



National conference on "New Imperatives in Drug Design and Discovery" (NIDDD-2019) was organized and hosted by Department of Chemistry, UkaTarsadia University, Surat (Gujarat-India) during 22nd-23rd November – 2019. This conference was organized in association with Indian Society of Chemists and Biologists (ISCB) Lucknow, India and The National Academy of Sciences, India (Mumbai Chapter).

The major aim of this conference was to provide opportunity to young researchers and students to interact with eminent speakers and also present their work in the form of posters and oral communications. The scientific sessions included several plenary lectures, oral communications and poster presentations from various subject areas of Chemical Sciences, Pharmaceutical sciences and Biological sciences.

Total of 350delegates across the country were registered for NIDDD-2019. Total 14 abstracts were accepted for oral presentations and 68 abstracts were accepted for poster presentations by scientific committee.

The NIDDD-2019 was financially supported by GUJCOST, DST and GSBTM (Government of Gujarat) funding agencies.

During inaugural session Dr. V. R. N. Pillai (Ex-Chairman and Vice Chairman University Grant Commission New Delhi) had graced the function as Chief Guest. Prof. D. R. Shah (Provost; UkaTarsadia University), Prof. Anamik K. Shah (Vice Chancellor of Gujarat Vidyapith and President of ISCB), Prof. A. K. Singh (Chairman of NASI), Prof. Evans Coutinho (Bombay college of Pharmacy), Prof. R. Krishnamurthy (Dean Faculty of Science, UTU), Prof. K. R. Desai (Former Director of Department of Chemistry, UTU), Prof. Paresh N. Patel (I/c Director of Department of Chemistry, UTU), Prof. Ajit Joshi (Department of Chemistry, UTU) were present and shared their feelings about the NIDDD-2019 during the inaugural session. NIDDD was started with our university anthem followed by Iamp lightning by present dignitaries. After inaugural session, all the technical sessions were followed as per the schedule.

The first technical session was chaired by Prof. K. R. Desai, in which Prof. Anamik K. Shah delivered his plenary talk. A group photo session was organized before lunch. After lunch, in the second technical session chaired by Prof. Shailesh Shah (Director Maliba Pharmacy College, UTU) there were two plenary lectures. Prof. Evans Coutinho and Prof. BajarangKumbhar gave their plenary talks in this session. After tea break in the first oral session chaired by Prof. A. K. Singh total six oral communications were presented.

The second day started with breakfast followed by two plenary lectures. This session was chaired by Prof. Evans Coutinho in which the first plenary talk was delivered by Prof. A. K. Singh while the second was by Prof. Hitesh D. Patel. In the second session chaired by Prof. R. Krishnamurthy, the first plenary talk was delivered by Prof. Rajesh K. Patel while the second by Dr. Vaibhav P. Mehta. There was a poster session organized during tea break followed by oral presentations. The oral session was again chaired by Prof. A. K. Singh where total six oral communications were presented. This was followed by Valedictory function where many dignitaries were present on the stage including Prof. A. K. Singh, Prof. Evans Coutinho, Prof. N. C. Shah, Shri Bhagubhai Patel (President, BPKM), Prof. K. R. Desai, Prof. Paresh Patel and Prof. Ajit Joshi. Some dignitaries were requested to say few words to motivate students. Some participants shared their experiences of the two days stay at the UkaTarsadia University and the quality of conference, all of which were high on appreciation for the hospitality and good arrangements as well as the scientific content of the conference. Dr. DharmeshChejara gave vote of thanks to all who contributed towards the success of the conference directly or indirectly. Prizes where distributed for the best oral and poster presentations in which total of 6 where awarded best oral prizes while 3 received best poster prizes. With this the conference was concluded.

Events with pictures and short description

Inauguration



















Day 1: (22/11/2019)

Plenary Session I: (Session Chair: Prof. K. R. Desai)

Plenary Lecture 1. Prof. Anamik Shah (Time 11.00 - 11.50 hrs.)



Prof. Prof. Anamik Shah delivered his interactive talk titled"*A facile journey of Medicinal Chemistry: Recent updates in small molecule drug discovery*". The talk was focused on pharmacopeia, bioinformatics, patents, medicinal value of small molecules, etc. He motivated the early stage researchers and students to work towards the upliftment of society through innovative research and discoveries. He talked about the tribal people having sickle cell anemia in and around Ahmadabad and Gandhinagar region. The major part of the talk was devoted towards the importance of small molecule heterocycles synthesis and their biological activities.

Plenary Session II: (Session Chair: Prof. Shailesh Shah)

Plenary Lecture 2. Prof. Evans Countinho (Time 13.30 - 14.10 hrs.)

Prof. Evans Countinhofrom Bombay college of Pharmacy explained in detail about a new formalism, developed by his group, called Eigen Value Analysis (EVANS) that can be used to



calculate physical and chemical properties of a chemical compound. He gave theoretical basis of the formalism and with some examples showed how it works and how the data obtained correlates with experimental values and observed bioactivity.

Plenary Lecture 3. Dr. BajarangKumbhar (Time 14.10 - 14.50 hrs.)

Dr. BajarangKumbhar gave a lecture titled "*Exploring the interaction of drug-resistant \alpha,\beta-tubulin isotypes with anticancer agents*" using the molecular modeling approach. He presented latest investigations of the different binding affinity of drug-resistant tubulin isotypes for DAMA-colchicine, combretastatin A4 and pelorusideA using homology modeling, molecular docking, molecular dynamics simulations and binding free-energy calculations.



Oral Session I: (Session Chair: A. K. Singh)

Oral Presentation: OP1-6 (Time 15.10 - 16.20 hrs.)

- 1. Dr. Abhishek Sharma,
- 2. Dr. RajalaxmiSubramaniyam,
- 3. Dr. Bhavin Vyas,
- 4. Dr. Ajay Sharma,
- 5. Mr. Bhrugesh Joshi,
- 6. Dr. Vilas Surana

Presenters delivered lecture on their area of expertise in chemistry, biology and bioinformatics. Each presenter was given 10 minutes of time for presentation.





Day 2: (23/11/2019)

Breakfast (Time 8.00 – 9.40 hrs.)

Plenary Session III: (Session Chair: Prof. Evans Coutinho)

Plenary Lecture 4. Prof. A. K. Singh (Time 9.40 – 10.20 hrs.)



Prof. Anil K. Singh delivered a lecture on "Design and Development of Radio protectants and Caged Compounds".He explained in detail Vitamin A and E related radio protective/antioxidant compounds - synthesis and assay of their antiradical abilities. Synthesis of novel photo triggers and their applications in caging of drugs and bioactive natural products. Prof. Singh also gave valuable information onsynthesing several donoracceptor diarylpolyenes as models of photo biologically active linear

polyenes and studied their photochemical and photo physical properties to further characterize the excited state structure and dynamics of photo biologically important linear polyenes.

Plenary Lecture 5. Dr. Hitesh Patel (Time 10.20 - 11.00 hrs.)

Dr. Hitesh Patel delivered a lecture titles "*Therapeutic and Diagnostic reagents development for MTB*". He highlighted the number of patients suffering from Tuberculosis worldwide and the big part of those is Indians. He talked about the present status of therapeutic and diagnostic compounds and methods available and need for improvements in them. His group's work on therapeutic and diagnostic reagents/chemicals for Mycobacterium Tuberculosis was presented well.



Plenary Session IV: (Session Chair: Prof. R. Krishnamurthy)

Plenary Lecture 6. Prof. Rajesh Patel (Time 11.00 – 11.40 hrs.)



Dr. Rajesh Patel delivered lecture titled "Concepts, opportunities and challenges of chemo informatics and bioinformatics augmented *in silico* drug discovery". The evolution of drug discovery process from classical pharmacology to high throughput screening and further to in sillico drug discovery was presented. The benefits of the later technique were highlighted in terms of medicinal chemistry, optimization of hit molecules to increase the affinity, selectivity, efficacy/potency, metabolic stability and oral bioavailability. The interplay and

interaction at interphase of bioinformatics and chemoinformatics for drug discovery process were nicely presented by the speaker.

Plenary Lecture 7. Dr. Vaibhav Mehta (Time 11.40 - 12.20 hrs.)

Dr. Vaibhav P. Mehta delivered lecture on "*Evaluation of EnablingSustainable Technology for Efficient Synthetic Organic Chemistry*". He explained how the enabling sustainable technologies are efficient compared to thetraditional way of research. Use of monomode and multimode microwave apparatuses for different cross-coupling reactions like Suzuki, Sonogashira, Kumada, Liebeskindschrogle, etc. was highlighted. Dr. Mehta presented some of his works in the field of microwave assisted organic synthesis, multicomponent reactions, crosscoupling reactions and transition metal catalysis in which the



efficiency, atom economy, reduced reaction times were key features. Flow chemistry, automation starting from reaction to characterization and other technologies were presented in a lucid manner.

Oral Session II: (Session Chair: A. K. Singh)

Oral Presentation: OP-8-14. (Time 13.30 - 14.40 hrs.)

- 7 Dr. RajamouliBoddula,
- 8 Dr. SandeshLodha,

- 9 Dr. Tapan K. Pal,
- 10 Mr. VaibhavNaik,
- 11 Mr. NileshPrajapati,
- 12 Dr. JigarSoni
- 13 Mr. SherifAdeyemi
- 14 Dr.SatyanarayanBattula

Presenters delivered lecture on their area of expertise in chemistry, biology and bioinformatics. Each presenter was given 10 minutes of time for presentation.

Poster Session: (Judges: Dr. Vaibhav P. Mehta, Dr. Hitesh D. Patel, Dr. Tapan K. Pal, Dr. Rajalakshmi Subramaniyam, Dr. Ajay Kumar Sharma, Dr. Ajit Joshi)



Along with oral presentations poster session also took place including 68 total posters. The above mentioned judges were grouped in to three and they evaluated all posters for their scientific merit and impact. Based on the evaluation provided by judges the best three posters were selected for prize.

Valedictory function: 15.15-16.00 hrs.

In the valedictory function many dignitaries were present on the stage including Prof. A. K. Singh, Prof. Evans Coutinho, Prof. N. C. Shah, Shri Bhagubhai Patel (President, BPKM), Prof. K. R. Desai, Prof. Paresh Patel and Prof. Ajit Joshi,&some dignitaries were requested to say few words to motivate students. In this valedictory function 255 participants were being present,some of them shared their experiences of the two days stay at the UkaTarsadia University and the quality of conference, all of which were high on appreciation for the hospitality and good arrangements as well as the scientific content of the conference. Dr. Dharmesh Chejara gave vote of thanks to all

who contributed towards the success of the conference directly or indirectly. Judges from the poster session were awarded certificate of appreciation and memento. Prizes where distributed for the best oral and poster presentations in which total of 6 where awarded best oral prizes while 3 received best poster prizes. With this the conference was concluded.







Glimpses of non-scientific events

