**Best Research Papers (10)**

1. **Sawant Ramesh**, Wadekar Jyoti, Ukirde Rushikesh and Barkade Ganesh. Synthesis, Molecular Docking and Anticancer Activity of Novel 1, 3-Thiazolidin-4-Ones. **Pharmaceutical Sciences**. Vol. 27(3), 345 - 352, (2021).

**[Cite Score – 1.7**]

In a present study series of 2-substituted-3-(1H-benzimidazole-2-yl)-thiazolidin-

4-ones were designed, synthesized by the microwave-assisted system, and characterized by melting point, IR, 1H NMR, and mass spectroscopy. All the newly synthesized compounds were examined for their in vitro anticancer activity against breast cancer cell line MCF-7 by Sulforhodamine B (SRB) assay.

The compounds AB-12 (GI50: 28.5 μg/ml) and AB-6 (GI50: 50.7 μg/ml) exhibited

significant cell growth inhibitory activity.

These results indicate that compound AB-12 and AB-6 as related polo-like kinase 1 inhibitors compounds could be lead compounds for further development of anticancer

agents.

1. **Ramesh L. Sawant**, Rahul Kale, Jyoti Wadekar, Amol Ghodechor, Abhijit Sherkar. Targeting VEGF to Design Pyrimidines against Breast Cancer and Diabetic Retinopathy. **Moroccan Journal of Chemistry**. Vol. 6(4), 689-699, (2018). **[IMPACT FACTOR – 0.552**].

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| A library of 900 pyrimidine derivatives was screened virtually on vascular endothelial growth factor (VEGF) using Vlife MDS 4.1 software to identify potential candidates with anticancer and anticataract activity. A series of 2,4,6-substituted pyrimidine derivatives were synthesized in good yields from chalcones, where chalcones have been prepared according to claisen - schimidt condensation by condensing various ketones with aromatic aldehyde in presence of ethanol and sodium or potassium hydroxide. Their structures were confirmed by IR, 1H NMR and mass spectra. Biological screening of the potential candidates was done for anticancer and anticataract activity. The present study reveals that a derivative of pyrimidine shows activity against breast cancer and diabetic retinopathy through inhibition of VEGF. |

1. **Ramesh L. Sawant**, Jyoti B. Wadekar, Santosh B. Kharat, Hitakshi S. Makasare. Targeting PPAR-γ to Design and Synthesize Antidiabetic Thiazolidines. **EXCLI Journal**. Vol. 17, 598-607, (2018). **[IMPACT FACTOR – 2.424**].

A series of thiazolidine derivatives were designed by docking into PPAR-γ active site. The structure of target was obtained from the protein data bank (PDB ID P37231). A library of 200 molecules was prepared on random basis. Molecular docking studies were performed using VLife MDS 4.3 software. After molecular docking studies, the

4-substituted-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylic acid N-[4-(2,4-dioxo-thiazolidin-5-ylidenemethyl)-phenyl]-hydrazides (**4a-4h**) were selected for synthesis. The progress of reaction and purity of the synthesized compounds were monitored by TLC and melting point. Structures of title compounds were confirmed by elemental analysis, IR, 1H NMR and mass spectral data. The antidiabetic activity of title compounds was performed using the Wistar rats by alloxan-induced method. The compounds have shown antidiabetic activity comparable with the standard drug pioglitazone. These findings suggest that potent antidiabetics can be generated by substituting nonpolar, electron withdrawing substituents at the fourth position of pyrimidine skeleton and hydrogen bond acceptor at the nitrogen of the thiazolidine nucleus, to inhibit peroxisome proliferator-activated receptor-γ.

1. **Ramesh L. Sawant\***, Prashant D. Lanke and Jyoti B. Wadekar. Tyrosinase Inhibitory Activity, 3D QSAR and Molecular Docking Study of 2, 5-Disubstituted-1, 3, 4-Oxadiazoles. **Journal of Chemistry.** Vol. 2013, Article ID 849782, 7 pages, (2013).

DOI: 10.1155/2013/849782. [**IMPACT FACTOR – 0.716**].

In continuation with our research program, in search of potent enzyme tyrosinase inhibitor, a series of synthesized 2,5-disubstituted 1,3,4-oxadiazoles have been evaluated for enzyme tyrosinase inhibitory activity. Subsequently, 3D QSAR and docking studies were performed to and optimum structural requirements for potent enzyme tyrosinase inhibitor from this series. e synthesized 20 compounds of 2,5-disubstituted-1,3,4-oxadiazole series were screened for mushroom tyrosinase inhibitory activity at various concentrations by enzyme inhibition assay. e percentage enzyme inhibition was calculated by recording absorbance at 492 nm with microplate reader. 3D QSAR and docking studies were performed using VLife MDS 3.5 software. In the series 2,5- disubstituted-1,3,4-oxadiazoles enzyme tyrosinase inhibitory activity was found to be dose dependent with maximum activity for compounds 4c, 4h, 4m, and 4r. 3D QSAR and docking studies revealed that more electropositive and less bulky substituents if placed on 1,3,4-oxadiazole nucleus may result in better tyrosinase inhibitory activity in the series.

1. **Ramesh L. Sawant\*,** Charusheela A. Bansode and Jyoti B. Wadekar.In vitro anti-inflammatory potential and QSAR analysis of oxazolo / thiazolo pyrimidine derivatives. **Medicinal Chemistry Research.** Vol. 22(4), 1884–1892, (2013). **[IMPACT FACTOR – 1.271**]

Twenty-six different benzylidene oxazolo/ thiazolo (3,2-a)-pyrimidine-6-carboxamide derivatives were synthesized and evaluated for their anti-inflammatory potential by protein denaturation method. The structures of title compounds were characterized by IR and NMR spectral data. The SAR studies reveal that compounds containing electron withdrawing polar group at para position of 5-phenyl ring and electron withdrawing non-polar group at para position of 2-benzylidene moiety of thiazolo pyrimidine nucleus have better anti-inflammatory potential. The 2DQSAR studies were performed on VLife MDS software which reveals that anti-inflammatory potential of benzylidene- 3-oxo-5H-oxazolo/thiazolo (3,2-a)-pyrimidine-6-carboxamides is dependent on estate contribution, alignment independent, individual and path count descriptors.

1. **Ramesh L. Sawant**\* and Manish S. Bhatia. QSAR Analysis of 2-Oxo-1,2,3,4-Tetrahydropyrimidine Analogues of Antibacterials. **Collect. Czech. Chem. Commun.** Vol. 74(9), 1361–1373 (2009).

**DOI:**10.1135/cccc2009054 **[IMPACT FACTOR – 0.784**]

The purpose of this study was to synthesize several 3-benzoyl-5-acyl-6-methyl-4-substituted-2- oxo/thioxo-1,2,3,4-tetrahydropyrimidines, evaluate them for their antibacterial activity and to establish correlation between the activity and physicochemical properties. 5-Acyl-6-methyl-4-substituted-2-oxo/thioxo-1,2,3,4- tetrahydropyrimidines (A) were synthesized by cyclocondensation reaction between appropriate aldehyde, acetoacetate and urea/thiourea in presence of aluminium chloride and hydrochloric acid which upon treatment with benzoyl chloride in presence of pyridine in benzene furnish the title compounds (1-28). The structures of all title compounds have been confirmed on the basis of their analytical, IR and NMR spectral data. The title compounds have been tested for antibacterial activity against Staphylococcus aureus. The compounds were divided into training and test sets. A quantitative structure activity relationship study was made using various descriptors. Several statistical expressions were developed using stepwise multiple linear regression analysis. The best quantitative structure activity relationship model was further cross validated. The study revealed that total positive partial charge (PC+) and total polar negative Van der Waals surface area (Q\_VSA\_PNEG) contributes negatively where as contribution of Van der Waals surface area to molar refractivity (SMR\_VSA7) contributes positively to the antibacterial activity. The compounds with improved antibacterial potential can be successfully designed with selected quantitative structure activity relationship model.

1. **Ramesh Sawant**\* and Deepali Kawade. Synthesis and biological evaluation of some novel 2-phenyl benzimidazole-1-acetamide derivatives as potential anthelmintic agents. **Acta Pharmaceutica**. Vol. 61 (3), 353-361, 2011.

DOI: 10.2478/v10007-011-0029-z **[IMPACT FACTOR – 2.23**].

The present study describes synthesis of a series of 2-phenyl benzimidazole-1-acetamide derivatives and their evaluation for anthelmintic activity using Indian adult earthworms, Pheretima posthuma. The structure of the title compounds was elucidated by elemental analysis and spectral data. The compounds 4-({[2-(4-nitrophenyl)-1H-benzimidazol-1-yl]acetyl}amino) benzoic acid (3a), N-ethyl-2-[2-(4-nitrophenyl)-1H-benzimidazol-1-yl] acetamide (3c), N-benzyl-2-[2-(4-nitrophenyl)-1H-benzimidazol-1-yl] acetamide (3d), N-(4-hydroxyphenyl)-2-[2-(4-nitrophenyl)-1H-benzimidazol-1-yl] acetamide (3f), 2-[2-(4-nitrophenyl)-1H-benzimidazol-1-yl]-N-phenyl acetamide (3h), 2-[2-(4-chlorophenyl)-1H-benzimidazol-1-yl]-N'-phenylacetohydrazide (3k), 2-[2-(4-chlorophenyl)-1H-benzimidazol-1-yl]-N-(4-nitrophenyl) acetamide (3n) and 2-[2-(4-chlorophenyl)-1H-benzimidazol-1-yl]-N-phenyl acetamide (3q) were found better to paralyze worms whereas N-ethyl-2-[2-(4-nitrophenyl)-1H-benzimidazol-1-yl] acetamide (3c), N-(4-nitrophenyl)-2-[2-(4-nitrophenyl)-1H-benzimidazol-1-yl] acetamide (3e), 4-({[2-(4-chlorophenyl)-1H-benzimidazol-1-yl] acetyl}amino) benzoic acid (3j), 2-[2-(4-chlorophenyl)-1H-benzimidazol-1-yl]-N-ethyl acetamide (31) and 2-[2-(4-chlorophenyl)-1H-benzimidazol-1-yl]-N-phenyl acetamide (3q) were better to cause death of worms compared to the anthelmintic drug albendazole.

1. **Ramesh Sawant**\* and Varsha Sarode. Synthesis, Spectral Characterization and Analgesic Activity of 2-Methylthio-1, 4- Dihydropyrimidines. **Iranian J. Pharm. Res**. Vol. 10 (4), 733-739, 2011. **[IMPACT FACTOR – 1.69**]

A series of 2-methylthio-1,4-dihydropyrimidine derivatives (II) were synthesized in good yields by alkylation of 1,2,3,4-tetrahydropyrimidines (I) with methyl iodide in the presence of pyridine. Their structures were confirmed by elemental analysis, IR and 1 H NMR spectra. The compounds were tested for analgesic activity by acetic acid induced writhing method. Compounds IIh, IIe, IIk and IIl showed excellent to good analgesic activity. Other compounds showed moderate analgesic activity. The observed analgesic activity is mainly because of inhibition of the peripheral pain mechanism by the title compounds.

1. **Ramesh Sawant**\*, Lokesh Bhangale, Jyoti Wadekar and Pandurang Gaikwad. Substituent selection for design and synthesis of antimicrobial 1,3 oxazines: A Topliss modified approach. **Redactia Revistei FARMACIA** Vol. 60 (1), 32-39, 2012. **[IMPACT FACTOR – 1.43**].

The purpose of the present work was to select substituents by using Topliss modified approach to synthesize new 1,3 oxazines with antimicrobial effect. In the series of 6-[4-substitutedphenyl]-4-phenyl-6H-1,3-oxazin-2-amines and N-[6-(4-substitutedphenyl)- 4-phenyl-6H-1,3-oxazinyl] acetamides, substituents at fourth position of the phenyl ring were selected according to the Topliss modified approach and the initial set of compounds was synthesized. The antimicrobial screening revealed that compounds with methoxy substituent having negative sigma (-0.04) and negative pi (-0.27) values are good antimicrobial agents showing low minimum inhibitory concentration (MIC). The hydroxyl group substituent with more negative sigma (-0.61) and pi (-0.37) values was selected to synthesize final set compounds and were found better antimicrobials than the initial set of compounds. The study revealed that electron donating polar substituents at fourth position of the phenyl ring are required to improve antimicrobial potential in the series of 6-[4- substitutedphenyl]-4-phenyl-6H-1,3-oxazin-2-amines and N-[6-(4-substitutedphenyl)-4- phenyl-6H-1,3-oxazinyl] acetamides.

1. **Ramesh L. Sawant**\*, Varsha I. Sarode, Ganesh D. Jadhav and Jyoti B. Wadekar. Synthesis, molecular docking and cardioprotective activity of 2-methylthio-1, 4-dihydropyrimidines. **Medicinal Chemistry Research**. Vol. 21(8), 1825–1832, (2012).

DOI: 10.1007/s00044-011-9700-7. **[IMPACT FACTOR – 1.96**].

A series of 2-methylthio-1,4-dihydropyrimidinederivatives (IIa–IIl) were synthesized in good yields byalkylation of 1,2,3,4-tetrahydropyrimidines (Ia–Il) withmethyl iodide in the presence of pyridine. Their structureswere conﬁrmed by elemental analysis, IR, and 1H NMRspectra. Molecular docking of title compounds was doneusing VLife MDS 3.5 on voltage-dependent calciumchannel b subunit functional core and its complex with thea1 interaction domain i.e. AID-b complex (PDB code1T3L) to identify potential candidat es with minimum dockscore for cardioprotective activity. Biological screening ofthe potential candidates (IIf and IIi) was done for cardio-protective activity. Adult Sprague–dawley rats were pre-treated with test compounds IIf and IIi. After the treatmentperiod, adrenaline was subcutaneously injected to rats at aninterval of 24 h for 2 days to induce myocardial injury.After 48 h, rats were anaesthetized and electrocardio-graphic (ECG) observations were performed. Poten tialcompounds IIf and IIi showed signiﬁcant cardioprotectiveactivity against adrenaline-induced myocardial infarction inrats. Adrenaline-induced ECG alterations such as reducedR–R interval, increased heart rate, reduced P duration, andST-segment elevation were brought to the near norm alvalues by pretreatment of compounds IIf and IIi.