[*Natural Medicines*, **52**, 529-532 (1998)] [Lab. Of Herbal Garden]

Cultivation of *Geranium thunbegii* in Vietnam (1) Morphological Characteristics and Geraniin Contents.

Masashi YOSHIDA, Jitsuo TANAKA, Eiji SAKAI, Yukio NORO, TOMOKO Kawamura, Ngyuen Van THUAN and Toshihiro TANAKA*

The morphological characteristics and geraniin contents of cultivated *Geranium thunbergii* in Vietnam were compared with those grown in Japan. The characteristics of the leaves of Vietnamese such as the blade size, the petiole lemgth, the number of stomata, the palisade ratio, the long glandular hair and the gerniin contents agred with the characteristics of Japanese *G, thunbergii*.

[*Cancer Res.*, **58**, 3806-3811(1998)] [Lab. of Radiochemistry]

High Susceptibility of *p53*(+/-) Knockout Mice in *N*-Butyl-*N*-(4-hydroxybutyl)nitrosamine Urinary Bladder Carcinogenesis and Lack of Frequent Mutation in Residual Allele.

Keisuke OZAKI, Tokuo SUKATA, Shinji YAMAMOTO, Satoshi UWAGAWA, Takaki SEKI, Hajime KAWASAKI, Akira YOSHITAKE, Hideki WANIBUCHI, Akihiro KOIDE, Yukio MORI* and Shoji FUKUSHIMA

Both heterozygote *p53*(+/-) knockout mice and C57BL/6 original parent strain were administered ~0.025% *N*-butyl-*N*-(4-hydroxybutyl)nitrosamine (BBN) in the drinking water for 20 weeks. As compared with the parent strain, greater lesion yields were observed in the knockout mice, and transitional cell carcinomas and preneoplastic lesions were also observed more frequently in the knockout mice. There was no significant difference in the mutation rates at the residual *p53* gene and in the urinary concentration of *N*-butyl-*N*-(3-carboxypropyl)nitrosamine (BCPN), a proximate carcinogenic metabolite, between the knockout and original strains. 5-Bromo-2'-deoxyuridine labeling indices were significantly higher in knockout mice than wild-type mice. In conclusion, knockout mice are distinctly more sensitive to urinary bladder carcinogenesis induced by BBN than the parent strain. It appeared to be related to the high level of cell proliferation rather than that of the mutations at the *p53* gene or that of BCPN in the urine.

[*J. Mol. Struct.*, **449**, 69-75 (1998)] [Lab. of Instrumental Center]

Molecular Structure of Methyl Phenylpyruvates Studied by ^{1}H NMR and IR Spectroscopies and Quantum Mechanical Calculations.

Ho-Hi LEE, Takatomo TAKAI, Hitoshi SENDA, Akio KUWAE and Kazuhiko HANAI*

Molecular structure of methyl phenylpyruvate (MPP) and its *p*-substituted derivatives has been investigated by ^{1}H NMR and IR spectroscopies. The spectral data indicate that MPPs take the enol form both in solution and in the solid state. The ab initio calculations were carried out to get information on the configurational and conformational preferences in the enol form. It is suggested from the calculation that the inter- and intra-molecular hydrogen bondings between the enol OH and the ester C=O are important for stabilization of the conformer.

[*Spectrosc. Lett.*, **31**, 379-395 (1998)] [Lab. of Instrumental Center]

Keto-Enol Tautomerism of Mono-substituted Phenylpyruvic Acids as Studied by NMR and PM3 Calculation.

Takatomo TAKAI, Hitoshi SENDA, Ho-Hi LEE, Akio KUWAE and Kazuhiko HANAI*

Keto-enol tautomerism of mono-substituted phenylpyruvic acids has been studied by the ^{1}H and ^{13}C NMR spectra. The equilibrium constants and the kinetic parameters for the tautomerism were obtained from the spectral data. The equilibrium constants are strongly dependent on the position of the substitution; the values for the *o*-substituted PPAs are several times larger than those of the *m*- or *p*-substituted derivatives. The PM3 calculations have been carried out to obtain the information on the preferred conformations of the tautomers and on the mechanism for the tautomerism. The results suggest the involvement of a solvent molecule in the equilibrium process.