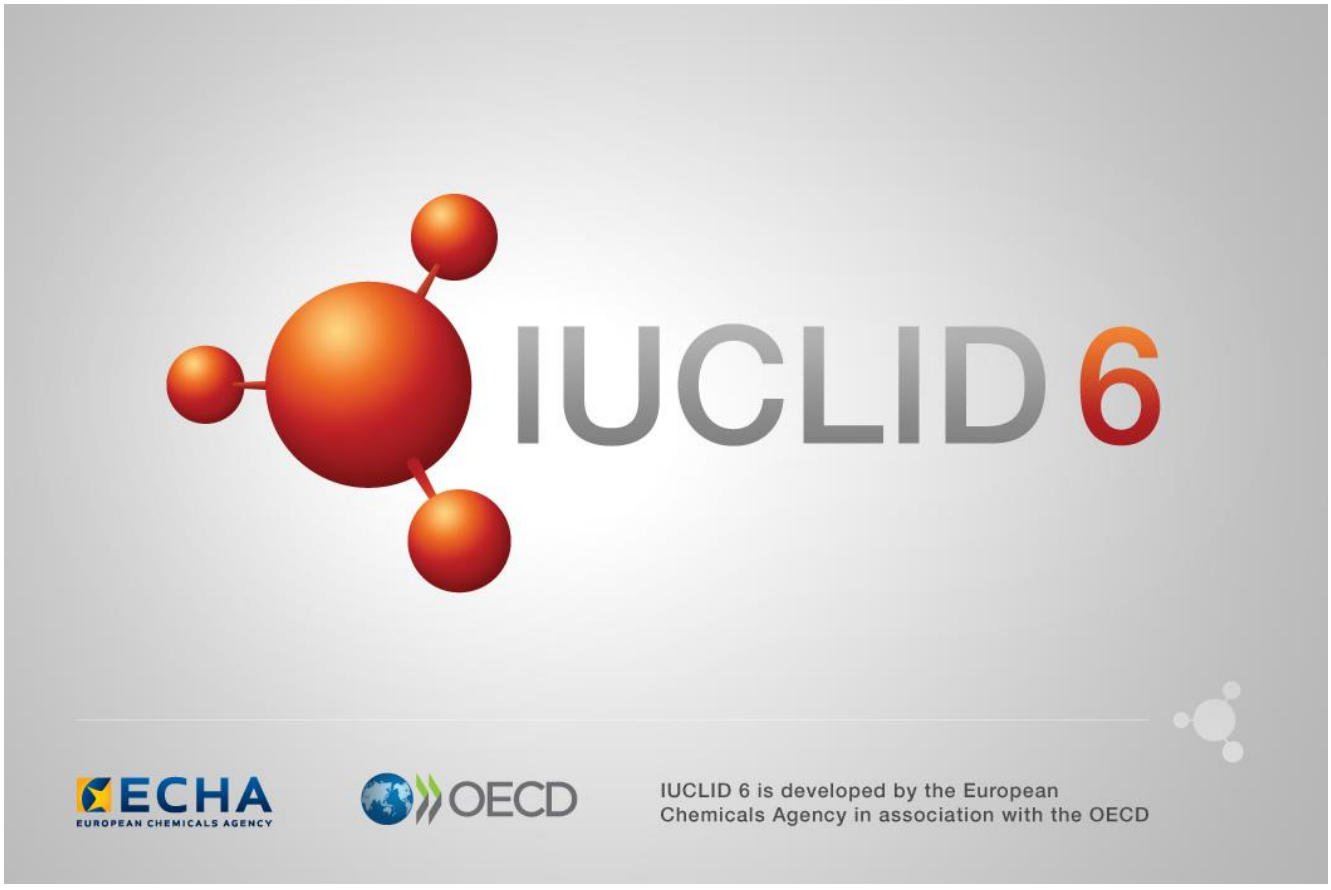
IUCLID 6

Webinar IUCLID 6 – Questions and Answers

IUCLID 6.6

10/11/2021



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1. INTRODUCTION

This IUCLID 6 webinar took place on the 10th November 2021. It was intended for users of IUCLID 6.

More information from the release can be found on the IUCLID website.

The presentations were followed by a question and answer session. The content of this session is reported in this document.

Please also have a look at the latest update of the Frequently Asked Questions page on the IUCLID 6 website: https://iuclid6.echa.europa.eu/faq.

2. CLASSIC INTERFACE

Q1: Can I just confirm that web based and classic are still linked platforms? Changes to data made in one platform will still be updated in the other platform.

A1: Yes, this is the same database, only with two different interfaces.

Q2: In the classic interface it was possible to link all relevant studies at once to a selected assessment entity. In the web interface, it seems that every study has to be selected separately, which takes quite a while. Am I doing something wrong or is there another easier way?

A2: Thank you for your feedback. We are indeed missing a multiselect or select all feature at this level in the web interface. We will check the prioritisation allocated to this improvement.

Q3: How are placed now all studies in the new interface vs the classical interface? I see much useful to find them in the classical version

A3: We would welcome your feedback on this describing what you prefer in the classic interface. You can contact the ECHA Helpdesk and we will take your comments into account for the next releases as the web interface is the only one we intend to maintain in the future.

Q4: The classic interface is way more fast to use, way more easy to navigate and shouldn't be abandoned.

A4: The performance of the web interface has been improved in this new release. The web interface is the only one meant to be used. We are keeping the classic interface in order to perform specific actions which have not been ported to the web interface yet and are used by a limited group of advanced users. We are monitoring the coverage of the web interface in terms of features and will decommission the classic interface as soon as it is possible. Please contact the Helpdesk if you identify issues with the navigation of the web interface as we are taking actions to continuously improve it.

3. VALIDATION

Q5: A new rule triggers quality check warnings in the Technical Completeness Check when the Test Material Information does not match the reference substance of the registered substance. For instance, for metals, where effect is ion-based, this is typically the case; is there a guidance on how to include this experimental data without triggering the checks?

A5: This is indeed a quality check introduced for REACH submissions. The test material information should be similar to the registered substance unless a read-across approach is used.

4. REPORTING

Q6: The report generator management is difficult to use. Is there some documentation available?

A6: More details on how to use the Report Management is in the IUCLID functionalities manual, section 21.1. (Hopefully, this gives you enough information to use the functionality.

Q7: We experience issues with CSR generation from a dataset containing attachments in a word-format. Are all attachments to be converted to a PDF?

A7: Attachments can be of any types in IUCLID, not only PDFs. We are not aware of any issues related to the generation of the CSR that would come from the type of attachments stored in a dataset.

Q8: When there will be a possibility to extract a draft PAR and SPC (BPR) from the IUCLID data?

A8: Currently, the creation of a draft PAR report from IUCLID is not prioritised by ECHA. However, we are interested to know users view on this topic, so if you could provide your comments on the importance of this report, via the Help Desk, we will analyse them. Regarding the SPC report, currently, it is possible to extract IUCLID data that are relevant for the SPC for a single product. An XML file is generated and can be uploaded to the SPC Editor.

5. INSTALLATION AND MIGRATION

Q9: Last time you've launched a new version of IUCLID (in April 2021), I have downloaded the upgrade and all the data I have had in IUCLID were erased. An IT expert had to move the settings of my PC before that date so he could restore my lost data. Why did it happen, and will it happen again now?

A9: If you are using a Desktop version, the updater takes a backup of your installation, including the data, before the upgrade. For a server version, the user has to back up the database beforehand. During upgrade, the data is obviously kept and migrated to a new version. In case you would like to verify the upgrade process before proceeding, you can contact us at the ECHA Helpdesk.

Q10: There appear to be multiple sub folders named .....\ glassfish \ glassfish4\glassfish\domains\domain1\config\ from previous IUCLID updates in the main IUCLID folder. Can you provide guidance to which sub-folders can be deleted after a new update and guidance to location of error log files.

A10: I have performed several updates to 6.2.0, and never seen the effect you describe. The files in use should be the most recent ones. Back up your data before deleting anything. If you need further help, please create a ticket with the helpdesk at https://echa.europa.eu/contact.

Q11: We use a standalone version of IUCLID. Will this also be updated at a new release?

A11: Users of the IUCLID standalone version have the application installed in their own computers. This means that, to have access to the latest version, you need to update your installation, yourself, using the updater, for instance, available at https://iuclid6.echa.europa.eu/de/download.
If you were using the IUCLID Cloud services, the upgrade, including the migration of the data, would be done automatically for you. You can find more information about it here https://echa.europa.eu/support/dossier-submission-tools/echa-cloud-services

Q12: When will IUCLID/ECHA support PostgreSQL officially as valid database? Especially for big databases this would improve the performance issue. We would like to change our database to PostgreSQL however only when ECHA supports PostgreSQL officially.

A12: We are making progress towards the official support of PostgreSQL. We are currently working on a tool that will support users migrating information from Derby or Oracle to PostgreSQL. Once it is ready (in the coming weeks) we will be able to officially support this new database type.

6. COPY FUNCTIONALITY

Q13: Coping and removing records/data in the classic interface was much easier than in the new one.

A13: The concept for copying records has indeed changed in the web interface. It is presented in this video tutorial: https://youtu.be/41B66VLpaag. In terms of records deletion, a bulk record deletion is still to be implemented indeed.

Q14: It appears to not be possible to copy an existing record (not a dataset) - is this the case, or am I missing the functionality?

A14: The copy of documents in the web interface is still possible. The process differs from the one used in the classic interface though. You need to access your target substance (the one you want to copy information to), then select the options available under the three dots in the top right corner, and select Copy data from. You can then select the dataset from which you want to copy data and select the relevant document(s) to be copied.

Q15: The "Copy data from" instrument is quite difficult to use in case of large databases: the classic "clipboard" is way more easy to use because you can select the data from the source dataset without having to search through a long list of substances. Are you planning on restore this function?

A15: In the classic interface or the web interface the user also has to find the source and the target dataset. The approach in the web interface is that the users stay in the dataset they are editing and access the relevant datasets to copy data from in a sliding window.

Q16: The classic interface is really useful to prepare fast clean dataset to share members with the bulk copy past content, by physchem, ecotox or tox section. the copy from is not clean way with the .copy suffix added

A16: The ‘Copy’ suffix is there to distinguish from the existing documents. If you copy into an empty dataset, you might want to use another possibility which is ‘Clone’. This functionality is available under three dots next to the substance displayed in the list of substances. It creates an identical dataset.

Q17: Will there be a "clipboard manager " for the web version in near future?

A17: The possibility to copy documents is already available in the web interface: 'Copy data from'. This is illustrated in a video tutorial: https://youtu.be/41B66VLpaag

7. WEB INTERFACE & FUNCTIONALITIES

Q18: Are you aware of any functional differences between the web version and the classic version? For example, options that appear greyed out and not available in one version but not so in the other version?

A18: In IUCLID 6.6 two features still appear 'greyed-out' in the web interface: inventory management and server administration. For the first feature, we will investigate the need to maintain this feature although we have not observed requests supporting this until now. For the server administration, the configuration is now maintained in configuration files at the server level and we will not maintain a specific user interface for these server administrator settings.

Q19: The new IUCLID does not accept the SMILES information, it gives all the time warning. Why this happens? How to solve this problem?

A19: This is not something that we have observed or that we have been made aware of. The SMILES field in the reference substance can store up to 2,000 characters, as in previous versions. Please contact the ECHA Helpdesk in case the issue persists.

Q20: Can we generate dossiers for multiple mixtures at once in the new release? Now we had to do it one by one and this takes a lot of time (certainly because the web version is so slow and not all QC is checked by the classic version) if you have > 250 submissions to do.

A20: Dossiers can be generated only one by one using the IUCLID interface. In case you would like to automate this step, I would suggest to have a look at the IUCLID Public API in order to script the creation of dossiers: https://iuclid6.echa.europa.eu/public-api. This solution would probably require the development of code.

Q21: From my experiences, when IUCLID server version 6.5 (July) is used by more people (est. 20 user), then it is not stable. Error message, server is not responding, occurs often, or I will be logged out automatically. Is this fixed in the newer version?

A21: The performance has been improved with the new version of IUCLID. However, other parameters can impact the performance such as the memory allocation or the type of database used. We have experience with databases containing thousands of datasets accessed by 100+ users.

Q22: Have you fixed the issues about long loading times for larger databases? When using the web version, it takes ages to load a substance/mixture and to navigate through the datasets if you have more than 50 substances and it's impossible to work.

A22: We indeed received feedback from users that the performance of the web interface was poor for databases containing a large number of substances or for substances containing many documents. In the past months we have implemented some fixes and improvements that were tested with users who reported the issues to us. IUCLID 6.6 released at the end of October contains these fixes so the situation should be better. In case you still experience performance issues, please contact the Helpdesk to get support on the ways to optimise the configuration of your installation.

Q23: Is it possible to export CLP notifications of several substances in one time and to submit it in the REACH-IT ?

A23: Currently, you can export in bulk the i6z files from IUCLID. However, in REACH-IT, you can only submit these CLP notifications one-by-one. In the first half of next year (2022), there will be a possibility to submit CLP notifications in bulk via system-to-system submissions.

Q24: Is it now possible to bulk-delete information? For example, if you want to delete uses and replace them with new ones (from a Consortium template for example) you had to manually delete the

uses one by one and with the current poor speed of the system, this could take hours. Any improvement here?

A24: The bulk deletion of documents is not supported yet in the web interface unfortunately. Each document has to be deleted one by one for the time being. However, if your uses are managed in a template, replacing the template in the dataset should be enough to reflect the changes.

Q25: Is there a feature to filter all substances that have the same working context (CLP Notification or CLP Poison Centre notification, ...)? Is the basic composition information automatically copied for the same substance that has several working context?

A25: You can filter all substance dossiers that have the same working context. You need to use the functionality Advanced search above the substance list (Dossiers) and select a working context from the pick list under 'Dossier Submission Type'. For the datasets this is not supported. However, when you reuse a dataset, and change a working context, the data inserted (for example composition) will remain there.

Q26: Is there a size limit for the attachments (previously it was 100MB)?

A26: You can filter all substance dossiers that have the same working context. You need to use the functionality Advanced search above the substance list (Dossiers) and select a working context from the pick list under 'Dossier Submission Type'. For the datasets this is not supported. However, when you reuse a dataset, and change a working context, the data inserted (for example composition) will remain there.

There is still a limit of 100MB to each individual attachment uploaded to IUCLID. This is a bug that will be fixed in the next released version though. However, we always recommend to make sure that the attachment size is optimised as much as possible before being uploaded to IUCLID. E.g. pdf files can be compressed. If this is not possible, the files > 100MB can be split and attached individually if needed.

Q27: Regarding the bulk import using csv files, do you really expect users to look for phrase codes, etc, in the excel table published in the IUCLID format? or are you planning to switch from csv to another format to allow for data validation before uploading?

A27: You are correct. This import using csv file is a first attempt to upload data in bulk in specific fields of IUCLID. We will work on improving this feature in the future.

Q28: The classic interface displays a detailed error report when for exampling trying to export a CSR or create a dossier. The web interface only displays an error but doesn't detail which one. Can this be adapted ?

A28: It is our intention to provide an enhanced background job report for report generation failure next year (2022).

Q29: The import csv function doesn't work for fields with numeric values where ranges can be provided or for fields with value + unit. This is unfortunate since these numeric fields are the most time-consuming and error prone. Is there any workaround for this? Is the data uploader an option?

A29: Attempting to use the data uploader is probably more work and complexity than this simple use-case warrants. The new import csv feature is a first version that will be enhanced in accordance with feedback from users.

Q30: The issues with exporting large tables containing merged cells from the rich-text fields in IUCLID seem to still be present (for both the PDF and RTF export formats). Will this be improved in the next releases?

A30: We have prioritised for this year a fix to the issue concerning the display of merged table cells in rich text fields (for both printing and reporting). The fix should be seen in the next release of IUCLID (IUCLID Cloud in January 2022, and in the public release of IUCLID in April 2022 at the latest).

Q31: The Opt-out section is really difficult to manage on the web version : time consuming; to avoid a major discrepancy, only the classic version allowed to select all the RSS and summary.

A31: Thank you for the feedback. The web interface is the only one we intend to maintain in the future, so we are analysing all the discrepancies reported by the users. For the Opt-out section, we will look into the possibility to make multiple selection of documents at once.

Q32: The release notes says you fixed the exporting of datasets > 2 Gb when using Derby. Is there a file size limit now?

A32: There is no file size limit imposed by IUCLID itself. However, there should be enough space on your drive to store the files.

Q33: The web interface demonstration in the presentation appears to have loading speeds to access a substance, open end points or set a working context etc. which are much quicker than the current web interface. Is this example real time or edited for presentation please?

A33: The database used for the demo contains only a limited number of datasets which could explain the observation - we did not edit the video to make it looks faster ;-). IUCLID 6.6 contains improvements in terms of performance. The type of database used (Derby or Oracle) and the memory allocated to IUCLID can also play a role with the performance observed.

Q34: We are hopeful that the performance improvements to IUCLID web mean we no longer need to rely on using classic, but please can you confirm your proposed timeline for decommissioning classic as stated in reply to another question posted in this thread.

A34: By the end of the year, we will review with the IUCLID team the feedback collected until now from the users still using the Classic interface. This will help us finalising the decommissioning plan with a target of then end of 2022.

Q35: We had an issue with version 5.15.0 that was not solved by support (INC000000351099). The issue was with web interface where newly added functionalities (manage report, User Management) were not available in MS Edge browser. Was it fixed in this new release?

A35: Yes, this issue has been fixed in the latest release.

Q36: We have experienced very slow system since last update. We have >500 substances in our server version and want to know how much the number of substances would slow down our IUCLID? Do we need to export and save dossiers elsewhere to save capacity?

A36: For larger databases like yours, we recommend either a Derby server or an Oracle database. Soon, we will also support PostgreSQL which could help achieving a better performance. Please contact the Helpdesk in case you face performance issues with the latest version of IUCLID.

Q37: When I want to switch the working legal entity in the web interface, it is not working directly but I have to log out and in again first. Is this fixed?

A37: Hi, we are not aware of this issue. Please can you contact the ECHA Helpdesk to report the problem, stating which IUCLID version you are using, and the steps you take?

Q38: Where do I find the codes for the csv files for the bulk import, i.e. to populate repeatable blocks from csv file'? The codes will translate into the description, e.g. in the csv there is a number in the column 'Reason purpose.code' and in IUCLID it translates then to 'assessment report'?

A38: Finding codes is described in the user manual in section "3.6.9.1. Import file into a table". To open the manual, click on the large round question mark icon located top right on the main page of the user interface, or from the IUCLID website.

Q39: Will you add the functionality to search by substance UUID again, like we could in the classic interface?

A39: You can search for the dossiers and datasets, by their UUID, from the dashboard.

8. PCN

Q40: Can you explain in detail which changes in mixture composition are allowed w/o requiring a new UFI? Feature announced: Additional update reasons, such as ‘cease product from the market’ and ‘change in mixture composition without requiring a new UFI’.

A40: In this session we answer question related to the features of IUCLID, not the use of IUCLID in a specific context such as PCN in this case. We have a specific webinar on PCN scheduled soon.

9. INTERNATIONAL

Q41: After Brexit the UK is still using IUCLID. Do you collaborate with them like with AUS and NZ?

A41: UK is a member of the OECD IUCLID Group, as Australia and New Zealand for example. We are cooperating with OECD countries for the further development of IUCLID.

10. IUCLID TOOLS

Q42: Can you let me know what the roadmap is for the data extractor tool? Will there be a release that is compatible with the next version of IUCLID?
(Data extractor - ECHA (europa.eu))

A42: We are currently testing a Data extractor version compatible with IUCLID 6.6 and we will publish it in the coming couple of weeks. This will be announced on the IUCLID website.

Q43: The data uploader requires to use Knime. However, it requires a licence in order to use this tool.

A43: Knime is an open-source software that can be downloaded and used free of charge. Some additional services are offered but they are linked to the Server version of Knime. More information on the Knime website.

11. IUCLID FORMAT

Q44: Could you please clarify if we can still continues submitting dossiers prepared in IUCLID 6.5 by the end of year? We have upcoming deadlines and we would like to postpone the update of the server until January 2022. Thank you.

A44: Yes you can still submit dossier created in version 6.5

Q45: I am interested to know more about adding to dossiers that were submitted in 6.5 but need to topped up in 6.6, and how to successfully submit these large (>2 GB) dossiers? Also how to completely import datasets that have been built in 6.5 into 6.6 without losing critical cross links.

A45: Datasets created in IUCLID 6.5 can be updated to the new version of IUCLID and be used to create dossier updates. In order to minimise the size of the dossier update, please use the 'Export as light dossier' feature. You can find more information in the IUCLID user manual, section 18.10. Links are made only inside a dataset. If you export the dataset, all relevant links are preserved.

Q46: I have a look at the Acute oral toxicity, and do not see major changes as indicated in the webinar. Do these changes are only on the OECD working context and not on the PPP?

Is the format of standalone version 100% compatible to cloud version? We have problems in cloud system to import files created with standalone version.

A46: Acute oral toxicity is an OECD harmonised template and is used by several working contexts. The content of a document is always the same. Changes might not be visible but there were major for the compatibility issues.

Q47: Is the format of standalone version 100% compatible to cloud version? We have problems in cloud system to import files created with standalone version.

A47: The Cloud installations have been updated to IUCLID 6.6 so there should be no issue importing any IUCLID 6 data from other IUCLID 6 installations. In case of issue, please contact the ECHA Helpdesk as we will need more information in order to investigate the problem.

Q48: There used to be a summary endpoint for endocrine disrupting properties (working context PPP CA - 5.8.3), this seems to not exist anymore, or has it been moved somewhere else?

A48: The summary document still exists in IUCLID but has been moved under section 11.4 of the table of contents, in the specified working context.

Q49: To prepare Reach-like registration, the flag are not take into account the future and mandatory scope : UK flag, K-Reach and KKIDK flag will be useful.

A49: Thank you for your feedback. We will take note of this requirement and bring it to the OECD IUCLID group to be discussed with UK, South Korea and Turkey respectively.

Q50: You presented the option to generate reports on attachments. In the classic IUCLID a remark field was available where additional information on the content of the attached file could be added. This field is still available, but it cannot be accessed with the Web UI. Can you make it available again?

A50: The remark field for attachment is available for attachments made to the record as a whole but not for attachment inserted in a document field. We will look into this. Thank you for your feedback.

Q51: What about attachments during migration from 6.5 to 6.6 (PPP working context). Will that be an issue?

A51: Attachments are migrated to the new IUCLID 6.6 format during an upgrade, for all types of working contexts.

12. MISCELLANEOUS

Q52: It was said that the webinar will be published on the YouTube channel. Will that include the Support Material and Live Demo part?

A52: Yes, the full content of the webinar is available on ECHA's YouTube channel.

Q53: The version you have presented seems to be called IUCLID 6.6, but in the website the version to be downloaded (also as updater) is called IUCLID 6 - v6.2.0. Is this an inconsistency?

A53: The latest version of the IUCLID 6 application that is available for download in our website and also available in the ECHA Cloud services is version 6.2.0. That is correct. The "full" name of the application with the version included is: IUCLID 6 v6.2.0, indeed.

Q54: What is the procedure to ask for confidentiality on the name of the registrant with the web interface?

A54: Hello, are you talking about confidentiality in the REACH regulation? If this is the case, please see the relevant manual.