

# Review of: "Molecular mechanisms of Huanglian jiedu decoction on ulcerative colitis based on network pharmacology and molecular docking"

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Overall, the experimental design is good, however we raise three points for consideration.

First, ingredient identification. Network pharmacology has been widely used to explore the complex action mechanism of traditional Chinese medicine. In this study, 54 active components related to UC were identified. The screening criteria of the compounds based on the Human oral bioavailability (OB)  $\geq 30\%$  and drug-likeness (DL)  $\geq 0.18$ . Indeed, a bioactive compound with  $\geq 30\%$  of the OB value has good absorption and slow metabolism after oral administration. In fact, these compounds may mainly distribute in the colon, rather than must absorbed into the blood, to exert their pharmacological activities for ulcerative colitis, such as anti-inflammatory effect, restore intestinal barrier, etc. This screening criteria might miss a lot of ingredients that  $< 30\%$  of the OB value but has good effect in the treatment of UC.

Further, contents of the identified compounds from HLJDD should be considered, including their concentrations in vitro and in vivo. However, this factor was not taken into account in the paper. Report showed that the compounds merely obtained from the TCMSP data. This is a speculated result. In fact, the contents of ingredients significantly affect the efficacy of HLJDD in the treatment of UC. In vitro, the determination of ingredient contents could use for the quality control, which ensures the stability of curative effect of HLJDD. In vivo, the distribution of ingredient could reflect their sites of action. In this study, whether the identified bioactive components distributed in the colon or the site related to the UC treatment, which is warrant to verified.

Finally, validation of the key pathways for HLJDD. Ten genes are very important to the protein-protein interaction network. Functional analysis showed that these target genes were mainly involved in the regulation of various immune regulatory pathways, such as IL-17 and TNF signal pathway. However, these results seem to be a speculation. It is better to verify these key pathways through further animal experiments, rather than just using another prediction method like molecular docking.