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DESIGN, SYNTHESIS, SPECTRUM CHARACTERIZATION AND BIOLOGICAL ESTIMATION OF NOVEL 1,3,4-OXADIAZOLE DERIVATIVE

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ABSTRACT

We report the synthesis, spectrum characterization and biological assessment of novel 1,3,4-oxadiazole derivative based on reaction between 5-(4-aminophenyl)-1,3,4- oxadiazol-2-amine, glacial acetic acid & chloroacetyl chloride. Further the synthesized compound was determined by spectrum characterization (UV, ATR FTIR) and screened for antimicrobial activity.

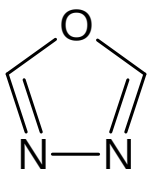
KEYWORDS: 1,3,4-oxadiazole derivative, 4-aminobenzoicacid, semicarbazide hydrochloride, n-(4-(5-amino-1,3,4-oxadiazol-2-yl)phenyl)-2-chloroacetamide, spectrum characterization, antimicrobial activity.

INTRODUCTION

In the branch of organic chemistry, the medicinal chemistry occupies the chief position because it involves design, development and synthesis of many new drugs. It is the major field of pharmaceutical science which the applies the principle of the chemistry and biology to the creation of knowledge leading to introduction of new drugs. The main objective of this field is to discover a new lead compounds or drug derivatives for use as a drug.[1]

Heterocyclic compounds are organic compounds with a ring structure that contains in the cycle at least one carbon atom and at least one other element, such as N, O, or S. The most common cycles contain five or six atoms, with the stability of these rings being higher than that of three, four, seven, or larger rings.[2]

Oxadiazole is a five-membered hetero cycle having two carbon atom, two nitrogen atom, one oxygen atom, and two double bonds. Oxadiazole is an important heterocyclic ring present in variety of biologically active molecules inclusive of fungicidal, bactericidal, anticancer, anti-tubercular, activities, etc. [3]



1,3,4-oxadiazole

METERIALS

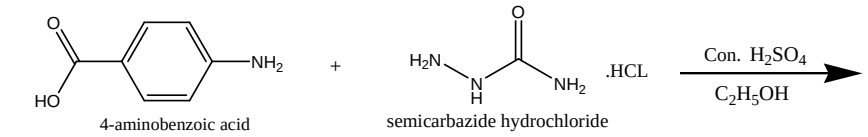
4-aminobenzoic acid, con. sulfuric acid, glacial acetic acid and other necessary chemicals were taken in Sri Vijay Vidyalaya college of Pharmacy, Nallampalli.

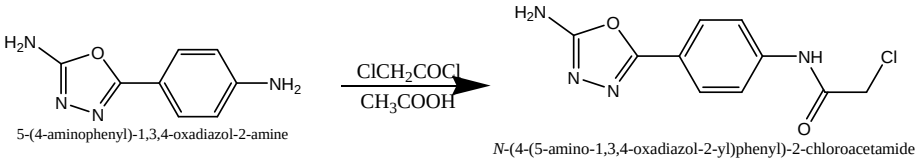
Semicarbazide, ethanol, and chloroacetyl chloride were purchased from Best Scientific Company, Dharmapuri.
The IR spectra of the compound were recorded on model- Bruker OPTIC ALPHA II (Germany) ATR FTIR spectrometer at Vinayaka Missions College of Pharmacy, Salem.

The absorption of compounds to be visualized in UV Spectro photometer, Brand- SHIMADZU, Model- 1601 at Vinayaka Missions College of Pharmacy, Salem.

The antimicrobial activity was performed by cup plate method in Sri Vijay Vidyalaya College of Pharmacy, Dharmapuri.

METHODS SCHEME





PROCEDURE

1. Synthesis of 5-(4-aminophenyl)-1,3,4-oxadiazole-2-amine

A mixture of semicarbazide Hydrochloride (11.15g, 0.1mol), 4-aminobenzoic acid (13.71g, 0.1 mol) and conc. Sulphuric acid 5 ml in 50 ml of ethanol was refluxed for 1.5 hour and poured onto crushed ice. The solid separated out was filtered, washed with cold water and recrystallized from ethanol to separate the first step product.

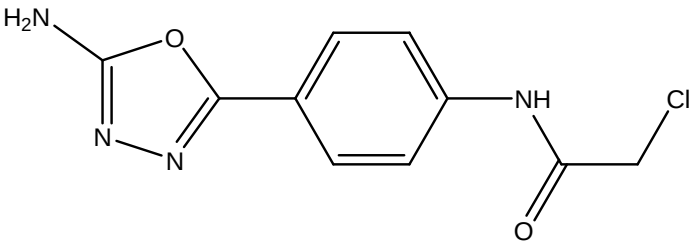
2. Synthesis of n-(4-(5-amino-1,3,4-oxadiazol-2-yl) phenyl)-2-chloroacetamide

A mixture of (1.76gm, 0.01mole) of 5-(4-aminophenyl)-1,3,4- oxadiazol-2-amine was dissolved in 10ml of glacial acetic acid to this (1.12ml, 0.01mole) of chloroacetyl chloride was added and the reaction mixture was refluxed for 1 hour. Cool the mixture to room temperature and pour into ice cold water the precipitate product was filtered and washed with water and dried. Then was recrystallized from ethanol.

INSTRUMEMTATION

The melting point of newly synthesized product determined by digital melting/boiling point apparatus. The completion of the reaction is confirmed by the using TLC method. The UV spectrum of newly synthesized compound is determined by using UV Spectro photometer, Brand- SHIMADZU, Model- 1601. The structure of compound is confirmed by model- Bruker OPTIC ALPHA II (Germany) ATR FTIR spectrometer.

RESULT AND DISCUSSION



N-(4-(5-amino-1,3,4-oxadiazol-2-yl)phenyl)-2-chloroacetamide

IUPAC name: N-(4-(5-amino-1,3,4-oxadiazol-2-yl)phenyl)-2-chloroacetamide
Molecular formula: $C_{10}H_9ClN_4O_2$
Molecular weight: 252.66
Boiling point: 872.12[k]
Appearance: appears like a powder form
Color: very light brown color

SPECTRUM CHARACTERIZATION

A) UV Spectrum

Sample: 1µg/ml

Blank: 0.1N NaOH

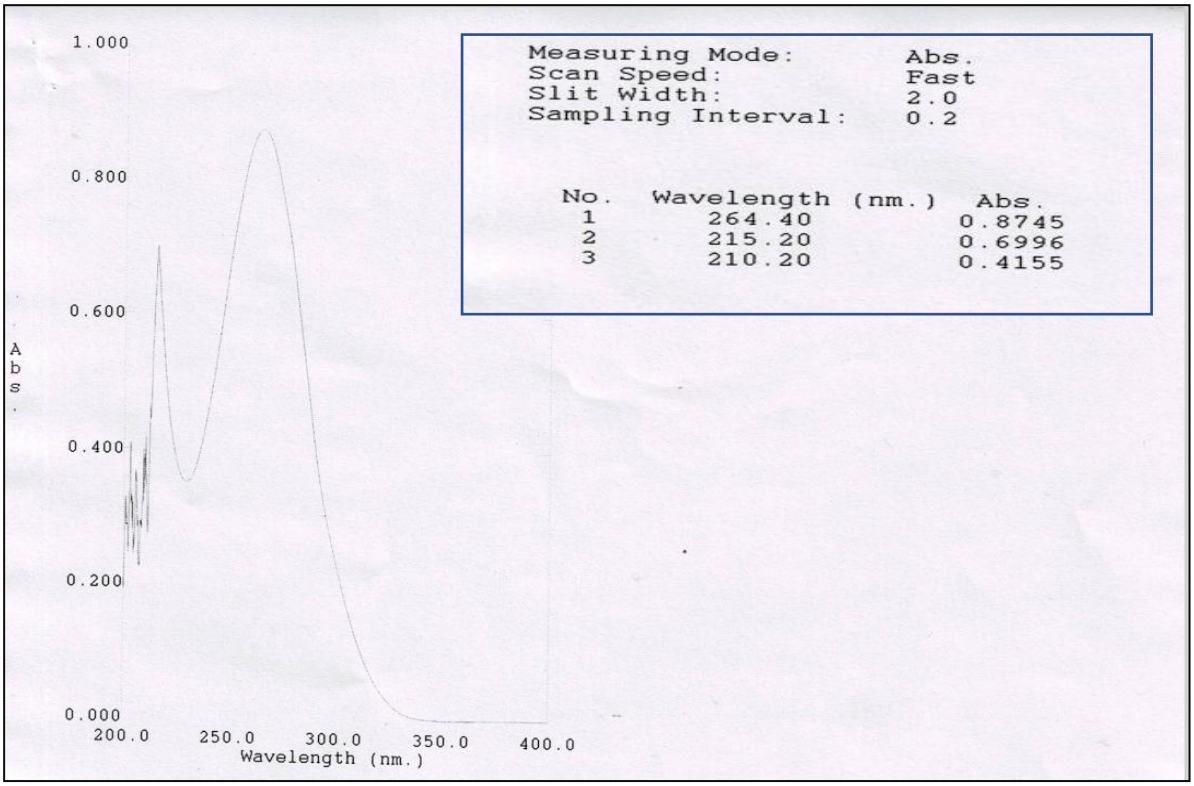


Fig. 1: UV spectrum of 1,3,4-oxadiazol derivative.

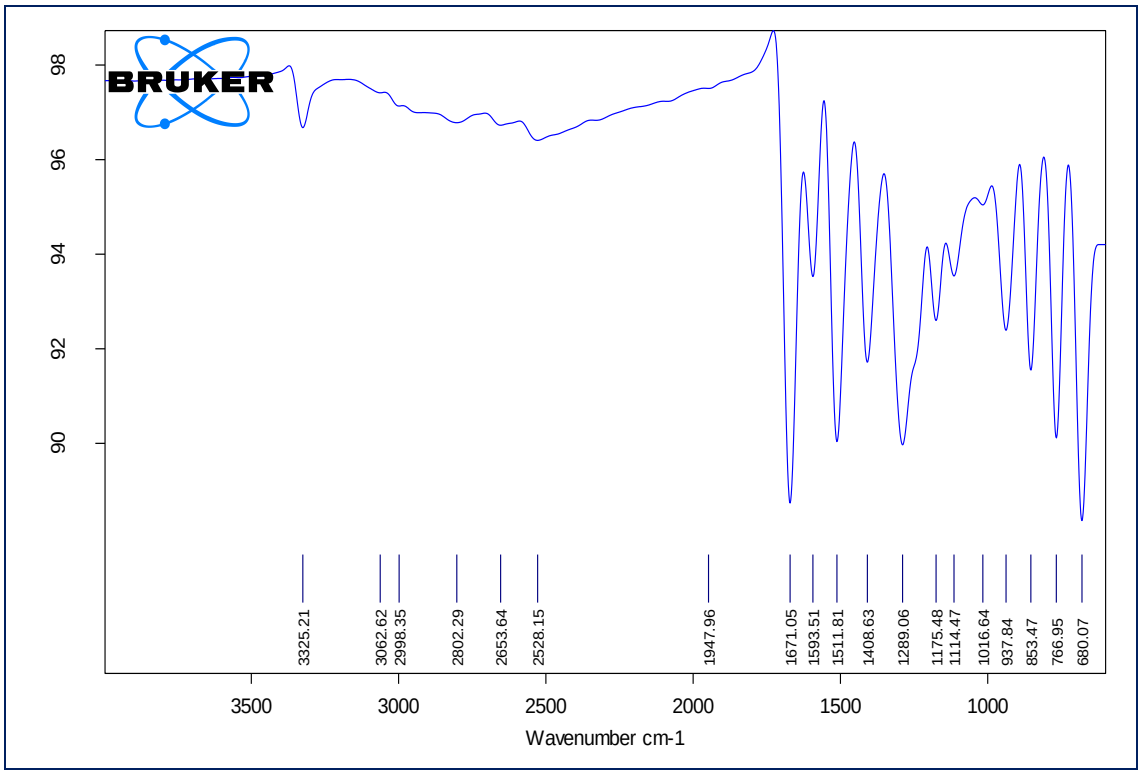


Fig. 2: ATR FTIR spectrum of 1,3,4-oxadiazol derivative.

B) IR SPECTRUM

Table 1: ATR FTIR interpretation of 1,3,4-oxadiazol derivative.

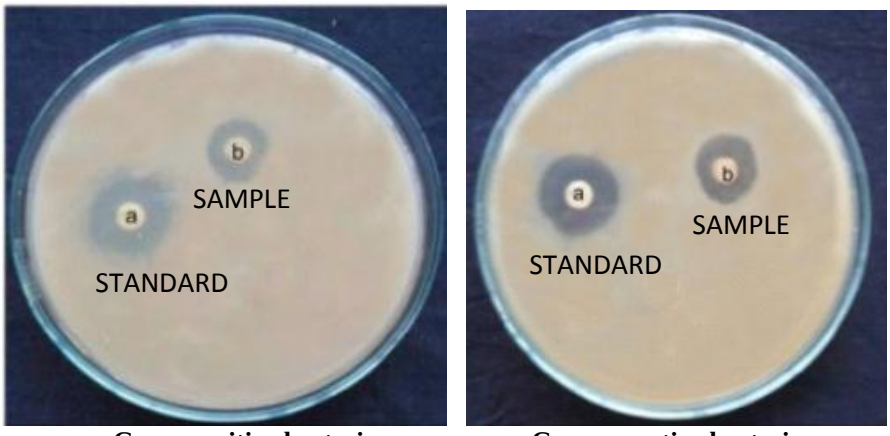
Radical	Wavelenth Literature	Atr Ftir Reading	Inference
C=C (Aromatic)	1450-1600 cm^{-1}	1511.81cm^{-1} 1593.51 cm^{-1}	C=C bond in a molecule
C-H (Aromatic)	~3030 cm^{-1}	3062.62 cm^{-1}	C-H bond in a molecule
C-H (Stretching) Alkane	2960-2850 cm^{-1}	2998.35	C-H bond in a molecule
C-O-C	1250-1050 cm^{-1}	1289.06 cm^{-1}	C-O-C bond in a molecule
C=N (Stretching)	1200-1350 cm^{-1}	1593.51 cm^{-1}	C=N bond in a molecule
C-Cl	850-550 cm^{-1}	680.07 cm^{-1}	C-Cl bond in a molecule
C=O (Amide)	1650-1700 cm^{-1}	1671.05 cm^{-1}	C=O bond in a molecule
N-H (Secondary Amide)	3100-3500 cm^{-1}	3325.21 cm-1	N-H bond in a molecule
N-H (Amine) bending	1500-1650 CM^{-1}	1593.51 cm^{-1}	N-H bond in a molecule

Antimicrobial Activity

Antibactrial Activity

Table 2: Minimum Inhibition Concentration of 1,3,4-oxadiazol derivative.

Microorganism	Reference Antibiotic	Concentration		Zone of inhibition (mm)	
		STD	SAMPLE	STD	SAMPLE
Gram positive bacteria *Staphylococcus aureus*	Streptomycin	0.75gm	10µg/ml	11mm	7mm
Gram negative bacteria *Escherichia coli*	Streptomycin	0.75gm	10µg/ml	12mm	9mm



Gram-positive bacteria **Gram-negative bacteria**

Fig. 3: Zone of Inhibition of 1,3,4-oxadiazol derivative.

CONCLUSION

In this work novel 1,3,4-oxadiazol derivative were synthesized. The synthesized compound was characterized by physicochemical, chromatographically and spectral analysis. The melting point and thin layer chromatography (TLC) were performed for check purity of the synthesized compound. Spectral studies i.e., UV and ATR FTIR were performed for peak absorption spectrum and structural conformation. The new synthesized compound was tested for antibacterial activity against gram positive & negative bacteria and shows less Minimum Inhibition Concentration (MIC) activity when compare with standard.

ACKNOWLEDGEMENT

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