A Quarterly News Letter of Krupanidhi College of Pharmacy, Bangalore I FOR PRIVATE CIRCULATION ONLY

# **SYNERGIA**

Updates Zeitgeist

Fun

## WORLD 25 SEPTEMBER PHARMACISTS DAY

## PHARMACISTS: caring for you

EDIT

#### Dear all.

During this quarter, KCP was abuzz with activities. Starting from the freshers induction to the first sessional examinations, every day was busy, fulfilling and rewarding. KCP is home to several innovative practices like the finishing school program mentored by Prakash V Mallya of Center for Pharmaceutical Professional Advancement, which creates industry coveted talents. In a proud note, KCP has bagged top academic laurels too, in doing so has scripted history in the highest number of academic laurels and pass percentages across all courses. This achievement is because of the unique "Gurukula" system of education followed here, where every student gets continuous individual attention and helps them achieve their academic goals.KCP, has also signed an MoU with Oiqihar Medical University in China will enable KCPlans to do research collaborations research and do exchange student and and teaching tenures with this top state university located in northern China. KCPlans had a fun during the Freshers and Teachers Day function and freshmen were guided by the invited luminaries. The World Pharmacists Day was too was marked with verve and was observed in a socially relevant manner. The NSS unit of KCP in collaboration with NIMHANS and Rotary International conducted a blod donation camp, in which the student and faculty volunteers donated blood to perpetuate the credo of this day – Pharmacists: Caring for You. **Rajeswari R, Editor** 

#### VOL.5 ISSUE 4

Brand Name ( Active Ingredient)	Indication	Sponsor	Approval
Musculoskelatal system			
Erelzi (Etanercept ) Injection	Rheumatoid Arthritis, Juvenile Idiopathic Arthritis, Psoriatic Arthritis, Ankylosing Spondylitis, Plaque Psoriasis	Sandoz Inc.	August 2016
Exondys 51 (Eteplirsen)	Duchenne Muscular Dystrophy	Sarepta Therapeutics	Sep, 2016
Endocrinology			
Adlyxin (Lixisenatide)	Improve blood glucose level in Diabetes Mellitus	Sanofi-Aventis US	Jul, 2016
Oncology			
Syndros (Dronabinol oral solution)	Anorexia associated with AIDS & nausea, vomiting associated with cancer chemotherapy	Insys Therapeutics	JUI, 2016
Sustol (Granisetron) Extended release injection	Chemotherapy induced nausea & vomiting	Heron Therapeutics	August 2016
Keytruda (Pembrolizumab)	Head and neck squamous cell cancer	Merck	August 2016
Arzerra (Ofatumumab)	Treatment of CLL	Genmab	August 2016
Ophthalmology			
Humira (Adalimumab)	Treatment of uveitis	Abbvie	July 2016
Xiidra (lifitegrast)	Treatment of dry eye disease	Shire US, Inc.	July 2016
Immunology			
Cuvitru (immune globulin subcutaneous (human)) Injection	Primary immunodeficiency	Shire US ,Inc	Sep, 2016
Neurology			
Yosprala (Aspirin and Omeprazole	Ischemic Stroke Prophylaxis, Gastric Ulcer Prophylaxis	Aralez Pharmaceuticals Inc.	Sep, 2016
Respiratory system			
Flonase sensimist (Fluticasone furoate)	Treatment of allergic rhinitis	GSK Consumer Healthcare	August 2016

Source: Centerwatch, USFDA, Current as on 28 Sep 2016. Compiled by Rejitha Thomas, Asst Prof, KCP.

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## Oncology Pharmacy Practice in India: A Need of the Hour



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Quality cancer care always remains a challenge in developing countries due to financial limitations, shortage of skills, limited research and diverse regulations for patient care. Cancer care in India has many challenges due to diverse patient populations, limited access to newer medicines, affordability of the patients to the existing cancer treatment, lack of medical insurance or insurance with limited benefits, limited financial support from government, poor awareness on importance of oncology pharmacy practice and oncology nursing care. Concept of oncology pharmacy services is in the developing stage in most of the Indian cancer hospitals. There are no residency programs available to build capacities to practice as oncology pharmacist. No structured training courses are available for nurses who want to gain exposure in the area of cancer care and hence, most of the nurses involved in cancer care are only general practitioners and not a specialist. Moreover, compare to other developed countries regulatory requirements to practice as nurse are limited in India and may also differ based on type of health care setting.

Due to this reality, over all burden of patient care remains on the oncology clinicians. Also, oncologists in India usually provide consultations to relatively higher number of patients compare to other clinicians in other developed countries. Clinicians also has limited opportunities to update their knowledge on newer drugs and updates on existing drugs. Moreover, Indian pharmaceutical market is highly influenced by pharmaceutical marketing and many clinicians even today relies upon medical representatives for pharmaceutical updates. In the backdrop of this reality, there is a great scope and demand for implementing oncology pharmacy services in Indian cancer hospitals.

Oncology Pharmacist has broad scope of providing various clinical pharmacy services to the cancer patients and health care professionals involved in cancer care. Due to abundant amount of research we have plenty of chemotherapeutic agents and targeted molecules in the market. Availability of high number of anti-cancer drugs in the market creates a demand for the most recent, critically evaluated and patient

specific information about drugs to the clinicians and patients. Clinical Pharmacist can meet this demand by being a part of health care team and by working as drug information provider. It is well evident that all the antineoplastic agents require safety monitoring before initiation of therapy and during therapy as well. Team work of clinical pharmacist with oncologists can always improve the quality of patient safety monitoring throughout the course of treatment. Clinical pharmacists can provide recommendations in form of dosage adjustments, additional supportive care and patient education to ensure patient safety while on cancer treatment. Due to complex nature of cancer care, there is high risk of medication errors to occur and oncology pharmacists can work together with nurses, clinicians and patients to minimize occurrence of these errors. Prevention of medication errors certainly benefits to reduce morbidity, mortality and health care expenditure. Oncology Pharmacist can always maintain their role as medication counsellor through active partnership with patients. Oncology Pharmacists can also involve in the patient centered, system centered and regulation centered research with ultimate aim of improving rational drug use. Unlike other clinical disciplines, oncology drugs needs more precautions while its preparation and administration and hence, pharmacist is the key person to manage required precautions by ensuring high quality aseptic transfer of anti-cancer drugs.

In India, JSS University College of Pharmacy, Mysore, had taken initiative to implement oncology pharmacy practice and research. Oncology pharmacy services in JSS practice includes services like medication therapy management, preparation of chemotherapy, biotherapy and IV admixtures, medicine & therapeutic information, patient medication counseling, adverse drug reaction reporting, monitoring and management. Oncology pharmacists are driving force to run medication errors reporting and prevention program in cancer patients. In general, Oncology Pharmacist can be a *practitioner, educator*, and *researcher* in order to promote rational drug use in cancer care.

KCP jointly organizes Indian Association of Colleges of Pharmacy, *Pharmacy Practice Advanced Leaning Module 10 - Oncology 2 -Hematology and Blood cancers* Nov 4, 5 & 6 at Bangalore. <u>www.iacp.org.in</u>

## Intravenous Medication Safety and Role of Pharmacist



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Safe and correct use of medication is one of the prime responsibilities of healthcare professionals in patient care. Medication safety involves giving the right person the right medication in the right dose at the right time and by the correct route. Though there are several strategies to improve patient safety within hospital settings, medical errors continue to increase. India reports 5.2 million medical injuries a year. Medication error is one of the most common medical errors. The Institute of Medicine (IOM) estimates that 98,000 people die every year in US at a cost of \$ 29 Billion due to medication errors. Since the prevalence of drug errors is high, it is crucial that all healthcare professionals understand the factors leading to errors, and avoid them to the best of their ability. Consequences of medication errors include permanent harm to patient, prolonged hospitalization, loss of trust and reliability about the provider and facility. Medication errors include prescribing error, administration error, dispensing error and documenting error.

Intravenous route is the most preferred route for drug administration when the patient is critically ill because it gives immediate therapeutic effect of medications but unfortunately this route is associated with high risk of patient harm. The number of available IV medications continues to expand. Several drug safety issues arising from intravenous drug administration are due to mistakes in dose calculations, incorrect route and rate of administration, incorrect diluents and dilution, Di (2ethylhexyl) phthalate (DEHP) release from medical devices, drug adsorption on the IV set and poor aseptic techniques. Several studies have reported the use of wrong diluents for IV drug reconstitution. Use of wrong diluents can cause drug solubility and stability problems. The most frequent IV medication errors are related to the administration rate, usually higher than that recommended. Rapid IV drug administration is associated with phlebitis, pain, and other complications. A proportion of drug is always lost between preparation and administration because of drug degradation, interaction with the diluents or with the giving set which in turn causes physical or chemical instability of drugs. Mixing of drugs becomes necessary when the patient is given with multiple medications. It is always better to avoid IV drug admixtures. If circumstances are so compelling, there should be evidence from published compatibility data. Two types of incompatibilities are commonly seen during IV drug administration: physical and chemical. Physical incompatibilities can be most easily detected and are evidenced by visible changes such as turbidity, precipitation, and colour change or gas formation. Some of the precipitates are lethal precipitates and they are potentially dangerous. Chemical incompatibilities can be detected using suitable analytical methods.

More than 300 drugs are light sensitive. This is because they can absorb UV and visible radiation, and causes the formation of free radicals. They can cause phototoxic or photoallergic reactions. Drugs like fluoroquinolones, tetracyclines, sulphonamides, and diuretics are extremely photosensitive. Among the fluoroquinolones, lomefloxacin is the most sensitive drug. Doxycycline is more sensitive than other tetracyclines. Furosemide and hydrochlorthiazide are highly photosensitive diuretics. This behaviour depends upon the presence of propionic acid group or chlorine atom or other susceptible groups in their chemical structure. Special attention should be given to the safe use of the group of medications designated as High Alert Medications as they can cause significant patient harm when used in error. Pharmacists have an integral role in ensuring safe. effective and appropriate use of intravenous medications through systematically conducted medication chart review, monitoring and evaluating intravenous drug related issues

as well as preparing and implementing IV drug preparation

and administration protocol.



## **Takayasu Arteritis - Case Report**

Takayasu Arteritis (TA) also known as aortoarteritis and pulseless disease is a rare condition. It is an inflammatory disease of the large arteries. The inflammation leads to narrowing of the arteries, and this can reduce blood flow to many parts of the body. TA particularly affects the aorta, and the pulmonary artery. The major arteries that arise from the aorta may also be affected. These include the subclavian arteries that supply the arms, renal arteries to the kidneys, coronary arteries in the heart and carotid arteries in the head and brain. It was first described in 1908, in a Japanese patient with retinal abnormalities. Although the disease has most often been reported in young East Asian women, it can affect both genders and all races.

The cause of TA is unknown. Examination of its characteristic acute vascular lesions reveals an infiltrative process with mononuclear macrophages and lymphocytes that enter vessel walls through the vasa vasorum. Takayasu arteritis patients constitute a management challenge because treatment options vary; depending on the stage of the disease at the time of its diagnosis.Sometimes patients with TA may have no symptoms, thus there is often a delay in detecting it, sometimes several years.

Here is a case report that describes a patient with Takayasu Arteritis. A 19 year old female patient known case of TA on Prednisolone tapering dose 15mg once daily reported to the general medicine department with chief complaints of intermittent fever for one month, along with cough with expectoration and pain in abdomen. Upon physical examination, patient was conscious and well oriented. Her body weight and height were 47kg and 160cm respectively with a BMI of 18.5/kg/m2.Her blood pressure was 130/90 mmHg in both arms and 120/100 mmHg in both legs. On systemic examination CVS S1 and S2 heard. Brachial artery, radial artery and abdominal aorta pulses were found to be absent on right and left side. Femoral artery, popliteal artery, posterior tibial artery and dorsalis pedis artery pulses were present on both right and left side. Carotid thrill was heard over the carotid artery area during auscultation.

Laboratory findings showed an elevated erythrocyte sedimentation rate (ESR) of 27 mm/hr. (normal value <20 mm/ 1 hr.) Carotid Doppler shows common carotid artery (CCA) wall thickening, longitudinal B mode of carotid bifurcation Internal carotid artery(ICA) and CCA shows increased systolic peak and decreased diastolic flow.Longitudinal B mode of carotid bifurcation External carotid artery (ECA) shows markedly increased systolic flow. CT angiography of carotids and upper limb shows concentric wall thickening in ascending arch and descending aorta. Focal short segment stenosis of proximal left carotid common artery, complete occlusion of left subclavian from origin to vertebral artery with reconstitution of distal subclavian by collaterals.

Long segment stenosis of right axillary artery from origin till brachial artery with near complete occlusion of proximal segment and reconstitution of distal artery by collaterals.The rest of the laboratory investigations, including serum creatinine, electrolytes and urinalysis, were normal.

Depending on the stage of the disease at the time of its diagnosis is an important factor in the therapeutic plan. A most often needs treatment to prevent further narrowing of affected arteries. Yet, the narrowing that has already occurred often does not improve, even with drug treatment. Glucocorticoids (prednisone, prednisolone or others), which are the first line treatment for TA .The dose and length of treatment depend on how bad the disease is and how long the patient has had it. Other treatment plan includes drugs that suppress the immune system and medications to regulate the immune system. If arteries become severely narrowed or blocked, need surgery to open or bypass these arteries to allow an uninterrupted flow of blood. Often this helps to improve certain symptoms, such as high blood pressure and chest pain. In some cases, though, narrowing or blockage may recur, requiring a second procedure. Also, in case of large aneurysms, surgery may be needed to prevent them from rupturing. Surgical options, which are best performed when inflammation of the arteries has been reduced, include: bypass surgery, blood vessel widening, aortic valve surgery.

The drugs prescribed throughout the hospital stay are Tab Prednisolone 10 mg OD and planned to continue with a gradual tapering schedule, Tab Folvite5 mg, Tab Livogen, Tab Neurobion Forte, Tab Pan 40mg, and Tab Shelcal all given once daily. Discharge medications were prescribed for 2 weeks. The drugs included Tab Prednisolone was given in tapered dose as 10mg OD for first week and followed by 5mg OD for second week, Tab Folitrax 7.5mg once a week, Tab Folvite 5 mg twice a week, Tab Livogen OD, Tab Neurobion Forte OD, Tab Pan 40mg OD.

Takayasu's requires periodic surveillance of the large arteries in the body and a multi-specialty care team. Frequent visits to the doctor may be needed. A vasculitis expert should be involved in the decision-making about drugs and the angiographic studies used to diagnose and follow the disease, as well as the frequency of the imaging studies. Blood studies including the erythrocyte sedimentation rate and the C-reactive protein are often used in monitoring the disease activity. A positive attitude and informed patient are keys to the success of treatment. It's essential to have a good relationship with your treating physician.

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## Life after Pharm D

Like most of my other classmates, I started my six year program entirely clueless about what was to come after I graduated. I suppose that is the case of every student that chooses a course that is new, hoping for something fresh and exciting. Most of us were told that the prospects were good abroad and that we should keep our minds focused on getting out of the country. Yet after the end of my program, I stand here in a small town called Vellore, working as a Clinical Pharmacist in one of India's prestigious mission hospitals, Christian Medical College and Hospital (CMCH).

What does it truly mean to be a Clinical Pharmacist? We are taught different concepts through our years in college about the different facets of clinical pharmacy, our roots in Pharmacology, Therapeutics and Pharmacokinetics are made strong. We learn how to implement these concepts during our Internship and the training we receive is crucial to our growth.

As a Clinical Pharmacist in CMCH, my main roles and responsibilities include- Patient Counseling, proving drug information, assessing prescriptions for appropriateness with a minor role in pharmacovigilance. My day to day schedule consists of a combination of these responsibilities with a main focus on patient counseling and prescription monitoring. Pharmacovigilance is carried out regularly since CMCH is an official pharmacovigilance centre. Work is carried out in collaboration with a government employed pharmacist who sends in suspected ADR reports to the CDSCO.

Hundreds of patients are catered to at the Outpatient department Pharmacy counseling desk; basic information regarding appropriate time to take medication, storage conditions, possible side effects and interactions are provided in a concise manner. Dispensing errors are picked up and clarifications are made before the patient is sent home. Likewise, there is a separate counseling desk that caters to pediatric as well as OB-GYN patients.

The main responsibility that distinguishes Clinical Pharmacists from any other Pharmacist is that of providing clinical information to the treating physician regarding a particular case in the ward and changing the drug dosing regimen when appropriate. This is precisely what happens in the MICU and MHDU on a regular basis. Ward rounds are conducted in order to assess every patient and the doses are then correlated with their CBC, lipid profile, respiratory gases, acid base profile, enzymes, hepatic and renal function tests to ensure individualized therapy; doses are subject to change as the blood profile changes . Cross referencing with standard dosing guidelines helps to confirm appropriateness of the particular regimen. If a particular prescription has an error, the respective physician is informed and valid evidence is provided from literature to prove our statement.



This process is easier when a good rapport is established between the clinical pharmacist and the physicians.

Drug related queries that arise during ward rounds are catered to and evidence based answers are provided after intensive reading in the Drug information service of the Hospital (DISH). Other queries come in during the day to DISH via the hospital hotline.

Monthly Journal clubs are customary and significant articles are discussed using critical appraisal techniques to further our knowledge. Research is welcomed and there are plenty of opportunities to learn from. The days I struggled to learn the different concepts of clinical research and biostatistics paid off. If you asked me if I dreamt of working in India as a Clinical Pharmacist during my days in college, I probably would have laughed until I cried seeing as I believed it to be impossible. But the times have changed, all you need is hard work and good mentors to guide you through the process. To my teachers- Thank you for shaping me into who I am, this would not be possible if not for your constant correction and encouragement. To my juniors- work hard and give it your best shot, it truly is worth all the trouble.

I find my work here fulfilling and am glad I can be of service to the patients that I come across each day. Yes, some people still look at you amusingly when they hear the word Pharm.D or our job description but do not let that stop you from pursuing it. It's up to us to prove them wrong and make a name for ourselves. Trust me when I tell you, Clinical Pharmacists are an essential part of the healthcare team and you will find your worth in time.

> **Dr. Judith Baskar,** Clinical Pharmacist Christian Medical College and Hospital, Vellore, TN

Judith Baskar is an alumna from the Pharm D 2010 - 2016 Batch, Krupanidhi College of Pharmacy. Synergia wishes her the best in her career and life - Editor.

The views expressed in this article are personal, and do not necessarily represent the views or policies of CMCH Vellore.

#### e n e r a е n S

Vitamin C or L-ascorbic acid, or simply ascorbate (the anion of ascorbic acid) is an essential nutrient for humans and certain other animal species.

It is a well-known component of Immunity

our immune system. Protects our body from infections and maintains healthy bone and teeth. Improves our body's ability to repair wounds and keeps us immune from baderia, viruses and infection. It is

necessary for collagen, the main structural protein found in connective tissue. Diabetes

Diabetic patients can also benefit from Vitamin C as it helps in regulating the sugar levels, reducing the risk of getting diabetes and improving the symptoms of the existing cases. Supplementing Vitamin C forces glucose in the body cells, where it protects against many complications of diabates

Vitamin C lowers the Hypertension blood pressure and de-

creases the probability of hypertension as well as serious health problems that may accompany high blood pressura

Vitamin C provides many benefits for the hair as following: Improves Hair Hair Growth: Low intake of Vitamin C may be a root cause for a number of hair-related problems that affect our hair growth. Its deficiency may result in dry hair and split ends. These condition are unlavourable for the regular growth of hair. Fights Danchuff it helps light the bacteria on the scalp. It wards of dandruff and helps to get rid of the folicles' debris and encour ages the growth of new hair. It also helps with dry and itohy scalps. Thicker Hair: It also helps improve the blood circulation and strengthens and repairs the capitaries too and this is particularly important for getting stronger, thicker hair. Fights Heir Disorders: it is an essential numerit for damaged hair and thus, treats and prevents a variety of hair disorders which can damage the hair follcles and affect the normal growth of hair. A clet containing significant levels of Vitamin C can help combat alopecia and baldness in men. Prevents Graying Of Hair: It not only helps combat hair loss but also helps retain the natura color by preventing the premature aging of the hair.

Vitamin C containg foods are Weight loss proven to help people lose fait and maintain healthy weight. Popular dieticians and nutritionists always include Vitamin C in diet charts because there is scientific evidence that shows that eating Vitamin C rich loods on a regular basis helps in losing weight significantly.



It reduces the severity of cold symptoms and acts as an effective antihistamine that lessens Common the unpleasant effects of the common cold, including inflam-



mation, runny nose and aches. It controls the allergy that causes the cold. It reduces the histamine level and often shortens the duration of the cold.

#### Heart disease



Vitamin C prevents heart disease by preventing free radicals from damaging the artery walls, which could lead to plaque formation. This nutrient also keeps the cholesterol from coldising, which can cause heart stroke. The problem of high blood pressure can also be resolved with this wonder nutrient. All these factors

combine to make Vitamin C an inexpensive and easy way to lower the risk of heart disease and strokes

It's antioxidant properties protect the cells from DNA damage and mutation and protect from cancer in the long run. It supports the body's immune system and prevents certain Cancer cancer forming compounds from



Skin

forming in the body. It reduces the risk of development of all types of cancers including lung, mouth, throat, colon, stomach and oesophagus. It also helps to regenerate Vitamin E which is another powerful anticxidant, it does not directly attack cancer that has already occurred but keeps the immune system nourished and enables to battle against cancer.

> It is the most important ingredient used in skin care treatments. Its ability to provide an effective shield against the sun has made it an indispensable ingredient used in the cosmetic industry. ts benefits for skin can be mentioned as: Sun Protec-

tion: Protects our skin from free radicals that develop due to excess exposure to the sun. Production Of Collagen. This, in turn, firms and tones the skin. Collagen deficiency makes the skin dull and Heless, Heals Wounds: The body uses Vitamin C to replace the damaged tissue and helps to heal the wound at a faster pace. Protects Against Skin Discolouration: Vitamin C protects DNA from photochemical reactions that can lead to tumor, skin discolouration and several kinds of skin cancer, improves Sky Texture Vitamin C improve the appearance and texture of the skin. Vitamin C increases the forms ion of clastin which thickens, protects and heals the skin ceta

#### TOP 10 FOODS RICH IN VITAMIN C



## Lucentis for proliferative diabetic retinopathy with diabetic macular edema: is it worth its price?

Generic name: Ranibizumab (Monoclonal Antibody)

Price in india : Approx Rs 25000 per vial

#### **Dosage forms and strengths:**

Single-use glass vial designed to provide 0.05 mL for intravitreal injection.

•10 mg/mL solution (LUCENTIS 0.5 mg) •6 mg/mL solution (LUCENTIS 0.3 mg)

#### Indications:

Neovascular (Wet) Age-Related Macular Degeneration (AMD)
Macular Edema Following Retinal Vein Occlusion (RVO)
Diabetic Macular Edema (DME)
Diabetic Retinopathy (Non Proliferative Diabetic Retinopathy (NPDR), Proliferative Diabetic Retinopathy (PDR)) in patients

with Diabetic Macular Edema (DME)

#### **Mechanism of Action:**

Wet macular degeneration occurs when abnormal blood vessels begin to grow underneath the retina and leak blood or fluid that blurs central vision. A chemical called vascular endothelial growth factor, or VEGF, causes this abnormal growth. Anti-VEGF treatments—Lucentis, Eylea and Avastin—work by seeking out harmful VEGF molecules and blocking them. This reduces abnormal growth and leakage, which helps to stabilize vision loss and, in some cases, can improve sight.

#### Is there an alternate drug?

Eylea (aflibercept) is made from a human antibody fragment. It works by keeping new blood vessels from forming under the retina (a sensory membrane that lines the inside of the eye). Eylea is used to treat wet age-related macular degeneration, swelling in the retina caused by a blockage in the blood vessels, diabetic retinopathy. But the price is comparatively similar to that of Lucentis.



Avastin, trade name of the drug bevacizumab, is a drug that has helped to treat cancers( FDA approved for colon cancer). It works in a similar way as Lucentis in that it helps to inhibit the growth of new blood vessels. Avastin is notably cheaper than Lucentis, but the drug has yet to be tested enough to be approved for use against diabetic madular oedema. There is a greater possibility of infection with Avastin due to potential contamination when the drug is being repackaged into smaller doses for the eye. So lucentis is worth its price to save vision.

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#### Heightened liver cancer risk linked to low blood selenium levels



In a recent study published in the *American Journal of Clinical Nutrition.* and NIH, selenium is essential for human health, with beneficial roles for reproduction, the immune system, and DNA synthesis. It is a trace element that occurs naturally in soil and plants, and enters the bodies of humans and animals via the food they ingest. Studies have also shown that selenium has antioxidant properties, meaning it can protect against oxidative stress - the process by which uncharged molecules called free radicals damage cells. Since oxidative stress has been associated with cancer development,

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#### Virtual High-Throughput Screening (vHTS) in CADD

Pharmaceutical companies are always searching for new leads to develop into drug compounds. One search method is virtual high-throughput screening. In vHTS, protein targets are screened against databases of small molecule compounds to see which molecule binds strongly to the target. If there is a "hit" with a particular compound, it can be extracted from the database for further testing. With today's computational resources, several million compounds can be screened in a few days on sufficiently large clustered computers. Pursuing a handful of promising leads for further development can save researchers considerable time and expense. ZINC is a good example of a vHTS compound library.

#### **Quantitative Structure-Activity Relationship Models**

Quantitative structure-activity relationship (QSAR) is essential component of (LB-CADD) Ligand-Based Computer-Aided Drug Design

These models describe the mathematical relation between structural features and target responses of a set of chemicals or drugs. The classic QSAR is known as the Hansch-Fujita approach which involves the correlation of various electronic, hydrophobic and steric features with biologic activity. In the early 1960s, Hansch and others began to establish QSAR models using various molecular descriptors like physical, chemical and biologic properties to provide computational estimates for the bioactivity of molecules. In 1964, Free and Wilson developed a mathematical model relating the presence of various chemical substituents to biologic activity (i.e, each type of chemical group was assigned as an activity contributor), and the two methods were later combined to create the Hansch/ Free-Wilson method.

The general workflow of a QSAR-based drug discovery project is to first collect a group of active and inactive ligands and then create a set of mathematical descriptors that describe the physicochemical and structural properties of those compounds. A model is then generated to identify the relationship between those descriptors and their experimental activity, maximizing the predictive power.

#### Approaches for QSAR

#### 1.Multidimensional QSAR: 4D and 5D Descriptors

Multidimensional QSAR (mQSAR) seeks to quantify all energy contributions of ligand binding which includes removal of solvent molecules, loss of conformational entropy and binding pocket adaptation. 4D-QSAR is an extension of 3D-QSAR that treats each molecule as an ensemble of spatial features such as different conformations, orientations, tautomers, stereoisomers and protonation states.

5D-QSAR has been developed to account for local changes in the binding site that contribute to an induced fit model of ligand binding. In this method induced fit is simulated by mapping a "mean envelope" for all ligands in a training set on to an "inner envelope" for each individual molecule. By using this information, the energetic cost for adaptation of the ligand to the binding site geometry is calculated.

#### 2.Receptor-Dependent 3D/4D-QSAR

Although QSAR methods are especially useful when structural information regarding target binding site is not available. One method, known as free energy force field 3D-QSAR is developed that describes all thermodynamic contributions for binding. Structurally, the analysis is focused solely on the site of interaction between the ligand and target, and all atoms of interest are assigned partial charges.

#### **3.Linear Regression and Related Methods**

Linear models used include multivariable linear regression analysis (MLR), principal component analysis (PCA), or partial least square analysis (PLS). MLR computes biologic activity as a weighted sum of descriptors or features. The method requires typically 4 or 5 data points for every descriptor used. PCA increases the efficiency of MLR by extracting information from multiple variables into a smaller number of uncorrelated variables.

PCA or PLS are commonly used for developing models for the molecular interaction field algorithm CoMFA and CoMSIA.

Advantage of these models is that they can be trained rapidly using the tools of linear algebra. The major drawback is that chemical structure often relates with biologic activity in a nonlinear fashion.

#### 4.Nonlinear Models Using Machine Learning Algorithms

Artificial neural networks (ANNs) are one of the most popular nonlinear regression models applied to QSARbased drug discovery. These models belong to the class of self organizing algorithms in which the neural network learns the relationship between descriptors and biologic activity through iterative prediction and improvement cycles.

A major drawback of neural networks is the fact that they are sensitive to overtraining, resulting in excellent performance within the training set but reduced ability to assess novel compounds. Therefore, care is taken to always measure ANN performance on "independent" data sets not used for model generation.

#### Conclusion

The extensive variety of computational tools used in drug discovery campaigns suggests that there are no fundamentally superior techniques. The performance of methods varies greatly with target protein, available data, and available resources. The successful stories of CADD application in drug discovery in recent years have demonstrated the potential value of CADD in drug development.

CADD approaches can provide valuable information for target identification and validation, lead selection, small-molecular screening and optimization. The latest technological advances (QSAR/ QSPR, structure-based design, combinatorial library design, chemoinformatics & bioinformatics); the growing number of chemical and biological databases; and an explosion in currently available software tools are providing a much improved basis for the design of ligands and inhibitors with desired specificity.

For example, Kruger and Evers completed a performance benchmark between structure- and ligand-based vHTS tools across four different targets, including angiotensin-converting enzyme, cyclooxygenase-2, thrombin and HIV-1 protease. Docking methods including Glide, GOLD, Surflex, and FlexX were used to dock ligands into rigid target crystal structures.

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#### Software for General Purpose Molecular Modeling

For workstations, minicomputers and supercomputers (SGI, Sun, Cray, etc.) AMBER—Peter Kollman and coworkers, UCSF. Computer assisted model building, energy minimization, molecular dynamics, and free energy perturbation calculations.

Midas Plus—UCSF Computer Graphics Laboratory. CHARMM—Martin Karplus and coworkers, Harvard. QUANTA/CHARMM—Molecular Simulations Inc. (MSI) molecular/drug design, QSAR, quantum chemistry. X-ray & NMR data analysis Insight/ DISCOVER— Biosym, Inc. Now MSI and Biosym became Accelrys Inc.

## For personal computers (Apple, Compaq, IBM, etc.)

- Alchemy III-Tripos, Inc.
- **SYBYL** Structure building and manipulation, energy minimization, molecular display, conformational searching Chem3D Pro—Cambridge Soft Corp.
- **Desktop Molecular Modeller**—Oxford Elec. Publishing Molecular Modeling Pro—WindowChem Software Energy minimization, QSAR (surface area,

#### Prof. Raman Dang, Principal, KCP assumes charge as secretary of APTI



Prof. Raman Dang, Principal of KCP, assumed charge as the secretary of Association of Pharmaceutical Teachers of India (APTI), an acclaimed body aimed at promoting the quality pharmaceutical education in India. APTI celebrated its 50th anniversary recently, and is an apex body representing the interests of pharmaceutical faculty in India. He is an internationally acclaimed academician and researcher in the domain of pharmacognosy and phytopharmaceuticals. He is also the present incumbent of the Chairman, Post Graduate Board of Studies of RGUHS, Karnataka. *Synergia* wishes him a fruitful tenure with APTI.

#### Department of Pharmaceutics conducts one day workshop on PK/PD Modelling

A one day workshop on Pharmacokinetic/Pharmacodynamic Modelling using Certara<sup>™</sup> Phoenix *WinNonlin* software: Concepts, Applications and Hands on Training was conducted on September 7th organized by the Department of Pharmaceutics, Krupanidhi College of Pharmacy, Bangalore and co sponsored by Rajiv Gandhi University of Health Sciences, Karnataka. Resource person for the workshop was Dr. Venkateswari Muthukrishnan, Senior Scientific Consultant, Certara<sup>™</sup>, South Asia Pacific. A Total 30 participants attended the workshop. Dr. Bharani S Sogali, HoD of the department was the convener of this workshop.



#### Oct - Dec 2016

## **Freshers Induction & Finishing school activities**





KCP has 6 courses from Diploma to Doctoral programs in pharmacy. Every year the freshmen of KCP are put through induction program to make them aware of their home environment and how to get the best of KCP experience.

The freshers were inducted in the various facets of functioning KCP, and day to day conduct and scheduling of academic and co curricular activities. The faculty of the induction program were Profs. MD Karvekar, PV Mallya - Directors, Dr.Raman Dang - Principal, Dr Sonal Dubey - Vice Principal, and professors Mahesh NM, Preeti Sudheer, M K Ranganath, Chandramouli R, Arsad Bashir Khan, Rajeswai R, Prabita, Ruchi Agrawal, Deepti and host of other faculties. The induction program helps the freshmen of KCP, to understand the systems and functioning of KCP better and help orient their academic and developmental goals better, The entire effort was oragnized to perfection by the finishing school committee.

The finishing school activities conducted by Center for Pharmaceutical Professional Advancement (CPPA)'s Director and Chief Mentor

Prof. Prakash V Mallya is a hallmark of the KCP experience. CPPA under his helm has conducted more than 250 world class interactions with the best in the industry. This year too the graduating batches of students underwent the finishing school routine mentored by Prof. Mallya and invited faculties Sri Ajit Kaikini and Prof. Anila. CPPA's efforts is well known and widely appreciated by the industry as well.

### **Freshers & Teachers day celebrations**

The Freshers Day and Teachers Day were celebrated on 15th September at the newly refurbished Hall of Fame.

The function was graced by the presence of Chief Guest Sri BT Khanapure Drug Controller, Drugs Control Department, Government of Karnataka ; Guest of honour Mr. Rajendran, CEO Green Chem, Herbal Extract and Formulation Bangalore; Mr. Ajit Kaikini, Special Invitee, Director Buoyance, Chairman Prof. Suresh Nagpal Krupanidhi group of Institution; Vice Chair person, Mrs. Geetha Nagpal; Director Academics Prof. M D Karvekar; Director, Center for Pharmaceutical Professional Advancement, Prof. Prakash V Mallya and Principal Raman Dang presided over the function.

The function started with invocation and traditional lamp lighting. Mrs. Ashwini welcomed the gathering followed by Keynote address by Dr. Raman Dang Principal, KCP. Professors Prakash V Mallya and Sonal Dubey Sharma were awarded the Teachers of Excellence for 2016.Cake cutting marked the Teachers Day Celebration. The program included solo songs, solo dance, group dance, and duet songs performed by a number of fresher and senior students.



#### KET inks MoU with Qiqihar Medical University, followed by faculty visits





Krupanidhi Educational Trust, the parent body of KCP inked a MoU with Qiqihar Medical University (QMU) and the Staff and Student exchange programs and finalizing the modalities of collaboration were on the offing.

QMU, located in the hometown of world-famous red-crowned cranes, stands by the scenic Nenjiang River and is a regular university of Heilongjiang Province, China.

Founded in 1946, the University held its 70 years' celebrations between 11th July – 17th July, 2016 for which professors Raman Dang, Principal and Sonal Dubey Sharma, Vice Principal of KCP, were the invited guests from Krupanidhi Group of institutions. The visit was marked with lot of cultural exchange, one to one meetings with the top officials and visit to their hospitals. A scientific conference was also held at the venue where an effective presentation made by theml. The entire program was arranged minute by minute and well organized. The University officials especially Dr. Sandeep took good care of then guests. Overall the visit had good deliberations with excellent outcomes and moving ahead. There is now scope for interested staff and students to move ahead for the exchange program which may start as early as end of November 2016.

### NSS Unit organizes blood donation camp to mark World Pharmacists Day



A blood donation camp was organized on 26th September 2016, at Krupanidhi College – Pharmacy Block, to observe the World Pharmacists Day. The programme was conducted by NSS cell, in association with Rotary International, Bangalore Indiranagar and NIMHANS Blood bank, Department Transfusion Medicine, Bangalore. Sensitization program was conducted on 24 September, 2016 in the seminar hall by Mrs. Lata Amashi, Chairman of Blood Donation, Rotary Bangalore Indiranagar. About 82 donors donated their blood for the social cause on this special day. Both NIMHANS team and Krupanidhi College of Pharmacy-NSS cell provided refreshments and Certificates for the donors.Dr Suverna Kirloskar Physician, Ms. Beena Tuysar, Social Worker,along with the team of NIMHANS Blood bank, Department Transfusion Medicine, organized the proceedings.



Patron: Dr. Suresh Nagpal, Mrs. Geetha Nagpal, Prof. Sunil Dhamangini, Ms. Neha Nagpal, Dr. Samuel Paul Isaac
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