



SATHYABAMA
Institute of Science and Technology
(Deemed to be University)
Accredited with Grade A by NAAC



DEPARTMENT OF CHEMISTRY

*Cordially invites you to the **DST-SERB**
sponsored five day workshop on
“CHALLENGES AND ADVANCES
IN COMPUTATIONAL
CHEMISTRY CACCh-2018”*

**To be held from 08-January-2018 to 12-January-2018 at
SATHYABAMA
Institute of Science and Technology**



ABOUT SATHYABAMA INSTITUTE OF SCIENCE AND TECHNOLOGY

Sathyabama is a pioneer in engineering education and was established with the aim of providing quality higher education in the areas of Engineering, Science and Technology on par with International standards. It persistently seeks and adopts innovative methods to improve the quality of higher education on a consistent basis. Having acquired excellence in the academic part of education with all sophisticated facilities available, Sathyabama has established several research centres in the field of Remote Sensing & Geo Informatics, Nano Technology, Ocean Research, Water Research, Robotics, Earth & Atmospheric Sciences, Non Destructive Testing & Waste Management in collaborations with esteemed National Research organizations and are progressively working towards innovation in the field of Science & Technology. Sathyabama has been accredited with 'A' grade by National Assessment and Accreditation Council (NAAC) and ISO 9001: 2008 Certification for Professional Quality Management Practices. It has undertaken various sponsored and collaborative research and development projects funded by national organizations such as Indian Space Research Organization (ISRO), Department of Science and Technology (DST), Indira Gandhi Centre for Atomic Research (IGCAR), Defence Research and Development Organization (DRDO), Department of Bio-Technology (DBT), Ministry of Environment and Forests (MoEF), Board of Research in Nuclear Sciences (BRNS) etc. Sathyabama holds great promise to expand the applications of space technology, benefiting the common man and enriching the quality of life. A step towards achieving this, the institution is successfully conducting non formal education programmes through 18 Village Resources Centre (VRCs) all over the state of Tamil Nadu.

ABOUT THE DEPARTMENT OF CHEMISTRY

The Department of Chemistry was started right from the inception of Sathyabama in the year 1988. It has well-established laboratories equipped with sophisticated instruments, which fulfil the needs of PG and Ph. D students. The department has highly qualified faculty and more than 20 Ph. D students. It has doctorates from reputed institutions like IIT, NIT CECRI, NML, etc. and published more than 75 research papers in reputed journals with high impact factor. The department has undertaken many research projects funded by CSIR, ISRO, DST and IGCAR.

NATIONAL ADVISORY COMMITTEE

Dr. Rajaraman, Associate Professor, IIT Bombay
Dr. Gunasekaran K, Associate Professor, University of Madras
Dr. Narahari Sastry G, Sr. Principal Scientist, Centre for Molecular Modelling, CSIR-IICT, Hyderabad.
Dr. Naresh Kandakatla, Manager R&D & Production at Helios Bio Nutrition Pvt. Ltd.
Dr. Geetha Swaminathan, Former Vice Principal, Stella Maris College, Chennai.
Dr. K. Shyamala, Former Head, Department of Bioinformatics, Stella Maris College
Dr. R. Karvembu, Associate Professor, Department of Chemistry, NIT Trichy
Dr. A. Nityananda Shetty, Professor, NITK, Suratkal

OBJECTIVES AND IMPORTANCE OF THE WORKSHOP

Chemists have been involved in computations for ages, but what we know as Computational Chemistry is a product of the digital age. However, Computational Chemistry did not come into its own until 1998 when Walter Kohn and John Pople won the Nobel Prize for Chemistry for their work in Density Functional Theory and Computational methods in Quantum Chemistry. It is a rapidly growing field of Chemistry and is now firmly established as an indispensable tool in the hands of researchers to carry out studies hitherto unachievable by conventional methodologies. This interesting field of study helps to create spectral profile simulations, modelling and designing molecules, understand structure activity relationships, homology modelling, design more productive and efficient processes, protein structure visualization, in molecular dynamics and in short to extract useful knowledge from oceans of data.

To bring about a better understanding of the scope of Computational Chemistry and its application in current research and education by UG and PG students and teachers, research scholars, etc., the Department of Chemistry has organized a five day Workshop on the Challenges and Advances in Computational Chemistry 2018 (CACCh-2018) that will focus on the molecular mechanism underlying human health and disease. This workshop will provide a comprehensive theoretical and practical hands-on training to all the participants on molecular modelling and drug design.

CONVENER

Ms. JANET SABINA X
Assistant Professor
Department of Chemistry
Sathyabama Institute of Science and Technology
Rajiv Gandhi Salai
Chennai – 600119

REGISTRATION FEE: RS. 2000 (For PG Students: Rs. 1000)

Kindly confirm your participation through phone or email. Registration through SMS to 9445362213.

Email: janetjeyakumar@gmail.com

Dr. Parthiban Srinivasan, Parthys Reverse Informatics, Chennai	Keynote Address
Dr. Gunasekaran, University of Madras	XRD: An inevitable partner of Chemistry
Dr. Naresh Kandakatla, Helios Pvt. Ltd., Hyderabad	Chemical structure drawing: 2D and 3D. Molecular Modelling – Discovery Studio
Dr. M. Karthikeyan, NCL, Pune	Chemoinformatics for drug discovery
Dr. Thiagarajan, IBAB, Bangalore	Virtual screening and rational drug design: principles and applications
Dr. Xavier Suresh, Sathyabama	Molecular modelling - AutoDock
Dr. Athi Naganathan, IIT Madras	Theoretical models of protein folding: myth or reality?
Dr. Madhavan Jacob, Loyola College	Fundamentals of Electronic structure calculations Role of computation on the signature and reactivity of molecules
Dr. Mukesh Dhoble, IIT Madras	Computer aided design of anti- inflammatory drugs Pharmacophore modelling
Dr. Rajaraman, IIT Bombay	Computing spectral parameters using ORCA
Dr. Deva Priyakumar, IIIT Hyderabad	Computational Studies on the Mechanism of Selection and Permeation Across Ion Channels

HIGHLIGHTS

- Eminent scientists from IIT Madras, Bombay, Hyderabad, Bangalore, Pune and the industry will deliver talks on various topics in Computational Chemistry
- Practical and interactive session with eminent personalities
- A highly comprehensive five day programme that will enrich all researchers in this field.



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JEPPIAR NAGAR, RAJIV GANDHI SALAI
CHENNAI - 600119



DEPARTMENT OF CHEMISTRY

This is to certify that Dr. / Mr. /Ms.

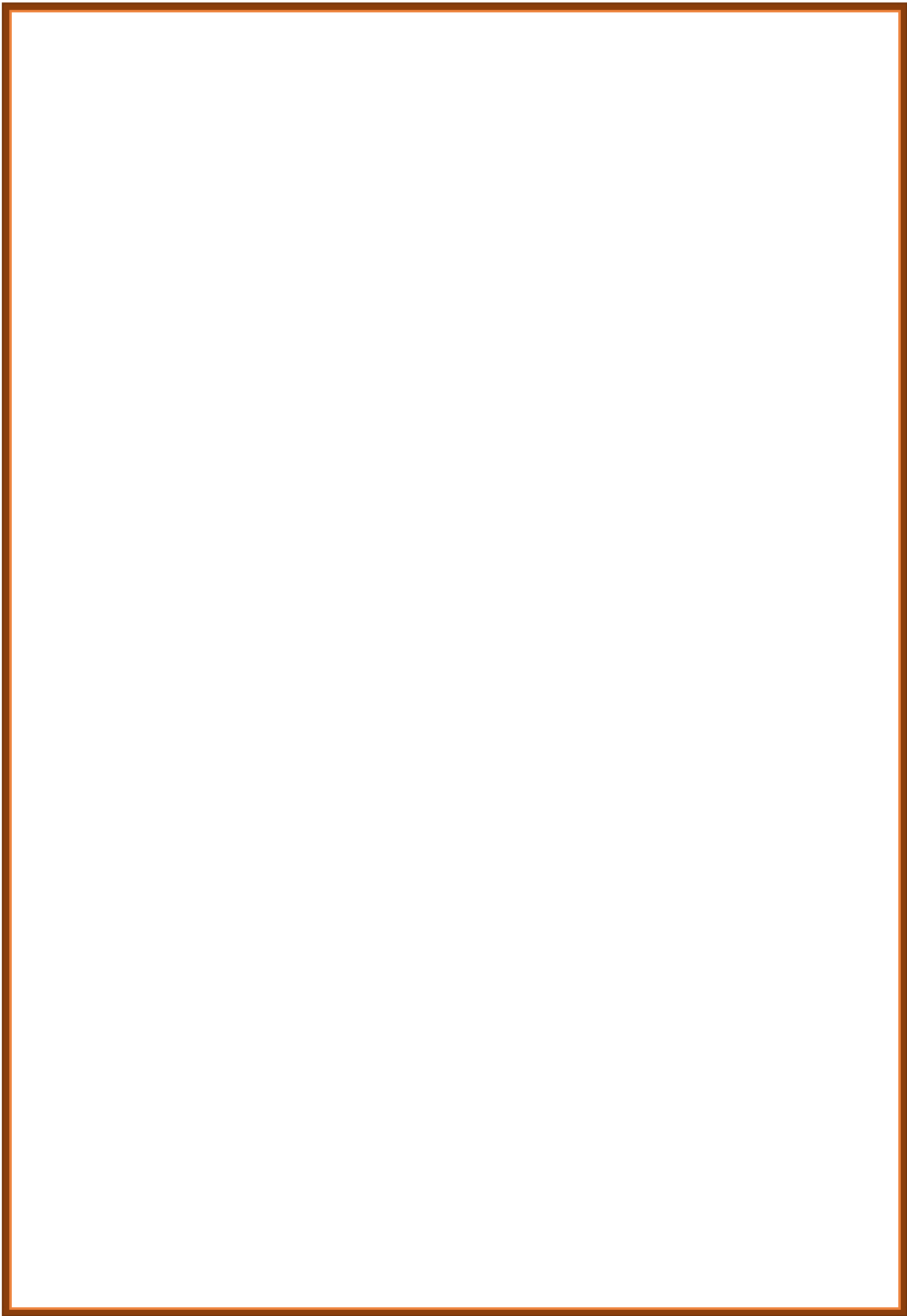
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has participated in the five day DST-SERB sponsored workshop on
“CHALLENGES AND ADVANCES IN COMPUTATIONAL CHEMISTRY
CACCh-2018” organized by the Department of Chemistry,
Sathyabama Institute of Science and Technology from 08th January
2018 to 12th January 2018.

Dr. J. Karthikeyan
Head, Department of Chemistry

Dr. M. Sundareswari
Dean, School of Science & Humanities

Ms. X. Janet Sabina
Convener, CACCh-2018



**DAYWISE SCHEDULE FOR THE FIVE DAY DST-SERB SPONSORED WORKSHOP ON
“CHALLENGES AND ADVANCES IN COMPUTATIONAL CHEMISTRY CACCh-2018”**

DAY I (08-01-2018)			
9:30 am – 10:00 am	Inauguration		
10:00 am – 10:15 am	Tea break		
10:15 am – 11:15 am	Lecture - 1	Dr. Parthiban Srinivasan, Parthys Reverse Informatics, Chennai	Keynote Address
11:15 am to 12:15 pm	Lecture – 2	Dr. Gunasekaran, University of Madras	XRD: An inevitable partner of Chemistry
12:15 pm – 1:00 pm	Lunch		
1:00 pm – 3:00 pm	Practical Session -1	Dr. Naresh Kandakatla, Helios Pvt. Ltd., Hyderabad	Chemical structure drawing: 2D and 3D. Molecular Modelling – Discovery Studio
DAY II (09-01-2018)			
9:30 am – 10:30 am	Lecture – 3	Dr. M. Karthikeyan, NCL, Pune	Chemoinformatics for drug discovery
10:30 am – 11: 00 am	Tea break		
11:00 am – 12:00 noon	Lecture – 4	Dr. Thiagarajan, IBAB, Bangalore	Virtual screening and rational drug design: principles and applications
12:00 noon – 1: 00 pm	Lunch		
1:00 pm – 3:00 pm	Practical Session -2	Dr. Xavier Suresh, Sathyabama	Molecular modelling - AutoDock
DAY III (10-01-2018)			
9:30 am – 10:30 am	Lecture – 5	Dr. Athi Naganathan, IIT Madras	Theoretical models of protein folding: myth or reality?
10:30 am – 11: 00 am	Tea break		
11:00 am – 12:00 noon	Lecture – 6	Dr. Madhavan Jacob, Loyola College	Fundamentals of Electronic structure calculations

12:00 noon – 1: 00 pm	Lunch		
1:00 pm – 3:00 pm	Lecture - 7	Dr. Madhavan Jacob, Loyola College	Role of computation on the signature and reactivity of molecules
DAY IV (11-01-2018)			
9:30 am – 10:30 am	Lecture - 8	Dr. Mukesh Dhoble, IIT Madras	Computer aided design of anti-inflammatory drugs
10: 30 am – 10:45 am	Tea break		
10:45 am – 12:30 pm	Practical Session - 3	Dr. Mukesh Dhoble, IIT Madras	Pharmacophore modelling
12:30 pm – 1: 30 pm	Lunch		
1:30 pm – 3:00 pm	Lecture - 9	Dr. Rajaraman, IIT Bombay	Computing spectral parameters using ORCA
Day V (12-01-2018)			
10:30 am – 11:00 am	Tea break		
11:00 – 12:00 noon	Lecture – 10	Dr. Deva Priyakumar, IIIT Hyderabad	Computational Studies on the Mechanism of Selection and Permeation Across Ion Channels
12:00 noon – 1: 00 pm	Lunch		
1:00 pm – 1: 30 pm	Valedictory		