QuantBio Express

ARTICLE TYPE

This is the title†

Full Name,*[a] Full Name,[b‡] and Full Name[a]

The abstract should be a single paragraph which summarises the content of the article. Any references in the abstract should be written out in full *e.g.* [Surname *et al., Journal Title*, 2000, **35**, 3523].

0.1 This is the subsection heading style

Section headings can be typeset with and without numbers.[1]

0.1.1 This is the subsubsection style.

These headings should end in a full point.

0.1.1.1 This is the next level heading. For this level please use `\paragraph`. These headings should also end in a full point.

1 Graphics and tables

1.1 Graphics

Graphics should be inserted on the page where they are first mentioned (unless they are equations, which appear in the flow of the text).[2]

Fig. 1 An example figure caption

1.2 Tables

Tables typeset in RSC house style do not include vertical lines. Table footnote symbols are lower-case italic letters and are typeset at the bottom of the table. Table captions do not end in a full point.[3,4]

Table 1 An example of a caption to accompany a table

Header one/units	Header two	Header three
1	2	3
4	5	6
7	8	9
10	11	12

Adding notes to tables can be complicated. Perhaps the easiest method is to generate these manually.§

2 Equations

Equations can be typeset inline *e.g.* $y = mx + c$ or displayed with and without numbers:

$$A = \pi r^2$$

$$\frac{\gamma}{\varepsilon x} r^2 = 2r \tag{1}$$

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† Electronic Supplementary Information (ESI) available: [details of any supplementary information available should be included here]. See DOI: 10.1039/b000000x/

‡ Additional footnotes to the title and authors can be included *e.g.* 'Present address:' or 'These authors contributed equally to this work' as above using the symbols: ‡, §, and ¶. Please place the appropriate symbol next to the author's name and include a `\footnotetext` entry in the the correct place in the list.

§ Footnotes should appear here. These might include comments relevant to but not central to the matter under discussion, limited experimental and spectral data, and crystallographic data.

Fig. 2 An image from the *Physical Chemistry Chemical Physics* cover gallery, set as a two-column figure.

$$T_{nn''}^{mm''} = \begin{cases} \dfrac{(q+p'')!\,(p-p'')!}{(q-q'')!\,(p+q'')!}\, a^{m-m''} b^{n''}\, P_{p-p''}^{(m-m'',n'')}(1-2A^2) P_{p-p''}^{(m-m'',n'')}(2B^2-1) \\ \text{when} \quad n-n'' \geq m-m'' \geq 0\,, \\ \\ \dfrac{(p+q'')!\,(q-q'')!}{(p-p'')!\,(q+p'')!}\, a^{m''-m} b^{n''}\, P_{q-q''}^{(m''-m,n'')}(1-2A^2)\, P_{q-q''}^{(m''-m,n'')}(2B^2-1) \\ \text{when} \quad n-n'' \geq m''-m \geq 0\,, \\ \\ 0 \quad \text{otherwise.} \end{cases} \tag{2}$$

You can also put lists into the text. You can have bulleted or numbered lists of almost any kind. The `mhchem` package can also be used so that formulae are easy to input: `\ce{H2SO4}` gives H_2SO_4.

For footnotes in the main text of the article please number the footnotes to avoid duplicate symbols. e.g. `\footnote[num]{your text}` the corresponding author `*` counts as footnote 1, ESI as footnote 2, e.g. if there is no ESI, please start at [num]=[2], if ESI is cited in the title please start at [num]=[3] etc. Please also cite the ESI within the main body of the text using †.

YOU CAN DELETE ALL THE ABOVE SECTIONS

3 Introduction

Explain the biological problem and briefly summarize what has been done before. Describe your aims for this project.

4 Methods

Present the computational methods that were used as succinctly as possible. Use references to papers, books, or other sources that you used to learn about them. Leave details for the appendix and submit your code as separate supplemental information files. If you obtained data for the project, provide the source here.

5 Results

Present your results, divided into sections for different portions of the project. Indicate who worked on each section. Illustrate your results with tables and figures and compare them to previously published results.

6 Discussion

Give some big-picture context for your work and speculate on its importance. Describe what you learned from doing this project and what you think about the future directions of this topic. This is where you can use more personal language and say fun things!

7 Conclusions

What is your takeaway from this project?

8 Acknowledgements

The acknowledgements come at the end of an article after the conclusions and before the notes and references.

References

1 C. D. Abernethy, G. M. Codd, M. D. Spicer and M. K. Taylor, *J. Am. Chem. Soc.*, 2003, **125**, 1128–1129.

2 F. A. Cotton, G. Wilkinson, C. A. Murillio and M. Bochmann, *Advanced Inorganic Chemistry*, Wiley, Chichester, 6th edn, 1999.

3 A. J. Arduengo, III, H. V. R. Dias, R. L. Harlow and M. Kline, *J. Am. Chem. Soc.*, 1992, **114**, 5530–5534.

4 L. N. Appelhans, D. Zuccaccia, A. Kovacevic, A. R. Chianese, J. R. Miecznikowski, A. Macchioni, E. Clot, O. Eisenstein and R. H. Crabtree, *J. Am. Chem. Soc.*, 2005, **127**, 16299–16311.