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

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Abstract In this study, twelve derivatives of Picroside were synthesized by introduction of different amino acid, electron withdrawing groups and electron repelling groups. And the derivatives were characterized by mass, 1H and 13C 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: Picroside; Derivatization; Anti-hepatic fibrosis; Virtual screening

Chemistry Electron withdrawing group halogen and acetyl groups were introduced into Picroside Ⅰ and Ⅱ, yielded b, c, d e, f. Electron repelling group methyl, methoxyl groups were introduced into Picroside Ⅰ and Ⅱ, yielded a, g. Besides, glycine and alanine were introduced into Picroside 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-ß1 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 Picroside 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.

	2A Z5	1KLC
c	+	-
d	+	+
f	+	+
g	+	+
h	+	-
i	+	+
j	+	-
k	+	+
l	-	+

Table 1 Interaction of Picroside Ⅱ derivatives and targets

Conclusion In this study, we use Picroside Ⅱ as leading compound, carried out alkylation, acetylation and amino acid linkage, and 12 derivatives were obtained. And the method of virtual screening was used to screening the hepatoprotective effect of the derivatives. Nine potentially reactive compounds were screened out of twelve derivatives. Compared with traditional cell or animal experiments, this method is simple and fast, saving a lot of time and material resources. Besides, the molecular docking method determine the way of interaction of the target and the compound, and its mechanism was initial explored. This study provides a reference for the further study of the pharmacokinetics and mechanism of action.

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EXPOSURE TO HIGH TEMPERATURE CONDITION ENHANCES THE ANTIPYRETIC, ANALGESIC AND ANTI-INFLAMMATORY OF SAPOSHNIKOVIA. DIVARICATA FRESH ROOT

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Abstract

It is an ecological environment that leads to the quality difference of Radix saposhnikoviae (RS) produced in different regions or environmental stress. Previous study revealed that exposure of S. divaricata fresh roots to high temperature has potential to increase the chromones content, but it is untrustwrothy to evaluate the quality only depending on components due to complexity. The pharmacokinetics parameters showed that only cimifugin was found in plasma after RS were administered to rats, heat-stress-RS (HRS) had a 50.6% increase of cimifugin concentration. The anti-pyretic effect of HRS was higher than that of RS at all the dosages, with HRS at 1 g/kg nearly equivalent to 2 g/kg RS. The analgesic effect of HRS was stronger than that of RS at all the dosages, with HRS at 1 g/kg nearly equivalent to 4 g/kg RS.The anti-inflammatory effects of the HRS and RS were both dose dependent. The anti-inflammatory effect of HRS was more potent than that of RS at all the dosages, with HRS at 1 g/kg nearly equivalent to 2 g/kg RS. High temperature dramatically advances the quality of RS.

Keywords: Radix Saposhnikoviae; chromone; pharmacokinetics; anti-pyretic; analgesic; anti-inflammatory.

Radix saposhnikoviae (RS) , widely used in Asian countries, is the dried root of non-bolting stage of Saposhnikovia divaricata (Turcz.) Schischk and mainly contains diverse chromone components, including cimifugin, prime-O-glucosylcimifugin (PGCN), and 4’-O-β-D-glucosyl-5-O-methylvisamminol (GML), but only cimifugin can be found in plasma after RS were administered to rats[1]. RS has anti-pyretic, analgesic and anti-inflammatory effects[2], Chromone contents varies tremendously according to the geographical origin or environmental stress, with PGCN varying from 0.11% to 0.48%, GML from 0.13% to 0.39%, and the total chromones from 0.18% to 6.8%[3]. Compared with cultivated RS, higher content of PGCN and GML was found in the wild one. Now, RS is nearly all obtained from the cultivated S. divaricata and the degradation of the quality is an undeniable fact. How to increase the content of the secondary metabolites in RS has become the focus of medicinal herb production.

Herbal medicine quality varied considerably according to the geographical origin or environmental stress, the good cultivated environment habitats can easily lead to reducing quality. Reactive oxygen species are the initial products produced under environmental stress conditions and represent key plant products that induce secondary metabolism, and secondary metabolites are often medicinal ingredients. High temperature must result in production