RESEARCH ARTICLE

Chemical Composition and QSRR Analysis of Essential Oil of Algerian *Scabiosa Daucoïdes* Desf

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ABSTRACT

The present study aimed to investigate, for the first time, the chemical composition of the essential oil from the aerial part of *Scabiosa daucoïdes* Desf (Caprifoliaceous) by GC-FID and GC-MS methods. The essential oil was extracted using the steam distillation technique. Thirty-eight components were identified, representing 76.49% of the total oil. The main constituents were spathulenol (8.95%), *cis*-α-copaene-8-ol (7.27%), *trans*-sesquisabinene hydrate (3.98%), germacrene B and germacrene D-4-ol (3.93%), caryophyllene alcohol (3.08%), and thujopsan-2-α-ol (3.04%). Moreover, a quantitative structure–retention relationship model was developed using multiple linear regression (MLR) after descriptor selection with a genetic algorithm employing variable subset selection (GA-VSS). The model attained demonstrates exceptional predictive ability with a cross-validated R-squared value of 98.36%, cross-validation of 97.47%, and external validation of 96.54%. These findings highlight model's accuracy concerning the retention index prediction and its application for studying essential oils. The molecular descriptors selected by GA-VSS, particularly QXXm, RDF060v, HATS4s, and s3_pathLength, significantly affected retention times.