

Indian Journal of Chemistry

Sect. B: Organic Chemistry including Medicinal Chemistry

VOL. 57B

NUMBER 6

June 2018

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Papers

- 811 Synthesis of novel 1,3-thiazole-triazole and 1,3-thiazole-isoxazole hybrids** A focused library of thirteen compounds, 3-((1-benzyl-1*H*-1,2,3-triazol-4-yl)methyl)-4-arylthiazol-2(3*H*)-ones (**6a-j**) and 4-aryl-3-((3-arylisoaxazol-5-yl)methyl)thiazol-2(3*H*)-one hybrids has been synthesized. Their chemical structures have been confirmed by HR-MS, IR, ¹H and ¹³C NMR spectra.

B Madhavilatha, Gowravaram Sabitha*, B V Subba Reddy, J S Yadav & B Jagan Mohan Reddy

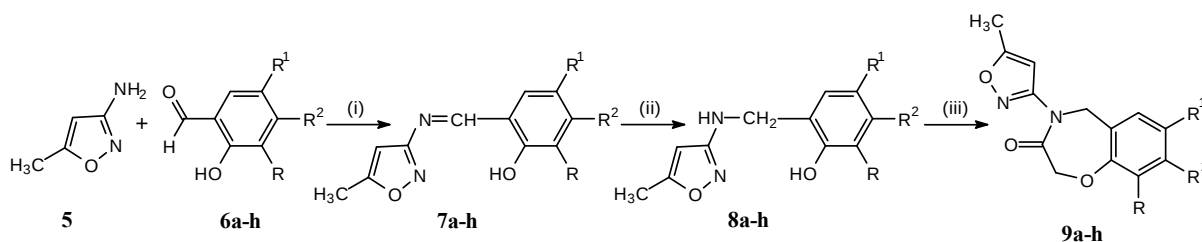
Natural Products Chemistry Division, CSIR-Indian Institute of Chemical Technology, Hyderabad 500 007, India

- 816 Mono-, di- and tri- substituted S-triazine as anti cancer agents: A comparative molecular docking study**

Arpita Prasantini Joshi, Anuj Tripathi & Chetti Prabhakar*

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- 823 A facile and simple synthesis of novel isoxazolyl benzo[*f*][1,4]oxazepin-3-(2*H*)-ones and their antimicrobial activity** A series of novel isoxazolyl benzo[*f*][1,4]oxazepin-3-(2*H*)-ones have been synthesized by adopting a facile and simple methodology. The reaction of 3-amino-5-methylisoxazole with salicylaldehydes, followed by reduction with NaBH₄, and *in situ* chloroacetylation and cyclization with chloroacetyl chloride and triethylamine afforded title compounds. Title compounds were evaluated for their *in vitro* antimicrobial activity against different bacterial and fungal strains.



Ramu Kakkerla*, Srinivas Marri, M P S Murali Krishna & M V Rajam

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- 830** **Advancements in BACE1 and non-peptide BACE1 inhibitors for Alzheimer's disease**

Nishita P Shah, Vivek S Solanki & Archana S Gurjar*

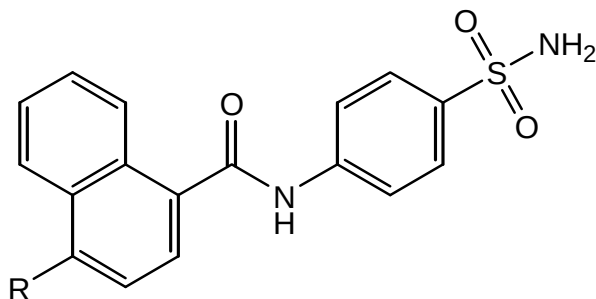
Prin. K. M. Kundnani College of Pharmacy, 23 Jote Joy, R. S. Marg, Cuffe Parade, Mumbai 400 005, India

- 843** **Four-component clean process for the eco-friendly synthesis of 1*H*-pyrazolo [1,2-*b*]phthalazine- 5,10-dione derivatives using Zn(OAc)₂.2H₂O as an efficient catalyst under solvent-free conditions**

Farzaneh Mohamadpour, Mojtaba Lashkari*, Reza Heydari & Nourallah Hazeri

Faculty of Science, Velayat University, Iranshahr, Iran

- 852** **Synthesis, antimicrobial and QSAR studies of novel benzenesulfonamide derivatives**



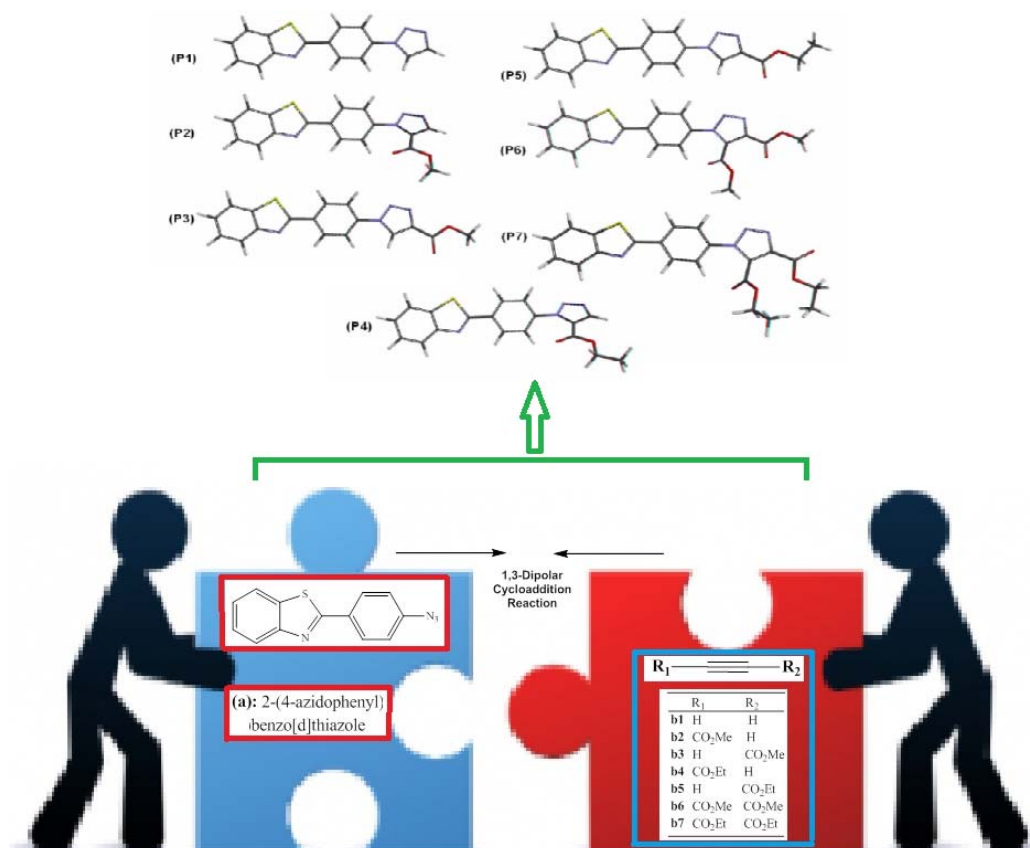
R: R = CH₃-, CH₃CH₂-, CH₃CH₂CH₂-, CH₃CH₂CH₂CH₂-

Gulay Zengin*, Huseyin Zengin, Hasan Turkmen & Metin Dıǵrak

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858 DFT study of 1,3-dipolar cycloaddition reaction of 2-(4-azidophenyl) benzo[d]thiazole with acetylene derivatives

In this study, the 1,3-dipolar cycloaddition reactions of azidophenyl derivatives fused to benzothiazole heterocyclic compound to $\text{C}\equiv\text{C}$ bonds of dipolarophiles such as functionalized acetylene derivatives have been investigated and discussed. The energy levels of the reactants, transition states (TS), products, the free energies of reaction ($\Delta_r G$ and $\Delta_r G^\ddagger$), HOMO and LUMO orbital levels, the $\Delta E_{\text{HOMO-LUMO}}$, rate constants by using Eyring's equation (k and k') and structural data have been calculated by DFT-B3LYP/6-31G* method.



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870 Design, synthesis and biological screening of N¹-(substituted pyridine-2-yl)-N³-(quinoline-2-yl) malonamide as novel anti-HIV-I agents

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