SYNOPSIS

“SYNTHESIS, CHARACTERIZATION & BIOLOGICAL EVALUATION OF SOME HETEROCYCLIC MOLECULES”

By

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Synopsis

Synopsis of the thesis is to be submitted to the Saurashtra University for the degree of Doctor of Philosophy in the Faculty of Science in Chemistry subject.

Faculty : Science

Subject : Chemistry

Title : “SYNTHESIS, CHARACTERIZATION & BIOLOGICAL EVALUATION OF SOME HETEROCYCLIC MOLECULES”

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Synopsis

Introduction

The heterocyclic compounds have always attracted an attention of chemists for their various and large pharmaceutical action & biological function.

The coumarine have diverse biological properties and various effects on the different cellular systems. Coumarine have important effects in plant biochemistry and physiology, acting as antioxidants, enzyme inhibitors and precursors of toxic substances. In addition, these compounds are involved in the actions of plant growth hormones and growth regulators, the control of respiration, photosynthesis, as well as defense against infection.

The coumarine have long been recognized to possess anti-inflammatory, antioxidant, antiallergic, hepatoprotective, antithrombotic, antiviral and anticarcinogenic activities. The coumarine are extremely variable in structure, due to the various types of substitutions in their basic structure, which can influence in their biological activity

Objectives

In present Ph.D. research work, the new coumarines have been synthesized using pyrimidine, 1,2,3-triazide, indol etc moieties to get better therapeutic agents, with following objectives.

1) To synthesise the heterocycles having coumarine moiety by various reported name reactions viz biginelli, passerini, click chemistry etc.

2) All the products have been characterized by elemental analyses, various spectroscopic techniques like IR, Mass & $^1$H NMR.

3) The purity of products have been checked by TLC.

4) All the products have been tested for their antimicrobial activity, using different strains of bacteria & fungi. some series of compound were also tested for their anti inflammatory activity.
Synopsis

The work to be presented in the thesis entitled “SYNTHESIS CHARACTERIZATION & BIOLOGICAL EVALUATION OF SOME HETEROCYCLIC MOLECULES” has been divided into six chapters as under.

CHAPTER-1
Multicomponent synthesis of 2-(2-hydroxybenzoyl)-6,6-dimethyl-3-phenyl-6,7-dihydro-1H-indol-4(5H)-one via Mannich reaction.

CHAPTER-2
Multicomponent synthesis of 4-phenyl-2-(pyrimidin-2-yl)-1H-chromeno[4,3-d]pyrimidin-5(2H)-one via Biginelli reaction.

CHAPTER-3
Synthesis and characterization of some 3-(2-(5-phenyl-1H-1,2,3-triazol-1-yl)acetyl)-2H-chromen-2-ones, using Click reaction.

CHAPTER-4
Synthesis and characterization of some 2-(tert-butylimino)-3-phenylchromeno[4,3-b][1,4]oxazin-5(2H)-ones, using Multicomponent Passerini types reaction.

CHAPTER-5
Multicomponent synthesis of 5-amino-6-phenyl-[2,2'-bipyrimidine]-4-carbonitrile.

CHAPTER-6
Biological evaluation of synthesized chemical entities.
Multicomponent synthesis of 2-(2-hydroxybenzoyl)-6,6-dimethyl-3-phenyl-6,7-dihydro-1H-indol-4(5H)-one via manich reaction.

Multicomponent reactions (MCR) are persuasive approach for developing a chemically diverse set of heterocyclic scaffolds with good yield. To this end, synthesis of a various 2-(2-hydroxybenzoyl)-6,6-dimethyl-3-substituted-6,7-dihydro-1H-indol-4(5H)-ones has been accomplished by MCR of 3-amino - 4-hydroxy coumarine, 5,5-Dimethyl-1,3-cyclohexanedione and various substituted aldehydes in presence of acid catalyst in organic solvents. The synthesized compounds were characterized by IR, $^1$H and $^{13}$C NMR and Mass spectrometry.

![Chemical structure](image)

Where $R= -\text{CH}_3$, -OCH$_3$, -Br, -Cl, etc

CHAPTER-2

Multicomponent synthesis of 4-phenyl-2-(pyrimidin-2-yl)-1H-chromeno[4,3-d]pyrimidin-5(2H)-one via Biginelli reaction.

In this chapter synthesis of a various 3,4-dihydro-1H-chromeno[4,3-d]pyrimidin-5(2H)-ones has been achieved by multicomponent cyclocondensation reaction of 6-nitro-4-hydroxy coumarine, various substituted aldehydes, and pyrimidine-2-carboximidamide in presence of acid catalyst in various organic solvents, The synthesized compounds were well characterized by IR, $^1$H and $^{13}$C NMR and Mass spectrometry.
CHAPTER-3

Synthesis and characterization of some 3-(2-(5-phenyl-1H-1,2,3-triazol-1-yl)acetyl)-2H-chromen-2-ones, using Click reaction.

This chapter deals with, synthesis of a various 3-(2-(5-phenyl-1H-1,2,3-triazol-1-yl)acetyl)-2H-chromen-2-ones, which are prepared by reaction of 3-(2-azidoacetyl)-2H-chromen-2-ones and various substituted phenyl acetylenes, using the Cu²⁺ and solvent mixture (Water : DMF : Butenol ). The synthesized compounds were characterized by IR, 1H and 13C NMR and Mass spectrometry.

CHAPTER-4

Synthesis and characterization of some 2-(tert-butylimino)-3-phenylchromeno[4,3-b][1,4]oxazin-5(2H)-ones, using Multi component Passerini types reaction.
Synopsis

Present work is related to passerini base cyclization reaction of 3-amino 4-hydroxycoumarine, substituted benzaldehydes and tert-butylisocyanide to furnish 2-(tert-butylimino)-3-phenylchromeno[4,3-b][1,4]oxazin-5(2H)-one. The synthesized compounds were characterized by IR, $^1$H and $^{13}$C NMR and Mass spectrometry.

\[ \text{Where, } R = \text{CH}_3, \text{OCH}_3, \text{Br}, \text{Cl}, \text{etc} \]

CHAPTER-5

**Multicomponent synthesis of 5-amino-6-phenyl-[2,2'-bipyrimidine]-4-carbonitrile.**

This chapter deals with synthesis of a various 5-amino-6-phenyl-[2,2'-bipyrimidine]-4-carbonitriles which are prepared by the reaction of pyrimidine-2-carboximidamide, malononitrile and various substituted aldehydes. The synthesized compounds were characterized by IR, $^1$H and $^{13}$C NMR and Mass spectrometry.

\[ \text{Where, } R = \text{-CH}_3, \text{-OH, -Cl, -NO}_2, \text{-CN, -Br, etc} \]
CHAPTER–6

BIOLOGICAL EVALUATION OF SYNTHESIZED CHEMICAL ENTITIES.

All the newly synthesized chemical entities have been screened for various biological activities using different strains of bacteria & fungi. Moreover, the compounds reported in chapter-2 have been screened for their anti-inflammatory activity.