

INSTRUCTIONS FOR SUBMISSION

Please read this in full, in particular regards tables and figures.

The abstracts for NIR-2019 are to be in the form of an extended abstract (2-4 pages) that clearly outlines the aim, methods, results and discussion.

Figures and Tables

Figures can be inserted using the icon in the text field menu

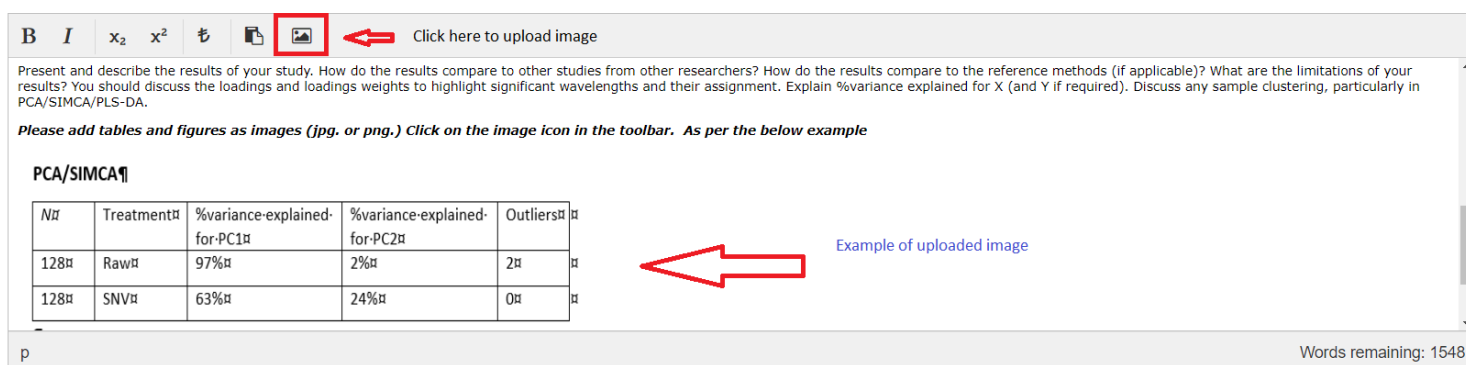
Tables are to be entered as figures.

Step 1. Use the word template to prepare your Tables ensuring you correctly enter the data.

Step 2. Copy the Table as normal and paste into a suitable image software package (e.g. Paint which comes with Windows, or a shareware such as Gimp (available for Windows, Mac, Linux)) Alternatively you can use the snipping tool in Office.

Step 3. Save the image as a .png or .jpg file

Step 4. Import the image using the "Import figure" icon in the text box menu.



Present and describe the results of your study. How do the results compare to other studies from other researchers? How do the results compare to the reference methods (if applicable)? What are the limitations of your results? You should discuss the loadings and loadings weights to highlight significant wavelengths and their assignment. Explain %variance explained for X (and Y if required). Discuss any sample clustering, particularly in PCA/SIMCA/PLS-DA.

Please add tables and figures as images (jpg. or png.) Click on the image icon in the toolbar. As per the below example

PCA/SIMCA

| N# | Treatment# | %variance-explained-for-PC1# | %variance-explained-for-PC2# | Outliers# |
|------|------------|------------------------------|------------------------------|-----------|
| 128# | Raw# | 97%# | 2%# | 2# |
| 128# | SNV# | 63%# | 24%# | 0# |

Words remaining: 1548

**Title of presentation to be 16-pt, centred, bolded in sentence case
with *Genus species* names in italics.**

Myname SURNAME, Yourname LASTNAME

Affiliation with address and postcode etc including Country

ABSTRACT

Begin with a few sentences to describe **what** you did, **why** you did it, **how** you did it and what the major results are. What is the impact of your results? Will it be used in the laboratory to replace or complement existing analyses? Will it allow you to collect spectra on-line?

INTRODUCTION

Provide some background to the study. Why is it important to develop a NIR method to do what you have done? Will this allow easier analysis of a difficult or costly task? What has been done before and how does your work improve on the earlier work?

METHODS AND MATERIALS

Only use the appropriate headings according to your type of study. Provide the most detail for the most relevant sub-heading. For example, if you are presenting a chemometric algorithm, you will probably talk more about the details of analysis than the sample selection.

Materials: Tell us about the samples you used. Where were they collected from? How were they collected? Were they prepared in anyway before lab analysis or NIR analysis (Were they dried – how? Were the milled to form a powder?)

Spectroscopy: Tell us about the instrument you used (Make/Model, Manufacturer). What is the spectral range and resolution of the instrument? How many scans were acquired for each spectrum? How many spectra were taken for each sample and was the sample re-packed between each spectrum? Was spectroscopy undertaken in transmission or diffuse reflectance? Fibre optic or integrating sphere?

Analysis: What software did you use for analysis (Version number, Supplier)? Were any in-house routines developed for special use (if so please describe)? What pretreatments did you use (SNV, MSC, DeTrend, derivatives, ...)? If derivatives were used describe the parameters (Gap-Segment, Norris-Gap, Savitzky-Gloay, 1st/2nd derivative, window/gap/segment size, polynomial order). What analyses did you perform (PCA, PLS regression, PLS-DA, MLR, PCR, SIMCA, ANN, ...)? How were outliers detected and removed? Were wavelength regions selected?

RESULTS

Present and describe the results of your study. How do the results compare to other studies from other researchers? How do the results compare to the reference methods (if applicable)? What are the limitations of your results? You should discuss the loadings and loadings weights to highlight significant wavelengths and their assignment. Explain %variance explained for X (and Y if required). Discuss any sample clustering, particularly in PCA/SIMCA/PLS-DA.

CONCLUSIONS

What is the impact of your results? Did you achieve what you set out to achieve? What needs to be done to move from the research stage to actual implementation and application of your results? How can you improve the study for next time?

REFERENCES

Examples of Journal, Proceedings and Book

Author ONE, Nother A and Last AT (1998) The best way to set up a NIR for solution-state analysis. *Journal of Near Infrared Spectroscopy*, 10(2), 112-117.

Student A and Supervisor B (2018) NIR Spectroscopy. In: Williams P and Saranwong S (Eds). Proceedings of 7th ICNIRS Meeting, A lovely place, Neverland. Pages 27-30.

Guru S (2006) The Ultimate Textbook of All Things Spectroscopic. Wonderous Press Ltd, New York. 376 pages. ISBN 123456789-00-X.

For assistance on preparing your abstract please see the tutorial by Phill Williams, Pierre Dardenne and Peter Flinn in JNIRS. It is a free download.

<http://journals.sagepub.com/doi/pdf/10.1177/0967033517702395>

To submit your abstract please click on the below link to be taken to the online abstract and registration system.

<https://yrd.currinda.com/register/event/1092>

Depending on the type of experiment, the following tables should be completed as well.

PCA/SIMCA

| N | Treatment | %variance explained for PC1 | %variance explained for PC2 | Outliers |
|-----|-----------|-----------------------------|-----------------------------|----------|
| 128 | Raw | 97% | 2% | 2 |
| 128 | SNV | 63% | 24% | 0 |

PLS – Reference Statistics

| Property | Units | Method | Standard | Mean | Median | SD | SEL |
|---------------|-------------------|------------------|--------------|--------|--------|-----|-------|
| Lignin | % m/m | Gravimetric | Tappi om-222 | 31.1 % | 30.5 % | 1.6 | 0.061 |
| Cellulose | % m/m | Gravimetric | Tappi om-222 | 43.8 % | 42.9 % | 3.8 | 0.023 |
| Hemicellulose | % m/m | LC | In-house | 27.6 % | 27.3% | 1.8 | 0.05 |
| Moisture | % m/m | Oven-dry basis | | 60.6% | 58.7 % | 5.2 | 0.2 |
| Density | kg/m ³ | Gravi-volumetric | | 472 | 459 | 27 | 0.5 |

PLS – Regression Statistics

| Property | N _{tot} | N _{train} | Treatment | Outliers | LVs | R ² _{cal} | RMSEC | r ² _{cv} | RMSECV |
|---------------|------------------|--------------------|-----------|----------|-----|-------------------------------|-------|------------------------------|--------|
| Lignin | 177 | 140 | 1der-SNV | 3 | 6 | 0.90 | 0.28 | 0.86 | 0.27 |
| Cellulose | 170 | 140 | 1der | 4 | 5 | 0.94 | 0.18 | 0.90 | 0.18 |
| Hemicellulose | 83 | 60 | 1der | 7 | 7 | 0.86 | 0.32 | 0.80 | 0.40 |
| Moisture | 177 | 140 | SNV | 1 | 3 | 0.988 | 0.09 | 0.97 | 0.10 |

R²_{cal} = R² for the calibration model

PLS – Prediction Statistics

| Property | N _{test} | r ² _{val} | RMSEP | RPD |
|---------------|-------------------|-------------------------------|-------|-----|
| Lignin | 37 | 0.88 | 0.31 | 2.9 |
| Cellulose | 37 | 0.91 | 0.21 | 3.3 |
| Hemicellulose | 23 | 0.79 | 0.44 | 2.0 |
| Moisture | 37 | 0.97 | 0.11 | 5.8 |

r²_{val} = r² for the validation samples (independent test set)