P-3: Blind Docking of Several Xanthone Compounds from Garcinia mangostana Linn. to HIV-1 Protease Reveals Two-Binding Mode (Poster Presentations) - The 3rd Gruber-Soedigdo Lecture 2010 : Molecular Biotechnology in Medicine & Bioindustry, 27-30 July 2010)

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ABSTRACT

Human Immunodeficiency Virus type 1 (HIV-1) is a retroviral virus that causes deadly disease, AIDS (Acquired Immunodeficiency Syndrome). The virus that mutates so fast, causes no drugs available to cure this disease totally yet. One of enzyme targets that can be inhibited to block the replication of this virus is HIV-1 protease. Inhibition to this enzyme causes the blocking of protein cleavage in virus maturation process. Several xanthone compounds from Garcinio mongostono Linn., a-, 􀀪-. dan y-mangostin, have shown inhibition activity to this enzyme. The structure, which is non-peptide based, gives possibility to different mechanism than other inhibitors. This research's aim is to search the binding modes of mangostin analogues. The method used in this research is in silica molecular docking. The result shows that there are two binding modes with higher affinity in the hydrophobic pocket active site (llG AutoDock 4 = (-9,64)-(-9.89) kcal/mo!; llG AutoDock Vina= (-8,7)-(-9,4) kcal/mo!) and molecular surface site which still shows good affinity (llG AutoDock 4 = (-5,85)·(-6,06) kcal/mol; llG AutoDock Vina = (-5,3)·(·5,9) kcal/mol).