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 ¹³C 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 ¹³C 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.

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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.
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✉ Michael G. Mueller
michael@access.net
Gregory C. Vain
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; [α]$^25_D + 92 (c 0.003, Py); UV (EtOH) $\lambda_{max}$

- 240 (4.15), 278 (4.30) nm; IR (KBr) $\nu_{max}$ 3382, 2877, 2925, 1736, 1701, 1630, 1606, 1517, 1445, 1374, 1276, 1117, 1070 cm$^{-1}$; $^1$H NMR (CDCl$_3$, 500 MHz): $\delta$ = 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-CH$_2$CH$_3$), 3.68 (1H, dq, $J$ = 6.8, 9.0 Hz, O-CH$_2$CH$_3$), 3.12 (3H, t, $J$ = 6.8, Hz, O-CH$_2$CH$_3$); $^{13}$C NMR (CDCl$_3$, 125 MHz): $\delta$ = 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 (CH$_2$, O-CH$_2$CH$_3$), 63.4 (CH$_2$, C-6), 14.5 (CH$_3$, O-CH$_2$CH$_3$); EIMS $m/z$ 326 [M]$^+$ (5), 308 (100); HRESIMS $m/z$ (pos): 349.0898 C$_{15}$H$_{20}$O$_2$Na (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.

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