



Indian Journal of Chemistry
Vol. 63, January 2024, pp. 72-79
DOI: 10.56042/ijc.v63i1.4424

International Journal of Science, Communication and Public Research
NISCP
सीएसआईआर-निरुपर

Synthesis, computational and biological activities of 2-[2-(4-arylamino)-4-methylphenylaminothiazol-5-oyl]naphthalenes

J Jebalenet^{a,b}, J Jenisha^{a,b}, Bojaxa A Rosy^c & T F Abbs Fen Reji^{*a}

^a Department of Chemistry and Research Centre, Nesamony Memorial Christian College, Marthandam 629 165, Tamil Nadu, India

^b Manonmaniam Sundaranar University, Tirunelveli 627 012, Tamil Nadu, India

^c Department of Botany & Research Centre, Holy Cross College (Autonomous), Nagercoil 629 004, Tamil Nadu, India

E-mail: abbsfen@gmail.com, jebalnetsujin@gmail.com

Received 28 July 2023; accepted (revised) 21 December 2023

2-[2-(4-Arylamino)-4-methylphenylaminothiazol-5-oyl]naphthalenes have been synthesized by the reaction of 2-bromoacetyl naphthalene and 1-aryl-3-(N,N¹-diarylamidino)thiourea in the presence of triethyl amine. The structures of the newly synthesized analogues have been confirmed by spectroscopic techniques. The *in vitro* antioxidant activity has been studied using DPPH assay and anticancer activity has been studied using MTT assay against cancer cells. *In silico* studies have been performed to predict the binding modes of the compounds with the cyclin-dependent kinase protein 6WUU. It is evident from the current results that all the synthesized compounds exhibit remarkable antioxidant and anticancer potential.

Keywords: Naphthalene, B3LYP/6-31G, DFT, SARS-CoVPLpro, Mulliken, DPPH, MTT