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- ❖ Address : Dept. of Pharmaceutical Chemistry, NMIMS, V.L. Mehta Road, Vile Parle (West), Mumbai-400056.
- ❖ Name of the International Conference/ Seminar/Symposium/ Workshop : International Conference on Pure and Applied Chemistry.
- ❖ Title of the abstract accepted : Investigational analysis using pharmacophore and docking studies on five-substituted 3, 3-diethyl-4, 5-dihydro-2(3H)- furanones and their homologs targeted as muscarinic receptor ligands.
- ❖ Date & Venue : 23-27th June 2014. Mauritius.
- ❖ Money sanctioned : ₹ 83,550/-
- ❖ Money reimbursed : ₹ 72,664/-

Participation Report

The International Conference on Pure and Applied Chemistry (ICPAC) is organized every two years. The 2014 conference was the third conference after it was started in the year 2010. This conference was held in Mauritius. ICPAC 2014 will particularly be important as the year is currently the International Year of Crystallography (IYCr2014). It was a four day event with total of 100 participants from 30 countries. The theme of ICPAC 2014 was "Crystallising Ideas: The Role of Chemistry". The theme was chosen in view of IYCr2014. The four day event was aimed at providing an international platform to participants for reporting their research (5 plenary lectures, 8 invited lectures, more than 40 oral lectures, 10 symposium lectures and 38 posters). Research holds the key to solving some of the important problems pertaining to energy, environment, health etc. The scientific program of ICPAC broadly covered all the disciplines of chemistry from fundamental to applied ones including multidisciplinary and related areas. The key note address was given by Ambassador Grace Asirwatham, the Deputy Director-General of Organisation for Prohibition of Chemical Weapons (OPCW) which was awarded the 2013 Nobel Peace Prize along with plenary and invited lectures by prominent scientists from around the world. A workshop on COSMO-RS: From Quantum Chemistry to Fluid Phase Thermodynamics and Drug Design was also conducted.

- Academic Highlights of the Training/Workshops, including major recommendation and the following: The highlight of the conference was on crystallography as it coincided with the year of crystallography. A lot of lectures, posters etc were presented in the area of material sciences, crystal structures and its application in multidisciplinary areas such as pharmaceutical sciences, medicinal/bioorganic/organic chemistry, energy, environment etc. It was fruitful conference which I strongly recommend for researchers.

i) New Development presented at the Training/Workshops

The conference aimed at providing the participants a platform for exchanging ideas on multidisciplinary Research. One aspect that was highlighted in the conference was the use of thermodynamics in drug design for which a training session was organized. Since it was the year of crystallography, there were many plenary, invited and poster presentations in material sciences. The knowledge was very helpful in inculcating the applicative role of crystals in drug delivery in Pharmaceutical sciences. Multidisciplinary areas of work were presented which ranged from Energy, Environment, Radiochemistry to Medicinal Chemistry.

(ii) New Development resulting from the Training/Workshops (200 words)

The conference was worthwhile to attend as it gave an opportunity to interact with eminent scientist and researchers from different parts of the world. It gave a platform for exchanging ideas and undertake research collaborations. The conference gave particular attention to the social programme, thereby giving an opportunity and an informal way of interaction and relaxation. The conference conducted a seminar and workshop on a software program COSMO-RS which discussed the applications of thermodynamics (enthalpy and entropy) in drug receptor interaction. The conference had many plenary lectures ranging from structural chemistry, radiochemistry, analytical chemistry to natural product chemistry. The invited lectures ranged from publishing research by springer, electrochemistry, use of chemistry in agriculture (sugarcane), to astrochemistry and dyes. The conference also included many organometallic based reactions and drug complexations for the treatment of different disorders. To keep up with the theme, the conference also organized lectures pertaining of crystals and their applications in different areas of research such as agriculture, pharmaceuticals, space, electronics etc.

(iii) Name of the Publication in case your work Is recommended for publications

The manuscript will be communicated to a suitable journal shortly

Participant's contribution to the Training/Workshops

The poster entitled "Investigational analysis using pharmacophore and docking studies on five-substituted 3,3-diethyl-4,5-dihydrofuranones and their homologs targeted as muscarinic receptor ligands" was accepted for presentation at the ICPAC-2014 conference in Mauritius. The poster was presented on June 26, 2014. The work depicted the importance of development of subtype selective muscarinic ligands for various disorders. The work highlighted manner in which the ligands were developed starting from the hypothesis to testing of the hypothesis by use of pharmacophore in the design of the ligands. The ligands designed were then properly synthesized by reported method, well characterized and evaluated in cell based radiolabelled binding assay. Further studies were carried out to evaluated the IC₅₀ and subtype selectivity of the selected compound. As muscarinic receptors belong to GPCR's, a pharmacophore building and docking experiments were conducted on the synthesized compounds to see their orientation in the binding pocket of the muscarinic subtype receptors. The compounds after pharmacophore generation docked well into the binding pocket which correlated well with the experimental binding data. The poster was well appreciated and lots of questions were asked. **I am happy to say that I have received the best poster award for my work**