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Abstract

Screening of Urea Transporter Inhibitors in Celery Seeds by UPLC-TOF-MS †

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Abstract: Urea transporters (UTs) are a kind of transmembrane protein that specifically permeate urea, and play an important role in the mechanism of urine concentration. Selective knockout of UT can concentrate urea without affecting water and electrolytes, resulting in selective diuresis, which is a promising new diuretic target. Most of the currently reported UT inhibitors are obtained from small molecular libraries screened. We subjected the methanolic extract of celery seed to silica gel column chromatography analysis, and screened the column chromatographic fractions of celery seed for UT-B inhibitory activity using the reported erythrocyte lysis model. The UT-B inhibitory activity was also screened for the fractions of celery seed separated by column chromatography, using the reported erythrocyte lysis model. The chemical composition of the active site was identified using UPLC-TOF-MS, and the active compounds were selected in combination with molecular docking and ADMET prediction. Screening of the extracted parts of celery seed, using an erythrocyte lysis model, yielded nine small molecules with good inhibitory activity, namely esters, phenols, and organic acids. This experiment shows that compounds with UT-B inhibitory effects can be found in ethnic medicinal materials, which not only provides new ideas for the discovery of UT-B inhibitors, but also contributes to the development of ethnic medicines.

Keywords: celery seed; UT-B inhibitor; erythrocyte lysis model

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