

N°1385 / PC

TOPIC(s) : Artificial intelligence / computational methods

EnzymeML-based workflow for FAIR enzyme kinetics

AUTHORS

Max HÄUSSLER / INSTITUTE OF BIOCHEMISTRY AND TECHNICAL BIOLOGY, ALLMANDRING 31, STUTTGART

Corresponding author : Juergen PLEISS / juergen.pleiss@itb.uni-stuttgart.de

PURPOSE OF THE ABSTRACT

Data management according to FAIR data principles is an emerging best practice in science.[1] In biocatalysis, the EnzymeML format implements these principles, enabling storing and working with biocatalytical (meta)data.[2] Furthermore, modeling results can be stored together with data on which the results are based on. Together with PyEnzyme, a Python interface for EnzymeML, powerful analysis workflows can be implemented, which exceed the capabilities of analysis in spreadsheet applications. Thus, the EnzymeML infrastructure supports the field by providing structured documentation to experimental data. Hence, enabling the implementation of FAIR analysis pipelines.

Here we present an EnzymeML-based workflow for kinetic parameter estimation, enabling a continuous data flow from raw data to kinetic parameters. Thereby, analytical raw data together with calibration data is used for accurate concentration calculation, enabling description of linear and non-linear relationships between the analytical signal and the analyte concentration. After calibration, the respective information is directly applied to the EnzymeML data model containing analytical raw data and yielding an EnzymeML data model with concentration data. Thereafter, concentration data from the EnzymeML data model is mapped to EnzymePynetics, a tool for kinetic parameter estimation based on time-course measurement data. EnzymePynetics enables time-course analysis of enzymatic reactions, assessing the inhibition constant K_i for potential substrate and product inhibition or an enzyme inhibitor apart from substrate and product. Furthermore, different enzyme inactivation models are applied. After fitting of different model combinations, the best fitting model is selected based on different statistical criteria and thus provides an insight into the kinetic mechanism of the enzymatic catalysis. Finally, the modeling results are written back to the EnzymeML data model and serialized to the standardized EnzymeML format.

FIGURES

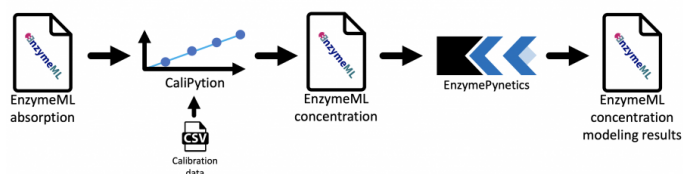


FIGURE 1

Workflow from raw data to kinetic parameters

Components of the kinetic parameter estimation workflow for enzyme reaction data.

FIGURE 2

KEYWORDS

FAIR | Kinetic parameter estimation | modeling

BIBLIOGRAPHY

[1] Wilkinson, M. D., Dumontier, M., Aalbersberg, I. J., Appleton, G., Axton, M., Baak, A., ... & Mons, B. . The FAIR Guiding Principles for scientific data management and stewardship. *Scientific data*, 3(1), 1-9 (2016).

[2] Lauterbach, S., Dienhart, H., Range, J. et al. EnzymeML: seamless data flow and modeling of enzymatic data. *Nat Methods* 20, 400-402 (2023).