

## Herbal Leads from HuangBai Plant for Development of CTM Based Potential SGLT2 Inhibitor for Treatment of Diabetes Induced Nephropathy

Hongyan MENG<sup>1,2</sup>, Min PENG<sup>2</sup>, Hongbo MA<sup>2</sup>, Qianqian LIU<sup>2</sup>, Guomin SI<sup>1,2\*</sup>, & Lihui CHEN<sup>3\*</sup>

<sup>1</sup>College of Traditional Chinese Medicine, Shandong University of Traditional Chinese Medicine, No. 4655, Daxue Road, Changqing District, Jinan 250355 China

<sup>2</sup>Department of Traditional Chinese Medicine, Shandong Provincial Hospital Affiliated to Shandong First Medical University, No. 324, Jingwu Road, Huaiyin District, Jinan 250021 China

<sup>3</sup>Department of Rheumatology and Immunology, Shandong Provincial Hospital Affiliated to Shandong First Medical University, No. 324, Jingwu Road, Huaiyin District, Jinan-250021 China

**SUMMARY.** The present study investigated methylene cycloartanol and cneorin-NP 36 for the treatment of diabetic-induced nephropathy. Diabetic-induced nephropathy is a type of kidney disease caused by diabetes complications. High blood sugar levels induce damage to the small blood vessels in the kidneys, resulting in this syndrome. A class of medications known as sodium-glucose cotransporter-2 (SGLT2) inhibitors are used to treat type 2 diabetes. They function by preventing glucose reabsorption in the kidneys, which helps to lower blood glucose levels. SGLT2 inhibitors have also been shown to benefit patients with diabetes-induced nephropathy. HuangBai is a traditional Chinese herbal medication that has been used to cure a variety of diseases for millennia. It has recently been discovered to have potential applications in the treatment of diabetes-induced nephropathy. In the current study paradigm, a ligand library based on the chemical elements of the HuangBai plant was created and computationally tested against human SGLT2. The results demonstrated that methylenecycloartanol and cneorin-NP 36 were discovered to have a possible inhibitory effect on human SGLT2 and may be a plant-based alternative medicine for the treatment of diabetic nephropathy. In summary, methylenecycloartanol and cneorin-NP 36 can be used for the development of novel therapeutics to benefit patients with diabetic-induced nephropathy.

**RESUMEN.** El presente estudio investigó el metileno cicloartanol y la cneorina-NP 36 para el tratamiento de la nefropatía inducida por la diabetes. La nefropatía inducida por la diabetes es un tipo de enfermedad renal causada por complicaciones de la diabetes. Los niveles altos de azúcar en la sangre inducen daño a los vasos sanguíneos pequeños en los riñones, lo que resulta en este síndrome. Una clase de medicamentos conocidos como inhibidores del cotransportador de sodio-glucosa-2 (SGLT2) se usan para tratar la diabetes tipo 2. Funcionan impidiendo la reabsorción de glucosa en los riñones, lo que ayuda a reducir los niveles de glucosa en sangre. También se ha demostrado que los inhibidores de SGLT2 benefician a los pacientes con nefropatía inducida por diabetes. HuangBai es un medicamento herbal chino tradicional que se ha utilizado para curar una variedad de enfermedades durante milenios. Recientemente se ha descubierto que tiene aplicaciones potenciales en el tratamiento de la nefropatía inducida por diabetes. En el paradigma de estudio actual, se creó una biblioteca de ligandos basada en los elementos químicos de la planta HuangBai y se probó computacionalmente contra SGLT2 humano. Los resultados demostraron que se descubrió que el metilencicloartanol y la cneorina-NP 36 tienen un posible efecto inhibitorio sobre el SGLT2 humano y pueden ser una medicina alternativa basada en plantas para el tratamiento de la nefropatía diabética. En resumen, el metilencicloartanol y la cneorina-NP 36 se pueden utilizar para el desarrollo de nuevos tratamientos que benefician a los pacientes con nefropatía inducida por la diabetes.

**KEY WORDS:** cneorin-NP 36, docking, herbal drug, HuangBai, nephropathy, SGLT2.

\* Authors to whom correspondence should be addressed. E-mails: sgm977@126.com; rubasu@163.com