Inhibitory and in silico molecular docking of Xeroderris stuhlmannii (Taub.) Mendonca & E.P. Sousa phytochemical compounds on human α-glucosidases

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Abstract

Ethnopharmacological relevance

Herbal traditional medicine is used by millions of people in Africa for treatment of ailments such as diabetes mellitus, stomach disorders and respiratory diseases. Xeroderris stuhlmannii (Taub.) Mendonca & E.P. Sousa (X. stuhlmannii (Taub.)) is a medicinal plant used traditionally in Zimbabwe to treat type 2 diabetes mellitus (T2DM) and its complications. However, there is no scientific evidence to support its inhibitory effect against digestive enzymes (α-glucosidases) that are linked to high blood sugar in humans.

Aim of the study

This work aims to investigate whether bioactive phytochemicals of crude X. stuhlmannii (Taub.) can scavenge free radicals and inhibit α-glucosidases in order to reduce blood sugar in humans.

Materials and methods

Here we examined the free radical scavenging potential of crude aqueous, ethyl acetate and methanolic extracts of X. stuhlmannii (Taub.) using the diphenyl-2-picrylhydrazyl assay in vitro. Furthermore, we carried out in vitro inhibition of α-glucosidases (α-amylase and α-glucosidase) by the crude extracts using chromogenic 3,5-dinitrosalicylic acid and p-nitrophenyl-α-D-glucopyranoside substrates. We also used molecular docking approaches (Autodock Vina) to screen for bioactive phytochemical compounds targeting the digestive enzymes.

Results

Our results showed that phytochemicals in X. stuhlmannii (Taub.) aqueous, ethyl acetate and methanolic extracts scavenged free radicals with IC50 values ranging from 0.002 to 0.013 μg/mL. Furthermore, crude aqueous, ethyl acetate and methanolic extracts significantly inhibited α-amylase and α-glucosidase with IC50 values of 10.5–29.5 μg/mL (versus 54.1 ±

0.7 μg/mL for acarbose) and 8.8–49.5 μg/mL (versus 161.4 ± 1.8 μg/mL for acarbose), respectively. In silico molecular docking findings and pharmacokinetic predictions showed that myricetin is likely a novel plant-derived α-glucosidase inhibitor.

Conclusion

Collectively, our findings suggest pharmacological targeting of digestive enzymes by X. stuhlmannii (Taub.) crude extracts may reduce blood sugar in humans with T2DM via inhibition of α-glucosidases.