



Chemometrics-assisted Comparative Chemical Profiling of Marketed *Nigella sativa* L. Seed Oils Using Spectroscopic Techniques

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SUMMARY. *Nigella sativa* L. seeds oil (NSO) also called as the black seeds oil is popularly known for its uses in a number of disease conditions and several NSO brands are available in the market as the folklore medicine. This study was designed to identify and compare the bioactive constituents present in two different brands of NSO preparations procured from local market. Fourier-Transform Infrared (FT-IR) and Gas Chromatography-Mass Spectrometry (GC-MS) techniques were employed to detect and quantify the constituents followed by chemometric analysis. The phytochemical analyses using GC-MS revealed presence of 40 and 33 constituents, respectively in the two tested oils. Among the major phytoconstituents, Thymoquinone (TQ), α -Pinene, *p*-Cymene, Nerol, Lavandulol, Carvacrol, (Z,Z)-9,12-octadecadienoic acid (Linoleic acid) and Squalene were present in both the samples showing high percent % peak area values. The FT-IR spectroscopic analysis showed presence of characteristic fingerprint functional groups confirming the authenticity of the procured samples. However, there were marked differences in the % area of different constituents making the two oils considerably different from each other. Using chemometric analysis, various dendrograms, heat maps (double dendrograms) and histograms were developed to compare and to make clusters of constituents with similar characteristics that might have originated from the same source.

RESUMEN. El aceite de semillas de *Nigella sativa* L. (NSO), también llamado aceite de semillas negras, es popularmente conocido por sus usos en una serie de enfermedades y varias marcas de NSO están disponibles en el mercado como medicina popular. Este estudio fue diseñado para identificar y comparar los componentes bioactivos presentes en dos marcas diferentes de preparaciones de NSO adquiridas en el mercado local. Se emplearon técnicas de infrarrojo por transformada de Fourier (FT-IR) y cromatografía de gases-espectrometría de masas (GC-MS) para detectar y cuantificar los constituyentes seguido de análisis quimiométrico. Los análisis fitoquímicos mediante GC-MS revelaron la presencia de 40 y 33 constituyentes, respectivamente, en los dos aceites probados. Entre los principales fitoconstituyentes, Thymoquinone (TQ), α -Pinene, *p*-Cymene, Nerol, Lavandulol, Carvacrol, (Z,Z)-9,12-octadecadienoic acid (Linoleic acid) y Squalene estaban presentes en ambas muestras mostrando un alto porcentaje % valores de área de pico. El análisis espectroscópico FT-IR mostró la presencia de grupos funcionales característicos de huellas dactilares que confirman la autenticidad de las muestras adquiridas. Sin embargo, hubo marcadas diferencias en el % de área de los diferentes constituyentes, lo que hizo que los dos aceites fueran considerablemente diferentes entre sí. Usando análisis quimiométricos, se desarrollaron varios dendrogramas, mapas de calor (dendrogramas dobles) e histogramas para comparar y hacer grupos de constituyentes con características similares que podrían haberse originado en la misma fuente.

KEY WORDS: black seed, chemometrics, FT-IR, GC-MS, *Nigella sativa*.

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