

Molecular Docking Simulation Based Screening for Revealing the Mechanism of Treating Eczema with *Lishi Xiaofeng Yin*

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SUMMARY. Eczema is a skin disorder characterized by inflammation, itching, and redness. *Lishi Xiaofeng Yin* is a traditional Chinese medicine formulation that has been used to treat eczema for centuries. However, the underlying mechanism of its therapeutic effect remains unclear. In this study, we used a molecular docking simulation approach to explore the potential plant-based leads of *Lishi Xiaofeng Yin* and predict the binding affinity of its active compounds against the macromolecular targets to investigate the potential mechanism of *Lishi Xiaofeng Yin* in treating eczema. Our results suggest that *Lishi Xiaofeng Yin* may exert its therapeutic effect on eczema by modulating multiple targets involved in the inflammatory response, immune regulation, and skin barrier function. These findings bring a scientific support for the clinical application of *Lishi Xiaofeng Yin* in the treatment of eczema and may also facilitate the development of new therapeutic strategies for this disorder.

RESUMEN. El eczema es un trastorno de la piel caracterizado por inflamación, picazón y enrojecimiento. *Lishi Xiaofeng Yin* es una formulación de la medicina tradicional china que se ha utilizado para tratar el eccema durante siglos. Sin embargo, el mecanismo subyacente de su efecto terapéutico sigue sin estar claro. En este estudio, utilizamos un enfoque de simulación de acoplamiento molecular para explorar los potenciales conductores de origen vegetal de *Lishi Xiaofeng Yin* y predecir la afinidad de unión de sus compuestos activos contra los objetivos macromoleculares para investigar el mecanismo potencial de *Lishi Xiaofeng Yin* en el tratamiento del eccema. Nuestros resultados sugieren que *Lishi Xiaofeng Yin* puede ejercer su efecto terapéutico sobre el eczema al modular múltiples objetivos involucrados en la respuesta inflamatoria, la regulación inmune y la función de barrera de la piel. Estos hallazgos brindan un respaldo científico para la aplicación clínica de *Lishi Xiaofeng Yin* en el tratamiento del eccema y también pueden facilitar el desarrollo de nuevas estrategias terapéuticas para este trastorno.

KEY WORDS: eczema, Lishi Xiaofeng, molecular docking, oleanolic acid

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