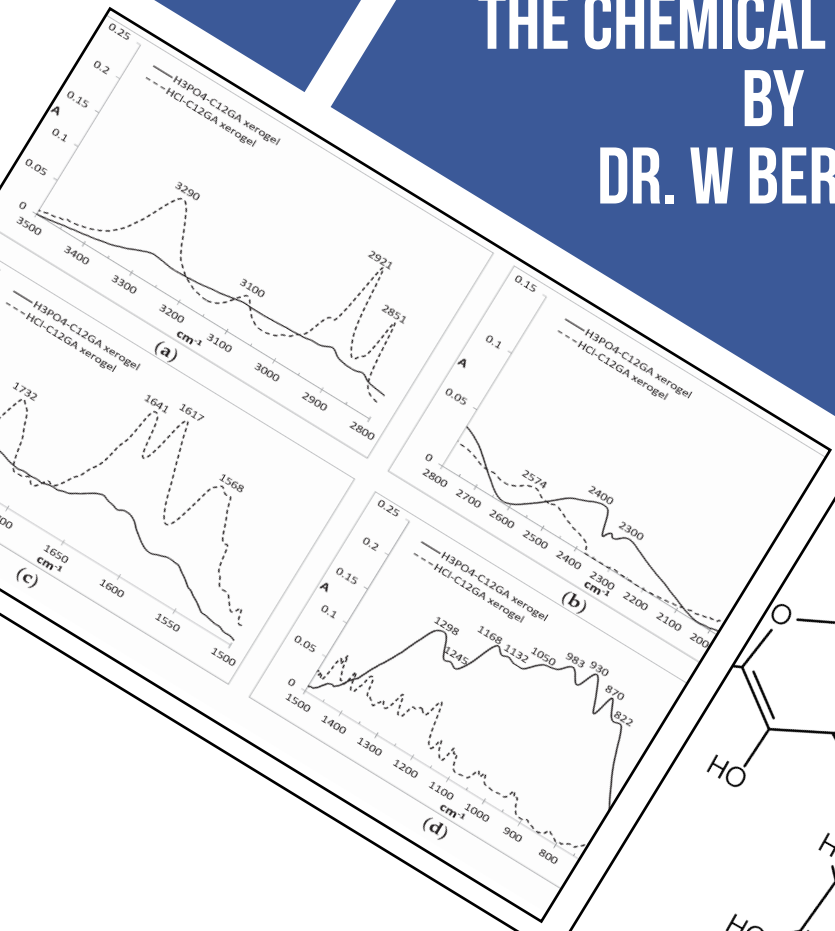
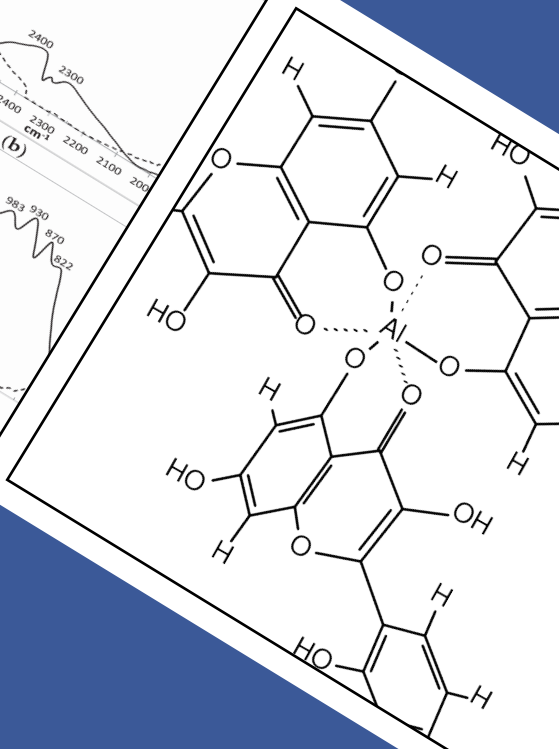
ARTICLE WRITING GUIDE: THE CHEMICAL SCIENCES BY DR. W BERGIUS





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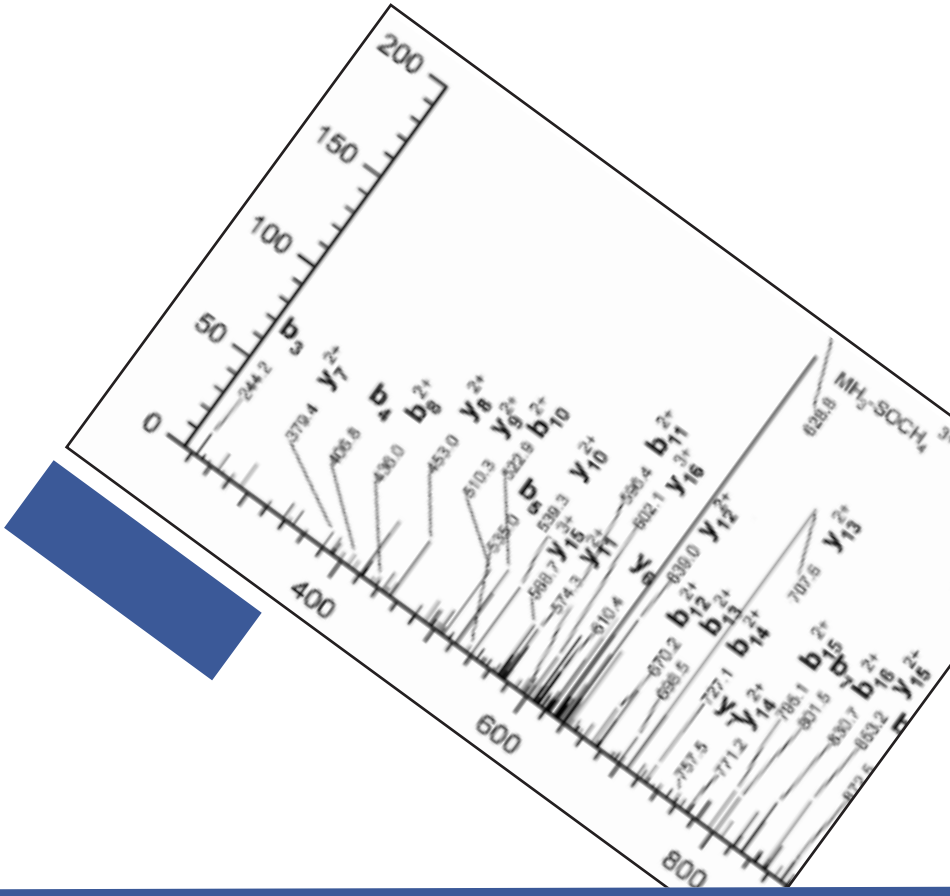
EDITORIAL

This guide is designed to assist authors and editors in the preparation of scholarly articles in the chemical sciences. The overall aims of a research article should be that it gives a comprehensive overview of the research it describes, presenting information clearly and accurately without excessive repetition or embellishment. This guide will give an overview of the main objectives of each article section, and pointers for how they should be constructed. Finally, the visual presentation and formatting of articles will also be discussed.

Ideally an article is presented neatly, consistently, error-free and ultimately as if it has been prepared with due care and attention to detail. These details are often treated as of secondary importance, but can affect how your paper is perceived, especially by editors and reviewers who may be pressed for time, so it is important to give the best impression possible.

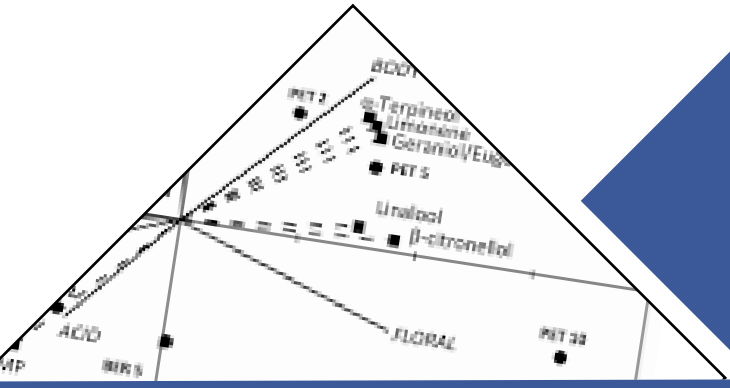


TITLE

The title of an article should use the fewest number of words possible that clearly and accurately reflect the contents of the article. It should describe what the research is about, also ideally mentioning the key result, e.g. ‘The use of lithium salts as electrolytes in Li–S batteries leads to increased cell capacity and stability’ is better than ‘Investigation into the use of lithium salts as electrolytes for use in Li–S batteries’. Avoid the use of undefined acronyms (unless very well known, e.g. NMR, SEM, etc.) and try to include relevant keywords that will help your article to appear in relevant searches.

Authors will often write their title first. Once you’ve finished your article, make sure to go back and re-read your title:

- Is it clear and concise?
- Does it accurately describe the key focus of the article?
- Does it allude to a key or interesting result?
- If somebody in your field was looking for a paper on this topic, what would they be typing into a search engine — would the title of your paper be easy to find?
- Is it free from errors and formatted correctly? Are chemical formulae correct, e.g. CO_2 vs. CO2? (See formatting section)

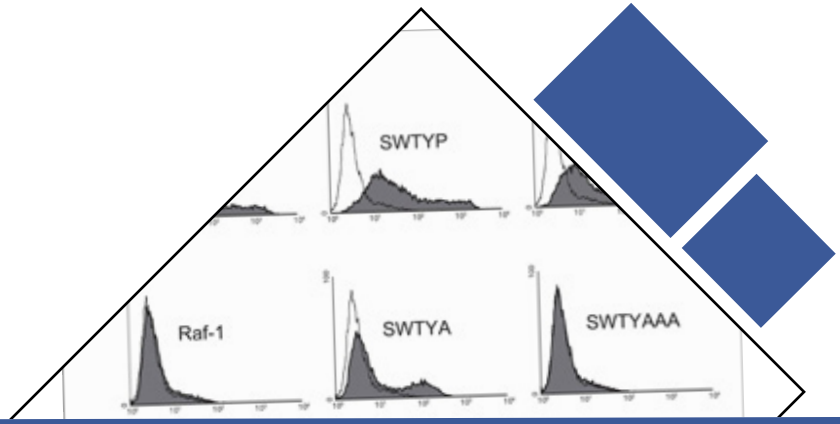


ABSTRACT

The abstract should be a brief, clear summary of your entire paper in approximately 100–250 words, containing a quick background of the topic and explaining the motivation for the research presented, how it was performed, the headline results and a concluding remark about implications for future research, potential applications and/or the field in general. As with the title, it is really important to get this part of the manuscript right, as it is often the only part a reviewer will have access to before deciding whether or not to review. It is also the first part any reader will look at, informing them of the quality and content of the paper. Again, it is beneficial to try and include keywords that will help your article to appear in relevant searches.

Once you have finished your whole article, it is very useful to return to the abstract to check that is still describes the text of the paper, clearly and accurately:

- Is it clear and concise?
- Does it accurately describe the key focus of the article?
- Does it accurately describe the main results of the paper and what has been achieved?
- Is it free from errors and formatted consistently and correctly? (See formatting section)

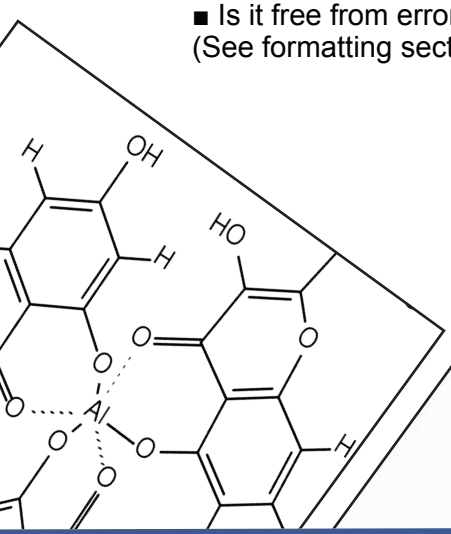


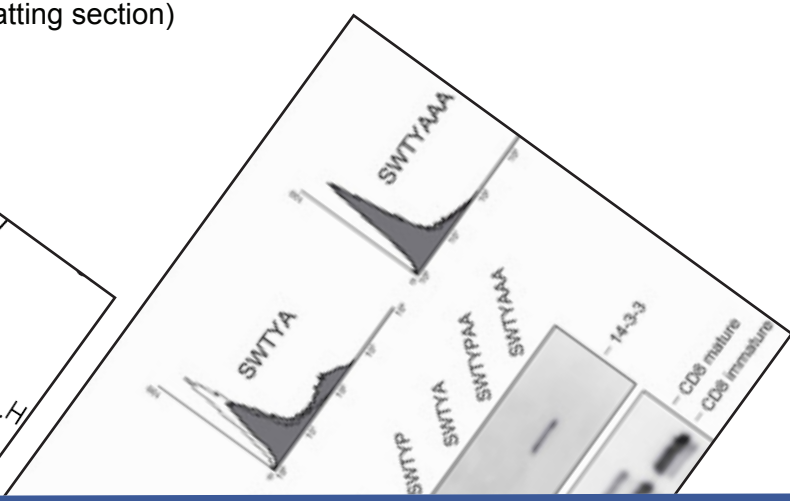
INTRODUCTION

An introduction should set your research into the context of the wider literature, explaining the background of the problem that you are trying to solve. The first paragraph should be a very broad introduction to the problem and why it is interesting in general (is it related to energy storage, drinking water, pharmaceuticals, specific diseases, consumer technology, sustainability, food production etc.?). The next 2–3 paragraphs should then describe in more detail the previous research in the literature surrounding this problem, and what has been achieved so far by both others and indeed your own previous research (try to reference this work in an appropriately balanced manner). By the end of these paragraphs it should be apparent that there is a shortcoming in our knowledge that needs to be addressed, which leads into the final paragraph outlining the aims and objectives of the article, and the overall hypothesis that you originally wanted to test.

When you have finished your introduction, read it through with the following questions in mind:

- Will the reader understand the significance of the work and why the research has been carried out?
- Does it provide the reader with an understanding of how the work fits into the broader literature?
- Are the aims and hypothesis of the research clearly explained?
- Are the references appropriate and balanced?
- Is it free from errors and formatted consistently and correctly? (See formatting section)





EXPERIMENTAL

The most important aspect of the experimental section is that it contains all of the necessary information required for another scientist to replicate your experiments and reproduce your results. Of course, knowledge of standard procedures can be assumed (e.g. drying of solvents, standard reaction setups, separation and purification techniques, etc.). However, precise conditions must be reported if relevant (e.g. temperature, pressure, mass, concentration, solvent, atmosphere, etc.). It is also acceptable to reference previously reported procedures, as long as this is done accurately and the reference given contains the complete information required.

Common practice is to have an initial subsection (1. Materials) describing a comprehensive list of the materials that were used in the research, their purity and where they were obtained from, as well as any appropriate discussion of further purification or storage procedures that were necessary. Then a subsection describing analytical procedures (2. Characterisation) should be included, detailing all characterisation techniques that were employed, the make and model number of instrumentation used as well as the exact operating parameters where appropriate (e.g. temperature, flow rate, wavelength, etc.). The following subsections should list experiments in a logical order, including all relevant experimental details and characterisation data for any compounds made. Finally, if any ethical statement is required, for example due to the use of laboratory animals or human volunteers, this should be included in the experimental section also.

When you have finished your experimental section, go back and read through it:

- Does it contain the details of all of the materials and instrumentation that were used?
- Does it contain all of the information required to replicate the complete set of experiments, in order that another scientist could produce the same results?
- Does it contain all necessary characterisation data?
  If necessary, does it contain an ethical statement?
- Is it free from errors and formatted consistently and correctly? (See formatting section)

RESULTS & DISCUSSION

Though other parts of the article have a certain importance with respect to gaining the attention of your readers, the Results & Discussion section is the heart of the article, containing the most important information detailing the outcome of your research and what the results mean. The results should be ordered logically and can either be presented in isolation prior to discussion, or interspersed with the discussion if this is more appropriate. While figures and tables can be used to include more complete data, only the data that bears direct relevance on the discussion should be included in the main text (if complete data are also lengthy and not required to read and understand the article, consider removing them from the article and instead submitting them as supplementary information).

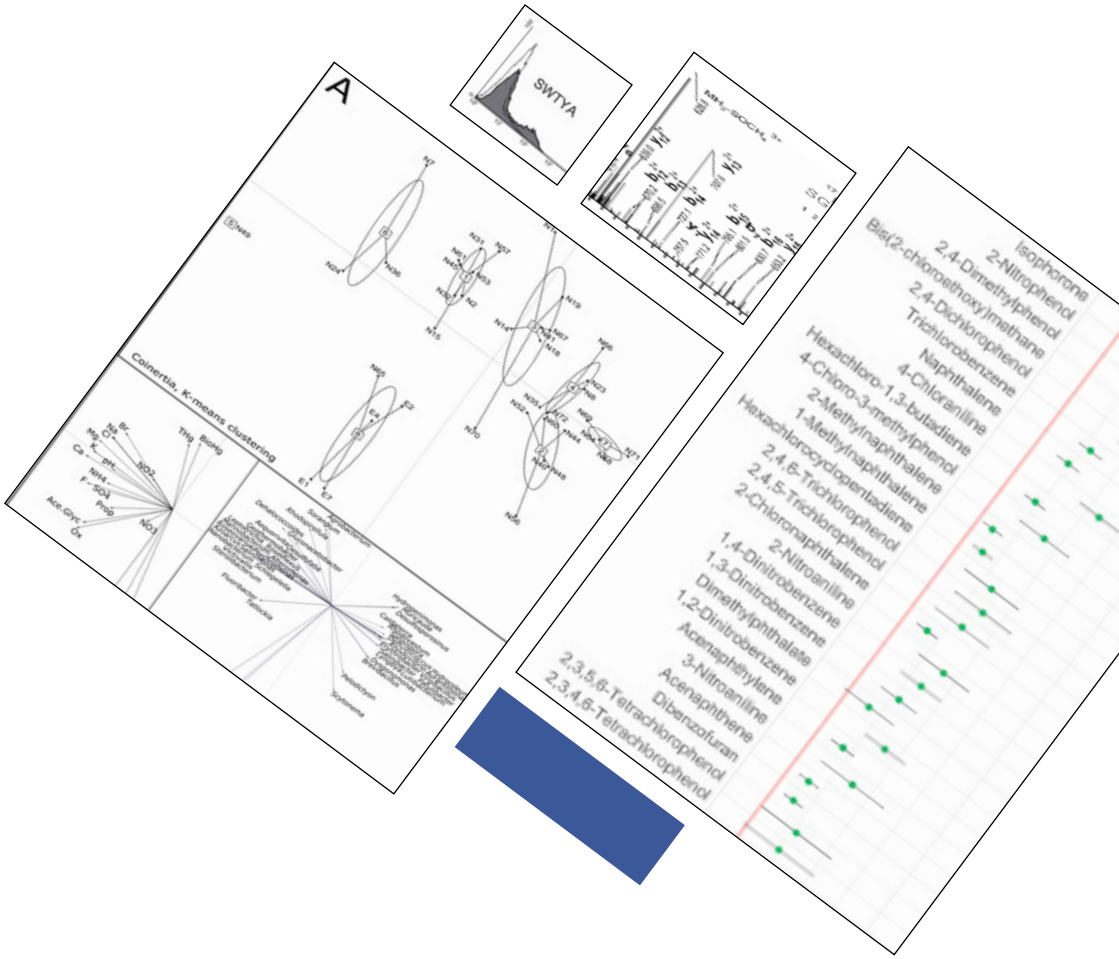
As you discuss your results make sure to keep the original purpose of the paper in mind and try to bring the discussion back to this point wherever possible. This will make the paper more focussed and reinforce the relevance of the work to the reader. While discussing the impact of your results, try also to compare them to other recent work, referencing as appropriate. Of course you should highlight the positive attributes of your research, but try also to be self-critical and clearly explain any shortcomings or areas that require improvement. Try also to avoid excessive repetition, and keep the discussion concise and to the point.

Reading back through your Results & Discussion section, ask yourself:

- Is it presented in a logical order that tells a complete story to the reader?
- Are complex arguments clearly explained and backed up by evidence?
- Is the impact of the work clearly explained and put into context with the wider literature?
- Are any potential points for improvement clearly discussed?
- Are any discussion points repeated too often?
- Does the focus of this section clearly relate back to the aims of the paper as outlined in the abstract and introduction?
- Is it free from errors and formatted consistently and correctly? (See formatting section)

CONCLUSIONS

The conclusions should ideally be a short and concise account of the key results of the paper and what has been achieved, with emphasis on why this is novel and the corresponding impact. It is customary to end this section with a few closing remarks on the broader significance and future directions of the presented research.



FORMATTING

Often overlooked and sometimes considered of secondary importance, formatting and consistency are important to present your research clearly to editors and reviewers, and instil confidence in them that the work has been prepared carefully and accurately. Make sure to thoroughly check through your manuscript for consistency in numbering and formatting of section headings and subheadings, spelling of chemical names, use of punctuation, use of font size and typeface, numbering of figures and tables, formatting of references, and consistency in use of American vs. British English (e.g. 'polymerise' vs. 'polymerize'). Always check for and follow any relevant guidelines supplied by the publisher of the journal to which you are going to submit your work. In general, here are some common pitfalls to try and avoid:

- Hyphenated terms — check your whole manuscript to ensure that you have not alternated between e.g. 'supercapacitor', 'super capacitor' and 'super-capacitor'. Make sure these terms are consistent throughout the manuscript. In this example case, only one is correct, but the mistake stands out much more if it is inconsistent with the rest of the text.

- Compound name spelling errors are not usually picked up by spell checking software unless you have added the spellings to your dictionary. Make sure to go through your paper and check that there are no hidden typos in chemical names and formulae.

- Acronyms and definitions —define an acronym once the first time that it is used in the article, then ensure to consistently use the acronym alone throughout the rest of the article. E.g. 'The monomer was polymerised using nitroxide mediated polymerisation (NMP). NMP was employed as it allowed careful control over the resulting molecular weight.'

- Use of hyphen (-), minus sign (−), en dash (–) and em dash (—). These symbols are not the same and they are not usually interchangeable. Try to make sure that they are used appropriately and consistently throughout your manuscript, particularly in the title and abstract. A hyphen is used when breaking a word between two lines, in a hyphenated phrase e.g. a benzene-derived compound, or in compound names e.g. 1,2,3-trimethylbenzene. A minus sign is a mathematical symbol and so should be used in units and equations, e.g. –ΔG or mol dm−3. An en dash is used to indicate a range, e.g. 'samples were centrifuged at 3000–6000 rpm', it can indicate a conflict or connection between two words,

FORMATTING CONT.

e.g. ‘reversible addition–fragmentation transfer polymerisation’ or ‘dose–response curve’, and it is also commonly used as a single chemical bond (whereas the equals sign, =, can be used as a double bond) in written chemical notation, e.g. CH3–CH=CH2. The em dash can be used parenthetically, e.g. ‘the previously synthesised compound — 3,5-dihydroxybenzyl alcohol — was added to the stirring solution’, and it can also be used in place of a colon, e.g. ‘the anode possessed excellent stability — it retained 95% of its initial capacity after 1000 cycles‘.

■ When stating temperatures, units are °F, °C or K (Kelvin does not have a degree symbol). Additionally, try to consistently use the degree symbol, and not superscript ‘o’ or ‘0’ as this can lead to formatting issues in publication.

■ Variables should always be in italics e.g. ‘pV = nRT’ or ‘n, where n is equal to a value between 1 and 3’.

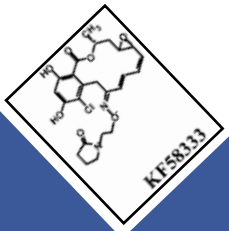
■ Latin abbreviations such as et al., e.g., i.e. or etc. should be in italic typeface — again, check for consistency.

■ Double check all citations in the main text to numbered figures, tables, equations and references to ensure that they refer to the correct piece of information.

■ Try to cite tables and figures consistently, i.e. do not alternate between ‘Figure 1’, ‘Fig. 1’ and ‘Fig 1’.

■ Try to cite references with a consistent format, using en dashes to indicate a range of references, e.g. ‘…has already been demonstrated in several recent studies.[12–15]’ Usually citations should go on the outside of punctuation, e.g. ‘studies.[12–15]’ and not ‘studies [12–15].’

■ References should be formatted consistently. Check for missing information (e.g. volume or page numbers, missing spaces or punctuation, incorrectly formatted text, etc.) and remember to use en dashes for page ranges. Make sure authors’ names are presented consistently and spelled correctly, including diacritical marks (e.g. é, ö, ñ, etc.).



FIGURES

Figures contribute significantly to the overall appearance of a manuscript and also contain much of the key data. As such, try to present them clearly, neatly and consistently. Where appropriate make sure to include axes labels, units, scale bars, error bars, legends and any other information that would be expected in a certain figure type. Check the spelling of any text contained in an image file, as these are often where spelling mistakes can creep in. Try to be consistent with use of typeface, font size, notation, alignment and scale where possible.