

DEVELOPMENT OF A CALIBRATION SYSTEM TO ASSESS THE REPRODUCIBILITY OF qNMR METABOLOMICS

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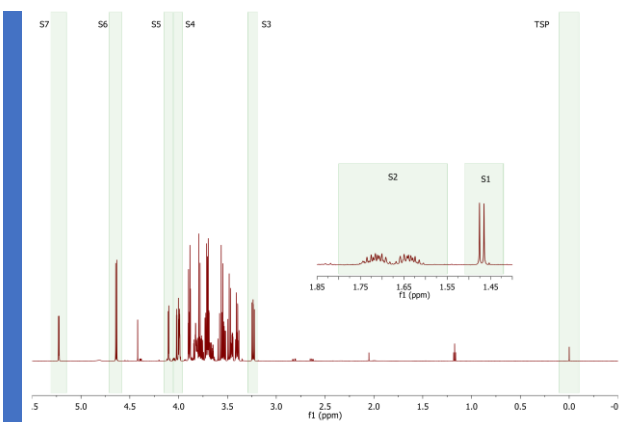
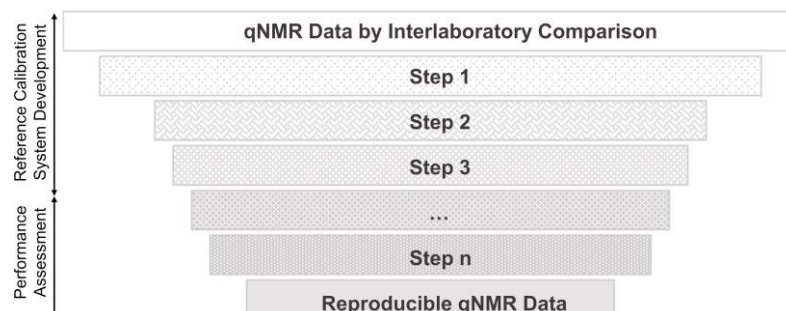
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Nowadays, qNMR method is widely applied to product identification and traceability thanks to the NMR spectroscopy ability to generate *statistically equivalent signals* regardless of the instrument configuration. Nevertheless, current literature still lacks official harmonized criteria to assess the reproducibility of qNMR data produced in diverse laboratories through differently configured spectrometers. The present study proposes a quality assurance protocol through the development of a community-built reference calibration system to be queried during the quantification of an analyte *via* NMR.

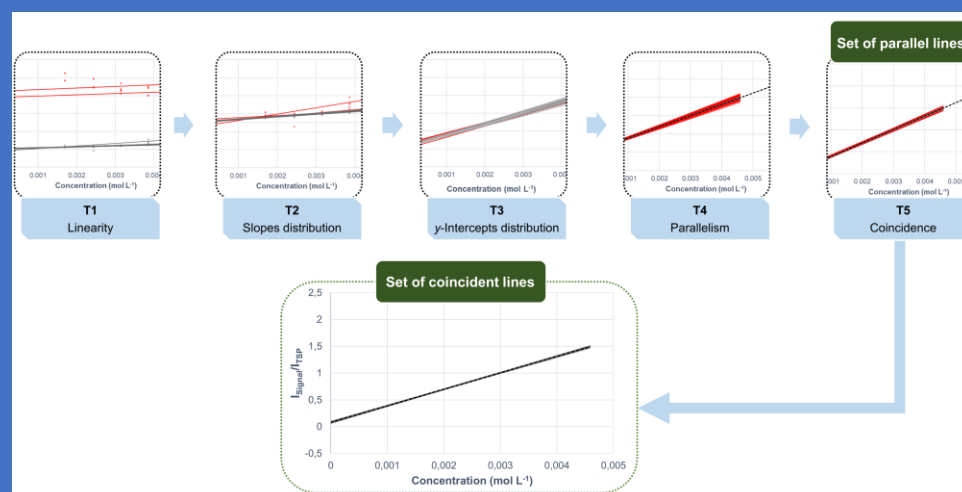
Introduction and scope of the study



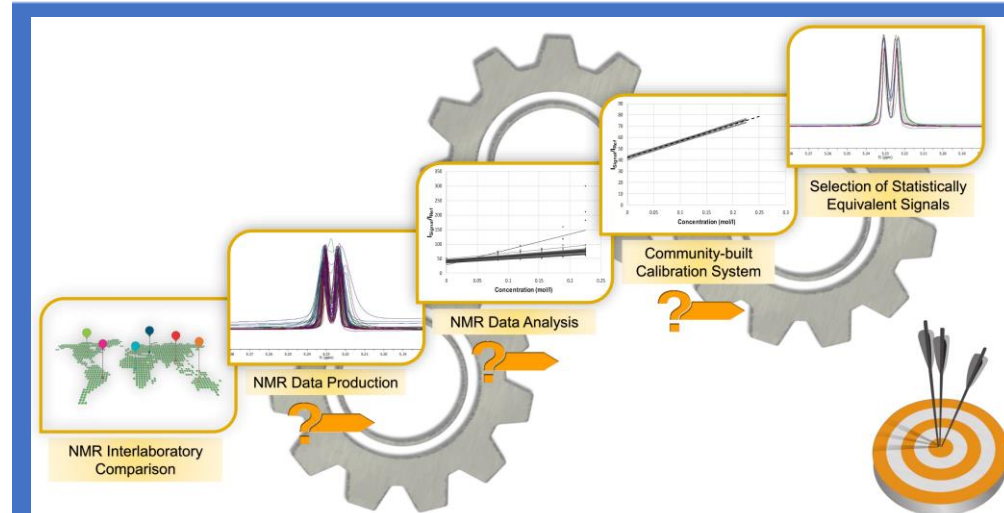
The well performing calibration data were used to build seven community-built calibration lines which acted as reference lines for the quantification of four selected metabolites (arginine, alanine, fructose, and glucose) in grape juice.

Results and discussion

The present study, exploiting the NMR data deriving from an interlaboratory comparison involving 65 participants from 15 countries, aimed at establishing the performance of the produced spectroscopic calibration data upon applying a multiple regression analysis and passing a sequence of five chemometric tests.



Conclusions and references



- A quality assurance protocol was developed to select the well performing calibration data among those produced by the interlaboratory comparison participants enabling the development of a community-built reference calibration system for each analyte taken under consideration.
- It was demonstrated the possibility to obtain statistically equivalent signals able to give high reproducibility in the prediction of metabolite concentrations in complex mixtures.

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