TITLE:

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ABSTRACT

Chemometric methods of experimental design associated with multivariate analysis were applied to spectroscopic data to discriminate different extracts from the leaves of the species Vernonia condensata Baker. For the extraction, four solvents (ethanol, ethyl acetate, dichloromethane and acetone) and their binary, ternary and quaternary mixtures were used. This approach allowed to determine the influence of the solvent extractor in the preparation of the extracts. Models of principal component analysis (PCA) and hierarchical analysis (AH), applied to data from the absorption spectroscopy in the infrared and ultraviolet-visible have proved to be useful tools in the investigation of the chemical composition of extracts. Besides the chemical investigation, we also evaluated in mice the antinociceptive activity of the different extracts through the abdominal constriction model as well as the lethal dose 50%, LD50, i.e., the dose that causes the death of half of the tested animals. The extracts that presented antinoceptive activity at all doses used were: Aqueous, ethanol pure, ethanol-ethyl acetate and dichloromethane-acetone binary mixtures and ethanol-ethyl acetatedichloromethane and ethanol-dichloromethane-acetone ternary mixtures. The application of models for areas of response with four components revealed that the extract obtained through the dichloromethane-acetone binary mixture showed the highest antinociceptive effect. In order to confirm the validity of the model, a new binary mixture of acetone- dichloromethane was prepared in the proportion 3:2 (v/v) and its antinociceptive activity was assessed. The results proved the validity of the model for the doses of 80 and 160 mg/kg.