NEAR INFRARED TRANSFLECTANCE SPECTROSCOPY (NIRS) IN PHYTOCHEMISTRY

C. W. Huck*, W. Guggenbichler, G.K. Bonn

Institute of Analytical Chemistry and Radiochemistry, Leopold-Franzens University, Innrain 52a, 6020-Innsbruck, Austria

During the last years phytochemistry and phytopharmaceutical applications have developed rapidly and so there exists a high demand for faster and more efficient analysis techniques. Therefore we have established a near infrared transflectance spectroscopy (NIRS) method that allows a qualitative and quantitative determination of new polyphenolic pharmacological active leading compounds within a few seconds. As the NIR spectrometer has to be calibrated the compound of interest has at first to be characterized by using one or other a combination of chromatographic or electrophoretic separation techniques such as thin layer chromatography (TLC), high performance liquid chromatography (HPLC), capillary electrophoresis (CE), gas chromatography (GC) and capillary electrochromatography (CEC)[1,2]. Both structural elucidation and quantitative analysis of the phenolic compound is possible by direct coupling of the mentioned separation methods with a mass spectrometer (GC-MS, LC-MS/MS, CE-MS, CEC-MS) and a NMR spectrometer (LC-NMR). Furthermore the compound has to be isolated (NPLC, MPLC, prep. TLC, prep. HPLC) and its structure elucidated by spectroscopic techniques (UV, IR, HR-MS, NMR) and chemical synthesis[3]. After that HPLC can be used to provide the reference data for the calibration step of the near infrared spectrometer. The NIRS calibration step is time consuming, which is compensated by short analysis times. After validation of the established NIRS method it is possible to determine the polyphenolic compound within seconds which allows to raise the efficiency in quality control and to reduce costs especially in the phytopharmaceutical industry[4].

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