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[Lab. of Manufacturing Pharmacy]

Reactivities of 1-Alkylthiabenzenes.

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The chemical reactivities of 1-alkylthiabenzenes were investigated. The electrophilic addition of dimethyl acetylenedicarboxylate (DMAD) to 1-alkylthiabenzenes afforded three types of 1:1-adducts, eight-membered ylidic compounds, norcaradiene compounds, and seven-membered compounds. Product distribution was affected with the solvents used. The mechanism for the formation of these products was discussed. The anion of 1-methylthiabenzene generated from treatment with LDA reacted with ketonic electrophiles to yield new thiabenzene derivatives having hydroxyalkyl substituents on the sulfur atom. On the other hand, treatment of the anion with carboxylic esters afforded no thiabenzenes bearing an acylated methyl group on the sulfur atom, but three kinds of acylmethyl group-migrated products.

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[Lab. of Manufacturing Pharmacy]

Two New Isoflavonoids from *Erythrina variegata*.

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Two new isoflavonoids, eryvarin A and eryvarin B were isolated from the wood of *Erythrina variegata* and their structures were elucidated on the basis of spectroscopic evidence.

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[Lab. of Radiochemistry]

Differences among Three Sister Strains of NON/Shi Mice in Sensitivity to Urinary Tract Carcinogenesis by *N*-Butyl-*N*-(4-hydroxybutyl)nitrosamine.

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We examined the susceptibility of three sister inbred strains of mice, NON/Shi, CTS/Shi, and NOD/Shi to *N*-butyl-*N*-(4-hydroxybutyl)nitrosamine (BBN) in an attempt to optimize our model for tumor induction and spontaneous metastasis. The incidences of renal pelvic and urinary bladder carcinomas in NON/Shi, CTS/Shi, and NOD/Shi were 52% and 44%, 16% and 63%, and 0% and 4%, respectively. Metastasis to lungs was only observed in renal pelvic carcinoma-bearing NON/Shi mice. Invasion of the prostate and/or intraperitoneal dissemination were observed in urinary bladder carcinoma-bearing NON/Shi and CTS/Shi mice. BBN intake was highest in NON/Shi mice but urinary concentrations of the carcinogen and *N*-butyl-*N*-(3-carboxypropyl)nitrosamine did not differ among the three strains. These results indicate that NON/Shi is the most sensitive of the three strains to carcinogenic effects of BBN on the urinary tract, particularly renal pelvis, and therefore the most suitable for our spontaneous metastasis model.

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[Lab. of Instrumental Center]

Polymorphism of 4-Fluorophenylpyruvic Acid Studied by X-Ray Crystallography and Vibrational Spectroscopy.

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Two polymorphic forms (I, mp 163.2 °C and II, mp 171.0 °C) of 4-fluorophenylpyruvic acid were obtained by crystallization from different solvents. Crystal structures of polymorphs I and II were determined by X-ray crystallography. These polymorphs show similar molecular and crystal structures to each other, except for the molecular geometries of the enol and carboxylic acid moieties. IR and Raman spectra of the two polymorphs were measured, and the spectral characteristics were compared with those of phenylpyruvic acid. Distinct IR spectral differences which result from the crystal field splitting were observed between the two forms.