

Undergraduate Research and Mentoring in New Biology

**Berry and citrus phenolic compounds can bind to hepatocyte nuclear factor-1 alpha**

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The research conducted includes computational docking of phenolic compounds into domains of hepatocyte nuclear factor 1-alpha (HNF-1 $\alpha$ ) to see the interactions that these compounds have with HNF-1 $\alpha$ . Western Blotting is also being done to detect the validity of the resulting computational models. HNF-1 $\alpha$  is a non-researched target with possible benefits in the management of Type-2-diabetes as it increases the transcription of dipeptidyl peptidase IV (DDP IV). High levels of DDP IV are associated with low levels of GLP-1 and GIP, which in turn, are associated with unregulated hyperglycemic states. The first of part of the study will include training on the use of computer docking software. This training will include learning the processes of how to run multiple docking simulations for different phenolic compounds. A simple step process of the docking simulations includes finding or drawing the chemical structure of the phenolic compounds as a three-dimensional model, obtaining a workable DPP IV crystal structure free of unnecessary ligands such as metal ions, and finally running the simulation. Studies will build on research that went into the study of berry and citrus phenolic compounds, but using HNF-1 $\alpha$  instead of DDP IV. Once the docking experiments are done, Western Blotting analysis will be done to see if the computational models have some validity.

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