

عنوان مقاله:

Bruguirea gymnorrhiza Leaf Extract Metabolites: Oral Bioavailability and GI Absorption Predictions

محل انتشار:

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خلاصه مقاله:

Background: Bruguirea gymnorrhiza is used to treat some diseases traditionally. Some scientific studies are important for its explanation and drug development. The aims of this study are to identify metabolites in B. gymnorrhiza leaf extract and predict their oral bioavailability and GI absorption associated with treating diseases. Methods: B. gymnorrhiza leaves were dried. Its flour was macerated in ethanol, then evaporated to produce an extract. The extract was analysed using Liquid Chromatography High Resolution-Mass Spectrophotometry (LCHR-MS) technique to identify its metabolites. The SwissADME tool was applied to predict their oral bioavailability and gastrointestinal (GI) absorption. Results: The LCHR-MS analysis resulted that B. gymnorrhiza leaf extract contained choline (۶۵.۱۸%) as the most dominant metabolite, followed by diisobutylphthalate (۷.۲۳%), isoleucine (۵.۶۲%), ۲,۲,۶,۶-tetramethyl-۱-piperidinol (TEMPO) (۴.۱۸%), valine (۳.۵۲%), L-phenylalanine (۲.۰۷%), d-(+)-proline (۱.۷۰%), ۲-[(۳S)-۱-(cyclohexylmethyl)-۳-pyrrolidinyl]-۱H-benzimidazole-۵-carbonitrile (۱.۴۴%), adenine (۱.۳۹%), ۲-[(۲-chlorobenzyl)sulfanyl]-۴,۶-dimethylnicotinonitrile (۱.۲۶%), L-norleucine (۱.۲۴%), dibenzylamine (۱.۲۶%) and wogonin (۱.۰۵%). Most of them were predicted not to be oral bioavailable, except diisobutylphthalate, TEMPO, ۲-[(۳S)-۱-(Cyclohexylmethyl)-۳-pyrrolidinyl]-۱H-benzimidazole-۵-carbonitrile, and wogonin. However, most of the metabolites were predicted to be absorbed by GI wall highly, except choline. Conclusion: The B. gymnorrhiza leaf extract contains ۱۳ main metabolites dominated by choline. They are mostly predicted not to be oral bioavailable and highly absorbed by GI tract. These results can be referred to direct and determine further steps of scientific studies of B. gymnorrhiza leaf extract and its metabolites as disease treating agents

کلمات کلیدی:

Bruguirea gymnorrhiza, Disease, prediction, SwissADME, treatment

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