Journal of Cheminformatics

LETTER RESPONSE

Open Access

Reply to "FAIR chemical structure in the Journal of Cheminformatics"

Rajarshi Guha[1], Nina Jeliazkova[2], Egon Willighagen[3*] and Barbara Zdrazil[4]

Schymanski and Bolton [1] requests the adoption of a FAIR approach to improve the FAIRness (findability, accessibility, interoperability, reusability) of chemical structures in the Journal of Cheminformatics. Currently, our journal encourages open science practices, but at the same time does not provide much guidance on how to implement these practices. Because FAIR chemical data is important [2], we welcome the open standard proposal and intend to adopt it as recommendation to authors.

Specifically, we will update the author guidelines that authors can improve the FAIRness by opting-in to provide chemical structures in open data associated with our journal articles in this format. For submissions where data is already provided in a FAIR format, an index file in this format can be provided. Second, we will make reviewers aware of this new, optional open standard.

While we agree with the importance of FAIR data, we also foresee practical complications when making this obligatory for all articles. Particularly, for the Database article type, the proposal may be both redundant to existing editorial standards as well as problematic for really large datasets as used in, for example, Probst and Reymond [3].

As a result, rather than require, we strongly recommend that authors include structure data in open, machine readable formats and identifiers, and point towards Schymanski and Bolton [1] as a means of doing so.

*Correspondence: egon.willighagen@maastrichtuniversity.nl
[3] Department of Bioinformatics-BiGCaT, NUTRIM School of Nutrition and Translational Research in Metabolism, Maastricht University, Maastricht, The Netherlands
Full list of author information is available at the end of the article

Authors' contribution
All authors were involved in designing and writing this reply and all read and approved the final manuscript.

Competing interests
All authors are editors for the Journal of Cheminformatics and have a contract with SpringerNature. Adoption of this new standard is expected to result in more data reuse, which has a positive impact on the number of citations that articles that provide the data get, which in turn benefits the journal and the publisher.

Author details
[1]Vertex Pharmaceuticals, Boston, MA 02129, USA. [2]Ideaconsult Ltd, Sofia, Bulgaria. [3]Department of Bioinformatics-BiGCaT, NUTRIM School of Nutrition and Translational Research in Metabolism, Maastricht University, Maastricht, The Netherlands. [4]Division of Pharmaceutical Chemistry, Department of Pharmaceutical Sciences, University of Vienna, Vienna, Austria.

Received: 25 May 2021 Accepted: 25 May 2021
Published online: 07 July 2021

References

1. Schymanski E, Bolton E (2021) FAIR Chemical structure in the Journal of Cheminformatics. J Cheminform. https://doi.org/10.1186/s13321-021-00520-4 **[cito:agreesWith] [cito:obtainsBackgroundFrom] [cito:repliesTo]**

2. Coles SJ, Frey JG, Willighagen EL, Chalk Stuart J (2020) Taking FAIR on the ChIN: the chemistry implementation network. Data Intell 2:131–8. https://doi.org/10.1162/DINT_A_00035 **[cito:citesAsAuthority] [cito:obtainsBackgroundFrom]**
3. Probst D, Reymond J-L (2020) Visualization of very large high-dimensional data sets as minimum spanning trees. J Cheminform 12(1):12. https://doi.org/10.1186/s13321-020-0416-x **[cito:citesAsDataSource]**

Publisher's Note