average daily intake of PCDDs/DFs via human milk for a baby weighing 5Kg could be calculated. The daily intake of PCDDs/DFs via breast-feeding was estimated to be 39 pg/kg body weight/day for 2,3,7,8-TeCDD and 86 pg/kg/day for TEQ. These levels are far above all virtually safe dose(VSD) or tolerable daily intake(TDI) values proposed by health authorities in various countries, ranging from 0.001 (US EPA) to 4 pg/kag/day (WHO).

[PD4-24] [10/19/2001 (Fri) 09:00 - 12:00 / Hall D]

Impurity profiling analysis of methamphetamine synthesized by three different methods

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Knowledge of impurities in methamphetamine is important that the impurities could have additional harmful effects on the methamphetamine users and the impurities can provide useful intelligence to forensic scientist concerning illicit methamphetamine products.
To investigate the pattern of impurity from illicit methamphetamines by various synthetic methods, methamphetamines were synthesized from ephedrine through three different methods - Nagai, Moscow and Emde. For the impurity profiling analysis, about 30mg of synthetic methamphetamine was dissolved in 1mL of phosphate buffer and extracted with 200 uL of ethylacetate which contains two different internal standards of dioctylsebacate and diphenylamine. The extract was analyzed by GC using Ultra-2 capillary column (0.2mm x 25m x 0.33um). The marker impurity (key product) also was identified of synthetic methamphetamines by GC/MS.

[PD4-25] [10/19/2001 (Fri) 09:00 - 12:00 / Hall D]

Pattern Recognition for Disease Diagnostics with Probabilistic Neural Network

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Early diagnosis of disease status is especially important in the cases of metabolic disorders and high resolution and rapidity in analysis can be achived with solid phase extraction and capillary gas chromatographic systems. In this study, plasma levels of saturated VLCFAs(Very Long Chain Fatty Acids) were determined by previously established analytical method. The saturated VLCFAs are known to be related with X-ALD (x-linked adrenoleuko-dystrophy).
For diagnosis of X-ALD with plasma level of the satuarated VLCFAs, an artificial neural network with radial basis transfer function and competitive transfer function was trained. The trained network, which is called PNN(Probabilistic Neural Network), was used to predict data of valdiation group and all of them were diagnosed correctly.
The architecture of PNN and data processing details will be presented. For comparison, results from dendrogram with K-nearest neighbor and K-means nearest group algorithm will be shown.

Poster Presentations - Field E1. Pharmaceutics

[PE1-1] [10/19/2001 (Fri) 09:00 - 12:00 / Hall D]

Mechanistic studies on peptide conjugate formation from GHRP-6 and PLGA polymer

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We previously reported that peptide conjugates were formed during in vitro release test of growth hormone releasing peptide-6 (GHRP-6, His-DTrp-Ala-Trp-DPhe-Lys-NH2) containing PLGA microspheres. LC/MS/MS analysis had confirmed that glycolic and lactic acids originated from PLGA polymer were conjugated to the free amino group of N-terminal His and epsilon amino group of Lys5 of GHPR-6. In this presentation, we studied the reaction mechanism of the conjugation formation more systemically by incubating GHRP-6 and a hydrophilic 50:50 PLGA polymer (RG502H, Boehringer Ingelheim) in various conditions. Two critical physico-chemical phenomena between GHRP-6 and PLGA polymer were determined as peptide binding to the polymer and glycolic/lactic acids conjugation to the peptide. From various experimental evidences including higher conjugate formation at alkaline pH, aminolysis of PLGA catalyzed by amino group of GHRP-6 is suggested as a plausible reaction mechanism.

[PE1-2] [10/19/2001 (Fri) 09:00 - 12:00 / Hall D]

Prediction method on the effect of transdermal enhancer II: Modeling by Artificial Neural Network-Partial Least Squares Regression

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The final goal of this work is to develope a proper regression model for the prediction of the effect of various enhancers on the transdermal flux. In order to carry out this task, flux data were obtained under homogeneous experimental condition. The effect of enhancers (2 hydrophobic and 2 hydrophilic) on the flux of model compounds (antipyrene, atropine, benzoic acid, chloraminophenamide, nicotinic acid) were studied.
Molecular descriptors of enhancers and model compounds were related with flux data of enhancer-drug combinations. Flux data were preprocessed in several different ways prior to regression analysis. Several regression models such as multiple linear regression(MLR), principal component regression (PCR), partial least squres regression(PLSR), continuum regression(CR), artificial neural network with non-linear transfer functions, and ANN-PLSR were tested and compared. The best prediction so far was obtained with ANN-PLSR(Artificial Neural Network-Partial Least Squares Regression).

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[PE1-3] [10/19/2001 (Fri) 09:00 - 12:00 / Hall D]

Solubilization of an anesthetic drug in nonionic surfactant systems

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