ScienceDirect

European Journal of Medicinal Chemistry

Volume 245, Part 1, 5 January 2023, 114889

Research paper

Design, synthesis, and biological evaluation of novel quinoline derivatives as small molecule mutant EGFR inhibitors targeting resistance in NSCLC: *In vitro* screening and ADME predictions

Ramakant A. Kardile [a], Aniket P. Sarkate [b], Deepak K. Lokwani [c], Shailee V. Tiwari [d], Rajaram Azad [e], Shankar R. Thopate [a]

Show more

https://doi.org/10.1016/j.ejmech.2022.114889

Get rights and content

Highlights

- Quinoline substituted sulphonamide (**9**–**21**) and amide (**23**–**29**) derivatives -to be anticancer agents.
- Compound **21** was found to be the most potent and exhibited promising inhibitory enzymatic activity.
- Docking studies revealed the binding of synthesised compounds is identical to binding patterns of EGFR-TK inhibitor's protein.
- MD simulation study was performed for EGFR-compound **21** complex, indicating the stability in both ATP and allosteric site of enzyme.

Polycyclic Aromatic Compounds >
Volume 43, 2023 - Issue 10

Research Articles

Molecular Docking Studies and Application of 6-(1-Arylmethanamino)-2-Phenyl-4*H*-Chromen-4-Ones as Potent Antibacterial Agents

Nitin M. Thorat, Vinayak Shahaji Khodade, Ajit P. Ingale, Deepak K. Lokwani, Aniket P. Sarkate & Shankar R. Thopate

Pages 8653-8666 | Received 01 Aug 2022, Accepted 16 Nov 2022, Published online: 09 Dec 2022

Cite this article https://doi.org/10.1080/10406638.2022.2150238 Check for updates

Abstract

The present article depicts the synthesis of the series of 6-(1-arylmethanamino)-2-phenyl-4H-chromen-4-ones and their antibacterial activity against the *S. aureus*. 6-(1-arylmethanamino)-2-phenyl-4*H*-chromen-4-ones (**1a–1n**) were obtained via reductive amination reaction of 6-aminoflavone with various commercially available aldehydes. Synthesized compounds and 6-aminoflavone (**1**) were assessed for their antimicrobial activities against the *S. aureus*. 6-aminoflavone (**1**) was found to have an MIC of 2 µg/mL. The compounds with side chains 4-fluorobenzyl (**1a**), 4-chlorobenzyl (**1b**), 4-nitrobenzyl (**1e**), 4-methoxybenzyl (**1g**) and (quinolin-2-yl)methyl (**1n**) were found to

Click chemistry inspired syntheses of new amide linked 1,2,3-triazoles from naphthols: biological evaluation and in silico computational study

Published: 30 March 2023

Volume 49, pages 2725–2753, (2023) Cite this article

Satish V. Akolkar, Mubarak H. Shaikh, Mininath K. Bhalmode, Prabhakar U. Pawar, Jaiprakash N. Sangshetti, Manoj G. Damale & Bapurao B. Shingate

Abstract

In search of new active molecules, a small focused library of new 1,2,3-triazoles derived from naphthols were efficiently prepared via the click chemistry approach. The synthesized triazole derivatives were evaluated for their antifungal, antioxidant and antitubercular activities. Furthermore, to rationalize the observed biological activity data, the molecular docking study has also been carried out against the active site of cytochrome P450 lanosterol 14α-demethylase of *C. albicans* to understand the binding

Archiv der Pharmazie / Volume 356, Issue 8 / 2300171

REVIEW ARTICLE

Curcumin-based bioactive heterocycles derived via multicomponent reactions

Amol A. Nagargoje, Mubarak H. Shaikh, Bapurao B. Shingate

First published: 12 June 2023
https://doi.org/10.1002/ardp.202300171
Citations: 3

Abstract

Curcumin is an important phytochemical, found in the Asian countries, especially in the Indian subcontinent. The use of this "privileged natural product" in the diversity-oriented synthesis of curcumin-based heterocycles via multicomponent reactions (MCRs) is the subject of interest for many medicinal chemists across the globe. This review particularly focuses on the reactions involving curcuminoids as one of the reactants in the MCRs of curcuminoid to synthesize curcumin-based heterocycles. Also, the various pharmacological activities of curcumin-based heterocycles generated via the MCR approach are discussed. The research work published in the last 10 years is in the focus of this review article.

CONFLICTS OF INTEREST STATEMENT

The authors declare no conflicts of interest.

REFERENCES

1 A. G. Atanasov, S. B. Zotchev, V. M. Dirsch, C. T. Supuran, *Nat. Rev. Drug Discov.* 2021, **20**, 200.

CAS | PubMed | Web of Science® | Google Scholar

2 A. Harvey, *Drug Discov. Today* 2008, **13**, 894.

Polycyclic Aromatic Compounds >
Volume 44, 2024 - Issue 9

Research Articles

New 1,2,3-Triazole-Tethered Chalcone Derivatives: Synthesis, Bioevaluation and Computational Study

Ramesh A. Kawale, Hemantkumar N. Akolkar, Mubarak H. Shaikh, Vijay M. Khedkar, Deepak N. Raut, Nirmala R. Darekar, ...show all

Pages 6232-6247 | Received 12 Dec 2022, Accepted 23 Oct 2023, Published online: 06 Nov 2023

Cite this article https://doi.org/10.1080/10406638.2023.2276239 Check for updates

Abstract

In search of new active molecules, a small focused library of novel 1,2,3-triazoles based chalcone derivatives has been efficiently prepared *via* the click chemistry approach. All the synthesized compounds were characterized with the help of IR, ^{1}H NMR, ^{13}C NMR and mass spectroscopic techniques. The synthesized novel 1,2,3-triazoles based chalcone derivatives evaluated for their anti-inflammatory and antioxidant activity. Furthermore, molecular modeling study could support these outcomes by demonstrating very good binding affinities at the active site of the cyclooxygenase 2 (COX-2) iterating the potential of this scaffold for further optimization.

Polycyclic Aromatic Compounds >
Volume 44, 2024 - Issue 4

Research Article

Antibacterial Activity of Novel 1-Cyclopropyl-6,7-Difluoro-8-Methoxy-4-Oxo-1,4-Dihydroquinoline-3-Carbohydrazide Derivatives

Zaki Ahmed B. Munshi, Mubarak H. Shaikh, Pravinsing S. Girase, Iqrar Ahmad, Harun Patel & Bhata R. Chaudhari

Pages 2703-2714 | Received 01 Dec 2022, Accepted 29 May 2023, Published online: 09 Jun 2023

Cite this article https://doi.org/10.1080/10406638.2023.2220866 Check for updates

Abstract

We have synthesized and characterized *N*-substituted-1-cyclopropyl-6,7-difluoro-8-methoxy-4-oxo-1,4-dihydroquinoline-3-carbohydrazide derivatives and were evaluated for their antibacterial activity against *Staphylococcus Aureus*, *Micrococcus Luteus*, *Bacillus subtilis* and Gram-negative *Escherichia Coli*, *Pseudomonas aeruginosa*

Journal of the Maharaja Sayajirao University of Baroda
ISSN :0025-0422

SYNTHESIS AND ANTIBACTERIAL SCREENING OF IMIDAZOLE CONTAINING SUBSTITUTED FLAVONES

Rupali S. Endait, Department of Chemistry, Radhabai Kale Mahila Mahavidyalaya, Ahmednagar-414001, Maharashtra, India
Pratibha V. Randhavane, Department of Chemistry, S. S. G. M. College, Kopargaon, Ahmednagar, 414001, Maharashtra, India

ABSTRACT
Imidazole anchored chromones (2) and chlorochromones (3) were synthesized from substituted chalcones (1) in Scheme I. Formation and structures of all the compounds were confirmed by spectroscopic techniques and elemental analytical data. All the synthesized compounds were screened for antibacterial activity against four bacterial strains (*Escherichia coli*, *Pseudomonas fluorescens*, *Staphylococcus aureus*, *Bacillus subtilis*) using Ampicillin as a standard drug.
KEYWORDS: Antibacterial activity, Chromones, Imidazole

INTRODUCTION
Due to biological importance of flavones chemists take good efforts for synthesis of their novel derivatives. Position and nature of substituents decides potential of biological activities associated with flavones.

Imidazole derivatives have occupied a predominant role in the field of medicinal chemistry. Incorporation of imidazole motif is significant synthetic strategy in drug chemistry. Imidazole containing compounds have shown activities like anticancer [1], antibacterial [1], antimicrobial [2], antioxidant [3], antitubercular [4], antirheumatoid arthritis [5] and antiviral [6].

Chromones are heterobicyclic compound occurred in nature as well as synthetic flavones are also reported by researchers. Both natural and synthetic flavone is an important building block in drug discovery. They are known for their diverse biological activities like antimicrobial [7], antiglycation [8], antioxidant [9-10], anti-inflammatory [11], analgesic [11], selective agonists for neuromedin U 2 receptor [12], etc.
Keeping in mind the biological activities associated with chromones, in present study we have synthesized biologically important imidazole containing substituted chromones with the evaluation of antibacterial potential.

RESULTS AND DISCUSSION
Dawane B S [13] have reported the synthesis of (*E*)-3-(2-butyl-4-chloro-1*H*-imidazol-5-yl)-1-phenylprop-2-en-1-ones (**1a-g**). Chalcones (**1**) in presence of DMSO/I_2 gave chromones (**2a-f**). IR spectrum of compound **2a** showed band at 1622 cm^{-1} due to carbonyl. The ^1H NMR spectrum of **2a** showed singlet for chromone proton at δ 6.77 ppm. Chalcones (**1**) in presence of copper chloride in DMSO gave 3-chlorochromones (**3a-g**). IR spectrum of compound **3a** showed a band at 1622 cm^{-1} due to carbonyl functional group.

EXPERIMENTAL SECTION
Physical constants were recorded in liquid paraffin bath with the help of capillaries and are uncorrected. IR spectra were recorded on *Shimadzu* IR Affinity-1S fourier transform infrared spectrophotometer. ^1H NMR spectra were recorded on Bruker Avance II 400 MHz NMR spectrometer with DMSO-d_6 as a solvent and TMS as an internal standard. Peak values are shown in δ (ppm). Mass spectra were recorded on Water acquity TQD mass spectrometer.

Polycyclic Aromatic Compounds ›
Volume 44, 2024 - Issue 9

Research Articles

New 1,2,3-Triazole-Tethered Chalcone Derivatives: Synthesis, Bioevaluation and Computational Study

Ramesh A. Kawale, Hemantkumar N. Akolkar, Mubarak H. Shaikh, Vijay M. Khedkar, Deepak N. Raut, Nirmala R. Darekar, ...show all

Pages 6232-6247 | Received 12 Dec 2022, Accepted 23 Oct 2023, Published online: 06 Nov 2023

Cite this article https://doi.org/10.1080/10406638.2023.2276239 Check for updates

Abstract

In search of new active molecules, a small focused library of novel 1,2,3-triazoles based chalcone derivatives has been efficiently prepared *via* the click chemistry approach. All the synthesized compounds were characterized with the help of IR, ^{1}H NMR, ^{13}C NMR and mass spectroscopic techniques. The synthesized novel 1,2,3-triazoles based chalcone derivatives evaluated for their anti-inflammatory and antioxidant activity. Furthermore, molecular modeling study could support these outcomes by demonstrating very good binding affinities at the active site of the cyclooxygenase 2 (COX-2) iterating the potential of this scaffold for further optimization.

Exploration of 2-(Substituted Phenyl)-thiazolidin-4-one as Anticancer Agents

Published: 10 January 2024

Volume 49, pages S81–S95, (2023) Cite this article

Russian Journal of Bioorganic Chemistry

Aims and scope

Submit manuscript

Rahul B. Shinde, Dattatraya N. Pansare, Aniket P. Sarkate, Shailee V. Tiwari, Rohini N. Shelke, Deepak Lokwani, Shirish Jain & Ashok M. Zine

Abstract

A facile synthesis of (2-(substituted phenyl)-thiazolidin-4-one by using recyclable catalyst β-cyclodextrinSO_3H has been achieved. It has been synthesized by successive three-component reaction of substituted benzaldehyde, 6/7-aminoflavone, thioglycolic acid with recyclable catalyst β-cyclodextrin-SO_3H. Our research team has performed *in vitro* anticancer study of all synthesized compounds. Among these synthesized compounds, (**IVf**) and (**IVn**) have demonstrated significant *in vitro* anticancer activity. The compound (**IVn**) was found to be very potent to standard drug Adriamycin. Additionally, the mechanism of anticancer activity was established by examining the inhibitory activity of synthesized compounds against Human Topoisomerase II (Topo-II). The compounds (**IVf**) and (**IVn**) was found to have a good ability to inhibit Topo-II

Synthesis of (Z)-5-((Substituted-2-(substituted phenyl)-quinoline-3-yl)methylene) Thiazolidinone as Antimicrobial and Anticancer Agent

Published: 23 November 2023

Volume 49, pages 1398–1407, (2023) Cite this article

Rahul B. Shinde, Dattatraya N. Pansare, Rohini N. Shelke, Mukund N. Bangal, Aniket P. Sarkate, Shailee V. Tiwari, Dhanraj Kamble, Pravin Chavan & Ashok M. Zine

Abstract

A simplistic synthesis of (Z)-5-((substituted-2-(substituted phenyl)quinolin-3-yl)methylene)-2-thioxothiazolidin-4-one derivatives has been accomplished by employing acetic acid as the solvent and sodium acetate as the catalyst. We used the Suzuki-Miyaura cross coupling reaction to create carbon-carbon bonds. Our method is practical and has many benefits, such as a quicker reaction time and a higher yield under reflux conditions. For their anticancer and antibacterial activities, all produced compounds were described and tested. Compounds are some of these (**IVa**), (**IVb**), and

ScienceDirect

Results in Chemistry

Volume 6, December 2023, 101134

A facile synthesis and characterization of some novel benzimidazole derivatives

Rahul B. Shinde [a], Dattatraya N. Pansare [b], Rohini N. Shelke [c], Aniket P. Sarkate [d], Shailee V. Tiwari [e], Mukund N. Bangal [a], Devidas S. Bhagat [f], Ashok M. Zine [a]

Show more

https://doi.org/10.1016/j.rechem.2023.101134

Get rights and content

Abstract

We successfully synthesized a series of novel benzimidazole derivatives with high yields in our current research study. The synthesis procedure involved condensing Ethyl 3-[[3-amino-4-(treiethylamino) benzoyl] (pyridine-5-yl) amino]-propanoate with various aromatic carboxylic acids, using EDC.HCl and a small amount of DMAP as catalysts. The resulting compounds underwent cyclization through coupling in the presence of acetic acid under reflux conditions. Notably, both the coupling and cyclization reactions were efficiently achieved, with the former occurring at room temperature and the latter at reflux temperature. Our synthesis method is both environmentally friendly and cost-effective. To characterize the synthesized compounds, we employed modern spectroscopic techniques such as FT-IR, ^{1}H NMR, ^{13}C NMR, and mass spectrometry. The compound **4i** shown the most potent *in vitro* anticancer activity. The compound **4e** and **4f** were also found to have good *in vitro* anticancer activity compared to other synthesized compounds. The result of *in vitro* anticancer activity says that the combination of pyridine, benzimidazole and thiophene ring best apposite for the development of novel anticancer agent. The other derivatives have also shown good activity such as compounds **4b, 4c, 4h** and **4j** with electron withdrawing group on phenyl ring.

Pyruvic acid-catalyzed one-pot three-component green synthesis of isoxazoles in aqueous medium: a comparable study of conventional heating versus ultra-sonication

Regular Article Published: 27 January 2022

Volume 134, article number 15, (2022) Cite this article

Santosh R Deshmukh, Archana S Nalkar & Shankar R Thopate

Abstract

A mild and efficient route for the one-pot synthesis of isoxazole derivatives has been developed using pyruvic acid as a catalyst under an aqueous medium. The reaction was carried out under conventional as well as ultrasonic conditions to afford the desired product in good yield. The features of this protocol are the use of environmental-friendly, commercially available, biodegradable catalyst, use of biologically safe solvent, simple experimental procedure and short reaction times. The given protocol can be a better alternative for the synthesis of 4*H*-isoxazol-5-one derivatives as compared to traditional methods.

Biosynthesis of Palladium Nanoparticles from *Moringa oleifera* Leaf Extract Supported on Activated Bentonite Clay and Its Efficacy Towards Suzuki–Miyaura Coupling and Oxidation Reaction

Published: 20 July 2022

Volume 12, pages 785–794, (2022) Cite this article

Satish B. Manjare ✉, Priyanka D. Pendhari, Sushil M. Badade, Shankar R. Thopate & Manali S. Thopate

Abstract

A biosynthesis of PdNPs was loaded on activated Bentonite clay. The catalyst was synthesised by using universal solvent water, $PdCl_2$ and *Moringa oleifera* leaves extract. The plant leaves extract acts both as a reducing agent and also as a capping agent. The synthesised PdNPs loaded on activated Bentonite clay were characterised by using FTIR, HR-TEM, ICP-AES, XRD and FESEM/EDX. The loaded PdNPs on activated Bentonite clay gave high rate of conversions of Suzuki–Miyaura coupling products and oxidation of

Polycyclic Aromatic Compounds >
Volume 42, 2022 - Issue 9

Research Articles

Ultrasound-Promoted Pyruvic Acid Catalyzed Green Synthesis of Biologically Relevant Bis(Indolyl)Methanes Scaffold under Aqueous Condition

Santosh R. Deshmukh, Archana S. Nalkar & Shankar R. Thopate

Pages 6501-6509 | Received 26 May 2021, Accepted 16 Sep 2021, Published online: 28 Sep 2021

Cite this article https://doi.org/10.1080/10406638.2021.1984259 Check for updates

Full Article Figures & data References Supplemental Citations

Metrics Reprints & Permissions Read this article

Abstract

An efficient and green protocol has been introduced for the synthesis of medicinally important bis(indolyl)methane derivatives using pyruvic acid catalyst in the presence of water. Pyruvic acid catalyzes the reaction of aldehyde with indole efficiently and products were obtained in good to excellent yields under sonication (50 °C) or under conventional heating (80 °C). The advantages of this synthetic methodology are use of environmental-friendly, commercially available, biodegradable catalyst, short reaction times, Lewis acid-free and metal-free mild reaction conditions with excellent yields and is compatible with a wide range of electronically diverse substrates. Pyruvic acid

Letters in Organic Chemistry

Editor-in-Chief

ISSN (Print): 1570-1786
ISSN (Online): 1875-6255

Letter Article

Water-Mediated Green Synthesis of Benzimidazoles Using Pyruvic Acid: A Comparable Study of Ultra-sonication *versus* Conventional Heating

Author(s): Santosh Rangnath Deshmukh*, Archana Subhash Nalkar and Shankar Ramchandra Thopate

Volume 19, Issue 7, 2022

Published on: 11 January, 2022

Page: [511 - 519] **Pages:** 9

DOI: 10.2174/1570178618666211105092142

Price: $65

Abstract

An efficient and green protocol has been introduced for the synthesis of benzimidazole derivatives using a pyruvic acid catalyst in the presence of water. Pyruvic acid catalyses the reaction of aromatic aldehydes with o-phenylenediamine efficiently, and products were obtained in good to excellent yields under sonication (50 °C) or under conventional heating (50 °C). The advantages of this synthetic methodology are the use of eco-friendly, commercially cheap, biodegradable catalyst, metal-free and Lewis acid-free mild reaction conditions with excellent yields, short reaction times, and compatible with a wide range of electronically diverse substrates. Pyruvic acid in water as a catalyst under ultrasound irradiation can be a better alternative to synthesize benzimidazole derivatives than some of the traditional methods.

Keywords: Pyruvic acid, benzimidazole, aldehyde, o-phenylenediamine, ultrasound irradiation, green chemistry, heterocyclic chemistry.

« Previous Next »

Graphical Abstract

[DBU][OAc]-mediated synthesis and anthelmintic activity of triazole–tetrazole conjugates

Published: 17 October 2022

Volume 48, pages 5187–5208, (2022) Cite this article

Madiha A. Siddiqui, Mubarak H. Shaikh, Amol A. Nagargoje, Tarannum T. Shaikh, Vijay M. Khedkar, Prathmesh P. Deshpande & Bapurao B. Shingate

Abstract

Tetrazoles and 1,2,3-triazoles are poorly understood regarding their anthelmintic activity. Therefore, an effort was taken to identify novel chemical scaffolds as anthelmintic agents; a series of 1,2,3-triazole–tetrazole conjugates were synthesized. The synthesis of 1,2,3-triazole based tetrazole derivatives has carried out via [2+3]-cycloaddition reaction of triazolyl nitriles with sodium azide. The present design and synthetic strategy offers excellent yields of the products in the presence of [DBU][OAc] under ultrasonic irradiations. The synthesized triazole–tetrazole conjugates were characterized by spectroscopic techniques and screened for their anthelmintic activity. Most of the

Analytical Chemistry Letters ›
Volume 12, 2022 - Issue 5

Research Article

Investigation of the Anti-inflammatory potential of Mono-carbonyl Analogues of Curcumin

Amol A. Nagargoje, Satish V. Akolkar, Mubarak H. Shaikh, Hemant kumar N. Akolkar, Deepak N. Raut, Parshuram M. Pisal, ...show all

Pages 586-598 | Received 18 Jun 2022, Accepted 30 Sep 2022, Published online: 23 Nov 2022

Cite this article https://doi.org/10.1080/22297928.2022.2132877 Check for updates

Abstract

In the present investigation, we report the synthesis, anti-inflammatory activity and molecular docking of monocarbonyl analogues of curcumin. The anti-inflammatory activity of the synthesized compounds was gauzed using the protein denaturation assay using Diclofenac sodium as reference standard. Among the tested compounds, **3d**, **3e**, **3f**, **3j**, **3k**, **3l** and **3m** displayed excellent anti-inflammatory activity by exhibiting good range of percentage inhibition as compared to the standard DFS. *In silico* binding affinity study against Cyclooxygenase (COX-2) enzyme could provide valuable insight into their plausible mechanism of action. Also, *in silico* ADME prediction of synthesized monocarbonyl curcumin analogues showed excellent pharmacokinetic parameters by not violating Lipinski's rule of five.

Polycyclic Aromatic Compounds >
Volume 43, 2023 - Issue 6

Research Articles

Design, Synthesis and Bioevaluation of Highly Functionalized 1,2,3-Triazole-Guanidine Conjugates as Anti-Inflammatory and Antioxidant Agents

Madiha A. Siddiqui, Amol A. Nagargoje, Mubarak H. Shaikh, Rashiqua A. Siddiqui, Amit A. Pund, Vijay M. Khedkar, ...show all

Pages 5567-5581 | Received 10 Mar 2022, Accepted 18 Jul 2022, Published online: 08 Aug 2022

Cite this article https://doi.org/10.1080/10406638.2022.2105904 Check for updates

Abstract

In search of new biologically potent molecules a small focused library of new guanidine-1,2,3-triazole hybrid derivatives were synthesized *via* Organocatalytic enolate- mediated azide-carbonyl [3 + 2] cycloaddition yielding a highly functionalized triazole core structure. The synthesis of all the derivatives were confirmed by spectral analysis ^{1}H NMR, ^{13}C NMR and MS. The new guanidine-1,2,3-triazole conjugates were found to exhibit promising anti-inflammatory and antioxidant activity. The anti-inflammatory activity screened by membrane stabilization method summarizes the four potential conjugates **5c**, **5f**, **5h** and **5g** to be potent in comparison with standard

Synthesis, Biological Activity, and Computational Study of 1-[5-(4-Methylthiazol-5-yl)-2-phenyl-1,3,4-oxadiazol-3(2*H*)-yl]ethanone Derivatives

Published: 15 September 2022

Volume 92, pages 1511–1518, (2022) Cite this article

Nirmala R. Darekar, Sushama J. Takate, Hemant N. Akolkar, Mubarak H. Shaikh, Vijay M. Khedkar, Bhausaheb K. Karale & Sadhana D. Mhaske

Abstract

A simple and efficient method of synthesis of 1-[5-(4-methylthiazol-5-yl)-2-phenyl-1,3,4-oxadiazol-3(2*H*)-yl]ethanone from (*E*)-*N*′-benzylidene-4-methylthiazole-5-carbohydrazides and acetic anhydride has been developed. Structures of the synthesized compounds have been confirmed by IR, ^{1}H and ^{13}C NMR, and mass spectra. All compounds have been tested for their in vitro antibacterial and antifungal activity. Molecular docking study has been carried out for deeper insight in the antimicrobial action and prediction of the binding modes of these compounds. In silico ADMET

CHEMISTRY JOURNAL OF MOLDOVA. General, Industrial and Ecological Chemistry. 2022, 17(2), 94-100
ISSN (p) 1857-1727 ISSN (e) 2345-1688
http://cjm.ichem.md
http://dx.doi.org/10.19261/cjm.2022.892

ONE-POT SYNTHESIS OF SUBSTITUTED BENZIMIDAZOLE DERIVATIVES UNDER ULTRASONIC IRRADIATION USING $ZnFe_2O_4$ REUSABLE CATALYST

Dhanraj Kamble [a], Anil Shankarwar [a], Yuvraj Sarnikar [b], Radhakrushna Tigote [c], Mubarak Shaikh [d], Pravin Chavan [e*]

[a] *Department of Chemistry, Sarswati Bhuvan Education Society's, College of Science, Paithan gate Road, Gulmandi-03, Aurangabad 431001, Maharashtra, India*
[b] *Department of Chemistry, Dayanand Science College, Barshi Road, Prakash nagar, Latur 413531, Maharashtra, India*
[c] *Department of Chemistry, Dr. B. A. M. University (Aurangabad) Sub-campus, Near to MIDC-Sector-2, Osmanabad 413501, Maharashtra, India*
[d] *Department of Chemistry, Radhabai kale Mahila Mahavidyalaya, near to Tarakpur road Bus stand, Ahemadnagar- 414001, Maharashtra, India*
[e] *Department of Chemistry, Doshi Vakil Arts College and G.C.U.B. Science & Commerce College, Goregaon, Lonere-Goregaon Road, Goregaon, Raigad 402103, Maharashtra, India*
[*] *e-mail: chemistryp141286@gmail.com; phone: (+91 90) 28 137 355*

Abstract. An efficient one-pot synthesis of benzimidazole derivatives by the condensation between various *o*-phenylenediamine and substituted aromatic aldehyde using $ZnFe_2O_4$ as a nano-catalyst under ultrasonic irradiation conditions was described. Remarkable advantages of the present synthetic strategy over the previously reported methods are shorter reaction times, higher isolated yields and simple work-up procedure. The presence of electron withdrawing and electron donating groups on the aromatic rings did not affect the yield of the product. The $ZnFe_2O_4$ catalyst was recycled after completion of reaction and was reused.

Keywords: one pot reaction, substituted benzimidazole, ultrasound irradiation, $ZnFe_2O_4$ catalyst, biological activity.

Received: 01 August 2022/ Revised final: 10 October 2022/ Accepted: 13 October 2022

Introduction

Nitrogen containing heterocycles are of great importance due to the synthetic utility and extensive attention in organic chemistry and benzimidazole is one amongst them [1-3]. The NH group in benzimidazole is very weakly basic and relatively strongly acidic and benzimidazoles are able to form salts [4]. Outstanding uses of benzimidazoles in medicinal as well pharmaceutical fields include treating fungus pathogens, to treat nematode and trematode infection in animals and humans, stopping hyphal growth. Other benzimidazoles play an important role as preservative agents in fruits, paints, textiles, leather industry, papermaking process. Various pharmaceutical drugs have been manufactured from benzimidazole ring such as astemizole, esomeprazole, nitazene, etonitazene, clonitazene, anti-tuberculosis *etc.* [5-7]. Several authors have reviewed the spectrum of benzimidazole's pharmacological activity [8-11]. Numerous of its derivatives exhibit pharmacological effects and thus have been promoted in commercialization of medications as shown in Figure 1, therefore there is a continuous inetrest in developing new methods of synthesis and improving the existing ones.

In recent years, various methods have described syntheses of substituted benzimidazoles using several catalysts, such as rose Bengal [12], *p*-tolunesulfonic acid/graphine and *N,N*-dimethyl aniline/graphine [13], NH_4Cl [14], $[Yb(OPf)_3]$ [15], $In(OTf)_3$ [16], $FeCl_3$ [17], $VO(acac)_2$ [18], I_2 [19], NH_4OAc [20], nano-catalyst such as $COFe_2O_4$ [21], Co/SBA-15 [22], ZnO [23], MNPs@Cu-PMT [24], MNP-IL [25], ZnS [26], $Co(OH)_2$/CoO(II) [27], CuMVs [28] and MIL-53(Fe) [29]. Many of these processes endure limitations, such as extreme reaction conditions, low yields, dreary work-up procedures and co-occurrence of several side reactions.

Polycyclic Aromatic Compounds ›
Volume 43, 2023 - Issue 2

Research Articles

Pyridine-1,3,4-Thiadiazole-Schiff Base Derivatives, as Antioxidant and Antimitotic Agent: Synthesis and *in Silico* ADME Studies

Amit A. Pund, Mubarak H. Shaikh, Badrinarayan G. Chandak, Vijay N. Bhosale & **Baban K. Magare**

Pages 1247-1262 | Received 20 Oct 2021, Accepted 30 Dec 2021, Published online: 17 Jan 2022

Cite this article https://doi.org/10.1080/10406638.2022.2026988 Check for updates

Abstract

An efficient method developed for the synthesis of asymmetric *(S)*-N-benzylidene-2-(benzyloxy)-1-(5-(pyridin-2-yl)-1,3,4-thiadiazol-2-yl)ethanamine derivatives with excellent yield in short reaction time. The antioxidant and antimitotic activities were estimated and strongly correlated with the potential of Ascorbic acid and Methotrexate respectively. All the synthesized molecules were characterized using various spectral techniques including FTIR, ^{1}H NMR, ^{13}C NMR, and Mass spectrometry. The drug-likeness properties were studied using *in silico* ADME parameters. All the compounds have an acceptable range of values which indicated good drug-like characteristics based on Lipinski's rule of five and to be orally active. The present

International Journal of Advance and Applied Research
www.ijaar.co.in
ISSN – 2347-7075 Impact Factor – 7.328
Peer Reviewed Bi-Monthly
Vol.9 No.6 July – Aug 2022

TRIAZOLE DERIVATIVES AND THEIR BIOLOGICAL POTENTIAL: A REVIEW

Rupali Somnath Endait
Assistant Professor, Department of Chemistry, Radhabai Kale Mahila Mahavidyalaya, Ahmednagar-414001, Maharashtra, India
***Corresponding Author*- Rupali Somnath Endait**
Email id: rupaliendait@gmail.com
DOI- 10.5281/zenodo.7069830

Abstract
Azoles are nitrogen containing cyclic compounds with great importance in the field of pharmacology. Almost all azoles and their compounds shows various vital biological properties like antimalarial, anti-tubercular, anti-inflammatory, antibacterial, antileishmanial, antifungal, etc. so synthesis of azoles is now adays interested area for the researchers. Triazole is five membered, nitrogen containing aromatic cyclic system. To synthesize azoles different methods are used and they possess different therapeutics properties. This review contains structural development in triazole with their various biological activities.

Introduction

In the recent era number of heteroaromatic compounds are known and are used to treat fungal infections, among them azole molecule shows better antifungal property. Albaconazole, Fluconazole, Voriconazole, etc are commonly used antifungal moieties.Fluconazole is first synthetic antifungal agent which contains triazole and it is used in the treatment of systemic candida infections, fungal infections as Cryptococcal meningitis, oropharyngeal and esophageal candidiasis. It is also acts as cytochrome P450 (CYPs) enzyme inhibitor[1] in human, Vitamin d3 25-hydroxylase activity with protein. Voriconazole is also good antifungal agent and used to cure fungal infections. It also shows invasive candidiasis caused by any kind of candida, Scedosporium, Penicilliosis and Fusarium. Due to its easy metabolism by hepatic cytochrome P450, it interacts with many kinds of drugs

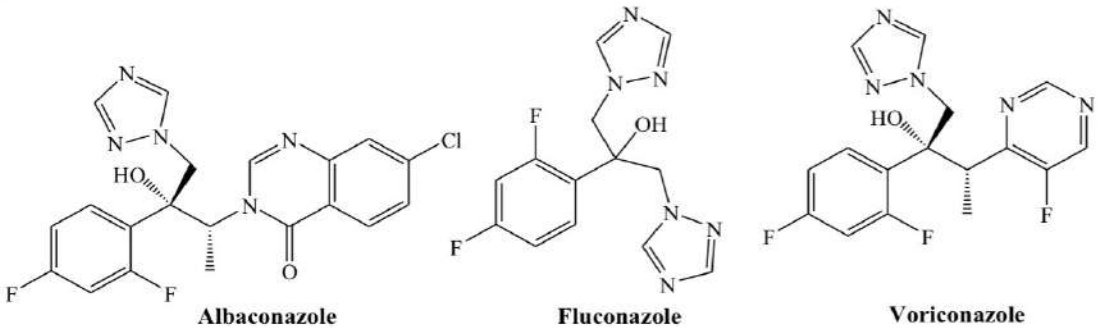


Figure 1: Common triazole containing antifungal agents

Along with antifungal activities triazole have broad spectrum of other biological activities like anti-tubercular[2], antitumor[3], anti-inflammatory[4], antimycobacterial[5], antiviral[6], antimalarial[7], antileishmanial[7], antioxidant[8], etc. Triazole motif attracts the most of the researchers due to their

SAMRIDDHI
A Journal of Physical Sciences, Engineering and Technology
ISSN(P): 2229-7111
ISSN(O): 2454-6767

A GREEN SYNTHESIS OF SCHIFF'S BASES WITH MULTIFLUORINATED CORE AND THEIR ANTIFUNGAL STUDY

Pratibha Randhavane*
Department of Chemistry, Shri Sadguru Gangageer Maharaj Science, Gautam Arts and Sanjivani Commerce College, Kopargaon, Dist. Ahmednagar, Maharashtra, India
Email- pvrandhavane@gmail.com

Rupali Endait
Department of Chemistry, Radhabai Kale Mahila Mahavidyalaya, Ahmednagar, Maharashtra, India, Email- rupaliendait@gmail.com

ABSTRACT- The present work explains an eco-friendly synthesis of Schiff's bases derived from the reaction of 2-(3,5-bis(trifluromethyl)phenoxy)acetohydrazide with different aromatic aldehydes. They were synthesized by environmentally benign methods like grinding, stirring and ultrasonication irradiation. The chemical structures of these new compounds were established by spectral analysis like IR, PMR and LCMS. The synthesized compounds were checked for their antifungal potential using C. Albicans and A.Niger Strains.

Keywords – Multifluorinated, Schiff's base, antifungal, grinding, stirring, ultrasound irradiation.

INTRODUCTION

Schiff's bases are subclass of imines which consists of –C=N- group. They are synthesized by condensation of carbonyl compounds like aldehydes or ketones with primary amines. Schiff's bases are the compounds with pharmaceutical importance like antiproliferative [1], anticonvulsant [2], antitubercular [3], antibacterial [4], anti-inflammatory [5] and acetylcholinesterase [6]. The schiffs bases of isonicotinoylhydrazide and their cobalt, copper, nickel and zinc complexes have shown antibacterial, antifungal and cytotoxic activity [7]. The carvone Schiff bases derived from isoniazid were studied for pharmacokinetic potential [8].

The Schiffs bases are not only biologically potent but are have many applications in dyes, pigments, electrical conductivity, agrochemical and analytical chemistry [9].

The schiffs base of pyridine-3-carbohydrazide were synthesized in basic medium [10]. Various green synthetic methods for the preparation of Schiffs bases have also reported in literature. Synthesis of Schiffs bases in aqueous medium with good yield was reported [11]. The green methods also include the use of nature derived catalyst like lemon juice [12], calcined egg shell [13], PEG-400 [14] and heteropolyacid PTA [15].

Indian Journal of Heterocyclic Chemistry
Vol. 32 - Number 04 (Oct-Dec 2022) 433-438
DocID: https://connectjournals.com/01951.2022.32.433

ISSN (Print) : 0971-1627
ISSN (Online) : 2456-4311

Synthesis, Characterization and Biological Evaluation of Thiazole Containing Chromones and Pyrazole Derivatives

Nirmala R. Darekar[1,2], Sushama J. Takate[2], Hemantkumar N. Akolkar[4]*, Supriya P. Salve[2], Bhausaheb K. Karale[1], Sadhana D. Mhaske[2,3]

[1]Department of Chemistry, Radhabai Kale Mahila Mahavidyalaya, Ahmednagar, Maharashtra, India
[2]Department of Chemistry, New Arts, Science and Commerce College, Ahmednagar, Maharashtra, India
[3]Department of Chemistry, Dadapatil Rajale Arts, Science and Commerce College, Adinathnagar, Ahmednagar, Maharashtra, India
[4]Department of Chemistry, Abasaheb Marathe Arts and New Commerce, Science College, Rajapur, Dist- Ratnagiri, Maharashtra, India

ABSTRACT A novel series of 2-(4-methylthiazol-5-yl)-4*H*-chromen-4-ones (**5**) and 2-(5-(4-methylthiazol-5-yl)-1*H*-pyrazol-3-yl)phenols (**6**) were synthesized by using 4-methylthiazole-5-carboxylic acid **1** and substituted 2-hydroxy acetophenone **2.** All the synthesized compounds were characterized with the help of spectral techniques and screened for their antimicrobial activities.

KEYWORDS Antimicrobial activity, Chromone, Pyrazole, Thiazole.

How to cite this article: Darekar NR, Takate SJ, Akolkar HN, Salve SP, Karale BK, Mhaske SD. Synthesis, Characterization and Biological Evaluation of Thiazole Containing Chromones and Pyrazole Derivatives, *Indian J. Heterocycl. Chem.*, **2022**, *32*, 433–438. (*DocID: https://connectjournals.com/01951.2022.32.433*)

INTRODUCTION

Among the various classes of heterocyclic compounds, azoles are extensively investigated from synthetic and bioactivity point of view. These have shown a broad spectrum of pharmacological activities and are useful in treatment of systemic as well as infectious diseases.

1,3-Thiazole containing compound found in many clinically used drugs such as Nizatidine, Meloxicam, Ritonavir, and Nitazoxanide. Molecules containing thiazole are having wide spectrum of biological activities such as anti-inflammatory,[1,2] antibacterial,[2] antimycobacterial,[3] antiproliferative,[4] adenosine receptor antagonists,[5] C-aryl glucoside SGLT2 inhibitors,[6] etc. Chromone derivatives exhibit wide range of pharmacological activities such as antiallergic,[7] antitumor,[8] neuroprotective,[9] antioxidant,[10] anti-inflammatory,[10] and antibacterial.[11]

Pyrazole containing compounds played important role in agricultural and medicinal field. Pyrazole and its derivatives are known to possess antibacterial,[12] antipyretic,[13] fungistatic,[14] anticancer,[15] antifungal,[16] and anti-inflammatory[17] activities.

Thiazolyl pyrazole clubbed compounds were found various biological activities such as antioxidant,[18] apoptosis inducers,[19] anti-infective,[19] fungicidal,[20] and anti-inflammatory.[21]

Activities associated with thiazole, chromone and pyrazole encouraged us to synthesize thiazole anchored chromones and pyrazoles.

RESULTS AND DISCUSSION

Chemistry

4-Methylthiazole-5-carboxylic acid **1** on reaction with substituted 2-hydroxyacetophenone **2** in pyridine and $POCl_3$ gave 2-acetylphenyl 4-methylthiazole-5-carboxylate **3**.[22] In the ^1H NMR spectrum of the compound **3a**, the three methyl group attached to phenyl ring, acetyl group and thiazole ring showed singlet peak at δ 2.38, 2.54 and 2.68

*Corresponding author: Email: hemantakolkar@gmail.com

Journal Homepage : www.connectjournals.com/ijhc
Published & Hosted by : CONNECT Journals www.connectjournals.com

Synthesis, Biological Activity, and Computational Study of 1-[5-(4-Methylthiazol-5-yl)-2-phenyl-1,3,4-oxadiazol-3(2*H*)-yl]ethanone Derivatives

Published: 15 September 2022

Volume 92, pages 1511–1518, (2022) Cite this article

Russian Journal of General Chemistry

Aims and scope

Submit manuscript

Nirmala R. Darekar, Sushama J. Takate, Hemant N. Akolkar, Mubarak H. Shaikh, Vijay M. Khedkar, Bhausaheb K. Karale & Sadhana D. Mhaske

Abstract

A simple and efficient method of synthesis of 1-[5-(4-methylthiazol-5-yl)-2-phenyl-1,3,4-oxadiazol-3(2*H*)-yl]ethanone from (*E*)-*N*′-benzylidene-4-methylthiazole-5-carbohydrazides and acetic anhydride has been developed. Structures of the synthesized compounds have been confirmed by IR, ^{1}H and ^{13}C NMR, and mass spectra. All compounds have been tested for their in vitro antibacterial and antifungal activity. Molecular docking study has been carried out for deeper insight in the antimicrobial action and prediction of the binding modes of these compounds. In silico ADMET

Heterocyclic Letters
Vol. 12| No.3|571-576|May-July|2022
ISSN : (print) 2231–3087 / (online) 2230-9632
CODEN: HLEEAI
http://heteroletters.org

SYNTHESIS AND ANTIBACTERIAL SCREENING OF THIAZOLYL PYRAZOLE CONTAINING CHROMONES AND AURONES

Nirmala R. Darekar[a], Bhausaheb K. Karale[a], Jaidip B. Wable[b], Hemantkumar N. Akolkar[c,*]

[a]*Department of Chemistry, Radhabai Kale Mahila Mahavidyalaya, Ahmednagar, 414 001, Maharashtra, India.*
[b]*Department of Chemistry, K.J.S.S.C. College, Vidyavihar, Mumbai, Maharashtra, India.*
[c]*Department of Chemistry, Abasaheb Marathe Arts and New Commerce, Science College, Rajapur, Dist- Ratnagiri, 416 702, Maharashtra, India.*
E-Mail: hemantakolkar@gmail.com (Corresponding Author)

ABSTRACT
Thiazolyl pyrazole anchored chalcones were converted into chromones and aurones. Formation of the target compounds was confirmed by spectral techniques like IR, ^{1}H NMR and mass spectrometry. The newly synthesized compounds were screened for their antibacterial activities.

KEYWORDS: Thiazole, pyrazole, chromones, aurones.

INTRODUCTION
1,3-Thiazole is well known sulphur and nitrogen containing five membered heterocyclic compound found in many clinically used drugs like Nizatidine, Meloxicam, Ritonavir, Tiazofurin, Bleomycin, Nitazoxanide, etc. Molecules containing thiazole nucleus are attractive targets for medicinal chemistry because of their wide spectrum of biological activities such as anti-inflammatory[i, ii], antibacterial[ii], antiproliferative[iii] and adenosine receptor antagonists[iv]. Pyrazole and its derivatives are known to possess antibacterial[v], fungistatic[vi], and anti-inflammatory[vii] activities. Chromone is an important class of oxygen-containing heterocyclic compounds and part of the flavonoid family. Chromone derivatives exhibit wide range of pharmacological activities such as antiallergic[viii], antitumor[ix], antimicrobial[x], antioxidant[xi], anti-inflammatory[xii], antiproliferative[xiii], *etc*. Aurones are found in some flowers, bark, seedlings, leaves and nectar of plant species. Recently aurones are known to have various biological activities such as anti-cancer[xiv], antioxidant[xv], anti-inflammatory[xvi] and antimicrobial[xvi].

Various biological activities associated with thiazole, pyrazole, chromones and aurones prompted us to synthesize thiazolyl pyrazole anchored fluorinated chromones and aurones.

Heterocyclic Letters
Vol. 12| No.2|281-293|February -April|2022
ISSN : (print) 2231–3087 / (online) 2230-9632
CODEN: HLEEAI
http://heteroletters.org

SYNTHESIS AND ANTIBACTERIAL SCREENING OF IMIDAZOLE ANCHORED PYRAZOLINES, BENZODIAZEPINES AND CHROMONES

Rajendra Deshmukh[a], Bhausaheb Karale[a], Nirmala Darekar[a], Pratibha Randhavane[b], Hemant kumar Akolkar[c,*]

[a]*Department of Chemistry, Radhabai Kale Mahila Mahavidyalaya, Ahmednagar, 414001, Maharashtra, India.*
[b]*Department of Chemistry, S. S. G. M. College, Kopargaon, 423601, Maharashtra, India.*
[c]*Department of Chemistry, Abasaheb Marathe Arts and New Commerce, Science College, Rajapur, Dist- Ratnagiri, 416 702, Maharashtra, India.*
E-Mail: hemantakolkar@gmail.com (Corresponding Author)

ABSTRACT
Imidazole anchored chalcones were converted into pyrazolines, benzodiazepines, chromones, chlorochromones and hydroxychromones. 3-*O*-alkylated-6-(4-fluorophenyl)chromones were synthesized from 3-*O*-alkylated-6-bromochromonesby Suzuki-Miyaura Reaction. Formation of the target compounds was confirmed by spectral tools like IR, ^{1}H NMR and mass spectrometry. The newly synthesized compounds were studied for their antibacterial potential using bacterial strains *Bacillus Subtilis* and *Escherichia Coli.*

KEYWORDS: Suzuki-Miyaura Reaction, pyrazolines, benzodiazepines, chromones, chlorochromones and hydroxychromones.

INTRODUCTION
Imidazole ring system is important biological building-block present in hormones such as histidine and the related hormone histamine. Many drugs contain an imidazole ring having antifungal[i], antibiotic[ii], anticancer[iii], andantiepilepsy[iv] properties. Some important marketed drugs which contain imidazole ring are Ketoconazole (antifungal), Miconazole (antifungal), Losartan (antihypertension) and Ondansetron (nausea).
Pyrazoline and imidazole are five membered heterocyclic compounds having high importance in synthetic chemistry due to their pharmacological activity and less toxicity. Pyrazolines have shown biological activities like antidepressant[v], anticonvulsant[vi], antimicrobial[vii], analgesic[viii] and anticancer[ix].
The importance of benzodiazepines has been increased in medicinal chemistry because of their wide range of biological activity, easily available raw material and high yield. In all benzodiazepines, 1,5-benzodiazepines and their derivatives are important because of their wide spectrum of biological and pharmacological activity. 1, 5-Benzodiazepines are known to have antimicrobial[x], antiHIV[xi] and antidepressive[xii] activities.

Development of a new chromogenic spray reagent for the detection and identification of synthetic pesticide carbaryl in biological material by high-performance thin-layer chromatography

Short Communication Published: 06 September 2022

Volume 35, pages 431–434, (2022) Cite this article

JPC – Journal of Planar Chromatography – Modern TLC

Aims and scope

Submit manuscript

Umakant D. Pawar, Dattatraya N. Pansare, Rohini N. Shelke, Chandrakant D. Pawar, Asif M. Pathan, Vijay J. Thakre, Bhagwan S. Dobhal & Rajendra K. Pardeshi

Indian Journal of Chemistry
Vol. 61, February 2022, pp. 225-228

Design, synthesis and characterization of novel fluorinated styryl chromones

S G Kundlikar*[a], P J Jojar[a], M S Tarade[a], Y R Thorat[a], D R Thube[a], B K Karale[b], H N Akolkar[b] & S D Mhaske[c]

[a]New Arts, Commerce and Science College Parner, Dist. Ahmednagar 414 302, India

[b]Radhabai Kale Mahila Mahavidyalaya, Dist. Ahmednagar 414 001, India

[c]Dadapatil Rajale Arts, Science and Commerce College, Pathardi, Dist. Ahmednagar 414 102, India

E-mail: saritakundlikar1@gmail.com

Received 1 June 2020; accepted (revised) 8 November 2021

(E)-3-(3-(Trifluoromethyl)-5-nitrophenyl)acrylic acid **1** when treated with substituted 2-hydroxyacetophenones **2** in dry pyridine and $POCl_3$ affords compound **3** which when reacted with pyridine/KOH by B. V. transformation gives **4**. Compound **4** on refluxing with acetic acid in HCl gives **5**. The structures of all synthesized compounds have been confirmed by spectroscopic techniques.

Keywords: Fluorine, diketone, styryl chromones

Substitution of hydrogen atom by fluorine into potentially active drug molecule alters lipophilic, electronic, steric parameters as well as pharmacokinetic and pharmacodynamic properties of drugs. Fluorine containing molecule is considered as an important tool in the design of new drugs[1]. Fluorine incorporated drugs are endowed with wide spectrum of biological activities such as insecticidal[2], anticoagulant[3], antimicrobial[4], antitumor[5] and anticancer[6].

β-Diketones are important intermediates in many drug syntheses[7]. The diketone derivatives are associated with broad spectrum of biological activities like corrosion inhibitor[8], antimicrobial[9], inhibition of amyloid α aggregation[10], antiinflammatory[11], *etc*.

Chromone moiety is a core fragment of different flavonoids like flavones, isoflavones and flavonols[12]. Large number of chromone derivatives are known for their pharmacological properties like such as anti-picornavirus capsid-binders[13], antitumor[14], anticancer[15]. Styryl chromones is one of the small family of chromone compounds exhibiting different biological activities like cytotoxicity[16], antiproliferative[17], monoamine oxidase inhibitors[18] and anti-noroviral agents[19].

Based on this valuable literature observations associated with fluorine, diketone and chromones the present work describes an attempt towards synthesis of fluorine containing different diketones and chromones (Scheme I).

Experimental Section

Melting points were determined in open capillaries in liquid paraffin bath and are uncorrected. Mass spectra were recorded on Waters Acquity TQD mass spectrometer. ^{1}H NMR spectra were recorded on Bruker Avance II 500 MHz NMR spectrometer in $CDCl_3$ as a solvent and TMS as an internal standard. Peak values are shown in δ (ppm). IR spectra were recorded on Shimadzu IR Affinity-1S spectrophotometer.

(E)-2-Acetylphenyl 3-(3-(trifluoromethyl)-5-nitrophenyl)acrylate, 3a-e

Equimolar quantities of 2-(4-fluorophenyl)-5-phenylbenzofuran-3-carboxylic acid **1** (0.004M) and substituted 2-hydroxyacetophenone **2** (0.004M) was dissolved in pyridine (20 mL) maintained at about 0°C then $POCl_3$ (0.004 M) was slowly added maintaining the temperature below 4°C. After complete addition the reaction mixture was kept overnight. Resulting reaction mixture was poured over crushed ice, solid thus obtained was separated by filtration and crystallized from ethanol to afford **3**.

(E)-2-Acetylphenyl 3-(3-(trifluoromethyl)-5-nitrophenyl)

acrylate, 3a: m.p. 68°C. Yield 90%. IR: 2929, 1690, 1521, 1351, 1154, 678 cm^{-1}; ^{1}H NMR ($CDCl_3$): δ 2.56 (s, 3H), 6.75 (d, J = 16 Hz, 1H), 7.19 (dd, J = 4.6 Hz, 1H), 7.29 (dd, J = 3 and 4.6 Hz, 1H), 7.54 (dd, J = 3 Hz, 1H), 7.58-7.79 (m, 4H), 7.93 (d, J = 16 Hz, 1H); MS:

Indian Journal of Chemistry
Vol. 61, February 2022, pp. 225-228

Design, synthesis and characterization of novel fluorinated styryl chromones

S G Kundlikar*[a], P J Jojar[a], M S Tarade[a], Y R Thorat[a], D R Thube[a], B K Karale[b], H N Akolkar[b] & S D Mhaske[c]

[a]New Arts, Commerce and Science College Parner, Dist. Ahmednagar 414 302, India

[b]Radhabai Kale Mahila Mahavidyalaya, Dist. Ahmednagar 414 001, India

[c]Dadapatil Rajale Arts, Science and Commerce College, Pathardi, Dist. Ahmednagar 414 102, India

E-mail: saritakundlikar1@gmail.com

Received 1 June 2020; accepted (revised) 8 November 2021

(E)-3-(3-(Trifluoromethyl)-5-nitrophenyl)acrylic acid **1** when treated with substituted 2-hydroxyacetophenones **2** in dry pyridine and $POCl_3$ affords compound **3** which when reacted with pyridine/KOH by B. V. transformation gives **4**. Compound **4** on refluxing with acetic acid in HCl gives **5**. The structures of all synthesized compounds have been confirmed by spectroscopic techniques.

Keywords: Fluorine, diketone, styryl chromones

Substitution of hydrogen atom by fluorine into potentially active drug molecule alters lipophilic, electronic, steric parameters as well as pharmacokinetic and pharmacodynamic properties of drugs. Fluorine containing molecule is considered as an important tool in the design of new drugs[1]. Fluorine incorporated drugs are endowed with wide spectrum of biological activities such as insecticidal[2], anticoagulant[3], antimicrobial[4], antitumor[5] and anticancer[6].

β-Diketones are important intermediates in many drug syntheses[7]. The diketone derivatives are associated with broad spectrum of biological activities like corrosion inhibitor[8], antimicrobial[9], inhibition of amyloid α aggregation[10], antiinflammatory[11], *etc*.

Chromone moiety is a core fragment of different flavonoids like flavones, isoflavones and flavonols[12]. Large number of chromone derivatives are known for their pharmacological properties like such as anti-picornavirus capsid-binders[13], antitumor[14], anticancer[15]. Styryl chromones is one of the small family of chromone compounds exhibiting different biological activities like cytotoxicity[16], antiproliferative[17], monoamine oxidase inhibitors[18] and anti-noroviral agents[19].

Based on this valuable literature observations associated with fluorine, diketone and chromones the present work describes an attempt towards synthesis of fluorine containing different diketones and chromones (Scheme I).

Experimental Section

Melting points were determined in open capillaries in liquid paraffin bath and are uncorrected. Mass spectra were recorded on Waters Acquity TQD mass spectrometer. ^{1}H NMR spectra were recorded on Bruker Avance II 500 MHz NMR spectrometer in $CDCl_3$ as a solvent and TMS as an internal standard. Peak values are shown in δ (ppm). IR spectra were recorded on Shimadzu IR Affinity-1S spectrophotometer.

(E)-2-Acetylphenyl 3-(3-(trifluoromethyl)-5-nitrophenyl)acrylate, 3a-e

Equimolar quantities of 2-(4-fluorophenyl)-5-phenylbenzofuran-3-carboxylic acid **1** (0.004M) and substituted 2-hydroxyacetophenone **2** (0.004M) was dissolved in pyridine (20 mL) maintained at about 0°C then $POCl_3$ (0.004 M) was slowly added maintaining the temperature below 4°C. After complete addition the reaction mixture was kept overnight. Resulting reaction mixture was poured over crushed ice, solid thus obtained was separated by filtration and crystallized from ethanol to afford **3**.

(E)-2-Acetylphenyl 3-(3-(trifluoromethyl)-5-nitrophenyl)

acrylate, 3a: m.p. 68°C. Yield 90%. IR: 2929, 1690, 1521, 1351, 1154, 678 cm^{-1}; ^{1}H NMR ($CDCl_3$): δ 2.56 (s, 3H), 6.75 (d, J = 16 Hz, 1H), 7.19 (dd, J = 4.6 Hz, 1H), 7.29 (dd, J = 3 and 4.6 Hz, 1H), 7.54 (dd, J = 3 Hz, 1H), 7.58-7.79 (m, 4H), 7.93 (d, J = 16 Hz, 1H); MS:

Indian Journal of Heterocyclic Chemistry
Vol. 32 - Number 04 (Oct-Dec 2022) 433-438
DocID: https://connectjournals.com/01951.2022.32.433

ISSN (Print) : 0971-1627
ISSN (Online) : 2456-4311

Synthesis, Characterization and Biological Evaluation of Thiazole Containing Chromones and Pyrazole Derivatives

Nirmala R. Darekar[1,2], Sushama J. Takate[2], Hemantkumar N. Akolkar[4]*, Supriya P. Salve[2], Bhausaheb K. Karale[1], Sadhana D. Mhaske[2,3]

[1]Department of Chemistry, Radhabai Kale Mahila Mahavidyalaya, Ahmednagar, Maharashtra, India
[2]Department of Chemistry, New Arts, Science and Commerce College, Ahmednagar, Maharashtra, India
[3]Department of Chemistry, Dadapatil Rajale Arts, Science and Commerce College, Adinathnagar, Ahmednagar, Maharashtra, India
[4]Department of Chemistry, Abasaheb Marathe Arts and New Commerce, Science College, Rajapur, Dist- Ratnagiri, Maharashtra, India

ABSTRACT A novel series of 2-(4-methylthiazol-5-yl)-4*H*-chromen-4-ones (**5**) and 2-(5-(4-methylthiazol-5-yl)-1*H*-pyrazol-3-yl)phenols (**6**) were synthesized by using 4-methylthiazole-5-carboxylic acid **1** and substituted 2-hydroxy acetophenone **2.** All the synthesized compounds were characterized with the help of spectral techniques and screened for their antimicrobial activities.

KEYWORDS Antimicrobial activity, Chromone, Pyrazole, Thiazole.

How to cite this article: Darekar NR, Takate SJ, Akolkar HN, Salve SP, Karale BK, Mhaske SD. Synthesis, Characterization and Biological Evaluation of Thiazole Containing Chromones and Pyrazole Derivatives, *Indian J. Heterocycl. Chem.*, **2022**, *32*, 433–438. (*DocID: https://connectjournals.com/01951.2022.32.433*)

INTRODUCTION

Among the various classes of heterocyclic compounds, azoles are extensively investigated from synthetic and bioactivity point of view. These have shown a broad spectrum of pharmacological activities and are useful in treatment of systemic as well as infectious diseases.

1,3-Thiazole containing compound found in many clinically used drugs such as Nizatidine, Meloxicam, Ritonavir, and Nitazoxanide. Molecules containing thiazole are having wide spectrum of biological activities such as anti-inflammatory,[1,2] antibacterial,[2] antimycobacterial,[3] antiproliferative,[4] adenosine receptor antagonists,[5] C-aryl glucoside SGLT2 inhibitors,[6] etc. Chromone derivatives exhibit wide range of pharmacological activities such as antiallergic,[7] antitumor,[8] neuroprotective,[9] antioxidant,[10] anti-inflammatory,[10] and antibacterial.[11]

Pyrazole containing compounds played important role in agricultural and medicinal field. Pyrazole and its derivatives are known to possess antibacterial,[12] antipyretic,[13] fungistatic,[14] anticancer,[15] antifungal,[16] and anti-inflammatory[17] activities.

Thiazolyl pyrazole clubbed compounds were found various biological activities such as antioxidant,[18] apoptosis inducers,[19] anti-infective,[19] fungicidal,[20] and anti-inflammatory.[21]

Activities associated with thiazole, chromone and pyrazole encouraged us to synthesize thiazole anchored chromones and pyrazoles.

RESULTS AND DISCUSSION

Chemistry

4-Methylthiazole-5-carboxylic acid **1** on reaction with substituted 2-hydroxyacetophenone **2** in pyridine and $POCl_3$ gave 2-acetylphenyl 4-methylthiazole-5-carboxylate **3**.[22] In the ^1H NMR spectrum of the compound **3a**, the three methyl group attached to phenyl ring, acetyl group and thiazole ring showed singlet peak at δ 2.38, 2.54 and 2.68

*Corresponding author: Email: hemantakolkar@gmail.com

Journal Homepage : www.connectjournals.com/ijhc
Published & Hosted by : CONNECT Journals www.connectjournals.com

Journal of the Chinese Chemical Society / Volume 68, Issue 4 / p. 657-668

ARTICLE

Synthesis of 3-(trifluoromethyl)-1-(perfluorophenyl)-1*H*-pyrazol-5(4*H*)-one derivatives via Knoevenagel condensation and their biological evaluation

Sujata G. Dengale, Hemantkumar N. Akolkar, Bhausaheb K. Karale, Nirmala R. Darekar, Sadhana D. Mhaske, Mubarak H. Shaikh, Dipak N. Raut, Keshav K. Deshmukh

First published: 26 November 2020
https://doi.org/10.1002/jccs.202000357
Citations: 5

Abstract

In search of new active molecules, a small focused library of the synthesis of 3-(trifluoromethyl)-1-(perfluorophenyl)-1*H*-pyrazol-5(4*H*)-one derivatives (**4a-d**, **5a-f**, and **6a-e**) has been efficiently prepared via the Knoevenagel condensation approach. All the derivatives were synthesized by conventional and nonconventional methods like ultrasonication and microwave irradiation, respectively. Several derivatives exhibited excellent anti-inflammatory activity compared to the standard drug. Furthermore, the synthesized compounds were found to have potential antioxidant activity. In addition, to rationalize the observed biological activity data, an in silico absorption, distribution, metabolism, and excretion (ADME) prediction study also been carried out. The results of the in vitro and in silico studies suggest that the 3-(trifluoromethyl)-1-(perfluorophenyl)-1*H*-pyrazol-5(4*H*)-one derivatives (**4a-d**, **5a-f**, and **6a-e**) may possess the ideal structural requirements for the further development of novel therapeutic agents.

CONFLICT OF INTEREST

The authors declare no conflict of interest, financial or otherwise.

Supporting Information

Polycyclic Aromatic Compounds >
Volume 42, 2022 - Issue 10

Research Articles

[DBUH][OAc]-Catalyzed Domino Synthesis of Novel Benzimidazole Incorporated 3,5-Bis (Arylidene)-4-Piperidones as Potential Antitubercular Agents

Dnyaneshwar D. Subhedar, Mubarak H. Shaikh, Amol A. Nagargoje, Dhiman Sarkar, Vijay M. Khedkar & **Bapurao B. Shingate**

Pages 7010-7024 | Received 02 May 2021, Accepted 13 Oct 2021, Published online: 23 Oct 2021

Cite this article https://doi.org/10.1080/10406638.2021.1995008 Check for updates

Abstract

A series of new benzimidazole incorporated 3,5-bis (arylidene)-4-piperidones were synthesized by using aryl aldehydes, piperidinone, 2-(chloromethyl)-benzimidazole and DBU acetate [DBUH][OAc] act as a catalyst under solvent free condition in excellent yields. The synthesized compounds were screened for their *in vitro* antimycobacterial activity against *M. tuberculosis* H37Ra (*MTB*) and *M. bovis* BCG strains. The compounds **4a**, **4b**, **4e**, **4i**, **4k** and **4l** are highly potent against both the strains. Most of the active compounds are non-cytotoxic against MCF-7, A549, HCT 116 and THP-1 cell lines. Furthermore, a molecular docking study of these compounds

Polycyclic Aromatic Compounds ›
Volume 42, 2022 - Issue 9

Research Articles

Synthesis and Biological Evaluation of 2-(4,5,6,7-Tetrahydrobenzo[*c*]Isoxazol-3-yl)-4*H*-Chromen-4-Ones

Sujata G. Dengale, **Hemantkumar N. Akolkar**, Nirmala R. Darekar, Mubarak H. Shaikh, Keshav K. Deshmukh, Sadhana D. Mhaske, ...show all

Pages 6337-6351 | Received 27 Feb 2021, Accepted 09 Sep 2021, Published online: 27 Sep 2021

Cite this article https://doi.org/10.1080/10406638.2021.1982733 Check for updates

Full Article Figures & data References Supplemental Citations
Metrics Reprints & Permissions Read this article

Abstract

A new series of 2-(4,5,6,7-tetrahydrobenzo[*c*]isoxazol-3-yl)-4*H*-chromen-4-ones **5a-e** were synthesized from 1-(2-hydroxyphenyl)-3-(4,5,6,7-tetrahydrobenzo[*c*]isoxazol-3-yl)propane-1,3-diones **4a-e** in presence of acetic acid and conc. HCl. Compounds **4a-e** were synthesized by Baker-Venkataraman rearrangement from 2-acetylphenyl 4,5,6,7-tetrahydrobenzo[c]isoxazole-3-carboxylate **3a-e** in presence of pyridine and KOH and compounds **3a-e** were synthesized from 4,5,6,7-tetrahydrobenzo[*c*]isoxazole-3-carboxylic acid **1** and substituted 2-hydroxy acetophenone **2a-e**. All the synthesized

Polycyclic Aromatic Compounds >
Volume 42, 2022 - Issue 9

Research Articles

$[Et_3NH][HSO_4]$-Catalyzed One-Pot Solvent Free Syntheses of Functionalized [1,6]-Naphthyridines and Biological Evaluation

Mubarak H. Shaikh, Dnyaneshwar D. Subhedar, Vijay M. Khedkar & **Bapurao B. Shingate**

Pages 6043-6059 | Received 13 Apr 2021, Accepted 14 Aug 2021, Published online: 02 Sep 2021

Cite this article https://doi.org/10.1080/10406638.2021.1970587 Check for updates

Abstract

We have developed a convenient one-pot multicomponent synthesis of highly functionalized [1,6]-naphthyridines under solvent free condition using $[Et_3NH][HSO_4]$ in excellent yield. This protocol offers several advantages, including short reaction time, simple experimental workup procedure and no toxic byproducts, avoids the use of toxic organic solvents and anhydrous conditions. Further. we have screened the synthesized naphthyridines for *in vitro* antibacterial, antifungal and antioxidant activity. Furthermore, a molecular docking study of these compounds was carried out to investigate their binding pattern with the target, β-Ketoacyl-acyl carrier protein synthase III (FabH). Finally, the ADME parameters for these compounds showed good drug like properties and can be developed as oral drug candidates.

Madje et al., J Adv Sci Res, 2021; 12 (3) Suppl 2: 265-26

ScienSage

Journal of Advanced Scientific Research

Available online through http://www.sciensage.info

SYNTHESIS, CHARACTERIZATION AND ANTIMICROBIAL EVALUATI(4R)-4-AMINOCYCLOHEXYL)-N6-(PHENYL)-9-CYCLOPENTYL-9H-PURI

Dhanraj Kamble[1], Anil Shankarwar[1], Radhakrishna Tigote[2], Mubarak Shaikh[4], Pravin Chavan[5], Balaji Mad

[1]*Department of Chemistry, S.B.E.S. College of Science, Aurangabad, M*

[2]*Department of Chemistry Dr. B. A. M. University Sub campus, Osmanabad*

[3]*Department of Chemistry Dayanand Science College, Latur, Dist. Latur,*

[4]*Department of Chemistry, Radhabai kale Mahila Mahavidyalaya, Ahemadna*

[5]*Doshi Vakil Arts College and G.C.U.B. Science & Commerce College, Goregaon-E*

[6]*Department of Chemistry Vasantrao Naik Mahavidyalaya, Aurangabad,*

**Corresponding author: drmadjebr@gmail.com*

ABSTRACT

In this study, we have synthesized N2-((1r,4r)-4-aminocyclohexyl)-N6-(substitutedp diamine derivatives **(7a-j)** from N-(-substituted phenyl)-9-cyclopentyl-2-fluoro-9H- diamine under microwave irradiation condition and examined for their antibacte *Streptococcus aureus* and *Bacillus subtilis* strains. All compounds **(7a-j)** displayed mode Minimum Inhibition Concentration (MIC).

Keywords: Purine, Purine fluoro-9H-purin-6-amine, N-9 Substituted-6-chl Cyclohexane-1,4-diamine.

1. INTRODUCTION

The Purine antimetabolites have been used in the development of many potent medicinal agents, which exhibited antineoplastic, antileukemic, antiviral, anti-bacterial and antifungal activities [1, 2]. The purine nucleoside analogs are also used in the treatment of autoimmune diseases [3]. 6-Mercapto purine is used therapeutically as an immunosuppressive agent [4] and inhibits the growth of bacterial and mammalian cells [5]. Other 6-mercapto purine, mercapto-pyridine and mercapto-pyrimidine derivatives also exhibit antibacterial

brains, meat extrac mackerel, scallops, g amount of purine is a fish and seafood, mushrooms, green oatmeal, wheat bran, infected cells have nucleotides which a synthesis and this r sensitive target for a 2-functionalized pu

ORIGINAL SCIENTIFIC PAPER

CROATICA CT CHEMICA

Croat. Chem. Acta 2021, *94*(1), 35–41
Published online: December 31, 2021
DOI: 10.5562/cca3758

UKD 1926

Synthesis and Biological Evaluation of Indolyl Bis-chalcones as Anti-Breast Cancer and Antioxidant Agents

Pravin S. Bhale,[1,*] Hemant V. Chavan,[2] Rupali S. Endait,[3] Ashok T. Kadam,[1] Rajesh J. Bopalkar,[1] Mandar S. Gaikwad[1]

[1] Department of Chemistry, Yeshwantrao Chavan Mahavidyalaya, Tuljapur, Dist-Osmanabad-413601, Maharashtra, India
[2] Department of Chemistry, A.S.P. College, Devrukh, Dist-Ratnagiri-415 804, Maharashtra, India
[3] Department of Chemistry, Radhabai Kale Mahila Mahavidyalaya, Ahmednagar-414001, Maharashtra, India
* Corresponding author's e-mail address: bhale.ps@gmail.com

RECEIVED: March 23, 2021 ★ REVISED: July 21, 2021 ★ ACCEPTED: July 28, 2021

Abstract: A series of novel α-cyano substituted indolyl bis-chalcones (3a–l) has been synthesized and evaluated for their *in vitro* antitumor activity against the human breast cancer MCF7 (estrogen receptor-positive) and normal Vero cell lines using sulforhodamine B (SRB) assay method. Compounds 3a, 3c and 3d showed potent activity (GI_{50} = 11.7, 15.3 and 17.9 μM respectively) against the human breast cancer MCF7 cell line, which was almost as good as that of adriamycin (GI_{50} = < 0.1 μM) whereas, screening against the normal Vero Monkey cell line showed moderate selectivity. Furthermore, all the synthesized compounds screened for their antioxidant potential against DPPH, NO, SOR, and H_2O_2 radicals. Most of the bis-chalcones exhibited significant DPPH (51.09–12.72 %) and NO (64.11–34.43 %) radical scavenging activity and modest activity against SOR (88.08–43.14 %) and H_2O_2 (80.13–56.0 %) radicals compared to the reference standard ascorbic acid (40.78 %, 42.63 %, 87.05 %, and 79.42 % respectively). Current study provides impetus for the development of highly potent indolyl bis-chalcone derivatives as anticancer leads.

Keywords: indolyl bis-chalcone, breast cancer, anti-cancer activity, antioxidant activity.

INTRODUCTION

PRESENTLY cancer is deemed to a principal worldwide health problem that leads to death.[1] Although considerable progress is made in controlling the progression of this devastating disease, till the date an entire cure for cancer remains a dream. Most of the cancer treatment is the use of surgery, radiation and chemotherapy.[2] Most of the marketed chemotherapeutic agents suffer from serious and sometimes intolerable toxic effects. So, the development of novel anticancer agents is a crucial need of time.[3,4] Chalcone is one of the important scaffold exhibiting diverse biological activities such as anti-inflammatory,[5] antimalarial,[6] antileishmanicidal, antiviral, antifungal, antibacterial and anticancer.[7,8] Different type of structural alterations was performed in the chalcones primary structure either by varying the aryl moieties or the enone linker. Another tactic which is not that typical in literature is to change the α-position of the α,β-unsaturated carbonyl system. This is a promising idea since it should have a direct and straightforward influence on the reactivity (Figure 1). Examples of the effect of α-alteration on biological activity are also present. First time Edwards et al. reported that α-substituted chalcones are more potent than their unsubstituted counter parts.[9] Lawrence et al. also improved cytotoxic effects of α-substituents such as phenyl, ester, cyano and fluoro groups on α,β-unsaturated carbonyl system.[10] Kumar et. al. also reported α-cyano bis-indolyl chalcones as novel anticancer agents.[11] Recently, our research group reported α-cyano substituted bis-indolyl chalcone[12] and extended conjugated indolyl chalcones as potent anti-breast cancer agents.[13] In continuation of our constant efforts to discover a potent anticancer agents,[14–18] herein we have synthesized a series of novel α-cyano substituted indolyl bis-chalcone having phenyl ring as a spacer and *in vitro* evaluated for their anti-breast cancer and anti-oxidant activity (Scheme 1).

Journal of the Chinese Chemical Society / Volume 68, Issue 4 / p. 657-668

ARTICLE

Synthesis of 3-(trifluoromethyl)-1-(perfluorophenyl)-1*H*-pyrazol-5(4*H*)-one derivatives via Knoevenagel condensation and their biological evaluation

Sujata G. Dengale, Hemantkumar N. Akolkar, Bhausaheb K. Karale, Nirmala R. Darekar, Sadhana D. Mhaske, Mubarak H. Shaikh, Dipak N. Raut, Keshav K. Deshmukh

First published: 26 November 2020
https://doi.org/10.1002/jccs.202000357
Citations: 5

Abstract

In search of new active molecules, a small focused library of the synthesis of 3-(trifluoromethyl)-1-(perfluorophenyl)-1*H*-pyrazol-5(4*H*)-one derivatives (**4a-d**, **5a-f**, and **6a-e**) has been efficiently prepared via the Knoevenagel condensation approach. All the derivatives were synthesized by conventional and nonconventional methods like ultrasonication and microwave irradiation, respectively. Several derivatives exhibited excellent anti-inflammatory activity compared to the standard drug. Furthermore, the synthesized compounds were found to have potential antioxidant activity. In addition, to rationalize the observed biological activity data, an in silico absorption, distribution, metabolism, and excretion (ADME) prediction study also been carried out. The results of the in vitro and in silico studies suggest that the 3-(trifluoromethyl)-1-(perfluorophenyl)-1*H*-pyrazol-5(4*H*)-one derivatives (**4a-d**, **5a-f**, and **6a-e**) may possess the ideal structural requirements for the further development of novel therapeutic agents.

CONFLICT OF INTEREST

The authors declare no conflict of interest, financial or otherwise.

Supporting Information

Polycyclic Aromatic Compounds ›
Volume 42, 2022 - Issue 9

Research Articles

Synthesis and Biological Evaluation of 2-(4,5,6,7-Tetrahydrobenzo[*c*]Isoxazol-3-yl)-4*H*-Chromen-4-Ones

Sujata G. Dengale, **Hemantkumar N. Akolkar**, Nirmala R. Darekar, Mubarak H. Shaikh, Keshav K. Deshmukh, Sadhana D. Mhaske, ...show all

Pages 6337-6351 | Received 27 Feb 2021, Accepted 09 Sep 2021, Published online: 27 Sep 2021

Cite this article https://doi.org/10.1080/10406638.2021.1982733 Check for updates

Abstract

A new series of 2-(4,5,6,7-tetrahydrobenzo[*c*]isoxazol-3-yl)-4*H*-chromen-4-ones **5a-e** were synthesized from 1-(2-hydroxyphenyl)-3-(4,5,6,7-tetrahydrobenzo[*c*]isoxazol-3-yl)propane-1,3-diones **4a-e** in presence of acetic acid and conc. HCl. Compounds **4a-e** were synthesized by Baker-Venkataraman rearrangement from 2-acetylphenyl 4,5,6,7-tetrahydrobenzo[c]isoxazole-3-carboxylate **3a-e** in presence of pyridine and KOH and compounds **3a-e** were synthesized from 4,5,6,7-tetrahydrobenzo[*c*]isoxazole-3-carboxylic acid **1** and substituted 2-hydroxy acetophenone **2a-e**. All the synthesized compounds were characterized with the help of IR, ^{1}H NMR, ^{13}C NMR and mass spectroscopic techniques. All the compounds were screened for their *in vitro* anti-

Journal of the Chinese Chemical Society / Volume 68, Issue 4 / p. 657-668

ARTICLE

Synthesis of 3-(trifluoromethyl)-1-(perfluorophenyl)-1*H*-pyrazol-5(4*H*)-one derivatives via Knoevenagel condensation and their biological evaluation

Sujata G. Dengale, Hemantkumar N. Akolkar, Bhausaheb K. Karale, Nirmala R. Darekar, Sadhana D. Mhaske, Mubarak H. Shaikh, Dipak N. Raut, Keshav K. Deshmukh

First published: 26 November 2020
https://doi.org/10.1002/jccs.202000357
Citations: 5

Abstract

In search of new active molecules, a small focused library of the synthesis of 3-(trifluoromethyl)-1-(perfluorophenyl)-1*H*-pyrazol-5(4*H*)-one derivatives (**4a-d**, **5a-f**, and **6a-e**) has been efficiently prepared via the Knoevenagel condensation approach. All the derivatives were synthesized by conventional and nonconventional methods like ultrasonication and microwave irradiation, respectively. Several derivatives exhibited excellent anti-inflammatory activity compared to the standard drug. Furthermore, the synthesized compounds were found to have potential antioxidant activity. In addition, to rationalize the observed biological activity data, an in silico absorption, distribution, metabolism, and excretion (ADME) prediction study also been carried out. The results of the in vitro and in silico studies suggest that the 3-(trifluoromethyl)-1-(perfluorophenyl)-1*H*-pyrazol-5(4*H*)-one derivatives (**4a-d**, **5a-f**, and **6a-e**) may possess the ideal structural requirements for the further development of novel therapeutic agents.

CONFLICT OF INTEREST

The authors declare no conflict of interest, financial or otherwise.

Supporting Information

Indian Journal of Heterocyclic Chemistry
Vol. 31 - Number 2 (Apr-Jun 2021) 177-182
DocID: https://connectjournals.com/01951.2021.31.177

ISSN (Print) : 0971-1627
ISSN (Online) : 2456-4311

Synthesis and Biological Screening of Some New 5,7-dihydro-4*H*-thieno[2,3-*c*] pyran-3-yl containing 1,2,4-Triazoles, 1,3,4-Oxadiazoles, and 1,3-Thiazoles

Ranjana K. Jadhav[1], Hemant N. Akolkar[2], Arun B. Nikumbh[3], Bhausaheb K. Karale[2]*

[1]Department of Chemistry, S. M. Joshi College, Hadapsar, Pune, Maharashtra, India
[2]Department of Chemistry, Radhabai Kale Mahila Mahavidyalaya, Ahmednagar, Maharashtra, India
[3]Department of Chemistry, Annasaheb Aawate College Manchar, Pune, Maharashtra, India

ABSTRACT Some new 5,7-dihydro-4*H*-thieno[2,3-c]pyran thiosemicarbazides (**2a-g**) were synthesized from 5,7-dihydro-4*H*-thieno[2,3-*c*]pyran-3-carbohydrazide (**1**) and aryl isothiocyanates in ethanol. The compounds **2** on refluxing with 1 N NaOH gave 5-(5,7-dihydro-4*H*-thieno[2,3-c]pyran-3-yl)-4-phenyl-4*H*-1,2,4-triazole-3-thiols **3a-g**. The reaction of **2** with 4N NaOH in presence of I_2/KI gave 5-(5,7-dihydro-4*H*-thieno[2,3-c]pyran-3-yl)-*N*-phenyl-1,3,4-oxadiazol-2-amines (**4a-g**). When **2** were reacted with 2-bromo-1-(4-fluorophenyl)ethanone, corresponding (11*Z*)-*N'*-(4-(4-fluorophenyl)-3-phenylthiazol-2(3*H*)-ylidene)-5,7-dihydro-4*H*-thieno[2,3-c]pyran-3-carbohydrazides (**5a-f**) were formed. The structures of the synthesized compounds were confirmed by using spectral techniques. The synthesized compounds were screened for their antifungal and antibacterial activity.

KEYWORDS Thiosemicarbazides, Triazoles, Oxadiazoles, Thiazoles, Antifungal and Antibacterial activity.

How to cite this article: Jadhav, R.K., Akolkar, H.N., Nikumbh, A.B., Karale, B.K. Synthesis and Biological Screening of Some New 5,7-dihydro-4*H*-thieno[2,3-*c*]pyran-3-yl containing 1,2,4-Triazoles, 1,3,4-Oxadiazoles, and 1,3-Thiazoles, *Indian J. Heterocycl. Chem.*, **2021**, *31*, 177–182. *(DocID: https://connectjournals.com/01951.2021.31.177)*

Biogenic synthesis of ZnO nanoparticles from *Parthenium histerophorus* extract and its catalytic activity for building bioactive polyhydroquinolines

Published: 05 January 2021

Volume 47, pages 1743–1758, (2021) Cite this article

Prasad Mane, Bipin Shinde, Pankaj Mundada, Bhausaheb Karale & Arvind Burungale

Abstract

In the present protocol, biogenic synthesis of ZnO nanoparticles using an aqueous extract of weed, i.e. *Parthenium* is efficiently carried out. The proficient and operationally simple catalytic application of biogenic ZnO nanoparticle is explored towards a synthesis of pharmaceutically relevant and densely functionalized polyhydroquinolines by condensation of four components viz. aromatic aldehyde, dimedone, ethyl acetoacetate, and ammonium acetate. The synthesized polyhydroquinolines were screened for their antimicrobial activity against bacteria and fungi; some of them exhibit better to excellent activity. The developed protocol is enriched with captivating advantages such as excellent

'In water' exploration of *Alpinia zerumbet*-fabricated CuO NPs in the presence of NaPTS at room temperature: green synthesis of 1,8-dioxooctahydroxanthene derivatives

Published: 04 January 2021

Volume 47, pages 1221–1237, (2021) Cite this article

Bipin Shinde, Santosh Kamble, Harsharaj Jadhav, Prasad Mane, Kalpesh Khude, Hern Kim, Bhausaheb Karale & Arvind Burungale

Abstract

The biogenic synthesis of copper oxide nanoparticles (CuO NPs) from the leaf extract of *Alpinia zerumbet* was investigated in this protocol. The basic nature of *A. zerumbet* leaf extract helps in CuO NPs synthesis. The catalytic activity of *A. zerumbet*-fabricated CuO NPs is explored in water at room temperature only in the presence of NaPTS hydrotrope. The green catalytic protocol is investigated via synthesis of 1,8-dioxooctahydroxanthene. The biogenic leaf extract fabricated CuO NPs are efficiently reactive, stable and recyclable in aqueous solution of sodium *p*-toluenesulfonate (NaPTS) hydrotrope. CuO/NaPTS

Indian Journal of Heterocyclic Chemistry
Vol. 31 - Number 2 (Apr-Jun 2021) 177-182
DocID: https://connectjournals.com/01951.2021.31.177

ISSN (Print) : 0971-1627
ISSN (Online) : 2456-4311

Synthesis and Biological Screening of Some New 5,7-dihydro-4*H*-thieno[2,3-*c*] pyran-3-yl containing 1,2,4-Triazoles, 1,3,4-Oxadiazoles, and 1,3-Thiazoles

Ranjana K. Jadhav[1], Hemant N. Akolkar[2], Arun B. Nikumbh[3], Bhausaheb K. Karale[2]*

[1]Department of Chemistry, S. M. Joshi College, Hadapsar, Pune, Maharashtra, India
[2]Department of Chemistry, Radhabai Kale Mahila Mahavidyalaya, Ahmednagar, Maharashtra, India
[3]Department of Chemistry, Annasaheb Aawate College Manchar, Pune, Maharashtra, India

ABSTRACT Some new 5,7-dihydro-4*H*-thieno[2,3-c]pyran thiosemicarbazides (**2a-g**) were synthesized from 5,7-dihydro-4*H*-thieno[2,3-*c*]pyran-3-carbohydrazide (**1**) and aryl isothiocyanates in ethanol. The compounds **2** on refluxing with 1 N NaOH gave 5-(5,7-dihydro-4*H*-thieno[2,3-c]pyran-3-yl)-4-phenyl-4*H*-1,2,4-triazole-3-thiols **3a-g**. The reaction of **2** with 4N NaOH in presence of I_2/KI gave 5-(5,7-dihydro-4*H*-thieno[2,3-c]pyran-3-yl)-*N*-phenyl-1,3,4-oxadiazol-2-amines (**4a-g**). When **2** were reacted with 2-bromo-1-(4-fluorophenyl)ethanone, corresponding (11*Z*)-*N'*-(4-(4-fluorophenyl)-3-phenylthiazol-2(3*H*)-ylidene)-5,7-dihydro-4*H*-thieno[2,3-c]pyran-3-carbohydrazides (**5a-f**) were formed. The structures of the synthesized compounds were confirmed by using spectral techniques. The synthesized compounds were screened for their antifungal and antibacterial activity.

KEYWORDS Thiosemicarbazides, Triazoles, Oxadiazoles, Thiazoles, Antifungal and Antibacterial activity.

How to cite this article: Jadhav, R.K., Akolkar, H.N., Nikumbh, A.B., Karale, B.K. Synthesis and Biological Screening of Some New 5,7-dihydro-4*H*-thieno[2,3-*c*]pyran-3-yl containing 1,2,4-Triazoles, 1,3,4-Oxadiazoles, and 1,3-Thiazoles, *Indian J. Heterocycl. Chem.*, **2021**, *31*, 177–182. *(DocID: https://connectjournals.com/01951.2021.31.177)*

Journal of the Chinese Chemical Society / Volume 68, Issue 4 / p. 657-668

ARTICLE

Synthesis of 3-(trifluoromethyl)-1-(perfluorophenyl)-1*H*-pyrazol-5(4*H*)-one derivatives via Knoevenagel condensation and their biological evaluation

Sujata G. Dengale, Hemantkumar N. Akolkar, Bhausaheb K. Karale, Nirmala R. Darekar, Sadhana D. Mhaske, Mubarak H. Shaikh, Dipak N. Raut, Keshav K. Deshmukh

First published: 26 November 2020
https://doi.org/10.1002/jccs.202000357
Citations: 5

Abstract

In search of new active molecules, a small focused library of the synthesis of 3-(trifluoromethyl)-1-(perfluorophenyl)-1*H*-pyrazol-5(4*H*)-one derivatives (**4a-d**, **5a-f**, and **6a-e**) has been efficiently prepared via the Knoevenagel condensation approach. All the derivatives were synthesized by conventional and nonconventional methods like ultrasonication and microwave irradiation, respectively. Several derivatives exhibited excellent anti-inflammatory activity compared to the standard drug. Furthermore, the synthesized compounds were found to have potential antioxidant activity. In addition, to rationalize the observed biological activity data, an in silico absorption, distribution, metabolism, and excretion (ADME) prediction study also been carried out. The results of the in vitro and in silico studies suggest that the 3-(trifluoromethyl)-1-(perfluorophenyl)-1*H*-pyrazol-5(4*H*)-one derivatives (**4a-d**, **5a-f**, and **6a-e**) may possess the ideal structural requirements for the further development of novel therapeutic agents.

CONFLICT OF INTEREST

The authors declare no conflict of interest, financial or otherwise.

Supporting Information

Issue 45, 2020

Previous Next

From the journal:
RSC Advances

Nanostructured N doped TiO_2 efficient stable catalyst for Kabachnik–Fields reaction under microwave irradiation †

Sachin P. Kunde,[ab] Kaluram G. Kanade,[*ac] Bhausaheb K. Karale,[a] Hemant N. Akolkar,[a] Sudhir S. Arbuj,[d] Pratibha V. Randhavane,[a] Santosh T. Shinde,[a] Mubarak H. Shaikh[a] and Aniruddha K. Kulkarni[e]

Author affiliations

Abstract

Herein, we report nitrogen-doped TiO_2 (N-TiO_2) solid-acid nanocatalysts with heterogeneous structure employed for the solvent-free synthesis of α-aminophosphonates through Kabachnik–Fields reaction. N-TiO_2 were synthesized by direct amination using triethylamine as a source of nitrogen at low temperature and optimized by varying the volume ratios of $TiCl_4$, methanol, water, and triethylamine, under identical conditions. An X-ray diffraction (XRD) study showed the formation of a rutile phase and the crystalline size is 10 nm. The nanostructural features of N-TiO_2 were examined by HR-TEM analysis,

Polycyclic Aromatic Compounds >
Volume 42, 2022 - Issue 5

Research Articles

Design, Synthesis and Biological Evaluation of Novel Furan & Thiophene Containing Pyrazolyl Pyrazolines as Antimalarial Agents

Hemantkumar N. Akolkar, Sujata G. Dengale, Keshav K. Deshmukh, Bhausaheb K. Karale, Nirmala R. Darekar, Vijay M. Khedkar & ...show all

Pages 1959-1971 | Received 07 Aug 2020, Accepted 05 Sep 2020, Published online: 14 Sep 2020

Cite this article https://doi.org/10.1080/10406638.2020.1821231 Check for updates

Abstract

In search for novel compounds targeting Malaria, based on the *in silico* molecular docking binding affinity data, the novel furans containing pyrazolyl chalcones (**3a-d**) and pyrazoline derivatives (**4a-d**) were synthesized. The formation of the synthesized compound were confirmed by spectral analysis like IR, ^{1}H NMR, ^{13}C NMR and mass spectrometry. Compounds with thiophene and pyrazoline ring **4b** (0.47 µM), **4c** (0.47 µM) and **4d** (0.21 µM) exhibited excellent anti-malarial activity against *Plasmodium falciparum* compared with standard antimalarial drug Quinine (0.83 µM). To check the selectivity furthermore, compounds were tested for antimicrobial activity and none of

Propargylated monocarbonyl curcumin analogues: synthesis, bioevaluation and molecular docking study

Original Research Published: 10 August 2020

Volume 29, pages 1902–1913, (2020) Cite this article

Medicinal Chemistry Research

Aims and scope

Submit manuscript

Amol A. Nagargoje, Satish V. Akolkar, Dnyaneshwar D. Subhedar, Mubarak H. Shaikh, Jaiprakash N. Sangshetti, Vijay M. Khedkar & Bapurao B. Shingate

Abstract

In the current experimental study, we have synthesised new monocarbonyl curcumin analogues bearing propargyl ether moiety in their structure and evaluated for in vitro antifungal and radical scavenging activity. The antifungal activity was carried out against five human pathogenic fungal strains such as *Candida albicans*, *Fusarium oxysporum*, *Aspergillus flavus*, *Aspergillus niger* and *Cryptococcus neoformans*. Most of the curcumin analogues displayed excellent to moderate fungicidal activity when compared with standard drug Miconazole. Also, synthesised analogues exhibited potential radical scavenging activity as compared with standard antioxidant Butylated hydroxyl toluene (BHT). Based on biological data, structure-activity relationship (SAR) were also

Archiv der Pharmazie / Volume 353, Issue 11 / 2000164

FULL PAPER

New *N*-phenylacetamide-linked 1,2,3-triazole-tethered coumarin conjugates: Synthesis, bioevaluation, and molecular docking study

Satish V. Akolkar, Amol A. Nagargoje, Mubarak H. Shaikh, Murad Z. A. Warshagha, Jaiprakash N. Sangshetti, Manoj G. Damale, Bapurao B. Shingate

First published: 09 August 2020
https://doi.org/10.1002/ardp.202000164
Citations: 20

Abstract

A series of new 1,2,3-triazole-tethered coumarin conjugates linked by *N*-phenylacetamide was efficiently synthesized *via* the click chemistry approach in excellent yields. The synthesized conjugates were evaluated for their in vitro antifungal and antioxidant activities. Antifungal activity determination was carried out against fungal strains such as *Candida albicans*, *Fusarium oxysporum*, *Aspergillus flavus*, *Aspergillus niger* and *Cryptococcus neoformans*. Compounds **7b**, **7d**, **7e**, **8b** and **8e** displayed higher potency than the standard drug miconazole, with lower minimum inhibitory concentration values. Also, compound **7a** exhibited potential radical scavenging activity as compared with the standard antioxidant butylated hydroxytoluene. In addition, a molecular docking study of the newly synthesized compounds was carried out, and the results showed a good binding mode at the active site of the fungal (*C. albicans*) P450 cytochrome lanosterol 14α-demethylase enzyme. Furthermore, the synthesized compounds were also tested for ADME properties, and they demonstrated potential as good candidates for oral drugs.

Supporting Information

Chemistry & Biology Interface, 2020, 10, 3, 73-86

RESEARCH PAPER ISSN: 2249 –4820

CHEMISTRY & BIOLOGY INTERFACE

An official Journal of ISCB, Journal homepage; www.cbijournal.com

Synthesis, evaluation and molecular docking of 1,2,3-triazolyl chalcones as potential antifungal and antioxidant agents

Amol A. Nagargoje[1,2], Satish V. Akolkar[1], Mubarak H. Shaikh[1,3], Dnyaneshwar D. Subhedar[1], Jaiprakash N. Sangshetti[4], Vijay M. Khedkar[5], Bapurao B. Shingate*[1]

[1]*Department of Chemistry, Dr Babasaheb Ambedkar Marathwada University, Aurangabad, 431004, India*
[2]*Department of Chemistry, Khopoli Municipal Council College, Khopoli, 410203, India*
[3]*Department of Chemistry, Radhabai Kale Mahila Mahavidyalaya, Ahmednagar, 414001, India*
[4]*Department of Pharmaceutical Chemistry, Y. B. Chavan College of Pharmacy, Rafiq Zakaria Campus, Aurangabad, 431001, India*
[5]*Department of Pharmaceutical Chemistry, School of Pharmacy, Vishwakarma University, Pune, 411048, India*
E-mail: bapushingate@gmail.com(B. B. Shingate)*
**Corresponding author. Tel.: (91-0240-2403312)*
Received 15 June 2020, Accepted 30 June 2020

Abstract: A series of new 1,2,3-triazolyl chalcones were efficiently synthesized and screened for in *vitro* antifungal activity against five different fungal strains such as *Candida albicans*, *Fusarium oxysporum, Aspergillus flavus*, *Aspergillus niger* and *Cryptococcus neoformans*. All the synthesized chalcones displayed potential antifungal activity against most of the tested fungal strains. Especially, compounds **9b, 9c, 9d** and **9g** are the most active chalcones and displayed excellent MIC values as compared to standard antifungal drug Miconazole. Based on the structural similarity to known triazole inhibitors of sterol 14α-demethylase (CYP51), molecular docking study was performed to gauze the binding affinity of these chalcones and gains an insight into the plausible mechanism of antifungal action. The synthesized chalcones were also evaluated for in *vitro* antioxidant activity. All compounds exhibited moderate to excellent antioxidant activity, particularly compounds **9e, 9f, 9g** and **9h** exhibited excellent antioxidant activity in comparison with standard butylated hydroxytoluene (BHT). Furthermore, the synthesized chalcones were analyzed for ADME properties and showed the potential to build up as good oral drug candidates.

Keywords: 1,2,3-triazole, Chalcone, Antifungal activity, Antioxidant activity, Molecular docking study, ADME prediction.

1. Introduction

The incidences of multidrug-resistant fungal infections in recent years have increased dramatically and commonly seen in patients with weak immune systems [1]. An increasing number

Polycyclic Aromatic Compounds >
Volume 42, 2022 - Issue 4

Research Articles

Tetrazoloquinoline-1,2,3-Triazole Derivatives as Antimicrobial Agents: Synthesis, Biological Evaluation and Molecular Docking Study

Mubarak H. Shaikh, Dnyaneshwar D. Subhedar, Satish V. Akolkar, Amol A. Nagargoje, Vijay M. Khedkar, Dhiman Sarkar & ...show all

Pages 1920-1941 | Received 21 Jun 2020, Accepted 05 Sep 2020, Published online: 16 Sep 2020

Cite this article https://doi.org/10.1080/10406638.2020.1821229 Check for updates

Abstract

In search of new active molecules, a small focused library of tetrazoloquinoline-based 1,2,3-triazoles has been efficiently prepared *via* click chemistry approach. Several derivatives were found to be exhibiting promising antimicrobial and antioxidant activity characterized by their lower minimum inhibitory concentration values. All the synthesized compounds exhibited excellent antibacterial activity against Gram negative bacteria *E. coli* and *F. devorans* and antifungal activity against *C. albicans* and *A. niger*. Further, these compounds were tested for their antitubercular activity against dormant *MTB H37Ra* and dormant *M. bovis BCG* using XRMA assay protocol and

Polycyclic Aromatic Compounds >
Volume 42, 2022 - Issue 5

Research Articles

Amide-Linked Monocarbonyl Curcumin Analogues: Efficient Synthesis, Antitubercular Activity and Molecular Docking Study

Dnyaneshwar D. Subhedar, Mubarak H. Shaikh, Amol A. Nagargoje, Satish V. Akolkar, Sujit G. Bhansali, Dhiman Sarkar & ...show all

Pages 2655-2671 | Received 14 Sep 2020, Accepted 25 Oct 2020, Published online: 09 Dec 2020

Cite this article https://doi.org/10.1080/10406638.2020.1852288 Check for updates

Abstract

An approach toward the synthesis of novel conjugates of 3,5-bis (arylidene)-4-piperidones (DAP) pharmacophore with amide-linkage has been developed *via* one-pot multicomponent reaction of aryl aldehydes, piperidinone and 2-chloro-*N*-phenylacetamide using $[Et_3NH][HSO_4]$ as a catalyst/medium. Both substitutions on arylidene rings and piperidinone nitrogen (substituted 2-chloro-*N*-phenylacetamide) were varied. The synthesized conjugates were evaluated for their *in vitro* antitubercular activity against *M. tuberculosis* $H_{37}Ra$ (*MTB*) and *M. bovis* BCG strains. Among the series, compounds **4f**, **4g, 4i** and **4j** showed remarkable broad spectrum

Polycyclic Aromatic Compounds >
Volume 42, 2022 - Issue 5

Research Articles

Design, Synthesis and Biological Evaluation of Novel Furan & Thiophene Containing Pyrazolyl Pyrazolines as Antimalarial Agents

Hemantkumar N. Akolkar, Sujata G. Dengale, Keshav K. Deshmukh, Bhausaheb K. Karale, Nirmala R. Darekar, Vijay M. Khedkar & ...show all

Pages 1959-1971 | Received 07 Aug 2020, Accepted 05 Sep 2020, Published online: 14 Sep 2020

Cite this article https://doi.org/10.1080/10406638.2020.1821231 Check for updates

Abstract

In search for novel compounds targeting Malaria, based on the *in silico* molecular docking binding affinity data, the novel furans containing pyrazolyl chalcones (**3a-d**) and pyrazoline derivatives (**4a-d**) were synthesized. The formation of the synthesized compound were confirmed by spectral analysis like IR, ^{1}H NMR, ^{13}C NMR and mass spectrometry. Compounds with thiophene and pyrazoline ring **4b** (0.47 µM), **4c** (0.47 µM) and **4d** (0.21 µM) exhibited excellent anti-malarial activity against *Plasmodium falciparum* compared with standard antimalarial drug Quinine (0.83 µM). To check the selectivity furthermore, compounds were tested for antimicrobial activity and none of

Microwave Assisted Synthesis and Antibacterial Activity of New 1,3,4-Thiadiazoles and 1,2,4-Triazoles Derived from 2-{2-[2-(4-Fluorophenyl)-4-methylthiazol-5-yl]-1*H*-benzo[*d*]imidazol-1-yl}acetohydrazide

Published: 12 October 2020

Volume 90, pages 1721–1726, (2020) Cite this article

N. R. Darekar, B. K. Karale, H. N. Akolkar & A. S. Burungale

Abstract

A series of novel derivatives of 1-(2-{2-[2-(4-fluorophenyl)-4-methylthiazol-5-yl]-1*H*-benzo[*d*]imidazol-1-yl}acetyl)-4-phenylthiosemicarbazide, 5-({2-[2-(4-fluorophenyl)-4-methylthiazol-5-yl]-1*H*-benzo[*d*]imidazol-1-yl}methyl)-4-phenyl-4*H*-1,2,4-triazole-3-thiol and 5-({2-[2-(4-fluorophenyl)-4-methylthiazol-5-yl]-1*H*-benzo[*d*]imidazol-1-yl}methyl)-*N*-phenyl-1,3,4-thiadiazol-2-amine have been synthesized by the conventional method as well as using MW irradiation. All newly synthesized compounds have been tested for antibacterial activity. Several products have demonstrated moderate activity against gram positive and gram negative bacterial strains.

Issue 45, 2020

Previous Next

From the journal:
RSC Advances

Nanostructured N doped TiO_2 efficient stable catalyst for Kabachnik–Fields reaction under microwave irradiation †

Sachin P. Kunde,[ab] Kaluram G. Kanade,[*ac] Bhausaheb K. Karale,[a] Hemant N. Akolkar,[a] Sudhir S. Arbuj,[d] Pratibha V. Randhavane,[a] Santosh T. Shinde,[a] Mubarak H. Shaikh[a] and Aniruddha K. Kulkarni[e]

Author affiliations

Abstract

Herein, we report nitrogen-doped TiO_2 (N-TiO_2) solid-acid nanocatalysts with heterogeneous structure employed for the solvent-free synthesis of α-aminophosphonates through Kabachnik–Fields reaction. N-TiO_2 were synthesized by direct amination using triethylamine as a source of nitrogen at low temperature and optimized by varying the volume ratios of $TiCl_4$, methanol, water, and triethylamine, under identical conditions. An X-ray diffraction (XRD) study showed the formation of a rutile phase and the crystalline size is 10 nm. The nanostructural features of N-TiO_2 were examined by HR-TEM analysis,

Journal of Heterocyclic Chemistry / Volume 57, Issue 4 / p. 1692-1697

ARTICLE

Synthesis and characterization of novel 2-(1-benzyl-3-[4-fluorophenyl]-1*H*-pyrazol-4-yl)-7-fluoro-4*H*-chromen-4-one derivatives

Kiran S. Hon, Hemantkumar N. Akolkar, Bhausaheb K. Karale

First published: 28 January 2020
https://doi.org/10.1002/jhet.3894
Citations: 6

Abstract

Novel 1-benzyl-3-(4-fluorophenyl)-1*H*-pyrazole-4-carbaldehydes **3a** to **3e** were synthesized via Vilsmeier-Haack reaction of the appropriate 1-benzyl-2-(1-(4-fluorophenyl)ethylidene)hydrazines, derived from 4-fluoroacetophenone **1** with substituted 2-benzylhydrazines **2a** to **2e**. The base catalyzed condensation of 1-benzyl-3-(4-fluorophenyl)-1*H*-pyrazole-4-carbaldehydes **3a** to **3e** with 1-(4-fluoro-2-hydroxyphenyl)ethanone **4** gave (*E*)-3-(1-benzyl-3-(4-fluorophenyl)-1*H*-pyrazol-4-yl)-1-(4-fluoro-2-hydroxyphenyl)prop-2-en-1-ones **5a** to **5e**. On cyclization with dimethyl sulfoxide (DMSO)/I_2, compounds **5a** to **5e** gave 2-(1-benzyl-3-(4-fluorophenyl)-1*H*-pyrazol-4-yl)-7-fluoro-4*H*-chromen-4-ones **6a** to **6e**. Structures of all novel compounds were confirmed by infrared (IR), proton nuclear magnetic resonance (^{1}H NMR), carbon nuclear magnetic resonance (^{13}C NMR), and mass spectral data. All the synthesized compounds were screened for their antibacterial activities.

Supporting Information

Filename	Description
jhet3894-sup-0001-Appendix S1.docx Word 2007 document , 5.7 MB	**Appendix S1**: Supporting information

Polycyclic Aromatic Compounds >
Volume 42, 2022 - Issue 5

Research Articles

Design, Synthesis and Biological Evaluation of Novel Furan & Thiophene Containing Pyrazolyl Pyrazolines as Antimalarial Agents

Hemantkumar N. Akolkar, Sujata G. Dengale, Keshav K. Deshmukh, Bhausaheb K. Karale, Nirmala R. Darekar, Vijay M. Khedkar & ...show all

Pages 1959-1971 | Received 07 Aug 2020, Accepted 05 Sep 2020, Published online: 14 Sep 2020

Cite this article https://doi.org/10.1080/10406638.2020.1821231 Check for updates

Abstract

In search for novel compounds targeting Malaria, based on the *in silico* molecular docking binding affinity data, the novel furans containing pyrazolyl chalcones (**3a-d**) and pyrazoline derivatives (**4a-d**) were synthesized. The formation of the synthesized compound were confirmed by spectral analysis like IR, ^{1}H NMR, ^{13}C NMR and mass spectrometry. Compounds with thiophene and pyrazoline ring **4b** (0.47 µM), **4c** (0.47 µM) and **4d** (0.21 µM) exhibited excellent anti-malarial activity against *Plasmodium falciparum* compared with standard antimalarial drug Quinine (0.83 µM). To check the selectivity furthermore, compounds were tested for antimicrobial activity and none of

Microwave Assisted Synthesis and Antibacterial Activity of New 1,3,4-Thiadiazoles and 1,2,4-Triazoles Derived from 2-{2-[2-(4-Fluorophenyl)-4-methylthiazol-5-yl]-1*H*-benzo[*d*]imidazol-1-yl}acetohydrazide

Published: 12 October 2020

Volume 90, pages 1721–1726, (2020) Cite this article

N. R. Darekar, B. K. Karale, H. N. Akolkar & A. S. Burungale

Abstract

A series of novel derivatives of 1-(2-{2-[2-(4-fluorophenyl)-4-methylthiazol-5-yl]-1*H*-benzo[*d*]imidazol-1-yl}acetyl)-4-phenylthiosemicarbazide, 5-({2-[2-(4-fluorophenyl)-4-methylthiazol-5-yl]-1*H*-benzo[*d*]imidazol-1-yl}methyl)-4-phenyl-4*H*-1,2,4-triazole-3-thiol and 5-({2-[2-(4-fluorophenyl)-4-methylthiazol-5-yl]-1*H*-benzo[*d*]imidazol-1-yl}methyl)-*N*-phenyl-1,3,4-thiadiazol-2-amine have been synthesized by the conventional method as well as using MW irradiation. All newly synthesized compounds have been tested for antibacterial activity. Several products have demonstrated moderate activity against gram positive and gram negative bacterial strains.

Indian Journal of Heterocyclic Chemistry
Vol. 30 - Number 04 (Oct-Dec 2020) 607-613
DocID: https://connectjournals.com/01951.2020.30.607

ISSN (Print) : 0971-1627
ISSN (Online) : 2456-4311

Synthesis of New Thiazole Anchored N'-Benzylidene Carbohydrazide and 1,3,4-Oxadiazole Derivatives by Conventional and Microwave Irradiation Methods

Vaibhav P. Landage[1], Hemantkumar N. Akolkar[2], Dilip R. Thube[1*], Bhausaheb K. Karale[2]

[1]Department of Chemistry, Ahmednagar Jilha Maratha Vidya Prasarak Samaj's New Arts, Commerce and Science College, Savitribai Phule Pune University, Parner, Ahmednagar, Maharashtra, India
[2]Department of Chemistry, Rayat Shikshan Sanstha's Radhabai Kale Mahila Mahavidyalaya, Savitribai Phule Pune University, Ahmednagar, Maharashtra, India

ABSTRACT The 2-(4-chlorophenyl)-4-methylthiazole-5-carbohydrazide (**3**) and aromatic aldehydes (**4**) were heated together in alcohol under reflux and microwave (MW) irradiation, to get new series of thiazolyl benzylidine carbohydrazides **5A-K**, which in turn under the influence of reflux and MW irradiation, cyclized with acetic anhydride and propionic anhydride to achieve thiazolyl 1,3,4-oxadiazole derivatives **6A-K** and **7A-K**, respectively. The structures of newly synthesized compounds were confirmed by spectral and elemental analysis.

KEYWORDS Benzylidinecarbohydrazide, Oxadiazole, Thiazole, MW irradiation.

How to cite this article: Landage, V.P., Akolkar, H.N., Thube, D.R., Karale B.K. Synthesis of New Thiazole Anchored N'-Benzylidene Carbohydrazide and 1,3,4-Oxadiazole Derivatives by Conventional and Microwave Irradiation Methods, *Indian J. Heterocycl. Chem.*, **2020**, *30*, 607–613. *(DocID: https://connectjournals.com/01951.2020.30.607)*

Indian Journal of Heterocyclic Chemistry
Vol. 30 - Number 03 (Jul-Sep 2020) 355-360
DocID: https://connectjournals.com/01951.2020.30.355

ISSN (Print) : 0971-1627
ISSN (Online) : 2456-4311

Microwave-assisted Synthesis, Characterization, and Antibacterial Screening of Some Pyrazolone Derivatives

Bhausaheb Kisan. Karale[1]*, Sarita G. Kundlikar[1], Hemantkumar N. Akolkar[1], Pratibha V. Randhavane[1], Sushama J. Takate[2]

[1]Department of Chemistry, Radhabai Kale Mahila Mahavidyalaya, Ahmednagar, Maharashtra, India
[2]Department of Chemistry, New Arts, Science and Commerce College, Ahmednagar, Maharashtra, India

ABSTRACT 1-(4-(4-Chlorophenyl)thiazol-2-yl)-3-propyl-1*H*-pyrazol-5(4*H*)-one **5** was prepared by the reaction of 1-(4-(4-chlorophenyl)thiazol-2-yl)hydrazine and ethyl 3-oxohexanoate. Compound **5** was condensed with different 4-formylpyrazoles **8a-f** to give product **9a-f** through Knoevenagel condensation. The reaction was carried out by both conventional and non-conventional methods. The structures of all the newly synthesized compounds were confirmed with the help of spectral techniques. All the compounds were screened for antibacterial activity. Compounds **9a**, **9d,** and **9e** exhibited good antibacterial activity against *Bacillus subtilis*.

KEYWORDS Knoevenagel condensation, Pyrazolone, Thiazoles, Thiophene.

How to cite this article: Karale, B.K., Kundlikar, S.G., Akolkar, H.N., Randhavane, P.V., Takate, S.J. Microwave-assisted Synthesis, Characterization, and Antibacterial Screening of Some Pyrazolone Derivatives, *Indian J. Heterocycl. Chem.*, **2020**, *30*, 355–360. *(DocID: https://connectjournals.com/01951.2020.30.355)*

Indian Journal of Heterocyclic Chemistry
Vol. 30 - Number 04 (Oct-Dec 2020) 525-530
DocID: https://connectjournals.com/01951.2020.30.525

ISSN (Print) : 0971-1627
ISSN (Online) : 2456-4311

Synthesis and Antibacterial Screening of Some New Pyrazolylchromones and Pyrazolylcoumaran-3-ones

Sushama J. Takate[1], Supriya P. Salve[1], Sushama B. Dare[1], Bhausaheb K. Karale[2], Hemantkumar N. Akolkar[2], Dnyaneshwar B. Falke[1], Rahul B. Ghungurde[1], Sadhana D. Mhaske[3]*

[1]Department of Chemistry, New Arts, Commerce and Science College, Ahmednagar; Affiliated to SPPU, Pune, Maharashtra, India

[2]Department of Chemistry, Radhabai Kale Mahila Mahavidyalaya, Ahmednagar; Affiliated to SPPU, Pune, Maharashtra, India

[3]Department of Chemistry, Dadapatil Rajale Arts, Science and Commerce College, Adinathnagar; Affiliated to SPPU, Pune, Maharashtra, India

ABSTRACT Some new pyrazolylchromones **4a-e** (flavone analogs) and pyrazolylcoumaran-3-ones **5a-e** (aurone analogs) were synthesized by refluxing chalcones **3a-e** in dimethyl sulfoxide/I_2 and Pyridine/$Hg(OAc)_2$, respectively. Spectral techniques such as infrared, proton nuclear magnetic resonance, and mass spectrometry were used to confirm the structures of newly synthesized compounds. These compounds were studied for their antibacterial activities toward *Bacillus subtilis, Staphylococcus aureus, Escherichia coli,* and *Salmonella typhi*. Some of these compounds showed promising activity against test organisms.

KEYWORDS: Pyrazoles, Flavones, Aurones, Antibacterial activity.

How to cite this article: Takate, S.J., Salve, S.P., Dare, S.B., Karale, B.K., Akolkar, H.N., Falke, D.B., Ghungurde, R.B., Mhaske, S.D. Synthesis and Antibacterial Screening of Some New Pyrazolylchromones and Pyrazolylcoumaran-3-ones. *Indian J. Heterocycl. Chem.*, **2020,** *30*, 525-530. *(DocID: https://connectjournals.com/01951.2020.30.525)*

INTRODUCTION

Treatment of various diseases is a worldwide serious issue. The emergence of newer infectious diseases, multidrug resistance developing in microbial strains, diseases due to homeostatic disturbances, toxicity associated with existing drugs have created a need of selective, potential therapeutic agents. In search of potential therapeutic agents, many natural and synthetic compounds have been investigated. Many of the natural products are heterocycles which possess medicinal properties and serve as lead molecules for drug discovery.[1] Lead modification is an important step in drug design and development.

Pyrazole containing compounds are medicinally useful because of their various therapeutic properties, including antimicrobial,[2,3] anti-inflammatory,[4] antitubercular,[5] antitumor,[6] antidiabetic,[7] and antiviral and antioxidant[8] properties.

Flavonoids are extensively studied plant products for their biological potential. Chalcones are important intermediates in the flavonoid synthetic pathway and also have medicinal properties.[9] These are known to exhibit antibacterial,[10] antitubercular,[11] anti-inflammatory,[12,13] antimalarial,[14] antifungal,[15] and antiviral[16] activities. Synthetic chalcones with heterocyclic rings have been investigated for medicinal properties and are also used in the synthesis of various heterocycles. Pyrazole containing chalcones exhibits potential antimicrobial,[17] antioxidant,[18] and anticancer[19] activities.

Flavones and aurones are medicinally useful members of the flavonoid family. Flavones are widely known for their interesting bioactivities. As a consequence of the

*Corresponding author: E-mail: mhaskesadhana@gmail.com

Published & Hosted by :
Journal Homepage :
www.connectjournals.com/ijhc
www.connectjournals.com

Indian Journal of Heterocyclic Chemistry
Vol. 30 - Number 04 (Oct-Dec 2020) 525-530
DocID: https://connectjournals.com/01951.2020.30.525

ISSN (Print) : 0971-1627
ISSN (Online) : 2456-4311

Synthesis and Antibacterial Screening of Some New Pyrazolylchromones and Pyrazolylcoumaran-3-ones

Sushama J. Takate[1], Supriya P. Salve[1], Sushama B. Dare[1], Bhausaheb K. Karale[2], Hemantkumar N. Akolkar[2], Dnyaneshwar B. Falke[1], Rahul B. Ghungurde[1], Sadhana D. Mhaske[3]*

[1]Department of Chemistry, New Arts, Commerce and Science College, Ahmednagar; Affiliated to SPPU, Pune, Maharashtra, India

[2]Department of Chemistry, Radhabai Kale Mahila Mahavidyalaya, Ahmednagar; Affiliated to SPPU, Pune, Maharashtra, India

[3]Department of Chemistry, Dadapatil Rajale Arts, Science and Commerce College, Adinathnagar; Affiliated to SPPU, Pune, Maharashtra, India

ABSTRACT Some new pyrazolylchromones **4a-e** (flavone analogs) and pyrazolylcoumaran-3-ones **5a-e** (aurone analogs) were synthesized by refluxing chalcones **3a-e** in dimethyl sulfoxide/I_2 and Pyridine/$Hg(OAc)_2$, respectively. Spectral techniques such as infrared, proton nuclear magnetic resonance, and mass spectrometry were used to confirm the structures of newly synthesized compounds. These compounds were studied for their antibacterial activities toward *Bacillus subtilis, Staphylococcus aureus, Escherichia coli,* and *Salmonella typhi*. Some of these compounds showed promising activity against test organisms.

KEYWORDS: Pyrazoles, Flavones, Aurones, Antibacterial activity.

How to cite this article: Takate, S.J., Salve, S.P., Dare, S.B., Karale, B.K., Akolkar, H.N., Falke, D.B., Ghungurde, R.B., Mhaske, S.D. Synthesis and Antibacterial Screening of Some New Pyrazolylchromones and Pyrazolylcoumaran-3-ones. *Indian J. Heterocycl. Chem.*, **2020,** *30*, 525-530. *(DocID: https://connectjournals.com/01951.2020.30.525)*

INTRODUCTION

Treatment of various diseases is a worldwide serious issue. The emergence of newer infectious diseases, multidrug resistance developing in microbial strains, diseases due to homeostatic disturbances, toxicity associated with existing drugs have created a need of selective, potential therapeutic agents. In search of potential therapeutic agents, many natural and synthetic compounds have been investigated. Many of the natural products are heterocycles which possess medicinal properties and serve as lead molecules for drug discovery.[1] Lead modification is an important step in drug design and development.

Pyrazole containing compounds are medicinally useful because of their various therapeutic properties, including antimicrobial,[2,3] anti-inflammatory,[4] antitubercular,[5] antitumor,[6] antidiabetic,[7] and antiviral and antioxidant[8] properties.

Flavonoids are extensively studied plant products for their biological potential. Chalcones are important intermediates in the flavonoid synthetic pathway and also have medicinal properties.[9] These are known to exhibit antibacterial,[10] antitubercular,[11] anti-inflammatory,[12,13] antimalarial,[14] antifungal,[15] and antiviral[16] activities. Synthetic chalcones with heterocyclic rings have been investigated for medicinal properties and are also used in the synthesis of various heterocycles. Pyrazole containing chalcones exhibits potential antimicrobial,[17] antioxidant,[18] and anticancer[19] activities.

Flavones and aurones are medicinally useful members of the flavonoid family. Flavones are widely known for their interesting bioactivities. As a consequence of the

*Corresponding author: E-mail: mhaskesadhana@gmail.com

Published & Hosted by :
Journal Homepage :
www.connectjournals.com/ijhc
www.connectjournals.com

Indian Journal of Heterocyclic Chemistry
Vol. 30 - Number 03 (Jul-Sep 2020) 355-360
DocID: https://connectjournals.com/01951.2020.30.355

ISSN (Print) : 0971-1627
ISSN (Online) : 2456-4311

Microwave-assisted Synthesis, Characterization, and Antibacterial Screening of Some Pyrazolone Derivatives

Bhausaheb Kisan. Karale[1]*, Sarita G. Kundlikar[1], Hemantkumar N. Akolkar[1], Pratibha V. Randhavane[1], Sushama J. Takate[2]

[1]Department of Chemistry, Radhabai Kale Mahila Mahavidyalaya, Ahmednagar, Maharashtra, India
[2]Department of Chemistry, New Arts, Science and Commerce College, Ahmednagar, Maharashtra, India

ABSTRACT 1-(4-(4-Chlorophenyl)thiazol-2-yl)-3-propyl-1*H*-pyrazol-5(4*H*)-one **5** was prepared by the reaction of 1-(4-(4-chlorophenyl)thiazol-2-yl)hydrazine and ethyl 3-oxohexanoate. Compound **5** was condensed with different 4-formylpyrazoles **8a-f** to give product **9a-f** through Knoevenagel condensation. The reaction was carried out by both conventional and non-conventional methods. The structures of all the newly synthesized compounds were confirmed with the help of spectral techniques. All the compounds were screened for antibacterial activity. Compounds **9a**, **9d,** and **9e** exhibited good antibacterial activity against *Bacillus subtilis*.

KEYWORDS Knoevenagel condensation, Pyrazolone, Thiazoles, Thiophene.

How to cite this article: Karale, B.K., Kundlikar, S.G., Akolkar, H.N., Randhavane, P.V., Takate, S.J. Microwave-assisted Synthesis, Characterization, and Antibacterial Screening of Some Pyrazolone Derivatives, *Indian J. Heterocycl. Chem.*, **2020**, *30*, 355–360. *(DocID: https://connectjournals.com/01951.2020.30.355)*

Indian Journal of Heterocyclic Chemistry
Vol. 30 - Number 04 (Oct-Dec 2020) 607-613
DocID: https://connectjournals.com/01951.2020.30.607

ISSN (Print) : 0971-1627
ISSN (Online) : 2456-4311

Synthesis of New Thiazole Anchored N'-Benzylidene Carbohydrazide and 1,3,4-Oxadiazole Derivatives by Conventional and Microwave Irradiation Methods

Vaibhav P. Landage[1], Hemantkumar N. Akolkar[2], Dilip R. Thube[1*], Bhausaheb K. Karale[2]

[1]Department of Chemistry, Ahmednagar Jilha Maratha Vidya Prasarak Samaj's New Arts, Commerce and Science College, Savitribai Phule Pune University, Parner, Ahmednagar, Maharashtra, India
[2]Department of Chemistry, Rayat Shikshan Sanstha's Radhabai Kale Mahila Mahavidyalaya, Savitribai Phule Pune University, Ahmednagar, Maharashtra, India

ABSTRACT The 2-(4-chlorophenyl)-4-methylthiazole-5-carbohydrazide (**3**) and aromatic aldehydes (**4**) were heated together in alcohol under reflux and microwave (MW) irradiation, to get new series of thiazolyl benzylidine carbohydrazides **5A-K**, which in turn under the influence of reflux and MW irradiation, cyclized with acetic anhydride and propionic anhydride to achieve thiazolyl 1,3,4-oxadiazole derivatives **6A-K** and **7A-K**, respectively. The structures of newly synthesized compounds were confirmed by spectral and elemental analysis.

KEYWORDS Benzylidinecarbohydrazide, Oxadiazole, Thiazole, MW irradiation.

How to cite this article: Landage, V.P., Akolkar, H.N., Thube, D.R., Karale B.K. Synthesis of New Thiazole Anchored N'-Benzylidene Carbohydrazide and 1,3,4-Oxadiazole Derivatives by Conventional and Microwave Irradiation Methods, *Indian J. Heterocycl. Chem.*, **2020**, *30*, 607–613. *(DocID: https://connectjournals.com/01951.2020.30.607)*

Microwave Assisted Synthesis and Antibacterial Activity of New 1,3,4-Thiadiazoles and 1,2,4-Triazoles Derived from 2-{2-[2-(4-Fluorophenyl)-4-methylthiazol-5-yl]-1*H*-benzo[*d*]imidazol-1-yl}acetohydrazide

Published: 12 October 2020

Volume 90, pages 1721–1726, (2020) Cite this article

N. R. Darekar, B. K. Karale, H. N. Akolkar & A. S. Burungale

Abstract

A series of novel derivatives of 1-(2-{2-[2-(4-fluorophenyl)-4-methylthiazol-5-yl]-1*H*-benzo[*d*]imidazol-1-yl}acetyl)-4-phenylthiosemicarbazide, 5-({2-[2-(4-fluorophenyl)-4-methylthiazol-5-yl]-1*H*-benzo[*d*]imidazol-1-yl}methyl)-4-phenyl-4*H*-1,2,4-triazole-3-thiol and 5-({2-[2-(4-fluorophenyl)-4-methylthiazol-5-yl]-1*H*-benzo[*d*]imidazol-1-yl}methyl)-*N*-phenyl-1,3,4-thiadiazol-2-amine have been synthesized by the conventional method as well as using MW irradiation. All newly synthesized compounds have been tested for antibacterial activity. Several products have demonstrated moderate activity against gram positive and gram negative bacterial strains.

Polycyclic Aromatic Compounds >
Volume 42, 2022 - Issue 5

Research Articles

Design, Synthesis and Biological Evaluation of Novel Furan & Thiophene Containing Pyrazolyl Pyrazolines as Antimalarial Agents

Hemantkumar N. Akolkar, Sujata G. Dengale, Keshav K. Deshmukh, Bhausaheb K. Karale, Nirmala R. Darekar, Vijay M. Khedkar & ...show all

Pages 1959-1971 | Received 07 Aug 2020, Accepted 05 Sep 2020, Published online: 14 Sep 2020

Cite this article https://doi.org/10.1080/10406638.2020.1821231 Check for updates

Abstract

In search for novel compounds targeting Malaria, based on the *in silico* molecular docking binding affinity data, the novel furans containing pyrazolyl chalcones (**3a-d**) and pyrazoline derivatives (**4a-d**) were synthesized. The formation of the synthesized compound were confirmed by spectral analysis like IR, ^{1}H NMR, ^{13}C NMR and mass spectrometry. Compounds with thiophene and pyrazoline ring **4b** (0.47 µM), **4c** (0.47 µM) and **4d** (0.21 µM) exhibited excellent anti-malarial activity against *Plasmodium falciparum* compared with standard antimalarial drug Quinine (0.83 µM). To check the selectivity furthermore, compounds were tested for antimicrobial activity and none of

Journal of Heterocyclic Chemistry / Volume 57, Issue 4 / p. 1692-1697

ARTICLE

Synthesis and characterization of novel 2-(1-benzyl-3-[4-fluorophenyl]-1*H*-pyrazol-4-yl)-7-fluoro-4*H*-chromen-4-one derivatives

Kiran S. Hon, Hemantkumar N. Akolkar, Bhausaheb K. Karale

First published: 28 January 2020
https://doi.org/10.1002/jhet.3894
Citations: 6

Abstract

Novel 1-benzyl-3-(4-fluorophenyl)-1*H*-pyrazole-4-carbaldehydes **3a** to **3e** were synthesized via Vilsmeier-Haack reaction of the appropriate 1-benzyl-2-(1-(4-fluorophenyl)ethylidene)hydrazines, derived from 4-fluoroacetophenone **1** with substituted 2-benzylhydrazines **2a** to **2e**. The base catalyzed condensation of 1-benzyl-3-(4-fluorophenyl)-1*H*-pyrazole-4-carbaldehydes **3a** to **3e** with 1-(4-fluoro-2-hydroxyphenyl)ethanone **4** gave (*E*)-3-(1-benzyl-3-(4-fluorophenyl)-1*H*-pyrazol-4-yl)-1-(4-fluoro-2-hydroxyphenyl)prop-2-en-1-ones **5a** to **5e**. On cyclization with dimethyl sulfoxide (DMSO)/I_2, compounds **5a** to **5e** gave 2-(1-benzyl-3-(4-fluorophenyl)-1*H*-pyrazol-4-yl)-7-fluoro-4*H*-chromen-4-ones **6a** to **6e**. Structures of all novel compounds were confirmed by infrared (IR), proton nuclear magnetic resonance (^{1}H NMR), carbon nuclear magnetic resonance (^{13}C NMR), and mass spectral data. All the synthesized compounds were screened for their antibacterial activities.

Supporting Information

Filename	Description
jhet3894-sup-0001-Appendix S1.docx Word 2007 document , 5.7 MB	**Appendix S1**: Supporting information

Issue 45, 2020

Previous Next

From the journal:
RSC Advances

Nanostructured N doped TiO_2 efficient stable catalyst for Kabachnik–Fields reaction under microwave irradiation †

Sachin P. Kunde,[ab] Kaluram G. Kanade,[*ac] Bhausaheb K. Karale,[a] Hemant N. Akolkar,[a] Sudhir S. Arbuj,[d] Pratibha V. Randhavane,[a] Santosh T. Shinde,[a] Mubarak H. Shaikh[a] and Aniruddha K. Kulkarni[e]

Author affiliations

Abstract

Herein, we report nitrogen-doped TiO_2 (N-TiO_2) solid-acid nanocatalysts with heterogeneous structure employed for the solvent-free synthesis of α-aminophosphonates through Kabachnik–Fields reaction. N-TiO_2 were synthesized by direct amination using triethylamine as a source of nitrogen at low temperature and optimized by varying the volume ratios of $TiCl_4$, methanol, water, and triethylamine, under identical conditions. An X-ray diffraction (XRD) study showed the formation of a rutile phase and the crystalline size is 10 nm. The nanostructural features of N-TiO_2 were examined by HR-TEM analysis, which showed they had rod-like morphology with a diameter of ~7 to 10 nm. Diffuse reflectance spectra show the extended absorbance in the visible region with a narrowing in the band gap of 2.85 eV, and the high resolution XPS spectrum of the N 1s region confirmed successful doping of N in the TiO_2 lattice. More significantly, we found that as-synthesized N-TiO_2 showed significantly higher catalytic activity than commercially available TiO_2 for the synthesis of a novel series of α-amino phosphonates *via* Kabachnik–Fields reaction under microwave irradiation conditions. The improved catalytic activity is due to the presence of strong and Bronsted acid sites on a porous nanorod surface. This work signifies N-TiO_2 is an efficient stable catalyst for the synthesis of α-aminophosphonate derivatives.

Indian Journal of Chemistry
Vol. 58B, April 2019, pp. 504-510

Synthesis, characterization and antibacterial screening of fluorinated benzofuran containing heterocycles

S G Kundlikar, P V Randhavane, H N Akolkar & B K Karale*
P G Department of Chemistry, Radhabai Kale Mahila Mahavidyalaya, Ahmednagar 414 001, India
E-mail: bkkarale@yahoo.com

Received 7 June 2017; accepted (revised) 26 December 2018

2-(4-Fluorophenyl)-5-phenylbenzofuran-3-carboxylic acid **1** when treated with substituted 2-hydroxyacetophenones **2** in dry pyridine and $POCl_3$ affords compound **3** which when reacted with pyridine/KOH by B. V. transformation gives **4**. Compound **4** on refluxing with different reagents Ac_2O in presence of sodium acetate, acetic acid in HCl, and hydrazinehydrate in alcohol gives **5**, **6** and **7** respectively. The structures of all synthesized compounds have been confirmed by spectroscopic techniques. All the synthesized compounds have been screened for their antibacterial activity.

Keywords: Benzofuran, chromones, pyrazoles, antibacterial activity

Benzofuran is considered as an important class of heterocyclic compound present in numerous bioactive natural products as well as pharmaceuticals and polymers[1]. Many of the clinically approved drugs are synthetic containing mono and fused benzofuran ring in conjunction with other heterocycles. They possess wide spectrum of biological activities such as TGR5 agonists[2], antimicrobial[3], antibacterial[4], anticoagulator[5], MAO-B enzyme inhibitor[6] and antioxidant[7].

Due to presence of two carbonyl groups, β-diketones are valueable substrates in many chemical syntheses. The functionalized derivatives of β-diketone are clinically important molecules and widely used due to their antibacterial[8], anti-HIV-1[9], insecticidal[10] and antiviral[11] activities.

Chromone and its derivatives have been studied for over century or more due to important biological activities such as cholesterol acyltransferase[12], antitumour[13], anticancer[14], topoisomerase II inhibitor[15], antioxidant[16] and antifungal[17]. Pyrazole derivatives occupy an important position in medicinal[18] and pesticide chemistry with having a wide range of bioactivities such as cytotoxic[19], analgesic[20], antibacterial[21] and urease inhibitors[22].

In view of biological activities associated with benzofuran, chromones and pyrazoles we decided to synthesize series of benzofuran containing different heterocycles and screened them for their antibacterial activity (Scheme I).

Experimental Section

Melting points were determined in open capillaries in liquid paraffin bath and are uncorrected. Mass spectra were recorded on Waters Acquity TQD mass spectrometer. ^{1}H NMR spectra were recorded on Bruker Avance II 400 MHz NMR spectrometer in DMSO-d_6 as a solvent and TMS as an internal standard. Peak values are shown in δ (ppm). IR spectra were recorded on Shimadzu IR Affinity-1S spectrophotometer.

2-Acetylphenyl-2-(4-fluorophenyl)-5-phenylbenzo furan-3-carboxylate, 3a-g

Equimolar mixture of 2-(4-fluorophenyl)-5-phenylbenzofuran-3-carboxylic acid **1** (0.003M) and substituted 2-hydroxyacetophenone **2** (0.003M) was dissolved in pyridine (15 mL) taken in dry beaker maintained at about 0°C. To this reaction mixture $POCl_3$ (0.003 M) was slowly added maintaining the temperature below 4°C. After complete addition the reaction mixture was kept overnight, then the resulting reaction mixture was poured over crushed ice. The product thus obtained was separated by filtration and crystallized from ethanol to afford **3**.

2-Acetylphenyl-2-(4-fluorophenyl)-5-phenylbenzo furan-3-carboxylate, 3a: m.p.176°C. Yield 76%. IR: 3080, 1748, 1686, 1604, 1504, 1165 cm^{-1}; ^{1}H NMR: δ 2.49 (s, 3H), 7.22 (s, 1H), 6.90-6.98 (m, 1H), 7.33-7.42 (m, 4H), 7.44-7.53 (m, 2H), 7.58-7.90 (m, 5H), 8.00 (dd, 1H), 8.10 (dd, 1H), 8.23 (d, 1H); MS: *m/z*

Indian Journal of Chemistry
Vol. 58B, August 2019, pp. 916-920

Synthesis, characterisation and antimicrobial screening of some new thiazolyl chromones and pyrazoles

V P Landage[a], D R Thube*[a] & B K Karale[b]

[a] P.G. Department of Chemistry, New Arts, Commerce and Science College, Parner, Ahmednagar 414 302, India
(Affiliated to Savitribai Phule Pune University, Pune)

[b] P.G. Department of Chemistry, Radhabai Kale Mahila Mahavidyalaya, Ahmednagar 414 001, India
(Affiliated to Savitribai Phule Pune University, Pune)

E-mail: drthube@rediffmail.com

Received 16 February 2018; accepted (revised) 2 May 2019

A series of substituted chromones and pyrazole derivatives have been synthesized from esterification of acid **1** with 2-hydroxy acetophenones **2** to give compounds **3** which is in turn converted in to β-diketones **4** in presence of excess of KOH by Baker-Venkatraman transformation. Acid catalysed cyclisation of β-diketones **4** yield a series of 2-substituted chromones **5**. 2-Substituted chromones **5** have been used to synthesise substituted pyrazole derivatives **6**. All the synthesised compounds have been characterised by spectral and analytical data. Chromones and pyrazoles have been evaluated for their antibacterial and antifungal activities.

Keywords: Baker-Venkatraman transformation, β-diketones, chromones, pyrazoles

In recent years it was found that microbial infections and drug resistivity of microbes have been increased enormously. Therefore it is necessary to develop a new and effective antimicrobial drug. The researcher's efforts have been made towards the designation of new agent. For designation of new agents heterocyclic molecules play important role because most of the heterocyclic compounds are biologically active. Chromones are found to be naturally occurring oxygen containing heterocyclic compounds and well known for their biological activities such as antitumor[1], antioxidant[2], antiinfective[3], antiallergic[4], antiinflammatory[5], anticancer[6], antiplatelate[7], antifungal[8] and antibacterial[9] activities. 3-formylchromones are important synthon for incorporating chromone moieties into heterocyclic system[10,11].

Pyrazole moiety is one of the most important biologically active heterocyclic compound. Pyrazole and its derivatives are associated with antibacterial[12] antifungal[13], antidiabetic[14], antiparasitic[15], anti-tubercular[16] and antiviral[17] activities (Figure 1 and Figure 2).

Thiazole is nitrogen and sulphur containing heterocyclic compound and found to be a structural fragment of naturally occurring vitamin, vitamin B1 (Thiamine). Thiazole derivatives are associated with wide range of biological activities including antibacterial[18], anticancer[19], anticonvulsant[20], antituberculousis[21], antifungal[22], antianaesthetic[23], antiinflamaratory[24] and antisedative[25]. Chlorinated heterocyclic compounds are found to be biological active and shows biological activities such as antioxidant[26], antiinflamaratory[26] and analgesic[26] (Figure 1).

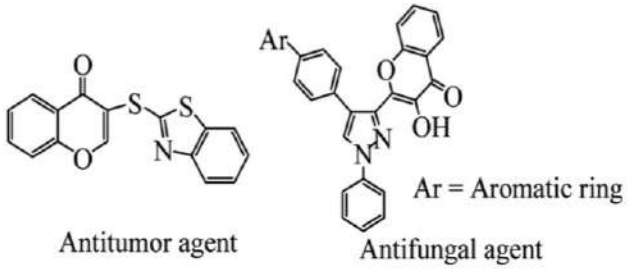


Figure 1

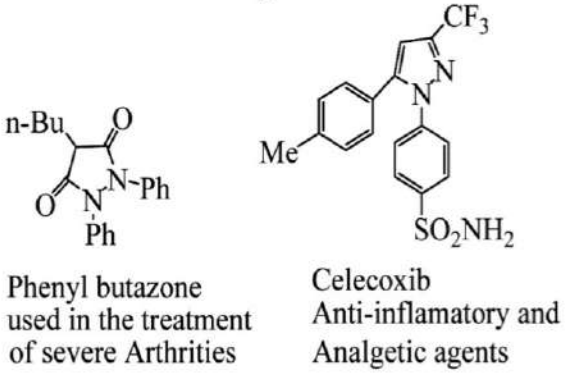


Figure 2

Est. 1984

ORIENTAL JOURNAL OF CHEMISTRY
An International Open Access, Peer Reviewed Research Journal

www.orientjchem.org

ISSN: 0970-020 X
CODEN: OJCHEG
2019, Vol. 35, No.(1):
Pg. 481-484

Brief Communication

Synthesis and Antibacterial Screening of Novel Thiazolyl Pyrazole and Benzoxazole

VAIBHAV PRABHAKAR LANDAGE[1], DILIP RAOSAHEB THUBE[1]* and BHAUSAHEB KISAN KARALE[2]*

[1]Department of Chemistry, New Arts, Commerce and Science College, Parner,Ahmednagar-414302, India,
[2]Department of Chemistry, Radhabai Kale Mahila Mahavidyalaya, Ahmednagar-414001, India,
*Corresponding author Email: drthube@rediffmail.com

http://dx.doi.org/10.13005/ojc/350164

Received: June 18, 2018; Accepted: December 10, 2018)

ABSTRACT

A new series of (2-hydroxyphenyl)(1-(4-p-tolylthiazol-2-yl)-1*H*-pyrazol-4-yl)methanone 3a-g, 2[(E)–{1-[4-(p-tolyl)-1, 3-thiazol-2-yl)]-1*H*-pyrazol-4-yl} (hydroxyimino)methyl]phenol 4a-g and 2-(1-(4-p-tolylthiazol-2-yl)-1*H*-pyrazole-4-yl)benzo[*d*]oxazole 5a-g have been synthesised. These synthesised compounds have been characterised by the spectral, analytical data and scanned for their antibacterial activities.

Keywords: Thiazole,3-formylchromone, Pyrazole, Benzo[*d*]oxazole.

INTRODUCTION

The introduction of heterocyclic moieties found in molecules have advantage in drug discovery and development because of its broad range of biological activities. Thiazole and its derivatives show biological activities such as anti-inflammatory[1], analgesic[2], antimicrobial[3,4], antioxidant[5], antitumor[6,7], anticonvulsant[8]. 3-formylchromone and its derivatives are known to associate in organic synthesis[9] and showing biological activities include antitumor[10], antibacterial[10], antitubulin[11], anti-helicobacter pylori[12], antiallergic[13], antioxidant[14], topoisomerase I inhibitor[15]. Pyrazole containing heterocyclic molecules are associated with wide range of biological activities such as antimicrobial[16], anticancer[17], antifungal[18], anti-inflammatory[19], antitumor[20], and anti-anxiety[21]. Benzoxazoles derivatives are found to be associated with anticancer[22], antimicrobial[23], HIV-1 reverse transcriptase Inhibitor Activity[24], inhibitors of lysophosphatidic acid acyltransferase-beta[25], anti-inflammatory[26], analgesic[26], antibacterial[27], antifungal[27], anticancer[28] activities. As a part of our interest in heterocyclic molecules have a extensive variety of biological activities and that have been explored for developing pharmaceutically important molecules, we here in report the synthesis of a set of new series of thiazolyl pyrazoles and benzoxazoles and their antibacterial activities.

ScienceDirect

Bioorganic & Medicinal Chemistry Letters

Volume 29, Issue 10, 15 May 2019, Pages 1199-1202

Thiazolyl-pyrazole derivatives as potential antimycobacterial agents

Sushma J. Takate [a e], Abhijit D. Shinde [b e], Bhausaheb K. Karale [c e], Hemant Akolkar [c e], Laxman Nawale [d], Dhiman Sarkar [d], Pravin C. Mhaske [b e]

Show more

https://doi.org/10.1016/j.bmcl.2019.03.020

Get rights and content

Abstract

Mycobacterium tuberculosis (*Mtb*) is an obligate aerobe that is capable of long-term persistence under conditions of low oxygen tension. A series of thiazolyl-pyrazole derivatives (**6a–f**, **7a–f**, **8c**, **8e**) were screened for antimycobacterial activity against dormant *M. tuberculosis* H37Ra (D-MTB) and *M. bovis* BCG (D-BCG). Nine thiazolyl-pyrazole analogs, **6c**, **6e**, **7a**, **7b**, **7c**, **7e**, **7f**, **8c** and **8e** exhibited promissing minimum inhibitory concentration (MIC) values (0.20–28.25 μg/mL) against D-MTB and D-BCG strains of *Mtb*. Importantly, six compounds (**7a**, **7b**, **7e**, **7f**, **8c** and **8e**) exhibited excellent antimycobacterial activity and low cytotoxicity at the maximum evaluated concentration of >250 μg/mL. Finally, the promising antimycobacterial activity and lower cytotoxicity profile suggested that, these compounds could be further subjected for optimization and development as a lead, which could have the potential to treat tuberculosis.

Graphical abstract

Journal of Heterocyclic Chemistry / Volume 56, Issue 6 / p. 1780-1786

Article

Synthesis and Characterization of Novel 1-Methyl-3-(4-phenyl-4*H*-1,2,4-triazol-3-yl)-1*H*-indazole Derivatives

Kiran S. Hon, Hemantkumar N. Akolkar, Bhausaheb K. Karale

First published: 15 April 2019
https://doi.org/10.1002/jhet.3545

Abstract

A series of novel 1-methyl-3-(4-phenyl-4*H*-1,2,4-triazol-3-yl)-1*H*-indazoles was synthesized in three steps from 5-(1-methyl-1*H*-indazol-3-yl)-4-phenyl-2*H*-1,2,4-triazole-3(4*H*)-thiones. 5-(1-Methyl-1*H*-indazol-3-yl)-4-phenyl-2*H*-1,2,4-triazole-3(4*H*)-thiones were converted into 1-methyl-3-(5-(methylsulfonyl)-4-phenyl-4*H*-1,2,4-triazol-3-yl)-1*H*-indazoles upon methylation followed by treatment with aq. $KMnO_4$. The reaction of 1-methyl-3-(5-(methylsulfonyl)-4-phenyl-4*H*-1,2,4-triazol-3-yl)-1*H*-indazoles with Raney nickel resulted in desulphonylation to afford corresponding 1-methyl-3-(4-phenyl-4*H*-1,2,4-triazol-3-yl)-1*H*-indazoles. All the new synthesized compounds were characterized by spectral techniques.

Supporting Information

Filename	Description
JHET_3545-sup-0001-Supplementary data JHC.docx Word 2007 document , 7.7 MB	Data S1: Supporting Information

Please note: The publisher is not responsible for the content or functionality of any supporting information supplied by the authors. Any queries (other than missing content) should be directed to the corresponding author for the article.

Microwave Assisted Synthesis and Antimicrobial Activity of Novel 1,3,4-Thiadiazoles and 1,2,4-Triazoles Derived from 2-(3-Fluorophenyl)-4-methylthiazole-5-carbohydrazide

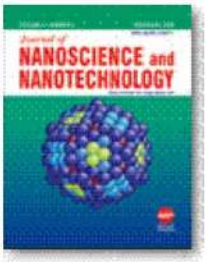
Published: 16 August 2019

Volume 89, pages 1535–1540, (2019) Cite this article

S. G. Dengale, B. K. Karale, H. N. Akolkar, N. R. Darekar & K. K. Deshmukh

Abstract

The precursors 2-{[2-(3-fluorophenyl)-4-methyl-1,3-thiazol-5-yl]carbonyl}-*N*-phenylhydrazinecarbothioamides are synthesized from 2-(3-fluorophenyl)-4-methylthiazole-5-carbohydrazide and aryl isothiocyanates. MW irradiation of the precursors under alkali or acidic conditions led to the products of cyclization 5-[2-(3-fluorophenyl)-4-methylthiazol-5-yl]-*N*-phenyl-1,3,4-thiadiazol-2-amine or 5-[2-(3-fluorophenyl)-4-methylthiazol-5-yl]-4-phenyl-4*H*-1,2,4-triazole-3-triiol, accordingly. Structures of the synthesized compounds are confirmed by IR, ^{1}H, and ^{13}C NMR, and mass spectra. All products are tested *in vitro* for their antibacterial and antifungal activity.



Nanocrystalline Cu–ZnO as an Green Catalyst for One Pot Synthesis of 4,4'-((phenyl)methylene)bis(3-methyl-1-phenyl-1H-pyrazol-5-ol) Derivatives

Authors: Shinde, Santosh [1] ; Karale, Bhausaheb [1] ; Bankar, Digambar [2] ; Arbuj, Sudhir [2] ; Moulavi, Mansur [2] ; Amalnerkar, Dinesh [2] ; Kim, Taesung [1] ;
Source: Journal of Nanoscience and Nanotechnology, Volume 19, Number 8, August 2019, pp. 4623-4631(9)
Publisher: American Scientific Publishers
DOI: https://doi.org/10.1166/jnn.2019.16490

Abstract | References | Citations | Supplementary Data | Suggestions

Synthesis of 4,4'-((phenyl)methylene)bis(3-methyl-1-phenyl-1H-pyrazol-5-ol) derivatives was successively carried out using Cu doped ZnO nanomaterials. The nanocrystalline Cu–ZnO was obtained by decomposing as-synthesized copper–zinc oxalate intermediate at 520 °C. The prepared Cu–ZnO nanostructured catalyst was characterized with FTIR, X-ray diffraction, field emission scanning electron microscope and electron diffraction techniques. XRD analysis indicates the formation of highly crystalline hexagonal phase of ZnO along with the presence of monoclinic CuO. FESEM photographs shows the existence of plate like structures made up of small spherical shaped particles having size in the range of 30–50 nm. As-synthesized Cu–ZnO was used as heterogeneous catalyst for one pot synthesis of 4,4'-((phenyl)methylene)bis(3-methyl-1-phenyl-1H-pyrazol-5-ol) derivatives using phenyl hydrazine, ethyl acetoacetate and aromatic aldehydes. The 3-methyl-1-phenyl-1H-pyrazol-5-ol was obtained as *in-situ* precursor to the series of bis-pyrazolone derivatives. The progress of reaction was monitored by thin layer chromatography. The obtained organic product was further characterized and confirmed by FT-IR, $_1$H-NMR, $_{13}$C-NMR and HRMS spectroscopic techniques. The Cu–ZnO catalyst confers upto 96% yield of pyrazolone derivatives in ethanol solvent at refluxing condition. The Cu–ZnO catalyst was used successfully up to 5 cycles without much loss of catalytic activity. Overall, the use of environmental friendly Cu–ZnO nano-structures as a heterogeneous catalyst shows higher yield and lower reaction time towards the synthesis of bispyrazolone derivatives by Tandem Knoevenagel/Michael reaction.

Keywords: Bispyrazolone; Heterogeneous Catalyst; Nanocrystalline Cu–ZnO; One Pot Synthesis; Tandem Knoevenagel/Michael Reaction

Document Type: Research Article

ScienceDirect

Arabian Journal of Chemistry

Volume 12, Issue 8, December 2019, Pages 5212-5222

Original article

Synthesis and characterization of nanostructured Cu-ZnO: An efficient catalyst for the preparation of (*E*)-3-styrylchromones

Sachin P. Kunde [a], Kaluram G. Kanade [a b], Bhausaheb K. Karale [a], Hemant N. Akolkar [a], Pratibha V. Randhavane [a], Santosh T. Shinde [a]

https://doi.org/10.1016/j.arabjc.2016.12.015

Get rights and content

Abstract

We have explored nanocrystalline ZnO and Cu-ZnO catalyst for the preparation of 3-styrylchromones with trans selectivity derived from 3-formylchromones. Synthesis of ZnO and Cu-ZnO nano flakes (NFs) was carried by precipitation technique. The analytical techniques such as UV-Visible spectroscopy, X-ray diffraction (XRD), Brunauer-Emmett-Teller (BET), field emission scanning electron microscopy (FESEM) and energy-dispersive analysis X-ray spectroscopy (EDAX) were used to characterize the catalysts. The XRD pattern showed highly pure wurtzite ZnO and Cu-ZnO. The FESEM images showed nano flakes such as sunflower seed morphology in the range width of 9–34nm and length 90–180nm. Doping of copper in ZnO was employed to study the selectivity of Knoevenagel and Knoevenagel-Doebner reactions. Knoevenagel condensation was catalyzed efficiently by pure ZnO nano flakes, whereas the Cu-ZnO nano flakes facilitate the Knoevenagel-Doebner reaction. Present synthetic protocols are novel, very clean and

ScienceDirect

Arabian Journal of Chemistry

Volume 12, Issue 8, December 2019, Pages 5212-5222

Original article

Synthesis and characterization of nanostructured Cu-ZnO: An efficient catalyst for the preparation of (*E*)-3-styrylchromones

Sachin P. Kunde [a], Kaluram G. Kanade [a b], Bhausaheb K. Karale [a], Hemant N. Akolkar [a], Pratibha V. Randhavane [a], Santosh T. Shinde [a]

https://doi.org/10.1016/j.arabjc.2016.12.015

Get rights and content

Abstract

We have explored nanocrystalline ZnO and Cu-ZnO catalyst for the preparation of 3-styrylchromones with trans selectivity derived from 3-formylchromones. Synthesis of ZnO and Cu-ZnO nano flakes (NFs) was carried by precipitation technique. The analytical techniques such as UV-Visible spectroscopy, X-ray diffraction (XRD), Brunauer-Emmett-Teller (BET), field emission scanning electron microscopy (FESEM) and energy-dispersive analysis X-ray spectroscopy (EDAX) were used to characterize the catalysts. The XRD pattern showed highly pure wurtzite ZnO and Cu-ZnO. The FESEM images showed nano flakes such as sunflower seed morphology in the range width of 9–34nm and length 90–180nm. Doping of copper in ZnO was employed to study the selectivity of Knoevenagel and Knoevenagel-Doebner reactions. Knoevenagel condensation was catalyzed efficiently by pure ZnO nano flakes, whereas the Cu-ZnO nano flakes facilitate the Knoevenagel-Doebner reaction. Present synthetic protocols are novel, very clean and

Microwave Assisted Synthesis and Antimicrobial Activity of Novel 1,3,4-Thiadiazoles and 1,2,4-Triazoles Derived from 2-(3-Fluorophenyl)-4-methylthiazole-5-carbohydrazide

Published: 16 August 2019

Volume 89, pages 1535–1540, (2019) Cite this article

S. G. Dengale, B. K. Karale, H. N. Akolkar, N. R. Darekar & K. K. Deshmukh

Abstract

The precursors 2-{[2-(3-fluorophenyl)-4-methyl-1,3-thiazol-5-yl]carbonyl}-*N*-phenylhydrazinecarbothioamides are synthesized from 2-(3-fluorophenyl)-4-methylthiazole-5-carbohydrazide and aryl isothiocyanates. MW irradiation of the precursors under alkali or acidic conditions led to the products of cyclization 5-[2-(3-fluorophenyl)-4-methylthiazol-5-yl]-*N*-phenyl-1,3,4-thiadiazol-2-amine or 5-[2-(3-fluorophenyl)-4-methylthiazol-5-yl]-4-phenyl-4*H*-1,2,4-triazole-3-triiol, accordingly. Structures of the synthesized compounds are confirmed by IR, ^{1}H, and ^{13}C NMR, and mass spectra. All products are tested *in vitro* for their antibacterial and antifungal activity.

Conventional and Non-Conventional Synthesis of Novel (4*E*)-4-((3-(2-(4-fluorophenyl)-4-methylthiazol-5-yl)-1-aryl-1*h*-pyrazol-4-yl) methylene)-3-alkyl-1-aryl-1*h*-pyrazol-5(4*h*)-ones

R. K. Jadhav[1], H. N Akolkar[2] and B. K. Karale[4*]
[1]Assistant Professor, Department of Chemistry, S. M. Joshi College, Hadapsar, Pune- 411028, India.
[2]Assistant Professor, Department of Chemistry, Radhabai Kale Mahila Mahavidyalaya, Ahmednagar- 414001.
[4]Principal, Chatrapati shivaji college, Satara- 415001.

Abstract : A conventional and non-conventional Knoevenagel condensation of 3-(2-(4-fluorophenyl)-4-methylthiazol-5-yl)-1-aryl-1*H*-pyrazole-4-carbaldehyde and 3-alkyl-1-aryl-1*H*-pyrazol-5(4*H*)-one gave (4*E*)-4-((3-(2-(4-fluorophenyl)-4-methylthiazol-5-yl)-1-aryl-1*H*-pyrazol-4-yl)methylene)-3-alkyl-1-aryl-1*H*-pyrazol-5(4*H*)-one. The structures of the synthesized compounds were confirmed with the help of spectral techniques.

IndexTerms – conventional, non-conventional, Knoevenagel condensation.

I. Introduction

Knoevenagel condensation is a reaction in which C-C bond formation takes place and extensively used in synthesis of olefins and pharmacologically active compounds. This condensation is catalysed by different catalysts such as L-tyrosine[1], [BmIm]OH[2], lipoprotein lipase[3], tetrabutylphosphonium prolinate[4], thermally decomposed mesoporous Ni-Fe hydrotalcite[5] etc. Fluorinated compounds are of great interest to synthetic and medicinal chemist due to unique physical biological properties imparted by fluorine[6]. Fluorinated compound possess variety of biological activities like antimicrobial[7], antibacterial[8] and anticancer[9].

Thiazole and its derivative have attracted many researchers due to their pharmacological potentials. Thiazole containing compounds exhibits EP_1 receptor antagonist[10], VEGF-A inhibitors[11], cytotoxic[12], C-aryl glucoside SGLT2 Inhibitor[13], vascular adhesion protein-1 (VAP-1) inhibitors[14] activities. Pyrazolone derivatives possess numerous biological activities like neuraminidase inhibitors[15], nonallergenic antipyretic analgesics[16], HIV-1 integrase inhibitors[17], anti-orthopoxvirus[18] and anti-bacterial agents[19].

Now a days microwave & ultrasound irradiations have been extensively used to activate organic reactions. It is a green approach which has many advantages over conventional methods[20, 21]. Many organic reactions have been carried out in higher yield, shorter reaction time and milder conditions under microwave and ultrasound irradiation[22-25].

In view of activities associated with fluorinated compounds, thiazole, pyrazolone and use of eco-friendly techniques we describes here the synthesis of (4*E*)-4-((3-(2-(4-fluorophenyl)-4-methylthiazol-5-yl)-1-aryl-1*H*-pyrazol-4-yl)methylene)-3-alkyl-1-aryl-1*H*-pyrazol-5(4*H*)-one derivatives by conventional and non-conventional methods.

II. Experimental Section

The melting points were determined by open capillary method and are uncorrected. IR spectra were recorded on Shimadzu IR Affinity-1S Fourier transform infrared spectrophotometer. ^{1}H NMR spectra were recorded on Bruker Avance II 400 MHz NMR spectrometer using TMS as an internal standard and $CDCl_3$ as a solvent. The mass spectra were recorded on Acquity TQD Waters mass spectrometer. Microwave irradiation was carried out in Raga synthetic microwave system and for ultrasound method Bio techno labs ultrasonicator was used.

(4*E*)-4-((3-(2-(4-Fluorophenyl)-4-methylthiazol-5-yl)-1-aryl-1*H*-pyrazol-4-yl)methylene)-3-alkyl-1-aryl-1*H*-pyrazol-5(4*H*)-one, 3a-j

Conventional method: Equimolar amounts of 3-(2-(4-fluorophenyl)-4-methylthiazol-5-yl)-1-aryl-1*H*-pyrazole-4-carbaldehyde **1** (0.002 mol) and pyrazolone **2** (0.002 mol) were taken in glacial acetic acid (15 mL). The reaction mixture was refluxed till completion of reaction (checked by TLC). After completion of reaction, contents were then poured into crushed ice. Solid obtained was filtered, dried and purified by recrystallization from acetic acid to get pure compounds **3a-j**. The physical data of compounds synthesized by above method is given in **Table 1**.

Microwave method: Equimolar amounts of 3-(2-(4-fluorophenyl)-4-methylthiazol-5-yl)-1-aryl-1*H*-pyrazole-4-carbaldehyde **1** (0.002 mol) and pyrazolone **2** (0.002 mol) were taken in glacial acetic acid (15 mL). Contents of flask were subjected for microwave irradiation at 350W for time as shown in table, till completion of reaction (checked by

SYNTHESIS AND CHARACTERIZATION OF SOME BENZOFURAN ANCHORED HETEROCYCLES

S. G. Kundlikar*[a], B. K. Karale[b], D. R. Thube[a], H. N. Akolkar[b], S. D. Mhaske[a] & P. G. Rohokale[a]
[a]Department of Chemistry and Research Center, New Art's, Commerce and Science College, Parner
P.G. Department of Chemistry, Radhabai Kale Mahila Mahavidyalaya, Ahmednagar, 414 001, India

Received: February 22, 2019 Accepted: March 29, 2019

ABSTRACT: *: 7-Bromo-5-chlorobenzofuran-2-carbohydrazide **1** was reacted with different aromatic aldehydes **2** to give benzofuranyl hydrazone derivative **3**. Compound **3**on refluxed with acetic anhydride gave corresponding oxadiazoline derivtive **4**. The structures of all the synthesized compounds were confirmed with the help of spectral techniques.*

Key Words: *Benzofuran, Hydrazone, Halogen, Oxadiazoline*

INTRODUCTION

Heteroaromatic compounds have attracted considerable attention in the design of biologically active molecules and advanced organic materials. So in the synthetic organic chemistrydifferent synthetic methods for the preparation of such compounds is of great interest. Oxygen, sulphur and nitrogen containing heterocycles are of great importance due to their broad spectrum of pharmacological activities.

Benzofuran nucleus contributes the core structure of several pharmacologically active natural products and their derivatives are active inhibitors against many diseases, fungus, viruses, enzymes and microbes. Benzofuran derivatives are endowed with various biological activities such as acetylcholinesterase inhibitors[1], anticancer[2],allosteric modulators of Hsp90[3], antibacterial[4] and inhibition of HIF-1[4].

Oxadiazoline derivatives are endowed with various biological activities like antitubulin[5], gamma secretase inhibitors[6], antimicrobial[7], anti-HIV[8], as novel potential inhibitors targeting chitin biosynthesis[9]*etc.*

Encouraged by the biological activities associated with different benzofuran, oxadizolines as mentioned above we have decided to synthesize benzofuran containing oxadiazolines.

Experimental Section

Melting points were determined in open capillary tubes in liquid paraffin bath and are uncorrected. Silica gel G TLC plates were used to check the purity of the compounds. The structures of all synthesized compounds were assigned on the basis of instrumental techniques such as IR and ^{1}H NMR spectrometry.

^{1}H NMR spectra were recorded on Bruker Avance II 400 MHz NMR spectrometer in $CDCl_3$ as a solvent and TMS as an internal standard. IR spectra were recorded on *Bruker Alpha* Eco-ATR. The schematic presentation of detailed scheme is presented in **Scheme-I** and M.P. and percentage yield data is presented in **Table-I**.

N'-(4-Chlorobenzylidene)-7-bromo-5-chlorobenzofuran-2-carbohydrazide.

Acid hydrazide (0.0017 mol) **1** and aldehyde (0.0017 mol) **2** were dissolved in alcohol and refluxed for 2 hrs. After completion of reaction, content were concentrated and allow at room temperature when solid substance was separated out and filtered. It was recrystallized from ethanol to afford compound **3**.

Formation of compound was confirmed by TLC, M.P. and spectral techniques.

3a: IR: 3080 (=CH), 1674 (C=O), 1552 (C=N), 1495 (C=C),1162 (C-O-C) cm^{-1}; ^{1}H NMR ($CDCl_3$): δ 7.31 (t, 2H,Ar-H), 7.33 (dd, 2H,Ar-H), 7.35 (dd, 1H,Ar-H), 7.62-7.67 (m, 3H,Ar-H), 8.39 (s, 1H,Ar-H), 9.69 (s, 1H,Ar-H);MS: *m/z* (M+1), 378.

3b: IR: 3076 (=CH), 1671 (C=O), 1556 (C=N), 1497 (C=C),1167 (C-O-C) cm^{-1}; ^{1}H NMR ($CDCl_3$): δ 7.41 (d, 2H,Ar-H), 7.62-7.67 (m, 3H,Ar-H), 7.76 (d, 2H,Ar-H), 8.39 (s, 1H,Ar-H), 9.69 (s, 1H,Ar-H);MS: *m/z* (M+1), 413.

3c: IR: 3079 (=CH), 1674 (C=O), 1555 (C=N), 1499 (C=C), 1350 (-NO_2), 1164 (C-O-C) cm^{-1}; ^{1}H NMR ($CDCl_3$): δ 7.48 (d, 2H,Ar-H), 7.66-7.71 (m, 3H,Ar-H), 7.78 (d, 2H,Ar-H), 8.42 (s, 1H,Ar-H), 9.72 (s, 1H,Ar-H);MS: *m/z* (M+1), 423.

INTERNATIONAL RESEARCH JOURNAL OF PHARMACY
www.irjponline.com
ISSN 2230 – 8407

Research Article

SYNTHESIS AND ANTIBACTERIAL SCREENING OF 1-(2-(2-CHLOROPHENYL)-2-(4-(6-FLUOROBENZO[D]ISOXAZOL-3-YL)PIPERIDIN-1-YL) CONTAINING 1,3,4-THIADIAZOLE, 1,2,4-TRIAZOLE AND 1,3,4-OXADIAZOLE DERIVATIVES

Rajendra Deshmukh, Hemantkumar Akolkar, Bhausaheb Karale *
P.G. Department of Chemistry, Radhabai Kale Mahila Mahavidyalaya, Ahmednagar, Maharashtra, India
*Corresponding Author Email: hemantakolkar@gmail.com

Article Received on: 25/11/18 Approved for publication: 07/01/19

DOI: 10.7897/2230-8407.100261

ABSTRACT

A series of novel 1,3,4-thiadiazole, 1,2,4-triazole and 1,3,4-oxadiazole have been synthesized from 1-(2-(2-chlorophenyl)-2-(4-(6-fluorobenzo[d]isoxazol-3-yl)piperidin-1-yl)acetyl)-4-phenyl thiosemicarbazide 6 and their antimicrobial activities were reported. Compounds 6b, 6c, 9a, 9b, 9d and 9e have shown moderate activity towards Bacillus Subtilis and Escherichia Coli bacterial species. The structure of synthesized compounds was confirmed by spectral analysis.

Keywords: Benzo[d]isoxazole, 1,3,4-Thiadiazole, 1,2,4-Triazole and 1,3,4-Oxadiazole

INTRODUCTION

Benzo[d]isoxazole is one of the oxygen and nitrogen containing heterocyclic compound. In recent years compounds containing benzo[d]isoxazole scaffold attracts many researchers due to their pharmacological activities. Benzo[d]isoxazole and their derivatives are associated with antitubercular[1], antimycobacterial[2], anti-inflammatory[3], antidiabetic[4] and c-Met kinase inhibitor[5] etc activities. Thiosemicarbazide is a versatile intermediate for the synthesis of heterocycles like triazole, thiadiazole, oxadiazole & thiazole. Thiosemicarbazide derivatives are associated with as antioxidant[6], cathepsin L inhibitors[7], metallo-β -lactamase inhibitors[8] etc activities.

1,3,4-Thiadiazole, 1,2,4-triazole and 1,3,4-oxadiazole are significant class of heterocyclic compound and posses variety of biological activities. 1,3,4-Thiadiazole derivatives have been investigated for antiinflammatory[9], antituberculosis[10], anxiolytic[11], antidepressant[12] and herbicidal[13] activities.. 1,2,4-Triazole and its derivatives exhibit antitumor[14], antioxidant[15], antitubercular[16], antifungal[17,18], antibacterial[17,19], anti-inflammatory[20] and etc activities. 1,2,4-Triazole nucleus found in many drugs such as Letrozole, Vorozole, Voriconazole, Itraconazole, Alprazolam, Etoperidone, etc. 1,3,4-Oxadiazole containing compounds possess various biological activities such as tyrosinase inhibitors[21], anti-inflammatory[22], analgesic[22], anticonvulsant[23], antiproliferative[24] and antitubercular[25].

Activities associated with above heterocycles, it is worthwhile to synthesize 1-(2-(2-chlorophenyl)-2-(4-(6-fluorobenzo[d] isoxazol-3-yl)piperidin-1-yl) bearing various heterocycles such as 1,3,4-thiadiazole, 1,2,4-triazole and 1,3,4-oxadiazole and to evaluate for their antibacterial activities against Bacillus Subtilis and Escherichia Coli bacterial species.

MATERIALS AND METHODS

Substituted 1-(2-(2-chlorophenyl)-2-(4-(6-fluorobenzo[d] isoxazol-3-yl)piperidin-1-yl)acetyl)-4-phenylthiosemicarbazide **6** was synthesized in five steps starting from 2-(2-chlorophenyl)acetic acid **1**. 2-(2-Chlorophenyl)acetic acid **1** was converted into 2-bromo-2-(2-chlorophenyl)acetic acid **2** by using NBS. Methyl ester **3** of compound **2** was treated with 6-fluoro-3-(piperidin-4-yl)benzo[d]isoxazole hydrochloride in presence of base to afford methyl 2-(2-chlorophenyl)-2-(4-(6-fluorobenzo [d]isoxazol-3-yl)piperidin-1-yl)acetate **4**. 2-(2-Chlorophenyl)-2-(4-(6-fluorobenzo[d]isoxazol-3-yl)piperidin-1-yl)acetohydrazide **5** was prepared by refluxing compound **4** with hydrazine hydrate. Condensation of compound **5** with different aryl isothiocynates in alcohol furnished the corresponding thiosemicarbazides **6**. Thiosemicarbazides undergoes cyclisation to give thiadiazoles in acidic condition whereas to triazoles in basic medium. Oxadiazoles were prepared by treating thiosemicarbazides with iodine and potassium iodide in NaOH. The spectral analysis supports these transformations.

The antibacterial activity of some of the newly synthesized compounds was carried out by agar well diffusion method. Two bacterial species were chosen for the study, one was Gram Positive Bacillus Subtilis and another was Gram Negative Escherichia Coli. Ampicillin was used as a standard drug for this study. Compounds **6b**, **6c**, **9a**, **9b**, **9d** and **9e** have shown moderate activity towards Bacillus Subtilis and Escherichia Coli bacterial species.

Journal of Heterocyclic Chemistry / Volume 56, Issue 6 / p. 1780-1786

Article

Synthesis and Characterization of Novel 1-Methyl-3-(4-phenyl-4*H*-1,2,4-triazol-3-yl)-1*H*-indazole Derivatives

Kiran S. Hon, Hemantkumar N. Akolkar, Bhausaheb K. Karale

First published: 15 April 2019
https://doi.org/10.1002/jhet.3545

Abstract

A series of novel 1-methyl-3-(4-phenyl-4*H*-1,2,4-triazol-3-yl)-1*H*-indazoles was synthesized in three steps from 5-(1-methyl-1*H*-indazol-3-yl)-4-phenyl-2*H*-1,2,4-triazole-3(4*H*)-thiones. 5-(1-Methyl-1*H*-indazol-3-yl)-4-phenyl-2*H*-1,2,4-triazole-3(4*H*)-thiones were converted into 1-methyl-3-(5-(methylsulfonyl)-4-phenyl-4*H*-1,2,4-triazol-3-yl)-1*H*-indazoles upon methylation followed by treatment with aq. $KMnO_4$. The reaction of 1-methyl-3-(5-(methylsulfonyl)-4-phenyl-4*H*-1,2,4-triazol-3-yl)-1*H*-indazoles with Raney nickel resulted in desulphonylation to afford corresponding 1-methyl-3-(4-phenyl-4*H*-1,2,4-triazol-3-yl)-1*H*-indazoles. All the new synthesized compounds were characterized by spectral techniques.

Supporting Information

Filename	Description
JHET_3545-sup-0001-Supplementary data JHC.docx Word 2007 document , 7.7 MB	Data S1: Supporting Information

Please note: The publisher is not responsible for the content or functionality of any supporting information supplied by the authors. Any queries (other than missing content) should be directed to the corresponding author for the article.

ScienceDirect

Bioorganic & Medicinal Chemistry Letters

Volume 29, Issue 10, 15 May 2019, Pages 1199-1202

Thiazolyl-pyrazole derivatives as potential antimycobacterial agents

Sushma J. Takate [a e], Abhijit D. Shinde [b e], Bhausaheb K. Karale [c e], Hemant Akolkar [c e], Laxman Nawale [d], Dhiman Sarkar [d], Pravin C. Mhaske [b e]

Show more

https://doi.org/10.1016/j.bmcl.2019.03.020

Get rights and content

Abstract

Mycobacterium tuberculosis (*Mtb*) is an obligate aerobe that is capable of long-term persistence under conditions of low oxygen tension. A series of thiazolyl-pyrazole derivatives (**6a–f**, **7a–f**, **8c**, **8e**) were screened for antimycobacterial activity against dormant *M. tuberculosis* H37Ra (D-MTB) and *M. bovis* BCG (D-BCG). Nine thiazolyl-pyrazole analogs, **6c**, **6e**, **7a**, **7b**, **7c**, **7e**, **7f**, **8c** and **8e** exhibited promissing minimum inhibitory concentration (MIC) values (0.20–28.25 μg/mL) against D-MTB and D-BCG strains of *Mtb*. Importantly, six compounds (**7a**, **7b**, **7e**, **7f**, **8c** and **8e**) exhibited excellent antimycobacterial activity and low cytotoxicity at the maximum evaluated concentration of >250 μg/mL. Finally, the promising antimycobacterial activity and lower cytotoxicity profile suggested that, these compounds could be further subjected for optimization and development as a lead, which could have the potential to treat tuberculosis.

Graphical abstract

Indian Journal of Chemistry
Vol. 58B, April 2019, pp. 504-510

Synthesis, characterization and antibacterial screening of fluorinated benzofuran containing heterocycles

S G Kundlikar, P V Randhavane, H N Akolkar & B K Karale*
P G Department of Chemistry, Radhabai Kale Mahila Mahavidyalaya, Ahmednagar 414 001, India
E-mail: bkkarale@yahoo.com

Received 7 June 2017; accepted (revised) 26 December 2018

2-(4-Fluorophenyl)-5-phenylbenzofuran-3-carboxylic acid **1** when treated with substituted 2-hydroxyacetophenones **2** in dry pyridine and $POCl_3$ affords compound **3** which when reacted with pyridine/KOH by B. V. transformation gives **4**. Compound **4** on refluxing with different reagents Ac_2O in presence of sodium acetate, acetic acid in HCl, and hydrazinehydrate in alcohol gives **5**, **6** and **7** respectively. The structures of all synthesized compounds have been confirmed by spectroscopic techniques. All the synthesized compounds have been screened for their antibacterial activity.

Keywords: Benzofuran, chromones, pyrazoles, antibacterial activity

Benzofuran is considered as an important class of heterocyclic compound present in numerous bioactive natural products as well as pharmaceuticals and polymers[1]. Many of the clinically approved drugs are synthetic containing mono and fused benzofuran ring in conjunction with other heterocycles. They possess wide spectrum of biological activities such as TGR5 agonists[2], antimicrobial[3], antibacterial[4], anticoagulator[5], MAO-B enzyme inhibitor[6] and antioxidant[7].

Due to presence of two carbonyl groups, β-diketones are valueable substrates in many chemical syntheses. The functionalized derivatives of β-diketone are clinically important molecules and widely used due to their antibacterial[8], anti-HIV-1[9], insecticidal[10] and antiviral[11] activities.

Chromone and its derivatives have been studied for over century or more due to important biological activities such as cholesterol acyltransferase[12], antitumour[13], anticancer[14], topoisomerase II inhibitor[15], antioxidant[16] and antifungal[17]. Pyrazole derivatives occupy an important position in medicinal[18] and pesticide chemistry with having a wide range of bioactivities such as cytotoxic[19], analgesic[20], antibacterial[21] and urease inhibitors[22].

In view of biological activities associated with benzofuran, chromones and pyrazoles we decided to synthesize series of benzofuran containing different heterocycles and screened them for their antibacterial activity (Scheme I).

Experimental Section

Melting points were determined in open capillaries in liquid paraffin bath and are uncorrected. Mass spectra were recorded on Waters Acquity TQD mass spectrometer. ^{1}H NMR spectra were recorded on Bruker Avance II 400 MHz NMR spectrometer in DMSO-d_6 as a solvent and TMS as an internal standard. Peak values are shown in δ (ppm). IR spectra were recorded on Shimadzu IR Affinity-1S spectrophotometer.

2-Acetylphenyl-2-(4-fluorophenyl)-5-phenylbenzo furan-3-carboxylate, 3a-g

Equimolar mixture of 2-(4-fluorophenyl)-5-phenylbenzofuran-3-carboxylic acid **1** (0.003M) and substituted 2-hydroxyacetophenone **2** (0.003M) was dissolved in pyridine (15 mL) taken in dry beaker maintained at about 0°C. To this reaction mixture $POCl_3$ (0.003 M) was slowly added maintaining the temperature below 4°C. After complete addition the reaction mixture was kept overnight, then the resulting reaction mixture was poured over crushed ice. The product thus obtained was separated by filtration and crystallized from ethanol to afford **3**.

2-Acetylphenyl-2-(4-fluorophenyl)-5-phenylbenzo furan-3-carboxylate, 3a: m.p.176°C. Yield 76%. IR: 3080, 1748, 1686, 1604, 1504, 1165 cm^{-1}; ^{1}H NMR: δ 2.49 (s, 3H), 7.22 (s, 1H), 6.90-6.98 (m, 1H), 7.33-7.42 (m, 4H), 7.44-7.53 (m, 2H), 7.58-7.90 (m, 5H), 8.00 (dd, 1H), 8.10 (dd, 1H), 8.23 (d, 1H); MS: *m/z*

Microwave Assisted Synthesis and Antimicrobial Activity of Novel 1,3,4-Thiadiazoles and 1,2,4-Triazoles Derived from 2-(3-Fluorophenyl)-4-methylthiazole-5-carbohydrazide

Published: 16 August 2019

Volume 89, pages 1535–1540, (2019) Cite this article

S. G. Dengale, B. K. Karale, H. N. Akolkar, N. R. Darekar & K. K. Deshmukh

Abstract

The precursors 2-{[2-(3-fluorophenyl)-4-methyl-1,3-thiazol-5-yl]carbonyl}-*N*-phenylhydrazinecarbothioamides are synthesized from 2-(3-fluorophenyl)-4-methylthiazole-5-carbohydrazide and aryl isothiocyanates. MW irradiation of the precursors under alkali or acidic conditions led to the products of cyclization 5-[2-(3-fluorophenyl)-4-methylthiazol-5-yl]-*N*-phenyl-1,3,4-thiadiazol-2-amine or 5-[2-(3-fluorophenyl)-4-methylthiazol-5-yl]-4-phenyl-4*H*-1,2,4-triazole-3-triiol, accordingly. Structures of the synthesized compounds are confirmed by IR, ^{1}H, and ^{13}C NMR, and mass spectra. All products are tested *in vitro* for their antibacterial and antifungal activity.

ScienceDirect

Arabian Journal of Chemistry

Volume 12, Issue 8, December 2019, Pages 5212-5222

Original article

Synthesis and characterization of nanostructured Cu-ZnO: An efficient catalyst for the preparation of (*E*)-3-styrylchromones

Sachin P. Kunde [a], Kaluram G. Kanade [a b], Bhausaheb K. Karale [a], Hemant N. Akolkar [a], Pratibha V. Randhavane [a], Santosh T. Shinde [a]

https://doi.org/10.1016/j.arabjc.2016.12.015

Get rights and content

Abstract

We have explored nanocrystalline ZnO and Cu-ZnO catalyst for the preparation of 3-styrylchromones with trans selectivity derived from 3-formylchromones. Synthesis of ZnO and Cu-ZnO nano flakes (NFs) was carried by precipitation technique. The analytical techniques such as UV-Visible spectroscopy, X-ray diffraction (XRD), Brunauer-Emmett-Teller (BET), field emission scanning electron microscopy (FESEM) and energy-dispersive analysis X-ray spectroscopy (EDAX) were used to characterize the catalysts. The XRD pattern showed highly pure wurtzite ZnO and Cu-ZnO. The FESEM images showed nano flakes such as sunflower seed morphology in the range width of 9–34nm and length 90–180nm. Doping of copper in ZnO was employed to study the selectivity of Knoevenagel and Knoevenagel-Doebner reactions. Knoevenagel condensation was catalyzed efficiently by pure ZnO nano flakes, whereas the Cu-ZnO nano flakes facilitate the Knoevenagel-Doebner reaction. Present synthetic protocols are novel, very clean and

Novel catalytic application of Ni@ZnO nanoparticles and ZnO nanoflakes in aqueous solution of NaPTS hydrotrope at room temperature via a green synthesis of 3,4-dihydropyrimidin-2(1H)-ones

Published: 30 January 2018

Volume 44, pages 3097–3113, (2018) Cite this article

Bipin Shinde, Santosh Kamble, Pramod Gaikwad, Vishvanath Ghanwat, Sagar Tanpure, Pavan Pagare, Bhausaheb Karale & Arvind Burungale

Abstract

We investigated a novel catalytic application of nickel-doped zinc oxide (Ni-ZnO) nanoparticles and zinc oxide (ZnO) nanoflakes at room temperature in an aqueous hydrotropic solution for the synthesis of biologically active dihydropyrimidones (DHPMs). Ni-ZnO is a stable, recyclable, green, efficient heterogeneous catalyst which

www.ijcps.org

IJCPS Vol. 7, Special Issue
RICES - Jan 2018

ISSN:2319-6602
International Journal of Chemical and Physical Sciences

Synthesis and Characterization of Chlorinated Thiophene Based Flavones

P. V. RANDHAVANE[1*], H. N. AKOLKAR[2], R. S. ENDAIT[2], R. K. JADHAV[1], A. B. NIKUMBH[1] and B. K. KARALE[2]

[1]Department of Chemistry, S. S. G. M. College, Kopargaon, (MS) India.
[2]Department of Chemistry, Radhabai Kale Mahila Mahavidyalaya, Ahmednagar, (MS) India.
Corresponding Author email: pvrandhavane@gmail.com

Abstract

(E)-3 -(3- (2,5-dichlorothiophen-3-yl) -1- (2,3-dimethylphenyl) -1H-pyrazol-4-yl) -1-(2-*hydroxyphenyl)prop-2-en-1-ones were synthesized by Claisen-Schmidt condensation reaction between 3-(2,5-dichlorothiophen-3-yl)-1-(2,3-dimethylphenyl)-1H-pyrazole-4-carbaldehyde and substituted 2-hydroxy acetophenones. 2-(3-(2,5-Dichlorothiophen-3-yl)-1-(2,3-dimethylphenyl)-1H-pyrazol-4-yl)-4H-chromen-4-ones were synthesized by oxidative cyclization of corresponding chalcones using DMSO/I_2.The structures of newly synthesized compounds were confirmed by some spectral analysis methods like, IR, NMR and Mass.*

Keywords: Chlorinated thiophene, oxidative cyclization,Claisen-Schmidt condensation.

Introduction

Thiophene is a five membered heteroaromatic compound with sulfur as a heteroatom. Thiophene and its derivatives exist in petroleum or coal. Thiophene moiety is found in certain natural products. It is also incorporated in several pharmacologically active compounds. The compounds containing thiophene moiety are reported to have antiproliferative [1], antibacterial [2], anticonvulsant [3] and antiprotozoal [4].

Chalcones are organic compounds possessing an enone moiety between two aromatic or heteroaromatic rings. These are the building blocks for the synthesis of various heterocyclic compounds like flavones, hydroxyl flavones, aurones and pyrazolines. Some chalcones are natural products found in various plant species around the world.Chalcones possess pharmacological activities like anticancer [5], anticancer [6] and antioxidant [6].

Flavones are group of naturally occurring oxygen containing heterocyclic compounds. They found in cereals and herbs. Flavones possess the activities such as antioxidant [7], antibacterial [8], antifungal [9] and antiviral [9].

Considering the biological importance of thiophene based heterocyclic compounds and in continuation of our work it was planned to synthesize chalcones and flavones containing chlorinated thiophene moiety.

Experimental

Melting points were recorded in open capillaries in liquid paraffin bath and are uncorrected. IR spectra were recorded on Perkin-Elmer FTIR spectrophotometer.^{1}H NMR spectra were recorded on Bruker Avance 400 MHz NMR spectrometer in DMSO as a solvent and TMS as an internal standard. Peak values are shown in σ (ppm). Mass spectra were recorded on Finnigan mass spectrometer.

www.ijcps.org

IJCPS Vol. 7, Special Issue
RICES - Jan 2018

ISSN:2319-6602
International Journal of Chemical and Physical Sciences

Synthesis and Characterization of Chlorinated Thiophene Based Flavones

P. V. RANDHAVANE[1*], H. N. AKOLKAR[2], R. S. ENDAIT[2], R. K. JADHAV[1], A. B. NIKUMBH[1] and B. K. KARALE[2]

[1]Department of Chemistry, S. S. G. M. College, Kopargaon, (MS) India.
[2]Department of Chemistry, Radhabai Kale Mahila Mahavidyalaya, Ahmednagar, (MS) India.
Corresponding Author email: pvrandhavane@gmail.com

Abstract

(E)-3 -(3- (2,5-dichlorothiophen-3-yl) -1- (2,3-dimethylphenyl) -1H-pyrazol-4-yl) -1-(2-*hydroxyphenyl)prop-2-en-1-ones were synthesized by Claisen-Schmidt condensation reaction between 3-(2,5-dichlorothiophen-3-yl)-1-(2,3-dimethylphenyl)-1H-pyrazole-4-carbaldehyde and substituted 2-hydroxy acetophenones. 2-(3-(2,5-Dichlorothiophen-3-yl)-1-(2,3-dimethylphenyl)-1H-pyrazol-4-yl)-4H-chromen-4-ones were synthesized by oxidative cyclization of corresponding chalcones using DMSO/I_2.The structures of newly synthesized compounds were confirmed by some spectral analysis methods like, IR, NMR and Mass.*

Keywords: Chlorinated thiophene, oxidative cyclization,Claisen-Schmidt condensation.

Introduction

Thiophene is a five membered heteroaromatic compound with sulfur as a heteroatom. Thiophene and its derivatives exist in petroleum or coal. Thiophene moiety is found in certain natural products. It is also incorporated in several pharmacologically active compounds. The compounds containing thiophene moiety are reported to have antiproliferative [1], antibacterial [2], anticonvulsant [3] and antiprotozoal [4].

Chalcones are organic compounds possessing an enone moiety between two aromatic or heteroaromatic rings. These are the building blocks for the synthesis of various heterocyclic compounds like flavones, hydroxyl flavones, aurones and pyrazolines. Some chalcones are natural products found in various plant species around the world.Chalcones possess pharmacological activities like anticancer [5], anticancer [6] and antioxidant [6].

Flavones are group of naturally occurring oxygen containing heterocyclic compounds. They found in cereals and herbs. Flavones possess the activities such as antioxidant [7], antibacterial [8], antifungal [9] and antiviral [9].

Considering the biological importance of thiophene based heterocyclic compounds and in continuation of our work it was planned to synthesize chalcones and flavones containing chlorinated thiophene moiety.

Experimental

Melting points were recorded in open capillaries in liquid paraffin bath and are uncorrected. IR spectra were recorded on Perkin-Elmer FTIR spectrophotometer.^{1}H NMR spectra were recorded on Bruker Avance 400 MHz NMR spectrometer in DMSO as a solvent and TMS as an internal standard. Peak values are shown in σ (ppm). Mass spectra were recorded on Finnigan mass spectrometer.