

Welcome

Data Uploader: converting your
chemical data into IUCLID format

19 October 2022

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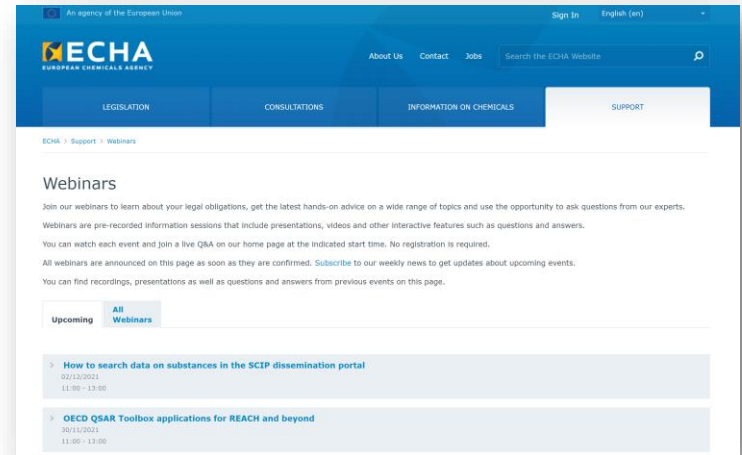


Live Q&A

- Join Q&A at: slido.com
Event code:
- Send questions from
11:00 to 13:00 (EEST, GMT +3)
- Only questions within scope
- Question not answered?
Contact us: echa.europa.eu/contact

Material available

- Video recording
- Presentations
- Q&A (soon after the event)



echa.europa.eu/webinars

Programme



Time	Topic	Speaker
11:00	Introduction	A les FRONTINI Data team, Computational Assessment, ECHA
11:05	First release: installation instructions and two use cases with example datasets and workflows	A les FRONTINI Data team, Computational Assessment, ECHA
11:15	First step: data mapping	A les FRONTINI Data team, Computational Assessment, ECHA
11:25	Data Uploader demo	A les FRONTINI Data team, Computational Assessment, ECHA
11:50	Further support	A les FRONTINI Data team, Computational Assessment, ECHA
11:55	Conclusions	A les FRONTINI Data team, Computational Assessment, ECHA
11:00 – 13:00	Webinar open for questions	

What you can expect today

- Get to know how to migrate data from legacy databases into IUCLID using Data Uploader
- Tips for building data migration workflows
- How to reach us for help

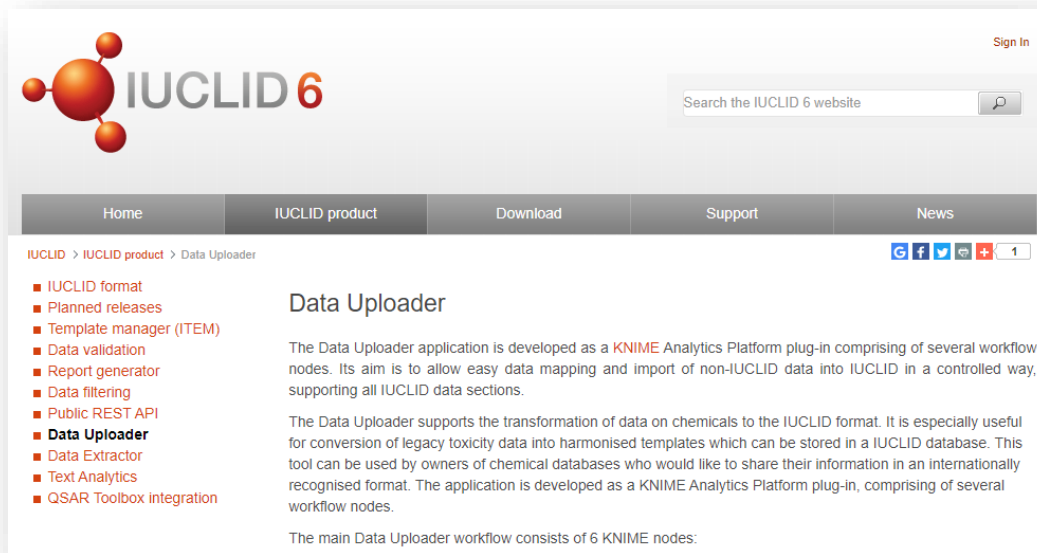


Motivation

- Transformation of data on chemicals to IUCLID format
- Conversion of legacy toxicity data into harmonised templates which can be stored in a IUCLID database
- Tool can be used by owners of chemical databases who want to share their information in an internationally recognised format
- Application developed as a KNIME Analytics Platform plug-in, comprising several workflow nodes

Ecosystem of tools: **Data Uploader**

- Migration of legacy data into IUCLID

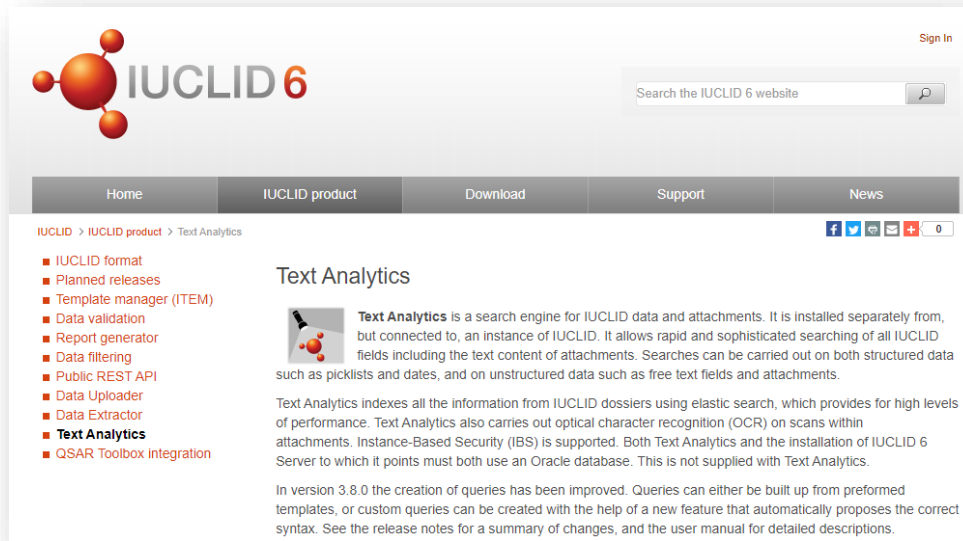


The screenshot shows the IUCLID 6 website interface. At the top left is the IUCLID 6 logo, consisting of three red spheres of varying sizes. To the right is a search bar with the placeholder text "Search the IUCLID 6 website" and a magnifying glass icon. In the top right corner, there is a "Sign In" link. Below the search bar is a navigation menu with five items: "Home", "IUCLID product", "Download", "Support", and "News". Below the navigation menu is a breadcrumb trail: "IUCLID > IUCLID product > Data Uploader". To the right of the breadcrumb trail are social media icons for Google+, Facebook, Twitter, LinkedIn, and YouTube, along with a notification icon showing the number "1". On the left side of the page, there is a list of links with red square bullet points: "IUCLID format", "Planned releases", "Template manager (ITEM)", "Data validation", "Report generator", "Data filtering", "Public REST API", "Data Uploader" (highlighted in bold), "Data Extractor", "Text Analytics", and "QSAR Toolbox integration". The main content area has the heading "Data Uploader" and two paragraphs of text. The first paragraph states: "The Data Uploader application is developed as a KNIME Analytics Platform plug-in comprising of several workflow nodes. Its aim is to allow easy data mapping and import of non-IUCLID data into IUCLID in a controlled way, supporting all IUCLID data sections." The second paragraph states: "The Data Uploader supports the transformation of data on chemicals to the IUCLID format. It is especially useful for conversion of legacy toxicity data into harmonised templates which can be stored in a IUCLID database. This tool can be used by owners of chemical databases who would like to share their information in an internationally recognised format. The application is developed as a KNIME Analytics Platform plug-in, comprising of several workflow nodes." At the bottom of the main content area, it says: "The main Data Uploader workflow consists of 6 KNIME nodes:"

iuclid6.echa.europa.eu/data-uploader

Ecosystem of tools: **Text Analytics**

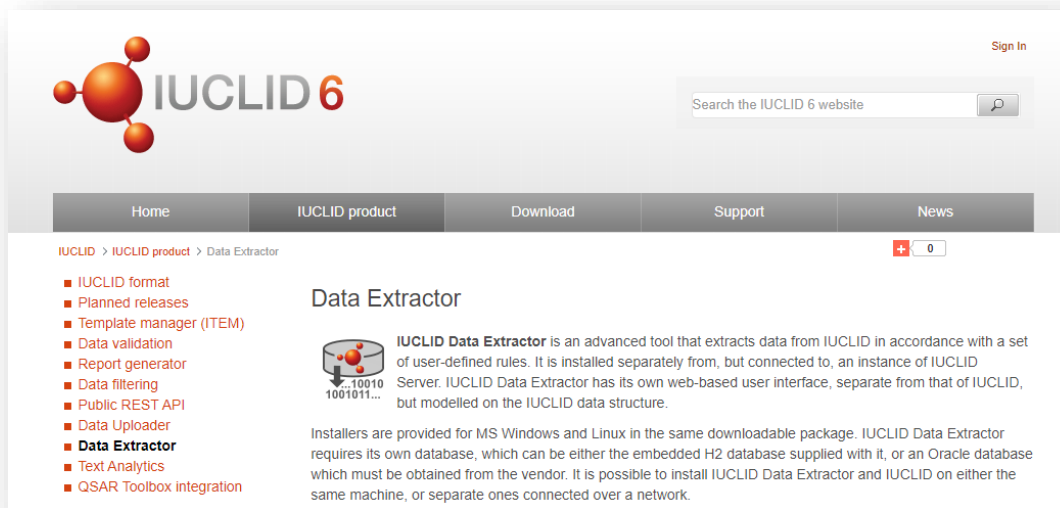
- Indexing and searching



The screenshot shows the IUCLID 6 website interface. At the top left is the IUCLID 6 logo, consisting of three orange spheres of varying sizes connected by lines. To the right of the logo is a search bar with the placeholder text "Search the IUCLID 6 website" and a magnifying glass icon. In the top right corner, there is a "Sign In" link. Below the search bar is a navigation menu with five items: "Home", "IUCLID product", "Download", "Support", and "News". Below the navigation menu is a breadcrumb trail: "IUCLID > IUCLID product > Text Analytics". To the right of the breadcrumb trail are social media icons for Facebook, Twitter, LinkedIn, YouTube, and a plus sign, followed by a notification icon showing "0". On the left side of the page, there is a list of links with orange square bullet points: "IUCLID format", "Planned releases", "Template manager (ITEM)", "Data validation", "Report generator", "Data filtering", "Public REST API", "Data Uploader", "Data Extractor", "Text Analytics", and "QSAR Toolbox integration". The main content area is titled "Text Analytics" and features a small icon of three orange spheres. The text below the icon reads: "Text Analytics is a search engine for IUCLID data and attachments. It is installed separately from, but connected to, an instance of IUCLID. It allows rapid and sophisticated searching of all IUCLID fields including the text content of attachments. Searches can be carried out on both structured data such as picklists and dates, and on unstructured data such as free text fields and attachments." Below this is a paragraph: "Text Analytics indexes all the information from IUCLID dossiers using elastic search, which provides for high levels of performance. Text Analytics also carries out optical character recognition (OCR) on scans within attachments. Instance-Based Security (IBS) is supported. Both Text Analytics and the installation of IUCLID 6 Server to which it points must both use an Oracle database. This is not supplied with Text Analytics." The final paragraph states: "In version 3.8.0 the creation of queries has been improved. Queries can either be built up from preformed templates, or custom queries can be created with the help of a new feature that automatically proposes the correct syntax. See the release notes for a summary of changes, and the user manual for detailed descriptions."

Ecosystem of tools: **Data Extractor**

- Data extraction and analytics



IUCLID 6


Search the IUCLID 6 website

Home IUCLID product Download Support News

IUCLID > IUCLID product > Data Extractor

- IUCLID format
- Planned releases
- Template manager (ITEM)
- Data validation
- Report generator
- Data filtering
- Public REST API
- Data Uploader
- **Data Extractor**
- Text Analytics
- QSAR Toolbox integration

Data Extractor

 **IUCLID Data Extractor** is an advanced tool that extracts data from IUCLID in accordance with a set of user-defined rules. It is installed separately from, but connected to, an instance of IUCLID Server. IUCLID Data Extractor has its own web-based user interface, separate from that of IUCLID, but modelled on the IUCLID data structure.

Installers are provided for MS Windows and Linux in the same downloadable package. IUCLID Data Extractor requires its own database, which can be either the embedded H2 database supplied with it, or an Oracle database which must be obtained from the vendor. It is possible to install IUCLID Data Extractor and IUCLID on either the same machine, or separate ones connected over a network.

A final note

- Beneficial if historically generated physicochemical, fate and (eco)toxicity data are available in the same harmonised IUCLID format
- We facilitate this by developing the Data Uploader and support data owners to migrate legacy data
 - KNIME gives the tools to extract information from the legacy source and the Data Uploader nodes simplify pushing the data into IUCLID
 - Published example workflows provide a framework
 - Migrating legacy data still requires mapping of fields from original source data to IUCLID document definitions. This can only be done by the data owner

oecd.org/ehs/templates

iuclid6.echa.europa.eu/format

Thank you

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[EUchemicals](https://www.youtube.com/EUchemicals)

Conclusions

Webinar: Using the data uploader
to convert and migrate data into
IUCLID

19 October 2022

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Regulatory Assistant
European Chemicals Agency



Conclusions

- [Download](#) Data Uploader
- Issues with installation? [Contact us](#)
- Check two use cases
- Map your data
- Check generated IUCLID schema
- Create workflows to transfer your data to csv files
- Check for potential errors and upload data to IUCLID



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