

Instruction to authors

1. Introduction

Medicinal Chemistry Research is a journal for the prompt disclosure of novel experimental achievements in the many facets of drug design, drug discovery, and the elucidation of mechanisms of action of biologically active compounds. Articles are sought which emphasize research in chemical biological relationships, especially with respect to: structure-activity relationships, investigations of biochemical and pharmacological targets of drug action, and correlations of structures with the mode of action of biologically active compounds. Studies will be welcomed that increase our understanding of biochemical interactions between drug molecules, ions, free radicals, and sterically important sections of macromolecular targets. The Journal is also dedicated to medicinal plants and to bioactive natural products of plant, fungal, mammalian and aquatic origin. The Journal publishes original contributions in seven major areas:

- Synthesis of bioactive compounds.
- Docking, molecular modeling, QSAR, SAR, and computational studies of bioactive interactions.
- Identification of targets and mechanism of activity of bioactive natural products isolated from plant, fungal, mammalian and aquatic origin.

Contributions reporting the following are not normally considered for publication:

- Biological activity on crude extracts that have not been characterized by analysis of their secondary metabolites (HPLC, ^1H and ^{13}C NMR including 2D NMR).
- Unexceptional and predictable bioactivity (e.g. antioxidant properties of phenolic or antibacterial activity of essential oils or antioxidant properties of metals such as iron, copper, etc.).
- Uncritical ethnopharmacological investigations, where a list of plants and their use are simply reported.
- Synthetic work in which the spectroscopic data is not complete (e.g., ^1H and ^{13}C NMR, HRMS, CHN, UV, IR, etc.).
- Computational work that simply discusses the docking, molecular modeling, QSAR, SAR, and computational studies of bioactive interactions without validation of the method (with experimental data).
- Biological activity that is low and insufficient to generate meaningful structure activity relationship.

Violation of any of the following rules will result in an immediate rejection:

RULE 1: The manuscript does not fall into any of the areas of interest of the Journal.

RULE 2: The manuscript is too preliminary (e.g data without comparison to a reference, or without a positive control).

RULE 3: The botanical source is not clearly identified, authenticated, or documented (voucher specimen).

RULE 4: The manuscript is too focused on a non-chemical subject (e.g., pharmacology, analytical studies of active ingredients, analytical studies of drug concentrations (ADME is suitable), etc.

RULE 5: Manuscripts that simply discuss antioxidant properties of phenols or other compounds known to possess antioxidant effects.

RULE 6: QSAR/modeling manuscripts that lack experimental biological validation of the proposed model(s).

RULE 7: The manuscript does not follow the formatting provided in this instruction to authors.

RULE 8: The manuscripts contains poor English and is difficult to read language.

2. General Consideration

Authors are strongly encouraged to provide their manuscript in an electronic format. The text must be in a single-column format and lines with double space. Use plain font 12 point Times New Roman and symbols (use internationally accepted signs and symbols for units, SI units). Use the automatic page numbering function to number all the pages. Ensure that all special characters are presented in the body of the text and do not use graphics. Abbreviations, except for very common ones, must be defined the first time they are used and a list supplied with the manuscript.

Using clear and concise English will help the editors and the reviewers concentrate on the scientific merit of the manuscript and thus smooth the peer review process. We reject manuscripts with good science that are poorly written. The following editing service provides language editing for scientific articles in all areas:

http://edanzediting.com/springer_lp?utm_source=springer&utm_medium=partner_link&utm_content=recommendation_page&utm_campaign=springer.

The text of a research manuscript should be divided into the following sections: **Introduction, Materials and Methods, Results and Discussion, Conclusions, Acknowledgements** (Funding), **Conflict of Interest**, and **References**. Tables, figures, and schemes, should be embedded in the text or be included right after the references on separate pages (one each per page). Do not upload tables, figures and schemes that are to be published in the manuscript into the electronic supplementary material. Authors are encouraged to provide supplementary material to keep the manuscript to a reasonable length.

3. Manuscript Organization

3.1. Title Page. A concise and informative title should appear on a separate page and avoid abbreviations and formulaes, and followed by the authors' first name, middle initial(s) and last name. Each name is followed by the digit(s) of the author's affiliation in superscript. For e.g:

Michael G. Mueller^{1,2} · Gregory C. Vain² · Alexander B. Smith³ · Diamond Club³

Each corresponding author's name is preceded by an envelope icon (✉) and the e-mail address should be indented by 5 mm. Authors with a supplied e-mail but who are not corresponding should have their name and e-mail content listed beneath the corresponding author's details, but without the envelope symbol. Each subsequent author and email will be separated by a blank line.

The affiliation list follows the corresponding authors and e-mail details and is separated from the email address by a blank line. It lists all affiliations within the author group. Each affiliation starts with a superscript number, which corresponds to the digit from the respective author names. Each subsequent affiliation will be separated by a blank line.

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3.2. Abstract. This should be presented as one paragraph detailing the purpose, experimental results and major conclusions, in a finding oriented format. This must be on the second page and no more than 250 words. The abstract should not contain any undefined abbreviations or unspecified references. Immediately after the abstract paragraph provide 4 to 6 keywords, which can be used for indexing purposes; use the heading Keywords before listing these words.

3.3. Introduction. The manuscript should start with an introduction where the rational and aims of the research are discussed. Be sure to include and reference similar investigations in support of the work.

3.4. Material and Methods. The author(s) are encouraged to be as concise as possible in the experimental description. Specific details about instruments used, sources of the reagents used should be incorporated in the text headed by the word experimental. In a separate paragraph experimental biological material should be used to describe the work and may include herbarium, voucher number, authenticated by, date of collection or cultivation, etc. Scientific names should be in italics (in manuscripts reporting natural product isolation) and the description of the isolation process, as well as other relevant data, should be provide in one paragraph. For synthetic papers all methodology used must be described.

The characterization of compounds should be presented in a separate paragraph. The peaks from the ¹³C NMR must be assigned to the corresponding carbon atom (i.e, if C-1 (carbon in position #1) has a NMR peak at 170.1 then the data should show that C-1 has the 170.1 peak (one decimal: do not use a range). There are a couple of ways to represent this information: ¹³C-NMR (DMSO-d₆): 170.1 (C=O) or 170.1 (C-1)). These assignments MUST be made before the work can be considered.

Under the material and methods section - compounds should be identified by IUPAC nomenclature and written using the following example:

Compound (or IUPAC name) (3a): Yellowish needles (MeOH) (This compound was prepared by.... It was obtained as a white solid, color, yield, etc); mp 85-86 °C; [α]_D²⁵ + 92 (c 0.003, Py); UV (EtOH) λ_{\max} (log ϵ) 240 (4.15), 278 (4.30) nm; IR (KBr) ν_{\max} 3382, 2877, 2925, 1736, 1701, 1630, 1606, 1517, 1445, 1374, 1276, 1165, 1117, 1070 cm⁻¹; ¹H NMR (CDCl₃, 500 MHz): δ = 7.84 (2H, d, J = 7.4 Hz, H-2', H-6'), 6.78 (2H, d, J = 7.4 Hz, H-3', H-5'), 5.15 (1H, d, J = 4.4 Hz, H-1), 4.60 (1H, dd, J = 2.4, 12.0 Hz, H-6a), 4.50 (1H, dd, J = 5.0, 12.0 Hz, H-6b), 4.38 (1H, dd, J = 1.2, 4.4 Hz, H-2), 4.24 (1H, dd, J = 1.6, 10.0 Hz, H-4), 3.92 (1H, ddd, J = 5.2, 7.4, 10.0 Hz, H-5), 3.49 (1H, dq, J = 6.8, 9.0 Hz, O-CH₂CH₃), 3.68 (1H, dq, J = 6.8, 9.0 Hz, O-CH₂CH₃), 1.12 (3H, t, J = 6.8, Hz, O-CH₂CH₃); ¹³C NMR (CDCl₃, 125 MHz): δ = 205.4 (C, C-3), 166.6 (C, COBz), 161.6 (C, C-4'), 131.8 (CH, C-2', C-6'), 120.8 (C, C-1'), 115.2 (CH, C-3', -5'), 100.8 (CH, C-1), 74.7 (CH, C-2), 73.2 (CH, C-5), 72.7 (CH, C-4), 64.3 (CH₂, O-CH₂CH₃), 63.4 (CH₂, C-6), 14.5 (CH₃, O-CH₂CH₃); EIMS m/z 326 [M]⁺ (5), 308 (100); HRESIMS m/z (pos): 349.0898 C₁₅H₁₈O₈Na (calcd. 349.0899); Anal. Calcd. for C₁₅H₁₅N₅: C, 67.90; H, 5.70; N, 26.40. Found: C, 67.84; H, 5.39; N, 26.12.

A paragraph with the pharmacological assays must be described in sufficient detail; positive and negative controls must be evaluated at the same concentration(s) to compare the effectiveness of the test compounds. With respect to the biological data, the concentration and doses must be presented as molar units, and presented as IC₅₀, EC₅₀, etc. References to statistical methods of calculation must be included in the manuscript. Also, the tested compounds, regardless if they are isolated as secondary metabolites, synthesized or purchased, must range between 95-100 % purity (TLC is not a reliable procedure for analysis). Materials and methods must include statements of human and animal welfare. Generic names of drugs and pesticides are preferred; if trade names are used, the generic name should also be provided.

Theoretical calculations (docking, molecular modeling, QSAR, SAR, computational studies, etc), software used, etc should be included in the material and methods section. All models must be validated with biological experimental data.

3.5. Results and Discussion. This section should concisely present the chemistry and medicinal/biological results. Tables, figures and schemes help to present the experimental data and design to maximize the comprehension and clarity of the results. The discussion should interpret the results, and significantly analyze the data.

3.6. Conclusion. This is an optional section where authors can highlight their results.

3.7. Acknowledgments. (Funding information) Acknowledgment of people, grants, funds, etc. should be placed in a separate section before the references. The complete names of funding organizations should be provided. In addition, please provide funding information, which includes a separate step in the submission process of the peer-review system. Funding providers should be selected from the standardized list provided during the submission of the manuscript. If the funding institution is not listed, it can be entered as free text. Funding information will be published as a searchable metadata for all accepted articles. Even so, acknowledgements of funding support should be described within the paper.

3.8. Conflict of Interest. Authors must disclose all relationships or interests that could have direct or potential influence or impart bias on the work. Although an author may not feel there is any conflict, disclosure of relationships and interests provides a more complete and transparent process, leading to an accurate and objective assessment of the work. Awareness of a real or perceived conflicts of interest is a perspective to which readers are entitled. This is not meant to imply that a financial relationship with an organization that sponsored the research or compensation received for consultancy work is inappropriate. Examples of potential conflicts of interests **that are directly or indirectly related to the research** may include but are not limited to the following:

- Research grants from funding agencies (please give the grant agency and the grant number)
- Honoraria for speaking at symposia
- Financial support for attending symposia
- Financial support for educational programs
- Employment or consultation
- Support from a project sponsor
- Position on an advisory board or a board of directors or other type of management relationships
- Multiple affiliations (the affiliation where the work is performed is what should be listed)
- Financial relationships (for example equity ownership or investment interest)
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- Holdings of spouse and/or children that may have financial interest in the work

In addition, interests that go beyond financial interests and compensation (non-financial interests) that may be important to readers, should be disclosed. These may include but are not limited to personal relationships or competing interests directly or indirectly tied to this research, or professional interests or personal beliefs that may influence your research.

The corresponding author collects the conflict of interest disclosure forms from all authors. In author collaborations, where formal agreements for representation allow it, it is sufficient for the corresponding author to sign the disclosure form on behalf of all authors. The corresponding author will include a summary statement in the text of the manuscript, in a separate section before the reference list, which reflects what is recorded in the potential conflict of interest disclosure form.

Conflict of Interest: Author A has received research grants from Company A. Author B has received a speaker honorarium from Company X and owns stock in Company Y. Author C is a member of committee Z.

If no conflict exists, the authors should state: Conflict of Interest: The authors declare that they have no conflict of interest.

3.9. References. In text citations appear in parentheses as (Author last name year); (Author and Coauthor, year); (Author et al., year).

Example: (Chang 1998); (Naik and Mohan, 2005); (Kime et al., 1987).

The list of references should only include works that are cited in the text and that have been published or accepted for publication. Personal communications and unpublished works should only be mentioned in the text. Do not use footnotes or endnotes as a substitute for a reference list.

Reference list entries should be listed alphabetically in the reference list. The format of listed references is: Last Name, Initial (year) Title. Journal Name (ISI Abbreviated) Volume No:ppp—ppp (no period).

For Journal articles:

León F, Gao J, Dale OR, Wu Y, Habib E, Husni AS, Hill RA, Cutler SJ (2013) Secondary metabolites from *Eupenicillium parvum* and their *in vitro* binding affinity for human opioid and cannabinoid receptors. *Planta Med* 79: 1756-1761

Li H, Liu T, Xuan H, Fang S, Zhao C (2014) A combination of pharmacophore modeling virtual screening, and molecular docking studies for a diverse set of colchicine site inhibitors. *Med Chem Res* 23:4713-4723

Articles by DOI (not publish yet):

Wright BD, Deblock MC, Wagers PO, Duah E, Robishaw NK, Shelton KL, Southerland MR, DeBord MA, Kersten KM, McDonald LJ, Stiel JA, Panzer MJ, Tessier CA, Paruchuri S, Youngs WJ (2015) Anti-tumor activity of lipophilic imidazolium salts on select NSCLC cell lines. *Med Chem Res*. doi:10.1007/s00044-015-1330-z

Books:

Youssef JA, Badr MZ (2013) Peroxisome proliferator-activated receptors Discovery and recent advances. Humana Press, Springer, New York

Book chapters:

Gogineni V, Leon F, Avery BA, McCurdy CR, Cutler SJ (2015) Phytochemistry of *Mitragyna speciosa*. In: Raffa RB (ed) *Kratom and other mitragynines: the chemistry and pharmacology of opioids from a non-opium source*. CRC press, Boca Raton, pp 77-94

Online documents:

National Institute on Drug Abuse Press Office (2014) Teen prescription opioid abuse, cigarette, and alcohol use trends down. NIH-NIDA news. <http://www.drugabuse.gov/news-events/news-releases/2014/12/teen-prescription-opioid-abuse-cigarette-alcohol-use-trends-down> Accessed 28 February 2015

Dissertations:

Gao J (2010) Fungi-derived natural products with binding affinities for human opioid or cannabinoid receptors. Dissertation, The University of Mississippi

Patents:

McCurdy CR, Mesangeau C, Chin FT, James ML, Shen B, Gambhir S, Biswal S, Behera D (2014) Highly selective sigma receptors ligands and radioligands as probes in nociceptive processing and the pathophysiological study of memory deficits and cognitive disorders. US Patent 2014-0328755, filed March 4, 2014, issued Nov 6, 2014

3.10. Tables. All tables are to be numbered using Arabic numerals. Tables should always be cited in the text and in consecutive numerical order. For each table, please supply a table caption (title) explaining the components of the table. Identify any previously published material by giving the original source in the form of a reference at the end of the table caption. Footnotes to tables should be indicated by superscript lower-case letters (or asterisks for significance values and other statistical data) and included beneath the table body.

3.11. Schemes and Figures. The use of illustrations to clarify information is encouraged. All figures and or schemes are to be numbered using Arabic numerals. Figures and/or schemes should always be cited in text in consecutive numerical order. Figures or schemes parts should be denoted by lowercase letters (a, b, c, etc.). If an appendix appears in your article and it contains one or more figures, continue the consecutive numbering of the main text. Do not number the appendix figures, "A1, A2, A3, etc." Figures in online appendices (Electronic Supplementary Material) should, however, be numbered separately. Each figure should have a concise caption describing accurately what the figure depicts. Include the captions in the text file of the manuscript, not in the figure file. Figure captions begin with the term Fig. in bold type, followed by the figure number, also in bold type. No punctuation is to be included after the number, nor is any punctuation to be placed at the end of the caption. Identify all elements found in the figure in the figure caption; and use boxes, circles, etc., as coordinate points in graphs. Identify previously published material by giving the original source in the form of a reference citation at the end of the figure caption.

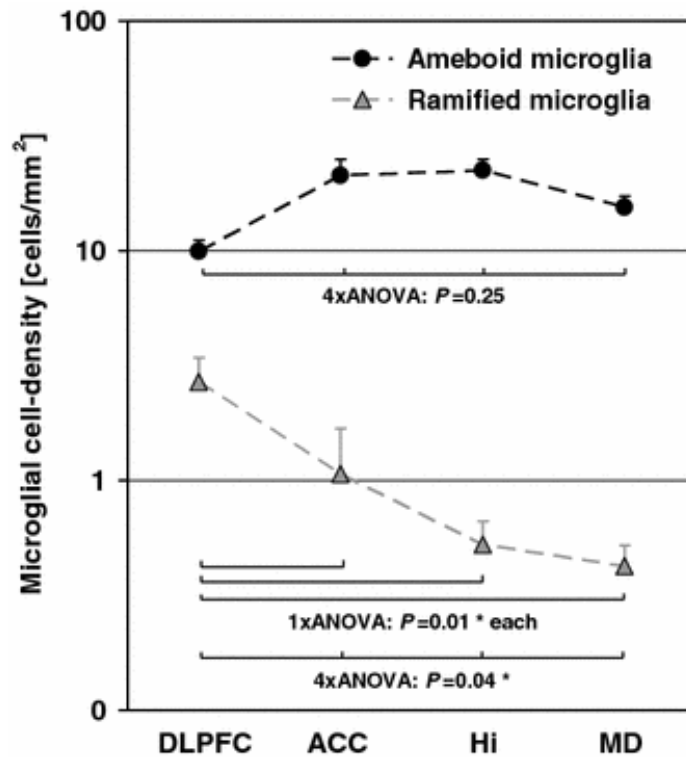
It is preferred that chemical structures be drawn using the ChemDraw program with preferences set for ACS 1996. Authors using other drawing packages should, modify their program's parameters to meet the ChemDraw ACS 1996 preferences.

If color is necessary then there is a charge for the print version of the manuscript. To facilitate the process, please follow the "artwork and illustrations guidelines":

Electronic Figure Submission

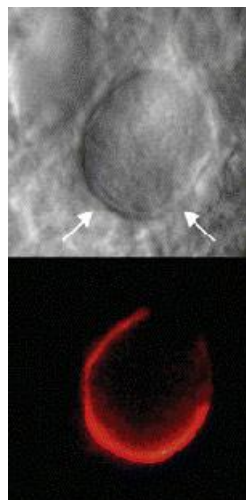
- Supply all figures electronically.
- Indicate what graphics program was used to create the artwork.
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- Vector graphics containing fonts must have the fonts embedded in the files.
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Line Art



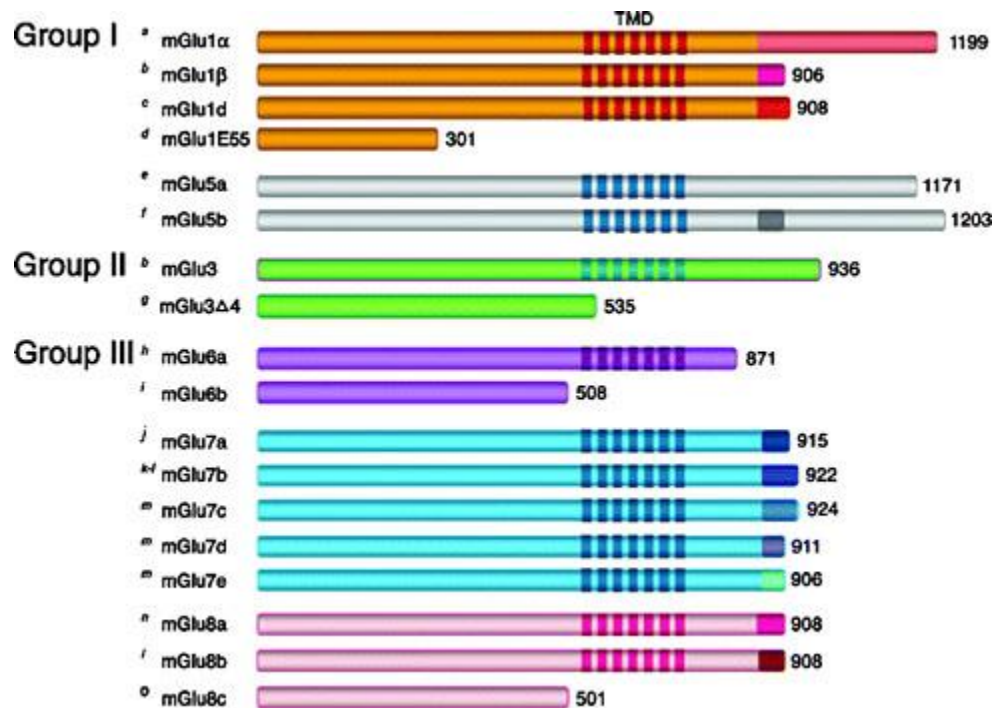
- Definition: Black and white graphic with no shading.
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- All lines should be at least 0.1 mm (0.3 pt) wide.
- Scanned line drawings and line drawings in bitmap format should have a minimum resolution of 1200 dpi.
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- Definition: Photographs, drawings, or paintings with fine shading, etc.
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Color art is free of charge for online publication while the print version has a charge for color. If black and white will be used in the print version, make sure that the main information will be visible. Many colors are not distinguishable from one another when converted to black and white format. A simple way to check this is to make a xerographic copy to see if the necessary distinctions between the different colors are still apparent. If the figures will be printed in black and white, do not refer to color in the captions of figures, schemes, etc. Color illustrations should be submitted as RGB (8 bits per channel).

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Submission:

- Supply all supplementary material in standard file formats.
- Please include in each file the following information: article title, journal name, author names; affiliation and e-mail address of the corresponding author.
- To accommodate user downloads, please keep in mind that larger-sized files may require very long download times and that some users may experience other problems during downloading.

Audio, Video, and Animations

- Always use MPEG-1 (.mpg) format.

Text and Presentations

- Submit your material in PDF format; .doc or .ppt files are not suitable for long-term viability.
- A collection of figures may also be combined in a PDF file.

Spreadsheets

- Spreadsheets should be converted to a PDF if no interaction with the data is intended.
- If the readers are encouraged to make their own calculations, spreadsheets should be submitted as .xls files (MS Excel).

Specialized Formats

- Specialized format such as .pdb (chemical), .wrl (VRML), .nb (Mathematica notebook), and .tex can also be supplied.

Collecting Multiple Files

- It is possible to provide multiple files in a .zip or .gz file.

Numbering

- If supplying any supplementary material, the text must make specific mention of the material as a citation, similar to that of figures and tables.
- Refer to the supplementary files as “Online Resource”, e.g., “... as shown in the animation (Online Resource 3)”, “... additional data are given in Online Resource 4”.
- Name the files consecutively, e.g. “ESM_3.mpg”, “ESM_4.pdf”.

Captions

- For each supplementary material, please supply a concise caption describing the content of the file.

Processing of supplementary files

- Electronic supplementary material will be published as received from the author without any conversion, editing, or reformatting.

Accessibility

In order to give people of all abilities and disabilities access to the content of your supplementary files, please make sure that

- The manuscript contains a descriptive caption for each supplementary material
- Video files do not contain anything that flashes more than three times per second (so that users prone to seizures caused by such effects are not put at risk)

4. Submission

Submission of a manuscript implies: that the work described has not been published before; that it is not under consideration for publication anywhere else; that its publication has been approved by all co-authors, if any, as well as by the responsible authorities – tacitly or explicitly – at the institute where the work has been carried out. The publisher will not be held legally responsible should there be any claims for compensation.

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This journal is committed to upholding the integrity of science. As a member of the Committee on Publication Ethics (COPE) the journal will follow the COPE guidelines on how to deal with potential acts of misconduct.

Authors should refrain from misrepresenting research results which could damage the trust in the journal, the professionalism of scientific authorship, and ultimately the entire scientific endeavor. Maintaining integrity of research and its presentation can be achieved by following the rules of good scientific practice, which include:

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- No data have been fabricated or manipulated (including images) to support your conclusions
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- Changes of authorship or in the order of authors are not accepted **after** acceptance of a manuscript.
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If there is a suspicion of misconduct, the journal will carry out an investigation following the COPE guidelines. If, after investigation, the allegation seems to raise valid concerns, the accused author will be contacted and given an opportunity to address the issue. If misconduct has been established beyond reasonable doubt, this may result in the Editor-in-Chief's implementation of the following measures, including, but not limited to:

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Compliance with Ethical Standards: To ensure objectivity and transparency in research and to ensure that accepted principles of ethical and professional conduct have been followed, authors should include information regarding sources of funding, potential conflicts of interest (financial or non-financial), informed consent if the research involved human participants, and a statement on welfare of animals if the research involved animals.

Authors should include the following statements (if applicable) in a separate section entitled "Compliance with Ethical Standards" before the References when submitting a paper:

- Disclosure of potential conflicts of interest
- Research involving human participants and/or animals
- Informed consent

Please note that standards could vary slightly per journal dependent on their peer review policies (i.e. double blind peer review) as well as per journal subject discipline. Before submitting your article check the Instructions for Authors carefully.

The corresponding author should be prepared to collect documentation of compliance with ethical standards and send if requested during peer review or after publication.

The Editors reserve the right to reject manuscripts that do not comply with the above-mentioned guidelines. The author will be held responsible for false statements or failure to fulfill the above-mentioned guidelines.

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If doubt exists whether the research was conducted in accordance with the 1964 Helsinki Declaration or comparable standards, the authors must explain the reasons for their approach, and demonstrate that the independent ethics committee or institutional review board explicitly approved the doubtful aspects of the study.

The following statements should be included in the text before the References section:

Ethical approval: “All procedures performed in studies involving human participants were in accordance with the ethical standards of the institutional and/or national research committee and with the 1964 Helsinki declaration and its later amendments or comparable ethical standards.”

For retrospective studies, please add the following sentence:

“For this type of study formal consent is not required.”

5.2. Statement on the welfare of animals. The welfare of animals used for research must be respected. When reporting experiments on animals, authors should indicate whether the international, national, and/or institutional guidelines for the care and use of animals have been followed, and that the studies have been approved by a research ethics committee at the institution or practice at which the studies were conducted (where such a committee exists).

For studies with animals, the following statement should be included in the text before the References section:

Ethical approval: “All applicable international, national, and/or institutional guidelines for the care and use of animals were followed.”

If applicable (where such a committee exists): “All procedures performed in studies involving animals were in accordance with the ethical standards of the institution or practice at which the studies were conducted.”

If articles do not contain studies with human participants or animals by any of the authors, please select one of the following statements:

“This article does not contain any studies with human participants performed by any of the authors.”

“This article does not contain any studies with animals performed by any of the authors.”

“This article does not contain any studies with human participants or animals performed by any of the authors.”

5.3. Informed consent. All individuals have individual rights that are not to be infringed. Individual participants in studies have, for example, the right to decide what happens to the (identifiable) personal data gathered, to what they have said during a study or an interview, as well as to any photograph that was taken. Hence it is important that all participants gave their informed consent in writing prior to inclusion in the study. Identifying details (names, dates of birth, identity numbers and other information) of the participants that were studied should not be published in written descriptions, photographs, and genetic profiles unless the information is essential for scientific purposes and the participant (or parent or guardian if the participant is incapable) gave written informed consent for publication. Complete anonymity is difficult to achieve in some cases, and informed consent should be obtained if there is any doubt. For example, masking the eye region in photographs of participants is inadequate protection of anonymity. If identifying characteristics are altered to protect anonymity, such as in genetic profiles, authors should provide assurance that alterations do not distort scientific meaning.

The following statement should be included:

Informed consent: “Informed consent was obtained from all individual participants included in the study.”

If identifying information about participants is available in the article, the following statement should be included:

“Additional informed consent was obtained from all individual participants for whom identifying information is included in this article.”

6. Additional Information

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