Editorial

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As Editor-in-Chief of this international journal, it is ultimately my responsibility to ensure that the papers accepted for publication clearly report findings which advance our understanding of the basic science and correct application of NIR spectroscopy. In this endeavour I am ably and willingly supported by experienced editors and a large team of dedicated reviewers.

Like all peer review journals, JNIRS receives many papers which must be rejected because they do not, and even with major revision will not, meet the required standard of a contribution to existing knowledge. At this point the author’s hopes, aspirations and possibly their careers have been diminished and the reviewers and the editorial team have nothing to show for the time that they have devoted to the paper.

JNIRS publishes reviews, original research papers, technical notes and letters. Technical notes are available to authors who wish to report novel findings which will stimulate discussion and more extensive investigation. Technical notes are a suitable avenue for publishing preliminary findings, sometimes based on a limited number of samples or where minimal validation of the results is possible due to the availability or cost of samples. However, Technical Notes should demonstrate a spectral basis for the conclusions offered and must clearly indicate the limitations of the study. Authors must avoid unsubstantiated claims of the value of the work. Technical notes often report feasibility studies using a limited number of samples and it may not be feasible to test the models, so there is an expectation that a more comprehensive paper will follow when more convincing evidence is available.

In an original research paper the authors are expected to explain why the study was initiated and state the hypothesis that they set out to test, describe what was done in the materials and methods so that other scientists could repeat the study, and present sufficient results to allow conclusions to be made after discussing their significance relative to current knowledge.

Dr Phil Williams advised me that he was concerned that only 6 of 19 key facts were routinely included in over 100 papers that he surveyed during 2013 which reported NIR calibrations. The full list of facts can be viewed in available publications. The omissions of greatest concern relate to (a) the testing of calibrations, (b) the identification of the spectral information used to develop a calibration and (c) the methods of assembly of samples.

Replicate spectra of a sample must be averaged—not divided into calibration and test set samples. Cross-validation is being over-used as a surrogate for rigorous testing of calibrations. Reviewers and readers are more inclined to accept that a new calibration is reliable if they see how it performed when used to test true validation samples. The validation samples must not have been used to develop the calibration and, preferably, not even “close” to the calibration set samples: e.g., they may be taken from a different season or factory. Actually the most rigorous test of a calibration is to see how it predicts the required data on completely new “real world” samples, after the calibration exercise has been completed, and the calibration has been installed for use in the field.

In addition to making thorough evaluations of their calibrations, authors should also identify the basis of the calibrations that they report. This includes identifying the absorbance peaks which relate in a meaningful way to the constituents in or properties of the samples being analysed. This can realise interesting and useful information on how an absorber influences a parameter such as texture, for which there are no “classical” absorbers.

When I first used a NIR spectrometer it was common for outsiders to label it as “black box” technology. Those days are far behind us.

NIR spectroscopy will continue to be the preferred technology for many analyses, but only if calibrations are thoroughly tested and subsequently prove reliable when used for routine analyses by non-specialist operators working in hostile environments.

My aim is to ensure that JNIRS, as the only peer-review journal dedicated to near infrared spectroscopy, only publishes
papers that report soundly conducted science and, for papers reporting calibrations, calibrations which are fully validated and supported by evidence which reveals the chemical or physical, as well as the statistical, basis of the calibration.

It would be more profitable in terms of researchers’ and reviewers’ time if fewer papers were rejected and fewer papers were returned for major revision. Authors writing papers for JNIRS are fortunate to have technical support from many experienced NIR scientists. The support is in the form of occasional articles, on-going publications, a discussion forum which attracts answers to day-to-day problems from many experienced NIR scientists, via links to valuable information on the IM Publications web site, and a series of lectures now being assembled by the University of Cordoba as the International Virtual Platform for Learning and Teaching of Near Infrared Spectroscopy. There are also comprehensive guidelines in international standards for certain products.

Of course, spending time with an experienced NIR spectroscopist is also highly recommended.

As a final comment, JNIRS and many other scientific journals are published in English. Workers for whom English is not the first language who seek to publish their findings in such journals, are encouraged to seek advice on the expression of their thoughts, results and conclusions in English.

References


5. Various authors of excellent articles on NIR calibrations in NIR news [1990 to present].


7. http://www.impublications.com/content/near-infrared-spectroscopy
