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RECENT TRENDS IN THE SEPARATION OF CHIRAL DRUGS

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Many of the currently used drugs in practice are mixtures of enantiomers. Although they have the same chemical structure, the enantiomeric forms of a drug can differ in potency, selectivity for receptors, transporters and/or enzymes, rate of metabolism, metabolites, excretion and toxicity, behavior in biological systems (like pharmacokinetics, bioavailability, efficacy and biopharmaceutical parameters). Therefore, it is important to promote the chiral separation and analysis racemic drugs in pharmaceutical industry in order to eliminate the unwanted isomer from the preparation. The use of single enantiomer drugs can potentially lead to simpler and more selective pharmacologic profiles included therapeutic indices, simpler pharmacokinetics due to different rate of metabolism and decreased drugs interactions. For example, Levorotary-isomer of all β -blockers is more potent in blocking β -adrenoceptors than their dextrorotary-isomer, such as S(-)-propranolol is 100 times more active than its R(+)-antipode. In the early period analytical chiral separation was a rather difficult task and separation methods were not as advanced as today. Nevertheless, it was clear that chiral drugs should be enantiomer separated and each isomer should be used separately. Enantiomers are separated by using the modern techniques like HPLC and Chiral HPLC has proven the best methods for the direct separation and analysis of enantiomers. The physical method and enantioselective immunoassays are used for characterization of chiral or racemic drugs. The chiral separation of racemic drugs is a necessary operation in pharmaceutical industry. Therefore the development of new chiral separation techniques and will be a topic subject in academic research as well as in industrial advance. It is also important to give more information about chiral drugs especially racemic form to health care professionals in order to help them to finding an optimal treatment and a right therapeutic control.

BIOGRAPHY

Sudha T has completed her PhD from Vels University, India. She is the Associate professor of Adhiparasakthi College of Pharmacy, affiliated to The Tamil Nadu Dr. MGR Medical University, Tamil Nadu, India. She has over 40 publications that have been cited over 15 times. She has been serving as an Editorial Board Member of reputed journals. She has published the book entitled "PHARMACEUTICAL ANALYSIS-I" by PV books.

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EVALUATION OF AN INVERSE MOLECULAR DESIGN ALGORITHM IN A MODEL BINDING SITE FOR THE IN SILICO DESIGN OF A YEATS2 GENE BLOCKADOR FOR THE DEPLETION OF YEATS2 AND ITS INTERACTIONS BETWEEN YEATS DOMAIN AND ACETYLATED HISTONES FOR THE REDUCTION OF THE ATAC COMPLEX-DEPENDENT H3K9AC PROMOTER LEVELS TARGETING TO THE DEACTIVATION OF THE ESSENTIAL NSCLC GENES

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Computational molecular design is a useful tool in modern drug discovery. Virtual screening is an approach that docks and then scores individual members of compound libraries. In contrast to this forward approach, inverse approaches construct compounds from fragments, such that the computed affinity or a combination of relevant properties is optimized. We have recently developed a new inverse approach to drug design based on the dead-end elimination and A* algorithms employing a physical potential function. It has recently been identified that the YEATS domain as a novel acetyllysine-binding module regulating the functional importance of YEATS domain-containing proteins in human non-small cell lung cancer (NSCLC) for cancer cell growth and survival. YEATS2 binds to acetylated histone H3 via its YEATS domain. Here, we have discovered for the first time an in silico predicted and computer-aided molecular designed YEATS2 gene blockador for the reduction of YEATS2-containing ATAC co-localized complex with H3K27 acetylation (H3K27ac) promoters of actively transcribed NSCLC genes as a histone H3K27ac inhibitor that regulates a transcriptional program essential for NSCLC tumorigenesis by utilizing the MicrocrylaqTM cluster of algorithms for Large-Scale Protein-Ligand Docking experiments. Computational chemistry, NSCLC genes, Protein-Ligand Docking experiments, ATAC complex-dependent H3K9ac promoter, acetylated histones, docking, compounds libraries, MicrocrylaqTM cluster of algorithms.

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HIBISCUS FLOWERS AND OLIVE LEAVES EXTRACTS-BASED FORMULATION IN NEURODEGENERATION: A NETWORK-BASED APPROACH

Matteo Micucci, Maria Frosini, Alberto Chiarini and Roberta Budriesi

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Despite high clinical heterogeneity, neurodegenerative disorders share many common etiologic features involving increased ROS formation and inflammation. ROS worsen the progression of the disease owing to oxidative damage and impaired mitochondrial function. Moreover, the accumulation of misfolded proteins contributes to the onset and progression of brain inflammatory response, which in turn, increases ROS release and subsequent oxidative stress (OS). Thus, the reduction of ROS levels may be a promising strategy to delay neurodegeneration. In this view many vegetal extracts and natural compounds endowed with antioxidant (but not only) properties are currently under clinical investigations. Pres Phytum[®] is a nutraceutical product composed by leaves- and flowers-extracts of *Olea europaea* L. and *Hibiscus sabdariffa* L., respectively, whose composition has already been characterized by HPLC coupled to a UV-Vis and QqQ-Ms detector. The effects of the components of this natural extracts are widely reported and most of them are mostly due to their antioxidant, antiapoptotic and anti-inflammatory properties. The aim of this study was to assess neuroprotective effects of PRES in *in vitro* models of OS-mediated injury. Human neuroblastoma SH-SY5Y cells or rat brain slices were treated with hydrogen peroxide and neuronal damage as well as Pres Phytum[®] neuroprotective effects was assessed. Results showed that Pres Phytum[®] treatment reverted the increase in sub-diploid, dapi-and annexin V-positive-cells caused by hydrogen-peroxide challenge in SHSY-5Y cells. Furthermore, Pres Phytum[®] reduced ROS formation, as well as changes in the mitochondrial potential ($\Delta\Psi_m$) and caspase-3, 8 and 9 activity caused by OS. Pres Phytum[®] neuroprotective effects were confirmed also in rat brain slices. In conclusion, natural compounds still present a great challenge in finding an appropriate treatment to these devastating diseases. In this regards, the present results suggest the possibility of Pres Phytum[®] as a new preventive strategy for patients with high risk of these pathologies.

NEW DEVELOPMENTS AND PROSPECTIVES IN CATALYSIS BY METAL OXIDES

Védrine J C

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This presentation deals with acid-base, redox, oxidation catalytic reactions and more general catalytic properties of metal oxides and their recent developments in the field of heterogeneous catalysis, a field of high applied interest. It includes a description of the main metal oxide catalysts used for acid-base (various reactions), redox (partial and total oxidations) and other reactions and of the main industrial processes using or expected to use them. Some case studies have been chosen as examples of recent progresses in metal oxides syntheses leading to new 2D, 3D materials and these reactions. Particular attention is borne on recent and future researches and perspectives, mainly monitored by actual society regulations related to environmental issues, uses of biomass derivatives, carbon neutral processes and sustainability.

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CONSTRUCTION OF NANOSTRUCTURED BINARY METAL OXIDES FOR ELECTRO-CATALYSIS AND BIOSENSORS

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Development of nanostructured materials with superior morphology by simple methodology has incessantly received a significant scientific interest due to their unique physical and chemical properties for the applications in electrochemical sensors and biosensors. Binary metal oxides, particularly, metal molybdates and tungstates possess enormous attentions due to their high electrical conductivity, excellent structural stability and reproducibility compared to single one. In this regard, author fabricated different metal molybdates and tungstates with well-defined morphology and utilized as chemical sensors and biosensors in real environment and biological fluids. For occasion, two-dimensional plate-like tin molybdate was fabricated via simple co-precipitation route and employed as an electrochemical for the detection of neurotoxicity drug clioquinol. Highly sensitive and selective electrochemical sensor for the identification of postharvest scald inhibitor diphenylamine was developed using seed-like strontium molybdate modified electrode. A flower-like neodymium molybdate was prepared and studied towards the selective electrochemical sensor for the antibiotic drug nitrofurantoin. The CoWO₄ nanospheres was prepared by low temperature chemical synthesis method and evaluated towards the sensitive detection of glucose biosensor. A novel nickel tungstate was synthesized using simple hydrothermal treatment without using any surfactant or templates and investigated for its electrochemical properties for the detection of glucose biosensor. Well-crystalline 2D cerium tungstate nanosheets were prepared by a simple wet chemical approach and used as an excellent electron mediator for the fabrication of nitrite sensor. A novel ruthenium nanoparticles decorated tungsten oxide based sensor was developed and its catalytic behavior was demonstrated towards the oxidation of hydrazine. The aforementioned nanomaterials were furnished a good electrocatalytic activity with appreciable stability towards the chemical sensors and biosensors when compared with the previously reported sensors. The analytical parameters such as linear response range, sensitivity, limit of detection and reproducibility of the devices also been carried out and compared with the current state of the art.