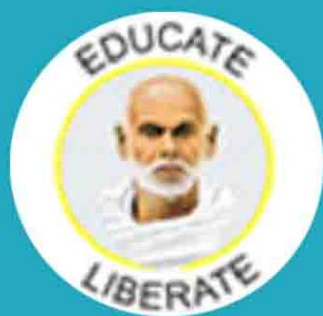


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SREE NARAYANA COLLEGE CHENGANNUR

Alappuzha, Kerala.

Aided College Affiliated to the University of Kerala
NAAC accredited with Grade 'B'

Two Day Workshop on

“Computational Modeling and Drug Design”

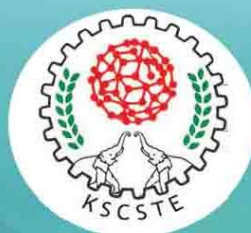
4th & 5th April 2018

Venue: SN COLLEGE, CHENGANNUR

Organised by
POST GRADUATE DEPARTMENT OF CHEMISTRY

In association with
Academy of Chemistry Teachers (ACT)

Supported & Sponsored by



Kerala State Council for Science, Technology and Environment (KSCSTE)
Sasthra Bhavan, Pattom, Thiruvananthapuram-695004, Kerala.

PROGRAMME

DAY I, 4/4/2018

9:00 am	: Registration
10.00 -10.45 am	: Inaugural Session
Prayer	: College choir
Welcome	: Dr. M S Latha Head, Department of Chemistry, SN College Chengannur
Presidential Address	: Dr. K Shiny Sreedhar Principal, SN College Chengannur
Inaugural Address	: Prof. Sabu Thomas Pro-Vice Chancellor Mahatma Gandhi University, Kottayam
Felicitation	: Dr. A V Anandaraj , (Chairman, RDC) : Dr. R. Raveendran UGC Emeritus Professor & Retd. Principal, SN College Chengannur
Vote of Thanks	: Dr. Manohar D Mullassery , General Secretary, ACT : Dr. Smitha Sasidharan Assistant professor, Department of Chemistry

Technical Session I

10.45-11.30 am	
Key note address	: Dr. Nandakumar Kalarikkal Director, IIUCNN, Mahatma Gandhi University, Kottayam
11.30-11.45 am	Tea Break
11.45-12.45 pm	Invited talk Dr. Sreejalakshmi , Associate Professor, IIST, Trivandrum "Fundamentals of computational modeling"
Topic	Lunch Break
12.45-1.45 pm	

Technical Session II

1.45-2.30 pm	
Topic	Dr. M S Latha , Head, Department of Chemistry "Introduction to Drug Designing"
2.30-4.00 pm	Training Programme on Computational Modeling I

Day II, 5/4/2018

Technical Session III

9.30-10.30 am	Training Programme on Computational Modeling II
10.30-11.15 am	Invited talk Dr. K Santhosh Kumar , Scientist F, RGCB, Trivandrum "Current Trends in Drug Designing"
Topic	Tea Break
11.15-11.30 am	Training Programme on Computer Aided Drug Design
11.30-12.45 pm	Lunch Break
12.45-1.45 pm	

Technical Session IV

1.45-2.30 pm	Invited talk Dr. Gopakumar G , Scientific Officer, IGCAR, Kalpakkam "Applications of Computational Modeling"
Topic	Discussion and Feed Back
2.30-3.00 pm	Tea Break
3.00-3.15 pm	
3.15-4.00 pm	Valedictory Function

Report of Two Day Workshop on "Computational Modeling and Drug Design"
on 4-5th April 2018 at Department of Chemistry, SN College Chengannur

Computational modeling techniques have long been used for the synthesis of molecular structure and cost-effective (virtual) experimental analysis prior to synthesis. Computational techniques, especially molecular modeling, play a vital role in the drug design process. Ideally, the computational method will be able to predict affinity before a compound is synthesized and hence save enormous time and cost. Although progress was being made in computer aided drug design, the potential for high-throughput screening had begun to take precedence as a means for finding novel therapeutics. The method has the advantage of requiring minimal compound design or prior knowledge, and technologies required to screen large libraries have become more efficient. Most importantly, drug design projects may fail without the efforts of experts in computational modeling. Our department is involved in the identification of phytochemical based leads using computational methods such as Schrodinger software. At this context we organized a workshop under the sponsorship of Kerala State Council for Science, Technology and Environment (KSCSTE) to promote the scientific aspirations of post graduate students, researchers and faculties from various colleges in Kerala. The workshop was also intended to provide a common platform for the delegates to share knowledge and to plan strategies for modern drug research by intellectual interaction with experts in the field.

The workshop started with the registration at 9.00 AM on 4th April 2018. The inauguration function of programme began with an invocation by the students of our college. Dr. Rejikumar, Associate Professor and Principal in Charge presided over the function. Dr. Smitha Sasidhran, Convenor of the workshop welcomed the distinguished guests, invited speakers, delegates, faculties and students to the workshop. Prof. Sabu Thomas, Pro-Vice Chancellor, Mahatma Gandhi University inaugurated the workshop by lighting up the lamp and he also delivered the inaugural address. He inspired the students with the motivational speech and he also emphasized the significance of computational methods for the development of new drugs. He also said that the proper usage and

implementation of the Schrodinger software can reduce the time and cost in the area of drug research.

Dr. M S Latha, Head, Department of Chemistry delivered vote of thanks in the inaugural function.

The inauguration function was followed by Key Note Address by Nandakumar Kalarikkal, Director, Inter University Centre for Nanoscience and Nanotechnology, Mahatma Gandhi University. He congratulated Department of Chemistry for taking initiative to organise the workshop which covers fundamental as well as advanced level of knowledge and hands on training on computational modeling and drug designing. He shared his views on the usage of software for drug designing. After the tea break Dr. M S Latha give an introductory talk on the workshop, Schrodinger software and its application for drug designing. Later Dr. Sreejalekshmi, Associate Professor from IIST, Trivandrum delivered an invited talk on "Fundamentals of Computational Modeling". The delegates and students were highly inspired by her way of presentation and fruitful discussion. After the lunch break hands on training on software continues till 4.00 pm. Mrs. Sruthy and Miss Nayana, Research Scholars of Department of Chemistry assisted the delegates during training sessions. Faculty of members of the Department of Chemistry and Dr. Sreejalekshmi were also available for technical assistance and discussion during training.

On the second day of workshop training programme started from 9.00 am. At 10.45 invited speaker Dr. K. Santhoshkumar from RGCB, Trivandrum delivered a talk on "Current Trends in Drug Designing". His talk was much interactive and delegates clarified the doubts as well. Later Dr. A Padmesh, Assistant Professor from IIT Palakkad delivered a talk on "Applications of Computational Modeling". After the lunch break training programme was continued and the delegates were supplied with course materials and study aids. During valedictory function, in the afternoon at 3.00 pm Dr. M S Latha, HOD, Chemistry Department congratulated delegates for active participation, fruitful discussions, support and cooperation during the two day workshop. She distributed the certificates to the participants. Delegates also and their views of the programme. Dr. Abu Thahir and Miss Saraswathy gave feedback of their programme and discussed the possibility to continue the collaboration and networking in the future. Dr. Smitha Sasidharan, Convenor of the programme acknowledged delegates, faculty members, students and KSCSTE for the support to organise the

programme. The Newspapers such as Mathrubhumi and Kerala Kaumudi also reported the event. The photographs and news clipping of the programme follows:-



Welcome speech by Dr. Smitha Sasidharan



Presidential address by Dr. Rejikumar



Lighting of the lamp at the inaugural function



Inaugural address by Prof. Sabu Thomas



Vote of Thanks by Dr. M S Latha



Key Note Address by Prof. Nandakumar Kalarikkal



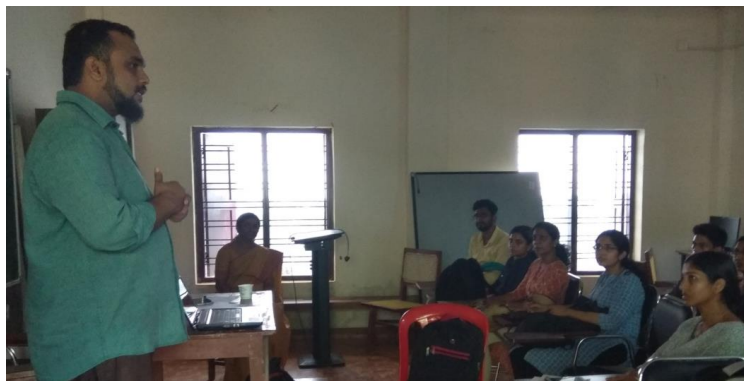
Photos from Inaugural Function



Invited Talk by Dr. A. Padmesh



Invited talk by Dr. Santhoshkumar



Valedictory function and feed back session



ചെങ്ങന്നൂർ ശ്രീനാരായണ കോളേജിൽ നടന്ന ശില്പശാല മഹാത്താഗാന്ധി സർവ്വകലാശാല പ്രോ.വൈസ് ചാൻസലർ പ്രൊഫ.ഡോ. സാബുതോമസ് ഉദ്ഘാടനം ചെയ്യുന്നു

Kerala Kaumudi, Pathanamthitta, 6th April

കമ്പ്യൂട്ടർ സഹായത്തോടെ മരുന്നുൽപാദനം വേഗത്തിലാക്കാം- സെമിനാർ

ചെങ്ങന്നൂർ കമ്പ്യൂട്ടർ സഹായത്തോടെ മരുന്നുൽപാദനവും പരീക്ഷണവും വേഗത്തിലാക്കാൻ സാധിക്കുമെന്ന് എം.ജി. സർവകലാശാല പ്രോ- വൈസ് ചാൻസലർ ഡോ. സാബു തോമസ്. ചെങ്ങന്നൂർ ശ്രീനാരായണ കോളേജിൽ 'കമ്പ്യൂട്ടേഷണൽ മോഡലിങ്ങ് ആൻഡ് ഡ്രഗ് ഡിസൈൻ' ശില്പശാല ഉദ്ഘാടനം ചെയ്യുകയായിരുന്നു അദ്ദേഹം. രോഗങ്ങളും അവയെ പ്രതിരോധിക്കുന്ന ഔഷധ മൂലകങ്ങളും കമ്പ്യൂട്ടറിൽ പരീക്ഷിക്കാൻ സാധിക്കും. പ്രത്യേകമായി രൂപവൽക്കരിക്കുന്ന സോഫ്റ്റ് വെയറില്ലെടയാണ് ഇതിന് കഴിയുക. പരീക്ഷണശാലയിൽനിന്ന് വിപണിയിലേക്ക് വേഗത്തിൽ മാറുന്നതിനാണ് ഇത് സഹായിക്കും- സാബു തോമസ് പറഞ്ഞു. പ്രിൻസിപ്പൽ ഇൻ. ചാർജ് ഡോ. രജി



ചെങ്ങന്നൂർ ശ്രീനാരായണ കോളേജിൽ നടന്ന ശില്പശാല എം.ജി. സർവകലാശാല പ്രോ- വൈസ് ചാൻസലർ ഡോ. സാബു തോമസ് ഉദ്ഘാടനം ചെയ്യുന്നു

കുമാർ അധ്യക്ഷത വഹിച്ചു. എം.ജി. യൂണിവേഴ്സിറ്റി നാനോ സെൻറർ ഡയറക്ടർ ഡോ. നന്ദകുമാർ കളരിക്കൽ, ഐ.ഐ.എസ്.ടി. തിരുവനന്തപുരം അസോസിയേറ്റ് ഡോ. ശ്രീജാലക്ഷ്മി, രാജീവ് ഗാന്ധി സെൻറർഫോർ ബയോടെക്നോളജിയിലെ ശാസ്ത്രജ്ഞൻ ഡോ. കെ. സന്തോഷ് കുമാർ, പാലക്കാട് ഐ.ഐ.ടി. അസി. പ്രൊഫ. ഡോ.പത്മേഷ്, കൺവീനർ ഡോ. സ്നീത ശശിധരൻ, കോളേജ് റസതന്ത്രവിഭാഗം മേധാവി ഡോ. എം.എസ്. ലത തുടങ്ങിയവർ പ്രസംഗിച്ചു.

The workshop was successful and interactive. We could train 35 delegates from various institutes. The delegates included post graduate students, researchers and faculty members. The possibility for further collaboration and networking is resulted as the outgrowth of workshop. The organisers acknowledge KSCSTE for funds and support.