Fw: letter of collaboration

From: Dr. B. C. Roy College of Pharmacy & A. H. S., Durgapur (bcrcp_dgp@yahoo.co.in)

To: souvik_basak1@yahoo.com

Date: Thursday, November 11, 2021 at 06:39 PM GMT+5:30

Sent from Yahoo Mail on Android

----- Forwarded message -----
From: "Dr. B. C. Roy College of Pharmacy & A. H. S., Durgapur" <bcrcp_dgp@yahoo.co.in>
To: "schakraborty111@yahoo.co.in" <schakraborty111@yahoo.co.in>, "debjani" <debjani@jcbose.ac.in>
Cc:
Sent: Thu, 11 Nov 2021 at 5:52 pm
Subject: Re: letter of collaboration

To

Dr. Debjani Roy,

Faculty,

Department of Biophysics,

Bose Institute, Kolkata

Sub: Acceptance of Proposal for collaborative research with reference to e-mail dated 9th November, 2021

Dear Madam,

We are in receipt of a mail from your end informing us that you would like to collaborate with Dr. Souvik Basak and his group at Dr. B.C. Roy College of Pharmacy & Allied Health Sciences, Durgapur, West Bengal regarding the experimental work on Alzheimer's disease funded by the grant of the Bose Institute.

The college authority is pleased to accept your proposal for the collaborative work between Bose Institute, Kolkata and Dr. B.C. Roy College of Pharmacy & Allied Health Sciences, Durgapur, West Bengal.

We are happy that you would bear the required chemical and consumable cost for the said project work at Dr. B.C. Roy College of Pharmacy & Allied Health Sciences. We will be further glad if you kindly provide some overhead cost required for the said work. We would extend our team's expertise in all the avenues of the project work to our best as mentioned by you.

We expect a letter of agreement/MOU with Bose Institute, Kolkata for the collaborative work at the earliest.

We would further appreciate your continuous endeavour for future collaborative works as well, along with the necessary fund support as Principal/co-investigator for further developments of our research team and faculty.

Thanking you for your kind co-operation,

Dr. B. C. Roy College of Pharmacy & AHS Durgapur

Prof. (Dr.) Samir Kumar Samanta
M. Pharm., Ph.D (J.U.)
Principal
Dr. B. C. Roy College of Pharmacy & AHS
Durgapur, West Bengal-713206

Sincerely,

Dr. Subrata Chakraborty,

Director,

Dr. B.C. Roy College of Pharmacy & Allied Health Sciences, Durgapur, West Bengal

On Tuesday, 9 November, 2021, 03:37:09 pm IST, debjani <debjani@jcbose.ac.in> wrote:

To
The Director
Dr. B.C. Roy College of Pharmacy & Allied Health Sciences
Durgapur
West Bengal.

November 9, 2021

Dear Sir,
I would like to collaborate with Dr. Souvik Basak and his group at Dr. B.C. Roy College of Pharmacy & Allied Health Sciences, Durgapur, WB, regarding the experimental work on Alzheimer's Disease. The emphasis will be given on protein fibrillation, biochemical assays, and protein characterization. For these experiments, I am sharing my purchased chemicals and consumables with his group. As a part of this collaboration, I will visit his laboratory in Durgapur and his group will be allowed to work at Bose Institute as well. We will carry out the experimental work at Dr. B. C. Roy College and Bose Institute, Kolkata. This experimental work will be funded by the Grant of Bose Institute. Your cooperation is required in order to make it a successful collaboration and ultimately a fruitful research endeavor for AD therapeutic development.

Sincerely,

Debjani Roy
Dr. Debjani Roy
Faculty, Department of Biophysics
Bose Institute
Kolkata

Dr. B. C. Roy College of Pharmacy & AHS * Durgapur

Prof. (Dr.) Samir Kumar Samanta
M. Pharm., Ph.D (J.U.)
Principal
Dr. B. C. Roy College of Pharmacy & AHS
Durgapur, West Bengal-713206

project

From: debjani roy (roydebjani13@gmail.com)

To: souvik_basak1@yahoo.com

Date: Wednesday, August 17, 2022 at 08:05 PM GMT+5:30

Title of the project: Biological motifs for Alzheimer's Disease: Understanding neurodegenerative disease and the biology of ageing.

In 2021 I received 22lakhs rupees for this project.
The collaborator of this Project is Dr. Souvik Basak, Associate Professor, Dr. B.C. Roy College of Pharmacy & Allied Health Sciences, Durgapur, WB, India.

We are working on protein fibrillation pathway. We are interested in the development of protein fibrillation inhibitors which has long been recognized as potential therapeutics for ageing diseases. The most part of this work will be attributed to big database screening and ex vivo validations of these screened efficacious inhibitors. We are trying to develop a unified method for accelerating hit-to-lead strategies. This study emanated from our previously developed methods and subsequently predicted repositioning drug scaffolds.

Dr. B. C. Roy College of Pharmacy & AHS * Durgapur

Prof. (Dr.) Samir Kumar Samanta
M. Pharm., Ph.D (J.U.)
Principal
Dr. B. C. Roy College of Pharmacy & AHS
Durgapur, West Bengal-713206

Gmail

Souvik Basak <souvikb9@gmail.com>

Fwd: Reminder: Your Revision for Journal of Biomolecular Structure & Dynamics is due in one month on 24-Aug-2023

1 message

amit halder <amitcsir2011@gmail.com> Fri, Jul 28, 2023 at 3:51 PM
To: Souvik Basak <souvikb9@gmail.com>, debjani roy <roydebjani13@gmail.com>, Puja Mishra <pujamay12@gmail.com>

---------- Forwarded message ---------
From: **Journal of Biomolecular Structure & Dynamics** <onbehalfof@manuscriptcentral.com>
Date: Fri, Jul 28, 2023 at 2:42 PM
Subject: Reminder: Your Revision for Journal of Biomolecular Structure & Dynamics is due in one month on 24-Aug-2023
To: <amitcsir2011@gmail.com>

28-Jul-2023

Dear Dr Amit Halder,

Recently, you received a decision on Manuscript ID TBSD-2023-1798, entitled "Structural insights into the interactions of known drugs with hen egg white lysozyme for repositioning in Alzheimer's disease." This email is simply a reminder that your revision is due in one month on 24-Aug-2023.

If it is not possible for you to submit your revision by 24-Aug-2023, we will consider your paper as a new submission.

Please contact the Editorial Office if you are unable to submit within this time.

Please see a copy of the decision letter below which contains details of how to submit your revision and any comments from the editor/reviewers:

27-Jul-2023

Dear Dr Amit Halder,

Your manuscript entitled "Structural insights into the interactions of known drugs with hen egg white lysozyme for repositioning in Alzheimer's disease", which you submitted to Journal of Biomolecular Structure & Dynamics, has been reviewed. The referee comments are included at the bottom of this letter.

The referee(s) would like to see some revisions made to your manuscript before publication. Therefore, I invite you to respond to the referee(s)' comments and revise your manuscript.

When you revise your manuscript please ensure you submit two versions of your revised mansucript wiht the "Manuscript-with author details" file designation. One version should have changes highlighted by using yellow highlight and/or the Track Changes function, and the other should be a clean copy without highlights or Track Changes enabled.

In accordance with our format-free submission policy, an editable version of the article must be supplied at the revision stage. Please submit your revised manuscript files in an editable file format.

Please provide a reply to the referee comments; summarizing the changes you have made within the body of the manuscript in response to the referee comments, and any other response that you want the editor and the referees to note. You should submit it as a separate document along with manuscript files "Response to Decision Letter and Reviewer Comments". Upload this as the first document. You indicate in the space provided in the response box that a separate document has been uploaded.

The changes should be presented IN the revised paper, explaining the changes in the response document does not help the reader. The only manuscript that you upload should be the revised one with changes highlighted in yellow. Any other versions of the manuscript should not be uploaded.

Dr. B. C. Roy College of Pharmacy & AHS Durgapur

Prof. (Dr.) Samir Kumar Samanta
M. Pharm., Ph.D (J.U.)
Principal
Dr. B. C. Roy College of Pharmacy & AHS
Durgapur, West Bengal-713206

To submit a revision, go to https://rp.tandfonline.com/submission/flow?submissionId=238234892&step=1. If you decide to revise the work, please submit a list of changes or a rebuttal against each point which is being raised when you submit the revised manuscript.

If you have any questions or technical issues, please contact the journal's editorial office at TBSD-peerreview@journals.tandf.co.uk.

Please enter your responses to the comments made by the referee(s) in the space provided. You can use this space to document any changes you made to the original manuscript. Please be as specific as possible in your response to the referee(s).

IMPORTANT: Your original files are available to you when you upload your revised manuscript. Please delete any redundant files before completing the submission.

Because we are trying to facilitate timely publication of manuscripts submitted to Journal of Biomolecular Structure & Dynamics, your revised manuscript should be uploaded by 24-Aug-2023. If it is not possible for you to submit your revision by this date, we may have to consider your paper as a new submission.

Once again, thank you for submitting your manuscript to Journal of Biomolecular Structure & Dynamics and I look forward to receiving your revision.

Sincerely,
Professor Sarma
Editor in Chief, Journal of Biomolecular Structure & Dynamics
rhs07@albany.edu

Referee(s)' Comments to Author:

Referee: 1

Comments to the Author
The authors used Six drugs (dapsone, diltiazem, timolol, rosiglitazone, mesalazine and milnacipran) to understand the anti-Alzheimer's nature using hen egg white lysozyme. They used computational techniques MD simulations in combination with the in vitro studies. The study has a potential and well-written manuscript. However, it requires additional evidence to show anti-alzheimer's.
Comments:
1. The molecules which you have used show not much significant effect on fibrillization. Usually, if really inhibiting the fibrillization, it is always better to show the TEM or AFM data. So that your study will have more value. You must show this in your revision.
2. Most of the data can be clubbed. Some of the data quality (font size is invisible) is poor. Improve the figures.
3. Figure legends should be expanded.

Referee: 2

Comments to the Author
1. The simulation length is small, please increase length of the simulation.
2. Please provide average RMSD valuse along with standard deviation for each system.
3. Please calculate average RMSD for each amino acid residue that are present around ligand-1 and ligand-2, so that we can understand which residue's contribution is more.
4. Could you please explain how milnacipram helps to retention of the α-helix?
5. Please increase the image quality.
6. The reference format should be same for all the references.

Referee: 3

Comments to the Author
The manuscript titled "Structural insights into the interactions of known drugs with hen egg white lysozyme for repositioning in Alzheimer's disease "by Prof Halder et al. investigates the anti-protein fibrillating activity of six drugs. The authors employed in both silico and in vitro evaluation techniques to assess the potential of six drugs as anti-Alzheimer's agents. Among these drugs, three candidates demonstrated stable binding within the fibrillating region of Hen Egg White Lysozyme (HEWL), a widely recognized model protein for studying amyloid fibril formation and related mechanisms.
Regarding the in vitro evaluation, the use of Congo red and ThT assay provides the essential data. The authors' approach of monitoring fluorescence intensity as a function of drug concentration is noteworthy. However, the reported inhibitory effects ranging from 20.95% to 27.03% were not found to be significant.
To complement the existing findings and contribute positively to the manuscript, several additional approaches are suggested:

Dr. B. C. Roy College of Pharmacy & A.H.R.C. Durgapur

Prof. (Dr.) Samir Kumar Samanta
M. Pharm., Ph.D (J.U.)
Principal
Dr. B. C. Roy College of Pharmacy & A.H.R.C.
Durgapur, West Bengal-713206

1. Capturing aggregation kinetics at different time points could offer a deeper understanding of the inhibitory effects. Exploring a wider range of drug concentrations, including higher concentrations, would provide a comprehensive view of the inhibition kinetics (Refer publication 1-4 in reference section).
2. Employing advanced microscopic techniques such as TEM, SEM, or AFM to study fibrillary inhibition and observe morphological changes in fibril formation could enhance the comprehensiveness of the study. These high-resolution methods would offer valuable complementary data to support the conclusions drawn from the fluorescence assays (Refer publication 1-4 in reference section).
3. Furthermore, analyzing the secondary structure changes through Circular Dichroism (CD) could provide valuable insights into the formation of the characteristic cross-β sheet structure in amyloid fibrils. This additional analysis would strengthen the evidence for the inhibitory effects of the tested drugs (Refer publication 1-4 in reference section).

In conclusion, Prof Halder et al.'s manuscript presents a potential anti-protein fibrillating drugs with implications for Alzheimer's disease research. By incorporating the suggested complementary approaches, the authors can further enrich the study and solidify the significance of their findings. Overall, this research contributes to the growing body of knowledge in the field of amyloid fibril formation and potential therapeutic interventions.

1. Mahdavimehr M,. Inhibition of HEWL fibril formation by taxifolin: Mechanism of action. PLoS One. 2017 Nov 13;12(11):e0187841. doi: 10.1371/journal.pone.0187841.
2. Bugg CW, et al. Structural features and domain organization of huntingtin fibrils. doi: 10.1074/jbc.M112.353839.
3. Belwal, V.K, The β-turn-supporting motif in the polyglutamine binding peptide QBP1 is essential for inhibiting huntingtin aggregation. FEBS Lett, 594: 2894-2903. https://doi.org/10.1002/1873-3468.13873
4. Morshedi, D., Rezaei-Ghaleh, N., Ebrahim-Habibi, A., Ahmadian, S. and Nemat-Gorgani, M. (2007), Inhibition of amyloid fibrillation of lysozyme by indole derivatives – possible mechanism of action. The FEBS Journal, 274: 6415-6425. https://doi.org/10.1111/j.1742-4658.2007.06158.x

Editor's Comments to Author:

Associate Editor
Comments to Author:
Both reviewers have concerns, especially about the quality of the data and the images. I am concerned about the large number of authors for such a straightforward manuscript.

If you have any questions or experience any difficulties submitting your revised manuscript, please contact the journal's editorial office at TBSD-peerreview@journals.tandf.co.uk.

Sincerely,
Nasreen Banu
Journal of Biomolecular Structure & Dynamics Editorial Office
TBSD-peerreview@journals.tandf.co.uk

--

Amit Kumar Halder
amit.halder@fc.up.pt

Investigador Pós-Doc
Laboratório Associado para a Química Verde

FACULDADE DE CIÊNCIAS DA UNIVERSIDADE DO PORTO
Rua do Campo Alegre, s/n, 4169-007 Porto, Portugal
www.fc.up.pt

Dr. B. C. Roy College of Pharmacy & AHS * Durgapur

Prof. (Dr.) Samir Kumar Samanta
M. Pharm., Ph.D (J.U.)
Principal
Dr. B. C. Roy College of Pharmacy & AHS
Durgapur, West Bengal-713206

Structural insights into the interactions of repositioning and known drugs for Alzheimer's disease with hen egg white lysozyme by MM-GBSA

Amit Kumar Halder[a,b*#], Puja Mishra[a], Souvik Basak[a#], Debjani Roy[c*], Anurag Das[a], Sucheta Karmakar[a], Ritam Mondal[a], Shrestha Banerjee[a], Prakarsha De[a], Ankit Chatterjee[a], Susmita Mallick[a], Abhijit Hazra[d]

[a]Dr. B. C. Roy College of Pharmacy & Allied Health Sciences, Durgapur, WB, India

[b]LAQV@REQUIMTE/Department of Chemistry and Biochemistry, Faculty of Sciences, University of Porto, 4169-007 Porto, Portugal.

[c]Department of Biological Sciences, Bose Institute, Kolkata, India

[d]National Institute of Pharmaceutical Education and Research, Kolkata, India

[#]equal contribution

*Joint corresponding author

E-mail: amit.halder@bcrcp.org, roydebjani13@gmail.com

Authors' contributions:

Amit, Puja, Souvik: Conceived, designed and performed the simulations and the entire experiments, *Amit:* MD and MMGBSA, writing the manuscript; *Souvik and Puja:* Experimentation and writing the manuscript; *Debjani Roy:* Provided molecules, simulations and financial support; *Abhijit Hazra:* CD experiments and data analyses; *Prakarsha, Sherstha, Anurag, Sucheta, Ritam, Ankit and Sushmita:* Setting up the drug-protein reactions, batch and concentration