Research in the Biochemistry and Molecular Biophysics Group

This group is distinguished by a highly interdisciplinary nature of the research topics. Research compasses several areas of modern biochemistry and molecular biophysics, which include (but not limited to) the following areas/topics:

- Protein Structure-Function Relationships; Structural Enzymology; Structural basis of Enzyme Properties; Protein Engineering; Structure and Mechanism of DNA Replication
- GPCR-mediated Signal Transduction; Biophysical Chemistry of Calcium-binding proteins
- Biophysics; Green Chemistry; Structure-based Drug Design
- Phospholipid Scramblases; Membrane Biochemistry; Biochemical and Biophysical Characterization of Industrial Enzymes
- Structure-Function Relationships and Regulation of Ion Channels
- Protein Folding and Function; Protein-Protein and Protein-DNA Binding; Downhill Folding, Molten-Globules and Intrinsically Disordered Proteins; Thermodynamics, Dynamics and Kinetics; Liquid-Liquid Phase Separation; Engineering Protein Stability, Barriers and Rates; Statistical-Mechanical Models; Coarse-Grained and All-Atom Molecular Dynamics Simulations; Multi-Domain Proteins; Allostery; Dynamic Allostery; Epistasis; Macromolecular Crowding
- Enzyme-mediated Biomass Conversion for Biofuel and Functional Oligosaccharides; Bioremediation; Carbohydrate Chemistry
- Targeted Drug Delivery: Development of Conjugation Strategies for Antibody-Drug and Polymer-Drug Conjugates; Development of New Biosimilars: Identification of Novel Clones for Biosimilars and Improvement of Therapeutic Index of Proteins by Lipidation and Glycosylation; Biophysical Chemistry of modified Nucleic acids

In addition to conventional experimental biochemical approaches, combined with methods from molecular biology, recombinant DNA technology and microbiology, the experimental techniques employed in the group include, Recombinant protein production and purification; X-ray crystallography; Bioinformatics analysis; Spectroscopy (Circular Dichroism, Fluorescence, Anisotropy, Fluorescence Life-Time, FRET, NMR and UV Absorption

spectroscopy); Calorimetry (Differential Scanning Calorimetry, Isothermal Titration Calorimetry); Mass spectrometry; AUC; SAXS; Stopped-Flow Kinetics; Engineering Mutations in Proteins, Coarse-Grained and All-Atom Molecular Dynamics, Statistical Mechanical Models; Membrane protein overexpression and purification; Biochemical reconstitution of membrane proteins; *in-vitro* phospholipid translocation assays; Electrophysiology and Patch clamp; Calcium imaging; Ion-chromatography; Protein-protein interactions; Molecular dynamics simulations; Protein-ligand docking; Small molecule synthesis; Biological assays; Mammalian cell culture; Microscopy (Fluorescence, Scanning and Cryo-EM), among others.

Research in the Biological Sciences group

Faculty in the Biological Sciences group work on diverse areas of biology with emphasis on the following research areas:

- Electrophysiology, Ion channel and receptor biology, Calcium signaling
- Molecular epigenetics, Infection Biology, Malaria
- Quantitative genetics and systems biology of yeast, Specialized ribosomes in yeast, Gene-gene and gene-environment networks in yeast
- Bio-ethanol production, Functional oligosaccharides, Molecular bioremediation
- Germline stem cells, Caenorhabditis elegans, Gene silencing
- Vascular biology, Endothelial dysfunction, Atherosclerosis
- Pancreatic cancer evolution, Cellular plasticity, Metastasis, Chemoresistance, developing preclinical model of pancreatic cancer.
- Cardiovascular biology, Metabolic syndrome, Neuromodulation, Transgenic mouse models
- Cardiovascular genetics, Biomarker discovery, Molecular basis of hypertension, type 2 diabetes, myocardial infarction, chronic kidney disease
- Molecular mechanisms of pattern formation in the cellular slime mold Dictyostelium, Estimating the types and rates of different classes of spontaneous mutations as a function of seed age and manipulation of meiotic recombination rates in Arabidopsis
- Molecular pathogenesis of HIV/AIDS, Cancer biology, Regulation of nucleo-cytoplasmic transport proteins
- Neuronal communication, Neuropeptides in facilitating neuronal function, Neuronal degeneration, Vision restoration
- Monoclonal and Polyclonal antibodies, Peptides targeting novel oncogenes, CRISPR/Cas9, Developing pre-clinical models of tumor progression
- Tuberculosis, Microbiology, Immunology, Host-pathogen interactions

Research in the Biological Engineering group

The focus of research in the Biological Engineering group is on two major areas: Bioprocess Engineering and Biomaterials Engineering

Bioprocess engineering:

The primary focus of this group is on the development of biomanufacturing platforms for

- conversion of lignocellulosic biomass to value added products like ethanol, xylitol, arabitol, biopolymers and 3-hydroxypropionic acid
- metabolic engineering strategies to improve the yields of industrially important metabolites
- production of industrially important biocatalysts such as L-asparaginase, esterases, oxidoreductases and caffeine degrading enzymes
- production of biopharmaceuticals and bioactive compounds from plants
- alternative food products (synthetic meat) and marine based bioproducts
- understanding biological systems and its manipulation

In these topics, a major focus will be on strain/cell-line development for the various products, including engineered strains using synthetic biology tools; development of process analytics for monitoring and control to ensure product quality and optimal yields; and development of integrated processes (including downstream processes) at lab-scale and validation at pilot-scale. Cell level strategies to improve bioprocess productivities, mainly reactive species-based ones; Reactive species-based strategies for treatment and management of diseases such as cancer and cardiovascular diseases

Biomaterials engineering:

This group largely focuses on

- Developing novel biomaterials for drug delivery and tissue regeneration
- Designing bioengineered microenvironments to study physiological and pathological niches
- Micro/Nanofabrication and 3D bioprinting technologies for the development of functional tissue scaffolds
- Engineering organoids and microfluidic tissue-on-a-chip platforms for disease modeling

- Extracellular matrix regulation to control cellular behavior
- Biochemical and biophysical stimulation for cells and tissues

This line of research is geared towards developing novel pharmaceutical agents, drug carriers, medical implants and drug-testing platforms for pharmaceutical companies, and clinical translation. In the future, we aim to develop therapies that modulate the immune system, musculoskeletal system, nervous system, cardiovascular system, and diseases like cancer, diabetes, amongst others.

Research in the Computational Biology group

The Computational Biology group focuses on diverse research areas which include (not limited to) the following:

- Protein structure and function; Protein stability; Protein interactions; Binding affinity; Transcriptome analysis; Disease-causing mutations; Development of databases and tools
- Molecular dynamics simulations of proteins and nucleotides; QSAR; Structure-based drug design
- Computational neuroscience
- Systems biology; Metabolic engineering
- Molecular evolution; Comparative genomics; Structural bioinformatics
- Protein assembly and aggregation; Design of drug delivery mechanisms