German Federal Institute for Risk Assessment

Proposed updates in the residues section

– OHT 85-5 and its endpoint summary

– OHT 85-9 and its endpoint summary

19.06.2023, Italy, Parma

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Development of structured data formats within IUCLID environment

EFSA-BfR collaboration (Framework Partnership Agreement)

Scope of the collaboration:

- Update of OHT 85-5 and EP summary on **Magnitude of Residues (MoR) in plants**
- Update of OHT 85-9 and EP summary on **MoR in processed commodities**
- Define migration rules where possible
- Update of backlog file
- Update of picklists

➔ **IN VIEW OF the IUCLID release of 2024**

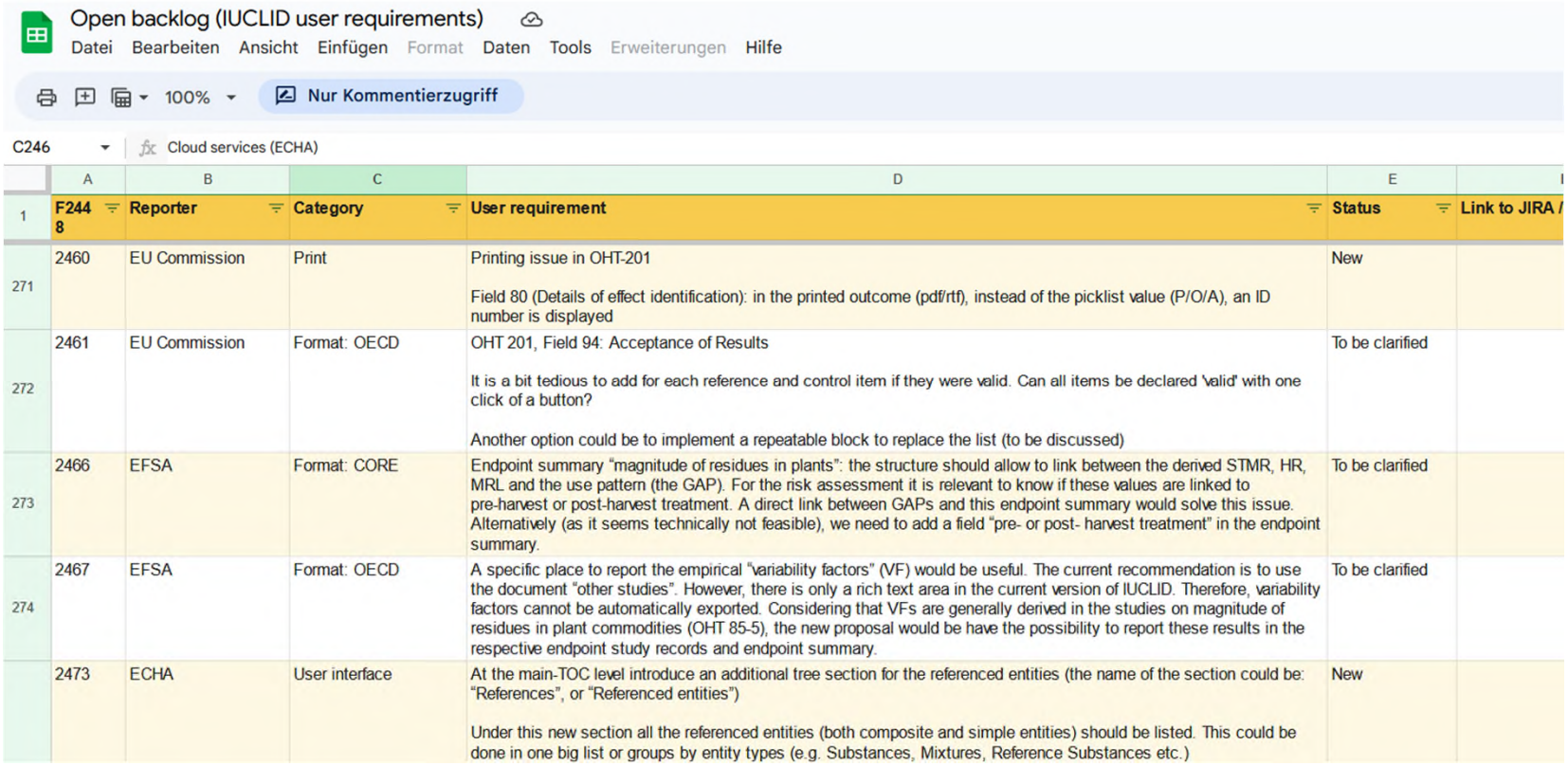
Backlog entries to be addressed, then proposals for structural change (Discussion)

Why an update of OHT 85-5 and OHT 85-9 is needed?

- **OHT 85-5 and OHT 85-9 are not often used by applicants:**
  - **Several negative feedback received from different user experiences** (reflected in the open backlog file)
    - Too complex formats
    - Impossible to fill-out manually
  - **Applicants still use the recommended xlsx-files** to report structured results on residue trials
    (but attachement files is not a sustainable solution in IUCLID)

Which updates are needed? it starts from the “open Backlog”

https://docs.google.com/spreadsheets/d/1kFkttA6rXtR2K6LlaauHozq9BSfv6a5EgFDM1GgtmfQ/edit#gid=0



Open backlog (IUCLID user requirements)

Datei Bearbeiten Ansicht Einfügen Format Daten Tools Erweiterungen Hilfe

100% Nur Kommentierzugriff

C246 Cloud services (ECHA)

	A	B	C	D	E	I
1	F2448	Reporter	Category	User requirement	Status	Link to JIRA /
271	2460	EU Commission	Print	Printing issue in OHT-201 Field 80 (Details of effect identification): in the printed outcome (pdf/rtf), instead of the picklist value (P/O/A), an ID number is displayed	New	
272	2461	EU Commission	Format: OECD	OHT 201, Field 94: Acceptance of Results It is a bit tedious to add for each reference and control item if they were valid. Can all items be declared 'valid' with one click of a button? Another option could be to implement a repeatable block to replace the list (to be discussed)	To be clarified	
273	2466	EFSA	Format: CORE	Endpoint summary “magnitude of residues in plants”: the structure should allow to link between the derived STMR, HR, MRL and the use pattern (the GAP). For the risk assessment it is relevant to know if these values are linked to pre-harvest or post-harvest treatment. A direct link between GAPs and this endpoint summary would solve this issue. Alternatively (as it seems technically not feasible), we need to add a field “pre- or post- harvest treatment” in the endpoint summary.	To be clarified	
274	2467	EFSA	Format: OECD	A specific place to report the empirical “variability factors” (VF) would be useful. The current recommendation is to use the document “other studies”. However, there is only a rich text area in the current version of IUCLID. Therefore, variability factors cannot be automatically exported. Considering that VFs are generally derived in the studies on magnitude of residues in plant commodities (OHT 85-5), the new proposal would be have the possibility to report these results in the respective endpoint study records and endpoint summary.	To be clarified	
	2473	ECHA	User interface	At the main-TOC level introduce an additional tree section for the referenced entities (the name of the section could be: “References”, or “Referenced entities”) Under this new section all the referenced entities (both composite and simple entities) should be listed. This could be done in one big list or groups by entity types (e.g. Substances, Mixtures, Reference Substances etc.)	New	

The open backlog file was screened:

- **8 relevant backlog items identifed within scope of OHT-85-5/9 revision**
- **Stratification/formatting issues:**
  - Reduce duplication of entries
  - Improve picklists (less free text fields)
  - Harmonise field names and structure
- **Data structure and user-friendliness:**
  - Reduce the use of nested blocks → Possible use of CSV upload
  - Simplified entry with more data granularity

Backlog update (I) “Additions”

#2487 (EFSA, Format: OECD): Add identifier for “Key results”

- A check box for key results has been implemented in several IUCLID formats (e.g. in mammalian tox section) but this concept is difficult to apply in the residue section, because key residue values are always identified in specific context (GAP, residue definitions…) → no changes proposed so far **(slido question 1)**

#2467 (EFSA, Format: OECD): Possibility to report Variability Factors (VF)

- Variability studies and VF derivation will not be implemented in OHT 85-5 (not OECD guided) but moved to default template OHT 85-7 (“other studies”) **(slido question 2a)**
- Variability Factors will be added to Endpoint Summary on Magnitude of Residues in plant commodities **(slido question 2b)**

Backlog update (II) “Streamline picklists and OHT-structure”

#2079 (EFSA, Format: OECD): Streamline picklists, less nested blocks, validation rules

- Picklists: alignment between different documents and existing databases, mapping
- Nested blocks: mitigate by csv upload (with long tables) to enter data into IUCLID
- Validation rules: mandatory fields (to be defined later)

#1786 (Finland, Format: OECD): Field names unclear, streamline structure

- Remove irrelevant fields, e.g. aspirated grain fractions, storage stability factor
- Residues in RAC/Processed to be amended by picklist or CSV Upload - not modified yet

#2073 (EFSA, Format: OECD): Streamline field name, stratify picklist

- Change of field name "Bulk raw agricultural commodity“ into “Commodity (RAC)“, picklist update (according to 396/2005)

Backlog update (III) “Linking of entries”

#2067 (EFSA, format: EU_PPP): Add linked picklist for processing based on commodity

- Development and use of hierarchical picklists for processed commodities

#2089 (EFSA, Format: OECD): Streamline material and methods section

- Deletion of fields not relevant for residue/processing trials , e. g. product type
- Crop group (line 74) to be in line with 396/2005
- Link with “method of analysis” to be harmonized with other OHTs, also considering the specificities of residues trials studies and possible need for further validation data

#2466 (EFSA, Format: CORE): Link GAP and STMR, HR, MRL

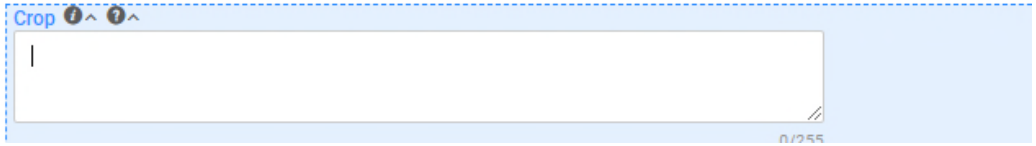
- Endpoint Summary: a direct link between GAP under assessment and the endpoints (STMR, HR, MRL) is relevant but is not technically possible → a field will be added to specify the type of use which is tested in the trials: “trial concept” (List values (multiple choice, one checkbox per treatment): seed treatment, pre-emergence, post-emergence, harvest, post-harvest, other)
- Endpoint Study record: Link with the GAP under assessment is not relevant but the field “trial concept” will also be added in the Study record

Picklist Updates

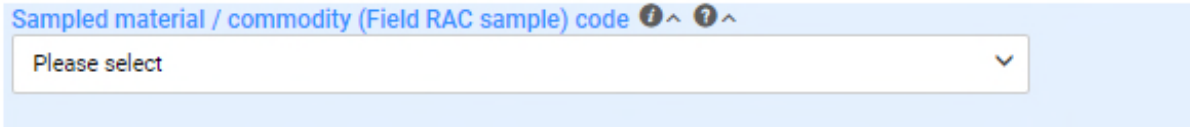
Picklist update in OHT 85-5:

In OHT 85-5, the following picklists shall be amended/created

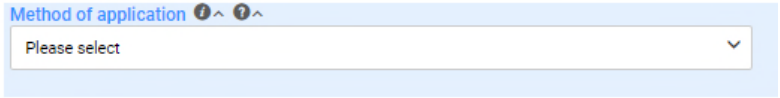
- “crop”: from free text to picklist aligned with the GAP table (using EPPO codes)



- “Samples material/ commodity (field RAC sample)”: from FAO Codex System to commodity list of “Annex I of Reg. (EU) 396/2005”



- “Trial concept” (new field to specify the type of use which is tested in the trials; NB: this is not covered by the method of application):



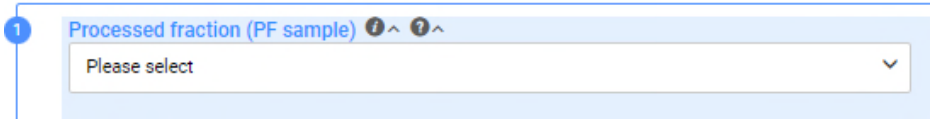
proposed picklist: seed treatment, pre-emergence, post-emergence, harvest, post-harvest, other

Picklist update in OHT 85-9

In OHT 85-9 fields with picklists shall be amended to support hierarchical picklist functions:

It is proposed modify the following picklists: **(slido question 3)**

- Processed fraction (PF sample): using **FoodEx2 codes/description** (picklist based on Processing Factor Database database, not from PRIMo 4)
- Sample processing

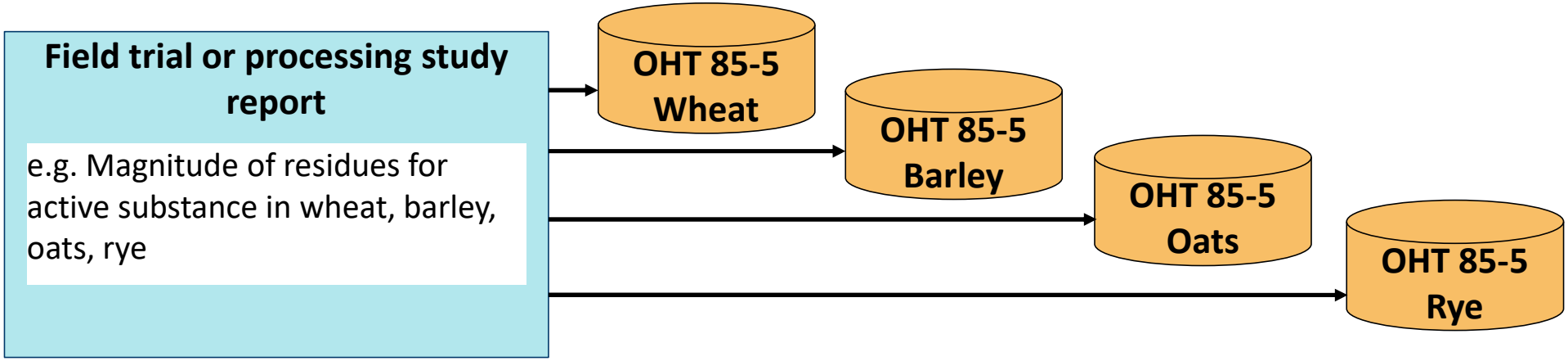


It is proposed to add the following picklists (from OHT 85-5):

- Country or territory
- State/Province
- Method of application
- Bulk raw agricultural commodity: FAO Codex System → Annex I of Reg. (EU) 396/2005
- Formulation type

Structure of OHT 85-5/85-9 and relationship with other OHTs (87 and 85-10)

Practical level of data granularity in OHT 85-5/9?



- More granular data → Easier data management and re-use
- One study report can lead to more than one Study Record
- Proposal for OHT 85-5: **1 Endpoint study record per crop** **(slido question 4)**

→ use the clone function to duplicate the common sections OHTs (trials site, methods...)

→ No nested blocks, less repeatable blocks

→ csv-upload-format can be supported by flat table format (long)

→ Pay attention to migration rules

A 85-5 (Commodities) is (should be?) the basis for a 85-9 (Processed commodities) (the samples require storage, 85-10 and analysis, 87)

Commodity (85-5)

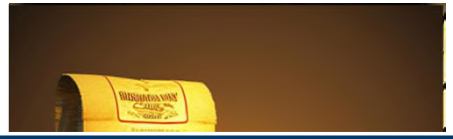
Processing

Processed commodity (85-9)

Storage stability (85-10)

Analysis (87)

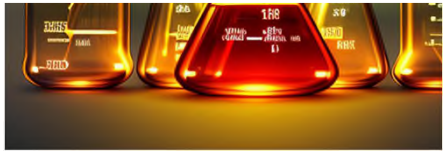
A 85-5 (Commodities) is (should be?) the basis for a 85-9 (Processed commodities) (the samples require storage, 85-10 and analysis, 87)



All are connected,
how should this be addressed in the future?

nodity (85-9)

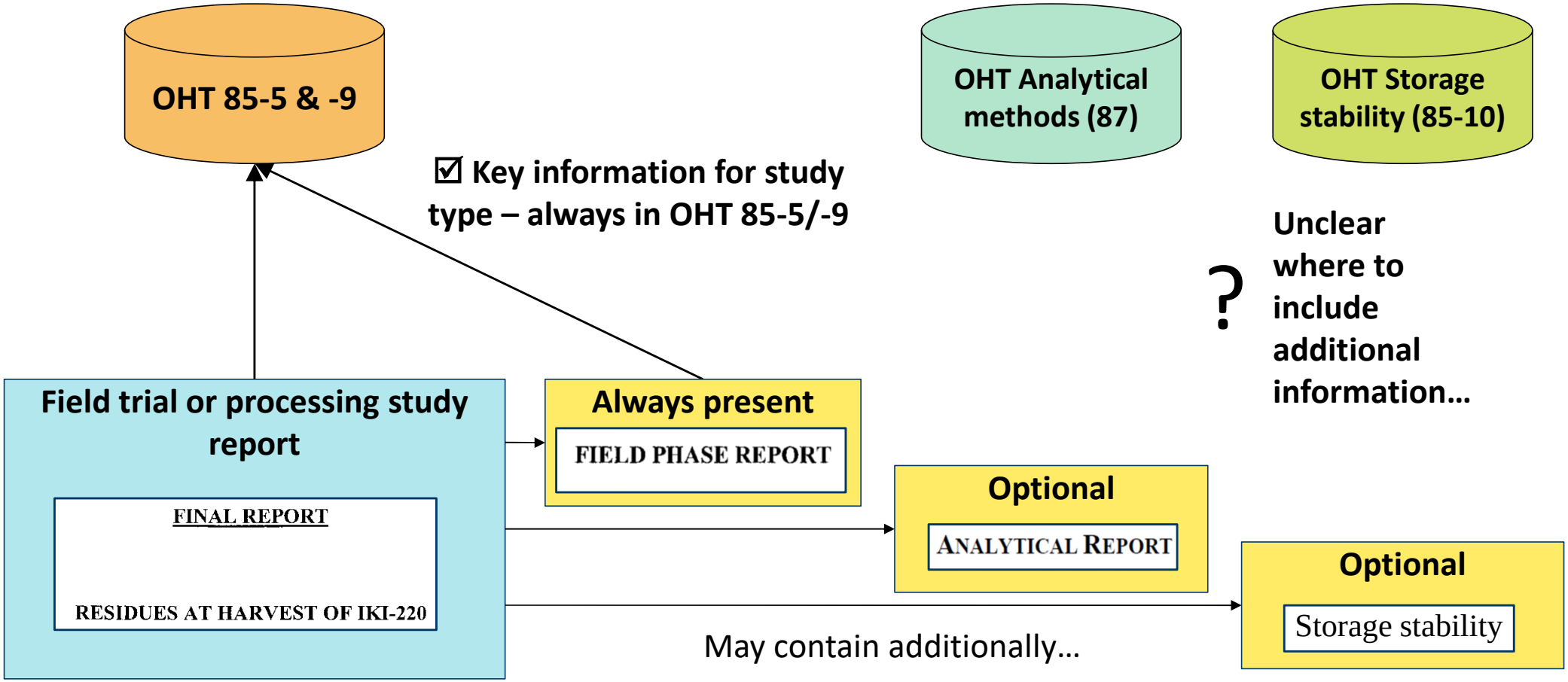
Storage stability (85-10)



Analysis (87)

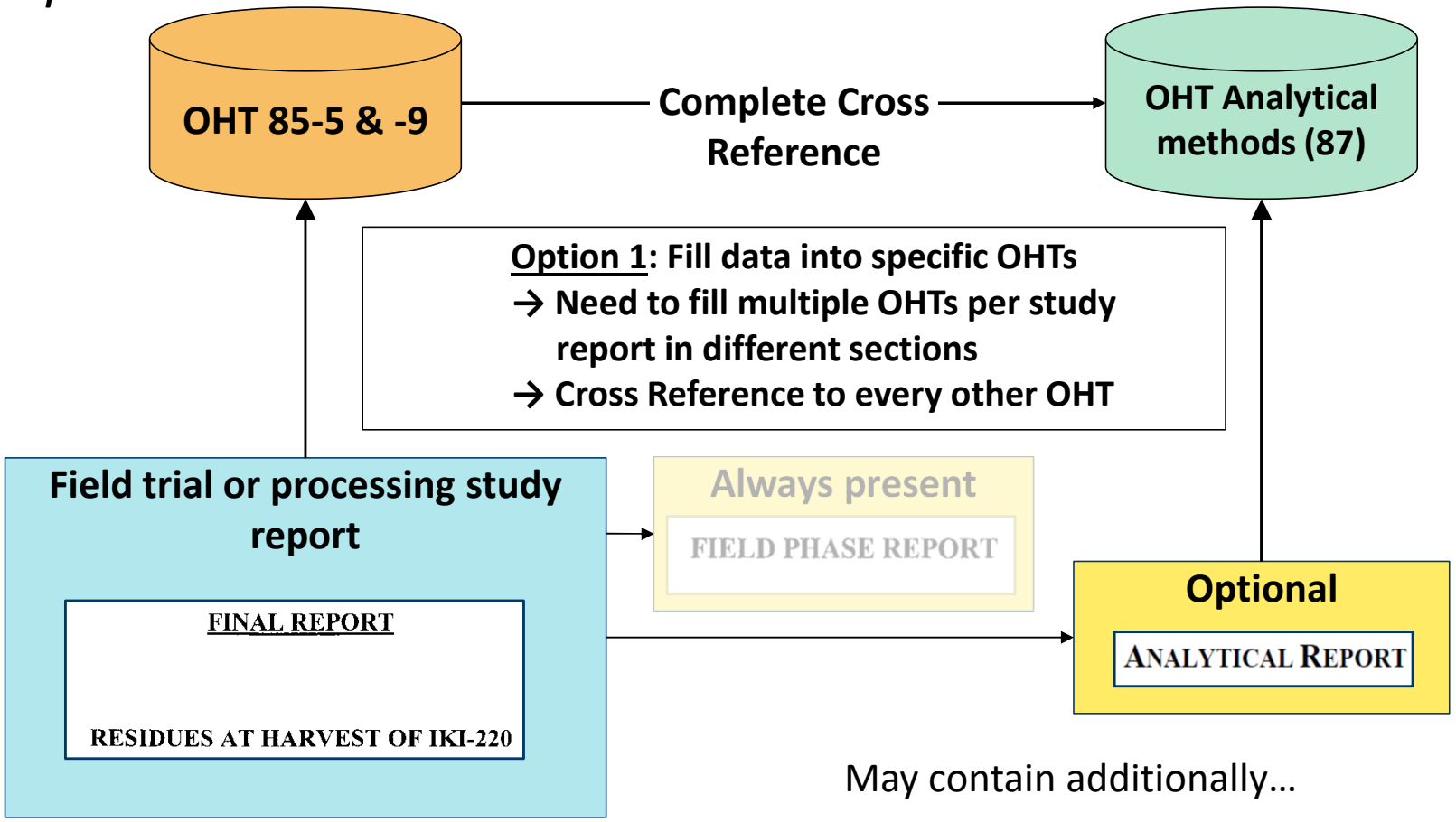
OHT 85-5 & 85-9 – Organisation of meta data related to other endpoints

General Structure



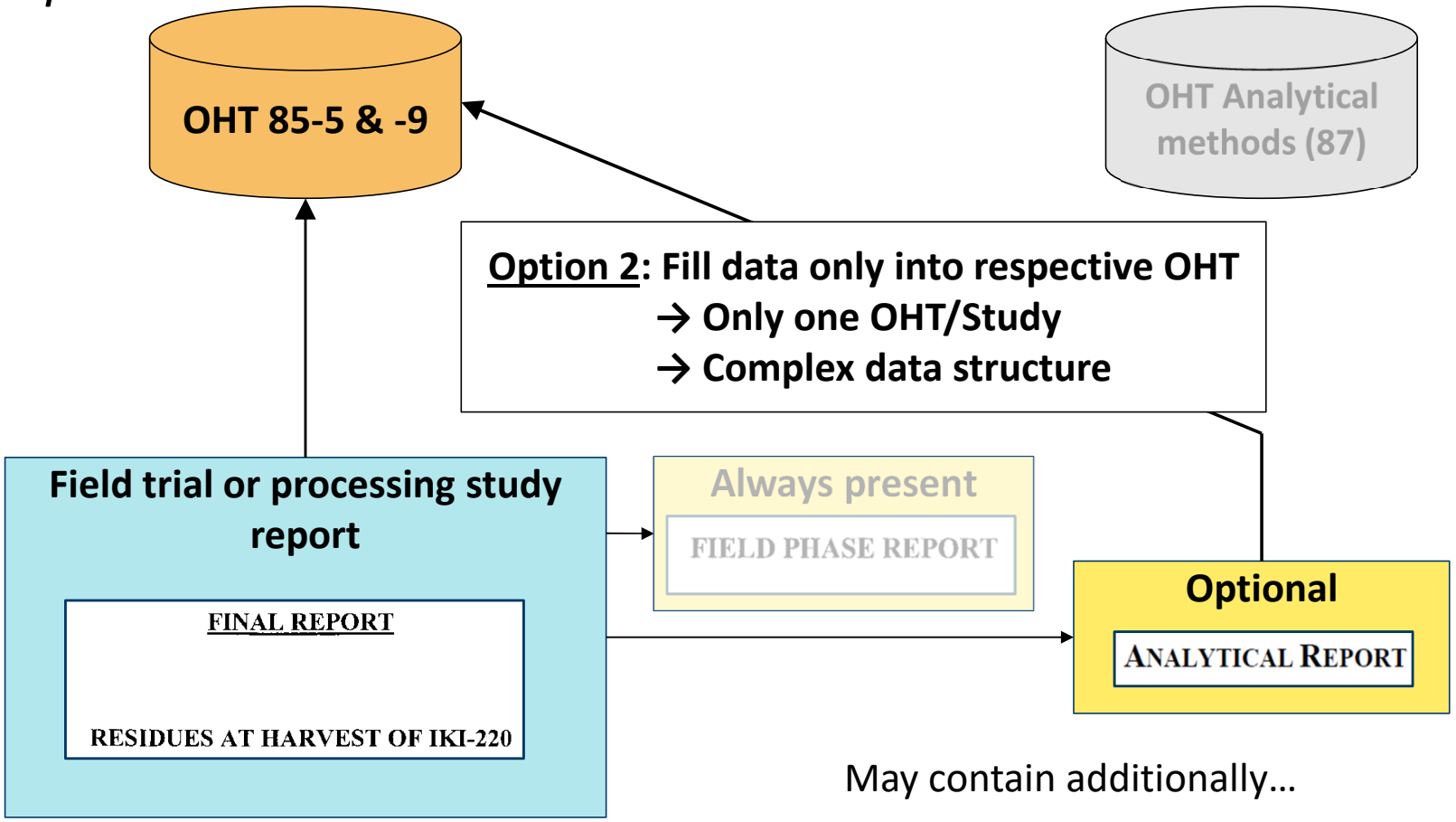
OHT 85-5 & 85-9 – Organisation of meta data related to other endpoints

Option 1



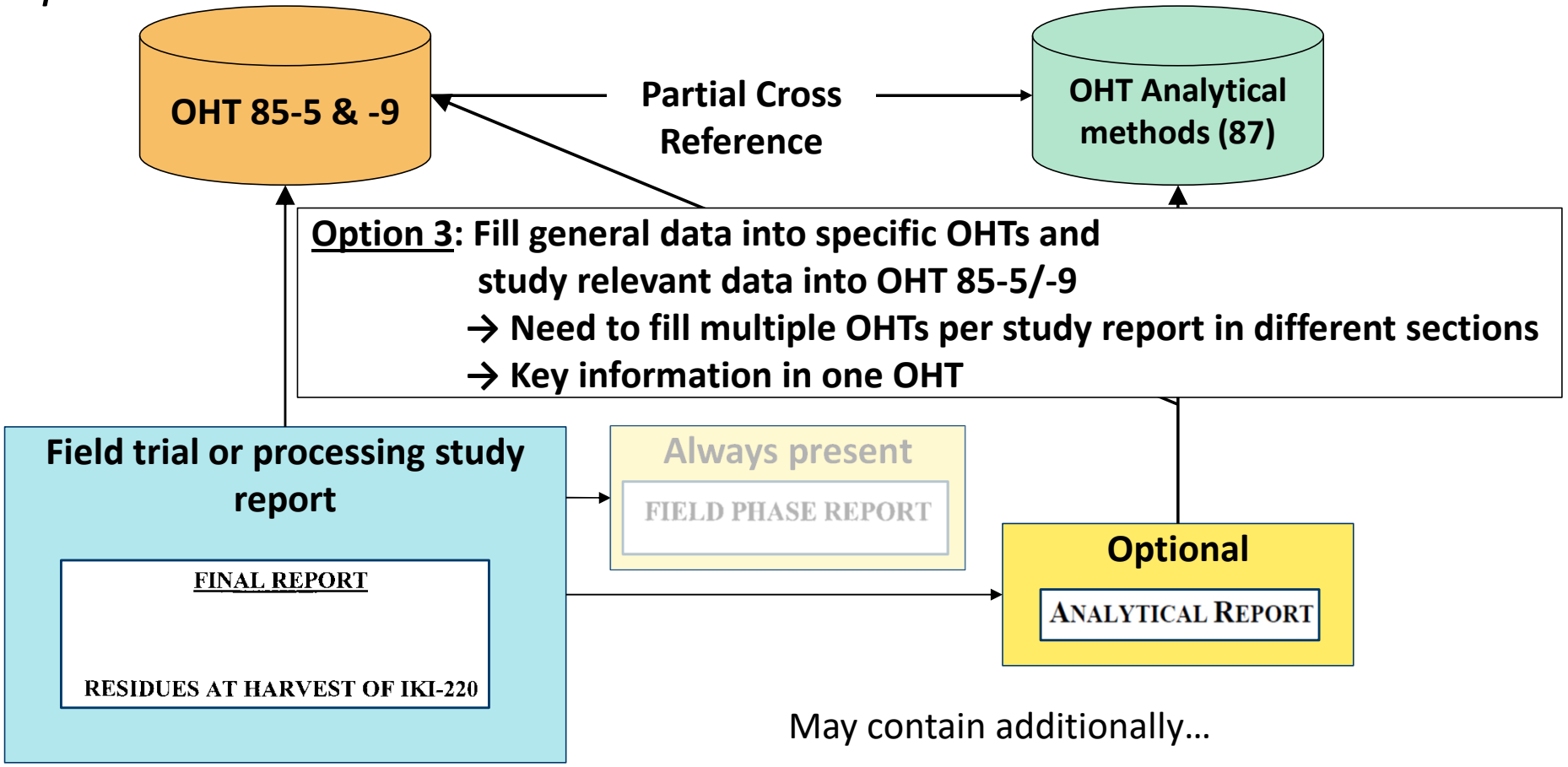
OHT 85-5 & 85-9 – Organisation of meta data related to other endpoints

Option 2



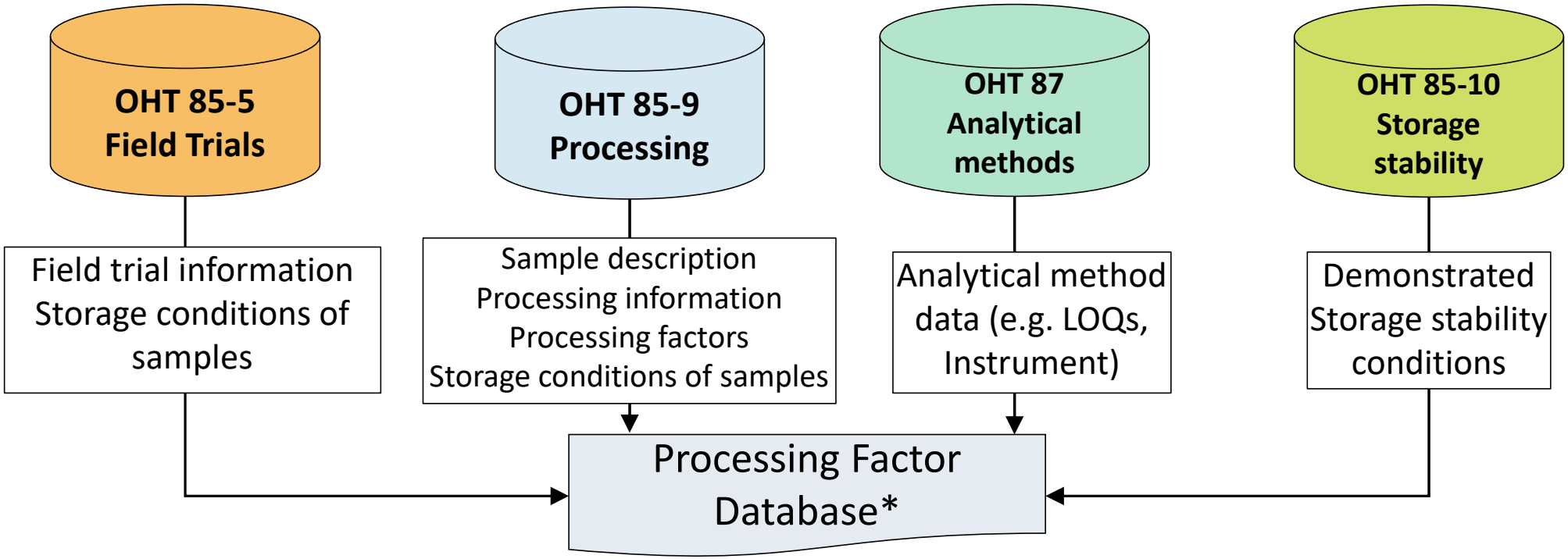
OHT 85-5 & 85-9 – Organisation of meta data related to other endpoints

Option 3



OHT 85-9 – Compatibility with EFSA/BfR Processing Factor Database

For compatibility of OHT 85-9 with the Processing Factor Database, specific meta-data are required, which are organised in different sections/OHTs:



*https://zenodo.org/record/6827098

Which option would you prefer?

1) **Fill data into specific OHTs**
   → Need to fill multiple OHTs per study report in different sections
   → Cross Reference many fields to each other OHT

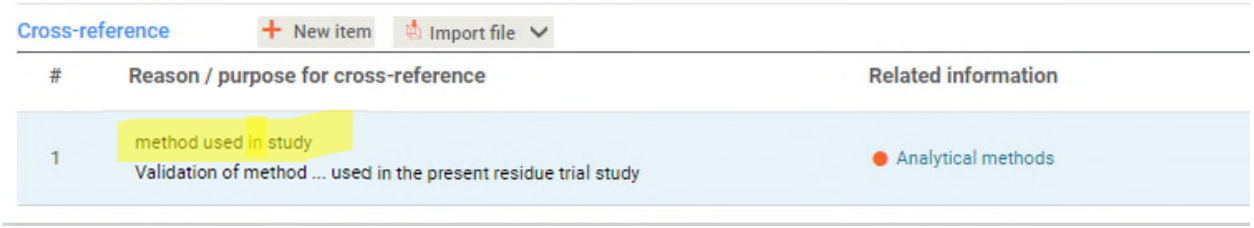
2) **Fill data only into respective OHT**
   → Only one OHT/Study
   → Complex data structure

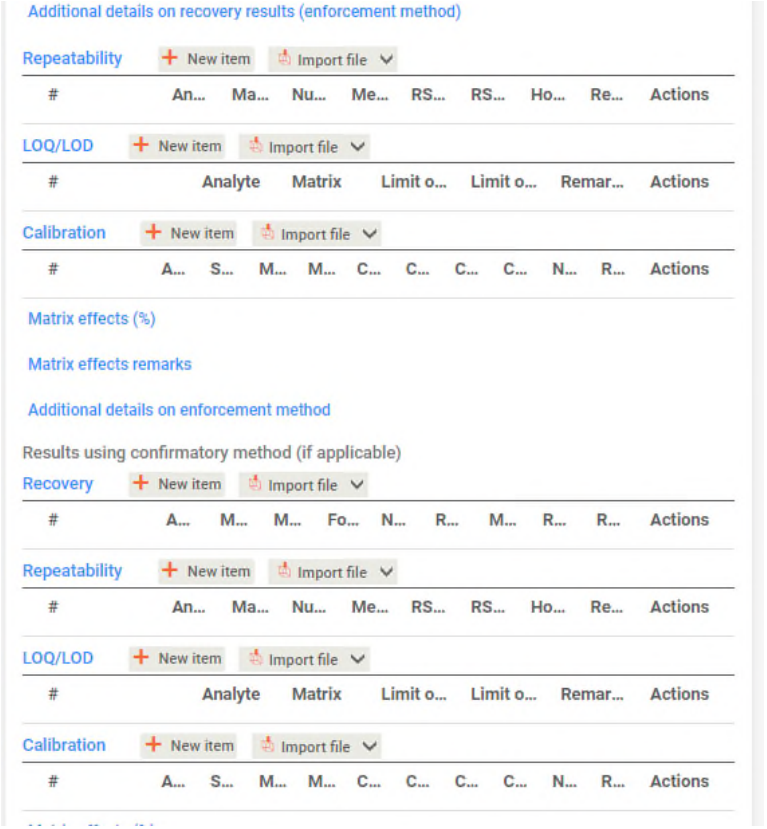
3) **Fill general data into specific OHTs and study relevant data into OHT 85-5/-9**
   → Need to fill multiple OHTs per study report in different sections
   → Key information in one OHT

Analytical method/Validation data

Concept: Everything that can be covered in OHT 87 (**extraction, calibration, measurement, LOQ…**) is kept in OHT 87

Using of the “cross-reference” feature to link with 85-5:





Additional information on method validation in the Specific trials might still be needed?

→ e.g. **Matrix, spike in (fortification level), recovery with the specific lab equipement?**

- To be added in 85-5/-9?
- What is the approach followed in OHTs of other sections?
- **slido question 5**

Thank you for your attention

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“Open Backlog”:
https://docs.google.com/spreadsheets/d/1kFkttA6rXtR2K6LlaauHozq9BSfv6a5EgFDM1GgtmfQ/edit#gid=0

slido questions:

N°	Question
1	Should we implement the “key results” boxes in OHT 85-5 and OHT 85-9?
2	a) Variability studies can be reported in default template OHT 85-7 (“other studies”) (not in OHT 85-5)? b) Variability Factors can be added to Endpoint Summary on Magnitude of Residues in plant commodities?
3	Implement FoodEx2 codes in the picklist used for the field “Processed fraction (PF sample)”?
4	Create 1 Endpoint study record per crop: OHT 85-5 should be designed for 1 crop (but possibly >1 commodity)?
5	How to report information on trials method validation? Option 1: All information can be reported in OHT 87 (with use of cross reference) Option 2: Additional fields need to be created in OHT 85 because OHT 87 cannot capture all information