Detecting effect of heat-related feed processing on molecular protein structure associated with nutrient utilization of barley grains in dairy cows by using vibrational molecular spectroscopy

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The objective of this study was to reveal the change from heat-related feed processing in the molecular protein structure of barley grains by using Attenuated Total Reflectance Fourier Transform vibrational molecular spectroscopy (ATR-Ft/VMS) with and correlate the molecular protein structure profile with rumen degradation. Barely grains (CDC Meredith) were sampled from harvested plots (n = 2) grown in 2013, 2014, and 2015. A sub-sample was coarsely crashed (gap size 1.78 mm) for in situ incubation and finely ground through 0.5 mm screen for the molecular spectral analysis. Amide I (1720 – 1577 cm^{-1}) and amide II (1577 – 1486 cm^{-1}) peak area intensities and peak heights, and secondary protein structures α-helices and β-sheets peak heights were measured in the region at ca. 1720 – 1486 cm^{-1} were quantified using OMNIC 7.3 software. Rumen degradation was performed by using rumen cannulated dairy cows. There was heat effect on the ratio of amide I to amide II area ($P < 0.001$), indicating that heat-related feed processing affected the molecular structure of protein as well as on α-helix to β-sheet ratio ($P = 0.008$). Correlation results showed that the bypass crude protein was negatively correlated to structural Amide I area ($P = 0.046$; $r = -0.71$) while the fraction potentially degradable (D) of protein was positively correlated to structural β-sheet height ($P = 0.22$; $r = 0.78$). This study has showed that heat-related feed processing affects the molecular protein structure differences and this difference can be detected by ATR-Ft/VMS. IMPLICATION: The ATR-Ft/VMS is a useful non-destructive technique that allows revealing molecular inherent structure in livestock feeds and the results could be associated with nutritive values.