RSC Advances

Home

Author

Submission Confirmation

Print

Thank you for your submission

Submitted to
RSC Advances

Manuscript ID
RA-ART-09-2020-007838

Title
In silico approach: Biological activities prediction of nordentatin derivatives as an anticancer agent in cAMP pathway inhibitors

Authors
Abdjan, Muhammad
Aminah, Nanik
siswanto, Imam
Thant, Tin
Kristanti, Alfinda Novi
Takaya, Yoshiaki

Date Submitted
13-Sep-2020

Author Dashboard

nanik siti aminah <nanik-s-a@fst.unair.ac.id>

Acknowledgement of your Submission to RSC Advances - RA-ART-09-2020-007838

1 message

RSC Advances <onbehalfof@manuscriptcentral.com> Sun, Sep 13, 2020 at 11:12 PM
Reply-To: advances@rsc.org
To: nanik-s-a@fst.unair.ac.id
Cc: muhammad.ikhlas.abdjan-2018@fst.unair.ac.id, nanik-s-a@fst.unair.ac.id, imamsiswanto@fst.unair.ac.id, tin.myo.thant-2017@fst.unair.ac.id, alfinda-n-k@fst.unair.ac.id, ytakaya@meijo-u.ac.jp

13-Sep-2020

Dear Dr Aminah:

TITLE: In silico approach: Biological activities prediction of nordentatin derivatives as an anticancer agent in cAMP pathway inhibitors

Thank you for your submission to RSC Advances, published by the Royal Society of Chemistry. This is an automatic acknowledgement that you have uploaded your files to our online submission system. Your manuscript ID is: RA-ART-09-2020-007838

Your manuscript will be passed to an editor for initial assessment as soon as possible. If there are any problems with your submission we will contact you.

RSC Advances is a gold open access journal. If accepted, your manuscript will be published open access and the article will be subject to the appropriate article processing charge (APC). Discounted APCs and full APC waivers for corresponding authors in certain countries are available. All authors are given the option to apply for a waiver after signing the open access licence - please see the following URL for more details: http://www.rsc.org/journals-books-databases/about-journals/rsc-advances

Please indicate the above manuscript ID when you contact us about this submission.

Do you have an ORCID iD? ORCID (Open Researcher and Contributor iD) is a unique researcher identifier that allows you to link your research output and other professional activities in a single record. We therefore encourage each researcher to sign up for their own ORCID account. Please edit your user account to link your ORCID iD or create a new one, ensuring that you have not linked your account to another researcher's ORCID iD. Please note that we are unable to do this on your behalf. If your article is accepted, you may choose to have your ORCID record updated automatically with details of the publication.

We already have the following information for authors of this manuscript: Abdjan, Muhammad - No ORCID iD Available, Aminah, Nanik - No ORCID iD Available, siswanto, Imam - No ORCID iD Available, Thant, Tin - No ORCID iD Available, Kristanti, Alfinda Novi - No ORCID iD Available, Takaya, Yoshiaki - No ORCID iD Available
If this is not how you want your name to appear on an Accepted Manuscript, please amend your ScholarOne account.

The Royal Society of Chemistry is a member of CrossCheck. Your submission may be compared against the CrossCheck database using the iThenticate plagiarism detection software. For further information, please see here: http://www.rsc.org/Publishing/Journals/guidelines/EthicalGuidelines/CrossCheck/CrossCheck.asp

This journal has a policy of sharing reviewer reports. Please note that the Editor's decision and copies of the reports will be shared with all reviewers who provide a recommendation on your manuscript.

Please contact us if we can be of any assistance.

Yours sincerely,
RSC Advances Editorial Office
advances@rsc.org
If you need to contact the journal, please use the email address advances@rsc.org

****

DISCLAIMER:

This communication is from The Royal Society of Chemistry, a company incorporated in England by Royal Charter

nanik siti aminah <nanik-s-a@fst.unair.ac.id>

Track the progress of your RSC Advances submission

1 message

RSC Advances <noreply@rsc.org> Sun, Sep 13, 2020 at 11:12 PM
To: Dr Nanik Siti Aminah <nanik-s-a@fst.unair.ac.id>

Dear Dr Nanik Siti Aminah

Thank you for submitting your manuscript to RSC Advances. We have safely received the files and information you have provided.

Our team are currently processing your submission and will be in touch shortly.

You can use the following link to track the status of your submission. You can also share this link with your co-authors so that they can keep track of the manuscript's progress too.

https://submissions.rsc.org/tracker/RA-ART-09-2020-007838?t=ZKN9CQL792Y3xdmpilszYUtWBJQ9szhUFsUTCVkp8B6CUg%3D%3D

Yours sincerely,
RSC Advances Editorial Office
advances@rsc.org

Please do not reply to this email.

nanik siti aminah <nanik-s-a@fst.unair.ac.id>

Decision on submission to RSC Advances - RA-ART-09-2020-007838

3 messages

RSC Advances <onbehalfof@manuscriptcentral.com> Fri, Oct 23, 2020 at 4:50 PM
Reply-To: advances@rsc.org
To: nanik-s-a@fst.unair.ac.id

23-Oct-2020

Dear Dr Aminah:

Manuscript ID: RA-ART-09-2020-007838
TITLE: In silico approach: Biological activities prediction of nordentatin derivatives as an anticancer agent in cAMP pathway inhibitors

Thank you for your submission to RSC Advances, published by the Royal Society of Chemistry. I sent your manuscript to reviewers and I have now received their reports which are copied below.

I have carefully evaluated your manuscript and the reviewers' reports, and the reports indicate that major revisions are necessary.

Please submit a revised manuscript which addresses all of the reviewers' comments. Further peer review of your revised manuscript may be needed. When you submit your revised manuscript please include a point by point response to the reviewers' comments and highlight the changes you have made. Full details of the files you need to submit are listed at the end of this email.

Please submit your revised manuscript as soon as possible using this link:

*** PLEASE NOTE: This is a two-step process. After clicking on the link, you will be directed to a webpage to confirm. ***

https://mc.manuscriptcentral.com/rscadv?URL_MASK=ec128da908f64bf882068de556d41e5d

(This link goes straight to your account, without the need to log on to the system. For your account security you should not share this link with others.)

Alternatively, you can log in to your account (https://mc.manuscriptcentral.com/rscadv) where you will need your case-sensitive user ID and password details.

You should submit your revised manuscript as soon as possible; please note you will receive a series of automatic reminders. If your revisions will take a significant length of time, please contact me.

Supporting our community through Covid-19
While our publishing services are running as usual, we also know that this is a very challenging time for everyone, for many different reasons. If any aspect of the publishing process is worrying you – for example you think you may struggle to meet a pre-determined deadline – please let us know, and we will work out an answer together.

RSC Advances is a gold open access journal. If accepted, your manuscript will be published open access and the appropriate article processing charge (APC) will apply. Discounted APCs and full APC waivers for corresponding authors in certain countries are available. All authors are given the option to apply for a waiver after signing the open access licence - please see the following URL for more details: http://www.rsc.org/journals-books-databases/about-journals/rsc-advances

The Royal Society of Chemistry requires the submitting author to provide their ORCID iD when they submit a revised manuscript. This is quick and easy to do as part of the revised manuscript submission process. We will publish this information with the article, and you may choose to have your ORCID record updated automatically with details of the publication.

Please also encourage your co-authors to sign up for their own ORCID account and associate it with their account on our manuscript submission system. Please note that we are unable to do this on behalf of your co-authors. For further information see: http://www.rsc.org/journals-books-databases/journal-authors-reviewers/processes-policies/#attribution-id.

I look forward to receiving your revised manuscript.

Yours sincerely,
Professor Yongjun Liu
Associate Editor, RSC Advances

****
REVIEWER REPORT(S):
Referee: 1

Recommendation: Major revisions

Comments:
In the present study the authors have employed Molecular docking and dynamics approach to assess the binding of a few (10) nordentatin derivatives against the PDE4 gene.

The manuscript needs the following revisions:
1. It is preferable that instead of using "biological activity", the authors should use the term "binding" as no experimental determination of activity is undertaken.
2. The term "activities" from the title should be removed.
3. The authors should rewrite abstract and stress on the observations and results obtained from this study, rather than the general statements. For example: the last sentence in the abstract "Consideration of several....." should either be reframed or deleted as it is a general statement.
4. The length of introduction should be reduced. It is too lengthy.
5. It is not clear why the authors have selected only 10 nordentatin derivatives. It is always preferable if more number of derivatives are taken for docking.
6. In general there are a lot of errors and the manuscript should be go through proof read carefully. For example: (a) instead of "Chimera", "himera" is written in methods. (b) Meanwhile, Linux-based software used Was..... should be "Linux based softwares Guassian.....etc were used." (c) Delete "Windows-based" from Windows-based Disovery Studio....
7. In the sentence "The results show that candidates PS-1, PS-2, PS-3, ..." replace smaller with better.
8. The analysis of total energy output during the simulation period.....Which total energy is being referred to? It is not clear.
9. Table 7. It should be specified what is MD and MDS.

Additional Questions:
Does the work significantly advance the understanding or development in this field?: Yes

Is this work of relevance to the chemistry community?: Yes

Are the conclusions of the work convincing and sufficiently supported by experimental evidence?: Yes

Is the experimental section sufficiently detailed to allow others to reproduce the work?: Yes

Are the reported claims adequately discussed in the context of the literature?: Yes

Are the number of tables and figures in the manuscript appropriate and clear?: Yes

Referee: 2

Recommendation: Minor revisions

Comments:
In this manuscript, the authors explored the binding of a series of nordentatin derivatives with the protein targets using a combination of molecular docking and molecular dynamic simulation. Some derivatives show strong binding with the target protein, which suggest the potential of these derivatives as drugs in inhibiting the cAMP pathway. In general, the used methods are appropriate, and results are reasonable. Thus, the manuscript is acceptable for publication.
Revision suggestions:
1). Please explain why the strong binding these dirivatives can inhibit the cAMP pathway, i.e., the relation of binding energy and activity.
2). Some figures, such as Figure 3, 4 and 5 are not clear.

Additional Questions:

Does the work significantly advance the understanding or development in this field?: Yes

Is this work of relevance to the chemistry community?: Yes

Are the conclusions of the work convincing and sufficiently supported by experimental evidence?: Yes

Is the experimental section sufficiently detailed to allow others to reproduce the work?: Yes

Are the reported claims adequately discussed in the context of the literature?: Yes

Are the number of tables and figures in the manuscript appropriate and clear?: Yes

****
FILES TO PROVIDE WITH YOUR REVISED MANUSCRIPT:
IMPORTANT: Your original files are available to you when you upload your revised manuscript. Please delete any redundant files before completing the submission. Please carefully check the spelling and format of all author names, affiliations and funding information. If your paper is accepted for publication, it is important this information is accurate to ensure your article is correctly indexed, which may affect citations and future funding evaluation.

- A point-by-point response to the comments made by the reviewer(s)
- Your revised manuscript with any changes clearly marked (.doc(x) or.pdf file)
- Your revised manuscript as a .doc(x) file including figures, without highlighting, track changes, etc. (If providing in TeX format instead, please also provide a final PDF version including figures). Please note that we cannot proceed with publication using a .pdf file only.

High quality figures
EITHER
embedded in a doc(x) file
OR
as numbered figures in separate files in .tif, or .eps format, with a resolution of 600 dpi or greater and structures preferably as ChemDraw files. Chemwindow files (.cwg/.cw2), ISIS/Draw exported in sketch format (.skc) and ChemSketch exported in ChemDraw format (.cdx) may also be supplied.

AND

• A table of contents entry: graphic maximum size 8 cm x 4 cm and one sentence of text, maximum 20 words, highlighting the novelty of the work
• Your revised Electronic Supplementary Information (if any)
• Your revised CheckCIF reports (if any). Please ensure that any revised cif files have been deposited with the Cambridge Crystallographic Data Centre (CCDC) via https://deposit.ccdc.cam.ac.uk/ before you submit your revised manuscript.

For Feature Articles/Review-type articles only:
• A photograph and biography of yourself and your co-authors. Separate photographs of each author may be supplied or if you prefer, a group photograph, saved as a .tif, .pdf or .jpeg file. The resolution of the photographs should be 600 dpi or higher. The dimensions of the photograph in the printed journal will be 4 cm wide x 5 cm high (individual photograph) or 8.3 cm wide x 5 cm high (group photograph). Individual photographs should be accompanied by a maximum of 100 words; a group photograph by a maximum of 200 words. There can be a maximum of 6 individual biographies per article.
• Copies of permissions required from other publishers to reproduce figures. Please ensure that necessary permissions are acknowledged in the figure captions in accordance with the publishers' instruction. Information on how to obtain permissions and rights that we require are given on our website at http://www.rsc.org/journals-books-databases/journal-authors-reviewers/licences-copyright-permissions/

****
If you need to contact the journal, please use the email address advances@rsc.org

****

nanik siti aminah <nanik-s-a@fst.unair.ac.id>

Acknowledgement of your revised manuscript submission to RSC Advances - RA-ART-09-2020-007838.R1

1 message

RSC Advances <onbehalfof@manuscriptcentral.com> Thu, Nov 5, 2020 at 1:11 PM
Reply-To: advances@rsc.org
To: nanik-s-a@fst.unair.ac.id
Cc: muhammad.ikhlas.abdjan-2018@fst.unair.ac.id, nanik-s-a@fst.unair.ac.id, imamsiswanto@fst.unair.ac.id, tin.myo.thant-2017@fst.unair.ac.id, alfinda-n-k@fst.unair.ac.id, ytakaya@meijo-u.ac.jp

05-Nov-2020

Dear Dr Aminah:

TITLE: In silico approach: Biological prediction of nordentatin derivatives as an anticancer agent in cAMP pathway inhibitors
AUTHORS: Abdjan, Muhammad; Aminah, Nanik; siswanto, Imam; Thant, Tin; Kristanti, Alfinda Novi ; Takaya, Yoshiaki

Thank you for your revised submission to RSC Advances, published by the Royal Society of Chemistry. This is an automatic acknowledgement that you have uploaded your files to our online submission system. Your manuscript ID is: RA-ART-09-2020-007838.R1

Your manuscript will be passed to an editor for initial assessment as soon as possible. If there are any problems with your submission we will contact you.

RSC Advances is a gold open access journal. If accepted, your manuscript will be published open access and the article will be subject to the appropriate article processing charge (APC). Discounted APCs and full APC waivers for corresponding authors in certain countries are available. All authors are given the option to apply for a waiver after signing the open access licence - please see the following URL for more details: https://www.rsc.org/journals-books-databases/about-journals/rsc-advances

Please indicate the above manuscript ID when you contact us about this submission.

If there have been any changes to the list of authors during this revision, please inform the Editorial Office of the reason for the change. All authors must confirm they are happy with the authorship change by emailing advances@rsc.org.

Do you have an ORCID iD? ORCID (Open Researcher and Contributor iD) is a unique researcher identifier that allows you to link your research output and other professional activities in a single record. We therefore encourage each researcher to sign up for their own ORCID account. Please edit your user account to link your ORCID iD or create a new one, ensuring that you have not linked your account to another researcher's ORCID iD. Please note that we are unable to do this on your behalf. If your article is accepted, you may choose to have your ORCID record updated automatically with details of the publication.

We already have the following information for authors of this manuscript: Abdjan, Muhammad - No ORCID iD Available, Aminah, Nanik - https://orcid.org/0000-0002-2767-6006, siswanto, Imam - No ORCID iD Available, Thant, Tin - No ORCID iD Available, Kristanti, Alfinda Novi - No ORCID iD Available, Takaya, Yoshiaki - No ORCID iD Available
If this is not how you want your name to appear on an Accepted Manuscript, please amend your ScholarOne account.

This journal has a policy of sharing reviewer reports. Please note that the Editor's decision and copies of the reports will be shared with all reviewers who provide a recommendation on your manuscript.

Please contact us if we can be of any assistance.

Yours sincerely,
RSC Advances Editorial Office
advances@rsc.org
If you need to contact the journal, please use the email address advances@rsc.org

****

DISCLAIMER:

nanik siti aminah <nanik-s-a@fst.unair.ac.id>

Decision on submission to RSC Advances - RA-ART-09-2020-007838.R1

1 message

RSC Advances <onbehalfof@manuscriptcentral.com> Fri, Nov 6, 2020 at 4:21 PM
Reply-To: advances@rsc.org
To: nanik-s-a@fst.unair.ac.id

06-Nov-2020

Dear Dr Aminah:

Manuscript ID: RA-ART-09-2020-007838.R1
TITLE: In silico approach: Biological prediction of nordentatin derivatives as an anticancer agent in cAMP pathway inhibitors

Thank you for submitting your revised manuscript to RSC Advances. After considering the changes you have made, I am pleased to accept your manuscript for publication in its current form.

You will shortly receive a separate email from us requesting you to submit a licence to publish for your article, so that we can proceed with publication of your manuscript.

RSC Advances is a gold open access journal. Your manuscript will be published open access and the article will be subject to the appropriate article processing charge (APC). Discounted APCs and full APC waivers for corresponding authors in certain countries are available. All authors are given the option to apply for a waiver after signing the open access licence - please see the following URL for more details: https://www.rsc.org/journals-books-databases/about-journals/rsc-advances

We are offering all corresponding authors not already members of the Royal Society of Chemistry one year's Affiliate membership as part of their APC. If you would like to find out more please email membership@rsc.org.

Learn all about our member benefits at https://www.rsc.org/membership-and-community/join/#benefit

We will email you information on how to access your RSC Advances article proofs shortly.

As an author you are entitled to a 25% discount on books published by the Royal Society of Chemistry. To receive this discount, enter the promotional code JLTH25 when purchasing from our online bookshop (pubs.rsc.org/bookshop). Please contact booksales@rsc.org if you have any problems.

Discover more Royal Society of Chemistry author services and benefits here:

https://www.rsc.org/journals-books-databases/about-journals/benefits-of-publishing-with-us/

Thank you for publishing with RSC Advances, a journal published by the Royal Society of Chemistry – connecting the world of science to advance chemical knowledge for a better future

With best wishes,

Professor Yongjun Liu
Associate Editor, RSC Advances

******

If you need to contact the journal, please use the email address advances@rsc.org

****

nanik siti aminah <nanik-s-a@fst.unair.ac.id>

Required: Licence to Publish - D0RA07838G

1 message

advances@rsc.org <advances@rsc.org>
To: nanik-s-a@fst.unair.ac.id

Fri, Nov 6, 2020 at 5:46 PM

Friday, November 6, 2020

Dear Dr Aminah,

TITLE: In silico approach: Biological prediction of nordentatin derivatives as an anticancer agent in cAMP pathway inhibitors
MANUSCRIPT ID: D0RA07838G

Before we can publish your manuscript in RSC Advances, we need you to sign a licence to publish.

Follow this link to choose and sign your licence to publish:

https://licences.rsc.org/email-link?id=D0RA07838G&t=ctICCWCY4mU2r5epjlovY0tTDJY1%2Bz8%3D

We are unable to publish your manuscript until a valid licence has been received, so please sign the licence as soon as possible to avoid delays. If you would like to publish your article open access, relevant licence options are also available through the above link. Please reply to this email if you have any questions.

Thank you for choosing to publish with RSC Advances, a journal published by the Royal Society of Chemistry.

Yours sincerely,
RSC Advances Editorial Office

****

nanik siti aminah <nanik-s-a@fst.unair.ac.id>

Confirmation: Licence to Publish signed - D0RA07838G

1 message

advances@rsc.org <advances@rsc.org> Mon, Nov 9, 2020 at 10:31 AM
To: nanik-s-a@fst.unair.ac.id

Monday, November 9, 2020

Dear Dr Aminah,

TITLE: In silico approach: Biological prediction of nordentatin derivatives as an anticancer agent in cAMP pathway inhibitors
MANUSCRIPT ID: D0RA07838G

We are pleased to confirm we have received your signed licence to publish for your article D0RA07838G.

Your article will be published gold open access. Our customer services team will contact you shortly if required.

You will receive a separate email explaining how to access your article proofs.

Yours sincerely,
RSC Advances Editorial Office

****

Your RSC Advances article (D0RA07838G) proof is ready for checking

3 messages

advances@rsc.org <advances@rsc.org> Thu, Nov 19, 2020 at 9:20 PM
To: nanik-s-a@fst.unair.ac.id

Follow us and stay in touch

ROYAL SOCIETY OF CHEMISTRY

Dear Dr Nanik Siti Aminah

In silico approach: Biological prediction of nordentatin derivatives as an anticancer agent in cAMP pathway inhibitors

We have prepared a proof of your article, which is now available at Proof Central.

Proof Central provides you with a user-friendly interface to help you manage your proofs quickly and efficiently. You can find out more about Proof Central here.

You can find instructions on the submission of your corrections at Proof Central.

Please return your corrections within 48 hours. If you are unable to return your corrections within 48 hours, please let us know.

Supporting our community through Covid-19
While our publishing services are running as usual, we also know that this is a very challenging time for everyone, for many different reasons. If any aspect of the publishing process is worrying you – for example you think you may struggle to meet a pre-determined deadline – please let us know, and we will work out an answer together. You can contact the journal at advances@rsc.org.

If you prefer to send your corrections by email, please download your proof using Proof Central and send your corrections to advances@rsc.org

The page numbers on the proof are not the final page numbers of your article, we will send these once your article is published in an issue of *RSC Advances*.

If you have a waiver request pending, please do not return your proof corrections; due to our fast publication times we will be unable to stop or delay the publication of your article. If your waiver is not granted you will be required to pay the Article Processing Charge according to the terms and conditions which you accepted when you submitted your article.

With best wishes,
From the Editors of *RSC Advances*
Royal Society of Chemistry
advances@rsc.org

If you are unable to access your proofs using the links above, please paste the following link into your browser: https://rscjournals.proofcentral.com/en-us/landing-page.html?token=4fb2facc050eb294c7f200608dff16

Your RSC Advances article page numbers are now available

1 message

advances@rsc.org <advances@rsc.org>
To: nanik-s-a@fst.unair.ac.id

Wed, Nov 25, 2020 at 6:59 PM

Dear Dr Nanik Siti Aminah

In silico approach: Biological prediction of nordentatin derivatives as an anticancer agent in cAMP pathway inhibitors

We have published your *RSC Advances* article in an issue on pages 42733 - 42743.

It can now be cited as:

RSC Advances, 2020, **10**, 42733 - 42743

We would like to hear your thoughts on the editing service provided for this article. Please give us your opinion through this short, 5-minute survey.

Access your PDF reprints here

Manuscript ID: D0RA07838G

Password: 471719 (this link will expire in 60 days)

You can now access the enhanced HTML version of your article here

We encourage you to share your article with the chemical sciences community. Share your article easily among colleagues, peers or students by downloading your free PDF reprint or by purchasing paper reprints here. Find out more about your deposition and sharing rights.

You can see all the latest papers published in RSC Advances by signing up to our email alerts service here

Thank you for publishing with *RSC Advances*, a journal published by the Royal Society of Chemistry – connecting the world of science to advance chemical knowledge for a better future.

With best wishes,
From the Editors of *RSC Advances*
Royal Society of Chemistry
advances@rsc.org