qData – a web-based FAIRification workflow for (eco)toxicological dose(concentration)-response data

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Introduction and objective

Effect-based methods generate heterogeneous data across biological levels, from molecular to apical, using diverse technologies. These data are often reported in isolated formats, limiting integration, reuse, and interpretation within AOP development and risk assessment frameworks.

The objective of this work was to develop a harmonized, multi-endpoint Data Reporting Format (DRF) and a prototype web-based interface (the qData UI) as a FAIRification workflow for structured (eco)toxicity Dose–Response (DR) data analysis. The workflow supports standardized data entry, repository submission, Point of Departure (POD) analysis for AOP-informed approaches (fig. 1).

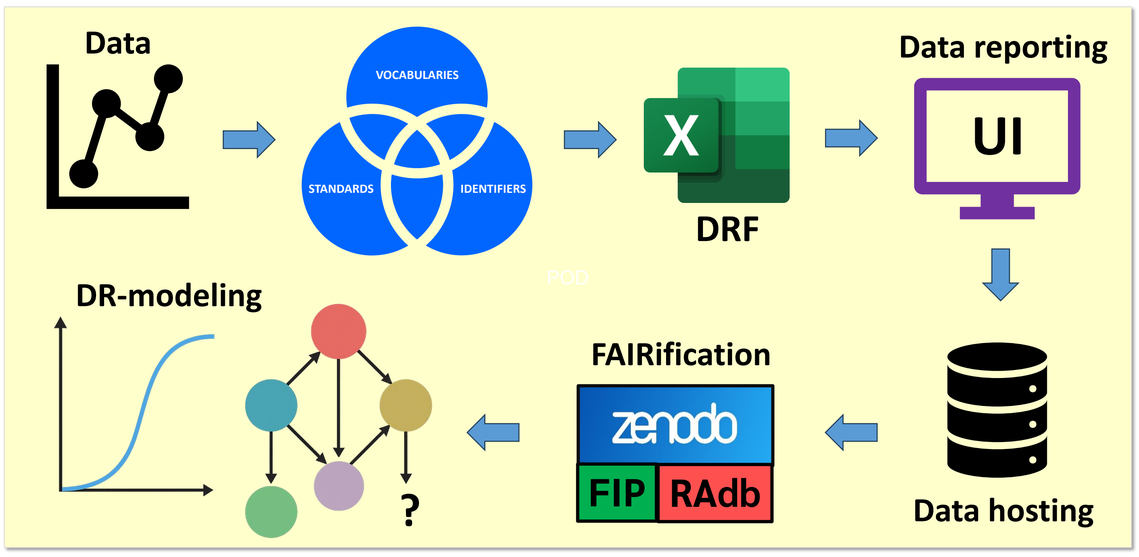

Fig 1. Workflow for (eco)toxicity data: data generation, alignment with vocabularies/standard/ontologies/ identifiers, development of multi-endpoint *Data Reporting Format (DRF), data import by a user interface (UI), data hosting, FAIRification, data sharing (Zenodo) & dose-response (DR) modeling.*

User Interface (UI)

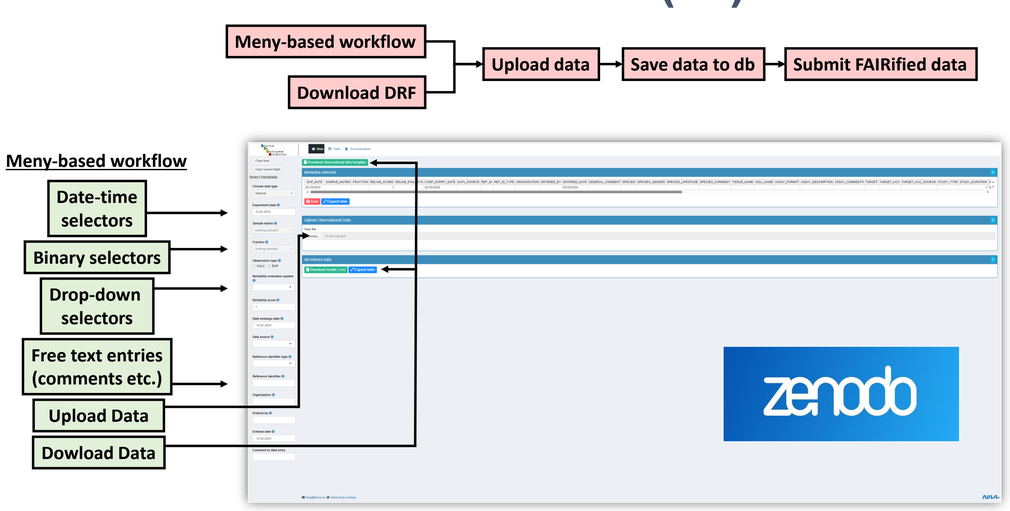

Fig 2. Data reporting user interface (UI) developed as a dashboard (qData) with upload and download functionality. The UI offers the option of reporting data by a menu-based workflow and uploading key metadata and data. The workflow is envisioned to support FAIRification processes and further processing of experimental data for dose-response analysis and AOP development.

Dose-response (DR) modeling

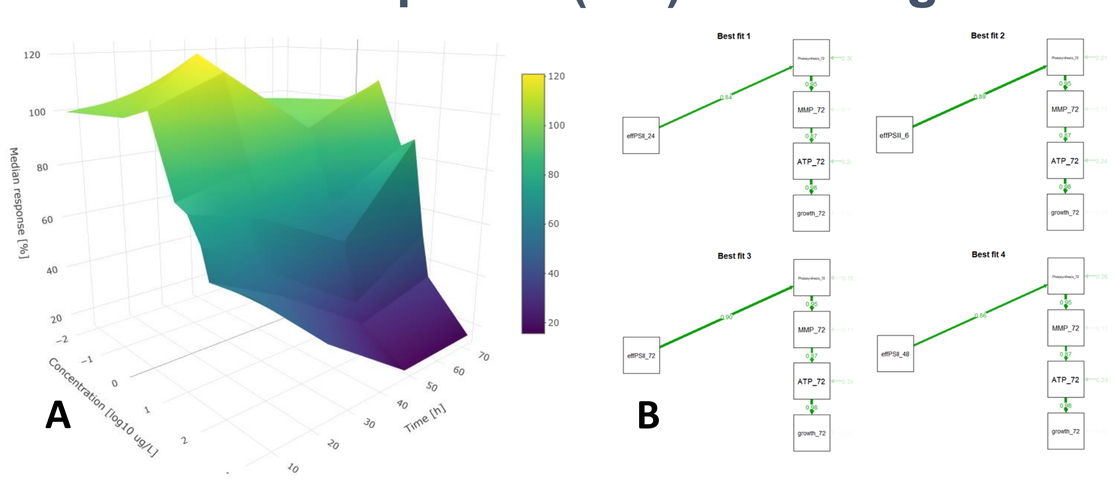

Fig 3. Analysis of dose-response (DR) data using (A) Point Of Departure (POD) assessment and (B) Structure Equation Modeling (SEM). The data display a case study on Diuron toxicity in the algae Chlamydomonas reinhardtii *spanning multiple biological levels and time points (endpoints: PSII inhibition, mitochondrial membrane potential, ATP content and growth).*

Summary and outlook

Summary

A workflow was developed for quantitative dose (concentration) response data from (eco)toxicological studies by:
1) Developing an xlsx-based multi-endpoint Data Reporting Format (DRF)
2) Prototyping a web-based user interface (UI) and a data-hosting database (db)
3) Establishing a FAIRification hub to support data sharing (e.g. by Zenodo) and further analysis of experimental data
4) Performing standardized POD and SEM analysis

Outlook

1) Harmonise/standardise the controlled vocabularies with commonly available standards, ontologies and identifiers
2) Release a beta-version for external testing
3) Integrate analysis workflow into risk assessment tools such as the Source To Outcome Predictor (STOPredictor)
4) Support qualitative & quantitative AOP development, data sharing & integrative modeling

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