

Applicable Models Based on Equi-Energetic Servings: Part 1 PLSR Based Models Predicting the Perceived Satiety of Common Food Products

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Abstract

Background: Partial Least Squares Regression (PLSR) was used to develop predictive regression models numerically relating either the macronutrient composition or the reciprocal energy density of individual food products to their perceived satiety.

Objective: To develop predictive PLSR models numerical relating the macronutrient composition and to product weight/MJ of a wide range of food products to their quantified perceived satiety.

Method: Published data on the perceived satiety of food products were used for model development using PLSR.

Results: Using PLSR the most relevant regression factors optimally relating the macronutrients to the perceived satiety are Total Dietary Fiber (TDF), protein and sugar ($r = 0.83$). The sample set could be divided into plant based samples, characterized by the presence of TDF and starch and non-plant based samples devoid of TDF by nature. For the non-plant based products protein is the most relevant regression factor ($r = 0.92$). For the plant based products, sugar and fiber are the most relevant regression factors ($r=0.86$). For the plant based products the perceived satiety could also be related to the product weight/MJ, which is the reciprocal of the energy density. Prerequisites to develop these predictive models are the use of a proper reference product, a sensitive and reliable scaling of the perceived satiety, in combination with equi-energetic servings of the food products analyzed.

Conclusions: PLSR is a suitable tool to relate the perceived satiety of food products to their macronutrient composition, and for plant base products also to their product weight/MJ. A prerequisite to come to these conclusions is the use of equi-energetic servings, a reference product and an adequate satiety scaling procedure.

Keywords: Perceived satiety; Predictive models; Equi-energetic servings; Macronutrient composition; Energy density

Abbreviations: IAUC: Average Integrated Area Under the Curve; PLSR: Partial Least Squares Regression; RMSEC/P: Root Mean Square Error of Calibration/Prediction; TDF: Total Dietary Fiber; SatS: Satiety Score

Introduction

The perceived satiating capability of food products is the result of a complex set of psycho-physiological mechanisms. Satiety is the process that inhibits further eating, causing a reduction in hunger and an increase in fullness after a meal is eaten; whereas, the inhibitory processes that lead to the termination of a meal refers to satiation [1]. This perceived satiating capability of singular food products, beverages and meals is influenced by their macronutrient composition, energy density, palatability, physical structure, digestibility and previous experiences [2-5]. In their research Holt, *et al.* [2-4] studied the relation between a range of fresh and processed food products, their macronutrient composition, their satiety-, glycemic-, and insulinemic responses and their subsequent food intake. Rather than using 50 gram carbohydrate servings [6] conventionally used to study the glycemic-, and insulinemic responses of food products, 1 MJ servings were used. This approach enabled the study of products virtually deviant in carbohydrates. Besides the elegance of these integrated

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studies [2-4], the results obtained are descriptive rather than predictive in nature. Results from other sensory studies with panelists have shown that, using PLSR, it is possible to relate sensory perceived texture and flavor attributes to instrumental measurements [7-11]. The resulting multivariate regression models are based on the statistical analysis of the relation between input (texture, flavor attributes) parameters and response variables (instrumental measurements); a dose-response relation. With these models one tries to integrate domain knowledge of specific products with a measuring technique to develop statistical based, predictive models. These type of models are, in general, well suited for practical applications since most of the time, they have a high predictive power, though their applicability in general remains limited to the measuring situation [12]. PLSR has received a great amount of attention in the field of chemometrics, due to its success resulting in applications in other scientific areas including bioinformatics, food research, medicine, pharmacology, social sciences, and physiology, to name but a few [13]. One of the reasons for the wide application of PLSR is that it can analyze (numerous) input data that are both strongly correlated and noisy, and simultaneously model one or several response variables [14]. In order to develop predictive, perceived satiety models based on the chemical composition of food products, a prerequisite is an adequate description of the macronutrient composition of these individual food products, together with a proper numerical scaling of the perceived satiety [15] relative to a standard reference product. The use of one standard reference product enables the comparison of the satiety results of different samples in time and origin. An additional requirement here is the use of equi-energetic servings to eliminate the effect of the total energy consumed on the perceived satiety. As far as our information goes, only the previous satiety research of Holt, *et al.* [2-4] meet these criteria. The estimation of the perceived satiety based on the macronutrient composition of food products could be useful for enabling the production of higher satiety food products as well as assisting dieticians and physicians in the development of diets with an enhanced satiety versus energy content ratio.

Material and Methods

Model development

PLSR was used to develop predictive models relating either the macronutrient composition, or physical product properties to the perceived satiety of a range of fresh and processed food products. PLSR based model formation and validation testing were performed as described previously [16]. The squared difference between the PLSR based predicted satiety values and measured satiety values is summed and averaged. The square root of this value is taken giving the root mean squares error of calibration (RMSEC), the modeling error. This latter value, together with the correlation coefficient between the measured and predicted satiety values, describes the predictive ability of this calibration model. To assess the predictive capability of a calibration model a new PLSR model was constructed based on two third of the randomly selected samples. The predictive capacity of this new PLSR model was tested on the remaining one third of the samples and expressed as the root means squares error of prediction, RMSEP [10,16]. Outliers (see below) were excluded both from model development and validation testing.

Data sources

Published satiety data [2-4] were used for PLS regression analysis using white bread as reference. In their manuscript [2,3] six different product groups were distinguished using white bread as reference for each group. However, the average Integrated Area Under the Curve (IAUC) of the white bread reference samples was different for each product group. Since the results of this latter study can be considered as one integrated experiment the data will be treated as one set. For this reason the number weighted average of the IAUC for white bread from these six product groups was calculated. This averaged IAUC value for the SatS of white bread was set at 100. The published satiety values of the other food products studied were adapted accordingly.

Outliers

Dixon's Q-Test at $P \leq 0.05$ [17] was used to define outliers using the critical values as worked out in greater detail [18]. This test can be used to determine whether a measured value, that is part of a set of measurements, can be defined as an outlier. In regression analysis the regression residual, the difference between the observed and predicted dependent variable, is used rather than the actual measured value. Here, the discordance tests TN7 ($TN7 = (x_n - x_{(n-1)}) / (x_n - x_1)$) was used [18].

Simulations

For simulation purposes the consequences of staling of bread and the processing of apples into either applesauce or apple juice on the perceived satiety were taken as examples. In case of bread staling [19] a major part of this effect is assumed to be caused by the formation of resistant starch [20]. Resistant starch can be considered as fiber since it escapes amylase-digestion in the small intestine [21]. Here it is assumed that the formation of 1g resistant goes at the expense of 1g digestible starch thereby decreasing the energy content of the bread with 17 kJ and enhancing the total amount of TDF with 1g. To compensate for this energy loss, the energy content of the original product has to restore to 1 MJ. In this example the energy content of all macronutrients has to be multiplied with 1000 MJ/ (1000-17) MJ. In case of bread staling, the data of Hung, Yamamori and Morita [22] were used describing the formation of resistant starch of white bread in time. The macronutrient composition of applesauce [23] and apple juice [24] originated from the USDA National Nutrient Database for Standard Reference.

Results and Discussion

PLSR models relating the perceived satiety of food products with their macronutrient composition

In first instance those macronutrients were identified that significantly contribute to the PLSR models relating the macronutrients of the individual food products to their corresponding satiety score (SatS). The results of the PLSR based modeling of all samples (Table 1, Model 1) shows that three regression factors, protein, sugar and TDF, are required to obtain an optimal fit. The relevance of these three macronutrients to contribute to the perceived satiety of food products is mentioned earlier [1]. Neither starch, nor fat are relevant regression factors for the PLSR models. Using Dixon's Q-test [17,18], one sample (4; low-fat high-moisture bread) was shown to be an outlier. A closer look to the food products analyzed showed that the original sample set could be divided into plant-based products, containing starch and fiber, (Table 1, Models 2A,B) and non-plant based products (Table 1, Models 3A,B) where, by nature, starch and fiber are absent. For the PLSR model of the plant based products it is obvious that the contribution of protein as regression factor has almost vanished (Table 1, Model 2A). Omitting protein from the regression analysis results in a slightly better PLSR model (Table 1, Model 2B). This suggests that protein is no relevant regression factor for the plant based, fiber containing products.

The predictive power of the regression factors sugar and fiber for the perceived satiety of the plant based food products, was tested by a training set, containing two-third of the randomly selected samples [16]. The predictive power [16] of this training set (Model 2C-1) was tested on the remainder of these samples, the validation set (Table 1, Model 2C-2; validation set). The regression models for the training and validation set do significantly ($P < 0.05$) not differ from each other. This is reflected by the similar values of the regression coefficients, correlation coefficient and values for the RMSEC, in combination with the observations that the training set is capable to adequately predict the samples contained within the validation set and *vice versa* (Table 1, See; "training set predicts validation set" and "validation set predicts training set").

Though the number of samples of the non-plant based samples is small, a PLSR analysis indicates both protein and sugar as regression factors. The negative value for sugar as regression factor (Table 1, Model 3A), the more sugar a sample contains the lower its perceived satiety, does not seem realistic. The use of protein as only regression factor hardly affects the regression results (Table 1, Model 3B). This suggests that for non-plant based samples the amount of protein within such a product can be directly related to its perceived satiety. In Figure 1 the graphical presentation of the measured versus the predicted satiety score values for plant based products (Table 1, Model 2B) and non-plant based products (Table 1, Model 3B), including the 95% confidence intervals of both models is presented.

The observation that Model 1, containing all samples, can be split into a plant based model, with only fiber and sugar as relevant regression factors, and a non-plant based model, with protein as major regression factor, is surprising. For example some of the samples within the plant based model contain more protein (e.g. lentils, baked beans) than some of the non-plant based samples. An explanation could be that for the plant based samples at increasing amounts of both protein and fiber, the fiber progressively annihilates the satiety behavior of protein. However, to research this assumption, a different experimental set-up is required than used in the studies cited here [2-4].

Satiety Score									
PLSR Model	Samples	Number of samples	Number of outliers	r	1RMSEC	Regression Factors			
						Protein (g)	2Sugar (g)	3TDF (g)	Starch (g/MJ)
1	All samples	45	1	0.83	44.8	0.33	0.22	0.77	4NR
2A	Plant based-A	39	1	0.86	42.5	-0.02	0.31	0.82	NR
2B	Plant based-B	39	1	0.87	42,1	NR	0.21	0.85	NR
2C-1	- Plant based-B "Training set"	26	1	0.83	45,4	NR	0.12	0.83	NR
2C-2	- Plant based-B "Prediction set"	13	0	0.95	45.6	NR	NR	NR	NR
2D-1	"Training set" predicts "Validation set"	NR	NR	0.83	35.4	NR	NR	NR	NR
2D-2	"Validation set" predicts "Training set"	NR	NR	0.86	48.0	NR	NR	NR	NR
3A	Non-plant based-A	6	0	0.99	8.0	0.57	-0.53	NR	NR
3B	Non-plant based-B	6	0	0.92	21,7	0.92	NR	NR	NR
4A	Bread	10	0	0.95	40.7	NR	NR	NR	NR
4B	Plant based-B, excl. bread	29	0	0.85	28,4	NR	NR	NR	NR
Product weight (g/MJ)									
5A	Bread	10	0	0.97	5.4	NR	0.28	0.84	0.15
5B	Plant based-B, excl. bread	29	0	0.80	85.4	NR	0.46	0.59	NR

Table 1: Results of the PLSR analysis relating the Satiety Score with either macronutrients or product weight (g/MJ), and product weight with macronutrients, and the numerical values of the relevant regression factors within a sample-set and the values of the regression correlation, R, and the RMSEC. ¹RMSEC/P; Root Mean Square Error of Calibration/Prediction, ²NR; Not Relevant

Exploring the boundaries of the PLSR models

To obtain information regarding the boundaries of the regression models developed for the three most relevant regression models (Table 1, Models 1, 2B and 3B) the consequences of the absence of protein and sugar, or the presence of either 1 MJ protein or 1 MJ sugar were estimated. These estimates were made in the presence or absence of 10g TDF (see Table 2). The first two rows of Table 2 represent the situation that neither protein, nor sugar is present as macronutrient, but just fat and/or starch; the offset of the regression analysis. For Model 3B, in all cases the offset is 80 SatS units. Not surprisingly, protein is the only macronutrient capable to enhance the SatS with 161 units. For Model 2B, in all cases TDF enhances the SatS with 100 units, sugar enhances the SatS with 65 units, and protein has no SatS enhancing effect. For Model 3B, the SatS enhancing effect by TDF is 89 units, by protein 164 units, and by sugar 65 units. For these 3 models, the SatS enhancing effect by TDF ranges between 89-100 units, for protein between 161-164 units, and for sugar a value of 65 units is observed. Using the SatS values from Model 1 for these three macronutrients, using 17 kJ per gram protein and sugar, the SatS value 2.79 units/g for protein and 1, 11 units/g for sugar. Ten gram TDF enhances the satiety score with 89 SatS units; this is 8.9 units/g TDF.

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With respect to the offset, this value represents the satiety score of any product not containing protein, sugar, or TDF. Since neither fat, nor starch are recognized to be relevant regression factors, the results of the models discussed above, suggest that any composition of starch and fat, with a total energy content of 1MJ will have a satiety score, in the absence of TDF, of 49 (Table 2, Model 1), of 61 (Table 2, Model 2B) and of 80 (Table2, Model 3B) respectively. The addition of fiber will enhance these satiety scores for these models with, 89, 100, and 0 SatS unit per ten gram TDF respectively.

Composition			Model		
			Non-plant based-B (Model 3B)	Plant based-B (Model 2B)	All samples (Model 1)
Protein (MJ)	Sugar (MJ)	TDF (g)	Regression Factors		
			Protein (g)	Sugar (g), TDF (g)	Protein (g), Sugar (g), TDF (g)
			Satiety Score predicted	Satiety Score predicted	Satiety Score predicted
Offset		0	80	61	49
Offset		10	80	161	138
1	0	0	241	61	213
1	0	10	241	161	302
0	1	0	80	126	114
0	1	10	80	226	203

Table 2: Estimate of the Satiety Score of either 1 MJ protein or sugar in the absence and presence of 10g TDF.

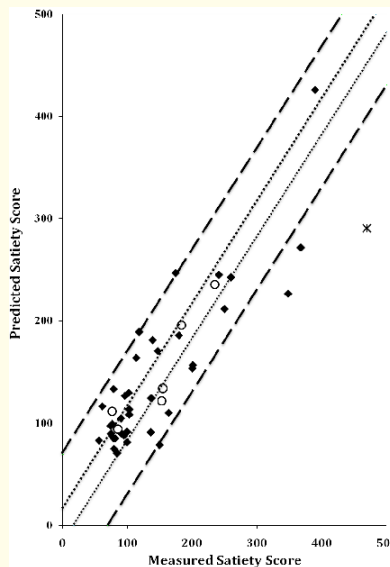


Figure 1: Measured satiety score versus predicted satiety score.

◆: Plant based samples; ○: Protein based samples, *: Outlier; ————: 95% confidence interval for the plant based samples;: 95% confidence interval for the non-plant based samples.

Assessing the Satiety Score of food products based on the SatS values of protein, sugar and TDF

The information obtained above leads to a different way to assess the satiety score of individual products. For example, white rice contains 5.0g protein, 0.1g sugar and 0.4g TDF [2]. Using the above given data for the satiety scores of protein, sugar and TDF per gram, the contribution of these macronutrients to the satiety score is $(5.0 \times 2.79 + 0.1 \times 1.11 + 0.4 \times 8.9) = 17,7$ SatS units. The value for the offset is 49 SatS units under the condition of an energy content of 1MJ. However, about 8% of this energy content is already occupied by the regression factors protein and sugar for which the offset value has to be compensated, resulting in an offset of $(0.92 \times 49) = 45, 1$ SatS units. In other words, an estimated SatS value for white rice is calculated of $(17, 7 + 45, 1 =) 63$ SatS units. The SatS values of all products [2,4] products contained in Model 1 were calculated in the way as described above. The relation between the measured satiety values and the values calculated in the way described above is:

$$\text{SatS-predicted} = 0.59 \text{ SatS-measured} + 37.9 \quad (r = 0.82; \text{RMSEC} = 58.9) \quad (\text{Eqn. 1})$$

This latter value for r is almost similar to the r value for Model 1 as described in Table 1. The relation between this way described calculated and the predicted satiety values, according Model 1, is:

$$\text{SatS-predicted} = 9.94 \text{ SatS-predicted (Model 1)} - 11,5 \quad (r = 0.98; \text{RMSEC} = 23.7) \quad (\text{Eqn. 2})$$

Representing an almost perfect fit between the calculated SatS values using PLSR and the SatS values calculated as described above. This almost perfect fit is, however, not surprising since the information for the two data sets was derived from the same source (Table 1, Model 1). These results described above show that it is possible to ascribe a numerical value to the PLSR regression factors, each value describing the numerical contribution of the regression factor to the SatS.

PLSR models relating the perceived satiety of food products to their product weight per MJ

In agreement with other observations [25] the perceived satiety of the plant based products can be related to the product weight/MJ. Which is the reciprocal value of the energy density of the food products? In Table 1 the results of the PLSR analysis between product weight/MJ and the perceived satiety is presented (Models 4A, B). No relation between the “Non-plant based” samples and the product weight/MJ could be established. These samples were omitted from further analysis. To obtain acceptable results the “Plant-based products”, have to be split into the bread samples (Model 4A) and the remainder of the samples (Model 4B). Using these two groups, for each group a linear relation could be established between the product weight per 1MJ and the satiety score. The results of this analysis are shown in Figure 2. It is obvious that in the analysis of weight/MJ versus perceived satiety, the bread samples, and the samples belonging to the remainder of the plant based products, belong, in contrast to the PLSR analysis of macronutrients against the perceived satiety, to two different groups. Noticeable is that, in contrast to Models 1 and 2, the low-fat high-moisture bread sample [4] is no outlier in Model 4A.

PLSR models relating the macronutrient composition to the product weight per MJ

Since adequate PLSR based relations could be established between both, the macronutrient composition and the perceived satiety, and between the product weight/MJ and the perceived satiety, the relation between the macronutrient composition and product weight/MJ was also addressed. For the plant based products without bread, sugar and TDF suffice as relevant regression factors (Model 5B), similar to Model 2. For the bread samples, in addition to sugar and TDF, starch was also a relevant regression factor; its contribution to Model 5B was relatively small, though relevant. Again, the low-fat high-moisture bread sample [4] is no outlier in this latter model.

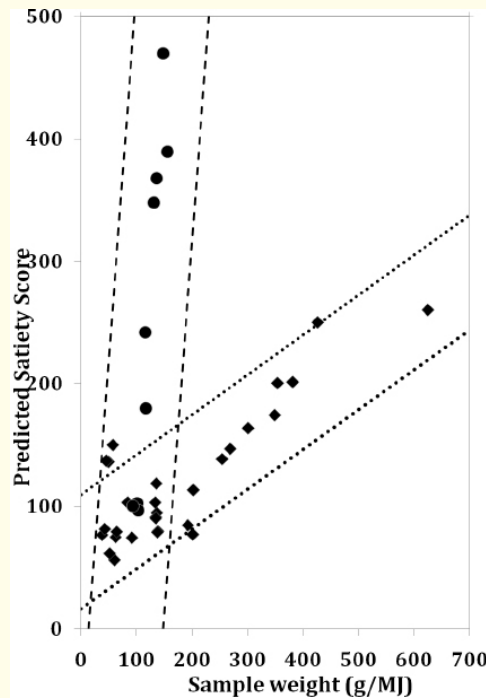


Figure 2: ●: Plant based samples without bread samples; ◆: Bread based samples;: 95% confidence interval for the plant based samples without bread; ———: 95% confidence interval for the bread samples

Simulation

Staling of bread is a complex phenomenon which is, to a major extent, caused by the retro gradation of starch, with emphasis on amylopectin [19] to form resistant starch, a fiber [20,21]. The consequences of this staling process is the conversion of (part of the) starch into resistant starch, at the expense of the total amount of starch. This process is characterized by a toughening and hardening of bread. Since white bread is used as reference product with a SatS of 100 (by definition) the formation of fiber, resistant starch, which latter macronutrient has, as shown above, a substantial impact on the perceived satiety of food products, the estimated effect the formation of resistant starch on the perceived SatS of white bread seems of sufficient relevance to be addressed here. The simulated consequences of the progress of the staling of bread in time on the perceived satiety are shown in Figure 3. This simulation clearly shows that due to the changed physicochemical properties of the reference product in time the perceived satiety of this product is also subject to changes.

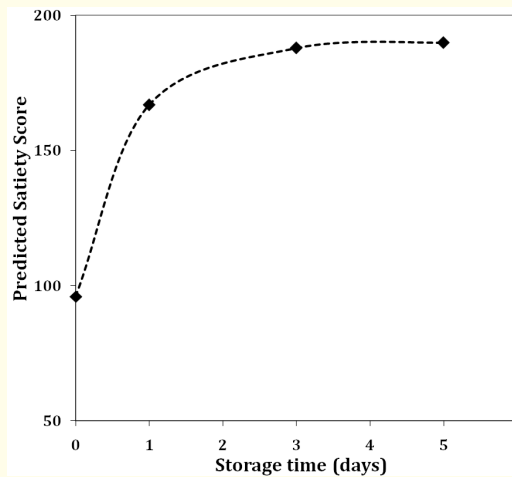


Figure 3: The staling of bread in time and the estimated consequences for the perceived satiety score.
◆: Estimated satiety score caused by the staling of bread.

An additional example is the processing of apples into apple sauce and apple juice. The difference in glycemic, insulinemic and satiety responses between apples, apple sauce and apple juice was shown previously [26-28]. For apples the measured and predicted value of the SatS are respectively 250 and 212. For apple sauce [23] and apple juice [24] the simulated perceived satiety values (Table 1 Model 2A) are respectively 234 and 161. Though, at 1MJ of product, the amount of sugar is virtually the same for apples, applesauce and apple juice, due to heat processing (applesauce), or the application of pectinases, (apple juice) the amount of TDF decreases from 8.9 to 6.7 and to 1.2g/MJ respectively. In other words the decrease in the simulated perceived satiety in the range apple, applesauce, and apple juice is probably mainly caused by the decrease in TDF. Earlier studies also showed that assessors' rating of satiety was significantly higher following the intake of fruit compared to juice [27-30].

Conclusions

Though the amount of samples analyzed in this study is relatively small, the product versatility is high, representing a broad spectrum of common fresh and processed food products. Three macronutrients, protein, sugar and TDF are relevant to develop PLSR models relating these macronutrients to the perceived satiety of the individual products. Samples containing no fiber by nature, the non-plant based products can be separated from the TDF containing, plant based samples, resulting in two independent regression models. However, in case of the plant based products it is not clear why protein loses its relevance as regression factor, in case of the non-plant based products the role of sugar is not clear. To address these questions requires a different research approach compared with the one researched in this study.

Only for the plant based samples a circular observation can be made; a PLSR model can be developed relating the mentioned macronutrients to the perceived satiety, between the perceived satiety and the product weight/MJ (g/MJ) and between the product weight/MJ and the mentioned macronutrients. For the last two models bread behaves differently compared to the remainder of the plant-based samples (see Figure 2). An explanation for this could be the substantial volume increase during dough preparation prior to baking to make bread. This increase in volume does not occur for the other processed products, also leading to a different range in product weight/MJ for bread.

With regard to the contribution of protein, sugar and TDF to the perceived satiety, the satiety score of these individual macronutrients can be estimated. Applying the boundaries of 0 or 1 MJ protein or sugar respectively either in the absence or presence of 0 or 10g TDF, estimates can be made about the SatS value of 1g protein, sugar or TDF. For Model 1 it is estimated that, per gram, the perceived satiety caused by TDF is 3.2 times that of protein and 8.0 times that of sugar. Using these values the SatS values of the individual products can be calculated. An excellent relation is observed between calculated satiety based on the contribution of protein, sugar and starch, and the satiety values predicted by the PLSR based model (Table 1, Model 1), suggesting the correctness of the individual calculated SatS values (per gram) for fiber, protein and sugar. Important to note is that these calculated SatS values are valid for both fresh as well as processed food products. Apparently processing has no noticeable intrinsic effect on the perceived satiety of the wide range of products studied here; the same model applies for e.g. fresh apples and processed beans. Despite the versatility in the overall chemical composition of the dietary fiber of the plant based food products and, in addition, the effects of processing on this composition [30] within this study TDF could be considered as one integral group, resulting in one regression factor. Addition of fiber increases the perceived satiety independent of its origin; e.g. exogenous fiber added to bread [4].

Next to the satiety measurements discussed here, white bread frequently serves as reference in the determination of the glycemic and insulinemic response of food products [31]. As shown here and mentioned earlier [32] the properties of white bread as reference material change in time accompanied by (simulated) changes in the perceived satiety of the reference material, with all its related consequences. These consequences of this staling process on the glycemic response of white bread will be discussed else [31]. Given the rapid starch retro gradation process, in combination with its substantial effects on the perceived satiety of white bread, it is furthermore suggested that the use of white bread as reference should be re-evaluated [32].

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