STRENDA Guidelines Level 1A

Version 1.8 doi:10.3762/strenda.18

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 1A) 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, a few essential parameters for the measurement of equilibrium constants are now included.

List Level 1A
defines data that are recommended for the methods section for publishing enzyme data.
This information should allow the reproducibility of the results.

Data	Comments
Identity of the enzyme	
Name of reaction catalyst	name, preferably the accepted name from the IUBMB Enzyme List
Fully balanced chemical reaction equation	elements and charges balanced. See convention in R.A. Alberty “Thermodynamics of Biochemical Reactions”, doi:10.1002/0471332607
EC number	
Oligomeric state	number of different subunits
Sequence or sequence accession number	
Organism/species & strain	NCBI Taxonomy ID
Additional information on the enzyme	
Isoenzyme	naturally occurring variant or indication of selection of alternative
Tissue	
Organelle	
Localization	within cell. Specify what localization is based on

STRENDA Guidelines Level 1A

Data	Comments
Post-translational modification	add only when determined
Preparation	
Description	e.g., commercial source, procedure used or reference along with modifications
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
Metalloenzyme	mutant, content, cofactors
Storage Conditions	
Storage temperature	if frozen, freezing method, *e.g.*, -20 °C flash
Atmosphere if not air	
pH	e.g., 7.0
At which temperature was the pH measured?	e.g., 25 °C
pH-Buffer & concentrations (including counter-ion)	e.g., 200 mM potassium phosphate, 100 mM HEPES-KOH. If pH is adjusted by addition of acid or base not shown in buffer name, make this clear – e.g., 50 mM sodium acetate adjusted with HCl.
Metal salt(s) & concentrations	e.g., 10 mM KCl, 1.0 mM $MgSO_4$
Other components	e.g., 1.0 mM EDTA, 1.0 mM dithiothreitol, 10% v/v glycerol, 20% w/w DMSO, 1 mg/ml PEG2000, 2 mg/ml BSA, peptidase inhibitors
Enzyme/protein concentration	molar concentration if known, (quote assumed molar mass), otherwise mass concentration, e.g., µM or mg ml^{-1}
Optional: Statement about observed loss of activity under the above conditions	e.g., less than 10% loss after 1 month

STRENDA Guidelines Level 1A

Data	Comments
Statement about the thawing procedure	e.g., on ice
Assay Conditions	
Identity and purity of all assay components	identified unambiguously, ideally by reference to ID from database (such as PubChem, ChEBI), or using a textual identifier (such as InChI) and/or showing chemical structure (or SMILES). Origin of compounds used with statement on purity.
Measured reaction	as a stoichiometrically balanced equation e.g., 2 mol substrate oxidized per mol O_2 consumed, with all products identified
Assay temperature	
Assay pressure	if it is not atmospheric; indicate if not aerobic
Atmosphere if not air	
Assay pH	How was it measured?
Buffer & concentrations	e.g., 100 mM Tris-HCl, 200 mM potassium phosphate, including counter-ion. If pH is adjusted by addition of acid or base not shown in buffer name, make this clear – e.g., 50 mM sodium acetate adjusted with HCl.
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 known, otherwise mass concentration. e.g., mg ml^{-1} or better: µM
Varied components	e.g., inhibitor concentration
Total assay mixture ionic strength	
Activity	

STRENDA Guidelines Level 1A

Data	Comments
Initial rates of the reaction measured	determine how established, estimate ranges in substrate/product concentrations at the last data point. e.g., true initial tangent or average over specified time
Proportionality between initial velocity and enzyme concentration	if available
Enzyme activity	Ideally k_{cat} (i.e. V_{max}/enzyme concentration), otherwise expressed as amount product formed per amount enzyme protein present per time unit. Activity is sometimes reported as enzyme unit or international unit (1 IU = 1 µmol min^{-1}). The katal (mol/s) may alternatively be used as a unit of activity (conversion factor 1 unit = 16.67 nkat). Specify at which (range of) enzyme concentration(s) this was determined.
Equilibrium measurements	
Evidence that reaction reached equilibrium	e.g., approached from both (or all if multiple substrates/products) directions
State which of all reactants were measured directly	e.g., glucose phosphate and glucose measured directly, excess phosphate estimated by mass balance
Range of starting material and product concentrations in the experiment	ideally a table of all initial and measured equilibrium concentrations
Complexing metal ions	if the reaction involved species that might bind these (e.g., phosphate esters), essential to report estimated pMg and/or pCa
Methodology	
Assay method	a literature reference may suffice for an established procedure but any modification should be detailed
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
Additional material desirable	
Free metal cation concentrations	e.g., of Mg^{2+} and Ca^{2+}, specify how calculated

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.

Members of the Commission are: **B.M. Bakker** (University Medical Center Groningen, The Netherlands), **A. Cornish-Bowden** (CNRS-BIP, Marseilles, France), **P. Fitzpatrick** (University of Texas Health Science Center at San Antonio, San Antonio, TX, USA), **P. Halling** (University of Strathclyde, Glasgow, UK), **T.S. Leyh** (The Albert Einstein College of Medicine, Bronx, NY, USA), **A.G. McDonald** (Trinity College Dublin, Ireland), **M. Neumann-Schaal** (Leibniz Institute DSMZ, Braunschweig, Germany), **C. O'Donovan** (EBI, Cambridge, UK), **J. Pleiss** (University of Stuttgart, Germany), **F.M.Raushel** (Texas A&M University, College Station, TX, USA), **J.M. Rohwer** (University of Stellenbosch, South Africa), **S. Schnell** (University of Notre Dame, IN, USA), **N. Swainston** (The University of Liverpool, UK), **M.-D. Tsai** (Academia Sinica, Taipeh, Taiwan), **K. Tipton** (Trinity College, Dublin, Ireland), **H.V. Westerhoff** (Universities of Amsterdam, The Netherlands), **U. Wittig** (Heidelberg Institute of Theoretical Studies, Germany) **R. Wohlgemuth** (Lodz University of Technology, Poland) and **C. Kettner** (co-ordination, Beilstein-Institut, Frankfurt, Germany).

More information: www.beilstein-strenda.org