

Author guidelines in chemistry through the lens of research data sharing

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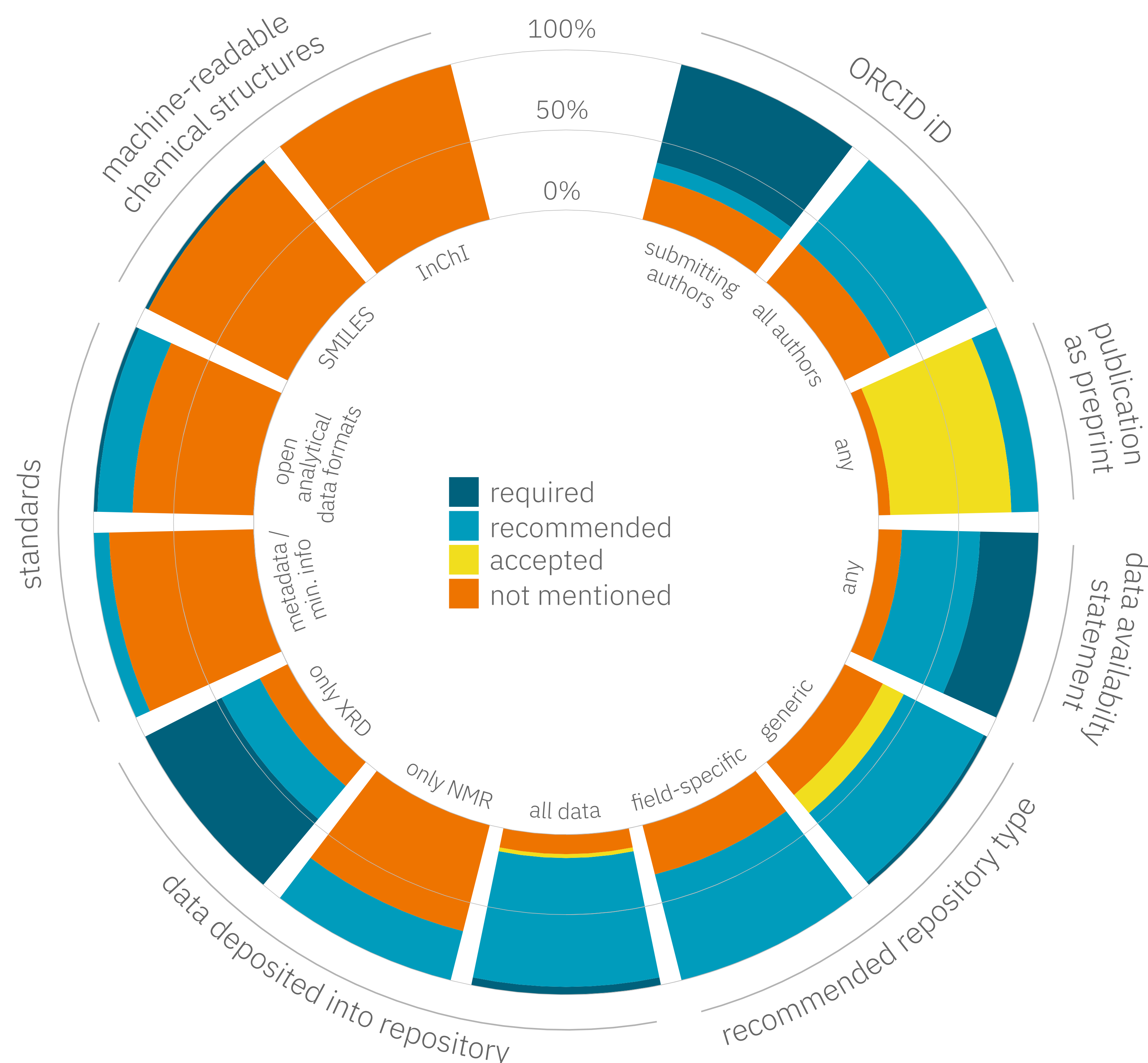
Background

Publishing research data is widely regarded as good scientific practice but is not yet as common as sharing results in scientific articles. With movements towards FAIR data and Open Science practices, various aspects of academic publishing need to be updated. To this end, the author guidelines put forth by scientific journals can pave the way and assist authors in data publication.

Survey: What Criteria did we Consider?

The table below summarizes the criteria considered in the survey of 42 chemistry-related journals from 13 publishers.

Category	Criterium	Relevance
ORCID iD	Whether authors and/or coauthors must submit their ORCID iD.	Promotes unambiguous and persistent author identification, which is part of rich and descriptive metadata.
Preprint servers	Whether manuscripts posted on open access preprint servers such as arXiv, bioRxiv, or ChemRxiv prior to publication in the journal will be considered or is encouraged.	Publishing on preprint servers before publication in a journal promotes transparency. This is a similar process to publishing research data prior publishing an article.
Data availability statement	Whether a journal expects a data availability statement. The exact wording of the statement was not taken into account.	Provides information on how underlying research data can be found and accessed.
Data deposition into repository	Whether journals expect underlying data to be published in a repository. Split into all data, NMR data, and XRD data.	Ensures research data are findable and accessible. XRD and NMR represent two of the most common analytical methods in chemistry.
Recommended repositories	Whether the journal explicitly suggests field-specific and/or generic repositories. Field-specific repositories include limited types of data but often have advanced features for data analysis or visualization; generic repositories may accept any type of research data regardless of subject, method, or format.	Assists authors in choosing suitable repositories for their data, thus enhancing accessibility and findability, while ensuring adherence to community standards.
Metadata / minimum information requirements	Whether the journal expects authors to follow (field-)specific guidelines and standards regarding minimal descriptive information with respect to the context of the research data.	Enhances findability and reusability of datasets.
Open analytical data formats	Whether the journal lists specific open file formats for analytical data.	Ensures the datasets are interoperable and reusable.
Machine readable structures (InChI, SMILES)	Whether a journal requires chemical structures to be reported in machine-readable formats	Ensures data provided on chemical structures is findable, interoperable and can be interpreted by machines.



Results: The Current Situation

- The use of ORCID iDs is common practice; approx. two-thirds of surveyed journals require them for submitting authors and the same amount recommending them for all authors.
- 82% of journals require or recommend the submission of data availability statements.
- Data sharing is a well-established practice for crystallography, with approx. 75% of journals requiring or recommending XRD data be shared in a research data repository.
- Sharing of all underlying data is recommended by 85 % journals, while only 5% require it.
- The use of standards for metadata / minimum information and analytical data formats were rarely mentioned in the guidelines (10%).
- Machine-readable chemical structures were only mentioned by a single journal.

This survey took place twice. The results of the second survey are reported here. Notable changes took place in terms of journals recommending or even requiring the use of data availability statements. A similar shift was seen for publishing all underlying research data.

Takeaways and Outlook

The results indicate a clear move towards research data sharing in chemistry in conjunction with publishing research results. Technical aspects in accordance with the FAIR data principles still require solutions and awareness. This means...

... for authors

- Provide rich metadata and comply with community standards
- Use identifiers for authors and to link datasets with articles

... for publishers and editors

- Guide researchers in making data FAIR
- Implement technical solutions to facilitate the submission processes from a data publication perspective

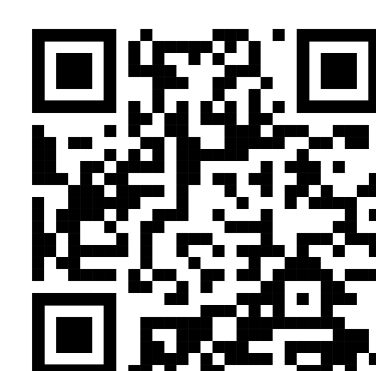
... for infrastructure providers

- Field-specific repositories are still lacking in some areas of chemistry
- Machine-readability of structures require further development

Read the paper in Pure and Applied Chemistry
DOI: [10.1515/pac-2022-1001](https://doi.org/10.1515/pac-2022-1001)



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