

# Indian Journal of Chemistry

VOL. 64

NUMBER 10

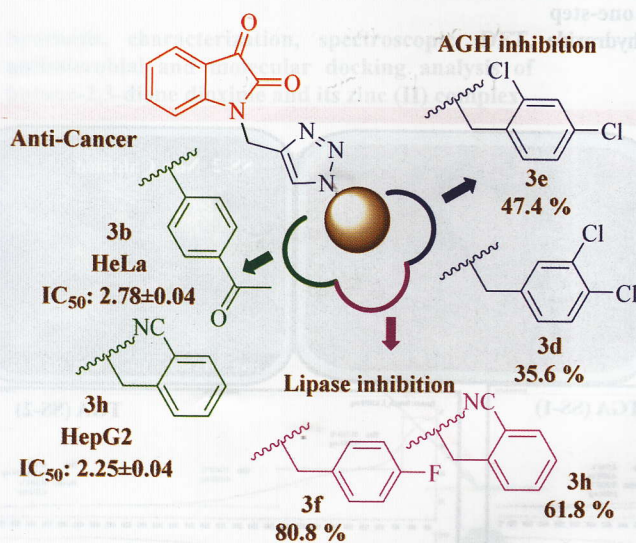
OCTOBER 2025

## CONTENTS

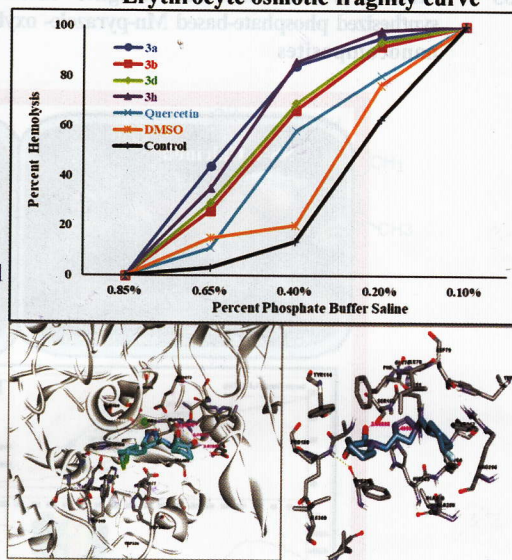
### Papers

933

Synthesis and evaluation of isatin-N-1,2,3-triazoles analogues for *in vitro* anticancer,  $\alpha$ -glucosidase inhibition properties via molecular hybridization approach



Erythrocyte osmotic fragility curve

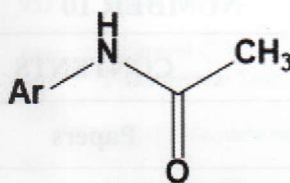


A Niranjana Kumar, J Kotesk Kumar\*, K V N S Srinivas\*, Srinivas Chinde, Anand Kumar Domatti, Yogesh Kumar, Paramjit Grover, Ashok Tiwari & Feroz Khan

Phytochemistry Division, CSIR-Central Institute of Medicinal and Aromatic Plants, Research Centre, Boduppal, Hyderabad 500 092, India

- 942 **Synthesis of bioactive aryl anilides using solid acidic  $\text{FeCl}_3$ -Bentonite catalyst: DFT analysis, molecular docking and ADMET property evaluation**

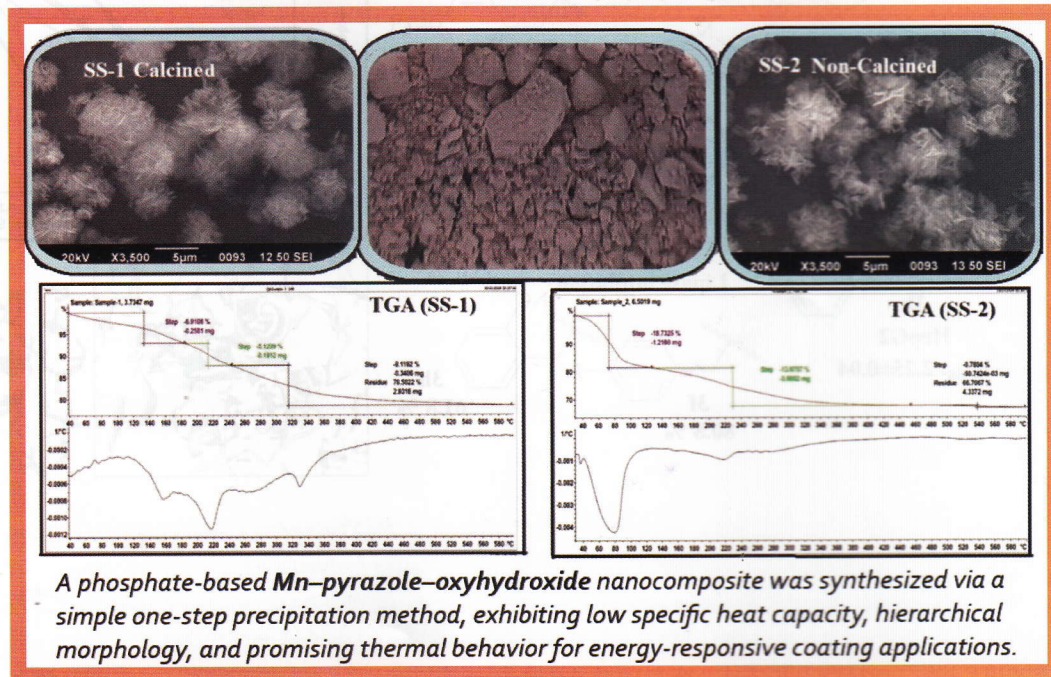
Two anilides have been synthesized with more than 85% yield by acid ferric chloride-bentonite catalyzed conversion-rearrangement of oxime in ethereal medium under sonication. The molecular docking, ADMET properties and antimicrobial activities of these anilides have been investigated.



I Muthuvel, J Divya, P Gayathri, S Balasundari, P Sudha, C Palanivel, B Krishnakumar, V Manikandan, Abdullah K Alanazi & G Thirunarayanan\*

Department of Chemistry, Annamalai University, Annamalainagar 608 002, Tamil Nadu, India

- 953 **Structural and thermal insights into one-step synthesized phosphate-based Mn-pyrazole- oxyhydroxide nanocomposites**

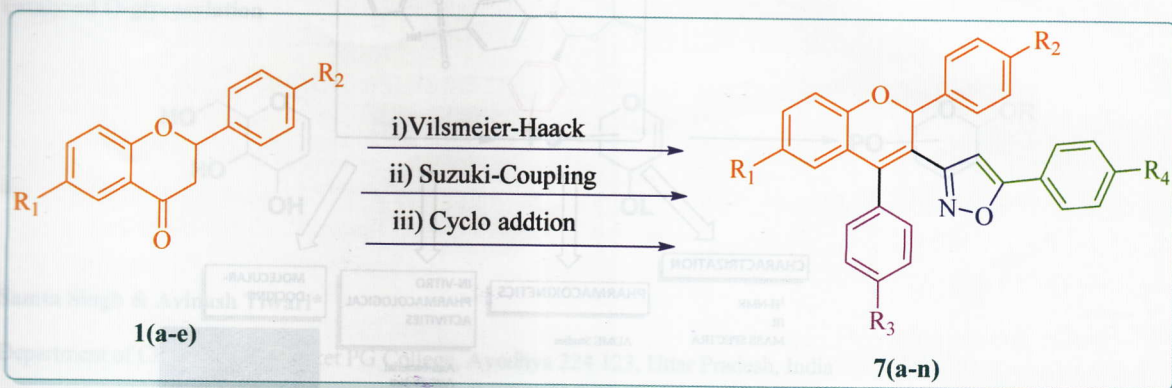


Sushree Priyadarshini, Gouri Sankhar Brahma & Suprava Nayak\*

School of Chemistry, Gangadhar Meher University, Sambalpur 768 004, Odisha, India

962

**Facile synthesis of highly functionalized aromatic novel 3-(2,4-substituted diaryl-2H-chromen-3-yl)-5-phenylisoxazole derivatives**

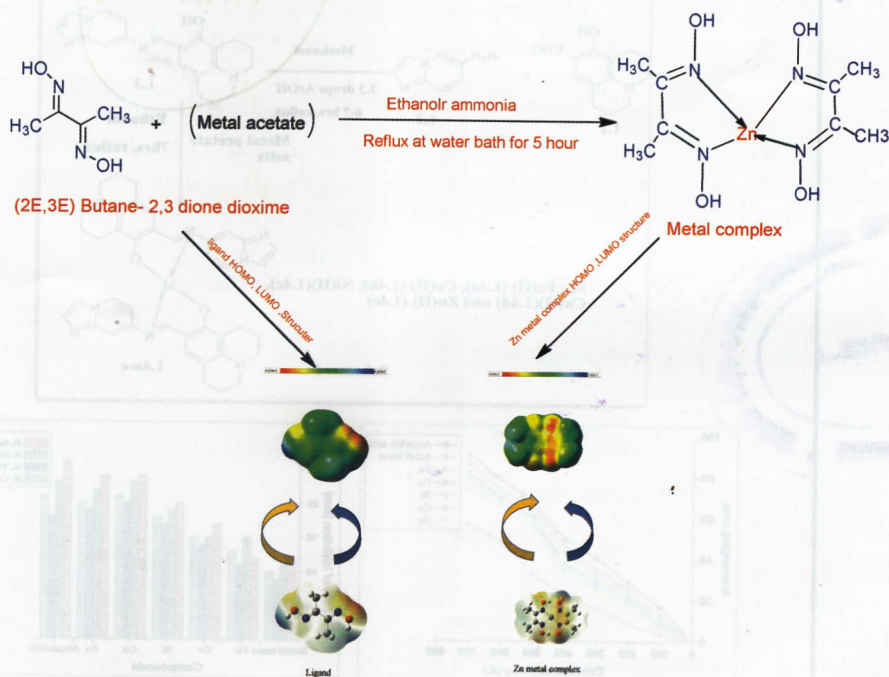


**Madhu Gutam, Santosh Kumar Konda, Naveen Reddy Vadiyala, Gangadhar Thalari, Jayaprakash Rao Yerrabelli & Prasad Rao Chitneni\***

Natural Products Laboratory, Department of Chemistry, Osmania University, Hyderabad 500 007, Telangana, India

966

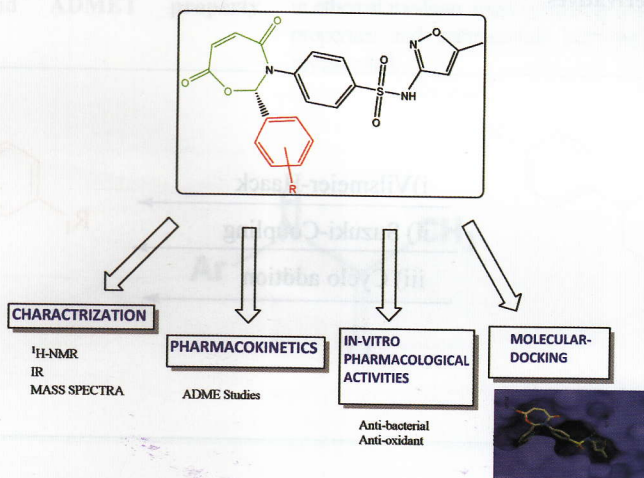
**Synthesis, characterization, spectroscopic, DFT, antimicrobial and molecular docking analysis of butane-2,3-dione dioxime and its zinc (II) complex**



**Reema Chand\*, Mohseen Ahmed & Bibhesh K Singh**

Department of Chemistry, M.B.G.P.G College, Haldwani 263 139, Nainital, Uttarakhand, India

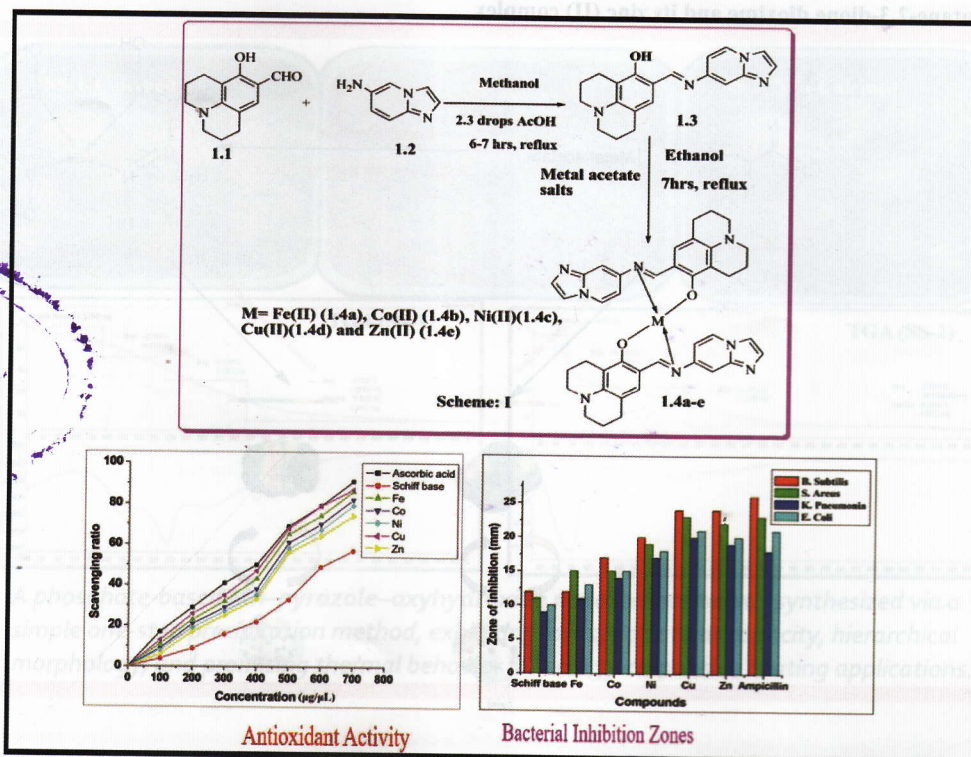
**979 Synthesis, characterization, antimicrobial and antioxidant screening of novel oxazepines**



**Rishabh Sheth, Tirth Thaker\*, Sweta Maurya & Anupam Jyoti**

Department of Chemistry, Parul Institute of Applied Sciences, Parul University, Vadodara 391 760, Gujarat, India

**988 Synthesis, spectral characterizations, antioxidant, and antibacterial studies of novel Schiff base and its metal complexes**

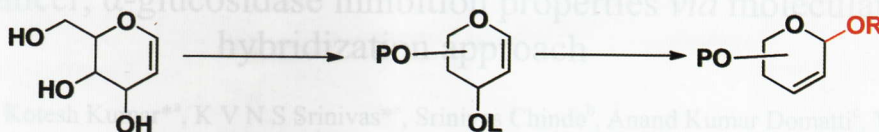


**Mamatharani Ravula**

Telangana Social Welfare Residential Degree College for Women, Warangal West 506 002, Telanagana, India

## Notes

- 995 **Synthesis of 6-isopropoxy-2-phenyl-4,4a,6,8a-tetrahydropyrano[3,2-d][1,3]dioxine via palladium catalysed O-glycosylation**



Samta Singh & Avinash Tiwari\*

Department of Chemistry, K S Saket PG College, Ayodhya 224 123, Uttar Pradesh, India

Authors for correspondence are indicated by (\*)

Received 18 August 2025; accepted (revised) 7 October 2025

The anticancer,  $\alpha$ -glucosidase inhibition profiles of isatin-1,2,3-triazole conjugates (9 Nos) are reported here. The compounds 3a ( $IC_{50}$  5.52 $\pm$ 0.04), 3b ( $IC_{50}$  2.78 $\pm$ 0.04  $\mu$ M), 3d ( $IC_{50}$  7.09 $\pm$ 0.037  $\mu$ M) and 3e ( $IC_{50}$  2.25 $\pm$ 0.04  $\mu$ M) have shown more potent anti-cancer activity against HeLa and HepG2 cell lines respectively compared to the standard Doxorubicin ( $IC_{50}$  9.03 $\pm$ 0.97 and 10.15 $\pm$ 0.003 respectively). While, compound 3e potentially inhibits  $\alpha$ -glucosidase enzyme (47.4%) when compared to the standard Acarbose (56.0%), compound 3f has shown potent lipase inhibition activity (88.8%) when compared to the standard Orlistat (91.1%). In *in silico* studies, the docking of derivatives with the respective anticancer, ALH and lipase targets have revealed their potential binding affinities. Also the plot of PSA vs ALogP has revealed the compounds with favorable physicochemical properties for CNS drug development or oral delivery.

**Keywords:** Isatin, 1,2,3-Triazole, Anticancer,  $\alpha$ -Glucosidase, Lipase, Docking studies

Isatin (1*H*-indole-2,3-dione moiety) is one of the most interesting class of heterocyclic molecule and consists of indole nucleus and two types of carbonyl groups (ketone and lactam groups). It can be found in plants like genus *Isatis*<sup>1</sup>, *Calceolaria discolor* LINDL<sup>2</sup>, and *Isatis purpurascens* Aubl<sup>3</sup>. Isatin also present in mammalian tissues, fluids<sup>4</sup> parotid gland of *Bufo* sp.<sup>5</sup> Isatin is an extensible substrate that may be utilized to synthesize a wide range of heterocyclic compounds, such as oxadiazoles and sulphonamides (carbonyl compounds), spiro compounds (antiproliferative)<sup>6</sup>, sulfonamide-based-derivatives (multi-kinase inhibitors), cyclic ureas and oximes (*in vivo* antitumour activity)<sup>7</sup>, indoles (antiproliferative)<sup>8</sup>, indirubin analogs (antiproliferative)<sup>9</sup>, di- or trisubstituted indoles (antiproliferative)<sup>10</sup>, dihydropyrazole hybrids (antiproliferative)<sup>11</sup>, Ciprofloxacin and Moxifloxacin derivatives (antibacterials)<sup>12</sup>, ferrocene-tethered indoles (antibacterials)<sup>13</sup>, etc. Several isatin-based conjugates have entered clinical studies, including two molecules, Sorafenib and Toleranib, that have been

authorized for clinical usage against tumors. Other derivatives, including Nintedanib, Vemurafenib, and Orantinib,<sup>14</sup> are now in clinical studies for their anticancer potential (Fig. 1).

Assuming that the presence of isatin derivatives have antiproliferative activity, therefore, several attempts to investigate the anticancer profile of isatin-1,2,3-triazoles (3 Nos) in addition to  $\alpha$ -glucosidase and lipase.

## Results and Discussion

### Chemistry

The synthetic strategy of isatin N-substituted 1,2,3-triazoles was outlined in our earlier studies<sup>15</sup>.

### In vitro anti-cancer activity

Anticancer activity of Isatin-N-1,2,3-triazole derivatives 3a-i were evaluated in *in vitro* mode<sup>16</sup> on the human cancer cell lines A549, HepG2, MCF-7, HeLa and SKOV3. The results of *in vitro* cytotoxic activity were expressed as the  $IC_{50}$  ( $\mu$ M) and doxorubicin was used as positive control (Table 1).