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Papers

1183 Influence of intramolecular ring-ring π,π interaction on crystal building in ternary compound of nickel(II) chelates of 2,2'-{[2-(4methylphenyl)ethyl]azanediyl} diacetic acid and 1,10-phenanthroline – Synthesis, spectral, optical and quantum chemical study

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Dheerendra Kumar Patel*, Duane Choquesillo-Lazarte, Josefa María González-Pérez & province de la administrative Juan Niclós-Gutiérrez

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Department of Physiological and Chemistry, College of Veterinary Medicine, Al-Shatrah University, 64007 Al-Shatrah, Iraq

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Synthesis of diversely substituted 5methylpyrazolo[1,5-a]pyrimidines assisted by ultrasound in aqueous media: Molecular docking for potential antiviral, anticancer activities Pyrazolo[1,5-*a*]pyrimidine derivatives have been synthesized using ultrasonication of 3-amino-1*H*-pyrazoles and enaminones in an aqueous medium with KHSO₄. Structural confirmation is achieved through spectral techniques and X-ray crystallography. Molecular docking studies identified potential antiviral and anticancer agents, with molecular dynamics confirming the stability of ligand **9c**.



Shunan Kaping, Rene Barbie Browne & Jai N Vishwakarma*

Organic Research Laboratory, Department of Chemistry, Assam Don Bosco University, Tapesia Gardens, Sonapur 782 402, Assam, India a transformed and the second

1222 Novel bioactive flavonoid 5-hydroxy-2-(8-hydroxy 4-0x0-4H-chromen-2-yl)-4-0x0-3,4-dihydro-2H-1-benzopyran-7-yl-N-[(2-methylpropoxy) carbonyl] carbamate from *Kalanchoe pinnata*



Latha Ophelia George*, RadhaH R, Pragasam A & Preeti N Tallur

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1228 Synthesis, biological evaluation, ADME studies and molecular docking of 1-(3-substituted phenylisoxazol-5-yl) naphthalen-2-ol moiety with VEGFR-2 and Caspase-3 enzymes inhibitors 1-(3-Substituted phenylisoxazol-5-yl) naphthalen-2-ol has been created by cyclizing chalcones and subjected to biological evaluation, ADME studies and molecular docking with VEFGR-2 and Caspase-3 enzymes inhibitors.



Dipen Panchani, Tirth Thaker* & Shaile Thakur

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1236 Synthesis, spectral characterization and antibacterial activities of heterocyclic complexes with Schiff base derived from 3-hydroxybenzofuran-2-carbaldehyde and (furan-2-yl)methanamine The Schiff base 2-((E)-((furan-2-yl)methylimino)methyl)benzofuran-3-ol has been prepared and evaluated by means of elemental analysis, infrared spectroscopy, nuclear magnetic resonance, mass spectroscopy and thermal analysis (TGA). The analytical findings of the complexes validate the synthesis of a 1:2 [M:L] ratio. Infrared spectra show that metal ions are bivalently bound to the Schiff base *via* azomethine-N and phenolic-oxygen groups. Studies have been conducted to determine if the ligand and its metal chelates have antibacterial effects against the designated microorganisms.



Suryasri Erukala & Sunkari Jyothi*

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1240 Identification of Sirtuin 1-targeted anti-Alzheimer agents using structure-based drug design and multi-database screening

Synthesis and antimicrobial activity of novel 4-(heazo[d]imidazoi-2-yi)-4,5-dihydra-heazo[/][1,4] vazepia-3(2H) ones



Preeti Chandel, Smita Jain, Ritu Singh, Mohammad Chand Jamali, Jaya Dwivedi* & Swapnil Sharma

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1263 Synthesis and antimicrobial activity of novel 4-(1*H*benzo[*d*]imidazol-2-yl)-4,5-dihydro-benzo[*f*][1,4]oxazepin-3(2*H*) ones

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G Prasoona, B Kishore, P Dharmender & G Brahmeshwari*

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1271 Multifaceted analysis of intermolecular interactions in α-terpineol-halobenzenes binary mixtures: Insights from thermophysical, acoustical, and spectral techniques, supported by quantum computational approaches

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1294 Synthesis and spectral properties of aromatically π coumarin-fused extended mesotetraphenylpyridoporphyrins Ph OH СНО NH₂ o-dichlorobenzene n 180 °C, 1 h Ph P Domino reaction approach Simple access to coumarin-fused pyridoporphyrins in good yields

Red-shifted absorption due to the extended π-conjugation

Pargat Singh & Mahendra Nath*

One-pot operation

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Authors for correspondence are indicated by (*)

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