TITLE:

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ABSTRACT

The performance of a chromatographic fingerprint obtained is closely dependent on the chromatographic separation degrees and concentration distributions of all the chemical components in herbal medicines. The purpose of this work is to investigate the influence of different solvents on the extraction medium and the mobile phase strength of reversed phase liquid chromatography and diode arrays detection using statistical mixture designs to improve the quality of chromatographic fingerprints of the unfractionated extract of the Bauhinia variegata L. For modeling, the number of peaks was used as a measure of fingerprint information. Methanol (MeOH) and acetonitrile (ACN) were used as the mobile phase modifying solvents. Dichloromethane, ethanol and acetone were used as extraction solvents. The results show that the dependence of the peak numbers on the solvent composition increases with increasing mobile phase strength. Three mobile phases, each with a chromatographic strength of two, produced good results. A MeOH: H2O (77:23 v/v) mixture results in 17 peaks in the chromatographic fingerprint whereas ACN:H2O (64,5:35,5 v/v) and MeOH:ACN:H2O (35:35:30 v/v) mixtures result in 18 and 20 peaks, respectively. The optimum solvent compositions to extract chemical substances in the three mobile phases from the chromatographic analysis of the Bauhinia variegata L. were acetone:ethanol (75:25 v/v) and dichloromethane:acetone (70:30 v/v) mixtures and 100% dichloromethane, respectively. Principal component analysis and hierarquical cluster analysis models were applied to chromatograms of different extracts and mobile phases, as well as on UV-VIS middle infrared (FTIR) spectral data for each extract and their models were correlated with the HPLC models. The mixture design methodology allows obtaining useful mathematical models for describing the effects of mobile phase and extraction mixture compositions on the chromatographic fingerprints.