150 ANOS PARA 118 ELEMENTOS – A TABELA PERIÓDICA

Livro de Resumos

O presente livro foi produzido a partir dos trabalhos submetidos diretamente pelos autores. Foram apenas introduzidas pequenas alterações de edição que de modo algum modificaram os conteúdos científicos. O modelo final de impressão foi estabelecido para o XXVI Encontro Nacional da Sociedade Portuguesa de Química de acordo com as normas divulgadas publicamente nos anúncios do evento. A responsabilidade dos conteúdos científicos é dos respetivos autores.

Health

Amino Acids Profile for Assessing Serra da Estrela Cheese Producers

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This work has the purpose to evaluate if the Serra da Estrela cheeses collected from 6 producers have typical chemical characteristics, with controlled variability, considering that cheeses were produced during different time periods, the raw milk comes from different animals, and that the cheese processing may slightly differ between cheesemaking producers. For this, the cheeses' amino acids profile was used, since it gives evidence at chemical level about cheese's nutritional characteristics.

In this study, 6 cheese certified producers located in different municipalities of the region of Serra da Estrela were selected, being collected 24 cheeses, which were stored in plastic tubes at -20°C until analyzed. For each cheese, two samples were evaluated by UPLC–MS/MS (Dionex Ultimate 3000 UPLC instrument from Thermo Scientific, USA) equipped with a diode-array detector and coupled to a mass detector Linear Ion Trap LTQ XL mass spectrometer (ThermoFinnigan, San Jose, CA, USA) equipped with an ESI source. The chromatographic separation was carried out on a U-VDSpher PUR C18-E 100mm×2.0 mm id, 1.8 µm column (VDS optilab, Germany) and its temperature was maintained at 40 °C. The mobile phase was composed of (A) 0.1% (v/v) formic acid in water and (B) 0.1% (v/v) formic acid in acetonitrile/water (50:50, v/v), using a multistep gradient program at a flow rate of 0.40 mL/min and an injection volume of 5 µL. Data acquisition was carried out with Xcalibur®data system (ThermoFinnigan, San Jose, CA, USA).

The overall quantitative amino acid profile, found in the studied cheese samples included the following compounds: arginine, histidine, lysine, cysteine, asparagine, glutamine, glutamic acid, serine, threonine, aspartic acid, valine, methionine, proline, isoleucine, tyrosine, phenylalanine and tryptophan. In general, for each amino acid, a linear regression coefficient of determination (R^2) greater than 0.98 was obtained. The experimental data were treated using a linear discriminant analysis (LDA), as the supervised pattern recognition method, aiming verifying if the amino acids profile (17 amino acids) could be used to correctly classify cheese samples according to their producer. An internal evaluation was considered using k-folds in order to minimize model over-fitting (reducing the risk of over-optimistic results) and the search included the evaluation of the optimal number of variables in the LDA model, between 2 to 17 independent variables, using a meta-heuristic simulated annealing variable selection algorithm.[1,2] Data was standardized (centered and scaled) and the obtained models in the cross-validation allowed an average classification accuracy superior to 90%, while the best model allowed correct classifications with a predictive sensitivity (proportion of positive correct classifications) and specificity (proportion of negatives correct classifications) greater than 95%.

Reference:
1. Kuhn M.; Johnson K. *Applied Predictive Modeling*, Springer **2013**.
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