NMR-Based Metabolomic Study of Antimalarial Plant Species Used Traditionally by Vha-Venda People in Limpopo Province, South Africa

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Abstract : Regardless of the significant advances accomplished in reducing the burden of malaria and other tropical diseases in recent years, malaria remains a major cause of mortality in endemic countries. This is especially the case in sub-Saharan Africa where 99% of the estimated global malaria deaths occurs on an annual basis. The emergence of resistant Plasmodium species and the lack of diversified chemotherapeutic agents provide the rationale for bioprospecting for antiplasmodial scaffolds. Crude extracts from twenty indigenous antimalarial plant species were screened for antimalarial activity and then subjected to 1H NMR-based metabolomic analysis. Ten plant extracts exhibited significant in vitro antiplasmodial activity (IC50 ≤ 5 µg/ml). The Principal Component Analysis (PCA) of the acquired 1H NMR spectra could not separate the analyzed plant extracts according to the detected antiplasmodial bioactivity. Application of supervised Orthogonal Projections to Latent Structures–Discriminant Analysis (OPLS-DA) to the 1H NMR profiles resulted in a discrimination pattern that could be correlated to bioactivity. A contribution plot generated from the OPLS-DA scoring plot illustrated the classes of compounds responsible for the observed grouping. Given the preliminary in vitro results, Tabernaemontana elegans Stapf. (Apocynaceae) and Vangueria infausta Burch. subsp. infausta (Rubiaceae) were subjected to further phytochemical investigations. Two indole alkaloids, dregamine and tabernaemontanine possessing antiplasmodial activity were isolated from T. elegans. Two compounds were isolated from V. infausta subsp. infausta and identified as friedelin (IC50 = 3.01 µg/ml) and morindolide (IC50 = 18.5 µg/ml). While these compounds have been previously identified, this is the first account of their occurrence in the genus Vangueria and their antiplasmodial activity. Based on the results of the study, metabolomics can be used to globally identify classes of plant secondary metabolites that are responsible for antiplasmodial activity.

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