Memorandum of Understanding

Between

Dr. Devidas S. Bhagat
Assistant Professor,
Department of Forensic Chemistry,
Government Institute of Forensic Science,
Aurangabad 431 004,
MS, INDIA.

Dr. Bapu Thorat,
Assistant Professor,
Department of Chemistry,
Government Arts and Science College,
Aurangabad 431 004,
MS, INDIA.

Memorandum of Understanding is signed with the mutual agreement of both the representatives of institutes as per:

Article 1:

The subject at present Memorandum of Understanding is the establishment of an educational cooperation between Dr. Devidas S Bhagat, Assistant Professor, Department of Forensic Chemistry, Government Institute of Forensic Science, Aurangabad 431 004, and Dr. Bapu Thorat, Assistant Professor, Department of Chemistry, Government Arts and Science College, Aurangabad 431 004. MS, INDIA.

Article 2:

Following terms and conditions agreed upon by both the parties agreed to endeavor to cooperate

1. To undertake collaborative research activities leading to research analysis
2. To work in collaboration leading to research findings and subsequent publication
3. To accomplish joint academic and research related activities
4. To work jointly on particular research areas for research projects, etc.
5. There will be no financial obligations/liabilities on both institutions.

Article 3:

The present MoU is intended for the next three years from **28** September **2021.**

Dr. D. S. Bhagat
Assistant Professor
Dr. D. S. Bhagat
Assistant Professor, Class-I Gazetted
Government Institute of Forensic Science,
Aurangabad 431 004.

Govt. Institute of Forensic Sciences Aurangabad सत्यमेव जयते

Dr. Bapu Thorat,
Assistant Professor
Dr. BAPU R. THORAT
M.E.S. Class-1
Government College of Arts
And Science, Aurangabad

Director
Govt. Institute of Forensic Science
Aurangabad.

Date:

TO WHOM IT MAY CONCERN

This is to certify, that there have been collaborative research activities between faculty members of *Government Institute of Forensic Science, Nipatniranjan Nagar, Caves Road, Aurangabad-431004* and *Dr. Bapu Thorat, Assistant Professor, Department of Chemistry, Government Arts and Science College, Aurangabad 431 004. MS, INDIA.*. The details of the collaborative research activities carried out are as follows:

Collaborators:

1. Dr. Bapu Thorat, Assistant Professor, Department of Chemistry, Government Arts and Science College, Aurangabad 431 004. MS, INDIA.

Between

2. Dr. Devidas S. Bhagat, Assistant Professor. Department of Forensic Chemistry. Government Institute of Forensic Science. Nipatniranjan Nagar. Caves Road. Aurangabad-431004, MS, India.

It is hence certified that there have been successful collaboration in term of research and resulted in the research paper publication during *2021-22.*

No. of Publications: **04**

Dr. Devidas S. Bhagat
Assistant Professor.
Dr. D. S. Bhagat
Assistant Professor, Class-I Gazetted
Government Institute of Forensic Science,
Aurangabad - 431 004.

Dr. Bapu Thorat
Assistant Professor
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Govt. Institute of Forensic Sciences ★ Aurangabad ★ सत्यमेव जयते

Director
Govt. Institute of Forensic Science
Aurangabad.

Following are the list of the publications;

Academic Year 2021-22

1. Thorat, Bapu, Vipul P. Purohit, Ramesh Yamgar, Devidas Bhagat, Swati Wavhal, and Suraj N. Mali. "Structural Insight into 2-Aryl-4-Quinoline Carboxylic Acid-Based Dihydroorotate Dehydrogenase (DHODH) and its Potential Anti-SARS-CoV-2 Activity through Pharmacophore Modeling, Multidimensional QSAR, ADME, and Docking Studies." *Physical Chemistry Research* 11, no. 4 (2023): 783-800
2. Chavan, Vilas A., Devidas S. Bhagat, Ajit K. Gangawane, Himani P. Khawashi, and Bapu R. Thorat. "Bimetallic Nanomaterials-Based Electroanalytical Methods for Detection of Pesticide Residues." (2022).
3. Thorat, Bapu R., Suraj N. Mali, Swati S. Wavhal, Devidas S. Bhagat, Ravikumar M. Borade, A. Chapolikar, Ajaykumar Gandhi, and Pawan Shinde. "L-Proline: A Versatile Organo-Catalyst in Organic Chemistry." *Combinatorial chemistry & high throughput screening* (2021).
4. Bhosale, Dinesh, Suraj N. Mali, Bapu R. Thorat, Swati S. Wavhal, Devidas S. Bhagat, and Ravikumar M. Borade. "Synthesis, Molecular Docking, and In vitro Antimycobacterial Studies on N'-arylidene-4-nitrobenzohydrazides." *Recent Advances in Anti-Infective Drug Discovery Formerly Recent Patents on Anti-Infective Drug Discovery* 17, no. 1 (2022): 69-83.

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Recent Patents on Anti-Infective Drug Discovery, 2022, *17*, 1-15

SHORT COMMUNICATION

Synthesis, Molecular Docking, and *In vitro* Antimycobacterial Studies on N'-arylidene-4-nitrobenzohydrazides

Dinesh Bhosale[1], Suraj N. Mali[2], Bapu R. Thorat[3,*], Swati S. Wavhal[1], Devidas S. Bhagat[4] and Ravikumar M. Borade[4]

[1]*Department of Chemistry, Government of Maharashtra's Ismail Yusuf College of Arts, Science and Commerce, Mumbai-410060 (MS), India;* [2]*Department of Pharmaceutical Sciences and Technology, Birla Institute of Technology, Mesra (835215), India;* [3]*Department of Chemistry, Government of Maharashtra, Government College of Arts and Science, Aurangabad-431001 (MS), India;* [4]*Department of Chemistry, Government Institute of Forensic Science, Aurangabad-431004, (MS), India*

Abstract: ***Background*:** *Mycobacterium tuberculosis (Mtb)* is an organism that causes tuberculosis (TB). In 2019, 10 million individuals worldwide contracted tuberculosis, with 1.4 million people dying from the disease each year (World Health Organization, 2021). Hydrazones-hydrazide-based drugs have been shown to be bactericidal against M. tuberculosis replication.

***Objectives*:** We herein intended to synthesize a series of acid hydrazones (**3a-3l**) by condensing 4-nitrobenzohydrazine with substituted aromatic acids in ethanol at room temperature.

***Materials and Methods*:** All newly synthesized compounds were characterized by standard spectroscopic techniques. Synthesized compounds were then tested for anti-mycobacterial activity against H37Rv strains. Molecular docking analysis was performed for three crystal structures of 1ENY, 1TED and 2FUM *Mycobacterium tuberculosis* receptors.

***Results*:** Among all tested molecules, **3i** (MIC: **50** µg/mL) and **3b** (MIC: **50** µg/mL) were found to be the best ligands for further development of new anti-TB drug. We found that our proposed molecules have higher docking scores, corresponding standard anti-TB agents, such as ciprofloxacin and isoniazid. Synthesized compounds were found to have drug-likeness properties when tested with Lipinski's filter for drug-likeness.

***Conclusion*:** Our current study proposes N'-arylidene-4-nitrobenzohydrazides as anti-TB agents. Agents with such system can be developed in future for development into active lead molecules.

ARTICLE HISTORY

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Keywords: Acid hydrazones, 4-nitrobenzohydrazide, molecular docking, 1ENY, 1TED, 2FUM.

1. INTRODUCTION

Tuberculosis (TB) is a disease caused by the bacteria Mycobacterium tuberculosis (Mtb) [1]. Lack of effective treatment can exacerbate symptoms while also increasing mycobacterial resistance to currently available antibiotics. Due to the socio-economic fragility of patients, the developing antibiotic resistance of Mtb strains, and the high number of annual deaths worldwide, this highly contagious disease is now considered a global emergency [2].

Acyl hydrazones are an old class of imine-based molecules. The first molecule of N-acylhydrazines was reported in 1850 and after that

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Combinatorial Chemistry & High Throughput Screening, XXXX, *XX*, 000-000

REVIEW ARTICLE

L-Proline: A Versatile Organo-Catalyst in Organic Chemistry

Bapu R. Thorat[1*], Suraj N. Mali[2*], Swati. S. Wavhal[3], Devidas S. Bhagat[4], Ravikumar M. Borade[4], A. Chapolikar[1], Ajaykumar Gandhi[1] and Pawan Shinde[1]

[1]*Government of Maharashtra, Government College of Arts and Science, Aurangabad - 431001 (MS), India;* [2]*Department of Pharmaceutical Sciences and Technology, Birla Institute of Technology, Mesra, India;* [3]*Department of Chemistry, Government of Maharashtra's Ismail Yusuf College of Arts, Science and Commerce, Mumbai - 410060 (MS), India; d.* [4]*Department of Chemistry, Government Institute of Forensic Science, Aurangabad 431 004, (MS), India*

ARTICLE HISTORY

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Abstract: ***Background*:** L-proline is a natural amino acid having secondary amine functionality and acts as a bifunctional catalyst (organo-catalyst). The amino-functional group acts as Lewis base type while carboxylic acids act as Brønsted acid type catalysts. It catalyzed different asymmetric syntheses, including known reactions such as Aldol condensation, Mannich reaction, Michael Addition, Knoevenagel condensation, Hantzsch synthesis, OXA-Michael Henry tandem, Ullmann reactions, Wieland-Miescher ketone synthesis, Robinson annulation, Biginelli reaction, α-amination. It is also an essential catalyst for synthesizing heterocyclic skeletons such as coumarin, spiro-oxindoles, imidazoles, benzimidazoles, quinoxalines, podophyllotoxin, benzothiazoles, isoxazolidines, phenothiazines, aziridine, indole, 1,5-benzodiazepines, pyridine, and quinazolines.

***Objective*:** In this review, we had the objective to critically summarize the use of proline and proline derivatives as catalysts of multicomponent reactions performed in various media and leading to synthetically and biologically relevant heterocycles, a very important class of compounds that constitutes over 60% of drugs and agrochemicals.

***Methods*:** All scholarly articles for L-Proline catalyzed reactions were retrieved from ScienceDirect, Google Scholar , PubMed, etc.

***Results and Conclusion*:** Given the importance of L-Proline based reactions, it has been observed to have tremendous applications in organic chemistry. It can also act as a 'Green catalyst'.

Keywords: L-proline, organo-catalyst, amino acids, bifunctional catalyst, asymmetric synthesis.

1. INTRODUCTION

Asymmetric metal catalysis has been widely explored in various fields such as materials science, medicinal chemistry, etc. and proved to be essential during the synthesis of newer molecules with higher catalytic efficiency. Moreover, "asymmetric organocatalysis" involves the use of organic compounds for such kinds of reactions. Thus, in consideration of the same organic catalyst, L-proline, a naturally occurring cyclic α-amino acid, has proved its significance in the past several decades to date [1]. From a recent literature survey, it has also been seen that various nanostructure-based catalysts have been explored for various organic reactions [2a-2e].

There are several structural features of L-proline that make it more beneficial as an organo-catalyst. Multiple catalytic roles of L-proline are due to various structural features, as shown in Fig. (1). It is the only natural amino acid having a secondary amine functionality, which raises the pKa value and better nucleophilicity of this amino acid compared to other amino acids. The L-proline is considered a bifunctional catalyst, i.e., it behaves as both Brønsted acid or base or shows both behaviors during a mechanism. The high stereoselectivity of this catalyst is well known. The feature of covalent catalysis is also shown by the nitrogen atom of the proline. In general, the presence of adjacent amino and carboxylic acid groups makes it an excellent chelating agent and therefore forms metal chelate in metal-catalyzed reactions. It is not the only catalyst for organic conversions, but it still seems the best for many organic conversions.

L-proline and its derivatives or salt are easy to handle, have excellent solubility, are cost-effective, nontoxic, and experimentally have simplicity. Most of the L-proline catalyzed reactions are carried out at room temperature, i.e., L-proline catalyzed reactions have a modest energy requirement, which is another advantage of such reactions. It is used for high stereoselective transitions, possibly due to its formation of well-organized transition states between proline

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Regular Article

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Structural Insight into 2-Aryl-4-Quinoline Carboxylic Acid-Based Dihydroorotate Dehydrogenase (DHODH) and its Potential Anti-SARS-CoV-2 Activity Through Pharmacophore Modeling, Multidimensional QSAR, ADME, and Docking Studies

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(Received 12 October 2022, Accepted 12 November 2022)

Dihydroorotate dehydrogenase (DHODH) is a rate-limiting enzyme in the biosynthesis of pyrimidine, which catalyzes the oxidation of dihydroorotate to orotate. Uridine monophosphate is biosynthesized by orotate. DHODH inhibitors have been shown to have antiviral activity against cytomegalovirus, Ebola, influenza, Epstein-Barr virus, and picornavirus. The anti-SARS-CoV-2 activity of DHODH inhibitors has also been investigated. DHODH inhibitors, including leflunomide and its metabolite teriflunomide, have been found to have anti-SARS-CoV-2 activity. In relation to the importance of this enzyme (*i.e.*, DHODH) in drug design, the present study aimed to develop statistically robust and interpretable 2D- and 3D-quantitative structure-activity relationship (QSAR) models based on a dataset of 92 molecules of biologically active 2-aryl-4-quinoline carboxylic acid analogs, reported as DHODH inhibitors. The correlation coefficient (R^2) values of the training set of the partial least squares (PLS) and all five Kernel-based PLS models for the respective fingerprints were found to be 0.7091, 0.8336 (linear), 0.7586 (radial), 0.8606 (dendritic), 0.6832 (desc), and 0.7670 (Molprint 2D), respectively ($R^2 \approx 0.9$). However, the external validation coefficient (Q^2) values of the test set were found to be 0.7009, 0.7503 (linear), 0.7737 (radial), 0.8250 (dendritic), 0.6756 (desc), and 0.7533 (Molprint 2D), respectively ($Q^2 > 0.6$). The developed 4-point pharmacophore model (ARRR_1), with one hydrogen bond acceptor and three aromatic rings, was found to be crucial in preserving the activity of 2-aryl-4-quinoline carboxylic acid analogs as DHODH inhibitors. Furthermore, the molecular docking of DHODH inhibitors against SARS-CoV-2 target proteins revealed the significant role of DHODH inhibitors.

Keywords: Dihydroorotate dehydrogenase, Molecular modeling, QSAR, CADD, Structural features, 2-Aryl-4-quinoline carboxylic acid analogs

INTRODUCTION

Dihydroorotate dehydrogenase (DHODH), as an iron-containing flavin-dependent enzyme found in the inner membrane of mitochondria, is the most researched and distinct therapeutic target among several viral agents [1]. Dihydroorotate was converted to orotate by the fourth enzyme for the de novo pyrimidine biosynthetic process [2]. These pyrimidines are necessary for the production of certain phospholipids and nucleic acids, such as RNA and DNA [2]. De novo synthesis and salvage are the two main mechanisms for the biosynthesis of pyrimidines.

Pyrimidines are biosynthesized *via* the salvage synthesis pathway in resting or fully differentiated cells whereas highly proliferative cells, such as tumor cells, where the demand for

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Review
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Bimetallic Nanomaterials-Based Electroanalytical Methods for Detection of Pesticide Residues

Vilas A. Chavan [1,2,3], Devidas S. Bhagat [2,*], Ajit K. Gangawane [3], Himani P. Khawashi [4], Bapu R Thorat [5]

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Abstract: The application of bimetallic nanoparticles-based electroanalytical techniques in forensic science for pesticide detection residues in various exhibits are the emphasis of this review paper. Although many pesticide detection methods have been developed, nanomaterial-based electroanalytical methods have several benefits, including rapid analysis, cost-effective analysis, downsizing to increase performance, and field deployability. Bimetallic nanoparticles such as gold, platinum, palladium, nickel, and iron-based nanomaterials have been widely used as electrode modification agents for electrocatalytic activities and the synergistic impact of two different metals in a single probe. This review first outlined the applicability of electroanalytical techniques based on the bimetallic sensor for detecting pesticide residue. To assess existing applications and use of bimetallic nanoparticles for pesticide detection, selected studies with sensitivity, the limit of detection (LOD), and analytical application were examined. Finally, the existing difficulties and possible prospects in pesticide detection employing electroanalytical methods were explored.

Keywords: pesticide; bimetallic nanoparticles; electroanalytical; forensic applications.

1. Introduction

Forensic science deals with the recognition, identification, individualization, and reconstruction of physical evidence collected from the crime scene and finding the truth on the alleged matter by applying theories, principles, laws, and techniques of all the basic sciences in crime scene investigation [1]. Forensic technology is the study, inspection, and identification of clue materials at crime scenes that establish clear connections to offenders and facilitate their quick capture. Forensic evidence is crucial for identifying offenders through examinations at crime sites and related forensic exhibits before a court ruling. Additionally, it's a better way to maintain accurate records of the clue materials against the accused [2].