Supplementary File (Appendix 1)

Comparative Evaluation of Phytochemical Screening, *in vitro* Antioxidant and α-Glucosidase Inhibitory Properties of *Ceiba pentandra* and *Basella rubra* Leaf Extracts: Identification of Active Principles by Q-TOF LCMS, ADMET Prediction and Molecular Docking Approach

ABSTRACT

Ceiba pentandra and *Basella rubra* leaves are traditionally used in Indonesia to treat ailments like diabetes. This study aimed to validate their use by assessing their antioxidant and α-glucosidase inhibitory properties. Initially, maceration of the leaves of both plants yielded DCM, MeOH, and aqueous extracts. These were phytochemically profiled, and the most active extracts underwent Q-TOF LCMS analysis to identify potential active principles, followed by molecular docking to ascertain their mechanism of action. The results revealed that the aqueous and methanol extracts of *C. pentandra* exhibited potent antioxidant activities, with IC_{50} values of 17.66 ± 0.7 and 53.58 ± 0.25 µg/mg AAE for FRAP, respectively. In comparison, the aqueous and methanol extracts of *B. rubra* showed lower antioxidant potential, with values of 8.73 ± 0.1 and 10.17 ± 0.08 µg/mg AAE, respectively. Additionally, the DPPH assay displayed that the aqueous and methanol extracts of *C. pentandra* had IC_{50} values of 157.32 ± 3.44 and 27.71 ± 1.54 µg/mL, respectively. In contrast, the aqueous and methanol extracts of *B. rubra* had higher IC_{50} values of 661.78 ± 1.8 and 253.76 ± 2.4 µg/mL, respectively. Owing to their significantly higher antioxidant activity, the aqueous and methanol extracts of *C. pentandra* leaves also displayed better α-glucosidase inhibitory effects compared to *B. rubra*, with IC_{50} values of 109.54 ± 1.72 and 10.78 ± 0.48 µg/mL, respectively. Q-TOF LCMS analysis of *C. pentandra*'s methanol extract identified significant bioactive compounds including *m*-coumaric acid (1), *cis*-β-D-Glucosyl-2-hydroxycinnamate (2), luteolin 7-rhamnosyl(1->6)galactoside (3), avenanthramide 2s (4), robinetin 3-rutinoside (5), melanoxetin (6), scutellarein 7-glucoside (7), torosaflavone B 3'-O-β-D-glucopyranoside (8), and 2"-O-α-L-rhamnosyl-6-C-fucosyl-3'-methoxyluteoiin (9). Molecular docking analysis showed that compounds 7, 8, and 3 were the most active with protein 3A4A, having affinity energies of -9.7, -10.0, and -10.3 kcal/mol, respectively. These phenolic compounds could be safe α-glucosidase inhibitors for diabetes treatment.

Keywords: *Ceiba pentandra*, *Basela rubra*, Phytochemical analysis, Antioxidants, DPPH, FRAP, α-glucosidase inhibitory effect, Q-TOF LCMS, *in silico*, molecular docking