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## Using ATR-FT/IR molecular spectroscopy to detect effects of blend DDGS inclusion level on the molecular structure spectral and metabolic characteristics of the proteins in hulless barley

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### HIGHLIGHTS

- ▶ Feed combination caused great effects on protein metabolic characteristics.
- ▶ Protein 2nd structure profile changed with increasing inclusion rate of blend DDGS.
- ▶ Increasing blend DDGS rate resulted in increase of truly absorbed protein supply.
- ▶ Feed combination process changed protein molecular structure spectral feature.

### GRAPHICAL ABSTRACT



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### ABSTRACT

The objectives of this study were to investigate the effects of inclusion of a bioethanol co-product of blend DDGS (wheat:corn = 70%:30%) on protein molecular structure spectral and metabolic characteristics in hulless barley-based feed using ATR-FT/IR molecular spectroscopy. Hulless barley grain with the blend DDGS were mixed in the five ratios. The results showed that when blend DDGS was included at an increased ratio, predicted truly absorbed protein supply was highly and linearly increased ( $P < 0.05$ ) from 98 to 245 g kg<sup>-1</sup> DM and degraded protein balance was increased ( $P < 0.05$ ) from -1 to 75 g kg<sup>-1</sup> DM. The ratio of amide I to II peak area was increased ( $P < 0.05$ ) in the original combination samples but decreased ( $P < 0.05$ ) in the in situ 48 h residue samples. The ratio of  $\alpha$ -helix to  $\beta$ -sheet peak height was quadratically changed with increasing inclusion rate of blend DDGS in the original samples, but no difference among the in situ 48 h residue samples, indicating completion of protein degradation. No correlation was found between protein 2nd structures and protein nutrient profiles not only for the original combination samples (except NPN) but also for in situ 48 h residue samples. This study may provide information on how protein molecular structure and metabolic characteristic changes after feed combination and how more effectively utilize hulless barley and blend co-products for dairy and beef cattle.

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### Introduction

To date, hulless barley grains and bioethanol co-products [such as wheat and corn dried distillers grains with solubles (DDGS)]

have become important ingredients of diets in ruminants. Because of their great scientific and financial interest, the studies on evaluation the nutritive values of hulless barley grains with altered carbohydrate traits [1,2] and various types of DDGS have become

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a global research focus [3–5]. Publications results show that there are big biological differences between hullless barley and bioethanol co-products [1–5], which are close related to not only their protein content and ruminal degraded behaviors, but also their inherent molecular structures [6]. By using standard in situ and in vitro techniques and NRC or DVE/OEB system, the truly digestible nutrients, the predicted truly absorbed protein supply (DVE) and the degraded protein balance (OEB) in various barley grains and DDGS have been estimated effectively [5,7]. At the same time, by using molecular spectroscopy techniques: SR-IMS, DRIFT, the differences of protein molecular structure makeup in different barley grains or DDGS have been detected [6,8]. However, studies on protein molecular structures in relation to nutritive value and digestive behaviors of protein in animals are still limited. To our knowledge, there was lack research on the effects of blend DDGS (NOT pure DDGS) inclusion on the molecular structure spectral profiles in original samples and rumen residue samples and metabolic characteristics of the proteins in hullless barley in beef and dairy cattle.

The objectives in this study were to investigate the effects of inclusion of a bioethanol co-product (wheat:corn blend DDGS = 70%:30%) on protein molecular structure spectral and the metabolic characteristics of hullless barley-based feeds mixture. The parameters assessed included (1) protein molecular structure makeup features; (2) traditional nutrient profiles; (3) protein fractions partitioned; (4) in situ nutrient degradation kinetics and effective degradability; (5) the predicted truly absorbed protein supply in the small intestine and the degraded protein balance; (6) relationship of protein molecular structure to nutrient profiles

and metabolic characteristics. The hypothesis of this study was that the feed combination changed protein molecular structural spectral profile, therefore changed the metabolic characteristics of protein.

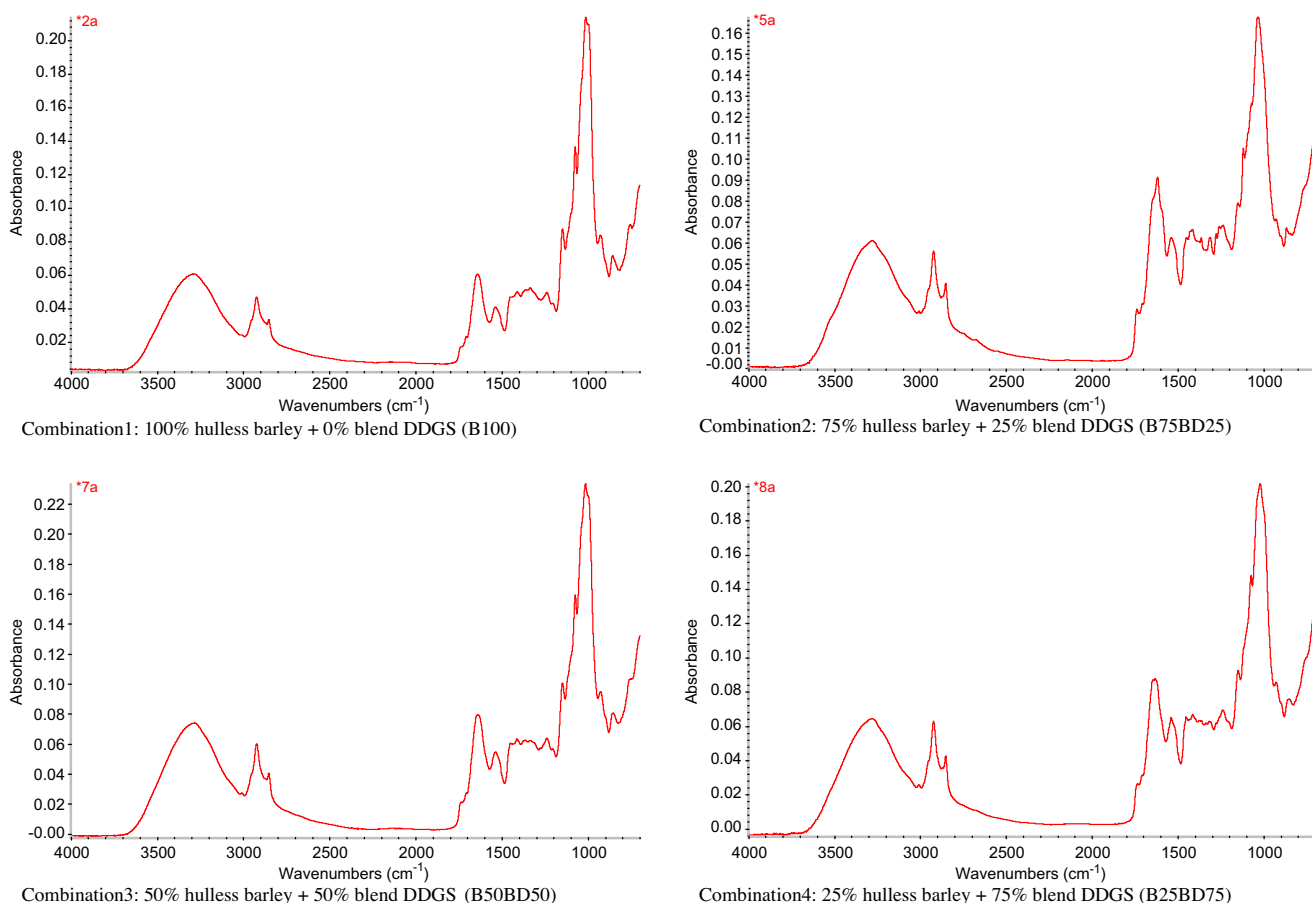
## Materials and methods

### Feed samples selected and test designed

In this study, hullless barley (cv. CDC McGwire) and blend DDGS (wheat:corn = 70%:30%) were used for studying the protein molecular structures and protein metabolic characteristics in combined feeds. Five feed combinations (hullless barley: blend DDGS percentage ratio) were combined by hand at the ratios of 100:0, 75:25, 50:50, 25:75, and 0:100. The combinations were named as B100, B75BD25, B50BD50, B25BD75, and BD100 according to hullless barley to blend DDGS ratio. Before chemical analysis, all samples were ground through a 1 mm screen (Retsch ZM-1, Brinkmann Instruments Ltd., Mississauga, ON, Canada).

### Molecular spectroscopic investigation

The spectroscopic experiments were conducted at the University of Saskatchewan. JASCO FT/IR-ATR-4200 (JASCO Corporation, Tokyo, Japan) was used to collect the molecular spectrum data of five hullless barley and blend DDGS combinations and their relative in situ 48 h residue samples. For each treatment, ten replicates were randomly set. Thirty-two scans per spectrum were collected



**Fig. 1.** Typical spectra of five combinations of hullless barley with co-products from bioethanol processing of blend DDGS: (a) common scale and offset scale; (b) whole mid-IR region, fingerprint region and amide I and amide II region.

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