Indian Journal of Chemistry
Vol. 64, March 2025, pp. 291-298
DOI: 10.56042/ijc.v64i3.16490

# Antiproliferative activity of triterpenoids of *Nelumbo nucifera* Gaetrn. rhizomes and their derivatives: *In vitro* and *in silico* studies

Deepika Singh*[a], Shiv Kumar[b], Mahendra P Darokar[b] & Prabir K Chaudhuri[a]

[a] Medicinal Chemistry Division
and
[b] Molecular Bioprospection Department, CSIR-Central Institute of Medicinal and Aromatic Plants, PO CIMAP, Lucknow 226 015, India
E-mail: deepika.sh25@yahoo.com

*Received 27 December 2024; accepted(revised) 27 February 2025*

Breast cancer and prostate cancer are the most common malignancy in women and men, respectively. In view of serious side effects of the available therapies, cost of the treatment and drug-resistance, the search for more effective anticancer drug is urgently needed. Triterpenoids present inedible rhizomes of *Nelumbo nucifera* Gaetrn which possess antiproliferative activities. To investigate the therapeutic effect of *N. nucifera* triterpenoids against breast and prostate cancers, the semi-synthetic derivatives of triterpenoids have been prepared and monitored for their *in vitro* bioassay, molecular docking, QSAR and ADMET studies. Compound 2α, 3β, 24-triacetoxy hyptatic acid-A(**3c**) show significant inhibitory activity against breast cancer (MCF-7, $IC_{50}$ = 9.77 ± 0.9 μM) along with the strong binding affinity towards the active site of 3ERT with docking score of –7.2 kcal/mol. The QSAR model suggests the importance of geometrical shape and dipole moment of triterpenoids for their antiproliferative activity against MCF-7 cells, while AlogP and DPSA_1 is crucial for showing the activity against PC-3 cells. The ADMET analysis demonstrates that the triterpenoids follow most of the physicochemical properties required for their optimum bioavailability and not showing any toxicity. In this study, hyptatic acid-A emerged as a good structural template to develop novel leads against different cancers and substitution at C24 hydroxyl group has important role in bioactivity.

**Keywords:** *Nelumbo nucifera* Gaertn., Triterpenoids, Antiproliferative activity, Estrogen receptor alpha, Androgen receptor