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Molecular docking of andrographolide to rennin, HIV-Protease and Tyrosine kinase enzymes

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AutoDock 3.0 was used to dock andrographolide, a diterpenoid from the herb Andrographis Paniculata Nees, to the active site of Renin, HIV -1 Protease, and Tyrosine kinase enzymes. The andrographolide structure was prepared using Insight's II Builder module. The partial charge for the atoms of the ligand and the enzymes were assigned using Discover module of Insight II. Autogrid were used to create affinity grid maps centered to the active site of each enzyme. The andrographolide was docked into the active site of each enzyme using AutoDock's Lamarckian Genetic algorithm to search for low energy binding orientations. Estimated free energy of binding of the docked andrographolide in the Renin active site was 8.16 kcal/mol. For the HIV-1 Protease enzyme, the free energy of binding were -11.07 kcal/mol. While the free energy of binding for the interaction of andrographolide with the tyrosine kinase enzyme was -5.64 kcal/mol. This shows that andrographolide might be able to inhibit the formation of angiotensin I from angiotensinogen which is catalyzed by Renin. The result for HIV -1 Protease enzyme showed that andrographolide might be able to block the enzyme's action in the cleavage of the HIV's long 'poly-protein' in the assembly of matured viruses. The results for tyrosine kinase enzyme showed that andrographolide might be able to function as a tyrosine kinase inhibitor. Tyrosine kinase is an important enzyme which is related to many diseases among others are diabetes.