


# KAKATIYA GOVERNMENT COLLEGE

HANUMAKONDA

Name : Dr. Alishala Ashok  
Designation : Asst. Professor of Chemistry  
Year of Award of Ph.D. : 2023  
Name of the University : Osmania University, Hyderabad, T.S.  
Year of entering into Govt. Service : 08-01-2005 as JL  
21-05-2013 as DL (21-05-2013)

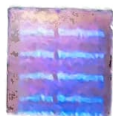
S. No.	Details of copies of Certificates	Remarks
1	Copy of Ph.D Certificate	Enclosed copy
2	Press note	Enclosed copy
3	Research work dates of seminars and Pre-Ph.D Date of joining in this college	Enclosed copy
4	Details of Ph.D Admission-part time or full time	16-03-2017 part time.
5	Copies of RDC Approval letters of Ph.D	Enclosed copy
6	Name of guide/supervisors with mobile number, email id	Prof. B. Sakvam, 9849530367, bschema@gmail.com
7	Copies of guide allotment letter	Enclosed copy
8	No. of increments sanctioned for Ph.D.	03
9	Published Research article-copies.	Enclosed copy
10	Original Ph.D Thesis.- Book.	Available in office.

  
PRINCIPAL  
KAKATIYA GOVT. COLLEGE  
Hanamkonda.

  
Signature  
Name & Designation  
Dr. Alishala Ashok  
Asst. Professor of Chemistry

OU 969798

# Osmania University



Faculty of Science

This is to certify that Ashok  
son / daughter of Rajaiah  
having pursued a course of study prescribed by this University  
and having passed the requirements by Examination and by  
thesis has been admitted to the Degree of

**Doctor Of Philosophy**

in the Subject of Chemistry

The title of the Thesis is :

Design, Molecular Modeling, Synthesis of some New 1,8-Naphthyridinyl  
Heterocycles and their Biological Evaluation

The candidate has been declared qualified for the award of the  
Degree of Ph.D. on 11 Oct 2023

Given under the seal of the University



CN102380989



Hyderabad, T.S.

Dated Kartika 9, 1945  
October 31, 2023

*Amis*  
Vice-Chancellor



CONFIDENTIAL SECTION  
EXAMINATION BRANCH  
NO. 783/Ph.D/Exams/2023

OSMANIA UNIVERSITY  
HYDERABAD-500 007, T.S.  
Dated: 11 Oct, 2023

**PRESS NOTE**

The following candidates who had presented the Thesis on the subject mentioned against each for the degree of Ph.D are declared qualified for the award of Degree of Doctor of Philosophy (Ph.D.) of Osmania University, Hyderabad.

**Ph.D.**

S.N	Reference No.	Name of the Candidate/ Father Name	Subject	Thesis Title	Supervisor/ Regn. Date
1	PHD44447	Mr. Ashok S/o. Rajaiah	Chemistry	Design, Molecular Modeling, Synthesis of some New 1,8- Naphthyridinyl Heterocycles and their Biological Evaluation	Prof. B Sakram Dept. of Chemistry, O.U., Hyd. (03/04/2017)
2	PHD44448	Mr. Lingaswamy Veeramalla S/o. Yadaiah	Geology	Petrology and Geochemical Studies of Spatially Related Carbonatites and Associated Rocks from Padavannoor, Karapatu, Kunnathur of Samalpatti and Sevathur Complexes Tamilnadu, India	Dr. K Sreenu Assoc. Professor, Dept. of Geology, O.U., Hyd. (03/10/2018)
3	PHD44449	Mr. N Mallesham S/o. Papaiah	History	B.N. Sastry: A Biographical Study (1932- 2002)	Prof. G Anjaiah(Retd.) Dept. of History, O.U., Hyd. (20/03/2017)
4	PHD44450	Ms. N Lakshmi Neelima D/o. N Madhava Rao	English	Revisiting the Institution of Family: A Study of the Selected Novels of Manju Kapur and Anita Nair	Dr. B Ashok Asst. Professor, Dept. of English, O.U., Hyd. (17/03/2017)
5	PHD44451	Ms. Rohini A D/o. Mohan Rao A	Environmental Science	Ecological Studies on Safilguda Lake with Reference to Water Quality	Prof. P Manikya Reddy Dept. of Botany, O.U., Hyd. (01/04/2017)
6	PHD44452	Ms. R Gayathri D/o. R Ramchander	English	Interpersonal and Intrapersonal Conflicts: A Psychoanalytical Study of the Selected Novels of Jane Austen, Charlotte Bronte and Virginia Woolf	Dr. J Madhavi Asst. Professor, Dept. of English, UCT, O.U., Hyd. (19/08/2017)

7	PHD44453	Ms. G Sumalata D/o. Guppa Niranjan	Nutrition	Studies on Identification and Characterization of Isolated Probiotics from Dairy Products and Human Breast Milk and to Develop Food Supplements for Human Health	Dr. M Shiva Prakash(Retd.) Sr. Scientist, ICMR, NIN, Hyd. (21/01/2016)
---	----------	---------------------------------------	-----------	--	---

*C.P. Vardhani* 11/10/23  
Addl. Controller of Examinations  
(Confidential)

Copy forwarded to:

1. The Candidate \_\_\_\_\_
2. P.A. to Controller of Examination, O.U.
3. The Dean, Faculty of Arts / Science / Social sciences , O.U.
4. The Chairperson, BOS in Chemistry/ English/ EnvironmentalScience/ Geology/ History/ Nutrition, O.U.
5. The Head Dept of Chemistry/ English/ EnvironmentalScience/ Geology/ History/ Nutrition/Journalism, O.U.
6. The Secretary to the Vice-Chancellor/P.A. to Registrar, O.U.
7. The Deputy Registrar/ Accounts/ Admin/ Academic/ UGC Cell, O.U.
8. The Librarian, General Library, O.U.
9. The Public Relations Officer, O.U.
10. The Cheif Warden, Hostel and Messes, O.U.
11. The ACOE(EDP), Examination Branch, O.U.
12. The Director, Infrastructure, Admin. Buildings, O.U.
13. The Secretary, Assoc. of Indian Universities, 16, Kotla Road, New Delhi-110002
14. The Director, Research Division, Assoc. of Indian Universities, 16, Kotla Road, New Delhi-110002
15. The Secretary, UGC, 35, Feroz Shah Road, New Delhi-110002
16. The Editor, University News, AIU Campus, Kotla Road, New Delhi-110002
17. The Senior Statistical Officer, U G C, (Info & Stats Bureau), 35, Feroze Shah Road, New Delhi - 110 221.
18. The Local Press (through DIPR), Govt. of T.S., Hyderabad.
19. The Examiner \_\_\_\_\_

With a request to send the remuneration bill dully filled in immediately and also to return the copy of the Thesis/Dissertation if it is not done so far.

**DEPARTMENT OF CHEMISTRY: UNIV. COLLEGE OF SCIENCE: O.U. Hyd.**

**Research Design Seminar Report**

The Research design seminar of **Mr. A. Ashok** was conducted in Lecture Hall No. II on 22.08.2022 at 10.00 A.M. in the Department of Chemistry, O.U on the topic "Design, Molecular modeling, synthesis of some new 1,8-naphthyridyl heterocycles and their biological evaluation." The candidate has presented detailed comprehensive literature review of the Research topic and the plan of work and progress of the work satisfactorily.



( Dr. B Sakram)

Supervisor Professor  
Asso. Professor  
Department of Chemistry  
Osmania University  
HYDERABAD - 500 007



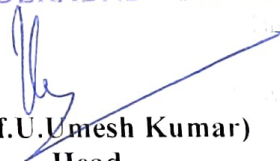
( Prof. P. Leelavathi)  
Chairperson BOS

Chairperson  
Board of Studies in Chemistry  
Dept of Chemistry  
Osmania University, Hyd-07.



( Dr. T. Gangadhar)

Subject Expert  
Asso. Professor  
Department of Chemistry  
Osmania University  
HYDERABAD - 500 007



( Prof. U. Umesh Kumar)  
Head

Department of Chemistry

Head  
Department of Chemistry  
UCS, Osmania University  
Hyderabad-007

**DEPARTMENT OF CHEMISTRY: UNIV. COLLEGE OF SCIENCE: O.U. HYD.**

**Pre – Submission viva Seminar Report**

The Pre-Viva examination of **Mr. A. Ashok** in the Department of Chemistry, O.U on 20.02.2023 at 11.00 A.M. The pre-viva was presented as a seminar, open to all Teachers and Research Scholars.

The candidate was asked to present the work carried out by him and then asked questions related to his topic of work “**Design, Molecular modeling, synthesis of some new 1,8-naphthyridinyl heterocycles and their biological evaluation**”. The candidate has answered all the questions satisfactorily.

An earlier Seminar was conducted and certified by the supervisor.

Based on the evaluation of the work done and satisfactory performance of the candidate in the pre-viva presentation, He is permitted to submit thesis for Ph.D in Chemistry, Osmania University.



**( Prof. B. Sakram )**  
**Supervisor**

Professor  
Department of Chemistry  
Osmania University  
HYDERABAD - 500 007



**( Prof. U. Umesh Kumar )**  
**I/c Chairperson BOS**

Chairperson  
Board of Studies  
Department of Chemistry  
Osmania University, Hyderabad



**( Prof. B. Yadagiri )**  
**Subject Expert**

Department of Chemistry  
Osmania University  
HYDERABAD - 500 007



**( Prof. U. Umesh Kumar )**  
**Head**

Department of Chemistry  
**Head**  
Department of Chemistry  
UCS, Osmania University  
Hyderabad-007

45



**OFFICE OF THE DEAN FACULTY OF SCIENCE  
OSMANIA UNIVERSITY HYDERABAD**

No. 3498/A / DFSc/2017

Date: 16.03.2017

ORDERS

**Sub :** FACULTY OF SCIENCE, OU – Admission to Ph.D. Course Category II  
2013-2014, Orders - Chemistry - Issued.

**Ref. No :** No 325 /F/Acad-III/2017

Dated 23.02.2017

\*\*\*

The candidates in the enclosed list are provisionally admitted to the Ph.D. course of Osmania University for the academic year 2013-2014 on the recommendation of the Admission Committee in the Faculty of Science in the subject mentioned against his/her name.

The selected candidates are required to fulfill the conditions, if mentioned against their names, and to submit their Joining Reports (Proforma provided), by **10. 04 . 2017** failing which their admission orders would be deemed to have been withdrawn. No further notice will be given. The Joining Reports along with the original D.D. and all necessary documents should be submitted in the concerned Departments. **No joining report will be accepted without the T.C. (Transfer Certificate) in original or a letter from the respective University where from the Post Graduate Degree has been obtained to the effect that no separate Transfer Certificate will be issued by that University.** The Dean's office shall then issue a list of names of the admitted candidates to the Heads of the Departments concerned, which shall be final.

The registration is valid for a period of four years for Full Time Research Scholars and five years for Part Time Research Scholars from the date of joining after which period it will be cancelled unless otherwise extended.

All the selected candidates both Full-Time and Part-Time have to pay the fee as under:

- |  |                  |
|--|------------------|
| 1. Both Full Time and Part Time Scholars working in the Osmania University | Rs.2000 per year |
| 2. Scholars working in recognised Research Centres outside the University  | Rs.5000 per year |

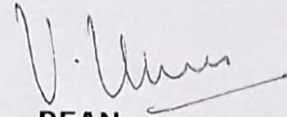
(P.T.O.)

through a demand draft in favour of "Dean, Faculty of Science, Osmania University". They should submit their Joining Reports in the concerned University Department in the prescribed proforma in triplicate along with the Original DD., and M.Sc., Certificate (Xerox Copy) in proof of satisfaction of the conditions stipulated. If the candidate fails to pay the fees mentioned above within the specified time his/her admission will be cancelled without further notice to the candidate.

The selected candidates are required to submit an undertaking to the effect that they do not ask for hostel facilities (Annexure II) along with their joining reports, failing which they will not be granted admission.

Candidates selected under the category "Part Time" are required to submit an undertaking in triplicate on the proforma provided (Annexure-III) that they would be taking necessary leave as per rules of the University. Their admission is conditional upon realization of dues to the University if any from the candidates. The admissions are made on the basis of the present occupation of the candidates. In case there is a change in occupation or place of work during the period of their candidature in the Ph.D., course, their admission is liable to be cancelled. Any change in their occupation should be brought to the notice of the Dean, through the Supervisor and the Head of the Department, and the Dean may permit the candidate to continue his/her Ph.D. course as per the rules.

The candidates who are admitted to the Ph.D. course shall not pursue any other course or appear for any other examination leading to any other Degree (both Full-Time and Part-Time) of this University or any other University. Any violation of this regulation will lead to the cancellation of admission.

  
DEAN

Faculty of Science, O.U.

DEAN

Faculty of Science  
OSMANIA UNIVERSITY

HYDERABAD-500 007

To

The Research Scholar concerned.

Copy forwarded for information and necessary action to:-

1. Principal, University College of Science, O.U.
2. The Vice Principal, Hostels, Univ College of Science, O.U.
3. The Head, Department of \_\_\_\_\_, O.U.
4. The Controller of Examinations, O.U.
5. The Asst. Registrar (Academic), O.U.
6. The Librarian, University Library, O.U.
7. The Secretary to Vice-Chancellor, O.U.
8. The Officer on Special Duty to Vice-Chancellor, O.U.
9. The P.A. to Registrar, O.U.
10. The Chief Warden, Hostels & Messes, O.U.



## Chemistry

21	Hareesh Reddy. B	M	OC	FT	Dr. M. Vasavi
22	M Bhargavi	F	BC-B	PT	Dr. P. Sarita Rajender
23	D Ravindra Reddy	M	OC	PT	Dr. B. Vijaya Kumar
24	Shaik Khaleel	M	BC-B	PT	Dr. P. Sarita Rajender
25	Bojja Anil Kumar	M	SC	PT	Dr. Y. Hemasri
26	Sreenu Daravath	M	ST	FT	Prof. P Shivraj
27	D. Govardhan	M	SC	PT	Prof. K.C. Rajanna
28	Aitha Shalini	F	OC	PT	Dr. P. Jalapathi
29	S Manasa	F	BC-B	FT	Prof. M. Vithal
30	Nagu Moodu	M	ST	PT	Dr. K. Shiva Kumar
31	Gaddam Sai Prasad	M	ST	PT	Dr. D.A. Padmavathy
32	H Smitha	F	OC	PT	Prof Ch. Sarala Devi
33	J Ravi Kumar	M	BC-B	PT	Prof. Ch. Prasad Rao
34	B Mounika	F	BC-D	FT	Dr. M. Vasavi
35	Ameena Husain	F	OC	PT	Prof Ch. Sarala Devi
36	A Vasantha	F	BC-B	PT	Dr. A. Haripadmasree
37	Kandula Kotaiah	M	SC	FT	Dr. A.K.D. Bhavani
38	Matkala Balakrishna	M	BC-D	PT	Dr. A. Haripadmasree
39	M Pallavi	F	BC-D	PT	Dr. P.V. Anantalaksmi
40	M. Keshavulu	M	BC-D	FT	Prof. Ch. Abraham Lincoln
41	MD Jakeer Pasha	M	BC-E	FT	Dr. P. Someshwar
42	K. Chandra Rekha	F	OC	PT	Dr. T.V.D. Prasad
43	M. Mallesh	M	BC-A	PT	Dr. A. Krishnam Raju
44	Haribabu	M	BC-A	PT	Dr. G. Vijaya Lakshmi
45	A Ashok	M	BC-A	PT	Dr. B. Sakram
46	S Prashanth	M	BC-A	FT	Prof. S. Satyanarayana
47	P Radhika	F	BC-A	FT	Dr. P. Someshwar

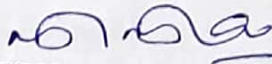
*V. Manu*  
**DEAN**  
 Faculty of Science  
 OSMANIA UNIVERSITY,  
 HYDERABAD-500 007.

ANNEXURE - III

PROFORMA TO BE FILLED BY THE CANDIDATE SELECTED UNDER THE  
CATEGORY "SUBJECT TO TAKING LEAVE AS PER RULES"


I, ALISHALA ASHOK have been provisionally  
selected for the Ph.D. course as Part Time Research Scholar in the Faculty of Science  
for the academic year 2013-2014 in the subject of Chemistry and I  
hereby agree that I would take leave for a minimum of one year for attending the  
classes of the Ph.D. work during the tenure of the Ph.D. course and a letter from the  
employer that the required leave will be sanctioned for the purpose stated.

HYDERABAD

  
SIGNATURE OF THE CANDIDATE


Date: 03-04-2017

Name:

  
Signature of the Supervisor  
Dr. B. KRAM  
Assistant Professor  
Department of Chemistry  
Osmania University  
HYDERABAD-500

Name:

Signature of the Head

  
Name: **HEAD**  
Department of Chemistry  
Osmania University  
Seal: Hyderabad-500 007.



**JOINING REPORT OF Ph.D. COURSE,  
FACULTY OF SCIENCE, OSMANIA UNIVERSITY**

- 1 Name & Phone No / Male / Female ALISHALA ACHOK, 9849767362, MALE
- 2 Father's Name RAJAI AH
- 3 Details of Scholarship if any NO
- 4 College/Institute at which the Candidate proposes to work Osmania University
- 5 Full-Time/Part-Time PART-TIME
- 6 Name of the Supervisor Dr. B. Sakram
- 7 Department Chemistry
- 8 State whether you being to OC/BC (A/B/C/D/E)SC/ST BC-A
- 9 Topic of Research Design, molecular modeling, synthesis of some new 1,8-Naphthyridyl heterocycles and their biological evaluation.

To  
The Dean,  
Faculty of Science

//Through Proper Channel//

Sir, Ref: Order No. 3498/A/DFSc/OU/20 Dt 16-03-2017

I am herewith submitting my joining report today i.e. on 03-04-2017

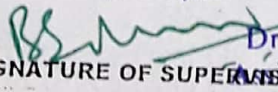
I have read the rules and regulations of the Ph.D. Course/ Course and I undertake to abide by them.

I understand that my admission may be cancelled, if the statements I made in my application are found to be false.

I have satisfied all conditions stipulated in my admission order and I am enclosing herewith the necessary certificates (if applicable).

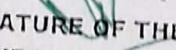
**LIST OF ENCLOSURES**


1. D.D. No: 120413 Date 22/3/2017 Amount 2000.00

  
**Dr. B SAKRAM**  
Assistant Professor  
Department of Chemistry  
Osmania University  
HYDERABAD-500

  
SIGNATURE OF CANDIDATE

SIGNATURE OF THE HEAD OF  
INSTITUTION IN WHICH  
CANDIDATE PROPOSES TO WORK

  
SIGNATURE OF THE HEAD  
OF THE UNIV. DEPARTMENT  
**HEAD**  
Department of Chemistry  
Osmania University  
Hyderabad-500 007.

  
SIGNATURE OF THE DEAN  
**DEAN**  
Faculty of Science  
OSMANIA UNIVERSITY,  
HYDERABAD-500 007.

## Structural elucidation of compounds using different types of spectroscopic techniques

Ashok Alishala\*

Department of Chemistry, Govt. Degree & PG College, Mancheril, Dist: Adilabad- 504208 (T.S.) India.

\*Corresponding author: E.Mail:alishala2010@gmail.com, Mobile: 9849767362

### ABSTRACT

Analytical techniques can be used for the purpose of identification of structure and composition of a chemical compound. Each analytical technique has a different method and mode of detection. An analytical process can be considered as a generation of information, however, unambiguous true identification especially that of unknown compound needs a large amount of information. The reason is that the results of the procedure are very often complex chemical compounds. Their molecules differ between each other in elements and the number of their atoms, types of chemical bonds, configurations and conformations. The complexity of a molecule increases with the number and diversity of atoms, bonds, molecular configurations/conformations. Correspondingly, the amount of information required for the full description of complex molecules and differentiation between them is also increased. Thus analytical techniques providing more information such as those of molecular spectrometry, are preferred for identification, other factors being equal. Using proper methods, higher selectivity is achieved, which also expressed in a larger number of identification points. At the same time, some techniques generating a lot of information such as emission spectral analysis are not applicable in molecular analysis with its numerous identification problems.

Spectroscopy studies the light absorbing properties of matter. Since each compound has its unique molecular or ionic structure, its light absorbing properties will also be unique. A quick method to obtain a lot of information about a compound's structure. Sometimes, with sufficient spectroscopic results, the compound's structure can be completely determined.

**Key words:** UV spectroscopy, Microwave spectroscopy, IR spectroscopy. Mass spectroscopy, NMR spectroscopy, different instruments of spectroscopy.

### INTRODUCTION

**Ultra Violet (UV):** Ultraviolet light is electromagnetic radiation with a wavelength shorter than that of visible light, but longer than X-rays, in the range 10 nm to 400 nm. It is so named because the spectrum consists of electromagnetic waves with frequencies higher than those that humans identify as the colour violet. These wavelengths of light cause electrons to be promoted to higher energy orbitals. Thus, information about a molecule's orbitals and bonding can be obtained.

**Microwave spectroscopy:** Microwaves cause molecules to rotate. In fact, the microwave oven works by causing the fast rotation of water molecules. This rotational kinetic energy is observed as the heating of the water.

**UV Spectroscopy: Instrumentation and Spectra**

**Instrumentation:** The construction of a traditional UV-Visible spectrophotometer requires sample handling, irradiation, detection and output. Here is a simple schematic that covers most modern UV spectrometers:

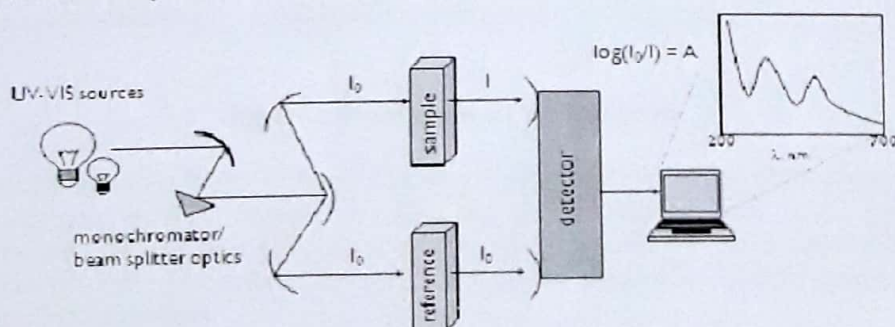
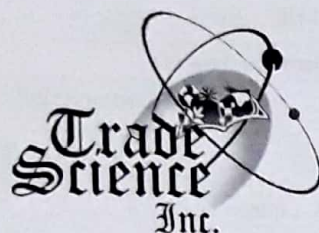


Figure.1.Schematic of UV-Visible spectrophotometer



# BioCHEMISTRY

*An Indian Journal*

*Regular Paper*

BCAIJ, 9(5), 2015 [165-168]

## **Analysis of microelements in the forest soil of the mahadevpur reserve forests of karimnagar east division, karimnagar district, telangana, India**

T.Karunakar<sup>1</sup>, A.Ashok<sup>2</sup>, M.Venkateshwarlu<sup>3</sup>, E.Ayshwarya<sup>4</sup>, T.Ugandhar<sup>5\*</sup>

<sup>1</sup>Department of Chemistry SRR Govt.Arts & Science College Karimnagar-505001, (INDIA)

<sup>2</sup>Department of Chemistry Govt Degree & P.G.College Mancherial—504208, (INDIA)

<sup>3</sup>Department of Botany, University College Kakatiya University Warangal-506009, (INDIA)

<sup>4</sup>Department of Biotechnology SRR Govt. Arts & Science College Karimnagar -505001, (INDIA)

<sup>5</sup>Department of Botany, SRR Govt.Arts & Science College Karimnagar - 505001, (INDIA)

E-mail: tugandharbiotech@gmailcom.in

### **ABSTRACT**

Mineral elements that are needed by plants in only trace amounts are known as micro-elements or micro-metals or trace elements or micro-nutrients. These elements are as important to the plant's health as macro-elements, but needed in lower quantities. Many of the microelements are enzyme co-factors, which are easily supplied to the plants through the soil. These microelements are Iron (Fe), Copper (Cu), Manganese (Mn), Boron (B), Molybdenum (Mo), Zink (Zn) and Chlorine (Cl).

The forest ecosystems are dominant ecosystems in the sheltered tropical forests of Mahadevpur Reserve Forests of Karimnagar East Division, Karimnagar District of Telangana, India. The various bio-geo-chemical processes that the trace elements undergo during their residence times in the forest ecosystem, ultimately determine their distribution in the forest environment. Different factors such as sediment characteristics, grain size, distribution, mineral composition and organic content may control the partitioning and also the bioavailability of the microelements in the soil.

In the present studies, it provides the information on the distribution of trace metals in the forest ecosystem of Mahadepur Reserve Forests in relation with the sediment organic carbon and their texture. Bimonthly collections of soil sediments are made from January 2014 to June 2014. Hydrographical parameters such as pH, salinity and dissolved oxygen were noted. The oven dried samples were subjected to the textural study by sieving and pipette method followed the Krumbein Pettijohn were analyzed and determined the microelements.

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### **INTRODUCTION**

Plants require air, water, light, temperature, soil and more than 40 elements to grow well. Out of this large number of elements 9 macroelements such as are Oxygen (O), Hydrogen (H), Carbon (C), Nitrogen (N), Phosphorus (P), Potassium (K), Calcium

(Ca), Magnesium (Mg), Sulphur (S) and 7 microelements such as Iron (Fe), Copper (Cu), Manganese (Mn), Boron (B), Molybdenum (Mo), Zink (Zn) and Chlorine (Cl) respectively are detected as essential for the growth and development of the plants.

As the science of chemistry progresses and the analytical techniques improved, as such the TABLE-



# OSMANIA UNIVERSITY

## MEMORANDUM OF MARKS

PA 254603

Ph.D. COURSE WORK SEPTEMBER 2018

Examination

REF NO.: 201926675

FACULTY OF SCIENCE

DATE: 22-06-2019

NAME: ALISHALA ASHOK

ROLL NO.: 900717540175

PARENT(S) NAME: ALISHALA RAJAIHAH

SL. NO.	SUBJECT NAME	UNIVERSITY EXAMINATION		RESULT
		MAXIMUM MARKS	MARKS SECURED	
	<b>ORGANIC CHEMISTRY</b>			
1	RESEARCH METHODOLOGY	100	56	PASS
2	SPECIALISATION (BROAD FIELD)	100	41	FAIL
TOTAL		200	97	
GRAND TOTAL		===	===	

TOTAL IN WORDS : \* NINE \* SEVEN \*

GRAND TOTAL AT THE END OF THE COURSE =

RESULT: **FAILED**

MINIMUM PASS MARKS: FIFTY

CLERK-INCHARGE

SUPERINTENDENT

CONTROLLER OF EXAMINATIONS



# OSMANIA UNIVERSITY

## MEMORANDUM OF MARKS

PA 255166

Examination Ph.D. COURSE WORK AUGUST 2019

REF NO.: 2019603

FACULTY OF SCIENCE

DATE: 31-08-2019

NAME: ALISHALA ASHOK

ROLL NO.: 900717540175

PARENT(S) NAME: ALISHALA RAJAJIAH

SL. NO.	SUBJECT NAME	UNIVERSITY EXAMINATION		RESULT
		MAXIMUM MARKS	MARKS SECURED	
1	ORGANIC CHEMISTRY SPECIALIZATION (BROAD FIELD)	100	53	PASS
TOTAL		100	53	
GRAND TOTAL		---	---	

TOTAL IN WORDS: \* FIVE \* THREE \*

GRAND TOTAL AT THE END OF THE COURSE: =====

RESULT: COMPLETED

MINIMUM PASS MARKS:FIFTY

CLERK-IN-CHARGE

SUPERINTENDENT

CONTROLLER OF EXAMINATIONS



**COPPER (II) ACETATE CATALYSED SYNTHESIS OF NOVEL 6-(2-CHLORO-4-FLUOROPHENYL)-9-PHENYL-[1,2,4] TRIAZOLO[4,3-a][1,8]NAPHTHYRIDINE DERIVATIVES UNDER MICROWAVE IRRADIATION AND THEIR BIOLOGICAL AND MOLECULAR DOCKING STUDIES**

**Alishala Ashok, Boda Sakram\***

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**ABSTRACT;**

An efficient, simple and eco-friendly synthetic route has been developed for the construction of 6-(2-chloro-4-fluorophenyl)-9-phenyl-[1,2,4]triazolo[4,3-a][1,8]naphthyridine derivatives using Cu(OAc)<sub>2</sub> catalyst under microwave irradiation successfully accomplished (**7a-h**) with good yields (85-94%). The molecular structures of the compounds confirmed by IR, <sup>1</sup>H NMR, <sup>13</sup>C NMR and mass spectral data as well as elemental analyses studies. All synthesized compounds evaluated for their antimicrobial activity. Among them compounds **7c** and **7h** showed high antibacterial and antifungal activities. In silico studies have proved that compounds **7c** and **7h** have strong binding affinity.

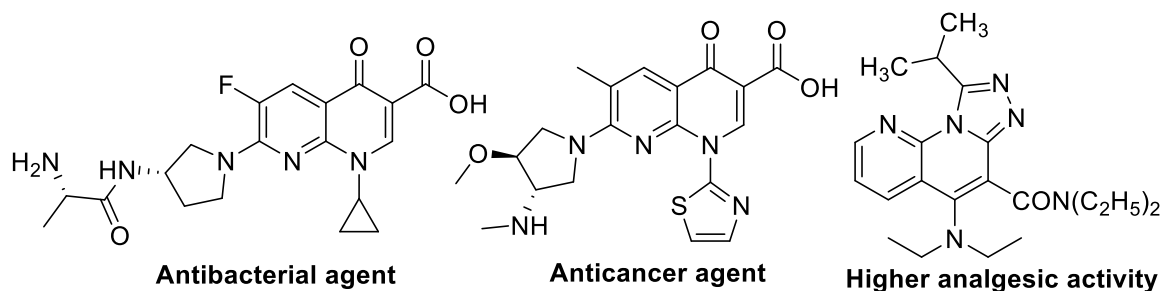
**KEYWORDS:** [1,8]naphthyridines, Cu(OAc)<sub>2</sub>, microwave irradiation, antimicrobial activity, molecular docking studies.

**INTRODUCTION**

Heterocyclic compounds containing 1,8-naphthyridine moiety are interesting as prospective biologically active substance and these are centre of attraction for the synthetic organic researcher and medicinal chemists because of the 1,8-naphthyridine group of products have gained special concentration of researchers on account of their demonstrating a variety of interesting biological activities that include anti-inflammatory<sup>i</sup>, antibacterial<sup>ii,iii</sup> antioxidant<sup>iv</sup> anti-HIV<sup>v</sup> anti-allergic,<sup>vi</sup> anticancer,<sup>vii</sup> anti-malarial,<sup>viii</sup> anti-micobacterial activity.<sup>ix</sup> A number of other remarkable applications have also been reported in the literature, for example potent inhibition of protein kinase C isozymes,<sup>x</sup> discriminatory inhibition of p38 mitogen-activated protein kinase,<sup>xi</sup> Acyl-CoA:cholesterolacyltransferase (ACAT) inhibitory activity<sup>xii</sup>.

1,8-Naphthyridine derivatives have also exhibited potential applications in neurological disorders such as Alzheimer's disease<sup>xiii</sup>. In recent year microwave assisted organic reaction has emerged as new tool in organic synthesis and significant advantages include that remarkably accelerated the reaction rate and decrease reaction time and enhancement the yield..<sup>xiv, xv</sup> Some of the medicinally potent 1,8-naphthyridine derivatives are shown in **Fig 1**.



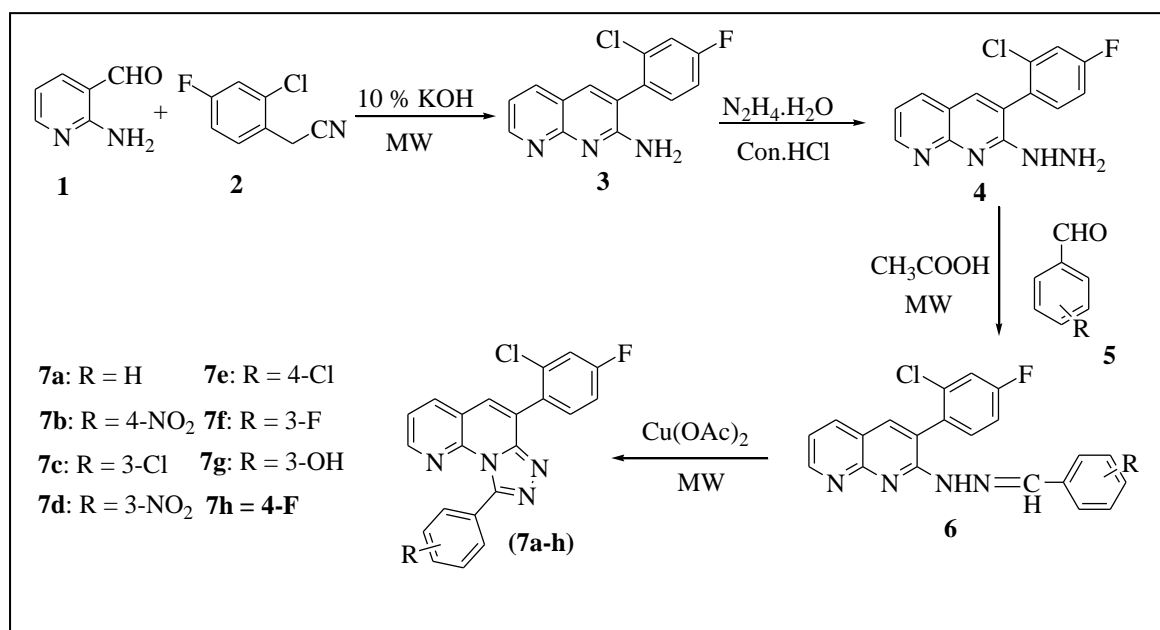


We have investigated a simple, convenient, and eco friendly process for the construction of 6-(2-chloro-4-fluorophenyl)-9-phenyl-[1,2,4]triazolo[4,3-a][1,8]naphthyridine derivatives. To the best of our knowledge there is no microwave method reported in the literature for these (7a-h) compounds using Copper (II) acetate catalyst under microwave irradiation.

## RESULTS AND DISCUSSION

A representation for the formation of 6-(2-chloro-4-fluorophenyl)-9-phenyl-[1,2,4]triazolo[4,3-a][1,8]naphthyridine derivatives (**7a-h**) catalyzed by  $\text{Cu}(\text{OAc})_2$  is shown in **Scheme 1**. To develop eco-friendly methodology we have utilized cheap and non-toxicity of the reagent Copper (II) acetate  $\text{Cu}(\text{OAc})_2$  through microwave irradiation method. The experimental procedure for these reactions is remarkably simple, short reaction times and does not require the use of expensive catalysts is significant improvement of this process.

**Scheme 1.**  $\text{Cu}(\text{OAc})_2$  catalyzed synthesis of 6-(2-chloro-4-fluorophenyl)-9-phenyl-



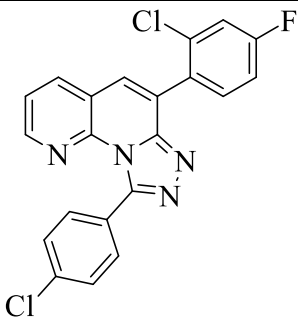
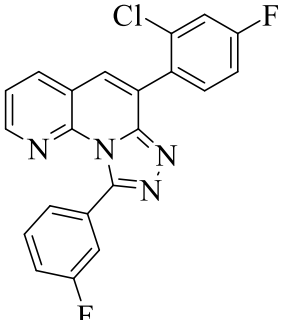
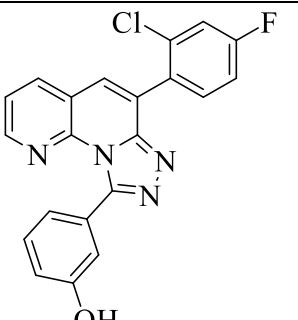
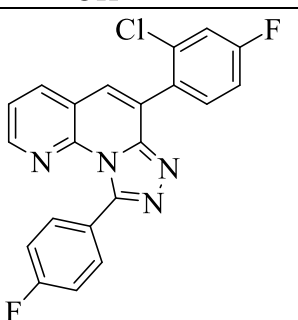
[1,2,4]triazolo[4,3-a][1,8]naphthyridine derivatives.

The reaction proceeds *via* Friedlander condensation of 2-aminonicotinaldehyde **1** with appropriate active methylene compound 2-(2-chloro-4-fluorophenyl)acetonitrile **2** in the presence of 10% KOH without any solvent under MW irradiation yielded 3-(2-chloro-4-fluorophenyl)-1,8-naphthyridin-2-amine **3**. Then compound **3** reacted with hydrazine hydrate in the presence of catalytic amount of Conc. HCl obtained 3-(2-chloro-4-fluorophenyl)-2-hydrazinyl-1,8-naphthyridine derivative **4**. In the presence of acetic acid various aromatic aldehydes reacted with compound **4** formed the corresponding compounds (E)-2-(2-

benzylidenehydrazinyl)-3-(2-chloro-4-fluorophenyl)-1,8-naphthyridines (**6a-h**), then in the presence of Cu(OAc)<sub>2</sub> **Copper (II) Acetate** intramolecular cyclization occurred and formed the 6-(2-chloro-4-fluorophenyl)-9-phenyl-[1,2,4]triazolo[4,3-a][1,8]naphthyridine derivatives (**7a-h**) with good yields in short reaction time.

**Table 1** Synthesis of 6-(2-chloro-4-fluorophenyl)-9-phenyl-[1,2,4]triazolo[4,3-a][1,8]naphthyridine derivatives (**7a-h**).

Entry	Analog	Aldehyde	Products	Time (m)	Yield <sup>a</sup> (%)
1	<b>7a</b>	Benzaldehyde		3	87
2	<b>7b</b>	4-Nitrobenzaldehyde		3.5	85
3	<b>7c</b>	3-Chlorobenzaldehyde		2.5	82
4	<b>7d</b>	3-Nitrobenzaldehyde		4	88

5	7e	4-Chlorobenzaldehyde		3.5	81
6	7f	3-Fluorobenzaldehyde		2.5	84
7	7g	3-Hydroxybenzaldehyde		4	87
8	7h	4-Fluorobenzaldehyde		3.5	94

<sup>a</sup>Isolated yields after purification

The reaction proceeds proficiently with very good yields in microwave condition and the reaction is clean and devoid of any by products. The products were formed with an elevated quantity of purity by this method. All the newly synthesized compounds were confirmed by IR, <sup>1</sup>H NMR and mass spectral data as well as elemental analyses studies.

The reaction proceeds efficiently in very good yields in mortar and pestle grinding and the reaction is clean and devoid of any by-products.

#### **BIOLOGICAL ACTIVITIES (ANTIBACTERIAL AND ANTIFUNGAL ACTIVITIES)**

**Antibacterial activity:** All these newly synthesized products (**7a–h**) were evaluated for their *in vitro* antibacterial activity against the Gram-positive bacteria *S. Epidermidis* and Gram-negative bacteria *Escherichia coli* at three diverse concentrations using standard reference

drug Amoxicillin. The products activity was tested by agar well diffusion procedure according to the developed earlier method<sup>xvi</sup>. All compounds displayed high inhibition activity, particularly

**7c** and **7h** demonstrated the highest antibacterial activity against all the tested strains (Table 2).

**Antifungal activity:** All the synthesized products (**7a–h**) were screened for their antifungal activity against two pathogenic fungal strains *Aspergillusniger* and *Candida metapsilosis* using standard reference drug Grieseofulvin. Activity was tested by using the disc diffusion technique <sup>xvii</sup>. All the compounds revealed high inhibition activity against the pathogenic fungal strains. Compounds **7c** and **7h** exhibited the highest antifungal activity (Table 2).

**Table 2** Antimicrobial activity screening data of the synthesized products (**7a–h**)

Compounds	Bacterial strains						Fungal strains					
	<i>S. epidermidis</i> (conc.in µg/mL)			<i>E. coli</i> (conc.in µg/mL)			<i>A. niger</i> (conc.in µg/mL)			<i>C.Metapsilosis</i> (conc. in µg/mL)		
	10	20	30	10	20	30	10	20	30	10	20	30
7a	3	4	7	3	5	9	5	7	11	5	9	12
7b	5	6	10	4	6	7	6	8	11	7	11	12
<b>7c</b>	<b>7</b>	<b>9</b>	<b>14</b>	<b>8</b>	<b>11</b>	<b>15</b>	<b>8</b>	<b>11</b>	<b>12</b>	<b>9</b>	<b>12</b>	<b>15</b>
7d	4	6	8	4	8	10	6	9	10	6	9	12
7e	6	8	9	5	9	11	5	8	12	7	10	11
7f	4	9	12	6	9	12	7	9	11	6	11	12
7g	5	8	9	5	8	10	6	9	12	6	9	11
<b>7h</b>	<b>7</b>	<b>11</b>	<b>16</b>	<b>9</b>	<b>12</b>	<b>14</b>	<b>9</b>	<b>12</b>	<b>15</b>	<b>9</b>	<b>12</b>	<b>16</b>
<b>Amoxicillin</b>	<b>10</b>	<b>14</b>	<b>18</b>	<b>12</b>	<b>15</b>	<b>17</b>	-	-	-	-	-	-
<b>Grieseofulvin</b>	-	-	-	-	-	-	<b>9</b>	<b>12</b>	<b>16</b>	<b>10</b>	<b>12</b>	<b>16</b>

**Molecular Docking Studies:** Auto Dock 4.0 suite was used as a molecular-docking<sup>xviii</sup> software for performing computerized docking of ligands to their macromolecular receptors. In the present study we used semi-flexible docking protocols. The three dimensional structure development of orally active 6-(2-chloro-4-fluorophenyl)-9-phenyl-[1,2,4]triazolo[4,3-a][1,8]naphthyridines as a potent Pde10inhibitor for the management of schizoprenia [PDB:3UI7] was obtained from Protein Data Bank (PDB)<sup>xix</sup>. The target protein, phosphodiesterase type 10(PDE10), was kept as rigid. The ligands being docked were set flexible, in order to discover an arbitrary number of torsional degrees of freedom in addition to the six spatial degrees of freedom spanned by the translational and rotational parameters. The Graphical User Interface program “Auto Dock Tools” was used to prepare, run, and analyze the docking simulations. Kollman united atom charges, salvation parameters and polar hydrogens were added into the receptor PDBfile (PDB ID: 3UI7) for preparation of protein indocking. This PDE10 enzyme structure did not have any water molecules and/or ligands to remove from its PDB file and make a free receptor. Since ligands were not peptides, Gasteiger charge was assigned and then non polar hydrogens were merged. Auto Grid 4.0Program, supplied with Auto Dock 4.0, was used to produce grid maps. Compounds **5c–5e** exhibited efficient interactions (Table 3 and Fig. 2, and 3).

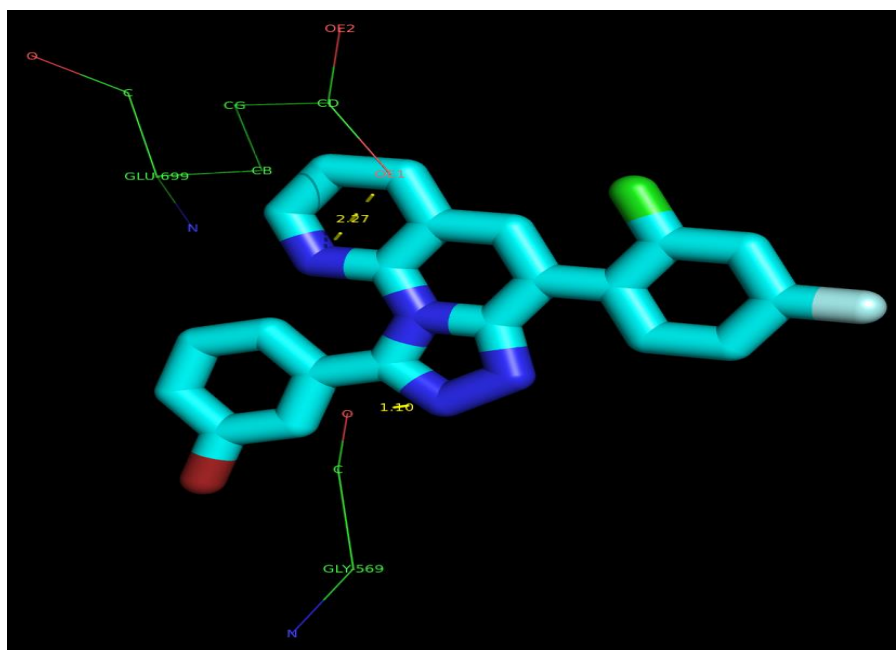


Fig .2 Binding mode of the synthesized molecule 7c molecule

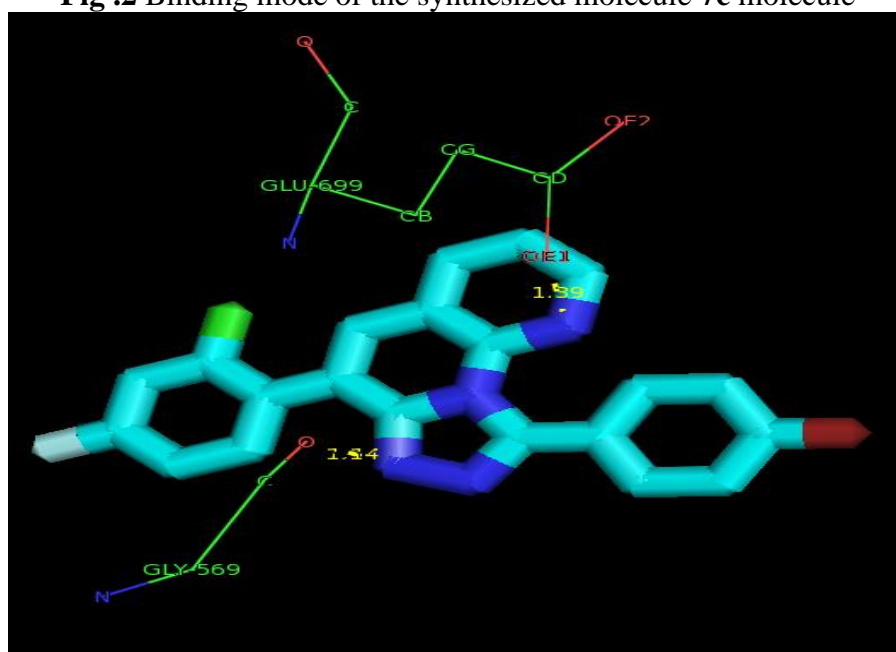


Fig .3 Binding mode of the synthesized molecule 7h molecule.

Table 3 Atoms involved in the interactions.

Analog	Receptor 3UI7 (Interacting atoms)	Ligand (Atoms)	H-bond Distance (Å°)	Docking energy (Kcal/mol)
7a	LY569O	NH	1.09	-87.6985
	GLU695OE2	NH	2.00	
7b	ASP674O	NH	2.93	-75.6218
	HIS525NE2	O	3.10	
7c	GLY569O	NH	1.10	<b>-88.7253</b>
	<b>GLU699OE1</b>	<b>NH</b>	<b>2.97</b>	

7d	TYR5240	NH	2.98	-79.8844
7e	GLY5690	O	1.15	-86.2321
	GLU699OE1	NH	2.14	
7f	GLY5690	NH	1.13	-77.8808
7g	GLY5690	NH	1.17	-85.2347
	GLU699OE1	NH	1.49	
7h	GLY5690	NH	1.14	<b>-87.8386</b>
	<b>GLU699OE1</b>	<b>NH</b>	<b>2.91</b>	

**EXPERIMENTAL** All the reagents and chemicals were purchased from Aldrich and used without further purification. Purity of the molecules was checked by F<sub>254</sub> silica-gel precoated TLC plates using hexane and ethyl acetate (7:3) as eluent. The melting points were resolute in an open capillary tube with a Buchi melting point apparatus and are uncorrected. <sup>1</sup>H NMR spectra were recorded on Bruker 400 MHz spectrometer using DMSO-*d*<sub>6</sub> as solvent. Mass spectra were recorded on ESI mass spectrometer. IR spectra were recorded with Bruker Tensor 27 series FT-IR spectrophotometer in KBr disks. Microanalyses were performed on a Carlo-Erba model EA1108 analytical unit.

**General procedure for the synthesis of 3-(2-chloro-4-fluorophenyl)-1,8-naphthyridin-2-amine (3)**

**Typical procedure via Microwave irradiation:** A mixture of **1** (1 mmol, 122.12 mg) active methylene compound **2** (1 mmol) and 10% KOH (5 drops) was exposed to MW irradiation at 200W intermittently at 30 sec for 2.0 min. On completion of the reaction, as monitored by TLC, the reaction mixture was cooled and treated with chilled water. The solid that separated was filtered, washed with water and purified by recrystallization from methanol to afford **3**.

**General procedure for the synthesis of 3-(2-chloro-4-fluorophenyl)-2-hydrazinyl-1,8-naphthyridine (4)**

3-(2-chloro-4-fluorophenyl)-1,8-naphthyridin-2-amine (1 mmol) **3** reacted with an excess of 80% hydrazine hydrate and Con HCl under microwave condition formed desired product **4**.

**General procedure for the synthesis of (E)-2-(2-benzylidenehydrazinyl)-3-(2-chloro-4-fluorophenyl)-1,8-naphthyridine (6)**

In the presence of acetic acid (15 mol%) 3-(2-chloro-4-fluorophenyl)-2-hydrazinyl-1,8-naphthyridine(**4**) reacted with aromatic aldehyde (1,mmol) obtained the products **6a-h**. On the completion of reaction (monitored by TLC) the mixture was poured into ice-cold water then resulting solid product was filtered, washed with water and purified by recrystallization from ethanol to furnished compound **6**.

**General procedure for the synthesis of 6-(2-chloro-4-fluorophenyl)-9-phenyl-[1,2,4]triazolo[4,3-a][1,8]naphthyridine derivatives(7a-h)**

Compound **7** (0.01 mol) and Cu(OAc)<sub>2</sub> (0.01 mol) were mixed thoroughly and exposed to MW at 800W intermittently at 30 sec intervals for the specified time (**Table I**). After complete conversion as indicated by TLC, the reaction mixture was cooled and treated with methanol (20 mL). The methanol solution was poured into ice cold water (40mL), the separated solid product was filtered and purified by re-crystallization from ethanol to obtained products (**7a-h**).

**6-(2-chloro-4-fluorophenyl)-9-phenyl-[1,2,4]triazolo[4,3-a][1,8]naphthyridine (7a)**

M.p.: 184-186 °C; IR: 1638 (C=C), 1591, (C=N), 1015 (C-F); 818 (C-Cl); cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ 9.3 (s, 1H), 9.19 (s, 1H), 8.92-8.7 (d, 2H, J = 7.2 Hz), 8.6-8.4 (d, 2H, J = 7.6 Hz), 7.97-7.70 (m, 6H). <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>): δ 158, 155, 153, 149,

147, 144, 140, 138 (2C), 137, 136, 135, 130(2C), 124, 118. ESI-MS:  $m/z$ 375.07 [M+H]<sup>+</sup> Anal. Calc. For C<sub>21</sub>H<sub>12</sub>ClFN<sub>4</sub>: C, 67.30; H, 3.23; N, 14.95; Found: C, 67.41; H, 3.19; N, 14.87; %.

**6-(2-chloro-4-fluorophenyl)-9-(4-nitrophenyl)-[1,2,4]triazolo[4,3-a][1,8]naphthyridine (7b)**  
M.p.: 240-242 °C; IR: 1638 (C=C), 1426, (C=N), 1015 (C-F); 915 (C-Cl); cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ 9.18-9.12 (s, 1H), 8.6-8.5 (m, 3H), 8.2-8.19 (m, 2H), 8.0-7.98 (m, 3H), 7.98-7.86 (m, 3H); <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>): δ 158.3, 155.6, 153.2, 149.4, **145.6**, **144.3**, 140.3, 138 (2C), 137, 132 2C, 129 2C, 122, 118. ESI-MS:  $m/z$ 420.06 [M+H]<sup>+</sup> Anal. Calc. For C<sub>21</sub>H<sub>11</sub>ClFN<sub>5</sub>O<sub>2</sub>: C, 60.08; H, 2.64; N, 16.68; Found: C, 60.13; H, 2.69; N, 16.63; %.

**6-(2-chloro-4-fluorophenyl)-9-(3-chlorophenyl)-[1,2,4]triazolo[4,3-a][1,8]naphthyridine (7c)**

M.p.: 218-220 °C; IR: 1655 (C=C), 1605, (C=N), 959 (C-F); 854 (C-Cl); cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ 9.28 (s, 1H), 8.9-8.6 (m, 2H), 8.31-8.27 (m, 3H), 8.10-7.96 (m, 3H), 7.95-7.87 (m, 3H); <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>): δ 162, 158, 152, 148, 144, 139 (2C), 135, 130 (2C), 129, 127, 126, 118. ESI-MS:  $m/z$ 409.14 [M+H]<sup>+</sup> Anal. Calc. For C<sub>21</sub>H<sub>11</sub>Cl<sub>2</sub>FN<sub>4</sub>: C, 61.63; H, 2.71; N, 13.69; Found: C, 61.68; H, 2.76; N, 13.71; %.

**6-(2-chloro-4-fluorophenyl)-9-(3-nitrophenyl)-[1,2,4]triazolo[4,3-a][1,8]naphthyridine (7d)**

M.p.: 238-239 °C; IR: 1659 (C=C), 1606, (C=N), 951 (C-F); 857 (C-Cl); cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ 8.96 (s, 1H), 8.48-8.46 (d, 2H, J = 7.2 Hz), 8.16 (s, 1H), 7.93-7.81 (m, 2H), 7.71- 7.69 (m, 4H); <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>): δ 159, 156, 153, **152**, 141, 140, 138 (2C), 137, 136, 134, 130, 129, 126, 124, 118. ESI-MS:  $m/z$ 420.10 [M+H]<sup>+</sup> Anal. Calc. For C<sub>21</sub>H<sub>11</sub>ClFN<sub>5</sub>O<sub>2</sub>: C, 60.08; H, 2.64; N, 16.68; Found: C, 60.11; H, 2.69; N, 16.71; %.

**6-(2-chloro-4-fluorophenyl)-9-(4-chlorophenyl)-[1,2,4]triazolo[4,3-a][1,8]naphthyridine (7e)**

M.p.: 221-223 °C; IR: 1655 (C=C), 1606, (C=N), 957 (C-F); 854 (C-Cl); cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ 8.97 (s, 1H), 8.43 (s, 1H), 8.02 (d, 2H, J = 7.2 Hz), 7.91-7.87 (m, 3H), 7.24-7.21 (m, 4H); <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>): δ 158, 155, 151, 141, 140, 138 (2C), 137, 136, 133, 130, 129, 126, 123, 118. ESI-MS:  $m/z$ 409.14 [M+H]<sup>+</sup> Anal. Calc. For C<sub>21</sub>H<sub>11</sub>Cl<sub>2</sub>FN<sub>4</sub>: C, 61.63; H, 2.71; N, 13.69; Found: C, 61.69; H, 2.77; N, 13.74; %.

**6-(2-chloro-4-fluorophenyl)-9-(3-fluorophenyl)-[1,2,4]triazolo[4,3-a][1,8]naphthyridine (7f)**

M.p.: 212-214 °C; IR: 1661 (C=C), 1608, (C=N), 952 (C-F); 858 (C-Cl); cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ 9.21 (s, 1H), 8.8 (s, 1H), 8.43 (s, 1H), 7.83-7.51 (m, 5H), 7.23-7.17 (m, 3H). <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>): δ 162, 158, 153, 148 (2C), 142, 139, 136, 131, 129.7 (2C), 128, 126, 125, 118.; ESI-MS:  $m/z$ 393.12 [M+H]<sup>+</sup> Anal. Calc. For C<sub>21</sub>H<sub>11</sub>ClF<sub>2</sub>N<sub>4</sub>: C, 64.21; H, 2.82; N, 14.26; Found: C, 64.31; H, 2.89; N, 14.36; %.

**3-(6-(2-chloro-4-fluorophenyl)-[1,2,4]triazolo[4,3-a][1,8]naphthyridin-9-yl)phenol (7g)**

M.p.: 210-212 °C; IR: 1650 (C=C), 1609, (C=N), 957 (C-F); 858 (C-Cl); cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ 9.8 (s, 1H), 8.80 (s, 1H), 8.17 (s, 1H), 8.17 (s, 1H), 8.16-7.82 (m, 7H), 7.19- 6.97 (m, 2H); <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>): δ 159, 152, **148**, 147. (2C), 142, 140, 133, 132, 130 (2C), 129 (2C), 128, 127, 125, 118; ESI-MS:  $m/z$ 393.07 [M+H]<sup>+</sup> Anal. Calc. For C<sub>21</sub>H<sub>11</sub>ClF<sub>2</sub>N<sub>4</sub>: C, 64.21; H, 2.82; N, 14.26; Found: C, 64.34; H, 2.89; N, 14.21; %.

**6-(2-chloro-4-fluorophenyl)-9-(4-fluorophenyl)-[1,2,4]triazolo[4,3-a][1,8]naphthyridine(7h)**

Pale brown solid; M.p.: 175-176 °C; IR: 1657 (C=C), 1608, (C=N),957 (C-F); 856 (C-Cl);  $\text{cm}^{-1}$ .

$^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ ):  $\delta$  9.11 (s, 1H), 8.3 (s, 1H), 8.41 (s, 1H), 7.94-7.84 (m, 5H), 7.33-7.27 (m, 3H).  $^{13}\text{C}$  NMR (100 MHz, DMSO- $d_6$ ):  $\delta$  158, 155, 152, 148, 145,143, 142, 138 2C, 136, 132, 130, 129 (2C), 128, 118. ESI-MS:  $m/z$  393.07  $[\text{M}+\text{H}]^+$  Anal. Calc. For  $\text{C}_{21}\text{H}_{11}\text{ClF}_2\text{N}_4$ : C, 64.21; H, 2.82; N, 14.26; Found: C, 64.27; H, 2.92; N, 14.31; %.

**CONCLUSION:**

The  $\text{Cu}(\text{OAc})_2$  catalyzed expedient and eco-friendly method developed for the synthesis of 6-(2-chloro-4-fluorophenyl)-9-phenyl-[1,2,4]triazolo[4,3-a][1,8]naphthyridine scaffolds under microwave irradiation. Antimicrobial activity of the synthesized products is evaluated against pathogenic bacterial and fungal strains. Among these compounds **7c** and **7h** displayed the maximum activity. Molecular modeling studies proved that their strong binding affinity and H-bond interactions.

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# Green synthesis of substituted 1,8-naphthyridin-thiazole scaffolds, molecular docking studies and biological evaluation

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## Abstract

Eco-friendly construction of N-(5-(2-methyl-1,8-naphthyridine)-thiazole-benzamide and 5-(2-methyl-1,8-naphthyridine)-N-(3-aryl-1,8-naphthyridine-thiazole-2-amine derivatives under microwave method afforded good yields in short reaction time with maximum selectivity compared with conventional method in the presence of triethylamine and, Pd(PPh<sub>3</sub>)<sub>4</sub>. This route can assimilate the concept of green chemistry because reaction process is very squatter reaction time and enhanced energy efficiency. Synthesized molecules are tested for their antimicrobial activity; among them, **7e** and **7b** compounds have shown good results and molecular modeling evaluation has been done by considering docking scores, hydrogen bond interactions, affinity, and the short distance between ligand and receptor. In silico studies also good complimented for these results.

**Keywords** Green synthesis · 1,8-naphthyridin-3-yl)thiazol-2-yl)benzamides · Antimicrobial screening · Molecular docking studies

## Introduction

Nitrogen atoms consisting heterocyclic 1,8-naphthyridine moiety play an important function in the medicinal chemistry [1]. 1,8-naphthyridine and substituted naphthyridine molecules have a broad range of beneficial pharmacological applications. A number of noteworthy biological activities like that anti-inflammatory [2, 3] anti-tumor activity [4], anti-proliferative [5] and antioxidant activity [6]. In current years, microwave-supported synthetic organic reactions have become more attractive and

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AND THEIR BIOLOGICAL EVALUATION**

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