

and benzyl benzoate was used as the internal standard. The separation of the six phthalates and internal standard was optimized, and the optimal analytical conditions were as follows : column, DB-1701 (I.D. 0.25mm); mobile phase, helium; oven temperature 200°C(10 min) → 10°C/min → 260°C(30min), injector temperature 230°C, detector temperature 280°C. The linearity of the method was investigated for the range 10–100µg/mL for the six phthalates and correlation coefficients were between 0.9950 and 0.9992. The limit of detection (LODs) of the six phthalates were between 0.27 and 0.95 µg/mL. Methanol, acetonitrile and hexane was used as extraction solvents. The recoveries of DEP and DEHP were about 96.5–105.7% when analyzed DEP and DEHP in cosmetics using hexane as a solvent. Hexane was proved to be the best solvent to extract phthalates in the lotions. Commercial lotions were analyzed by the above analytical method, and no phthalates was detected in them.

[PD4-29] [10/18/2002 (Fri) 13:30 – 16:30 / Hall C]

Simultaneous determination of seven major human cytochrome P450 activities using LC/MS/MS

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A LC/MS/MS method for the simultaneous determination of the activities of seven major human drug-metabolizing cytochrome P450s (CYP3A4, CYP2D6, CYP2C9, CYP1A2, CYP2C19, CYP2A6, and CYP2C8) was developed. This method used an in vitro cocktail of specific substrates (midazolam, bufuralol, diclofenac, ethoxyresorufin, S-mephenytoin, coumarin, and paclitaxel) and LC/MS/MS. The assay incubation time is 20 min and the analysis time is 8 min/sample. The seven metabolites were quantified by multiple reaction monitoring (MRM) method. Potent specific inhibitors of the seven enzymes (ketoconazole, quinidine, sulfaphenazole, tranilcypromine, quercetin, furafylline, and 8-methoxypsoralen) were evaluated in cocktail and individual substrate incubations. This cocktail method offers an efficient, robust way to determine the cytochrome P450 inhibition profile of large numbers of compounds. The enhanced throughput of this method greatly facilitates its use to assess CYP inhibition as a drug candidate selection criteria. This method was successfully applied to the screening of new drug screening.

[PD4-30] [10/18/2002 (Fri) 13:30 – 16:30 / Hall C]

Studies on the evaluation of efficacy of functional cosmetics(I) –Studies on the in vitro SPF test method of sunscreen products

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The present study was undertaken to develop the in vitro sun protection factor(SPF) test method having good correlation with in vivo method using human, 8% homomentyl salicylate, P3 reference standard and commercially available sunscreen products were measured by the in vitro method using SPF 290S analyzer, and the SPF_s were compared with the SPF_s measured by in vivo test method. In vitro SPF_s of 8% HMS and P3 reference standard were 4.59 ±0.12 and 14.94 ±0.83. There are good correspondence, correlation coefficients were 0.9506 and 0.9769 respectively, between the in vitro and in vivo SPF_s for the sunscreen creams and lotions. Correlation coefficients of makeup base/liquid foundation, lotion labeled with "shake before use" and compact powder were 0.8812, 0.8632 and 0.5984 respectively. The optimum mixture ratio of compact powder and cream base represents 1:0.8. These results suggest that the in vitro SPF test method will be able to be used as an alternative method for in vivo SPF in case of lotion and cream.

[PD4-31] [10/18/2002 (Fri) 13:30 – 16:30 / Hall C]

Comparison of CE and HPLC as analytical methods of (-)-yatein enantiomer from Cupressaceae plants

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Cupressaceae plants are used in traditional folk medicine, whose extracts have been found to possess some bioactivities. (-)-Yatein is a lignan of the dibenzyl-butyrolactone type, that has been isolated from some Cupressaceae plants. It was reported that (-)-yatein, isolated from plants, showed different activities from the synthetic yatein [3]. Hence, the enantioselective determination of yatein from synthetic materials and natural products would be necessary.

A capillary electrophoretic and high performance liquid chromatographic procedure was developed for the enantioselective determination of yatein from Cupressaceae plants. The separation by CE was done by using borate buffer (100 mM, pH 10.5) containing 30v/v% methanol and 20 mM CM-b-CD on a fused silica capillary (75 μ m i.d. x 34.6 cm, 30 cm to detector). (-)-Yatein enantiomers were also separated by HPLC using 81 % methanol on (R,R)-Whelk-O1 column (4.6 x 250 mm). The contents of (-)-yatein in Juniperus, Thuja and Chamaecyparis species, belonged to Cupressaceae plants, were 7.13, 0.24 and 0.11 mg/g, respectively, indicating this method could be applied for the quality control of (-)-yatein.

[PD4-32] [10/18/2002 (Fri) 13:30 - 16:30 / Hall C]

Determination of the water content in Citrus leaves by portable near infrared (NIR) system

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The amount of water for the cultivation of citrus is different based on the growing period. The water content in the leaves of citrus can be a index for watering during cultivation. The purpose of this study is to determine non-destructively the water content of Citrus leaves by using near infrared spectroscopy (NIRS). Citrus leaves were prepared from satsuma mandarin leaves (Citrus unshiu Marc. var. okitsu) ranging from 62.20 to 69.98% of water content by loss on drying, NIR reflectance spectra of Citrus leaves were acquired by using a fiber optic probe. It was found that the variation of absorbance band due to OH vibration of water depending on the water content change around 1450nm in the second derivatives spectra. Partial least squares regression (PLSR) was applied to develop a calibration model over the spectral range 1100-1700nm. The calibration model predicted the water content for validation set with a standard errors of prediction (SEP) of 0.97%. In order to validate the developed calibration model, routine analyses were performed using newly prepared Citrus leaves. The NIR routine analyses showed good results with determination of water content with a SEP 0.81% compared with those of loss on drying. This study showed that the rapid and non-destructive determination of the water content in Citrus leaves was successfully performed by portable NIR system.

[PD4-33] [10/18/2002 (Fri) 13:30 - 16:30 / Hall C]

Classification based on Near-IR spectra with application to Cnidium Rhizome

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A near infrared (NIR) method was developed to analyze specious diversity for morphologically similar umbelliferous herbal medicine, Cnidium officinale Makino. This herbal medicine has been widely used as 'chungung' without any discrimination of its quality and original plants, though it has the ambiguous origins of plants between various countries especially Korea, China and Japan. It is named by Cnidium officinale Makino in Korea and Japan, in comparison with Ligusticum chuanxiong Hort. in China. The rapid and accurate analytical method to classify according to its different genus name mentioned before, NIR spectroscopy with a reflectance fiber optic probe and a photo-diode array type InGaAs detector was also demonstrated. In order to select the best identification method, a pattern recognition technique using soft independent modeling of class analogy (SIMCA) was applied. In overall, NIR spectroscopy using pattern recognition technique is shown to have significant potential as a rapid and accurate method for identification of herbal medicines.

[PD4-34] [10/18/2002 (Fri) 13:30 - 16:30 / Hall C]