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Final Report on SSD2 pilot results in Denmark

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EXTERNAL SCIENTIFIC REPORT

DTU Food
National Food Institute

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Final Report on SSD2 pilot results in Denmark

National Food Institute, Technical University of Denmark

Jens Hinge Andersen, Kevin Jørgensen, Louise Grønhøj Hørbye Jensen, Birgitte Helwigh, Jytte Butters

Abstract

This document is the "Report on SSD2 pilot results" of the project OC/EFSA/DCM/2013/05: "Pilot project on the implementation of SSD2 in the frame of the electronic transmission of harmonised data collection of analytical results to EFSA". The report includes a description of the software and tools used, a description of the challenges encountered in migrating data structure from SSD1/XML to SSD2 in the national data repositories, a summary of the experience gained in testing SSD2 and recommendations for EFSA on effectiveness and suitability of the SSD2 in the different domains. The following domains are included: Pesticides Residues (under Regulation (EC) No 396/2005), Contaminants (under Regulation (EC) 1881/2006), Food Additives (under Regulation (EC) 1333/2008) and Microbiological data (under Directive 2003/99/EC).

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Key words: Standard sample description, SSD2, XML transfer of data, FoodEx2, EFSA data models, Denmark

Question number: EFSA-Q-2015-00607

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Summary

This document is the "Report on SSD2 pilot results" of the project OC/EFSA/DCM/2013/05: "Pilot project on the implementation of SSD2 in the frame of the electronic transmission of harmonised data collection of analytical results to EFSA". The report includes a description of the software and tools used, a description of the challenges encountered in migrating data structure from SSD1/XML to SSD2 in the national data repositories, a summary of the experience gained in testing SSD2 and recommendations for EFSA on effectiveness and suitability of the SSD2 in the different domains. The following domains are included: Pesticides Residues (under Regulation (EC) No 396/2005), Contaminants (under Regulation (EC) 1881/2006), Food Additives (under Regulation (EC) 1333/2008) and Microbiological data (under Directive 2003/99/EC).

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1. Introduction

1.1. Background and Terms of Reference as provided by the requestor

This contract was awarded by EFSA to: National Food Institute, Technical University of Denmark

Contractor: Christine Nellemann

Contract: Pilot project on the implementation of SSD2 in the frame of the electronic transmission of harmonised data collection of analytical results to EFSA.

Contract number: OC/EFSA/DCM/2013/05

1.2. Background as provided by EFSA

In 2010 the SSD Guidance Document (EFSA, 2010a) and the Guidance on Data Exchange (EFSA, 2010b) were published defining a standard format to transmit chemical occurrence analytical data in food and feed samples to European Food Safety Authority (EFSA). These guidance documents describe the data model and data interchange protocol[1] for reporting the results of laboratory tests on food and feed samples in several food domains (contaminants, pesticides, etc.).

Since 2010, the use of the Standard Sample Description (SSD) has been fully implemented and used in the national competent authorities and laboratories in 27 Member States and two EFTA countries (Iceland and Norway) involved in the pesticide monitoring data collection. In addition to the general SSD Guidance Document mentioned above, an EFSA Guidance Document on the use of the SSD specific for pesticide data reporting (EFSA, 2012) has been produced and is reviewed on a yearly basis.

For chemical contaminants data collection, through Article 3614 grant procedures EFSA has provided funding to official reporting organisations in Member States to implement the SSD within their data management systems.

In 2011, the Biological Monitoring Unit (BIOMO) ran a pilot study [EFSA-Q-2011-00174] for the collection of Antimicrobial Resistance (AMR) data at isolate-based level. The existing SSD model could not be entirely adopted and consequently a preliminary ad-hoc data model was developed for the pilot. As the two data models were similar, as an outcome of the pilot study, the "Working group for the provision of zoonoses data in XML and Excel format" [EFSA-Q-2011-00226] proposed to extend the SSD to be compatible with the current draft format on Antimicrobial Resistance data at isolate-based level.

A working Group on SSD Extension (WG-SSD2) was established in 2012 to extend the SSD to include zoonotic agents in food and animals, antimicrobial resistance and food additives, and to provide a framework for the collection of harmonised analytical measurement data on chemical and microbiological contaminants in different matrices (e.g. food, feed, animals, water, environmental samples, food contact materials). The amended standard proposed by the working group WG-SSD2 is called Standard Sample Description version 2 (SSD2).

1.3. Additional information

This document is the "Report on SSD2 pilot results" for the project OC/EFSA/DCM/2013/05: "Pilot project on the implementation of SSD2 in the frame of the electronic transmission of harmonised data collection of analytical results to EFSA"

The objective of the project was to establish a system to export data from the Danish data repositories in compliance with the published EFSA SSD2 data models and control terminologies for the following data categories:

[1] Electronic data interchange: is the structured transmission of data between organizations by electronic means. It is used to transfer electronic documents or business data from one computer system to another computer system.

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- Pesticides Residues (under Regulation (EC) No 396/2005[2])
- Contaminants (under Regulation (EC) 1881/2006[3])
- Food Additives (under Regulation (EC) 1333/2008[4])
- Microbiological data (under Directive 2003/99/EC[5])

The objective for this document was to report on SSD2 pilot results:

- Describe software and tools used and/or developed,
- Describe challenges encountered in migrating data structure from SSD, respectively data formats currently used for antimicrobial resistance, to SSD2 in the national data repositories,
- Summarize the experience gained in testing SSD2, and
- Provide recommendations for EFSA on effectiveness and suitability of the SSD2 in the different domains.

2. Applied methodology and software

2.1. Pesticides residues, contaminants and food additives domains

2.1.1. Data structure mapping between the national database data elements and the SSD2 data elements

The configuration file for transformation of the Danish Veterinary and Food Administration (DVFA) Laboratory information management system (LIMS) dataset to a SSD2 compatible SAS dataset is described in Appendix A.

2.1.2. Challenges encountered in migrating data structure from national repositories to SSD2

The national repository at the DVFA was based on a new LIMS as of 1st January 2014. For this reason, a new data extraction system had to be implemented for the pilot transmissions of 2014 data.

Initially, the data extraction from the DVFA repository included some transformations of data in order to align values with SSD2 specifications for the initial transmission of pesticide data. However, this system turned out to be incompatible with transmission of data on chemical occurrences and additives because several data fields where translated to EFSA SSD2 codes by 'hard coding' in the database; this made a flexible recoding for other data domains difficult. Consequently a new data extraction system was implemented, making the original, unchanged, repository data available for further processing at the Technical University of Denmark (DTU) .

[2] Regulation (EC) NO 396/2005 of the European Parliament and of the Council of 23 February 2005 on maximum residue levels of pesticides in or on food and feed of plant and animal origin and amending Council Directive 91/414/EEC

[3] Commission Regulation (EC) No 1881/2006 of 19 December 2006 setting maximum levels for certain contaminants in foodstuffs

[4] Regulation (EC) No 1333/2008 of the European Parliament and of the Council of 16 December 2008 on food additives

[5] Directive 2003/99/EC of the European Parliament and of the Council of 17 November 2003 on the monitoring of zoonoses and zoonotic agents, amending Council Decision 90/424/EEC and repealing Council Directive 92/117/EEC

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2.1.1.1. General remarks

Handling of SSD2 catalogue changes

During the pilot project we experienced difficulties in finding the correct information on data structure and catalogue versions from EFSA sources. Access to updated Excel versions of catalogues was described in the SSD2 guideline (8.1. Maintenance and versioning of SSD2 controlled terminology catalogues) would also have made data transformation easier.

Handling of LIMS limitations

The mandatory element 'Type of matrix' (E.01 sampMatType) does not have an equivalent element in LIMS, and cannot be deducted from the categorised product identification code in LIMS. For the pilot, reporting was restricted to samples from the category "Food".

The element 'Type of limit for the result evaluation' (N.03 evalLimitType) has so far been established based on project identification, since the element is not unambiguously defined in LIMS.

The elements for date of analysis (F.03 analysisY, F.04 analysisM, F.05 analysisD) has been reported as the date of the final analysis of the sample in order to be compliant with section F (Sample analysed), not as the actual date of analysis, since this value could be dependent on each method used for the sample (section L, Analytical method or M Result).

Handling of FoodEx2 related issues

Our initial transmission failed due to errors in the EFSA food classification and description system (FoodEx2) coding for several samples. The major part of these samples was correctly coded at the time when our product catalogue was set up, but the FoodEx2 coding had changed since then (e.g. A0EYT#F26.A07XE$F27.A02BV 'Salt-preserved fish, GEN=Other, RAWSRC=Cod' replaced by A0FCB 'Salted cod'). Maintenance and versioning of FoodEx2 should involve methodology on how to handle changes in FoodEx2 e.g. deprecated FoodEx2 codes. We suggest to include a "FoodEx2 Change Log" on new releases describing major/minor changes to be aware of.

Harmonisation document on specific requirements on contaminants and additives in SSD2

The release of the final Specific Requirements Document (EFSA 2015a) was published for internal SSD2 project members after the Data Collection deadlines, leaving no time to cover these requirements for the Data Transmission.

In many cases we cannot recognize the stated requirements from the discussions or suggestions from the group of pilot participants.

It is suggested to revise the requirements in the above mentioned document, in particular the parts, where mandatory reporting of information has been suggested. Furthermore, EFSA should consider whether a real need exists for some of the requirements with very detailed dependencies on food matrices, since checking as well as fulfilling of such business rules may be difficult to implement for data providers. It is our opinion that such requirements should be only recommended since a missing mandatory field will prevent reporting of the result.

Examples:

Nitrate: 'Additional sampling event information' (C.06) has been stated as mandatory for information that presently is not available in all cases (harvest date, type of cultivation). In addition, a free text field like C.06 is not recommended for mandatory information.

Polycyclic aromatic hydrocarbons (PAH): 'Coded description of the analysed matrix' (G.01): It is stated that "It is mandatory to describe the container or wrapper that holds the product. Commission

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Regulation (EC/333/2007)[6] gives specific instruction to avoid certain containers when analysing PAHs." It is our opinion that the description of container or wrapper in G.01 is reserved to the container or wrapper for the product on the market, not after sampling. Element B.05 Sampling programme can be used to report whether the sampling has been done according to legislation.

Furthermore, for 'Expression of result percentage' (M.13) is stated (as mandatory): "For PAH determining in cocoa grain and cocoa derived products, including chocolate, field M.13 Expression of result percentage type compound should additionally refer to the method of determining fat in cocoa products." Presently M.13 is composed of three numerical fields, and method of determining fat cannot be reported here. Also here, validating information depending on detailed product description may be problematic for the data provider.

Perchlorates: 'Coded description of the matrix of the sample taken' (E.02), Attribute F21: 'Production method' has been classified as mandatory.

Dioxins: 'Coded description of the matrix of the sample taken' (E.02) (and 'Coded description on the analyzed matrix' (G.01)) It is stated that "The appropriate descriptor field E.02 should specify species of the tested fish, and the descriptor field G.01 should state the part of fish body tested (ex: liver, muscle tissue, etc.)". According to the general guideline, data providers are not required to report G.01 if an expected difference between E.02 and G.01 can be derived from the legislation specified in 'Sampling program' (B.05). Furthermore, it should be mentioned that these two facets normally are predefined as implicit facets to the FoodEx2 base code.

Bisphenol and additives: We cannot understand the reasons why the mandatory fields 'Sampling strategy' (B.03) and 'Sampling method' (B.05) must be specified as "Not specified" according to Table 1 in the Specific Requirements Document (EFSA 2015a).

2.1.1.2. Pesticides

Handling of free text fields

Some challenges related to description of samples were due to uncategorised information on detailed information, e.g. for fruit and vegetables not common on the Danish market. Such samples could be categorised as e.g. "Exotic vegetable" from the DVFA LIMS product catalogue while more detailed information (e.g. "Lotus Roots") was given in various free text fields. As these fields in other cases contained classified information in DVFA LIMS on e.g. the identity of shop owners, these fields cannot be transmitted EFSA as they cannot be made public available since this could undermine commercial interests of a natural or legal person, including intellectual property.

A general problem (in DVFA LIMS) for all domains is that some of the information needed as categorised information in SSD2 are either only available from free text fields or the information has been registered in free text fields instead of in the assigned list fields with categorised values.

Handling of reporting of substances

The method templates in the DVFA LIMS includes all substances analysed for in the method, but for multi methods, only substances that was detected are reported in the data set describing the results for a sample. For this reason major manual maintenance of method/substance catalogues is necessary. SAS procedures unfold the reported analytical method to the full analytical scope for each sample.

Pesticide residue reporting includes complex residues definitions which in addition may depend on the analysed matrix. The DVFA LIMS method templates do not reflect this in all cases. Tools have not yet been made available from EFSA to manage this automatically, but the recently developed EFSA

[6] Commission Regulation (EC) No 333/2007 of 28 March 2007 laying down the methods of sampling and analysis for the official control of the levels of lead, cadmium, mercury, inorganic tin, 3-MCPD and benzo(a)pyrene in foodstuffs

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"Matrix tool" has been used in combination with our own "Matrix table C" to define and validate both the residue definition and the value of parameter type for each result. "Matrix table C" lists, for each residue definition relevant for our reporting, the possible parameter codes that can be part the reporting of the residue definition, while the EFSA "Matrix table A" lists the possible combinations of product code (from MATRIX catalogue) and residue definition (from PARAM catalogue). These tools have shown through the EFSA "advanced validation" to code correctly (provided that catalogues are correct) except for some uncommon residue definitions (e.g. Flucythrinate where same substance/analyte has to be reported with two different paramCodes depending on the matrix or Fenpropimorph where the 'mother compound' are not part of the residue definition). An automatic solution for these situations has still to be found.

Handling of "Action Taken" results

Results for "Action taken" are not part of the information in DVFA LIMS, and are supplied in an Excel table from the DVFA based on a SAS report of non-compliant results. The information received are manually coded and joined to the SSD2 dataset based on sample identity and parameter code (result identification code).

Handling of new guidelines

The specialised pesticide guideline for pesticides was published very late in the process (Draft version April/May 2015, final version July 2015 (EFSA 2015b)). Since new specific requirements were introduced in the guideline, revision of already recoded results had to be performed.

2.1.1.3. Chemical occurrences

Acrylamide:

Classification based on Commission Recommendation 2010/307/EU[7] on the monitoring of acrylamide and Commission Recommendation 2013/647/EU[8] on investigations into the levels of acrylamide in food was added manually to an Excel table and joined to the SSD2s dataset based on sample identification.

Dioxins:

Information on fat content was missing for several sample types where results were based on fat content. In some cases (fats, whole eggs) fat content from food composition tables were used, but 1300 results from 40 samples (meat, milk, liver) were not reported.

In case of duplicate analyses only the result from the first analysis are reported to EFSA. This requires some manual corrections by the laboratory since LIMS is reporting the average in such cases.

Metals:

Limit of quantification (resLOQ) is defaulted to 3 × resLOD (Limit of detection).

Dioxins:

The dioxin limit of quantification was mistakenly reported as limit of detection in resLOD.

PAHs:

Information on treatment (smoking, cooking etc.) is entered manually in an Excel sheet. This information is joined to SSD2 (sampMatInfo.com) based on sample identification.

[7] Commission Recommendation of 2 June 2010 on the monitoring of acrylamide levels in food
[8] Commission Recommendation of 8 November 2013 on investigations into the levels of acrylamide in food

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2.1.1.4. Additives

Subsampling

The structure for reporting of subsamples in DVFA LIMS is not directly compatible with the structure of SSD2. However, with a few exceptions, it was possible to implement automatic procedures to align LIMS reporting to SSD2. The exceptions could be identified by business rules and then manually corrected.

Qualitative analysis

For e.g. added colours both qualitative (positive or negative) and quantitative results may be reported as valid results in LIMS. Automatic procedures were implemented to filter off screening results where these were supplemented by quantitative results. In case of conflicting qualitative and quantitative results, quantitative results were given priority.

2.1.3. Summarised experience gained in testing SSD2

In the pesticide domain, 709,734 results from 2510 samples were reported successfully as XML files in SSD as well as SSD2 format were to the DCF.

In the domain of chemical occurrences, a total of 17,734 results from 1116 samples were reported, while results from 40 samples were discarded due to missing information on fat content.

For additives, 1529 results from 384 samples were reported, including results from sub samples.

Excluding the efforts in setting up the system, we expect that the major efforts in keeping the system running will be updating of our local method/substance catalogues and product catalogues.

The major efforts for each data transmission will be finding and categorising information in free text fields for elements that need to be categorised in SSD2.

2.2. Microbiological domain - Antimicrobial resistance table

2.2.1. Challenges encountered in migrating data structure from XML reporting system to SSD2

In this report we differentiate between the existing reporting system called XML and this pilot project called SSD2.

Using the temporary and not completed XSD-file was made virtually impossible as specifics as usage and definitions for "body elements" are missing. "body elements" are the elements defining the result rows in section <dataset>. The output was generated using this XSD-file as well as SSD_STRUCTURE 131030 - TILRETTET jf SSD Guide pr 150107.xls in order to extract the file format and upload successfully. An easier road to completion of the task would have needed completed XSD-file and manual as these are essential to complete the task efficiently.

Migrating to the codes from the new catalogues created challenges which we need to address once the SSD2 format becomes permanent and the catalogue structure becomes fixed and more stable. Particularly catalogues MTXTYP "MTXTYP" and MTX "FoodEx2 Matrix" needed recoding/redefining from XML codes in the MATRIX catalogue to SSD2 codes as frequently used codes were discontinued ie. pigs/unspecified or pigs/mixed herds. The consequence is that the results reported in SSD2 format are less specific than the reported results in XML format. As stated in section 4.1.1 Microbiological domain it was cumbersome for the scientific staff to pick valid codes for terms already translated into suitable codes which was rendered discontinued. Here a mapping tool from present codes to SSD2 allowed codes is absolutely essential. Unless there are no restrictions on which values can be used in which table the catalogues need and addition of "usage flags".

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Having to access catalogues/pick lists in XML format instead of excel is a challenge that will remain unsolved until SSD2 format becomes permanent. The catalogues will be implemented as external list read from the Oracle RDBMS using known technology... However XML files are not easy to read for recipients who need overview in order to pick the correct candidate rows. They will need to import the file/catalogue to office tools or other xml tools. We suggest that the basic idea for changing the catalogue entries becomes available to the user of the system, so mistakes are minimised.

The ever changing formats in the excel picklists used in the XML system are seen as problems that are unnecessarily introduced by EFSA every year. This is seen every year when the new picklists from excel are imported into the Oracle RDBMS structures (tables). It is not an immediate import as columns or structure of the spreadsheet often change. This make the implementation of the new picklists a manual process and therefore operator heavy

2.2.2. Summarised experience gained in testing SSD2

It was possible to migrate and upload valid output files to transfer the 2014 AMR and 2014 prevalence datasets from the XML reporting system to the SSD2 using the catalogues, definitions files, voluminous description documents and the spreadsheet mentioned.

3. Conclusions

The design of data structure and terminology mapping between the national database data elements and the SSD2 data elements has been successfully carried out for the data on pesticides, antimicrobial resistance, chemical occurrences and additives.

For the **chemical domains** we find from the data provider side that SSD could be replaced by SSD2. The major effort would be updating LIMS product catalogues to FoodEx2 codes.

For pesticides, implementation of 'MRL applicability' could be a more clear indication of the MRL used for evaluation than the present use of 'product treatment'. This, and the availability of MATRIX codes from FoodEx2, would make SSD2 acceptable for pesticide data analysis.

For the **microbiological domain** it will be feasible to transform the present structure of the XML output to SSD2 formatted output.

However we need stable formats of catalogues/picklists in order to ease the yearly maintenance of these. The catalogues will be implemented as external list read from the Oracle RDBMS using known technology.

In order to "translate" present codes to valid SSD2 codes we need a mapping tool and the described ideology behind the code changes in particularly Foodex2 matrix, which was fundamentally changed.

In order to ease the upload of tables it is essential that data dictionaries are stables as well as XSD files and that they are available in good time before that yearly deadline.

4. Recommendations

4.1. Chemical domains

1) Update user friendly versions of catalogues (Excel) synchronously with machine readable versions (XML)
2) Embed specific requirements in legal documents. EFSA should coordinate with EU Commission in order to bind authorities to report in accordance to specific requirements.
3) EFSA should continue work on solving the problems related to complex residue definitions either by simplifying residue definitions or by setting up tools to aid reporting and/or validation of residue definitions and parameter type.

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4) It should be clarified if and how information on applicability of the MRL should be reported; this information is reported in the SSD element prodTreat, which is not available. We suggest that an attribute is created for this purpose, e.g. anMatInfo.MRLapplicable (with acceptable values "Y" or "N" from YESNO catalogue) unless FoodEx2 codes can supply this information.

5) By default the element "anMatCode" has the same value as "sampMatCode". It should be clarified whether the same relation exists between sampMatInfo.com and anMatInfo.com, and between sampMatText and anMatText. This is important for the placement of information related to specific requirements.

6) Presently, reporting of fat percent is required for results reported on fat basis; i.e. such results cannot be reported, although they could still be of value for exposure assessment. Thus, the consequence of this lack of information should be a warning, not an error.

7) Publish a "FoodEx2 Change Log" on new releases describing major/minor changes to be aware of (e.g. e.g. A0EYT#F26.A07XE$F27.A02BV 'Salt-preserved fish, GEN=Other, RAWSRC=Cod' replaced by A0FCB 'Salted cod').

8) EFSA should consider whether a real need exists for some of the specific requirements with very detailed dependencies on food matrices, since fulfilling and checking of such business rules may be difficult to implement for data providers. It is our opinion that such requirements should be only recommended since a missing mandatory field will prevent reporting of the result (see 2.1.1.1. General remarks for examples).

9) Include the two texts "analysed as such" and "analysed after hydrolysis, derivatisation" in the controlled terminology SSD_CAT_ANLYMD e.g. as facet values.

10) Likewise, the listed methods for hydrolysis and derivatisation as well as the three AOCS methods should be included in the controlled method terminology.

11) Procedure for error reporting after DCF upload should be optimised – possibly in cooperation with the network groups for reporting.

4.1.1. Microbiological domain

The XSD-file is containing elements for the related fact table. All body-elements should be defined completely incl. reference to validation catalogues, data element definitions and usage in the specific tables (AMR, prevalence). By usage is meant if the element is mandatory for the table and if the element is required to be delivered in the specific table. This will ease the creation of output.

Catalogues in XML format is a challenge as new tools has to be introduced to staff. Particularly for the FoodEx2 catalogue we suggest that EFSA provides list of translations between the amalgamated codes from the XML picklists and the new code structure in this very large catalogue. We unfortunately found several code options to be correct choices for discontinued XML picklist codes.

In the XML pick lists we have found the usage flags for valid code options in specific tables. This makes valid codes easily obtainable when using our applications, and makes the reporting more efficient. It is important that the usage flags are also included in the SSD2 catalogues.

In the uploading process we have the following recommendations: When EFSA is validating the data upload we only receive one error at a time. For structural errors this is understandable, but for validation and code errors it would be more efficient and time saving if we could receive a full feedback containing all errors, so the number of upload attempt would be minimized before a valid status could be obtained.

We would like to receive an overview table with information on legislation that states which data reporting is mandatory, e.g. the new reporting on pig herds, reporting of AMR data. Then Member State (MS) indicate that data are collected and analysed according to a specific harmonised legislation. This would make data more comparable between MSs.

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For efficient implementation of changes to the catalogues it is very important that all catalogues will remain available and up to date so they can be downloaded into the national reporting system automatically. The formats of the catalogues must be stable and not be changed. Further, some kind of automatic information should be pushed forwarded to the Member States when catalogues are updated so we always know when to download new catalogues into our national system.

A document with a translation from the old XML system to the new SSD2 is important for comparability of data between MS and over time. We foresee that the reported data will be very difficult to interpretate once MS move on to using the FoodEx2. The challenge will be comparing data between MS as well as over time.

Until now, the final version of the picklist (catalogues) and information about the changes to the reporting system has always been provided shortly before the reporting period. Therefore there has always been limited time for implementation and validation at national level. For future reporting years, EFSA should consider a longer period for MS to implement the annual changes and to develop the updated national reporting system accordingly.

Right now the condition "mandatory" is added to some variable that are not mandatory for all types of data. This should be corrected in the reporting system as data providers do not have the time and resources to collate and validate date that are not mandatory.

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Abbreviations

AMR	Antimicrobial resistance
AOCS	American Oil Chemists' Society
BIOMO	EFSA biological monitoring unit
DCF	EFSA Data Collection Framework
DTU	Technical University of Denmark
DVFA	Danish Veterinary and Food Administration
EFSA	European Food Safety Authority
EFTA	European Free Trade Association
Excel	Microsoft® Excel 2010
FoodEx2	EFSA food classification and description system
LIMS	Laboratory information management system
MRL	Maximum residue limit
MS	EU member state
PAH	Polycyclic aromatic hydrocarbons
RDBMS	Relational database management system
SAS	SAS® Statistical Analysis Software
SSD	Standard Sample Description
SSD2	Standard Sample Description version 2
WG-SSD2	EFSA working group on SSD extension
XML	Extensible Markup Language
XSD	XML Schema Definition

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Appendix A – SSD Structure DTU table

Description of columns in table 1 and 2:

- Element Name: SSD2
- Element name/Attribute name: SSD2
- DTU: Actions
  - Constant: Value in column LIMS is inserted in SSD2 Element/Attribute
  - Direct: Value of LIMS element is inserted in SSD2 Element/Attribute
  - Table: Value of LIMS element is used as key for lookup in translation catalogue. Lookup value is inserted in SSD2 Element/Attribute
  - Join: Concatenated value of listed LIMS elements (separated by $) is inserted in SSD2 Element/Attribute
  - -: See note
  - (empty): Not included in SSD2 file (elements are not shown in table)
- LIMS: Name of element in LIMS file
- LIMS_cat: Reference to translation catalogue
- Cat_key: Name of column in LIMS_cat serving as key for lookup
- Cat_Lookup: Name of column in LIMS_cat serving as output for lookup

Table 1: SSD2 elements

Element Code	Element Name	DTU	LIMS	LIMS_cat	Cat_key	Cat_lookUp	Note
M.01	resId	Constant	(empty)				See note 1
A.01	localOrgId	Constant	Danish Veterinary and Food Administration (DVFA)				See note 2
A.02	localOrgCountry	Constant	DK				
B.01	progId	Direct	PROJEKT_NR				
B.02	progLegalRef	Table	PROJEKT_NR	REG.EFSAproj	PROJEKTNR	Lovgivning_kode	
B.03	sampStrategy	Table	PROJEKT_NR	REG.EFSAproj	PROJEKTNR	Udtagningsstrategi_kode	
B.04	progType	Table	PROJEKT_NR	REG.EFSAproj	PROJEKTNR	Projekttype_kode	
B.05	sampMethod	Table	PROJEKT_NR	REG.EFSAproj	PROJEKTNR	Prøveudtagningsmetode_kode	
B.06	sampler	Constant	CX02A				See note 3
B.07	sampPoint	Table	BRANCHEGRP_NIV_2_KONTROLOBJEKT	REG.L_SAMPNT	L_name	code	

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Element Code	Element Name	DTU	LIMS	LIMS_cat	Cat_key	Cat_lookUp	Note
C.05	sampUnitIds	Compound	(empty)				See note 4
D.01	sampId	Direct	PROEVE_ID_HOVEDPROEVE				
D.02	repCountry	Constant	DK				
D.03	sampCountry	Constant	DK				
D.05	repYear	Function	Year(DATO_UDTAGET)				
D.06	sampY	Function	Year(DATO_UDTAGET)				
D.07	sampM	Function	Month(DATO_UDTAGET)				
D.08	sampD	Function	Day(DATO_UDTAGET)				
E.01	sampMatType	Constant	(empty)				See note 5
E.02	sampMatCode	Table	PRODUKT_ID	REG.LIMSvare	Produkt_ID	FoodEx2_Code	See note 6
E.03	sampMatText	Table	PRODUKT_ID	REG.LIMSvare	Produkt_ID	UKvare	
E.04	origCountry	Table	OPRINDELSE_LAND_KODE_ATTRIBUT	REG.L_COUNTRY	u_fvstcountryid	COUNTRY_code	
E.07	origFishAreaText	Direct	FANGSTOMRAADE_ATTRIBUT				
E.10	sampMatInfo	Compound	(empty)				See note 4
F.01	sampAnId	Direct	PROEVE_ID				
F.03	analysisY	Function	Year(DATO_ANALYSE_AFSLUTTET)				
F.04	analysisM	Function	Month(DATO_ANALYSE_AFSLUTTET)				
F.05	analysisD	Function	Day(DATO_ANALYSE_AFSLUTTET)				
G.01	anMatCode	Compound	(empty)				See note 4
G.02	anMatText	Constant	(empty)				See note 7
H.01	anPortSeq	Direct	DATASAET				
J.01	labId	Direct	LABORATORIUM_ENHED_MED_NR				
J.02	labAccred	Constant	L001A				See note 8
J.03	labCountry	Constant	DK				See note 9
K.01	paramType	Constant					See note 10
K.02	paramCode	Table	PARAMETER_ID	REG.LIMSstof	limsName	code	
K.03	paramText	Table	PARAMETER_ID	REG.LIMSstof	limsName	UKstof	
L.01	anMethRefId	Direct	TESTMETODE_ID				
L.02	anMethRefCode	Table	TESTMETODE_ID	REG.LIMSmet	Testmetode_ID	AnlyRefMDcode	
L.03	anMethType	Table	TESTMETODE_ID	REG.LIMSmet	Testmetode_ID	AnlyTypCode	
L.04	anMethCode	Table	TESTMETODE_ID	REG.LIMSmet	Testmetode_ID	AnlyMDcode	
L.05	anMethText	Direct	PROEVNINGS_PRINCIP				

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Element Code	Element Name	DTU	LIMS	LIMS_cat	Cat_key	Cat_lookUp	Note
M.02	accredProc	Table	AKKREDITERING_PARAM_RESULTAT	REG.L_MDACC	L_name	termCode	
M.03	resUnit	Table	ANALYSERESULTAT_VISNING_ENHED	REG.L_UNIT	L_Name	code	
M.04	resLOD	Direct	LOD_VAERDI_TAL				
M.05	resLOQ	Direct	LOQ_VAERDI_TAL				See note 11
M.10	resVal	Direct	ANALYSERESULTAT_INDTASTET_TAL				
M.11	resValRec	Constant	.				See note 12
M.12	resValRecCorr	Constant	E				
M.13	exprResPerc	Compound	(empty)				See note 4
M.14	exprResType	Table	ANALYSERESULTAT_VISNING_ENHED	REG.L_EXPRRES	L_Name	code	
M.15	resQualValue	Table	ANALYSERESULTAT_VISNING_TEKST	REG.L_POSNEG	L_name	code	
M.16	resType	Constant					See note 13
M.17	resValUncert	Direct	USIKKERHED_EKSPANDERET				
M.20	resInfo	Constant	(compound)				
N.01	evalLowLimit	Constant					See note 14
N.03	evalLimitType	Constant	W002A				See note 14
N.04	evalCode	Constant					See note 15
N.05	actTakenCode	Constant					See note 16
N.06	evalInfo	Compound	(empty)				See note 4
X.001	lang	Constant	da				See note 17
X.004	Packaging	Table	EMBALLERING_ATTRIBBUT	REG.L_PRODPAC	L_name	code	See note 18
X.013	Projekt_Oplysning_1	Direct	PROJEKT_OPLYSNING_1_ATTRIBUT				See note 19
X.014	Projekt_Oplysning_2	Direct	PROJEKT_OPLYSNING_2_ATTRIBUT				See note 19
X.015	Projekt_Oplysning_3	Direct	PROJEKT_OPLYSNING_3_ATTRIBUT				See note 19
X.016	Projekt_Oplysning_4	Direct	PROJEKT_OPLYSNING_4_ATTRIBUT				See note 19
X.017	Projekt_Oplysning_5	Direct	PROJEKT_OPLYSNING_5_ATTRIBUT				See note 19
X.018	Projekt_Oplysning_6	Direct	PROJEKT_OPLYSNING_6_ATTRIBUT				See note 19
X.019	Projekt_Oplysning_7	Direct	PROJEKT_OPLYSNING_7_ATTRIBUT				See note 19
X.020	Produkt_ID	Direct	PRODUKT_ID				See note 20
X.021	FoodEx2vare_Name	Table	PRODUKT_ID	REG.LIMSvare	Produkt_ID	FoodEx2_Name	
X.022	UKvare	Table	PRODUKT_ID	REG.LIMSvare	Produkt_ID	UKvare	
X.023	UKvareOKO	Constant					
X.024	DKvare	Table	PRODUKT_ID	REG.LIMSvare	Produkt_ID	DKvare	

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Element Code	Element Name	DTU	LIMS	LIMS_cat	Cat_key	Cat_lookUp	Note
X.025	DKvareOKO	Constant					
X.026	Vgruppe	Table	PRODUKT_ID	REG.LIMSvare	Produkt_ID	Vgruppe	
X.027	prodCode	Table	PRODUKT_ID	REG.LIMSvare	Produkt_ID	prodCode	
X.028	prodTreat	Table	PRODUKT_ID	REG.LIMSvare	Produkt_ID	prodTreat	
X.029	Vtype	Table	PRODUKT_ID	REG.LIMSvare	Produkt_ID	Vtype	
X.030	MRLapplic	Table	PRODUKT_ID	REG.LIMSvare	Produkt_ID	MRLapplic	
X.036	prodCom_pliste	Table	PRODUKT_POSITIVLISTE_NR	REG.Pliste	Pliste	code	
X.037	sampMatCode_pliste	Table	PRODUKT_POSITIVLISTE_NR	REG.Pliste	Pliste	FoodEx2	
X.041	Saerlige_Ordninger_1	Direct	SAERLIGE_ORDNINGER_1_ATTRIBUT				See note 21
X.042	Saerlige_Ordninger_2	Direct	SAERLIGE_ORDNINGER_2_ATTRIBUT				See note 21
X.043	OKO	Table	SAERLIGE_ORDNINGER_1_ATTRIBUT	REG.L_PRODMD	L_name	OKO	See note 21
X.044	OKO2	Table	SAERLIGE_ORDNINGER_2_ATTRIBUT	REG.L_PRODMD	L_name	OKO	See note 21
X.045	F21_prod	Table	SAERLIGE_ORDNINGER_1_ATTRIBUT	REG.L_PRODMD	L_name	foodexCode	See note 21
X.046	F21_prod2	Table	SAERLIGE_ORDNINGER_2_ATTRIBUT	REG.L_PRODMD	L_name	foodexCode	See note 21
X.049	FoodEx1	Table	PRODUKT_ID	REG.LIMSvare	Produkt_ID	FoodEx	
X.050	PROEVE_NIVEAU	Direct	PROEVE_NIVEAU				See note 22
X.056	DATO_UDTAGET	Direct	DATO_UDTAGET				
X.058	FE2delprv	Function	FE2delprv				See note 7
X.059	FE2delprv_navn	Function	FE2delprv_navn				See note 7
X.060	UKdelprv	Function	UKdelprv				See note 7
X.061	DKdelprv	Function	DKdelprv				See note 7
X.062	FE2_AA	Function	FE2_AA				See note 23
X.063	FE2_AA_name	Function	FE2_AA_name				See note 23
X.064	sampMatCode_packmat_name	Table	EMBALLERING_ATTRIBBUT	REG.L_PRODPAC	L_name	F19PackMat_Name	
X.065	DKland	Table	OPRINDELSE_LAND_KODE_ATTRIBUT	REG.L_COUNTRY	u_fvstcountryid	fvstcountrydesc	
X.066	UKland	Table	OPRINDELSE_LAND_KODE_ATTRIBUT	REG.L_COUNTRY	u_fvstcountryid	COUNTRY_name	
X.067	Eustatus	Table	OPRINDELSE_LAND_KODE_ATTRIBUT	REG.L_COUNTRY	u_fvstcountryid	EUstatus	
X.070	DATO_PRODUKTION_ATTRIBUT	Direct	DATO_PRODUKTION_ATTRIBUT				
X.071	DATO_HOLDBARHED_ATTRIBUT	Direct	DATO_HOLDBARHED_ATTRIBUT				
X.072	DATO_ANALYSE	Direct	DATO_ANALYSE_AFSLUTTET				
X.073	Parameter_ID	Direct	PARAMETER_ID				
X.074	DKstof	Table	PARAMETER_ID	REG.LIMSstof	limsName	Dkstof	

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Element Code	Element Name	DTU	LIMS	LIMS_cat	Cat_key	Cat_lookUp	Note
X.081	GENFINDINGS_PROCENT	Direct	GENFINDINGS_PROCENT				
X.088	evalCode1	Table	VURD_KODE_PAA_PARAMETER_KODE_1	REG.L_RESEVAL	L_name	Code	See note 15
X.089	evalCode2	Table	VURD_KODE_PAA_PARAMETER_KODE_2	REG.L_RESEVAL	L_name	Code	See note 15
X.090	evalCode3	Table	VURD_KODE_PAA_PARAMETER_KODE_3	REG.L_RESEVAL	L_name	Code	See note 15
X.097	INDGREBSVAERDI_VAERDI_TEKST	Direct	INDGREBSVAERDI_VAERDI_TEKST				See note 14
X.098	ML_VAERDI_TEKST	Direct	ML_VAERDI_TEKST				See note 14
X.099	MRL_VAERDI_TAL	Direct	MRL_VAERDI_TAL				See note 14
X.100	MRPL_VAERDI_TEKST	Direct	MRPL_VAERDI_TEKST				See note 14
X.101	AKTIONSVAERDI_VAERDI_TEKST	Direct	AKTIONSVAERDI_VAERDI_TEKST				See note 14
X.114	Dato_Oracle	Direct	INDS_DATO				See note 24

Note 1: Synthesized from sampId, sampAnId, paramCode. To be expanded with sampEventId and anPortSeq if relevant.
Note 2: Earlier transmissions used "DK_DTU_08"
Note 3: Only official samling ("CX02A") is foreseen
Note 4: Placeholder for compound element
Note 5: Placeholder for sample matrix type
Note 6: Codes for F21 (Production-method) and F19 (Packaging-material) added in code in special cases.
Note 7: Placeholder for subsample information
Note 8: Only results from laboratories with an accreditation are foreseen by the Food Authority
Note 9: Presently only results from Danish laboratories are relevant
Note 10: paramType assigned in code in combination with tables (Matrix Table A, Matrix Table C)
Note 11: Pesticides: LOQ for summed RDs handled in method/substance catalogues
Note 12: Not implemented
Note 13: resType is assigned in code, based on anMethType, resVal, resLOD, resLOQ
Note 14: Limit values as reported in five different elements in the LIMS file. The correct type is selected in translation program.
Note 15: evalCode is assigned in code, based on evalCode1, evalCode2, evalCode3
Note 16: actTakenCode is joined in code, based on Excel sheet with resID and actTakenCode from Competent Authority
Note 17: For parallel coding in SSD1
Note 18: Coding of packMat facet
Note 19: Ad hoc coding of program specific information
Note 20: Elements for FE2 facet production method
Note 21: Coding of subsamples
Note 22: Placeholder for acrylamide codes
Note 23: Date and time for transfer from DVFA to DTU

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Table 2: Elements for compound fields

Element Code	Element name	Attribute name	DTU	LIMS	LIMS_cat	Cat_key	Cat_lookUp	Notes
C.05	sampUnitIds	animalId	Direct	CHR_NR_ATTRIBUT				Note 1
C.05	sampUnitIds	herdId	Direct	FLOK_ID_ATTRIBUT				Note 1
C.05	sampUnitIds	batchId						Note 1
C.05	sampUnitIds	sampHoldingId	Direct	BESAETNINGS_ID_ATTRIBUT				Note 1
C.05	sampUnitIds	slaughterHouseId						Note 1
C.05	sampUnitIds	sampPlantId						Note 1
E.02	sampMatCode	packformat	Constant					Note 2
E.02	sampMatCode	packmat	Table	EMBALLERING_ATTRIBBUT	REG.L_PRODPAC	L_name	F19PackMat	Note 2
E.02	sampMatCode	prod	Constant					Note 3
E.02	sampMatCode	foodAdditiveLegislativeClass	Table		REG.LIMSpliste	LIMS	Code	
E.10	sampMatInfo	brandName	Direct	HANDELSNAVN				
E.10	sampMatInfo	manuf	Direct	NAVN_KONTROLOBJEKT				Note 4
E.10	sampMatInfo	com	Direct	SUPPLERENDE_PROEVEBESKRIVELSE				Note 4
E.10	sampMatInfo	prodY	Function	Year(DATO_PRODUKTION_ATTRIBUT)				
E.10	sampMatInfo	prodM	Function	Month(DATO_PRODUKTION_ATTRIBUT)				
E.10	sampMatInfo	prodD	Function	Day(DATO_PRODUKTION_ATTRIBUT)				
E.10	sampMatInfo	expiryY	Function	Year(DATO_HOLDBARHED_ATTRIBUT)				
E.10	sampMatInfo	expiryM	Function	Month(DATO_HOLDBARHED_ATTRIBUT)				
E.10	sampMatInfo	expiryD	Function	Day(DATO_HOLDBARHED_ATTRIBUT)				
M.13	exprResPerc	fatPerc	Function	fatPerc				Note 5
M.13	exprResPerc	moistPerc	Function	moistPerc				Note 6
M.13	exprResPerc	alcoholPerc	Constant					Note 7
M.20	resInfo	com	Direct	VURD_PR_PARAM_PAA_ANALYSEATT				Note 8
N.06	evalInfo	sampAnAsses						Note 9
N.06	evalInfo	sampTkAsses	Constant					Note 10
N.06	evalInfo	sampEventAsses						Note 9
N.06	evalInfo	com	Constant					Note 8

Note 1 Partly available; not yet implemented. Relevant for veterinary drug residues only

Note 2 FE2 attributes can be ad hoc coded using information for special project from LIMS element EMBALLERING_ATTRIBBUT

Note 3 Coded based on extra elements X.041 - X.046

Note 4 The Food Authority considers this information as classified. Information will not be transmitted.

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Element Code	Element name	Attribute name	DTU	LIMS	LIMS_cat	Cat_key	Cat_lookUp	Notes
Note 5	Implementation will rely on specific analysis of fat in sample or value from food composition table as was the case for SSD1 implementation.							
Note 6	Implementation will rely on specific analysis of dry matter in sample or value from food composition table							
Note 7	Implementation will rely on specific analysis of alcohol in sample or value from food composition table							
Note 8	Reported on ad hoc basis							
Note 9	Not yet implemented							
Note 10	Calculated based on resType, resVal, evalLowLimit							

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