1159-92-203 **Nayoung Ko**, CRG NJ, Cresskill, NJ , and **Richard Kyung*** (nycrick@gmail.com), CRG NJ, Cresskill, NJ. *Study on thermodynamic stability and geometrical optimization of phytoncide molecules.*

Based on variational method for density functional theory, the correlation between flavanon molecules and the effectiveness in antioxidant activity was studied in this research. For the flavanon or phytoncide molecules to have better effect, molecules with higher thermodynamic stability, better geometrical optimization and higher activity are needed for their anti-inflammatory effects and effective activity in radical scavenging. In this project, the geometrical and molecular properties of different molecules in phytoncides were studied. Electrostatic potential maps were also used to interpret the activity of the molecules. A molecular software was used to measure the optimization energy and the dipole moment of each molecule tested in this experiment. Molecules with lower optimization energies were predicted to be more thermodynamically stable than those with higher optimization energies. Molecules with higher dipole moment were predicted to be more active than those with lower dipole moment. The purpose of this research was to determine the safety of the components used in the phytoncides for their antioxidant activity by checking whether there was any noticeable difference in molecular energies and activities of the different molecules or structural isomers. (Received August 04, 2020)