# DEVELOPMENT OF NANOEMULSION ALOE VERA EXTRACT AS ANTI-AGING THROUGH IN VITRO STUDY AND THE MECHANISM OF INHIBITION OF COLLAGENASE PROTEIN BY IN SILICO

**by Sri Atun, Nirfina Aznam, Retno Arianingrum, Adity Sangal**

ABSTRACT

Bright and youthful skin is one of the beauty standards in the world. *Aloe vera* is a species from the xanthorrhoeaceae family, which is known to have extraordinary therapeutic properties, especially for healthy skin, hair and digestion. Currently, *Aloe vera* is a plant that is widely used in various beauty products. However, several studies have shown activity that is less effective for dealing with various skin problems*.* **The problem of this research** is how to develop the potential of *Aloe vera* to become a basic ingredient for beauty to lighten and prevent skin aging.**The aims of this study** were to carry out qualitative and quantitative phytochemical analyzes of *Aloe vera* extract (ethanol and water), to make *Aloe vera* extract nanoemulsions, to test their activity as antioxidants and absorbent of UV rays, and to predict the mechanism of inhibition of collagenase protein receptors *in- silico.* **The research methods** to be carried out include (1) making extracts (ethanol and water) from *Aloe vera*; (2) qualitative analysis of phytochemicals which included tests for terpenoids, saponins, flavanoids, alkaloids, tannin extracts and fractions of *Aloe vera*; (3) quantitative analysis of phenolic and flavonoid content; (4) preparation of nanoemulsion extract *Aloe vera* by means of spontaneous emulsion using coconut oil and surfactant (Tween 80) in various compositions; (5) To characterize particle size, polydesperity index, and zeta potential using a Particle Size Analyzer (PSA); (6) to test the activity as an antioxidant using the DPPH (1.1-diphenyl-2-Picrylhydrazyl-Hydrazine) method; (7) To test of activity as an absorber of UV light by spectrophotometric; (8) to predic the mechanism of activity of compounds previously found in *Aloe vera* (Pubmed data based) against collagen protein receptors *in- silico*. Investigation of *in-silico* docking activity was done for ROS (PDB 3ZBF), collagenase (PDB ID 966C), hyaluronidase (PDB ID 1FCV) receptors downloaded from the RCSB PDB Database page (www.rcsb.org). All compounds then minimize their energy using the Avogadro application. Molecular docking simulation was carried out with AutoDock Vina's default settings (Vina). The best-docked conformation determined by vina scoring was employed for the visual analysis, by Pymol, ligplus (Interaction ligand-receptor), and GIMB 2.10 to visualize the interaction between the ligand and the receptor. From this research it can be concluded that:Ethanol extract and *Aloe vera* gel contain phenolic, flavonoid and saponin compounds.The total phenolic compound content of Aloevera ethanol extract was 379.138 ± 0.335 mg/g GAE sample; Meanwhile, *Aloe vera* Gel contains 0.0619 ± 0.038 mg/g GAE sample.Nanoemulsion of *Aloevera* ethanol extract can be made at varying ratios of extract-VCO-Tween 80 (0.1: 0.5 :2.0) with the addition of distilled water to a total volume of 100 mL with a particle size of 497 nm (67.2%) and 61, 2 nm (17.2%). Meanwhile, *Aloe vera* gel nanoemulsion can be made in varying ratios of -VCO-Tween 80 gel (0.2: 0.5: 2.0) with the addition of distilled water to a total volume of 100 mL with a particle size of 111.3 nm (74.1%). Each sample was made by stirring using a magnetic stirrer and heated at 70$^{o}$ C for 1 hour. *Aloe vera* ethanol extract and nanoemulsion form have medium antioxidant activity, while Aloevera gel has low antioxidant activity. Ethanol extracts, gels, and in the form of nanoemulsions *Aloe vera* can generally absorb UV-A, UV-B, and UV-A light. Isovitexin has an energy affinity for ROS receptor model targets (PDB 3ZBF), collagenase (PDB 966C), hyaluronidase (PDB 1FCV) receptors), which is higher than other compounds found in *Aloe vera* plants.

Kata Kunci: *Aloe vera, nanoemulsion, antioxidant, antiaging, collagenase*