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Physical Analysis of the Biomolecules Causing Periodontitis JEHUN SHIN, SEONG HYEON LEE, CHAI RIN KIM, Choice Research Group — Periodontitis caused by microorganisms that adhere to and grow on the tooth's surfaces, is an inflammatory diseases causing gum infection. The disease damages the soft tissues that surround and support the teeth and destroys the bone that supports teeth and finally causes tooth loss. An increased risk of stroke and heart attack problems are related to the periodontitis as well. Most bacteria or pathogens attach to gum surface where they form a biofilm. Bacterial cells in biofilms are well protected against antibiotics. The mechanisms of action are still unknown, and it is difficult to control pathogens with antibiotics in biofilm infections and thus the study on the antibiotics is needed. In this research, a number of natural water soluble, small-sized antibiotics molecules and their derivatives are studied. Molecular editing programs such as Gamess, Chemcraft and Avogadro, with an auto-optimization feature that determines the theoretical values of the structures atomic properties are used to build virtually any molecule with the optimized geometry according to various force field options. The UFF (Universal Force Field) is used for optimizing most molecules.

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