2nd International Conference on

PHARMACEUTICAL CHEMISTRY AND DRUG DISCOVERY

June 12-13, 2019 | Bangkok, Thailand

PHARMA CHEM CONGRESS 2019



ACCEPTED ABSTRACTS

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J Pharm Chem Chem Sci 2019, Volume 3

APPLICATION OF THE STANDARDIZED FORM MAGNETITE NANOPARTICLES (ICNB) IN CREATURE SIMPLE AND PRACTICAL METHOD OF ADDITIVE MODERNIZATION OF PRESERVATION SOLUTIONS FOR RED BLOOD CELLS

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This study was devoted to the learning of the use of nanotechnology to correct the functional activity of red blood cells (RBCs) at the storage stages at a positive temperature. It was established that saline NaCl, which had previously been processed by magnetite nanoparticles (ICNB) had a marked membrane-stabilizing effect, inhibits hemolysis and increasing the sedimentation stability of preserved RBCs. The complex analysis of the obtained data allowed determining the primary mechanisms effect of the saline NaCl, which had previously been processed by ICNB on the preserved RBCs. The proposed method of additive modernization of preserved RBCs was adapted to the production process. The optimization results were obtained in creating a simple and practical method of additive modernization of preservation solutions that does not violate the compliance requirements, improves the quality, efficiency and safety transfusion of RBCs.

Note:

J Pharm Chem Chem Sci 2019, Volume 3

SYNTHESIS OF MONODISPERSE LATEXES TO CREATE IMMUNODIAGNOSTIC DRUGS

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Monodisperse latexes are the main raw material for the production of immunodiagnostic drugs. Doing a search in scientific journals and on the internet one can find plenty of publications in which provided recipes are synthesis of monodisperse latex. After reading these recipes, one can make a conclusion that the monodisperse latex is prepared likely intuitively than using programmed recipes. The main method for producing monodisperse latexes is polymerization in a highly dispersed monomer-water system (emulsion polymerization). The report presents the results of the study of the mechanism of formation of latex particles in the polymerization of different monomers in a heterogeneous static monomer-water system. Based on this study, author has developed recipes for the synthesis of monodisperse latexes. The report demonstrates electron photographs of particles of the latexes synthesized based on chloroprene, styrene and vinyl acetate.

Note:

J Pharm Chem Chem Sci 2019, Volume 3

ROLE OF ACUPUNCTURE IN CANCER AND WINDOW CANCER RESEARCH

Rahul Hajare
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Background: Acupuncture in cancer care with intermediate outcomes among really feasible and attractive therapeutic option. Complementary and alternative medicine (CAM) is commonly used by cancer patients. Recent randomized controlled trials showed that acupuncture is safe, effective and feasible for the management of cancer-related fatigue and other adverse events of anti-neoplastic therapies.

Materials & Methods: Since November 2012, author has been offering a supportive care program of 20 minutes weekly session of acupuncture for the management of chemotherapy-induced nausea/vomiting, hot flashes, cancer-related fatigue and xerostomia. A brochure regarding indications and techniques was offered to all cancer patients who received a systemic antiblastic therapy (chemotherapy, target therapy and endocrine treatment) and/or radiation therapy.

Results: More than 500 patients affected by solid tumours or lymphoma were treated in our operative unit during the period of the project. None of them preferred to receive acupuncture in addition to the specific pharmacological treatment.

Note:

J Pharm Chem Chem Sci 2019, Volume 3

PHARMA CHEMISTS, CAN YOU COLLABORATE WITH OUR BIOINORGANIC HYBRID SYSTEMS USING AI?

Takashiro Akitsu
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Recently, author has published new bioinorganic hybrid materials composed of Schiff base complexes and laccase (A metalloprotein to reduce molecular oxygen to water). In recent conference, he was presented molecular design and preliminary data of new Cu(II/I) or Mn(III/II) Schiff base complexes having redox active (anthraquinone) ligands and photochromic (azobenzene) ligands by means of electrochemical and computational methods (DFT calculations and docking simulation of protein-ligand employed in drug chemistry commonly). Thus, not only experimental methods but also computational methods may be useful to develop such bioinorganic materials. Furthermore, to decrease empirical trial-and-error using high-cost biomolecules as well as to realize sophisticated molecular design beyond the computational method or crystal structure database, he would like to employ AI (machine learning) for searching and prediction in bioinorganic studies.

Note:

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PARAMETRIC CONTRIBUTION IN PHARMACOPHORE MODELING OF BENZODIAZEPINE DERIVATIVES: A CHEM BIOINFORMATIC APPROACH

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Present study is aimed to describe the pharmacophoric requirements in reference to anti-hypertensive activity of the benzodiazepine derivatives. A set of seventy benzodiazepine derivatives with inhibitory concentration (logIC50) and verity of structural features, electronic properties, dimensional features and quantum chemical parameters are subjected to the studies using *in silico* drug design approach.

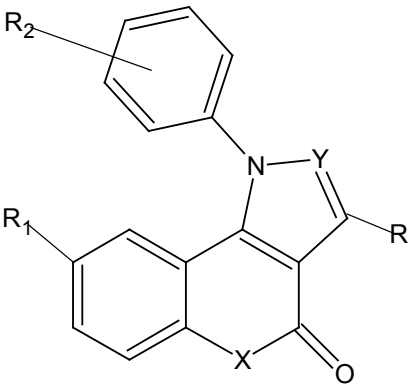

Fig.1. Parent structures of Benzodiazepine derivatives

In the process of analysis, role of structural, quantum chemical and dimensional features have been studied in respect to the pharmacophoric behavior of the benzodiazepine derivatives and their biological activity. To see more inside out about the role of electronic and energy parameters in modeling of pharmacophore for the anti-hypertensive activity of benzodiazepine derivatives, conformational study is performed using Huckel molecular orbital theory and quantum molecular mechanics method applying MM+ force field, to find out the suitable confirmer with respect to the energy and electronic features for desired biological function. Energy and other modeling parameters like electron density, net charge and stabilization factor are tested in multiple linear regression analysis helped in finding out the combination of parameters emphasizing the pharmacophoric features and can be used for the modeling of pharmacophors in benzodiazepine derivatives. Pharmacophoric features are also verified by performing docking studies using receptor ligand docking process.

Note: