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HPLC/LC-MS guided phytochemical screening of African medicinal plants and prediction of possible cytochrome P450 interactions

Saneesh Kumar[1], Nontombi Sephule[2], Charles Awortwe[1], Patrick J Bouic[1, 2] and Bernd Rosenkranz[1]
[1]University of Stellenbosch, South Africa
[2]Synexa Life Sciences, South Africa

Introduction: The dried roots of *Withania somnifera (Solanaceae), Glycyrrhiza glabra (Fabaceae) and Astragalus membranaceus* (Fabaceae) are used as folklore medicines for multifarious diseases including HIV/AIDS in Africa.

Objective: To determine the phyto-constituents present in the roots of *W. somnifera, G. glabra and A. membranaceu*s using methanol, ethanol, aqueous and ethyl acetate solvent extractions and assess the potential of each extract in altering the activity of cytochrome P450 enzymes.

Methods: Exhaustive extraction of the dried roots of *W. somnifera, G. glabra and A. membranaceu*s was done using water, methanol, ethanol and ethyl acetate, and qualitative analysis was completed using biochemicals tests, HPLC analysis and multiple reaction monitoring HPLC combined with electrospray ionisation and tandem MS (HPLC-ESCI/MS/MS) using quercetin, caffeine, coumarin, lanatoside C and gallic acid as reference standards for flavonoids, alkaloids, coumarins, cardiac glycosides and phenols.

Results: The biochemical tests confirmed the presence of alkaloids, saponins, phenols, glycosides, terpenoids, flavonoids and coumarins in almost all the plants, the methanol extracts having the most compared to the other solvent extracts. Based on the reaction color intensity, G. glabra had the most quantity of flavonoids. The HPLC analysis baseline quercetin, coumarin, lanatoside C, caffeine and gallic acid standards with retention times 0.71 min, 1.23 min, 1.93 min, 1.25 min and 0.79 min, respectively and all plant extracts with retention times ±0.63 min, ±0.96 min, ±0.55 min, ±0.35 min and ±0.77 min on the average with respect to their equivalent standards. The LC/MS analysis further confirmed the presence of flavonoids, phenols, glycosides and coumarins in most extracts with MRM scan retention times in close proximity with the masses of the daughter ions of the standards; 1.64 min for quercetin, 2.44 min for caffeine, 6.92 min for lanatoside C, 2.08 min for coumarin and 1.3 min for gallic acid. Alkaloids with masses matching caffeine daughter ions were least observed in all the extracts. Full scans both positive and negative ion modes also showed the presence of many phyto-constituents in the same class of compounds as the internal standards. The assessment model was baseline flavonoids (quercetin) as potential inducers, terpenoids and coumarins as potential inhibitors, the alkaloid caffeine as an inducer and glycoside derivates as inhibitors. The phyto-chemical fingerprints of the extracts from *W. somnifera, G. glabra and A. membranaceu*s projected the possibility of their inhibitory/inducive effect on the cytochrome P450 enzymes.

Conclusions: The results show that the consumption of the investigated plants together with conventional drugs may present a risk of possibly relevant herb-drug interaction.

saneesh.7.kumar@gmail.com

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