STRENDA Guidelines Level 1B

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as approved on 30th November 2021

The STRENDA Commission (Standards for Reporting Enzymology Data) compiled the following Guidelines, as a service to the community, to define the minimum amount of information that should accompany any published enzyme activity data.

The current STRENDA Guidelines (List Level 1B) was reviewed on the STRENDA meeting in November 2021 in terms of consistency of form and content, as well as of the order and plausibility of the list entries. In addition, it now includes recommendations for reporting on the accuracy and deposition of data as well as those parameters which should be reported when equilibrium measurements have been performed.

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defines those data that are required to allow a quality check on the data and to ensure their value to others. In principle, this is the minimum information to describe enzyme activity data.

Information required	Comments
Required data for all enzyme functional data	
Reproducibility, number of independent experiments	Indicate how many times the measurement was reproduced and what changed between replicates; just repeat reactions, different enzyme preparations, different ways, alternative staff, different laboratories
Precision of measurement	e.g., standard error of the mean, standard deviation, confidence limits, quartiles. Comments on possible systematic errors are also useful.
Specification whether relative to subunit or oligomeric form	

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Information required	Comments
Preferably deposit measured/raw data (e.g., time course of product concentrations) to enable re-analysis	Make data findable by citing DOI or URL, accessible by making it open, interoperable by structuring and describing the data by using formats such as EnzymeML
Data necessary for reporting kinetic parameters	(choose which ones are available from your experiments)
Kinetic equation (which will then define parameters)	Name or state the model or equation used and the variable in it, e.g., Michaelis-Menten, varying concentration of ATP, fixed glucose or $v = V_{max} / (1 + K_A/[2\text{-aminopropane}] + K_B/[2\text{-butanone}])$
k_{cat}	V_{max} in terms of mol reaction per mol enzyme per time, so units often reported as s^{-1} or min^{-1}
V_{max}	Should be as a specific activity, with units like mol min^{-1}(g enzyme)$^{-1}$, or (mol product) min^{-1} (g protein in the preparation)$^{-1}$, *see* List Level 1A
k_{cat}/K_m	k_{cat}/K_m given as per concentration per time e.g., $mM^{-1}s^{-1}$
K_m	units or concentration necessary, e.g., mM, define how K_m was defined operationally (e.g. as $S_{0.5}$)
$S_{0.5}$	concentration, e.g., mM
Hill coefficient, saturation ratio (RS) or other coefficients of cooperativity	with equation defining the parameter as noted above
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:** if commercial computer programs are used, determine which were used
K_{M2}	Michaelis constants for all co-substrates, inclusive the coenzymes

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Information required	Comments
K_P	K_m for reverse operation or product inhibition constants (with equation above showing definition). This is for all products inclusive of cofactors. If information is absent, indicate at what product concentrations there was no effect on enzyme rate.
Choice of model used to determine the parameters	Report any measures of quality of fit, and for any alternative models considered.
High-substrate inhibition, if observed, with K_i value	with defining equation above
Data required for reporting inhibition data	
Time-dependence and reversibility	with method described
Inhibition	K_i units necessary
types:	
reversible	e.g., competitive, uncompetitive, etc., with units and how values were determined
tight-binding	association/dissociation rates; estimates OK if small
irreversible	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. McDonald, A.G. & Tipton, K.F. In: Nature Encyclopedia of Life Sciences London (2020). doi:10.1002/9780470015902.a0000601.pub3
	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 details, e.g., by Cortes, A. *et al.* (2001) *Biochem. J.* **357**:263-268. doi:10.1042/bj3570263
Data required for reporting activation data	similar to the requirements for inhibition data

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Information required	Comments
Data required for reporting equilibrium measurement	See further details in IUBMB document: Alberty R.A. *et al.* (2011) *Biophys. Chem.* **155**:89-103. doi:10.1016/j.bpc.2011.03.007
Measured equilibrium concentrations	preferred that these are tabulated
K_{eq}' or K' (i.e. the pH dependent equilibrium constant)	with reference to full reaction equation presented and direction identified.
	with units where not symmetrical, e.g. M, mM^{-1}, mol kg^{-1} (molality). Explain any reactants not treated by way of dissolved concentrations, e.g., water, gases as partial pressures, activities for reactants not behaving as infinitely dilute.
	Estimates of equilibrium constants may sometimes also be obtained by fitting to kinetic (progressive) data. If so, follow the recommendations as for other kinetic parameters, including stating the equation fitted.
Convention used	by default assume biochemical convention using total concentrations of ionising or complexing compounds. But state clearly if using defined chemical species.

About the STRENDA Commission:

The STRENDA Commission is formed by an international panel of highly-regarded scientists who bring in diverse expertises such as biochemistry, enzyme nomenclature, bioinformatics, systems biology, modelling, mechanistic enzymology and theoretical biology.

The Commission was founded in 2003 and is supported by the Beilstein-Institut since then.

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More information: www.beilstein-strenda.org