Journal of Kermanshah University of Medical Sciences
Volume 26 · Issue 4 · e131043

OPEN PEER REVIEW

Evaluation of Molecular Docking and Cytotoxicity by *Pycnocycla bashagardiana* Fruit Essential Oil in Colon Cancer Cell Lines

Zahra Ghazazani, masoumeh heshmati, Jinous Asgarpanah, Sanaz Pashapour

SUBMITTED	REVISED	ACCEPTED	DOI
26 Aug 2022	19 Dec 2022	21 Dec 2022	10.5812/jkums-131043

About this report

This open peer review (OPR) report shows the public comments made on this article during peer review, by the reviewers, the associate editor and the editor-in-chief, for every revision round, together with the authors' replies. Comments appear only with the consent of the people who wrote them. Reviewers who chose to sign their report are named; the others are shown as "Referee". Comments are edited for language only, and confidential remarks to the editors are not included.

More about open peer review: brieflands.com/knowledgebase/opr

Contents

1 **Original submission** Editor-in-Chief 2
2 **Revision 1** Editor-in-Chief 3
Authors' reply to reviewers 4
Reviewer and editor comments 7
3 **Revision 2** Associate Editor, Editor-in-Chief 8
Authors' reply to reviewers 9
Reviewer and editor comments 10
4 **Revision 3** Editor-in-Chief 11
Authors' reply to reviewers 12
Reviewer and editor comments 13

1 Original submission

1 comment · 1 Nov 2022

Editor-in-Chief

MAJOR REVISION 1 Nov 2022

Revision is needed.

2

Revision 1

AUTHORS' RESPONSE TO REVIEWERS

Authors' reply to reviewers

The next pages contain the authors' point-by-point reply to the comments of this revision round, as submitted with the revised manuscript. It is published as the authors wrote it.

1:

-1 Title
Evaluation of Molecular docking, cytotoxicity by essential oil from Pycnocycla bashagardianaFruits in colon cancer cell line
-2 Persian and English abstract (Explanation: the abstract contains the Background, Methods, Results and Conclusion sections and has a maximum of 250 words):

The full name of the plant should be stated in the title Mozaff) bashagardiana

Pycnocycla).

The full name of the plant is Pycnocycla bashagardiana, which was italicized in the text.

-3 Keywords: Appropriate.

-4 Introduction:

-1 Abbreviations should be written in full the first time, including RPMI, MTT, PBS ...

Thank you for the respected reviewer's comment; the corrections were made .

-2 The geographical details (longitude and latitude) of the area where the plant was collected should be written.

Thank you for the reviewer's comment; unfortunately, no information on the geographical area is available .

-3 It has many writing and grammatical errors.

Thank you for the respected reviewer's comment; the corrections were made

-5 Materials and Methods :

-4 In RNA extraction, in addition to NanoDrop, RNA quality should have been measured by agarose gel electrophoresis.

Including the agarose gel for RNA extraction in an article is not at all customary. Therefore, it has not been included in this article either.

-5 The temperature conditions of the PCR Real-time should be stated.

Thank you for the respected reviewer's comment; the corrections were made.

-6 Results :
In the graphs of Figure 4, with which group were the groups compared? There is no control column. The horizontal axis does not show the concentration. On what basis were the significance marks placed? It is not clear whether Bcl-2 increased or decreased relative to the control group? It appears to have increased.

In real-time analysis, fold change means comparison with the control, which is always the value 1. Therefore, drawing the control bar in the graph was avoided. Also, the text related to this section states that the comparison was made with the control group (untreated). The concentrations are indicated in the graph.

Given that a series of flow cytometry images has been included in the article, was this test repeated, given that error bars appear on the graphs?

Yes, but one series of the images has been included.

Why were 6 concentrations selected in the MTT test, 3 concentrations in flow cytometry and two concentrations in the real-time PCR test? It would have been better to select the concentrations based on the IC50.

Based on the flow cytometry results, one of the concentrations was removed because of high necrosis

In the graphs of Figure 4, with which group were the groups compared? There is no control column. The horizontal axis does not show the concentration. On what basis were the significance marks placed? It is not clear whether Bcl-2 increased or decreased relative to the control group? It appears to have increased

In real-time analysis, fold change means comparison with the control, which is always the value 1. Therefore, drawing the control bar in the graph was avoided. Also, the text related to this section states that the comparison was made with the control group (untreated). The concentrations are indicated in the graph.

-7 Discussion:
The Discussion heading should be written

Thank you for the respected reviewer's comment; the corrections were made.

9. The first line of the Discussion relates to the Introduction and should be deleted (

Thank you for the respected reviewer's comment; the corrections were made.

reference.) Thank you for the respected reviewer's comment; the corrections were made.

10

-8 Conclusion : Appropriate.

-9 References should be corrected according to the journal format. Thank you for the respected reviewer's comment; the corrections were made.

2 Revision 1

1 comment · 8 Nov 2022

Editor-in-Chief

MINOR REVISION 8 Nov 2022

Comparative expert's comments
The geographical characteristics (longitude and latitude) of the plant collection area should be written. 3- There are many spelling and grammar mistakes.
4- In RNA extraction, in addition to nanodrops, RNA quality should be measured by agarose gel electrophoresis. 5- Temperature conditions should be mentioned in real-time PCR.
6- In the graphs of Figure 4, what group were the groups compared with? There is no control column. The horizontal axis does not show the concentration. What are the significance symbols based on? It is not clear whether Bcl-2 increased or decreased compared to the control group.
It seems to increase.
7- Considering that there is a series of flow cytometry photos in the article, has this test been repeated, given that an error bar is shown on the graphs?
8- Why were 6 concentrations selected in MTT, 3 concentrations in the flow cytometry test and two concentrations in the real-time PCR test? It would have been better to choose concentrations based on IC50.

3

Revision 2

AUTHORS' RESPONSE TO REVIEWERS

Authors' reply to reviewers

The next pages contain the authors' point-by-point reply to the comments of this revision round, as submitted with the revised manuscript. It is published as the authors wrote it.

he geographical characteristics (longitude and latitude) of the plant collection area should be written. 3- There are many spelling and grammar mistakes.

Was corrected.

4- In RNA extraction, in addition to nanodrops, RNA quality should be measured by agarose gel electrophoresis.

Checking RNA quality is not necessary in gene expression studies using real-time PCR, because if the RNA quality is low, DNA is not synthesized and no peak is observed.

It is not necessary to check the quality of RNA in gene expression studies with real-time PCR, because if the quality of the RNA is low, DNA will not be synthesized in real-time and the peak will not be seen.

5- Temperature conditions should be mentioned in Real-time PCR.

Was corrected.

6- In the graphs of Figure 4, what group were the groups compared with? There is no control column. The horizontal axis does not show the concentration.

What are the significant signs based on? It is not clear whether Bcl-2 increased or decreased compared to the control group.It seems to increase.

The graphs were corrected.

Was corrected

7- Considering that there is a series of flow cytometry photos in the article, has this test been repeated that the error bar is shown on the graphs?

Yes . The analyzes were repeated 3 times and the error bar is shown in the graphs.

8- Why were 6 concentration selected in MTT, 3 concentrations in the flow cytometry test and two concentrations in the real-time PCR test? It would have been better to choose concentrations based on IC50.

Based on the results of the MTT test, the percentage of apoptosis of the normal cell line L929 and the cancer cell line HT29 treated with PBFEO at three concentrations of 50, 100, and 250 for 48 hours was examined. Because significant necrosis was observed at a concentration of 250 µg/mL compared with untreated cells, we excluded the 250 concentration from the gene expression analysis.

Based on the results of the MTT test, the percentage of apoptosis of normal cell line L929 and cancer cell line HT29 treated with PBFEO with three concentrations of 50, 100, 250 in 48 hours was investigated. Also, significant necrosis was observed in comparison with untreated cells at a concentration of 250 µg/ml. Therefore, we excluded the concentration of 250 from the study to check gene expression.

[Translated from Persian by the Brieflands editorial office.]

3 Revision 2

2 comments · 14 Dec 2022 – 14 Dec 2022

Associate Editor

MINOR REVISION 14 Dec 2022

1- The article should be fundamentally revised in terms of grammar and spelling.
2- Essential oil analysis should be compared with similar studies such as https://doi.org/10.22038%2FIJBMS.2017.20860.5426 and https://dx.doi.org/10.22092/jmpb.2021.343038.1213 and the difference in myristicin percentage should be explained.
3- The purpose of the docking study is not clear. It would have been better for the authors to use modeling studies to investigate anticancer mechanisms. It is also recommended that the authors report ADMET studies for myristicin.
4- In the introduction and discussion sections, the innovation of this study has not been addressed, and the manuscript cannot be published until these items are added.

Editor-in-Chief

MINOR REVISION 14 Dec 2022

The following points require correction:

1- The article should be fundamentally revised in terms of grammar and spelling.
2- Essential oil analysis should be compared with similar studies such as https://doi.org/10.22038%2FIJBMS.2017.20860.5426 and https://dx.doi.org/10.22092/jmpb.2021.343038.1213 and the difference in myristicin percentage should be explained.
3- The purpose of the docking study is not clear. It would have been better for the authors to use modeling studies to investigate anticancer mechanisms. It is also recommended that the authors report ADMET studies for myristicin.
4- In the introduction and discussion sections, the novelty of the study has not been addressed, and the manuscript cannot be published until these items are added.

4

Revision 3

AUTHORS' RESPONSE TO REVIEWERS

Authors' reply to reviewers

The next pages contain the authors' point-by-point reply to the comments of this revision round, as submitted with the revised manuscript. It is published as the authors wrote it.

- The article should be fundamentally revised in terms of grammar and spelling.

Was corrected

2- Essential oil analysis should be compared with similar studies such as https://doi.org/10.22038%2FIJBMS.2017.20860.5426 and https://dx.doi.org/10.22092/jmpb.2021.343038.1213 and the difference in myristicin percentage should be explained.

Was corrected

3- The purpose of the docking study is not clear. It would have been better for the authors to use modeling studies to investigate anticancer mechanisms. It is also recommended to report ADMET studies for myristicin.

There are limited studies in this field. The purpose of this study is to investigate the essential oil of PBFEO plant fruit.

4- In the section introduction and discussion, the innovation of its study has not been addressed and the manuscript cannot be published until these items are added.

Was corrected

4 Revision 3

1 comment · 21 Dec 2022

Editor-in-Chief

ACCEPT 21 Dec 2022

Accept