ABSTRACT BOOK ABSTRACTS



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ATOPIC ECZEMA/DERMATITIS

AN IN-SILICO APPROACH ON VIRGIN COCONUT OIL (VCO) FOR ATOPIC DERMATITIS TREATMENT

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Introduction: Virgin Coconut Oil (VCO) has traditionally been used as a moisturizer for centuries in the tropics. Virgin Coconut Oil is a therapy for atopic dermatitis because it has a function in skin barrier repair and anti-inflammation.

Objective: To evaluate computationally the content of VCO acting as atopic dermatitis treatment.

Material and Methods: Active compounds of Cocos nucifera were extracted from KnapSack database. SMILE format was retrieved from PUBCHEM database. Predictions of skin barrier repair, anti-inflammatory inhibitor histamine and anti-eczema were conducted using PASS SERVER. Molecular mechanism of active compounds in the human body was retrieved from STITCH (Search Tool for Interacting Chemicals) which were experimentally predicted, then were analyzed computationally. Further Pathway analysis used Cytoscape software.

Results: There were 19 active compounds found in VCO. Most of the compounds acted as anti-eczema repair with the Probability score (Pa) 0.872. In addition, VCO was also potential for anti-inflammatory (Pa: 0.608). It indicated that the specific compounds had potential computationally. The result of pathway analysis showed linoleic acid a protein target Free Fatty Acid (FFA) acting as a receptor for medium and long chain saturated and unsaturated fatty acids.

Conclusion: In our study suggested that VCO could be used as atopic dermatitis therapy by activating FFA and inhibiting occurrence atopic dermatitis.

Keyword: Atopic dermatitis, Free Fatty Acid, In-silico, Virgin Coconut Oil





