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Manuscript Number: JAFR-D-23-00344R1

Green Seaweed *Caulerpa racemosa* - Chemical Constituents, Cytotoxicity in Breast Cancer Cells and Molecular Docking Simulation

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I am pleased to inform you that your manuscript has been accepted for publication.

My comments, and any reviewer comments, are below.

Your accepted manuscript will now be transferred to our production department. We will create a proof which you will be asked to check, and you will also be asked to complete a number of online forms required for publication. If we need additional information from you during the production process, we will contact you directly.

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Kind regards,
Yangchao Luo, Ph.D.
Editor-in-Chief
Journal of Agriculture and Food Research

Editor and Reviewer comments:

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Manuscript Number: JAFR-D-23-00344

Green Seaweeds *Caulerpa racemosa* - Chemical Constituents, Cytotoxicity in Breast Cancer Cells and Molecular Docking Simulation

Thank you for submitting your manuscript to Journal of Agriculture and Food Research.

I have completed my evaluation of your manuscript. The reviewers recommend reconsideration of your manuscript following revision. I invite you to resubmit your manuscript after addressing the comments below. Please resubmit your revised manuscript by May 21, 2023.

When revising your manuscript, please consider all issues mentioned in the reviewers' comments carefully: please outline in a cover letter every change made in response to their comments and provide suitable rebuttals for any comments not addressed. Please note that your revised submission may need to be re-reviewed.

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Journal of Agriculture and Food Research values your contribution and I look forward to receiving your revised manuscript.

Kind regards,
Yangchao Luo, Ph.D.
Editor-in-Chief

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Editor-in-Chief
Journal of Agriculture and Food Research

Editor and Reviewer Comments:

Reviewer #1: Dear Editors,

I have carefully and thoroughly evaluated the manuscript/Submission "Green Seaweeds *Caulerpa racemosa* - Chemical Constituents, Cytotoxicity in Breast Cancer Cells and Molecular Docking Simulation".

Marine resources, such as algae, seaweed, and invertebrates are indeed a promising food and health research trend because of their potential sustainability and availability.

This article presents the results of study aimed at determining the anticancer activity of *C. racemosa* extracts in breast cancer cells, identify compounds, and determine the mechanism using computational models. Metabolites that have been observed in this work will potentially become a reference for other researchers in exploring functional foods and drug candidates. Interestingly, this manuscript has succeeded in presenting an integrated in silico and in vitro study of the benefits of green seaweed in combating cancer and their anti-free radical potential.

This manuscript can be considered for acceptance to publication, but the reviewer note minor issues that need to be corrected by the Authors:

1. Title, don't use "S" in the suffix of Seaweeds, it should be "Seaweed" because only one species is used in this study.
2. It is not necessary to write "molecular docking" in italics.
3. I notice in Introduction section "Other molecules in seaweeds with antioxidant and antitumor properties include proteins and carotenoids (Burritt et al., 2002; Hwang et al., 2008)", this should be added with the latest relevant references, as an alternative: <https://doi.org/10.3390/molecules28073267>.
4. In figure 2, "(15.625, 31.25, 62.5, 125, 250, and 500 µg/mL, for 4 h" is missing the closing parenthesis.
5. Writing: In Vitro, In Silico, and In Vivo please pay attention to writing in italics; check in the main manuscript.
6. In the conclusion, please provide conclusions regarding the results of in vitro antioxidants and anticancer (the current format does not emphasize these results); and change "green algae" to "green seaweed" to match the title.

Reviewer #2: The manuscript "Green Seaweeds *Caulerpa racemosa* - Chemical Constituents, Cytotoxicity in Breast Cancer Cells and Molecular Docking Simulation" explores the potential of green seaweeds as functional food candidates. Metabolite data were obtained through metabolomic profiling using the liquid chromatography-electrospray ionization quadrupole time-of-flight mass spectrometry (LC-ESI-QTOF-MS) system, an advanced method in the characterization of new food and drug research. The conclusion is supported by comprehensive data and studies, with antioxidant and anticancer properties examined through two approaches (In Silico and In Vitro). Therefore, this manuscript presents data and results that are scientifically sound and can be considered for publication after minor revisions:

1. Please change "2.3 Cytotoxicity Activity Analysis via MTT Assay" to "2.3 Cytotoxicity Analysis via MTT Assay."
2. In the "Characterization of compounds" section, please change the sentence "The characterization of metabolites in extract is important to education their mechanism of actions and standardization purposes."

Reviewer #2: The manuscript "Green Seaweeds *Caulerpa racemosa* - Chemical Constituents, Cytotoxicity in Breast Cancer Cells and Molecular Docking Simulation" explores the potential of green seaweeds as functional food candidates. Metabolite data were obtained through metabolomic profiling using the liquid chromatography-electrospray ionization quadrupole time-of-flight mass spectrometry (LC-ESI-QTOF-MS) system, an advanced method in the characterization of new food and drug research. The conclusion is supported by comprehensive data and studies, with antioxidant and anticancer properties examined through two approaches (In Silico and In Vitro). Therefore, this manuscript presents data and results that are scientifically sound and can be considered for publication after minor revisions:

1. Please change "2.3 Cytotoxicity Activity Analysis via MTT Assay" to "2.3 Cytotoxicity Analysis via MTT Assay."
2. In the "Characterization of compounds" section, please change the sentence "The characterization of metabolites in extract is important to education their mechanism of actions and standardization purposes." to "The characterization of metabolites in extract is important to understand their mechanism of actions and standardization purposes."
3. "Table 2. Characterization of compounds in hexane, ethyl acetate, and ethanol extract of *C. racemosa* by using LC-ESI-QTOF-MS." should be changed to "Table 2. Observed compounds in hexane, ethyl acetate, and ethanolic extract of *C. racemosa* via LC-ESI-QTOF-MS screening."
4. In table 2, there is a comma (,) error that should be a period (.).
5. In the conclusion, please state the potential as functional food or anticancer nutraceuticals and their potential in capturing free radicals.
6. In table 2, compound number 7 has redundant writing of "C18H34O".
7. In table 2, provide an appropriate legend underneath; for example, RT:?
8. In "3.6. Data Management and Statistical Analysis," please provide information on the software used for data processing.

Reviewer #3: In this manuscript, the authors aimed to . This study aimed to determine the anticancer activity of *C. racemosa* extracts in breast cancer cells, identify compounds, and determine the mechanism using computational models. The topic is very interesting, and the study is well designed and written.

I do have some minor comments:

The Abstract: English language and style are fine/minor spell check required.

Keywords: Recommended to be sorted alphabetically.

Introduction: It provides sufficient background and includes all relevant references.

Figures

Figure 2, caption it is ethyl acetate not acetic.

Figure 3, in the X axis it is also ethyl acetate not acetic.

Figure 4, caption is the same mistake.

The text after figure 4, remove the repeated word database.

Tables:

Table 2, adjust the molecular formula of compound 13. and also, the table size to fit to the contents or you can try to draw the structure of the identified compounds in a separate figure away from the table if it is

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Table 4 title ethyl acetate not acetic and adjust the table size to fit with the contents.

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Green Seaweed *Caulerpa racemosa* - Chemical Constituents, Cytotoxicity in Breast Cancer Cells and Molecular Docking Simulation

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