

ABOUT THE COLLEGE

Sree Narayana College, Varkala in the name of the visionary Sree Narayana Guru follows His doctrines closely to its heart in all its teaching learning process. The college established in 1964 is affiliated to University of Kerala and ever since the inception, the institution has made an indelible impression in the realm of higher education in Kerala.

ABOUT THE WORKSHOP

Materials science is considered to play a central role in supporting the development of the technological foundations in the 21st century. To meet the ever-increasing demand for novel materials, and at the same time satisfy the growing public concern for the energy/power consumption and environmental impacts, novel routines other than relying on the traditional trial-and-error would be necessary. With recent developments in computational techniques, coupled with the rapid progress in computer efficiency, ab-initio/first principles-based computational materials design is now a reality.

Bioinformatics and cheminformatics are scientific disciplines that have evolved in recent decades at the interface between chemistry, biology, and computer science. Predictive informatics methods employ statistical techniques to mine this data for hidden correlations and to retrieve molecules, genes or patterns with specific properties or desirable biological activities from large databases. Informatics methods have been especially valuable in drug design and development, but are also increasingly employed in several other disciplines which are governed by the science of complex systems.

NATIONAL ADVISORY COMMITTEE

- **Prof Achuthsankar S Nair**
Dept of Computational Biology and Bioinformatics,
University of Kerala, Karyavattom
- **Dr. SMA Shibli,**
Professor, Department of Chemistry, University of Kerala
- **Dr. Mangala Sunder Krishnan,**
Professor Emeritus and Former Head of the Dept of,
Chemistry, IIT Madras
- **Dr. Parameswaran Pattiyil,**
Professor, Department of chemistry, NIT, Calicut
- **Dr. Jayasree Elambalassery**
Professor, Dept. of Applied Chemistry CUSAT
- **Dr Abi T G,**
Asst. Professor Dept. of Chemistry
Sacred Heart College Thevara

ORGANIZING COMMITTEE

- Sri. Vellapally Natesan,**
Manager (Patron)
Dr. K.C Preetha, Principal (Chairperson)
Sri. Aji SRM (SN Trust Executive Member)
Dr. Archana. S.R (HoD & Convenor)
Smt. Lija P Lakshmanan (Asst Professor)
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Smt. Shibitha Thampi (Asst Prof & Co-Convenor)
Smt. Induja P (Asst Professor)
Smt. Saritha. S.J (Asst Professor)
Dr. Reshma. R (Asst Professor)
Smt. Lekshmi S Dharan (Asst Professor)
Miss. Dhanya U R (Guest Faculty)

SREE NARAYANA COLLEGE

Sivagiri, Varkala

Affiliated to University of Kerala
NAAC Reaccredited with B++ Grade



National Workshop on COMPUTATIONAL MATERIAL DESIGN & INFORMATICS

2nd & 3rd March 2023
Venue: Conference Hall



Jointly Organized by
P G Department of Chemistry
(DBT Star Scheme Supported), IQAC
&
**Kerala State Council for Science,
Technology and Environment
(KSCSTE)**

THEME OF THE WORKSHOP

- Introducing Simulation Tools
- Multiscale Modeling
- Physico-chemical properties and nanoscale processes.
- Molecular Docking
- Computer Aided Drug Design & Delivery Systems
- Computational Nanotechnology

INSTRUCTIONS

*Registration Fees: Rs. 500/- for Research Scholar/ Faculty /Student (**Spot payment only**)

*Registration deadline: 25th Feb 2023
Number of participants are limited to 50
Participant confirmation on first come first serve basis.

*Participation Certificate, Program kit, Snacks and Lunch will be provided

*Participants are requested to bring their laptop

REGISTRATION LINK

<https://forms.gle/TjMQrGNDWRbL4Koa6>

CONTACT US

Dr. Archana. S.R
Convenor
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Technical support

PROMINENT A PERFECT SOLUTION



Inauguration & Inaugural Address

Prof. Achuthsankar S Nair

Dept of Computational Biology and Bioinformatics,
University of Kerala, Karyavattom



Topic: "Exploring Computational Chemistry for Research in Interdisciplinary Science"

Dr Abi T G

Asst. Professor & Research Guide, Dept. of Chemistry, Sacred Heart College Thevara



Topic: "Drug discovery challenges and opportunities"

Dr. Sherin DR

Research Scientist, School of Digital Sciences
Kerala University of Digital Sciences,
Innovation and Technology



Topic: Deep drug design using computational techniques-OPEN CADD

Dr. P. K. Krishnan Namboori

Head, Computational Chemistry Group
Amrita Molecular Modeling And Synthesis
Research lab, Coimbatore

PROGRAMME SCHEDULE

Day 1 (2nd March 2023)

8.45 A.M	: Registration
9.30 AM –10.45 AM	: Inaugural session
Prayer	: Chemistry Choir
Welcome	: Dr. Archana. S.R, HOD (Convenor)
Presidential address:	Dr. K.C Preetha, Principal
Inauguration and inaugural address	: Prof. Achuthsankar S Nair Dept of Computational Biology and Bioinformatics
Felicitations	: Sri. Aji SRM (SN Trust Ex. Member) Dr. Preetha Krishna (IQAC Co-ordinator) Dr. Leji , (HOD, Zoology) Sri.G. Sivakumar (PTA Vice President)
Vote of Thanks	: Mrs. Shibitha Thampi (Co-convenor)
10.45 AM -11.00 AM:	Tea Break

Technical Sessions

11.00 AM- 1.00 PM	: Keynote address Dr. Abi TG , Asst. Professor, Dept. of Chemistry, Sacred Heart College, Thevara
1.00 PM-1.55 PM	: Lunch Break
2.00 PM-3.30 PM	: Dr. Sherin DR , Research Scientist, Digital University, Kerala

Day 2 (3rd March 2023)

10.00 AM-11.20 AM	: Invited Talk Dr. P.K. Krishnan Namboori Head, Amrita Molecular Modeling & Synthesis lab, Coimbatore
11.20AM- 11.30 AM	: Tea Break
11.30 AM -1.00 PM	: Hands-on training
1.00 PM – 2.00 PM	: Lunch Break
2.00 PM – 3.00 PM	: Hands-on training
3.00 PM – 3.30 PM	: Valedictory Session