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Towards efficient use of data, models and tools in food microbiology

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Food microbiology researchers, risk assessment agencies and food business operators rely heavily on the reuse of knowledge that is available as data, models and tools. Unfortunately, such knowledge reuse remains challenging, as food safety data sets, models and tools are usually only available in platform-dependent or software-dependent formats that rarely comply to the Findability, Accessibility, Interoperability, and Reusability data principles. In recent years, the Risk Assessment Modelling and Knowledge Integration Platform (RAKIP) Initiative developed the so-called Food Safety Knowledge Exchange (FSKX) format. This development was accompanied by the creation of open-source software that facilitates the adoption of FSKX. Future work within RAKIP will focus on creating semantic interoperability in FSKX-related solutions and on the extension of the FSKX format towards other food microbiology knowledge.

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Abbreviations: FSK, Food Safety Knowledge; FSKX, Food Safety Knowledge Exchange; FMJ, Food and Ecological Systems Modelling Journal; QMRA, Quantitative Microbial Risk Assessment; RAKIP, Risk Assessment Modelling and Knowledge Integration Platforms; WGS, Whole-Genome Sequencing; BfR, Bundesinstitut für Risikobewertung; Anses, French Agency for Food, Environmental and Occupational Health & Safety; DTU-Food, National Food Institute at the Technical University of Denmark; SSI, Statens Serum Institut; EFSA, European Food Safety Authority; WHO, World Health Organization; GUI, Graphical User Interface; GMS, Generic Metadata Schema; VRE, Virtual Research Environment; FAIR, Findable, Accessible, Interoperable, Reusable

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Introduction

Food safety is a major challenge for the increasingly globalized food sector [1]. This challenge requires the adoption of methods for analyzing new and increasingly complex food systems. Modeling is an integral part of the scientific evidence used to guide the response of risk managers to address the food safety associated with these food systems. Food systems can largely benefit from the ever-improving IT-based technologies and data from the food and related sectors [2]. Therefore, there is a continuous interest in developing new solutions that help to exploit the potential of IT-based technologies in the food sector [2–11].

The Risk Assessment Modelling and Knowledge Integration Platform (RAKIP) Initiative aims at supporting researchers from the food sector in their efforts to increase the transparency and reusability of experimental data and mathematical models [12]. RAKIP was initiated in 2016 and is continuously funded by three institutions with food safety risk assessment mandates: ANSES, BfR and DTU Food. Over the years, RAKIP followed the strategy outlined by Plaza-Rodriguez et al. in 2015 [13] and created critical resources that enable efficient exchange of risk assessment models and data [14–18]. For example, during the generation of risk assessments, there might be the need to combine a

consumer phase model for exposure assessment from one author with the dose–response model created by another. If these models are only available in different formats or tools, their re-use by risk assessors might be hampered. For that purpose, missing resources that could facilitate the efficient exchange of data and models between software solutions were developed. This strategy takes into account that numerous software solutions exist in the field that may only slowly take up the new RAKIP resources.

The RAKIP Initiative and activities in other bioscience disciplines [19] also support the Farm to Fork Strategy at the heart of the European Green Deal by enabling efficient information exchange on the basis of harmonized information exchange formats [6]. This EU strategy aims at transforming food systems to better readjust food security, food safety, biodiversity, environmental costs and ethical objectives. Efficient information exchange and integration of knowledge between sectors and disciplines is an important element to reach the shared goals of the European Green Deal [5]. A transformation of such impact needs to be facilitated by IT-based resources for information exchange, which are currently not available. The RAKIP Initiative has exemplified a strategy for future information exchange and integration for the microbial risk assessment domain [14].

Another important driver of change in information exchange and data management are the Findable, Accessible, Interoperable, and Reusable (FAIR) principles [20] that ultimately aim at implementing Tim Berners-Lee's vision of a 'Web of Data' [21]. Despite the increasing adoption of these principles by governmental, research and funding agencies [22], there are still significant barriers to their full implementation, specifically for researchers [23] and agencies [24].

One of the key barriers is that critical resources for providing semantically interoperable metadata, like domain-specific ontologies, are often missing. This is specifically true for information on the food sample, its handling during the experiments, the data generation step, and the data modification steps applied after the measurements were taken, although first initiatives are also underway in this domain [25,26]. If data would be provided in semantically interoperable ways, this would support researchers and even allow computer-based algorithms to integrate available data from different sources in a meaningful way.

Large international initiatives like EOSC Life (https://www.eosc-life.eu/) create new solutions: for example, the RO-Crate standard for packaging research data with its metadata [27], which will be taken into account by the RAKIP Initiative in decisions to further enhance the resources supporting efficient knowledge exchange in the food microbiology sector. This also includes considerations of what tools need to be developed to reduce the workload for knowledge creators.

Available resources facilitating knowledge exchange in the domain of food safety risk assessment

For the food safety risk assessment domain, the RAKIP project created the following infrastructural resources to enable efficient exchange of domain-specific data and models:

1. A file format called Food Safety Knowledge Exchange (FSKX) that allows for the exchange of executable models, for example, microbial growth and inactivation models, source attribution models, and risk assessment models, together with linked information like metadata, underlying experimental or observational data, simulation scenarios, and simulation results, in a standardized way (https://foodrisklabs.bfr.bund.de/fskx-food-safety-knowledge-exchange-format/). The FSKX file format can also comprise 'joined' models, that is, models that are composed of several model modules, where each module is an individual FSKX file.
2. A community-driven harmonized annotation schema for food safety knowledge (e.g. data and models), called Generic Metadata Schema (GMS), with integrated controlled vocabularies that make use of existing code lists and information exchange standards [14]. GMS also allows the easy creation of knowledge-type specific metadata schemata. This helps to capture only relevant meta-information that is specific to certain model classes or knowledge domains.
3. A Minimum Information guideline Consultative Group on International Agricultural Research (CGIAR) called Minimum Information Required to Annotate Food Safety Risk Assessment Models (MIRARAM) [17] that supports model creators, journal editors, and reviewers as well as curators of model repositories on what minimum meta-information should be provided for risk assessment models.
4. A number of web-based and desktop software solutions to facilitate the adoption of FSKX and MIRARAM by knowledge creators and knowledge users. The most feature-complete software is FSK-Lab [16], which is an extension to the open-source data analytics platform KNIME (www.knime.org). This platform was also used to establish a number of web services for execution, creation, editing, and joining of FSKX models [18]. All 'FSK-Lab'-based software solutions currently support the execution of models created in the scripting language R (www.r-project.org) and Python (www.python.org) and the joining of FSKX models.

5. A number of online repositories for the collection and execution of models were established, for example, the RAKIP-Web model repository (https://knime.bfr.berlin/landingpage/RAKIP-Model-Repository) and the Food and Ecological Systems Modelling Journal (FESMJ) (https://fmj.pensoft.net/) [28]. These online resources can even be linked to each other; for example, the executable model feature in FESMJ makes use of a model execution service provided within a Virtual Research Environment (VRE) named 'FMJ_Lab' (https://aginfra.d4science.org/group/fmj_lab) and a simulation configuration service provided by RAKIP-Web.
6. A number of 3rd party software solutions allow import or export of FSKX files, for example, MicroHibro (https://www.microhibro.com) [29] and BioinactivationFE (https://foodlab-upct.shinyapps.io/bioinactivationFE/) [30]

The RAKIP project website https://foodrisklabs.bfr.bund.de/rakip-web-portal/ provides more details on these resources.

Development needs to extend the Food Safety Knowledge Exchange (FSKX) format into a standard facilitating data-driven innovations in food microbiology

So far, RAKIP has primarily been focused on microbiological food safety and risk assessment knowledge. As the idea to promote knowledge exchange is relevant in other domains as well, the RAKIP Initiative plans to expand its scope, for example, towards the One Health sector, which implies the involvement of a broader range of experts and expertise. In order to adopt the available FSKX-related resources also in various other food microbiology domains, a number of additional infrastructural developments are needed. This work must target four main areas:

1. the FSKX format itself,
2. the software supporting FSKX,
3. FSKX-compliant content in knowledge repositories,
4. training and support for information providers and users.

For area 1, the work will address three aspects: a) make the necessary adjustments so that FSKX can be used for information objects from other food disciplines, such as microbial data analysis pipelines, food tracing data, food authenticity data, whole-genome sequencing (WGS) data, and so on; b) extend FSKX such that the provisioning of semantically interoperable meta-information is supported, that is, via linking the controlled vocabularies in GMS to relevant ontologies; and c) provide options to use FSKX for the exchange of protected data and models, for example, as encrypted information objects.

For area 2, investments need to be made into a) the automated generation of open-source software libraries in different popular programming languages, which can be integrated into new and existing software tools and reduce the maintenance effort for software developers (including the support for backward compatibility between different FSKX versions), b) the improvement of the usability and functionalities of the existing FSKX-compliant software solutions (a significant development effort must thereby be directed towards technical solutions, e.g. Application Programming Interfaces (APIs), that make use of the semantically interoperable meta-information provided within FSKX objects in the future), and c) the provisioning of secure, cloud-based computational resources that allow to combine and execute FSKX information objects from different programming languages.

For areas 3 and 4, an ongoing investment in human resources will be required to create a critical quantity of knowledge in FSKX-based knowledge repositories like RAKIP-Web (https://knime.bfr.berlin/landingpage/RAKIP-Model-Repository) and to provide training and education. Collaborative international support will be essential to assure continued commitment.

Semantic interoperability of Food Safety Knowledge Exchange (FSKX) formatted information objects

The full adoption of the FAIR principles remains a significant challenge for researchers not only in the food microbiology sector. Even if data and models were provided with appropriate metainformation, for example, using the FSKX format, this meta-information is in many cases not captured in a semantically interoperable way [31]. As a consequence, the currently available food microbiology knowledge is not directly exploitable by semantic web technologies, for example, to automatically enrich food microbiology data sets with information from related disciplines, like food nutrition, food consumption, food technology or public health (for an illustrative example, see http://www.rxnfinder.org/frcd/ [32]). This lack of interoperability is in our opinion partly due to a lack of knowledge and adoption of food-related ontologies like FoodOn [33] and a lack of customized software tools like SciLite [34] or 'ISA tools' (https://isa-tools.org/ [35]) that support food microbiology researchers in their knowledge-sharing efforts. Also, tools and platforms facilitating the easy exploitation of semantically interoperable metainformation, as it is available in other disciplines (e.g. like DisGeNET-RDF (https://www.disgenet.org/rdf) or Omics DI https://www.omicsdi.org/), are missing in the food microbiology sector. As a consequence, it will be necessary to bring together several stakeholders from the food microbiology community to work synergistically towards the objective of FAIR data.

A roadmap towards open infrastructural resources enabling data-driven innovations in food microbiology

In order to accomplish the development goals outlined above, it is important to implement measures that can provide long-term financial and organizational support. The foundation of the RAKIP Initiative by DTU Food, ANSES and BfR is therefore an opportunity for the food microbiology sector, as this initiative allows the linking of long-term governmental support with the developments funded by research grants. Specifically, the RAKIP Initiative is committed to supporting the development and provisioning of infrastructural resources that facilitate efficient information exchange in microbial and chemical risk assessment, risk–benefit analysis and food microbiology. It is already planned to expand the RAKIP Initiative network towards other risk assessment institutions (e.g. EFSA, SSI, WHO) and universities (e.g. University Cordoba, University of Donja Gorica etc.). An open-access knowledge base and a well-defined standardized knowledge exchange format will also be beneficial for the private sector and may support collaboration where possible. A combination of efforts of the RAKIP Initiative with existing European infrastructure providers like ELIXIR (https://elixir-europe.org/) [19] would further open up new opportunities for funding, synergistic development, visibility, and end-user support.

On a technical level, the following development tasks will be addressed by the RAKIP Initiative in the near future:

- Creation of a technical framework to maintain and extend the FSKX format. This framework provides a) an intuitive graphical user interface (GUI) for collaborative curation of the GMS and the data/model-class specific metadata schemata and b) an automated software code generation pipeline that transforms agreed FSKX changes into software code libraries for different programming languages and tools, also maintaining backward compatibility wherever possible.
- Maintain and improve the functions and user-friendly application of existing FSKX-related software tools, like RAKIP-Web, FSK-Lab, the FSK2R R library, the services offered via the D4Science VREs [36], as well as 3rd party tools.

In parallel, the RAKIP Initiative will continuously extend the amount of FSKX-compliant content in, for example, the RAKIP-Web model repository and provide individual support for researchers who wish to convert their own data or models into the FSKX format even if this will not be deposited in RAKIP-Web. This includes the organization of regular workshops, webinars and e-learning courses, and the active communication and dissemination of results at relevant international conferences. In the mid-term perspective, the RAKIP Initiative aims at developing into a service provider for infrastructural resources that supports interoperability of data and services and that is closely connected to similar initiatives from other life science and One Health domains.

An important issue when sharing models remains the model code quality verification. Indeed, the computer programs used in risk assessment modeling are often complex and expensive to develop. However, the model code is rarely formally verified. So far, the main code review approach is to compare the generated model results with the ones from the original publication. Even though other and better solutions can be envisaged, this responsibility will stay with any platform owner or journal reviewer in the foreseeable future. The resources generated by the RAKIP Initiative will support their work, as the original model code can be shared with FSKX, even if it was created in various programming languages.

Conclusion and recommendations

All stakeholders of the food sector need to adapt to new technological opportunities and the societal, ecological and business transformations ahead. For risk assessment agencies, this implies that there is an increased demand for timely and transparent risk assessments, which in turn require the development of adequate infrastructural resources facilitating this transformation. Here, the establishment of harmonized information exchange formats for data and models from the food microbiology sector, together with solutions that facilitate the implementation of modular modeling frameworks as described in Refs. [37–39] are fundamental building blocks.

In order to create synergies between the development work driven by risk assessment agencies and the broader food microbiology research community, RAKIP is open to collaborations with other risk assessment agencies and research institutions. Only in this way, strong synergies between academic, governmental and private sector development can be created. In addition, the RAKIP Initiative could evolve into an infrastructure provider that is closely interlinked with other international networks and initiatives like ELIXIR (https://elixir-europe.org/) or the Ontologies Community of Practice of the CGIAR Platform for Big Data in Agriculture [40] and also provide support for the often-difficult long-term maintenance of infrastructural resources. In the long run, the RAKIP Initiative will work towards the establishment of a truly interoperable, modular food microbiology knowledge ecosystem that can support all food sector stakeholders.

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Author contributions

Matthias Filter: Conceptualization, Writing – original draft. **Maarten Nauta**: Writing – review & editing. **Sara M. Pires**: Writing – review & editing. **Laurent Guillier**: Writing – review & editing. **Tasja Buschhardt**: Writing – original draft.

Conflict of interest statement

None.

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