

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

Reaction conditions provided

- | | |
|---|--|
| <input checked="" type="checkbox"/> Cell type (H-cell, gas-diffusion type, etc.) | <input checked="" type="checkbox"/> Currents |
| <input checked="" type="checkbox"/> Cell, electrode, and membrane material | <input type="checkbox"/> Dependence of current on scan or stir rate |
| <input checked="" type="checkbox"/> Electrode geometric area (cm ²) | <input checked="" type="checkbox"/> Treatment or polishing of the electrode |
| <input checked="" type="checkbox"/> Scan rate for cyclic voltammograms | <input type="checkbox"/> pH for aqueous solutions (start, during reaction, end) |
| <input checked="" type="checkbox"/> Reactants | <input checked="" type="checkbox"/> Electrolyte |
| <input checked="" type="checkbox"/> Three-electrode or two-electrode configuration (half-cell or full cell, respectively) | <input type="checkbox"/> Mass transfer conditions (rotation rate for rotating disc electrode; stir bar, flow rate in flow cells) |
| <input type="checkbox"/> Bias potential and, for three-cell configuration, the reference electrode used | |

Data reported

- | | |
|---|---|
| <input checked="" type="checkbox"/> Vendor information, photographs, and/or schemes of any custom apparatus | <input type="checkbox"/> Polarization plot (cell voltage versus current or current density) |
| <input type="checkbox"/> Normalized electrochemical surface area activity | <input type="checkbox"/> Electrochemically active surface area (ECSA, A/cm ² _{ECSA}) |
| <input type="checkbox"/> Electrochemical impedance spectroscopy (EIS) | <input type="checkbox"/> Stability test conditions |
| <input type="checkbox"/> Mass activity | <input checked="" type="checkbox"/> Current densities |
| <input type="checkbox"/> Specific activity | <input type="checkbox"/> Faradaic efficiency |
| <input type="checkbox"/> Mass balance | <input type="checkbox"/> 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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- The [General Catalysis checklist](#) has been completed

Reaction conditions provided

- | | |
|---|---|
| <input type="checkbox"/> Vendor information, photographs, and/or schemes of any custom apparatus and reaction setup | <input type="checkbox"/> Total optical power impinging on the sample if liquid ($\text{mW}\cdot\text{mL}^{-1}$) |
| <input type="checkbox"/> Photocatalyst loading | <input type="checkbox"/> Source and wavelength of light used for illumination |
| <input type="checkbox"/> Substrate concentration | <input type="checkbox"/> Wavelength distribution of light |
| <input type="checkbox"/> Sacrificial donor | <input type="checkbox"/> Hole or electron scavengers |
| <input type="checkbox"/> Other additives | <input type="checkbox"/> Optical irradiance at the sample ($\text{mW}\cdot\text{cm}^{-2}$) |
| <input type="checkbox"/> Reaction vessel size, material, and thickness of glassware | |

Data reported

- | | |
|--|---|
| <input type="checkbox"/> Quantum yields | <input type="checkbox"/> Apparent quantum yields or photonic efficiencies |
| <input type="checkbox"/> Photocatalytic efficiencies | |

Control experiments conducted

- | | |
|---|--|
| <input type="checkbox"/> Reaction without catalyst | <input type="checkbox"/> Stern-Volmer or other quenching experiments |
| <input type="checkbox"/> Reaction without light (on/off test and reaction conducted completely in the dark) | |

Other

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