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Experimental validation, anyone?

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Even though *Nature Computational Science* is a computational-focused journal, some studies submitted to our journal might require experimental validation in order to verify the reported results and to demonstrate the usefulness of the proposed methods.

At *Nature Computational Science*, we focus on the development and use of computational techniques and mathematical models, as well as their application across a range of scientific disciplines to address complex, real-world challenges. We strive to publish manuscripts that advance their respective fields, both conceptually and practically, which means that verified predictions and well-validated methodologies are a must. Validation can come in many different forms – depending on the nature of the research topic – and may include comparisons to experimental data.

Experimental and computational research have worked hand-in-hand in many disciplines, helping to support one another in order to unlock new insights in science. We recognize the importance of these collaborations, particularly since experimental work may provide 'reality checks' to models. Although we are a computational science journal, this does not mean that experimental validations are outside of our scope. On the contrary, we believe that it is important to provide validations with real experimental data – when appropriate – in order to demonstrate that the method being proposed by a manuscript is practically useful, as well as to confirm that the claims put forth in the study are valid and correct.

We certainly understand that, in some fields, identifying an experimentalist with whom to collaborate can be challenging, and that performing the necessary experiments can be an arduous task – such as in the biological sciences – but there might be other viable alternatives, as there is much existing experimental data that are available to researchers. As an example, in evolutionary biology, experiments can be expensive and time-consuming due to the use of model organisms that need to be observed over long periods of time, while in neuroscience, experiments can be invasive and also raise ethical concerns. However, in both cases, recent advancements in experimental techniques have allowed for the generation of experimental datasets that are within reach of scientists, such as those put forth by MorphoBank and The BRAIN Initiative. For studies in genome informatics, data is much easier to come by, for example with the availability of the Cancer Genome Atlas and the many datasets put forth by the National Library of Medicine. Drug design and discovery research also poses unique challenges in terms of validation, as clinical experiments on drug candidates can take years to conclude. In these cases, it may be sufficient to compare a proposed drug candidate to the structure, property, and efficacy of existing drugs. Without reasonable experimental support, claims that a drug candidate may outperform those on the market can be difficult to substantiate.

In the physical sciences, experimental validation is also an essential task for verifying the performance of a proposed computational method. In some areas, such as chemistry, there may be an expectation from the community that the computational work is paired with an experimental component. For instance, in molecular design and generation studies, experimental data that confirms the synthesizability and validity of the newly generated molecules can help to verify the computational findings and demonstrate the practical usability of the proposed model. Of course, it may not always be possible to collaborate with an experimentalist, and therefore, quantifications of the synthesizability and comparisons to the structure and properties of existing molecules, such as those reported in PubChem or OSCAR databases, may be sufficient. However, if the work suggests that the generated molecules have a better performance within a given application, such as catalysis or medicinal chemistry, these claims may require a more thorough experimental study. Similarly, in materials science, if a theoretical prediction points to a domain of new materials systems with exotic properties, then experimental synthesis, materials characterization, and sometimes tests within real devices would be required to support the prediction. Notably, there is a growing amount of experimental data becoming available across the materials science community, for instance through the High Throughput Experimental Materials Database or the Materials Genome Initiative. The increasing availability of experimental data presents exciting times for computational scientists, as this makes it possible to validate models and predictions more effectively than ever before.

Naturally, this is not a comprehensive discussion of all of the areas that *Nature Computational Science* covers, and it is not a set of rigid rules either, but rather a general guidance to err on the side of including an experimental validation when feasible and appropriate. Of course, specific requests for additional comparisons or experiments might be made on a case-by-case basis, since, as a multidisciplinary journal, we recognize that different disciplines have different standards and requirements when it comes to experimental validation. Moving forward, we hope that these guidelines help to avoid any 'surprises' in the event that we ask for experimental validation and better clarify our rationale for making these requests.

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