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**Dr. Rajiv Dahiya** Ph.D, D.Sc, FAPP, FICCE

**Proceedings of APP 4th Annual National Convention**

Theme: 'Industry Participation in Academic Intervention: Need for Overall' Upgradation of Pharmacy Profession'

Venue: Invertis Institute of Pharmacy, Invertis University, Bareilly (UP), India

(31<sup>st</sup> January, 2015)



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[31<sup>st</sup> January, 2015 – Invertis Institute of Pharmacy, Invertis University, Bareilly (UP), India]



# ASSOCIATION OF PHARMACY PROFESSIONALS (APP)

4<sup>TH</sup> ANNUAL NATIONAL CONVENTION

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INTERVENTION: NEED FOR OVERALL UPGRADATION OF  
PHARMACY PROFESSION

Venue: Invertis Institute of Pharmacy, Invertis University, Bareilly (UP)  
(31<sup>st</sup> January, 2015)

## PLENARY & INVITED LECTURES

*E-mail: [appconv2015@gmail.com](mailto:appconv2015@gmail.com)  
Website: [www.appconnect.in](http://www.appconnect.in)*

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[31<sup>st</sup> January, 2015 – Invertis Institute of Pharmacy, Invertis University, Bareilly (UP), India]



PL-01

## DISCOVERY OF A SMALL MOLECULE IN A DISEASE INDICATION

**Dr. Krishna Menon\***

*President & Chief Scientific Officer, Cellceutix Corporation, Beverly,  
Massachusetts, United States of America*

[krishna.menon@cellceutix.com](mailto:krishna.menon@cellceutix.com)

*Received: December 16, 2014*

The term "Disease" usually refers to any condition that causes pain, dysfunction, distress, social problems or death to the person that effects or similar problems for those in contact with the person afflicted. Therefore, it includes injuries, disabilities, disorders, syndromes, infections, isolated symptoms, deviant behaviors and atypical variations of structure and function. Disease affects, not only physically, but also emotionally. Compounds used as medicines are most often organic compounds, which are often divided into the broad classes of small organic molecules (e.g., atorvastatin, fluticasone, clopidogrel) and "biologics" (infliximab, erythropoietin, insulin glargine), the latter of which are most often medicinal preparations of proteins (natural and recombinant antibodies, hormones, etc.). Ligand design includes design of a small molecule that will bind tightly to its target. Although modeling techniques for prediction of binding affinity are reasonably successful, there are many other properties, such as bioavailability, metabolic half-life, side effects, etc., that first must be optimized before a ligand can become a safe and efficacious drug. These other characteristics are often difficult to predict using rational drug design techniques. Structure-based drug design (or direct drug design) relies on knowledge of the three dimensional structure of the biological target obtained through methods such as x-ray crystallography or NMR spectroscopy. The structures of a compound and the functions of each moiety or the active groups in a compound should be known. Different moieties may be responsible for intrinsic activity and affinity. Present presentation will cover ADMET, synthesis in small quantities in milligram, synthesis in gram quantities, regulatory toxicity studies, IND submission, clinical trials, cGMP manufacturing of API and drug product, pharmacovigilance, the molecule and its life.

PLENARY LECTURE

【A1】



PL-02

## FUTURISTICS OF INDIAN PHARMA INDUSTRY: GROWTH AND PROSPECTS

**Dr. Ashutosh Kar\***

*Guest Professor, School of Pharmaceutical Sciences, Apeejay Stya University, Gurgaon, Haryana*

[ashukar1@yahoo.com](mailto:ashukar1@yahoo.com)

*Received: January 20, 2015*

The Indian Pharma Industry has made a quantum leap forward in the recent past in different fields. It has become one of the front runners in the production of high quality Generic Drugs. Importantly, India's rich client markets e.g. U.S. and E.U. Nations have accomplished a gallant success. Besides, being the world's choicest nation with special reference to: Manufacturing Locations, Outsourcing activities, R & D profile, Clinical trial facilities, Low wages and excellent administrative centres. India has the tremendous potential and opportunities for: Generics (also Biotechnology generics), Biotechnology, Outsourcing (Contract manufacturing) and R & D outsourcing as well. India claims to be the third largest nation in the world in terms of volume. India Brand Equity Foundation (IBEF) has projected the India Pharma Market to grow at a compound annual growth rate (CAGR) of 14-17% between 2012-16. India joined the league of top 10 Global Pharma Markets in sales by 2020 (with a turnover reaching USD 50 billion). India's top-notch status in the domain of outsourcing, IT and clinical data management hub based on: Rich resource and talent pool, Technological innovation, Creditable quality operations flexibility, Cost effectiveness, Time to market and competitive advantages. Leading the pack Indian players getting set to attain high-risk high-return field of new drug research activities.

PLENARY LECTURE

**[ A2 ]**



PL-03

## MUCUNA PRURIENS VERSUS LEVODOPA IN PARKINSON'S DISEASE: AN INDUSTRIAL PERSPECTIVE

**Dr. Sanjay Kasture\*** Post-doc (Italy)

*Principal & Professor, Sanjivani College of Pharmaceutical Education and Research,  
Kopargaon, Ahmednager, Maharashtra  
[principal@sanjivanipharm.org.in](mailto:principal@sanjivanipharm.org.in)*

*Received: November 25, 2014*

Mucuna pruriens (MP) has long been used in Indian traditional medicine as support in the treatment of Parkinson's disease. In our endeavor to evaluate and compare the antiparkinsonian activity of Mucuna pruriens with levodopa, two sets of experiments were carried out. In rat model of Parkinson's disease (PD), an extensive evaluation of the antiparkinsonian effects of an extract of MP seeds known to contain, among other components, 12.5% L: -dihydroxyphenylalanine (L: -DOPA), as compared to equivalent doses of L: -DOPA. The study revealed that an acute administration of MP extract at a dose of 16 mg/kg (containing 2 mg/kg of L: -DOPA) consistently antagonized the deficit in latency of step initiation and adjusting step induced by a unilateral 6-hydroxydopamine lesion, whereas L: -DOPA was equally effective only at the doses of 6 mg/kg. At the same dosage, MP significantly improved the placement of the forelimb in vibrissae-evoked forelimb placing, suggesting a significant antagonistic activity on both motor and sensory-motor deficits. The effects of MP extract were moreover investigated by means of the turning behavior test and in the induction of abnormal involuntary movements (AIMs) after either acute or subchronic administration. MP extract acutely induced a significantly higher contralateral turning behavior than L: -DOPA (6 mg/kg) when administered at a dose of 48 mg/kg containing 6 mg/kg of L: -DOPA. On subchronic administration, both MP extract (48 mg/kg) and L: -DOPA (6 mg/kg) induced sensitization of contralateral turning behavior; however, L: -DOPA alone induced a concomitant sensitization in AIMs suggesting that the dysknetic potential of MP is lower than that of L: -DOPA. MP (48 mg/kg) was also effective in antagonizing tremulous jaw movements induced by tacrine, a validated test reproducing parkinsonian tremor.

PLENARY LECTURE

【 A3 】



IL-01

## OVERVIEW OF GMPs

**Mr. P. P. Sharma\***

*Ex-Deputy Drugs Controller, Delhi & Ex-Vice President, Pharmacy Council of India (PCI)  
Pharmaceutical Consultant and Guest Faculty, Amity School of Pharmacy, Amity University, Noida, Uttar Pradesh  
[ppsharma@gmail.com](mailto:ppsharma@gmail.com)*

*Received: November 11, 2014*

Earlier approach to quality control of drugs was to manufacture them and test at the end. This approach could not prevent mishaps including those where some lives were lost. K. Harris amendment in 1962 in US law stipulated that a drug shall be considered adulterated, if methods used in its mfg./processing, testing, packaging or storing did not conform to GMP. In 1968, first draft of WHO GMP appeared. In 1973, Guide to Good Pharmaceutical Manufacturing practice (Orange Guide) appeared in UK. In India, GMPs were included in Schedule M to the Drugs and Cosmetics Rules. All these guidelines have been reviewed and updated. WHO GMPs are international Guidelines. The current version appears in the WHO Technical Report Series 961. The main objectives of GMP are: conformance to the predetermined specifications, to minimize contamination, to eliminate error and to produce product of consistent quality. WHO GMPs have main principles and supplementary guidelines. The main principles have been covered in various elements which include Quality Assurance, Good Manufacturing Practices for Pharmaceutical Products, Sanitation and Hygiene, Qualification and Validation, Complaints, Product Recalls, Contract Production and Analysis, Self-inspection, Quality Audits and Supplier's Audits and Approval, Personnel, Training, Personal Hygiene, Premises, Equipment, Materials, Documentation, Good Practices in Production, Good Practices in Quality Control. There are various supplementary guidelines e.g. Supplementary GMP for Sterile Products, Supplementary GMP for active pharmaceutical ingredients (APIs).

INVITED LECTURE

**【A4】**



IL-02

## MEDICINAL CHEMIST'S PERSPECTIVE OF MOLECULAR MODELING

**Dr. Ranganathan Balasubramanian\*** Post-doc (USA)

*Head, Department of Pharmaceutical Chemistry, Amrita School of Pharmacy,  
Amrita Vishwa Vidyapeetham University, Health Sciences Campus, Kochi, Kerala*  
[ranganathanb@aims.amrita.edu](mailto:ranganathanb@aims.amrita.edu)

*Received: November 25, 2014*

Today's presentation will focus on how the field of computational chemistry in general, and molecular modeling in particular, have served the drug discovery endeavor. Coming from a medicinal chemist, the narration provides an overview of some of these tools as a bench chemist would perceive them and would hopefully prepare the audience for the technical session(s) to follow. Beginning with a question of whether medicinal chemists should engage in molecular modeling, and if so, what benefits it would bring in terms of productivity to the drug creation process, the lecture aims to cover the different arms of drug design with a focus on sensitizing the listeners to the commonly used terminology in this discipline as well as alerting them about the availability of some free downloadable software for simple applications. Since the entire drug development process from lead identification to commercialization is practiced in big pharma, a strong industrial flavor is sustained throughout the lecture and the evolution of different ideas or their applications is portrayed in that sense. While hailing computer-aided molecular design as a viable alternate model in drug discovery that nicely complements classic screening, the lecture notes that the caveats of these techniques ought to be kept at the back of one's mind while applying them and concludes by reiterating the importance of chemical intuition in this fascinating art.

INVITED LECTURE

【A5】



IL-03

## QSAR AND PHARMACOPHORE MAPPING: CASE STUDIES

**Dr. Vipin Kumar\***

*Head, Department of Pharmacy, School of Chemical Sciences and Pharmacy,  
Central University of Rajasthan, Bandersindri, Ajmer, Rajasthan*

[vipkumar@curaj.ac.in](mailto:vipkumar@curaj.ac.in)

*Received: November 04, 2014*

QSAR and Pharmacophore mapping are the key tools of ligand based drug design techniques. In the present talk, the case studies of working with both of these tools have been discussed. Quantitative structure activity relationship studies have been performed with 32 synthetically derived analogues for their inhibitory effects on monoamine oxidase-A using two-dimensional topological descriptors. The statistical analysis has shown that excellent results are obtained by using multiple linear regression method. The best model was selected based on the highest  $R^2$  value (0.904). The results are discussed critically using variety of statistical parameters such as squared correlation coefficient ( $R^2$ ), adjusted  $R^2$ , predicted residual sum of square (PRESS) and Pogliani's quality factor (Q). The models were validated by using the method of leave-one and leave-many out cross-validation methods. Secondly, a dataset of pyrrolopyridine derivatives inhibiting mitogen-activated protein kinase activated protein kinase-2 (MK2) has been selected to perform three dimensional pharmacophore mapping studies. To understand the essential structural features for MK2 inhibitors, pharmacophore hypothesis were built on the basis of a set of known MK2 inhibitors selected from literature using PHASE program. Three pharmacophore models with one hydrogen-bond acceptor (A), two hydrogen-bond donors (D), one hydrophobic group (H) and one aromatic ring (R) as pharmacophoric features were developed. Amongst them the pharmacophore hypothesis ADDHR1 yielded a statistically significant 3D-QSAR model with 0.926 as  $R^2$  value and was considered to be the best pharmacophore hypothesis. The developed pharmacophore model was externally validated by predicting the activity of test set molecules. The squared predictive correlation coefficient of 0.882 was observed between experimental and predicted activity values of test set molecules.

INVITED LECTURE

**[A6]**





IL-04

## MOLECULAR SELF ASSEMBLY FOR CREATING THE NANOSTRUCTURES AND THEIR APPLICATIONS IN DRUG DELIVERY

**Dr. Atindra D. Shukla\*** Post-doc (Israel)

*Associate Professor, Shah-Schulman Center for Surface Science & Nanotechnology,*

*Dharamsinh Desai University, Nadiad, Gujarat*

[atindra.sscssn@ddu.ac.in](mailto:atindra.sscssn@ddu.ac.in)

*Received: November 25, 2014*

Molecular level control over self-assembled system is the ultimate desire of researchers across the world to achieve perfect or near perfect drug delivery satisfying all the pre-requisites. Understanding of molecular functionality influencing the molecular interactions giving rise to molecular self-assembly is the key to design effective drug carrier system. Nano scale drug carriers are found to be potent, safe and versatile and hence getting popularity rapidly. Self-assembly is proving to be a viable route to create nano structured drug delivery vehicles. The USP of self assembled architecture adopted for drug delivery is control over size, better bioavailability and greater compatibility with human body, targeted and tunable drug release profile. Here in we have attempted to develop new polymer/surfactant blends for use in improved drug delivery system. Surfactant and polymer mixtures in solution are used for various pharmaceutical drug delivery systems as well as many industrial applications in the cosmetic, food, paint, enhanced oil recovery, and other sectors. It is particularly the combination of a certain polymer with a specific surfactant at well-chosen concentrations that determines the fine tuning of the rheology of its aqueous solutions. Polymer-surfactant mixtures are increasingly being used in a wide range of domestic, industrial and technological applications. The mixtures are in general aqueous-based and polymers are added to the systems to control rheology and stability and to manipulate surface adsorption. Interactions within (such formulations) are driven by hydrophobic, dipolar and electrostatic forces. The complex nature of these interactions and the desire to understand them has led to a wealth of research on the subject, both experimental and theoretical.

INVITED LECTURE

【A7】



IL-05

## OPHTHALMIC NANO-PHARMACEUTICALS: VISIONARY APPROACH

**Dr. Kashyap Nagariya\***

*Associate Research Scientist, Zydus Cadila Healthcare Limited, Ahmedabad, Gujarat*

[bschhikara@gmail.com](mailto:bschhikara@gmail.com)

*Received: November 17, 2014*

With the development in nanotechnology, it is now possible to produce drug formulation as nanopharmaceuticals that can be utilized in a variety of innovative ways. New drug delivery pathways can now be used that can increase drug efficacy and reduce side effects. These nano formulations offer several advantages including elimination of toxicity because of nonionic surfactants and improved efficacy due to the greater dose of the drug that can be administered and delivered. For better development of the ocular nanopharmaceutical systems, it is essential to understand the pharmaceutically relevant properties of nanopharmaceuticals. Nanopharmaceuticals offer unique properties as compared to micro or macroparmaceuticals. Salient features include small size, high surface area, easy to suspend in liquids, deep access to cells and organelles, variable optical and magnetic properties, particles smaller than 200 nm can be easily sterilized by filtration with a 0.22  $\mu$ m filter. Nanopharmaceutical delivery systems have potential applications for ocular drug delivery. However, nanopharmaceuticals are not a universal solution for all problems associated with ocular drug delivery. Many of the problems associated with the delivery of ocular therapeutics including rapid clearance, short duration of action, and inefficient uptake can in part be addressed using Nanopharmaceutical systems. Nanopharmaceuticals coated or prepared with mucoadhesive or bioadhesive polymers will likely prolong precorneal residence time of the drug in the tear film and help increase drug uptake into the cornea and conjunctiva following topical administration.

INVITED LECTURE

**【A8】**



IL-06

## BONE DEPOSITION STUDY OF ANTI-LEPROTIC DRUG CLOFAZIMINE BY A SENSITIVE REVERSE PHASE LIQUID CHROMATOGRAPHY METHOD

**Dr. Jiaur R. Gayen\***

*Scientist, Pharmacokinetics and Metabolism Division, CSIR- Central Drug Research Institute,*

*Lucknow, Uttar Pradesh*

[jr.gayen@cdri.res.in](mailto:jr.gayen@cdri.res.in)

*Received: October 30, 2014*

Clofazimine (CLF) is a rhimino phenazine dye with a wide antimycobacterial spectrum and an important constituent of the triple-drug regimen (dapsone + rifampicin + clofazimine) recommended by WHO for the treatment of leprosy. CLF has been reported to be highly distributed in various tissues like liver, spleen, brain, lungs, kidneys, heart, adrenal glands, gall bladder, small intestine and placenta in the form of reddish-orange crystals. CLF on multiple dosing causes clastogenic effect due to genotoxicity and becomes toxic itself by accumulating into the body. We developed a simple, sensitive and precise reverse phase liquid chromatographic (RP-HPLC) method coupled with an extraction procedure for the quantification of CLF from rat bone marrow cells as well as from plasma. CLF and chlorzoxazone (internal standard) were extracted by liquid-liquid extraction from plasma and rat bone marrow cells. The chromatographic separation was performed in isocratic mode by the mobile phase consisting of 10 mM ammonium formate (pH 3.0 with formic acid) and acetonitrile in a ratio of 50:50 (v/v). The method was accurate and precise in the linear range of 15.6–2000.0 ng/ml. After single oral dose of 20 mg/kg, the maximum concentration of CLF in plasma and bone marrow cells were obtained at 12 h with the concentrations of 600.94 and 915.42 ng/ml respectively. The  $AUC_{0-72h}$  and mean elimination half life ( $t_{1/2}$ ) of CLF in bone marrow cells were 40516.59 h.ng/ml and 45.69 h respectively, which signified the low body clearance and high deposition of CLF in bone marrow cells. The pharmacokinetic investigation confirmed that the CLF endure for a long period in circulation even after single oral dose may be due to deposition in bone marrow.

INVITED LECTURE

**[ A9 ]**



IL-07

## PRESCRIPTION MEDICINES

**Dr. Suresh V. Chennupati\***

*Principal & Professor, Mother Teresa Pharmacy College, Sathupally, Khammam, Telangana*  
[sureshchennupati@rediffmail.com](mailto:sureshchennupati@rediffmail.com)

*Received: December 05, 2014*

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Medicines can help you feel better and get well when you are sick. The two main types of medicine are prescription and over-the-counter (OTC). Prescription drugs can be used to treat a variety of health complications but can also be abused and become dangerous. But if you don't follow the directions, medicines can hurt you. You can lower the chances of side effects (unwanted or unexpected effects) from medicines by following directions carefully. Side effects may be mild, like an upset stomach. Other side effects can be more serious, like damage to your liver. Follow the directions from pharmacist or doctor to get the best results.

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INVITED LECTURE

**[A10]**



IL-08

## ENTREPRENEURSHIP AND INTELLECTUAL PROPERTY RIGHTS

**Mr. Rahul Taneja\***

*Scientist - IPR, Patent Information Centre, Department of Science and Technology,  
Government of Haryana, Panchkula, Haryana*

[rahulipr@hotmail.com](mailto:rahulipr@hotmail.com)

*Received: January 07, 2015*

There was a time when property of any individual or organization was measured in terms of physical tangible assets like land, buildings, valuables like cars, gold, machinery etc. But with passage of time, intangible assets also got recognition, and now we know these intangible assets as Intellectual Property or IP. Now, in modern concept of ownership, we count both intangible and tangible property as property associated with an individual or an organization. Intellectual Property is the Property, which has been created by exercise of Intellectual Faculty. It is the result of persons Intellectual Activities. Thus Intellectual Property refers to creation of mind such as inventions, designs for industrial articles, literary, artistic work, symbols which are ultimately used in commerce. Intellectual Property rights allow the creators or owners to have the benefits from their works when these are exploited commercially. These rights are statutory rights governed in accordance with the provisions of corresponding legislations. A Patent is a statutory right for an invention granted for a limited period of time to the patentee by the Government, in exchange of full disclosure of his invention for excluding others, from making, using, selling, importing the patented product or process for producing that product for those purposes without his consent. Patent protection is territorial right and therefore it is effective only within the territory of India. However, filing an application in India enables the applicant to file a corresponding application for same invention in convention countries, within or before expiry of twelve months from the filing date in India. It is granted for Invention provided invention must be novel, technically advanced or economic significant and industrially useful. India is far behind in terms of Patent filing in healthcare as compared to other countries such as United States of America, China, and European Countries etc.

INVITED LECTURE

【A11】



IL-09

## NOVEL MULTIPARTICULATES TECHNOLOGY

**Dr. Vipin Saini\***

Dean, M. M. College of Pharmacy, M. M. University, Mullana, Ambala, Haryana  
[vipinsaini31@rediffmail.com](mailto:vipinsaini31@rediffmail.com)

Received: January 07, 2015

Controlled release formulations in tablet form are many but over the years the spheroids/multiparticulates or pellet formulations have gained immense popularity owing to their superiority over the former in several respects: controlled absorption with resulting reduction in peak to trough ratios, targeted release of the drug to specific areas within the gastrointestinal tract, absorption of drug irrespective of the feeding state, minimal potential for dose dumping, facility to produce combination of dosage form, etc. Spherical oral dosage forms such as pills have been used in the pharmaceutical industry for a long time, but the full impact of systematically agglomerated spherical units or pellets on controlled release oral dosage form design and performance was not realized till early 1970s. These solid oral dosage forms consists of a multiplicity of small discrete particulates, which include pellet and granules. These systems provide flexibility during formulation development and therapeutic benefits to patients in last two decades. The significant advantage of multiparticulates is that they can be divided into desired doses without formulation or process changes. Furthermore, controlled-release multiple-unit dosage forms are less susceptible to dose dumping than the reservoir or matrix type, single unit tablet since the drug release profile does not depend on the drug release properties of a single unit. Technological advances in dosage form design, the advent of highly specialized equipments, and the popularity of controlled-release dosage forms as a means of drug delivery have made multiparticulates a viable and attractive alternative to single dosage forms. Multiparticulates (pellets) also have numerous therapeutic advantages over single unit dosage forms. When taken orally, multiparticulates generally disperse freely in the gastrointestinal tract, maximize absorption, minimize side effects, and reduce inter-and intra patient variability.

INVITED LECTURE

**[A12]**



IL-10

## HELMINTHIC MANIFESTATION IN UTTAR PRADESH : CURRENT SCENARIO

**Dr. Emdad Hossain\***

*Head, Department of Pharmacology, Pharmacy College, Azamgarh, Uttar Pradesh*

[emdad@rediffmail.com](mailto:emdad@rediffmail.com)

*Received: January 07, 2015*

Helminths are specific type of parasites which are responsible of foremost cause of different life threatening manifestation for mammals including human round the globe specifically in third world countries. In the recent survey it was found that more than one-third of the world population is helminth-infected. Uttar Pradesh comes under the backward category in India for poor health and sanitation system. Eastern area is more affected than western part of the state. Whipworm, roundworm and hookworm together affected major people in the state. School-going children have affected much more by the hookworm. The morbidity associated with heavy hookworm infection is predominantly manifested as impaired physical and cognitive development in children. Infertility was observed with human infected by lymphatic filariasis. Numerous meat-eating people also affected by tape worm due to improper cooking. Currently trematodes also affected domestic animals and human as well; liver fluke, blood fluke, intestinal fluke are main parasites manifested them. The study explained details about current scenario of helminthic manifestation in Uttar Pradesh, will be useful for the preventive measures.

INVITED LECTURE

**【A13】**



IL-11

## PHARMACEUTICAL PATENT SYSTEM IN INDIA

**Dr. Saurabh Dahiya\***

*Department of Pharmaceutics, School of Pharmaceutical Sciences, Apeejay Stya University, Gurgaon, Haryana*  
[saurabhdahiya@gmail.com](mailto:saurabhdahiya@gmail.com)

*Received: January 09, 2015*

A patent is a grant by the government of exclusive rights in a new, useful and non-obvious invention in exchange for the disclosure of that invention. The patent system in India is governed by the Patents Act, 1970 as amended by the Patents (Amendment) Act, 2005 and the Patents Rules, 2003 as amended by the Patents (Amendment) Rules, 2006. The latest amendment in the year 2005 was made in order to bring the patent law in India into compliance with the TRIPS Agreement and to introduce patents for drugs, medicines and food products. The Patent system is administrated under Department of Industrial Policy and Promotion, Ministry of Commerce and Industry, Government of India. There are four patent offices in India, located at Delhi, Kolkata, Mumbai and Chennai, headed by the Controller General of Patents, Designs and Trade Marks. The latest Amendment enabled Patent Act to grant Product Patent for Pharmaceutical substances and brought deletion of exclusive marketing rights from the act. Patent rights are territorial in nature. It is important that applicants file in India as early as possible, as India follows a "first to file" system that gives priority to the first inventor to file an application. This is irrespective of when the applicant plans to commence use of the invention in India. The term of a patent is twenty years from the date of the application, irrespective of whether it is filed with provisional or complete specifications. To keep the patent valid for the term of 20 years a renewal fee has to be paid every year. If the renewal fee is not paid within the prescribed time, the patent will cease to have effect. In some cases, India has granted a compulsory license to a local manufacturer to supply a patented drug at a lower cost than the price of innovator company, where reasonable requirements of the public were not being met viz. patented drug not available at reasonable price or granted patent not being fully commercially exploited thus paving the way for access to affordable medicines for all.

INVITED LECTURE

**[A14]**





IL-12

## SUSTAINED RELEASE DOSAGE FORMS

**Mr. Abhishek Raj\***

*Deputy Manager (R & D), Quest Pharmaceuticals Private Limited, Birgunj, Nepal*  
[abhishekr4@gmail.com](mailto:abhishekr4@gmail.com)

*Received: January 14, 2015*

The aim of present study is to develop oral sustained release dosage forms with different techniques like wet granulation, dry granulation and direct compression. Various polymers and fillers are used at varying concentration to control the drug release. The dissolution studies for these formulations are carried out and it is indicated that the drug release can be modulated by varying the concentration of polymers and fillers. Another approach to control the drug release is by coating with suitable polymer. These types of drug delivery systems are designed to achieve prolonged therapeutic effect by continuously releasing medication over an extended period of time after administration of single dose. In case of injectable dosage form, this period may vary from days to month. In case of orally administered forms, however, this period is measured in hours and critically depends on the residence time of the dosage form in gastro intestinal tract. The basic goal of this therapy is to achieve steady state blood level that is therapeutically effective and non toxic for an extended period of time. Maximum bioavailability with a minimum dose can be achieved by these types of formulations. Some of the SR tablet formulation like Metformin, Metoprolol Succinate, Alfuzosin will be discussed in this study.

INVITED LECTURE

**【A15】**



IL-13

## MAGNETIC NANOPARTICLES MEDIATED TARGETED DRUG DELIVERY SYSTEMS

**Dr. S. Latha\*, P. Selvamani, C. Prabu, M. Arputha Bibiana**

*Department of Pharmaceutical Technology & Centre for Excellence in Nanobio Translational Research,  
Anna University, BIT Campus, Tiruchirappalli, Tamil Nadu*

[lathasuba@yahoo.co.in](mailto:lathasuba@yahoo.co.in)

*Received: January 19, 2015*

The presentation would include fundamentals of magnetic nanoparticles that have been exploited for targeted drug delivery. Further the results of the development of a sustained-release dosage form for methotrexate that could be used for the magnetic targeted drug therapy of rheumatoid arthritis were included in detail.  $\text{CaCO}_3$  microparticles were prepared by biomimetic mineralization method *i.e.* by addition of 50 ml of 0.2 M calcium chloride solution to 50 ml of 0.2 M sodium carbonate solution mixed earlier with 200 mg of polystyrene sulphonate. Size of  $\text{CaCO}_3$  / PSS were characterized by SEM was found to be ~5 microns and exhibited spherical and porous morphology with a zeta potential of -11 mV. Methotrexate was loaded to  $\text{CaCO}_3$  microparticles using solvent evaporation technique 200 mg of methotrexate was dissolved in 10 ml of absolute ethanol. Drug solution was added to prepared microparticles of  $\text{CaCO}_3$  (400 mg) that was previously dispersed in water under stirring (400 r.p.m.) at room temperature for 12 h and further evaporated to dryness. The drug loaded microspheres were coated with anionic and cationic polyelectrolytes by layer-by-layer technique alternatively for three times using polyallylamine hydrochloride and polystyrene sulphonate respectively. The electrolyte coating over the surface of microparticles was confirmed by zeta potential measurements.

INVITED LECTURE

**【A16】**



IL-14

## MEDICAL DEVICES AND AIDS TO DAILY LIVING FOR GERIATRIC PATIENTS: A PHARMACISTS PERSPECTIVE

**Dr. Pankaj Jain\***

*Consultant (Pharmacolegal), Vertex Solutions, Rohtak, Haryana*

[jainp7@gmail.com](mailto:jainp7@gmail.com)

*Received: January 21, 2015*

Treatment in hospitals is expensive and improved technology enables individuals to stay at home or to go home earlier from hospital, and also permits earlier diagnosis and self-care management. Both medical and assistive devices allow less costly home-based treatment. Medical devices include a wide range of items. Any article, instrument, apparatus, or contrivance, including any component, part or accessory thereof, manufactured, sold or represented for use in the diagnosis, treatment, mitigation or prevention of a disease, disorder or abnormal physical state or its symptoms. When choosing a medical or assistive device, several factors need to be considered such as the physical, the cognitive and the emotional characteristics. Types of medical devices include for bathroom safety, mobility and transfer, patient comfort aids, incontinence aids, home diagnostic tools, respiratory aids, wound care products, surgical sundries, home intravenous products, sensory aids, sports and orthopedic products and home safety equipment. As pharmacist is the first health care professional approached by patient before the start of use of any medical device or for best use of medical device a pharmacist must be well verse with all the medical devices available especially in geriatric healthcare setup.

INVITED LECTURE

**【A17】**



IL-15

## APPLICATION OF MOLECULAR DOCKING IN DRUG DESIGN

**Dr. Jainendra Jain\***

*Principal, RamEesh Institute of Vocational and Technical Education, Greater Noida, Uttar Pradesh*

[jainendrem@gmail.com](mailto:jainendrem@gmail.com)

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Docking based drug design is one of the most logical approaches in drug discovery paradigm. The structured knowledge of the binding capabilities of the active site residues to specific groups on the agonist and antagonist leads to proposals for synthesis of very specific agents with a high probability of biological action. Molecular docking and molecular mechanics are the two most commonly used methodologies in CADD. In the present study, VLife MDS 4.3.3 was employed for virtual screens of most active compounds (J<sub>14</sub>, J<sub>26</sub>, J<sub>30</sub>, J<sub>32</sub>, J<sub>33</sub>, RNH<sub>4</sub> and RNH<sub>12</sub>) which have shown promising anticonvulsant results in animal studies. These compounds were studied for selective inhibition of gamma amino butyrate aminotransferase (GABA AT), a potential anticonvulsant drug target. All these compounds have shown strong H-bonding interactions with LYS 329A residue of GABA AT, thus strongly suggesting GABA AT inhibition as possible mechanism of action.

INVITED LECTURE

**【 A18 】**



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## ASSESSMENT OF DRUG USE PATTERNS AND INTERVENTIONS TO PROMOTE THE RATIONAL USE OF MEDICINES

**Dr. Saurabh Kumar Banerjee\***

*School of Pharmaceutical Management, The IIPHMR University, Jaipur, Rajasthan*

[saurabh@iihmr.edu.in](mailto:saurabh@iihmr.edu.in)

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Irrational use of medicines is an extremely serious global problem that is uneconomical and detrimental to a nation's economy. Medicine use is rational (appropriate, proper, correct) when patients receive the appropriate medicines, in doses that meet their own individual requirements, for an adequate period of time, and at the lowest cost both to them and the community. Common types of irrational medicine use are: The use of too many medicines per patient (Polypharmacy); inappropriate use of antimicrobials, often in inadequate dosage, for non-bacterial infections; over-use of injections when oral formulations would be more appropriate; failure to prescribe in accordance with clinical guidelines. The objective of this study is to suggest the methodology which could be undertaken to measure the type and degree of irrational use of medicines in context to general prescribing and quality of care problems at primary health care facilities and suggest interventions which could be undertaken for promoting the rational use of the medicines. The following WHO drug use indicators can be used to identify general prescribing and quality of care problems at primary health care facilities. These are namely Prescribing Indicators: Average number of medicines prescribed per patient encounter, percent medicines prescribed by generic name, percent encounters with an antibiotic prescribed; Patient Care Indicators: Average consultation time, Average dispensing time, percent medicines actually dispensed; Facility Indicators: Availability of essential medicines list or formulary to practitioners, availability of clinical guidelines; Complementary Drug Use Indicators: Average medicine cost per encounter, percent prescriptions in accordance with clinical guidelines. Four types of interventions strategies to improve drug use can be distinguished as educational, managerial, financial and regulatory. Monitoring medicine use and using the collected information to develop, implement and evaluate strategies to change irrational medicine use behavior are fundamental to any national programme to promote rational use of medicines.

INVITED LECTURE

**【 A19 】**