

NMR, ¹³C-NMR, HPLC and LC/MS/MS. The treatment of GSH and S-9 fraction with 1- or 2-bromopropane at a physiological condition (pH 7.4, 37 °C) for 1hr produced GSH metabolites, which were identified by UV, HPLC and ESI LC/MS/MS analyses. In addition, time-response and dose-response effects of formation of GSH metabolites were investigated. The present results suggest that 1- and 2-bromopropane might form GSH metabolites at in vivo condition. Detection of GSH metabolites formed by 1- and 2-bromopropane at in vivo experimental models is on progress.

[PD1-11] [2003-10-10 14:00 - 17:30 / Grand Ballroom Pre-function]

Practical Synthesis of α -Galactosyl Ceramide, KRN 7000.

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Galactosyl ceramides play important roles in biological system as immunomodulator and essential constituents of membranes and cell walls. An efficient synthesis of α -galactosyl ceramide, KRN 7000, derived from marine sponge *Agelas mauritanus* as accomplished via a short reaction involving the coupling ceramide moiety and trichloroacetimidate as glycosylation donor. We could synthesize α -galactosyl ceramide stereoselectivity without β -anomer formation on a multigram scale.

[PD1-12] [2003-10-10 14:00 - 17:30 / Grand Ballroom Pre-function]

Design of Novel Ras Farnesyltransferase Inhibitors Based on Virtual Screening and Docking Studies

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Inhibition of the protein-modifying enzyme farnesyltransferase is considered as a major emerging strategy in cancer therapy because of the involvement of farnesylated proteins in oncogenesis. We studied the structure-activity relationship of a novel class of CAAX-peptidomimetic farnesyltransferase inhibitors based on the benzophenone scaffold. FlexX docking of inhibitors confirmed reasonable fit of the molecule into the peptide binding site of farnesyltransferase. We also performed a virtual screening with LeadQuest chemical library databases to identify novel inhibitors of farnesyltransferase. Finally, detail docking studies were performed using these compounds which showed high scoring from the virtual screening experiment.

[PD1-13] [2003-10-10 14:00 - 17:30 / Grand Ballroom Pre-function]

Synthesis of 2-phenyl-1,8-naphthyridin-4-ones

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2-Phenyl-1,8-naphthyridin-4-ones had been synthesized for their cytotoxic activity. Substituted acetophenone was treated with NaH and diethyl carbonate to give ethyl benzoylacetates, which was reacted with substituted 2-aminopyridine and PPA to yield 2-phenylpyridopyrimidine-4-ones. These compounds was heated at 350 °C in liquid paraffin to afford final compounds, 2-phenyl-1,8-naphthyridin-4-ones.

[PD1-14] [2003-10-10 14:00 - 17:30 / Grand Ballroom Pre-function]

Wogonin and Its Analogs

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