

ABSTRACT

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Title of Diploma Thesis: UHPLC-HRMS in analysis of food supplements containing ginsenosides

The aim of this work was to develop an analytical method for the analysis of the main components of a dietary supplement, in which the following plant extracts are contained: fenugreek seed, roseroot root, Asian ginseng root and damiana leaf. The ultra-high performance liquid chromatography coupled to high-resolution mass spectrometry (UHPLC-HRMS) was used. Another goal was to determine whether prohibited testosterone is present in the dietary supplement. Measurements were carried out with ACQUITY UPLC I-Class System. A quadrupole time-of-flight mass analyzer SYNAPT G2-Si was used for mass spectrometric detection. Continuous data were collected. The data independent acquisition method (DIA) was used to collect data. The library of MS spectra of potentially predicted substances was created and ginsenosides were identified as major compounds.

In the first step, the preparation of food supplement samples was optimized. Water, acetonitrile, methanol, ethanol and ethyl acetate were tested as solvents. In the next step, the chromatographic conditions were optimized. 5 chromatography columns were compared. The Atlantis Premier BEH C18 AX column was selected for the final measurements. The following parameters were optimized for the MS setup: desolvation temperature, capillary voltage, desolvation gas flow rate, cone voltage, and collision energy for DIA. The calibration curve of testosterone was measured. The limit of detection was 0.5 ng/ml. Testosterone has not been identified in the dietary supplement samples.

Keywords: ginsenosides; testosterone; UHPLC-HRMS; dietary supplements; method development; optimization