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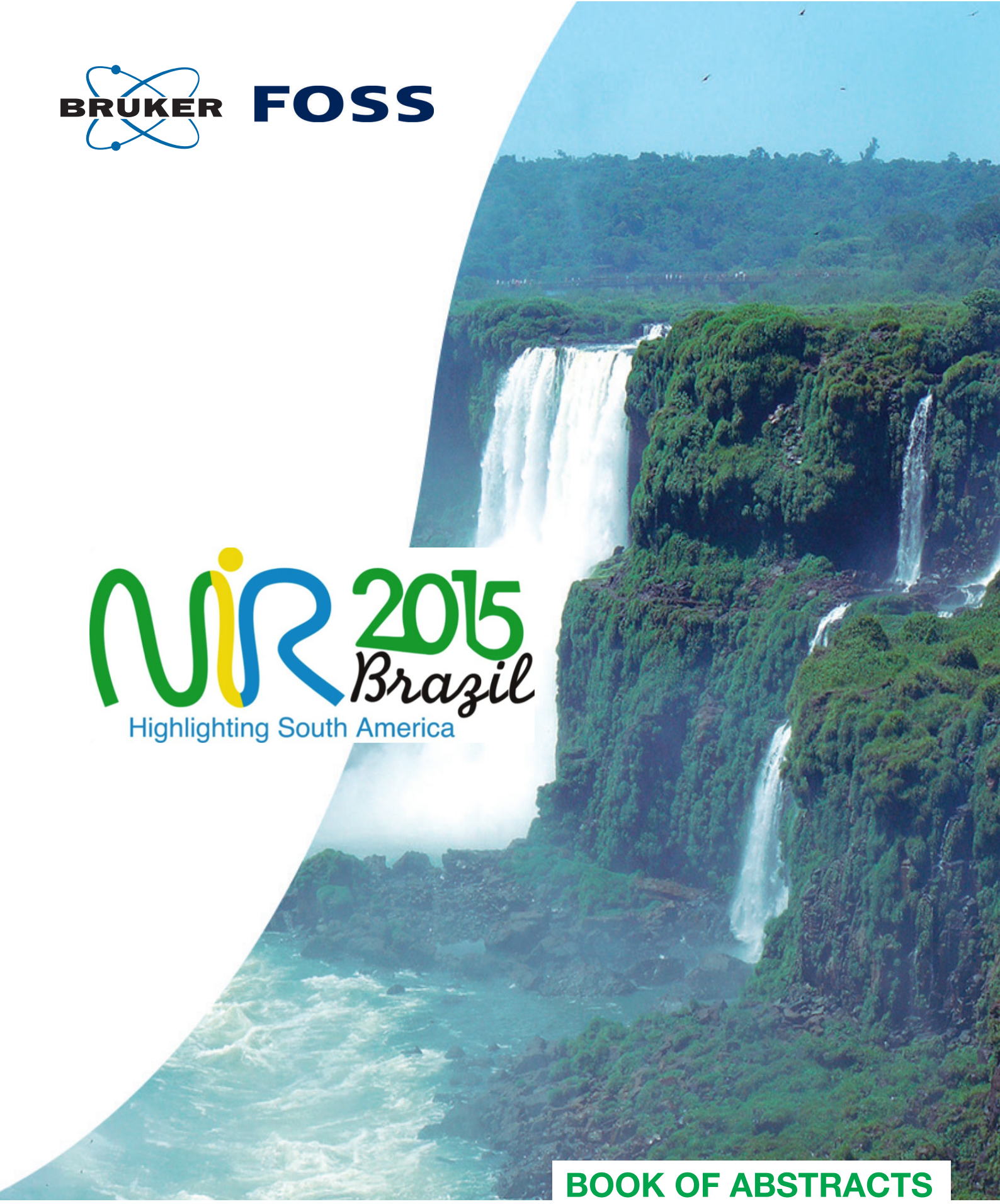

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Development of Calibration Model for Measuring Stilbene Content of Wood Samples by NIRS

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Topic: Agriculture and food

Fast and accurate methods are needed to measure durability related chemical characteristics from wood. In the field of forest tree breeding, the measurements would be performed from increment core samples collected from standing trees. In this study, we have assessed the potential of Near Infrared Spectroscopy (NIRS) for evaluating the content of stilbenes pinosylvin (PS) and its monomethyl ether (PSM) from heartwood samples of Scots pine, Pinus sylvestris L. Scots pine wood samples used were collected from a 43-year-old half-sib progeny trial at Leppävirta in eastern Finland in 2009. Heartwood samples with length of 20-30 mm including the annual rings from 5 to 8 (counted from the pith) were taken from a random side of the increment cores. Each heartwood sample was halved longitudinally. The other half was milled for chemical analysis, and the other half was subjected to optical measurements. The PS and PSM concentrations were analyzed in milled heartwood samples by gas chromatography – mass spectrometry (GC-MS). The sum of their content, total stilbenes (STB), in wood was used as reference for NIRS measurements. Their concentrations varied from 1.81 to 23.02 mg/g (average=10.83 mg/g and standard deviation 4.08 mg/g). Before NIRS measurements, the heartwood samples were stabilized at 22 RH% at room temperature and spectra were acquired on a PerkinElmer Spectrum 400 spectrometer. Depending on the length of the individual sample two to five measurements per sample in every five millimeters were taken and averaged. Each measurement consisted in 64 averaged scans with a resolution of 8 cm^{-1} within a circle with radius of about 4 mm. Resulting spectra ranged between 4000 and 10000 cm^{-1} with an extrapolated step size of 2 cm^{-1}. Total number of samples measured by NIRS was 474 and they were divided into calibration (212) and validation (262) sets. First, statistical pretreatments have been applied to the spectra in order to improve the signal quality resulting in 7 spectra modalities: raw (no statistical pre-treatment), norm (normalization), der1 (first derivative on raw spectra), der2 (second derivative on raw spectra), norm_der1 (first derivative on normalized spectra), norm_der2 (second derivative on normalized spectra). Second, partial-least square (PLS) regressions have been carried out for each spectra modality to build calibration models. The number of components of each PLS regression was optimized within a 4-fold cross-validation sampling scheme repeated 100 times (Monte-Carlo Cross-Validation, MCCV). Additionally, an automatic selection of wavenumbers was carried out using the competitive adaptive reweighted sampling (CARS) approach (Li et al. 2009a). Model accuracy was evaluated both within the calibration set through the cross-validation procedure and the validation set, using the coefficient of determination (R^2) and the root mean square error (RMSE) of prediction. The best PLS regression model corresponded to the second derivative on normalized spectra pretreatment. It was characterized by R^2 and RMSE of 0.90 and 1.29 mg/g in the calibration set and of 0.87 and 1.54 mg/g in the validation set. This obtained model demonstrates the usefulness of NIRS for evaluating the stilbene content in massif wood.

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