

and thus may potentially be beneficial in the treatment of gastric lesions. However a dose response study is required to illustrate if these beneficial effects will help in the healing of gastric lesions.

Poster Presentation PG16

Docking of Different Enzymes with Quercetin

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Flavonoids are a group of polyphenols that widely exists as colourful pigment for fruits, vegetables and herbs. Quercetin is one of the major components of flavonoids. The objective of this study was to investigate the anticancer properties of flavonoids. In this study, we investigated the binding mode of quercetin with a PTK receptor (PDB code 2HCK) by using Autodock3.0. Ligand quercetin was prepared using InsightII (program distributed by Molecular Simulations, Inc.). Besides that, 14 other enzymes (1CX2, 1QOR, 1D7K, 1EH6, 1UTG, 1ABK, 1GP5, 1GP6, 1GP6, 1E90, 2RNR, 1POA, 1HYT, 1A28 and 2TSR) were also studied. Grid parameters files and docking parameters files were created to run autogrid and autodock. For the experiment when quercetin was docked with the PTK receptor, the RMSD of the structure resulted from Autodock procedure was 0.143 Å different from the X-ray structure. The top clusters (those with the most favorable ΔG_{bind}) appeared to have high frequency of occurrence. To conclude, protein 2HCK, 1CX2, 1QOR, 1EH6, 1GP5, 1GP6, 1A28 and 2TSR showed strong interaction. Moderate interaction occurred between quercetin with protein 1D7K, 1UTG, 1ABK, 2RN2, 1POA and 1HTY. There was only weak interaction between 1E90 with quercetin.