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Protein network module-based identification of key pharmacological pathways of *Curcuma phaeocaulis* Val. acting on hepatitis

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Abstract:

Ethnopharmacological relevance: Curcuma phaeocaulis Val. (*CP*), as the vital medicines for blood-breaking and disorder-eliminating, has been widely used for hepatitis with good curative effects. Owing to the complexity of traditional Chinese medicine, the pharmacological mechanism of *CP* remains unclear. To solve this problem, a protein network module-based approach was proposed in this study.

Materials and methods: Firstly, the content of active components of *CP* was detected based on HPLC-DAD. Then the liver protection of *CP* on Con A-induced hepatitis was validated via the analysis of serum levels of ALT, AST and LDH and histological findings. Next, the targets of *CP* components obtained from TCMD database were predicted by STITCH and ChEMBL retrieval. In addition, the protein interaction network (PIN) of *CP* was constructed by Cytoscape based on protein-protein interaction of targets obtained from STRING database. Following the topological analysis of *CP* PIN, it showed to exhibit the properties of scale-free, small world, and modularity matched with the property of complex biological networks. Finally, the functional modules were

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Abbreviations: CP, *Curcuma phaeocaulis* Val.; ALT, Alanine aminotransferase; AST, Aspartate transaminase; LDH, Lactate dehydrogenase; PIN, Protein interaction network; HBV, Hepatitis B virus; HCV, Hepatitis C virus; TCM, Traditional Chinese medicine; PPIs, Protein-protein interactions; NFKB1, Nuclear factor kappa B subunit 1, p50; RELA, Transcription factor p65, p65; NFKBIA, NF-κB inhibitor alpha; NFKBIB, NF-κB inhibitor beta; IKBKB, inhibitor of nuclear factor kappa-B kinase subunit beta; CHUK, Conserved helix-loop-helix ubiquitous kinase; TGFB1, Transforming growth factor beta 1; TGFBR1, TGF beta type I receptor; TGFBR2, TGF beta type II receptor; SMAD3, Mothers against decapentaplegic homolog 3; SMAD4, Mothers against decapentaplegic homolog 4; ZFYVE9, SMAD anchor for receptor activation

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