[*Mutagenesis*, **16**, 479-486 (2001)] [Lab. of Radiochemistry]

N-Benzylimidazole for preparation of S9 fraction with multi-induction of metabolizing enzymes in short-term genotoxicity assays.

Yukio Mori,* Akihiro Koide, Kohji Fuwa and Yoshinori Kobayashi

To evaluate the usefulness of *N*-benzylimidazole (BI) as an inducer with wide spectrum detection of precarcinogens in short-term bioassays, rats were orally treated with BI and BI plus ethanol or acetone. BI markedly induced cytochrome P450 (CYP) 1A1, 2B1 and constitutive CYP1A2, 2B2, 2E1 and 3A2 in rats. BI plus ethanol or acetone specifically induced CYP2E1 and 2B1 levels when compared with BI alone. The combined treatments also elevated mutagenic activities of eight heterocyclic amines, aflatoxin B_1, benzo[*a*]pyrene and 2-aminofluorene in strain TA98 and those of five *N*-nitrosamines in strain TA100. In addition, BI induced UDP-glucuronyltransferase activities towards 4-nitrophenol and testosterone. These results demonstrate that BI has a bifunctional action, with wide spectrum induction of phase I and II enzymes, and combined treatment with ethanol or acetone would be a pertinent inducer for metabolic enzymes in *in vitro* bioassays, the potential being comparable with or superior to other typical ones.

[*Spectrochim. Acta, Part A*, **57**, 265-271 (2001)] [Lab. of Instrumental Center]

Molecular Structure and Vibrational Spectra of Phenolphthalein and its Dianion.

Ko-Ki KUNIMOTO, Hiromasa SUGIURA, Toshiyuki KATO, Hitoshi SENDA,
Akio KUWAE and Kazuhiko HANAI*

Infrared and Raman spectra of phenolphthalein (PP) and its dianion form (sodium and potassium salts) were studied both in the solid state and in aqueous solution. Band assignments were carried out on the basis of the isotope shifts of the ring deuterated and ^{13}C-substituted derivatives. Spectral analyses reveal that the PP dianion exists as mixtures of the benzenoid form (colorless) and the quinoid form (colored) in the solid state and in aqueous solution, while the neutral PP solely takes the γ-lactone form. This work provideds the first vibrational spectroscopic evidence for the coexistence of the two species in the PP dianions.

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A Comparative Vibrational and NMR Study of *cis*-Cinnamic Acid Polymorphs and *trans*-Cinnamic Acid.

Kazuhiko HANAI,* Akio KUWAE, Takatomo TAKAI, Hitoshi SENDA and Ko-Ki KUNIMOTO

The IR and Raman spectra of the two polymorphic forms (58°- and 68°-forms) of *cis*-cinnamic acid were measured, and the spectral differences were discussed on the basis of the crystal structures of the two forms. The IR bands related to the COOH group differ in the frequencies and band shape, reflecting differences in the hydrogen bonding between the two modifications. These spectra were compared with those of *trans*-cinnamic acid. The IR, Raman, and NMR spectra of the isotopic compounds, including the deuterated and ^{13}C analogs of the cis and trans acids, were also recorded in the solid state and in solution to confirm the spectral assignments.

[*Atherosclerosis*, **159**, 307-312 (2001)] [Lab. of Clinical Pharmaceutics]

Heparin-stimulated expression of extracellular-superoxide dismutase in human fibroblasts.

Tetsuo ADACHI,* Hirokazu HARA, Harutaka YAMADA, Naoya YAMAZAKI, Masayuki YAMAMOTO,
Tadashi SUGIYAMA, Arao FUTENMA and Yoshihiro KATAGIRI

Extracellular-superoxide dismutase (EC-SOD) is the major SOD isozyme in the arterial wall and may be important for antioxidation capability of the vascular wall and normal vascular function. EC-SOD is expressed in various cell types in the vascular wall, and the synthesis of EC-SOD by human fibroblasts is known to be highly responsive to various inflammatory cytokines. Heparin is a highly sulfated glycosaminoglycan with many functions such as antithrombotic, antilipemic and antiatherosclerotic effects. Heparin induced EC-SOD expression at both the mRNA and protein levels. The stimulatory effect seemed to increase roughly with the degree of glysosaminoglycan sulfation. The enhanced expression of EC-SOD by heparin must contribute to the antiatherosclerotic effect of heparin.