The Journal of Supercritical Fluids 214 (2024) 106393

Contents lists available at ScienceDirect

The Journal of Supercritical Fluids

journal homepage: www.elsevier.com/locate/supflu

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

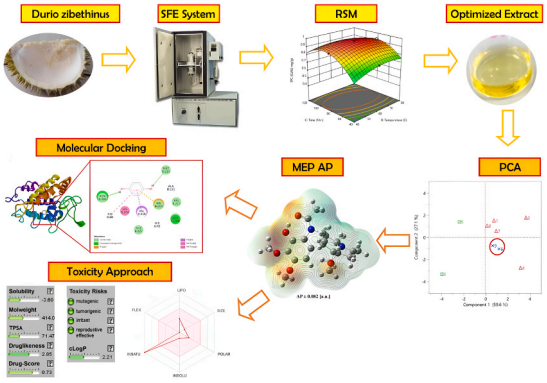
Sofiyyah Ismail [a], Erna Normaya [a,b], Syamimi Sulfiza Shamsuri [a], Anwar Iqbal [c], Mohd Bijarimi Mat Piah [d], Sharifuddin Md Zain [e], Mohammad Norazmi Ahmad [a,b,*]

[a] *Experimental and Theoretical Research Lab (ETRL), Department of Chemistry, Kulliyyah of Science, IIUM Kuantan, Pahang, Malaysia*
[b] *Sustainable Nanotechnology and Computational Modelling (SuNCoM) Research Group, Kulliyyah of Science, IIUM Kuantan, Pahang, Malaysia*
[c] *School of Chemical Sciences, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia*
[d] *Faculty of Chemical and Process Engineering Technology, University Malaysia Pahang Al-Sultan Abdullah, 26300 Kuantan, Pahang Malaysia*
[e] *Department of Chemistry, Faculty of Science, Universiti of Malaya (UM), Kuala Lumpur 50603, Malaysia*

HIGHLIGHTS

- Chemometric-assisted SFE identified the *Durio zibethinus* rind as the cosmetic's source.
- The optimal extraction of TPC was obtained at 62 °C, 34.4441 MPa, 86 min of extraction.
- The PCA-assisted GC MS classified AP as an effective natural cosmetic ingredient.
- ADME-Tox and OSIRIS Property Explorer predict the AP's safety as a natural cosmetic.
- Molecular docking revealed the non-covalent interaction during tyrosinase inhibition.

GRAPHICAL ABSTRACT



ARTICLE INFO

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

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_2 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

* Corresponding author at: Experimental and Theoretical Research Lab (ETRL), Department of Chemistry, Kulliyyah of Science, IIUM Kuantan, Pahang, Malaysia.
E-mail addresses: mnorazmi@iium.edu.my, mnorazmi85@gmail.com (M.N. Ahmad).

https://doi.org/10.1016/j.supflu.2024.106393
Received 16 April 2024; Received in revised form 22 August 2024; Accepted 23 August 2024
Available online 26 August 2024