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#### **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

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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

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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

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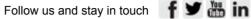


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