Antidiabetic, antioxidant and *in silico* molecular docking of *Xeroderris stuhlmannii* (Taub.) Mendonca & E.P. Sousa phytochemical compounds on human pancreatic α-amylase and human lysosomal acid-α-glucosidase

Brilliant Nyathi, Jonathan Tatenda Bvunzawabaya, Emily Manzombe, Kudakwashe Tsotsoro, Major Allen Selemani, Gadzikano Munyuki and Freeborn Rwere

ABSTRACT

Millions of people in developing nations rely on herbal traditional medicine for the treatment of ailments such as diabetes mellitus, stomach disorders and respiratory diseases. *Xeroderris stuhlmannii* (Taub.) Mendonca & E.P. Sousa is a medicinal plant used traditionally in Zimbabwe to treat diabetes mellitus and its complications. However, there is no scientific evidence to support its role as an antidiabetic medicinal plant. Here we hypothesized that *Xeroderris stuhlmannii* (Taub.) Mendonca & E.P. Sousa contain bioactive phytochemicals that can scavenge free radicals, and inhibit digestive enzymes that contribute to type 2 diabetes mellitus (T2DM). To test this hypothesis, we examined the free radical scavenging potential of crude extracts using the diphenyl-2-picrylhydrazyl assay *in vitro*. Furthermore, we carried out *in vitro* antidiabetic activity of crude extracts using chromogenic 3,5-dinitrosalicylic acid and p-nitrophenyl-alpha-D-glucopyranoside substrates on alpha-amylase and alpha-glucosidase. In addition, we used molecular docking approaches to screen for bioactive phytochemical compounds targeting the digestive enzymes. Our results showed that phytochemicals in *Xeroderris stuhlmannii* (Taub.) Mendonca & E.P. Sousa extracts scavenged free radicals with IC_{50} values ranging from 0.011-0.013 micrograms/mL. Further, the crude extracts significantly inhibited alpha-amylase and alpha-glucosidase with IC_{50} values of 12.9-21.1 micrograms/mL and 8.8-16.0 micrograms/mL, respectively. *In silico* molecular docking findings and pharmacokinetic predictions showed that myricetin is a novel inhibitor of the digestive enzymes that contributes to high blood glucose. Collectively, our findings suggest pharmacological targeting of digestive enzymes by *Xeroderris stuhlmannii* (Taub). Mendonca & E.P. Sousa crude extracts could lesion type 2 mellitus complications in humans.