[PC1-5] [10/19/2001 (Fri) 09:00 - 12:00 / Hall D]

Antitumor activity of carboxyethylgermanium sesquioxide on cancer cell lines in vitro

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The purpose of this study was to investigate the antitumor effect of Ge-132, on organo germanium with several cancer cell lines (SK-Mel-2,B16-F10,SK-N-MC,Hep-G2 and Human normal skin fibroblast CCD-986sk) in vitro. It was examined by MTT assay. Also, combination of Ge-132 with antioxidants were studied by MTT assay. As a result, Ge-132 produced a dose-related (0.85mg/ml, 0.41mg/ml, 0.2mg/ml, 0.1mg/ml) reduction of viability on each cancer cell lines.Ge-132,significantly inhibited proliferation under the conc.of 0.85mg/ml but it was not toxic on human normal fibroblast cell, In addition, we were used an antioxidant as Vit.E ,Vit C, Glutathione, L-Cysteine. L-Cysteine with Ge-132 complex was significantly inhibited cell viability.

[PC1-6] [10/19/2001 (Fri) 09:00 - 12:00 / Hall D]

Docking of thiosemicarbazone derivatives into dihydrofolate reductase using FlexiDock

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Dihydrofolate reductase(DHFR) is a successful drug target for anticancer and antibacterial treatments bacause of its important role in the synthesis of DNA. N4-(2-Acetoxyethoxymethyl)-2-acetylpyridine thiosemicarbazone(AATSC) has been reported to have inhibitory activity against bovine DHFR. In this experiment, three thiosemicarbazone derivatives including AATSC were docked into DHFR of three different species using FlexiDock. Human, Escherichia coli, Candida albicans DHFR were used as target proteins. The ligands were docked into DHFR alone, DHFR-NADPH binary complex, and DHFR-inhibitor binary complex to find out the exact location where the ligands bind to the enzyme. As the results, all three derivatives were docked sucessfully into DHFRs with different binding spaces implying that the ligands can either bind to the coenzyme site or substrate site. The results also show that each ligand has different binding modes to the enzymes of the same species and the same ligand demonstrates specific binding modes to the enzymes of different species.

[PC1-7] [10/19/2001 (Fri) 09:00 - 12:00 / Hall D]

Docking of 1,1-dioxo-6-(substituted) methylene penicillanic acid into Enterobacter cloacae β-lactamase with QXP.

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Bacterial β-lactamases provide resistance to β-lactams by hydrolyzing the β-lactam bond. Many β-lactamase inhibitors have been clinically used usually in combination with β-lactams. Developing therapeutically effective β-lactamase inhibitors has been an importance to the antibiotic therapy. Recently, a series of 1,1-dioxo-6-(substituted) methylene penicillanic acid have been synthesized as