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Antibacterial, antiparasitic and *in-silico* studies of *Dichapetalum madagascariense* Poire

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Dichapetalum madagascariense (Dichapetalaceae) is used to treat bacterial infections, jaundice, urethritis, and viral hepatitis. Its root has been investigated to contain broad-spectrum biologically active *dichapetalins*. To evaluate the plant's antibacterial and antiparasitic potentials coupled with in silico methods, we isolated and identified the known *dichapetalins* A and M from the roots. Both dichapetalins were tested together with the leaf (DML) and root (DMR) ethanol extracts on six ATCC bacteria strains *(Shigella flexneri, Bacillus cereus, Salmonella paratyphi* B*, Listeria monocytogenes, Escherichia coli, Staphylococcus aureus)* and three parasites; *Trypanosoma brucei brucei, Leishmania donovan*i and *Plasmodium falciparum* 3D7 strain using the Alamar Blue Assay. *Dichapetalins* A and M were potent against *B. cereus* with IC_{50}, 11.15 and 3.15µg/ml respectively compared with ampicillin (IC_{50}, 1.70µg/ml). DML (IC_{50}, 0.45µg/ml) was threefold more potent than ampicillin (IC_{50}, 1.5µg/ml) against *S. paratyphi* B and more active (IC_{50}, 12.65µg/ml) against S. *flexneri* than ampicillin (IC_{50}, 14.02µg/ml). *Dichapetalins* A (IC_{50}, 74.22µg/ml) and M (IC_{50}, 72.34µg/ml) were only active against T. b. brucei compared to the standard extract of *Coptis japonica* (IC_{50}, 3.6µg/ml) and suramin (IC_{50}, 4.96µg/ml). *Dichapetalin* M showed moderate activity against *L. donovani* (IC_{50}, 0.21µg/ml) with IC50, 16.80µg/ml. DML and DMR gave IC50, 9.66 and 11.17µg/ml respectively against T. b. brucei when compared with *C. japonica* (IC_{50}, 3.6µg/ml) and suramin (IC_{50}, 4.96µg/ml). Target prediction with PIDGIN software indicated NR1I2 as a plausible target for *dichapetalin* A. Protein blasting the protein sequence of this xenobiotic sensor nuclear receptor to the used species suggested that *dichapetalin* A may have a bacteriostatic effect through the nucleotide hydrolase NUDIX (T. brucei), or the uncharacterized protein YagA or ydbH (S. *flexneri*). However, the understanding of the exact mechanism of the *dichapetalin's* antibiotic effect requires further research.

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