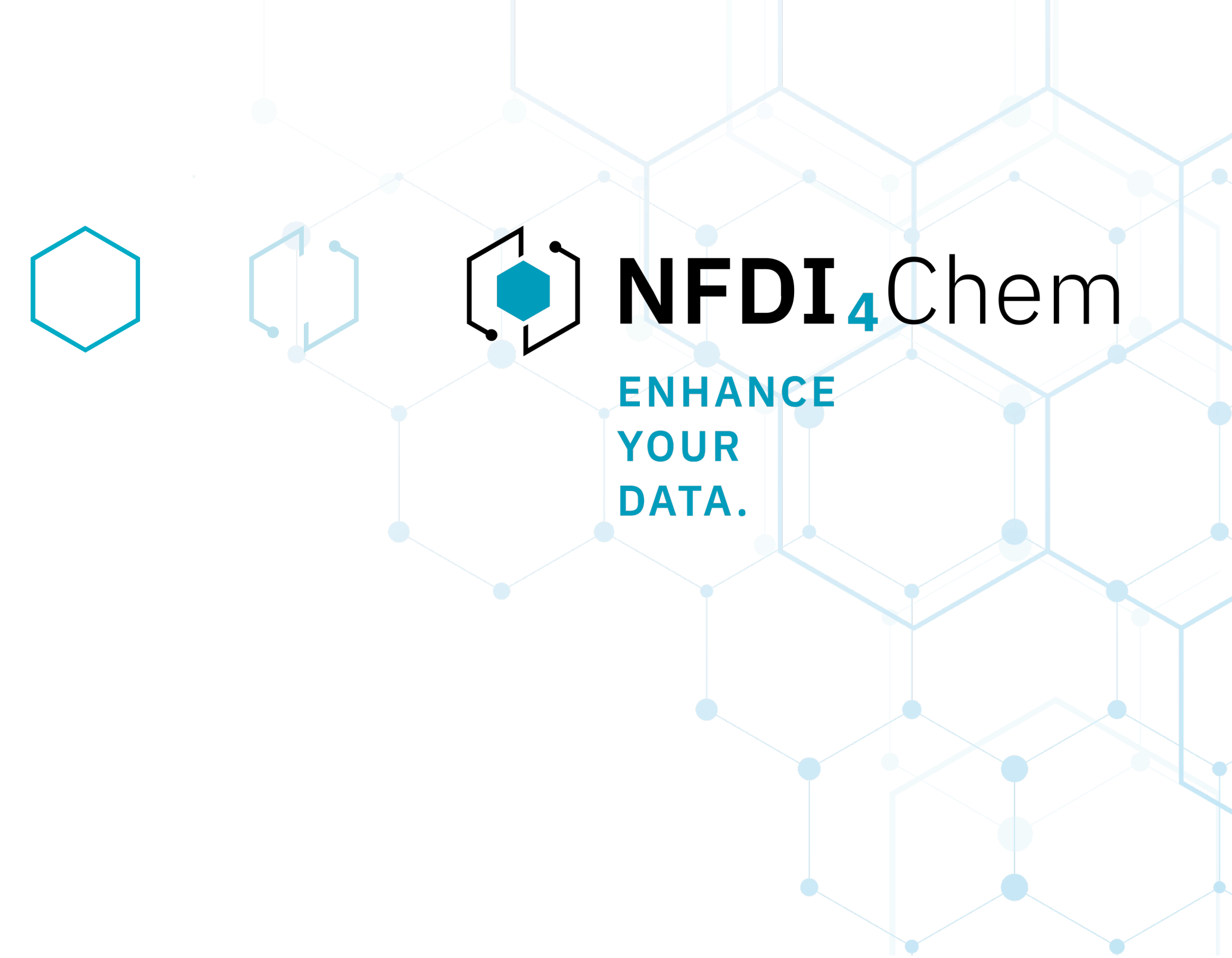


# Publishing Standards in Chemistry and Beyond



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## Advancing Research Data Publication

NFDI4Chem sets standards for authors, publishers, and infrastructure providers, ensuring research data is seamlessly linked to published findings in a human- and machine-readable way. These standards support policy, decision-making, and technical solutions from manuscript submission to article publication.

	Scientific Authors	Academic Publishers	Research Data Repositories
Manuscript Submission	<p><b>For your Dataset</b></p> <ul style="list-style-type: none"><li>✓ Identify yourself </li><li>✓ Identify your institution </li><li>✓ Choose a license </li><li>✓ Utilize collection DOIs</li></ul> <p>To identify yourself, your collaborators and your institution, ensure you use ORCID IDs and RORs in the dataset metadata. Then, choose a license to define how others may reuse your data; opt for the most open license possible to ensure wide reuse. For <b>multiple datasets</b>, generate a collection DOI to clearly wrap them and associate them to your manuscript.</p> <p><b>For your Manuscript</b></p> <ul style="list-style-type: none"><li>✓ <b>Data Availability Statement</b> with the dataset PID</li><li>✓ Cite and reference dataset</li><li>✓ Cite others' data with PID</li><li>✓ Provide <b>reviewer link</b> for datasets</li></ul> <p>Include a Data Availability Statement with your dataset PID (usually a DOI) upon submission to help readers access the underlying data. Cite your dataset in the manuscript where relevant and include it in your references. If you reused others' datasets, cite them using the PID instead of just citing their paper. If you have not yet published your dataset, be sure to set it to read-only and include a review link with the manuscript submission, allowing reviewers a <b>full picture of your research</b>.</p>	<ul style="list-style-type: none"><li>✓ Recommend chemistry-friendly repositories</li></ul> <div></div> <ul style="list-style-type: none"><li>✓ Include <b>Data Availability Statements</b> and provide templates</li><li>✓ Integrate Data Availability Statement into <b>submission system</b></li><li>✓ Encourage dataset pre-submission</li></ul> <p>Assist authors in selecting <b>research data repositories</b> by suggesting trusted, chemistry-friendly options. Require Data Availability Statements and guide authors by providing editable templates as well as integrating these items into your submission system. Encourage authors to publish their data prior to manuscript publication, which enables them to provide an <b>active DOI</b> with the manuscript, as is common practice with crystallographic data. This can assist in automated workflows with your publication system, such as DOI quality checks.</p>	<ul style="list-style-type: none"><li>✓ Group licenses</li><li>✓ Encourage <b>least restrictive license</b> </li><li>✓ Dataset abstract ≠ manuscript abstract </li><li>✓ Label Creator metadata field as Authors/Creators</li><li>✓ Provide <b>collection DOIs</b></li><li>✓ Autofill publisher field with repository name</li></ul> <p>At this stage, researchers are uploading their data and filling out their metadata. Inform them about potential copyright issues when using the manuscript abstract for the dataset, emphasizing that datasets should have their own descriptions—this information can be included as a tooltip in the metadata editor. To assist in selecting licenses, group them by type, distinguishing between those for research data and software. By pre-selecting open Creative Commons licenses like CC0 or CC BY, guide authors in choosing licenses that ensure flexible data reuse. Ensure they understand the metadata form by labeling the creator field as <i>Creator/Author</i> and prefill the repository name as publisher, adding the re3data identifier. This ensures unambiguous identification as well as correct citations creation. If you use separate identifier for reactions, molecules, and analyses, provide the option to generate collection DOIs to facilitate data submission alongside a manuscript.</p>
Manuscript Review & Acceptance	<ul style="list-style-type: none"><li>✓ Add article DOI to dataset as <i>IsSupplementTo</i></li><li>✓ <b>Publish dataset</b> upon manuscript acceptance</li></ul> <p>Once your manuscript has been accepted it is time to publish your dataset to ensure the DOI is active as soon as your manuscript is published. When provided the article DOI, add this to your dataset as a <b>related identifier</b> using the relation <i>IsSupplementTo</i>, creating a human and machine-readable link.</p>	<ul style="list-style-type: none"><li>✓ Include <b>dataset in review</b></li><li>✓ Require data publication upon acceptance</li></ul> <p>Explicitly encourage dataset review in your author guidelines and ensure that access to datasets is provided alongside manuscripts. If datasets have not been pre-submitted, communicate the <b>requirement for publication</b> within the acceptance notification. This ensures that an active dataset identifier is established, facilitating automated metadata quality checks prior to publication.</p>	<ul style="list-style-type: none"><li>✓ Provide <b>URLs for dataset review access</b></li><li>✓ Encode access credential in URL</li></ul> <p>To facilitate a dataset's inclusion in the review process, provide a read-only review status option that include a URL for reviewer access. Access credentials should be encoded to avoid having to explicitly communicate these.</p>
Article Publication	<ul style="list-style-type: none"><li>✓ <b>Relax and Celebrate !</b></li><li>✓ Maybe announce on social media, and mention that the manuscript comes with data</li><li>✓ Consider submitting your dataset to the next FAIR4Chem award</li></ul> <p>The <b>FAIR4Chem Award</b> honors researchers in chemistry who publish their research data. The award is given for published chemistry research datasets that best meet the FAIR principles (findable, accessible, interoperable, and reusable). NFDI4Chem will award the FAIRest dataset with a <b>monetary price</b> of 500 €, supported by the Fonds der Chemischen Industrie (FCI).</p>	<ul style="list-style-type: none"><li>✓ <b>Link</b> datasets to articles in Crossref DOI Metadata using <i>is-supplemented-by</i></li><li>✓ Utilize <b>Scholix Framework</b></li></ul> <p>Ensure a <b>machine-readable link</b> between the article and its underlying data by including the dataset DOI as a related identifier with the relation <i>is-supplemented-by</i> in the Crossref metadata. Use the information provided by Scholix, a framework to improve linking between scientific literature and research data, to discover datasets that relate to already published articles. Ensure Crossref DOI metadata is correctly enriched with this information.</p>	<ul style="list-style-type: none"><li>✓ Dataset includes <b>data &amp; metadata</b></li><li>✓ Include structured, domain specific metadata</li><li>✓ Allow metadata corrections and updates</li><li>✓ Contribute to <b>Scholix.org</b></li><li>✓ Embargoed data has <b>accessible</b> metadata</li></ul> <p>A dataset downloaded by and exchanged with others should include both data and structured, domain-specific metadata. <b>BagIt</b> can be used as a packaging format, while <b>RO-Crate</b> helps capture this comprehensive metadata. Researchers should be able to correct and update metadata as needed, with versioning providing transparency. This allows the addition of related identifiers post-publication. Contributing to Scholix.org enhances the visibility of research outputs and engaging with Scholix hubs like <b>DataCite</b> or <b>OpenAire</b> help others discover connected objects. For data published with embargo, metadata must remain accessible for findability.</p>

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