Medicinal Chemistry Communications

Guidelines for Authors†

Also see: www.rsc.org/authorguidelines

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1.0 General policy

Medicinal Chemistry Communications (*MedChemComm*) is a monthly, peer-reviewed journal for the publication of original research articles and reviews in medicinal chemistry research. Main research areas include:

- Design, synthesis and biological evaluation of novel chemical or biochemical entities leading to new pharmacological agents, probes and/or potential drugs
- Computational, biophysical, physicochemical, molecular biological, proteomic studies of chemical or biochemical entities and their interaction with their biological environment
- Pharmacokinetic behaviour, pharmacodynamics, and drug safety and toxicology
- Chemical biology studies that enable drug discovery
- Chemical modifications of known chemical or biochemical entities that improve pharmacological properties

Authors should note that papers that mainly emphasise novel organic synthetic routes or are directed more towards an organic audience may be more suited for submission to *Organic & Biomolecular Chemistry*, and work focussing on the chemical interface with the -omic sciences and systems biology to *Molecular BioSystems*.

There is no page charge for papers in *MedChemComm*. The use of colour to enhance figures is encouraged. We are happy to print figures in colour, free of charge, where the use of colour enhances the scientific understanding of the figure. In addition, for the online version of the journal, colour is provided at no cost in both the PDF and HTML versions.

Notes and details of criteria for publication, and on RSC policy on the initial assessment of submissions can be found on ReSourCe.‡

2.0 Article types

2.1 Concise Articles

MedChemComm publishes all original research work in one format, 'Concise Article'. Authors are strongly encouraged to report their work in a succinct way, although scholarly discussion of results is expected. Lengthy introductions, extensive data, and excessive experimental details and conjecture should not be included. Authors are encouraged to place experimental procedures and characterisation data in the Supplementary Information where appropriate and it is expected that most Concise Articles will be 3–7 printed journal pages in length.

The Royal Society of Chemistry strongly discourages the fragmentation of a substantial body of work into a number of short publications. Unnecessary fragmentation is a valid reason for rejection of manuscripts. All reported measurements should have their uncertainties and limitations clearly stated. Sufficient experimental details should be included such that a scientist skilled in the art would be able to reproduce the results presented.§ **It is**

† For more detailed information on this topic, including guidelines for article layout, preparation of illustrations, presentation of experimental data, and supplementary information deposition, as well as links to useful websites, templates and other software resources, and authoring tools, see: http://www.rsc.org/authorguidelines.

‡ See http://www.rsc.org/resource

§ Experimental procedures and characterisation should be included as Electronic Supplementary Information. See section 3.3

mandatory to justify and/or reference claims regarding health impairments or toxic consequences and indicate adherence to funding body and country specific guidelines regarding animal welfare; as stated in the Royal Society of Chemistry ethical guidelines on human and animal welfare.¶

2.2 Reviews

Reviews may be a concise and critical appraisal or a personal viewpoint of activity in a specialist area of medicinal chemistry, or a short, personal account of a new area of research. Reviews will be easy-to-read articles covering current areas of interest and not comprehensive reviews of the literature. These are normally published by invitation of the *MedChemComm* Editorial Board. However, suggestions from authors are welcome and enquiries should be directed to the relevant Associate Editor. Potential writers should contact the relevant Associate Editor before embarking on their work.

To aid the Associate Editors to judge the suitability of a proposed review for the journal, authors may be asked to submit a synopsis. The aim is not to provide an extra burden for the author, but to ensure the article will appeal to the journal's intended readership. **Acceptance of the synopsis by the Associate Editor does not guarantee publication of the final manuscript.** Synopses should include:

- A paragraph explaining the current importance of the field, its implications for the wider scientific community, and the communities of readers who will find the article of interest.
- A structured outline of the review, giving section headings and expanding on each of these
- A selection of representative references to indicate its breadth and timeliness

All reviews undergo a rigorous and full peer-review procedure, in the same way as regular research articles.

3.0 Submission

3.1 Initial submission

Articles should be submitted using the RSC file upload service, RSC Manuscript Central.‖ On submitting their manuscripts, authors are encouraged to supply the names and addresses of two or three potential referees. Rapid publication is aided by careful preparation of text and illustrations. Particular attention is drawn to the use of (i) SI units and associated conventions, (ii) IUPAC nomenclature for compounds and (iii) standard methods of literature citation. The RSC Manuscript Central service allows up to five files to be uploaded at a time, alternatively a ZIP file containing up to 20 files can be uploaded. All files relating to a single manuscript should be uploaded simultaneously during one transaction. Files uploaded separately will result in more than one manuscript number being assigned and may subsequently be lost. Authors should not forward more than one version of their manuscript or submit the manuscript by e-mail to avoid errors in manuscript handling by the relevant Editorial Office. If however, authors experience problems using the submission system and are unable to submit their manuscript, they should e-mail it by file attachment directly to the Editorial Office explaining the difficulties.

All authors submitting work for publication are required to agree a Licence to Publish. Authors submitting online will be asked to agree a Licence to Publish as part of the process. Alternatively, a downloadable PDF version is available, which can be completed and forwarded to the Editorial Office.

After submission your file will be acknowledged by the relevant Editorial Office as soon possible. Authors should contact the Editorial Office if they have not received an acknowledgement within four working days.

3.2 Submission of revised articles and material for proof preparation

Revised manuscripts should be sent to the Editorial Office by file upload *via* RSC Manuscript Central. Please check the manuscript carefully for consistency, particularly in the representation of chemical formulae, compound names and words with alternative spellings. Successful use of your electronic files should speed up the production process and avoid errors being introduced. Authors should ensure that files submitted at this stage contain the final version of their manuscript. Proof corrections should only correct errors from the Production process and should not be used to make general changes to the text. We try to use the supplied data in our production process, but mathematical equations and tables in particular may be re-keyed by the typesetter. It is imperative that authors check their proofs (including any tabulated data and figures) very carefully. Papers are published as Advance Articles on the web as soon as possible after the return of proof corrections. Late corrections cannot be incorporated after publication of the Advance Article.

4.0 Characterisation of new compounds

Sufficient experimental details should be included such that a scientist skilled in the art would be able to reproduce the results presented. The synthesis of all new compounds must be described in detail.

4.1 Organic compounds

Synthetic procedures must include the specific reagents, products and solvents and must give the amounts (g, mmol, for products: %) for all of them, as well as clearly stating how the percentage yields are calculated. Characterisation should include: (i) proton NMR data backed up with LC-MS data with a minimum purity criteria of 95% evidenced from these two techniques; (ii) disclosure of final physical state: solid; amorphous; liquid; solution; (iii) additional data such as CHN data and HRMS data where available; (iv) for chiral compounds, evidence of enantiomeric purity via chiral HPLC or derivatisation to diastereoisomeric compounds/use of chiral shift reagents; (v) for known compounds, an original reference should be cited; (vi) for compounds made as part of an array, LC-MS data is sufficient providing that full data is made available for key compounds. For compounds generated through combinatorial methods, lead compounds should be characterised to the same standards as compounds generated through standard synthetic procedures.

4.2 Biomolecules (*e.g.* enzymes, proteins, DNA/RNA, oligosaccharides, oligonucleotides)

Authors should provide rigorous evidence for the identity and purity of the biomolecules described. The techniques that may be employed to substantiate identity include mass spectrometry, LC-MS, sequencing data (for proteins and oligonucleotides), high field ^{1}H or ^{13}C NMR and X-ray crystallography. Purity must be established by one or more of the following: HPLC, gel electrophoresis, capillary electrophoresis, or high field ^{1}H or ^{13}C NMR. Sequence verification should also be provided for nucleic acid cases involving molecular biology.

For organic synthesis involving DNA, RNA oligonucleotides, their derivatives or mimics, purity must be established using HPLC and mass spectrometry as a minimum. For new derivatives comprising modified monomers, the usual organic chemistry analytical requirements for the novel monomer must be provided (see 4.1: Organic compounds). It is not however necessary to provide this level of characterisation for the oligonucleotide into which the novel monomer is incorporated.

4.3 Biological data

Doses and concentrations should be expressed as molar quantities (*e.g.*, mol kg^{-1}, μmol kg^{-1}, M, mM). Forms of administration as well as physical states and formulations should be noted. For those compounds found to be inactive, the highest concentration (*in vitro*) or dose level (*in vivo*) tested should be indicated.

Quantitative biological data are required for all test compounds. Biological test methods should be described in sufficient detail such that a scientist skilled in the art would be able to reproduce the results presented. Known or standard compounds or drugs should be tested under the same experimental conditions for the purpose of comparison. Data may be presented tabulated or as graphs; extensive data for compounds is best presented in tabulated within the

¶ http://www.rsc.org/Publishing/ReSourCe/EthicalGuidelines
‖ See http://mc.manuscriptcentral.com/rsc

Electronic Supplementary information. Active compounds from combinatorial syntheses should be resynthesised and retested to verify biological activity. Some indication of the variability and reliability of any data presented must be given. It is expected that all tested compounds would be 95% pure and shown to be so using standard methods.

4.4 Small molecule single crystal X-ray crystallographic data
Crystallographic work will be assessed for its chemical interest. Thus crystallographic work carried out as part of a wider chemical study should not normally be submitted separately from the results of that study. The description of a crystallographic structure determination should be as brief as possible, consistent with the following guidelines, and should be included at the end of the paper.**

4.4.1 Deposition of material at the Cambridge Crystallographic Data Centre. Supplementary crystallographic data will be deposited by the Royal Society of Chemistry with the Cambridge Crystallographic Data Centre (CCDC) as part of the assessment process. Each structure will be assigned a separate CCDC number that will be quoted in the subsequent crystallographic report. Data will be held in the CCDC's confidential archive until publication of the article, when data for organic and metallo-organic compounds will be entered into the Cambridge Structural Database. Post-publication requests for individual data sets should be directed to: CCDC, 12 Union Road, Cambridge, UK CB2 1EZ. Fax: +44 (0)1223 336033. deposit@ccdc.cam.ac.uk

If the article is not published by the Royal Society of Chemistry, supplementary crystallographic data will remain in the CCDC's confidential archive. If the crystal structure(s) are subsequently published elsewhere, the CCDC Deposition Number(s) provided in the Royal Society of Chemistry crystallographic report should be quoted in that publication, and the CCDC advised of the new journal and the appropriate reference. Data will then enter the appropriate database as described above.

4.5 Macromolecular structure determination and sequence data
All manuscripts that report novel macromolecular three-dimensional structures at the level of individual atomic positions must be accompanied by deposition of the required structural data in the appropriate database to support the conclusions drawn. For X-ray structures, atomic coordinates and structure factor data are required. For NMR structures, data should include all resonance assignments and restraints used in structure determination (NOEs, spin–spin coupling constants, amide exchange rates, etc.) as well as atomic coordinates derived for both an individual/average structure and an acceptable family of structures. Sufficient information must be supplied to satisfy referees of the validity of the conclusions drawn.

Deposited files must be released immediately on publication. A six-month delay will be considered only in exceptional circumstances. Articles will not be published until the relevant PDB or NDB accession number has been provided. These codes should be quoted both in the experimental section of the manuscript and in the abstract so that abstracting services will access them.

Newly reported nucleic acid or protein sequences must be deposited with the appropriate database. Deposited files must be released immediately on publication of the article, which will not be published until an accession number is quoted in the experimental section of the manuscript and the abstract.††

5.0 Publication of theoretical and computational work

Authors should ensure that the purpose of the work and the precise objectives of the calculations performed are clearly stated; the results obtained should be reported only in so far as they relate to those objectives.‡‡

6.0 Molecular modelling guidelines

Molecular modelling studies should be subject to the same rigorous scientific standard required of other types of experiment, such that objective evaluation by independent investigators is possible. Authors are therefore strongly encouraged to provide sufficient details of any computationally assisted modelling results they report that might assist in any such evaluation.

7.0 Administration

Receipt of a paper will be acknowledged, and the paper will be given a reference number which authors are asked to quote on all their subsequent correspondence. If no such acknowledgement has been received after a reasonable period of time, authors should check with the Editorial Office as to whether the paper or the acknowledgement has gone astray.

7.1 Editorial policy
All manuscripts will be processed in an efficient, fair and timely manner. Papers that are accepted must not be published elsewhere except by permission of the Royal Society of Chemistry. Submission of a manuscript will be regarded as an undertaking that the same material is not being considered for publication by another journal. Every paper deemed suitable for consideration as a submission will be assessed by at least two independent referees, except under exceptional circumstances. Authors who disagree strongly with the resulting editorial decision may appeal to the *MedChemComm* Editorial Board through the Editor-in-Chief. RSC policy on the initial assessment of submissions, and details of criteria for publication, can be found on ReSourCe.

7.2 Copyright

7.3 Reprints
A PDF reprint of each paper will be supplied free of charge. Authors may print and distribute hardcopies of their article on demand. Authors may also send the electronic file to individuals, as one would send a printed reprint. However, the electronic file may not be distributed *via* an e-mail listserver and it may not be placed on any website.

** For a full explanation and instructions for publication of crystallographic work visit http://www.rsc.org/Publishing/ReSourCe/AuthorGuidelines/Techniques/index.asp

†† Protein Data Bank: http://pdb.rutgers.edu/, deposit@deposit.rcsb.org or http://www.ebi.ac.uk/pdbe/, pdbhelp@ebi.ac.uk; Nucleic Acids Database: http://ndbserver.rutgers.edu, ndbadmin@ndbserver.rutgers.edu; EMBL Nucleotide Sequence Submissions: http://www.ebi.ac.uk/Submissions/, datasubs@ebi.ac.uk; National Center for Biotechnology Information (GenBank): http://www.ncbi.nlm.nih.gov/, info@ncbi.nlm.nih.gov; DNA Data Bank of Japan: http://www.ddbj.nig.ac.jp/, ddbj@ddbj.nig.ac.jp; Protein Information Resource (Protein Sequence Database, PSD): http://pir.georgetown.edu/, pirmail@nbrf.georgetown.edu

‡‡ Full guidelines are available here: http://www.rsc.org/Publishing/ReSourCe/AuthorGuidelines/Techniques/