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809 Synthesis of ethyl 2-((4-phenyl-1*H*-1,2,3-triazol-1-yl)methyl)-4*H*/2*H*-chromene-3-carboxylates by cyclo- addition of ethyl 2-(azidomethyl)-4*H*-chromene-3-carboxylates with alkynes

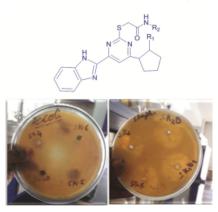
The cycloaddition reaction of ethyl 2-(azidomethyl)-4H-chromene-3-carboxylates with phenylacetylene/4-fluoro phenylacetylene have provided mixture of 2H- and 4H-triazobylchromene-3-carboxylates. 4-Methoxy-3-methyl-phenylacetylene and acetylenedicarboxylates have provided exclusively 2H-triazobylchromene-3-carboxylates. Interestingly, prop-2-yn-1-ol and ethyl propiolate have provided exclusively 4H-triazobylchromene-3-carboxylates.

Sairam Mudulkar, Sai Teja Kolla & China Raju Bhimapaka*

Department of Organic Synthesis and Process Chemistry, CSIR-Indian Institute of Chemical Technology, Hyderabad 500 007, India

816 Synthesis and antimicrobial activity of 2-((4-(1H-benzo[d]imidazol-2-yl)-6-(2-ethylcyclopentyl) pyrimidin-2-yl)thio)-N-methylacetamide

2-((4-(1H-Benzo[d]imidazol-2-yl)-6-(2-ethylcyclopentyl)- pyrimidin-2-yl)thio)-N alkylacetamide **4a-h** have been synthesized and show the best profile of activity against *Staphylococcus aureus*, *Escherichia coli* and *Aspergillus fumigatus*.

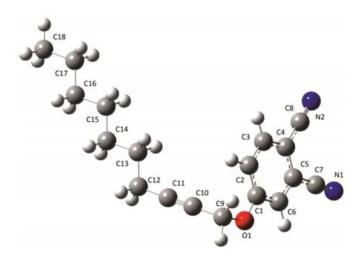


Sunitha Ch & Brahmeshwari G*

Department of Chemistry, Kakatiya University, Warangal 506 009, India

823 (dec-2yn-1-yloxy)phthalonitrile

DFT quantum chemical calculations (Fukui The optimized molecular geometry of title molecule is computed functions, NLO, TDOS, OPDOS, DNA/ECT) on 4- using B3LYP/DFT in gas phase.

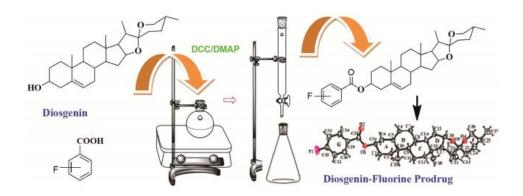


Serap Uzun

Department of Basic Sciences, Faculty of Engineering, Samsun University, Samsun, Turkey

831 Expeditious synthesis of isolated steroids-fluorine prodrugs, their single crystal X-ray crystallography, DFT studies and mathematical modeling

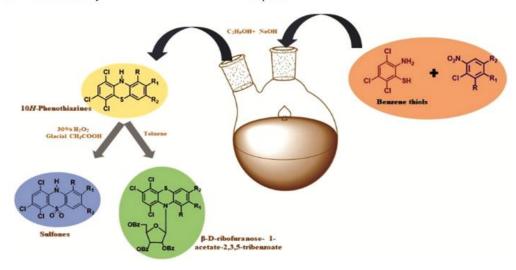
Novel steroidal-fluorine prodrugs using cholesterol (1), stigmasterol (4) and hydrocortisone acetate (7) is isolated from the flowers of Allamanda violacea.



Arun Sethi*, Amandeep, Ranvijay Pratap Singh, Rachana Pathak, Rohit Prakash, Sonia Sharma & Rajni Kant

Department of Chemistry, University of Lucknow, Lucknow-226 007, Uttar Pradesh, India

842 Synthesis of bioactive chlorinated 10*H*phenothiazines, sulfones, ribofuranosides and their antimicrobial activity Synthesis of some biologically active 10*H*-phenothiazines, their sulfones and ribofuranosides using substituted 2-aminobenzenethiol is reported.



Arun Goyal*, Shikha Agarwal* & D C Gautam

Department of Chemistry, Govt P.G. College Rajgarh Alwar-301 408, Rajasthan, India

849 Synthesis, characterisation and evaluation of some 1,5-benzodiazepine quinolin-2-one derivatives as possible hypnotic agents A series of novel 3-(2-(phenyl/substituted phenyl)-1*H*-benzo[*b*][1,5]-diazepin-4-yl)-4-methoxy-1-phenyl/ methylquinolin-2(1*H*)-one derivatives are synthesised by condensation of 3-substituted cinnamoyl-4-methoxy-1-phenyl/methylquinolin-2(1*H*)-one with *o*-phenylenediamine.

Sleep latency of
$$26.67 \pm 2.629$$
 minutes
Sleeping time of 111.00 ± 6.028 minutes
NH

NH

NH

OCH₃ increases Hypnotic activity

Molecular docking score -149.448

Reema R Raiturkar, Shivalingrao N Mamle Desai, Vanessa M Gracias, Aneka D Shenvi Sangavkar, Chrislyne Fernandes, Bheemangouda S Biradar & Sachin K Chandavarkar*

Department of Pharmacognosy, ASPM College of Pharmacy, Sangulwadi, Dist. Sindhudurg 416 810, Maharashtra, India

858 Synthesis and molecular characterization with DFT study of 2-chloro-1-(3-methyl-3-mesityl-cyclobutyl)-ethanone

The molecular elucidation of 2-chloro-1-(3-methyl-3-mesityl-cyclobutyl)—ethanone is conducted by FT-IR and NMR. DFT is used to stimulate and confirm the structure and molecular characteristics, using the DFT/B3LYP/cc-pVDZ method.

Pelin Koparir, Rebaz Omar* & Metin Koparir

Department of Chemistry, Faculty of Science and Health, Koya University, Koya KOY45, Kurdistan Region, F R Iraq

866 Synthesis and spectral analysis of 5,7-dihydroxy-3-(4-hydroxybenzyl)-6,8-dimethylchroman-4-one An efficient and concise synthetic route is designed based on 5,7-dihydroxy-3-(4-hydroxybenzyl)-6,8-dimethylchroman-4-one, an important active ingredient extracted from *Polygonatum Odoratum* (Mill.) Druce.

Zhen Lv*, Jifang Yang & Lu Han

College of Pharmacy, Qiqihar Medical University, Qiqihar, 161006 China

870 Triton-B/CS₂ mediated novel synthesis of substituted thioureas: A novel class of anti-cancer agents A novel method for the synthesis of substituted thioureas through reaction of corresponding amines with CS₂, methyl iodide using Triton-B as phase transfer catalyst, is reported.

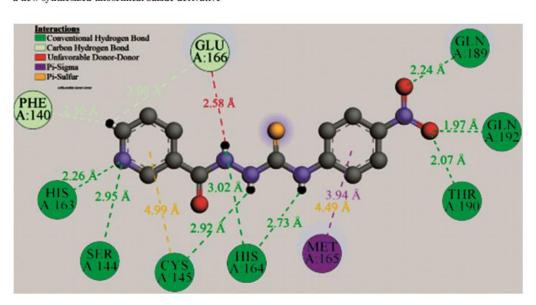
$$R_{1} = \bigcap_{CF_{3}} F^{Q} \text{ etc } R_{3} = CH_{3}, C_{2}H_{5}, C_{6}H_{13}, PhCH_{2} \text{ etc } R_{4} = H, CH_{3}, C_{2}H_{5}, etc$$

Nitin Srivastava, Devdutt Chaturvedi*, Ram Kishore, Manpreet Kaur & Raminderjit Kaur

Department of Chemistry, School of Physical Sciences, Mahatma Gandhi Central University, Motihari (East Champaran)-845 401, Bihar, India

878 Structural, spectral, bioactivity, antioxidant and molecular docking (with SARS-CoV-2) analyses on a new synthesized thiosemicarbazide derivative

The interactions between the docked ligand compound and the target macromolecule of SARS-CoV-2 Mpro

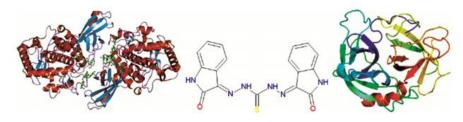


Aytaç Güder*, Nuri Öztürk, Can Alaşalvar, Halil Gökce, Emre Menteşe, Hakan Bektaş & Canan Albay

Giresun University, Vocational School of Health Services, 28100, Giresun, Turkey

895 Anti-tyrosinase, anti-elastase, and antioxidant activities of some symmetric bisthiocarbohydrazone compounds

The symmetric bisthiocarbohydrazones have been evaluated in terms of their anti-tyrosinase, anti-elastase and antioxidant potentials *in vitro*. All the tested compounds exhibit anti-tyrosinase and anti-elastase activities

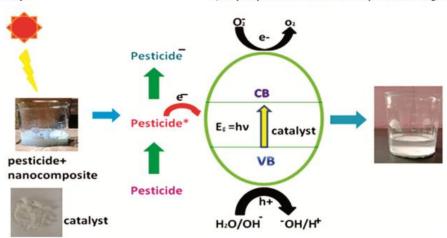


Yeliz Kaya, Ozlem Sacan, Ayşe Erçağ* & Refiye Yanardag

Istanbul University-Cerrahpaşa, Faculty of Engineering, Department of Chemistry, Inorganic Chemistry Division, 34320 Avcılar – Istanbul, Turkey

901 An efficient photocatalytic degradation of Quinalphos pesticide under visible light using zinc oxide/magnesium oxide nanocomposites as a novel photocatalyst

The development of an efficient and energetic photocatalyst is required for the eradication of pollutants present in water. In this study ZnO/MgO nanocomposite has been prepared for the degradation of Quinalphos pesticide in 40 minutes in the presence of sunlight.



S Sibmah* & E K Kirupavasam

Department of Chemistry & Research Centre, Nesamony Memorial Christian College, Marthandam 629 165, Tamil Nadu, India

Authors for correspondence are indicated by (*)

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