

# International Journal of Drug Design and Discovery

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## Guide for Authors

The *International Journal of Drug Design and Discovery* publishes studies on all aspects in the field of drug design and discovery that include drug design by rational approach, QSAR, molecular modelling, target-based design, pharmacophore modelling, drug synthesis, process development, medicinal chemistry, drug metabolism, pharmacokinetics, ADME, clinical research, biotechnology and nanotechnology related to drug discovery.

### Manuscripts Accepted for Submission

- Original research articles.
- Reviews: comprehensive, authoritative, descriptions of any subject within the journal's scope.
- Brief Communications: short reports of data from original research.

### Manuscript Submission

Authors should submit their manuscripts to the chief editor via the email [[dsriram@bits-hyderabad.ac.in](mailto:dsriram@bits-hyderabad.ac.in) & [pyogee@bits-hyderabad.ac.in](mailto:pyogee@bits-hyderabad.ac.in)]. All correspondence, including notification of the editor's decision and requests for revision, takes place by e-mail. A printed copy of the manuscript is not required at any stage of the process.

### The Following Items should be Supplied at First Submission

- *Manuscript*: Complete manuscript with graphical abstract content
- *Cover letter*: (i) highlighting the novelty, significance, and urgency of the submitted work, which merits rapid publication; (ii) names of potential referees.

**Language:** Articles must be written in clear, concise, grammatical English. Any author who is not fluent in idiomatic English is urged to gain assistance with manuscript preparation. Reviewers are not expected to correct grammatical errors and any deficiency in this area may detract from the scientific content of the paper.

**Journal policy:** Submission of an article implies that the work described has not been published previously (except in the form of an abstract or as part of a published lecture or academic thesis), that it is not under consideration for publication elsewhere, that its publication is approved by all authors and tacitly or explicitly by the responsible authorities where the work was carried out, and that, if

accepted, it will not be published elsewhere in the same form, in English or in any other language, without the written consent of the publisher. Authors accept full responsibility for the factual accuracy of the data presented and should obtain any authorization necessary for publication. As such the contents of the papers are the sole responsibility of the authors and publication shall not imply the concurrence of the editors or publisher. All papers are submitted to referees who advise the editor on the matter of acceptance in accordance with the high standards required, on the understanding that the subject matter has not been previously published and is not under consideration elsewhere. Referees will be asked to distinguish contributions meeting the above requirements and having an element of novelty, timeliness, and urgency that merits publication in the journal. We ask referees to help in the selection of articles that have this breadth and suggest that papers covering narrower aspects of the field be sent to journals specializing in those areas. Referee names are not disclosed, but their views are forwarded by the editor to the authors for consideration. Authors are encouraged to suggest names of several experts in the field when papers are first submitted.

### Manuscript Preparation

**General requirements:** The corresponding author's full mailing address, including mail codes, phone number, fax number, and e-mail address should be included. Authors are asked to provide four keywords, which will be used for indexing purposes. The manuscript should be compiled in the following order: Graphical Abstract, Title, Authors, Affiliations, Abstract, Keywords, Introduction, Results, Discussion, Conclusion, Experimental, References and Notes, Tables, Figures, and Schemes.

**Graphical abstracts:** Authors must supply a graphical abstract at the time the paper is first submitted. The abstract should summarize the contents of the paper in a concise, pictorial form designed to capture the attention of a wide readership and for compilation of databases. Carefully drawn chemical structures that serve to illustrate the theme of the paper are desired.

**Title:** The title should be brief, specific, and rich in informative words; it should not contain any literature references or compound numbers.

**Authors and affiliations:** Where possible, supply given names, middle initials, and family names for complete identification. Use superscript lowercase letters to indicate different addresses, which should be as detailed as possible and must include the country name. The corresponding author should be indicated with an asterisk, and contact details (fax, e-mail) should be placed in a footnote. Information relating to other authors (e.g., present addresses) should be placed in footnotes indicated by an appropriate symbol.

**Abstracts:** Authors must include a short abstract of approximately four to six lines that states briefly the purpose of the research, the Principal results, and major conclusion(s). References and compound numbers should not be mentioned in the abstract.

**Text:** It should be subdivided in the simplest possible way consistent with clarity. Headings and subheadings should reflect the relative importance of the sections, and all headings should be numbered. In the *introductory section* of the manuscript, the author should strive to define the significance of the work and the justification for its publication. Any background discussion should be brief and restricted to pertinent material. Ensure that all tables, figures, and schemes are cited in the text in numerical order. *The preferred position for chemical structures should be indicated.* All measurements and data should be given in SI units where possible, or in other internationally accepted units. Abbreviations should be used consistently throughout the text, and all nonstandard abbreviations should be defined on first usage.

**Reviews:** When submitting a review article, the corresponding author should include a biographical information as well as a black-and-white photograph. Biography should be one paragraph (approximately 150-200 words) and should include date and place of birth, universities attended, degrees obtained, major professional posts held, present title, a line or two about the major research interests, and anything else professionally relevant and of special interest.

**Experimental section:** Authors should be as concise as possible in experimental descriptions. The Experimental section must contain all the information necessary to guarantee reproducibility. An *introductory paragraph* containing information concerning solvents, sources of less common starting materials, special equipment, etc., should be provided. The procedures should be written in the past tense and include the weight, mmol, volume, etc., in parentheses after the names of the substances or solvents. General reaction conditions should be given only once. The title of an experiment should include the chemical name and compound number of the product prepared; subsequently, this compound should be identified by its number. Details of the workup procedure must be

included. Physical and spectroscopic data, including NMR, high-resolution mass analysis and elemental analysis, can be included in the experimental section or presented in tables.

**Acknowledgments:** An acknowledgment section may be included. It should be placed after the manuscript text and before the references.

**Abbreviations:** Standard ACS abbreviations should be used throughout the manuscript and are employed without periods. The preferred forms for some of the more commonly used abbreviations are mp, bp, °C, K, min, h, mL, µL, g, mg, µg, cm, mm, nm, mol, mmol, µmol, M, mM, µM, ppm, HPLC, TLC, GC, <sup>1</sup>H NMR, GC-MS, HRMS, FABHRMS, UV, IR, EPR, ESR, DNase, ED<sub>50</sub>, ID<sub>50</sub>, IC<sub>50</sub>, LD<sub>50</sub>, im, ip, iv, mRNA, RNase, rRNA, tRNA, cpm, Ci, dpm,  $V_{max}$ ,  $K_m$ ,  $k$ ,  $t_{1/2}$ . All non-standard abbreviations should be defined following the first use of the abbreviation.

**References and notes:** In the text, references should be indicated by superscript Arabic numerals which run consecutively through the paper and appear after any punctuation. Please ensure that all references are cited in the text and vice versa. The reference list should preferably contain only literature references, although other information (e.g., experimental details) can be placed in this section. Preferably, each reference should contain only one literature citation. Authors are expected to check the original source reference for accuracy. Formatting for common references are shown below.

**Scientific articles:** Qiao, C.; Gupte, A; Boshoff, H.I.; Wilson, D.J.; Bennett, E.M.; Somu, R.V.; Barry, C.E.; Aldrich, C.C. *J. Med. Chem.* 2007, 50, 6080.

**Books:** Doe, J. S.; Smith, J. In *Medicinal Chemistry*; Roe, P., Ed.; Pergamon Press: Oxford, 1990; Vol. 1, pp 301-383.

**Patent:** Lyle, F. R. U.S. Patent 6,973,257, 1995.

**Tables:** All tables should be cited in the text, and numbered in order of appearance with Arabic numerals. All table columns should have a brief explanatory heading and, where appropriate, units of measurement. Vertical lines should not be used. Footnotes to tables should be typed below the table and should be referred to by superscript letters. Each table should have a descriptive heading, which, together with the individual column headings, should make the table, as nearly as possible, self-explanatory.

**Legends:** Legends for figures and schemes should be grouped together separately.

**Artwork:** Figures, schemes, and equations must be cited in the text and numbered in order of appearance with Arabic numerals. Other graphics, such as structures, do not need

to be numbered, but please indicate in the text where these are to appear. All graphics (including chemical structures) must be provided at the actual size that they are to. Legends should not be included as part of the graphic; instead all legends should be supplied at the end of the text.

**Color:** Color figures may be printed in the journal at no charge to the author, provided that the editor considers the color necessary to convey scientific information.

**Nomenclature:** It is the responsibility of the authors to provide correct nomenclature. Chemical names for drugs are preferred. If these are not practical, generic names, names approved by the U.S. Adopted Names Council, or those approved by the World Health Organization may be used.

**Characterization of new compounds:** All new compounds should be fully characterized with relevant spectroscopic data. Microanalyses should be included whenever possible. Under appropriate circumstances, high-resolution mass spectra may serve in lieu of microanalysis, if accompanied by suitable NMR criteria for sample homogeneity.

**Biological data:** Biological test methods must be referenced or described in sufficient detail to permit the experiments to be repeated by others. Standard compounds and established drugs/agents should be tested in the same system for comparison. Statistical limits (statistical significance) for the biological data are usually required. If statistical limits cannot be provided, the number of

determinations and an indication of the variability and reliability of the results should be given. References to statistical methods of calculation should be included. Doses and concentrations should be expressed in molar quantities when comparisons of potencies are made with compounds having substantial differences in molecular weights. For inactive agents, the highest concentration or dose level tested should be indicated. Detailed descriptions of biological methods should be placed in the Experimental section.

**Software:** Software used as part of computer-aided drug/agent design (e.g., molecular modeling, QSAR, conformational analysis, molecular dynamics) should be readily available from accepted sources and the authors may specify where the software can be obtained. Assurance of the quality of the parameters employed for the relevant potential functions should be detailed in the manuscript.

**Proofs:** Proofs will be dispatched via e-mail and should be returned with corrections as quickly as possible, normally within 48 hours of receipt. Authors should ensure that corrections are returned in one communication and are complete, as subsequent corrections will not be possible.

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