**[PD4-4] [ 2003-10-10 14:00 - 17:30 / Grand Ballroom Pre-function ]**

## Metabonomic Studies on The Time-Related Metabolic Effects of α-Naphtylisothiocyanate on Urine in The Rats by Liquid Chromatography-Mass Spectrometry

La Sookie°, Kim Dong-Hyun
*Bioanalysis and Biotransformation Research Center, Korea Institute of Science and Technology*

Metabonomic analysis using Liquid Chromatography-Mass Spectrometry (LC-MS) was employed to test the feasibility to predict chemical-induced toxicity. Time-dependent metabolic variations were evaluated in rats treated with the model hepatotoxin, α- naphthylisothiocyanate (ANIT). Urine samples of ANIT treated group and control group were collected up to 7 days postdose. Urine samples were analyzed by gradient HPLC combined with electrospray mass spectrometry. The chromatographic results were data-reduced and analyzed using principal component analysis to show the time dependent biochemical variations induced by ANIT toxicity. These preliminary results suggest that LC-MS-based approaches may have a useful tool in metabonomic analysis that complements existing approaches.

**[PD4-5] [ 2003-10-10 14:00 - 17:30 / Grand Ballroom Pre-function ]**

## Metabolism of Eupatilin in the Rats Using Liquid Chromatography/Electrospray Mass Spectrometry

Ji Hye Young°, Lee Hye Won, Lee Hong Il, Kim Hae Kyoung, Shim Hyun Joo, Kim Soon Hoe, Kim Won Bae, Lee Hye Suk
*Wonkwang University, Dong-A Pharmaceutical Co. LTD., 47-5, Sanggal-ri, Kiheung-up, Yongin-si, Kyunggi-do, 449-905, Korea*

Eupatilin (5,7-dihydroxy-3",4",6-trimethoxyflavone) is an active ingredient of an ethanol extract of Artemisia asiatica (DA-9601) that is used in the treatment of gastritis. In vitro and in vivo metabolism of eupatilin in the rats has been studied by LC-electrospray mass spectrometry. Rat liver microsomal incubation of eupatilin in the presence of NADPH and UDPGA resulted in the formation of four metabolites (M1-M4). M1, M2, M3 and M4 were tentatively identified as 3"- or 4"-O-demethyl-eupatilin glucuronide, eupatilin glucuronide, 6-O-demethyleupatilin and 3"- or 4"-O-demethyl-eupatilin glucuronide, respectively. Those metabolites from in vitro study were also characterized in bile, plasma or urine samples after an intravenous administration of eupatilin to rats. In rat bile, plasma and urine samples, eupatilin glucuronide (M2) was a major metabolite, whereas M3, M4 and M4 glucuronide (M1) were the minor metabolites.

**[PD4-6] [ 2003-10-10 14:00 - 17:30 / Grand Ballroom Pre-function ]**

## Simultaneous enantioseparation of β-blockers by chiral capillary electrophoresis in reversed polarity mode

Jiyung Kim°, Jung Han Kim, Kyoung Rae Kim*
*School of Life Science and Engineering, Yonsei University and College of pharmacy, Sungkyunkwan University **

The chiral separation of multiple β-blockers is described for their accurate chiral discrimination by chiral capillary electrophoresis (CE). The cyclodextrin-modified CE system was operated in the reversed polarity mode. In this mode, fairly good enantiomeric resolutions were achieved. Relative migration times to internal standard under optimum conditions were characteristic of each enantiomer with good precision. Therefore, in this study, the usefulness for the chiral separation and accurate identification will be discussed.

**[PD4-7] [ 2003-10-10 14:00 - 17:30 / Grand Ballroom Pre-function ]**

## Advanced HPLC Diagnostic Method for Galactosemia Using 8-Amino-2-naphthalenesulfonic acid.

Lee Sang-Soo°, Hong Seon-Pyo, Yoon Hye-Ran
*College of Pharmacy, Kyung Hee University, Department of Oriental Pharmaceutical Science, Kyung Hee University, Seoul Medical Science Institute*

In galactose metabolic pathway : there are three inborn metabolic disorders galactokinase deficiency (galactosemia type Ⅱ), galactose-1-phosphate uridyl transferase(GALT) daficiency (galactosemia type Ⅰ), uridine diphosphate galactose-4-epimerase deficiency (galactosemia typeⅢ). Among these disorders GALT deficiency is the most severe and common. Infants with GALT deficiency fail to metabolize galactose-1-phosphate. As a consequence, galactose-1-phosphate and galactose are accumulated in blood in which GALT enzyme plays the role of a pathognomonic marker.In the previous paper, we reported a reversed-phase HPLC method using 8-Amino-2-naphthalenesulfonic acid as derivatization reagent for the determination of galactosemia. But, this method has the defects such as a relatively longer pretreatment, the reduction of sensitivity.We developed a advanced diagnostic method for galactosemia by shortening pretreatment and increasing the sensitivity.

**[PD4-8] [ 2003-10-10 14:00 - 17:30 / Grand Ballroom Pre-function ]**

## Indirect chiral separation of α-arylmethylpropionic acids by liquid chromatography

Min ChungSik°, Jang SeungJae, Choi BoKyung, Kim YoungLim, Jung HaeYun, Bak KyungMin, Lee KyungHee, Jo KeangIn, Gu YouNi
*KFDA*

A various α-arylmethylpropionic acids(profen) have been widely used as non-steroidal anti-inflammatory drugs for the relief of acute and chronic rheumatoid arthritis and osteoarthritis, as well as for other connective tissue disorders and pains. Example is fenoprofen, ibuprofen, ketoprofen, and naproxen. All are chiral and, except for naproxen and ibuprofen, are marketed in racemic form. Enantioseparations of profens have been of considerable interest because their anti-inflammatory and analgesic effects have been attributed almost exclusively to their (S)-enantiomer. A simple method for determination of optical purity of (+) and (-)-α-arylmethylpropionic acids has been developed. By means of EEDQ, α-arylmethylpropinic acids was coupled to (S)-napthylethylamide. The diasteoisomeric derivatives was then separated by normal-phase liquid chromatography. And separation process of diastreomeric isomer was interpreted by molecular mechanics and quantum mechanics calculation of diasteromeric conformation.

**[PD4-9] [ 2003-10-10 14:00 - 17:30 / Grand Ballroom Pre-function ]**

## Studies on the tyrosinase inhibitory comound of Potentilla bifurca L. var. glabrata Lehm

Piao Xiang Lan°, Lim Geun Sil, Lee Youn Ju, Kim Bak Kwang, Park Man Ki, Park Jeong Hill
*College of Pharmacy, Seol National University, Seoul 151-742, Korea*

Tyrosinase is an important enzyme involved in the transition steps from tyrosine to melanin. Inhibition of the tyrosinase activity could block melanin formation from tyrosine and thus prevent melanin pigmentation on skin. This may contribute to the development of new whitening agent that would be useful in the prevention of pigmentation. in this study, we isolated tyrosinase inhibitory compound from BuOH fraction of Potentilla bifurca L. var. glabrata Lehm by activity guided fractionation method. Based on spectroscopic data, the active compound was identified as a quercetin 4''-O-glucopyranoside.

**[PD4-10] [ 2003-10-10 14:00 - 17:30 / Grand Ballroom Pre-function ]**

## Physical properties and determination of eupatilin, a new antigastritic agent, by high performance liquid chromatography

Jang Ji Myun°, Shim Hyun Joo, Ahn Byung Ok, Kim Soon Hoe, Kim Won Bae
*Dong-A Pharmaceutical Co. LTD., 47-5, Sanggal-ri, Kiheung-up, Yongin-si, Kyunggi-do, 449-905, Korea*