

Collaborative Project: Development of a system for collection, analysis and utilization of product data for authenticity in the food sector (FoodAuthent)

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Food crises can constitute a health risk to the population, and can influence consumer trust in manufacturers, retailers and the authorities. To confirm that goods comply with their label descriptions, analytical methods are used as part of the food authentication process. As products grow more diverse and goods flows more complex, however, assessing the accuracy of labelling is becoming increasingly difficult. Food authentication experts therefore need analytical methods and IT solutions that are flexible and suitable for day-to-day use, and which can be utilised by all of the stakeholders along a product chain. Such stakeholders include manufacturers, suppliers, retailers and regional authorities. To resolve this problem, the 'FoodAuthent' project has developed the 'fAuthent' software package, which facilitates the use of analytical 'fingerprint' methods for application in the collaborative authentication of food (www.foodauthent.de).

Specifically, the project investigated analytical methods that determine the composition of food products by mapping out their individual chemical 'fingerprint'. This fingerprint can then be compared with samples of unadulterated foods. This method allows the detection both of adulterations such as added substances as well as the verification of geographical origin, for example, the specific variety of a product that is used or certain manufacturing processes. For its part, 'fAuthent' is the first IT platform capable of storing 'fingerprints', product master data and data analysis methods, and making these available for shared use. In the future, platforms of this kind will be useful for the efficient discovery and prevention of fraudulent or misleading practices in relation to food products, since the initial technical foundations for networking and the exchange of data between all stakeholders in the product chain—such as companies, retailers and authorities—have now been created.

The platform developed in the FoodAuthent project, 'fAuthent', is based on open and standardised interfaces as well as open source software components. This platform has been trialled by using typical measurement data from goods in the product groups of hard cheese, seed oils and spirits. This work involved investigating key aspects of standardisation in nontargeted analysis for use in day-to-day applications.

Project activities undertaken by the BfR included analytical aspects (e.g. the development of non-targeted analytical methods for food authentication and of statistical models for spectrum comparability and quality assurance) as well as the development of a system architecture and open source software solutions for the day-to-day usage of the collected data as part of the 'System model and end-user services' work package.

1 Brief summary of research project

1.1 BfR task specification/activities

The primary project goal for FoodAuthent was the development of a computerised demonstration system for food authentication, known as the 'fAuthent system'. This software system can be used to manage and evaluate analytical results and product master data (metadata) of individual food samples, and share this data with other facilities and institutions. The system itself is built around analytical results/data that have been taken from non-targeted food analysis, a technique known as food 'fingerprinting'. The project therefore aimed to establish the initial general technical conditions required for the routine application of fingerprinting



techniques in quality assurance, quality control and food monitoring work. Alongside the development of the fAuthent system itself, this included basic issues related to standardisation in non-targeted food analysis (standardised analysis including sample preparation, data analysis, comparability of spectra and quality assurance). In the process, the German Federal Institute for Risk Assessment (BfR) was involved in almost all of the project work packages.

The primary focus of the BfR's work in relation to 'Fingerprinting analyses and data mining' (part A of the project) involved the development of analytical methods for the selected scenarios on the one hand—the detection of geographical origin (*FoodRegio-Detect*) and the identification of food fraud (*FoodFraud-Detect*)—as well as the various scenario foods. Other points of focus included providing support for the creation of statistical evaluation models as well as investigations relating to spectra comparability and quality assurance.

The work of the BfR in relation to the 'System model and end-user services' (part B of the project) primarily involved the following:

- Development of a system architecture based on IT standards for the integration and evaluation of analytical food fingerprint data
- Development of specialised open source software solutions for end users to ensure easy use of the collected data

Models for ensuring the long-term improvement and continuity of the solutions were also developed.

1.2 General project conditions and framework

The FoodAuthent project received funding from the innovation programme operated by the German Federal Ministry of Food and Agriculture (BMEL), and specifically to promote innovations in detecting the geographical origin of food. The project commenced on 15 September 2016 and concluded on 31 December 2019.

1.3 Project planning and timeline

During the FoodAuthent project, work packages were completed in accordance with the work planning set out in the project application, with only slight adjustments to this timetabling (fig. 1). The achievement of project goals was supported by milestone planning (tab. 1) with project work in both parts of the project—part A (fingerprinting analysis and data mining) and part B (system model and end-user services)—being completed simultaneously.

Achieving these milestones (tab. 1, fig. 1) and results (tab. 2) according to the overall project proposal (OPP) was the responsibility of the respective project partners, and ensured primarily by the work of the GS 1 Consortium Lead Germany and project managers for parts A and B. As well as the milestones agreed in the consortium, the BfR also set a number of additional goals and milestones within its sub-project (S-P).



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Teil A Fingerprinting-Analysen & Dataining													
A1 Anforderungsanalyse (Lastenheft)													
A1.1 Auswahl des "Szenario"-Lebensmitteln													
A1.2 Anforderungen an Fingerprinting-Analyseverfahren													
A1.3 Anforderungen an Analysedaten-Standards													
A1.4 Anforderungen an die Referenzdaten in der fAuthent-Cloud													
A2 Konzepterstellung sowie analytische/statistische Vorarbeiten													
A2.1 Entwicklung von Fingerprinting-Analyseverfahren													
A2.2 Standard für Analysedaten													
A2.3 Untersuchung eines Pilotprobensatzes													
A2.4 Multivariate Statistik und W orkflows			-										
A2.5 Qualitätssicherung in der Analytik													
A2.6 Vergleichbarkeit der Daten													
A3 Komponentenentwicklung													
A3.1 Datenformate und Datamining													
A3.2 Authentischer Datensatz													
A3.3 fAuthent Referenz daten Cloud													
A 3 4 Datananalyce-Workflow-Verzeichnie													
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A4 Valuationing A 4 A Micht outhontionto Drohon													
A4.2 Optimierung Datenanalyse-W orkflows							_						
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Teil B Systemkonzept & Endnutzer-Dienste													
B5 Anforderungsanalyse (Lastenheft)													
B5.4 Erarhaitinna R9R/ R9C/ R9C/ Itaa Casas													L
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B.5.2 Antorgerungen 1A ument-Gesamtsystem													
B5.3 Lastenheftvalidierung		-			_		_					_	
B6 fAuthent Systemarchitektur-, Prozess- und Schnittstellenkonzept													
B6.1 Konzept Discovery-Service													
B6.2 Konzept EPCIS-/CBV-basiertes Eventsystem													
B6.5 Prozess-/Service-/Schnittstellen-Design													
B7 Komponentenentwicklung													
B7.1 Machbarkeitsstudie für das FoodAuthent Gesamtsystem													
B7.2 Realisierung zweier B2G Use Cases													
B7.3 Realisierung der B2B Use Cases													
B8 Validierung					╞	E							
B8.1 Erarbeitung eines Konzepts für Validierung und Tests													
B8.2 Prüfung auf Anforderungen der Stakeholder													
B8.3 Durchführung von Integrationstests und Workshops													
B8.4 Erstelling von Emnfahlungen zur Ortimierung													
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B9.1 Entwicklung eines Transfer- und V erstetigungskonzepts												_	
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Figure 1: Project schedule – with the exception of work packages 6.3, 6.4, 6.6 and 7.4, the BfR was actively involved throughout.



 Table 1: Milestone planning (MS).

MS as per OPP	Goals achieved	Planned achievement (month)	Delay (months)
MS1	Submission of requirements analyses from parts A and B	M12	-
MS2	Submission of software components from parts A and B	M33	3
MS3	Submission of evaluation reports from parts A and B	M36	3
MS as per S-P			
MS BfR1	Submission of a standard test specification for the analysis methods applied in the project	M18	-
MS BfR2	Submission of the 'B2G app' software solution	M33	3
MS BfR3	Report on the implementation and updating of the continuity model	M36	3

Table 2: Work goals (R) for which the BfR was responsible.

Result	Description	Achievement (month)
R2.1	Submission of standard test specifications for the analysis methods applied in the project	M18
R7.2	Software component – 'B2G app'	M36

1.4 Scientific and technical situation used as a starting-point

Food fraud is a growing risk for both companies and consumers, not least as a result of the increasing globalisation of the food and feed trade, coupled with the simultaneous increases in complexity affecting international product chains. At the same time, cases of food fraud—such as diluting wine with water—are primarily economically motivated [1,2]. The reliable authentication of products and the detection of cases of food fraud have always presented major challenges to both regulators and the food industry itself. Key aspects here include the establishment of flexible and reliable analytical methods, as well as the collection of authentic reference samples for routine analysis work.

Non-targeted analysis of food products

Non-targeted analysis (also including subsequent statistical data analysis) facilitates a correlation of the spectral signature ('fingerprint') of food products with their advertised product characteristics. This process involves comparing the signature recorded from a sample with reference data (signatures of food products with known product characteristics). These fingerprinting technologies can be used to answer pertinent questions relating to the authenticity of food products—both as a parallel process and even retrospectively. Examples here include the detection of unlawful food additives as well as verifying a food's origin [2,3]. Despite its broad range of potential applications, non-targeted analysis is currently utilised by only a few commercial providers. In one example, one provider offers a product for testing the authenticity of wine, fruit juice and honey as a commercial solution. This solution can be used to collect quantitative data on ingredients in order to verify certain food characteristics as advertised (e.g. species, year of harvest). This involves conducting the corresponding sample analysis (using nuclear magnetic resonance (NMR) spectroscopy) in customer laboratories according to the provider's specified procedures. The data analysis is conducted centrally using a shared data model, based on a proprietary database operated by the provider



[4-7]. The use of non-targeted analysis in food control conducted by the authorities is currently limited as a result of an absence or lack of the following factors [8,9]:

- Strategies for achieving the validation and quality assurance of procedures, including:
 (i) standardised analytical methods and sampling protocols; and (ii) validated, automated statistical methods (workflows) for data analysis
- Uniform data exchange formats
- > (Publicly) accessible databases with measurement data for representative samples
- User-friendly open source software, for the effective exchange of authenticity data between laboratories for the purpose of shared processing/analysis

System models and end-user services

To achieve the efficient deployment of resources with the aim of avoiding and combating food fraud, the establishment of a close-meshed network based on the confidential exchange of data between all product chain stakeholders as well as the authorities is a highly promising approach [8]. Systems available to date, known as traceability systems—for which product authenticity can be understood as a subset of the features offered—can be classified into one of four approaches:

- (i) One step forwards/one step backwards
- (ii) Centralised database
- (iii) Forwarding of information ('pedigree')
- (iv) Distributed/local data storage

In terms of current and future requirements, the first three approaches are proving increasingly inadequate, however, for reasons such as limited real-time capability and reaction speed, limited scalability and/or failure to maintain data ownership for data owners. As a result, a distributed/local architecture seems to be more promising. One important standard for distributed data storage is EPC Information Services (EPCIS): this can be applied to ensure that each piece of information along a product chain is recorded electronically and provided to application systems. The corresponding EPCIS specification (https://www.gs1.org/standards/epcis) is an important and established exchange format for event-based product tracing/process documentation—in the food retail sector, for example. Data on the origin and processing of food products can be recorded by applying this standard, and made available to (legitimate) user groups. The object identities recorded (such as the identification number for an article or a consignment, for example) are also linked to the current local time, the locality, the corresponding status and the business process. This works to create a consecutive series of events leading back to the origin of the raw materials used. In this context, state-of-the-art traceability solutions are based on the EPCIS standard. As part of the Food-Authent project, models and technical solutions have now been developed that aim to build on the existing standards to also achieve the exchange of information about product-specific analysis data.

As regards the development of publicly accessible databases with reference measured values and product master data, it is also clear that conventional database models (and relational database management systems in particular) have only limited capability for meeting contemporary requirements for distributed data storage. In particular, such solutions must be readily scalable: in a crisis, for example, they must be able to handle very large data volumes



with a simultaneously large user base (as is the case with traceability applications). Databases of the 'NoSQL'¹ type (implemented by fTRACE, for example; https://web.ftrace.com/en/) are an appropriate technology option here and were trialled for the first time in this project in the context of fingerprint data.

In terms of the development of end-user services, the project applied existing open source software solutions such as the KNIME Analytics Platform (<u>www.knime.com</u>), OpenChrom® (<u>https://lablicate.com/platform/openchrom</u>) and Eclipse (www.eclipse.org).

The activities within the FoodAuthent project in relation to improvements to non-targeted analytical methods, as well as the creation of a system model and end-user services, are based on the circumstances as presented here. In particular, spectroscopic fingerprinting methods were utilised. Key points of focus here involved standardisation aspects (quality assurance and spectra comparability). Supplementing this work, groundwork was also completed for automated data processing—with a particular focus on processing NMR spectra—by using the open source software KNIME and OpenChrom. Once complete, the software components developed were provided as a modular extension to the new open source fAuthent system. A demonstration model for the fAuthent system was also developed and tested. In contrast to currently available commercial solutions, this system makes it possible for any user to manage their own analytical results, together with product-related information, and obtain statistical reports and share relevant information as required transparently with other system partners. In this way, the limiting factors as described above are properly accounted for (including future-proof data management software and effective techniques for data exchange).

1.5 Cooperation with other bodies

Alongside consortium activities conducted jointly with GS1 Germany GmbH (GS1G), Benelog Betriebs GmbH & Co. KG (BENE), Lablicate GmbH (LAB), University of Konstanz (UKO) and Eurofins Analytik GmbH (EF), members of the project advisory board were involved in discussions about the implementation of the proposed system approach. In addition, project results were also submitted regularly to board members, made available for discussion and presented at relevant scientific conferences.

With the objective of implementing the tasks assigned in A2.6 on the topic of 'data comparability', the BfR made use of its existing contacts and partnerships to organise the temporary secondment of a scientific research assistant hired by the project to the Walloon Agricultural Research Centre (CRA-W, Belgium). This secondment was used to complete analyses at a third Fourier Transform Infrared (FT-IR) spectrometer, and the opportunity was also taken to discuss research with the Centre's specialists on subjects such as multivariate statistics.

In terms of ensuring the continuity of the system approach, the BfR and several German state agencies for consumer and health protection (LUAs) laid the groundwork for close collaboration (exchange and shared analysis of measurement data) by harmonising the authenticity testing of wine with NMR spectroscopy in parallel to the project. This work forms the initial starting-point for a submitted follow-up project.

¹ NoSQL stands for 'not only SQL' and refers to database systems that follow a non-relational approach. These databases, which can be based on a variety of database models, are horizontally scalable and can therefore be used for Big Data applications.



2 Detailed presentation

2.1 Use of the project grant and the results achieved in detail, including a comparison with the specified goals

The following section presents the work/activities of the BfR and the results achieved in accordance with work packages.

A1 – Requirements analysis (requirements specification)

A1.1 Selection of the 'scenario' food

All project partners mutually agreed to investigate the following three food matrices: hard cheese (e.g. Emmentaler), spirits originating from viticulture (e.g. wine spirits and brandy) and seed oils (e.g. rapeseed oil, pumpkin seed oil).

A1.2 Requirements for analytical fingerprinting methods

A requirements analysis was conducted concerning the criteria for the analytical fingerprinting methods to be developed. The primary focus here was on the general applicability of the analytical methods for the various matrices, while accounting for the two scenarios of *Food-Regio-Detect* and *FoodFraud-Detect*. As a first step, analytical insights concerning experience with fingerprinting analysis were discussed. The following aspects were taken into account as part of this requirements analysis: instruments/equipment available in testing laboratories, method practicability, costs incurred by the analysis, uniform sample preparation and choice of instrument parameters to ensure use of comparable data. The results of the requirements analysis were documented in a requirements specification by the due date (E1.1).

A1.3 Requirements for analysis data standards (lead: BfR)

To develop an agreed documentation for the requirements and the data standards currently in use, the BfR organised operational coordination meetings between consortium partners while conducting literature searches on existing data standards. As a result of this work and activities, it was decided that the fAuthent system for defining the analysis data should be based on the extant ISA (Investigation Study Assay) data standard (https://isa-tools.org/for-mat/specification.html). As a supplementary step, a web-based glossary was developed, so as to synchronise the consistent descriptions necessary for the interdisciplinary development of the fAuthent system and wording between the project partners.

A1.4 Requirements for reference data in the fAuthent cloud

As part of this coordinated analysis/discussion, the required types of reference data were determined, classified and assigned to eight categories. A strategy for integrating/interconnecting required external (reference data) services was also defined. A decentralised storage strategy was decided on, which meets the requirements for roles/rights and data ownership, as well as accounting for data volumes, while also confirming the need for a *discovery services* model. A key contribution from the BfR here was to ensure that the particular requirements of government agency system partners were properly accounted for in the requirements analysis.



A2 - Conceptual design and preliminary analytical/statistical work; lead: BfR

A2.1 Development of analytical fingerprinting methods (lead: BfR)

For the 'scenario' food products, analytical methods based on NMR spectroscopy, FT-IR spectroscopy and isotope-ratio mass spectrometry (IRMS) were developed, in accordance with requirements identified in A1.2.

Hard cheese samples were embrittled with liquid nitrogen, shredded and then homogenised. An aliquot of the sample was then utilised for extracting the fat phase and the casein (for IRMS analysis, for example) (according to [10]). For the FT-IR spectroscopic analysis, the sample was used directly, as well as the sample's fat extract. For the NMR spectroscopic analysis, the samples were extracted with deuterated chloroform. Following centrifugation, the supernatant was removed and analysed.

Following their homogenisation, it was possible to analyse **seed oil** samples directly using FT-IR spectroscopy as well as IRMS. For the NMR spectroscopic analysis, the homogenised samples were dissolved in deuterated chloroform.

For the NMR spectroscopic investigation of **spirits**, an aliquot of the samples was diluted with deionised water to an alcohol concentration of 28% by volume, to which a phosphate buffer prepared with deuterium oxide was then added.

A detailed description of the individual analytical methods was documented using standard operating procedures (E2.1, MS BfR1).

A2.2 Standard for analysis data

For the subsequent data analysis and the creation of classification models (e.g. for the *Food-Regio-Detect* and *FoodFraud-Detect* scenarios), product-related metadata, information about sampling and sample preparation, the generated spectra and device-specific settings are all of fundamental importance. An existing, open data standard, ISA, was utilised in order to be able to exchange these kinds of information in a standardised format between project partners (and later, between fAuthent system partners). The BfR also contributed significantly to the conceptual development of an initial fAuthent metadata standard (*FoodAuthent Knowledge Exchange* (FAKX)), which enables the exchange of all of the information types processed within the fAuthent system (including metadata, measured values, data analysis methods and models) between the individual fAuthent instances.

A2.3 Investigation of a pilot sample set

As the first step, the analytical fingerprinting methods developed in A2.1 by both laboratories (BfR, EF) were tested for their general applicability on a limited number of samples. Among other aspects, this included the comparability of spectra (A2.6). To this end, 15 hard cheese samples, 23 seed oil samples and 15 spirits were analysed by the BfR using FT-IR and NMR spectroscopy, and IRMS. In addition, the datasets and associated metadata were provided to project partners for A2.4, A.3 and A.4.

A2.4 Multivariate statistics and workflows

Analysis data and metadata were exchanged between BfR and UKO on a continual basis. In addition, various data pre-processing steps and chemometrical methods were tested by BfR on the KNIME server provided, and proposals for improvements were submitted in the form of reports.



A2.5 Quality assurance in analysis (lead: BfR)

In this work package, strategies for analytical quality assurance (QA) in fingerprinting analysis were investigated and developed. With the goal of establishing basic criteria for data analysis, reference samples (with a known composition, e.g. citric acid standard or an adequately characterised seed oil, e.g. refined rapeseed oil) were exchanged between the laboratories and analysed in the course of a working day.

One initial measure for studying precision over time is the convention of maintaining control charts, as is established practice in traditional, targeted analysis. To do this, the integrals of individual signals from a reference sample (e.g. the fatty acid signals in the case of seed oil) were entered onto a control chart. In this process, there is an opportunity to specify limit values, i.e. warning and control limits based on the standard deviation of the measured values observed over time. However, only individual parameters (integrals of selected signals) can be accounted for from a sample-and not the entire metabolome. A second approach utilises all of the parameters detected in a sample, by performing an exploratory analysis of the data using multivariate data analysis methods and observing their variance across a multi-dimensional space. In the process, deviations or trends can be detected, whereby the criterion that the variance of the quality control sample (QC sample) must be smaller than the variance of the authentic samples must be fulfilled [11]. Since this requires a representative set of authentic samples to have been analysed in order to evaluate the QC sample, this approach is only conditionally suitable as a means of verifying method precision. In addition, no concrete limit values can be determined and applied here in terms of decision-making. The evaluation is based on the experience of the person conducting the analysis.

A further strategy for analytical quality assurance, first investigated and developed in this project, also takes into account the entire metabolome of the QC sample. In this case, the evaluation is made using *one class classifiers* (OCCs) as well as distance- and density-based models [12]. In an approach similar to the control chart described above, a mathematical model as well as warning/control limits are determined by using a pre-period of measurements of the QC sample [13]. The investigations revealed that *local outlier factor* and *k-nearest neighbour* models are particularly suited to the task of verifying the precision of the method. It should be noted, however, that the identification of deviations over time is only conditionally possible, since only a unilateral test of deviations is performed.

A2.6 Comparability of data

NMR spectroscopy: The investigations were based on the samples analysed in the two laboratories (BfR and EF) according to the agreed standard operating procedures (MS BfR1). One option for ensuring the comparability of NMR spectra between individual laboratories is based on integral determination within a specific area from the spectrum of a reference sample (e.g. QC sample) followed by calculation of the ERETIC factor (according to [14]). The ratio of these factors from both laboratories is then applied to the spectral data from the remaining samples in order to minimise device-specific differences (different intensities).

FT-IR spectroscopy: Seed oil samples were analysed using three FT-IR spectrometers (BfR and CRA-W). To minimise device-specific intensity differences between spectra, three approaches were investigated [15]:

- *(i)* Spectra pre-processing
- *(ii)* Application of a correlation coefficient
- (iii) Piecewise direct standardisation (PDS)

Using the *FoodFraud-Detect* example scenario (pumpkin seed oil adulterated with rapeseed oil), the approaches were tested by comparison with the respective classification results. This



permits the following conclusion to be drawn: data correction with the application of a correlation coefficient is a suitable approach for utilising spectra from separate FT-IR spectrometers within a shared database, since—in contrast to *(i)* and *(iii)*—no spectral information is lost.

A3 – Component development

A3.1 Data formats and data mining

Contributions made by the BfR ensured that the concept of semi-automated derivation of the data mining parameters (e.g. details of origin, source or production) based on product master data was accounted for as part of component development. This was achieved by the continual exchange of insights between partners and the provisioning of analysis data.

A3.2 Authentic dataset

Samples of the three food matrices were procured by BfR from retail sources; the associated metadata were compiled and subsequently provided to project partners. EF was provided with sample material. Based on the two scenarios (*FoodFraud-Detect* and *FoodRegio-Detect*), the BFR performed analyses of all food samples in order to construct an authentic measurement dataset. All measurement data and product-related information were made available to project partners.

A3.3 fAuthent reference data cloud

The BfR provided support for the development of the fAuthent reference data repository, particularly in terms of the interface definition and testing of the technical implementation.

A3.4 Data analysis workflow register

Activities relating to the installation and update of a KNIME server instance were completed.

A4 – Validation

A4.1 Non-authentic samples (lead: BfR)

To test the data analysis workflows and mathematical models developed (A2.4), relevant topics were identified for both of the scenarios (*FoodFraud-Detect* and *FoodRegio-Detect*), and corresponding analyses of 'non-authentic' samples were performed:

Food	FoodFraud-Detect	FoodRegio-Detect
Seed oil	Authentication of pumpkin seed oil (adulteration by the addition of cheaper oil not affecting the overall taste)	Authentication of German rapeseed oil
Spirits	Adulteration by the addition of antifreeze, methanol, denatured ethanol	
Hard cheese		Authentication of Emmentaler and 'Bergkäse' from the Allgäu region

A4.2 Optimisation of data analysis workflows

Analysis data and metadata (A4.1) were exchanged between BfR and UKO on a continual basis. The BfR provided support for the validation of the chemometric models and tested the jointly developed workflows; proposals for improvements were submitted.



B5 – Requirements analysis (requirements specification)

B5.1 Authoring of B2B/B2G/B2C use cases

The BfR worked with other project partners to draw up detailed descriptions of the use cases relevant for the overall fAuthent system while accounting for the corresponding business and data processing processes; these use cases were then signed off and prioritised. A comprehensive, harmonised glossary was prepared, together with the derivation of all functional requirements for the overall fAuthent system.

B5.2 Requirements for overall fAuthent system (lead: BfR)

The functional requirements for the overall fAuthent system were derived from a detailed analysis of the use cases. A process analysis was used to depict the core processes. By analysing their interplay, together with a text-based process description and a discussion conducted with software developers and end users, all of the functional requirements for the overall fAuthent system were derived and documented. The results of the requirements analysis were documented as a requirements specification.

B5.3 Requirements specification validation

Validation of the requirements specification was completed by the Project Advisory Board. To this end, the results of the requirements analysis were presented and discussed with the Board.

B6 – FoodAuthent system architecture, process and interface model

B6.1 Discovery service model

Workshops (BfR, GS1G and BENE) were organised to discuss the technical solution strategies and to compare these with the requirements from B5. It transpired that the discovery service not only can and should handle tasks for data discovery itself (data availability) but also tasks for the detection and protection of access privileges to these same data, while properly accounting for a 'chain of custody' (CoC). Support was also provided for work investigating and assessing the use of hashing technologies, for example.

B6.2 Model for an EPCIS-/CBV-based event system

In particular, the BfR was involved in assuring the mutual exchange of data, and the 'translation' between experts from the 'lab work packages' and software developers. As part of this work, the BfR was responsible for ensuring that the system model developed was appropriate for the requirements of government end users, especially as these are subject to more stringent criteria (e.g. concerning internet access, fewer infrastructural facilities, etc.).

B6.5 Process/service/interface design

The BfR contributed actively to the design of the system interfaces. These interfaces were documented using a YAML file (*markup language*), and can be accessed and executed online via Swagger. Points of focus in this work included interfaces for data analysis workflows, fingerprint sets, and the import and export of FAKX files.



B7 – Component development

B7.1 Feasibility study for the overall FoodAuthent system

The focus of the BfR's work here was the development of user interface components that permit users to access data from the fAuthent system via the interfaces implemented previously. The BfR participated actively in discussions about fAuthent system implementation and developed open source components in the form of FSKX plug-ins based on KNIME.

B7.2 Implementation of B2G use cases: 'Assessment of product chain risks' and 'find-ings density' (lead: BfR)

A web-based service for assessing product chain risks and visualising the 'findings density' was implemented as a KNIME workflow. Also designated as the 'B2G app', this workflow permits government authorities (and, where access is authorised, other stakeholders from the supply chain and research institutions) to discover how often a product batch, product or product group has undergone authentication checking. In a further step, authorised users are also able to review the results of these assessments for the existing classification models or even the measured values in comparison to the reference data utilised. The prototypical web service was installed and tested on a BfR KNIME server instance as a web service, although it is also available as a local PC application within the open source KNIME software.

B7.3 Implementation of B2B use cases

The BfR provided support as required for work focusing on extending the OpenChrom software and implementing OpenChrom functionalities as a KNIME extension.

B8 – Validation

B8.1 Development of a model for validation and testing

Together with GS1G, a model was designed for the validation of the software components developed: this model was then presented to the software team and optimisations completed with the developers. Following this, the validation and test tasks devised were then input into the Confluence project management software.

B8.2 Testing against stakeholder requirements (lead: BfR)

In the course of workshops with the Board and special hackathons with other project partners, the software component demo instances were tested to verify their ability to meet the requirements of potential users (e.g. stakeholders in the supply chain, government authorities and research institutions). As a result of this work, it was possible to derive recommendations for optimisation, especially in terms of the usability and visualisation of measurement data and data analysis steps.

B8.3 Completion of integration tests and workshops

The BfR participated actively in the execution of integration tests and the organisation of expert workshops. The BfR was involved in particular in testing and improving the functionality offered by the core fAuthent API (interface), as well as the ISA and FAKX data exchange formats.

B8.4 Drawing up recommendations for optimisation

In the course of this work, the BfR was able to derive a wide range of recommendations for improving both its own 'B2G app' and the overall fAuthent system. The results are available to project partners in potential follow-on projects.



B9 – Continuity model

B9.1 Development of a transfer and continuity model

The BfR was actively involved in the preparation of a high-level specification, which was adopted and documented as planned by the Consortium. During the project, this model was optimised on a continual basis, serving as a means of coordinating measures for publication and dissemination.

B9.2 Implementation of the transfer and continuity model

The BfR initiated the production of the logo and flyer, implementing both in agreement with project partners, and commissioned the explainer video on the fAuthent system while also providing a substantial amount of content

(<u>https://www.youtube.com/watch?v=gzglh1sBlfw</u>).Press enquiries were answered in consultation with the project coordinator. Participation in research events resulted in the identification of new and relevant information and resources, while offering an opportunity to present project results.

B9.3 Cross-sectional tasks

The BfR provided support to project coordination work by participating in conference calls, Consortium sessions and meetings of the Advisory Board. In addition, the BfR worked with the Project Coordinator to organise and host the project wrap-up conference on 26 November 2019.

2.2 Necessity and appropriateness of work contributed

The funds provided were utilised effectively from both a scientific and economic perspective, the milestones and results were achieved in full, knowledge transfer was completed, and the availability of insights and results was ensured for both research and practice. Research work has been and will be published (see section 3). The BfR remains active in communicating the results to ensure their effective implementation.

The project results contribute to improving the safety, quality and competitiveness of the food sector, while offering an immediate benefit to stakeholders in the field of food safety and management (government agencies, retailers and businesses). With the achievement of the project goals and the continuity achieved by the pilot version of the project approach, urgent requirements from the food sector have been met by computerised, practical solutions for the collective use of fingerprinting technologies and local data storage.

The research and development tasks that were addressed in this project were associated with considerable financial risks for all project partners. None of those involved would have been able to bear these risks without support from the state. At the same time, feedback from third parties received in the course of the project demonstrate that the generic solution strategy pursued by this project has enormous potential for applications in both a public and private sector context.

2.3. Estimated benefit, with particular reference to the utility of the results in the sense of the updated utilisation plan

The BfR plans to further develop the project solutions with the aim of deploying them in the long term for the fulfilment of its official duties and for research purposes. The results will



also be made available to other government agencies, such as the state agencies for consumer and health protection. The BfR will also continue working on the establishment of uniform data standards and further improvements to open source software solutions in this field. Taking developments in the FoodAuthent project as a starting-point, the development of a prototype is now being pursued with the aim of trialling this for wine authenticity testing within selected government agencies at federal and state level. The BfR and several German state agencies for consumer and health protection (LUAs) have therefore laid the groundwork for close collaboration (exchange and shared analysis of measurement data) by harmonising the authenticity testing of wine with NMR spectroscopy in parallel to the project.

For the BfR itself, the open analytical, software-based and non-technical systems are an important aspect, since the BfR as a public-sector agency is especially dependent upon these kinds of cooperatively developed solutions. The BfR will therefore develop these project results after the end of the project and contribute to their continuation.

2.4 Progress in the project field achieved by other parties, such as became known to the grant recipient during the course of the project

Since the start of the project, no new results have transpired that could potentially collide with FoodAuthent's own goals. The European Union adopted an action plan to combat food fraud as a response to the horsemeat scandal involving beef products. Regulation (EU) 2017/625 (EU Controls Regulation) established the possibility of naming reference laboratories within the European Union for establishing the authenticity and integrity of the food chain. As a consequence, the BMEL announced the formation of a corresponding National Reference Centre for Authentic Food ('NRZ-Authent') at the Max Rubner Institute in May 2017. The remit of this National Reference Centre includes the coordination and concentration of national activities in the field of food authenticity, the (further) development of analytical methods for assessing the authenticity of food products, and the standardisation and validation of such methods. As regards these activities, further improvements in the analytical field as well as the setup of the fAuthent instance could be of particular interest. To support the activities of the National Reference Centre, and in the sense of ensuring the continuity of the overall fAuthent system, the project results were therefore presented at an expert conference (https://www.bfr.bund.de/en/press information/2019/49/ fingerprint helps to convict food counterfeiters-243298.html).

3 Scientific publications and scientific work resulting from the project

Publications:

- 1. Esslinger, S, Filter, M, Bartram, T: FoodAuthent Wegbereiter einer harmonisierten Echtheitsprüfung von Lebensmitteln (2020) Lebensmittelchemie 74, 61–99 (2020)
- 2. Bartram, T, Esslinger, S: Lebensmittelfälschungen unter der Lupe (2019) FOOD-Lab 01/2019

Presentations:

1. Esslinger, S: FoodAuthent - Fingerprinting-Analysen und Datamining (2019), Abschlusskonferenz, Berlin



- 2. Filter, M., Schüler, T., Valentin, L.: Software-Demonstratoren für behördliche Endnutzer (2019), Abschlusskonferenz, Berlin
- 3. Lörchner, C: Qualitätssicherung in der nicht-zielgerichteten Authentizitätsprüfung- am Beispiel von Rapsöl mittels FT-IR (2019), Abschlusskonferenz, Berlin
- Fauhl-Hassek C, Esslinger S, Lörchner C, Valentin L, Filter M.: fAuthent an open source framework for distributed food authenticity data and knowledge management (2019), 2nd technical workshop of the EC Knowledge Centre for Food Fraud and Quality, Geel
- 5. Lörchner, C: Wege zur Harmonisierung in der nicht-zielgerichteten Analytik spektroskopie-basierter Gerätevergleich (2019) Dt. Lebensmittelchemikertag, Dresden
- 6. Esslinger, S: Ansatz für die gemeinsame Nutzung spektroskopischer Daten das FoodAuthent-Projekt (2019) Experten-Treffen, Berlin
- 7. Lörchner, C: FoodAuthent Ein Fortschrittsbericht (2019) Next-NMR, Karlsruhe
- Lörchner, C: Comparable fingerprinting data an analytical approach towards comprehensive food authentication on the example of edible oils (2018) PreDoc-Symposium, Berlin
- 9. Lörchner, C: Investigations on the comparability of fingerprinting data Learn to walk before you run (2018) Food Integrity Conference, Nantes
- 10. Esslinger, S: Tracking Down Food Fraud NMR Spectroscopy in Wine Authentication (2018)-, BIT's 6th Annual Conference of AnalytiX-2018 Miami
- 11. Fauhl-Hassek, C: Lebensmittelverfälschung und Verbraucherschutz. (2018) Workshop Food Fraud Berlin
- Bartram, T, Esslinger, S: FoodAuthent Entwicklung eines Systems zur Sammlung, Analyse und Verwertung von Produktauthentizitätsdaten im Lebensmittelbereich (2018) BLE Innovationstage 2018, Bonn
- Lörchner, C: Analytische Authentizitätsprüfung im Lebensmittelbereich Verfahrensentwicklung und Harmonisierungsaspekte (2018) Vortragsreihe – Symposium Universität Halle, Halle
- 14. Fauhl-Hassek, C: Validation and reporting of non-targeted "fingerprinting" approaches for food authentication (2017) Workshop RAFA, Prag
- 15. Esslinger, S, Fauhl-Hassek, C.: Vorstellung des BMEL-Projektes FoodAuthent (2017) NEXT-NMR-AG, Karlsruhe
- 16. Lörchner, C: Vorstellung des Projektes FoodAuthent (2017) Wein- und Fruchtsaft-Analysenkommission, Berlin
- 17. Fauhl-Hassek, C: Analytische Authentizitätsprüfung von der Forschung in die Routine (2017) BVL Konferenz Food Fraud, Berlin



- 18. Esslinger, S: Vorstellung des Projektes "FoodAuthent" (2017) 5. Wissenschaftliche Veranstaltung der BMEL-Ressortforschung im Bereich Ernährung, Lebensmittelsicherheit und Tiergesundheit, Berlin
- 19. Esslinger, S: Authentizitätsprüfung in der amtlichen Überwachung Möglichkeiten und Herausforderungen (2016) Fortbildung für den Öffentlichen Gesundheitsdienst, Berlin
- 20. Esslinger, S, Filter, M: Planned project: FoodAuthent (2016) Treffen der Heads of Agencies, Berlin

Posters:

- 1. Lörchner, C, Fauhl-Hassek, C, Horn, M, Esslinger, S: A jointly used database a long way in non-targeted analysis (2019) RAFA, Prag
- 2. Valentin L, Horn M, Böckelmann S, Bartram T, Tröger R, Esslinger S, et al.: fAuthent -An open source platform to share scientific data (2019) 9th International Symposium on RECENT ADVANCES IN FOOD ANALYSIS, Prague, Czech Republic
- Valentin L, Horn M, Böckelmann S, Bartram T, Tröger R, Esslinger S.: fAuthent An Open Source Framework For Distributed Food Authenticity Data And Knowledge Management (2019) 11th International Conference of Predictive Modelling in Food (ICPMF11), Braganza, Portugal
- 4. Lörchner, C, Fauhl-Hassek, C, Baeten, V, Fernandez, J, Esslinger, S: Steps toward harmonization in non-targeted analysis (2019) RAFA, Prag (*Posterpreis*)
- Lörchner, C, Fauhl-Hassek, C, Drescher, S, Esslinger, S: Untersuchungen der Vergleichbarkeit von Fingerprinting-Daten – Learn to walk before you run (2018) Lebensmittelchemikertag, Berlin
- Lörchner, C, Fauhl-Hassek, C, Berger, F, Esslinger, S: Food Fingerprinting An analytical approach towards comprehensive food authentication (2018), One Health & Food Safety Congress, Helsinki
- 7. Esslinger, S, Drescher, S, Fauhl-Hassek, C, Lörchner, C: Authentication of edible oils using non-targeted spectroscopic fingerprinting techniques (2018) ASSET 2018, Belfast
- 8. Lörchner, C, Fauhl-Hassek, C, Berger, F, Esslinger, S: FoodAuthent: Collection, analysis and utilization of analytical food fingerprints (2017) RAFA, Prag
- Lörchner, C, Fauhl-Hassek, C, Berger, F, Filter, M, Esslinger, S: The FoodAuthent project – Steps forward harmonized analytical authentication (2017) Joint International Symposium, Berlin (*Posterpreis*)
- Lörchner, C, Fauhl-Hassek, C, Berger, F, Esslinger, S: FoodAuthent: Sammlung, Analyse und Verwertung analytischer Lebensmittel-Fingerprints (2017) Lebensmittelchemikertag, Würzburg
- 11. Lörchner, C, Fauhl-Hassek, C, Berger, F, Esslinger, S: Food Fingerprinting An analytical approach towards comprehensive food authentication (2017) ANUGA, Köln



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Further information on the subject of food authenticity from the BfR website

About the research project

https://www.bfr.bund.de/en/development_of_a_system_for_the_collection_analysis_and_utilisation_of_product_authenticity_data_foodauthent_-202679.html

https://www.bfr.bund.de/en/press_information/2019/49/_fingerprint__helps_to_convict_food_counterfeiters-243298.html

https://www.bfr.bund.de/en/press information/2016/47/tracking down the food fraudsters-199280.html



BfR 'Opinions app'

About the BfR

The German Federal Institute for Risk Assessment (BfR) is a scientifically independent institution within the portfolio of the Federal Ministry of Food and Agriculture (BMEL) in Germany. The BfR advises the Federal Government and the States ('Laender') on questions of food, chemical and product safety. The BfR conducts its own research on topics that are closely linked to its assessment tasks.

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