



**ANRF/DST-SERB  
Sponsored**

International Conference on

**RESILIENT INNOVATIONS  
FOR SUBSISTENCE ENVIRONMENT**

21<sup>st</sup> , 22<sup>nd</sup> NOVEMBER

**ICRISE  
2025**



**SOUVENIR**



**GCRJY**

**GOVERNMENT COLLEGE, RAJAHMUNDRY**

**AUTONOMOUS - NAAC - A+**



**DST-SERB/ANRF Sponsored  
International Conference on Resilient Innovations For  
Subsistence Environment (ICRISE-25)  
21st,22nd November, 2025**

## **FOREWORD**

We are delighted to welcome all participants to the DST-SERB/ANRF Sponsored International Conference on Resilient Innovations for Subsistence Environment (ICRISE-25), being held on 21st–22nd November 2025. In an era marked by climate unpredictability, resource constraints, and environmental challenges, building resilience has become a vital foundation for sustainable development.

ICRISE-25 provides a global platform for scientists, academicians, researchers, industry professionals, and policymakers to exchange ideas and explore innovative solutions that empower subsistence-level communities while safeguarding ecological balance. This conference emphasizes transformative, interdisciplinary approaches in areas such as green technologies, climate-smart agriculture, renewable energy, environmental biotechnology, AI-enabled sustainability tools, and socio-economic strategies for community resilience.

We express our sincere gratitude to DST-SERB/ANRF for their generous support and to all contributors and participants whose involvement enriches the scientific value of this conference.

### **Editorial Board**

**Dr N Baby Nirmala**

**Dr L Rajeswari**

**Dr CH Rajani**

**Dr P Surekha**

**Dr G Tejaswini**

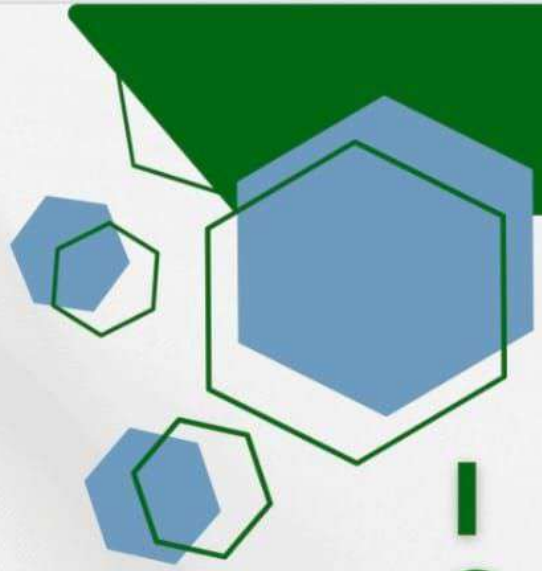
**Dr V Durga Praveena**

**Dr P Surya Sree**



**Department of Chemistry  
GCARJY**

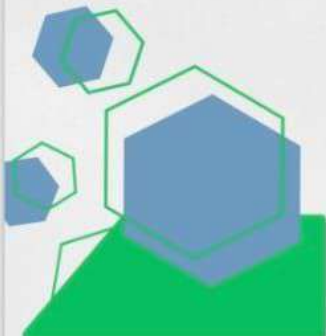
13	<b>Rational ligand designs for the isolation of coinage metal complexes and their utility in homogeneous catalysis</b> Maksood Alam, Adinarayana Doddi	13
14	<b>Exploring Si–H Functionalized Phosphines as Ambiphilic Ligands in transition metal complexes and their utilisation in Homogenous Catalysis</b> Rageshree Dasha, Amiya Sahooa, Adinarayana Doddi	15
15	<b>Dandelion-like <math>\text{Co}_3\text{O}_4\text{--ZnMn}_2\text{O}_4/\text{ZnMnO}_3</math> Heterostructures Nanocomposite as a Battery-Type Electrode with High Specific Capacity for Hybrid Supercapacitors</b> Mulla Jakeer Hussain, G. Madhavi	17
16	<b>Nature-Based Solutions for Biodiversity Conservation</b> V. Geetha	18
17	<b>Smart Water Management and Clean Energy Transitions</b> D. Jeevitha, Kiranmai Tamma, P. Bhavani, G. Suswara Deepika	19
18	<b>Design, synthesis, and apoptotic evaluation of spiro[indoline-3,3'-pyrazolo[1,2-a]indazole] derivatives via [3 + 2] N,N-cycloaddition</b> Rapeti Thrinadh Kumar, Sohel C. Mulani, Shaik Anwar and Ravi K. Kottalanka	20
19	<b>Nanotechnology Implications in Health and the Environment</b> Dr. K. Vijaya Lakshmi	21
20	<b>Artificial intelligence in environmental monitoring: Advancements, challenges, and future directions</b> K. R. Shanmugam, M. Guru Sekhar	22
21	<b>From UV to Visible Light and Conventional to Green methods: Photocatalysis by Modified TiO<sub>2</sub> Semiconductors</b> Winnie Teja Dokka, Beebi Shaik	23
22	<b>Design and Computational Docking Exploration of Innovative Thiadiazole Analogues Targeting Cancer Activity</b> Indhumathy. P, Gandhimathi. R	24
23	<b>A Green sustainable RP-HPLC method for simultaneous estimation of atazanavir and ritonavir: development, validation and environmental impact assessment</b> K. Archana, M. Sumithra	25
24	<b>Spatial distribution of Uranium water quality on seasonal basis around proposed Nuclear Power Plant (NPP) site at Kovvada, Srikakulam District, Andhra Pradesh, India.</b> Yugandhar. M, G.V. Subba Reddy, D. Ramarao, S.K. Sahoo, A. Vinod Kumar, P. V. S. Machiraju	26
25	<b>Resilient Water Innovations for Subsistence Communities: Pathways Toward Decentralized and Climate-Adaptive Security</b> N. Baby Nirmala, M. Santha Kumari, Ch. Rajani	27



# ICRISE 2025



**“Let us permit Nature to have her way,  
She understands her business better than us”**



**ISBN NUMBER**



## Design and Computational Docking Exploration of Innovative Thiadiazole Analogues Targeting Cancer Activity

Indhumathy. P<sup>1</sup>, Gandhimathi. R\*

<sup>1,\*</sup>Department of Pharmaceutical Chemistry and Analysis, School of Pharmaceutical Sciences, Vels Institute of Science, Technology and Advanced Studies, Chennai, Tamil Nadu, India.

Corresponding author: \*e-mail:

### ABSTRACT

Melanoma, arising from uncontrolled melanocyte proliferation, is treatable in its early stages but poses significant challenges in advanced cases. This study aimed to design and evaluate novel thiadiazole derivatives as potential anti-cancer agents targeting the BRAF protein using 3D-QSAR modeling and molecular docking. A dataset of 51 reported BRAF inhibitors was analyzed using the Schrödinger suite, and the Gaussian-based QSAR model showed strong predictive reliability ( $r^2 = 0.93$ ,  $r^2_{cv} = 0.47$ ,  $SE = 0.2$ ,  $F \text{ ratio} = 80.3$ ), with field contributions of steric (0.29), hydrophobic (0.24), hydrogen bond donor (0.18), electrostatic (0.188), and hydrogen bond acceptor (0.08). Guided by these findings, 25 novel thiadiazole derivatives were designed and subjected to docking studies in PyRx. Among them, compound IA25 demonstrated the best binding affinity ( $-9.7 \text{ kcal/mol}$ ), comparable to the standard Dabrafenib, forming two hydrogen bonds with Asn221 and Phe209 residues. Other derivatives showed scores ranging from  $-8.0$  to  $-9.6 \text{ kcal/mol}$ , with 10 shortlisted for further study. These results highlight the critical role of hydrogen bond donor and acceptor substituents on the thiadiazole ring in BRAF inhibition and suggest IA25 as a promising anti-cancer lead.

**Keywords:** Thiadiazole, BRAF enzyme, Quantitative structure–activity relationship, Docking studies.