

## Predictive Modelling of Curcuminoid Bioaccessibility as a Function of Food Formulation and Associated Properties

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**Abstract :** Background: The bioaccessibility of bioactive compounds is a critical determinant of the nutritional quality of various food products. Despite its importance, there is a limited number of comprehensive studies aimed at assessing how the composition of a food matrix influences the bioaccessibility of a compound of interest. This knowledge gap has prompted a growing need to investigate the intricate relationship between food matrix formulations and the bioaccessibility of bioactive compounds. One such class of bioactive compounds that has attracted considerable attention is curcuminoids. These naturally occurring phytochemicals, extracted from the roots of *Curcuma longa*, have gained popularity owing to their purported health benefits and also well known for their poor bioaccessibility. Project aim: The primary objective of this research project is to systematically assess the influence of matrix composition on the bioaccessibility of curcuminoids. Additionally, this study aimed to develop a series of predictive models for bioaccessibility, providing valuable insights for optimising the formula for functional foods and provide more descriptive nutritional information to potential consumers. Methods: Food formulations enriched with curcuminoids were subjected to in vitro digestion simulation, and their bioaccessibility was characterized with chromatographic and spectrophotometric techniques. The resulting data served as the foundation for the development of predictive models capable of estimating bioaccessibility based on specific physicochemical properties of the food matrices. Results: One striking finding of this study was the strong correlation observed between the concentration of macronutrients within the food formulations and the bioaccessibility of curcuminoids. In fact, macronutrient content emerged as a very informative explanatory variable of bioaccessibility and was used, alongside other variables, as predictors in a Bayesian hierarchical model that predicted curcuminoid bioaccessibility accurately (optimisation performance of 0.97 R<sup>2</sup>) for the majority of cross-validated test formulations (LOOCV of 0.92 R<sup>2</sup>). These preliminary results open the door to further exploration, enabling researchers to investigate a broader spectrum of food matrix types and additional properties that may influence bioaccessibility. Conclusions: This research sheds light on the intricate interplay between food matrix composition and the bioaccessibility of curcuminoids. This study lays a foundation for future investigations, offering a promising avenue for advancing our understanding of bioactive compound bioaccessibility and its implications for the food industry and informed consumer choices.

**Keywords :** bioactive bioaccessibility, food formulation, food matrix, machine learning, probabilistic modelling

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