Minutes of the

13th STRENDA Meeting

18 September, 2017

Hotel Jagdschloss Niederwald

Rüdesheim, Germany

by Carsten Kettner

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(as approved by the participants)

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Participants

(in alphabetical order)

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Unfortunately absent

- Athel Cornish-Bowden, CNRS-BIP, Marseille, France,
- Dietmar Schomburg, Technical University Braunschweig, Germany

Introduction in STRENDA (for invited guests)

CK gave a short introduction in the STRENDA project, its roots and goals for invited guests who were not aware in detail of both the Commission and its missions, i.e.

- Development of experimental standard conditions;
- Definition of minimum information for reporting functional enzyme data (STRENDA Guidelines);
- Generation of a comprehensive data acquisition and storage system (STRENDA DB)

For further details, please refer to the web site of STRENDA, i.e. http://www.beilstein-strenda.org.

Report on past and future STRENDA activities

Suggestion

Antonio Baici (University of Zurich) to become appointed member of the STRENDA Commission.

After a short self-introduction from AB and explanation of the reasons for the appointment by CK, the Commission agreed to apoint AB a member of the Commission.

BioCatNet

BioCatNet is a database system for the integration of enzyme sequences and biocatalytic experiments and includes kinetic data from enzyme experiments. The difference between BioCatNet and STRENDA DB is that the data input in BioCatNet is carried out mainly using Excel sheets with time-course data. There is no GUI for query nor for data input. The first contact of CK with the Stuttgart-based PI (Jürgen Pleiss) showed that there are overlaps and synergies between both projects. More discussions are planned for the near future.

Promotion

on ResearchGate

- updates on the STRENDA project regularly published
- >800 reads, >90 followers

Presentations (given and planned)

- eScience Days, Heidelberg, March 2017
- Beilstein Open Science Symposium, May 2017
- [BC]2 Biological Computional Conference, Basel, September 2017
- MPDL Open Science Days MPDL, Berlin, October, 2017
- PTB, Braunschweig, November 2017

DOIs registered for STRENDA Guidelines

- List level 1A (Description of the Experiment): 10.3762/strenda.17
- List level 1B (Description of the Enzyme Activity Data): 10.3762/strenda.27
- Generic text on STRENDA Guidelines (for inclusion in instructions for authors by journals): 10.3762/strenda.3

Recommendations and Registrations

(a) STRENDA DB is recommended by

- Archives in Biochemistry and Biophysics
- Beilstein Journal of Organic Chemistry
- eLife
- Nature (including Biotechnology, Chemistry, Microbiology, Pharmacology, Systems Biology)
- PLoS (relevant journals, e.g. One, Biology, Computational Biology, Medicine)
- Scientific Data
- The Journal of Biological Chemistry

(b) STRENDA DB is registered with:

- re3data.org (Registrty of Research Data Repositories)

- OpenDOAR (Directory of Open Access Repositories)
- OpenAIRE (Collection of Open Access resources for results/data from EU-funded projects)
- FAIRsharing.org (successor of BioSharing.org, formerly MIBBI)

- STRENDA Poster (available at Materials to be used by the STRENDA Commission, http://www.beilstein-institut.de/en/projects/strenda/meetings)
- STRENDA slide (includes the most important information on the STRENDA project, to be included in regular presentations), also available at the URL given above.
- STRENDA T-shirts for all members of the Commission

Manuscript on STRENDA DB

NS guided through the pre-final version of the STRENDA DB manuscript to be submitted to FEBS J. A few paragraphs have been discussed and reformulated. Corrections for some figures have been sorted out and agreements have been made for improvements.

NS and CK will finalize the manuscript and submit it as soon as possible. SS suggested his graphics designer for the last polishing of the figures. This suggestion was accepted.

Note: the paper entitled "STRENDA DB: enabling the validation and sharing of enzyme kinetics data" as been published online after peer-review in March 2018.

https://febs.onlinelibrary.wiley.com/doi/epdf/10.1111/febs.14427.

STRENDA DB

Report, progress and comments

CK gave an overview of the general idea of STRENDA DB regarding both the data being captured and the workflow of interactions between authors, journals and STRENDA DB. In addition, he summarized the latest developments, i.e. mainly change requests, testing and

bug fixing since the last STRENDA meeting in September 2016. The system was launched in the last days of December 2016 and is fully operable since then. Data sets are coming in and are cited in publications as well.

A discussion was started by MH with regards to a quicker filling of STRENDA DB using data from recent publications in order to make STRENDA DB useful for the community. The more data are offered the more acceptance is the project gaining from the community. After a long discussion the Commission decided not to enter “old” data but only new, future data from coming publications. It was recognized that the number of datasets will increase more slowly when only new data are entered but this was accepted. MH made clear that the future support of STRENDA by Beilstein-Institut is dependent of the progress (in terms of number of data sets in the database) and success of the project. The Commission took note of this comment.

Simplification of terminology used (Experiment, ESS)

PH suggested to simplify the terminology used in STRENDA DB, in particular 'Experiment' to be renamed 'Enzyme' and 'Experimental Subset (ESS)' to be replaced by 'Conditions'. This issue was discussed and the Commission agreed to ease the input process as far as possible, in particular for first-time-users.

CK will check.

Result: A deeper investigation of the implications and consequences of the change of the terminology showed that the replacement of 'Experiment' by 'Enzyme' is fine but there are serious issues with the replacement of ESS. Thus, in a after-the-meeting electronic correspondence, the Commission agreed on replacing ESS by 'Dataset'. This modification was specified in a change request document and carried out subsequently by the IT specialists at Beilstein-Institut.

Extension: Inhibition and activation parameters (Modifiers)

AB gave an overview of inhibition and activation of enzymes and presented mathematical and graphical representations of 17 different inhibition and activation types. He proposes an extension of STRENDA DB which currently just can cover inhibition data for five linear inhibition mechanisms but leaving out any allosteric interactions. A detailed introduction along with many examples from the literature is provided on www.enzyme-modifier.ch.

In addition to his presentation, AB provides the Commission with detailed suggestions on how to modify STRENDA DB in order to enable the system to capture enzyme-ligand interaction data accurately and comprehensively (see appendix).

The Commission is not convinced that this extension will be a necessary one due to the following reasons (AFAIR):

- STRENDA DB already covers 80% of all enzyme data
- suggested terminologies do not strictly follow IUBMB recommendations (maybe true – but can be easily modified)
- not a use-case of the members of the Commission (but of clinical enzymologists)
- maybe too complicated, often users are not aware of the variety of modifying mechanisms (but help provided by STRENDA DB)

In order to broaden the potential target groups which will be invited to use and enter data in STRENDA DB the directors of the Beilstein-Institut decided to implement this extension proposed in a way that the user will have the choice between entering data following the current path or entering data on modified activities in a more detailed way.

Future plans

Manuscript on missing information in the literature

Initiated by PH and CK this manuscript is circulating within those in the Commission who are interested to contribute. Ideally, members of the Commission contribute with examples from own papers where important information has been overlooked to be included. This is considered an important indication that the members of the Commission are not impeccable, either. Finalization is expected in the first quarter 2018. CK will send a presubmission inquiry to first Science and then Biochemistry since publications from these journals have been inspected in detail. These journals should have the first chance to discuss with us on how to proceed. A joint publication with the editors-in-chiefs is well conceivable.