International Journal of Trend in Innovative Research (IJTIIR)
Available Online @ www.ijtiir.com | ISSN: 2582-0354

Computer-Aided Research on Chemical Constituents and Biological Activities of Chinese Medicinal Plants under the Background of "Internet+"

Ming Zhang
Chuxiong Medical College, Chuxiong, Yunnan, China

***Abstract*—**Based on computer-aided research on the chemical components and biological activities of Chinese medicinal plants, we have used a variety of chromatographic separation techniques (including MCI resin, normal phase silica gel column chromatography, Sephadex LH-20 gel, preparative high performance liquid phase, etc.) The chemical components of each plant were systematically separated. In this work, a total of 133 compounds were isolated from these three medicinal plants. Their structure types include phenanthrene (9,10-dihydrophenanthrene and phenanthrene), carzanane type two Terpenes, flavonoids, high isoflavones, phenylpropanoids, etc., among which 76 new compounds, 3 of them showed good activity. This study was the first to discover the neuroprotective activity of phenanthrene compounds in Juncus the reagents provide possible lead compounds.

Keywords*—Computer-Aided Research, Chemical Constituents, Biological Activities, Medicinal Plants*

I. INTRODUCTION

It was first published in "Shen Nong's Materia Medica" and was regarded as an essential medicine for life and was listed as the top grade. Materia Medica has been recorded in the past dynasties, and it has been commonly used by doctors since ancient times. The Polygala tenuifolia included in the Chinese Pharmacopoeia is the root of the genus Polygala tenuifolia and Polygala tenuifolia. It has the effects of calming nerves, nourishing the mind, eliminating phlegm, and reducing swelling. It is used for the symptoms of insomnia, dreaminess, forgetfulness and palpitations, trance, uncomfortable expectoration, sore swelling and poison, breast swelling and pain caused by the incompatibility of heart and kidney. Modern pharmacological studies have shown that Polygala has the pharmacological effects of expectorant, sedation, soothe the nerves and nourish the mind, treat Alzheimer's disease, anti-aging, anti-cancer and anti-mutation, lowering blood pressure, regulating coolness, inhibiting bacteria and anti-inflammatory. Elsholtzia is a commonly used traditional Chinese medicine. The whole plant of Elsholtzia fragrans can be used for medicinal purposes. It has a pungent taste and mild in nature. It has the functions of sweating and relieving heat, promoting water and dispersing dampness, warming the stomach and regulating the middle. Disease and other effects [1-6].

Many Elsholtzia plants are tea plants, and can be used as tea for drinking for disease prevention and treatment. For example, East Perilla can be used as a tea, which has the effect of clearing away heat and detoxification; Yebazi is used as a tea for local hospitality among Yunnan ethnic minorities and has the effect of preventing colds. At the same time, Elsholtzia is also one of the "food and medicine" varieties announced by the Ministry of Health. In addition, Elsholtzia is also one of the good nectar plant species, such as Yebazi, Elsholtzia densiflora, Elsholtzia, Yecaoxiang and Dongperilla are all excellent. The most famous source of nectar, especially the wild trifoliate honey-"Yunnan hard honey". The Dictionary of Chinese Medicine records that the traditional Chinese medicine rush is the dried stem pith or whole plant of the genus Rush, the same genus J. Setchuensis Buchen (J. Setchuensis Buchen) J. leschenaultii Gay. is also used as medicine. It has the effects of clearing the heart, lowering fire, diuresis and drenching, and is used to treat gonorrhea, edema, dysuria, damp-heat jaundice, upset and insomnia, night crying, throat palsy, Trauma etc. [7-14]

At present, scholars at home and abroad have conducted more detailed studies on the chemical constituents of four plants of the genus Juncus, J. effusus, J. setchuensis, J. acutus and J. roemerianus, and a large amount of phenanthrene has been isolated from them. Class (including 9,10-dihydrophenanthrene, phenanthrene, and dimers), benzocoumarin, dihydrodiphenoxy, triterpenes, glycerides, flavonoids, steroids, phenols and other compounds. Astragalus membranaceus (Astragalus membranaceus) is a legume perennial herb, widely distributed in temperate regions around the world (Jia et al. 2012; Zhong et al. 2012). Astragalus, first recorded in Shennong's Materia Medica, is the most popular health medicine and has a history of more than 2,000 years in China (Fan et al. 2012). Astragalus is also commonly used in traditional Chinese medicine prescriptions. It is used as an immunomodulator, the treatment of colds, diarrhea, fatigue and loss of appetite, as well as the treatment of cardiovascular diseases (Liu et al. 2011). In the past two decades, the pharmacological effects of the chemical constituents of Astragalus have been deeply studied, especially the activity of its polysaccharide constituents has been systematically studied [15-21].

Studies have shown that Astragalus polysaccharide has immunomodulation (Qiu et al. 2010; Li et al 2009), anti-oxidation (Li et al. 2010; Li et al. 2012; Niu et al. 2011), and anti-tumor (Zhu et al. 2011) ; Li et al. 2009), anti-diabetic (Liu et al. 2010), anti-viral (Jiang et al. 2010; Zhuge et al. 2012), liver protection (Qin et al. 2012), anti-inflammatory (He et al. al. 2012; Jiang et al. 2010), anti-atherosclerosis (Wang et al. 2010; Cheng et al. 2012) and neuroprotection (Hanrui et al. 2012). In addition to the above two kinds of Polygala, a variety of plants of the genus Polygala are widely used in the folk and have been recorded in writing for a long time. For example, melon seed gold, first appeared in "Plant Name Real Map". It has been used for hundreds of years in foreign countries. It has been recorded in the tenth edition of the American formulary, the annual edition of the British subsidiary pharmacopoeia, the eighth edition of the Japanese Pharmacopoeia, and the eighth edition of the former Soviet Union Pharmacopoeia [22-24].

II. The Proposed Methodology

A. Chinese Medicinal Plant Chemical Composition

Ketone compounds are a class of active ingredients in Polygala medicinal plants, which are generally divided into simple canone, canoneoxoxib, ketoxib and dicanone. Among them, simple auxiliary ketones are the most common, and there is a position that can be substituted on the nucleus. At present, only three substituents of hydroxyl, methoxy and methylenedioxy are present. The probability of N-position being substituted is high. For methylene for the dioxy group, the substitutions are mainly in the, and, positions of the straight type, and angle type substitutions are rare. According to the number of oxygen-containing substituents, the oral cavity compounds can be divided into five types: di-substituted, tri-substituted, tetra-substituted, penta-substituted and hexa-substituted. A variety of auxiliary ketone components have been isolated and identified from plants of this genus.

$$H_2\text{-}14 \Leftrightarrow H\text{-}6 \tag{3}$$

$$RI = a + b/C \tag{4}$$

The casanane diterpene is derived from the pimranane diterpene precursor, which has a basic tricyclic diterpene skeleton, and is substituted by an ethyl group at 13 and a methyl substituted at position 14. It can be regarded as a piramane type the 13-position methyl group of the diterpenoids migrates to the 14-position. Caesalpinia spinosa, Caesalpinia volkensii and other plants have been reported as carshanane diterpenes. Among them, the five species of C. sylvestris, Yunshi of South China, Yunshi of beak, buttercup, and hematoxylin are the most widely reported. Castane-type diterpenes have complex and variable structural types, and are a hot field in the research of natural products in recent years. According to the structural characteristics of castane-type diterpenes, they can be divided into the following types: Folin-Ciocalteu's) color method (Singleton and Rossi 1965). The principle is that polyphenol compounds in alkaline solution, tungstomolybdic acid can quantitatively oxidize polyphenol compounds, and itself is reduced to produce blue compounds. The intensity of the blue color is proportional to the number of phenolic groups, thus the content of total phenolics in the sample can be determined.

Gallic acid mother liquor and standard solution: Weigh 27.645 mg of gallic acid, which is 25 mg gallic acid (FW170.12), and distilled water to a 25 ml volumetric flask to make a mother liquor with a concentration of 1000 ug/mL. The mother liquor is diluted into a gallic acid standard solution with a concentration gradient of 0.0, 20.0, 40.0, 60.0, 80.0, 100.0, 150.0, 200.0, 250.0, 300.0 ug/mL. Karsanane diterpenes with furan rings are prone to rearrangement. There are a large number of rearrangements reported at present, and their rearrangements are mainly manifested in methyl migration and ring destruction. For example: caesalbonducin D (11) and E (12) derived from Hematoxylin, spirocaesalmin B (13), caesalpinimin A (14), caesalminaxin E (15), macrocaesalmin (16), neocaesalminin A (17) etc.

B. Analysis of Biological Activity of Medicinal Plants

With the continuous deepening of research on Polygala plants, scholars at home and abroad have successively reported on the biological activities of the genus plants, especially in the central nervous and cardiovascular system, anti-aging, anti-tumor and other aspects. The major progress is summarized as follows: A large number of castane-type diterpenes have been reported in the genus Yunshi, and many literatures have reported the cytotoxic activity of castane-type diterpenes. Xu Xudong et al. found that the caesalpin A in the beak pod cloud had a very good inhibitory effect on HepG-2 (IC50 4.7 μM) and MCF-7 (IC50 2.1 μM), and caesalpin B and caesalpin D were respectively against MCF-7 (IC50 7.9 μM) and AGS (IC50 6.5 μM) cell lines have a selective inhibitory effect. Norcaesalpinin I shows good activity on HepG-2 cell lines (IC50 16.4 μM).

Research by Xuan Lijiang et al. found that caesalminaxin D and caesalminaxin H in Rhizoma Ceratoides showed better cytotoxic activity against K562 cell lines. The electron-withdrawing effect of nitro and nitro is a kind of stable free radical, and its lone pair electron has strong absorption near 517 nm (dark purple in alcohol solution). When there is a scavenger, the lone pair of electrons are paired, and the absorption disappears or weakens. By measuring the degree of weakening of the absorption, the activity of the free radical scavenger can be evaluated. IC50 refers to the concentration of the sample needed to remove 50% DPPH and is also used as an indicator of antioxidant capacity. The DPPH method is a fast (reaction time only takes about 20 min), simple, sensitive and feasible method to evaluate the antioxidant activity of natural antioxidants. Ammonia-induced cough method and colorimetric method were used to observe Shengyuanzhi and various processed products. The decoction has antitussive and expectorant effects on mice.

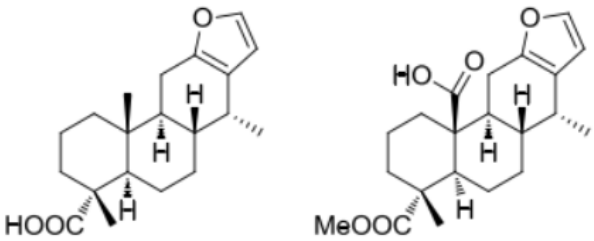
$$\rho_{out} = \sum_{m,n=0}^{k} e^{i\pi J} \times e^{-(\tau a^T a)} \tag{3}$$

$$\rho(t) = \sum_{n=0}^{m} \frac{(2\Gamma t)^n}{n!} e^{-(ta)^2} \tag{4}$$

The results showed that Polygala Sheng, Honey Polygala, Ginger Polygala, and Zhigancao Polygala have significant antitussive effects. High-dose Polygala, low-dose Polygala, and high-dose Zhi Polygala also have significant expectorant effects. The casanane diterpenes in the genus Rhododendron showed good antimalarial activity. Thai scholar Amorn Petsom et al. isolated 16 casanane diterpenes from the pits of the thorn fruit hematoxylin and tested these compounds Inhibition of multi-drug resistant Plasmodium falciparum (Plasmodium falciparum), the results show that bonducellepins E–G show good antimalarial effects, and the IC50 values of these three compounds are between 1.6–5.8 μM.

C. Computer-Aided Analysis of Chemical Constituents and Biological Activities of Medicinal Plants

It can significantly prolong the plasma recalcification time of rabbits in vitro, significantly prolong the fibrin clotting time caused by thrombin, and significantly prolong the partial thromboplastin time has no significant effect on the plasma prothrombin time. Pre-administration significantly prolonged the clotting time of mice, reduced the length of thrombus formed in the tail caused by carrageenan, and significantly inhibited the swelling of the foot extension. Therefore, it may exert anticoagulant and antithrombotic effects by affecting the endogenous coagulation system. The water extract of P. sibiricum can significantly reduce the whole blood specific viscosity and reduction specific viscosity of rats with acute blood cancer caused by dextrose, and greatly expand the auricular arterioles and venules of mice, and increase the number of capillary openings.



62 63

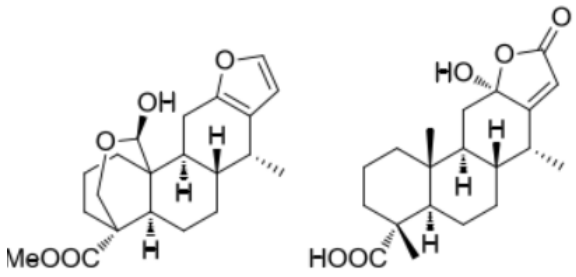
Fig.1. Biological Activities of Medicinal Plant

Elsholtzia is a commonly used traditional Chinese medicine in summer in our country. Li Shizhen's "Compendium of Materia Medica" records: "Elshollandia is a medicine for relieving the appearance of summer moon, such as ephedra in winter moon". Elsholtzia has a high medicinal value. Scholars at home and abroad have conducted research on medicinal Elsholtzia plants and found that it has anti-inflammatory, antipyretic, analgesic, sedative, anti-epidemic, strengthened immunity, antibacterial and bactericidal effects, and has direct Inhibition of influenza virus, etc., and the extraction and separation of other chemical components from Elsholtzia plants have laid the foundation for the development and utilization of Elshollandia plants. However, the current research mainly concentrates on Elsholtzia, Osmanthus oleracea, Elsholtzia scoparia, etc., and mainly focuses on the volatile oil components, which is not comprehensive and in-depth.

Compound 84 is a white powder, [α]24D-61.8 (c 0.2, CHCl3). The ESIMS of the compound showed the quasi-molecular ion peak m/z 523.3 [M + H]+, and the HRESIMS showed the quasi-molecular ion peak m/z 545.1982 [M + Na]+ (calcd for C26H34O11Na, 545.1993).

III. Experiment

The chemical composition analysis of medicinal plants is shown in the figure.



64 65

Fig.2. Analysis of chemical constituents of medicinal plants

The biological activity analysis of medicinal plants is shown in the figure.

Position	δ_H	δ_C
1		173.1
2		131.8
3	3.02 (1H, ddd, *J* = 2.4, 13.2, 9.6 Hz) 2.70 (1H, dd, *J* = 13.2, 4.0 Hz)	29.1
4	4.24 (1H, dd, *J* = 9.6, 4.0 Hz)	54.2
5	6.37 (1H, dd, *J* = 6.8, 2.4 Hz)	130.5
6	1.70 (3H, d, *J* = 6.8 Hz)	14.8
7		173.9
8	4.08 (2H, t, *J* = 9.6 Hz)	66.5
9	1.55 (2H, dt, *J* = 9.6, 3.2 Hz)	31.7
10	1.31 (2H, dt, *J* = 7.2, 3.2 Hz)	20.1
11	0.86 (3H, t, *J* = 7.2 Hz)	14.0

Fig.3. Analysis of biological activity of medicinal plants

The computer-aided analysis of the chemical composition of medicinal plants is shown in the figure.

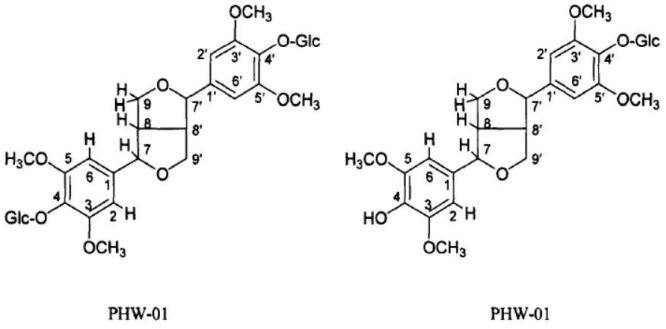


Fig.4. Computer aided analysis

CONCLUSION

Based on computer-aided research on the chemical components and biological activities of Chinese medicinal plants, we have used a variety of chromatographic separation techniques (including MCI resin, normal phase silica gel column chromatography, Sephadex LH-20 gel, preparative high performance liquid phase, etc.) The chemical components of each plant were systematically separated. In this work, a total of 133 compounds were isolated from these three medicinal plants. Their structure types include phenanthrene (9,10-dihydrophenanthrene and phenanthrene), carzanane type two Terpenes, flavonoids, high isoflavones, phenylpropanoids, etc., among which 76 new compounds, 3 of them showed good activity.

References

[1] Liu Bo. Study on the chemical constituents and biological activities of five medicinal plants. Nanjing University, 2018.
[2] Qu Zhengyi, Jin Yinping, Zhang Yuwei, et al. Research progress in chemical constituents, biological activity and clinical application of genus Lysate[J]. Chinese Journal of Experimental Formulas, 2018, 24(01):209-216.
[3] Zhu Jihua, Hu Haobin, Lu Jie. Study on chemical constituents and biological activities of Rosaceae medicinal woody plants in Ziwuling forest area[J]. 2021(2014-1):29-31.
[4] Liao Tianlu, Liao Tianjiang, Lv Linhua. Study on the chemical constituents and pharmacology of the medicinal plant Phyllostachys edulis[J]. Rural Science & Technology, 2018(20): 2.
[5] Zhang Lu. Study on the chemical constituents and biological activities of two Elsholtzia plants[D]. Kunming University of Science and Technology, 2019.
[6] Chen Hongjiang, Liu Jianan, Li Xiang, et al. Research progress on the chemical constituents and biological activities of Gymnospora[J]. Chinese Patent Medicine, 2018, v.40(05):148-153.
[7] Liu Hongdong, Pan Lingling, Zhou Xiang, et al. Research progress on the chemical constituents and pharmacological activities of alkaloids in orchid plants[J]. Chinese and Herbal Medicine, 2019(3):14.
[8] Xie Shuangshuang, Wu Ye, Zhang Na, et al. Study on the chemical composition and biological activity of the endophytic fungus Phomopsis sp.TJ507A from Phyllanthus chinensis [J]. Natural Products Research and Development, 2019, 31(1): 8 .
[9] Yang Yumeng, Zhang Zhiguo. Research progress on the chemical constituents and pharmacological effects of Polygonum medicinal plants[J]. Journal of Science & Economics Guide, 2018(4): 2.
[10] Wu Peiqian. Study on the chemical composition and anti-AD activity of two medicinal plants[D]. Lanzhou University, 2019.
[11] Wang Shoujun. Study on the chemical constituents and pharmacology of the medicinal plant Yinchen[J]. Systems Medicine, 2019, 4(9):3.
[12] Liang Wenxian, Ni Lin, Zou Xiaoxing, et al. Research progress on the chemical constituents and pharmacological activities of Phalaenopsis plants[J]. Chinese Herbal Medicine, 2018, 49(5):7.
[13] Zhou Xueming, Song Xiaoping, Han Changri, Chen Guangying. Discovery of active ingredients from characteristic tropical medicinal plants in Hainan [C]// The 20th National Symposium on Organic Analysis and Biological Analysis of the Chinese Chemical Society. 2019.
[14] Guo Ziyan, Yu Jianqing. Research progress on the chemical constituents and biological activities of piperine alkaloids[J]. 2018.

[15] Deng Yanqiu, Zhao Lichun, Tang Hongzhen, et al. Research progress on the chemical constituents and biological activities of Bitterwood[J]. Chinese Patent Medicine, 2020, 42(5):6.
[16] Zeng Yuanyuan, Tong Tao, Huang Kunlun. Research progress on extraction process, composition analysis and biological activity evaluation of Ulva polyphenols[J]. Food Industry Science and Technology, 2021, 42(20):386-392.
[17] Li Yameng. Study on the chemical constituents and biological activity of Chinese onion[D]. Jilin University, 2019.
[18] Wang Dan. Study on the biological activity of secondary metabolites and the chemical composition of n-butanol from the endophytic fungi of Huoxiang[D]. Lanzhou University of Technology, 2019.
[19] Zhao Siqi, Meng Hong, Yi Fan. Recommendations for computer-aided drug design in the screening of cosmetic botanical functional raw materials[J]. Daily Chemical Industry, 2019, 49(04):51-56+72.
[20] Wu Qihao. Study on the chemical composition and biological activity of six marine biological samples[D]. Zhejiang University of Technology, 2019.
[21] Su Boyuan, Liu Yan, Xue Yanyu, et al. Research on anti-tumor activity of Magnolia vulgaris and Magnolia sinensis based on reverse molecular docking[J]. Computers and Applied Chemistry, 2019, 36(4):8.
[22] Luo Ting. Study on the chemical constituents and activities of Shi Yanfeng, Xiaoji and Motherwort [D]. Yunnan University, 2019.
[23] Hou Yong. Study on the chemical constituents and biological activity of poplar flowers [D]. Anhui Medical University, 2019.
[24] Wei Wenjun. Study on terpenoids and their biological activities in three medicinal plants [D]. 2019.