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2nd November 2022.

Prof. Feng Zhu
Associate Editor
Journal of Chemical Information and Modeling

RE: Second response to reviewers for manuscript identifier ci-2022-00779z.R1

Dear Prof. F. Zhu,

Reference is made to following manuscript:

Manuscript ID:	**ci-2022-00779z.R1**
Title:	**Few-Shot Learning for Low-Data Drug Discovery**
Author(s):	Vella, Daniel; Ebejer, Jean-Paul

Many thanks for your and the reviewer's helpful comments on our submission. We believe this process has helped improve the overall quality of our manuscript. We addressed the requested changes as commented next (comments in shaded areas).

Reviewer #1 Comments

1. The authors have addressed the points in the initial reviews. The paper is of interest to the journal readership and should be published.

We thank the reviewer for their detailed and insightful comments.

Reviewer #2 Comments

2. The authors have addressed all my questions, I recommend the manuscript to be accepted for publication.

We thank the reviewer for their comments.

Editor's Comments

You have indicated that you have used at least one figure or table in my manuscript or supplementary information that was previously published. Please indicate what has been previously published and provide permissions to use this figure or table.

Permission to use this has now been sought and approved (footnote on pg. 12).

Figures 3 and 6 need to be cited in the text.

All figures and tables are now cited in text.

JCIM is now accepting images to appear on the front cover of the journal. If you have a visually arresting and scientifically interesting image, please upload it and a brief (80 word) description of the image as part of your revised submission.

We are submitting a front cover image (ci-2022-00779z-coverpage-art.png) together with our revised submission. The 80-word blurb is as follows:

Supervised Machine learning is typically data-hungry, which is in stark contrast to the limited data for new disease targets. We explore few-shot machine learning which aims to "learn how to learn" from just a few examples. Our proposed architecture makes use of embeddings created through graph convolutional networks, achieving better results than the state-of-the-art on Tox21 data. We classified molecules as active or otherwise, within a previously unseen experimental assay using only 1-10 molecules and a model trained on related assays.

JCIM has a Twitter feed (@JCIM_ACS; https://twitter.com/jcim_acs) covering the latest news and highlights in the field. If you would like us to feature your manuscript on this platform, please share a Tweet of no more than 140 characters.

We suggest the following tweet:

Few-shot learning using GCNs and Prototypical Networks tested on Tox21, MUV and DUD-E datasets. @UMmalta @dr_jpe @danvlla

ACS Publications uses Crossref Similarity Check Powered by iThenticate to detect instances of similarity in submitted manuscripts. In publishing only original research, ACS is committed to deterring plagiarism, including self-plagiarism. Your manuscript may be screened for similarity to published material.

We welcome these checks.

Once again, we thank you and the reviewers for their helpful and constructive feedback: it has strengthened the manuscript, and we look forward to its publication in JCIM.

If you require further details or clarifications, please do not hesitate to get in touch.

Sincerely yours,

Dr Jean-Paul Ebejer
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