Registration starts on 14.09.2022

Date of Workshop	:	24.09.2022
Duration	:	9.00 am to 5.00 pm
Venue	:	Seminar Hall, Loyola Institute of Frontier Energy, Loyola College, Nungambakkam, Chennai-600034

Registration Link:

https://forms.gle/dj6maH9P8c8XpMG66

Payment Details:

Indian Overseas Bank
M/S DIRECTOR LIFE
Account No: 171201000009998
IFSC: IOBA0001712
Branch: Loyola College Campus

Registration Fees Per Candidate: Rs.500/-

Expected Numbers of Participants: **40**
Candidates are asked to bring their own lap tops and pen drives.

LOYOLA INSTITUTE OF FRONTIER ENERGY (LIFE)

LIFE is an interdisciplinary and collaborative research institute in Loyola College started by **Rev. Dr. Francis Xavier**, S.J, in 1995 with a team of six like-minded Professors from Chemistry, Physics and Zoology. The basic tenet of LIFE is border-less, collaborative, and interdisciplinary research in science with a balance between pure and applied sciences with the ultimate view of translating the fruits of research for improving the quality of life of the society. The thrust areas are: Energy, Environment, Material Science, Bioethics, Awareness Education to Students and the Masses.

Today, 11 voluntary faculties from the departments of Chemistry, Physics, and Life Sciences are engaged in active research with 36 research scholars pursuing Ph.D. besides a number of M.Phil. and M.Sc. project students. It is recognized as one of the Centers of Excellence in Loyola and also one of the two research institutes of Loyola enjoying the benefit of 175% tax-exemption.

LIFE's immediate focus is to consolidate its activities in interdisciplinary and collaborative research projects among its own members first and then finding collaborative partners with other institutions in Loyola Campus such as Entomology Research Institute **(ERI)**, LOYOLA-ICAM College of Engineering and Technology **(LICET)** and Loyola Institute of Business Management **(LIBA)**

Convener

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PATRONS:

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Secretary & Correspondent, Loyola College, Chennai.

Rev. Dr.A. Thomas SJ
Principal, Loyola College, Chennai.

Dr.J.A.Charles
Deputy Principal, Loyola College, Chennai.

LIFE Faculty:

Dr. George Johnson, Dr. J. Merlyn Shyla
Dr. Jaccob, Dr. Jaqueline
Dr. Pushparani, Dr. Victor Antonyraj
Dr. Johnmary

LOYOLA INSTITUTE OF FRONTIER ENERGY

LOYOLA COLLEGE, CHENNAI.

ORGANISES

Workshop On

COMPUTATIONAL CHEMISTRY FOR BIOTECHNOLOGY

Title

National Workshop on "Emerging Trends *in silico* Molecular Docking Drug Designing, Prediction of Toxicity Profile by ADMED Analysis, Density Function Theory as applied to Optimized Structure of Organic Molecules and pharmacokinetic Properties of Synthetic Novel Organic, Herbal, and Phytochemical Compounds"

Background

Owing to its impact on society, the design of novel drugs has the potential to interest a wide audience, and offers a rare opportunity to introduce numerous concepts in chemistry and biochemistry. Drug design can be seen as a multi objective cyclic optimization process. Indeed, it is significant to develop the understanding not only that a drug is generally an effective ligand for a protein of therapeutic interest, but also that these molecules need to have drug-like properties. Computer-aided drug design and bioinformatics methods play an essential role in addressing these different challenges. Here we introduce **synthesized novel organic compounds, Herbal based compounds as well as phytochemical compounds** and their affinities are performed by using freely available **Auto Dock vina 4.0**. Educational tool Software. Drug Design Workshop, which presents the basics of drug design and provides anyone with access to computational methods and resources to conceive and evaluate molecules for their potential to become actual drugs. One pedagogical **ADME or toxicity properties of small drug-like** molecules objective is done by multi objective nature of the optimization process in (computer-assisted) drug design. This implies that, besides affinity, the pharmacokinetic and the pharmacodynamic properties of the small molecules will be performed by SwissADME free online software.

The college students, research scholars, industry personals and teachers are certainly beneficiaries. The doctoral students, have always shown great interest and enthusiasm whatever their scientific background and level. The subject not only is timely, but also concerns each and every one. Our workshop provides a simplified view of complex notions and allows a wide audience to discover the key stages in drug discovery as well as the importance of bio informatics in life science today.

Objectives of Workshop

- ***In silico*** Drug Designing pertaining to Cancer, Arboviruses, Nipha virus, and chronic diseases are performed by using Novel organic synthetic compounds, Herbal as well as phytochemical compounds.
- By developing collaborations with other centres, Institutions and universities to validate all the ***in silico*** lead molecules with performing high end ***in vitro*** studies.
- Extension of pharmacophore and pharmacophore QSAR modelling studies against Anticancer, Anti diabetic and Anti-inflammatory targets.
- To perform Molecular dynamics and simulations studies for specific phytochemicals leading to the discovery of potential lead molecules.
- To perform Immuno informatic cum validating studies on the viral proteins of different viruses with special importance to arboviruses and Nipha virus.
- Assessment of quantum chemical parameters of the Phytochemical compounds with reference to standard drugs available for diseases.
- ADME Pharmacokinetic and pharmacodynamic properties are carried out.
- Molecular recognition is the ability of biomolecules to recognize other biomolecules and selectively interact with them. Examples are transcription, translation, signal transduction, transport, regulation, enzymatic catalysis, viral and bacterial infection and immune response.
- Molecular docking is the process that involves placing molecules in appropriate configurations to interact with a receptor. Molecular docking is a natural process which occurs within seconds in a cell.
- In molecular modeling the term “molecular docking” refers to the study of how two or more molecular structures fit together.

Organizing secretary

Dr. M. F .VALAN

ASSISTANT PROFESSOR

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Speakers/ Resource Persons

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TOPIC:

PHYTO CHEMISTRY AND NATURAL PRODUCT ISOLATION

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TOPIC:

MOLECULAR DOCKING AND ORGANIC SYNTHESIS

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TOPIC:

PHYTOCHEMICAL METHODS AND NATURAL PRODUCT ISOLATION