

Chemometric analysis of grass pea (*Lathyrus sativus* L.) using ATR-FTIR spectroscopy: Predictive models for ODAP and Homoarginine contents

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Grass pea (*Lathyrus sativus* L.) is a resilient cool-season legume that tolerates environmental and biotic stresses. Neuro lathyrism, a neurological disorder, is associated with the presence of a neurotoxin called β -N-oxalyl-L- α , β -diaminopropionic acid (β -ODAP) in grass pea seeds [1]. ODAP exists in two isomeric forms (α and β), with the β isomer being the toxic variant, accounting for 95% of total ODAP [2]. Grass pea is also a unique source of homoarginine, a nonproteinogenic amino acid involved in the production of nitric oxide (NO), a vasodilator that prevents cardiovascular and renal dysfunctions. This study aimed to develop chemometric prediction models for grass pea ODAP and homoarginine contents using a rapid spectroscopic FTIR screening method coupled with mass spectrometry and supported by statistical analysis. Dried grass pea seeds, harvested over three years under similar conditions, were milled, and resulting flours analyzed using HPLC-ESI-MS/MS [3]. For quick screening, Attenuated Total Reflectance – Fourier Transformed Infrared Spectroscopy, ATR-FTIR (Thermo Nicolet 6700 spectrometer with an ATR crystal diamond) was performed on the samples. Partial least square regression multivariate analysis was conducted using Unscrambler X 10.4.1 software to explore the correlations between spectral data and quantified ODAP isomers and homoarginine. Calibration models were designed using flour samples from the three harvesting years, with selected spectral regions based on relevant literature. The models were validated through random cross-validation, achieving good correlation (above 0.5) between predicted and observed values for most parameters. Further experiments are ongoing to increase data variability explanation and reduce the root mean square error of the models. ATR-FTIR, combined with multivariate analysis, offers an alternative method for accurately quantifying parameters that impact health positively (e.g., homoarginine) or pose challenges to incorporating grass pea into the diet (e.g., ODAP).

[1] Gonçalves et al. (2022). <http://10.3390/agronomy12061324>.

[2] Das et al. (2021) <http://10.3389/fpls.2021.703275>.

[3] Bento-Silva et al. (2019) <http://10.3390/molecules24173043>.