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**Chemometric assisted green extraction of tyrosinase inhibitor from Durio zibethinus rind for skin whitening agents in cosmetic products**

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**Abstract**

Cosmetics typically contain artificial substances that could be harmful to people's health. Extended usage and exposure to these harmful substances are frequently linked to a number of negative impacts and illnesses. This study processed a Durio zibethinus rind, rich in natural antityrosinase properties, with a chemometric-assisted green extraction system. The TPC value was obtained at the optimum conditions (34.4 MPa, 62°C, and 86 min). GC-MS and FTIR spectroscopy were performed to identify the phenolic compounds and their functional group, respectively. The optimized extract contains 77 % of the mushroom tyrosinase activity. PCA shows that aspidospermidin-17-ol,1-acetyl-19,21-apoxy-15,16-dimethoxy- (AP) resembles the similar cluster with hydroquinone. COSMO-RS was used to investigate the extraction mechanism of CO<sub>2</sub> and AP during the SFE process. DFT and molecular docking were used to calculate the chemical reactivity and explain the tyrosinase inhibition mechanism, respectively. ADME-Tox and OSIRIS Property Explorer showed no violation of Lipinski's rule, and toxicity with AP. In conclusion, a high-value, natural and safe cosmetic ingredient (AP) for cosmetopea was discovered using an innovative green extraction system. © 2024 Elsevier B.V.

**Author Keywords**

ADMEX Tox; Chemometric (RSM and PCA); Durio zibethinus; Molecular docking; Supercritical fluid extraction (SFE); Tyrosinase

**Index Keywords**

Supercritical fluid extraction, Supercritical fluids; ADMEX tox, Chemometric (RSM and PCA), Chemometrics, Durio zibethinus, Fluid extraction, Green extractions, Molecular docking, Supercritical, Supercritical fluid extraction, Tyrosinase; Fourier transform infrared spectroscopy

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