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CONTENTS

Papers

Green synthesis of 5-methylpyridinium derivatives by C2-functionalization of pyridine-1-oxide derivatives and their antibacterial activity

An innovative green economic route has been developed for one pot multicomponent synthesis of 5-methylpyridinium derivatives by the reaction of 3-methylpyridine-1-oxide, aromatic aldehyde and β -ketoester catalysed by different ionic liquids (ILs), [BMIM][OH], [BMIM][C1], [BMIM][Ac] in good to excellent yields. A relative study reinforced that [BMIM][OH] is the best IL for this C2-functionsalization reaction.



Surbhi Dhadda, Prakash G Goswami, Kalpana Yadav, Anjali Guleria, Dinesh K Jangid* & Chandra L Khandelwal

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Medicinally important pyranopyrazoles have been synthesized using methods having environment friendly features such as energy efficiency, aqueous medium, no hazardous solvent, no chromatography, in addition to the short reaction time, catalyst reusability and substrate tolerance without affecting yield.



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Anti-inflammatory, analgesic and antitubercular activity of 4,6-diphenyl-4,5,6,7-tetrahydro-3-selena-1,2,5-triazo-indene derivatives Synthesis of new quinazolinone-based Mannich bases in good yields *via* a three-step procedure is reported. The bio-assay results show that some synthesized bases exhibited weak to moderate cytotoxic activity against SKLu-1 and MCF-7 cell lines.



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207 A novel approach to determine anti-proliferative, anti-migratory and anti-microbial properties of 2phenylethylammonium carboxylate molecular salts 2-Phenylethylammonium (PEA) salt derivatives have been prepared between 2-phenylethylamine with various aromatic carboxylic acids (nicotinic, benzoic, salicylic, and γ -resorcylic and confirmed by spectroscopic analyses.



Hüseyin Akbaş*, Seçil Erden Tayhan & Sema Bilgin

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Interaction of dpyatriz and Cu/Zn-dpyatriz complexes with human telomere DNA: The role of G-quadruplex formation and its effect on antitumor and antitelomerase activity

The dpyatriz, Cu-dpyatriz and Zn-dypatriz compounds induce and stabilize antiparallel G-quadruplex conformations in telomeric sequences, resulting in efficient antitelomerase and anticancer activity *in vitro*.



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Chemical studies of chromanone-thiadiazole, pyridazine and thiosulfin hybrid A spiro[chroman-3,2'-[1,3,4]-thiadiazole]-4-one,3', aspiro [chroman-3,2'- piprazine]-4-one, and a mixture of 1,3,4oxadithiins, 1,3,4,5,6-oxatetrathiocins, 1,2,4-trithiolanes, 1,2,4,5tetrathiins derivatives were synthesized.



Mohamed I Hegab*, Hala E M Tolan, Farouk A Gad & Farouk M E Abdel-Megeid

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Synthesis and characterization of bioactive Linear synthesis of a biheterocylic framework having anti-fungal isoxazole and 1,3,4-oxadiazole heterocycle and anti-bacterial activity in good overall yield.



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244 New quinazolinone-based Mannich Synthesis and *in vitro* cytotoxic evaluation

bases: New quinazolinone-based Mannich bases **4a-c** and **5a-e** have been synthesized in good yields *via* a three-step procedure, starting from 6-hydroxyanthranilic acid 1. The research suggests that the presence of the Mannich group in the phenyl ring has more beneficial effect on the cytotoxic activity than in the quinazolinone nucleus.



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Synthesis, characterization, cytotoxicity evaluation and molecular docking study of new bis-chalcone, fused-pyrimidine and fused-pyrazoline derivatives

It involves synthesis of new bis-chalcone compounds and further cyclization into fused-pyrimidine and fused-pyrazoline that tested for cytotoxicity activity against breast cancer cell lines (MCF-7 & MD-MB-231) and molecular docking study with 3ERT protein.



Bazri Izwan Bakar, Mohammad Murwih Alidmat, Melati Khairuddean*, Wan Nuaralia Asyikin Wan Ibrahim, Kwan Wai Mun, Nik Nur Syazni Nik Mohammad Kamal & Musthahimah Muhammad

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265 Synthesis, electrical conductivity and NIR absorption of some metal dithiolene complexes: Some recent developments

From the very beginning of this research work on metal dithiolene chemistry, at early 1960's, it naturally attracts researchers. In this present endeavour we have discussed the summery of research from near past to upcoming future exclusively based on solid state electrical conductivity and Near infrared (NIR) absorption study of metal dithiolene complexes.



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278 Antioxidant properties of capsaicin analogues: A DFT study

Twelve capsaic analogues with functional groups -SH, $-NH_2$, $-OCH_3$ and -F in the aromatic ring, have been proposed and studied using DFT methodologies in order to analyse their antioxidant properties.



Porras-Alvarado M, Bautista-Renedo J, Reyes Pérez H, Cuevas Yáñez E & González-Rivas N*

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284 3D-QSAR, design, docking and in silico ADME studies The 3D-QSAR models were generated to support the of indole-glyoxylamides and indolyl oxoacetamides as molecular interactions and biological property of Indole glyoxylamide and Indolyl oxoacetamide. New analogues

The 3D-QSAR models were generated to support the molecular interactions and biological property of Indole glyoxylamide and Indolyl oxoacetamide. New analogues were designed based on the predictions, validation & visualization results. These were then docked and analyzed for binding affinity, and based on the 3D-QSAR model, docking scores, and ADMET findings, the hypothesis was established that further novel agents can be synthesized as potential PL-inhibitors.



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