Development and optimization of gas chromatography method for the determination of Selina-1,3,7(11)-trien-8-one and Selina-1,3,7(11)-trien-8-one epoxide in *Eugenia uniflora* essential oil by central composite design.

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Eugenia uniflora is a perennial tree, named in Brazil as Pitanga, belonging to the *Myrtaceae* family and native from the central part of Brazil to the north of Argentina. The essential oil of *E. uniflora* has been largely studied in several reports. Rodrigues *et al*. have studied the *in vitro* anti-leishmania activity of this oil with promising results (1). Jung *et al*. have investigated the application of this essential oil as an insecticide against *Atta laevigatta* ants, demonstrating a good potential (2). Barbosa *et al*. have determined the antibacterial properties of *E. uniflora* essential oil (3). The main constituents of *E. uniflora* are selina-1,3,7(11)-trien-8-one and selina-1,3,7(11)-trien-8-one epoxide (4). The isolation of these sesquiterpenoids by countercurrent chromatography is currently the subject of a project conducted by our research group. To optimize the analysis of samples from the isolation process development, a fast gas chromatography method was developed. Central composite design was applied, based in an original method used in our lab, to three different columns in order to determine the best suited. The chosen columns were the DB-5, DB-35 and DB-17ht, all of which have phenyl-methylpolysiloxane stationary phases, the differences between them been the amount of phenyl groups present. DB-5 have 5% of phenyl groups, DB-35 have 35% of phenyl and DB-17ht have 50% of phenyl groups. Phenyl groups in this phases interact with the more polar oxygenated terpenes resulting in better shaped peaks and faster and reliable analysis. The three columns were tested with 15 different methods generated by the central composite design using initial oven temperature, heating rate and flow as factors. Evaluation of the chromatograms indicated the DB-35 column as the most suited for the analysis. Method optimization for this column was carried out using initial oven temperature, heating rate and carrier gas flow as factors. Two conditions were selected for validating the model generated: (1) 72.89 ºC initial temperature, 4.71 ºC/min heating rate and 1.27 ml/min of carrier gas flow; (2) 70 ºC initial temperature, 6.49 ºC/min heating rate and 1.46 ml/min carrier gas flow. Results fell within the predicted values with the exception of selina-1,3,7(11)-trien-8-one in the second condition which have a higher than expected resolution and was then considered suitable for analysis. These conditions were selected because they have a lower analysis time. This method was validated for the determination of selina-1,3,7(11)-trien-8-one and selina-1,3,7(11)-trien-8-one epoxide.

1. Rodrigues, K.A.F. et al. Evid. Based Compl. Alt., 2013, 279726.
2. Jung, P.H. et al. Floresta e ambiente, 2013, **20**, 191-196.
3. Barbosa, L.N. et al. J. Oleo Sci., 2015, **64**, 289-298.
4. Costa, D.P. et al. J. Braz. Chem. Soc., 2009, **20**, 1287-1293.

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