docking studies were performed against the PARP-1 enzyme (PDB ID: 4ZZZ), a key target in anticancer therapy. Compounds A2, A3, and A5 exhibited strong binding affinities with Glide scores comparable to the reference drug Olaparib. ADME predictions further supported their drug-likeness and suitability as lead candidates. The *in vitro* anticancer activity of all compounds was assessed against human breast cancer cell lines MCF-7 and MDA-MB-231 using the MTT assay. Notably, compounds A3 and A5 demonstrated significant cytotoxicity, with IC_{50} values in the low micromolar range, closely aligning with Olaparib. The remaining compounds showed moderate activity, indicating a structure-activity relationship (SAR) influenced by the nature of the aldehyde substituents. Overall, the findings highlight compounds A3 and A5 as promising PARP-1 inhibitors with potential for further development in anticancer drug discovery.

Keywords: Schiff bases, 1,2,4-Triazole, PARP-1 inhibitors, green synthesis, Anticancer activity, Molecular docking

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CENTRAL COMPOSITE DESIGN ASSISTED HPLC METHOD DEVELOPMENT FOR HIGH-THROUGHPUT ANALYSIS OF TELMISARTAN, CHLORTHALIDONE AND METOPROLOL SUCCINATE

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Optimization for the estimation of drug combinations by HPLC is essential and superior in terms of efficient, cost, accuracy and regulatory compliance comparing normal method development making it high quality pharmaceutical analysis. Optimization by Central Composite Design is highly significant due to its advanced and systematic approach of multiple variables evaluation and their interaction providing minimal number of experimental runs by giving an accurate mathematical models like Response surface method which predicts method performance under various conditions. The present study uses Telmisartan, Chlorthalidone and Metoprolol Succinate. In their combined tablet dosage forms for method development and validation using CCD as an Optimization tool by HPLC. For Optimization, acetonitrile concentration as mobile phase, pH of the phosphate buffer and flow rate were selected as factors with chosen responses from capacity factor, retention time and resolution between the peaks. The results obtained from CCD experiments were presented as perturbation and response surface plots to get visual representation of individual and multiple factors. Overall, the method gets a desirability value of 0.770 indicating best method performance. Retention time of Telmisartan, Chlorthalidone and Metoprolol Succinate. were 5.239, 7.692- and 10.623-minutes using acetonitrile and 0.05M phosphate buffer in the ratio 30:70 %V/V and pH of 6.2 at a flow rate 1.0 ml/min at a detection wavelength of 215 nm. Validation parameters according to ICH guidelines were done and found to be within limits. The method may be adopted for routine analysis of these drugs in pharmaceutical industry.

Keywords: Optimization, Central Composite design, HPLC, Validation, ICH guidelines

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NOVEL ZINGERONE-DERIVED CHALCONES AS POTENTIAL NEUROPROTECTIVE LEADS: SYNTHESIS, *IN SILICO* DOCKING, AND *IN VITRO* EVALUATION

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Chalcones are open-chain flavonoids with antioxidant and neuroprotective potential. Zingerone, a phenolic alkanone from Zingiber officinale, has demonstrated beneficial neuroprotective effects. This study reports the synthesis of novel Zingerone-derived chalcones, their structural characterisation, *in silico* docking, and evaluation of neuroprotective activity. A series of six Zingerone-derived chalcones were synthesised via Claisen–Schmidt condensation using substituted benzaldehydes. Structures were confirmed by FT-IR, 1H/13C NMR, and mass spectrometry. *In silico* docking was performed against acetylcholinesterase (AChE), monoamine oxidase-B (MAO-B), and GSK-3β using AutoDock Vina. ADMET profiles were predicted *in silico*. Neuroprotective effects were evaluated in SH-SY5Y neuronal cells exposed to H_2O_2-induced oxidative stress, using MTT, ROS, caspase-3, and mitochondrial potential assays. The synthesised chalcones exhibited good yields (62–83%). Docking scores ranged from −7.8 to −10.2 kcal/mol for AChE and −7.1 to −9.4 kcal/mol for MAO-B, with the methoxy-substituted derivative (C4) showing the best binding (−10.2 kcal/mol for AChE). ADMET analysis predicted BBB penetration, logP values between 2.5–3.8, and no hepatotoxicity or mutagenicity risk. In SH-SY5Y cells, H_2O_2 reduced viability to 48 ± 3.2%, whereas pretreatment with chalcones (10 µM) restored viability to 78–91% ($p < 0.01$). ROS generation decreased by 65%, caspase-3 activity was reduced by 45%, and mitochondrial membrane potential was preserved at 82% of control levels compared to 51% in untreated stressed cells. Zingerone-derived chalcones display favourable drug-likeness, strong binding affinity to neurodegeneration-related targets, and significant neuroprotective effects *in vitro.* These findings suggest their potential as leads for developing novel therapeutics against neurodegenerative disorders.

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SYNTHESIS, CHARACTERIZATION, AND BIOLOGICAL EVALUATION OF 2-PHENYL-1,3-OXAZOL-5-ONE DERIVATIVES AS POTENTIAL BREAST CANCER THERAPEUTICS: A COMBINED APPROACH OF MICROWAVE SYNTHESIS, MOLECULAR DOCKING, AND CYTOTOXIC STUDY

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Oxazolone derivatives have gained significant attention due to their wide spectrum of biological activities, particularly anticancer potential. Breast cancer continues to be a leading cause of mortality among women, necessitating the development of novel therapeutic agents. In this study, 36 derivatives of 2-Phenyl-1,3-Oxazol-5-One were designed as potential PARP-1 inhibitors. Molecular docking against PARP-1 (PDB ID: 4UND) revealed that several compounds exhibited favourable binding affinities, with strong hydrogen bonding and hydrophobic interactions comparable to standard drugs such as niraparib, veliparib, and Olaparib. Three top-ranking derivatives (OV1, OV2, and OI30) were synthesized using an efficient microwave-assisted method involving hippuric acid and substituted benzaldehydes. Structural confirmation was achieved through FT-IR, ^{1}H-NMR, and mass spectrometry. Biological evaluation by MTT assay demonstrated dose-dependent cytotoxicity, with certain derivatives showing moderate to potent activity against breast cancer cells. In addition, *in silico* ADME profiling indicated favourable drug-likeness and pharmacokinetic potential. The present work establishes 2-Phenyl-1,3-Oxazol-5-One derivatives as promising scaffolds for anticancer drug discovery targeting PARP-1. The combination of rational design, docking validation, eco-friendly microwave-assisted synthesis, spectral characterization, and preliminary biological evaluation highlights their potential as lead candidates. Further optimization and pharmacological studies are warranted to advance these oxazolone derivatives toward breast cancer therapy.

Keywords: 2-Phenyl-1,3-Oxazol-5-One, Oxazolone derivatives, PARP-1 inhibition, Microwave-assisted synthesis, Anticancer agents

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ANTIMICROBIAL POTENTIAL OF NOVEL 3,5-DISUBSTITUTED 1,3,4-OXADIAZOLE-2-THIONE DERIVATIVES: AN IN-SILICO AND *IN-VITRO* APPROACH

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Infectious diseases remain a significant health concern, accounting for approximately 41% of the global disease burden. One of the main causes of this problem is bacterial resistance to antibiotics. The current antibiotic therapies are often accompanied by a range of toxic effects. Antimicrobial drugs may produce adverse effects like an allergic reaction and hypersensitivity upon consumption. Additionally, a major concern is

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