



Isolation, characterization, in silico ADMET prediction of novel Xanthone Glycoside derivative from Egyptian *Mangifera Indica* having promising antiaging activity

Naglaa S. Ashmawy^{1, 5, 6*}, Heba Al nashar^{1, 2}, Eman M El- Labbad^{3, 4}

¹Pharmacognosy Department, Faculty of Pharmacy, Ain Shams University, Cairo, Egypt

²Center for Drug Discovery Research and Development, Ain Shams University, Egypt

³Pharmaceutical Chemistry Department, Faculty of Pharmacy, Ain Shams University, Abbassia, 11566, Cairo, Egypt

⁴Department of Pharmaceutical Sciences, College of Pharmacy, Gulf Medical University, Ajman, United Arab Emirates

⁵Pharmacy Department, City University College of Ajman, Ajman, United Arab Emirates

⁶Rochester Institute of Technology-Dubai. Dubai, United Arab Emirates

Abstract

Mangifera indica (MI), has been an important medicinal herb for over 4000 years. This genus *Mangifera* comprises about 30 species of fruiting trees of family Anacardiaceae. *Mangifera* was widely used in traditional medicine for therapeutic purposes by several cultures. Various parts of *Mangifera* tree were utilised for the treatment of a variety of ailments.

Mangifera indica leaves extract grown in Egypt was subjected to successive chromatography techniques resulted in isolation of a novel non-reported xanthone derivative (TM-1). The in-vitro ability of TM-1 to inhibit elastase and tyrosinase enzymes activities was assessed. The novel compound exhibited remarkable anti-elastase and anti-tyrosinase inhibitory effects with IC₅₀ values of 1.064 µg/mL and 1.336 µg /mL respectively compared to the positive controls. In order to assess the drugability and formulation consideration of TM-1, in silico, ADMET prediction was conducted using the SwissADME server. This included Lipinski's rule of five, such as lipophilicity, solubility, and Pharmacokinetic properties as GIT absorption, distribution, metabolism, and skin permeation. All the physicochemical properties of TM-1 are within desirable ranges except for high polarity which may be attributed to the presence of the sugar moiety. TM-1 showed promising predicted topological aqueous solubility and reasonably predicted skin penetration suggesting the suitability of TM-1 for topical formulation. This is coherent with the in-vitro Antiaging evaluation.

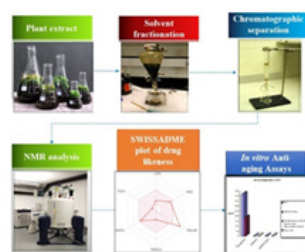


Figure1: Chromatographic isolation, NMR analysis followed by structure elucidation and ADMET study then in vitro anti-aging evaluation

Biography

Naglaa Saad is an Assistant Professor, Faculty of Pharmacy, and Ain Shams University. She received her Master and Ph.D. degrees in Pharmaceutical Sciences from Faculty of Pharmacy, Ain Shams University. Currently, she is an active researcher in various fields related to drug discovery with special emphasis on isolation, structure elucidation and biological screening of secondary metabolites from natural sources with application of molecular modelling to design new active drug molecules. She is currently conducting a group of studies in metabolomics field especially for discovering the metabolites and related pathways underlying some types of cancer. Dr. Saad has good experience in chemical analysis field with the ability to work with different high technology analysis devices including NMR, GC-MS, LC-MS and HPTLC and efficiently working with advanced software programs like; Mestronova (Mesterlab 11), Xcalibur 3.1, EndNote X7, AMDIS 2.6 (NIST MS Library), Chemomx and MetaboAnalyst 4.0.

Recent Publications

1. October 2021- Ola D.A. Shammout, Naglaa S. Ashmawy, Sarra B. Shakartalla, Alaa M. Altaie , Hany A. Omar and Sameh S. M. Soliman. Comparative sphingolipidomic analysis reveals significant differences between doxorubicin-sensitive and -resistance MCF-7 cells. Accepted manuscript-PLOS ONE journal.
2. 2021- Sarra B Shakartalla, Razan B Alhumaidi , Ola D A Shammout , Zainab M Al Shareef , Naglaa S Ashmawy , Sameh S M Soliman. Dyslipidemia in breast cancer patients increases the risk of SAR-CoV-2 infection. Infection, genetics and evolution journal, 104883.
3. 2021- Moza Mohamed Alzaabi, Rania Hamdy, Naglaa S. Ashmawy, Alshaimaa M. Hamoda, Fatemah Alkhatay, Neda Naser Khademi, Sara Mahmoud Abo Al Joud, Ali A. El-Keblawy & Sameh S. M. Soliman. Flavonoids are promising safe therapy against COVID-19. Phytochemistry reviews, P1-3.
4. 2021- Alshaimaa M. Hamoda, Bahgat Fayed, Naglaa S. Ashmawy, Abdel-Nasser A. El-Shorbagi, Rania Hamdy and Sameh S. M. Soliman. Marine Sponge is a Promising Natural Source of Anti-SARS-CoV-2 Scaffold. Frontiers in pharmacology
5. 2020-Naglaa S. Ashmawy, Haidy A. Gad, Sherweit H. El-Ahmady, Mohamed L. Ashour and Abdel Nasser B. Singab. The genus *Polyscias* (Araliaceae): A phytochemical and biological review. Journal of Herbal Medicine, 100377.

3rd Global Experts Meeting on Medicinal Chemistry and Drug Design
Webinar | March 14, 2022

Citation: Naglaa S. Ashmawy, Isolation, characterization, in silico ADMET prediction of novel Xanthone Glycoside derivative from Egyptian *Mangifera Indica* having promising antiaging activity, Medicinal Chemistry 2022, 3rd Global Experts Meeting on Medicinal Chemistry and Drug Design, Webinar | March 14, 2022