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Do **NOT** write outside the grey boxes. Any text or images outside the boxes **will** be deleted.

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Title:

Predicting food digestion behavior by food breakdown classification system class using micro-CT images

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Abstract: (Your abstract must use **Normal style** and must fit in this box. Your abstract should be no longer than 300 words. The box will 'expand' over 2 pages as you add text into it.)

Preparation of Your Abstract

1. The title should be as brief as possible but long enough to indicate clearly the nature of the study. Capitalise the first letter of the first word **ONLY** (place names excluded). No full stop at the end.
2. Abstracts should state briefly and clearly the purpose, methods, results and conclusions of the work.

Introduction: Clearly state the purpose of the abstract

Methods: Describe your selection of observations or experimental subjects clearly

Results: Present your results in a logical sequence

Discussion: Emphasize new and important aspects of the study and conclusions that are drawn from them

Introduction: Understanding how foods behave post-consumption without relying on *in vivo* or *in vitro* trials is needed. The food breakdown classification system (FBCS) predicts food digestion behaviour based on initial hardness and softening rate during static *in vitro* digestion. This study aims to develop a machine learning model to classify foods into the six FBCS classes using features extracted from micro-computed tomography images of undigested foods.

Methods: Texture- and shape-based features were extracted from micro-computed tomography images from 43 different foods and used to train four machine learning models: decision trees, k-nearest neighbour, random forest and support vector machine. For model testing and validation, multiple data splitting methods were examined: stratified versus leave-out sampling for train/test splits, and 5-fold versus leave-one-out cross validation for train/validation splits. Accuracy, precision, recall and F1-score were determined for both the validation and test sets for each machine learning model.

Results: Stratified sampling with 5-fold cross validation resulted in high F1-scores for validation (0.91–0.95) and test (0.92–0.96) sets across the four different machine learning models. Leave-out sampling with 5-fold cross validation gave higher validation scores (0.85–0.97), but lower test scores (0.51–0.63) across the four different machine learning models. Leave-out sampling and leave-one-out cross validation resulted in poor performance (validation: 0.45–0.51; test: 0.04–0.50). The trends in F1 score were consistent across accuracy, precision, and recall.

Discussion: Stratified sampling with 5-fold cross validation resulted in strong model performance, where models could classify foods into their FBCS class using microstructural information. However, this sampling and validation method does not reflect applications in which new foods would be classified. Leave-out methods better simulate such conditions but have lower performance. Overall, this study demonstrates the possibility to classify food digestion behaviour based on initial properties, which may be a future tool in streamlining development of foods with targeted digestion behaviour.