Laboratory intercomparison for biocrystallization (crystallization with additives) applied to different wheat varieties

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Zusammenfassung

Für die Methode der Empfindlichen Kupferchloridkristrallisation ist ein standardisiertes Dokumentationsprotokoll entwickelt und auf verschiedene Proben landwirtschaftlicher Produkte angewendet worden. Auf dieser Grundlage wurde mit Weizenproben ein Vergleich zwischen verschiedenen Labors durchgeführt. Bei standardisierten und nicht-standardisierten Vorgehensweisen in fünf verschiedenen europäischen Labors wurde getestet, ob kodierte Proben nach verschiedenen Weizensorten gruppiert werden können. Die Gruppierung erfolgte nach Kriterien, die aufgrund der visuellen Bewertung der Kristallisationsmuster definiert worden waren.

Alle Labore konnten die codierten Proben erfolgreich in Übereinstimmung mit den definierten Klassen gruppieren. Dies deutet darauf hin, dass mit der Methode ein zuverlässiges Verfahren gegeben ist. Weitere Forschung sollte sich auf den Einfluss verschiedener Faktoren im Zuge des Laborprozesses beziehen wie auch auf ein vertieftes Verständnis der Grundlagen der Methode.

Summary

After the biocrystallization method has been documented, standardized and applied on various agricultural and food samples, laboratory intercomparison is performed on wheat samples. Standardized and non-standardized approaches in five different laboratories throughout Europe are compared based on their ability to group coded samples according different wheat varieties as classes. The grouping is based on defined criteria from visual evaluation of the crystallization patterns. All laboratories can successfully group coded samples according to defined classes. This indicates a robust method principle, which needs further research work. Next research challenges may be investigations on the influence of different factors along the laboratory process as well as insights in the methods principle.

Keywords: biocrystallization, laboratory intercomparison, method, wheat

Introduction

The principle in biocrystallization can be described as dendritic growth of dihydrate cupric chloride (a self-organization system) in the presence of an additive, the sample under study (*Busscher et al*. 2014, *Kahl et al*. 2014a). The results are emerging crystal patterns, which can be evaluated by different

algorithms (*Andersen et al.* 1999; *Doesburg & Nierop*, 2013). In addition to computer assisted pattern evaluation, the patterns can be evaluated visually by standardized operations using single morphological criteria (*Huber et al.* 2010). The biocrystallization method was applied for organic wheat authentication (*Kahl et al.* 2014b) as well as for following product changes during food processing (*Seidel et al.* 2015; *Kahl et al.* 2009; *Kahl et al.* 2013a). The method was standardized for samples of carrot (*Busscher et al.* 2010a), wheat (*Kahl et al.* 2013b) and milk (*Kahl et al.* 2013a). The standardization process mainly consists of documentation of the laboratory procedures, followed by testing the influence of different factors, such as grinding, filtering, mixing ratio of amounts of cupric chloride and additive. The evaporation process was investigated in detail with different additives (*Busscher et al.* 2010b). For milk and wheat samples, comparison between different laboratories was made, based on the same equipment (crystallization chamber) and standardized laboratory procedures (*Kahl et al.* 2013a; *Kahl et al.* 2013b). Patterns derived from the same samples but crystallized in different laboratories were comparable with respect to structure variables. Conditions and procedures must, however, be standardized and documented. The biocrystallization approach was also successfully applied without these laboratory standardization processes (*Fritz et al.* 2011). Here, patterns from wheat samples derived from different farming systems could be grouped and classified, when biocrystallization was used together with other image forming methods. The patterns were evaluated by grouping them, based on similar image features and classifying them, based on qualitative visual comparisons to reference patterns. Samples from the same field trial could be significantly differentiated according to the farming treatments organic versus non-organic, when samples from three different years, including field replication, were crystallized with the standardized approach using image analysis (*Kahl et al.* 2015). The objective of the present study was to determine to what degree standardized and non-standardized biocrystallization approaches, used in different laboratories, are able to group coded wheat samples in a laboratory comparison. Since 2002, laboratories in Germany (Bonn, Darmstadt and Witzenhausen) as well as Denmark and the Netherlands have been exchanging knowledge and information regarding biocrystallization. In 2006, the groups started to perform laboratory intercomparisons. After two years of training, coded wheat samples were sent to each laboratory for differentiating and grouping the patterns. The results from 2009 and 2010 have already been reported for the standardized method using a structure algorithm (*Kahl et al.* 2014b). Here, the intercomparison with visual evaluation is reported for standardized and non-standardized biocrystallization.