

Abstract Submitted
for the FWS19 Meeting of
The American Physical Society

Study on the Flavanon for Their Effectiveness in the Treatment of Periodontitis Using Bio-chemical and Computational Analysis NAYOUNG KO, The Masters School in Dobbs Ferry, RICHARD KYUNG, Choice Research Group — There is a strong association between flavanon molecules and the effectiveness in dental disease treatment. The molecules are widely used in clinical applications in dentistry for their anti-inflammatory effects and effective activity in radical scavenging. The primary purpose of this research is to analyze the thermodynamical and stereochemical safety of several types of nano-scaled flavanon molecules and to find thermo-chemical properties of their derivatives that could be used as biological agents in the periodontitis treatment. The reactivity and conductivity were also measured through the dipole moments to calculate the activity level the molecule could have with other nearby molecules. Lastly, electrostatic potential maps were utilized to visualize the polarization and assess the reactivity level of each molecule. As an antioxidant and having a disease inhibitory effect, the Flavanois and a few other derivatives showed good activity and stability. A molecular editing program was used to model, optimize, and compare the resulting molecular optimization energies and other characteristics of the molecules.

Richard Kyung
Choice Research Group

Date submitted: 05 Oct 2019

Electronic form version 1.4