

TRENDS IN MEDICINAL AND ENVIRONMENTAL SCIENCE: AN INTRODUCTION

Editors:

Dr. Iqbal Azad

Department of Chemistry, Integral University, Lucknow

Dr. Jamal Akhtar Ansari

Department of Chemistry, Integral University, Lucknow

Prof. Malik Nasibullah

Department of Chemistry, Integral University, Lucknow

Prof. Abdul Rahman Khan

Department of Chemistry, Integral University, Lucknow



No part of this publication may be reproduced, transmitted, or stored in a retrieval system, in any form or by any means, electronic, mechanical, photocopying, recording, or otherwise, without the prior permission of the author.

Published by: Book Rivers

Website: - <https://www.bookrivers.com>

Email: publish@bookrivers.com

1st Print Edition - 2026

Copyright©: Editors

Title: Trends In Medicinal and Environmental Science: An Introduction

Editors: Dr. Iqbal Azad, Dr. Jamal Akhtar Ansari, Prof. Malik Nasibullah, Prof. Abdul Rahman Khan

All Rights Reserved

ISBN: 978-93-6884-737-3

MRP: 370/-INR

(Printed in India)

TABLE OF CONTENTS

S. NO.	CHAPTER TITLE	PAGE NO.
Chapter 1	Nutritional Analysis and Evaluation of Food Products Made from Date Seed Powder <i>Mantasha Mirza, Abdul Rahman Khan, Iqbal Azad</i>	1 - 24
Chapter 2	Synthesis, and Computational Studies of Methyl 6-Amino-5-Cyano-2-Oxo-2' h-Spiro[Indoline-3'4'-Pyrano(2,3-C) Pyrazole]-3'-Carboxylate <i>Umme Habiba Malik, Ayesha Anwer, Mohammad Amir, Malik Nasibullah</i>	25 – 39
Chapter 3	Studies of ZnBi ₂ O ₄ Nanoparticles for the Removal of Amido Black Dye <i>Neda Afreen, Naseem Ahmad, Nafees Ahmad</i>	41 – 49
Chapter 4	Assessment of Heavy Metal Contamination in Polymeric Disposable Items <i>Nafees Ahmad, Arshad Iqbal, Iqbal Azad, Naseem Ahmad</i>	50 – 65
Chapter 5	Ecofriendly Synthesis of Zinc Oxide Nanoparticles Using Moringa Oleifera Leaves Extract and Its Characterizations <i>Mohd. Samiullah, Mohd Arsh Khan, Qazi Inamur Rahman, Abdul Rahman Khan</i>	66 – 85

Chapter 6	Utilization of Peels of Citrus Fruit for Extracting Essential Oil Using Steam Distillation and Soxhlet Extraction	86 – 103
	<i>Saimah Khan, Yusra Khatoon</i>	
Chapter 7	Geo-Polymerization with Particular Emphasis on Fly Ash for Construction Material Applications	104 – 118
	<i>Deepak Mallah, Tahmeena Khan</i>	
Chapter 8	Azole Derivatives and Their Biological Activities	119 – 137
	<i>Vaishnavi Dubey, Mohd Arsh Khan, Neda Fatima, Sabahat Yasmeen Sheikh, Firoj Hassan</i>	

CHAPTER - 2

SYNTHESIS, AND COMPUTATIONAL STUDIES OF METHYL 6'-AMINO-5'-CYANO-2-OXO-2'H- SPIRO[INDOLINE-3'4'- PYRANO(2,3-C) PYRAZOLE]-3'-CARBOXYLATE

*Umme Habiba Malik^a, Ayesha Anwer^a, Mohammad Amir^a, Malik
Nasibullah^{a*}*

*^aDepartment of Chemistry, Integral University, Lucknow (U.P.),
India*

**Corresponding email: malik@iul.ac.in*

Abstract

Pyrazole derivatives are important heterocyclic compounds known for their wide range of biological activities, including antibacterial, antifungal, anti-inflammatory, analgesic, anticancer, and antidiabetic properties. In this study, a novel spiro pyranopyrazole derivative, methyl 6'-amino-5'-cyano-2-oxo-2'H-spiro[indoline-3,4'-pyrano[2,3-c]pyrazole]-3'-carboxylate, was synthesized through a one-pot multicomponent reaction using dimethyl acetylene dicarboxylate (DMAD), hydrazine monohydrate, malononitrile, and isatin in PEG:EtOH medium with TBAI as a catalyst at room temperature. The synthesized compound was obtained in good yield and characterized by spectroscopic methods. Pharmacokinetic and ADMET studies indicated favourable drug-likeness, oral bioavailability, and acceptable absorption properties according to Lipinski's rule of five. Biological activity prediction also suggested promising pharmacological potential.

Keywords: Pyrazole, Pyranopyrazole, Isatin, Multicomponent reaction, ADMET study, Drug-likeness

- [14] Halliday RS, Huey R, Hart WE, Belew RK. Automated docking using a Lamarckian genetic algorithm and empirical binding free energy function. *J Comput Chem.* 1998;19(14):1639-1662.
- [15] Mortelmans K, Zeiger E. The Ames Salmonella/microsome mutagenicity assay. *Mutat Res.* 2000;455(1-2):29-60.
- [16] Srimai V, Ramesh M, Parameshwar KS, Parthasarathy T. Computer- aided design of selective cytochrome P450 inhibitors and docking studies of alkylresorcinol derivatives. *Med Chem Res.* 2013;22(11):5314-5323.
- [17] Veber DF, Johnson SR, Cheng HY, Smith BR, Ward KW, Kopple KD. Molecular properties that influence the oral bioavailability of drug candidates. *J Med Chem.* 2002;45(12):2615-2623.