

Infrared Spectroscopy Fingerprinting of Herbal Products- Application of the Hypericum perforatum L. Supplements

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Abstract : Infrared spectroscopy (FT-IR) is an advanced technique frequently used to authenticate both raw materials and final products using their specific fingerprints and to determine plant extracts biomarkers based on their functional groups. In recent years the market for Hypericum has grown rapidly and also has grown the cases of adultery/replacement, especially for Hypericum perforatum L. specie. Presence/absence of same biomarkers provides preliminary identification of Hypericum species in safe use in the manufacture of food supplements. The main objective of the work was to characterize the main biomarkers of Hypericum perforatum L. (St. John's wort) and identify this species in herbal food supplements after specific FT-IR fingerprint. An experimental program has been designed in order to test: (1) raw material (St. John's wort); (2) intermediate raw materials (St. John's wort dry extract); (3) the finished products: tablets based on powders, on extracts, on powder and extract, hydroalcoholic solution from herbal mixture based on St. John's wort. The analyze using FTIR infrared spectroscopy were obtained raw materials, intermediates and finished products spectra, respectively absorption bands corresponding and similar with aliphatic and aromatic structures; examination was done individually and through comparison between Hypericum perforatum L. plant species and finished product The tests were done in correlation with phytochemical markers for authenticating the specie Hypericum perforatum L.: hyperoside, rutin, quercetin, isoquercetin, luteolin, apigenin, hypericin, hyperforin, chlorogenic acid. Samples were analyzed using a Shimatzu FTIR spectrometer and the infrared spectrum of each sample was recorded in the MIR region, from 4000 to 1000 cm^{-1} and then the fingerprint region was selected for data analysis. The following functional groups were identified -stretching vibrations suggests existing groups in the compounds of interest (flavones-rutin, hyperoside, polyphenolcarboxylic acids - chlorogenic acid, naphthodianthrones- hypericin): oxidril groups (OH) free alcohol type: rutin, hyperoside, chlorogenic acid; C = O bond from structures with free carbonyl groups of aldehyde, ketone, carboxylic, ester: hypericin; C = O structure with the free carbonyl of the aldehyde groups, ketone, carboxylic acid, esteric/C = O free bonds present in chlorogenic acid; C = C bonds of the aromatic ring (condensed aromatic hydrocarbons, heterocyclic compounds) present in all compounds of interest; OH phenolic groups: present in all compounds of interest, C-O-C groups from glycoside structures: rutin, hyperoside, chlorogenic acid. The experimental results show that: (I)The six fingerprint region analysis indicated the presence of specific functional groups: (1) 1000 - 1130 cm^{-1} (C-O-C of glycoside structures); (2) 1200-1380 cm^{-1} (carbonyl C-O or O-H phenolic); (3) 1400-1450 cm^{-1} (C=C aromatic); (4) 1600- 1730 cm^{-1} (C=O carbonyl); (5) 2850 - 2930 cm^{-1} (-CH₃, -CH₂-, =CH-); (6) 338-3920 cm^{-1} (OH free alcohol type); (II)Comparative FT-IR spectral analysis indicate the authenticity of the finished products (tablets) in terms of Hypericum perforatum L. content; (III)The infrared spectroscopy is an adequate technique for identification and authentication of the medicinal herbs , intermediate raw material and in the food supplements less in the form of solutions where the results are not conclusive.

Keywords : Authentication, FT-IR fingerprint, Herbal supplements, Hypericum perforatum L.

Conference Title : ICMPPN 2018 : International Conference on Medicinal Plants and Natural Products

Conference Location : San Francisco, United States

Conference Dates : June 06-07, 2018