

Hanxue

## 1. Materials and Methods

### 1.1 General information

60 cases of patients with anal perianal pruritus to our hospital between July 2012 - July 2013 according to the sequence are divided into control group and treatment group, 30 patients in each group, treatment group, 18 cases were male, 12 female patients, age between 31-55, duration of 6 months to 3 years, control group, 19 cases were male, 11 female cases, age between 34-57, duration of half a year to 3 years. Two groups in terms of age, gender, disease duration, severity by statistical test are no significant difference.

### 1.2 Diagnostic and inclusion criteria

#### 1.2.1 Diagnostic criteria

With reference to 2002 "Chinese medicine" in anorectal perianal pruritus diagnosis standard:

- (1) The disease occurred in the anus around, mainly to itching.
- (2) No primary skin rash performance and Poor diet sleep can aggravate the disease.
- (3) The skin often white or hypopigmentation, thickening of the skin wrinkles serious, chapped, exudation, moss, pigmentation.

#### 1.2.2 Inclusion criteria

Between the age of 18-60 years old, in accordance with the diagnostic criteria, voluntarily accept the signed informed consent, no drug allergies and cardiovascular disease, etc.

### 1.3 Therapeutic method

#### 1.3.1 Drug composition

Treatment group: compound methylene blue preparation by methylene blue 2ml, 2.5 ml of 2% lidocaine, bupivacaine 5ml and 5% NaHCO<sub>3</sub> 0.5 ml, 5 ml of water for injection preparation.

Control group: cetirizine provided by the Western Medicine Bureau, Suzhou Dawnrays pharmaceutical production, Approval number: Chinese medicine standard word H19980014.

#### 1.3.2 Treatment process

Treatment group: Compound methylene blue inject Huiyin Acupoint, Long strong point, Two times a week.

control group: cetirizine 10mg qd.po, 1 week for a period of treatment

### 1.4 Observation index and curative effect judgment standard

#### 1.4.1 Observation index

Observing the subjective sensation of itching and the objective index of the degree of mucus, According to the severity of the disease is divided into three degrees.

#### 1.4.2 Criterion of curative effect

Recovery: The symptoms and signs disappeared, the integral is reduced more than 85%

Excellent: The symptoms and signs were improved, the integral is reduced more than 50%.

Effective: The symptoms and signs were improved, the integral is reduced more than 20%.

Inefficacy: Symptoms, signs of improvement is not obvious, or even worse, the symptom integral reduced less than 20%.

1.5 statistical method: Using SPSS17.0 software, Measurement data using T test, count data using chi square test.

2. Result: After 1 weeks treatment, IN the treatment group: 7 cases were cured, 15 cases were markedly effective, 5 cases were effective, and 3 cases were ineffective; In the control group, 3 cases were cured, 14 cases were markedly effective, 10 cases were effective, and 3 cases were ineffective. The total effective rate of both were 90%, The treated group had an effectual rate of 73%, more than the control group: 56%. The treatment group was significantly better than the control group,  $p < 0.05$ . 5 cases of recurrence in the treatment group after 1 weeks of drug withdrawal and 12 cases of recur-

rence in the control group. In long-term efficacy The treatment group was significantly better than the control group too.

### 3. discuss

Perianal pruritus is a pruritic, chronic, recurrent skin disease with a complex aetiology and unclear pathogenesis. The mechanism of the itch is related to the involvement of histamine, pg, 5- hydroxytryptamine, Leukotrienes, enzymes, platelet activating factor and protein decomposition products. Modern treatment uses external and oral anti histamine drugs, the effect is not good. Traditional Chinese medicine treatment of various means, but more than a long course of treatment, the effect is difficult to exact.

Methylene blue is mainly used for the treatment of nitrite and cyanide poisoning. In recent years, with the development of pharmacological research, it is found that methylene blue has a pro nerve and directly hinders the electrical conduction of nerve fibers. By participating in the sugar metabolism and promote oxidation to pyruvate, changes in acid-base balance and membrane potential of nerve endings of inside and outside, thus affecting the excitability and conduction of nerve impulses[3]. By blocking nerve conduction plays antipruritic, analgesic effect . Lidocaine can relieve local pain of the needle. Bupivacaine can maintain long-term antipruritic, analgesic. Sodium bicarbonate can neutralize the methylene blue local nerve block caused by burning pain. The drug combination to the antipruritic effect is good for perianal itching . Huiyin is an important point of human body, It can dredge the body and promote the transfer and circulation of yin and Yang Qi to play the antipruritic effect. Long strong point is located at the midpoint of the coccyx and anus tip line. The posterior branch of the caudal nerve and the distribution of the anal nerve are below it, so Point injection can play a role in nerve block. It is suitable for clinical application.

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### **VIRTUAL SCREENING OF ANTI-HEPATIC FIBROSIS AGENTS FROM NOVEL PICROSIDE DERIVATIVES**

**Hua Han, ZhengQ Li, Xin Ying**

Key Laboratory of Chinese Materia Medica, Ministry of Education, Heilongjiang University of Chinese Medicine, Harbin, 150040, China E-mail: lizhengqing1125@163.com

**Abstract** In this study, twelve derivatives of Picoside were synthesized by introduction of different amino acid, electron withdrawing groups and electron repelling groups. And the derivatives were characterized by mass, <sup>1</sup>H and <sup>13</sup>C Nuclear magnetic resonance (NMR) techniques. Virtual screening method was used to evaluate the anti-hepatic fibrosis effect of the derivatives. Two pivotal proteins during liver anti-hepatic fibrosis occurring were selected as the targets, and their marketed inhibitors were chosen as reference. The LibDock Score of nine derivatives were higher than the marketed inhibitors. Indicated that the nine derivatives may have pharmacological effects similar to those of marketed inhibitors, and can be used as anti-hepatic fibrosis medicine for further research and development.

**Keywords:** Picoside; Derivatization; Anti-hepatic fibrosis; Virtual screening

**Chemistry** Electron withdrawing group halogen and acetyl groups were introduced into Picoside I and II , yielded b, c, d e, f. Electron repelling group methyl, methoxyl groups were introduced into Picoside I and II , yielded a, g. Besides, glycine and alanine were introduced into Picoside II , yielded h, i, j, k, l.

**Docking study** Docking study was carried out using the Libdock mode of software Discovery Studio 2.5 (DS 2.5). The two key targets in liver injury (TGF-β1 and TNF-α) were obtained from the RCSB Protein Data Bank (<http://www.rcsb.org/pdb/home/home.do>).[1] The protein preparation was carried out in DS 2.5 in four steps, deleted original ligand, added hydrogen, forced CHARMM field, and prepared using 'Prepare Protein'. After preparation, defined the protein as receptor and find sites, defined sphere from site which original ligand bonded. Save the proteins as docking receptor.[2]

The structures of Picoside derivatives were charted by Chem3D Ultra 9.0, and preparation were carried out in DS 2.5 in three steps, added hydrogen, forced CHARMM field and minimization. Save as ligands.

The marketed inhibitors of the four targets were obtained from the DrugBank database (<https://www.drugbank.ca/>),[3] preparation as the ligands and save as reference.

The prepared ligands and marketed inhibitors were selected and docked into the sphere of the target. The docking result was evaluated with LibDock Score, the LibDock Score of marketed inhibitors was set as threshold. The derivatives which LibDock Score was higher than the threshold was retained as candidate compounds.[4,5]

### Docking results

Screened derivatives which LibDock Score higher than the threshold as candidate compounds, deleted duplicate item, eight compounds were got in Table 1.