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Docking of protein tyrosine with flavonoids

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Flavonoids are a group of polyphenols widely occurring in colorful pigment for fruits, vegetables and herbs (Lee, *et. al.* 2000). Quercetin is one of the major components of flavonoids. It has been identified as a Protein Tyrosine Kinase (PTK) inhibitor (Filipeanu, *et. al.* 1995). Besides that, it is also a strong antioxidant due to its ability to scavenge oxygen free radicals (Movileanu, *et. al.* 2000). In this study, we investigate the binding mode of quercetin with a PTK receptor (PDB code 2HCK) by using Autodock3.0. Besides that, 14 others different flavonoids such as eupatorin, luteolin, genistein, myricetin, rhamnetin, apigenin, kaempherol, naringenin, tricin, hesperetin, daidzein, isohamnetin, sinensetin and morin also being studied. Grid parameters files and docking parameters files have been created to run autogrid and autodock. For experiment when quercetin docked with PTK receptor, clustering histogram of docking showed that 32 conformers were in the cluster that has lowest docked energy -5.97 kcal/mol. It was noted that hydrogen bonds formed by PHE340 and MET341 of 2HCK to quercetin. Furthermore, we also found that the aromatic ring bond between PHE340 and quercetin also help to stabilize the binding conformations.