

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

### **Metabonomic Studies on The Time-Related Metabolic Effects of $\alpha$ -Naphthylisothiocyanate on Urine in The Rats by Liquid Chromatography-Mass Spectrometry**

La Sookie<sup>o</sup>, 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,  $\alpha$ -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<sup>o</sup>, 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 $\beta$ -blockers by chiral capillary electrophoresis in reversed polarity mode**

Jiyung Kim<sup>o</sup>, 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  $\beta$ -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.**