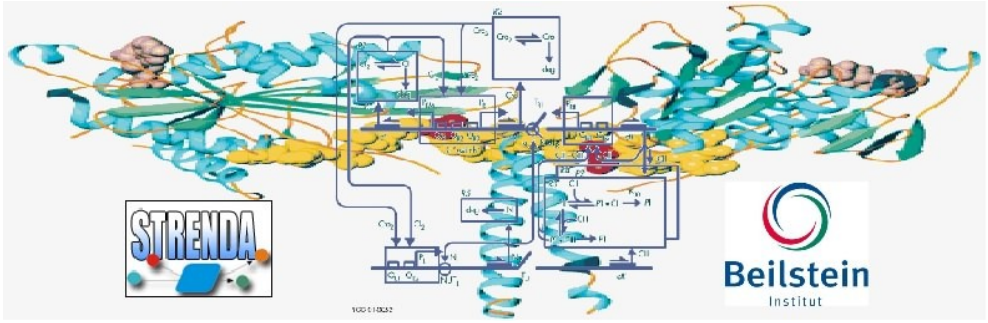

Minutes of the

STRENDA Meeting 2008

September 14th – 17th, Rüdesheim/Rhein, Germany

by Carsten Kettner

Agenda

(as approved by the participants)

1 Opening, Expectations and Aims
2 STRENDA Overview
3 STRENDA Checklists Level 1 A and B
4 Guidelines of the European Section of Applied Biocatalysis (ESAB, a task group of the European Federation of Biotechnology, EFB)
5 STRENDA Checklist Level 2
6 Checklists and guidelines to be adopted by journals
7 The electronic enzyme data submission system
8 Revised STRENDA Manuscript
9 4th ESCEC Symposium

Participants

(in alphabetical order)

- Richard N. Armstrong, Vanderbilt University, Dept. of Biochemistry, Nashville, TN, U.S.A.;
- Athel Cornish-Bowden, CNRS-BIP, 13402 Marseille, France;
- Gunter S. Fischer, Max Planck Research Unit for Enzymology of Protein Folding, 06120 Halle, Germany;
- F. Peter Guengerich, Dept. of Biochemistry, Vanderbilt University, Nashville, TN, U.S.A.;
- Peter Halling, University of Strathclyde, Dept. of Pure and Applied Chemistry, Glasgow G1 1XL, Scotland;
- Jan-Hendrik Hofmeyr, University of Stellenbosch, Dept. of Biochemistry, 7602 Stellenbosch, South Africa;
- Carsten Kettner, Beilstein-Institut, 60487 Frankfurt/Main, Germany (co-ordination);
- Thomas S. Leyh, The Albert Einstein College of Medicine, Dept. of Biochemistry, Bronx, NY, U.S.A.;
- Dietmar Schomburg, Technical University Braunschweig, Dept. of Bioinformatics and Systems Biology, 38106 Braunschweig, Germany;
- Willy Stalmans, Katholieke Universiteit Leuven, Afdeling Biochemie, B-3000 Leuven, Belgium;
- Christoph Steinbeck, EMBL Outstation – European Bioinformatics Institute, Hinxton CB10 1SD, United Kingdom;
- Roland Wohlgemuth, SIGMA-ALDRICH Chemie GmbH, CH-9470 Buchs, Switzerland;

Absent: Keith Tipton, Trinity College, Dept. of Biochemistry, Dublin 2, Ireland

Appendix:

(List of Attachments)

- Keith Tipton's suggestions for the meeting
- updated STRENDA checklists Level 1A and B
- Guidelines for reporting of biocatalytic reactions
- Subsets of the STRENDA guidelines for the electronic submission system

Expectations and Aims

The proposed agenda corresponded well with those topics which were of greatest importance to the participants with the exception of database related topics such as data quality, databases for enzyme assays, curation workflows, interoperability of databases and data semantics. Since these aspects would require a separate meeting there was general agreement to omit this subject from the discussions during the current meeting. The following topics and goals were suggested by the participants were covered by the agenda:

- closing discussion of the STRENDA checklists Level 1B and B („finalisation of the finalised checklists"),
- starting concrete discussions on Level 2,
- journal requirements, policies, formats and acceptance of checklists from the community,
- harmonisation and consolidation of various standards and recommendations,
- electronic data submission to databases and journals, rapid consideration of new enzymes,
- and a series of single aspects concerning structure-function relationships, enzymology teaching ways, data artefacts and reproducibility of experiments.

The overall goal of the meeting was to increase the visibility of STRENDA for journals and societies, hence the reason that members of editorial boards from journals (*Biochemistry*, *Journal of Biological Chemistry* and *Biological Chemistry*) as well as representatives from IUBMB and EFB were invited to attend the meeting.

STRENDA Overview

Carsten Kettner gave a brief overview of the STRENDA missions which include a long term vision i.e. the establishment of experimental standard conditions to ensure the generation of reliable, validated and comparable enzyme data and two shorter term visions namely, the definition of guidelines for good scientific publication and the generation of a comprehensive data acquisition system which takes into account the requirements stated in the STRENDA guidelines. It is obvious that STRENDA needs support and input from the scientific community, biochemical journals, funding agencies and scientific societies.

One of the major steps taken by STRENDA was to register with MIBBI. MIBBI is an acronym for „Minimum Information for Biological and Biomedical Investigations" and was initiated by Chris Taylor, Susanna-Assunta Sansone (both EBI, Hinxton) and Dawn Field (Natural Environment Research Council, Oxford). This project aims at – at a first glance – the improvement of communication, the transfer of knowledge and the integration between checklist developers. The standardization checklists which are in relative isolation to each other will be coordinated and made more visible.

Therefore, MIBBI considers itself as an integrated checklist ressource for the community to avoid repetitive re-invention of the „standardization" wheel. To support this ressource idea, a web-based, freely accessible site is maintained at EBI to develop in principle three kinds of reporting standards: Minimum information lists, syntax (formats), controlled vocabularies and ontologies (semantics). The MIBBI project is described in detail in Taylor *et al*., *Nat. Biotechnol.* 2008, **26**(8):889-896. Cooperation with the MIBBI project participants is still ongoing.

STRENDA Checklists Level 1A and 1B

Athel Cornish-Bowden described the STRENDA checklists Level 1A and 1B and. He commented and explained the individual aspects. The checklists were then discussed in terms of consistency of form and content, as well as the order and plausibility of the list entries. Some aspects were indicated as requiring minor changes. After introduction of the suggested changes both lists were approved by the participants and these are now regarded as „completed". The updated version of the lists will be published on the STRENDA web site and can alos be found as attachement of these minutes.

ESAB/EFB Guidelines for Reporting Biocatalytic Reactions

Peter Halling outlined the differences between the requirements for the description of experiments in applied biocatalysis and those for general enzymology.
The basic requirement of biocatalysis reactions in industrial applications is the availability of recipes that fully describe reproducible processes. The emphasis in these reactions is reproducibility of reactions as opposed to full characterisation of the enzymes used. Therefore, for example, biocatalysts do not need to be identified through their reactions but simply from their commercial product codes. Since there are examples where impurity are crucial for successful reactions, crude or impure enzymes are acceptable. For any reaction it is valuable to compare the results obtained with alternative catalysts or reaction conditions. Thus when searching for the optimal conditions, wide ranges of operating conditions are studied which often lead to compromises between activity and stability. These conditions include unusual rather than physiological conditions with both high substrate concentration (e.g. 3 M) used and high product concentrations obtained. Non-physiological conditions such as the use of non-aqueous media - organic solvents, gases, supercritical fluids and ionic liquids – can also be investigated. The same considerations can be extended to both immobilised enzymes for which a proper description of the preparation together with the results of characterisation are required and for multi-phase systems that need efficient agitation. Further details on the requirements and proposed guidelines are provided in the corresponding attachement.

Even although applied purposes must address other issues for system description other than basic functional enzymology due to their different aims, there is a common intersection of requirements when catalytic reactions are reported.
During their efforts to create guidelines for reporting biocatalytic reactions the working group set up by the ESAB noted that – in addition to a number of publications which deal specifically with some of the biocatalysis issues - the STRENDA group was also aiming to set up guidelines for reporting enzymology data. In the course of the current STRENDA meeting discussions were held about possible co-operations to create data reporting guidelines that would meet the needs for all scientists working with enzymes. The participants reached a general agreement to co-operate closely with the ESAB and consequently, have extended an invitation to the ESAB for the admission of a representative of the ESAB group to join the STRENDA group. This person will be nominated on the forthcoming ESAB meeting in January 2009.

STRENDA Checklist Level 2

The participants were in agreement that the diverse groups concerned with functional enzymology of certain organisms would have different views on standards of experimental conditions. For example, plant systems biologists require different standardized protocols than those working with micro-organism or human cells. For this reason it was suggested that representatives from the various systems biology consortia such as YSBN, SysMo, HepatoSys, BRAIN, E.coli, Arabidopsis etc. should be invited to give a talk at the forthcoming ESCEC Symposium in September 2009. Moreover, it was also suggested that pharmaceutical companies, groups involved with drug metabolism and biodegradation should be invited to give their views. Short discussions of around 15 minutes duration to present an overview of the possibilities and impossibilities of standardizing experimental procedures are envisaged. It is anticipated that these people will also provide helpful advice during the discussions to create a draft version of the Level 2 checklist.
Furthermore, it will be proposed that STRENDA could co-ordinate the works on this checklist. This may result in the creation of one organism-independent Level 2A list and several organism-dependent Level 2B lists, both in close contact to the communities.

Adoption of the STRENDA Guidelines by Journals

The question was discussed how journals – better: the editorial boards of the journals – could be convinced to adopt the STRENDA guidelines in their instructions to authors. It was some surprise and delight that we learned that the editorial board of JBC has adopted the STRENDA guidelines in May 2008 in their instructions to authors (http://www.jbc.org/misc/ifora.shtml#_Enzyme_Activity_Data).

It is hoped that further journals will follow. This process could be accelerated by direct contact of STRENDA with the editors and by the active demand of the community that functional enzyme data in publications should be standardized.

Action: Tom Leyh will compose a letter on behalf of STRENDA presenting the recommendations of the working group. After approval by STRENDA, the letter will be sent to the editors of selected biochemistry journals.

Action: Richard Armstrong and Fred Guengerich will write a letter on behalf of the scientific community to biochemistry journals to express the demand mentioned above.

Action: Carsten Kettner will check the access log file of the STRENDA web site to see if access has increased after the adoption of the lists by JBC.

Action: All, check the instructions to authors in the major biochemistry journals

The question remained open as to whether the journals require to make the consideration of checklists by the authors mandatory or optional.

However, authors should be encouraged to download the lists from the STRENDA web-site (www.strenda.org/documents.html). The participants were in complete agreement that the checklists must keep the balance between setting the definitions at too rigorous a level and too low a level. To increase the possibility that the rules will be observed, they need to be as "painless" as possible to avoid friction. This could be done by providing an Excel sheet to authors and editors that contains the checklists definitions which can be filled in with the determined data.

Since the STRENDA checklists require higher visibility to be accepted by the community the following suggestions were made:

- creating a brochure about STRENDA for conferences;
- presentation of the guidelines on meetings, e.g. FEBS Meeting in Prague (Czech Republic), July 2009, and IUBMB congress in August 2009 in Shanghai (China);
- further discussion at the 4th ESCEC Symposium in September 2009 in Ruedesheim (Germany);
- providing a brochure/flyer on STRENDA at the Biotrans Conference, held in Bern (Switzerland), July 2009 and at selected Gordon Conferences (Richard Armstrong is willing to leave the flyer there).

Electronic Data Submission System

The second short-term vision of STRENDA is to define the requirements for the deposition of data in journals and databases (as mentioned above). The objective is to develop a comprehensive data acquisition system that allows authors to submit electronically their experimental data to public databases prior to publication (see also: Apweiler et al. *Trends*

Biochem. Sci., 2005, **30:**11-12; PMID: 15653320). Co-operations with journal editors and publishers should ensure that a commonly accepted design will be created which enables both databases producers and journals to access functional enzyme data.

Dietmar Schomburg gave a brief overview of the information stored in the BRENDA database to point out on the one hand grade of coverage of the STRENDA guidelines by the database's data structure and the requirements that should be fulfilled by an electronic data submission system. An existing draft of an submission system, developed by Schomburg's group at the University of Cologne in 2006, is online and is accessible at https://strenda.bioinfo.nat.tu-bs.de/strenda2/index.php?option=com_wrapper&Itemid=8. Dietmar Schomburg also introduced the participants the process of data input. This data submission system is intentionally ver close to the structure and content of the STRENDA guidelines. A discussion about this draft on the 2007 ESCEC Symposium resulted in a few strong points which are worth to be considered during the subsequent development.

- too complicated to be used
- too many fields to be entered
- how to make use by scientists easier?
- How to convince scientists to enter their data prior/after publication?

Due to the 1:1 implementation of the submission system according to the guidelines, the first two points and – in principle the third point, too - are easy to asnwer. The fourth point poses more of a problem.

At the STRENDA meeting the participants agreed that any processes to enter data into forms must be less time-consuming and must not constitute a burden for the authors. The following points were raised:

- *What is missing?*
  - → figures and diagrams in a machine-readable format (required meta data);
  - → auto-save function upon tab switching (tab = sub-menu line on top of the forms)
  - → default values are not specified
  - → offline data input in downloaded (Excel?) sheets; these files can be uploaded in the system and automatically read.

- *Which fundamental data is the user interested in?*

This question led to the decision to create three subsets of the STRENDA guidelines. The form has in total three subsets – „required", „recommended", „optional" data – and are individual tables. The user can decide in which detail she/he will enter her/his functional data. The „required data" will compose the mandatory data basis which can be extended by further available functional data. „Recommended data" will both help the referees to keep in mind what data may be missing and support the addition of any missing data by the authors. „Optional data" are nice-to-have data.

The selection of the appropriate aspects from the lists was made immediately after the discussions and are provided in the corresponding attachement.

Actions: Dietmar Schomburg will be concerned with the modification of the technical platform of the presented submission form within about two months upon approval of these minutes. After the implementation has been finished, he will notify the participants of this STRENDA meeting for evaluation and tests. Test reports will be sent to Dietmar Schomburg to be considered for further adjustments.
Note that this system is not yet in use, so it is still possible to introduce either minor changes or to re-build the system completely.

Actions: to inform the scientific community a manuscript will be prepared to present this submission system (who? - n.d.). A brief article will be submitted to *ASBMB Today* immediately after the main manuscript appears in print. It was suggested that the submission tool should to be advertised on the SIGMA-Aldrich web page.

- *How to convince users to enter data/to contribute?*

This question has not been answered in a satisfactory way that any meaningful action could be instigated. There some consensus that all groups involved in publication: authors, referees, editors and readers/users must be involved. The participants were in agreement that the potential advantages of such a submission tool appear to be dependent on an increased contribution of the users – a classical hen-and-egg problem. The more users submit their data in a structured way by using the submission tool the more the users will benefit from the entered data and then hopefully, the more users will participate. This seems to be a self-regulating and self-motivating system and therefore providing this tool appears to be a worthwhile excercise.

The Revised STRENDA Manuscript

Dietmar Schomburg (as corresponding author) reported the evolution of the STRENDA manuscript which describes the pre-requisites for the development of the guidelines, presents the guidelines themselves and introduces the idea of an electronic submission system for functional enzyme data. Acting on a suggestion by Rolf Apweiler, the manuscript was submitted to *Nature Biotechnology* (NBT) in fall of 2006 since at that time NBT decided to give the diverse standardization groups a platform. Dietmar Schomburg received comments from six reviewers to which the group responded. However, the editor of NBT insisted that the responses should be included in the manuscript. After this was done subsequent contacts with the editor have proved disappointing.
Recently, Keith Tipton took over the work on the manuscript and presented a revised version which was discussed at the STRENDA meeting.

The group greatly appreciated the efforts spent by Keith Tipton but the general opinion was that we should focus on just one issue (as KT argues himself, see his suggestions),

i.e. the STRENDA guidelines and ensuring data quality. It was suggested that the data submission issue should be put into another manuscript (see above). It was also noted that we should weaken the focus on the systems biology community and to concentrate more the entire enzymology / biochemistry community.
There was also general agreement that only persons who contributed to the manuscript will be listed as authors. Alternatively, contributors and supporters could be acknowledged according to NBT.

Actions: Tom Leyh will contact first the editor of *Nat. Biotechnol.* for reasons and comments on our last version of the manuscript. Provided with this information he will revise the manuscript according to the suggestions made by the group.

4th ESCEC Symposium

The 4th ESCEC Symposium will be held 13th to 16th September, 2009 in Ruedesheim. One focus will be on the discussion of possible ways to standardize the experimental conditions. Considering this topic it was suggested to invite speakers from diverse systems biology groups such as Drosophila ("fly"), C. elegans, E. coli, SysMo, Brain, HepatoSys etc. Carsten Kettner, the organizer of this symposium, asked for suggestions for further speakers.

Appendix

1 Keith Tipton's Suggestions for the Meeting

STRENDA – Some thoughts on the way forward

In going through the reviewers' comments on our Nature Biotechnology submission, it was clear that several of their points reflected a lack of clarity in our own objectives. The simple goal of standards for reporting enzyme data has become confused by mixing it up with the desires of the systems biologists to define organism standard conditions, and the databases, which would like to be able to import their data directly. As a result we have ended up trying to do everything at once, whereas it might have been better to have concentrated on the completing and 'marketing' the main objective, before considering the other aspects. That would have established the reputation of STRENDA and avoided a lot of criticism.

Some of the reviewers seemed to feel that we were trying to coerce research workers to obey the dictats of systems biologists. We must make it clear that we accept the there are several reasons for studying an enzyme that do involve using physiological conditions – all we can do is to establish guidelines for those who would like their results to be useful for this wider application. We should try to identify appropriate systems biology groups, working with different organisms and send them a copy of our Level 2 document asking them to provide suitable assay conditions and suggest any other material that should be included. It is hopeless simply relying on individuals accessing our web pages. Jannie, and others, should be able to suggest some suitable systems biologists and we may find other groups through Carsten's MIBBI contacts.

A common feeling amongst those who do experiments is that their work is already time-consuming and it is unreasonable to suggest that they should do additional work just to make life easier for the database people. We must recognize those feelings and accept that researchers will only enter data if they think it worth their while to do so. They will certainly not wish to waste their time completing overly complex web forms. While it is far from perfect, the Kineticon approach of asking what type(s) of information is to be added and then providing tailored entry forms should be investigated.

A final thought is that the limericks should be removed from the STRENDA homepage. They do not convey the impression that we take our task seriously and, worse, they can be taken to imply that STRENDA is not really independent but simply a tool of BRENDA, which was an inference that drew adverse comment from some of the reviewers.

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2 Updated STRENDA Checklists Level 1A and B

Level 1, List A:

Required data for the methods section for publishing of enzyme activity data.

The data are required to allow the reproducibility of the results.

Version 1.5
Date: October 9th, 2008

Data	Comments
Identity of the enzyme	
Name of Reaction Catalyst	Name, preferably the accepted name from the IUBMB Enzyme List
EC number	
Sequence accession number	
Organism/species & strain	
Isoenzyme	
Additional information on the enzyme	
Tissue/organelle	
Localization	Within cell or experiment? Specify what localization is based on
Post-translational modification	Add only when determined
Preparation	
Description	*e.g., commercial source, procedure used or reference*
Artificial modification	*e.g. Truncated, His-tagged, fusion protein, lacking native glycosylation*
Enzyme or protein purity	purity defined by which criteria. Specify whether protein or enzyme was purified. *e.g., apparently homogeneous by PAGE, crude mitochondrial fraction, determined by MS*
Substrate purity	Determine origin of substrate
Assay Conditions	

Data	Comments
Measured reaction	as a stoichiometrically balanced equation.
Assay temperature	
Assay pressure	If it is not atmospheric; indicate if not aerobic
Assay pH	Description of confirmation
Buffer & concentrations	*e.g., 100 mM Tris-HCl, 200 mM potassium phosphate*
Metal salt(s) & concentrations	*e.g., 10 mM KCl, 1.0 mM $MgSO_4$*
Other assay components	*e.g., 1.0 mM EDTA, 1.0 mM dithiothreitol*
Coupled assay components	If relevant
Substrate & concentration ranges	*e.g., 1 - 100 mM glucose, 5 mM ATP*
Enzyme/protein concentration	Molar concentration if number of active sites known, otherwise mass concentration. *e.g. nmol ml^{-1} or mg ml^{-1} or better: µmol l^{-1} or g l^{-1}*
Variable components	
Total assay mixture ionic strength	
Activity	
Initial rates of the reaction measured	Determine how established
Proportionality between initial velocity and enzyme concentration	If available
Specific activity	Units necessary: Expressed as amount product formed per amount enzyme protein present - sometimes referred to as enzyme unit or international unit (1 U = 1 µmol min^{-1}). The katal (mol/s) may alternatively be used as a unit of activity (conversion factor 1 unit = 16.67 nkat).
Methodology	
Assay method	a literature reference may suffice for an established procedure that is used without modification
Type of assay	*e.g., continuous or discontinuous, direct or coupled*
Reaction stopping procedure	in the case of discontinuous assays
Direction of the assay	With respect to the reaction equation provided *e.g., NAD reduction by alcohol dehydrogenase; alcohol + NAD^+ → aldehyde or ketone + NADH + H^+*
Reactant determined	*e.g., NADH formation, O_2 utilization*

Data	Comments
Reaction stoichiometry	*e.g., 2 mol substrate oxidized per mol O_2 consumed*
Additional material desirable	
Free metal cation concentrations	e.g. *of Mg^{2+} and Ca^{2+}*
Reaction equilibrium constant K	Define conditions and reaction direction

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Level 1, List B

Additional information required for reporting enzyme kinetic data.

The information is required to allow a quality check on the data and to ensure their value to others.

Version 1.5
Date: October, 9th, 2008

Information required	Comments
Required data for all enzyme functional data	
Number of independent experiments	Problems of reproducibility?
Indication of accuracy	*e.g. standard error of the mean, standard deviation, confidence limits, quartiles*
Specification whether relative to subunit or oligomeric form	
Data necessary for reporting kinetic parameters	Units necessary:
V_{max}	V_{max} given as units or katal, as defined in List 1,
k_{cat}	V_{max} may be divided by the specific activity units (moles per unit time per unit enzyme mass) of the enzyme to give k_{cat}, measured in s^{-1} or min^{-1}
k_{cat}/K_m	k_{cat}/K_m given as per time per concentration, *e.g.* $s^{-1}.mM^{-1}$
K_m	Units necessary
$S_{0.5}$	Both are concentrations*, e.g. mM*
Hill coefficient, saturation ratio (R_S) or other coefficients of cooperativity	
How was the given parameter obtained?	*e.g. non-linear curve fitting using least squares, non-parametric method such as direct linear plot, linear regression to transformed form of rate equation* **Note**: The use of linear transformations for determining Michaelis-Menten parameters is recognised to be inaccurate.

Information required	Comments
s/K_m range used	*e.g. 0.1 to 10*
Model used to determine the parameters	With explanation of why is the chosen model considered to be the “right“ model
High-substrate inhibition, if observed, with K_I value	
Data required for reporting inhibition data	
Time-dependence and reversibility	With method described
For reversible inhibitors: type and K_I *values*	*e.g. competitive, uncompetitive, etc.,* With units and how values were determined
For tight-binding inhibitors: association/dissociation rates, *inhibition type and* K_I *values*	Units necessary
For irreversible inhibitors: type Appropriate kinetic parameters	*e.g., non-specific, mechanism-based, "suicide substrate”.* There are too many alternative parameters to list here. The reference to a quite comprehensive source is recommended: *Enzymes:Irreversible Inhibition*. Tipton, K.F. In: *Nature Encyclopedia of Life Sciences* London, (2001). http://www.els.net/ [doi:10.1038/npg.els.0000601] **NOTE:** IC_{50} values These have been used for both reversible or irreversible inhibition. However the use is not recommended because these values are without a consistent meaning. The relationship of these values to inhibition constants is analysed in detail e.g. by Cortes, A. *et al.* (2001) *Biochem. J.* **357**:263-268.
Data required for reporting activation data	Similar to the requirements for inhibition data
Additional material desirable	
Kinetic mechanism	*e.g. ordered bi-bi,*
Data for cooperative behaviour: model used	With equation given *e.g. Monod-Wyman-Changeux, etc.*
Time-dependency of enzyme reactions	i.e., duration of initial-rate conditions at defined substrate concentrations etc.
Example of at least one experiment together with raw data	

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3 Guidelines for Reporting of Biocatalytic Reactions (EFB-ESAB)

Draft for checklist

Description of the reaction system used

- Specify all concentrations present in the actual reaction medium pH
- pH electrode calibration basis
- Temperature
- Pressure (if not atmospheric)
- Nature of biocatalyst specified unambiguously, including any additives
- Available information on impurities in biocatalyst, post-translational modifications, etc
- Amount or concentration of biocatalyst presented on clear basis
- For non-aqueous media (e.g. based on organic solvents, ionic liquids, gases, supercritical fluids), residual water content or water activity
- For any system that is not certainly single phase - agitation conditions

Reporting on the reaction progress

- Termination procedure for stopped assay
- Specify what concentration(s) are actually measured
- Which phase(s) analysed if multiple
- Evidence of linearity if rates estimated from single time point
- Other observations on reaction mixtures, e.g. phase separation

Presentation and analysis of kinetic data

- Rates presented on scale independent basis (e.g. biocatalyst specific activity units)
- Biocatalyst amount basis clear
- Reference rate specified if others shown relative
- Rates compared with best known alternative?

- Acceptable method for fitting kinetic models
- Appropriate model discrimination tests
- Implied comparison clear in statements on specificity/selectivity
- Show E values, not just ee

Reporting of stability studies

Clear statement of conditions for both:

- pre-treatment
- assay

(especially critical when different)

Reproducibility

Measure of scatter and numbers performed for

- replicate sample analyses
- replicate reactions

Clear basis for error estimates in parameters from whole data sets <back to l.o.a.>

4 Subsets of the STRENDA Guidelines for the Electronic Data Submission System

4.1 Required Data

Description of the Experiment (Level 1A)

	Comments
Identity of the Enzyme	
Name of Reaction Catalyst, EC number	
Organism/species & strain	
Additional Information on the Enzyme	
Tissue/organelle	If applicable
Localization	If applicable
Preparation	
Description	
Artificial modification	
Enzyme or protein purity	
Assay Conditions	
Measured reaction	
Assay temperature	
Assay pressure	If it is not atmospheric; indicate if not aerobic
Assay pH	

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Description of Enzyme Activity Data (Level 1B)

	Comments
Required Information for All Functional Enzyme Data	
Indication of accuracy	
Data necessary for Reporting Kinetic Parameters	As many of these parameters as measured
V_{max}	
k_{cat}	
k_{cat}/K_m	
K_m	
$S_{0.5}$	
Hill coefficient, saturation ratio (R_s) or other coefficients	
How was the given parameter obtained?	
s/K_m range used	
Model used to determine the parameters	
High-substrate inhibition, if observed, with K_I value	
Data Required for Reporting Inhibition Data	
Time-dependence and reversibility	
For reversible inhibitors:	
Type and KI values	
For tight-binding inhibitors:	
association/dissociation rates, inhibition type and K_I values	
For irreversible inhibitors: type	
Appropriate kinetic parameters	
Data Required for Reporting Activation Data	Similar to the requirements for inhibition data

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4.2 Recommended Data

Description of the Experiment (Level 1A)

Identity of the Enzyme

Sequence accession number

Isoenzyme

Required Information for All Functional Enzyme Data

Number of independent experiments

Preparation

Substrate purity

Assay Conditions

Buffer & Concentrations

Metal salt(s) & concentrations

Other assay components

Substrates & concentration ranges

Enzyme/protein concentration

Coupled assay components — If relevant

Variable components

Activity

Specific activity (indicate substrate and concentrations)

Initial rates of the reaction measured

Proportionality between initial velocity and enzyme concentration

Methodology

Assay method

Type of assay

Reaction stopping procedure

Direction of the assay

Reactant determined

Reaction stoichiometry

4.3 Optional Data

Description of the Experiment (Level 1A)

Additional Information on the Enzyme

Post-translational modification

Additional Material Desirable

Total assay mixture ionic strength

Free metal cation concentrations

Reaction equilibrium constant K

Activity

Initial rates of the reaction measured

Proportionality between initial velocity and enzyme concentration

Description of Enzyme Activity Data (Level 1B)

Required Information for All Functional Enzyme Data

Specification whether relative to subunit or oligomeric form

Additional Material Desirable

Kinetic mechanism

Data for cooperative behaviour: model used

Time-dependency of enzyme reactions

Example of at least one experiment together with raw data

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