Isoniazid (INH) is one of the most successful tuberculosis medications on the market today. In particular, isoniazid is used as a prophylaxis medication to avoid resurgence of illness in those who have underlying Mycobacterium tuberculosis (MTB) infection. The mode of action of isoniazid is complicated and incorporates a number of distinct aspects in which various biomolecular routes are impacted, including mycolic acid production. Catalase-peroxidase (KatG) activates the prodrug isoniazid and enzymes such as β-ketoacyl ACP synthase (KasA) and enoyl acyl carrier protein (ACP) reductase target the active isoniazid products. Various genes in diverse biochemical networks and pathways are involved in the physiological mechanisms of isoniazid resistance. Isoniazid resistance is the most common of all clinical drug-resistant isolates, with incidence in some areas of up to 20 to 30%. In this review article, several existing components that may influence the complexities of isoniazid function including mechanism of action, resistance mechanisms in MTB, along with their history, different synthetic procedures, uses, dosage forms, side effects, adverse drug reactions, physico-chemical characteristics, ADME properties, contraindications as well as future perspectives are discussed. Studies of pharmacokinetics have found that the cause of the drug mediated hepatotoxicity is possible by metabolism of isoniazid. Because of inter-individual heterogeneity of polymorphism that affect isoniazid metabolism rates, customized medicines may be required in various populations to prevent hepatotoxicity. The isoniazid multidrug combination treatment which would proved to be effective tuberculosis treatment in future. Further exploration is needed for better comprehension of pathogenesis mechanism of Mycobacterium tuberculosis (MTB) and drug resistance studies are required for building up better therapeutics and diagnostic against tuberculosis.

Keywords: Mycobacterium tuberculosis, Drug resistance mechanisms, Isoniazid, Catalase-peroxidase, β-Ketoacyl ACP synthase.
A Retrospective Study of Synthesis, Structure-Activity Relationship and Antimicrobial Activity of 4-Formyl Pyrazole Containing Isoniazid Moiety

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4-Formyl pyrazole is nitrogen containing heterocyclic aromatic molecule containing isoniazid moiety. The molecule is formed by fusion of two heterocyclic ring i.e. pyrazole and isoniazid. The current paper covers a vast range of methods for synthesis of 4-formyl pyrazole containing isoniazid moiety and its derivatives using variety of catalyst, solvent medium and microwave irradiation with a goal of achieving a high yield and rapid separation of products. This work describes 4-formyl pyrazole and isoniazid antimicrobial activity as well as their structural-activity relationship. It also includes the mechanism of action of pyrazole and isoniazid and includes the list of current patents linked to various pharmacological activities in previous past years.

Keywords: 4-Formyl pyrazole, Isoniazid, Pharmacological activity, Heterocyclic, Mechanism of action, Pyrazole
Microwave Assisted a Highly Atom Economic, Chemo-, Regio- and Stereoselective Synthesis and Evaluation of Dispiro[1\(H\)-indene-2,3\(′\)′'-pyrrolidine-2,3\(′′\)′'-[3\(H\)]indole]-1,2\(′′\)′'(1\(''\)H)diones as Antibacterial and Antifungal Agents

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1,3-Dipolar cycloaddition of \textit{in situ} generated non-stabilized azomethine ylides through the decarboxylative condensation of sarcosine and substituted isatin with 2-(arylmethylene)-2,3-dihydro-1\(H\)-inden-1-ones in microwave produced dispiro[1\(H\)-indene-2,3\(′\)′'-pyrrolidine-2,3\(′′\)′'-[3\(H\)]indole]-1,2\(′′\)′'(1\(''\)H)diones in a highly stereo- and regio-selective fashion. The synthesized compounds were subjected to antibacterial and antifungal studies. It was found that many compounds possess a considerable antibacterial and antifungal activity against all the tested organisms.

Keywords: 1,3-Dipolar cycloaddition, Azomethine, Ylides, Dispiro compounds, Antibacterial activity, Antifungal activity.
Pharmacological Investigation of Fluoro, Iodo and Hydroxy Derivative of Chloro Substituted Homoisoflavonoids

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In present study, the synthesized substituted homoisoflavonoid derivatives were screened for their in vivo/in vitro antiarthritic activity, in vitro anti-inflammatory and DPPH free radical scavenging activity. The male Wistar rats were used for investigation of in vivo antiarthritic activity against complete freund’s adjuvant (CFA) induced arthritis and assessment was done for change in paw volume, serum marker enzymes (ALP, SGOT and SGPT) and membrane stabilization potential. in vitro anti-inflammatory activity was assessed by the protein denaturation method. In vitro free radical scavenging activity was assessed by the DPPH method. The result indicated that compound HIFa showed a significant antiarthritic activity as compared to other substituted homoisoflavonoid derivatives. The significant membrane stabilization and inhibition of protein denaturation showed in vitro antiarthritic and anti-inflammatory activity of substituted homoisoflavonoid derivatives. The substituted homoisoflavonoid derivatives showed dose dependent DPPH free radical scavenging activity. From the present study, it was observed that the iodo derivative of substituted homoisoflavonoid derivatives have significant pharmacological activities as compared to floro and hydroxyl derivatives.

Keywords: Homoisoflavonoid derivatives, Anti-inflammatory activity, DPPH assay, Antiarthritic activity, Homoisoflavonoid derivatives.
Chloroquine derivatives were one of the medications tested against the coronavirus pandemic in 2020 and they appeared to be effective. In this present work, \((2E,2'E)-2,2'-(\text{propane-1,2-diyldiene})\text{bis}(N\text{-methylhydrazinecarbothio-amide})\) (PMTSC) has been postulated as a possible antiviral for the treatment of COVID-19 by using 1-Click docking. Compound PMTSC has been synthesized by the condensation reaction between pyruvaldehyde and \(N\)-methylthiosemicarbazide. The synthesized PMTSC was confirmed by elemental analysis and NMR spectral study. The binding interaction of PMTSC has been performed with SARS-CoV main protease (PDB code: 2GZ7 and 2GZ8). The docking results showed good binding energies and interactions.

**Keywords:** Thiosemicarbazone, Schiff’s base, SARS-CoV, Docking, Protein-Ligand binding interaction.
Exploring 3D QSAR Study of Pyridone-Pyrimidone Derivatives as Glucokinase Activators in Treatment of Diabetes Mellitus by using CoMFA Method

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In this work, we have performed 3D QSAR study of reported pyridone-pyrimidone derivatives. CoMFA was applied to generate 3D QSAR models. Total eight QSAR models were generated. Model 2 was close to standard set criteria. Effect of steric and electrostatic substituents on biological activity was observed on contour maps. This study will be helpful for future researchers in designing new pyridine-pyrimidone derivatives.

Keywords: Glucokinase, Pyridone-Pyrimidone, 3D QSAR, Diabetes mellitus.
Computer-Aided Drug Design Boon in Drug Discovery

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An innovative sequential step of detecting new medicines or drugs dependent on the information of a target is called drug design. The drug is a small molecule that alters the capacity of a bimolecular, example, protein, receptor or catalyst that leads to restorative incentive for patients. Designing of drug by computational method helped steady use of computational science to find, improve and study drugs as well as biologically related active molecules. The displaying examines like the structure-based plan; ligand-based drugs structure; database looking and restricting partiality dependent on the information of a biological target. In this article, we present the zones where CADD (computer aided drug design) devices uphold the medication disclosure measure.

Keywords: CADD, Biological target, Molecular docking, Drug discovery.
Prediction of *in silico* ADMET Properties and Molecular Docking Study of Substituted Thiadiazole for Screening of Antibacterial and Antifungal Activities against Protein Targets *Helicobacter pylori* α-Carbonic Anhydrase and *Trypanosoma brucei* Pteridine Reductase

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The aim of this work was to evaluate the physico-chemical, pharmacokinetic parameters (absorption, distribution, metabolism, excretion and toxicity) and pharmacodynamic parameters (bioactivity and adverse reactions) of substituted thiadiazole by means of *in silico* computational prediction. Online softwares such as Pre-ADMET, Molinspiration and rule of five were used for the analysis. Substituted thiadiazole fits the characteristics of drug-likeness, pharmacokinetic properties appropriate to the predicted patterns and activities within the scope for the treatment of infection in the stomach or duodenum (first part of the small intestine), gastritis and trypanosomiasis. Therefore, *in silico* results allow us to conclude that substituted thiadiazole is predicted to be a potential future drug candidate, due to its relevant Drug-likeness profile, bioavailability, excellent liposolubility and adequate pharmacokinetics, including at the level of CNS, penetrating the blood-brain barrier. Molecular docking studies have also been performed to screen the antibacterial and antifungal activities of the 50 designed compounds against protein targets *Helicobacter pylori* α-carbonic anhydrase (PDB: 5TUO) and *Trypanosoma brucei* Pteridine Reductase (PTR1) (PDB: 4WCD) respectively. Among all the compounds C11 exhibited the most significant affinity score against *Helicobacter pylori* α-carbonic anhydrase and C37 exhibited the most significant affinity score against *Trypanosoma brucei* pteridine reductase (PTR1) best significant hydrogen bonds interaction at the active site of protein.

*Keywords:* Toxicity prediction, Molecular Docking, Molinspiration, PreADMET, Rule of five, Substituted thiadiazole.
Ultrasound Assisted New Imines of 3E-3-(4-Substituted benzylidene)-4-(substituted-1,3,4-thiadiazole-2-ylimino)pentane-2-one and their Antimicrobial Studies

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A new series of Schiff bases of 3-(4-substituted benzylidene)-4-(substituted-1,3,4-thiadiazole-2-ylimino)pentane-2-one having various substituents of aryl attached to acetoacetone by Knoevenagel condensation and substituted 1,3,4-thiadiazole were synthesized by using solid supported tetrabutylammonium hydrogen sulfate in microwave irradiation. The synthesized Schiff bases have been evaluated by ¹H NMR, elemental analysis, FTIR, mass spectroscopy. All Schiff bases have been screened for their antimicrobial activities. These compounds possess good result of antimicrobial studies.

Keywords: Schiff base, Acetoacetone, Thiazole, Ultrasound.
Synthesis and Anti-inflammatory Activity of Newer Indolyl Pyrazolines and Indolyl Isoxazolines

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Various 5-substituted aryl-3-(2′-carboxy-5′-methoxyindolyl)-2-pyrazolines (9-15) and 5-substituted aryl-3-(2′-carboxy-5′-methoxyindolyl)isoxazolines (16-22) have been synthesized by the cyclization of compounds 1-(2′-carboxyl-5′-methoxyindolyl-3-arylidenyl chalcones (2-8) by treating them with hydrazine hydrate/glacial acetic acid and hydroxylamine hydrochloride/2% NaOH, respectively and TLC checked for their purity. Structure of all these newly synthesized compounds was characterized by elemental (C, H, N) analysis and IR and ¹H NMR spectroscopy. All the synthesized compounds were tested for their anti-inflammatory and ulcerogenic activities and acute toxicity and found to possess varying degrees of these activities. Compound 15 is 5-(3′′-methoxy-4′′-hydroxyphenyl)-3- (2′-carboxy-5′-methoxyindolyl)-2-pyrazoline found to be the most potent compound of the series, more potent than the standard drug phenylbutazone.

Keywords: Indoles, Pyrazolines, Isoxazolines, Ulcerogenic activity, Anti-inflammatory activity.
Synthesis and Characterization of Thiadiazole Pyrazolene Anthranilic Acid Derivatives as Potent Anti-inflammatory Agents

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Several new substituted thiadiazole pyrazolene anthranilic acid derivatives were synthesized. These compounds also evaluated for their anti-inflammatory and analgesic activities. Compound 2-((5-(3-(2,6-dichloro)acrylamido)-1,3,4-thiadiazol-2-yl)methyl amino)-benzoic acid (5b) and 2-((5-(1-acetyl-5-(2,6-dichloro)-4,5-dihydro-1H-pyrazol-3-ylamino)-1,3,4-thiadiazol-2-yl)methyl amino)benzoic acid (6b) were found to be most active compounds of this series, which exhibits 38.10 & 48.50% anti-inflammatory activity while, 36.24 & 40.10 % analgesic activity, respectively. The structures of all the compounds were characterized by analytical data, IR, ¹H NMR and mass spectrometry.

Keywords: Thiadiazoles, Pyrazolene, Anthranilic acid derivatives, Analgesic activity, Anti-inflammatory activity.
Synthesis, Characterization and Bioactivity of Propranolol and its Derivatives

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Herein, the conventional method used for β-blocker synthesis is initiated by refluxing biphenyl-2-ol (1) with an epoxy ring (2) in the presence of K$_2$CO$_3$ to obtain 2-[(biphenyl-2-yloxy)methyl]oxirane (3). Compound (3) was then reacted with 99% isopropylamine (4) and various substituted phenols (6a-i) to form 1-(biphenyl-2-yloxy)-3-(propan-2-ylamino)propan-2-ol (5) and 1-(2,6-dimethyl-4-methoxy-4-chloro-3-hydroxy-/2,6-dimethoxy-/3,4-dimethyl-4-amine-/4-bromo/3,4-dinitro-/2,4-dihydroxyphenoxy)-3-(biphenyl-2-yloxy)-propan-2-ols (7a-i), respectively. The synthesized compounds were analyzed by $^1$H NMR and FTIR spectroscopy to determine their structure and also evaluated for their antifungal activity against *Rhizoctonia solani* and *Aspergillus niger* using the food poison technique. From the activity data, it was found that compound 1-(biphenyl-2-yloxy)-3-(propan-2-ylamino)-propan-2-ol (5) was most active against both the fungi *Rhizoctonia solani* and *Aspergillus niger*. The antibacterial activity was also determined against *Bacillus* species by zone of inhibition method. The compounds (5, 7a-i) were also evaluated for its herbicidal activity.

Keywords: Propranolol, β-Blockers, Antifungal activity, Herbicidal activity, Antibacterial activity.
PM3 Method based QSAR Study of the Derivatives of Thiadiazole and Quinoxaline for Antiepileptic Activity using Topological Descriptors

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QSAR study of the derivatives of thiadiazole and quinoxaline has been performed for the antiepileptic activity using the topological descriptors viz., molar refractivity, shape index (basic kappa, order 1), shape index (basic kappa, order 2), shape index (basic kappa, order 3), valence connectivity index (order 0, standard), valence connectivity index (order 1, standard) and valence connectivity index (order 2, standard). In the best QSAR model, the descriptors are molar refractivity, shape index (basic kappa, order 1), shape index (basic kappa, order 3) and valence connectivity index (order 0, standard).

In this QSAR model, the regression coefficient is 0.872435 and cross-validation coefficient is 0.832189, which indicate that this QSAR model can be used to predict the antiepileptic activity of any compound belonging to this series. QSAR model developed using single descriptor shape index (basic kappa, order 1) or shape index (basic kappa, order 3) or valence connectivity index (order 2, standard) also has good predictive power.

Keywords: QSAR models, Thiadiazole, Quinoxaline, Descriptors, Antiepileptic activity, Computational chemistry.
PM3 Method based QSAR Study of the Derivatives of Thiadiazole and Quinoxaline for Antiepileptic Activity using Quantum Mechanical and Energy Descriptors

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QSAR analysis of the derivatives of thiadiazole and quinoxaline has been made for antiepileptic activity (pED₅₀) using quantum mechanical and energy descriptors. The descriptors ionization potential, HOMO energy, LUMO energy, electron affinity, total energy, conformation minimum energy and log P have been used for QSAR analysis. The PM3 method has been employed for the calculation of descriptors. The best QSAR model has been obtained by using the descriptors electron affinity, total energy, conformation minimum energy and log P in which regression coefficient is 0.836651 and cross-validation coefficient is 0.761455. Also the single descriptor total energy is able to produce good QSAR model and hence the antiepileptic activity of any compound of the series can be predicted by calculating the value of total energy.

Keywords: Descriptors, QSAR analysis, PM3 method, Antiepileptic activity, Regression coefficient, Cross-validation coefficient.
Synthesis, Characterization, Antimalarial and Anticancer Activities of Few New Amino Analogues of 1,4-Naphthoquinone

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Present study involves the synthesis, characterization, antimalarial and anticancer activities of some novel substituted amino analogues of 1,4-naphthoquinone. The chloro group present in the key starting materials like 2,3-dichloro-1,4-naphthoquinone (1) and 2-chloro-3-[trans-4-(4-chlorophenyl)cyclohexyl]-1,4-naphthoquinone (2) was replaced by substituted amines. These analogues were isolated, purified and screened for antimalarial and anticancer activities. A few of the novel compounds were found to possess substantial biological activity and are reasonably potent.

Keywords: Naphthoquinone derivatives, Synthesis, Characterization, Antimalarial activity, Anticancer activity.
Synthesis of bis Azo Disperse Dyes derived from 2-Amino-4(4'-nitro phenyl)thiazole having tertiary-Amines as Coupling Component, their Characterization and Evolution of Dyeing Characteristics

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2-Amino-4(4'-nitro phenyl)-1,3-thiazole was used to couple with diazotized 2-amino-5(4'-nitro phenyl)-1,3,4-thiadiazole to gave mono azo disperse dye with good yield. This mono azo disperse dye was further diazotized and coupled with different tertiary amines which were couplers that yielded bis azo disperse dyes (AJ1-AJ15). The synthesized dyes were analyzed via elemental analysis, IR, ¹H NMR spectral analysis. All the synthesized dyes were applied on polyester fiber by using HTHP method and their dyeing performance and their fastness characteristics were studied.

Keywords: 2-Amino-5(4'-nitro phenyl)-1,3,4-thiadiazole, 2-Amino-4(4'-nitro phenyl)-1,3-thiazole, bis azo dyes, Polyester.
in silico Analysis of 4-((1-(3-Nitrophenyl)-5-oxo-3-phenyl-4,5-dihydro-1H-pyrazol-4-yl)methyl)benzoic Acid: An Emerging 3-CLpro Non-peptidic Inhibitors for COVID-19

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Existing study involves effort to forecast absorption, distribution, metabolism, excretion, toxicity and polypharmacological profile of 4-((1-(3-nitrophenyl)-5-oxo-3-phenyl-4,5-dihydro-1H-pyrazol-4-yl)-methyl)benzoic acid (NPOPPBA), a 3CLpro non-peptidic inhibitors with the aid of by means of in silico methods. In the beginning, PASS online computational software’s utilized to investigate pharmacological action of NPOPPBA. Followed by, Swiss ADME online tool utilized to estimate of physical parameters, chemical properties, log P, solubility, absorption, distribution, metabolism, excretion, drug like property and medicinal chemistry. Lastly, XUNDRUG eMolTox online tool utilized to forecast toxicity. End result of PASS online prediction tool confirmed that NPOPPBA may be used as Fusarinine-C ornithinesterase inhibitor, which may be beneficial in most cancers treatment; Swiss ADME end outcome confirmed molecule may orally absorbable but not able to pass lipophilic membrane of brain and hence will not able to show undesirable effect centrally. Observations of bioavailability study shows NPOPPBA may be taken into consideration as a drug like because it shows all parameters falls inside red location of graph. The log P become observed about 3.7 signifying NPOPPBA may absorb on oral administration, solubility in water was found to be poor demonstrating need of attempts to enhance it in formulation development. This molecule can also additionally inhibits CYP2C19 which performs an essential function in metabolism of drugs live omeprazole, which are utilized to cure of gastrointestinal disorder and need to take precaution in the course of use of proton pump inhibitors. It is also CYP2C9 inhibitor therefore due care need to be taken for drugs undergoing phase I metabolism. XUNDRUG online resource outcomes confirmed hepatic and nephron toxicity possibility of NPOPPBA. Here from this existing analysis, it may be confirmed that the beneficial absorption, distribution, metabolism, excretion, drug like property and easy in synthesis of current molecule recommended that NPOPPBA may be an amazing medicinal agent in upcoming COVID-19 treatment.

Keywords: COVID-19, Drug likeness, 3CLpro non-peptidic inhibitors.