

## Abstracts

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The Properties and Application of a Novel Amphiphilic Polymer as an Active Interfacial Modifier

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A peptide/silicone hybrid functional polymer composed of silk peptide and silicone resin with a hydrophobic alkyl group was investigated for its compatibility and functionality as a cosmetic ingredient. We have found this polymer provides characteristic functions to modify and control various interfacial properties and named it Active Interfacial Modifier (AIM-FN). At the liquid/liquid interface, AIM-FN worked as an excellent W/O emulsifier for various oils, polar or non-polar, and even for silicone oil. In principle AIM-FN stays at the interface between the aqueous phase and lipid phase because it isn't compatible with either phase. At liquid/solid interfaces, the peptide moiety of AIM-FN attaches to the hydrophilic solid surface and makes it water repellent and water proof with its hydrophobic silicone and alkyl residue. An emulsion formulated with AIM-FN gives a non-oily and non-tacky skin feeling as AIM-FN improves the solid/solid (skin/skin) surface property.

Development of an In Silico Prediction System for the Risk Assessment of Chemicals —Development of a Prediction Model for Skin Irritation—

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In order to develop a prediction system for the safety of chemicals, many attempts have been made by examining quantitative structure-activity relationships (QSAR). The results, however, were not always satisfactory enough in view of predictability when it is assumed that they are used in actual situations. In the present study, therefore, we have attempted to develop an in silico prediction system enabling the risk assessment of cosmetic raw materials by combining a molecular orbital calculation method and an artificial neural network system. Human patch test data on 161 samples were collected from a past publication and experiment results in our laboratory. Molecular weight, polarizability $\alpha$ , polarizability $\gamma$ , dipole moment, and ionization potential were obtained from molecular orbital calculations as descriptors to predict the skin irritation. In addition, concentration and exposure time were added as descriptors. A neural network system was employed for the analysis. Consequently, by using leave-one-out cross-validation methods, it was shown that the neural network model can predict the positive rate in a human patch test with reasonable accuracy (root mean square error was

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0.352). The above results suggest that their combinational use will enable us not only to predict the toxicological potential of cosmetic raw materials but also to make the risk assessment possible.

#### Development of an Amino Acid-Responsive Fine Liposome

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In this study, we attempted to develop a liposome which showed a responsiveness to membrane-fluidity to amino acids as a NMF component in the human skin. Amino acids have an amphoteric charge in solution. Therefore, we considered that the liposomes were given a one-sided electrical charge and controlled on the surface charge, so that their membrane-properties were varied by electrostatic forces of attraction or repulsion with the electric charges of amino acids. First, we investigated the constituent of the liposome with responsiveness to outer conditions. It was found that the liposomes containing the Dipalmitoyl phosphatidic acid (PA) showed the most effective responsiveness to 5, (6) -Carboxyfluorescein (CF) leakage. Further, it was indicated that the surface charge and the microfluidity in the vicinity of the polar group affected the CF leakage. Next, we investigated the membrane-fluidity in the presence of amino acids, expecting that the membrane-fluidity was controlled by neutralization or the increase of the surface charge with the electrical charges of amino acids. As a result, the promotion of the leak was seen in the presence of an acidic amino acid (Asp) having a negative charge. On the other hand, the depression of the leak was seen in the presence of a neutral amino acid (Gly) or a basic amino acid (Lys) having a neutral or a positive charge, respectively. Lys was the most effective on the depression of the leak. Moreover, we found that the microfluidity in the vicinity of the polar group affected the depression of CF leakage. It was assumed that the depression of leakage was due to the neutralization of the surface charge and the decrease of the microfluidity in the presence of the neutral amino acid or the basic amino acid. In conclusion, we confirmed that the liposome which showed responsiveness to amino acids was prepared by mixing PA into PC liposome.

#### The Effects of Licorice Leaf Extract on Ceramide and Hyaluronan Synthesis

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Both water-holding and permeability barrier function in the stratum corneum (SC) are essential for keeping skin moisture. Intercellular lipids in SC, which are composed mainly of cholesterol, fatty acids, and ceramides, play a crucial role for maintaining the function in SC. The object of our study is to find active ingredients from plant extracts for enhancing the abilities of skin hydration and barrier repair by focusing on the synthesis of ceramides. As a result, we found that licorice leaf extract is a promising ingredient showing not only an increase of mRNA expression levels of serine palmitoyltransferase (SPT) and sphingomyelinase related to ceramide biosynthesis in keratinocytes but also syntheses of ceramides in a 3D skin model and in human skin. Furthermore, licorice leaf extract showed an increase of mRNA expression levels of HMG-CoA reductase (HMGR) related to cholesterol biosynthesis and an increase of hyaluronan (HA) production in in vitro tests. One of the principles isolated from licorice leaf extract, 6-prenyl-naringenin, was thought to be one of the active components. These results suggested that licorice leaf extract may be a useful ingredient for skin care due to the synthesis of intercellular lipids and HA.

#### The Effects of Coptis japonica Root Extract and Its Key Component, Berberine, on Human Subcutaneous Adipocytes

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An increase of subcutaneous fat presses lymph vessels and blood vessels in skin tissues, and results in not only causing skin troubles such as skin sagging and swelling but also forming cellulite that makes bodylines worse. To expand

further application of plant extracts to cosmetics, we focused on inhibitory effects of subcutaneous preadipocyte differentiation and facilitating lipolysis in adipocytes. In this study, in a screening test of a number of plant extracts, *Coptis japonica* root extract and its key component, berberine, showed potent inhibition of triglyceride accumulation and subcutaneous preadipocyte differentiation. Furthermore, *Coptis japonica* root extract

and berberine down-regulated the mRNA expression level of several differentiation factors derived from subcutaneous preadipocytes. *Coptis japonica* root extract and berberine in subcutaneous adipocytes facilitated lipolysis in mature adipocytes. Our study suggested that *Coptis japonica* root extract and its key component, berberine, is expected to be useful for slimming and related skin troubles such as skin sagging, swelling, cellulite, and so on.

