compare biological activities with the normal ribonucleoside. An amino group serves as a bioisostere of a hydroxyl group and 2'-hydroxyl substituted 3'-aminonucleosides apparently have a higher population of N-type nucleoside conformations. Here, we report the synthesis of the azido- and amino-substituted tiazofurin derivatives, starting from 1,2;5,6-di-O-isopropylidene-D-glucose.

[PD1-43] [2003-10-10 14:00 - 17:30 / Grand Ballroom Pre-function]

Cytotoxic activity of 1-phenyl-2-alkylsulfonylamido propanol derivatives

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The 20 alkylsulfonylamido propanol derivatives had been investigated for their cytotoxic activity against HT-29 colon cancer, Caki-2 renal cancer, A549 lung cancer, PC-3 prostate cancer, HL-60 leukemia cell using MTT assay. Cytotoxic activity was strongly influenced by the substituted alkyl chain length and the optimal alkyl chain length for cytotoxicity was C11. Some of alkylsulfonylamido propanol derivatives showed stronger activity than reference compound, B13.

[PD1-44] [2003-10-10 14:00 - 17:30 / Grand Ballroom Pre-function]

The docking and searching approach to hit COX-2 inhibitors

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The typical approach of virtual screening is to prepare a 3D database and dock each member to the receptor, and carry out a post-analysis to make a final selection of compounds to be tested. The biological test of these compounds leads to 'hit'. The size of the 3D database is rate-determining factor because the docking process is still time-consuming method. The number of compounds for biological testing is cost-determining factor because the materials used in the test are cost-consuming. The use of the representative subsets derived from the entire database help reduce runtime of docking procedure. The representative subset was made by the method of chemistry space selection. The flexible docking was applied to 3D subset database for the screening of COX-2 inhibitor. The compounds derived from this docking study were sent for the COX-2 inhibition test. Three compounds were hit. Several substructure queries from three compounds were searched into the entire database. The compounds derived from substructure searching were sent for the COX-2 inhibition test. We obtained more hits. Such strategies, that use the docking to subset and the substructure-searching, possibly reduce the runtime of the docking and the number of total compounds sent for biological test.

[PD1-45] [2003-10-10 14:00 - 17:30 / Grand Ballroom Pre-function]

Antifungal activities of juglone and naphthazarine derivatives

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Juglone and naphthazarine derivatives were newly systhesized for the evaluation of antifungal activities. These derivatives were prepared by methylation of juglone and 2,3-dichloro-5,8-dihydroxy-1,4-naphthoquinone, and by regioselective nucleophilic subsitution with arylthiols. All compounds were tested in vitro for their growth inhibitory activities against pathogenic fungi by the standard method. The MIC values were determined by comparison to flucytosine as a standard agent. In general, most juglone derivatives shows in vitro antifungal activities. Among them, 2-arylthio-5-methoxy-juglones showed the most potent antifungal activities against all pathogenic fungi.