

Revision 1.1, Last updated: November 08, 2021

- » *Chem Catalysis* has compiled these checklists to foster improved rigor and reproducibility in research and increased clarity and transparency in data reporting.
- » Authors are encouraged to include the completed checklists as supplemental information at the time of submission. The checklists will be included in the supplemental information of published articles.
- » Rather than check off all items on the list, authors should mark only those items that apply to their article.

The following checklists are relevant for this manuscript:

General catalysis checklist

Please note: the general catalysis checklist should be completed for all submissions, including those with biocatalysts, electrochemistry, and photocatalysts

Biocatalysis checklist

Electrochemistry checklist

Photocatalysis checklist

Sustainability remarks

"Principles of green chemistry" have been considered in designing and conducting the research

For more information, please see <https://www.acs.org/content/acs/en/greenchemistry/principles/12-principles-of-green-chemistry.html>.

I verify that, to the best of my knowledge, this form is completed accurately in agreement with all co-authors

Submitting author name:

For general queries or feedback regarding this form, please email catalysis@cell.com

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Catalyst synthesis

Novel methods are provided in full detail
Chemical vendor provided if catalyst was purchased

Comprehensive literature references are included if the synthesis has been previously reported

Catalyst and new materials characterization

Elemental analysis
NMR spectroscopy
High-resolution mass spectrometry (HRMS)
Infrared spectroscopy
Crystallography
Phase and crystallinity
Morphology
Chemical composition of the catalyst

Thickness analysis for two-dimensional materials
Particle size and size distribution
Characterization and analysis of pore size
Exposed facets and orientation
Defect structure
Analysis of edge or vertex sites
Analysis of valence state
Data are available in a repository

Catalyzed reaction

Reaction conditions and complete experimental procedure provided
Size and type of reactor (e.g., flow, batch, semi-batch)
Operating temperature
Operating pressure
Solvent

Catalyst loading (mass and/or concentration and reaction volume)
Atmosphere
Mass balance
Reactant concentration at the beginning of reaction
Mass and/or heat transfer and mixing effects

Catalytic activity

Reaction kinetics
Turnover frequency
Turnover number

Product selectivity
Space-time yield
Kinetics of deactivation

Catalyst stability assessment

Long-term stability test, including test conditions
Recyclability test
Catalyst identity, loading, or purity were assessed post reaction (e.g. SEM, TEM, XRD, ICP, etc; details provided)

Control and benchmarking experiments

Reaction without catalyst
Reaction without additives
Benchmarking table or figure (either other catalysts investigated in this study or previous literature reports with references)

Product or compound characterization

Identity

Integrated ^1H and ^{13}C NMR spectra provided
Multiplicity and coupling constants provided in-text
Other NMR experimentation provided
High resolution mass spectral data
Infrared (IR) absorption spectroscopy
UV-vis spectroscopy
Chiral chromatography (GC and/or HPLC)
X-ray diffraction (powder and/or single crystal)

Purity

Isolated yields
High-field ^1H NMR spectra
1D proton-decoupled ^{13}C NMR spectra
Combustion elemental analysis
Quantitative GC or HPLC analytical data
Electrophoretic analytical data
Sequence (biomacromolecules)
Dispersity (polymers)

Quantification and statistical analysis

The paper reports statistical analysis

There is a statement as to what (if any) methods were used to determine if the data met the assumptions of the statistical approach

The statistical parameters (e.g., exact value of n samples, standard error of the mean, standard deviation) are reported in the paper

Computational analysis

Calculations were conducted
Software details, including version number
Details of all basis sets and exchange-correlation functionals or wave function methods
Force-field parameters
Temperature and/or pressure (if non-standard conditions)
Coordinates, calculated energies, and lowest frequency of all stationary points
Intrinsic reaction coordinate to confirm transition states

Data and code are available in a repository
Convergence criteria of the force and energy
Definitions of computed physical quantities and description of all corrections to electronic energies
Ensemble
k-point and supercell size
Simulation cell details (if periodic calculations) or details if using molecular dynamics or Monte Carlo
Pseudopotential

Other

The [biocatalysis checklist](#) is relevant for this work

The [photocatalysis checklist](#) is relevant for this work

Other information is relevant for the general catalysis or general characterization reported in this manuscript (if so, please provide details below)

The [electrochemistry checklist](#) is relevant for this work

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General conditions

The [General Catalysis checklist](#) has been completed

Catalyst identity

The name from the IUBMB Enzyme List to identify the enzyme is provided

The NCBI Taxonomy ID is provided

A naturally occurring variant

The localization within the cell

Any post-translational modification are detailed

The full protein sequence and the appropriate NCBI GenBank or UniProt accession code is provided

Gene identifiers

Expression modules (i.e., regulatory sequences)

Plasmids used for expression

Mutations within the gene or protein sequence (and an indication of whether the sequences are wild-type, synthetic and/or evolved)

Preparation

Novel methods are provided in full

Metalloenzyme

Comprehensive literature references are included if the synthesis has been previously reported

Artificial modification

Enzyme or protein purity

Storage and Propagation conditions

Storage solution

Storage temperature

Atmosphere if not air

pH (if stored in solution)

Buffer and concentrations (including counter-ion)

Metal salt(s) and concentrations

Enzyme or protein concentration

Details regarding thawing procedure

Propagation medium

Propagation temperature

Antibiotic resistances

Statement about observed loss of activity under any of the preceding conditions

Assay conditions

Substrate identity, purity, and concentrations

Buffer and concentrations

Metal salt(s) and concentrations

Total ionic strength of assay mixture

Enzyme or protein concentration

Coupled assay components

Assay temperature, pressure, medium, and pH

Atmosphere if not air

Culture vessel (e.g., flask, bioreactor, microtiter plate)

Measured reaction provided as stoichiometrically balanced equation

Activity/Performance

Measurements of initial rates of the reaction
Specific substrate consumption rate q_s (in mol/g_{CDW}/h)
Volumetric productivity Q_p (in kg/L/h or mol/L/hr)
Proportionality between initial velocity and enzyme concentration

Turnover number
Specific product formation rate q_p (in mol/g_{CDW}/h)
Enzyme activity expressed as k_{cat} (in s⁻¹ or min⁻¹) or international unit (1 IU = 1 μmol min⁻¹); katal (mol/s) may alternatively be used as a unit of activity (conversion factor 1 unit = 16.67 nkat)

Methodology

Assay method
Type of assay
Reaction-stopping procedure
Direction of the assay
Reactant determined
Concentrations of free metal cations

Reaction equilibrium constant
Pathway intermediates
By-products
Analytic methods for the detection of metabolites
If applicable: molecular cloning techniques
If applicable: recombinant DNA delivery techniques

Kinetic or physiological parameters

k_{cat} (in s⁻¹ or min⁻¹)
 V_{max}
 $S_{0.5}$ as concentration (e.g., mM)
High-substrate inhibition, if observed, with K_i value
Biomass yield on carbon substrate $Y_{x/s}$ (either g_{CDW}/g or g_{CDW}/mol)
Substrate toxicity (minimum inhibitory concentration - MIC in g/L or mol/L)
If applicable: tolerance to solvent concentrations (minimum inhibitory concentration - MIC in g/L or mol/L)

K_m units or concentration necessary (e.g., mM)
 k_{cat}/K_m as concentration per time (e.g., mM⁻¹ s⁻¹)
Model used to determine the parameters
Growth rate μ (in h⁻¹) or doubling time t_D in h
Hill coefficient, saturation ratio (RS), or other coefficients of cooperativity
(By-)product toxicity (minimum inhibitory concentration - MIC in g/L or mol/L)

Inhibition or activation data

Time dependence and reversibility

Inhibition (K_i units necessary)

Other

Other information is relevant for the biocatalysis reported in this manuscript (if so, please provide details below)

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General conditions

The [General Catalysis checklist](#) has been completed

Reaction conditions provided

Cell type (H-cell, gas-diffusion type, etc.)

Cell, electrode, and membrane material

Electrode geometric area (cm²)

Scan rate for cyclic voltammograms

Reactants

Three-electrode or two-electrode configuration (half-cell or full cell, respectively)

Bias potential and, for three-cell configuration, the reference electrode used

Currents

Dependence of current on scan or stir rate

Treatment or polishing of the electrode

pH for aqueous solutions (start, during reaction, end)

Electrolyte

Mass transfer conditions (rotation rate for rotating disc electrode; stir bar, flow rate in flow cells)

Data reported

Vendor information, photographs, and/or schemes of any custom apparatus

Normalized electrochemical surface area activity

Electrochemical impedance spectroscopy (EIS)

Mass activity

Specific activity

Mass balance

Polarization plot (cell voltage versus current or current density)

Electrochemically active surface area (ECSA, A/cm²_{ECSA})

Stability test conditions

Current densities

Faradaic efficiency

Overpotential (including clear information about how the thermodynamic potential was determined, estimated, or calculated)

Other

Other information is relevant for the electrochemistry reported in this manuscript (if so, please provide details below)

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General conditions

The [General Catalysis checklist](#) has been completed

Reaction conditions provided

Vendor information, photographs, and/or schemes of any custom apparatus and reaction setup

Photocatalyst loading

Substrate concentration

Sacrificial donor

Other additives

Reaction vessel size, material, and thickness of glassware

Total optical power impinging on the sample if liquid ($\text{mW}\cdot\text{mL}^{-1}$)

Source and wavelength of light used for illumination

Wavelength distribution of light

Hole or electron scavengers

Optical irradiance at the sample ($\text{mW}\cdot\text{cm}^{-2}$)

Data reported

Quantum yields

Photocatalytic efficiencies

Apparent quantum yields or photonic efficiencies

Control experiments conducted

Reaction without catalyst

Reaction without light (on/off test and reaction conducted completely in the dark)

Stern-Volmer or other quenching experiments

Other

Other information is relevant for the photocatalysis reported in this manuscript (if so, please provide details below)