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Hassanuddin, N.A.^a, Normaya, E.^{a b}, Ismail, H.^a, Iqbal, A.^c, Piah, M.B.M.^d, Abd Hamid, S.^e, Ahmad, M.N.^{a b}

Methyl 4-pyridyl ketone thiosemicarbazone (4-PT) as an effective and safe inhibitor of mushroom tyrosinase and antibrowning agent

(2024) *International Journal of Biological Macromolecules*, 255, art. no. 128229, .

DOI: 10.1016/j.ijbiomac.2023.128229

^a Experimental and Theoretical Research Lab (ETRL), Department of Chemistry, Kulliyah of Science, IIUM, Pahang, Kuantan, Malaysia

^b Sustainable Nanotechnology and Computational Modelling (SuNCoM) Research Group, Kulliyah of Science, International Islamic University Malaysia, Pahang, Kuantan, 25200, Malaysia

^c School of Chemical Science, Universiti Sains Malaysia, Penang, 11800, Malaysia

^d Faculty of Chemical & Natural Resources Engineering, Universiti Malaysia Pahang, Kuantan, Malaysia

^e Department of Chemistry, Kulliyah of Science, IIUM, Pahang, Kuantan, Malaysia

Abstract

Enzymatic browning is of concern as it can affect food safety and quality. In this study, an effective and safe tyrosinase inhibitor and anti-browning agent, methyl 4-pyridyl ketone thiosemicarbazone (4-PT), was synthesised and characterised using Fourier-transform infrared (FTIR) spectroscopy, CHNS elemental analysis, and proton (1H) and carbon-13 (13C) nuclear magnetic resonance (NMR) spectroscopy. The vibrational frequencies of 4-PT were studied theoretically using vibrational energy distribution analysis (VEDA). Density functional theory (DFT) was applied to elucidate its chemical properties, including the Mulliken atomic charges, molecular electrostatic potential (MEP), quantum theory of atoms in molecules (QTAIM) and reduced density gradient non-covalent interactions (RDG-NCIs). Moreover, 4-PT was compared with kojic acid in terms of its effectiveness as a tyrosinase inhibitor and anti-browning agent. The toxicity and physicochemical properties of 4-PT were predicted via ADME evaluation, which proved that 4-PT is safer than kojic acid. Experimentally, 4-PT (IC₅₀ = 5.82 μM, browning index (10 days) = 0.292 ± 0.002) was proven to be an effective tyrosinase inhibitor and anti-browning agent compared to kojic acid (IC₅₀ = 128.17 μM, browning index (10 days) = 0.332 ± 0.002). Furthermore, kinetic analyses indicated that the type of tyrosinase inhibition is a mixed inhibition, with Km and Vmax values of 0.85 mM and 2.78 E-09 μM/s, respectively. Finally, the mechanism of 4-PT for tyrosinase inhibition was proven by 1D, second derivative and 2D IR spectroscopy, molecular docking and molecular dynamic simulation approaches. © 2023 Elsevier B.V.

Author Keywords

Antibrowning agent; Density functional theory (DFT); Spectroscopy; Thiosemicarbazone; Tyrosinase inhibitor

Index Keywords

Fourier transform infrared spectroscopy, Ketones, Molecular dynamics, Molecular modeling, Nuclear magnetic resonance, Nuclear magnetic resonance spectroscopy, Phenols, Physicochemical properties, Quantum theory, Spectrum analysis; Anti - Browning agents, Antibrowning agent, Browning index, Density functional theory, Density-functional-theory, Kojic acid, Pyridyl, Thiosemicarbazones, Tyrosinase inhibition, Tyrosinase inhibitors; Density functional theory; kojic acid, methyl 4 pyridyl ketone thiosemicarbazone, monophenol monooxygenase, thiosemicarbazone derivative, unclassified drug; Article, carbon nuclear magnetic resonance, controlled study, density functional theory, elemental analysis, enzyme inhibition, evaluation study, Fourier transform infrared spectroscopy, kinetics, nuclear magnetic resonance spectroscopy, physical chemistry, proton nuclear magnetic resonance, quantum theory, static electricity, synthesis

Chemicals/CAS

kojic acid, 501-30-4; monophenol monooxygenase, 9002-10-2

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Correspondence Address

Ahmad M.N.; Experimental and Theoretical Research Lab (ETRL), Pahang, Malaysia; email: mnorazmi85@gmail.com

Publisher: Elsevier B.V.

ISSN: 01418130

CODEN: IJBMD

PubMed ID: 37981274

Language of Original Document: English

Abbreviated Source Title: *Int. J. Biol. Macromol.*

2-s2.0-85177757354

Document Type: Article

Publication Stage: Final

Source: Scopus

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