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.) Sanjay 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

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

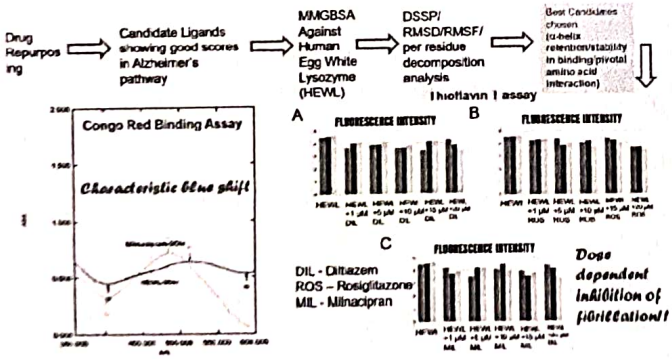
Amit Kumar Halder[a,b]*, Puja Mishra[a], Souvik Basak[a]*, Debjani Roy[c], Anurag Das[a], Sucheta Karmakar[a], Ritam Mondal[a], Shrestha Banerjee[a], Prakarsha De[a], Ankit Chatterjee[a], Susmita Mallick[a] and Abhijit Hazra[d]

[a]Dr. B. C. Roy College of Pharmacy & Allied Health Sciences, Durgapur, India; [b]LAQV@REQUIMTE/Department of Chemistry and Biochemistry, Faculty of Sciences, University of Porto, Porto, Portugal; [c]Department of Biological Sciences, Bose Institute, Kolkata, India; [d]National Institute of Pharmaceutical Education and Research, Kolkata, India

Communicated by Ramaswamy H. Sarma

ABSTRACT

Six drugs (dapsone, diltiazem, timolol, rosiglitazone, mesalazine, and milnacipran) that were predicted by network-based polypharmacology approaches as potential anti-Alzheimer's drugs, have been subjected in this study for *in silico* and *in vitro* evaluation to check their potential against protein fibrillation, which is a causative factor for multiple diseases such as Alzheimer's disease, Parkinson's disease, Huntington disease, cardiac myopathy, type-II diabetes mellitus and many others. Molecular docking and thereafter molecular dynamics (MD) simulations revealed that diltiazem, rosiglitazone, and milnacipran interact with the binding residues such as Asp52, Glu35, Trp62, and Asp101, which lie within the fibrillating region of HEWL. The MM-GBSA analysis revealed −7.86, −5.05, and −10.29 kcal/mol as the binding energy of diltiazem, rosiglitazone, and milnacipran. The RMSD and RMSF calculations revealed significant stabilities of these ligands within the binding pocket of HEWL. While compared with two reported ligands inhibiting HEWL fibrillation, milnacipran depicted almost similar binding potential with one of the known ligands (Ligand binding affinity −10.66 kcal/mol) of HEWL. Furthermore, secondary structure analyses revealed notable inhibition of the secondary structural changes with our candidate ligand; especially regarding retention of the 3/10 α-helix both by DSSP simulation, Circular dichroism, and FESEM-based microscopic image analyses. Taking further into experimental validation, all three ligands inhibited fibrillation in HEWL in simulated conditions as revealed by blue shift in Congo red assay and later expressing percentage inhibition in ThioflavinT assay as well. However, dose-dependent kinetics revealed that the antifibrillatory effects of drugs are more pronounced at low protein concentrations.



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KEYWORDS
Protein fibrillation; drug repositioning; MM-GBSA; Congo Red; ThioflavinT

1. Introduction

Protein fibrillation is a process characterized by the structural integration of a series of unfolded or misfolded proteins resulting in the formation of fibril-like structures. This fibril-like structure is often mediated by the formation of β-sheet as the core protein monomer, which by end to joining, forms fibril-like oligomers leading to protein aggregation and plaque formation (Arnaudov & de Vries, 2015; Athar et al., 2021; Ban et al., 2018; Borana et al., 2014; Chiti & Dobson, 2006; Dobson, 2003; Faramarzian et al., 2020; Harada et al., 2008). This process, known as amyloidogenesis, often results in tissue dysfunction by

CONTACT Amit Kumar Halder amit.halder@bcrcp.org, amitcsir2011@gmail.com; Debjani Roy roydebjani13@gmail.com
Equal contribution
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