
Fw: Revision Requested for Manuscript ID ac-2022-02913m.R2

Nagy Tibor <nagy.tibor@science.unideb.hu>
Címzett: Máté Benedek <bmate01@gmail.com>

2023. május 3. 19:19

Tibor Nagy, Ph.D.
senior lecturer
Department of Applied Chemistry
Faculty of Science and Technology
University of Debrecen
[Hungary, H-4032 Debrecen, Egyetem ter 1,](#)
Phone: +36 52 512-900/22454

Feladó: Nagy Tibor <nagy.tibor@science.unideb.hu>
Elküldve: 2023. május 3., szerda 13:47
Címzett: Dr. Kuki Ákos <kuki.akos@science.unideb.hu>
Tárgy: Fw: Revision Requested for Manuscript ID ac-2022-02913m.R2

Tibor Nagy, Ph.D.
senior lecturer
Department of Applied Chemistry
Faculty of Science and Technology
University of Debrecen
[Hungary, H-4032 Debrecen, Egyetem ter 1,](#)
Phone: +36 52 512-900/22454

Feladó: Dr. Kéki Sándor <keki.sandor@science.unideb.hu>
Elküldve: 2023. május 3., szerda 13:01
Címzett: Nagy Tibor <nagy.tibor@science.unideb.hu>
Tárgy: Fw: Revision Requested for Manuscript ID ac-2022-02913m.R2

Feladó: Analytical Chemistry <onbehalf@manuscriptcentral.com>
Elküldve: 2023. május 3., szerda 12:43
Címzett: Dr. Kéki Sándor <keki.sandor@science.unideb.hu>
Tárgy: Revision Requested for Manuscript ID ac-2022-02913m.R2

FIGYELEM: Ez a levél külső feladótól származik. Ne kattintson semmire a levélben, és ne nyissa meg a csatolmányt, amennyiben a küldő e-mail címét nem ismeri fel!

03-May-2023

Journal: Analytical Chemistry

Manuscript ID: ac-2022-02913m.R2

Title: "Enhanced Copolymer Characterization for Poloxamers Using Gel Permeation Chromatography Combined with Artificial Neural Network"

Author(s): Nagy, Tibor; Roth, Gergo; Benedek, Máté; Kuki, Ákos; Timári, István; Zsuga, Miklos; Kéki, Sándor

Dear Dr. Kéki:

Thank you for submitting your manuscript for publication in Analytical Chemistry.

The reviewers' comments were generally quite positive; however, as indicated in the enclosed comments, minor improvements are suggested. I will be pleased to consider for publication a revised manuscript that addresses the reviewers' concerns.

Please submit your revision on your ACS Paragon Plus homepage, along with a cover letter containing your point-by-point response to the reviewers' comments, by 02-Jun-2023. A revision received after this period will be considered a new submission and will be subject to a complete review process. Even in this case, a detailed response to the previous review and description of the revisions made are still required.

The following list should be reviewed carefully for important manuscript submission requirements. Missing items or incorrect format may delay the acceptance of your manuscript. For more details, please refer to the author guidelines at: <http://pubs.acs.org/page/ancham/submission/index.html>.

Please provide the following required files:

- A clean .doc/.docx file designated as the "Manuscript File" (see * detail below for contents).
- A highlighted/tracked changes version of the manuscript showing the changes made, uploaded separately and designated as "Supporting Information for Review Only".
- Supporting Information (SI) for Publication (if applicable). I do not require a highlighted version of the SI; this must be uploaded as a clean copy. SI may not be included in the Manuscript File (see ** detail below for additional requirements).

* Manuscript .doc/.docx file content:

- Title page must include an accurate list of each author's complete name, identical to the author names as entered into the ACS Paragon Plus system; also include the corresponding author's full contact information on the title page.
- Indicate the breakdown among and within sections with center heads and side heads; do not number manuscript sections.
- Figure captions. (Note that in ACS Paragon Plus, you have the option of embedding graphics into the manuscript or supplying graphics separately, but the captions must be in the Word document.)
- Tables with captions.
- References formatted as per ACS style; if you use Endnote, an updated style is available at https://endnote.com/style_download/american-chemical-society-acs/.
- A Table of Contents graphic must be included; for information on what we require, see: http://pubs.acs.org/paragonplus/submission/toc_abstract_graphics_guidelines.pdf.

** Supporting Information: If the manuscript is accompanied by any supporting information for publication, a brief description of the supplementary material is required in the manuscript. The appropriate format is: Supporting Information. Brief statement in nonsentence format listing the contents of the material supplied as Supporting Information.

- The first page of the SI should be a cover page that lists the authors' names and affiliations, the title of the primary article, and an abstract and/or a table of contents that describes the nature of the materials therein. All pages, including the cover page, should be numbered consecutively starting with page S-1.
- All SI files of the same type should be prepared as a single file (rather than submitting a series of files containing individual images or structures). ACS does not edit S

Other Information:

- When revising the manuscript in order to address the reviewers' comments, please keep in mind the

overall length requirements for your manuscript type. Graphics should be sized at the final production size. Single-column graphics are preferred and can be sized up to 240 points wide (3.33 in). Double-column graphics must be sized between 300 and 504 points (4.167 in and 7 in). Graphics have a maximum height of 660 points (9.167 in) including the caption (please allow 12 pts for each line of caption text).

- A request to extend the deadline requires Editor's approval. Special circumstances will be considered.

Funding Sources: Authors are required to report ALL funding sources and grant/award numbers relevant to this manuscript. Enter all sources of funding for ALL authors relevant to this manuscript in BOTH the Open Funder Registry tool in ACS Paragon Plus and in the manuscript to meet this requirement. See http://pubs.acs.org/page/4authors/funder_options.html for complete instructions.

ORCID: Authors submitting manuscript revisions are required to provide their own validated ORCID iDs before completing the submission, if an ORCID iD is not already associated with their ACS Paragon Plus user profiles. This iD may be provided during original manuscript submission or when submitting the manuscript revision. You can provide only your own ORCID iD, a unique researcher identifier. If your ORCID iD is not already validated and associated with your ACS Paragon Plus user profile, you may do so by following the ORCID-related links in the Email/Name section of your ACS Paragon Plus account. All authors are encouraged to register for and associate their own ORCID iDs with their ACS Paragon Plus profiles. The ORCID iD will be displayed in the published article for any author on a manuscript who has a validated ORCID iD associated with ACS Paragon Plus when the manuscript is accepted. Learn more at <http://www.orcid.org>.

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.

Thank you for considering Analytical Chemistry as a forum for the publication of your work.

With sincere regards,

Prof. Emily F. Hilder
Associate Editor
Analytical Chemistry
Phone: +1 (202) 600-9615
Email: hilder-office@anchem.acs.org

Reviewer(s)' Comments to Author:
Reviewer: 1

Recommendation: Publish either as is or subject to minor revisions as indicated.

Comments:
Review ac-2022-02913m.R2

First of all, I would like to sincerely apologize to the Authors and the Editor for submitting my review 10 days late.

I will make sure this situation does not happen again, especially if I have the chance to review another great article from these Authors.

I did review the first version of this draft (ac-2022-02913m) about which I was quite enthusiastic, but I did not review the first revision submitted (ac-2022-02913m.R1). Reading all three versions, the Authors have improved their draft and modified their ANN models in this second revision (ac-2022-02913m.R2), taking into consideration the important comment of the Referee indicated in the cover letter about the small training set.

However, it is remarkable that except for Mn (Fig 5A), all the correlations in the parity plots (Fig 5b for %EO, Fig 7 for n n/w EO/PO) are of lower quality in this second version with a higher number of samples and less input parameters than in the previous drafts.

I would really like the Authors to comment on these results: is this decrease of correlation due to the reduction of the number of input parameters, or due to the increase of the number of samples ? It seems like the comment of the Referee reported in the cover letter about a reduced number of training set leading to an overconfidence in the model accuracy is somehow validated here with the decrease of the

correlation.

I think it would be a great addition to the manuscript (or to the Supporting Information) to briefly discuss the variation of the correlation plots from the first to the second ANN models, adding reasons for this change. It will be of great added values for the researchers interested in pursuing this work, especially in the spirit of an "open source" database mentioned by the Authors.

Minor comments:

I was suggesting in my first review that a bit more data should be added to the Supporting Information (e.g. SEC chromatograms, NMR and MALDI spectra, especially for the n n/w EO/PO section with reflectron TOF data). it would be of particular importance for the mix and fractionations conducted to increase the number of samples (these samples are no longer commercial samples that other researchers can easily get).

As a very minor comment, I think that the new title proposed by the Authors now reduces the scope of the paper a bit too much. The term "poloxamer" normally refers to the triblock EO-PO-EO only, not the reversed configuration PO-EO-PO. And the Authors have also analyzed PEO and PPO homopolymers and discuss the presence of minor diblock EO-PO, so I would suggest finding another title not as broad as "copolymer" but more inclusive than just 'poloxamer'.

Additional Questions:

Significance: Top 5% (suitable for Analytical Chemistry)

Originality: Top 5% (suitable for Analytical Chemistry)

Broad Interest: High (suitable for Analytical Chemistry)

Technical Quality: High (suitable for Analytical Chemistry)

Are the conclusions adequately supported by the data?: Yes

Are the references appropriate and correct?: Yes

Is the English adequate?: Yes

Is the quality of the figures sufficient?: Yes

Are the data statistically significant with appropriate controls included?: In Part

To Revise Your Manuscript on the Web:

To revise your manuscript, log in to ACS Paragon Plus with your ACS ID at <http://acsparagonplus.acs.org/> and select "My Authoring Activity". There you will find your manuscript title listed under "Revisions Requested by Editorial Office." Your original files are available to you when you upload your revised manuscript. If you are replacing files, please remove the old version of the file from the manuscript before uploading the new file.

When submitting your revised manuscript through ACS Paragon Plus, you will be able to respond to the comments made by the reviewer(s) in the text box provided or by attaching a file containing your response letter.

FOR ASSISTANCE WITH YOUR MANUSCRIPT SUBMISSION PLEASE CONTACT:

ACS Publications Customer Services & Information (CSI)

Email: support@services.acs.org

Phone: 202-872-4357

Toll Free Phone: 800-227-9919 (USA/Canada only)

PLEASE NOTE: This email message, including any attachments, contains confidential information

related to peer review and is intended solely for the personal use of the recipient(s) named above. No part of this communication or any related attachments may be shared with or disclosed to any third party or organization without the explicit prior written consent of the journal Editor and ACS. If the reader of this message is not the intended recipient or is not responsible for delivering it to the intended recipient, you have received this communication in error. Please notify the sender immediately by e-mail, and delete the original message.

As an author or reviewer for ACS Publications, we may send you communications about related journals, topics or products and services from the American Chemical Society. Please email us at pubs-comms-unsub@acs.org if you do not want to receive these. Note, you will still receive updates about your manuscripts, reviews, or future invitations to review.

Thank you.