STREND A DB - The ‘PDB’ for Enzyme Function Data?

STREND A Commission* and Carsten Kettner
Trakehner Str. 7-9, 60487 Frankfurt/Main, Germany, oketner@beilstein-institut.de

Difficulties with Enzyme Data
Enzyme activity data can be found in large quantities in the scientific literature and databases. However, samples show that the data were measured under different experimental conditions (e.g., temperatures, pH, ionic strength, enzyme and substrate concentrations, activators and inhibitors) which makes any comparisons difficult.

Without a comprehensive description of the experiment including materials and methods, the comparison, interpretation and reproduction of enzyme activity data is not possible [1,2]. This seriously hampers the progress of the research enterprise due to its intrinsic complexity.

The difficulties become even more acute for those wishing to use such experimental data for the definition of system models, cellular behavior and the interaction of cells within tissues and organs. However, the case is the same for systems and synthetic biology, which requires reliable data to create high-quality simulation data.

How to Make this Data Useful?

The integration of enzyme functional data with data from genomic, transcriptomic, metabolomic and proteomic analyses requires that

- the data must be of high quality and should be accompanied with information on statistical variability.
- the data must have been obtained under comparable experimental conditions, which requires a definition of minimum experimental data.
- the data reported in the literature must be unambiguous, which requires the proper description of materials and methods.
- the data should be comprehensive and readily accessible by other scientists.

STREND A Provides Assistance
STREND A (Standards for Reporting Enzymology Data) is a data standardization project supported by the Beilstein Institute.

The STREND A Commission focuses on three main areas:

(A) Standardization of Assay Conditions
The derivation of uniform assay reporting protocols for the standardization of data for single enzymes and groups of enzymes presents a great challenge since the conditions under which an enzyme operates depend on the organism and organelle in which it occurs.

The basis of initial assay standards can be the physiological conditions, which are those conditions in which cells, tissues, organs or even the whole organism are present. However, these conditions need to be determined.

First important steps toward the definition of these conditions have been carried out in collaboration with a number of Dutch working groups. A standard protocol for the enzyme from the glycogen synthase of baker’s yeast has been defined and tested in obtaining the essential kinetics of all enzymes involved in this pathway.

This approach can be regarded as proof-of-principle and can be applied with modifications for the characterization of additional metabolic pathways [3].

(B) Publication Standards for Functional Enzyme Data

The STREND A Guidelines were developed through extensive interactions with the biochemistry community to define the minimum information that needs to be rigorously described in an assay paper (List Level 1A) and enzyme activity data (List Level 1B). However the STREND A Guidelines neither dictate or limit the experimental techniques used in enzymology experiments nor establish a metric for judging the quality of experimental data, but rather encourage that data sets are complete and validated, allowing scientists to review, revise and verify them. The emphasis is on providing useful and reliable information [4].

With the aim to support authors to comprehensively report kinetic and equilibrium data from their investigations of enzyme activities, currently more than 50 international biochemistry journals include the STREND A Guidelines in their instructions for Authors.

List Level 1A: Data required for a complete description of an experiment. This information should render the results reproducible.

List Level 1B: Description of Enzyme Activity Data. This is the minimum information required to describe enzyme activity data.
Version 1.7, September 22, 2016, doi:10.3762/btend.27

(C) STREND DB - an Electronic Validation and Storage System for Functional Enzyme Data

Authors (and journals) benefit from the use of STREND DB since it

- is an online storage and search platform,
- incorporates the STREND A Guidelines,
- checks submitted manuscript data on compliance with Guidelines,
- ensures that data are complete and valid,
- points to missing protocol information.

Many journals are already recommending their authors to store their enzyme assay and activity data in STREND DB, among them are eLife, Journal of Biochemistry, Beilstein Journal of Organic Chemistry, Research Data, Nature, and Archives of Biochemistry and Biophysics.

A successful formal compliance is followed by

- issuance of a STREND A Registry Number (SRN),
- generation of a fact sheet (PDF) containing all input data that can be submitted with the manuscript to the journal,
- assignment of a DOI for each dataset that allows reference and tracking of the dataset,
- public availability of data in the database only after the corresponding article has been peer-reviewed and published in a journal.

http://www.strenda-db.org/

References

* Members of the STREND A Commission: Richard N. Armstrong, Vanderbilt University, USA; Ancha Barcik, Swiss Institute of Bioinformatics, Barbara Baker, University of Groningen, The Netherlands; Athel Cornish-Bowden, GfK MANIAC, France; Paul F. Botella, University of Texas Health Science Center, USA; Peter Haring, Strathclyde University, UK; Thomas S. Leigh, Albert Einstein College of Medicine, USA, China, France, Germany; EMBL – European Bioinformatics Institute, UK; Frank W. Maniatis, Penn W. University, USA; John P. Rutten, University of Stellenbosch, South Africa; Bernd Brücher, GlaxoSmithKline, UK and Germany; Guenter Schiltz, University of Manchester, UK; Ulrich Wehling, University of Würzburg, Germany; Norbert Wuchter, University of Kiel, Germany; Michael Delahunty, University of Birmingham, England; Guido Fiehn, University of Potsdam, Germany; Oliver Titova, UCD Dublin, Ireland; Caroline Gehrke (reconstruction), Freiburg, Germany.

For more information, visit http://www.beilstein-strenda.org. The STREND A project is primarily supported by the Beilstein-Institut.