## Quality of organic legumes – prediction of main ingredients and amino acids by Near-Infrared Spectroscopy

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#### Abstract

The analytical potential of Near-Infrared Spectroscopy (NIRS) for predicting the chemical composition and the amino acid contents of grain legumes was evaluated. Pea and bean samples from field trials of different organically-managed experimental locations in Germany were analysed with reference methods. The reference data were used for developing calibration equations for the main ingredients and for the estimation of the amino acids. The calibration equations were validated on a remaining sample set. The statistics of NIRS calibrations showed that the predictions were successful or satisfactory for all main ingredients. The predictions of the essential amino acids were successful and respectively, for cystine in beans satisfactory as well. The obtained results indicated that the NIRS could be successfully used for the prediction of the main ingredients and amino acids in field beans and peas and therefore to evaluate the feed quality quickly and easy. The exact calculation of feed rations seems to be possible if the samples are analysed by NIRS directly after harvesting.

Key words: feed quality, legumes, near-infrared spectroscopy, amino acids, main ingredients

#### Introduction

The quality evaluation of organic feeds, especially the quick and easy determination of the main ingredients and the amino acid pattern in locally grown legumes, is very important to fulfil the requirements regarding the protein and amino acid supply of organically fed animals, especially monogastric animals. The analytical data of organic feeds, as compared with conventional table values, shows a clear deviation of protein and amino acids between conventional and organic feeds. The standard tabular values (DLG 1991) are not sufficient for the calculation of the feed rations in organic monogastric nutrition. Therefore the ability of NIRS to predict the chemical composition and the amino acids of organically grown legumes was tested.

#### Material and methodology

Pea and bean samples from field trials of different organically managed experimental locations in Germany, collected over two years, were used for the investigations. The main ingredients of the beans were determined according to VDLUFA methods (VDLUFA 1997) and amino acids by HPLC (EG 1998, Cohen and Michaud 2004). NIRS analysis was carried out with the ground samples using the Fourier-Transform NIR spectrometer (NIRLab N-200, Fa. Büchi, Essen) in the spectral range from 1000 to 2500 nm. Spectral data were exported to the NIRCal chemometric software (Fa. Büchi, Essen) and different mathematical pre-treatments were performed. Calibration equations for crude nutrients and each amino acid were developed by partial least square regression (PLS) on about two-thirds of the pea or bean samples using the results from the analytical reference methods. The calibration equations were than validated on the remaining sample sets (1/3 of pea or bean samples). The performance of the calibrations was evaluated in terms of standard error of prediction and coefficient of determination.

## Results

The statistical summary of the best calibration and prediction for the main ingredients in peas and beans is shown in Table 1.

	Field Peas (n=350)					Field Beans (n=233)					
	content of ingredient (g/kg DM)			NIRS perfor- mance data		content of ingredient (g/kg DM)			NIRS performance data		
Ingredient	mean	min	max	R <sub>K</sub>	SEP	mean	min	max	R <sub>K</sub>	SEP	
crude	229	180	267	0.96	3.7	292	247	355	0.98	4.8	
protein											
crude fat	20.3	16.6	27.8	0.86	0.83	18.3	14.1	25.7	0.86	0.96	
crude fiber	69.0	50.3	87.9	0.89	3.3	95.0	79.8	117	0.78	3.9	
crude ash	30.9	23.4	36.7	0.94	0.90	38.1	24.3	52.9	0.86	2.1	
starch	522	474	553	0.92	5.9	434	360	530	0.91	7.6	
sugar	74.2	62.5	86.5	0.93	1.8	53.4	44.4	69.1	0.88	2.1	

 Table 1.
 NIRS calibration statistics for prediction of main ingredients in field peas and beans

DM: dry matter

RK: regression coefficient of calibration, SEP: standard error of prediction

The statistics of NIRS calibrations for the main ingredients in peas showed that the predictions were successful for protein, minerals, starch and sugar. The prediction accuracy for fat and fiber was satisfactory. For field beans the predictions were successful for protein and starch and satisfactory for fat, fiber, minerals and sugar.

The statistical summary of the best calibration and prediction for the amino acids in peas and beans is shown in Table 2.

		Field	Peas (n=3	50)		Field Beans (n=233)					
	content o	f amino aci	ds (g/kg	NIRS	perfor-	content of	f amino ao	NIRS performance			
	DM)			mane	ce data		DM)	data			
amino acids	mean	min	max	R <sub>K</sub>	SEP	mean	min	max	R <sub>K</sub>	SEP	
lysine	17.2	14.6	19.6	0.95	0.32	19.4	15.9	25.0	0.93	0.61	
methionine	2.25	1.85	2.67	0.93	0.065	2.15	1.74	2.44	0.90	0.049	
cystine	3.02	2.06	3.78	0.85	0.17	3.40	2.03	4.1	0.94	0.11	
threonine	8.75	7.10	9.84	0.96	0.14	10.4	9.08	11.9	0.96	0.15	
arginine	18.8	12.3	24.1	0.96	0.55	26.9	20.2	34.9	0.98	0.67	
histidine	5.58	4.12	6.47	0.97	0.10	7.33	6.38	8.63	0.98	0.11	
isoleucine	10.1	7.76	11.7	0.97	0.16	12.3	10.3	14.9	0.97	0.23	
leucine	16.6	12.5	19.4	0.98	0.25	21.2	17.5	25.8	0.97	0.37	
phenylalanine	11.2	8.72	13.2	0.97	0.17	12.3	10.9	15.4	0.97	0.20	
valine	11.5	8.95	13.0	0.97	0.17	13.7	11.8	16.2	0.97	0.19	

Table 2. NIRS calibration statistics for prediction of amino acids in field peas and beans

DM: dry matter

RK: regression coefficient of calibration, SEP: standard error of prediction

The predictions of the essential amino acids in peas and beans were successful. The prediction accuracy for the sulphur-containing amino acid cystine is satisfactory and should be improved in further investigations.

#### Discussion

The deviations in the contents of the main ingredients, described in previous investigations (e.g., Böhm et al. 2007), were confirmed in our study.

The obtained results indicated that the NIRS could be successfully used for the prediction of the main ingredients and amino acids in field peas and bean, and therefore to evaluate the feed quality quickly and easilyy. The exact calculation of feed rations seems to be possible if the samples are analysed directly after harvesting by NIRS.

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