RAPID PREDICTION OF ENERGY CONTENT IN CEREAL FOOD PRODUCTS WITH NIRS.

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Energy content, expressed as calories per gram, is an important part of the evaluation and marketing of foods in developed countries. Currently accepted methods of measurement of energy by U.S. food labeling legislation include measurement of gross calories by bomb calorimetry with an adjustment for undigested protein and by calculation using specific factors for the energy values of protein, carbohydrate less the amount of insoluble dietary fiber, and total fat. The ability of NIRS to predict the energy value of diverse, processed and unprocessed cereal food products was investigated. NIR spectra of cereal products were obtained with an NIRSystems monochromator and the wavelength range used for analysis was 1104-2494 nm. Gross energy of the foods was measured by oxygen bomb calorimetry (Parr Manual No. 120) and expressed as calories per gram (CPG1, range 4.05-5.49 cal/g). Energy value was adjusted for undigested protein (CPG2, range 3.99-5.38 cal/g) and undigested protein and insoluble dietary fiber (CPG3, range 2.42-5.35 cal/g). Using a multivariate analysis software package (ISI International, Inc.) partial least squares models were developed for the prediction of energy content. The standard error of cross validation and multiple coefficient of determination for CPG1 using modified partial least squares regression (n=127) was 0.060 cal/g and 0.95, respectively, and the standard error of performance, coefficient of determination, bias and slope using an independent validation set (n=59) were 0.057 cal/g, 0.98, -0.027 cal/g and 1.05 respectively. The PLS loading for factor 1 (Pearson correlation coefficient 0.92) had significant absorption peaks correlated to C-H stretch groups in lipid at 1722/1764 nm and 2304/2346 nm and O-H groups in carbohydrate at 1434 and 2076 nm. Thus the model appeared to be predominantly influenced by lipid and carbohydrate. Models for CPG2 and CPG3 showed similar trends with standard errors of performance, using the independent validation set, of 0.058 and 0.088 cal/g, respectively, and coefficients of determination of 0.96. Thus NIRS provides a rapid and efficient method of predicting energy content of diverse cereal foods.