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Non Destructive Prediction of Lake Sediment by Near-infrared Spectroscopy

Tetsuya Inagaki[1], YOSHITSUGU SHINOZUKA[2*], kazuyoshi yamada[3], Akira Hayashida[4], Hitoshi Yonenobu[3], Satoru Tsuchikawa[1], Timo Saarinen[5], Akihiro Yoshida[6], Katsuya Gotanda[7], Yasuharu Hoshino[6], Motonari Ohyama[6], Hirotaka Oda[8], Yoshinori Yasuda[9]

[1]Nagoya university, [2]Hokkaido University, [3]Naruto University of Education, [4]Doshisha University, [5]University of Turku, [6]Tohoku University, [7]Faculty of Policy Informatics, [8]Nagoya university, [9]Research center for Japanese studies

The feasibility of near-infrared (NIR) reflectance spectroscopy with aid of multivariate analysis, which is rapid, inexpensive, non-destructive and correct technology, for the prediction of organic and inorganic fraction in lake sediment is reported.

The core samples were collected in Lake Ogawara (40 49 06 N, 141 19 55 E, 0 m a.s.l.) which is a 25 m deep brackish water lake formed on along the Pacific coast in Aomori Prefecture, northeastern Japan. The lake sediment consisted of well-preserved annually formed lamina. This suggests that the long cores are possibly a high-resolution record of past environmental changes. In December 2009, three parallel cores of ˜20 m in length were drilled nearly at the center of the lake. A continuous composite profile was established from these cores, which were all divided using plastic cubes (2.3 cm on a side). A total of 2,800 cubes were obtained.

Of the 2,800, 145 cubes (at about each 10 cm interval in core length up to 15 m in depth) were used for conventional and destructive geochemical analyses. Total organic carbon (TOC), total nitrogen (TN), total sulfur (TS) and C/N ratio were measured using an element analyzer (1108, Calbo Erba) and other inorganic compounds were measured using an inductively-coupled plasma atomic emission spectroscopy (ICP-AES, SPS 7700, Seiko Instruments Inc.).

NIR spectra were acquired in a diffuse reflectance mode using a FT-NIR spectrometer (MATRIX-F, Bruker) with fiber optics. To improve the signal-to-noise ratio, 64 scans were accumulated at a spectral resolution of 8 cm-1 over the wavenumber range of 10,000-4000 cm-1. Sediment samples used for conventional analysis were dried at the 100 OC for 24 hours before NIR spectral measurement to avoid the influence of strong absorption due to water.

Each sediments property was predicted from NIR spectra using partial least square (PLS) regression analysis. From the relationship between measured values and predicted values by PLS for each parameter and the observation of statistical results calculated, it is known that PLS analysis provided good regression models. The correlation for determinant for cross-validation of water content, TN, TOC, TS, Al2O3, Na2O/Al2O3, S/Al2O3, Fe2O3/Al2O3 and Sc/Al2O3 were 0.68, 0.80, 0.77, 0.58, 0.81, 0.53, 0.68, 0.68 and 0.65, respectively. The root mean square error of cross-validation (RMSECV) for each PLS regression model was adequately small. These calibrations demonstrate the ability of NIR spectroscopy for accurately prediction of multiple sediment parameters without any conventional and destructive geochemical analysis.