDH	gene
MMP1	gene
STAT1	gene
CDK1	gene
HMOX1	gene
CYP3A4	gene
CYP1A2	gene
CYP1A1	gene
ICAM1	gene
SELE	gene
NR1I2	gene
CYP1B1	gene
ALOX5	gene
GSTP1	gene
AHR	gene
PSMD3	gene
INSR	gene
GSTM1	gene
GSTM2	gene
AKR1C3	gene
SLPI	gene
RXRG	gene
NFKBIA	gene
IL1B	gene
CASP1	gene
IFNG	gene
ADCYAP1	gene
MAP2K4	gene
NR3C1	gene
PTPN1	gene

KCNMA1	gene
KDR	gene
PYGM	gene
PPARD	gene
RXRB	gene
MET	gene
MMP3	gene
EGFR	gene
VEGFA	gene
CCND1	gene
BCL2L1	gene
FOS	gene
CDKN1A	gene
EIF6	gene
MMP2	gene
MMP9	gene
MAPK1	gene
IL10	gene
EGF	gene
RB1	gene
IL6	gene
CDKN2A	gene
TP53	gene
ELK1	gene
POR	gene
ODC1	gene
TOP1	gene
RAF1	gene
SOD1	gene
HIF1A	gene
RUNX1T1	gene
HERC5	gene
HSPA5	gene
ERBB2	gene
ACACA	gene
CAV1	gene
MYC	gene
F3	gene
GJA1	gene
CCL2	gene
PTGER3	gene
CXCL8	gene
PRKCB	gene
BIRC5	gene
HSPB1	gene
IL2	gene
CCNB1	gene
PLAT	gene
THBD	gene

SERPINE1	gene
COL1A1	gene
PTEN	gene
IL1A	gene
MPO	gene
TOP2A	gene
ABCG2	gene
NFE2L2	gene
NQO1	gene
PARP1	gene
CHEK2	gene
CLDN4	gene
PPARA	gene
HSF1	gene
CRP	gene
CXCL10	gene
SPP1	gene
RUNX2	gene
RASSF1	gene
E2F1	gene
E2F2	gene
CTSD	gene
IGFBP3	gene
IGF2	gene
CD40LG	gene
IRF1	gene
ERBB3	gene
HK2	gene
RASA1	gene
SAA1	gene
CA2	gene
FASN	gene
CAT	gene
PLA2G4A	gene
ABCC2	gene
MTOR	gene
DRD2	gene
CDK4	gene
MDM2	gene
PCNA	gene
CASP7	gene
MCL1	gene
XIAP	gene
PTGES	gene
NUF2	gene
STAT3	gene
EDN1	gene
EDNRA	gene
NPM1	gene

ECE1	gene
PARP4	gene
ITGB3	gene
D1	mol
D2	mol
D3	mol
D4	mol
D5	mol
D6	mol
D7	mol
D8	mol
D9	mol
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D96	mol
D97	mol
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D99	mol
D100	mol
D101	mol
D102	mol
D103	mol
D104	mol
D105	mol
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D108	mol
D109	mol
D110	mol
D111	mol
D112	mol
D113	mol
D114	mol
D115	mol
D116	mol
D117	mol