Design, Synthesis, and Anticancer Evaluation of Novel N-[5-(1,3,4,5-tetrahydroxycyclohexyl)-1,3,4-thiadiazol-2-yl] Benzamide Analogues Through Integrated Computational and Experimental Approaches

Sujaritha Jayaraj
Saveetha Institute of Medical and Technical Sciences, Thandalam, Chennai

Background: The main aim of the current study is to develop, synthesize, in silico, in vitro and in vivo potentials of N-[5-(1,3,4,5tetrahydroxycyclohexyl)-1,3,4-thiadiazol-2-yl] benzamide derivatives for a possible anticancer drug to improve their efficiency and selectivity against cancer cells, computational approaches aided in the rational design of these chemicals. Spectroscopic methods verified the chemical structures of the target compounds. The structures of the synthesized analogs were determined by elemental analysis, IR, 1H NMR, 13C NMR and MS. Structure shows the presence of 1,3,4, thiadiazol also responsible for anticancer activity. The 10 analogs were synthesized and showed encouraging anticancer efficacy in preliminary biological evaluation, suggesting they might be suitable lead candidates for more optimization and preclinical exploration.

Result: N-[5-(1,3,4,5tetrahydroxycyclohexyl)-1,3,4-thiadiazol-2-yl] benzamide derivatives were synthesized (5a-5j) showed an optimum IC50 value in in vitro activity by SRB assay using MCF-7 as a strain, the few selected analogs 5b,5g & 5h were subjected for in vivo anticancer activity by DMBA induction of tumors in mice.

Conclusion: Through a computational and experimental approach this study's results a way for newer derivatives for the class of anticancer drugs

Keywords:1,3,4,5tetrahydroxycyclohexylderivatives, Molecular docking, topoisomerase, SRB assay, DMBA, anticancer evaluations

Biography

Sujaritha J, a passionate researcher, and academic achiever. I have always been driven by a curiosity for knowledge and a dedication to excellence. I have always fascinated by drug design and development. This early interest laid the foundation for my academic journey. I pursued my UG and PG in The Tamil Nadu Dr. Medical and research institute where I developed a deeper understanding of drug design and development.