

Industry Stress Test of IUCLID

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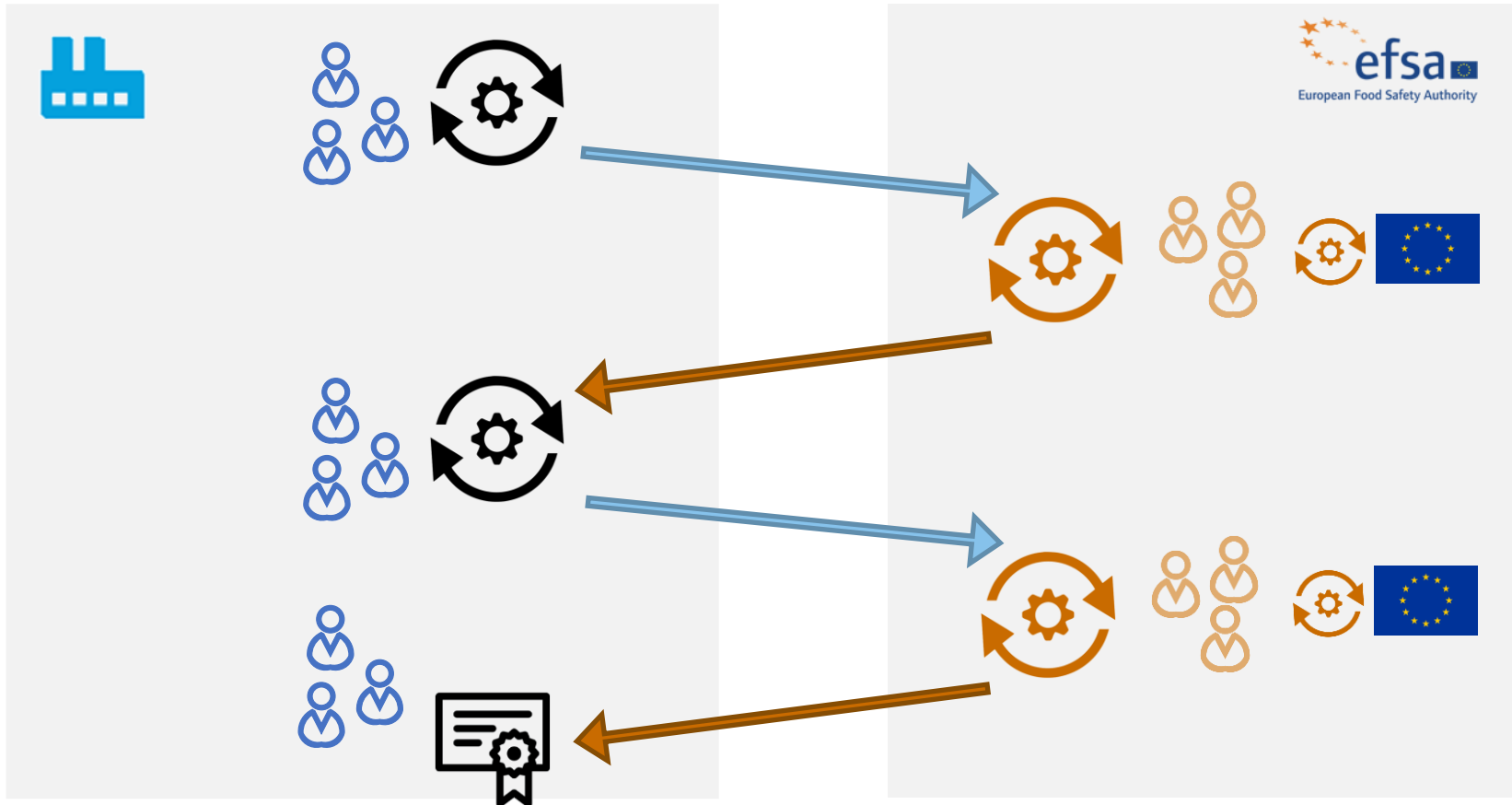
Agenda

- **IUCLID in PPP industry context**
- **Relevant integration use cases for industry**
- **Results of testing the integration use cases**
- **Performance of attachment handling**



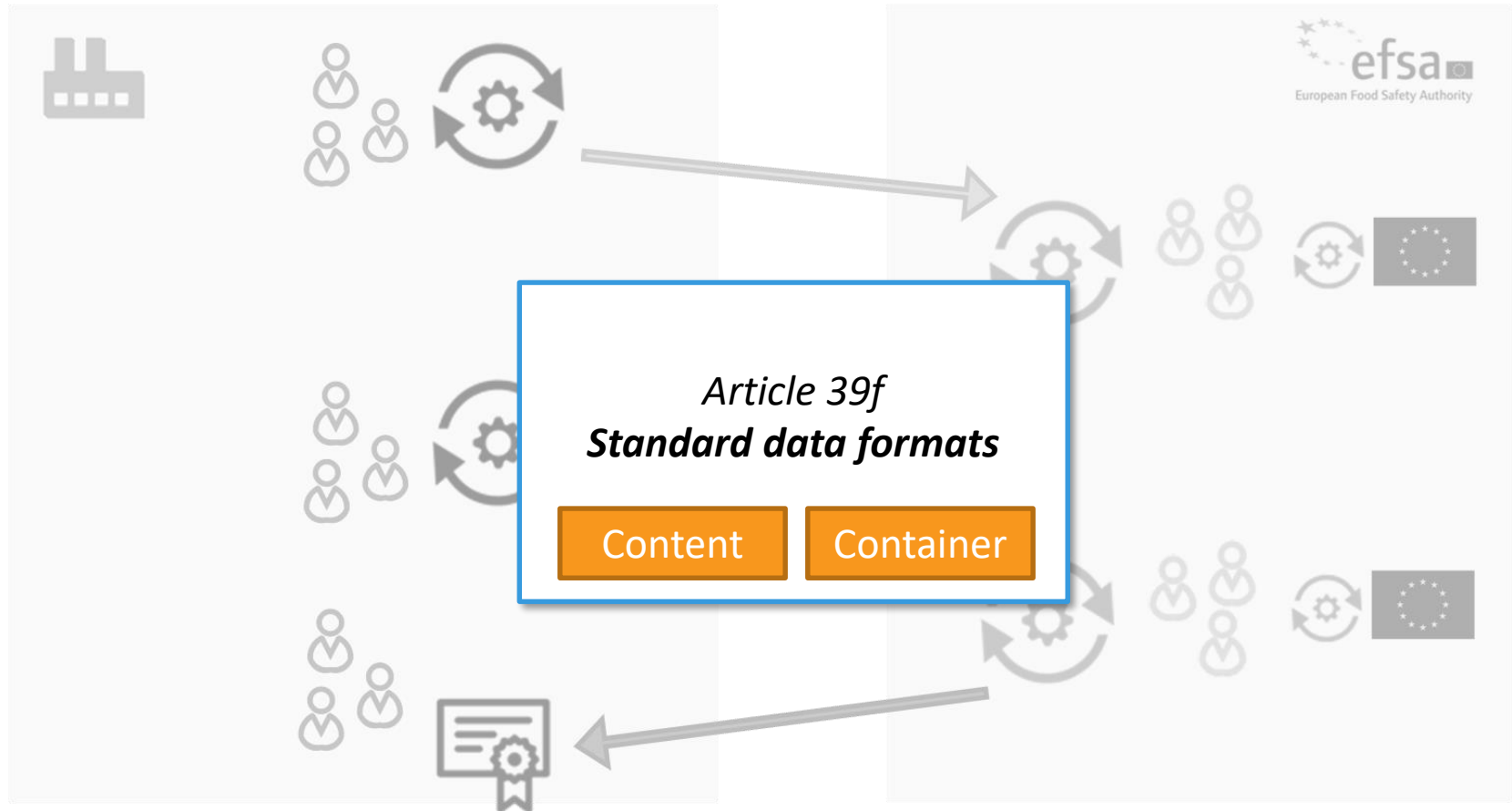
IUCLID in the PPP industry context

Simplified regulatory action



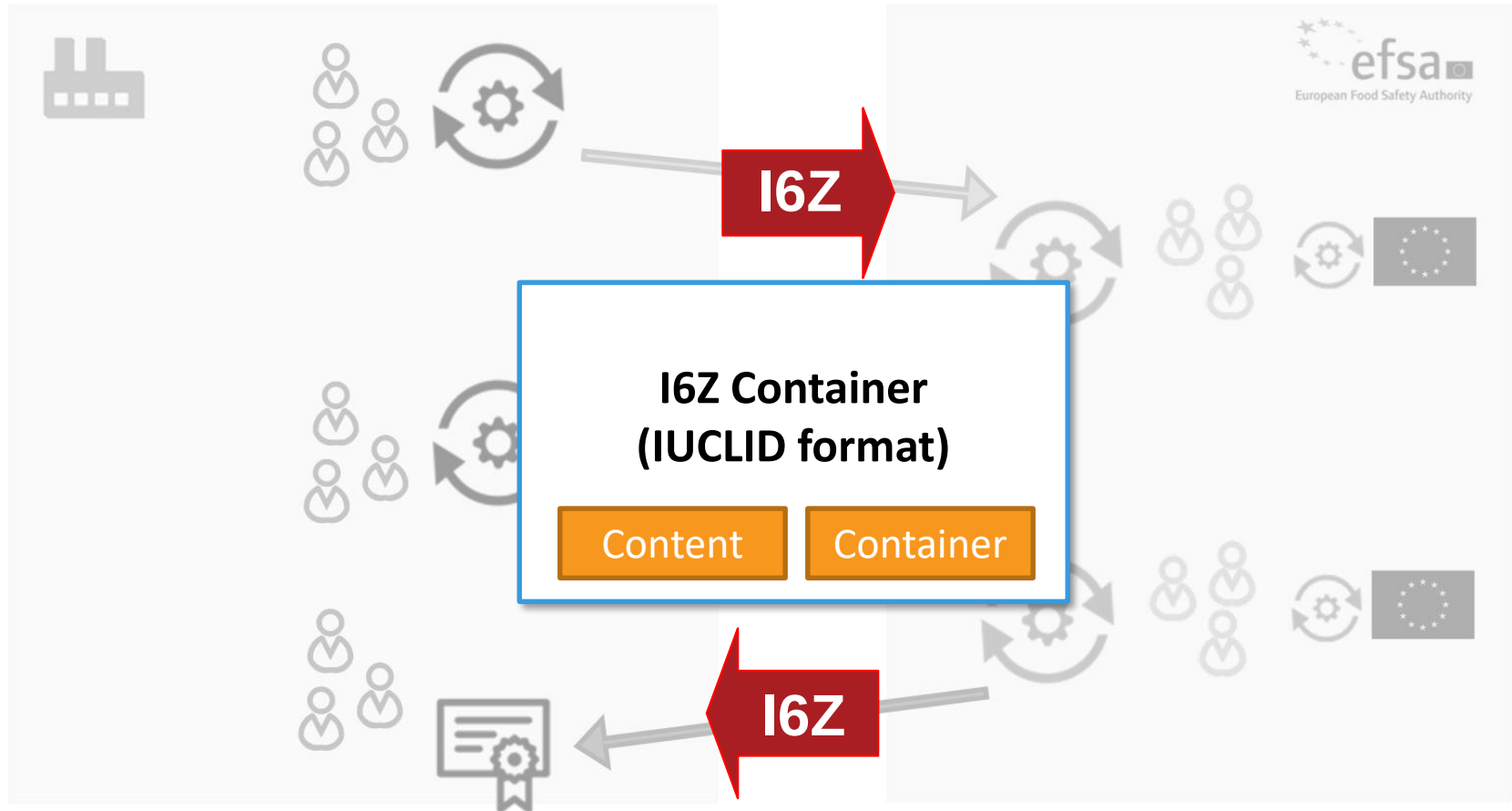
IUCLID in the PPP industry context

Simplified regulatory action

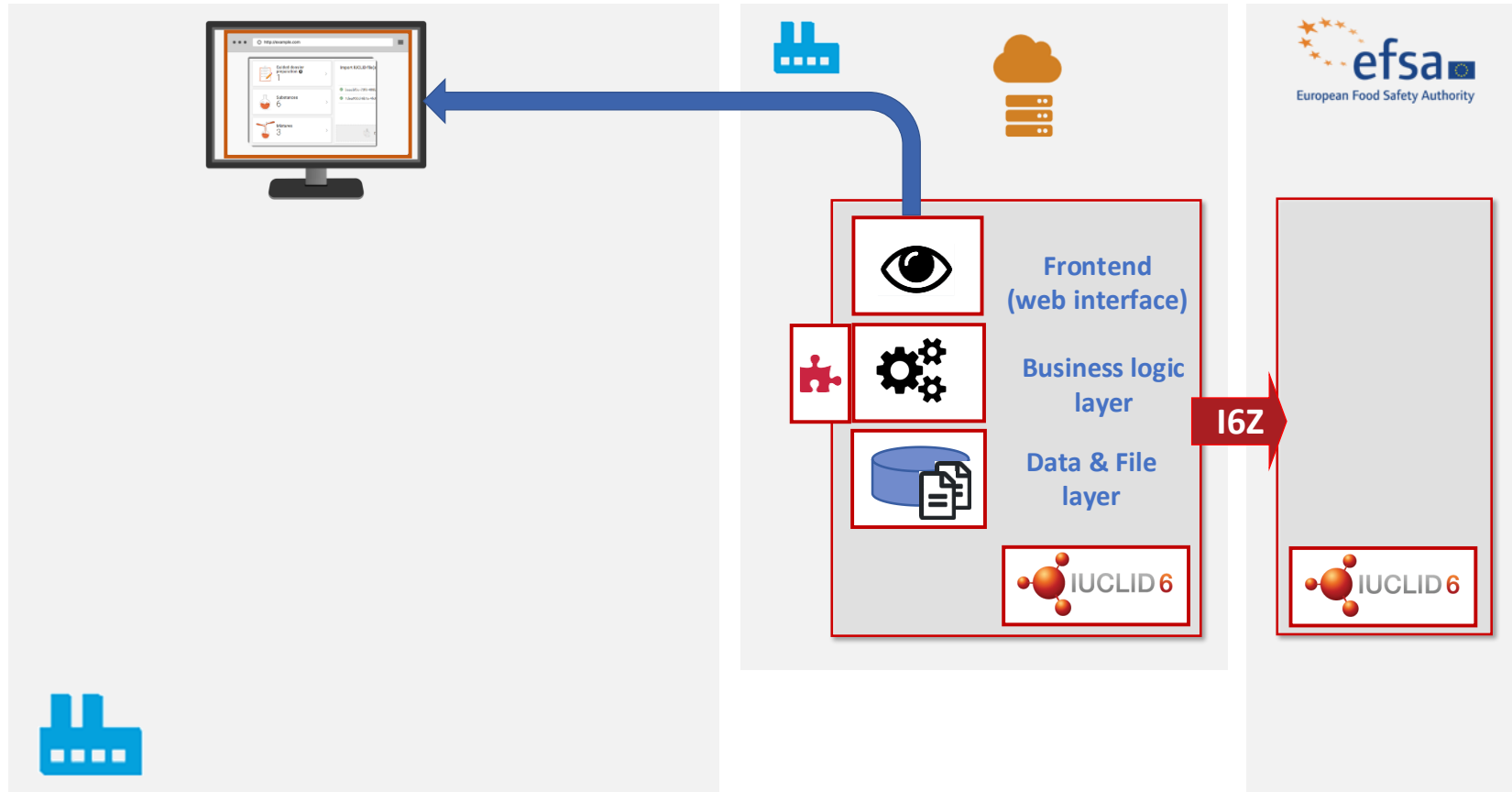


IUCLID in the PPP industry context

Simplified regulatory action

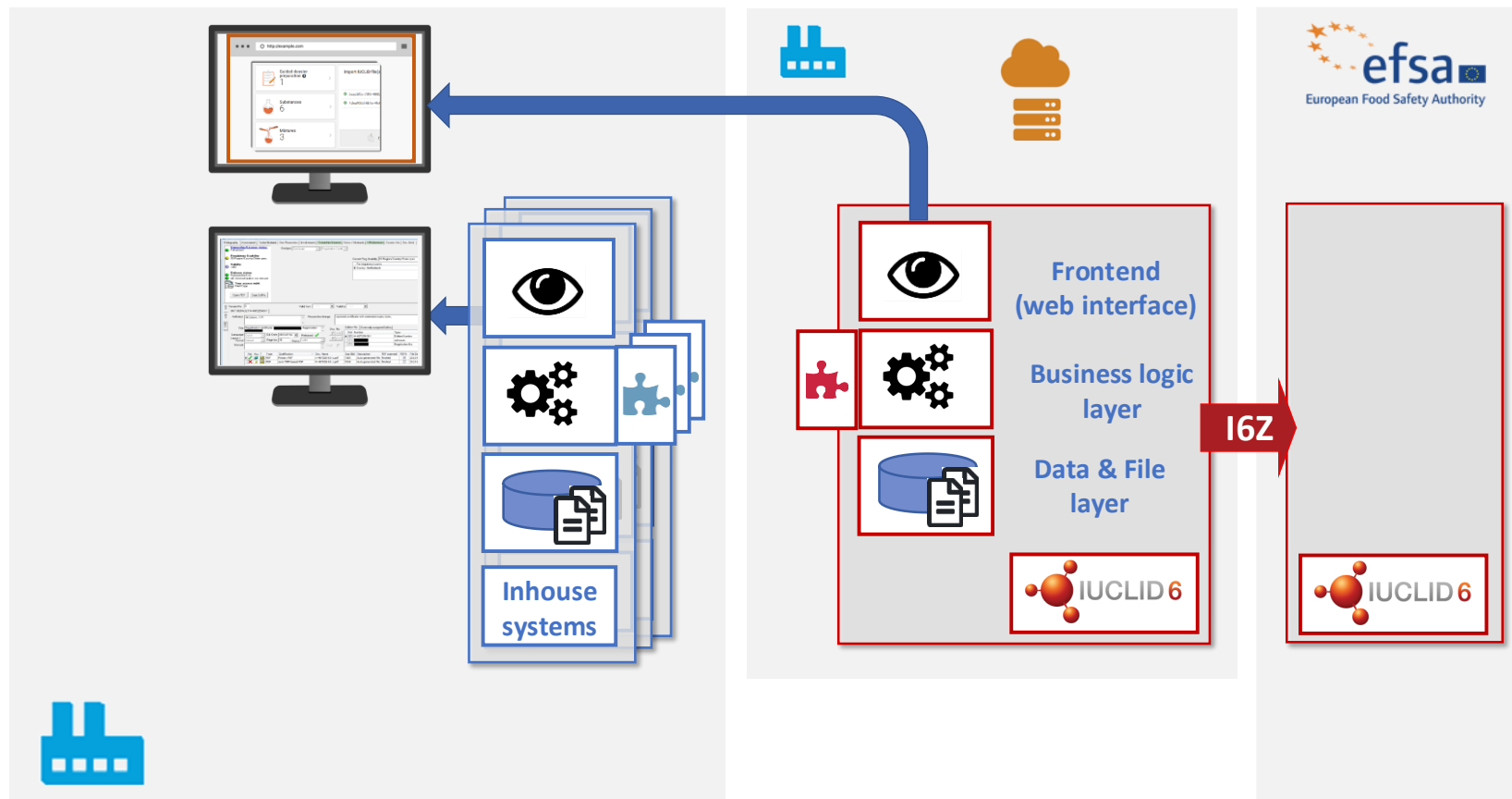


IUCLID in the PPP industry context



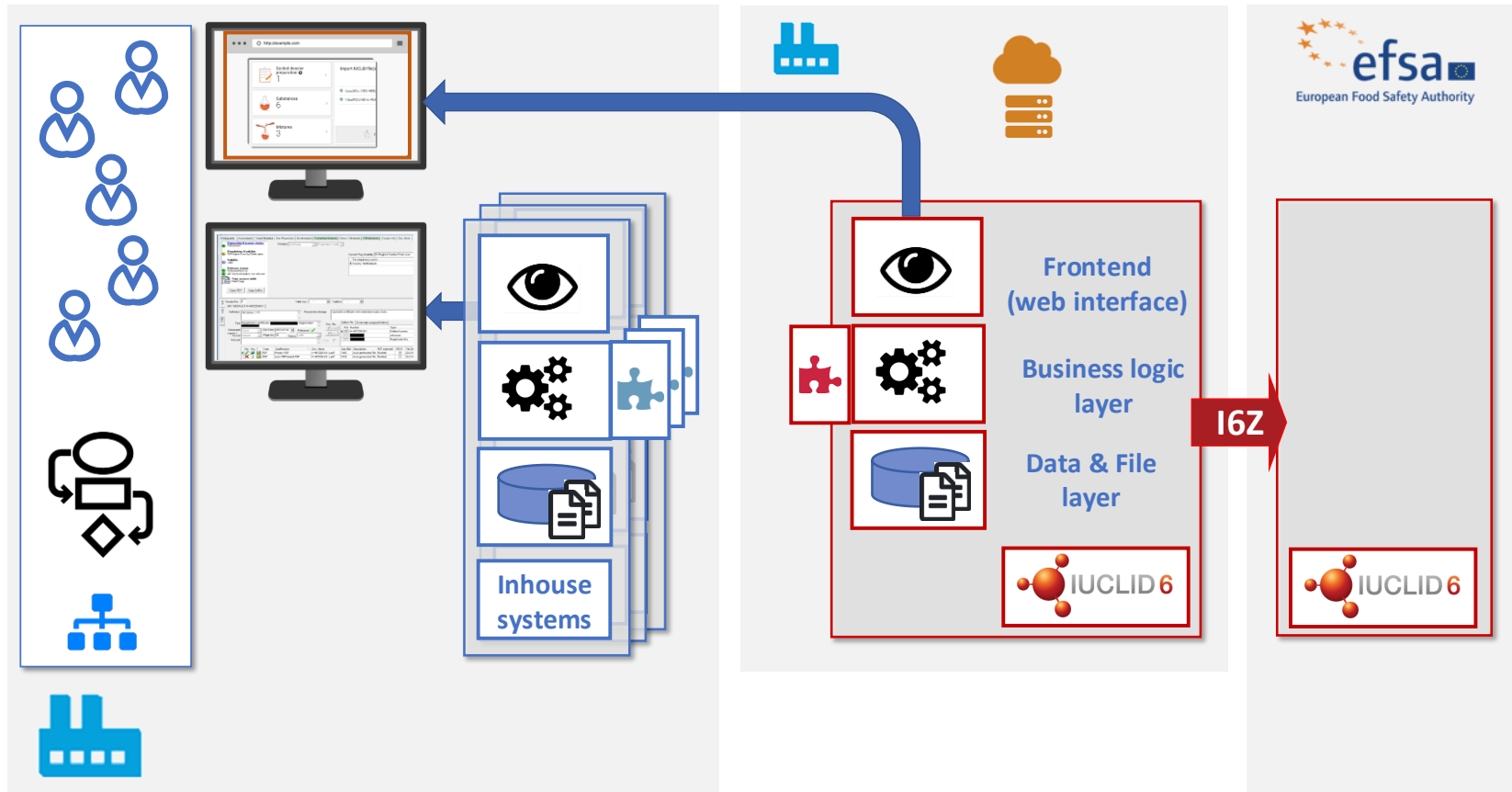
IUCLID in the PPP industry context

Inhouse systems



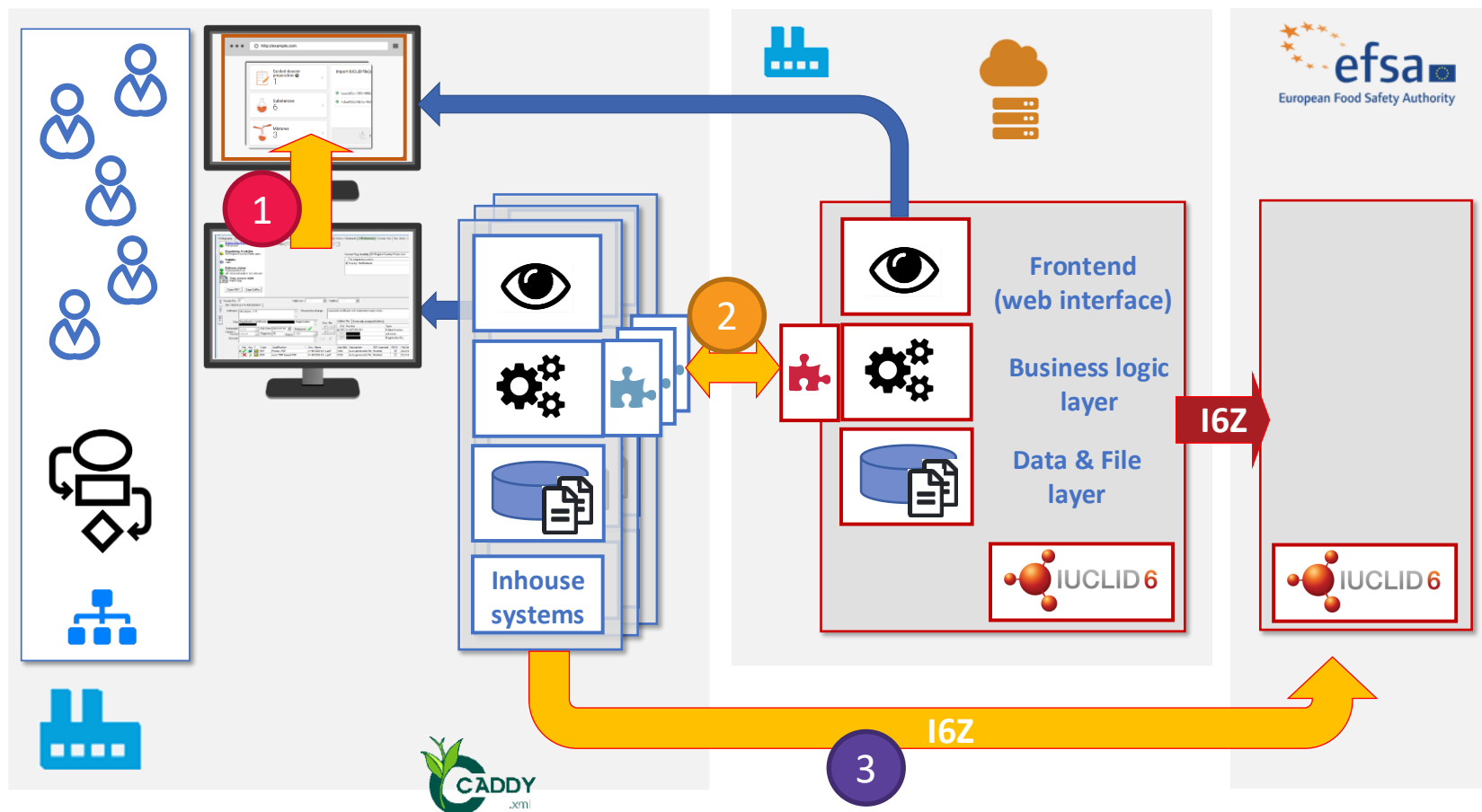
IUCLID in the PPP industry context

Inhouse systems & organizations



IUCLID in the PPP industry context

Required integration options



IUCLID in the PPP industry context

Integration possibilities

1 Manual / no integration

- Usability
- Functionality
- Robustness / stress test



2 API integration

- Feature completeness
- Robustness / stress test



3 Direct generation of IUCLID 6 data format

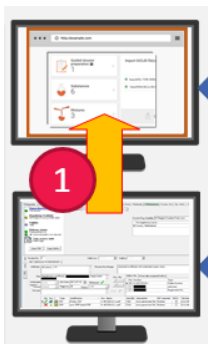
- Specification / availability of supporting information



IUCLID in the PPP industry context

1 Manual / no integration

- Rich-text control
 - Target: Retain formatting of content from existing sources to the extent possible (copy / paste)



PPP Spare, W.C. (2001) (summary)

Information

8

33

8

22

67

56

52

28

14

Please refer to "Any other information on results incl. tables"

[Results with reference substance](#)

None

Any other information on results incl. tables

Edit Format Table

B *I* U ~~S~~ $\times^2$ $\times_2$ $\equiv$ $\equiv$ $\equiv$ $\equiv$ $\equiv$

Paragraph A A $\equiv$ $\equiv$ $\equiv$ $\equiv$ $\equiv$

The obtained half-lives and DT90 values are shown in the tables below.

Table 7.2.1.1-2: Preliminary test: Distribution of radioactivity in different buffers at 50°C (values as % of applied)

Sampling	Percent of Analysis	Analytical	System
P			

IUCLID in the PPP industry context

1 Rich-text control

- **Pasting information**

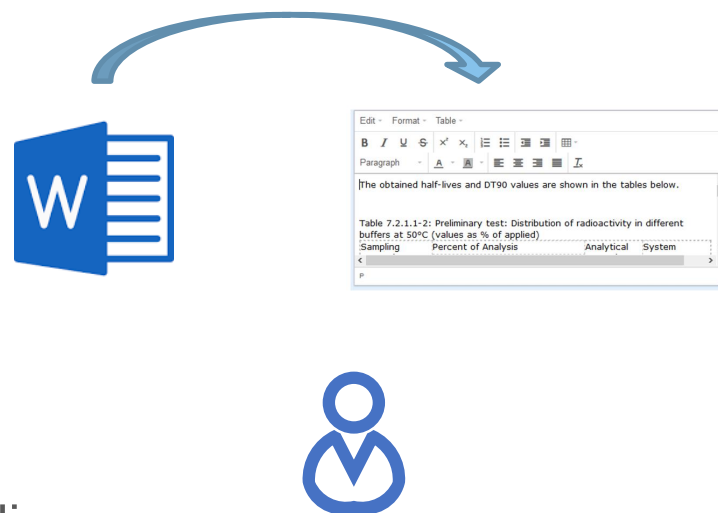
- **Format loss**

- Bulleted lists, Tabs
 - Font color / font highlighting
 - Images
 - Table borders / table cell shading

- **Functional loss**

- Fields (Headings, cross-references)
 - Hyperlinks

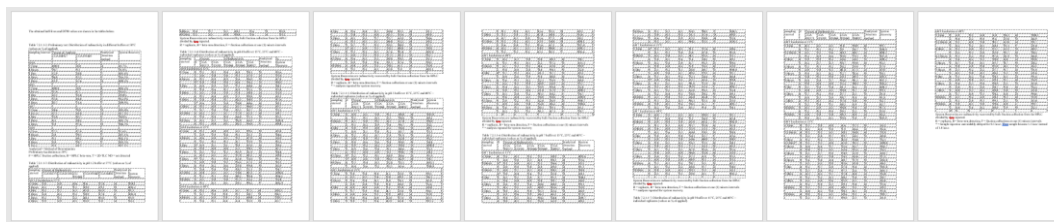
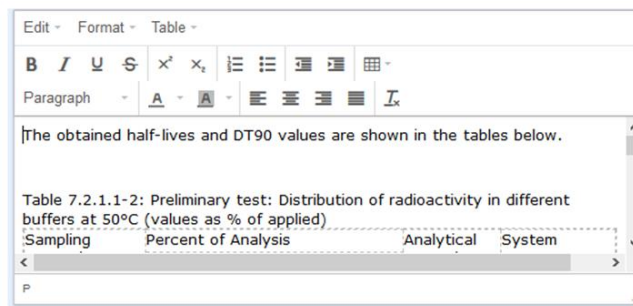
- **Note: Source application will impact pasting result**



IUCLID in the PPP industry context

1 Rich-text control

- Usability
 - Display of control too small for larger content
 - Control not fully and permanently resizableable
 - No navigation aids for large content
 - Scrollbar „jumps“ in web browser
 - See e.g. „7.2.1.1 Spare, W.C. (2001) (summary)”



IUCLID in the PPP industry context

1 Rich-text control

- Display / Rendering

- Web interface

- Cropping of tables
- Differences in formatting between edit mode and display mode

- PDF version

- illegible table content

Mean recovery (%)1	
Mean recovery (%)2	0.21038094744
Standard error (mg/ kg) matrix)	0.00000000000000007
	0.00000000000000007
Mean recovery (mg/ kg)	0.00000000000000007
Mean recovery (%)1	0.21038094744
Mean recovery (%)2	0.21038094744

IUCLID in the PPP industry context

1 Rich-text control

- **Suggested improvements**
 - Define structured content elements (e.g. tables) to decrease size of rich-text content
 - For remaining unstructured content: Retain formatting during copy / paste as far as possible
 - Improve usability
 - Improve rendering in web interface and PDF
 - Differentiate between editing mode and evaluation mode in the web interface

IUCLID in the PPP industry context

1 Tabular data (residue data) in Word

RESIDUE DATA SUMMARY FROM SUPERVISED TRIALS (SUMMARY)															
Active substance (common name)								Commercial Product (name)			-				
Crop/crop group:				Barley (Cereals)				Producer of commercial product							
Responsible body for reporting (name, address)								Indoor/Glasshouse/Outdoor			outdoor				
Country				Germany				Other active substance in the formulation							
Content of active substance (g/kg or g/L)				150 g/L				(common name and content)							
Formulation (e.g. WP)				EC (code)				Residues calculated as:							
1	2	3	4	5	6	7	8	9	10	11					
Report-No. Location (trial no.)	Commodity/ Variety	1. 2. 3.	Date of Sowing / planting Flowering Harvest	Method of treatment	Application rate per treatment			No of treat- ment(s) and last date	Growth stage at last treat. or date BBCH	Portion analysed	Residues as parent equivalents (mg/kg)			DALA (days)	Remarks
					kg a.s./hL	Water L/ha	kg a.s./ha						Total²		
419891 2013/1282605 Germany (L120228)	GC 0640/ Propino	1	03.03.2012	foliar	0.06*	200	0.113*	2	69	whole plant³	4.6	0.13	4.8	0	
		2	05.06- 18.06.2012	application	0.11**		0.225**	15.06.2012		ears	0.11	0.060	0.17	27	Method No
										rest of plant³	1.4	0.29	1.7	27	
		3	23.07.2012							grain	0.040	0.020	0.060	34	
										straw	1.9	0.46	2.3	34	LOQ
										grain	0.043	0.023	0.066	41	0.01 mg/kg
									straw	1.7	0.50	2.2	41		
419891 2013/1282605 France (N) (L120229)	GC 0640/ Cervoise	1	17.10.2012	foliar	0.06*	200	0.113*	2	69	whole plant³	3.6	0.16	3.7	0	
		2	25.05.- 31.05.2012	application	0.11**		0.225**	31.05.2012		ears	0.78	0.36	1.1	28	Method No
										rest of plant³	1.4	0.33	1.7	28	
		3	10.07.- 18.07.2012							grain	0.25	0.089	0.34	36	(535/1)
										straw	1.2	0.30	1.5	36	LOQ
										grain	0.22	0.072	0.29	47	0.01 mg/kg
									straw	1.4	0.39	1.7	47		
419891 2013/1282605 Spain (L120230)	GC 0640/ Pewter	1	28.12.2011	foliar	0.06*	200	0.113*	2	69	whole plant³	5.1	0.028	5.1	0	
		2	02.05.- 11.05.2012	application	0.11**		0.225**	17.05.2012		ears	0.69	0.25	0.94	28	Method No
										rest of plant³	0.52	0.14	0.66	28	
		3	28.06.2012							grain	0.21	0.066	0.28	36	
										straw	0.80	0.20	1.0	36	
										grain	0.27	0.082	0.35	42	0.01 mg/kg
									straw	0.81	0.23	1.0	42		

IUCLID in the PPP industry context

1 Tabular data (OHT 85-5) in IUCLID and PDF

Residues in crops (field trials) and rotational crops (limited field studies).001

1 Growth stage (BBCH) at sampling
123

1 Date of sampling
2010-01-01

1 Sampling information
sampling information

1 Sampled material / commodity (Field RAC sample)
AF 0162 - Grass forage

Residue levels + New item

4 Analyte identity
Cloquintocet-mexyl | Cloquintocet-mexyl | 99007-70-2

Analysis sample description
Sample 123

Extraction date
2020-01-02

Analysis date
2020-01-03

Method ID
foliar

Storage stability factor
12

Use of factor
yes

Correction by storage stability
yes

Recovery
2

Correction by recovery
yes

Reference portion
13

Residue level (measured)
> 12 <= 14 µg/g

Residue level (calculated)
12 ppm

Residue level (calculated and corrected)
11 ppm

One table
row

Sampling no.
#1

Sampling timing
DALA - Days after last application

Growth stage (BBCH) at sampling
123

Date of sampling
2010-01-01

Sampling information
sampling information

Sampled material / commodity (Field RAC sample)
AF 0162 - Grass forage

Residue levels

Analyte identity
Cloquintocet-mexyl | Cloquintocet-mexyl | 99007-70-2

EC number
99007-70-2

CAS number
IUPAC name
Cloquintocet-mexyl

EC name
CAS name

1

Analysis sample description
Sample 123

Extraction date
2020-01-02

Analysis date
2020-01-03

Method ID
foliar

Storage stability factor
12

Use of factor
yes

Correction by storage stability
yes

Recovery
2

Correction by recovery
yes

Reference portion
13

Residue level (measured)

> 12	<= 14	µg/g
12		ppm

Residue level (calculated and corrected)

11	ppm
11	ppm

Analyte identity
2-hydroxy-3-fluoro-5-chloro-pyridine, 5-chloro-3-fluoro-2(1H)pyridinone / 2-hydroxy-3-fluoro-5-chloro-pyridine, 5-chloro-3-fluoro-2(1H)pyridinone

EC number
CAS number
IUPAC name
2-hydroxy-3-fluoro-5-chloro-pyridine, 5-chloro-3-fluoro-2(1H)pyridinone

EC name
CAS name

Analysis sample description
description 2

IUCLID in the PPP industry context

2

API integration

- **Target: Automatic prefill to the extent possible**
 - Interface: „Public REST API“



- **Requirements**

- Specification and publication of (machine-readable)
- Complete technical document definitions
- Phrasegroups
- Validation rules (incl. Dynamic content)
- Migration rules
- Error codes
- Complete API definition



IUCLID in the PPP industry context

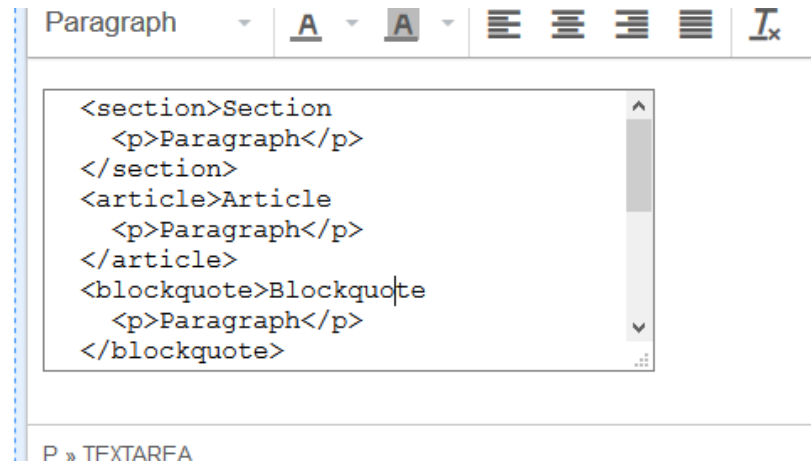
2

API integration



• Complete technical document definitions

- Example:
 - Accepted HTML syntax not defined
 - HTML5 syntax not correctly rendered in web interface



```
<section>Section
  <p>Paragraph</p>
</section>
<article>Article
  <p>Paragraph</p>
</article>
<blockquote>Blockquote
  <p>Paragraph</p>
</blockquote>
```

P » TFX TARFA



- Required: HTML syntax definition for rich-text areas (including OECD OHT definitions)

IUCLID in the PPP industry context

3

Direct generation of data format

- **Required**



- Standalone comprehensive I6Z format specification

- Container definition
- Complete document definitions (see above)
- Validation tool for I6Z package
 - Container definition validation



- Business & technical document validation

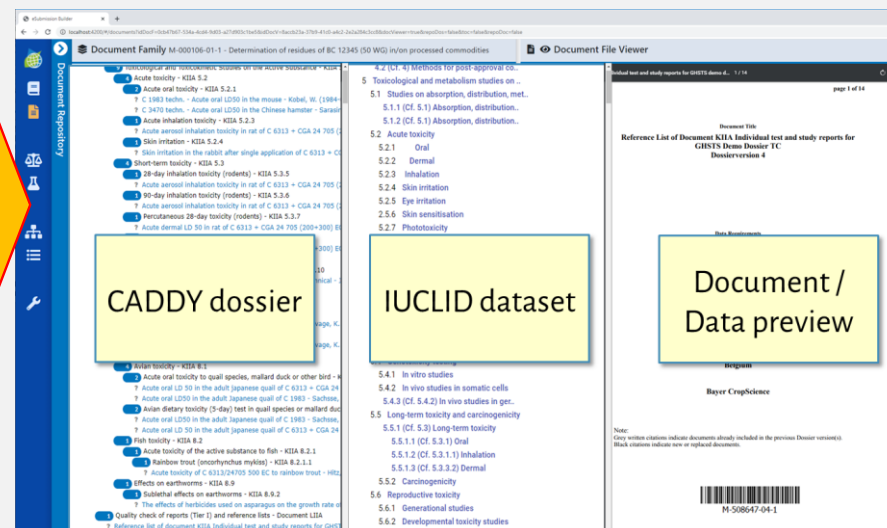


- Machine-readable detailed validation messages to correct erroneous I6Z package and/or content

3

IUCLID in the PPP industry context

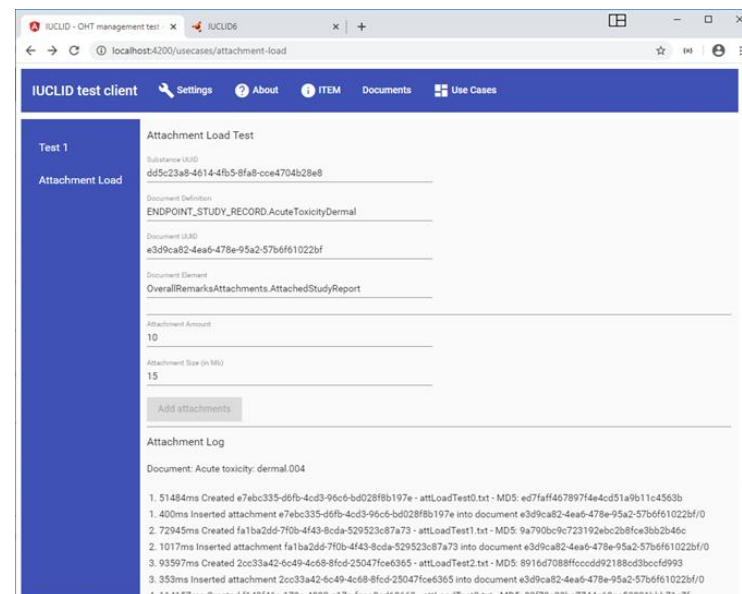
CADDY-xml cross-compiler



The screenshot displays the CADDY-xml cross-compiler interface. On the left, a 'Document Repository' sidebar lists various document types. The main area shows a 'Document Family' with a list of documents. A yellow box labeled 'CADDY dossier' is overlaid on the left side of the document list. A yellow box labeled 'IUCLID dataset' is overlaid on the right side of the document list. A yellow box labeled 'Document / Data preview' is overlaid on the right side of the document list. A red arrow labeled '16Z' points from the 'Document / Data preview' box to the right.

Performance of attachment handling

- 😊 • Datasets up to 3,6 GB created
- 😊 • Upload / Download of I6Z packages up to 3,6 GB
- 😐 • Availability of IUCLID instances after period of inactivity



Conclusions

Topics for improvement

- **Manual / no integration**
 - Rich-text control: Preservation of text formatting
 - Usability (rich-text & tabular information)
- **API integration & direct generation of data format**
 - Completion of technical specifications
 - Availability of external validation
 - Goal: Ensure interoperability
- **Availability of cloud instances**

A photograph of a field of golden wheat in the foreground, with a blue sky and white clouds in the background. The wheat stalks are in sharp focus, showing their golden-brown heads and thin stems. The sky is a pale blue with soft, white clouds.

Thank you !

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