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IUCLID-Decoder: Python code to extract the chemical property data for the substances registered under REACH

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Summary

The IUCLID-Decoder is a package in python that enables users to extract chemical property data from registration dossiers that have been submitted to the EU Regulation on Registration, Evaluation, Authorization and Restriction of Chemicals (REACH). The data is extracted from files that the European Chemicals Agency (ECHA) offers for download. These files, the so called 'REACH Study Results' contain more than 4 million IUCLID 6 format (i6d) files with study results. The 'decrypt_reach_results' function in the IUCLID Decoder package extracts and decodes the data and standardizes the units. The output is an SQLite database and (if set to 'True') an excel file with the database.

Statement of need

ECHA publishes on its website (ECHA, 2024b) the non-confidential substance data that have been submitted by the registrants under REACH. However, ECHA reserves the right to block systematic automated data collection activities including scraping, data mining, and extraction and re-utilization of the whole or a substantial part of the website and the ECHA databases, where justified and subject to applicable law. To be still able to access the data, ECHA offers to download the 'REACH Study Results' via the IUCLID website (ECHA, 2024a). The REACH Study Results contain results from studies that relate to physicochemical properties, environmental fate and pathways, and ecotoxicology and toxicological information. Data form free text fields are not provided, but most of the other data. As the data of the currently more than 20 000 substances come in over 4 million i6d-files, with a strucutre similar to xml-files, a script is needed to import them into a database. The IUCLID-Decoder package provided here enables the user to extract the information from the i6d-files and to compile them into a database or optionally an excel file. In addition, the information that is available in the REACH Study Results as numerical code including information on units, methods, reliability or study types is converted into text and the units of the study results are standardized as far as possible.

Description

The REACH Study Results come as zipped i6z-file. When using Linux or Mac, the path to the unzipped i6z-file can be given to the decrypt_reach_results function and the function can be run without considering where to place it. Under Windows, all i6z-files should be unzipped before running the function und the decrypt_reach_results should be place in the same folder as the REACH Study Results. More information on the expected document structure is provided in the GitHub repository.

The REACH Study Results contain one main folder per registered substance. This folder then contains the so-called 'manifest' as well as individual study results and the files that are needed to decode the results. The decrypt_reach_results function extracts the information property by property. To do this, it first opens the manifest of each substance and looks up the file ID for the property of interest. This property file is then opened and the data for the property of interest are read out. This is done with a recursive funtion which calls itself up until all the information has been retrieved. Additionally, data on the substance identidy such as the European Community (EC) number, the Chemical Abstract Service Registry Number® (CAS RN®) and the substance name are extracted. SMILES are not available and would need to be added later on seperatly. Before saving the data into a dataframe, the data are decoded, and the units are standardized.

It is recommended to check the IUCLID website regularly, as updated REACH Study Results are uploaded once or twice a year. This data can be easily transferred to a new database using the IUCLID decoder package.

The decrypt_reach_results function has already been used in our previous work where we analyzed the physicochemcial property data (Glüge & Scheringer, 2023) and the bioconcentration data (Glüge, Escher, et al., 2023) in the ECHA database. We have also used it in Körner et al. (2024) to check certain REACH study results on ready-biodegradation. Information on SMILES and curated SMILES for most of the organic mono-constituent substances registered under REACH are available in Glüge, McNeill, et al. (2023).

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