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, ^{1}H 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., ^{1}H 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:

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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. Vain[2] ·Alexander B. Smith[3] · Diamond Club[3]

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 ^{13}C 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: ^{13}C-NMR (DMSO-d_6): 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; $[\alpha]^{25}_{D}$ + 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 ($CDCl_3$, 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-C$\underline{H}_2$CH$_3$), 3.68 (1H, dq, *J* = 6.8, 9.0 Hz, O-C$\underline{H}_2$CH$_3$), 1.12 (3H, t, *J* = 6.8, Hz, O-CH$_2$C$\underline{H}_3$); ^{13}C NMR ($CDCl_3$, 125 MHz,): δ = 205.4 (C, C-3), 166.6 (C, $\underline{C}$OBz), 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 (CH_2, O-$\underline{CH}_2$CH$_3$), 63.4 (CH_2, C-6), 14.5 (CH_3, O-CH$_2\underline{CH}_3$); EIMS *m/z* 326 $[M]^+$ (5), 308 (100); HRESIMS *m/z* (pos): 349.0898 $C_{15}H_{18}O_8Na$ (calcd. 349.0899); Anal. Calcd. for $C_{15}H_{15}N_5$: 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 $IC_{50,}$ $EC_{50,}$ 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:

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- Financial support for attending symposia
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- Employment or consultation
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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).
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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, cigarrete, 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-derives 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 pathphysiological study of memory deficits and cognitive disorders. US Patent 2014-0328755, filled 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.

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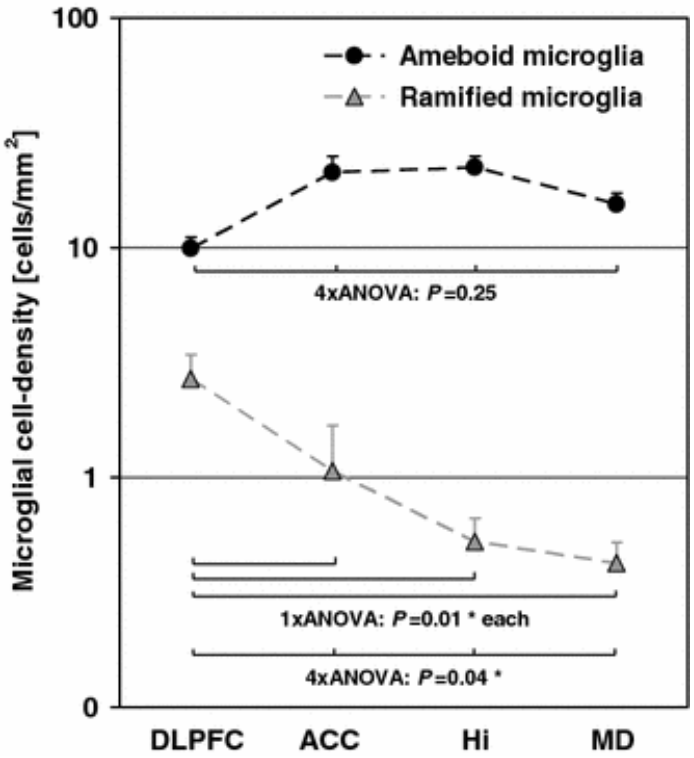

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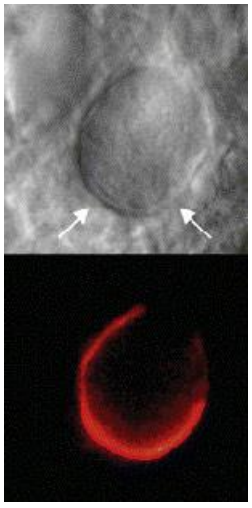

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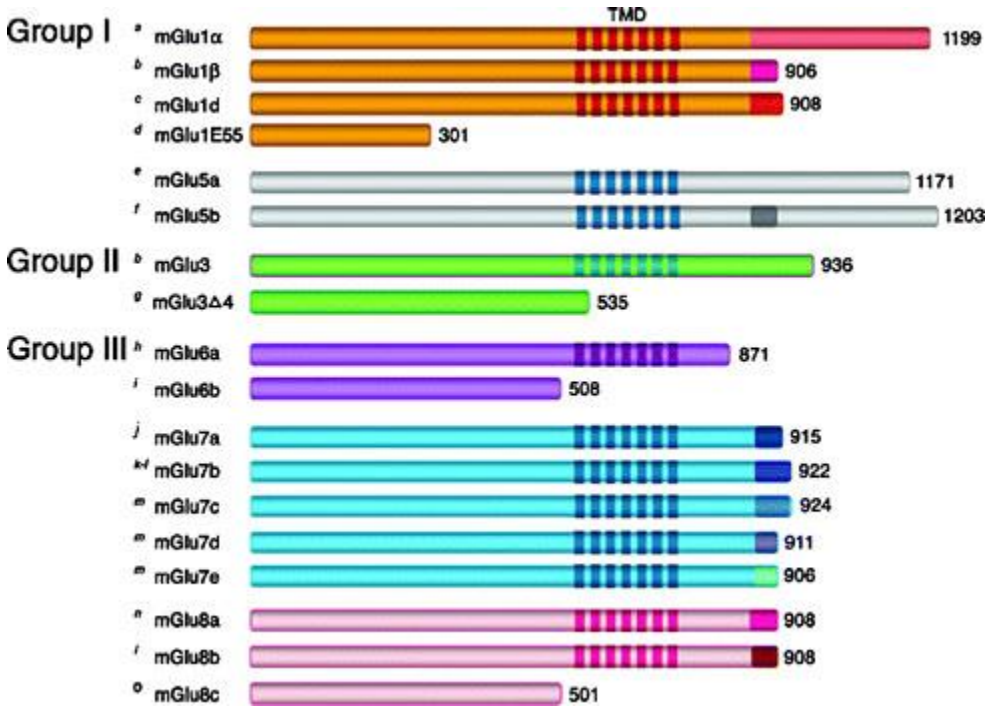

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Submission:

- Supply all supplementary material in standard file formats.
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- 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.

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

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

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

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- 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)

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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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- Disclosure of potential conflicts of interest
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- 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.

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"For this type of study formal consent is not required."

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

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