

## RESEARCH FACILITIES

### List of Research Facilities laboratory

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#### FTIR Spectrophotometer

FTIR spectrophotometer is used for the identification of unknown compounds, quantitative information, such as additives or contaminants, the identification of functional groups of organic compounds, polymer materials, petrochemical products, biological compounds, the pharmaceutical products and for academic research

#### Technical Description and Major Specifications

Model: PerkinElmer spectrum two FTIR spectrometer

Wavenumber Range: 4000 to 350 cm<sup>-1</sup>

Detector: TGS detector

Resolution: 0.5 cm<sup>-1</sup>

S/N ratio: 2000:1 ppm for 1 minute scan.

Wavelength accuracy: 0.01 cm<sup>-1</sup>

Sample requirement: Solid: ~0.2 (powder)

#### UV-Vis Spectrophotometer

The Varian Cary 50 Scan UV Visible Spectrophotometer is designed to analyze microlitre volumes of chemical and biological samples. With a maximum scan rate of 24,000 nanometers per minute, the Varian Cary 50 can scan the whole wavelength range of 190 to 1100 nm in less than 3 seconds. Additionally, the Varian Cary 50 features a data

collection rate of 80 points per seconds and can measure samples up to 3 Abs to reduce the need for frequent dilution. The Varian Cary 50's super-concentrated beam makes it ideal for fiber optic work, offering excellent coupling efficiency.

**Technical Description and Major Specifications:**

Model Cary 50 UV

Source: Deuterium lamp (UV region)

Beam splitting system: Beam splitter

Detectors: Bandwidth dual Detector

UV-Vis limiting resolution:  $\leq 1.5$  nm

Wavelength range: 190 to 1100 nm

Photometric range: 3.3 abs

Cell Holder: Single cell holder

Resolution:  $\geq 1.65$  nm (UV/Vis)

Spectral bandwidth: Fixed at 1.5 nm

Maximum scan rate: 24,000 nm/min

Dimensions (W x D x H): 50 x 59 x 20.5 cm

Data acquisition modes: Spectrum, kinetics and photometric with facilities such as % Abs, %T, %R, absolute %R, log Abs, 1st-4th derivative

**Note:**

**Instructions for UV-VIS users:**

- Please specify the mode of measurement (% A,%T,%R etc)
- Solvents must be specified for recording solution spectra

**Sample requirement:**

- Solid:  $\sim 0.2$  (powder)
- Thin film: 1.0-1.5 cm
- Solution:  $\sim 5$  ml

## Central Instrumentation Center

### UV-Vis Spectrophotometer



### Impedance Analyser

#### General Information-

Model: Impedance Analyzer (N4L, PSM1735)

#### Specification-

Frequency Range: 10 $\mu$ Hz to 35MHz

Temperature Range: Room temperature to 600°C

Functions: L, C, R (ac), Q, tan delta, impedance, phase - Series or Parallelcircuit

Current Shunt: External or N4L active head or IAI (Impedance Analysis Interface)



#### About Instrument and its applications

The impedance analyzer (N4L, PSM 1735 LCR Meter) is designed to study the dielectric properties of the samples in the frequency range of 10 $\mu$ Hz to 35MHz. in the temperature range from Room temperature to 600°C. The impedance data contains Tan  $\delta$ , Impedance, Cp, Rp, Lp, Cs, Rs, Ls, reactance, phase from which dielectric parameters such as dielectric constant, loss, complex permittivity, complex impedance, complex modulus and conductivity can be obtained.

#### Sample Requirements-

1. Powder samples should be pelletized ( $\approx$ 10 mm diameter and  $\approx$ 1mm thickness).
2. Crystals with dimension ( $\approx$ 10 mm length,  $\approx$ 10 mm Breath,  $\approx$ 2 mm thickness) should be polished in all the sides.

**Instrument Fabrication Centre**

**Photoacoustic Spectrophotometer**



The Photoacoustic Spectrophotometer fabricated in this centre was already sold to other research institute such as SSN research centre and Loyala College, Chennai.

### **Semi-automatic Reddy Tube**

Table-top semi-automatic Reddy Tube is the product of Sacred Heart Instrumentation Centre, Sacred Heart College. This shock tube is capable of producing shock waves of Mach number ranging from 1 to 4.5. It has three sections as that of driver, driven and diaphragm sections. An air compressor is used to supply driver gas into the driven section. The driver and driven sections consist of long seamless stainless-steel tubes of 48 cm and 180 cm, respectively and both have an inner diameter of 1.5 cm. While the atmospheric air is compressed into the driver section, at the critical pressure, the diaphragm is ruptured and the shock wave is generated and moves along the driven section. The sample holder is placed at 1 cm away from the open end of the driven section. The shock tube is capable to produce up to 500 shocks per hour as well as we can vary the Mach number by suitable diaphragms. More than 20 institutions including research laboratories from abroad used this shock tube and made more than 75 research publications in reputed international journals.



## Powder X-Ray Diffractometer

### General Information

Model: Bruker D2-Phaser

Year of Installation: 2018

### Specification

X-Ray Source: 2.2kW Cu anode, 40 kV/40 mA

Detector: LYNXEYE XE

Step size: 0.0002°

2Theta range: 4° to 80°

### About Instrument and its applications

X-ray Diffraction (XRD) is a high-tech, non-destructive technique for analyzing a wide range of materials, including metals, polymers, catalysts, plastics, pharmaceuticals, thin-film coatings, ceramics, solar cells and semiconductors. The Bruker D2 X-ray diffractometers can be used for nearly all X-ray diffraction application, such as structure determination, phase analysis, stress and texture measurement. The D2 PHASER delivers good data quality and due to its compact size, low weight, and ease-of-use design, the system is conveniently mobile, without the need for complicated infrastructure. A standard power outlet and a few minutes is required to take for the system for an outstanding result. The D2 PHASER is a well-equipped instrument with the unique LYNXEYE XE-T detector, energy resolution of 380 eV allows a unique, digital monochromator mode to efficiently remove - unwanted radiation, such as sample fluorescence, - K - beta radiation, and Bremsstrahlung - background scattering, without losses in detection speed.

## Sample Requirements-

Amount- approximately 1g (in fine powder form)



## Structural Biochemistry Lab

Recent progress in X-ray crystallography and in particular cryo-EM (cryo- electron microscopy) has greatly advanced our understanding of the structure and dynamics of biomolecules. Although structures of several proteins have been solved in different conformational states, the dynamics and the functional mechanism of how these macromolecules operate cannot be understood from static snapshots obtained experimentally. Molecular dynamics (MD) simulations can be used to understand the dynamic nature of biomolecular systems with high spatial and temporal resolution. The lab utilizes both coarse-grained models and all-atom MD simulations to understand conformational dynamics in proteins and protein folding.

Our research interest includes understanding the conformational changes and dynamics of periplasmic binding proteins. We also probe for structural features that guide the mechanism of ligand binding in these proteins. The lab also studies ligand transport mechanism in membrane proteins, particularly glucose transporters and ATP-binding cassette (ABC) transporters. The lab also focuses on understanding protein folding and domain-swapping. Our attention here is focused on probing the folding mechanism of proteins, particularly those that domain-swap and relate this to understand the crucial mechanism that triggers folding as a domain- swapped dimer as against a monomer.

### Lab facility

The lab is well equipped with 6 GPU and 6 high-end workstations, network access storage, printer, separate internet connection. The lab has close collaborations with NCBS

(Bengaluru) and IIT-Madras.

### Research funding

1. Teacher Associateship for Research Excellence (TARE) award (Science & Engineering Research Board (SERB), Govt. of India), in collaboration with Dr. Athi Naganathan (Dept. of Biotechnology, IIT-Madras)

Duration: Three years(Dec. 2020-Nov. 2023)

Title: “Understanding the functional dynamics and drug efflux mechanism of ABC transporters”

Funds Sanctioned: Rs. 8,25,000

2. Early Career Research (ECR) award (SERB, Govt. of India), Apr. 2017-Mar.2020 @ Sacred Heart College, Tirupattur

Duration: Three years (Mar. 2017-Mar. 2020)

Title: “Multiscale Modelling to Gain Mechanistic Insights into GlucoseTransporters”

Funds Utilized: Rs. 18,90,010

### Online Journals

In addition to the existing Sacred Heart Journal of Science and Humanities, the following five biannual online open access journals have been started from January 2017 with complete online journal submission system. All the five journals have been already assigned online ISSN. Each journal is unique with separate editorial board comprising subject experts from different Research institutes in India and abroad from some of our own staff serving as an editorial board member.



### Infrastructure Development

A Dell Power Edge R749 Server and fifteen computers (desktop) were purchased and placed in the digital library for the effective usage of networking. Wi -Fi is provided for all Research Scholars (PG, M.Phil. and Ph.D. Students). In the browsing centre, 25 high configuration computers are added for UG students. College updated its official website by adding a number of modules to offer more online services to both staff and students. Thus, e – Governance has been enhanced towards paperless office. Also added high speed server and necessary equipments for networking through FIST and management fund to conduct online exams and automation of college administration.

#### **Department of Mathematics:**

Licenced MATLAB2021a Version was installed in Ramanujam Computational Lab for the study of solution in difference equations, differential equations, linear and non- linear programming, mathematical statistics, matrices, Numerical methods, applied mathematics and etc.,



#### **E-Learning: Ramanujan Computational Laboratory**

#### **Department of Physics:**

Purchased the following nine new experimental setups and introduced them in the recently revised PG curriculum for the students admitted in the year 2021 -22 and thereafter.

1. Digitalized constant deviation spectrograph for the study of Iron / Copper arc spectrum.
2. Laurentz half shade polarimeter for the study of specific rotation of sugar solutions.
3. Thomson's experimental setup for the study of  $e/m$  of an electron.
4. Millikan's drop experimental setup for the determination of the charge of an electron.
5. Zeeman effect setup for the determination of  $e/m$ , and Lande  $g$  – fatcor of



electrons.

6. Frank – Hertz experiment for the study of critical potentials.
7. Michalson's interferometer for the determination of wavelengths and separation of wavelengths of sodium light.
8. Susceptibility of solids by Guoy's method.
9. Determination of Planck's constant by photoelectric effect.

In addition to servicing of few electronics kits utilizing the maintenance grant, the old and ageing computers have been replaced with six new desktop computers for doing C programming and simulation studies.

#### **Department of Chemistry:**

Department of chemistry upgraded its teaching and research facilities through the following equipments bought through the FIST funding.

1. Electrochemical analyzer and workstation which is used to perform electrochemical reactions that are used in analytical chemistry and battery applications.

##### **Details about Instrument**

Model	- CHI6005E
High Frequency (Hz)	- 1e+5
Low Frequency (Hz)	- 1
Amplitude (V)	- 0.005
Quite Time (sec)	- 2

2. Visible spectrometer that is very helpful in conducting light absorption experiments.
3. Muffle furnace which is utilized as a subsidiary instrument to sintered materials.
4. A rotavapor which is used to demonstrate the solvent separation process.

These instruments are used to upgrade the practical curriculum and thereby offer the students an opportunity to provide the research enhancements and to get familiarized with the principles of electrochemistry, preparation of chemical compounds, analysis of different types of solutions and for solvent separation processes.

#### **Department of Biochemistry and Microbiology:**

The equipment purchased under DST – FIST scheme is utilized for the following purposes.

1. The PCR Machine (Model – WEE32) is used to diagnosis of COVID 19

infection in humans.

2. The ELISA Reader (Model – Robonik) is used for immunology Practicals for analyse the reactions within the multi -tier wells of the plate reader.
3. The Lyophilizer (Model – SZ042B) is used for the preservation of microbial cultures by Deep freezing method.
4. The Semi Auto analyser reader (Model – Robonik Prietest) for the analysis of blood, serum, plams, cerebrospinal fluids and urine samples.
5. The UV chamber (Model – BCAD – IH222) for inoculate the fungi in the culture medium without air contaminants.